**Supplementary data 2**

What is in the fish? Collaborative trial in suspect and non-target screening of organic micropollutants using LC- and GC-HRMS

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**Table S11.** The full list of compounds identified by the participants through suspect or non-suspect screening.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **Smiles** | **m/z** | **Method of identification** | **Site** | **Method of analysis** | **Method of sample preparation** | **Lab** |
| Frescolat MGA | CC1CCC(C2(C1)OCC(O2)CO)C(C)C | 228.17300 | Suspect screening | Canal | LC-HRMS | In house | B |
| L-Valine | O=C(O)C(N)C(C)C | 117.07919 | Suspect screening | Canal | LC-HRMS | In house | C |
| Niacinamide | O=C(N)C=1C=NC=CC1 | 122.04832 | Suspect screening | Canal | LC-HRMS | In house | C |
| Creatinine | O=C(O)C(N)C(C)C | 113.05928 | Suspect screening | Canal | LC-HRMS | In house | C |
| Allopurinol | O=C1NC=NC=2NN=CC12 | 136.03867 | Suspect screening | Canal | LC-HRMS | In house | C |
| 4H-3a,7-Methanoazulen-4-one, 1,2,3,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, (3R,3aR,7S,8aS)- | OCC12CCC(=CC2OC3CC(O)C1(C)C43OC4)C | 218.16722 | Suspect screening | Canal | LC-HRMS | In house | C |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17766 | Suspect screening | Canal | LC-HRMS | In house | C |
| Drofenine | CCN(CC)CCOC(=O)C(C1CCCCC1)C2=CC=CC=C2 | 317.23552 | Suspect screening | Canal | LC-HRMS | In house | C |
| Linoleic acid | CCCCCC=CCC=CCCCCCCCC(=O)O | 280.24041 | Suspect screening | Canal | LC-HRMS | In house | C |
| Eicosapentaenoic acid | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O | 302.22460 | Suspect screening | Canal | LC-HRMS | In house | D |
| Docosahexaenoic acid | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O | 328.24020 | Suspect screening | Canal | LC-HRMS | In house | D |
| 2-Ethylhexanoic anhydride | CCCCC(CC)C(=O)OC(=O)C(CC)CCCC | 270.21950 | Suspect screening | Canal | LC-HRMS | In house | D |
| 12,13-epoxy-9Z-octadecenoic acid | CCCCCC1C(O1)CC=CCCCCCCCC(=O)O | 296.23510 | Suspect screening | Canal | LC-HRMS | In house | D |
| 9-Oxononanoic acid | C(CCCC=O)CCCC(=O)O | 172.10990 | Suspect screening | Canal | LC-HRMS | In house | D |
| 11-Aoctadecenoic acid | CCCCCCC=CCCCCCCCCCC(=O)O | 282.25590 | Suspect screening | Canal | LC-HRMS | In house | D |
| Azelaic acid | C(CCCC(=O)O)CCCC(=O)O | 188.10490 | Suspect screening | Canal | LC-HRMS | In house | D |
| 4-oxonon-2-enoic Acid | CCCCCC(=O)C=CC(=O)O | 170.09430 | Suspect screening | Canal | LC-HRMS | In house | D |
| 7-Ketooctanoic acid | CC(=O)CCCCCC(=O)O | 158.09430 | Suspect screening | Canal | LC-HRMS | In house | D |
| Propanoic acid, 3-(2-butoxyethoxy)- | CCCCOCCOCCC(=O)O | 190.12050 | Suspect screening | Canal | LC-HRMS | In house | D |
| Butyl 3-hydroxy-3-4-dimethyl-5-(2-6-6-trimethyl-2-cyclohexen-1-yl)pent-4-en-1-oate | CCCCOC(=O)CC(C)(/C(=C/C1C(=CCCC1(C)C)C)/C)O | 322.25080 | Suspect screening | Canal | LC-HRMS | In house | D |
| (E)-2-(3-5-hexadienyl)-5-methylfuran | CC1=CC=C(O1)CC/C=C/C=C | 162.10450 | Suspect screening | Canal | LC-HRMS | In house | D |
| Linolenic acid | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O | 278.22460 | Suspect screening | Canal | LC-HRMS | In house | D |
| Cyclopropanecarboxylic acid- 2-[1-(3-3-dimethylcyclohexyl)ethoxy]-2-methylpropyl ester | CC(C1CCCC(C1)(C)C)OC(C)(C)COC(=O)C2CC2 | 296.23510 | Suspect screening | Canal | LC-HRMS | In house | D |
| 13-keto-9Z,11E-octadecadienoic acid | CCCCCC(=O)C=CC=CCCCCCCCC(=O)O | 294.21950 | Suspect screening | Canal | LC-HRMS | In house | D |
| Prednienic acid | CC12CC(C3C(C1CCC2(C(=O)O)O)CCC4=CC(=O)C=CC34C)O | 346.17800 | Suspect screening | Canal | LC-HRMS | In house | D |
| Leucylproline | CC(C)CC(C(=O)N1CCCC1C(=O)O)N | 228.14740 | Suspect screening | Canal | LC-HRMS | In house | D |
| Acridine | c1ccc2nc3ccccc3cc2c1 | 179.07350 | Suspect screening | Canal | LC-HRMS | In house | F |
| 1,2,3-Benzotriazole | C1=CC=C2C(=C1)NN=N2 | 119.04835 | Suspect screening | Canal | LC-HRMS | In house | F |
| 4-Octylphenol | CCCCCCCCc1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | In house | F |
| Bisphenol A diglycidyl ether | CC(C)(C1=CC=C(C=C1)OCC2CO2)C3=CC=C(C=C3)OCC4CO4 | 340.16746 | Suspect screening | Canal | LC-HRMS | In house | F |
| Benzyldimethyldodecylammonium | CCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1 | 304.30043 | Suspect screening | Canal | LC-HRMS | In house | F |
| Benzothiazole | C1=CC=C2C(=C1)N=CS2 | 135.01427 | Suspect screening | Canal | LC-HRMS | In house | F |
| 2-hydroxy-Benzothiazole | C1=CC=C2C(=C1)NC(=O)S2 | 151.00918 | Suspect screening | Canal | LC-HRMS | In house | F |
| Perfluorodecanoic acid | O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 513.96731 | Suspect screening | Canal | LC-HRMS | In house | F |
| Perfluoroundecanoic acid | OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 563.96412 | Suspect screening | Canal | LC-HRMS | In house | F |
| Perfluorooctanesulfonic acid (PFOS) | C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 499.93750 | Suspect screening | Canal | LC-HRMS | In house | F |
| Irbesartan | C12(C(N(Cc3ccc(c4c(c5[nH]nnn5)cccc4)cc3)C(=N1)CCCC)=O)CCCC2 | 428.23246 | Suspect screening | Canal | LC-HRMS | In house | F |
| (R)-1-phenylpropylamine  BMPEA  3-Phenylpropylamine  N-Methylphenethylamine  N-Ethylbenzylamin  benzyldimethylamine  N-Ethyl-4-methylaniline N,N,3-Trimethylaniline N-Ethyl-2-methylaniline N,N,2-Trimethylaniline | CCC(C1=CC=CC=C1)N  CC(CN)C1=CC=CC=C1  NCCCC1=CC=CC=C1  CNCCC1=CC=CC=C1  CCNCC1=CC=CC=C1  CN(C)CC1=CC=CC=C1  CN(C)C1=CC(C)=CC=C1 CCNC1=C(C)C=CC=C1 CN(C)C1=C(C)C=CC=C1 | 135.10480 | Suspect screening | Canal | LC-HRMS | In house | I |
| N,N,3,5-Tetramethylaniline | CN(C)C1=CC(C)=CC(C)=C1 | 149.12045 | Suspect screening | Canal | LC-HRMS | In house | I |
| Tetrahydro-1,3,5,5-tetramethyl-1H-pyrimidin-2-one | CN1CC(C)(C)CN(C)C1=O | 156.12626 | Suspect screening | Canal | LC-HRMS | In house | I |
| Fenuron | CN(C)C(=O)NC1=CC=CC=C1 | 164.09496 | Suspect screening | Canal | LC-HRMS | In house | I |
| 1-[(1R,2S)-2,6,6-trimethylcyclohex-3-en-1-yl]ethanone | CC1C=CCC(C1C(=O)C)(C)C | 166.13577 | Suspect screening | Canal | LC-HRMS | In house | I |
| Levetiracetam | CC[C@H](N1CCCC1=O)C(N)=O | 170.10553 | Suspect screening | Canal | LC-HRMS | In house | I |
| 1-(3-Aminopropyl)azepan-2-one | NCCCN1CCCCCC1=O | 170.14191 | Suspect screening | Canal | LC-HRMS | In house | I |
| 1,2,3,4-Tetrahydronaphthalene-1-ethanol 1-Phenylcyclohexan-1-ol 1,2,3,4-Tetrahydronaphthalene-2-ethanol. | C1CC(C2=CC=CC=C2C1)CCO OC1(CCCCC1)C1=CC=CC=C1 C1CC2=CC=CC=C2CC1CCO | 176.12012 | Suspect screening | Canal | LC-HRMS | In house | I |
| 3-[(4R)-4-(propan-2-yl)cyclohex-1-en-1-yl]propanal | CC(C)C1CCC(=CC1)CCC=O | 180.15142 | Suspect screening | Canal | LC-HRMS | In house | I |
| methyprylon | CCC1(CC)C(=O)NCC(C)C1=O | 183.12593 | Suspect screening | Canal | LC-HRMS | In house | I |
| Endothal | OC(=O)C1C2CCC(O2)C1C(O)=O | 186.05282 | Suspect screening | Canal | LC-HRMS | In house | I |
| 1-(1H-Indol-3-yl)butan-1-one 3-(3-Oxobutyl)-1H-indole | CCCC(=O)C1=CNC2=CC=CC=C12 CC(=O)CCc1c[nH]c2c1cccc2 | 187.09971 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2,2,5,7-Tetramethylindan-1-one | CC1=CC(C)=C2C(CC(C)(C)C2=O)=C1 | 188.12012 | Suspect screening | Canal | LC-HRMS | In house | I |
| Benzyl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OCC1=CC=CC=C1 | 192.11503 | Suspect screening | Canal | LC-HRMS | In house | I |
| Sedanolide | CCCCC1C2CCCC=C2C(=O)O1 | 194.13068 | Suspect screening | Canal | LC-HRMS | In house | I |
| Gabapentin | NCC1(CC(O)=O)CCCCC1 | 171.12593 | Suspect screening | Canal | LC-HRMS | In house | I |
| Endothal | OC(=O)C1C2CCC(O2)C1C(O)=O | 186.05282 | Suspect screening | Canal | LC-HRMS | In house | I |
| Methyl 2-acetyl-2-allylpent-4-ene-1-oate | COC(=O)C(CC=C)(CC=C)C(C)=O | 196.10994 | Suspect screening | Canal | LC-HRMS | In house | I |
| 4-Octylmorpholine | CCCCCCCCN1CCOCC1 | 199.19361 | Suspect screening | Canal | LC-HRMS | In house | I |
| alpha,alpha-Dicyclopropyl-4-methylbenzyl alcohol | CC1=CC=C(C=C1)C(O)(C1CC1)C1CC1 | 202.13577 | Suspect screening | Canal | LC-HRMS | In house | I |
| N-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Canal | LC-HRMS | In house | I |
| 3,3'-[butane-1,4-diylbis(oxy)]bispropanamine | C(CCOCCCN)COCCCN | 204.18378 | Suspect screening | Canal | LC-HRMS | In house | I |
| N,N-Dibutylaniline | CCCCN(CCCC)C1=CC=CC=C1 | 205.18305 | Suspect screening | Canal | LC-HRMS | In house | I |
| Ibuprofen | CC(C)CC1=CC=C(C=C1)C(C)C(O)=O | 206.13068 | Suspect screening | Canal | LC-HRMS | In house | I |
| 4-tert-octylphenol | CC(C)(C)CC(C)(C)c1ccc(cc1)O | 206.16707 | Suspect screening | Canal | LC-HRMS | In house | I |
| MDEA / 3,4-Methylenedioxyethamphetamine | CCNC(C)CC1=CC2=C(C=C1)OCO2 | 207.12593 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2,4,4,7-Tetramethylnona-6,8-dien-3-one oxime | CC(C)C(=NO)C(C)(C)CC=C(C)C=C | 209.17796 | Suspect screening | Canal | LC-HRMS | In house | I |
| 3-(Decyloxy)propionitrile 3-(isodecyloxy)propiononitrile | CCCCCCCCCCOCCC#N CC(C)CCCCCCCOCCC#N | 211.19361 | Suspect screening | Canal | LC-HRMS | In house | I |
| hexaminolevulinic acid | CCCCCCOC(=O)CCC(=O)CN | 215.15214 | Suspect screening | Canal | LC-HRMS | In house | I |
| 4-tert-butyl-3-hydroxy-2,6-xylylacetonitrile | CC1=CC(=C(C(=C1CC#N)C)O)C(C)(C)C | 217.14666 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | In house | I |
| Ritalinic acid | OC(=O)C(C1CCCCN1)C1=CC=CC=C1 | 219.12593 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-(3,4-dimethoxyphenyl)-3-methylbutyronitrile | COC1=CC=C(C=C1OC)C(C#N)C(C)C | 219.12593 | Suspect screening | Canal | LC-HRMS | In house | I |
| Precocene II | COC1=CC2=C(C=CC(C)(C)O2)C=C1OC | 220.10994 | Suspect screening | Canal | LC-HRMS | In house | I |
| Benzoic acid, 2-amino-, hexyl ester | CCCCCCOC(=O)C1=CC=CC=C1N | 221.14158 | Suspect screening | Canal | LC-HRMS | In house | I |
| 3,4-methylenedioxypropylamphetamine | CCCNC(C)CC1=CC2=C(C=C1)OCO2 | 221.14158 | Suspect screening | Canal | LC-HRMS | In house | I |
| ethyl 2-allyl-2-cyano-3-methylhexanoate | CCCC(C)C(CC=C)(C#N)C(=O)OCC | 223.15723 | Suspect screening | Canal | LC-HRMS | In house | I |
| 3-Phenyl-2,3-dihydro-1,3-benzothiazol-2-imine | C1=CC=C(C=C1)N2C3=CC=CC=C3SC2=N | 226.05647 | Suspect screening | Canal | LC-HRMS | In house | I |
| 7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole | CCC12COC(N1C(OC2)C(C)C)C(C)C | 227.18853 | Suspect screening | Canal | LC-HRMS | In house | I |
| (2S)-1-(tert-butoxycarbonyl)-4-oxopyrrolidine-2-carboxylic acid | CC(C)(C)OC(=O)N1CC(=O)CC1C(=O)O | 229.09502 | Suspect screening | Canal | LC-HRMS | In house | I |
| diethyl 4-oxopentane-1,2-dicarboxylate | CCOC(=O)CC(CC(=O)C)C(=O)OCC | 230.11542 | Suspect screening | Canal | LC-HRMS | In house | I |
| (Acetylazanediyl)di(ethane-2,1-diyl) diacetate | CC(=O)OCCN(CCOC(C)=O)C(C)=O | 231.11067 | Suspect screening | Canal | LC-HRMS | In house | I |
| 5,6,7,8-Tetrahydro-gamma-oxonaphthalene-2-butyric acid | OC(=O)CCC(=O)C1=CC2=C(CCCC2)C=C1 | 232.10994 | Suspect screening | Canal | LC-HRMS | In house | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Suspect screening | Canal | LC-HRMS | In house | I |
| Pentylone Dibutylone | CCCC(NC)C(=O)C1=CC=C2OCOC2=C1 CCC(N(C)C)C(=O)C1=CC=C2OCOC2=C1 | 235.12084 | Suspect screening | Canal | LC-HRMS | In house | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Canal | LC-HRMS | In house | I |
| viloxazine | CCOC1=C(OCC2CNCCO2)C=CC=C1 | 237.13649 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate | CC1(COC(=O)C2CC=CCC2C(=O)OC1)C | 238.12051 | Suspect screening | Canal | LC-HRMS | In house | I |
| N-Dodecylacrylamide | CCCCCCCCCCCCNC(=O)C=C | 239.22491 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-((2-Methyl-1-oxoallyl)oxy)ethyl 6-hydroxyhexanoate | CC(=C)C(=O)OCCOC(=O)CCCCCO | 244.13107 | Suspect screening | Canal | LC-HRMS | In house | I |
| Celestolide | CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C | 244.18272 | Suspect screening | Canal | LC-HRMS | In house | I |
| Bisnortilidin | CCOC(=O)C1(CCC=CC1N)C2=CC=CC=C2 | 245.14158 | Suspect screening | Canal | LC-HRMS | In house | I |
| Ethyl 1-benzylpiperidine-4-carboxylate | CCOC(=O)C1CCN(CC2=CC=CC=C2)CC1 | 247.15723 | Suspect screening | Canal | LC-HRMS | In house | I |
| alprenolol | CC(C)NCC(O)COC1=C(CC=C)C=CC=C1 | 249.17288 | Suspect screening | Canal | LC-HRMS | In house | I |
| (Z)-9-Cycloheptadecen-1-one. | O=C1CCCCCCC\C=C/CCCCCCC1 | 250.22967 | Suspect screening | Canal | LC-HRMS | In house | I |
| Tricyclo(3.3.1.13,7)dec-1,3-diyldi(acetic acid) | [H]C12CC3([H])CC(CC(O)=O)(C1)CC(CC(O)=O)(C2)C3 | 252.13616 | Suspect screening | Canal | LC-HRMS | In house | I |
| N-(3-Acetyl-4-hydroxyphenyl)heptan-1-amide | CCCCCCC(=O)NC1=CC(C(C)=O)=C(O)C=C1 | 263.15214 | Suspect screening | Canal | LC-HRMS | In house | I |
| triisobutyl phosphate | CC(C)COP(=O)(OCC(C)C)OCC(C)C | 266.16470 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-(3,5-dimethylhex-3-en-2-yloxy)-2-methylpropyl cyclopropanecarboxylate | CC(C)C=C(C)C(C)OC(C)(C)COC(=O)C1CC1 | 268.20384 | Suspect screening | Canal | LC-HRMS | In house | I |
| Tridecyl methacrylate Isotridecyl methacrylate tetradecyl acrylate | CCCCCCCCCCCCCOC(=O)C(C)=C CC(C)CCCCCCCCCCOC(=O)C(C)=C CCCCCCCCCCCCCCOC(=O)C=C | 268.24023 | Suspect screening | Canal | LC-HRMS | In house | I |
| N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine | COCCCNCC1=CC(OC)=C(OC)C(OC)=C1 | 269.16271 | Suspect screening | Canal | LC-HRMS | In house | I |
| Decyl 5-oxo-L-prolinate | CCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 269.19909 | Suspect screening | Canal | LC-HRMS | In house | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Canal | LC-HRMS | In house | I |
| Octanoic anhydride | CCCCCCCC(=O)OC(=O)CCCCCCC | 270.21949 | Suspect screening | Canal | LC-HRMS | In house | I |
| Alphameprodine [INN:BAN:DCF] | CC[C@H]1CN(C)CC[C@]1(OC(=O)CC)C1=CC=CC=C1 | 275.18853 | Suspect screening | Canal | LC-HRMS | In house | I |
| 5alpha-Androstan-3beta-ol | C[C@@]12CCC[C@H]1[C@@H]1CC[C@H]3C[C@@H](O)CC[C@]3(C)[C@H]1CC2 | 276.24532 | Suspect screening | Canal | LC-HRMS | In house | I |
| Terbucarb | CNC(=O)OC1=C(C=C(C)C=C1C(C)(C)C)C(C)(C)C | 277.20418 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-(Decanoylamino)ethanesulfonic acid | CCCCCCCCCC(=O)NCCS(O)(=O)=O | 279.15043 | Suspect screening | Canal | LC-HRMS | In house | I |
| Brefeldin A | [H][C@@]12C[C@H](O)C[C@@]1([H])[C@H](O)\C=C\C(=O)O[C@@H](C)CCC\C=C\2 | 280.16746 | Suspect screening | Canal | LC-HRMS | In house | I |
| p-(1-(p-Pentylphenyl)vinyl)anisole | CCCCCC1=CC=C(C=C1)C(=C)C1=CC=C(OC)C=C1 | 280.18272 | Suspect screening | Canal | LC-HRMS | In house | I |
| Methyl 3-oxohexadecanoate | CCCCCCCCCCCCCC(=O)CC(=O)OC | 284.23514 | Suspect screening | Canal | LC-HRMS | In house | I |
| Sodium N-methyl-N-(1-oxododecyl)-ß-alaninate | CCCCCCCCCCCC(=O)N(O)CCC(=O)[O-]·[Na+] | 285.23039 | Suspect screening | Canal | LC-HRMS | In house | I |
| norethisterone | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C | 298.19328 | Suspect screening | Canal | LC-HRMS | In house | I |
| Sodium decyl phthalate diisopentyl phthalate CROMOPHTAL DPP RED TFP | [Na+].CCCCCCCCCCOC(=O)C1=CC=CC=C1C([O-])=O CC(C)CCOC(=O)C1=CC=CC=C1C(=O)OCCC(C)C CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCC | 306.18311 | Suspect screening | Canal | LC-HRMS | In house | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Canal | LC-HRMS | In house | I |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Canal | LC-HRMS | In house | I |
| homodihydrocapsaicin-I | CC(C)CCCCCCCC(=O)NCC1=CC(=C(C=C1)O)OC | 321.23039 | Suspect screening | Canal | LC-HRMS | In house | I |
| 15-(tert-Butyl)-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecine | CC(C)(C)C1=CC2=C(C=C1)OCCOCCOCCOCCO2 | 324.19367 | Suspect screening | Canal | LC-HRMS | In house | I |
| hydrogen N-(1-oxododecyl)-L-glutamic acid | CCCCCCCCCCCC(=O)NC(CCC(=O)O)C(=O)O | 329.22022 | Suspect screening | Canal | LC-HRMS | In house | I |
| ETHYL ARACHIDONATE | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OCC | 332.27153 | Suspect screening | Canal | LC-HRMS | In house | I |
| Pentadecyl 5-oxo-L-prolinate | CCCCCCCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 339.27734 | Suspect screening | Canal | LC-HRMS | In house | I |
| MEGESTROL | [H][C@@]12CC[C@](O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(C)C2=CC(=O)CC[C@]12C | 342.21949 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-Hydroxypropane-1,3-diyl bis(2-propylvalerate) | CCCC(CCC)C(=O)OCC(O)COC(=O)C(CCC)CCC | 344.25627 | Suspect screening | Canal | LC-HRMS | In house | I |
| Bis(tert-butyl) 1,4-dihydro-2,6-dimethyl-4-propylpyridine-3,5-dicarboxylate | CCCC1C(C(=O)OC(C)(C)C)=C(C)NC(C)=C1C(=O)OC(C)(C)C | 351.24096 | Suspect screening | Canal | LC-HRMS | In house | I |
| GLYCERYL LINOLENATE | CCC=CCC=CCC=CCCCCCCCC(=O)OCC(O)CO | 352.26136 | Suspect screening | Canal | LC-HRMS | In house | I |
| PEG-2 OLEAMIDE N,N-bis(2-hydroxyethyl)oleamide | CCCCCCCCC=CCCCCCCCC(=O)NCCOCCO CCCCCCCC\C=C/CCCCCCCC(=O)N(CCO)CCO | 369.32429 | Suspect screening | Canal | LC-HRMS | In house | I |
| eplerenone | COC(=O)[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@@]23O[C@@H]2C[C@@]2(C)[C@@H](CC[C@@]22CCC(=O)O2)[C@H]13 | 414.20424 | Suspect screening | Canal | LC-HRMS | In house | I |
| Budesonide | CCCC1O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)C=C[C@]5(C)[C@H]4[C@@H](O)C[C@]3(C)[C@@]2(O1)C(=O)CO | 430.23554 | Suspect screening | Canal | LC-HRMS | In house | I |
| Isodecyl isononyl phthalate Decyl nonyl phthalate | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC© CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC | 432.32396 | Suspect screening | Canal | LC-HRMS | In house | I |
| Glyceryl phosphate | OCC(O)COP(O)(O)=O | 172.01367 | Suspect screening | Canal | LC-HRMS | In house | I |
| Acamprosate | CC(=O)NCCCS(O)(=O)=O | 181.04088 | Suspect screening | Canal | LC-HRMS | In house | I |
| Sulfuric acid, monohexyl ester, sodium salt | [Na+].CCCCCCOS([O-])(=O)=O | 182.06128 | Suspect screening | Canal | LC-HRMS | In house | I |
| 4-morpholineethanesulfonic acid | OS(=O)(=O)CCN1CCOCC1 | 195.05653 | Suspect screening | Canal | LC-HRMS | In house | I |
| 3-Amino-4-methoxybenzenesulfonic acid 2-Amino-5-methoxybenzenesulfonic acid 5-Amino-6-hydroxytoluene-3-sulphonic acid | COC1=CC=C(C=C1N)S(O)(=O)=O COC1=CC(=C(N)C=C1)S(O)(=O)=O CC1=CC(=CC(N)=C1O)S(O)(=O)=O | 203.02523 | Suspect screening | Canal | LC-HRMS | In house | I |
| 3-morpholin-4-ylpropane-1-sulfonic acid | C1COCCN1CCCS(=O)(=O)O | 209.07218 | Suspect screening | Canal | LC-HRMS | In house | I |
| 1-(2,5-Dihydroxyphenyl)octan-1-one | CCCCCCCC(=O)C1=C(O)C=CC(O)=C1 | 236.14124 | Suspect screening | Canal | LC-HRMS | In house | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Canal | LC-HRMS | In house | I |
| Loxoprofen alcohol | CC(C1=CC=C(C=C1)CC2CCCC2O)C(=O)O | 248.14124 | Suspect screening | Canal | LC-HRMS | In house | I |
| Propachlor ESA | CC(C)N(C(=O)CS(O)(=O)=O)C1=CC=CC=C1 | 257.07218 | Suspect screening | Canal | LC-HRMS | In house | I |
| Hydroxypethidine | CCOC(=O)C1(CCN(C)CC1)C1=CC(O)=CC=C1 | 263.15214 | Suspect screening | Canal | LC-HRMS | In house | I |
| Ethyl 3-(3,4,5-trimethoxyphenyl)propionate Butyl 3,4,5-trimethoxybenzoate | CCOC(=O)CCC1=CC(OC)=C(OC)C(OC)=C1 CCCCOC(=O)C1=CC(OC)=C(OC)C(OC)=C1 | 268.13107 | Suspect screening | Canal | LC-HRMS | In house | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Canal | LC-HRMS | In house | I |
| Efavirenz | FC(F)(F)[C@]1(OC(=O)NC2=CC=C(Cl)C=C12)C#CC1CC1 | 315.02739 | Suspect screening | Canal | LC-HRMS | In house | I |
| Triaziflam | CC(COC1=CC(C)=CC(C)=C1)N=C1NC(=N)N=C(N1)C(C)(C)F | 333.19649 | Suspect screening | Canal | LC-HRMS | In house | I |
| NONOXYNOL-4 | CCCCCCCCCC1=CC=CC=C1OCCOCCOCCOCCO | 396.28757 | Suspect screening | Canal | LC-HRMS | In house | I |
| simvastatin hydroxyl acid | CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 436.28249 | Suspect screening | Canal | LC-HRMS | In house | I |
| Perfluorooctanesulfonic acid | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | In house | I |
| N-Ethylperfluorooctane-1-sulfonamide | CCNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 526.98478 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-Methylene-3-butyn-1-ol 1-Methoxybut-1-en-3-yne | OCC(=C)C#C COC=CC#C | 82.04186 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-(1,1-Dimethylethyl)-4-(1-methyl-1-phenylethyl)phenol | CC(C)(C)C1=C(O)C=CC(=C1)C(C)(C)C1=CC=CC=C1 | 268.18272 | Suspect screening | Canal | LC-HRMS | In house | I |
| 2-((2-Hydroxyethyl)(3-methoxypropyl)amino)ethyl methacrylate | COCCCN(CCO)CCOC(=O)C(C)=C | 245.16271 | Suspect screening | Canal | LC-HRMS | In house | I |
| 4-O-Desmethyl 4-O-Ethyl Trimethoprim | CCOC1=C(OC)C=C(CC2=CNC(=N)NC2=N)C=C1OC | 304.15354 | Suspect screening | Canal | LC-HRMS | In house | I |
| 4-Acetamidoantipyrine | CN1N(C(=O)C(NC(C)=O)=C1C)C1=CC=CC=C1 | 245.11643 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-Formylaminoantipyrine | CN1N(C(=O)C(NC=O)=C1C)C1=CC=CC=C1 | 231.10078 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5-Methylbenzotriazole | CC1=CC=C2NN=NC2=C1 | 133.06400 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Benzotriazole | N1N=NC2=CC=CC=C12 | 119.04835 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Diphenhydramine | CN(C)CCOC(C1=CC=CC=C1)C1=CC=CC=C1 | 255.16231 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Lidocaine | CCN(CC)CC(=O)NC1=C(C)C=CC=C1C | 234.17321 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Metoprolol | COCCC1=CC=C(OCC(O)CNC(C)C)C=C1 | 267.18344 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| *N*-Desmethylvenlafaxine | CNCC(C1=CC=C(OC)C=C1)C1(O)CCCCC1 | 263.18853 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Terbutryn | CCNC1=NC(NC(C)(C)C)=NC(SC)=N1 | 241.13612 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Galaxolidone | CC1C(C)(C)C2=CC3=C(C=C2C1(C)C)C(=O)OCC3C | 272.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Venlafaxine | COC1=CC=C(C=C1)C(CN(C)C)C1(O)CCCCC1 | 277.20418 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4,6-Bis(propylamino)-s-triazin-2-ol | CCCNC1=NC(=NC(=O)N1)NCCC | 211.14331 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Methadone | CCC(=O)C(CC(C)N(C)C)(C1=CC=CC=C1)C1=CC=CC=C1 | 309.20926 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Propranolol | CC(C)NCC(O)COC1=CC=CC2=CC=CC=C12 | 259.15723 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-[4-(2-aminoethyl)phenyl]-*N*,*N*-dimethylacetamide | CN(C)C(=O)CC1=CC=C(C=C1)CCN | 206.14191 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1-Phenyl-1,3-octadecanedione | CCCCCCCCCCCCCCCC(=O)CC(=O)C1=CC=CC=C1 | 358.28718 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-imidazol-1-yl-2-methylpyridine | CC1=C(C=CC=N1)N2C=CN=C2 | 159.07965 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Bortezomib | B(C(CC(C)C)NC(=O)C(CC1=CC=CC=C1)NC(=O)C2=NC=CN=C2)(O)O | 384.19689 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| a-Hydroxymetoprolol | CC(C)NCC(COC1=CC=C(C=C1)C(COC)O)O | 283.17836 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-imidazol-1-yl-2-methylpyridine | CC1=C(C=CC=N1)N2C=CN=C2 | 159.07965 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 10-Hydroxydecanoic acid | C(CCCCC(=O)O)CCCCO | 188.14124 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,4,4,7-Tetramethylnona-6,8-dien-3-one oxime | CC(C)C(=NO)C(C)(C)CC=C(C)C=C | 209.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(N-Ethyl-p-toluidino)ethanol | CCN(CCO)C1=CC=C(C)C=C1 | 179.13101 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate | CCOCCOCCOCCOC(=O)C(C)=C | 246.14672 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Arachidonoyl glycerol | CCCCC/C=C\\C/C=C\\C/C=C\\C/C=C\\CCCC(=O)OC[C@H](CO)O | 378.27701 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-cyclohexylidene-2-phenylacetonitrile | N#CC(=C1CCCCC1)C1=CC=CC=C1 | 197.12045 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Undecyl-1H-imidazole-4-carboxylic acid | CCCCCCCCCCCC1=NC(=CN1)C(O)=O | 266.19943 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-(2-(2-Hydroxyethoxy)ethylimino)-2,2-dimethylpropyl dodecanoate | CCCCCCCCCCCC(=O)OCC(C)(C)C=NCCOCCO | 371.30356 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (7aR)-3a,7a-dihydro-3H-1-benzofuran-2-one | C1C2C=CC=C[C@H]2OC1=O | 136.05243 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-Nitrophenylacetylene | [O-][N+](=O)C1=CC=CC(=C1)C#C | 147.03203 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-Heptylbenzoic acid | CCCCCCCC1=CC=C(C=C1)C(O)=O | 220.14633 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5-Fluoro ADBICA | CC(C)(C)C(C(=O)N)NC(=O)C1=CN(C2=CC=CC=C21)CCCCCF | 361.21656 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Aliskiren | COCCCOC1=CC(C[C@@H](C[C@H](N)[C@@H](O)C[C@@H](C(C)C)C(=O)NCC(C)(C)C(N)=O)C(C)C)=CC=C1OC | 551.39344 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| alprenolol | CC(C)NCC(O)COC1=CC=CC=C1CC=C | 249.17288 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Azithromycin | CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O | 748.50853 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| CGP 2160 |  | 492.32396 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Heterocodeine | CN1CC[C@]23[C@@H]4[C@H]1CC5=C2C(=C(C=C5)O)O[C@H]3[C@H](C=C4)OC | 299.15214 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Deschloralachlor |  | 235.15723 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Deschlormetolachlor |  | 249.17288 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Ethyl N-(2,3-dimethyl-2-isopropyl-1-oxobutyl)glycinate | CCOC(=O)CNC(=O)C(C)(C(C)C)C(C)C | 243.18344 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| arachidonamide | CCCCC/C=C\\C/C=C\\C/C=C\\C/C=C\\CCCC(=O)N | 303.25621 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1-(3-methoxypropyl)piperidin-4-one | COCCCN1CCC(=O)CC1 | 171.12593 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| hexa-2,4-dienoic acid | CC=CC=CC(O)=O | 112.05243 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| hexacarbacholine |  | 375.29713 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-[4-(3-aminocyclohexyl)phenyl]propan-1-ol | CC(CO)C1=CC=C(C=C1)C2CCCC(C2)N | 233.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| thymine | CC1=CNC(=O)NC1=O | 126.04293 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 16-Hydroxyhexadecanoic acid | OCCCCCCCCCCCCCCCC(O)=O | 272.23514 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Methylacenaphthylene | CC1=CC2=CC=CC3=C2C1=CC=C3 | 166.07825 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| N-Dodecyl-N-methylaniline | CCCCCCCCCCCCN(C)C1=CC=CC=C1 | 275.26130 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Nicotine met 7-192 |  | 192.12626 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5-Methoxybenzothiazole-2(3H)-thione | COC1=CC=C2SC(=S)NC2=C1 | 196.99691 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| carbetapentane | CCOC(=O)C1(CCCC1OCCN(CC)CC)C1=CC=CC=C1 | 333.23039 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| O-Desmethyltramadol | CN(C)CC1CCCCC1(O)C1=CC=CC(O)=C1 | 249.17288 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Bakuchiol | CC(=CCC[C@@](C)(C=C)/C=C/C1=CC=C(C=C1)O)C | 256.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| ethyl 4-[(3-ethoxy-3-oxopropyl)(methyl)amino]butanoate | CCOC(=O)CCCN(C)CCC(=O)OCC | 245.16271 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| pentadecan-15-olide | C1CCCCCCCOC(=O)CCCCCC1 | 240.20893 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| N'-(5-methoxy-1,2,3,4-tetrahydroquinolin-8-yl)propane-1,3-diamine | COC1=C2CCCNC2=C(C=C1)NCCCN | 235.16846 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Prolintane | CCCC(CC1=CC=CC=C1)N1CCCC1 | 217.18305 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Fosinopril | CCC(=O)OC(C(C)C)OP(=O)(CCCCC1=CC=CC=C1)CC(=O)N2C[C@@H](C[C@H]2C(=O)O)C3CCCCC3 | 563.30119 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Venlafaxine | CN(C)CC(C1=CC=C(C=C1)OC)C2(CCCCC2)O | 277.20418 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-(5-Methyl-1-methylene-4-hexenyl)-1-(4-methylpent-3-enyl)cyclohexene. | CC(=CCCC1=CCC(CC1)C(=C)CCC=C(C)C)C | 272.25040 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Ethylestrenol | CC[C@]1(O)CC[C@H]2[C@@H]3CCC4=CCCC[C@@H]4[C@H]3CC[C@]12C | 288.24532 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-(2,2-dimethyl-3,4-dihydro-2h-chromen-6-yl)-2-methylbutan-2-ol | CC1(CCC2=C(O1)C=CC(=C2)CCC(C)(C)O)C | 248.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (14S)-14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid | CC12CCCC(C1CCC(=C)C2CCC(=C)C(CO)O)(C)C(=O)O | 336.23006 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Quinuclidin-3-one | O=C1CN2CCC1CC2 | 125.08406 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-[(Undec-10-en-1-yl)oxy]propanenitrile | C=CCCCCCCCCCOCCC#N | 223.19361 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 15-Hydroperoxyeicosa-8Z,11Z,13E-trienoate | CCCCCC(/C=C/C=C\\C/C=C\\CCCCCCC(=O)O)OO | 338.24571 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Mebeverine | CCN(CCCCOC(=O)C1=CC(=C(C=C1)OC)OC)C(C)CC2=CC=C(C=C2)OC | 429.25152 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| rac-threo-Dihydrobupropion |  | 241.12334 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(Dimethylamino)-3,5,5-trimethylcyclohex-2-en-1-one | CN(C)C1=C(C)CC(C)(C)CC1=O | 181.14666 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5-(4-Aminophenyl)imidazolidine-2,4-dione | C1=CC(=CC=C1C2C(=O)NC(=O)N2)N | 191.06948 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-((((2-Amino-6-chlorophenyl)methyl)methylamino)acetyl)morpholine | CN(CC(=O)N1CCOCC1)CC1=C(N)C=CC=C1Cl | 297.12440 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5-(2-Aminopropyl)indole (5-API, 5-IT) | CC(CC1=CC2=C(C=C1)NC=C2)N | 174.11570 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| brompheniramine | CN(C)CCC(C1=CC=C(Br)C=C1)C1=CC=CC=N1 | 318.07316 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Icaridine | CC1(CC2(CC(N1)(C)C)OCC(O2)CO)C | 229.16779 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 12-hydroxystearic acid | CCCCCCC(CCCCCCCCCCC(=O)O)O | 300.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Myristoleic acid methyl ester | CCCCC=CCCCCCCCC(=O)OC | 240.20893 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Prednisolone tebutate | CC(C)(C)CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@]12C | 458.26684 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| retinol | C\C(=C/CO)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C | 286.22967 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Methylamino-1-(3,4-Methylenedioxyphenyl)propan-1-one (bkMDMA, methylone) |  | 207.08954 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| DL-alpha Tocopheryl nicotinate | CC1=C(C(=C(C2=C1OC(CC2)(C)CCCC(C)CCCC(C)CCCC(C)C)C)OC(=O)C3=CN=CC=C3)C | 535.40255 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3,4-Diacetylhexane-2,5-dione | CC(=O)C(C(C(C)=O)C(C)=O)C(C)=O | 198.08921 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Hexanedioic acid, diethenyl ester | C=COC(=O)CCCCC(=O)OC=C | 198.08921 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| beta.-Alanine, N-ethyl-N-phenyl-, methyl ester | CCN(CCC(=O)OC)C1=CC=CC=C1 | 207.12593 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1-Monopalmitin | CCCCCCCCCCCCCCCC(=O)OCC(CO)O | 330.27701 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-(2-Hydroxyethoxy)phenol | OCCOC1=CC=CC(O)=C1 | 154.06299 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-[Ethyl(3-methylphenyl)amino]propane-1-sulfonic acid | CCN(CCCS(O)(=O)=O)C1=CC(C)=CC=C1 | 257.10856 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5-Oxomyristic acid | CCCCCCCCCC(=O)CCCC(O)=O | 242.18819 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Benz(c)acridine | C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4N=C32 | 229.08915 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Cyclohexaneacetic acid | OC(=O)CC1CCCCC1 | 142.09938 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| dimethyl cyclohexane-1,4-dicarboxylate | C1CC2(CCC1CC(=O)O)OCCO2 | 200.10486 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Ethyl cyanocycloheptylideneacetate | CCOC(=O)C(C#N)=C1CCCCCC1 | 207.12593 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| JWH 122 N-(4-pentenyl) analog | CC1=CC=C(C2=CC=CC=C12)C(=O)C3=CN(C4=CC=CC=C43)CCCC=C | 353.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 17ß-hydroxy-17-(3-hydroxypropyl)androst-4-ene-4-one |  | 346.25080 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,4-Tridecadienal | C[C@]12CC[C@H]3[C@@H](CCC4C(=O)CCC[C@]34C)[C@@H]1CC[C@]2(O)CCCO | 194.16707 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,5-Dioctylbenzene-1,4-diol | CCCCCCCCC=CC=CC=O | 334.28718 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Acridin | CCCCCCCCC1=CC(O)=C(CCCCCCCC)C=C1O | 179.07350 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,4-Di-tert-butyl-5-nitrophenyl methyl carbonate | CC(C)(C)C1=CC(=C(C=C1[N+](=O)[O-])OC(=O)OC)C(C)(C)C | 309.15762 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-Methyldodecanonitrile | CCCCCCCCCC(C)CC#N | 195.19870 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-ethyl-2-methyl-2-isopentyl-1,3-oxazolidine | CCC1COC(N1)(C)CCC(C)C | 185.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Brinzolamide | CCNC1CN(S(=O)(=O)C2=C1C=C(S2)S(=O)(=O)N)CCCOC | 383.06433 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (1alpha,2beta,5alpha)-5-Methyl-2-(1-methylethyl)cyclohexyl (R)-N-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-beta-alaninate | CC1CCC(C(C1)OC(=O)CCNC(=O)C(C(C)(C)CO)O)C(C)C | 357.25152 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl (ethylamino)(oxo)acetate | CN(C)CCOC1=CC=CC=C1CC2=CC=CC=C2 | 255.18344 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (3,4-diethoxyphenyl)acetonitrile | CCOC1=C(OCC)C=C(CC#N)C=C1 | 205.11028 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1,4:3,6-Dianhydro-D-glucitol monostearate | CCCCCCCCCCCCCCCCCC(=O)OC1COC2C1OCC2O | 412.31888 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 12-hydroxystearic acid | CCCCCCC(O)CCCCCCCCCCC(O)=O | 300.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,2'-dimorpholinyldiethyl ether |  | 244.17869 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,3,5,6,8,9,11,12,14,15-Decahydro-4,13-(ethanoxyethanoxyethano)-4H,13H-1,7,10,16,4,13-benzotetraoxadiazacyclooctadecine | C1COCCOCCN2CCOCCOCCN1CCOC3=CC=CC=C3OCC2 | 424.25734 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,6-diethyl-p-toluidine | CCC1=CC(C)=CC(CC)=C1N | 163.13610 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,6-Dihydroxyethylaminotoluene | CC1=C(NCCO)C=CC=C1NCCO | 210.13683 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(Dimethylamino)-3,5,5-trimethylcyclohex-2-en-1-one | CN(C)C1=C(C)CC(C)(C)CC1=O | 181.14666 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(Methylthio)benzothiazol | CSC1=NC2=CC=CC=C2S1 | 181.00199 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-hydroxy-10-undecenoic acid | C=CCCCCCCCC(C(=O)O)O | 200.14124 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-phenyl ethyl propionate | CCOC(=O)C(C)C1=CC=CC=C1 | 178.09938 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3,7-Bis(1-methyl-1-phenylethyl)-10H-phenothiazine | CC(C)(C1=CC=CC=C1)C1=CC2=C(NC3=CC=C(C=C3S2)C(C)(C)C2=CC=CC=C2)C=C1 | 435.20207 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-cyclohexyl-2-cyclohexylimino-oxazolidin-4-one | O=C1COC(=NC2CCCCC2)N1C1CCCCC1 | 264.18378 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-Dodecylaniline | CCCCCCCCCCCCC1=CC=C(N)C=C1 | 261.24565 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5,6-Dimethyl-1H-benzotriazole | CC1=CC2=C(C=C1C)N=NN2 | 147.07965 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 6-(nonylamino)-6-oxoperoxyhexanoic acid | CCCCCCCCCNC(=O)CCCCC(=O)OO | 287.20966 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Acridone | O=C1C2=CC=CC=C2NC2=CC=CC=C12 | 195.06841 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Ametoctradin | CCCCCCCCC1=C(N)N2N=CN=C2N=C1CC | 275.21100 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| artemether | CO[C@H]1O[C@@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3 | 298.17802 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Bufencarb |  | 221.14158 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Lobendazole | CCOC(=O)NC1=NC2=CC=CC=C2N1 | 205.08513 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Coniine | CCC[C@H]1CCCCN1 | 127.13610 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| cyclododecanol | OC1CCCCCCCCCCC1 | 184.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Cytochalasin B | C[C@H]1[C@H]2[C@H](CC3=CC=CC=C3)NC(=O)[C@]22OC(=O)\C=C\[C@H](O)CCC[C@@H](C)C\C=C\[C@H]2[C@H](O)C1=C | 479.26717 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Desoxycodeine C | CN1CCC23C4C1CC5=C2C(=C(C=C5)OC)OC3C=CC4 | 283.15723 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Dimethyl 4,4'-(1,6-hexanediylbis(iminocarbonyl))bisbenzoate |  | 440.19474 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Dimetridazole | CN1C(C)=NC=C1N(=O)=O | 141.05383 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| echothiopate |  | 256.11363 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Ethyl hexahydro-1H-azepine-1-propionate | CCOC(=O)CCC1CCCCCN1 | 199.15723 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| JWH-081 | CCCCCN1C=C(C2=CC=CC=C21)C(=O)C3=CC=C(C4=CC=CC=C43)OC | 371.18853 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Mepronil | CC(C)OC1=CC=CC(=C1)\N=C(/O)C1=CC=CC=C1C | 269.14158 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| methyl 5-(dimethylamino)-2-methyl-5-oxopentanoate | COC(=O)C(C)CCC(=O)N(C)C | 187.12084 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| nicomorphine | CN1CC[C@@]23[C@H]4OC5=C2C(C[C@@H]1[C@@H]3C=C[C@@H]4OC(=O)C1=CC=CN=C1)=CC=C5OC(=O)C1=CC=CN=C1 | 495.17942 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| PEG-12 |  | 546.32515 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| PEG-13 |  | 590.35136 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Ranitidine TP 45 |  | 139.09971 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Streptolin | C1C(C2C(C(=O)N1)N=C(N2)NC3C(C(C(C(O3)CO)OC(=O)N)O)NC(=O)CC(CCCNC(=O)CC(CCCN)N)N)O | 630.34492 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Zolmitriptan | CN(C)CCC1=CNC2=CC=C(C[C@H]3COC(=O)N3)C=C12 | 287.16338 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| artemether | CO[C@H]1O[C@@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3 | 298.17802 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-hydroxybenzaldehyde | OC1=CC=C(C=O)C=C1 | 122.03678 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Oxitropium | CC[N+]1(C2CC(CC1C3C2O3)OC(=O)C(CO)C4=CC=CC=C4)C | 332.18618 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Telbivudine | CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)O | 242.09027 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (3aS,4R,5S,6S,8R,9R,9aR,10R)-6-ethenyl-5-hydroxy-4,6,9,10-tetramethyl-1-oxodecahydro-3a,9-propanocyclopenta[8]annulen-8-yl[(methylsulfonyl)oxy]acetate |  | 456.21818 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| N-[4-[2-[4-(3-cyanophenyl)piperazin-1-yl]ethyl]cyclohexyl]-3-methoxypropanamide | COCCC(=O)NC1CCC(CC1)CCN2CCN(CC2)C3=CC=CC(=C3)C#N | 398.26818 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (epoxyethyl)benzene | C1OC1C1=CC=CC=C1 | 120.05751 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1,3,3a,4,5,6,7,8,9,10,11,13a-Dodecahydrocyclododeca( c)furan. | C1CCCCC2COCC2C=CCCC1 | 208.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1,6-Octadiene, 8-methoxy- | COCC=CCCCC=C | 140.12012 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-hydroxy-1-(4-methoxyphenyl)-4-methylpentan-3-one | CC(C)C(=O)C(CC1=CC=C(C=C1)OC)O | 222.12559 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1-Hydroxy-N-[2-(tetradecyloxy)phenyl]naphthalene-2-carboxamide | CCCCCCCCCCCCCCOC1=C(NC(=O)C2=CC=C3C=CC=CC3=C2O)C=CC=C1 | 475.30864 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1-Nonyne | CCCCCCCC#C | 124.12520 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,4,5-Triphenylimidazole | N1C(=NC(=C1C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1 | 296.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,6,6-trimethylbicyclo[3.1.1]heptane-3-carbaldehyde | CC1C2CC(CC1C=O)C2(C)C | 166.13577 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(Ethylanilino)ethyl benzoate | CCN(CCOC(=O)C1=CC=CC=C1)C1=CC=CC=C1 | 269.14158 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Butanone, 1-(4-chlorophenoxy)-1-(1H-imidazol-1-yl)-3,3-dimethyl- = Climbazole | CC(C)(C)C(=O)C(OC1=CC=C(Cl)C=C1)N1C=CN=C1 | 292.09786 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-chloro-5-sec-hexadecylhydroquinone | CCCCCCCCCCCCCCC(C)C1=CC(O)=C(Cl)C=C1O | 368.24821 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-ethylhexyl nonanoate | CCCCCCCCC(=O)OCC(CC)CCCC | 270.25588 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Octylfuran | CCCCCCCCC1=CC=CO1 | 180.15142 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3,3',5,5'-tetra-tert-butylbiphenyl-2,2'-diol | CC(C)(C)C1=CC(=C(O)C(=C1)C(C)(C)C)C1=C(O)C(=CC(=C1)C(C)(C)C)C(C)(C)C | 410.31848 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-[Ethyl(3-methylphenyl)amino]propane-1-sulfonic acid | CCN(CCCS(O)(=O)=O)C1=CC(C)=CC=C1 | 257.10856 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-Methylcyclopentadecan-1-one | CC1CCCCCCCCCCCCC(=O)C1 | 238.22967 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-[4-[4-(Hydroxydiphenylmethyl)-1-piperidinyl]-1-oxobutyl]-a,a-dimethyl-ethyl ester benzeneacetic acid |  | 527.30356 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-Methyl-2-nonylphenol | CCCCCCCCCC1=C(O)C=CC(C)=C1 | 234.19837 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 9,14-dihydroxyoctadecanoic acid | CCCCC(CCCCC(CCCCCCCC(=O)O)O)O | 316.26136 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 9,10-Dihydroxystearic acid | CCCCC(CCCCC(CCCCCCCC(=O)O)O)O | 316.26136 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Cambendazole | CC(C)O\C(O)=N\C1=CC=C2N=C(NC2=C1)C1=CSC=N1 | 302.08375 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Arfendazam | CCOC(=O)N1CCC(=O)N(C2=CC=CC=C2)C2=CC(Cl)=CC=C12 | 344.09277 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| artemether | CO[C@H]1O[C@@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3 | 298.17802 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| azelaic acid | OC(=O)CCCCCCCC(O)=O | 188.10486 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Benzeneacetic acid, 4-[4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]-1-oxobutyl]-a,a-dimethyl- |  | 499.27226 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Benzenesulfonic acid, 4-methyl-, butyl ester | CCCCOS(=O)(=O)C1=CC=C(C)C=C1 | 228.08202 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Bis(2-phenylvinyl)phenol | C1=CC=C(C=C1)C=CC2=C(C(=CC=C2)O)C=CC3=CC=CC=C3 | 298.13577 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Calcium Ionophore A23187 | CC1CCC2(C(CC(C(O2)C(C)C(=O)C3=CC=CN3)C)C)OC1CC4=NC5=C(O4)C=CC(=C5C(=O)O)NC | 523.26824 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Chlorcyclizine | CN1CCN(CC1)C(C1=CC=CC=C1)C1=CC=C(Cl)C=C1 | 300.13933 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Dehydroxy Ractopamine | CC(CCC1=CC=C(C=C1)O)NCCC2=CC=C(C=C2)O | 285.17288 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| dibutyl 2,2'-thiobisacetate | CCCCOC(=O)CSCC(=O)OCCCC | 262.12388 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-(o-Butoxyphenoxy)-1,2-propanediol | CCCCOC1=CC=CC=C1OCC(CO)O | 240.13616 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Diisopropyl undecanedioate | CC(C)OC(=O)CCCCCCCCCC(=O)OC(C)C | 300.23006 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Dimethyl (3-oxo-2-pentylcyclopentyl)malonate | CCCCCC1C(CCC1=O)C(C(=O)OC)C(=O)OC | 284.16237 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Equilin | C[C@]12CC[C@H]3C(=CCC4=CC(O)=CC=C34)[C@@H]1CCC2=O | 268.14633 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid | C1=CC(=CC=C1CC(C(=O)O)O)O | 182.05791 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Herbimycin A | CO[C@H]1C[C@H](C)[C@@H](OC)C2=CC(=O)C=C(NC(=O)\C(C)=C\C=C/C(OC)[C@@H](OC(N)=O)\C(C)=C\[C@H](C)C1OC)C2=O | 574.28903 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-[2-[(1R,2R)-1-amino-2-hydroxypropyl]-5-hydroxy-4-[(4-hydroxyphenyl)methyl]imidazol-1-yl]acetaldehyde | C[C@H]([C@@H](C1=NC(=C(N1CC=O)O)CC2=CC=C(C=C2)O)N)O | 305.13756 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Isopentadecyl methacrylate | CC(C)CCCCCCCCCCCCOC(=O)C(C)=C | 296.27153 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Isopimaric acid | C[C@@]1(CC[C@H]2C(C1)=CC[C@@H]1[C@]2(C)CCC[C@@]1(C)C(O)=O)C=C | 302.22458 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Isopropyl L-methionate hydrochloride | CC(C)OC(=O)C(CCSC)N.Cl | 191.09800 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| alpha-Oxothiophen-2-acetonitrile | C1=CSC(=C1)C(=O)C#N | 136.99354 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Decylthioacetic acid | CCCCCCCCCCSCC(=O)O | 232.14970 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Florfenicol amine | CS(=O)(=O)C1=CC=C(C=C1)C(C(CF)N)O | 247.06784 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Chlorpheniramine, Desmethyl |  | 260.10803 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,3-Dihydroxypropyl 3-(hexylthio)propionate | CCCCCCSCCC(=O)OCC(O)CO | 264.13953 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Olanzapine, N-desmethyl | CC1=CC2=C(S1)NC3=CC=CC=C3N=C2N4CCNCC4 | 298.12522 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Oxazolam | C[C@@H]1CN2CC(=O)NC3=CC=C(Cl)C=C3[C@@]2(O1)C1=CC=CC=C1 | 328.09786 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| sulfapyrazole | CC1=NN(C(NS(=O)(=O)C2=CC=C(N)C=C2)=C1)C1=CC=CC=C1 | 328.09940 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-{2-hydroxy-6-[5-(1,4,5-trihydroxyundecyl)tetrahydrofuran-2-yl]hexyl}-5-methylfuran-2(5h)-one | CCCCCCC(C(CCC(C1CCC(O1)CCCCC(CC2=CC(OC2=O)C)O)O)O)O | 470.32435 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Desoxycortone 21-(3-phenylpropionate) |  | 462.27701 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Dipropylmalonic-acid | CCCC(CCC)(C(=O)O)C(=O)O | 188.10486 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Diethyl 4-oxoheptanedioate | CCOC(=O)CCC(=O)CCC(=O)OCC | 230.11542 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2'-methylacetoacetanilide | CC(=O)CC(=O)NC1=CC=CC=C1C | 191.09463 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Methyl 2-[(aminosulfonyl)methyl]benzoate | COC(=O)C1=C(CS(N)(=O)=O)C=CC=C1 | 229.04088 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Methyl dodec-9-enoate | CCC=CCCCCCCCC(=O)OC | 212.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| methyl palmitate | CCCCCCCCCCCCCCCC(=O)OC | 270.25588 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (2S)-2-methyl-3-oxooctadecanoic acid | CCCCCCCCCCCCCCCC(=O)[C@H](C)C(=O)O | 312.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(4-methylpiperazin-1-yl)-5-phenyl-1,3,4-thiadiazole | CN1CCN(CC1)C2=NN=C(S2)C3=CC=CC=C3 | 260.10957 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| O-Octyl hydrogen dithiocarbonate | CCCCCCCCOC(=S)S | 206.07991 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Oct-1-yne | CCCCCCC#C | 110.10955 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Phthalic Acid,Bis-N-Heptyl Ester | CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC | 362.24571 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| retinyl propionate | CCC(=O)OC\C=C(/C)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C | 342.25588 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| methyl docosa-4,7,10,13,16,19-hexaenoate | CC/C=C/C/C=C/C/C=C/C/C=C/C/C=C/C/C=C/CCC(=O)OC | 342.25588 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Sodium 2-(nonanoyloxy)benzenesulfonate | CCCCCCCCC(=O)OC1=CC=CC=C1S(=O)(=O)[O-].[Na+] | 314.11880 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Aminobenzimidazol | NC1=NC2=CC=CC=C2N1 | 133.06400 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Tenatoprazole | COC1=CC=C2NC(=NC2=N1)S(=O)CC1=NC=C(C)C(OC)=C1C | 346.10996 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| tetradecanedioic acid | OC(=O)CCCCCCCCCCCCC(O)=O | 258.18311 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Thiamine thiazolone | CC1=C(SC(=O)N1CC2=CN=C(N=C2N)C)CCO | 280.09940 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Torsemide | CC(C)NC(=O)NS(=O)(=O)C1=CN=CC=C1NC1=CC=CC(C)=C1 | 348.12561 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| DIMYRISTYL THIODIPROPIONATE | CCCCCCCCCCCCCCOC(=O)CCSCCC(=O)OCCCCCCCCCCCCCC | 570.46818 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Methyl 3-oxooctadecanoate | CCCCCCCCCCCCCCCCC(=O)CC(=O)O | 312.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 30-Methyl-2,5,8,11,14,17,20,23,26,29-decaoxahentriacontane | COCCOCCOCCOCCOCCOCCOCCOCCOCCOC(C)C | 470.30910 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-hydroxy-10-undecenoic acid | C=CCCCCCCCC(C(=O)O)O | 200.14124 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Mercaptoethyl nonanoate | CCCCCCCCC(=O)OCCS | 218.13405 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3,5,5-trimethylcyclohex-3-en-1-one | CC1=CC(C)(C)CC(=O)C1 | 138.10447 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Carbaprostacyclin | CCCCCC(C=CC1C(CC2C1CC(=CCCCC(=O)O)C2)O)O | 350.24571 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Methyl (cyclohexyloxy)acetate | COC(=O)COC1CCCCC1 | 172.10994 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Cytochalasin D | C[C@H]1[C@H]2[C@H](CC3=CC=CC=C3)NC(=O)[C@@]22[C@@H](\C=C\C[C@H](C)C(=O)[C@](C)(O)\C=C\[C@H]2OC(C)=O)[C@H](O)C1=C | 507.26209 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| isodecyl acrylate | CC(C)CCCCCCCOC(=O)C=C | 212.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Prostaglandin F2&#945; 1-11-lactone | CCCCC[C@H]1/C=C/[C@@H]2[C@@H](C/C=C\\CCCC(=O)O1)[C@H](C[C@H]2O)O | 336.23006 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Methoxycyclododecane | COC1CCCCCCCCCCC1 | 198.19837 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran. |  | 150.10447 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 6,10-Dimethylundecen-2-one |  | 196.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Octadecanoic acid, 3-oxo-, ethyl ester | CCCCCCCCCCCCCCCCCC(=O)CC(=O)O | 326.28210 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| tris(butylsulfanyl)phosphane | CCCCSP(SCCCC)SCCCC | 298.10125 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Aminomethanetricarbonitrile | NC(C#N)(C#N)C#N | 106.02795 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Nonanone | CCCCCCCC(C)=O | 142.13577 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Indoline | C1CNC2=CC=CC=C21 | 119.07350 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Carbetapentane | CCN(CC)CCOCCOC(=O)C1(CCCC1)C2=CC=CC=C2 | 333.23039 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| p-Cumenesulfonic acid | CC(C)C1=CC=C(C=C1)S(=O)(=O)O | 200.05072 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-Methoxy-4'-pentyl-1,1'-bi(cyclohexane) | CCCCCC1CCC(CC1)C1CCC(CC1)OC | 266.26097 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| epoprostenol | CCCCC[C@H](O)\C=C\[C@H]1[C@H](O)C[C@@H]2O\C(C[C@H]12)=C/CCCC(O)=O | 352.22497 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Gentian violet | CN(C)C1=CC=C(C=C1)C(C1=CC=C(C=C1)N(C)C)=C1C=CC(C=C1)=[N+](C)C | 372.24342 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| N~1~-[2-(Morpholin-4-yl)ethyl]ethane-1,2-diamine |  | 242.16707 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| stearoyl chloride | CC(CCCC(C)CC(=O)O)CC1CCCC2=CC=CC=C12 | 302.23764 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-{2-hydroxy-6-[5-(1,4,5-trihydroxyundecyl)tetrahydrofuran-2-yl]hexyl}-5-methylfuran-2(5h)-one | CCCCCCC(C(CCC(C1CCC(O1)CCCCC(CC2=CC(OC2=O)C)O)O)O)O | 470.32435 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| methylcyclohexane | CC1CCCCC1 | 98.10955 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| tetroxoprim | COCCOC1=C(OC)C=C(CC2=CN=C(N)N=C2N)C=C1OC | 334.16411 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Isopentyl p-methoxycinnamate | CC(C)CCOC(=O)C=CC1=CC=C(C=C1)OC | 248.14124 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Hydroxypropane-1,3-diyl bis(2-propylvalerate) | CCCC(CCC)C(=O)OCC(COC(=O)C(CCC)CCC)O | 344.25627 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Butalamine | CCCCN(CCCC)CCNC1=NC(=NO1)C2=CC=CC=C2 | 316.22631 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Endo-8-isopropyl-8-azabicyclo[3.2.1]octan-3-ol | CC(C)N1C2CCC1CC(C2)O | 169.14666 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Diisopropylbenzenesulphonic acid | CC(C)C1=C(C(=CC=C1)S(=O)(=O)O)C(C)C | 242.09767 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1-methyl-1,2-ethanediyl dioleate | CCCCCCCCC=CCCCCCCCC(=O)OCC(C)OC(=O)CCCCCCCC=CCCCCCCCC | 604.54306 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-Morpholino-5-(1H-pyrrol-1-yl)benzoic acid | C1COCCN1C2=C(C=C(C=C2)N3C=CC=C3)C(=O)O | 272.11609 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| (2E,4E)-4-(3,5-Dimethyl-1,3,4-oxadiazol-2(3H)-ylidene)-2-(pyrrolidine-1-carbothioyl)but-2-enenitrile | CN1N=C(C)O\C1=C\C=C(/C#N)C(=S)N1CCCC1 | 276.10448 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1,10-Decanediol dimethacrylate | CC(=C)C(=O)OCCCCCCCCCCOC(=O)C(=C)C | 310.21441 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 1-Benzyl-4-(methylamino)piperidine-4-carbonitrile | CNC1(CCN(CC2=CC=CC=C2)CC1)C#N | 229.15790 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2,3,5,6,8,9,11,12-Octahydro-1,4,7,10,13-benzopentaoxacyclopentadecine | C1COCCOC2=CC=CC=C2OCCOCCO1 | 268.13107 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 2-(Dodecane-1-sulfonyl)acetamide | CCCCCCCCCCCCS(=O)(=O)CC(N)=O | 291.18682 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropionate | CC(C)(CO)COC(=O)C(C)(C)CO | 204.13616 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-(2,4,4-trimethylpentylcarbonyloxy)benzenesulfonic acid | CC(CC(=O)OC1=CC=C(C=C1)S(O)(=O)=O)CC(C)(C)C | 314.11880 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-(2,4,4-trimethylpentylcarbonyloxy)benzenesulfonic acid | CC(CC(=O)OC1=CC=C(C=C1)S(O)(=O)=O)CC(C)(C)C | 314.11880 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-methyl-4-(methylthio)pentan-2-one | CSC(C)(C)CC(C)=O | 146.07654 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 4-Oxo-3,4-dihydroquinazoline-2-carbohydrazide | NNC(=O)C1=NC2=C(C=CC=C2)C(=O)N1 | 204.06473 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 5-Phenyl-1-pentyne | C#CCCCC1=CC=CC=C1 | 144.09390 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| LPE(20:5) | CC/C=C\\C/C=C\\C/C=C\\C/C=C\\C/C=C\\CCCC(=O)OC[C@H](COP(=O)(O)OCCN)O | 499.26989 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| butalamine | CCCCN(CCCC)CCNC1=NC(=NO1)C1=CC=CC=C1 | 316.22631 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Cytochalasin D | C[C@H]1[C@H]2[C@H](CC3=CC=CC=C3)NC(=O)[C@@]22[C@@H](\C=C\C[C@H](C)C(=O)[C@](C)(O)\C=C\[C@H]2OC(C)=O)[C@H](O)C1=C | 507.26209 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Dibutyl Succinate | CCCCOC(=O)CCC(=O)OCCCC | 230.15181 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| dimethyl cyclohexane-1,4-dicarboxylate | COC(=O)C1CCC(CC1)C(=O)OC | 200.10486 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| furan | O1C=CC=C1 | 68.02621 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| hexadecyl 4-chloro-3-[2-(5,5-dimethyl-2,4-dioxo-1,3-oxazolidin-3-yl)-4,4-dimethyl-3-oxopentamido]benzoate | CCCCCCCCCCCCCCCCOC(=O)C1=CC(=C(C=C1)Cl)NC(=O)C(C(=O)C(C)(C)C)N2C(=O)C(OC2=O)(C)C | 648.35413 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Ibuprofenol | CC(C)CC1=CC=C(C=C1)C(C)(C(=O)OOC(=O)C)O | 192.15142 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| 3-Isocyanopropyl toluene-p-sulphonate |  | 243.09292 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| N,N''-hexane-1,6-diylbis[N'-benzylurea] | O=C(NCCCCCCNC(=O)NCC1=CC=CC=C1)NCC1=CC=CC=C1 | 382.23688 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Phosphorothioic acid, O,O-bis(2-methylpropyl) ester, sodium salt | CC(C)COP(=S)([O-])OCC(C)C.[Na+] | 226.07926 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Styrene | C=CC1=CC=CC=C1 | 104.06260 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Lovastatin | CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12 | 404.25627 | Suspect screening | Canal | LC-HRMS | In house | K\_1 |
| Benzotriazole | N1N=NC2=CC=CC=C12 | 119.04835 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Diphenhydramine | CN(C)CCOC(C1=CC=CC=C1)C1=CC=CC=C1 | 255.16231 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Metoprolol | COCCC1=CC=C(OCC(O)CNC(C)C)C=C1 | 267.18344 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N-Desmethylvenlafaxin | CNCC(C1=CC=C(C=C1)OC)C2(CCCCC2)O | 263.18853 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| peak tail of galaxolidone | CC1C(C)(C)C2=CC3=C(C=C2C1(C)C)C(=O)OCC3C | 272.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Terbutryn | CCNC1=NC(NC(C)(C)C)=NC(SC)=N1 | 241.13612 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Galaxolidone | CC1C(C)(C)C2=CC3=C(C=C2C1(C)C)C(=O)OCC3C | 272.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Venlafaxine | COC1=CC=C(C=C1)C(CN(C)C)C1(O)CCCCC1 | 277.20418 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Hydroxybenzonitrile | OC1=CC=C(C=C1)C#N | 119.03711 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Terbutylazine-2-hydroxy | CCNC1=NC(=O)NC(=N1)NC(C)(C)C | 211.14331 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| O-desmethylvenlafaxine | CN(C)CC(C1=CC=C(C=C1)O)C2(CCCCC2)O | 263.18853 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-[4-(2-aminoethyl)phenyl]-N,N-dimethylacetamide | CN(C)C(=O)CC1=CC=C(C=C1)CCN | 206.14191 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Phenyl-1,3-octadecanedione | CCCCCCCCCCCCCCCC(=O)CC(=O)C1=CC=CC=C1 | 358.28718 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Flavanone | C1C(OC2=CC=CC=C2C1=O)C3=CC=CC=C3 | 224.08373 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-methylcinnolin-5-amine | CC1=CC2=C(C=CC=C2N=N1)N | 159.07965 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| a-Hydroxymetoprolol | CC(C)NCC(COC1=CC=C(C=C1)C(COC)O)O | 283.17836 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (14R\*,18R\*)-14,18-Dimethyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane | CC1CNCC(OCCOCCOCCOCCO1)C | 291.20457 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (RS)-9,10-difluoro-3-methyl-7-oxo-2,3-dihydro-7H-pyrido[1,2,3-de][1,4]benzoxazine-6-carboxylic acid (FPA) | CC1COC2=C3N1C=C(C(=O)C3=CC(=C2F)F)C(=O)O | 281.04996 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Phenyl-1H-pyrazol-5-amine | CC1=CC2=C(C=CC=C2N=N1)N | 159.07965 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 10-Hydroxycarbazepine | OC1CC2=CC=CC=C2N(C(O)=N)C2=CC=CC=C12 | 254.10553 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-[(Propylamino)methyl]octahydro-1H-inden-1-one | CCCNCC1CC2CCCCC2C1=O | 209.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| tyrosylphenylalanine | C1=CC=C(C=C1)CC(C(=O)O)NC(=O)C(CC2=CC=C(C=C2)O)N | 328.14231 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Tecomine | C[C@H]1CN(C[C@@H]2C1=CC(=O)[C@H]2C)C | 179.13101 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate | CCOCCOCCOCCOC(=O)C(C)=C | 246.14672 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Arachidonoyl-sn-glycerol | CCCCC/C=C\\C/C=C\\C/C=C\\C/C=C\\CCCC(=O)OC[C@H](CO)O | 378.27701 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-cyclohexylidene-2-phenylacetonitrile | N#CC(=C1CCCCC1)C1=CC=CC=C1 | 197.12045 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-Undecyl-1H-imidazole-4-carboxylic acid | CCCCCCCCCCCC1=NC(=CN1)C(O)=O | 266.19943 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-(2-(2-Hydroxyethoxy)ethylimino)-2,2-dimethylpropyl dodecanoate | CCCCCCCCCCCC(=O)OCC(C)(C)C=NCCOCCO | 371.30356 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-[4-(3-aminocyclohexyl)phenyl]propan-1-ol | CC(CO)C1=CC=C(C=C1)C2CCCC(C2)N | 233.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Heptylbenzoic acid | CCCCCCCC1=CC=C(C=C1)C(O)=O | 220.14633 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-vinylcyclohexene | C=CC1CCC=CC1 | 108.09390 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 5-Fluoro ADBICA | CC(C)(C)C(C(=O)N)NC(=O)C1=CN(C2=CC=CC=C21)CCCCCF | 361.21656 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 5-Nitroindoline | [O-][N+](=O)C1=CC=C2NCCC2=C1 | 164.05858 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| aliskiren | COCCCOC1=CC(C[C@@H](C[C@H](N)[C@@H](O)C[C@@H](C(C)C)C(=O)NCC(C)(C)C(N)=O)C(C)C)=CC=C1OC | 551.39344 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| alprenolol | CC(C)NCC(O)COC1=CC=CC=C1CC=C | 249.17288 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Azithromycin | CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O | 748.50853 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Benzeneacetamide | NC(=O)CC1=CC=CC=C1 | 135.06841 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Bisoprolol | CC(C)NCC(O)COC1=CC=C(COCCOC(C)C)C=C1 | 325.22531 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Butralin | CCC(C)NC1=C(C=C(C=C1[N+]([O-])=O)C(C)(C)C)[N+]([O-])=O | 295.15321 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| CGP 2160 |  | 492.32396 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Codeine | CN1CC[C@]23[C@@H]4[C@H]1CC5=C2C(=C(C=C5)OC)O[C@H]3[C@H](C=C4)O | 299.15214 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-(4-methoxyphenyl)-N-methyl-N-[(3-methyloxetan-3-yl)methyl]methanamine | CC1(COC1)CN(C)CC2=CC=C(C=C2)OC | 235.15723 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ethyl N-(2,3-dimethyl-2-isopropyl-1-oxobutyl)glycinate | CCOC(=O)CNC(=O)C(C)(C(C)C)C(C)C | 243.18344 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N-ethyl-N-[(4-prop-2-enoxy-3,5-dipropylphenyl)methyl]ethanamine | CCCC1=CC(=CC(=C1OCC=C)CCC)CN(CC)CC | 303.25621 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Fexofenadine | CC(C)(C1=CC=C(C=C1)C(CCCN2CCC(CC2)C(C3=CC=CC=C3)(C4=CC=CC=C4)O)O)C(=O)O | 501.28791 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-(3-methoxypropyl)piperidin-4-one | COCCCN1CCC(=O)CC1 | 171.12593 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| hexa-2,4-dienoic acid | CC=CC=CC(O)=O | 112.05243 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Leucylproline | CC(C)C[C@H](N)C(=O)N1CCC[C@H]1C(O)=O | 228.14739 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| thymine | CC1=CNC(=O)NC1=O | 126.04293 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 16-Hydroxyhexadecanoic acid | OCCCCCCCCCCCCCCCC(O)=O | 272.23514 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| octahydro-4(1h)-quinolinone | C1CCC2C(C1)C(=O)CCN2 | 153.11536 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N-{3-[Bis(2-hydroxyethyl)amino]phenyl}benzamide | OCCN(CCO)C1=CC=CC(NC(=O)C2=CC=CC=C2)=C1 | 300.14739 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| tetradecasphingosine | CCCCCCCCC/C=C/[C@H]([C@H](CO)N)O | 243.21983 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 17 alpha Dihydroequilin | CC12CCC3C(=CCC4=C3C=CC(=C4)O)C1CCC2O | 268.14633 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| ETHYL DIISOPROPYLCIN- NAMATE |  | 260.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Methyl-(S)-3-(tert-butoxycarbonyl)-2,2-dimethyl-4-oxazolidinecarboxylate | COC(=O)[C@@H]1COC(C)(C)N1C(=O)OC(C)(C)C | 259.14197 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Methylacenaphthylene | CC1=CC2=CC=CC3=C2C1=CC=C3 | 166.07825 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| tert-butyl 1,9-diazaspiro[5.5]undec-3-ene-9-carboxylate | CC(C)(C)OC(=O)N1CCC2(CC1)CC=CCN2 | 252.18378 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| tolicaine |  | 278.16304 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| MYRISTAMIDE DEA | CCCCCCCCCCCCCC(=O)N(CCO)CCO | 315.27734 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N-Dodecyl-N-methylaniline | CCCCCCCCCCCCN(C)C1=CC=CC=C1 | 275.26130 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 5-Methoxybenzothiazole-2(3H)-thione | COC1=CC=C2SC(=S)NC2=C1 | 196.99691 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| carbetapentane | CCOC(=O)C1(CCCC1OCCN(CC)CC)C1=CC=CC=C1 | 333.23039 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| O-Desmethyltramadol | CN(C)CC1CCCCC1(O)C1=CC=CC(O)=C1 | 249.17288 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Bakuchiol | CC(=CCC[C@@](C)(C=C)/C=C/C1=CC=C(C=C1)O)C | 256.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| ethyl 4-[(3-ethoxy-3-oxopropyl)(methyl)amino]butanoate | CCOC(=O)CCCN(C)CCC(=O)OCC | 245.16271 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| pentadecan-15-olide | C1CCCCCCCOC(=O)CCCCCC1 | 240.20893 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Perfluoropentanal | C(=O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 247.98837 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| piperidine-2-methylamine | CNC1CCCCN1 | 114.11570 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| procainamide | CCN(CC)CCNC(=O)C1=CC=C(N)C=C1 | 235.16846 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| PYR\_302.1865\_11.2|Pyrilamine N-oxide|2-[(4-methoxyphenyl)methyl-pyridin-2-ylamino]-N,N-dimethylethanamine oxide |  | 301.17903 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| SORBITAN CAPRYLATE | CCCCCCCC(=O)O[C@H](CO)C1OC[C@H](O)[C@H]1O | 290.17294 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N-ethyl-N-[(4-prop-2-enoxy-3,5-dipropylphenyl)methyl]ethanamine | CCCC1=CC(=CC(=C1OCC=C)CCC)CN(CC)CC | 303.25622 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| sphinga-4E,8E-dienine | CCCCCCCCC/C=C/CC/C=C/[C@H]([C@H](CO)N)O | 297.26678 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Fosinopril | CCC(=O)OC(OP(=O)(CCCCC1=CC=CC=C1)CC(=O)N1C[C@@H](C[C@H]1C(O)=O)C1CCCCC1)C(C)C | 563.30119 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-[(dimethylamino)methyl]-1-(3-methoxyphenyl)cycloheptan-1-ol | CN(C)CC1CCCCCC1(C2=CC(=CC=C2)OC)O | 277.20418 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (1R-(1a,4aß,4ba,10aa))-1,2,3,4,4a,4b,5,6,10,10a-Decahydro-7-isopropyl-1,4adimethylphenanthren- |  | 330.25588 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-(2,2-dimethyl-3,4-dihydro-2h-chromen-6-yl)-2-methylbutan-2-ol | CC1(CCC2=C(O1)C=CC(=C2)CCC(C)(C)O)C | 248.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,2-Benzenedicarboxylic acid, isooctyl nonyl ester |  | 404.29266 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-(2-Methylpentyl)cyclohexanecarboxylic acid | CCCC(C)CC1CCC(CC1)C(=O)O | 212.17763 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-methyl-1-piperidin-1-yloct-4-yn-3-ol | CCCC#CC(C)(CCN1CCCCC1)O | 223.19361 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Carbocyclic thromboxane A2 | CCCCC[C@@H](/C=C/[C@H]1CC2CC(C2)[C@@H]1C/C=C\\CCCC(=O)O)O | 348.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| dofamium | CCCCCCCCCCCC(=O)N(C)CC[N+](C)(C)CC(=O)NC1=CC=CC=C1 | 418.34280 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,3-Dioxolane, 2,4-dimethyl-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naph thalenyl)-, trans- | CC1COC(C)(O1)C1=CC2=C(C=C1)C(C)(C)CCC2(C)C | 288.20893 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Aphidicolin | C[C@]12CC[C@H]([C@@]([C@@H]1CC[C@@H]3[C@@]24CC[C@@]([C@H](C3)C4)(CO)O)(C)CO)O | 338.24571 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Acetyl-2,3,5,6,7,8-hexahydro-1,1-dimethyl-1H-benz(f)indene | CC(=O)C1=C2CCCCC2=CC3=C1CCC3(C)C | 242.16707 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Spiroxamine | CCCN(CC)CC1COC2(CCC(CC2)C(C)(C)C)O1 | 297.26678 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Mebeverine | CCN(CCCCOC(=O)C1=CC(=C(C=C1)OC)OC)C(C)CC2=CC=C(C=C2)OC | 429.25152 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| rac-threo-Dihydrobupropion | CC(C(C1=CC(=CC=C1)Cl)O)NC(C)(C)C | 241.12334 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ranitidine TP 45 |  | 139.09971 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| tetradecasphinga-4E,6E-dienine | CCCCCCC/C=C/C=C/[C@H]([C@H](CO)N)O | 241.20418 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 5-(4-Aminophenyl)imidazolidine-2,4-dione | C1=CC(=CC=C1C2C(=O)NC(=O)N2)N | 191.06948 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-((((2-Amino-6-chlorophenyl)methyl)methylamino)acetyl)morpholine | CN(CC(=O)N1CCOCC1)CC1=C(N)C=CC=C1Cl | 297.12440 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Dihydro-3-(octadecenyl)-2,5-furandione | CCCCCCCCCCCCCCCCC=CC1CC(=O)OC1=O | 350.28210 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Icaridine | CCC(C)OC(=O)N1CCCCC1CCO | 229.16779 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 12-hydroxystearic acid | CCCCCCC(O)CCCCCCCCCCC(O)=O | 300.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Myristoleic acid methyl ester | CCCCC=CCCCCCCCC(=O)OC | 240.20893 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| pirprofen | CC(C(O)=O)C1=CC=C(N2CC=CC2)C(Cl)=C1 | 251.07131 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Piperidinecarboxylic acid, 1-(1H-benzimidazol-4-yl)-, ethyl ester | CCOC(=O)C1CCN(CC1)C2=CC=CC3=C2N=CN3 | 273.14773 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Fosinopril | CCC(=O)OC(OP(=O)(CCCCC1=CC=CC=C1)CC(=O)N1C[C@@H](C[C@H]1C(O)=O)C1CCCCC1)C(C)C | 563.30119 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| DL-alpha Tocopheryl nicotinate | CC1=C(C(=C(C2=C1OC(CC2)(C)CCCC(C)CCCC(C)CCCC(C)C)C)OC(=O)C3=CN=CC=C3)C | 535.40255 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| cis-5,6-Dihydroxy-4-isopropylcyclohexa-1,3-dienecarboxylic acid | CC(C)C1=CC=C([C@H]([C@H]1O)O)C(=O)O | 198.08921 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| cis-5,6-Dihydroxy-4-isopropylcyclohexa-1,3-dienecarboxylic acid | CC(C)C1=CC=C([C@H]([C@H]1O)O)C(=O)O | 198.08921 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ethyl 2-Methyl-4-oxo-6-pentylcyclohex-2-ene-1-carboxylate. | CCCCCC1CC(=O)C=C(C1C(=O)OCC)C | 252.17255 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ethyl ricinoleate | CCCCCC[C@H](C/C=C\\CCCCCCCC(=O)OCC)O | 326.28210 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| bencyclane | CN(C)CCCOC1(CC2=CC=CC=C2)CCCCCC1 | 289.24056 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,3,5-tris(2-methyl-2-propenyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione | CC(=C)CN1C(=O)N(CC(C)=C)C(=O)N(CC(C)=C)C1=O | 291.15829 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Rimiterol | C1CCNC(C1)C(C2=CC(=C(C=C2)O)O)O | 223.12084 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (dibutylcarbamothioyl)sulfanide |  | 205.09589 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| beta.-Alanine, N-ethyl-N-phenyl-, methyl ester | CCN(CCC(=O)OC)C1=CC=CC=C1 | 207.12593 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-[Ethyl(3-methylphenyl)amino]propane-1-sulfonic acid | CCN(CCCS(O)(=O)=O)C1=CC(C)=CC=C1 | 257.10856 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Cyclohexaneacetic acid | OC(=O)CC1CCCCC1 | 142.09938 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| dimethyl cyclohexane-1,4-dicarboxylate | C1CC2(CCC1CC(=O)O)OCCO2 | 200.10486 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ethyl cyanocycloheptylideneacetate | CCOC(=O)C(C#N)=C1CCCCCC1 | 207.12593 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| ethylecgonine |  | 213.13649 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| hydrogen N-(1-oxododecyl)-L-glutamic acid | CCCCCCCCCCCC(=O)N[C@@H](CCC(O)=O)C(O)=O | 329.22022 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| JWH 122 N-(4-pentenyl) analog | CC1=CC=C(C2=CC=CC=C12)C(=O)C3=CN(C4=CC=CC=C43)CCCC=C | 353.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 17ß-hydroxy-17-(3-hydroxypropyl)androst-4-ene-4-one | C[C@]12CC[C@H]3[C@@H](CCC4C(=O)CCC[C@]34C)[C@@H]1CC[C@]2(O)CCCO | 348.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,4-Tridecadienal | CCCCCCCCC=CC=CC=O | 194.16707 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Acridin | C1=CC2=CC3=CC=CC=C3N=C2C=C1 | 179.07350 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,4-Di-tert-butyl-5-nitrophenyl methyl carbonate | CC(C)(C)C1=CC(=C(C=C1[N+](=O)[O-])OC(=O)OC)C(C)(C)C | 309.15762 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-Methyldodecanonitrile | CCCCCCCCCC(C)CC#N | 195.19870 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,3,5-triisopropyl-2,4-dinitrobenzene | CC(C)C1=CC(=C(C(=C1[N+](=O)[O-])C(C)C)[N+](=O)[O-])C(C)C | 294.15796 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-ethyl-2-methyl-2-isopentyl-1,3-oxazolidine | CCC1COC(N1)(C)CCC(C)C | 185.17796 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Brinzolamid | CCNC1CN(S(=O)(=O)C2=C1C=C(S2)S(=O)(=O)N)CCCOC | 383.06433 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (1alpha,2beta,5alpha)-5-Methyl-2-(1-methylethyl)cyclohexyl (R)-N-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-beta-alaninate | CC1CCC(C(C1)OC(=O)CCNC(=O)C(C(C)(C)CO)O)C(C)C | 357.25152 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl (ethylamino)(oxo)acetate | CCNC(=O)C(=O)O[C@@H]1C[C@H](C)CC[C@H]1C(C)C | 255.18344 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (3,4-diethoxyphenyl)acetonitrile | CCOC1=C(OCC)C=C(CC#N)C=C1 | 205.11028 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (undec-10-enoylamino)acetic acid | OC(=O)CNC(=O)CCCCCCCCC=C | 241.16779 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,3,5-Tri(tert-butyl)-2-nitrosobenzene | CC(C)(C)C1=CC(=C(N=O)C(=C1)C(C)(C)C)C(C)(C)C | 275.22491 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,4:3,6-Dianhydro-D-glucitol monostearate | CCCCCCCCCCCCCCCCCC(=O)OC1COC2C1OCC2O | 412.31888 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-(2,3-dihydro-1,3,3,6-tetramethyl-1-(1-methylethyl)-1H-inden-5-yl)ethanone | CC(C)C1(C)CC(C)(C)C2=CC(C(C)=O)=C(C)C=C12 | 258.19837 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 12-hydroxystearic acid | CCCCCCC(O)CCCCCCCCCCC(O)=O | 300.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,2'-dimorpholinyldiethyl ether | C1COCCN1CCOCCN2CCOCC2 | 244.17869 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,2,4-trimethylhexanedinitrile | CC(CC#N)CC(C)(C)C#N | 150.11570 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,5-bis(1,1-dimethylbutyl)hydroquinone | CCCC(C)(C)C1=CC(O)=C(C=C1O)C(C)(C)CCC | 278.22458 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,5-xylenol | CC1=CC(O)=C(C)C=C1 | 122.07316 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,6-diethyl-p-toluidine | CCC1=CC(C)=CC(CC)=C1N | 163.13610 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,6-Dihydroxyethylaminotoluene | CC1=C(NCCO)C=CC=C1NCCO | 210.13683 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-(2-(4-Nonylphenoxy)ethoxy)acetic acid (NPE2C) | CCCCCCCCCC1=CC=C(C=C1)OCCOCC(=O)O | 322.21441 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-(Dimethylamino)-3,5,5-trimethylcyclohex-2-en-1-one | CN(C)C1=C(C)CC(C)(C)CC1=O | 181.14666 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-(Methylthio)benzothiazol | CSC1=NC2=CC=CC=C2S1 | 181.00199 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-hydroxy-10-undecenoic acid | C=CCCCCCCCC(C(=O)O)O | 200.14124 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-nitro-2-phenyl-1,3-propanediol | OCC(CO)(C1=CC=CC=C1)[N+]([O-])=O | 197.06881 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-phenyl ethyl propionate | CCOC(=O)C(C)C1=CC=CC=C1 | 178.09938 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3,6,9,12-Tetraoxatridecylamine | COCCOCCOCCOCCN | 207.14706 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3,7-Bis(1-methyl-1-phenylethyl)-10H-phenothiazine | CC(C)(C1=CC=CC=C1)C1=CC2=C(NC3=CC=C(C=C3S2)C(C)(C)C2=CC=CC=C2)C=C1 | 435.20207 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3,7-dimethylnona-1,6-dien-3-ol | CCC(C)=CCCC(C)(O)C=C | 168.15142 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-cyclohexyl-2-cyclohexylimino-oxazolidin-4-one | O=C1COC(=NC2CCCCC2)N1C1CCCCC1 | 264.18378 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Dodecylaniline | CCCCCCCCCCCCC1=CC=C(N)C=C1 | 261.24565 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Methyl-7-diethylaminocoumarine | CCN(CC)C1=CC=C2C(C)=CC(=O)OC2=C1 | 231.12593 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 5,6-Dimethyl-1H-benzotriazole | CC1=CC2=C(C=C1C)N=NN2 | 147.07965 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 5-{(E)-(3-Carboxy-5-methyl-4-oxocyclohexa-2,5-dien-1-ylidene)[4-(diethylamino)phenyl]methyl}-2-hydroxy-3-methylbenzoic acid | CCN(CC)C1=CC=C(C=C1)C(\C1=CC(C(O)=O)=C(O)C(C)=C1)=C1\C=C(C)C(=O)C(=C1)C(O)=O | 461.18384 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Acridone | O=C1C2=CC=CC=C2NC2=CC=CC=C12 | 195.06841 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| allyl acetoacetate | CC(=O)CC(=O)OCC=C | 142.06299 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ametoctradin | CCCCCCCCC1=C(N)N2N=CN=C2N=C1CC | 275.21100 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| artemether | CO[C@H]1O[C@@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3 | 298.17802 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Bufencarb | CCCC(C)C1=CC(=CC=C1)OC(=O)NC.CCC(CC)C1=CC(=CC=C1)OC(=O)NC | 221.14158 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Lobendazole | CCOC(=O)NC1=NC2=CC=CC=C2N1 | 205.08513 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Coniine | CCC[C@H]1CCCCN1 | 127.13610 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| cyclododecanol | OC1CCCCCCCCCCC1 | 184.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Cytochalasin B | C[C@H]1[C@H]2[C@H](CC3=CC=CC=C3)NC(=O)[C@]22OC(=O)\C=C\[C@H](O)CCC[C@@H](C)C\C=C\[C@H]2[C@H](O)C1=C | 479.26717 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Decoquinate | CCCCCCCCCCOC1=C(OCC)C=C2NC=C(C(=O)OCC)C(=O)C2=C1 | 417.25152 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Desoxycodeine C | CN1CCC23C4C1CC5=C2C(=C(C=C5)OC)OC3C=CC4 | 283.15723 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| diethyl 1,2-cyclopentanedicarboxylate | CCOC(=O)C1CCCC1C(=O)OCC | 214.12051 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Dimethyl 4,4'-(1,6-hexanediylbis(iminocarbonyl))bisbenzoate | COC(=O)C1=CC=C(C=C1)C(=O)NCCCCCCNC(=O)C2=CC=C(C=C2)C(=O)OC | 440.19474 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Dimetridazole | CN1C(C)=NC=C1N(=O)=O | 141.05383 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| DISPERSE RED 17 | CC1=CC(=CC=C1\N=N\C1=CC=C(C=C1)[N+]([O-])=O)N(CCO)CCO | 344.14846 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| echothiopate |  | 256.11363 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ethyl hexahydro-1H-azepine-1-propionate | CCOC(=O)CCC1CCCCCN1 | 199.15723 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| JWH-081 | CCCCCN1C=C(C2=CC=CC=C21)C(=O)C3=CC=C(C4=CC=CC=C43)OC | 371.18853 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 6-Dehydroestrone | C[C@]12CC[C@H]3[C@H]([C@@H]1CCC2=O)C=CC4=C3C=CC(=C4)O | 268.14633 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Methyl 3-[4-[bis[2-(benzoyloxy)ethyl]amino]phenyl]-2,3-dicyanoacrylate | COC(=O)C(C#N)=C(C#N)C1=CC=C(C=C1)N(CCOC(=O)C1=CC=CC=C1)CCOC(=O)C1=CC=CC=C1 | 523.17434 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Methyl-(S)-3-(tert-butoxycarbonyl)-2,2-dimethyl-4-oxazolidinecarboxylate | COC(=O)[C@@H]1COC(C)(C)N1C(=O)OC(C)(C)C | 259.14197 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N-Decylimidazole | CCCCCCCCCCN1C=CN=C1 | 208.19395 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N-{2-[(E)-(2,6-Dicyano-4-nitrophenyl)diazenyl]-5-(diethylamino)phenyl}butanamide | CCCC(=O)NC1=C(C=CC(=C1)N(CC)CC)\N=N\C1=C(C=C(C=C1C#N)[N+]([O-])=O)C#N | 433.18624 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N2-(1-Oxobutyl)-L-lysine | CCCC(=O)N[C@@H](CCCCN)C(O)=O | 216.14739 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N2-(1-Oxobutyl)-L-lysine | CCCC(=O)N[C@@H](CCCCN)C(O)=O | 216.14739 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| nicomorphine | CN1CC[C@@]23[C@H]4OC5=C2C(C[C@@H]1[C@@H]3C=C[C@@H]4OC(=O)C1=CC=CN=C1)=CC=C5OC(=O)C1=CC=CN=C1 | 495.17942 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Oleandrin | CO[C@H]1C[C@H](O[C@H]2CC[C@@]3(C)[C@H](CC[C@@H]4[C@@H]3CC[C@]3(C)[C@H]([C@H](C[C@]43O)OC(C)=O)C3=CC(=O)OC3)C2)O[C@@H](C)[C@@H]1O | 576.32983 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| PEG-12 |  | 546.32515 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| PEG-13 |  | 590.35136 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| rimexolone | CCC(=O)[C@@]1(C)[C@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@]12C | 370.25080 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| SODIUM OLEOYL LACTY- LATE |  | 426.29814 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Streptolin | C1C(C2C(C(=O)N1)N=C(N2)NC3C(C(C(C(O3)CO)OC(=O)N)O)NC(=O)CC(CCCNC(=O)CC(CCCN)N)N)O | 630.34492 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Alachlor-OXA+Acetochlor OXA | CCC1=C(C(=CC=C1)CC)N(COC)C(=O)C(=O)O + CCC1=CC=CC(=C1N(COCC)C(=O)C(=O)O)C | 265.13141 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Tegaserod | CCCCCNC(=N)N\N=C\C1=CNC2=CC=C(OC)C=C12 | 301.19026 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Tegaserod | CCCCCNC(=N)N\N=C\C1=CNC2=CC=C(OC)C=C12 | 301.19026 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| tolicaine | CCN(CC)CC(=O)NC1=C(C=CC=C1C(=O)OC)C | 278.16304 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Valpromide | CCCC(CCC)C(N)=O | 143.13101 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Zolmitriptan | CN(C)CCC1=CNC2=CC=C(C[C@H]3COC(=O)N3)C=C12 | 287.16338 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| LAURETH-5 | CCCCCCCCCCCCOCCOCCOCCOCCOCCO | 406.32944 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| artemether | CO[C@H]1O[C@@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3 | 298.17802 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-hydroxybenzaldehyde | OC1=CC=C(C=O)C=C1 | 122.03678 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Telbivudine | CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)O | 242.09027 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (1S,4R,6R)-1-[(3E)-5-Hydroxy-3-methylpent-3-en-1-yn-1-yl]-2,2,6-trimethylcyclohexane-1,4-diole |  | 252.17255 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (3aS,4R,5S,6S,8R,9R,9aR,10R)-6-ethenyl-5-hydroxy-4,6,9,10-tetramethyl-1-oxodecahydro-3a,9-propanocyclopenta[8]annulen-8-yl[(methylsulfonyl)oxy]acetate |  | 456.21818 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,3,3a,4,5,6,7,8,9,10,11,13a-Dodecahydrocyclododeca( c)furan. | C1CCCCC2COCC2C=CCCC1 | 208.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,4:3,6-Dianhydro-D-glucitol monolaurate | CCCCCCCCCCCC(=O)OC1COC2C1OCC2O | 328.22497 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,6-Octadiene, 8-methoxy- | COCC=CCCCC=C | 140.12012 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)butan-1-one | CCCC(=O)C1=C(C)CCCC1(C)C | 194.16707 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-(Methoxymethyl)-1H-benzotriazole | COCN1N=NC2=C1C=CC=C2 | 163.07456 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Cyclohexyl-2-propen-1-one | C=CC(=O)C1CCCCC1 | 138.10447 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Cyclohexyl-4-hexylbenzene | CCCCCCC1=CC=C(C=C1)C1CCCCC1 | 244.21910 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Hydroxy-N-[2-(tetradecyloxy)phenyl]naphthalene-2-carboxamide | CCCCCCCCCCCCCCOC1=C(NC(=O)C2=CC=C3C=CC=CC3=C2O)C=CC=C1 | 475.30864 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Nonyne | CCCCCCCC#C | 124.12520 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,4,5-Triphenylimidazole | N1C(=NC(=C1C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1 | 296.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,6,6-trimethylbicyclo[3.1.1]heptane-3-carbaldehyde | CC1C2CC(CC1C=O)C2(C)C | 166.13577 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-(Ethylanilino)ethyl benzoate | CCN(CCOC(=O)C1=CC=CC=C1)C1=CC=CC=C1 | 269.14158 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-ethylhexyl nonanoate | CCCCCCCCC(=O)OCC(CC)CCCC | 270.25588 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3,3',4',5,7-pentahydroxyflavone | OC1=CC(O)=C2C(OC(=C(O)C2=O)C2=CC(O)=C(O)C=C2)=C1 | 302.04265 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,11-bis(prop-2-ynoxy)undecane | C#CCOCCCCCCCCCCCOCC#C | 264.20893 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-[Ethyl(3-methylphenyl)amino]propane-1-sulfonic acid | CCN(CCCS(O)(=O)=O)C1=CC(C)=CC=C1 | 257.10856 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-[4-[4-(Hydroxydiphenylmethyl)-1-piperidinyl]-1-oxobutyl]-a,a-dimethyl-ethyl ester benzeneacetic acid |  | 527.30356 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Methyl-2-nonylphenol | CCCCCCCCCC1=C(O)C=CC(C)=C1 | 234.19837 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 9,14-dihydroxyoctadecanoic acid | CCCCC(CCCCC(CCCCCCCC(=O)O)O)O | 316.26136 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 9,10-Dihydroxystearic acid | CCCCCCCCC(O)C(O)CCCCCCCC(O)=O | 316.26136 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Cambendazole | CC(C)O\C(O)=N\C1=CC=C2N=C(NC2=C1)C1=CSC=N1 | 302.08375 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-(3-Chlorophenyl)-4-hydroxymethyl-7,8-dimethoxy-5H-2,3-benzodiazepine | COC1=C(C=C2C(=C1)CC(=NN=C2C3=CC(=CC=C3)Cl)CO)OC | 344.09277 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| artemether | CO[C@H]1O[C@@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3 | 298.17802 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| PE(20:5(5Z,8Z,11Z,14Z,17Z)/0:0) | CC/C=C\\C/C=C\\C/C=C\\C/C=C\\C/C=C\\CCCC(=O)OC[C@H](COP(=O)(O)OCCN)O | 499.26989 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Benzenesulfonic acid, 4-methyl-, butyl ester | CCCCOS(=O)(=O)C1=CC=C(C)C=C1 | 228.08202 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Bis(2-phenylvinyl)phenol | C1=CC=C(C=C1)C=CC2=C(C(=CC=C2)O)C=CC3=CC=CC=C3 | 298.13577 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Calcium Ionophore A23187 | CC1CCC2(C(CC(C(O2)C(C)C(=O)C3=CC=CN3)C)C)OC1CC4=NC5=C(O4)C=CC(=C5C(=O)O)NC | 523.26824 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Celastrol | CC1=C(O)C(=O)C=C2C1=CC=C1[C@@]2(C)CC[C@@]2(C)[C@@H]3C[C@@](C)(CC[C@]3(C)CC[C@]12C)C(O)=O | 450.27701 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Chlorcyclizine | CN1CCN(CC1)C(C1=CC=CC=C1)C1=CC=C(Cl)C=C1 | 300.13933 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ciclesonide | CC(C)C(=O)OCC(=O)[C@@]12O[C@@H](O[C@@H]1C[C@H]1[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@]21C)C1CCCCC1 | 540.30870 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| DEXTRIN | OC[C@H]1OC(O[C@H]2[C@H](O)[C@@H](O)C(O[C@H]3[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]3CO)O[C@@H]2CO)[C@H](O)[C@@H](O)[C@@H]1O | 504.16904 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| dibutyl 2,2'-thiobisacetate | CCCCOC(=O)CSCC(=O)OCCCC | 262.12388 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Cyclohexene-1-ethanol, 4-(formyloxy)-4-(1-methylethyl)-, formate | CC(C)C1(CCC(=CC1)CCOC=O)OC=O | 240.13616 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Diisopropyl undecanedioate | CC(C)OC(=O)CCCCCCCCCC(=O)OC(C)C | 300.23006 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Dimethyl (3-oxo-2-pentylcyclopentyl)malonate | CCCCCC1C(CCC1=O)C(C(=O)OC)C(=O)OC | 284.16237 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Docosahexaenoic acid | CC/C=C\\C/C=C\\C/C=C\\C/C=C\\C/C=C\\C/C=C\\CCC(=O)O | 328.24023 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Metazachlor | CC1=CC=CC(C)=C1N(CN1C=CC=N1)C(=O)CCl | 277.09819 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| ethyl 3-ethoxypropionate | CCOCCC(=O)OCC | 146.09429 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,3-Dioxolane-4-methanol | CC(=CCCC(=CC1OCC(O1)CO)C)C | 226.15690 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Herbimycin A | CO[C@H]1C[C@H](C)[C@@H](OC)C2=CC(=O)C=C(NC(=O)\C(C)=C\C=C/C(OC)[C@@H](OC(N)=O)\C(C)=C\[C@H](C)C1OC)C2=O | 574.28903 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-[2-[(1R,2R)-1-amino-2-hydroxypropyl]-5-hydroxy-4-[(4-hydroxyphenyl)methyl]imidazol-1-yl]acetaldehyde | C[C@H]([C@@H](C1=NC(=C(N1CC=O)O)CC2=CC=C(C=C2)O)N)O | 305.13756 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Imolamine | CCN(CC)CCN1C(=N)ON=C1C1=CC=CC=C1 | 260.16371 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Indoleacetamide | NC(=O)CC1=CNC2=CC=CC=C12 | 174.07931 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2H-Pyran, tetrahydro-2-(9-tetradecenyloxy)- | CCCCC=CCCCCCCCCOC1CCCCO1 | 296.27153 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Isopimaric acid | C[C@@]1(CC[C@H]2C(C1)=CC[C@@H]1[C@]2(C)CCC[C@@]1(C)C(O)=O)C=C | 302.22458 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Isopropyl L-methionate hydrochloride | CC(C)OC(=O)C(CCSC)N.Cl | 191.09800 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Decylthioacetic acid | CCCCCCCCCCSCC(=O)O | 232.14970 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Florfenicol amine | CS(=O)(=O)C1=CC=C(C=C1)C(C(CF)N)O | 247.06784 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Chlorpheniramine, Desmethyl |  | 260.10803 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2,3-Dihydroxypropyl 3-(hexylthio)propionate | CCCCCCSCCC(=O)OCC(O)CO | 264.13953 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Olanzapine, N-desmethyl | CC1=CC2=C(S1)NC3=CC=CC=C3N=C2N4CCNCC4 | 298.12522 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Oxazolam | C[C@@H]1CN2CC(=O)NC3=CC=C(Cl)C=C3[C@@]2(O1)C1=CC=CC=C1 | 328.09786 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| sulfapyrazole | CC1=NN(C(NS(=O)(=O)C2=CC=C(N)C=C2)=C1)C1=CC=CC=C1 | 328.09940 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 30-Methyl-2,5,8,11,14,17,20,23,26,29-decaoxahentriacontane | COCCOCCOCCOCCOCCOCCOCCOCCOCCOC(C)C | 470.30910 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Diethyl 4-oxoheptanedioate | CCOC(=O)CCC(=O)CCC(=O)OCC | 230.11542 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Icosapent | CC\C=C/C\C=C/C\C=C/C\C=C/C\C=C/CCCC(O)=O | 302.22458 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Methyl 2-[(aminosulfonyl)methyl]benzoate | COC(=O)C1=C(CS(N)(=O)=O)C=CC=C1 | 229.04088 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (2S)-2-methyl-3-oxooctadecanoic acid | CCCCCCCCCCCCCCCC(=O)[C@H](C)C(=O)O | 312.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N,N-Diethyl-4-[(E)-(1,3-thiazol-2-yl)diazenyl]aniline | CCN(CC)C1=CC=C(C=C1)\N=N\C1=NC=CS1 | 260.10957 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| O,O-Didodecyl hydrogen dithiophosphate | CCCCCCCCCCCCOP(=S)(OCCCCCCCCCCCC)S | 466.30681 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| O-Octyl hydrogen dithiocarbonate | CCCCCCCCOC(=S)S | 206.07991 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Oct-1-yne | CCCCCCC#C | 110.10955 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Phthalic Acid,Bis-N-Heptyl Ester | CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC | 362.24571 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| retinyl propionate | CCC(=O)OC\C=C(/C)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C | 342.25588 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Sodium 2-(nonanoyloxy)benzenesulfonate | CCCCCCCCC(=O)OC1=CC=CC=C1S(=O)(=O)[O-].[Na+] | 314.11880 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-Aminobenzimidazol | NC1=NC2=CC=CC=C2N1 | 133.06400 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Cytarabin | NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O | 243.08552 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Tenatoprazole | COC1=CC=C2NC(=NC2=N1)S(=O)CC1=NC=C(C)C(OC)=C1C | 346.10996 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| [(Z)-undec-9-enyl] (2R)-2,3-dihydroxypropanoate | C/C=C\\CCCCCCCCOC(=O)[C@@H](CO)O | 258.18311 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Thiamine thiazolone | CC1=C(SC(=O)N1CC2=CN=C(N=C2N)C)CCO | 280.09940 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Torsemide | CC(C)NC(=O)NS(=O)(=O)C1=CN=CC=C1NC1=CC=CC(C)=C1 | 348.12561 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (2S)-2-methyl-3-oxooctadecanoic acid | CCCCCCCCCCCCCCCC(=O)[C@H](C)C(=O)O | 312.26645 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| L-tryptophan | C1=CC=C2C(=C1)C(=CN2)C[C@@H](C(=O)O)N | 204.08988 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (-)-2,7-Dolabelladiene-6beta,10alpha,18-triol | C[C@@H]\\1C[C@H](/C=C(/C[C@@H]([C@H]2[C@@H](CC[C@@]2(/C=C1)C)C(C)(C)O)O)\\C)O | 322.25080 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 30-Methyl-2,5,8,11,14,17,20,23,26,29-decaoxahentriacontane | COCCOCCOCCOCCOCCOCCOCCOCCOCCOC(C)C | 470.30910 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-Mercaptoethyl nonanoate | CCCCCCCCC(=O)OCCS | 218.13405 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-[(2-tert-butylcyclohexyl)oxy]butan-2-ol | CCC(O)COC1CCCCC1C(C)(C)C | 228.20893 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Methyl (cyclohexyloxy)acetate | COC(=O)COC1CCCCC1 | 172.10994 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Prostaglandin F2&#945; 1-11-lactone |  | 336.23006 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Methoxycyclododecane | COC1CCCCCCCCCCC1 | 198.19837 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 6,10-Dimethylundecen-2-one |  | 196.18272 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 3-oxoicosanoic acid | CCCCCCCCCCCCCCCCCC(=O)CC(=O)O | 326.28210 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| tris(butylsulfanyl)phosphane | CCCCSP(SCCCC)SCCCC | 298.10125 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-methyl-2,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-cyclopenta[12]annulene |  | 220.21910 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Methoxy-4'-pentyl-1,1'-bi(cyclohexane) | CCCCCC1CCC(CC1)C1CCC(CC1)OC | 266.26097 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1-Heptyne | CCCCCC#C | 96.09390 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| methyl trans-3-oxo-2-pentylcyclopentanecarboxylate | CCCCCC1C(CCC1=O)C(=O)OC | 212.14124 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N~1~-[2-(Morpholin-4-yl)ethyl]ethane-1,2-diamine |  | 242.16707 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-Hydroxypropane-1,3-diyl bis(2-propylvalerate) | CCCC(CCC)C(=O)OCC(COC(=O)C(CCC)CCC)O | 344.25627 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| (2E,4E)-4-(3,5-Dimethyl-1,3,4-oxadiazol-2(3H)-ylidene)-2-(pyrrolidine-1-carbothioyl)but-2-enenitrile | CN1N=C(C)O\C1=C\C=C(/C#N)C(=S)N1CCCC1 | 276.10448 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 1,10-Decanediol dimethacrylate | CC(=C)C(=O)OCCCCCCCCCCOC(=O)C(=C)C | 310.21441 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-(2-Ethylphenyl)-5-methyl-2,4-dihydro-3H-pyrazol-3-one | CCC1=C(C=CC=C1)N1N=C(C)CC1=O | 202.11061 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 2-(Dodecane-1-sulfonyl)acetamide | CCCCCCCCCCCCS(=O)(=O)CC(N)=O | 291.18682 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-((4-Aminophenyl)azo)-5-methyl-2-methoxyaniline | COC1=C(N)C=C(C)C(=C1)N=NC1=CC=C(N)C=C1 | 256.13241 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-(2,4,4-trimethylpentylcarbonyloxy)benzenesulfonic acid | CC(CC(=O)OC1=CC=C(C=C1)S(O)(=O)=O)CC(C)(C)C | 314.11880 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-methyl-4-(methylthio)pentan-2-one | CSC(C)(C)CC(C)=O | 146.07654 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| 4-Phenyl-1,2,4-triazoline-3,5-dione | O=C1NNC(=O)N1C1=CC=CC=C1 | 177.05383 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Dibutyl Succinate | CCCCOC(=O)CCC(=O)OCCCC | 230.15181 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| dimethyl cyclohexane-1,4-dicarboxylate | COC(=O)C1CCC(CC1)C(=O)OC | 200.10486 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| domoic acid | C[C@H](\C=C\C=C(/C)[C@H]1CN[C@@H]([C@H]1CC(O)=O)C(O)=O)C(O)=O | 311.13689 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Fexofenadine | CC(C)(C(O)=O)C1=CC=C(C=C1)C(O)CCCN1CCC(CC1)C(O)(C1=CC=CC=C1)C1=CC=CC=C1 | 501.28791 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| hexadecyl 4-chloro-3-[2-(5,5-dimethyl-2,4-dioxo-1,3-oxazolidin-3-yl)-4,4-dimethyl-3-oxopentamido]benzoate | CCCCCCCCCCCCCCCCOC(=O)C1=CC(=C(C=C1)Cl)NC(=O)C(C(=O)C(C)(C)C)N2C(=O)C(OC2=O)(C)C | 648.35413 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Ibuprofenol | CC(C)CC1=CC=C(C=C1)C(C)(C(=O)OOC(=O)C)O | 192.15142 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N',2-Diphenylhydrazine-1-carbohydrazide | NNC(=O)NN(C1=CC=CC=C1)C1=CC=CC=C1 | 242.11676 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| N,N''-hexane-1,6-diylbis[N'-benzylurea] | O=C(NCCCCCCNC(=O)NCC1=CC=CC=C1)NCC1=CC=CC=C1 | 382.23688 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Phosphorothioic acid, O,O-bis(2-methylpropyl) ester, sodium salt | CC(C)COP(=S)([O-])OCC(C)C.[Na+] | 226.07926 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Taurolithocholic acid 3-sulfate | CC(CCC(=O)NCCS(=O)(=O)O)C1CCC2C1(CCC3C2CCC4C3(CCC(C4)OS(=O)(=O)O)C)C | 563.25866 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Tetrahydrofurfuryl acrylate | C=CC(=O)OCC1CCCO1 | 156.07864 | Suspect screening | Canal | LC-HRMS | In house | K\_2 |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17763 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| Methoprene | CC(C)OC(=O)C=C(C)C=CCC(C)CCCC(C)(C)OC | 310.25079 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| Terbutryn | CCNC1=NC(=NC(=N1)SC)NC(C)(C)C | 241.13612 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| Fenuron | CN(C)C(=O)NC1=CC=CC=C1 | 164.09496 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| Proxyphylline | CC(CN1C=NC2=C1C(=O)N(C(=O)N2C)C)O | 238.10659 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| Metalaxyl | CC1=C(C(=CC=C1)C)N(C(C)C(=O)OC)C(=O)COC | 279.14706 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| carbachol | C[N+](C)(C)CCOC(=O)N | 147.11335 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| Benzotriazole -4-Me | CC1=CC=CC2=NNN=C12 | 133.06400 | Suspect screening | Canal | LC-HRMS | In house | H\_1 |
| Sabril | CC(CC1=CC(=C(C=C1)O)OC)NC | 195.12593 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| PFUnA | OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 563.96410 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| PFOS | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93750 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| PFOA | OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 413.97370 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| PFHxS | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 399.94390 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| PFDoA | OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 613.96090 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| PFDeA | C(=O)(C(C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)O | 513.96730 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| Ibuprofen | CC(C)CC1=CC=C(C=C1)C(C)C(O)=O | 206.13070 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| Alachlor-OXA | CCC1=C(C(=CC=C1)CC)N(COC)C(=O)C(=O)O | 265.13140 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| Thiabendazole | C1=CC=C2C(=C1)NC(=N2)C3=CSC=N3 | 201.03607 | Suspect screening | Canal | LC-HRMS | In house | H\_2 |
| Acridine | C1=CC=C2C(=C1)C=C3C=CC=CC3=N2 | 179.07350 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | A |
| 1-Methylbenzotriazole | CN1C2=CC=CC=C2N=N1 | 133.06400 | Suspect screening | Canal | LC-HRMS | Reference | A |
| 2-(Methylthio)benzothiazol | CSC1=NC2=CC=CC=C2S1 | 181.00199 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Terbutryn | CCNC1=NC(=NC(=N1)SC)NC(C)(C)C | 241.13612 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Cetrimonium | CCCCCCCCCCCCCCCC[N+](C)(C)C | 283.32373 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Benzotriazole | C1=CC2=NNN=C2C=C1 | 119.04835 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Perfluoro-1-octanesulfonic acid (PFOS) | C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Hypoxanthine | C1=NC2=C(N1)C(=O)NC=N2 | 136.03851 | Suspect screening | Canal | LC-HRMS | Reference | A |
| 2'-Deoxyinosine | C1C(C(OC1N2C=NC3=C2N=CNC3=O)CO)O | 252.08585 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Perfluorododecanoic acid | C(=O)(C(C(C(C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)O | 613.96093 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Perfluorotetradecanoic acid | C(=O)(C(C(C(C(C(C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)O | 713.95454 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Docosyltrimethylammonium | CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C | 368.42480 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Benzyldimethylhexadecylammonium (Cetalkonium) | CCCCCCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1 | 360.36240 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Dihexadecyldimethylammonium | CCCCCCCCCCCCCCCC[N+](C)(C)CCCCCCCCCCCCCCCC | 494.56580 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Benzyldimethyl(octadecyl)ammonium | CCCCCCCCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1 | 388.39360 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Benzyldimethyltetradecylammonium (Miristalkonium) | CCCCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1 | 332.33110 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Benzyldodecyldimethylammonium (Benzododecinium) | CCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1 | 304.29980 | Suspect screening | Canal | LC-HRMS | Reference | A |
| Didecyldimethylammonium | CCCCCCCCCC[N+](C)(C)CCCCCCCCCC | 326.37796 | Suspect screening | Canal | LC-HRMS | Reference | A |
| PEG n12 | C(COCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)O | 546.32520 | Suspect screening | Canal | LC-HRMS | Reference | A |
| PEG n13 | C(COCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)O | 590.35153 | Suspect screening | Canal | LC-HRMS | Reference | A |
| L-Valine | O=C(O)C(N)C(C)C | 117.07919 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Niacinamide | O=C(N)C=1C=NC=CC1 | 122.04832 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Creatinine | O=C(O)C(N)C(C)C | 113.05928 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Allopurinol | O=C1NC=NC=2NN=CC12 | 136.03867 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Fenuron | O=C(N)C=1C=NC=CC1 | 164.09508 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Venlafaxine met 2-248 | O=C(NC=1C=CC=CC1)N(C)C | 248.14129 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Verrucarol | OC1(CCCCC1)C(C2=CC=C(OC)C=C2)CN(C)C | 266.15185 | Suspect screening | Canal | LC-HRMS | Reference | C |
| 4H-3a,7-Methanoazulen-4-one, 1,2,3,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, (3R,3aR,7S,8aS)- | OCC12CCC(=CC2OC3CC(O)C1(C)C43OC4)C | 218.16722 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17766 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Drofenine | CCN(CC)CCOC(=O)C(C1CCCCC1)C2=CC=CC=C2 | 317.23552 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Linoleic acid | CCCCCC=CCC=CCCCCCCCC(=O)O | 280.24041 | Suspect screening | Canal | LC-HRMS | Reference | C |
| Docosahexaenoic acid | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O | 328.24020 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Eicosapentaenoic acid | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O | 302.22460 | Suspect screening | Canal | LC-HRMS | Reference | D |
| 12,13-epoxy-9Z-octadecenoic acid | CCCCCC1C(O1)CC=CCCCCCCCC(=O)O | 296.23510 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Docosa-4,8,12,15,19-pentaenoic acid | CCC=CCCC=CCC=CCCC=CCCC=CCCC(=O)O | 330.25590 | Suspect screening | Canal | LC-HRMS | Reference | D |
| 11-Aoctadecenoic acid | CCCCCCC=CCCCCCCCCCC(=O)O | 282.25590 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Methoxydienone | CCC12CCC3C(C1CCC2=O)CCC4=C3CC=C(C4)OC | 300.20890 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Linolenic acid | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O | 278.22460 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Laurocapram | CCCCCCCCCCCCN1CCCCCC1=O | 281.27190 | Suspect screening | Canal | LC-HRMS | Reference | D |
| 1-Dodecyl-2-pyrrolidinone | CCCCCCCCCCCCN1CCCC1=O | 253.24060 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Linoleamide | CCCCCC=CCC=CCCCCCCCC(=O)N | 279.25620 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Leucylproline | CC(C)CC(C(=O)N1CCCC1C(=O)O)N | 228.14740 | Suspect screening | Canal | LC-HRMS | Reference | D |
| Acridine | c1ccc2nc3ccccc3cc2c1 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| 1,2,3-Benzotriazole | C1=CC=C2C(=C1)NN=N2 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| 4-Octylphenol | CCCCCCCCc1ccc(O)cc1 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Bisphenol A diglycidyl ether | CC(C)(C1=CC=C(C=C1)OCC2CO2)C3=CC=C(C=C3)OCC4CO4 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Benzyldimethyldodecylammonium | CCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Benzothiazole | C1=CC=C2C(=C1)N=CS2 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| 2-hydroxy-Benzothiazole | C1=CC=C2C(=C1)NC(=O)S2 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Perfluorodecanoic acid | O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Perfluoroundecanoic acid | OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Perfluorooctanesulfonic acid (PFOS) | C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Irbesartan | C12(C(N(Cc3ccc(c4c(c5[nH]nnn5)cccc4)cc3)C(=N1)CCCC)=O)CCCC2 |  | Suspect screening | Canal | LC-HRMS | Reference | F |
| Ethyl thiocyanate | CCSC#N | 87.01427 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 6-Methylhepta-3,5-dien-2-one. | CC(C)=CC=CC(C)=O | 124.08881 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 1-Naphthol | OC1=CC=CC2=CC=CC=C12 | 144.05751 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Fenuron | CN(C)C(=O)NC1=CC=CC=C1 | 164.09496 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 1-[(1R,2S)-2,6,6-trimethylcyclohex-3-en-1-yl]ethanone | CC1C=CCC(C1C(=O)C)(C)C | 166.13577 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Octyl thiocyanate | CCCCCCCCSC#N | 171.10817 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 3-[(4R)-4-(propan-2-yl)cyclohex-1-en-1-yl]propanal | CC(C)C1CCC(=CC1)CCC=O | 180.15142 | Suspect screening | Canal | LC-HRMS | Reference | I |
| methyprylon | CCC1(CC)C(=O)NCC(C)C1=O | 183.12593 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 1-(1H-Indol-3-yl)butan-1-one 3-(3-Oxobutyl)-1H-indole | CCCC(=O)C1=CNC2=CC=CC=C12 CC(=O)CCc1c[nH]c2c1cccc2 | 187.09971 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Benzyl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OCC1=CC=CC=C1 | 192.11503 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Methyl 2-acetyl-2-allylpent-4-ene-1-oate | COC(=O)C(CC=C)(CC=C)C(C)=O | 196.10994 | Suspect screening | Canal | LC-HRMS | Reference | I |
| alpha,alpha-Dicyclopropyl-4-methylbenzyl alcohol | CC1=CC=C(C=C1)C(O)(C1CC1)C1CC1 | 202.13577 | Suspect screening | Canal | LC-HRMS | Reference | I |
| N-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 3,3'-[butane-1,4-diylbis(oxy)]bispropanamine | C(CCOCCCN)COCCCN | 204.18378 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Ibuprofen | CC(C)CC1=CC=C(C=C1)C(C)C(O)=O | 206.13068 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 4-tert-octylphenol | CC(C)(C)CC(C)(C)c1ccc(cc1)O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Precocene II | COC1=CC2=C(C=CC(C)(C)O2)C=C1OC | 220.10994 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 3,4-methylenedioxypropylamphetamine | CCCNC(C)CC1=CC2=C(C=C1)OCO2 | 221.14158 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 3-Phenyl-2,3-dihydro-1,3-benzothiazol-2-imine | C1=CC=C(C=C1)N2C3=CC=CC=C3SC2=N | 226.05647 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Tetradecanamide N,N-dimethyldodecanamide | CCCCCCCCCCCC(=O)N(C)C CCCCCCCCCCCC(=O)N(C)C | 227.22491 | Suspect screening | Canal | LC-HRMS | Reference | I |
| (2S)-1-(tert-butoxycarbonyl)-4-oxopyrrolidine-2-carboxylic acid | CC(C)(C)OC(=O)N1CC(=O)CC1C(=O)O | 229.09502 | Suspect screening | Canal | LC-HRMS | Reference | I |
| diethyl 4-oxopentane-1,2-dicarboxylate | CCOC(=O)CC(CC(=O)C)C(=O)OCC | 230.11542 | Suspect screening | Canal | LC-HRMS | Reference | I |
| (Acetylazanediyl)di(ethane-2,1-diyl) diacetate | CC(=O)OCCN(CCOC(C)=O)C(C)=O | 231.11067 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 5,6,7,8-Tetrahydro-gamma-oxonaphthalene-2-butyric acid | OC(=O)CCC(=O)C1=CC2=C(CCCC2)C=C1 | 232.10994 | Suspect screening | Canal | LC-HRMS | Reference | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Suspect screening | Canal | LC-HRMS | Reference | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Canal | LC-HRMS | Reference | I |
| viloxazine | CCOC1=C(OCC2CNCCO2)C=CC=C1 | 237.13649 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate | CC1(COC(=O)C2CC=CCC2C(=O)OC1)C | 238.12051 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2-((2-Methyl-1-oxoallyl)oxy)ethyl 6-hydroxyhexanoate | CC(=C)C(=O)OCCOC(=O)CCCCCO | 244.13107 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Celestolide | CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C | 244.18272 | Suspect screening | Canal | LC-HRMS | Reference | I |
| (Z)-9-Cycloheptadecen-1-one. | O=C1CCCCCCC\C=C/CCCCCCC1 | 250.22967 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Tricyclo(3.3.1.13,7)dec-1,3-diyldi(acetic acid) | [H]C12CC3([H])CC(CC(O)=O)(C1)CC(CC(O)=O)(C2)C3 | 252.13616 | Suspect screening | Canal | LC-HRMS | Reference | I |
| N-(dodecyl)pyrrolidinone | CCCCCCCCCCCCN1CCCC1=O | 253.24056 | Suspect screening | Canal | LC-HRMS | Reference | I |
| LAURYL HYDROXYETHYL IMIDAZOLINE | CCCCCCCCCCCC1=NCCN1CCO | 268.25146 | Suspect screening | Canal | LC-HRMS | Reference | I |
| N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine | COCCCNCC1=CC(OC)=C(OC)C(OC)=C1 | 269.16271 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Terbucarb | CNC(=O)OC1=C(C=C(C)C=C1C(C)(C)C)C(C)(C)C | 277.20418 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2-((Dimethylamino)methyl)-4-isononylphenol | CC(C)CCCCCCC1=CC(CN(C)C)=C(O)C=C1 | 277.24056 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Brefeldin A | [H][C@@]12C[C@H](O)C[C@@]1([H])[C@H](O)\C=C\C(=O)O[C@@H](C)CCC\C=C\2 | 280.16746 | Suspect screening | Canal | LC-HRMS | Reference | I |
| p-(1-(p-Pentylphenyl)vinyl)anisole | CCCCCC1=CC=C(C=C1)C(=C)C1=CC=C(OC)C=C1 | 280.18272 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2,5-bis(tert-butylperoxy)-2,5-dimethylhexane | CC(C)(C)OOC(C)(C)CCC(C)(C)OOC(C)(C)C | 290.24571 | Suspect screening | Canal | LC-HRMS | Reference | I |
| N-Hexadecylacrylamide | CCCCCCCCCCCCCCCCNC(=O)C=C | 295.28751 | Suspect screening | Canal | LC-HRMS | Reference | I |
| norethisterone | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C | 298.19328 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Sodium decyl phthalate diisopentyl phthalate CROMOPHTAL DPP RED TFP | [Na+].CCCCCCCCCCOC(=O)C1=CC=CC=C1C([O-])=O CC(C)CCOC(=O)C1=CC=CC=C1C(=O)OCCC(C)C CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCC | 306.18311 | Suspect screening | Canal | LC-HRMS | Reference | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate | COC(C)(C)CCCC(C)C\C=C\C(\C)=C\C(=O)OC(C)C | 310.25079 | Suspect screening | Canal | LC-HRMS | Reference | I |
| LAURETH-3 | CCCCCCCCCCCCOCCOCCOCCO | 318.27701 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 15-(tert-Butyl)-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecine | CC(C)(C)C1=CC2=C(C=C1)OCCOCCOCCOCCO2 | 324.19367 | Suspect screening | Canal | LC-HRMS | Reference | I |
| hydrogen N-(1-oxododecyl)-L-glutamic acid | CCCCCCCCCCCC(=O)NC(CCC(=O)O)C(=O)O | 329.22022 | Suspect screening | Canal | LC-HRMS | Reference | I |
| ETHYL ARACHIDONATE | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OCC | 332.27153 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Pentadecyl 5-oxo-L-prolinate | CCCCCCCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 339.27734 | Suspect screening | Canal | LC-HRMS | Reference | I |
| MEGESTROL | [H][C@@]12CC[C@](O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(C)C2=CC(=O)CC[C@]12C | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | I |
| GLYCERYL LINOLENATE | CCC=CCC=CCC=CCCCCCCCC(=O)OCC(O)CO | 352.26136 | Suspect screening | Canal | LC-HRMS | Reference | I |
| (Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine | CCCCCCCCC=CCCCCCCCC(=O)N(C)CC(=O)O | 353.29299 | Suspect screening | Canal | LC-HRMS | Reference | I |
| N-Phenyloctadecanamide | CCCCCCCCCCCCCCCCCC(=O)NC1=CC=CC=C1 | 359.31881 | Suspect screening | Canal | LC-HRMS | Reference | I |
| N-Stearylbenzylamine | CCCCCCCCCCCCCCCCCCNCC1=CC=CC=C1 | 359.35520 | Suspect screening | Canal | LC-HRMS | Reference | I |
| PEG-2 OLEAMIDE N,N-bis(2-hydroxyethyl)oleamide | CCCCCCCCC=CCCCCCCCC(=O)NCCOCCO CCCCCCCC\C=C/CCCCCCCC(=O)N(CCO)CCO | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | I |
| PALMITOYL GLUTAMIC ACID | CCCCCCCCCCCCCCCC(=O)N[C@@H](CCC(O)=O)C(O)=O | 385.28282 | Suspect screening | Canal | LC-HRMS | Reference | I |
| eplerenone | COC(=O)[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@@]23O[C@@H]2C[C@@]2(C)[C@@H](CC[C@@]22CCC(=O)O2)[C@H]13 | 414.20424 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Isodecyl isononyl phthalate Decyl nonyl phthalate | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC© CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC | 432.32396 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one-6'-(dibutylamino)-3'-methyl-2'-(phenylamino)- | CCCCN(CCCC)C1=CC2=C(C=C1)C3(C4=CC=CC=C4C(=O)O3)C5=C(O2)C=C(C(=C5)NC6=CC=CC=C6)C | 532.27259 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Glyceryl phosphate | OCC(O)COP(O)(O)=O | 172.01367 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Acamprosate | CC(=O)NCCCS(O)(=O)=O | 181.04088 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 3-Hydroxyphthalic acid 4-Hydroxybenzene-1,2-dicarboxylic acid | OC(=O)C1=C(C(O)=O)C(O)=CC=C1 OC(=O)C1=C(C=C(O)C=C1)C(O)=O | 182.02152 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 4-morpholineethanesulfonic acid | OS(=O)(=O)CCN1CCOCC1 | 195.05653 | Suspect screening | Canal | LC-HRMS | Reference | I |
| benzothiazole sulfonic acid | C1=CC=C2C(=C1)N=C(S2)S(=O)(=O)O | 214.97108 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 1-(2,5-Dihydroxyphenyl)octan-1-one | CCCCCCCC(=O)C1=C(O)C=CC(O)=C1 | 236.14124 | Suspect screening | Canal | LC-HRMS | Reference | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Loxoprofen alcohol | CC(C1=CC=C(C=C1)CC2CCCC2O)C(=O)O | 248.14124 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Ethyl 3-(3,4,5-trimethoxyphenyl)propionate Butyl 3,4,5-trimethoxybenzoate | CCOC(=O)CCC1=CC(OC)=C(OC)C(OC)=C1 CCCCOC(=O)C1=CC(OC)=C(OC)C(OC)=C1 | 268.13107 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Triaziflam | CC(COC1=CC(C)=CC(C)=C1)N=C1NC(=N)N=C(N1)C(C)(C)F | 333.19649 | Suspect screening | Canal | LC-HRMS | Reference | I |
| cefaloram | CC(=O)OCC1=C(N2[C@H](SC1)[C@H](NC(=O)CC1=CC=CC=C1)C2=O)C(O)=O | 390.08856 | Suspect screening | Canal | LC-HRMS | Reference | I |
| NONOXYNOL-4 | CCCCCCCCCC1=CC=CC=C1OCCOCCOCCOCCO | 396.28757 | Suspect screening | Canal | LC-HRMS | Reference | I |
| simvastatin hydroxyl acid | CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 436.28249 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Bis(p-(1,1,3,3-tetramethylbutyl)phenyl) hydrogen phosphate | CC(C)(C)CC(C)(C)C1=CC=C(OP(O)(=O)OC2=CC=C(C=C2)C(C)(C)CC(C)(C)C)C=C1 | 474.28990 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Perfluorooctanesulfonic acid | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Reference | I |
| N-Ethylperfluorooctane-1-sulfonamide | CCNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 526.98478 | Suspect screening | Canal | LC-HRMS | Reference | I |
| Octyl thiocyanate | CCCCCCCCSC#N | 171.10817 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2-Methylene-3-butyn-1-ol 1-Methoxybut-1-en-3-yne | OCC(=C)C#C COC=CC#C | 82.04186 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2-(1,1-Dimethylethyl)-4-(1-methyl-1-phenylethyl)phenol | CC(C)(C)C1=C(O)C=CC(=C1)C(C)(C)C1=CC=CC=C1 | 268.18272 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 2-((2-Hydroxyethyl)(3-methoxypropyl)amino)ethyl methacrylate | COCCCN(CCO)CCOC(=O)C(C)=C | 245.16271 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 4-O-Desmethyl 4-O-Ethyl Trimethoprim | CCOC1=C(OC)C=C(CC2=CNC(=N)NC2=N)C=C1OC | 304.15354 | Suspect screening | Canal | LC-HRMS | Reference | I |
| 19-Norandrostenedione | CC12CCC3C(C1CCC2=O)CCC4=CC(=O)CCC34 | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Galaxolidone | CC2(C)c1cc3C(=O)OCC(C)c3cc1C(C)(C)C2C | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17alpha-Estradiol | C[C@]12CC[C@H]3[C@@H](CCC4=C3C=CC(O)=C4)[C@@H]1CC[C@H]2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17b-hydroxyestra-4,6-diene-3-one;d6n;delta-6-nandrolone;6-dehydronandrolone;17-hydroxyestra-4,6-dien-3-one;4,6-estradien-17beta-ol-3-one;17b-hydroxyestra-4,6-diene-3-one d6n delta-6-nandrolone 6-dehydronandrolone 17-hydroxyestra-4,6-dien-3-one 4,6-estradien-17beta-ol-3-one | CC12CCC3C4CCC(=O)C=C4C=CC3C1CCC2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl phenylacetate | O=C(OC1CC2CCC1(C)C2(C)C)CC=3C=CC=CC3 | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl phenylacetate | O=C(OC(C)(C)C1CC=C(C)CC1)CC=2C=CC=CC2 | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Oestr-5(10)-ene-3,17-dione | O=C1CC2=C(CC1)C3CCC4(C(=O)CCC4C3CC2)C | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (1E)-2,6-Dimethylhepta-1,5-dien-1-yl phenylacetate | CC(C)=CCC/C(C)=C/COC(=O)Cc1ccccc1 | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17B-hydroxyestra-4,6-diene-3-one | C[C@]12CC[C@@H]3[C@H]4CCC(=O)C=C4C=C[C@H]3[C@@H]1CC[C@@H]2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| estr-4-ene-3,17-dione | C[C@]12CC[C@H]3[C@H]([C@@H]1CCC2=O)CCC4=CC(=O)CC[C@H]34 | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17beta-Estradiol | [H][C@@]12CC[C@H](O)[C@@]1(C)CC[C@]1([H])C3=CC=C(O)C=C3CC[C@@]21[H] | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9,10-Dehydro-19-nortestosterone | CC12CCC3=C4CCC(=O)C=C4CCC3C1CCC2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Estr-5-ene-3,17-dione | O=C1CC2=CCC3C(CCC4(C(=O)CCC34)C)C2CC1 | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzeneacetic acid, 1-ethenyl-1,5-dimethyl-4-hexen-1-yl ester | CC(C)=CCCC(C)(OC(=O)Cc1ccccc1)C=C | 272.17763 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cholest-4-en-3-one | CC(C)CCCC(C)C2CCC1C3CCC4=CC(=O)CCC4(C)C3CCC12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-a-cholesta-8,24-dien-3-ß-ol | OC1CCC2(C3=C(CCC2C1)C4CCC(C(C)CCC=C(C)C)C4(C)CC3)C | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cholest-5-en-3-one | CC(C)CCCC(C)C1CCC2C3CC=C4CC(=O)CCC4(C)C3CCC12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cholesta-4,6-diene-3ß-ol | OC1C=C2C=CC3C(CCC4(C)C3CCC4C(C)CCCC(C)C)C2(C)CC1 | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Desmosterol | C[C@H](CCC=C(C)C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (3ß,6Z)-9,10-secocholesta-5(10),6,8-trien-3-ol | OC1CC(C=CC2=CCCC3(C)C2CCC3C(C)CCCC(C)C)=C(C)CC1 | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Vitamin D3 | CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2C(CCC[C@]12C)=CC=C1/C[C@@H](O)CCC1=C | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 7,8-Didehydrocholesterol | CC(C)CCCC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1,2,3,5,6,7-hexahydrotetramethyl-s-indacenyl)ethanone | O=C(C)C1(C2=CC3=C(C=C2C(C)C1(C)C)CCC3)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-Bis(1,1-dimethylethyl)-2-naphthol | CC(C)(C)c1cc2c(cccc2)c(c1O)C(C)(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,4,5,6,7,8-Hexahydro-5,5,8,8-tetramethylanthracen-1(2H)-one | CC1(C)CCC(C)(C)c2cc3c(CCCC3=O)cc12 | 256.18272 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Octyl-2-naphthol | CCCCCCCCc1c(O)ccc2c1cccc2 | 256.18272 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Buten-1-one, 1-(2,3-dihydro-1,1,3,3,6-pentamethyl-1H-inden-5-yl)- | C/C=C/C(=O)c1c(C)cc2c(c1)C(C)(C)CC2(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Reference | L |
| as-Indacen-3(2H)-one, 1,6,7,8-tetrahydro-1,4,6,6,8,8-hexamethyl- | CC1CC(=O)c2c(C)cc3c(c12)C(C)(C)CC3(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,5,6,7-tetrahydro-3,5,5,6,7,7-hexamethyl-s-indacen-1(2H)-one | O=C1C=2C=C3C(=CC2C(C)C1)C(C)(C)C(C)C3(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Etc-588 | CCCCCCCC/C=CCCCCCCCC(=O)OC[C@H](CO[P@](=O)(O)OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC | 760.58563 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Nonenoic acid | CCCCC/C=C/CC(=O)O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Prenyl isobutyrate | CC(C)C(=O)OCC=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4,6-Nonanedione | CCCC(=O)CC(=O)CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Nonenoic acid | CCCCCC/C=CC(=O)O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,3-Diethylpentane-2,4-dione | CCC(CC)(C(=O)C)C(=O)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Butylpentane-2,4-dione | CCCCC(C(=O)C)C(=O)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,7-Dioxaspiro[5.5]undecane | C1CCC2(CCCCO2)OC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| tert-Butyl 3-methyl-2-butenoate | CC(=CC(=O)OC(C)(C)C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Neopentyl methacrylate | CC(=C)C(=O)OCC(C)(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2-Dimethyl-1,3-bis(vinyloxy)propane | CC(C)(COC=C)COC=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Pentenoic acid, 3,3-dimethyl-, ethyl ester | CCOC(=O)CC(C)(C)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl trans-2-methylcyclohexanecarboxylate | COC(=O)[C@@H]1CCCC[C@H]1C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isopentyl methacrylate | CC(C)CCOC(=O)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Prenyl butyrate | CCCC(=O)OCC=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Butanoic acid, 2-methylene-, 2-methylpropyl ester | CCC(=C)C(=O)OCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclopentyl isobutyrate | CC(C)C(=O)OC1CCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclopentyl butyrate | CCCC(=O)OC1CCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Nonane-2,4-dione | CCCCCC(=O)CC(=O)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Butyl 3-methyl-2-butenoate | CCCCOC(=O)C=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Methylpentyl acrylate | CC(C)CCCOC(=O)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Propene, 3,3'-[(1-methylethylidene)bis(oxy)]bis- | CC(C)(OCC=C)OCC=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Oxononan-1-al | CCCCCC(=O)CCC=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclohexyl propionate | CCC(=O)OC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| cis-4-methylcyclohexyl acetate | O=C(OC1CCC(C)CC1)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-cyclohexylpropionic acid | O=C(O)C(C)C1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1-methoxyisopropoxy)pent-2-yne | C(#CCC)COC(OC)(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methoxy-2-methylhept-4-yn-3-ol | OC(C#CCC)C(OC)(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1-ethoxyethoxy)pent-2-yne | C(#CCC)COC(OCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-methylpent-3-en-1-yl propionate | O=C(OCCC(=CC)C)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(hydroxymethyl)-6-methylhept-5-en-2-one | O=C(C)C(CO)CC=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methylallyl 2-methylbutyrate | O=C(OCC(=C)C)C(C)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-methyl-2-(1-methyl-1-butenyl)-1,3-dioxolane | O1CC(OC1C(=CCC)C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (Z)-1-methylhex-3-enyl acetate | O=C(OC(C)CC=CCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (E)-4-methyl-2-(pent-1-enyl)-1,3-dioxolane | O1CC(OC1C=CCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-methylbutyl methacrylate | O=C(OC(C)CCC)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| But-2-enyl 2-methylbutyrate | O=C(OCC=CC)C(C)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Isopropyl-5-oxohexanal | CC(C)C(CCC(C)=O)C=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-Methyl-3-propan-2-yloxan-2-one | CC1CCC(C(=O)O1)C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclohexanecarboxylic acid, 3-methyl-, methyl ester, (1R,3S)-rel- | COC(=O)C1CCCC(C)C1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(cyclohexyloxy)acetone | O=C(C)COC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Allyl hexanoate | CCCCCC(=O)OCC=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclohexanepropionic acid | OC(=O)CCC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methylcyclohexyl acetate | CC1CCCCC1OC(C)=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methylcyclohexylacetate | COC(=O)CC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| gamma-Nonanolactone | [C@H]1(OC(CC1)=O)CCCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (2Z)-3-Methyl-4-methylideneoct-2-ene | CCCCOC(=O)C(/C)=CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (Z)-Hept-3-enyl Acetate. | CCC/C=C/CCOC(C)=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (3Z)-Hex-3-en-1-yl propanoate | CCC=C/CCOC(=O)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclohexanecarboxylic acid, ethyl ester | CCOC(=O)C1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Octenoic acid, methyl ester | CCCCC/C=C/C(=O)OC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Hexen-1-ol, 1-propanoate, (2E)- | CCC/C=C/COC(=O)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Methylbutyl 2-Butenoate. | C/C=C/C(=O)OCCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Butenoic acid, 2-methyl-, 2-methylpropyl ester, (2E)- | CC=C(/C)C(=O)OCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2(3H)-Furanone, 5-butyldihydro-4-methyl- | CCCCC1OC(=O)CC1C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2H-Pyran-2-one, 6-butyltetrahydro- | CCCCC1CCCC(=O)O1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (4R,6R)-4-Hydroxy-2,2,6-trimethylcyclohexanone / 60046-50-6 | CC1CC(O)CC(C)(C)C1=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| g-Nonalactone | CCCCCC1CCC(O1)=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dihydro-3-(3-methylbutyl)furan-2(3H)-one | O=C1OCCC1CCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hept-1-enyl acetate | O=C(OC=CCCCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methyl-1,4-dioxaspiro[4.5]decane | O1CC(OC12CCCCC2)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| trans-2-pentylcyclopropanecarboxylic acid | O=C(O)C1CC1CCCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4,6,6-trimethyloxepan-2-one | O=C1OCC(C)(C)CC(C)C1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Allyl 2-ethylbutyrate | O=C(OCC=C)C(CC)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methylpentyl acrylate | O=C(OCC(C)CCC)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-methyloctan-4-olide | O=C1OC(C)(CC1)CCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [(cyclohexyloxy)methyl]oxirane | O1CC1COC2CCCCC2 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-ethylbutyl acrylate | O=C(OCC(CC)CC)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl 5-methylhex-2-enoate | O=C(OCC)C=CCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methylcyclohexyl acetate | O=C(OC1(C)CCCCC1)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Pentyl 2-butenoate | O=C(OCCCCC)C=CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl (*Z*)-oct-4-enoate | O=C(OC)CCC=CCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(tetrahydro-4-methyl-2H-pyran-2-yl)acetone | O=C(C)CC1OCCC(C)C1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hexyl acrylate | CCCCCCOC(=O)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-vinylpentyl acetate | O=C(OC(C=C)CCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclooctyl formate | O=COC1CCCCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-dimethylbutyl acrylate | O=C(OC(C)CC(C)C)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bicyclo[2.2.1]heptane-2,2-dimethanol | OCC1(CO)CC2CCC1C2 | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Propyl (E)-hex-2-enoate | O=C(OCCC)C=CCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(1-ethoxyethoxy)pent-1-yne | C#CCCCOC(OCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (E)-hept-2-enyl acetate | O=C(OCC=CCCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 7,7-dimethoxyhept-3-yne | C(#CCCC(OC)OC)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methylbutyl methacrylate | O=C(OCC(C)CC)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,3,5-trimethyloxepan-2-one | O=C1OCCC(C)CC1(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl (*E*)oct-3-enoate | O=C(OC)CC=CCCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-methyl-2-(2-methyl-1-propenyl)-1,3-dioxane | O1CCC(OC1C=C(C)C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-methylpentyl acrylate | O=C(OC(C)CCCC)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (*Z*)-pent-2-enyl butyrate | O=C(OCC=CCC)CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (*Z*)-non-6-enoic acid | O=C(O)CCCCC=CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl (*E*)-hept-4-enoate | O=C(OCC)CCC=CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-dimethylheptane-3,5-dione | O=C(CC(=O)C(C)C)C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Pentenoic acid, 2,4-dimethyl-, ethyl ester, (2*E*)- | CCOC(=O)/C(=C/C(C)C)/C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Pentyl methacrylate | CCCCCOC(=O)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isobutyl 3-methyl-2-butenoate | CC(C)COC(=O)C=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2'-Bipyrimidine | c1cnc(nc1)c1ncccn1 | 158.05925 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Chlorophthalic anhydride | Clc1ccc2C(=O)OC(=O)c2c1 | 181.97707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Chlorophthalic anhydride | Clc1cccc2C(=O)OC(=O)c12 | 181.97707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-(3-hydroxypropyl)stearamide | O=C(NCCCO)CCCCCCCCCCCCCCCCC | 341.32938 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Sodium N-octadecyl-ß-alaninate | [Na+].O=C([O-])CCNCCCCCCCCCCCCCCCCCC | 341.32938 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Octadecanamide, N-(2-hydroxypropyl)- | CCCCCCCCCCCCCCCCCC(=O)NCC(C)O | 341.32938 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dioleoyl phthalate | O=C(OC(=O)CCCCCCCC=CCCCCCCCC)C=1C=CC=CC1C(=O)OC(=O)CCCCCCCC=CCCCCCCCC | 694.51724 | Suspect screening | Canal | LC-HRMS | Reference | L |
| *N,N*-dimethyladenosine | OCC1OC(N2C=NC=3C2=NC=NC3N(C)C)C(O)C1O | 295.12805 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-D-Gluconoyl-L-valine | CC(C)[C@H](NC(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO)C(O)=O | 295.12672 | Suspect screening | Canal | LC-HRMS | Reference | L |
| p-amino-DL-phenylalanine hydrate | O=C(O)C(N)CC1=CC=C(N)C=C1.O | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-diisocyanato-2-methylcyclohexane | O=C=NC1CCCC(N=C=O)C1C | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-hydroxy-N-propylpyridine-2-carboxamide | O=C(NCCC)C1=NC=CC=C1O | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Acetanilide, mono(aminomethoxy) derivative | O=C(NC=1C=CC=CC1)COCN | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-hydroxy-N-isopropylpyridine-2-carboxamide | O=C(NC(C)C)C1=NC=CC=C1O | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dulcin | CCOc1ccc(NC(=O)N)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-(2-aminoethyl)-4-hydroxybenzamide monohydrochloride | Cl.O=C(NCCN)C1=CC=C(O)C=C1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tyrosinamide | NC(=O)[C@@H](N)Cc1ccc(O)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methoxy-4,6-dimethylpyridine-3-carboxamide | CC1=CC(=NC(=C1C(=O)N)OC)C | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| *N*-methyl-2-(4-nitrophenyl)ethanamine | CNCCC1=CC=C(C=C1)[N+](=O)[O-] | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Methoxy-1-methyl-3-phenylurea | CON(C)C(=O)Nc1ccccc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Carbamic acid, [[3-(aminomethyl)phenyl]methyl]- | NCc1cccc(CNC(=O)O)c1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,4-diisocyanato-1-methylcyclohexane | O=C=NC1CCC(C)C(N=C=O)C1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(((2-Hydroxyphenyl)methyl)amino)acetamide | NC(=O)CNCc1ccccc1O | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzenamine, N-ethyl-2-methyl-5-nitro- | CCNc1c(C)ccc(c1)[N+](=O)[O-] | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl 3,5-diaminobenzoate | CCOC(=O)c1cc(N)cc(N)c1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzenamine, *N*-(1-methylethyl)-4-nitro- | CC(C)Nc1ccc(cc1)[N+](=O)[O-] | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Amino-*N*-(2-hydroxyethyl)benzamide | Nc1c(cccc1)C(=O)NCCO | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2-Furoyl)piperazine | O=C(N1CC[NH2+]CC1)c1ccco1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(1H-Imidazol-1-yl)ethyl methacrylate | CC(=C)C(=O)OCCn1ccnc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| *N*-(3-Amino-4-methoxyphenyl)acetamide | COc1c(N)cc(NC(=O)C)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-((3-Hydroxy-4-methylphenyl)amino)acetamide | Cc1c(O)cc(NCC(=O)N)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(2-Hydroxyphenyl)-1,1-dimethylurea | CN(C)C(=O)Nc1c(O)cccc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2-Hydroxyethyl)-3-phenylurea | OCCNC(=O)Nc1ccccc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Dicyclopentyl-3,5-xylenol | Cc1cc(C)c(C2CCCC2)c(O)c1C1CCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Dicyclohexylphenol | Oc1c(cccc1C1CCCCC1)C1CCCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-cyclohexylidene-6-(1-cyclohexen-1-yl)cyclohexan-1-one | O=C1C(=C2CCCCC2)CCCC1C3=CCCCC3 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-bis(1-cyclohexen-1-yl)cyclohexan-1-one | O=C1C(C2=CCCCC2)CCCC1C3=CCCCC3 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Oestr-4-en-17-one | O=C1CCC2C3CCC4=CCCCC4C3CCC12C | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Di(cyclohexylidene)cyclohexan-1-one | O=C1C(=C2CCCCC2)CCCC1=C1CCCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Acetylethyltetramethyltetralin | CCc1c(cc2c(c1)C(C)(C)CCC2(C)C)C(=O)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-Cyclopentyl-1,1,3,3-tetramethylindan-5-ol | CC1(C)CC(C)(C)c2cc(C3CCCC3)c(O)cc12 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[2,3-Dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-inden-5-yl]ethan-1-one | CC(C)C1C(C)C(C)(C)c2cc(C)c(cc12)C(C)=O | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Xibornol | CC1=CC(=C(C=C1C)O)C2CC3CCC2(C3(C)C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-ethyl-1,3,4,6,7,8-hexahydro-4,6,8,8-tetramethylcyclopenta[g]-2-benzopyran | O1CC=2C=C3C(=CC2C(C)C1)C(C)(CC)CC3(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[1,3,3,6-Tetramethyl-1-(propan-2-yl)-2,3-dihydro-1H-inden-5-yl]ethan-1-one | CC(C)C1(C)CC(C)(C)c2cc(C(C)=O)c(C)cc12 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(4-(trans-4-butylcyclohexyl)phenyl)ethanone | CCCC[C@H]1CCC(CC1)c1ccc(cc1)C(C)=O | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1H-Naphtho[2,3-c]pyran, 3,4,6,7,8,9-hexahydro-4,6,6,9,9-pentamethyl- | CC1COCc2cc3c(cc12)C(C)(C)CCC3(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 8-ethyl-1,3,4,6,7,8-hexahydro-4,6,6,8-tetramethylcyclopenta[g]-2-benzopyran | O1CC=2C=C3C(=CC2C(C)C1)C(C)(C)CC3(C)CC | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1'-Biphenyl, 4-cyclohexyl- | OC1CCC(CC1)c1cccc(c1)C1CCCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl- | CC1C(C)(C)c2cc3COCC(C)c3cc2C1(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-Acetyl-1,1,2,4,4,7-hexamethyltetralin | CC1CC(C)(C)c2cc(C(C)=O)c(C)cc2C1(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Choline chloride | [Cl-].C[N+](C)(C)CCO | 139.07639 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Arachidoyl glycine | CCCCCCCCCCCCCCCCCCCC(=O)NCC(=O)O | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Oxiranylmethyl octadecylcarbamate | O=C(OCC1OC1)NCCCCCCCCCCCCCCCCCC | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(15-methylhexadecyl)-2-oxazoline-4,4-dimethanol | OCC1(N=C(OC1)CCCCCCCCCCCCCCC(C)C)CO | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-[(2-hydroxyethyl)amino]ethyl oleate | O=C(OCCNCCO)CCCCCCCC=CCCCCCCCC | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Heptadecyl-4,4(5H)-oxazoledimethanol | CCCCCCCCCCCCCCCCCC1=NC(CO)(CO)CO1 | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Stearoyl methyl beta-alanine | CCCCCCCCCCCCCCCCCC(=O)N(C)CCC(=O)O | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9-Octadecenamide, N-[2-(2-hydroxyethoxy)ethyl]-, (9Z)- | CCCCCCCCC=C/CCCCCCCC(=O)NCCOCCO | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (9Z)-N,N-Bis(2-hydroxyethyl)octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N(CCO)CCO | 369.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2-dimethylpropane-1,3-diyl dinonanoate | O=C(OCC(C)(C)COC(=O)CCCCCCCC)CCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Propylene didecanoate | O=C(OCC(OC(=O)CCCCCCCCC)C)CCCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [isopropylidenedicyclohexane-4,1-diyl]bis(tert-butyl) peroxide | O(OC(C)(C)C)C1CCC(CC1)C(C)(C)C2CCC(OOC(C)(C)C)CC2 | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-dihydroxypropan-2-yl (Z)-icos-11-enoate | CCCCCCCCC=CCCCCCCCCCC(=O)OC(CO)CO | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tetradecyl hydrogen azelate | CCCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)O | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diethyl cetylmalonate | CCCCCCCCCCCCCCCCC(C(=O)OCC)C(=O)OCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [2-(1-ethylpentyl)-1,3-dioxolan-4-yl]methyl laurate | O=C(OCC1OC(OC1)C(CC)CCCC)CCCCCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(1-ethylpentyl)-1,3-dioxan-5-yl laurate | O=C(OC1COC(OC1)C(CC)CCCC)CCCCCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Reference | L |
| trans-4-(4-propylcyclohexyl)phenyl trans-4-pentylcyclohexanecarboxylate | O=C(OC1=CC=C(C=C1)C2CCC(CCC)CC2)C3CCC(CCCCC)CC3 | 398.31848 | Suspect screening | Canal | LC-HRMS | Reference | L |
| trans-4-propylcyclohexyl trans-p-(4-pentylcyclohexyl)benzoate | O=C(OC1CCC(CCC)CC1)C2=CC=C(C=C2)C3CCC(CCCCC)CC3 | 398.31848 | Suspect screening | Canal | LC-HRMS | Reference | L |
| C12 Fatty acid methyl ester (MEE), 1 EO | CCCCCCCCCCCCOCCC(OC)=O | 272.23514 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 8-(2,2-diethoxyethoxy)-2,6-dimethyloct-2-ene | O(CCC(C)CCC=C(C)C)CC(OCC)OCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-hydroxyethyl myristate | O=C(OCCO)CCCCCCCCCCCCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-hydroxypalmitic acid | O=C(O)C(O)CCCCCCCCCCCCCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 16-Hydroxypalmitic acid | C(CCCCCCCC(=O)O)CCCCCCCO | 272.23514 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,4,4-Trimethylpentan-2-yl 2-ethylhexaneperoxoate | CCCCC(CC)C(=O)OOC(C)(C)CC(C)(C)C | 272.23514 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dodecanoic acid, 2-ethoxyethyl ester | CCCCCCCCCCCC(=O)OCCOCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Reference | L |
| a,a'-dimethylpiperazine-1,4-diethanol | OC(C)CN1CCN(CC1)CC(O)C | 202.16813 | Suspect screening | Canal | LC-HRMS | Reference | L |
| *N*-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,5-dimethylpiperazine-1,4-diethanol | OCCN1CC(N(CCO)CC1C)C | 202.16813 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (3s)-3-Amino-1-(cyclopropylamino)heptane-2,2-Diol | CCCC[C@H](N)C(O)(O)CNC1CC1 | 202.16813 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Doxercalciferol | C=C1/C(=C/C=C2CCC[C@@]3(C)[C@H]2CC[C@@H]3[C@H](C)/C=C/[C@H](C)C(C)C)C[C@@H](O)C[C@@H]1O | 412.33413 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-{2-[1-(5,6-dimethylhept-3-en-2-yl)-7a-methyl-octahydro-1h-inden-4-ylidene]ethylidene}-4-methylidenecyclohexane-1,3-diol | C=C1/C(=C/C=C2CCC[C@@]3(C)[C@H]2CC[C@@H]3[C@H](C)/C=C[C@H](C)C(C)C)C[C@@H](O)C[C@@H]1O | 412.33413 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(3,3,5-trimethylcyclohexyl) hydrogen 2-octadecenylsuccinate | O=C(OC1CC(C)CC(C)(C)C1)CC(C(=O)[O-])CC=CCCCCCCCCCCCCCCC | 492.41786 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-phenyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-one | O=C(C=CCC1CC=C(C)C1(C)C)C=2C=CC=CC2 | 254.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Estra-1(10),2,4,16-tetraen-3-ol | CC12CCC3C(C1CC=C2)CCC4=C3C=CC(=C4)O | 254.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Enzacamene | Cc1ccc(C=C2/C3CCC(C)(C2=O)C3(C)C)cc1 | 254.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-methylbenzylidene camphor | CC12C(/C(C(C(C)2C)CC1)=CC3=CC=C(C)C=C3)=O | 254.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(1-methylpropyl)-2-(1-phenylethyl)phenol | OC1=CC=C(C=C1C(C=2C=CC=CC2)C)C(C)CC | 254.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [4-[[4-(dimethylamino)phenyl]imino]cyclohexa-2,5-dien-1-ylidene]dimethylammonium chloride | CN(C)c1ccc(cc1)N=C2C=CC(=[N+](C)C)C=C2.[Cl-] | 254.16572 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethanone, 1-[(3R,3aR,7R,8aS)-2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl]- | C[C@@H]1CC[C@H]2C(C)(C)[C@H]3C[C@@]12CC(C(C)=O)=C3C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [3R-(3Î±,3aÎ²,7Î²,8aÎ±)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)ethan-1-one | CC1CCC2C(C)(C)C3CC12CC(C(C)=O)=C3C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethanone, 1-(1,3,4,4a,5,6,7-hexahydro-2,5,5-trimethyl-2H-2,4a-ethanonaphthalen-8-yl)- | CC(=O)C1=C2CC3(C)CCC2(CC3)C(C)(C)CC1 | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1H-Indene-5-ethanol, 2,3-dihydro-beta,1,1,2,3,3-hexamethyl- | CC(CO)c1ccc2c(c1)C(C)(C)C(C)C2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 2,6,10-trimethylcyclododeca-2,5,9-trien-1-yl ketone | CC(=O)C1CCC(=CCCC(=C/C/C=C1/C)C)/C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2,4,6-Tris(1-methylethyl)phenyl)ethan-1-one | CC(C)c1cc(C(C)C)c(C(=O)C)c(c1)C(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4,6-Bis(isopropyl)-3,3-dimethylindan-5-ol | CC(C)c1cc2c(c(C(C)C)c1O)C(C)(C)CC2 | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Phenylundecanone | CCCCCCCCCCC(=O)c1ccccc1 | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-(tert-Butyl)-1,1,3,3-tetramethylindan-5-ol | CC(C)(C)c1cc2c(cc1O)C(C)(C)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Cyclohexyl-6-isobutyl-p-cresol | CC(C)Cc1cc(C)cc(C2CCCCC2)c1O | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-Isobutyl-1,1,3,3-tetramethylindan-5-ol | CC(C)Cc1c(O)cc2c(c1)C(C)(C)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (3R-(3alpha,3abeta,7beta,8aalpha))-1-(2,3,4,7,8,8a-Hexahydro-3,8,8-trimethyl-1H-3a,7-methanoazulen-6-yl)acetone | C[C@H]1CC[C@@H]2C(C)(C)[C@@H]3C[C@]12CC=C3CC(C)=O | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[10,10-dimethyl-2,6-bis(methylene)bicyclo[7.2.0]undec-5-yl]ethan-1-one | O=C(C)C1C(=C)CCC2C(C(=C)CC1)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-2H-2,4a-methanonaphthalen-8-yl)ethan-1-one | O=C(C1=C2C(C)(C)C3CCC2(C3)C(C)(C)CC1)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(octahydro-7,7,8,8-tetramethyl-2,3b-methano-3bH-cyclopenta[1,3]cyclopropa[1,2]benzen-4-yl)ethanone | O=C(C)C1CCC(C)(C)C23CC4CC2C13C4(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| trans-p-(4-propylcyclohexyl)phenetole | O(C1=CC=C(C=C1)C2CCC(CCC)CC2)CC | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-[7-isopropyl-3,5-dimethylbicyclo[2.2.2]oct-5-en-2-yl]-3-buten-2-one | O=C(C=CC1C2C=C(C)C(CC2C(C)C)C1C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Di-tert-butyl-4-(prop-2-en-1-yl)phenol | CC(C)(C)C1=CC(CC=C)=CC(=C1O)C(C)(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethanone, 1-(2,6,10-trimethyl-2,5,9-cyclododecatrien-1-yl)- | CC(=O)C1CCC(C)=CCCC(C)=CCC=C1C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1,3,3-tetramethyl-6-(1-methylpropyl)indan-5-ol | OC=1C=C2C(=CC1C(C)CC)C(C)(C)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(6,6,9-trimethyl-2-methylenecycloundeca-4,8-dien-1-yl)ethan-1-one | O=C(C)C1C(=C)CC=CC(C)(C)CC=C(C)CC1 | 246.19837 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diazidodimethylsilane | [N-]=[N+]=N[Si](N=[N+]=[N-])(C)C | 144.05797 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Naphthalenol | Oc1ccc2ccccc2c1 | 144.05751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Phenyl-3-butyn-2-one | CC(=O)C#Cc1ccccc1 | 144.05751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Naphthol | Oc1cccc2ccccc12 | 144.05751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Acetylgalactosamine 4-sulfate | CC(=O)NC1C(C(C(OC1O)CO)OS(=O)(=O)O)O | 301.04675 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Acetyl-D-galactosamine 6-sulfate | CC(=O)N[C@H]1[C@H](O)O[C@H](COS(=O)(=O)O)[C@H](O)[C@@H]1O | 301.04675 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [5-acetamido-4,6-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxidanesulfonic acid | CC(=O)N[C@H]1[C@@H](O)O[C@H](CO)[C@H](OS(=O)(=O)O)[C@@H]1O | 301.04675 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Amino-5,6-dimethyl-1,2,4-triazine | Cc1c(C)nc(N)nn1 | 124.07490 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isooctyl nonyl phthalate | CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCC(C)C | 404.29266 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-ethylhexyl nonyl phthalate | O=C(OCCCCCCCCC)C=1C=CC=CC1C(=O)OCC(CC)CCCC | 404.29266 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (20S)-5a-pregnane-3ß,20-diol diacetate | O=C(OC(C)C1CCC2C3CCC4CC(OC(=O)C)CCC4(C)C3CCC12C)C | 404.29266 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 12a-hydroxy-3-oxo-5ß-cholan-24-oate | O=C(OC)CCC(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CC(O)C12C | 404.29266 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2(3H)-Benzothiazolethione, 3-methyl- | Cn1c(=S)sc2c1cccc2 | 181.00199 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(Methylthio)benzothiazole | CSc1nc2ccccc2s1 | 181.00199 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2-dimethoxy-1-methylethylamine | O(C)C(OC)C(N)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[(2-hydroxyethyl)amino]propan-2-ol | OCCNCC(O)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-((Hydroxymethyl)amino)-2-methyl-1-propanol | CC(C)(CO)NCO | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(ethylamino)propane-1,2-diol | OCC(O)CNCC | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-dimethylaminopropane-1,2-diol | OCC(O)CN(C)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-((2-Hydroxyethyl)amino)propanol | OCCCNCCO | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2-Dimethoxyethyl(methyl)amine | CNCC(OC)OC | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(dimethylamino)propane-1,3-diol | OCCC(O)N(C)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-amino-2-methylbutane-2,3-diol | C[C@@H](O)[C@@](C)(O)CN | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Amino-2-ethyl-1,3-propanediol | CCC(N)(CO)CO | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methanamine, 1,1-dimethoxy-N,N-dimethyl- | COC(OC)N(C)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Methyldiethanolamine | CN(CCO)CCO | 119.09463 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,3'-((1-Methylethylidene)bis(4,1-phenyleneoxy))dipropionodihydrazide | CC(C)(c1ccc(OCCC(=O)NN)cc1)c1ccc(OCCC(=O)NN)cc1 | 400.21106 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Pieristoxin G | C[C@@]1(O)CC23[C@@H](O)[C@@H]1CC[C@@]2(O)[C@@](C)(O)[C@@H]1[C@@H]2O[C@@H]2C(C)(C)[C@@]1(O)[C@H](O)[C@H]3O | 400.20972 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Hydroxy-2,4,6-triiodobenzoic acid | OC(=O)c1c(I)c(O)c(I)cc1I | 515.72162 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-Bis(((3-(aminomethyl)phenyl)methyl)amino)propan-2-ol | NCc1cc(CNCC(O)CNCc2cc(CN)ccc2)ccc1 | 328.22631 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,4:3,6-Dianhydro-D-glucitol monolaurate | CCCCCCCCCCCC(=O)OC1COC2C(O)COC12 | 328.22497 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Corchorifatty acid F | CC/C=CCC(C(/C=C/C(CCCCCCCC(=O)O)O)O)O | 328.22497 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(3,5-di-sec-butylcyclopent-1-enyl)-2,3,5-trihydroxyvaleric acid | O=C(O)C(O)C(O)CC(O)C1=CC(CC1C(C)CC)C(C)CC | 328.22497 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethanol, 2-decylthio- | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-mercaptododecan-2-ol | OC(CS)CCCCCCCCCC | 218.17044 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-methoxyundecane-3-thiol | SC(CCOC)CCCCCCCC | 218.17044 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dimethoxymethyloctylsilane | O(C)C(OC)[SiH2]CCCCCCCC | 218.17021 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-[(2-hydroxyethyl)[4-[(6-methoxybenzothiazol-2-yl)azo]-3-methylphenyl]amino]propiononitrile | N#CCCN(C1=CC=C(N=NC2=NC=3C=CC(OC)=CC3S2)C(=C1)C)CCO | 395.14160 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-[(1R,2R)-2-(Dimethylamino)cyclohexyl]-N-methyl-1,3-benzodioxole-5-carboxamide hydrochloride (1:1) | CN(C)[C@@H]1CCCC[C@H]1N(C)C(=O)c2ccc3c(c2)OCO3.Cl | 340.15537 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(hydroxymethyl)-2-[[(2-methyl-1-oxoallyl)oxy]methyl]-1,3-propanediyl bismethacrylate | O=C(OCC(CO)(COC(=O)C(=C)C)COC(=O)C(=C)C)C(=C)C | 340.15220 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Deacetylneosolaniol | CC1=C[C@@H]2[C@](C[C@@H]1O)([C@]3([C@@H]([C@H]([C@H]([C@@]34CO4)O2)O)O)C)COC(=O)C | 340.15220 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2'-Thiobisethanol | OCCSCCO | 122.04015 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-methylthiopropane-1,2-diol | OCC(O)CSC | 122.04015 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diethyl sulphone | O=S(=O)(CC)CC | 122.04015 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Trimethoxysilane | O(C)[SiH](OC)OC | 122.03992 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tripotassium propylsilanetriolate | [K+].[K+].[K+].[O-][Si]([O-])([O-])CCC | 122.03992 | Suspect screening | Canal | LC-HRMS | Reference | L |
| MEGESTROL | CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C=C(C)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6,7-DIHYDROCANRENONE | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@]21CCC(=O)O1 | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Endrisone | O=C1C=CC2(C(=C1)C(C)CC3C4CCC(C(=O)C)C4(C)CC(O)C32)C | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17Î²-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CCC2(O)C#CCO | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-oxopregna-1,4-diene-20-carboxylic acid | O=C1C=CC2(C(=C1)CCC3C2CCC4(C)C(CCC34)C(C(=O)O)C)C | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| retinol acetate;retinol, acetate;retinyl acetate;o~15~-acetylretinoic acid;[(2e,4e,6e,8e)-3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)nona-2,4,6,8-tetraenyl] acetate;retinol acetate retinol, acetate retinyl acetate o~15~-acetylretinoic acid [(2e,4e,6e,8e)-3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)nona-2,4,6,8-tetraenyl] acetate | CC1CCCC(C)(C)C=1C=CC(C)=CC=CC(C)=CC(=O)OC(C)=O | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 16a-ethyl-21-hydroxy-19-norpregna-4,9-diene-3,20-dione | O=C1C=C2C(=C3CCC4(C)C(C(=O)CO)C(CC)CC4C3CC2)CC1 | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Trimegestone | C[C@H](O)C(=O)[C@@]1(C)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3CC[C@@]21C | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Estra-1,3,5(10)-triene-3,17ß-diol 17-butyrate | O=C(OC1CCC2C3CCC4=CC(O)=CC=C4C3CCC12C)CCC | 342.21949 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methylene dibutyldithiocarbamate | CCCCN(CCCC)C(=S)SCSC(=S)N(CCCC)CCCC | 422.19178 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5'-Methylthioadenosine | CSC[C@H]1O[C@@H](n2cnc3c2ncnc3N)[C@H](O)[C@@H]1O | 297.08956 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-Benzodioxol-2-one | O=c1oc2c(o1)cccc2 | 136.01604 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Ethyl-2-benzothiazolamine | C1=CC=CC2=C1SC(=N2)NCC | 178.05647 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Amino-5,6-dimethylbenzothiazole | Cc1cc2c(cc1C)nc(N)s2 | 178.05647 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Amino-4,5,6,7-tetrahydrobenzo(b)thiophene-3-carbonitrile | Nc1c(C#N)c2c(CCCC2)s1 | 178.05647 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isothiocyanic acid, p-dimethylaminophenyl ester | CN(C)c1ccc(cc1)N=C=S | 178.05647 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Etisazole | C1=CC=CC2=C1C(=NS2)NCC | 178.05647 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Picolinic acid | C1=CC=NC(=C1)C(=O)O | 123.03203 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Nitrosophenol | Oc1ccc(cc1)N=O | 123.03203 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isonicotinic acid | OC(=O)c1ccncc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isonicotinaldehyde 1-oxide | [O-][n+]1ccc(C=O)cc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Nicotinic acid | OC(=O)c1cccnc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Nitrobenzene | O=N(=O)c1ccccc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(Hydroxymethyl)furan-2-carbonitrile | OCc1ccc(o1)C#N | 123.03203 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hexadecanamide, N,N-dimethyl- | CCCCCCCCCCCCCCCC(=O)N(C)C | 283.28751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isooctadecanoic acid, monoamide with 2-[(2-aminoethyl)amino]ethanol | O=C(N)CCCCCCCCCCCCCCC(C)C.OCCNCCN | 283.28751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Octadecanamide | CCCCCCCCCCCCCCCCCC(N)=O | 283.28751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Amines, C14-18; C16-18-unsaturated, alkyl, ethoxylated | CCOCCCCCCC=CCCCCCCCCN | 283.28751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Morpholine, 4-tetradecyl- | CCCCCCCCCCCCCCN1CCOCC1 | 283.28751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Aldimorph | C(N1CC(OC(C1)C)C)CCCCCCCCCCC | 283.28751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(Hexadecyl((1-hydroxy-2-naphthyl)carbonyl)amino)isophthalic acid | CCCCCCCCCCCCCCCCN(C(=O)c1ccc2ccccc2c1O)c1cc(cc(c1)C(=O)O)C(=O)O | 575.32469 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-Diphenylguanidine | N=C(Nc1ccccc1)Nc2ccccc2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Varenicline | c1cnc2cc3c(cc2n1)[C@H]1CNC[C@@H]3C1 | 211.11095 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Anthranilaldehyde phenylhydrazone | N(=CC=1C=CC=CC1N)NC=2C=CC=CC2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Varenicline | C1C2CNCC1C3=CC4=NC=CN=C4C=C23 | 211.11095 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Methyl-4-aminoazobenzene | CNc1ccc(cc1)N=Nc1ccccc1 | 211.11095 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(p-tolylazo)aniline | N(=NC1=CC=C(C=C1)C)C2=CC=C(N)C=C2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9-Methyl-9H-carbazole-3,6-diamine | Cn1c2c(cc(N)cc2)c2c1ccc(N)c2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Fosinopril | CCC(=O)O[C@@H](C(C)C)O[P@](=O)(CCCCc1ccccc1)CC(=O)N2C[C@@H](C[C@H]2C(=O)O)C3CCCCC3 | 563.30119 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methyl-1-o-tolylpent-1-en-3-one | O=C(C(=CC=1C=CC=CC1C)C)CC | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2,3,6-trimethylphenyl)-2-buten-1-one | O=C(C=CC)C=1C(=CC=C(C1C)C)C | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-phenylcycloheptan-1-one | O=C1CCCCCC1C=2C=CC=CC2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| a,a-dicyclopropylbenzyl alcohol | OC(C=1C=CC=CC1)(C2CC2)C3CC3 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-benzylcyclohexan-1-one | O=C1CCCCC1CC=2C=CC=CC2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4,4-dimethyl-1-phenylpent-1-en-3-one | O=C(C=CC=1C=CC=CC1)C(C)(C)C | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Hexen-3-one, 5-methyl-1-phenyl- | CC(C)CC(=O)C=Cc1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzenepropanal, .beta.-methyl-3-(1-methylethenyl)- | CC(CC=O)c1cccc(c1)C(C)=C | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| p-Cumenyl cyclopropyl ketone | CC(C)c1ccc(cc1)C(=O)C1CC1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2,5,7-Tetramethylindan-1-one | Cc1cc2c(C(=O)C(C)(C)C2)c(C)c1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Propenal, 2-methyl-3-[2-(1-methylethyl)phenyl]- | CC(C)c1c(/C=C(C)/C=O)cccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| p-Cyclohexylbenzaldehyde | O=Cc1ccc(cc1)C1CCCCC1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Methyl-4-methylidene-6-phenyltetrahydro-2H-pyran | CC1CC(=C)CC(O1)c2ccccc2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| p-tert-butylcinnamaldehyde | CC(C)(C)c1ccc(C=CC=O)cc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| alpha-Butylcinnamaldehyde | CCCCC(C=O)=C/c1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Octahydro-8,8-dimethylnaphthalene-2-carbaldehyde | CC1(C)CCCc2ccc(C=O)cc12 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Propenal, 2-methyl-3-[4-(1-methylethyl)phenyl]- | CC(C)c1ccc(cc1)C=C(/C)C=O | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2H-Pyran, 3,6-dihydro-2,4-dimethyl-6-phenyl- | CC1CC(=CC(O1)c2ccccc2)C | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2H-Pyran, 3,6-dihydro-4,6-dimethyl-2-phenyl- | CC1OC(CC(=C1)C)c2ccccc2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-Methyl-2-phenyl-2-hexenal | CC(C)CC=C(C=O)/c1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclohexylphenylketone | O=C(C1CCCCC1)c1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tetrahydrofurfuryl oleate | O=C(OCC1OCCC1)CCCCCCCC=CCCCCCCCC | 366.31340 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (tetrahydro-3-furyl)methyl oleate | O=C(OCC1COCC1)CCCCCCCC=CCCCCCCCC | 366.31340 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[[1-(isopropyl)cyclohexyl]carbonyl]pyrrolidine | O=C(N1CCCC1)C2(CCCCC2)C(C)C | 223.19361 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(3,7-dimethylocta-1,6-dien-1-yl)morpholine | O1CCN(C=CC(C)CCC=C(C)C)CC1 | 223.19361 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Propanenitrile, 3-(10-undecenyloxy)- | C=CCCCCCCCCCOCCC#N | 223.19361 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-hydroxy-1,2,3,4-tetrahydropyrimidin-2-one | O=C1NC=C[C@H](O)N1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,5-Piperazinedione | C1C(=O)NCC(=O)N1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dimethyl cyanoimidocarbonate | N#CN=C(OC)OC | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Maleamide | O=C(N)C=CC(=O)N | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,4(1H,3H)-Pyrimidinedione, dihydro- | O=C1CCNC(=O)N1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Muscimol | NCc1cc(=O)[nH]o1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Methylhydantoin | O=C1NC(=O)N(C)C1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,4-imidazolidinedione, 5-methyl- | CC1NC(=O)NC1=O | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Sodium ethyl cyanocarbamate | [Na+].N#CNC(=O)OCC | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (3S)-3-Aminopyrrolidine-2,5-dione | N[C@H]1CC(=O)NC1=O | 114.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Decanedioic acid, di-2-propenyl ester | C=CCOC(=O)CCCCCCCCC(=O)OCC=C | 282.18311 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethylene bis(cyclohexanecarboxylate) | O=C(OCCOC(=O)C1CCCCC1)C1CCCCC1 | 282.18311 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,10-Decanediyl diacrylate | C=CC(=O)OCCCCCCCCCCOC(=O)C=C | 282.18311 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dibutyl cyclohex-4-ene-1,2-dicarboxylate | O=C(OCCCC)C1CC=CCC1C(=O)OCCCC | 282.18311 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-ethyl-1-propyl-1,3-propanediyl bismethacrylate | O=C(OCC(CC)C(OC(=O)C(=C)C)CCC)C(=C)C | 282.18311 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2-bis(allyloxymethyl)butyl methacrylate | O=C(OCC(COCC=C)(COCC=C)CC)C(=C)C | 282.18311 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-isopropyl-2,2-dimethylpropane-1,3-diyl bismethacrylate | O=C(OCC(C)(C)C(OC(=O)C(=C)C)C(C)C)C(=C)C | 282.18311 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 11-nor-delta(9)-tetrahydrocannabinol-9-carboxylicacid | CCCCCc1cc(O)c2[C@@H]3CC(=CC[C@H]3C(C)(C)Oc2c1)C(O)=O | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6H-Dibenzo[b,d]pyran-9-carboxylic acid,6a,7,8,10a-tetrahydro-1-hydroxy-6,6-dimethyl-3-pentyl- | CCCCCc1cc(O)c2C3C=C(CCC3C(C)(C)Oc2c1)C(O)=O | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bisphenol A bis(2-hydroxypropyl) ether | CC(O)COc1ccc(cc1)C(C)(C)c1ccc(OCC(C)O)cc1 | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 21-hydroxypregn-4-ene-3,11,20-trione | O=C1C=C2CCC3C(C(=O)CC4(C)C(C(=O)CO)CCC34)C2(C)CC1 | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 16a,17-epoxy-11a-hydroxypregn-4-ene-3,20-dione | O=C1C=C2CCC3C4CC5OC5(C(=O)C)C4(C)CC(O)C3C2(C)CC1 | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Anecortave | C[C@]12CCC(=O)C=C1CC[C@@H]1C2=CC[C@@]2(C)[C@H]1CC[C@]2(O)C(=O)CO | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,3'-[isopropylidenebis(p-phenyleneoxy)]dipropanol | OCCCOC1=CC=C(C=C1)C(C2=CC=C(OCCCO)C=C2)(C)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Deprodone | O=C1C=CC2(C(=C1)CCC3C4CCC(O)(C(=O)C)C4(C)CC(O)C32)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Formebolone | O=CC1=CC2(C(=CC1=O)CCC3C4CCC(O)(C)C4(C)CC(O)C32)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 21-Deoxycortisone | CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3C(=O)C[C@]12C | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (isopropylidene)bis(1-methyl-1-phenylethyl) peroxide | O(OC(C=1C=CC=CC1)(C)C)C(OOC(C=2C=CC=CC2)(C)C)(C)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [isopropylidenebis(p-phenyleneoxy)]dipropanol | OC(OC1=CC=C(C=C1)C(C2=CC=C(OC(O)CC)C=C2)(C)C)CC | 344.19876 | Suspect screening | Canal | LC-HRMS | Reference | L |
| EPTC | CCCN(CCC)C(=O)SCC | 189.11873 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dromostanolone proprionate | CCC(=O)O[C@H]1CC[C@H]2[C@@H]3CC[C@H]4CC(=O)[C@H](C)C[C@]4(C)[C@H]3CC[C@]12C | 360.26644 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (3ß,17ß)-17-hydroxy-17-methylandrost-5-ene-3-ol propionate | O=C(OC1CC2=CCC3C(CCC4(C)C3CCC4(O)C)C2(C)CC1)CC | 360.26644 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cholan-24-oic acid, 3,6-dihydroxy-, methyl ester, (3alpha,5beta,6alpha)- | COC(=O)CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3C[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C | 406.30831 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Irisoquin | CCCCCCCCCCCCCCCCCCC1=C(O)C(=O)C=C(OC)C1=O | 406.30831 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 3-a,12-a-dihydroxy-5-ß-cholan-24-oate | O=C(OC)CCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CC(O)C12C | 406.30831 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,3,5,6,8,9,11,12,14,15-Decahydro-4,13-(ethanoxyethanoxyethano)-4H,13H-1,7,10,16,4,13-benzotetraoxadiazacyclooctadecine | C1COCCN2CCOCCOCCN(CCO1)CCOc1ccccc1OCC2 | 424.25734 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ppi-2458 | CO[C@H]1[C@H]([C@@]2(C)O[C@@H]2CC=C(C)C)[C@]2(CC[C@H]1OC(=O)N[C@@H](C(N)=O)C(C)C)CO2 | 424.25734 | Suspect screening | Canal | LC-HRMS | Reference | L |
| ruscogenin | C[C@H]1[C@H]2[C@H](C[C@H]3[C@@H]4CC=C5C[C@@H](O)C[C@@H](O)[C@]5(C)[C@H]4CC[C@]23C)O[C@]11CC[C@@H](C)CO1 | 430.30831 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3beta,17-Dihydroxypregn-5-en-20-one 17-hexanoate | CCCCCC(=O)O[C@@]1(CC[C@H]2[C@@H]3CC=C4CC(O)CC[C@]4(C)[C@H]3CC[C@]12C)C(=O)C | 430.30831 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hecogenin | C[C@H]1[C@H]2[C@H](C[C@H]3[C@@H]4CC[C@H]5C[C@@H](O)CC[C@]5(C)[C@H]4CC(=O)[C@]23C)O[C@@]21CC[C@@H](C)CO2 | 430.30831 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [2-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl]ethylamino]ethyl](2-hydroxyethyl)dimethylammonium acetate | O=C([O-])C.O=[N+]([O-])C1=CC=C(N=NC2=CC=C(C=C2)N(CC)CC[N+](C)(C)CCO)C(Cl)=C1 | 421.18807 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(benzoylamino)-2-[(ethoxycarbonyl)methylamino]-5-methoxybenzenediazonium tetrachlorozincate (2:1) | N#[N+]C=1C=C(OC)C(=CC1N(C(=O)OCC)C)NC(=O)C=2C=CC=CC2.N#[N+]C=1C=C(OC)C(=CC1N(C(=O)OCC)C)NC(=O)C=2C=CC=CC2.Cl[Zn-2](Cl)(Cl)Cl | 355.14063 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-(p-tolyl)butyramide | O=C(NC1=CC=C(C=C1)C)C(N=NC2=CC=C(C=C2[N+](=O)[O-])C)C(=O)C | 355.14063 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Testosterone isocaproate | CC(C)CCC(=O)OC1CCC2C1(CCC3C2CCC4=CC(=O)CCC34C)C | 386.28209 | Suspect screening | Canal | LC-HRMS | Reference | L |
| HU-210 | CCCCCCC(C)(C)C1=CC2=C(C3CC(=CCC3C(O2)(C)C)CO)C(=C1)O | 386.28209 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dexanabinol | CCCCCCC(C)(C)c1cc(O)c2c(c1)OC(C)(C)[C@H]1CC=C(CO)C[C@H]21 | 386.28209 | Suspect screening | Canal | LC-HRMS | Reference | L |
| HU 210 | CCCCCCC(C)(C)c1cc(c2c(c1)OC([C@H]3[C@H]2CC(=CC3)CO)(C)C)O | 386.28209 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17beta-Hydroxyandrost-4-en-3-one 3,3-dimethylbutyrate | CC(C)(C)CC(=O)OC1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C | 386.28209 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17ß-hydroxyandrost-4-en-3-one hexanoate | O=C(OC1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C)CCCCC | 386.28209 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-amino-6-hydroxy-2-pyridone hydrochloride | Cl.O=C1NC(O)=CC=C1N | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-methylisoxazole-3-carboxamide | O=C(N)C1=NOC(=C1)C | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-Methyluracil | Cc1cc(=O)[nH]c(=O)[nH]1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,6-Pyridazinedione, 1,2-dihydro-1-methyl- (8CI)(9CI) | CN1C(=O)C=CC(=O)N1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Furoic acid hydrazide | NNC(=O)c1ccco1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Imidazole-1-acetic acid | OC(=O)Cn1ccnc1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-Methyl-1H-4-carboxylic acid | Cc1c(nc[nH]1)C(=O)O | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Methyl-1H-imidazole-4-carboxylic acid | Cc1ncc([nH]1)C(=O)O | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Methyl-1H,5H-pyrimidine-4,5-dione | Cc1nc(O)cc(=O)[nH]1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Imidazole-4-acetic acid | C1=C(N=CN1)CC(=O)O | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Methyloxazole-5-carboxamide | Cc1ncoc1C(N)=O | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Methylpyridazine-3,6-diol | Cc1cc(=O)[nH][nH]c1=O | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Thymine | Cc1c[nH]c(=O)[nH]c1=O | 126.04293 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Triisobutylphosphine sulphide | S=P(CC(C)C)(CC(C)C)CC(C)C | 234.15711 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tributylphosphine sulphide | S=P(CCCC)(CCCC)CCCC | 234.15711 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Chlorodecyldimethylsilane | Cl[Si](C)(C)CCCCCCCCCC | 234.15706 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tributylchlorosilane | Cl[Si](CCCC)(CCCC)CCCC | 234.15706 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(methylsulphinyl)decane | O=S(C)CCCCCCCCCC | 204.15479 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dibutoxy(dimethyl)silane | O(CCCC)[Si](OCCCC)(C)C | 204.15456 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bis(1,1-dimethylethoxy)dimethylsilane | O(C(C)(C)C)[Si](OC(C)(C)C)(C)C | 204.15456 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Arachidonoyl glycerol | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OC(CO)CO | 378.27701 | Suspect screening | Canal | LC-HRMS | Reference | L |
| GLYCERYL ARACHIDO- NATE | CCCCC/C=CCC=C/C/C=CCC=C/CCCC(=O)OCC(O)CO | 378.27701 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bolenol | OC1(CC)CCC2C3CC=C4CCCCC4C3CCC21C | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethylestrenol | CC[C@]1(O)CC[C@H]2[C@@H]3CCC4=CCCC[C@@H]4[C@H]3CC[C@]12C | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Abietyl alcohol | CC(C)C1=CC2=CCC3C(C)(CO)CCCC3(C)C2CC1 | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(p-cumenyl)-2-octylpropionaldehyde | O=CC(CC1=CC=C(C=C1)C(C)C)CCCCCCCC | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tetradecanophenone | O=C(C=1C=CC=CC1)CCCCCCCCCCCCC | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-methyl-5-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthyl)pent-2-en-1-al | O=CC=C(C)CCC1=C(C)CCC2C1(C)CCCC2(C)C | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [1R-(1a,4aß,10aa)]-1,2,3,4,4a,5,6,9,10,10a-decahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol | OCC1(C)CCCC2(C3=C(C=C(CC3)C(C)C)CCC21)C | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1,3-trimethyl-6-(1,1,3,3-tetramethylbutyl)indan-5-ol | OC=1C=C2C(=CC1C(C)(C)CC(C)(C)C)C(C)(C)CC2C | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Desoxymethyltestosterone | [H][C@@]12CC[C@](C)(O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC[C@@]2([H])CC=CC[C@]12C | 288.24532 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (1-methylethylidene)di-4,1-cyclohexanediyl bismethacrylate | O=C(OC1CCC(CC1)C(C)(C)C2CCC(OC(=O)C(=C)C)CC2)C(=C)C | 376.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (5ß)-3ß,14-dihydroxycardanolide | O=C1OCC(C1)C2CCC3(O)C4CCC5CC(O)CCC5(C)C4CCC23C | 376.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hexyl nonyl phthalte | O=C(OCCCCCCCCC)C1=CC=CC=C1C(OCCCCCC)=O | 376.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2,6-diisopropyl-3,5-dimethyl- | CC(C)c1c(O)c(C(C)C)c(C)cc1C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Diisopropyl-3,4-xylenol | CC(C)c1c(O)c(C(C)C)c(C)c(C)c1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[3-methyl-2-(3-methyl-2-butenyl)-3-cyclohexen-1-yl]ethan-1-one | O=C(C)C1CCC=C(C)C1CC=C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(tert-butyl)-2,3,4,5,6,7-hexahydro-2-methyl-1H-inden-1-one | O=C1C2=C(CC1C)CC(CC2)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(4-isopropyl-1-cyclohexen-1-yl)pent-4-enal | O=CCCC=CC1=CCC(CC1)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(5-isopropyl-2-methyl-1-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1=C(C)CCC(C1)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-ethyl-5,9-dimethyldeca-2,4,8-trienal | O=CC(=CC=C(C)CCC=C(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Octahydro-a-methyl-4,7-methano-1H-indene-5-propionaldehyde | O=CC(C)CC1CC2CC1C3CCCC23 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Decahydro-5-methylspiro[furan-2(3H),5'-[4,7]methano[5H]indene] | O1C(C)CCC12CC3CC2C4CCCC34 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2-ethyl-4,4-dimethyl-2-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1C(=CC(C)(C)CC1)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-(4-methyl-3-cyclohexen-1-yl)hept-4-enal | O=CCCC=CC(C)C1CC=C(C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Penten-2-one, 3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)- | CC(C=C/C1CC=C(C)C1(C)C)C(C)=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2-(1-ethylhexyl)- | CCCCCC(CC)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 4-(1-ethylhexyl)- | CCCCCC(CC)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Penten-2-one, 3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)- | CC(=O)C(C)=CCC1CC=C(C)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2-(1-propylpentyl)- | CCCCC(CCC)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(1,1,3,3-Tetramethylbutyl)phenol | CC(C)(C)CC(C)(C)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methyl-1-(1-methylbicyclo[2.2.1]hept-5-en-2-yl)pent-1-en-3-ol | OC(C(=CC1CC2C=CC1(C)C2)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-bicyclo[2.2.1]hept-2-yl-2,4-dimethylpent-2-en-1-al | O=CC(=CC(C)CC1CC2CCC1C2)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1,2,3,5,6,7,8,8a-octahydro-8,8-dimethyl-2-naphthyl)ethan-1-one | O=C(C)C1CC=C2CCCC(C)(C)C2C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-(1,1-dimethylethyl)-3,4,5,6,7,8-hexahydronaphthalen-2(1H)-one | O=C1CC2=C(CC1)CC(CC2)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,4,4a,5,6,7-hexahydro-3,3,5,5-tetramethylnaphthalene-2(1H)-one | O=C1CC2=CCCC(C)(C)C2CC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-(2,2,3-trimethylcyclopent-3-en-1-yl)hex-5-en-3-one | O=C(CC=CC1CC=C(C)C1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[4-methyl-5-(3-methyl-2-butenyl)-3-cyclohexen-1-yl]ethan-1-one | O=C(C)C1CC=C(C)C(CC=C(C)C)C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,4-Di-tert-butylphenol | Oc(c(cc(c1)C(C)(C)C)C(C)(C)C)c1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,4,5,6,7,8-hexahydro-3,3,5,5-tetramethylnaphthalene-2(1H)-one | O=C1CC2=C(CC1(C)C)C(C)(C)CCC2 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,3,4,5,6,7-hexahydro-4-isopropyl-2,7-dimethyl-1H-inden-1-one | O=C1C2=C(CC1C)C(CCC2C)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hexahydro-2,5,5-trimethyl-2H-2,4a-methanonaphthalen-1(5H)-one | O=C1C2CCCC(C)(C)C32CCC1(C)C3 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- | CC(=O)C(C)=CC1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Buten-2-one, 4-(1,2,6,6-tetramethyl-2-cyclohexen-1-yl)- | CC1=CCCC(C)(C)C1(C)/C=C/C(=O)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Di-tert-butylphenol | CC(C)(C)C1=C(C(=CC=C1)C(C)(C)C)O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 4-(1-propylpentyl)- | CCCCC(CCC)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one | CCC(=O)C=CC1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-tert-butyl-2-sec-butylphenol | CCC(C)c1cc(ccc1O)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Octylphenol | CCCCCCCCc1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(1,1,3,3-Tetramethylbutyl)phenol | CC(C)(C)CC(C)(C)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| o-(1-methylheptyl)phenol | CCCCCCC(C)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6,9,10-trimethylundeca-3,5,9-trien-2-one | CC(C)=C(C)CCC(C)=CC=CC(C)=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, (1-methylheptyl)- | CCCCCCC(C)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, (2-ethylhexyl)- | CCCCC(CC)Cc1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2-octyl- | CCCCCCCCc1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methylionone | CCC(=O)C=CC1C(C)=CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzenepropanol, 4-(1,1-dimethylethyl)-.beta.-methyl- | CC(CO)Cc1ccc(cc1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dihydro-1,1,2,3,3-pentamethyl-4(5H)-indanone | CC1C(C)(C)C2=C(C(=O)CCC2)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Di(butan-2-yl)phenol | CC[C@H](C)c1cccc([C@H](C)CC)c1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Butenal, 2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)- | CCC(C=O)=CCC1CC=C(C)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| alpha-Isomethylionone | CC(=O)C(C)=CC1C(C)=CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, isooctyl- | CC(C)CCCCCc1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Methyl-4-(2,6,6-trimethyl-1-cyclohexenyl)-3-buten-2-one; | CC(=O)C(C)=C/C1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(5(or 6)-Methyl-7(or 8)-(1-methylethyl) bicyclo[2.2.2]oct-5-en-2-yl)ethan-1-one. | CC(C)C1CC2=C(C)CC1C(C2)C(C)=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)- | CC1CCC(=C(C=CC(C)=O)C1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| alpha-Irone | C[C@@H]1CC=C(C)[C@H](C=CC(C)=O)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-tert-Octylphenol | OC1=CC=C(C(C)(C)CCCCC)C=C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)- | CC(=O)C=C(C)C1C(C)=CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2,3,3a,4,5,6-hexahydro-1,1,3-trimethyl-1H-inden-5-yl)ethan-1-one | O=C(C)C1CC=C2C(C1)C(C)CC2(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzenepropanol, .beta.-pentyl- | CCCCCC(CO)Cc1ccccc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[4-(4-methyl-3-pentenyl)-3-cyclohexen-1-yl]ethan-1-one | O=C(C)C1CC=C(CCC=C(C)C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | O=CC1CC=C(CCC=C(C)C)CC1C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 8-isopropyl-6-methylbicyclo[2.2.2]oct-5-en-2-yl methyl ketone | O=C(C)C1CC2C=C(C)C1CC2C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-(2,2,3-trimethylcyclopent-3-en-1-yl)hex-4-en-3-one | O=C(C=CCC1CC=C(C)C1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (E)-1-(2-ethyl-6,6-dimethyl-1-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1=C(CC)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(5,5-dimethylcyclohex-1-en-1-yl)hex-4-en-1-one | O=C(C1=CCCC(C)(C)C1)CCC=CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,5-diisobutylphenol | OC=1C=C(C=C(C1)CC(C)C)CC(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(5,5-dimethyl-1-cyclohexen-1-yl)-3-methylpent-4-en-1-one | O=C(C1=CCCC(C)(C)C1)CC(C=C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(3,3,5-trimethyl-1-cyclohexen-1-yl)pent-4-en-1-one | O=C(C1=CC(C)(C)CC(C)C1)CCC=C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(3,5,5-trimethyl-1-cyclohexen-1-yl)pent-4-en-1-one | O=C(C1=CC(C)CC(C)(C)C1)CCC=C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (E,E)-1-(6-ethylidene-2,2-dimethylcyclohexyl)-2-buten-1-one | O=C(C=CC)C1C(=CC)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2,2-dimethyl-6-methylenecyclohexyl)pent-1-en-3-one | O=C(C=CC1C(=C)CCCC1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (E)-1-(2-ethyl-6,6-dimethyl-2-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1C(=CCCC1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diisobutylphenol | OC1=CC=CC(=C1CC(C)C)CC(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Di-sec-butylphenol | OC1=CC=CC(=C1C(C)CC)C(C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-methyl-4-(2,2-dimethyl-6-methylenecyclohexyl)-3-buten-2-one | O=C(C(=CC1C(=C)CCCC1(C)C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methyl-2-phenylheptan-4-ol | OC(CCC)CC(C=1C=CC=CC1)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,6,10-trimethylundeca-3,5,9-trien-2-one | O=C(C(=CC=C(C)CCC=C(C)C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)pent-1-en-3-one | O=C(C=CC1C(C=CCC1(C)C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(3,3-dimethylbicyclo[2.2.1]hept-2-ylidene)-2-methyl-2-buten-1-ol | OCC(=CC=C1C2CCC(C2)C1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(2,2,3-trimethyl-6-methylenecyclohexyl)-3-buten-2-one | O=C(C=CC1C(=C)CCC(C)C1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Methyl-1-(2,4,4-trimethylcyclohexen-1-yl)-2-buten-1-one | CC(=CC(=O)C1=C(C)CC(C)(C)CC1)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Penten-3-ol, 2-methyl-1-(methylbicyclo[2.2.1]hept-5-en-2-yl)- | C[C@@]1([C@@H]2C=C[C@@H](C1)C2)C=C([C@@H](O)CC)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2,4-bis(2-methylpropyl)- | CC(C)Cc1cc(CC(C)C)c(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,2,3,4,5,6,7,8-octahydro-2,5,5-trimethylnaphthalene-2-carbaldehyde | O=CC1(C)CC2=C(CC1)C(C)(C)CCC2 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,5-Diisopropyl-3,4-xylenol | CC(C)c1c(C)c(C)c(C(C)C)c(O)c1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-butenal | O=CC(C=CC1=C(C)CCCC1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| alpha,alpha-Diisopropylphenethyl alcohol | CC(C)C(O)(Cc1ccccc1)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)-2,2-dimethylpropanal | CC(C)(CC1=CCC2CC1C2(C)C)C=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Buten-2-one, 3-methyl-4-(3,5,6-trimethyl-3-cyclohexen-1-yl)- | CC1C=C(C)CC(C=C(/C)C(C)=O)C1C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Buten-2-one, 3-methyl-4-(2,4,6-trimethyl-3-cyclohexen-1-yl)- | CC1CC(=CC(C)C1C=C(/C)C(C)=O)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Butenal, 2-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- | CC(C=O)C=C/C1C(=CCCC1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Butenal, 2-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- | CC(C=O)=C/CC1C(=CCCC1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-butenal | CC(C=O)=C/CC1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Penten-3-one, 1-(2,4,6-trimethyl-3-cyclohexen-1-yl)- | CCC(=O)/C=C/C1C(C)CC(=CC1C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | CC(C)=CCCC1=CCC(C)(CC1)C=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1,2,3,4,5,6,7,8-octahydro-8,8-dimethyl-2-naphthyl)ethan-1-one | O=C(C)C1CC2=C(CCCC2(C)C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,2,3,4,5,6,7,8-octahydro-2,8,8-trimethylnaphthalene-2-carbaldehyde | O=CC1(C)CC2=C(CCCC2(C)C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-methyl-3-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | O=CC1CC(=CCC1C)CCC=C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(p-tert-butylphenyl)butan-2-ol | OC(C)CCC1=CC=C(C=C1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1,2,3,4,6,7,8,8a-octahydro-8,8-dimethyl-2-naphthyl)ethan-1-one | O=C(C)C1CCC2=CCCC(C)(C)C2C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hexahydro-3,5,5-trimethyl-2H-2,4a-methanonaphthalen-1(5H)-one | O=C1C2CC3(CC2C)C1CCCC3(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Cyclohexene-1-carboxaldehyde, 1-methyl-3-(4-methyl-3-penten-1-yl)- | CC(C)=CCCC1=CCCC(C)(C1)C=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2,6-bis(2-methylpropyl)- | CC(C)Cc1cccc(CC(C)C)c1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Penten-3-one, 1-(3,5,6-trimethyl-3-cyclohexen-1-yl)- | CCC(=O)/C=C/C1CC(=CC(C)C1C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Oxaspiro[4.5]deca-3,6-diene, 2,7-dimethyl-10-(1-methylethyl)- | CC(C)C1CCC(C)=CC11OC(C)C=C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,5-Di-tert-butylphenol | CC(C)(C)c1cc(cc(O)c1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (1S-(1alpha(E),5beta))-1-(5-Isopropyl-2-methyl-2-cyclohexen-1-yl)-2-buten-1-one | CC=CC(=O)C1CC(CC=C1C)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, p-isooctyl- | CC(C)CCCCCc1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dibutylphenol | CCCCc1cccc(O)c1CCCC | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 7,11-dimethyldodeca-4,6,10-trien-3-one | CCC(=O)/C=C/C=C(C)/CCC=C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Oxaspiro[4,5]deca-3,6-diene,6-ethyl-2,10,10-trimethyl- | CCC1=CCCC(C)(C)C21OC(C)C=C2 | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2,5-bis(1,1-dimethylethyl)- | CC(C)(C)c1cc(O)c(cc1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4,7-Dimethylindan | CC1=CC=C(C)C2=C1CCC2 | 146.10955 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1-Dimethylindan | CC1(C)CCc2ccccc12 | 146.10955 | Suspect screening | Canal | LC-HRMS | Reference | L |
| p-Isopropylstyrene | CC(C)c1ccc(C=C)cc1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,4,6-Trimethylstyrene | Cc1cc(C)c(C=C)c(C)c1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Phenyl-1-pentene | CC(CC=C)C1=CC=CC=C1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-pentenylbenzene | C=1C=CC(=CC1)C=CCCC | 146.10955 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1H-Indene, 2,3-dihydro-4,6-dimethyl- | CC1=CC2=C(CCC2)C(C)=C1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4,4a,5,6,7,8-hexahydro-6-(1-methylethyl)naphthalen-2(3H)-one | O=C1C=C2CCC(CC2CC1)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-3-en-2-one | O=C(C=CCC1CC=C(C)C1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| a-ethyl-5-isopropyl-2-methylbenzyl alcohol | OC(C1=CC(=CC=C1C)C(C)C)CC | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-[1-(1-methylethyl)allyl]cyclohex-2-ene-1-carbaldehyde | O=CC1C=CCCC1C(C=C)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| a,2-dimethyl-5-(1-methylvinyl)cyclohex-2-en-1-acetaldehyde | O=CC(C)C1C(=CCC(C(=C)C)C1)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)-2-butenal | O=CC=C(C)C1C2CCC(C2)C1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| a-methyl-4-(1-methylvinyl)cyclohexene-1-propan-1-al | O=CC(C)CC1=CCC(C(=C)C)CC1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| a,3,3-trimethyl-a-vinylbicyclo[2.2.1]hept-5-ene-2-methanol | OC(C=C)(C)C1C2C=CC(C2)C1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (1a,2ß,5ß)-4,5-dimethyl-2-(2-methylpropen-1-yl)cyclohex-3-ene-1-carbaldehyde | O=CC1CC(C(=CC1C=C(C)C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Butanone, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- | CC(=O)CCC1=C(C)C=CCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(2,4,4-Trimethyl-2-cyclohexenyl)-2-buten-1-one. | C/C=C/C(=O)C1CCC(C)(C)C=C1C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (Z)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one | CC=C/C(=O)C1C(=CCCC1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(4,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1CC=C(C)CC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Naphthalenecarboxaldehyde, 1,2,3,4,5,6,7,8-octahydro-5,5-dimethyl- | CC1(C)CCCC2=C1CCC(C2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,2,3,4,5,6,7,8-Octahydro-8,8-dimethyl-2-naphthaldehyde | CC1(C)CCCC2=C1CC(CC2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(4-Methyl-3-penten-1-yl)-3-cyclohexene-1-carbaldehyde | CC(C)=CCCC1=CCCC(C1)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 6-methyl-8-(1-methylethyl)- | CC(C)C1CC2C(CC1C=C2C)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 4-methyl-1-(1-methylethyl)- | CC(C)C12CCC(C)(CC1C=O)C=C2 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 1-methyl-4-(1-methylethyl)- | CC(C)C12CCC(C)(C=C1)C(C2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5(or 6)-Methyl-7(or 8)-(1-methylethyl)bicyclo[2.2.2]oct-5-ene-2-carbaldehyde | CC(C)C1CC2=C(C)CC1C(C2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(4-Methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | CC(C)=CCCC1=CCC(CC1)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Methylbutyl 2-phenylethyl ether | CC(C)CCOCCc1ccccc1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Octahydro-5,5-dimethylnaphthalene-2-carbaldehyde | CC1(C)CCC=C2CC(CCC12)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methyl-1-(4-methyl-3-cyclohexen-1-yl)pent-1-en-3-one | O=C(C(=CC1CC=C(C)CC1)C)CC | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3a,4,5,6,7,7a-hexahydro-6-methoxydimethyl-4,7-methano-1H-indene | O(C)C1CC2CC1C3C2C=CC3(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 7-isopropyl-5-methylbicyclo[2.2.2]oct-5-ene-2-carbaldehyde | O=CC1CC2C(=CC1C(C2)C(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6,10,10-tetramethyl-1-oxaspiro[4.5]deca-3,6-diene | O1C(C=CC12C(=CCCC2(C)C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-methyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-butenal | O=CC(=CCC1CC=C(C)C1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one | O=C(C)CC=CC1CC=C(C)C1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-allyl-octahydro-4,7-methano-1H-inden-5-ol | OC1(CC=C)CC2CC1C3CCCC23 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6,9,10-Tetramethyl-1-oxaspiro[4.5]deca-3,6-diene | CC1OC2(C=C1)C(C)C(C)CC=C2C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Heptylphenol | CCCCCCCC1=CC=C(C=C1)O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Buten-2-one, 4-(3,5,6-trimethyl-3-cyclohexen-1-yl)- | CC1C=C(C)CC(C=CC(C)=O)C1C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| α-Damascone | CC1=CCCC(C)(C)C1C(=O)CC=C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Methyl-9-(1-methylethylidene)bicyclo[3.3.1]nonan-2-one | [H]C12CCCC(C)(C(=O)CC1)C2=C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (4r,s)-4-(2-butyl)-cis-bicyclo[4.3.0]-2-nonen-8-one | CCC(C)C1CC2CC(=O)CC2C=C1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)- | CC=CC(=O)C1C(C)C=CCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (2E)- | CC=CC(=O)C1C(C)=CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (2Z)- | CC=C/C(=O)C1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- | CC(=O)C=CC1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [2-(2-methylbutoxy)ethyl]benzene | O(CCC=1C=CC=CC1)CC(C)CC | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3a,4,5,6-tetrahydro-1,3,3-trimethylindancarbaldehyde | O=CC1(C2=CCCCC2C(C)(C)C1)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3a,4,5,6-tetrahydro-2,2,3a-trimethylindancarbaldehyde | O=CC1C2=CCCCC2(C)CC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3a,4,5,6,7,7a-hexahydromethoxydimethyl-4,7-methano-1H-indene | O(C)C1(C(=CC2C3CCC(C3)C21)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,2-dimethyl-1-phenylpentan-3-ol | OC(CC)C(C)(C)CC=1C=CC=CC1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(2,4,6-Trimethyl-3-cyclohexen-1-yl)-3-buten-2-one | CC1CC(=CC(C)C1C=CC(C)=O)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| alpha-Ionone | CC(=O)/C=C/C1C(=CCCC1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-allyl-2,4,6-trimethylcyclohex-3-ene-1-carbaldehyde | O=CC1(CC=C)C(C=C(C)CC1C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Decahydrospiro[furan-2(3H),5'-[4,7]methano[5H]indene] | C1COC2(C1)CC3CC2C4CCCC34 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (2-(Pentyloxy)ethyl)benzene | CCCCCOCCc1ccccc1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 2-tert-butyl-4-isopropyl- | CC(C)c1cc(c(O)cc1)C(C)(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,6-Diisopropyl-3-methylphenol | CC(C)c1ccc(C)c(C(C)C)c1O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-Azulenemethanol, 1,2,3,3a,4,5,6,7(or 1,2,3,4,5,6,7,8)-octahydro-.alpha.,.alpha.,3,8-tetramethyl- | C[C@@H]1CC=C2[C@@H]1C[C@H](CO)CC=C2C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(3-Butenyl)-2,4,4-trimethylcyclohex-2-en-1-one | CC1=C(CCC=C)C(C)(C)CCC1=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(2,2-Dimethyl-6-methylenecyclohexyl)-3-buten-2-one | CC(=O)/C=C/C1C(=C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (4-methyl-3-pentenyl)cyclohexenecarbaldehyde | O=CC1=C(CCC=C(C)C)CCCC1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-butyraldehyde | O=CCCCC1=CCC2CC1C2(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(3,3-dimethyl-2-norbornyl)-3-buten-2-one | O=C(C=CC1C2CCC(C2)C1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(5,5-Dimethyl-1-cyclohexen-1-yl)pent-4-en-1-one | CC1(C)CCC=C(C1)C(=O)CCC=C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Isobutyl-2-isopropylphenol | CC(C)Cc1cc(C(C)C)c(O)cc1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ibuprofenol | CC(C)Cc1ccc(cc1)C(C)CO | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| beta-Ionone | CC(=O)C=CC1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6,7,8,8a-tetrahydro-2,5,5,8a-tetramethyl-5H-1-benzopyran | O1C(=CC=C2C1(C)CCCC2(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Pseudoionone | CC(C)=CCCC(C)=CC=CC(C)=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (2E)-1-[(1R,2S)-2,6,6-Trimethylcyclohex-3-en-1-yl]but-2-en-1-one | CC=CC(=O)C1C(C)C=CCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(2,2-dimethyl-6-methylenecyclohexyl)methacrylaldehyde | O=CC(=CC1C(=C)CCCC1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(2,6,6-trimethyl-2-cyclohexen-1-yl)methacrylaldehyde | O=CC(=CC1C(=CCCC1(C)C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Damascone | CC=CC(=O)C1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (E,Z,Z)-trideca-2,4,7-trienal | O=CC=CC=CCC=CCCCCC | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (E)-3-(2-butenyl)-2,4,4-trimethylcyclohex-2-en-1-one | O=C1C(=C(CC=CC)C(C)(C)CC1)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diisopropyl-m-cresol | OC1=CC=C(C(=C1C(C)C)C)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-methyl-5-phenylhexan-3-ol | OC(CC)CC(C=1C=CC=CC1)(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(p-cumenyl)-2-methylpropanol | OCC(C)CC1=CC=C(C=C1)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| TP\_2690 | Cc1cc(c(O)c(C)c1C)C(C)(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Chlorpheniramine,Â Desmethyl | CNCCC(c1ccc(Cl)cc1)c1ccccn1 | 260.10803 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1,3,3,5,5-hexamethyl-1,5-divinyltrisiloxane | O([Si](O[Si](C=C)(C)C)(C)C)[Si](C=C)(C)C | 260.10841 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Buturon | CC(C#C)N(C)C(=O)Nc1ccc(Cl)cc1 | 236.07164 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diacetoxydiethoxysilane | O=C(O[Si](OC(=O)C)(OCC)OCC)C | 236.07161 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(2-chloroethyl)-2,8-dimethyl-4H-pyrido[1,2-a]pyrimidin-4-one | O=C1C(=C(N=C2C=C(C=CN12)C)C)CCCl | 236.07164 | Suspect screening | Canal | LC-HRMS | Reference | L |
| oxybis(methyl-2,1-ethanediyl) diacrylate | CC(COCC(C)OC(=O)C=C)OC(=O)C=C | 242.11542 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Di(ethylene glycol) dimethacrylate | C(OC(C(C)=C)=O)COCCOC(C(C)=C)=O | 242.11542 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Propenoic acid, 2-ethyl-2-(hydroxymethyl)-1,3-propanediyl ester | CCC(CO)(COC(=O)C=C)COC(=O)C=C | 242.11542 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (4aalpha,5abeta,9aalpha,10abeta)-Octahydro-5aH,10aH-4a,9a-epoxydibenzo(b,e)(1,4)dioxin-5a,10a-diol | OC12CCCCC31OC1(O)CCCCC1(O2)O3 | 242.11542 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-hydroxy-1,6-hexanediyl diacrylate | O=C(OCCCCC(O)COC(=O)C=C)C=C | 242.11542 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tributyl citrate | CCCCOC(=O)CC(O)(CC(=O)OCCCC)C(=O)OCCCC | 360.21480 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Triisobutyl citrate | CC(C)COC(=O)CC(O)(CC(=O)OCC(C)C)C(=O)OCC(C)C | 360.21480 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dodecyl dihydrogen 2-hydroxypropane-1,2,3-tricarboxylate | O=C(O)CC(O)(C(=O)O)CC(=O)OCCCCCCCCCCCC | 360.21480 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tetracosahydrodibenz[b,n][1,4,7,10,13,16,19,22]octaoxacyclotetracosin | O1CCOCCOC2CCCCC2OCCOCCOCCOC3CCCCC3OCC1 | 460.30362 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 7-chloro-5-cyclohexyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one | O=C1NC=2C=CC(Cl)=CC2C(=NC1)C3CCCCC3 | 276.10294 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [3-(2,3-epoxypropoxy)propyl]triethoxysilane | O(CCC[Si](OCC)(OCC)OCC)CC1OC1 | 278.15495 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isooctyl [(2,3-dihydroxypropyl)thio]acetate | O=C(OCCCCCC(C)C)CSCC(O)CO | 278.15518 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 13,20,22-trihydroxy-8,14-dimethoxy-4,10,12,16-tetramethyl-3-oxo-19-[(prop-2-en-1-yl)amino]-2-azabicyclo[16.3.1]docosa-1(21),4,6,10,18(22),19-hexaen-9-yl carbamate | C=CCNc1c(O)cc2c(O)c1C[C@@H](C)C[C@H](OC)[C@H](O)[C@@H](C)C=C(C)[C@H](OC(N)=O)[C@@H](OC)C=CC=C(C)C(=O)N2 | 587.32067 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Merphos | CCCCSP(SCCCC)SCCCC | 298.10125 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(acryloyloxy)-1-propanesulfonic acid | OS(=O)(=O)CCCOC(=O)C=C | 194.02489 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Acetamide, N-(4-chlorophenyl)-2-cyano- | Clc1ccc(NC(=O)CC#N)cc1 | 194.02469 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Propenoic acid, 2-methyl-, 2-sulfoethyl ester, sodium salt | [Na+].CC(=C)C(=O)OCCS(=O)(=O)[O-] | 194.02489 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-chloro-2-(1H-pyrazol-3-yl)phenol | ClC=1C=CC(O)=C(C1)C2=NNC=C2 | 194.02469 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Sulphoethyl methacrylate | O=C(OC(C)S(=O)(=O)O)C(=C)C | 194.02489 | Suspect screening | Canal | LC-HRMS | Reference | L |
| sulphoethyl methacrylate | CC(=C)C(=O)OCCS(O)(=O)=O | 194.02489 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Perfluorooctanesulfonic acid | C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isooctanesulfonic acid, heptadecafluoro-, lithium salt | [Li+].[O-][S](=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tetrakis[(phosphonooxy)methyl]urea | OP(=O)(O)OCN(COP(=O)(O)O)C(=O)N(COP(=O)(O)O)COP(=O)(O)O | 499.93994 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Heptadecafluorooctane-2-sulfonic acid | OS(=O)(=O)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Reference | L |
| D-Glucitol monoacetate monopalmitate | CCCCCCCCCCCCCCCC(=O)O[C@@H](COC(C)=O)[C@@H](O)[C@H](O)[C@H](O)CO | 462.31927 | Suspect screening | Canal | LC-HRMS | Reference | L |
| D-glucitol mono(12-hydroxyoleate) | O=C(OCC(O)C(O)C(O)C(O)CO)CCCCCCCC=CCC(O)CCCCCC | 462.31927 | Suspect screening | Canal | LC-HRMS | Reference | L |
| ST50987637 | O=C(NC1CCCCC1)Nc1ccc(Cc2ccc(NC(=O)NC3CCCCC3)cc2)cc1 | 448.28383 | Suspect screening | Canal | LC-HRMS | Reference | L |
| alpha-Amylcinnamyl alcohol | CCCCCC(CO)=Cc1ccccc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(4-Tert-Butylbenzyl)propionaldehyde | CC(Cc1ccc(cc1)C(C)(C)C)C=O | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4'-tert-Butyl-2',6'-dimethylacetophenone | CC(=O)c1c(C)cc(cc1C)C(C)(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(3-tert-Butylphenyl)-2-methylpropanal | CC(Cc1cccc(c1)C(C)(C)C)C=O | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Methyl-3-[4-(2-methylpropyl)phenyl]propanal | CC(C)Cc1ccc(CC(C)C=O)cc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzene, [2-(cyclohexyloxy)ethyl]- | C1CCC(CC1)OCCc2ccccc2 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,2,3,4,5,6,7,8,9,10-Decahydro-5,9-methanobenzocycloocten-11-one | CC1C2CCCC(C2=O)C3=C1CCCC3 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,4,4a,5,8,8a-Hexahydro-3',6-dimethylspiro[1,4-methanonaphthalene-2(1H),2'-oxirane] | CC1OC12CC3CC2C4CC=C(C)CC34 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,4,4a,5,8,8a-Hexahydro-3',7'-dimethylspiro[1,4-methanonaphthalene-2(1H),2'-oxirane] | CC1OC12CC3CC2C4CC(=CCC34)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Butanone, 3-methyl-2-(1-methylethyl)-1-phenyl- | CC(C)C(C(C)C)C(=O)c1ccccc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(Octahydro-5H-4,7-methanoinden-5-ylidene)butanal | O=CCCC=C1/CC2CC1C3CCCC23 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Cyclohexyl-2,6-xylenol | Cc1cc(cc(C)c1O)C1CCCCC1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Phenol, 4-methyl-2-(1-methylcyclohexyl)- | Cc1cc(c(O)cc1)C1(C)CCCCC1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Octanophenone | CCCCCCCC(=O)c1ccccc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-Benzylcycloheptan-1-ol | OC1(Cc2ccccc2)CCCCCC1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(Dipropylamino)benzenediazonium tetrafluoroborate | [B+++].[F-].[F-].[F-].[F-].CCCN(CCC)c1ccc(cc1)[N+]#N | 204.15007 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1,3,3,6-Pentamethylindan-4-ol | Cc1cc2c(c(O)c1)C(C)(C)CC2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1,3,3,7-Pentamethylindan-5-ol | Cc1cc(O)cc2c1C(C)(C)CC2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cyclomenol [INN:DCF] | Cc1cc(O)c(C2CCCCC2)c(C)c1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(1,1-Dimethylethyl)-5,6,7,8-tetrahydro-2-naphthol | CC(C)(C)c1c(O)ccc2c1CCCC2 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethanone, 1-[2-(1,1-dimethylethyl)-4,6-dimethylphenyl]- | CC(=O)c1c(cc(C)cc1C)C(C)(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Cyclopentyl-6-isopropylphenol | CC(C)c1cccc(C2CCCC2)c1O | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(3,4-Bis(1-methylethyl)phenyl)ethan-1-one | CC(C)c1c(cc(cc1)C(=O)C)C(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-(phenylmethyl)heptan-4-one | O=C(CCC)C(CC=1C=CC=CC1)CC | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bornelone | O=C(C=CC=C1C2CCC(C2)C1(C)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-methyl-4-(4-isopropylphenyl)butan-2-one | O=C(C)C(C)CC1=CC=C(C=C1)C(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tetraallyloxirane | O1C(CC=C)(CC=C)C1(CC=C)CC=C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,2,3,3',3a,4,4',6,7,7a-decahydrospiro[4,7-methano-5H-indene-5,2'-[2H]pyran] | O1C=CCCC12CC3CC2C4CCCC34 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(bicyclo[2.2.1]hept-5-en-2-ylmethylene)hexenal | O=CC(=CC1CC2C=CC1C2)CCCC | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-ethyl-1,3,3-trimethylindan-5-ol | OC1=CC=C2C(=C1)C(C)(C)CC2(C)CC | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(3,7,7-trimethylbicyclo[4.1.0]hept-3-en-2-yl)-2-buten-1-one | O=C(C=CC)C1C(=CCC2C1C2(C)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[2,4-bis(1-methylethyl)phenyl]ethan-1-one | O=C(C1=CC=C(C=C1C(C)C)C(C)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-tert-butyl-a-cyclopropylbenzyl alcohol | OC(C1=CC=C(C=C1)C(C)(C)C)C2CC2 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,1,2,3,3-pentamethylindan-5-ol | OC1=CC=C2C(=C1)C(C)(C)C(C)C2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3'a,4,4',5,6',7',7'a-octahydro-4-methylspiro[furan-2(3H),5'-[4,7]methano[5H]indene] | O1CC(C)CC12CC3CC2C4C=CCC43 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-2-naphthol | OC1CC2=CC=C(C=C2CC1)C(C)(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(4,7,7-trimethylbicyclo[4.1.0]hept-3-en-3-yl)-2-buten-1-one | O=C(C=CC)C1=C(C)CC2C(C1)C2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Butyl-1,2,3,4-tetrahydro-1-naphthol | OC1(C=2C=CC=CC2CCC1)CCCC | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(3a,4,5,6,7,7a-hexahydrodimethyl-4,7-methano-1H-indenyl)ethanone | O=C(C)C1(C(=CC2C3CCC(C3)C21)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-(4-methylphenyl)heptanal | O=CCCCC(C1=CC=C(C=C1)C)CC | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,3,3a,4,7,7a-hexahydro-a-methyl-4,7-methano-1H-indene-5-propionaldehyde | O=CC(C)CC1=CC2CC1C3CCCC23 | 204.15142 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Rimexolone | CCC(=O)[C@@]1(C)[C@H](C)CC2C3CCC4=CC(=O)C=C[C@]4(C)C3[C@@H](O)C[C@]12C | 370.25080 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-ethoxypregna-3,5-diene-21,17a-carbolactone | CCOC1=CC2=CC[C@H]3[C@@H]4CC[C@@]5(CCC(=O)O5)[C@@]4(C)CC[C@@H]3[C@@]2(C)CC1 | 370.25080 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 16-methyl-20-oxopregna-5,16-dien-3-ß-yl acetate | O=C(OC1CC2=CCC3C4CC(=C(C(=O)C)C4(C)CCC3C2(C)CC1)C)C | 370.25079 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3ß-hydroxypregna-5,16-dien-20-one 3-propionate | O=C(OC1CC2=CCC3C4CC=C(C(=O)C)C4(C)CCC3C2(C)CC1)CC | 370.25079 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-methyl-20-oxopregna-5,16-dien-3-ß-yl acetate | O=C(OC1CC2=C(C)CC3C4CC=C(C(=O)C)C4(C)CCC3C2(C)CC1)C | 370.25079 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Rimexolone | Vexol | CCC(=O)[C@@]1(C)[C@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C | 370.25079 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-Cyanopurine | N#Cc1ncnc2c1[nH]cn2 | 145.03885 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-[formyl(6-methoxyquinolin-8-yl)amino]pentanoic acid | COC1=CC2=CC=CN=C2C(=C1)N(C=O)C(C)CCC(O)=O | 302.12666 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-[(benzoyl-5-oxopyrrolidin-2-yl)carbonyl]morpholine | O=C(C=1C=CC=CC1)N2C(=O)CCC2C(=O)N3CCOCC3 | 302.12666 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dnc008126 | CC[C@@H](C)Nc1ncc(C(=O)Nc2cc(C(=O)NC)ccc2C)s1 | 346.14635 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dicofol | OC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl | 367.90960 | Suspect screening | Canal | LC-HRMS | Reference | L |
| o,p'-Dicofol | OC(c1ccc(Cl)cc1)(c1ccccc1Cl)C(Cl)(Cl)Cl | 367.90960 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Viminol | CCC(C)N(CC(O)c1cccn1Cc1ccccc1Cl)C(C)CC | 362.21249 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (9Z)-17-carboxy-9-heptadecene-1-sulfonic acid | OC(=O)CCCCCCCC=CCCCCCCCCS(O)(=O)=O | 362.21270 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-Fluoro ADB-PINACA | CC(C)(C)C(C(=O)N)NC(=O)C1=NN(C2=CC=CC=C21)CCCCCF | 362.21180 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-Fluoro ADB-PINACA isomer 2 | O=C(N[C@H](C(N)=O)[C@H](CC)C)C1=NN(CCCCCF)C2=C1C=CC=C2 | 362.21180 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-Fluoro-2-ADB-PINACA isomer 2 | CC[C@H](C)[C@@H](C(=O)N)NC(=O)c1c2ccccc2nn1CCCCCF | 362.21180 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Sodium hydrogen sulphonatooleate | [Na+].O=C([O-])C(CCCCCCC=CCCCCCCCC)S(=O)(=O)[O-] | 362.21270 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9-sulpho-9-octadecenoic acid | O=C(O)CCCCCCCC(=CCCCCCCCC)S(=O)(=O)O | 362.21270 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Sodium hydrogen 9-sulphonatooctadecenoate | [H+].[Na+].O=C([O-])C=CCCCCCC(CCCCCCCCC)S(=O)(=O)[O-] | 362.21270 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,4-Dioxaspiro[4.5]decane-2-methanol, 9-methyl-6-(1-methylethyl)- | CC(C)C1CCC(C)CC11OCC(CO)O1 | 228.17255 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Glycidyl neodecanoate | CCC(C)(CCC(C)C)C(=O)OCC1CO1 | 228.17255 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Propanoic acid, 2-hydroxy-, 5-methyl-2-(1-methylethyl)cyclohexyl ester | CC(C)C1CCC(C)CC1OC(=O)C(C)O | 228.17255 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-tert-Butylcyclohexyl ethyl carbonate | CCOC(=O)OC1CCCCC1C(C)(C)C | 228.17255 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-Methylbutyl 1-hydroxycyclohexaneacetate | CC(C)CCOC(=O)CC1(O)CCCCC1 | 228.17255 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 12-oxotridecanoic acid | O=C(O)CCCCCCCCCCC(=O)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dihydro-5-(5-methoxy-1,5-dimethylhexyl)furan-2(3H)-one | O=C1OC(CC1)C(C)CCCC(OC)(C)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl menthyl carbonate | O=C(OCC)OC1CC(C)CCC1C(C)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl 2-hydroxycyclopentanehexanoate | O=C(OCC)CCCCCC1CCCC1O | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl 2-acetylnonan-1-oate | O=C(OCC)C(C(=O)C)CCCCCCC | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 3-oxododecanoate | O=C(OC)CC(=O)CCCCCCCCC | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-dioxacyclopentadecan-2-one | O=C1OCCCCCCCCCCCCO1 | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-hydroxyethyl 2-(isopropyl)-5-methylcyclohexanecarboxylate | O=C(OCCO)C1CC(C)CCC1C(C)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl 1-hydroxy-3,3,5-trimethylcyclohexaneacetate | O=C(OCC)CC1(O)CC(C)CC(C)(C)C1 | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-ethylhexyl 4-oxovalerate | O=C(OCC(CC)CCCC)CCC(=O)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| neodecanoic acid, oxiranylmethyl ester;oxiran-2-ylmethyl 2,2-dimethyloctanoate;neodecanoic acid, oxiranylmethyl ester oxiran-2-ylmethyl 2,2-dimethyloctanoate | CCCCCCC(C)(C)C(=O)OCC1CO1 | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4s,6R-Dimethyl-7R-acetoxy-3-nonanone | CCC([C@@H](C)C[C@@H](C)[C@H](OC(C)=O)CC)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4s,6s-Dimethyl-7R-acetoxy-3-nonanone | CCC([C@@H](C)C[C@H](C)[C@H](OC(C)=O)CC)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4s,6s-Dimethyl-7s-acetoxy-3-nonanone | CCC([C@@H](C)C[C@H](C)[C@@H](OC(C)=O)CC)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| trans-5-Isopropyl-6,7-epoxy-8-hydroxy-8-methylnonan-2-one | CC(CCC(C(C)C)[C@H](O1)[C@@H]1C(C)(O)C)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9,10-Anthracenedione, 1-amino-2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]-4-[(2,4,6-trimethylphenyl)amino]- | Cc1cc(C)c(Nc2cc(Oc3ccc(cc3)C(C)(C)CC(C)(C)C)c(N)c3c2C(=O)c2c(cccc2)C3=O)c(C)c1 | 560.30389 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzenediazonium, 4-(ethylamino)-3-methyl-, tetrafluoroborate(1-) | F[B-](F)(F)F.CCNc1c(C)cc(cc1)[N+]#N | 162.10312 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(ethylamino)-m-toluenediazonium trichlorozincate | N#[N+]C1=CC(=CC=C1NCC)C.Cl[Zn-](Cl)Cl | 162.10312 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(ethylamino)-2-methylbenzenediazonium hexafluoroarsenate | N#[N+]C1=CC=C(C=C1C)NCC.F[As-](F)(F)(F)(F)F | 162.10312 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Xanthurenic acid | C1=CC2=C(C(=C1)O)NC(=CC2=O)C(=O)O | 205.03751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Phthalylglycine | OC(=O)CN1C(=O)c2c(cccc2)C1=O | 205.03751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1H-Indole-2,7-dicarboxylic acid | OC(=O)c1cc2c([nH]1)c(ccc2)C(=O)O | 205.03751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Norverapamil | COc1ccc(CCNCCCC(C#N)(C(C)C)c2ccc(OC)c(OC)c2)cc1OC | 440.26751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-(3,4-dimethoxyphenyl)-5-{[2-(4-hydroxy-3-methoxyphenyl)ethyl](methyl)amino}-2-(propan-2-yl)pentanenitrile | COc1cc(CCN(C)CCCC(C#N)(C(C)C)c2ccc(OC)c(OC)c2)ccc1O | 440.26751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| M3 | COc1ccc(CCN(C)CCCC(C#N)(C(C)C)c2ccc(OC)c(OC)c2)cc1O | 440.26751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (+)-[3-cyano-3-(3,4-dimethoxyphenyl)hex-6-yl](5,6-dimethoxyphenethyl)methylammonium chloride | [Cl-].N#CC(C1=CC=C(OC)C(OC)=C1)(CC)CCC[NH+](C)CCC=2C=CC=C(OC)C2OC | 440.26751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (-)-[3-cyano-3-(3,4-dimethoxyphenyl)hex-6-yl][2-(3,4-dimethoxyphenyl)ethyl]methylammonium chloride | [Cl-].N#CC(C1=CC=C(OC)C(OC)=C1)(CC)CCC[NH+](C)CCC2=CC=C(OC)C(OC)=C2 | 440.26751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 6-{4-[(4-ethylpiperazin-1-yl)methyl]phenyl}-n-(1-phenylethyl)-7h-pyrrolo[2,3-d]pyrimidin-4-amine | CCN1CCN(Cc2ccc(-c3cc4c(N[C@H](C)c5ccccc5)ncnc4[nH]3)cc2)CC1 | 440.26885 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Norverapamil | COc1ccc(CCNCCC[C@](C#N)(c2ccc(OC)c(OC)c2)C(C)C)cc1OC | 440.26751 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diethyl 4,4'-[hexamethylenebis(oxy)]dibenzimidate | N=C(OCC)C1=CC=C(OCCCCCCOC2=CC=C(C=C2)C(=N)OCC)C=C1 | 412.23621 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-[2-(diethylamino)ethyl]-a-[(2,4,5-trimethoxyphenyl)methylene]phenylacetamide monohydrochloride | Cl.O=C(NCCN(CC)CC)C(=CC1=CC(OC)=C(OC)C=C1OC)C=2C=CC=CC2 | 412.23621 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tribufos | CCCCSP(=O)(SCCCC)SCCCC | 314.09616 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Tris(trimethylsilyl) phosphate | O=P(O[Si](C)(C)C)(O[Si](C)(C)C)O[Si](C)(C)C | 314.09548 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-(2,4-dichlorophenyl)-ß-methylpiperidin-1-propionamide monohydrochloride | Cl.O=C(NC1=CC=C(Cl)C=C1Cl)CC(N2CCCCC2)C | 314.09527 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Clibucaine | CC(CC(=O)Nc1ccc(cc1Cl)Cl)N2CCCCC2 | 314.09527 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-[(4-Cyclopropyl-5-hydroxy-4H-1,2,4-triazol-3-yl)sulfanyl]-1-(4-morpholinophenyl)-1-ethanone | C1CC1N2C(=O)NN=C2SCC(=O)C3=CC=C(C=C3)N4CCOCC4 | 360.12561 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-ethylhexyl 4-(2,4-dichlorophenoxy)butyrate | O=C(OCC(CC)CCCC)CCCOC1=CC=C(Cl)C=C1Cl | 360.12590 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isooctyl 4-(2,4-dichlorophenoxy)butyrate | O=C(OCCCCCC(C)C)CCCOC1=CC=C(Cl)C=C1Cl | 360.12590 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Nonyl 2-(2,4-dichlorophenoxy)propionate | O=C(OCCCCCCCCC)C(OC1=CC=C(Cl)C=C1Cl)C | 360.12590 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,4-Dioxane-2,3-diol | OC1OCCOC1O | 120.04226 | Suspect screening | Canal | LC-HRMS | Reference | L |
| L-Erythrose | OCC(O)C(O)C=O | 120.04226 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Trimethyl(methylthio)silane | S(C)[Si](C)(C)C | 120.04290 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Acetic acid, 2-hydroxy-2-methoxy-, methyl ester | O=C(OC)C(O)OC | 120.04226 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Digitoxigenin | C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@@]1(O)CC[C@@H]2C1=CC(=O)OC1 | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-ß,21-dihydroxypregn-5-en-20-one 21-acetate | O=C(OCC(=O)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Androst-5-ene-(3ß,17ß)-diyl diacetate | O=C(OC1CC2=CCC3C(CCC4(C)C(OC(=O)C)CCC34)C2(C)CC1)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-ß,17-a-dihydroxypregn-5-en-20-one 3-acetate | O=C(OC1CC2=CCC3C(CCC4(C)C3CCC4(O)C(=O)C)C2(C)CC1)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 11,20-dioxo-5-ß-pregnan-3-a-yl acetate | O=C(OC1CCC2(C)C3C(=O)CC4(C)C(C(=O)C)CCC4C3CCC2C1)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-hydroxy-20-oxo-5-pregnen-17a-yl acetate | O=C(OC1(C(=O)C)CCC2C3CC=C4CC(O)CCC4(C)C3CCC21C)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [3-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy]propyl](2-hydroxyethyl)dimethylammonium chloride | [Cl-].N#CC(=CC1=CC=C(C=C1)N(CC)CC)C(=O)OCCC[N+](C)(C)CCO | 374.24437 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [2-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy]ethyl](3-hydroxypropyl)dimethylammonium chloride | [Cl-].N#CC(=CC1=CC=C(C=C1)N(CC)CC)C(=O)OCC[N+](C)(C)CCCO | 374.24437 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-benzyl hydrogen 2-dodecenylsuccinate | O=C(OCC=1C=CC=CC1)CC(C(=O)[O-])CC=CCCCCCCCCC | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Rostafuroxin | C[C@]12CC[C@H](O)C[C@H]1CC[C@@H]1[C@@H]2CC[C@@]2(C)[C@]1(O)CC[C@]2(O)c1ccoc1 | 374.24571 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (5ß)-3ß,14-dihydroxycardanolide | O=C1OCC(C1)C2CCC3(O)C4CCC5CC(O)CCC5(C)C4CCC23C | 376.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (1-methylethylidene)di-4,1-cyclohexanediyl bismethacrylate | O=C(OC1CCC(CC1)C(C)(C)C2CCC(OC(=O)C(=C)C)CC2)C(=C)C | 376.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Hexyl nonyl phthalte | O=C(OCCCCCCCCC)C1=CC=CC=C1C(OCCCCCC)=O | 376.26140 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-{2-[(4-fluorophenyl)methyl]-1,3-dioxo-decahydropyrrolo[3,4-a]pyrrolizin-4-yl}benzene-1-carboximidamide | N=C(N)c1ccc([C@H]2[C@H]3C(=O)N(Cc4ccc(F)cc4)C(=O)[C@H]3[C@@H]3CCCN32)cc1 | 406.18050 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dicyclohexyl sulfosuccinic acid | OS(=O)(=O)C(CC(=O)OC1CCCCC1)C(=O)OC1CCCCC1 | 362.13992 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Marbofloxacin | Fc4cc1c2N(/C=C(C1=O)C(=O)O)N(COc2c4N3CCN(C)CC3)C | 362.13903 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-[2-(1-amino-2-hydroxypropyl)-4-[(4-fluoro-1h-indol-3-yl)methyl]-5-hydroxy-1h-imidazol-1-yl]acetic acid | C[C@H](O)[C@H](N)c1nc(Cc2c[nH]c3cccc(F)c23)c(O)n1CC(=O)O | 362.13903 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3'H-Cycloprop[15,16]androsta-6,15-dien-17-one, 3-(2,2-dimethyl-1-oxopropoxy)-15,16-dihydro-5-hydroxy-, (3ÃŸ,5ÃŸ,15a,16a)- | CC(C)(C)C(=O)O[C@H]1CC[C@]2(C)[C@H]3CC[C@@]4(C)[C@@H]([C@@H]5C[C@@H]5C4=O)[C@@H]3C=C[C@]2(O)C1 | 400.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (2S,4aR,4bS,6aS,7aS,8aS,8bS)-9-Hydroxy-4a,6a-dimethyl-7-oxo-1,2,3,4,4a,4b,5,6,6a,7,7a,8,8a,8b,8c,9-hexadecahydrocyclopropa[4,5]cyclopenta[1,2-a]phenanthren-2-yl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OC1CCC2(C)C3CCC4(C)C(C5CC5C4=O)C3C(O)C=C2C1 | 400.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,20-bis(ethylenedioxy)pregna-5,7-diene | CC12CCC3C(=CC=C4CC5(CCC34C)OCCO5)C1CCC2C1(C)OCCO1 | 400.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Heliotrope B | [Cl-].CCN(CC)C1=C[CH+]c2nc3ccc(cc3n(c3ccccc3)c2=C1)N(CC)CC | 400.26270 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 17-hydroxy-3-methoxy-6-methylpregna-3,5-dien-20-one acetate | O=C(OC1(C(=O)C)CCC2C3CC(=C4C=C(OC)CCC4(C)C3CCC21C)C)C | 400.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-ethoxy-17-hydroxypregna-3,5-dien-20-one 17-acetate | O=C(OC1(C(=O)C)CCC2C3CC=C4C=C(OCC)CCC4(C)C3CCC21C)C | 400.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Lenabasum | CCCCCCC(C)(C)c1cc(O)c2c(c1)OC(C)(C)[C@@H]1CC=C(C(=O)O)C[C@@H]21 | 400.26136 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-(4-Butyl-2-methylphenyl)-N&#39;-(2-chlorobenzoyl)urea | CCCCC1=CC(=C(C=C1)NC(=O)NC(=O)C2=CC=CC=C2Cl)C | 344.12916 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-(3-amino-2h-indazol-5-yl)-n-tert-butylbenzene-1-sulfonamide | CC(C)(C)NS(=O)(=O)c1ccc(-c2ccc3n[nH]c(N)c3c2)cc1 | 344.13070 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Fluprednidene acetate | CC(=O)OCC(=O)[C@@]1(O)C(=C)CC2C3CCC4=CC(=O)C=CC4(C)[C@@]3(F)C(O)CC12C | 432.19482 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9ß,11ß-epoxy-6a-fluoro-17,21-dihydroxy-16a-methylpregna-1,4-diene-3,20-dione 21-acetate | O=C1C=CC2(C(=C1)C(F)CC3C4CC(C)C(O)(C(=O)COC(=O)C)C4(C)CC5OC532)C | 432.19482 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[[4-[(dimethylphenyl)azo]dimethylphenyl]azo]-2-naphthol | OC=1C=CC=2C=CC=CC2C1N=NC3=CC=C(N=NC4=CC=CC(=C4C)C)C(=C3C)C | 408.19501 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[2,5-dimethyl-4-(2,5-dimethylphenylazo)phenylazo]-2-naphthol | OC=1C=CC=2C=CC=CC2C1N=NC3=CC(=C(N=NC4=CC(=CC=C4C)C)C=C3C)C | 408.19501 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-[[2,5-dimethyl-4-[(dimethylphenyl)azo]phenyl]azo]-2-naphthol | OC=1C=CC=2C=CC=CC2C1N=NC3=CC(=C(N=NC4=CC=CC(=C4C)C)C=C3C)C | 408.19501 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzoic acid, 2-[(octadecylamino)carbonyl]-, monosodium salt | [Na+].CCCCCCCCCCCCCCCCCCNC(=O)c1ccccc1C([O-])=O | 417.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (9E)-N-[2-(3,4-Dihydroxyphenyl)ethyl]octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)NCCC1=CC(=C(C=C1)O)O | 417.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| CB-52 | CCCCCCC1=C(C=C(C=C1)O)OCCCCCCCCCCC(=O)NC2CC2 | 417.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Cyclopropyl-8-[3-hydroxy-5-(2-methylheptan-2-yl)phenoxy]octanamide | CCCCCCC(C)(C)C1=CC(=CC(=C1)OCCCCCCCC(=O)NC2CC2)O | 417.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzoic acid, 4-[(octadecylamino)carbonyl]-, monosodium salt | [Na+].CCCCCCCCCCCCCCCCCCNC(=O)c1ccc(cc1)C(=O)[O-] | 417.32429 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,4-Benzenediol, 2,5-dioctyl- | CCCCCCCCc1cc(O)c(CCCCCCCC)cc1O | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-Benzenediol, 4-methyl-5-pentadecyl- | CCCCCCCCCCCCCCCc1c(C)c(O)cc(O)c1 | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diisooctylhydroquinone | CC(C)CCCCCc1c(CCCCCC(C)C)c(O)ccc1O | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,5-Bis(1,1,3,3-tetramethylbutyl)hydroquinone | CC(C)(C)CC(C)(C)c1cc(O)c(cc1O)C(C)(C)CC(C)(C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,5-diisooctylhydroquinone | OC=1C=C(C(O)=C(C1)CCCCCC(C)C)CCCCCC(C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bis(1,1,3,3-tetramethylbutyl)hydroquinone | OC1=CC=C(O)C(=C1C(C)(C)CC(C)(C)C)C(C)(C)CC(C)(C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Butyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate | O=C(OCCCC)CCCCCCCC=CCC=CCC=CCC | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9,12-octadecadienyl methacrylate | O=C(OCCCCCCCCC=CCC=CCCCCC)C(=C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 8,11,14-Eicosatrienoic acid ethyl ester | CCCCC/C=CC/C=CC/C=CCCCCCCC(=O)OCC | 334.28718 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Elmustine | OCCNC(=O)N(CCCl)N=O | 195.04107 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,3-Dihydroxypropyl 3-(hexylthio)propionate | CCCCCCSCCC(=O)OCC(O)CO | 264.13953 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Carbamic acid, (hydroxymethyl)-, 2-hydroxyethyl ester | OCCOC(=O)NCO | 135.05316 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl dimethylolcarbamate | COC(=O)N(CO)CO | 135.05316 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzenamine, 2,4-dinitro-N-phenyl- | [O-][N+](=O)c1cc(c(Nc2ccccc2)cc1)[N+](=O)[O-] | 259.05931 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Cloethocarb | CNC(=O)Oc1c(OC(CCl)OC)cccc1 | 259.06114 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Pyridine, 2-[(2,4-dinitrophenyl)methyl]- | [O-][N+](=O)c1cc(c(Cc2ncccc2)cc1)[N+](=O)[O-] | 259.05931 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Nitro-N-(4-nitrophenyl)aniline | [O-][N+](=O)c1ccc(Nc2ccc(cc2)[N+](=O)[O-])cc1 | 259.05931 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Nitro-N-(2-nitrophenyl)aniline | [O-][N+](=O)c1c(Nc2c(cccc2)[N+](=O)[O-])cccc1 | 259.05931 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4,4'-Dinitro-2-biphenylamine | Nc1cc(ccc1c1ccc(cc1)[N+](=O)[O-])[N+](=O)[O-] | 259.05931 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-Nitro-N-(4-nitrophenyl)aniline | [O-][N+](=O)c1ccc(Nc2c(cccc2)[N+](=O)[O-])cc1 | 259.05931 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-(4,6-Dichloro-1,3,5-triazin-2-yl)benzenesulphonamide | Clc1nc(NS(=O)(=O)c2ccccc2)nc(Cl)n1 | 303.95885 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (isopropylidene)bis(4,1-phenyleneoxyethylene) dilaurate | O=C(OCCOC1=CC=C(C=C1)C(C2=CC=C(OCCOC(=O)CCCCCCCCCCC)C=C2)(C)C)CCCCCCCCCCC | 680.50159 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Thioinosine | OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1cnc2c1[nH]cnc2=S | 284.05793 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3,9-diethoxy-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane | O(P1OCC2(CO1)COP(OCC)OC2)CC | 284.05786 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Testosterone enanthate | CCCCCCC(=O)OC1CCC2C1(CCC3C2CCC4=CC(=O)CCC34C)C | 400.29775 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3ß-hydroxyandrost-5-en-17-one heptanoate | O=C(OC1CC2=CCC3C4CCC(=O)C4(C)CCC3C2(C)CC1)CCCCCC | 400.29775 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Inecalcitol | C[C@H](CC#CC(C)(C)O)[C@H]1CC[C@@H]2/C(=C/C=C3C[C@@H](O)C[C@H](O)C3)CCC[C@@]21C | 400.29775 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Retinyl propionate | CCC(=O)OCC=C(/C)C=CC=C(/C)C=CC1=C(C)CCCC1(C)C | 342.25588 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (17ß)-17-allyl-3-methoxyandrosta-3,5-dien-17-ol | OC1(CC=C)CCC2C3CC=C4C=C(OC)CCC4(C)C3CCC21C | 342.25588 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Docosahexaenoic acid methyl ester | CC/C=CC/C=CC/C=CC/C=CC/C=CC/C=CCCC(=O)OC | 342.25588 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Toreforant | Cc1cc(C)c2nc(-c3cnc(NCCCC4CCN(C)CC4)nc3C)[nH]c2c1 | 392.26885 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Atenolol met 4 - 223 | O(c1ccc(CC(N)=O)cc1)CC(C=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bendiocarb | CNC(=O)Oc1cccc2OC(C)(C)Oc12 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2,4-Pyridinedicarboxylic acid, diethyl ester | CCOC(=O)c1ccnc(c1)C(=O)OCC | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dioxacarb | CNC(=O)Oc1ccccc1C1OCCO1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Acetyl-L-tyrosine | CC(=O)NC(Cc1ccc(O)cc1)C(O)=O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| L-Aspartic acid &#946;-benzyl ester | N[C@H](C(=O)O)CC(=O)OCc1ccccc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Benzyloxycarbonyl-beta-alanine | C1=CC=C(C=C1)COC(=O)NCCC(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-[3-(Dimethylamino)acryloyl]-4-hydroxy-6-methyl-2H-pyran-2-one | Cc1cc(c(c(=O)o1)C(=O)/C=C/N(C)C)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Mephenoxalone | COC1=CC=CC=C1OCC2CNC(=O)O2 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Benzyloxycarbonyl-L-alanine | C[C@H](NC(=O)OCc1ccccc1)C(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Butyl 4-nitrobenzoate | CCCCOC(=O)c1ccc(cc1)[N+](=O)[O-] | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl N-benzyloxycarbonylglycinate | COC(=O)CNC(=O)OCc1ccccc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diethyl dipicolinate | CCOC(=O)c1cccc(n1)C(=O)OCC | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Benzene, 1,4-dimethoxy-2-(2-nitro-1-propenyl)- | COc1cc(/C=C(C)/[N+](=O)[O-])c(OC)cc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Isopropyl 3-nitro-p-toluate | CC(C)OC(=O)c1cc(c(C)cc1)[N+](=O)[O-] | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Dimethyl 2,6-dimethylpyridine-3,5-dicarboxylate | COC(=O)c1cc(C(=O)OC)c(C)nc1C | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Benzylaminodiacetic acid | OC(=O)CN(CC(=O)O)Cc1ccccc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 4-acetamido-o-anisate | COC(=O)c1ccc(NC(=O)C)cc1OC | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Nitrophenyl trimethylacetate | CC(C)(C)C(=O)Oc1ccc(cc1)[N+](=O)[O-] | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Diethyl pyridine-3,5-dicarboxylate | CCOC(=O)c1cc(cnc1)C(=O)OCC | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 2-((ethoxycarbonyl)amino)benzoate | CCOC(=O)Nc1ccccc1C(=O)OC | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 3-((4-methoxyphenyl)amino)-3-oxopropionate | COC(=O)CC(=O)Nc1ccc(OC)cc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-benzyl-DL-aspartic acid | O=C(O)CC(NCC=1C=CC=CC1)C(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-benzoyl-DL-threonine | O=C(O)C(NC(=O)C=1C=CC=CC1)C(O)C | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-aminobenzylsuccinic acid | O=C(O)CC(C(=O)O)CC1=CC=C(N)C=C1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Methyl 5-(acetylamino)-o-anisate | O=C(OC)C1=CC(=CC=C1OC)NC(=O)C | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| [2-(2,5-dimethoxyphenyl)-1-methyl-2-oxoethylidene]hydroxyammonium chloride | [Cl-].O=C(C1=CC(OC)=CC=C1OC)C(=[NH+]O)C | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-({[(1z)-(2-methoxyphenyl)methylidene]amino}oxy)propanoic acid | COc1ccccc1/C=NOCCC(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N-Acetyl-L-tyrosine | CC(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (+)-Taxifolin | C1=CC(=C(C=C1C2C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O | 304.05830 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Sodium 2,4-dihydroxy-5-[(4-nitrophenyl)azo]benzoate | [Na+].O=C([O-])C1=CC(N=NC2=CC=C(C=C2)[N+](=O)[O-])=C(O)C=C1O | 304.05696 | Suspect screening | Canal | LC-HRMS | Reference | L |
| (2R-trans)-2,3-dihydro-3,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4-benzopyrone | O=C1C2=CC=C(O)C=C2OC(C3=CC(O)=C(O)C(O)=C3)C1O | 304.05830 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 2-[(2-methyl-1-oxoallyl)oxy]ethyl 1,3-dihydro-1,3-dioxoisobenzofuran-5-carboxylate | O=C1OC(=O)C2=CC(=CC=C12)C(=O)OCCOC(=O)C(=C)C | 304.05830 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4H-1-Benzopyran-4-one, 2-(2,6-dihydroxyphenyl)-2,3-dihydro-3,5,7-trihydroxy-, (2R,3R)- | C1=CC(=C(C(=C1)O)[C@@H]2[C@H](C(=O)C3=C(C=C(C=C3O2)O)O)O)O | 304.05830 | Suspect screening | Canal | LC-HRMS | Reference | L |
| n:1:2 fluorotelomer betaine-related, n=3 | C[N+](CC(O)=O)(C)CCC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 532.07690 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 9,10-bis(acetoxy)octadecanoic acid | O=C(OC(CCCCCCCC(=O)O)C(OC(=O)C)CCCCCCCC)C | 400.28249 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-amino-N-(2,5-dichloropentyl)-5-(ethylsulphonyl)-2-methoxybenzamide | O=C(NCC(Cl)CCCCl)C=1C=C(C(N)=CC1OC)S(=O)(=O)CC | 396.06773 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,2-Benzenedicarboxamide, 4-nitro- | NC(=O)c1ccc(cc1C(=O)N)[N+](=O)[O-] | 209.04366 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,3-Benzenedicarboxamide, 5-nitro- | NC(=O)c1cc(cc(c1)C(=O)N)[N+](=O)[O-] | 209.04366 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3-{[(E)-(nitromethylidene)amino]amino}benzoic acid | OC(=O)C1=CC(NN=C[N+]([O-])=O)=CC=C1 | 209.04366 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 3beta,5alpha,6beta,17-Tetrahydroxy-16alpha-methylpregnan-20-one 3-acetate | C[C@@H]1C[C@H]2[C@@H]3C[C@@H](O)[C@@]4(O)C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@@]1(O)C(=O)C)OC(=O)C | 422.26684 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Mevinolinic Acid | CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H](O)C[C@@H](O)CC(=O)O)[C@H]21 | 422.26684 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 7-{2,6-Dimethyl-8-[(2-methylbutanoyl)oxy]-1,2,6,7,8,8a-hexahydro-1-naphthalenyl}-3,5-dihydroxyheptanoic acid | CCC(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 422.26684 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Docosahexaenoic acid ethyl ester | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)OCC | 356.27153 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 4-Hydroxyphenobarbital | CCC1(C(=O)NC(=O)NC1=O)c1ccc(O)cc1 | 248.07971 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 5-methyl-5-piperonylhydantoin | O=C1NC(=O)C(N1)(C)CC2=CC=C3OCOC3=C2 | 248.07971 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,2-dihydro-3-oxo-2-phenyl-3H-pyrazol-1-yl ethyl carbonate | O=C(ON1C=CC(=O)N1C=2C=CC=CC2)OCC | 248.07971 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Censavudine | C#C[C@@]1(CO)C=C[C@H](n2cc(C)c(=O)[nH]c2=O)O1 | 248.07971 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Topiroxostat | N#Cc1cc(-c2n[nH]c(-c3ccncc3)n2)ccn1 | 248.08104 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Ethyl (2E)-2-(3-acetyloxy-1H-pyridin-2-ylidene)-2-cyanoacetate | CCOC(=O)/C(=C/1C(=CC=CN1)OC(=O)C)/C#N | 248.07971 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1-(propan-2-yl)-3-(quinolin-6-yl)-1h-pyrazolo[3,4-d]pyrimidin-4-amine | CC(C)n1nc(-c2ccc3ncccc3c2)c2c(N)ncnc21 | 304.14364 | Suspect screening | Canal | LC-HRMS | Reference | L |
| CETETH-8 PHOSPHATE | CCCCCCCCCCCCCCCCOCCO[P](O)(O)=O | 366.25351 | Suspect screening | Canal | LC-HRMS | Reference | L |
| N,N,N',N',N'',N''-hexaallyl-1,3,5-triazine-2,4,6-triamine | N=1C(=NC(=NC1N(CC=C)CC=C)N(CC=C)CC=C)N(CC=C)CC=C | 366.25320 | Suspect screening | Canal | LC-HRMS | Reference | L |
| Bis(2-ethylhexyl) 2-hydroxyethyl phosphate | O=P(OCCO)(OCC(CC)CCCC)OCC(CC)CCCC | 366.25351 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 1,12-Octadecanediol, phosphate | O=P([O-])([O-])OCCCCCCCCCCCC(O)CCCCCC | 366.25351 | Suspect screening | Canal | LC-HRMS | Reference | L |
| 20-hydroxy LTB4 | C(CCC=CCC(C=CC=CC=CC(CCCC(=O)O)O)O)CCO | 352.22720 | Suspect screening | Canal | LC-HRMS | Reference | N |
| (±)20-HDoHE | CCC(C=CC=CCC=CCC=CCC=CCC=CCCC(=O)O)O | 344.23750 | Suspect screening | Canal | LC-HRMS | Reference | N |
| LTB4 | CCCCCC=CCC(C=CC=CC=CC(CCCC(=O)O)O)O | 336.23260 | Suspect screening | Canal | LC-HRMS | Reference | N |
| Adrenic Acid | CCCCCC=CCC=CCC=CCC=CCCCCCC(=O)O | 332.27360 | Suspect screening | Canal | LC-HRMS | Reference | N |
| (±)11-HEDE | CCCCCC=CC=CC(CCCCCCCCCC(=O)O)O | 324.26890 | Suspect screening | Canal | LC-HRMS | Reference | N |
| 15(R)-HETE | CCCCCC(C=CC=CCC=CCC=CCCCC(=O)O)O | 320.23750 | Suspect screening | Canal | LC-HRMS | Reference | N |
| 5(R)-HETE | CCCCCC=CCC=CCC=CC=CC(CCCC(=O)O)O | 320.23750 | Suspect screening | Canal | LC-HRMS | Reference | N |
| 17(18)-EpETE | CCC1C(O1)CC=CCC=CCC=CCC=CCCCC(=O)O | 318.22180 | Suspect screening | Canal | LC-HRMS | Reference | N |
| 5(S)-HEPE | CCC=CCC=CCC=CCC=CC=CC(CCCC(=O)O)O | 318.22180 | Suspect screening | Canal | LC-HRMS | Reference | N |
| 5-Oxo-ETE | CCCCCC=CCC=CCC=CC=CC(=O)CCCC(=O)O | 318.22180 | Suspect screening | Canal | LC-HRMS | Reference | N |
| Eicosapentaenoic Acid | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O | 302.22730 | Suspect screening | Canal | LC-HRMS | Reference | N |
| 9,10-Epoxystearic acid | CCCCCCCCC1C(O1)CCCCCCCC(=O)O | 298.25300 | Suspect screening | Canal | LC-HRMS | Reference | N |
| cis-9,10-Epoxystearic acid | CCCCCCCCC1C(O1)CCCCCCCC(=O)O | 298.25300 | Suspect screening | Canal | LC-HRMS | Reference | N |
| 13(R)-HODE | CCCCCC(C=CC=CCCCCCCCC(=O)O)O | 296.23740 | Suspect screening | Canal | LC-HRMS | Reference | N |
| Inosine | C1=NC2=C(C(=O)N1)N=CN2C3C(C(C(O3)CO)O)O | 268.08290 | Suspect screening | Canal | LC-HRMS | Reference | N |
| Stearidonic Acid | CCC=CCC=CCC=CCC=CCCCCC(=O)O | 276.21140 | Suspect screening | Canal | LC-HRMS | Reference | N |
| Niacinamide | C1=CC(=CN=C1)C(=O)N | 122.04720 | Suspect screening | Canal | LC-HRMS | Reference | N |
| Fenuron | CN(C)C(=O)NC1=CC=CC=C1 | 164.09360 | Suspect screening | Canal | LC-HRMS | Reference | N |
| Choline | C[N+](C)(C)CCO | 104.10660 | Suspect screening | Canal | LC-HRMS | Reference | N |
| w/o MS2:Perfluorooctanesulfonic acid | C(C(C(C(C(F)(F)S(O)(=O)=O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 291.649 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:MLS000860046-01!Nocodazole | O=C(OC)Nc1nc2cc(ccc2[nH]1)C(=O)c3sccc3 | 302.053 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(20:4(5Z,8Z,11Z,14Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCC=CCC=CCC=CCC=CCCCCC | 544.336 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Estradiol | OC1=CC=C2C(=C1)CCC3C2CCC4(C)C(O)CCC34 | 273.181 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD147979 | O=C1OC(CC)C(C=C(C=CC(=O)C(C)CC(C)C(OC2OC(C)CC(N(C)C)C2O)C(C)C(O)C1)C)CO | 588.328 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(22:5(4Z,7Z,10Z,13Z,16Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCC=CCC=CCC=CCC=CCC=CCCCCC | 570.353 | Suspect screening | Canal | LC-HRMS | Reference | O |
| (R)-3-Hydroxy-tetradecanoic acid | O=C(O)CC(O)CCCCCCCCCCC | 243.196 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD97894 | O=C1NC=CC=2C=CC(OC3CCN(C(=O)C(NC(=O)C(N(C)C)C)CC(C)C)C3C(=O)NC1CC=4C=CC=CC4)=CC2 | 588.324 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(20:5(5Z,8Z,11Z,14Z,17Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCC=CCC=CCC=CCC=CCC=CCC | 542.321 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-{6-[(2,2-diphenylethyl)amino]-2-({[1-(propan-2-yl)piperidin-4-yl]amino}methyl)-9H-purin-9-yl}-5-(methoxymethyl)oxolane-3,4-diol | OC1C(O)C(OC1N2C=NC=3C(=NC(=NC32)CNC4CCN(CC4)C(C)C)NCC(C=5C=CC=CC5)C=6C=CC=CC6)COC | 614.342 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Unknown (carbon number 14); PlaSMA ID-378 |  | 243.192 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(20:2(11Z,14Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCCCC=CCC=CCCCCC | 548.367 | Suspect screening | Canal | LC-HRMS | Reference | O |
| drilodefensin 1 | O=S(=O)(O)C=1C=C(OC1CCCCCC)CC | 259.097 | Suspect screening | Canal | LC-HRMS | Reference | O |
| lauric acid [(3R,5R)-5-[2-[4-fluoro-2-[2-(3-methoxyphenyl)ethyl]phenoxy]ethyl]-1-methyl-pyrrolidin-3-yl] ester;hydrochloride | Cl.O=C(OC1CN(C)C(CCOC2=CC=C(F)C=C2CCC=3C=CC=C(OC)C3)C1)CCCCCCCCCCC | 590.341 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-{1-hydroxy-9a,11a-dimethyl-7-oxo-1H,2H,3H,3aH,3bH,4H,5H,7H,8H,9H,9aH,9bH,10H,11H,11aH-cyclopenta[a]phenanthren-1-yl}-2-oxoethyl 3-{[(oxolan-2-yl)methyl]carbamoyl}propanoate | O=C(OCC(=O)C1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3CCC21C)CCC(=O)NCC5OCCC5 | 528.301 | Suspect screening | Canal | LC-HRMS | Reference | O |
| hexyl 7a-{4-[7-(2-aminopyridin-4-yl)-2-(methylamino)-4,5,6,7-tetrahydro-1H-1,3-diazepin-7-yl]-3-methylbut-2-en-1-yl}-2,7-dioxo-1aH,2H,7H,7aH-naphtho[2,3-b]oxirene-1a-carboxylate | O=C(OCCCCCC)C12OC2(C(=O)C=3C=CC=CC3C1=O)CC=C(C)CC4(NC(=NCCC4)NC)C=5C=CN=C(N)C5 | 586.308 | Suspect screening | Canal | LC-HRMS | Reference | O |
| "(4S)-4-amino-5-[[(2S,3S)-1-[[(2S)-1-[[(2S)-3-carboxy-1-[[(1S)-1-carboxy-2-methylpropyl]amino]-1-oxopropan-2-yl]amino]-4-methyl-1-oxopentan-2-yl]amino]-3-methyl-1-oxopentan-2-yl]amino]-5-oxopentanoic acid" | O=C(O)CCC(N)C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)O)C(C)C)CC(=O)O)CC(C)C)C(C)CC | 586.311 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:cyclododecanol | OC1CCCCCCCCCCC1 | 185.188 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(20:3(5Z,8Z,11Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCC=CCC=CCC=CCCCCCCCC | 546.352 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(18:2(9Z,12Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCC=CCC=CCCCCC | 520.336 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Seneciphylline | O=C1OC2CCN3CC=C(COC(=O)C(O)(C(=C)CC1=CC)C)C32 | 356.144 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:"MLS001158085-01!(2S)-2-[[(2S)-2-(1,2-dihydroimidazo[1,2-a]benzimidazole-3-carbonylamino)-3-methylbutanoyl]amino]-2-phenylacetic acid" | O=C(O)C(NC(=O)C(NC(=O)N1c2nc3ccccc3n2CC1)C(C)C)c4ccccc4 | 436.203 | Suspect screening | Canal | LC-HRMS | Reference | O |
| N-[(3R,9S,10R)-9-[[cyclopropylmethyl(methyl)amino]methyl]-12-[(2S)-1-hydroxypropan-2-yl]-3,10-dimethyl-13-oxo-2,8-dioxa-12-azabicyclo[12.4.0]octadeca-1(14),15,17-trien-16-yl]-2-phenylacetamide | O=C1C2=CC(=CC=C2OC(C)CCCCOC(CN(C)CC3CC3)C(C)CN1C(C)CO)NC(=O)CC=4C=CC=CC4 | 614.34 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:2-methyl-4-(pyridin-2-yl)but-3-yn-2-ol | OC(C#CC1=NC=CC=C1)(C)C | 184.07 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-(2-{2-[({1-ethynyl-1-hydroxy-9a,11a-dimethyl-1H,2H,3H,3aH,3bH,4H,5H,7H,8H,9H,9aH,9bH,10H,11H,11aH-cyclopenta[a]phenanthren-7-ylidene}amino)oxy]acetamido}-3-methylbutanamido)pentanedioic acid | O=C(O)CCC(NC(=O)C(NC(=O)CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O)C#C)C2(C)CC1)C(C)C)C(=O)O | 612.325 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:LPC 18:2; PlaSMA ID-1556 | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCC=CCC=CCCCCC | 564.327 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-{1-[({3-[(1-carbamoyl-3-methylbutyl)carbamoyl]-5,6-dihydroxycyclohex-2-en-1-yl}carbamoyl)methyl]cyclopentyl}acetic acid | O=C(O)CC1(CC(=O)NC2C=C(C(=O)NC(C(=O)N)CC(C)C)CC(O)C2O)CCCC1 | 476.236 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Perfluorooctylsulfonic acid | O=S(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 498.924 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Amlexanox | O=C(O)C1=CC=2C(=O)C3=CC(=CC=C3OC2N=C1N)C(C)C | 297.089 | Suspect screening | Canal | LC-HRMS | Reference | O |
| CNP0430869 | O=C(CC(=O)CCCCCCC)CCC1=CC(OC)=C(O)C(=C1)C2C3CCNC4NCCC(=CC2(CO)CC5=CC=CN5)C43 | 640.355 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD173499 | O=CC(NC(=O)C(NC(=O)C(NC(=O)CC(O)CCCCCCCCC)CC(=O)N)C(O)CC(=O)N)CC(C)C | 572.365 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(18:1(9Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCC=CCCCCCCCC | 522.352 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Asperunguisin E | OC1CC2C3(C(=CCC2(C)C4CCC(O)(C)C(O)C(O)C14C)C(CC3)C(C)C)C | 407.312 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Valine | O=C(O)C(N)C(C)C | 118.085 | Suspect screening | Canal | LC-HRMS | Reference | O |
| C00051353 | O=CC(=C)C1C(C=O)=C(CO)C(OC(=O)C=CC2=CC=C(O)C=C2)C1 | 381.074 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 3-[[4-cyclohexyl-1-[[(3R)-3-(4-fluorophenyl)-1-isopropyl-4-piperidyl]methyl]-4-piperidyl]methyl]-4,4-dimethyl-oxazolidin-2-one | O=C1OCC(N1CC2(CCN(CC2)CC3CCN(CC3C4=CC=C(F)C=C4)C(C)C)C5CCCCC5)(C)C | 550.378 | Suspect screening | Canal | LC-HRMS | Reference | O |
| N-[3-(dibutylamino)propyl]-3-{2-methyl-3,5-dioxo-4,6,16-triazatetracyclo[7.7.0.0?,?.0??,??]hexadeca-1(9),10,12,14-tetraen-4-yl}benzamide | O=C(NCCCN(CCCC)CCCC)C1=CC=CC(=C1)N2C(=O)N3CCC=4C=5C=CC=CC5NC4C3(C2=O)C | 566.314 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:N-Caffeoylputrescine, (E)- | O=C(C=CC1=CC=C(O)C(O)=C1)NCCCCN | 273.118 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 1-[(3S,9R,10R)-12-[(2S)-1-hydroxypropan-2-yl]-3,10-dimethyl-9-[[methyl(pyridin-4-ylmethyl)amino]methyl]-13-oxo-2,8-dioxa-12-azabicyclo[12.4.0]octadeca-1(14),15,17-trien-16-yl]-3-phenylurea | O=C(NC=1C=CC=CC1)NC2=CC=C3OC(C)CCCCOC(CN(C)CC=4C=CN=CC4)C(C)CN(C(=O)C3=C2)C(C)CO | 616.353 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPE(22:4(7Z,10Z,13Z,16Z)/0:0) | O=C(OCC(O)COP(=O)(O)OCCN)CCCCCC=CCC=CCC=CCC=CCCCCC | 528.307 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:reynosin | O=C1OC2C(C1=C)CCC3(C)C(O)CCC(=C)C23 | 249.155 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD12261 | OC1=CC=2C=C3CCCC(C)(C)C3CCC2C=C1C | 257.187 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-({4-[(2-{[(tert-butoxy)carbonyl]amino}-4-methylpentanamido)methyl]cyclohexyl}formamido)-3-methylbutanoic acid | O=C(OC(C)(C)C)NC(C(=O)NCC1CCC(C(=O)NC(C(=O)O)C(C)C)CC1)CC(C)C | 470.319 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Terphenyl, hydrogenated | OC1CCC(C=2C=CC=C(C2)C3CCCCC3)CC1 | 259.205 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 1-benzoyl-4-{2-[(diethylamino)methyl]-1,3-thiazol-4-yl}piperidin-4-ol | O=C(C=1C=CC=CC1)N2CCC(O)(C=3N=C(SC3)CN(CC)CC)CC2 | 396.172 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Barbatic acid | O=C(O)C1=C(O)C(=C(OC(=O)C2=C(O)C(=C(OC)C=C2C)C)C=C1C)C | 359.109 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Isocurcumenol | OC12OC3(CC1=C(C)C)C(C(=C)C2)CCC3C | 257.145 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 4-(2-{4-[2-(2-acetamido-3-methylbutanamido)-3-methylbutanamido]-3-hydroxy-6-methylheptanamido}propanamido)-3,7-dihydroxy-6-methylheptanoic acid | O=C(O)CC(O)C(NC(=O)C(NC(=O)CC(O)C(NC(=O)C(NC(=O)C(NC(=O)C)C(C)C)C(C)C)CC(C)C)C)CC(C)CO | 660.42 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:INOSINE 5'-MONOPHOSPHATE | O=C1N=CNC2=C1N=CN2C3OC(COP(=O)(O)O)C(O)C3O | 349.051 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 7-Dehydrocholesterol | OC1CC2=CC=C3C(CCC4(C)C3CCC4C(C)CCCC(C)C)C2(C)CC1 | 385.342 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:"MLS001158023-01!4-phenyl-1-[2-(3,4,7-trimethyl-2-oxochromen-5-yl)oxyacetyl]piperidine-4-carboxylic acid" | O=c1oc2cc(cc(OCC(=O)N3CCC(C(=O)O)(c4ccccc4)CC3)c2c(c1C)C)C | 450.186 | Suspect screening | Canal | LC-HRMS | Reference | O |
| CNP0443897 | O=C([O-])C1=C2CC3C4C#CCN=C(NC)[N+]5=CCC(CNCCO)C3(C5)C2(CC1(O)COC6CCCC(NC)C6)C(C)C4 | 594.369 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 19-(azidomethoxy)nonadecanoic acid [4-[3-(4-fluorophenyl)-3-keto-prop-1-enyl]phenyl] ester | [N-]=[N+]=NCOCCCCCCCCCCCCCCCCCCC(=O)OC1=CC=C(C=CC(=O)C2=CC=C(F)C=C2)C=C1 | 592.356 | Suspect screening | Canal | LC-HRMS | Reference | O |
| PS(21:0/0:0) | O=C(OCC(O)COP(=O)(O)OCC(N)C(=O)O)CCCCCCCCCCCCCCCCCCCC | 566.344 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-({4-[(2-{[(tert-butoxy)carbonyl]amino}-3-phenylpropanamido)methyl]cyclohexyl}formamido)butanedioic acid | O=C(OC(C)(C)C)NC(C(=O)NCC1CCC(C(=O)NC(C(=O)O)CC(=O)O)CC1)CC=2C=CC=CC2 | 502.253 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(20:4(8Z,11Z,14Z,17Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCC=CCC=CCC=CCC=CCC | 566.323 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 17'-amino-16'-(hydroxymethyl)-9'-methyl-8'-oxaspiro[cyclopentane-1,4'-octacyclo[19.6.2.1?,?.1?,??.1?,??.0?,??.0??,??.0??,??]dotriacontane]-22',24',26',28'-tetraen-19'-yn-24'-ol | OC1=CC=C2C(=C1)C3C#CC4C5(OC6(C)CCCC7(CCC(CO)C4(N)C67)C5)C8CC(CC9(CCCC9)C8)C2C=C3 | 588.326 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:\_130036 | O=C1NC(C(=O)C1=C(O)C(C)CC(C)CC=CC)C(O)C2=CC=C(O)C=C2 | 396.175 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Detoxin D4 | O=C(O)CC(OC(=O)C(NC(=O)C(C)CC)CC=1C=CC=CC1)C2N(C(=O)C(N)C(C)C)CCC2OC(=O)CCC | 576.327 | Suspect screening | Canal | LC-HRMS | Reference | O |
| N-[4-(heptyloxy)phenyl]dispiro[cyclohexane-1,4'-[3,5,7,10,12]pentaoxatricyclo[7.3.0.0?,?]dodecane-11',1''-cyclohexane]-8'-carboxamide | O=C(NC1=CC=C(OCCCCCCC)C=C1)C2OC3OC4(OC3C5OC6(OC25)CCCCC6)CCCCC4 | 582.286 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:8,9-Dihydropiplartine | O=C1C=CCCN1C(=O)CCC2=CC(OC)=C(OC)C(OC)=C2 | 342.127 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Glycochenodeoxycholic acid 3-glucuronide | O=C(O)CNC(=O)CCC(C)C1CCC2C3C(O)CC4CC(OC5OC(C(=O)O)C(O)C(O)C5O)CCC4(C)C3CCC12C | 624.336 | Suspect screening | Canal | LC-HRMS | Reference | O |
| "(2R)-3-(carboxymethylsulfanyl)-2-[[(4R)-4-[(3R,5S,7S,10S,13R,17R)-3,7-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoyl]amino]propanoic acid" | O=C(O)CSCC(NC(=O)CCC(C)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CCC12C)C(=O)O | 552.304 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:3-(1H-indol-1-yl)-1-(8-methoxy-3,4-dihydro-1H-pyrido[4,3-b]indol-2(5H)-yl)propan-1-one | O=C(N1CC=2C=3C=C(OC)C=CC3NC2CC1)CCN4C=CC=5C=CC=CC54 | 396.172 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:Sibiromycin hemiaminal | O=C1C2=CC(OC3OC(C)C(NC)C(O)(C)C3O)=C(C(O)=C2NC(O)C4N1C=C(C=CC)C4)C | 476.238 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD55110 | O=C(O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(N)CC1=CNC=2C=CC=CC21)C(C)CC)C(C)C)CC(C)C)CCCNC(=N)N | 686.433 | Suspect screening | Canal | LC-HRMS | Reference | O |
| N-[(2R,3S)-5-[(2S)-1-hydroxypropan-2-yl]-2-[[(4-methoxyphenyl)methyl-methylamino]methyl]-3-methyl-6-oxo-2,3,4,7-tetrahydro-1,5-benzoxazonin-9-yl]-2-phenylacetamide | O=C(NC1=CC=C2OC(CN(C)CC3=CC=C(OC)C=C3)C(C)CN(C(=O)CC2=C1)C(C)CO)CC=4C=CC=CC4 | 560.309 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD136360 | O=C(OC1C(O)C(=C(CCC(=CCO)C)C2(C)CCCC(C)(C)C12)C)CC(C)C | 389.302 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Vignatic acid B | O=C(O)C1NC(=O)C(NC(=O)C(NC(=O)C(O)CC(C)C)C(OC2=CC=C(C=C2)C1)C(C)C)CC(C)C | 542.284 | Suspect screening | Canal | LC-HRMS | Reference | O |
| [5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl octadec-9-enoate | O=C1N=C(N)C=CN1C2OC(COC(=O)CCCCCCCC=CCCCCCCCC)C(O)C2O | 508.334 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-(2-{2-[({1-ethynyl-1-hydroxy-9a,11a-dimethyl-1H,2H,3H,3aH,3bH,4H,5H,7H,8H,9H,9aH,9bH,10H,11H,11aH-cyclopenta[a]phenanthren-7-ylidene}amino)oxy]acetamido}propanamido)hexanoic acid | O=C(O)C(NC(=O)C(NC(=O)CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O)C#C)C2(C)CC1)C)CCCC | 570.349 | Suspect screening | Canal | LC-HRMS | Reference | O |
| PE(17:2(9Z,12Z)/12:0) | O=C(OCC(OC(=O)CCCCCCCCCCC)COP(=O)(O)OCCN)CCCCCCCC=CCC=CCCCC | 646.442 | Suspect screening | Canal | LC-HRMS | Reference | O |
| CNP0446418 | O=C(N(C)CCN(C)C)C(C)C1CCC2(C)CC=3SC(=NC3C(C)C2C1O)CSC=4C=CC=CC4 | 516.273 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Leualacin F | O=C1OC(C(=O)NC(C(=O)OC(C(=O)NC(C(=O)NCC1)CC2=CC=C(O)C=C2)CC(C)C)CC(C)C)CC(C)C | 576.327 | Suspect screening | Canal | LC-HRMS | Reference | O |
| N-{6,13,14-trihydroxy-3-[(1H-indol-3-yl)methyl]-4,5,10,12-tetramethyl-1,17-dioxo-1H,2H,3H,3aH,6H,6aH,9H,10H,13H,14H,15H,16H,17H-cyclotrideca[d]isoindol-15-yl}acetamide | O=C(NC1CC(=O)C23C(=O)NC(CC4=CNC=5C=CC=CC54)C3C(=C(C)C(O)C2C=CCC(C=C(C)C(O)C1O)C)C)C | 590.319 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:bakuchiol | OC1=CC=C(C=C1)C=CC(C=C)(C)CCC=C(C)C | 257.186 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 5,8,11-Eicosatrienoic acid | O=C(O)CCCC=CCC=CCC=CCCCCCCCC | 305.245 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 1-(10Z-heptadecenoyl)-sn-glycero-3-phosphocholine | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCCC=CCCCCCC | 508.335 | Suspect screening | Canal | LC-HRMS | Reference | O |
| w/o MS2:NCGC00347533-02\_C31H40O11\_7,11-Methano-2H,4H-oxireno[1,8]cycloocta[1,2-f][2]benzopyran-8-acetic acid, 4-(3-furanyl)dodecahydro-alpha,11-dihydroxy-4a,7,9,9-tetramethyl-10-(2-methyl-1-oxopropoxy)-2,13-dioxo-, methyl ester, (alphaR,4R,4aR,7S,8S,10S,11S,11aR,12aS)- | O=C1OC(C2=COC=C2)C3(C)CCC4C5(OC5C6(O)C(=O)C4(C)C(C(O)C(=O)OC)C(C)(C)C6OC(=O)C(C)C)C3C1 | 606.293 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(20:1(11Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCCCC=CCCCCCCCC | 550.382 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD182078 | O=C1C(OC(O)C(O)C(O)C(O)CO)=C(OC2=CC(O)=C(O)C(O)=C12)C=3C=CC(O)=C(O)C3 | 469.098 | Suspect screening | Canal | LC-HRMS | Reference | O |
| N-[2-[2-[2-(N'-diazohydrazino)-2-keto-ethoxy]ethoxy]ethyl]-16-(2H-tetrazol-5-yl)palmitamide | [N-]=[N+]=NNC(=O)COCCOCCNC(=O)CCCCCCCCCCCCCCCC=1N=NNN1 | 510.35 | Suspect screening | Canal | LC-HRMS | Reference | O |
| (2S,4S)-2-[N'-[(1S,3S,4R,5S)-4-ethoxy-3,5-dihydroxy-1-isopropyl-nonyl]amidino]-4-propyl-pyrrolidine-1-carboxylic acid (2-keto-5-methyl-1,3-dioxol-4-yl)methyl ester | O=C1OC(=C(O1)COC(=O)N2CC(CCC)CC2C(=NC(CC(O)C(OCC)C(O)CCCC)C(C)C)N)C | 554.343 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Ginsenoyne J | OC(C=C)C=CC#CCC=CCCCCCCC | 247.208 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 3-(acetyloxy)-1-{4-[(4-hydroxy-3-methoxyphenyl)methyl]piperidin-4-yl}octyl 2,3-bis(methylamino)propanoate | O=C(OC(CCCCC)CC(OC(=O)C(NC)CNC)C1(CC2=CC=C(O)C(OC)=C2)CCNCC1)C | 560.305 | Suspect screening | Canal | LC-HRMS | Reference | O |
| LysoPC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCC=CCC=CCC=CCC=CCC=CCC=CCC | 590.321 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 2-{2-[(6-amino-4-{2-[3-(2-phenylethyl)phenyl]ethyl}pyridin-3-yl)methyl]-4-hydroxy-5-methoxyphenyl}-1-hydroxy-12-methyl-13-(methylamino)tridec-2-ene-4,6-dione | O=C(C=C(C1=CC(OC)=C(O)C=C1CC2=CN=C(N)C=C2CCC=3C=CC=C(C3)CCC=4C=CC=CC4)CO)CC(=O)CCCCCC(C)CNC | 704.405 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 12-[(3,4-dihydroxycyclohexyl)methyl]-1-hydroxy-12,16,24,28-tetramethyl-11,29-dioxa-4-azatricyclo[23.3.1.0?,?]nonacosa-17,21-diene-2,3,10,23-tetrone | O=C1C(=O)C2(O)OC(CCC2C)C(C(=O)C=CCCC=CC(C)CCCC(OC(=O)C3N1CCCC3)(C)CC4CCC(O)C(O)C4)C | 682.395 | Suspect screening | Canal | LC-HRMS | Reference | O |
| 3-methyl-2-propylpentanamide | O=C(N)C(CCC)C(C)CC | 158.151 | Suspect screening | Canal | LC-HRMS | Reference | O |
| UNPD183792 | O1CC2C3CC4N(CCC45C2N(C1C6C7C(=CC)CC8C(C=9NC=%10C=CC=CC%10C9CC86)C7)C%11CCCCC%115)CC3CC | 578.411 | Suspect screening | Canal | LC-HRMS | Reference | O |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | A |
| Acridine | C1=CC=C2C(=C1)C=C3C=CC=CC3=N2 | 179.07350 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | A |
| Perfluoro-1-octanesulfonic acid (PFOS) | C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | A |
| CAPSO (3-(cyclohexylamino)-2-hydroxy-1-propanesulfonic acid) | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | A |
| Perfluorododecanoic acid | C(=O)(C(C(C(C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)O | 613.96093 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | A |
| Docosyltrimethylammonium | CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C | 368.42460 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | A |
| Icosyltrimethylammonium | CCCCCCCCCCCCCCCCCCCC[N+](C)(C)C | 340.39380 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | A |
| 4-Methylbenzylidene Camphor | Cc1ccc(cc1)C=C2C3CCC(C)(C2=O)C3(C)C | 254.16700 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Cinoxate | CCOCCOC(=O)/C=C/c1ccc(OC)cc1 | 250.12050 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 6-Methylhepta-3,5-dien-2-one. | CC(C)=CC=CC(C)=O | 124.08881 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 1-Naphthol | OC1=CC=CC2=CC=CC=C12 | 144.05751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| N,N,3,5-Tetramethylaniline | CN(C)C1=CC(C)=CC(C)=C1 | 149.12045 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 1-[(1R,2S)-2,6,6-trimethylcyclohex-3-en-1-yl]ethanone | CC1C=CCC(C1C(=O)C)(C)C | 166.13577 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| methyprylon | CCC1(CC)C(=O)NCC(C)C1=O | 183.12593 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 1-(1H-Indol-3-yl)butan-1-one 3-(3-Oxobutyl)-1H-indole | CCCC(=O)C1=CNC2=CC=CC=C12 CC(=O)CCc1c[nH]c2c1cccc2 | 187.09971 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2,2,5,7-Tetramethylindan-1-one | CC1=CC(C)=C2C(CC(C)(C)C2=O)=C1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Benzyl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OCC1=CC=CC=C1 | 192.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Methyl 2-acetyl-2-allylpent-4-ene-1-oate | COC(=O)C(CC=C)(CC=C)C(C)=O | 196.10994 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| alpha,alpha-Dicyclopropyl-4-methylbenzyl alcohol | CC1=CC=C(C=C1)C(O)(C1CC1)C1CC1 | 202.13577 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| N-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 3,3'-[butane-1,4-diylbis(oxy)]bispropanamine | C(CCOCCCN)COCCCN | 204.18378 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Ibuprofen | CC(C)CC1=CC=C(C=C1)C(C)C(O)=O | 206.13068 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 4-tert-octylphenol | CC(C)(C)CC(C)(C)c1ccc(cc1)O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2,4,4,7-Tetramethylnona-6,8-dien-3-one oxime | CC(C)C(=NO)C(C)(C)CC=C(C)C=C | 209.17796 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 3-(Decyloxy)propionitrile 3-(isodecyloxy)propiononitrile | CCCCCCCCCCOCCC#N CC(C)CCCCCCCOCCC#N | 211.19361 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Ritalinic acid | OC(=O)C(C1CCCCN1)C1=CC=CC=C1 | 219.12593 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2-(3,4-dimethoxyphenyl)-3-methylbutyronitrile | COC1=CC=C(C=C1OC)C(C#N)C(C)C | 219.12593 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Precocene II | COC1=CC2=C(C=CC(C)(C)O2)C=C1OC | 220.10994 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Benzoic acid, 2-amino-, hexyl ester | CCCCCCOC(=O)C1=CC=CC=C1N | 221.14158 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 3,4-methylenedioxypropylamphetamine | CCCNC(C)CC1=CC2=C(C=C1)OCO2 | 221.14158 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| ethyl 2-allyl-2-cyano-3-methylhexanoate | CCCC(C)C(CC=C)(C#N)C(=O)OCC | 223.15723 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| diethyl 4-oxopentane-1,2-dicarboxylate | CCOC(=O)CC(CC(=O)C)C(=O)OCC | 230.11542 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| (Acetylazanediyl)di(ethane-2,1-diyl) diacetate | CC(=O)OCCN(CCOC(C)=O)C(C)=O | 231.11067 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 5,6,7,8-Tetrahydro-gamma-oxonaphthalene-2-butyric acid | OC(=O)CCC(=O)C1=CC2=C(CCCC2)C=C1 | 232.10994 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Pentylone Dibutylone | CCCC(NC)C(=O)C1=CC=C2OCOC2=C1 CCC(N(C)C)C(=O)C1=CC=C2OCOC2=C1 | 235.12084 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| viloxazine | CCOC1=C(OCC2CNCCO2)C=CC=C1 | 237.13649 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate | CC1(COC(=O)C2CC=CCC2C(=O)OC1)C | 238.12051 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| N-Dodecylacrylamide | CCCCCCCCCCCCNC(=O)C=C | 239.22491 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2-((2-Methyl-1-oxoallyl)oxy)ethyl 6-hydroxyhexanoate | CC(=C)C(=O)OCCOC(=O)CCCCCO | 244.13107 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Celestolide | CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C | 244.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2,2'-[oxybis(methylene)]bis[2-ethylpropane-1,3-diol] | CCC(CO)(CO)COCC(CC)(CO)CO | 250.17802 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| (Z)-9-Cycloheptadecen-1-one. | O=C1CCCCCCC\C=C/CCCCCCC1 | 250.22967 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Tricyclo(3.3.1.13,7)dec-1,3-diyldi(acetic acid) | [H]C12CC3([H])CC(CC(O)=O)(C1)CC(CC(O)=O)(C2)C3 | 252.13616 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| N-(dodecyl)pyrrolidinone | CCCCCCCCCCCCN1CCCC1=O | 253.24056 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| N-(3-Acetyl-4-hydroxyphenyl)heptan-1-amide | CCCCCCC(=O)NC1=CC(C(C)=O)=C(O)C=C1 | 263.15214 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2-(3,5-dimethylhex-3-en-2-yloxy)-2-methylpropyl cyclopropanecarboxylate | CC(C)C=C(C)C(C)OC(C)(C)COC(=O)C1CC1 | 268.20384 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine | COCCCNCC1=CC(OC)=C(OC)C(OC)=C1 | 269.16271 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Decyl 5-oxo-L-prolinate | CCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 269.19909 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Octanoic anhydride | CCCCCCCC(=O)OC(=O)CCCCCCC | 270.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Alphameprodine [INN:BAN:DCF] | CC[C@H]1CN(C)CC[C@]1(OC(=O)CC)C1=CC=CC=C1 | 275.18853 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Brefeldin A | [H][C@@]12C[C@H](O)C[C@@]1([H])[C@H](O)\C=C\C(=O)O[C@@H](C)CCC\C=C\2 | 280.16746 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| p-(1-(p-Pentylphenyl)vinyl)anisole | CCCCCC1=CC=C(C=C1)C(=C)C1=CC=C(OC)C=C1 | 280.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Methyl 3-oxohexadecanoate | CCCCCCCCCCCCCC(=O)CC(=O)OC | 284.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Sodium N-methyl-N-(1-oxododecyl)-ß-alaninate | CCCCCCCCCCCC(=O)N(O)CCC(=O)[O-]·[Na+] | 285.23039 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| norethisterone | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C | 298.19328 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Sodium decyl phthalate diisopentyl phthalate CROMOPHTAL DPP RED TFP | [Na+].CCCCCCCCCCOC(=O)C1=CC=CC=C1C([O-])=O CC(C)CCOC(=O)C1=CC=CC=C1C(=O)OCCC(C)C CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCC | 306.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| homodihydrocapsaicin-I | CC(C)CCCCCCCC(=O)NCC1=CC(=C(C=C1)O)OC | 321.23039 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 15-(tert-Butyl)-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecine | CC(C)(C)C1=CC2=C(C=C1)OCCOCCOCCOCCO2 | 324.19367 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| hydrogen N-(1-oxododecyl)-L-glutamic acid | CCCCCCCCCCCC(=O)NC(CCC(=O)O)C(=O)O | 329.22022 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| ETHYL ARACHIDONATE | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OCC | 332.27153 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Pentadecyl 5-oxo-L-prolinate | CCCCCCCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 339.27734 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Bis(tert-butyl) 1,4-dihydro-2,6-dimethyl-4-propylpyridine-3,5-dicarboxylate | CCCC1C(C(=O)OC(C)(C)C)=C(C)NC(C)=C1C(=O)OC(C)(C)C | 351.24096 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| GLYCERYL LINOLENATE | CCC=CCC=CCC=CCCCCCCCC(=O)OCC(O)CO | 352.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| (Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine | CCCCCCCCC=CCCCCCCCC(=O)N(C)CC(=O)O | 353.29299 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Isodecyl isononyl phthalate Decyl nonyl phthalate | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC© CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC | 432.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Glyceryl phosphate | OCC(O)COP(O)(O)=O | 172.01367 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Acamprosate | CC(=O)NCCCS(O)(=O)=O | 181.04088 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 3-Hydroxyphthalic acid 4-Hydroxybenzene-1,2-dicarboxylic acid | OC(=O)C1=C(C(O)=O)C(O)=CC=C1 OC(=O)C1=C(C=C(O)C=C1)C(O)=O | 182.02152 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 4-morpholineethanesulfonic acid | OS(=O)(=O)CCN1CCOCC1 | 195.05653 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| benzothiazole sulfonic acid | C1=CC=C2C(=C1)N=C(S2)S(=O)(=O)O | 214.97108 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 1-(2,5-Dihydroxyphenyl)octan-1-one | CCCCCCCC(=O)C1=C(O)C=CC(O)=C1 | 236.14124 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Loxoprofen alcohol | CC(C1=CC=C(C=C1)CC2CCCC2O)C(=O)O | 248.14124 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Hydroxypethidine | CCOC(=O)C1(CCN(C)CC1)C1=CC(O)=CC=C1 | 263.15214 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Ethyl 3-(3,4,5-trimethoxyphenyl)propionate Butyl 3,4,5-trimethoxybenzoate | CCOC(=O)CCC1=CC(OC)=C(OC)C(OC)=C1 CCCCOC(=O)C1=CC(OC)=C(OC)C(OC)=C1 | 268.13107 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Triaziflam | CC(COC1=CC(C)=CC(C)=C1)N=C1NC(=N)N=C(N1)C(C)(C)F | 333.19649 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| NONOXYNOL-4 | CCCCCCCCCC1=CC=CC=C1OCCOCCOCCOCCO | 396.28757 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| simvastatin hydroxyl acid | CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 436.28249 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| Perfluorooctanesulfonic acid | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2-(1,1-Dimethylethyl)-4-(1-methyl-1-phenylethyl)phenol | CC(C)(C)C1=C(O)C=CC(=C1)C(C)(C)C1=CC=CC=C1 | 268.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| triisobutyl phosphate | CC(C)COP(=O)(OCC(C)C)OCC(C)C | 266.16470 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 2-((2-Hydroxyethyl)(3-methoxypropyl)amino)ethyl methacrylate | COCCCN(CCO)CCOC(=O)C(C)=C | 245.16271 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 4-O-Desmethyl 4-O-Ethyl Trimethoprim | CCOC1=C(OC)C=C(CC2=CNC(=N)NC2=N)C=C1OC | 304.15354 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | I |
| 4-Formylaminoantipyrine | CC1=C(C(=O)N(N1C)C2=CC=CC=C2)NC=O | 231.10078 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 5-Methylbenzotriazole | CC1=CC2=NNN=C2C=C1 | 133.06400 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Benzotriazole | C1=CC2=NNN=C2C=C1 | 119.04835 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Caffeine | CN1C=NC2=C1C(=O)N(C(=O)N2C)C | 194.08038 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Citalopram | CN(C)CCCC1(C2=C(CO1)C=C(C=C2)C#N)C3=CC=C(C=C3)F | 324.16379 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Diazinon | CCOP(=S)(OCC)OC1=NC(=NC(=C1)C)C(C)C | 304.10105 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Diphenhydramine | CN(C)CCOC(C1=CC=CC=C1)C2=CC=CC=C2 | 255.16231 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Enilconazole = Imazalil | C=CCOC(CN1C=CN=C1)C2=C(C=C(C=C2)Cl)Cl | 296.04832 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Icaridine | CCC(C)OC(=O)N1CCCCC1CCO | 229.16779 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Lidocaine | CCN(CC)CC(=O)NC1=C(C=CC=C1C)C | 234.17321 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Metoprolol | CC(C)NCC(COC1=CC=C(C=C1)CCOC)O | 267.18344 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N-Desmethylvenlafaxine | CNCC(C1=CC=C(C=C1)OC)C2(CCCCC2)O | 263.18853 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Galaxolidone (peak tail) | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Terbutryn | CCNC1=NC(=NC(=N1)SC)NC(C)(C)C | 241.13612 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Venlafaxine | CN(C)CC(C1=CC=C(C=C1)OC)C2(CCCCC2)O | 277.20418 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Fluoren-9-one hydrazone | C1=CC=C2C(=C1)C3=CC=CC=C3C2=NN | 194.08440 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| HET0016 | CCCCC1=CC(=C(C=C1)N=CNO)C | 206.14191 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (2R,3S)-1-[(7-methyl-2,3-dihydro-1H-inden-4-yl)oxy]-3-(propan-2-ylamino)butan-2-ol | CC1=C2CCCC2=C(C=C1)OC[C@@H]([C@H](C)NC(C)C)O | 277.20418 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-amino-N-(5,6,7,8-tetrahydroisoquinolin-1-yl)benzamide | C1CCC2=C(C1)C=CN=C2NC(=O)C3=CC=C(C=C3)N | 267.13716 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate | CCOCCOCCOCCOC(=O)C(C)=C | 246.14672 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2'-Aminoacetophenone phenylhydrazone | CC(=NNC1=CC=CC=C1)C2=CC=CC=C2N | 225.12660 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-cyclohexylidene-2-phenylacetonitrile | N#CC(=C1CCCCC1)C1=CC=CC=C1 | 197.12045 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 17alpha-Dihydroequilin | C[C@]12CC[C@H]3C(=CCC4=C3C=CC(=C4)O)[C@@H]1CC[C@H]2O | 270.16198 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-tert-butylcyclohexanone | CC(C)(C)C1CCC(=O)CC1 | 154.13577 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Promucosine | COC1=C(C2=C3C(CC24C=CC(=O)C=C4)N(CCC3=C1)C(=O)OC)OC | 355.14197 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 5-Fluoro ADBICA | CC(C)(C)C(C(=O)N)NC(=O)C1=CN(C2=CC=CC=C21)CCCCCF | 361.21656 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Benzedrone | CC(NCC1=CC=CC=C1)C(=O)C1=CC=C(C)C=C1 | 253.14666 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Cyromazine | NC1=NC(NC2CC2)=NC(N)=N1 | 166.09669 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| di-p-tolyl sulphone | CC1=CC=C(C=C1)S(=O)(=O)C1=CC=C(C)C=C1 | 246.07145 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| thymine | CC1=CNC(=O)NC1=O | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 11-Hydroxyhexadecanoic acid | CCCCCC(CCCCCCCCCC(=O)O)O | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-(2-chloro-3-methoxyphenyl)-N-cyclohexylpropanamide | COC1=CC=CC(=C1Cl)CCC(=O)NC2CCCCC2 | 295.13391 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N,O-Didesmethylvenlafaxine | CNCC(C1=CC=C(O)C=C1)C1(O)CCCCC1 | 249.17288 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Tecostanine | CC1CCC2C1CN(CC2CO)C | 183.16231 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| nalbuphine | O[C@H]1CC[C@@]2(O)[C@H]3CC4=CC=C(O)C5=C4[C@@]2(CCN3CC2CCC2)[C@H]1O5 | 357.19401 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,6,7,8-Tetrahydro-1,4,6,6,8,8-hexamethyl-as-indacen-3(2H)-one | CC1CC(=O)C2=C1C3=C(C=C2C)C(CC3(C)C)(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| ethyl 4-[(3-ethoxy-3-oxopropyl)(methyl)amino]butanoate | CCOC(=O)CCCN(C)CCC(=O)OCC | 245.16271 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Sodium Lauroyl taurate | CCCCCCCCCCCC(=O)NCCS(=O)(=O)[O-].[Na+] | 329.16367 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| tetramethylthiuram monosulphide | CN(C)C(=S)SC(=S)N(C)C | 208.01626 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Olivetol | CCCCCC1=CC(O)=CC(O)=C1 | 180.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (1R-(1a,4aß,4ba,10aa))-1,2,3,4,4a,4b,5,6,10,10a-Decahydro-7-isopropyl-1,4adimethylphenanthren- |  | 330.25588 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ethylestrenol | CC[C@]1(O)CC[C@H]2[C@@H]3CCC4=CCCC[C@@H]4[C@H]3CC[C@]12C | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 5-Pentadecylbenzene-1,3-diol | CCCCCCCCCCCCCCCC1=CC(O)=CC(O)=C1 | 320.27153 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-(2,2-Dimethyl-3,4-dihydro-2h-chromen-6-yl)-2-methylbutan-2-ol | C1(CCC2=C(O1)C=CC(=C2)CCC(C)(C)O)C | 248.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methandriol | C[C@]1(O)CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C | 304.24023 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (14R\*,18R\*)-14,18-Dimethyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane | CC1CNCC(OCCOCCOCCOCCO1)C | 291.20457 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-Heptadecyl-1H-imidazole-4-carbodithioic acid | CCCCCCCCCCCCCCCCCC1=NC(=CN1)C(S)=S | 382.24764 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 16-methyl-6Z,9Z-heptadecadienoic acid | CC(C)CCCCC/C=C\\C/C=C\\CCCCC(=O)O | 280.24023 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3S,4R-Epoxy-6Z,9Z-nonadecadiene | CCCCCCCCC/C=C\\C/C=C\\C[C@@H]1[C@@H](O1)CC | 278.26097 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,2-Benzenedicarboxylic acid, isooctyl nonyl ester | CCCCCCCCCOC(=O)C1=C(C=CC=C1)C(=O)OCCCCCC(C)C | 404.29266 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Acetylated glycol stearate | CCCCCCCCCCCCCCCCCC(=O)OCCOC(C)=O | 370.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Diethyl cetylmalonate | CCCCCCCCCCCCCCCCC(C(=O)OCC)C(=O)OCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Prostaglandin A1 | CCCCC[C@H](O)\C=C\[C@H]1C=CC(=O)[C@@H]1CCCCCCC(O)=O | 336.23006 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (trans,trans)-4-(4-Ethoxy-2,3-difluorophenyl)-4'-propyl-1,1'-bi(cyclohexane) | CCCC1CCC(CC1)C2CCC(CC2)C3=C(C(=C(C=C3)OCC)F)F | 364.25777 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| PEG-16 |  | 722.43001 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (1R-(1a(R\*),2b,4aß,8aa))-2-Hydroxy-a,2,5,5,8a-pentamethyl-a- |  | 308.27153 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-Ethoxy-4'-propyl-1,1'-bi(cyclohexane) | CCCC1CCC(CC1)C1CCC(CC1)OCC | 252.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Carbocyclic thromboxane A2 | CCCCC[C@@H](/C=C/[C@H]1CC2CC(C2)[C@@H]1C/C=C\\CCCC(=O)O)O | 348.26645 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ethanaminium, 2-[[2-cyano-3-[4-[ethyl(phenylmethyl)amino]phenyl]-1-oxo-2-propenyl]oxy]-N,N,N-trimethyl-, chloride | CCN(CC1=CC=CC=C1)C2=CC=C(C=C2)C=C(C#N)C(=O)OCC[N+](C)(C)C.[Cl-] | 427.20266 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Iprovalicarb | CC(C)OC(=O)N[C@@H](C(C)C)C(=O)NC(C)C1=CC=C(C)C=C1 | 320.20999 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-Methoxyestra-2,5(10)-dien-17beta-ol | C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2O)CCC4=C3CC=C(C4)OC | 288.20893 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 15-Hydroperoxyeicosa-8Z,11Z,13E-trienoate | CCCCCC(/C=C/C=C\\C/C=C\\CCCCCCC(=O)O)OO | 338.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Heptyl-2-naphthol | CCCCCCCC1=C(C=CC2=CC=CC=C21)O | 242.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 9-Hexadecenamide | CCCCCCC=CCCCCCCCC(=O)NCCO | 297.26678 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-CYCLOHEXEN-1-OL, 2,6-DIMETHYL-4-(2,2,3-TRIMETHYL-3-CYCLOPENTEN-1-YL)- | CC1CC(C=C(C1O)C)C2CC=C(C2(C)C)C | 234.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1-O-(2R-methoxy-4Z-pentadecenyl)-sn-glycerol | CCCCCCCCCC/C=C\\C[C@H](COC[C@H](CO)O)OC | 330.27701 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-Amino-N-(4-(aminocarbonyl)phenyl)-4-methoxybenzamide | COC1=C(C=C(C=C1)C(=O)NC2=CC=C(C=C2)C(=O)N)N | 285.11134 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| rac-threo-Dihydrobupropion | CC(C(C1=CC(=CC=C1)Cl)O)NC(C)(C)C | 241.12334 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ranitidine TP 45 |  | 139.09971 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (S)-2-((tert)-butoxycarbonyl)amino)butanoic acid | CCC(C(=O)O)NC(=O)OC(C)(C)C | 203.11576 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (S)-2-((tert-Butoxycarbonyl)amino)-3,3-dimethylbutanoic acid | CC(C)(C)OC(=O)N[C@H](C(O)=O)C(C)(C)C | 231.14706 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ketocainol | CCCC(C1=CC=CC=C1OCCN(C(C)C)C(C)C)O | 293.23548 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-((((2-Amino-6-chlorophenyl)methyl)methylamino)acetyl)morpholine | CN(CC(=O)N1CCOCC1)CC1=C(N)C=CC=C1Cl | 297.12440 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Acetoin dimer |  | 176.10486 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| brompheniramine | CN(C)CCC(C1=CC=C(Br)C=C1)C1=CC=CC=N1 | 318.07316 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (2R)-2-[(E)-oct-4-enoxy]-3-octoxypropan-1-ol | CCCCCCCCOC[C@@H](CO)OCCC/C=C/CCC | 314.28210 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Dihydro-3-(octadecenyl)-2,5-furandione | CCCCCCCCCCCCCCCCC=CC1CC(=O)OC1=O | 350.28210 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ethyl N-(2,3-dimethyl-2-isopropyl-1-oxobutyl)glycinate | CCOC(=O)CNC(=O)C(C)(C(C)C)C(C)C | 243.18344 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 12-hydroxystearic acid | CCCCCCC(O)CCCCCCCCCCC(O)=O | 300.26645 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| retinol | C\C(=C/CO)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C | 286.22967 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-ethyl-2-methyl-2-isopentyl-1,3-oxazolidine | CCC1COC(N1)(C)CCC(C)C | 185.17796 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| benzothiazole sulfonic acid | OS(=O)(=O)C1=NC2=CC=CC=C2S1 | 214.97109 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methyl (3alpha,5beta,6alpha)-3,6-dihydroxycholan-24-oate |  | 406.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N,N-bis(2-hydroxyethyl)dodecanamide | CCCCCCCCCCCC(=O)N(CCO)CCO | 287.24604 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 17ß-hydroxy-17-(3-hydroxypropyl)androst-4-ene-4-one |  | 346.25080 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,4-Tridecadienal | CCCCCCCCC=CC=CC=O | 194.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,5-Dioctylbenzene-1,4-diol | CCCCCCCCC1=CC(O)=C(CCCCCCCC)C=C1O | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3,7-Bis(1-methyl-1-phenylethyl)-10H-phenothiazine | CC(C)(C1=CC=CC=C1)C1=CC2=C(NC3=CC=C(C=C3S2)C(C)(C)C2=CC=CC=C2)C=C1 | 435.20207 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| ACRIDINE | C1=CC=C2C(=C1)C=C3C=CC=CC3=N2 | 179.07350 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Benzenediazonium, 2,5-dibutoxy-4-(4-morpholinyl)-, tetrafluoroborate(1-) |  | 334.21307 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Chuangxinmycin | CC1C(SC2=CC=CC3=C2C1=CN3)C(=O)O | 233.05105 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,4-Di-tert-butyl-5-nitrophenyl methyl carbonate | CC(C)(C)C1=CC(=C(C=C1[N+](=O)[O-])OC(=O)OC)C(C)(C)C | 309.15762 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N-Acetylsulfapyridin | CC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=CC=N2 | 291.06776 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methyl 4-cyano-4-((4-fluorophenyl)amino)piperidine-1-carboxylate | COC(=O)N1CCC(CC1)(C#N)NC2=CC=C(C=C2)F | 277.12266 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-Methyldodecanonitrile | CCCCCCCCCC(C)CC#N | 195.19870 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Aleuritic acid | C(CCCC(C(CCCCCCO)O)O)CCCC(=O)O | 304.22497 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (1alpha,2beta,5alpha)-5-Methyl-2-(1-methylethyl)cyclohexyl (R)-N-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-beta-alaninate | CC1CCC(C(C1)OC(=O)CCNC(=O)C(C(C)(C)CO)O)C(C)C | 357.25152 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (1alpha,2beta,5alpha)-5-Methyl-2-(1-methylethyl)cyclohexyl (R)-N-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-beta-alaninate | CC1CCC(C(C1)OC(=O)CCNC(=O)C(C(C)(C)CO)O)C(C)C | 357.25152 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,4:3,6-Dianhydro-D-glucitol monostearate | CCCCCCCCCCCCCCCCCC(=O)OC1O[C@@H]2[C@H](O)CO[C@@H]2[C@H]1O | 412.31888 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1-(2,3-dihydro-1,3,3,6-tetramethyl-1-(1-methylethyl)-1H-inden-5-yl)ethanone | CC(C)C1(C)CC(C)(C)C2=CC(C(C)=O)=C(C)C=C12 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,2,3,3,4,4,5,5-octafluorovaleric acid (EINECS) | C(C(C(C(C(=O)O)(F)F)(F)F)(F)F)(F)F | 245.99271 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate | CC1(COC(=O)C2CC=CCC2C(=O)OC1)C | 238.12051 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,3,5,6,8,9,11,12,14,15-Decahydro-4,13-(ethanoxyethanoxyethano)-4H,13H-1,7,10,16,4,13-benzotetraoxadiazacyclooctadecine | C1COCCOCCN2CCOCCOCCN1CCOC3=CC=CC=C3OCC2 | 424.25734 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,4,6,8-Tetranitro-2,4,6,8-tetraazanonane-1,9-diyl diacetate | CC(=O)OCN(CN(CN(CN(COC(=O)C)[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-] | 428.08877 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,5-bis(1,1-dimethylbutyl)hydroquinone | CCCC(C)(C)C1=CC(O)=C(C=C1O)C(C)(C)CCC | 278.22458 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,6-Dihydroxyethylaminotoluene | CC1=C(NCCO)C=CC=C1NCCO | 210.13683 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-(2-(2-(2-Phenoxyethoxy)ethoxy)ethoxy)ethanol | OCCOCCOCCOCCOC1=CC=CC=C1 | 270.14672 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-(2-(4-Nonylphenoxy)ethoxy)acetic acid (NPE2C) | CCCCCCCCCC1=CC=C(C=C1)OCCOCC(=O)O | 322.21441 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-(Methylthio)benzothiazol | CSC1=NC2=CC=CC=C2S1 | 181.00199 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-hydroxy-10-undecenoic acid | C=CCCCCCCCC(C(=O)O)O | 200.14124 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-phenyl ethyl propionate | CCOC(=O)C(C)C1=CC=CC=C1 | 178.09938 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-phenyl-2-imidazoline | C1CN=C(N1)C1=CC=CC=C1 | 146.08440 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-piperidin-2-ylethanol | OCCC1CCCCN1 | 129.11536 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3'H-Cycloprop[15,16]androsta-6,15-dien-17-one, 3-(2,2-dimethyl-1-oxopropoxy)-15,16-dihydro-5-hydroxy-, (3ß,5ß,15a,16a)- |  | 400.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-Methyl-1-(4-methylphenyl)-1H-pyrazol-5-amine | CC1=NN(C(N)=C1)C1=CC=C(C)C=C1 | 187.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4,4'-(4-iminocyclohexa-2,5-dienylidenemethylene)dianiline | NC1=CC=C(C=C1)C(C1=CC=C(N)C=C1)=C1C=CC(=N)C=C1 | 287.14225 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 7-ethoxyacridine-3,9-diamine | CCOC1=CC2=C(N)C3=CC=C(N)C=C3N=C2C=C1 | 253.12151 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Acriflavinium |  | 209.09530 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Benzamide, 4-amino-N-(3-aminophenyl)- | NC1=CC=C(C=C1)C(=O)NC1=CC(N)=CC=C1 | 227.10586 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Benzenediazonium, 3-methoxy-4-(1-pyrrolidinyl)-, tetrafluoroborate(1-) |  | 204.11369 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Bromhexine | CN(CC1=CC(Br)=CC(Br)=C1N)C1CCCCC1 | 373.99933 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| CP 47,497-C8 homolog |  | 332.27153 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| cyclododecanol | OC1CCCCCCCCCCC1 | 184.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Cytochalasin B | C[C@H]1[C@H]2[C@H](CC3=CC=CC=C3)NC(=O)[C@]22OC(=O)\C=C\[C@H](O)CCC[C@@H](C)C\C=C\[C@H]2[C@H](O)C1=C | 479.26717 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Diethyl (2-(phenylthio)ethyl)malonate | CCOC(=O)C(CCSC1=CC=CC=C1)C(=O)OCC | 296.10823 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Dimethyl 4,4'-(1,6-hexanediylbis(iminocarbonyl))bisbenzoate | COC(=O)C1=CC=C(C=C1)C(=O)NCCCCCCNC(=O)C2=CC=C(C=C2)C(=O)OC | 440.19474 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Dioctylmaleate | CCCCCCCCOC(=O)C=CC(=O)OCCCCCCCC | 340.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ecgonine-methyl-ester (EME) | CN1C2CCC1C(C(C2)O)C(=O)OC | 199.12084 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| echothiopate |  | 256.11363 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ethyl hexahydro-1H-azepine-1-propionate | CCOC(=O)CCC1CCCCCN1 | 199.15723 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Gibberellin A7 | C[C@@]12[C@H]3[C@H](C(O)=O)[C@@]45C[C@@H](CC[C@H]4[C@]3(OC1=O)C=C[C@@H]2O)C(=C)C5 | 330.14672 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Glycine, N-[2-(carboxymethoxy)ethyl]-N-[2-[(1-oxododecyl)amino]ethyl]-, disodium salt | CCCCCCCCCCCC(=O)NCCN(CCOCC(=O)[O-])CC(=O)[O-].[Na+].[Na+] | 446.23688 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ibuprofen-methylester | CC(C)CC1=CC=C(C=C1)C(C)C(=O)OC | 220.14633 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methyl (3alpha,5beta,6alpha)-3,6-dihydroxycholan-24-oate |  | 406.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| methyl 5-(dimethylamino)-2-methyl-5-oxopentanoate | COC(=O)C(C)CCC(=O)N(C)C | 187.12084 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N-Stearylbenzylamine | CCCCCCCCCCCCCCCCCCNCC1=CC=CC=C1 | 359.35520 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Nobiletin | COC1=CC=C(C=C1OC)C1=CC(=O)C2=C(OC)C(OC)=C(OC)C(OC)=C2O1 | 402.13147 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Nonyl 3,4,5-trihydroxybenzoate | CCCCCCCCCOC(=O)C1=CC(O)=C(O)C(O)=C1 | 296.16237 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Palmitic acid, diester with 5-hydroxy-6-methylpyridine-3,4-dimethanol | CCCCCCCCCCCCCCCC(=O)OCC1=CN=C(C(=C1COC(=O)CCCCCCCCCCCCCCC)O)C | 645.53322 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| PEG-12 |  | 546.32515 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ramipril | CCOC(=O)[C@H](CCC1=CC=CC=C1)N[C@@H](C)C(=O)N1[C@H]2CCC[C@H]2C[C@H]1C(O)=O | 416.23112 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Rimexolone | CCC(=O)[C@@]1(C)[C@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@]12C | 370.25080 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Streptolin | C1C(C2C(C(=O)N1)N=C(N2)NC3C(C(C(C(O3)CO)OC(=O)N)O)NC(=O)CC(CCCNC(=O)CC(CCCN)N)N)O | 630.34492 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Tangeritin | COC1=CC=C(C=C1)C1=CC(=O)C2=C(OC)C(OC)=C(OC)C(OC)=C2O1 | 372.12090 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| TBEP (Tris(2-butoxyethyl) Phosphate) | CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC | 398.24334 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Terbutaline | CC(C)(C)NCC(O)C1=CC(O)=CC(O)=C1 | 225.13649 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Testosterone 17-Phenylpropionate | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2OC(=O)CCC1=CC=CC=C1 | 420.26645 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Tofisopam | CCC1C2=CC(OC)=C(OC)C=C2C(=NN=C1C)C1=CC=C(OC)C(OC)=C1 | 382.18926 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| trans-2-isopropyl-5-carboxy-1,3-dioxane | CC(C)C1OCC(CO1)C(=O)O | 174.08921 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Tricyclohexylmethanol | OC(C1CCCCC1)(C1CCCCC1)C1CCCCC1 | 278.26097 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| artemether | CO[C@H]1O[C@@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3 | 298.17802 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-hydroxybenzaldehyde | OC1=CC=C(C=O)C=C1 | 122.03678 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Telbivudine | CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)O | 242.09027 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (1R)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-ethanol | CC1(C)C2C[C@H]1C(CCO)=CC2 | 166.13577 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (1S,4R,6R)-1-[(3E)-5-Hydroxy-3-methylpent-3-en-1-yn-1-yl]-2,2,6-trimethylcyclohexane-1,4-diole |  | 252.17255 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (3R,3aR,6S,6aR)-hexahydrofuro[3,2-b]furan-3,6-diyl dioctanoate | CCCCCCCC(=O)OC1COC2C1OCC2OC(=O)CCCCCCC | 398.26684 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (R,Z)-5-(1-decenyl) dihydro-2(3H) furanone = Japonilure | CCCCCCCC\C=C/[C@H]1CCC(=O)O1 | 224.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,2,3,4,4a,7,8,8a-Octahydro-2,4a,5,8a-tetramethyl-1-naphthyl Formate. |  | 236.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,4-dioxacyclohexadecane-5,16-dione | O=C1CCCCCCCCCCC(=O)OCCO1 | 256.16746 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1-((1-Hydroperoxymethylcyclohexyl)dioxy)methylcyclohexan-1-ol | C1CCC(CC1)(COOC2(CCCCC2)COO)O | 274.17802 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,4,5-Triphenylimidazole | N1C(=NC(=C1C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1 | 296.13135 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-chloro-5-sec-hexadecylhydroquinone | CCCCCCCCCCCCCCC(C)C1=CC(O)=C(Cl)C=C1O | 368.24821 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3(or 4)-(4-Methylpenten-3-yl)cyclohex-3-ene-1-methyl Acetate. | - | 236.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,11-bis(prop-2-ynoxy)undecane | C#CCOCCCCCCCCCCCOCC#C | 264.20893 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1- enyl)cyclopropanecarboxylate | CC=CCC1=C(C)C(CC1=O)OC(=O)C1C(C=C(C)C)C1(C)C | 316.20384 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-Pregnen-20b-ol-3-one, 20b-Hydroxyprogesterone | C[C@H]([C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CCC4=CC(=O)CC[C@]34C)C)O | 316.24023 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1-O-(2R-Methoxy-4Z-tetradecenyl)-sn-glycerol | CCCCCCCCC/C=C\\C[C@H](COC[C@H](CO)O)OC | 316.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Cambendazole | CC(C)OC(=O)NC1=CC2=C(C=C1)N=C(N2)C3=CSC=N3 | 302.08375 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Arfendazam | CCOC(=O)N1CCC(=O)N(C2=CC=CC=C2)C2=CC(Cl)=CC=C12 | 344.09277 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3,9-dimethyl-2,4,8,10-tetraoxaspiro[5.5]undecane | CC1OCC2(CO1)COC(OC2)C | 188.10486 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 18-Sulfooleic acid | C(CCCCS(=O)(=O)O)CCCC=CCCCCCCCC(=O)O | 228.08202 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (9Z)-17-carboxy-9-heptadecene-1-sulfonic acid | C(CCCCS(=O)(=O)O)CCC/C=C\\CCCCCCCC(=O)O | 362.21270 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Bis(2-phenylvinyl)phenol | C1=CC=C(C=C1)C=CC2=C(C(=CC=C2)O)C=CC3=CC=CC=C3 | 298.13577 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Decyl 3-mercaptopropionate | CCCCCCCCCCOC(=O)CCS | 246.16535 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| dibutyl 2,2'-thiobisacetate | CCCCOC(=O)CSCC(=O)OCCCC | 262.12380 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-Octadec-9-enoxy-4-oxobut-2-enoic acid | CCCCCCCCC=CCCCCCCCCOC(=O)C=CC(=O)O | 366.27701 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1-Cyclohexene-1-ethanol, 4-(formyloxy)-4-(1-methylethyl)-, formate | CC(C)C1(CCC(=CC1)CCOC=O)OC=O | 240.13616 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Malonic acid, tetradecyl- | CCCCCCCCCCCCCCC(C(=O)O)C(=O)O | 300.23006 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| ditetradecyl fumarate | CCCCCCCCCCCCCCOC(=O)\C=C\C(=O)OCCCCCCCCCCCCCC | 508.44916 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Metazachlor | CC1=C(C(=CC=C1)C)N(CN2C=CC=N2)C(=O)CCl | 277.09819 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Ethyl 5,5,7-Trimethyl-1-oxaspiro(2.5)octane-2-carboxylate. | CCOC(=O)C1C2(O1)CC(CC(C2)(C)C)C | 226.15690 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Lauryl stearyl 3,3'-thiodipropionate | CCCCCCCCCCCCCCCCCCS(CCCCCCCCCCCC)(CCC([O-])=O)CCC([O-])=O | 598.50058 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Loxoprofen alcohol | CC(C1=CC=C(C=C1)CC2CCCC2O)C(=O)O | 248.14124 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| alpha-Oxothiophen-2-acetonitrile | C1=CSC(=C1)C(=O)C#N | 136.99354 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-Amino-6,7-dimethylpteridin-4-ol | CC1=NC2=NC(N)=NC(O)=C2N=C1C | 191.08071 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Decylthioacetic acid | CCCCCCCCCCSCC(=O)O | 232.14970 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Florfenicol amine | CS(=O)(=O)C1=CC=C(C=C1)C(C(CF)N)O | 247.06784 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Chlorpheniramine, Desmethyl |  | 260.10803 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Imolamine | CCN(CC)CCN1C(=N)ON=C1C1=CC=CC=C1 | 260.16371 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2,3-Dihydroxypropyl 3-(hexylthio)propionate | CCCCCCSCCC(=O)OCC(O)CO | 264.13953 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Olanzapine, N-desmethyl | CC1=CC2=C(S1)NC3=CC=CC=C3N=C2N4CCNCC4 | 298.12522 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Chlorcyclizine | CN1CCN(CC1)C(C1=CC=CC=C1)C1=CC=C(Cl)C=C1 | 300.13933 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Oxazolam | C[C@@H]1CN2CC(=O)NC3=CC=C(Cl)C=C3[C@@]2(O1)C1=CC=CC=C1 | 328.09786 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| sulfapyrazole | CC1=NN(C(NS(=O)(=O)C2=CC=C(N)C=C2)=C1)C1=CC=CC=C1 | 328.09940 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| MEGESTROL | CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C=C(C)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methandienone | C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3CC[C@]12C | 300.20893 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methyl 2-[(aminosulfonyl)methyl]benzoate | COC(=O)C1=C(CS(N)(=O)=O)C=CC=C1 | 229.04088 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N-benzyl-2-bromo-3-methoxypropanamide | COCC(Br)C(=O)NCC1=CC=CC=C1 | 271.02079 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N-methyltoluene-4-sulphonamide | CNS(=O)(=O)C1=CC=C(C)C=C1 | 185.05105 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Oct-1-ene-3-ol | CCCCCC(O)C=C | 128.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| PEG-2 LAURATE | CCCCCCCCCCCC(=O)OCCOCCO | 288.23006 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| retinyl propionate | CCC(=O)OC\C=C(/C)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C | 342.25588 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Sodium 2-(nonanoyloxy)benzenesulfonate | CCCCCCCCC(=O)OC1=CC=CC=C1S(=O)(=O)[O-].[Na+] | 314.11880 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3,9-dimethyl-2,4,8,10-tetraoxaspiro[5.5]undecane | CC1OCC2(CO1)COC(OC2)C | 188.10486 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Tenatoprazole | COC1=CC=C2NC(=NC2=N1)S(=O)CC1=NC=C(C)C(OC)=C1C | 346.10996 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Thiamine thiazolone | CC1=C(SC(=O)N1CC2=CN=C(N=C2N)C)CCO | 280.09940 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Torsemide | CC(C)NC(=O)NS(=O)(=O)C1=CN=CC=C1NC1=CC=CC(C)=C1 | 348.12561 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-(Furfurylthio)ethylamine | NCCSCC1=CC=CO1 | 157.05614 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Lauroyl 2-methyl isethionate | CCCCCCCCCCCC(=O)OC(C)CS(=O)(=O)O | 256.20384 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,5-Pentanediyl diacrylate | C=CC(=O)OCCCCCOC(=O)C=C | 212.10486 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| DIMYRISTYL THIODIPROPIONATE | CCCCCCCCCCCCCCOC(=O)CCSCCC(=O)OCCCCCCCCCCCCCC | 570.46818 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| methyl 12-hydroxyoctadec-9-enoate | CCCCCCC(CC=CCCCCCCCC(=O)OC)O | 312.26645 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (-)-2,7-Dolabelladiene-6beta,10alpha,18-triol | C[C@@H]\\1C[C@H](/C=C(/C[C@@H]([C@H]2[C@@H](CC[C@@]2(/C=C1)C)C(C)(C)O)O)\\C)O | 322.25080 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 30-Methyl-2,5,8,11,14,17,20,23,26,29-decaoxahentriacontane | COCCOCCOCCOCCOCCOCCOCCOCCOCCOC(C)C | 470.30910 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-hydroxy-10-undecenoic acid | C=CCCCCCCCC(C(=O)O)O | 200.14124 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 7-methylocta-1,6-diene | CC(C)=CCCCC=C | 124.12520 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-Mercaptoethyl nonanoate | CCCCCCCCC(=O)OCCS | 218.13405 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| diethyl dipropylmalonate | CCCC(CCC)(C(=O)OCC)C(=O)OCC | 244.16746 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| decan-4-olide | CCCCCCC1CCC(=O)O1 | 170.13068 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | N#CC1=CC=C(C=CC2=CC=C(C=CC3=CC=CC(=C3)C#N)C=C2)C=C1 | 332.13135 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3,5,5-trimethylcyclohex-3-en-1-one | CC1=CC(C)(C)CC(=O)C1 | 138.10447 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-(ethoxymethyl)-2-methoxyphenol | CCOCC1=CC(OC)=C(O)C=C1 | 182.09429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 6-cyclohexyl-4-methyl-2H-pyran-2-one | CC1=CC(=O)OC(=C1)C1CCCCC1 | 192.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 6-tert-butyl-m-cresol | CC1=CC=C(C(O)=C1)C(C)(C)C | 164.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 7-Butyloxepan-2-one | CCCCC1CCCCC(=O)O1 | 170.13068 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Carbaprostacyclin | CCCCCC(C=CC1C(CC2C1CC(=CCCCC(=O)O)C2)O)O | 350.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Halofenozide | CC(C)(C)N(NC(=O)C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1 | 330.11351 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-((3,4-Dimethoxyphenyl)methylene)-6-methylcyclohexanol | CC1CCC/C(=C\\C2=CC(=C(C=C2)OC)OC)/C1O | 262.15689 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| isooctyl acrylate | CC(C)CCCCCOC(=O)C=C | 184.14633 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methyl-iso-propylcyclohexenone, Carvone |  | 150.10447 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1-[(2-tert-butylcyclohexyl)oxy]butan-2-ol | CCC(O)COC1CCCCC1C(C)(C)C | 228.20893 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate. |  | 292.24023 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methyl (cyclohexyloxy)acetate | COC(=O)COC1CCCCC1 | 172.10994 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Mixture of (E)-Oxacyclohexadec-12-en-2-one, (E)-Oxacyclohexadec-13-en-2-one, (Z)-Oxacyclohexadec-(12)-en-2-one and (Z)-Oxacyclohexadec-(13)-en-2-one |  | 238.19328 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Cytochalasin D | C[C@H]1[C@H]2[C@H](CC3=CC=CC=C3)NC(=O)[C@@]22[C@@H](\C=C\C[C@H](C)C(=O)[C@](C)(O)\C=C\[C@H]2OC(C)=O)[C@H](O)C1=C | 507.26209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| isodecyl acrylate | CC(C)CCCCCCCOC(=O)C=C | 212.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| N4-(2-Hydrazino-2-oxoethyl)-2,1,3-benzothiadiazole-4-sulfonamide | NNC(=O)CNS(=O)(=O)C1=CC=CC2=NSN=C12 | 287.01468 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Oct-1-ene-3-ol | CCCCCC(O)C=C | 128.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Octahydro-7,7,8,8-tetramethyl-2,3b-methano-3bHcyclopenta |  | 262.19328 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Dinordeoxycholic acid | C[C@@H]([C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C)C(=O)O | 364.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Prostaglandin F2&#945; 1-11-lactone |  | 336.23006 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| DL-menthol | CC1CCC(C(C1)O)C(C)C | 156.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Methoxycyclododecane |  | 198.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-(2-{4-[2-(4-cyanophenyl)vinyl]phenyl}vinyl)benzonitrile | C1=CC(=CC(=C1)C#N)C=CC2=CC=C(C=C2)C=CC3=CC=C(C=C3)C#N | 332.13135 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1-Dodecanesulfonamide, N-(4-methylphenyl)- | CCCCCCCCCCCCS(=O)(=O)NC1=CC=C(C)C=C1 | 339.22320 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-Ketoapotrichothecene | CC1=CC2C(CC1)(C3(CC(=O)CC3(O2)CO)C)C | 250.15690 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran. |  | 150.10447 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-Hexylphenol | CCCCCCC1=CC=C(O)C=C1 | 178.13577 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 6,10-Dimethylundecen-2-one |  | 196.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 3-Butylphthalide | CCCCC1C2=CC=CC=C2C(=O)O1 | 190.09938 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Octadecanoic acid, 3-oxo-, ethyl ester | CCCCCCCCCCCCCCCC(=O)CC(=O)OCC | 326.28210 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| tris(butylsulfanyl)phosphane | CCCCSP(SCCCC)SCCCC | 298.10125 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (E,E)-8,10-Dodecadien-1ol | C\C=C\C=C\CCCCCCCO | 182.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| methylcyclohexane | CC1CCCCC1 | 98.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (2,2-Bis(undecyloxy)ethyl)benzene | CCCCCCCCCCCOC(CC1=CC=CC=C1)OCCCCCCCCCCC | 446.41238 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (2E,4E)-4-(3,5-Dimethyl-1,3,4-oxadiazol-2(3H)-ylidene)-2-(pyrrolidine-1-carbothioyl)but-2-enenitrile | CN1N=C(C)O\C1=C\C=C(/C#N)C(=S)N1CCCC1 | 276.10448 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| (E)-2-benzylideneoctanal, alpha-Hexyl Cinnamic Aldehyde, (2E)-2-(phenylmethylidene)octanal |  | 216.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 1,2,4-Benzenetricarboxylic acid, decyl octyl ester |  | 602.45464 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-(Dodecane-1-sulfonyl)acetamide | CCCCCCCCCCCCS(=O)(=O)CC(N)=O | 291.18682 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-Amino-6,7-dimethylpteridin-4-ol | CC1=NC2=NC(N)=NC(O)=C2N=C1C | 191.08071 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-Naphthylmyristate | CCCCCCCCCCCCCC(=O)OC1=CC2=CC=CC=C2C=C1 | 354.25588 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 2-Thiocyanatoethyl dodecanoate | CCCCCCCCCCCC(=O)OCCSC#N | 285.17625 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-(2,4,4-trimethylpentylcarbonyloxy)benzenesulfonic acid | CC(CC(=O)OC1=CC=C(C=C1)S(O)(=O)=O)CC(C)(C)C | 314.11880 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-(2,4,4-trimethylpentylcarbonyloxy)benzenesulfonic acid | CC(CC(=O)OC1=CC=C(C=C1)S(O)(=O)=O)CC(C)(C)C | 314.11880 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 4-methyl-4-(methylthio)pentan-2-one | CSC(C)(C)CC(C)=O | 146.07654 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 6,6'-(2-Methylpropane-1,3-diyl)di(1,3,5-triazine-2,4-diamine) | CC(CC1=NC(N)=NC(N)=N1)CC1=NC(N)=NC(N)=N1 | 276.15594 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Alpha-Ergocryptine | CC(C)C[C@@H]1N2C(=O)[C@](NC(=O)[C@H]3CN(C)[C@@H]4CC5=CNC6=CC=CC(=C56)C4=C3)(O[C@@]2(O)[C@@H]2CCCN2C1=O)C(C)C | 575.31077 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Cytochalasin D | C[C@H]1[C@H]2[C@H](CC3=CC=CC=C3)NC(=O)[C@@]22[C@@H](\C=C\C[C@H](C)C(=O)[C@](C)(O)\C=C\[C@H]2OC(C)=O)[C@H](O)C1=C | 507.26209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Dibutyl Succinate | CCCCOC(=O)CCC(=O)OCCCC | 230.15181 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| diethyl dipropylmalonate | CCCC(CCC)(C(=O)OCC)C(=O)OCC | 244.16746 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Exo-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol | CC1(C)C2CCC1(C)C(O)C2 | 154.13577 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Perindopril | CCC[C@H](N[C@@H](C)C(=O)N1[C@H]2CCCC[C@H]2C[C@H]1C(O)=O)C(=O)OCC | 368.23112 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Octadecanoic acid, [[4,6-bis[bis(methoxymethyl)amino]-1,3,5-triazin-2-yl](methoxymethyl)amino]methyl ester | CCCCCCCCCCCCCCCCCC(=O)OCN(COC)C1=NC(=NC(=N1)N(COC)COC)N(COC)COC | 642.46800 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Phosphorothioic acid, O,O-bis(2-methylpropyl) ester, sodium salt | CC(C)COP(=S)([O-])OCC(C)C.[Na+] | 226.07926 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| Lovastatin | CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12 | 404.25627 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | K |
| 19-Norandrostenedione | CC12CCC3C(C1CCC2=O)CCC4=CC(=O)CCC34 | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Galaxolidone | CC2(C)c1cc3C(=O)OCC(C)c3cc1C(C)(C)C2C | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17alpha-Estradiol | C[C@]12CC[C@H]3[C@@H](CCC4=C3C=CC(O)=C4)[C@@H]1CC[C@H]2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17b-hydroxyestra-4,6-diene-3-one;d6n;delta-6-nandrolone;6-dehydronandrolone;17-hydroxyestra-4,6-dien-3-one;4,6-estradien-17beta-ol-3-one;17b-hydroxyestra-4,6-diene-3-one d6n delta-6-nandrolone 6-dehydronandrolone 17-hydroxyestra-4,6-dien-3-one 4,6-estradien-17beta-ol-3-one | CC12CCC3C4CCC(=O)C=C4C=CC3C1CCC2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl phenylacetate | O=C(OC1CC2CCC1(C)C2(C)C)CC=3C=CC=CC3 | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl phenylacetate | O=C(OC(C)(C)C1CC=C(C)CC1)CC=2C=CC=CC2 | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Oestr-5(10)-ene-3,17-dione | O=C1CC2=C(CC1)C3CCC4(C(=O)CCC4C3CC2)C | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (1E)-2,6-Dimethylhepta-1,5-dien-1-yl phenylacetate | CC(C)=CCC/C(C)=C/COC(=O)Cc1ccccc1 | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17B-hydroxyestra-4,6-diene-3-one | C[C@]12CC[C@@H]3[C@H]4CCC(=O)C=C4C=C[C@H]3[C@@H]1CC[C@@H]2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| estr-4-ene-3,17-dione | C[C@]12CC[C@H]3[C@H]([C@@H]1CCC2=O)CCC4=CC(=O)CC[C@H]34 | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17beta-Estradiol | [H][C@@]12CC[C@H](O)[C@@]1(C)CC[C@]1([H])C3=CC=C(O)C=C3CC[C@@]21[H] | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9,10-Dehydro-19-nortestosterone | CC12CCC3=C4CCC(=O)C=C4CCC3C1CCC2O | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Estr-5-ene-3,17-dione | O=C1CC2=CCC3C(CCC4(C(=O)CCC34)C)C2CC1 | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzeneacetic acid, 1-ethenyl-1,5-dimethyl-4-hexen-1-yl ester | CC(C)=CCCC(C)(OC(=O)Cc1ccccc1)C=C | 272.17763 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cholest-4-en-3-one | CC(C)CCCC(C)C2CCC1C3CCC4=CC(=O)CCC4(C)C3CCC12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-a-cholesta-8,24-dien-3-ß-ol | OC1CCC2(C3=C(CCC2C1)C4CCC(C(C)CCC=C(C)C)C4(C)CC3)C | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cholest-5-en-3-one | CC(C)CCCC(C)C1CCC2C3CC=C4CC(=O)CCC4(C)C3CCC12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cholesta-4,6-diene-3ß-ol | OC1C=C2C=CC3C(CCC4(C)C3CCC4C(C)CCCC(C)C)C2(C)CC1 | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Desmosterol | C[C@H](CCC=C(C)C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (3ß,6Z)-9,10-secocholesta-5(10),6,8-trien-3-ol | OC1CC(C=CC2=CCCC3(C)C2CCC3C(C)CCCC(C)C)=C(C)CC1 | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Vitamin D3 | CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2C(CCC[C@]12C)=CC=C1/C[C@@H](O)CCC1=C | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 7,8-Didehydrocholesterol | CC(C)CCCC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC12C | 384.33922 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1,2,3,5,6,7-hexahydrotetramethyl-s-indacenyl)ethanone | O=C(C)C1(C2=CC3=C(C=C2C(C)C1(C)C)CCC3)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-Bis(1,1-dimethylethyl)-2-naphthol | CC(C)(C)c1cc2c(cccc2)c(c1O)C(C)(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,4,5,6,7,8-Hexahydro-5,5,8,8-tetramethylanthracen-1(2H)-one | CC1(C)CCC(C)(C)c2cc3c(CCCC3=O)cc12 | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Octyl-2-naphthol | CCCCCCCCc1c(O)ccc2c1cccc2 | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Buten-1-one, 1-(2,3-dihydro-1,1,3,3,6-pentamethyl-1H-inden-5-yl)- | C/C=C/C(=O)c1c(C)cc2c(c1)C(C)(C)CC2(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| as-Indacen-3(2H)-one, 1,6,7,8-tetrahydro-1,4,6,6,8,8-hexamethyl- | CC1CC(=O)c2c(C)cc3c(c12)C(C)(C)CC3(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,5,6,7-tetrahydro-3,5,5,6,7,7-hexamethyl-s-indacen-1(2H)-one | O=C1C=2C=C3C(=CC2C(C)C1)C(C)(C)C(C)C3(C)C | 256.18272 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Etc-588 | CCCCCCCC/C=CCCCCCCCC(=O)OC[C@H](CO[P@](=O)(O)OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC | 760.58563 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Nonenoic acid | CCCCC/C=C/CC(=O)O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Prenyl isobutyrate | CC(C)C(=O)OCC=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4,6-Nonanedione | CCCC(=O)CC(=O)CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Nonenoic acid | CCCCCC/C=CC(=O)O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,3-Diethylpentane-2,4-dione | CCC(CC)(C(=O)C)C(=O)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Butylpentane-2,4-dione | CCCCC(C(=O)C)C(=O)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,7-Dioxaspiro[5.5]undecane | C1CCC2(CCCCO2)OC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| tert-Butyl 3-methyl-2-butenoate | CC(=CC(=O)OC(C)(C)C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Neopentyl methacrylate | CC(=C)C(=O)OCC(C)(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2-Dimethyl-1,3-bis(vinyloxy)propane | CC(C)(COC=C)COC=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Pentenoic acid, 3,3-dimethyl-, ethyl ester | CCOC(=O)CC(C)(C)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl trans-2-methylcyclohexanecarboxylate | COC(=O)[C@@H]1CCCC[C@H]1C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isopentyl methacrylate | CC(C)CCOC(=O)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Prenyl butyrate | CCCC(=O)OCC=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Butanoic acid, 2-methylene-, 2-methylpropyl ester | CCC(=C)C(=O)OCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclopentyl isobutyrate | CC(C)C(=O)OC1CCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclopentyl butyrate | CCCC(=O)OC1CCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Nonane-2,4-dione | CCCCCC(=O)CC(=O)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Butyl 3-methyl-2-butenoate | CCCCOC(=O)C=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Methylpentyl acrylate | CC(C)CCCOC(=O)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Propene, 3,3'-[(1-methylethylidene)bis(oxy)]bis- | CC(C)(OCC=C)OCC=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Oxononan-1-al | CCCCCC(=O)CCC=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclohexyl propionate | CCC(=O)OC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| cis-4-methylcyclohexyl acetate | O=C(OC1CCC(C)CC1)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-cyclohexylpropionic acid | O=C(O)C(C)C1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1-methoxyisopropoxy)pent-2-yne | C(#CCC)COC(OC)(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methoxy-2-methylhept-4-yn-3-ol | OC(C#CCC)C(OC)(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1-ethoxyethoxy)pent-2-yne | C(#CCC)COC(OCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-methylpent-3-en-1-yl propionate | O=C(OCCC(=CC)C)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(hydroxymethyl)-6-methylhept-5-en-2-one | O=C(C)C(CO)CC=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methylallyl 2-methylbutyrate | O=C(OCC(=C)C)C(C)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-methyl-2-(1-methyl-1-butenyl)-1,3-dioxolane | O1CC(OC1C(=CCC)C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (Z)-1-methylhex-3-enyl acetate | O=C(OC(C)CC=CCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (E)-4-methyl-2-(pent-1-enyl)-1,3-dioxolane | O1CC(OC1C=CCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-methylbutyl methacrylate | O=C(OC(C)CCC)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| But-2-enyl 2-methylbutyrate | O=C(OCC=CC)C(C)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Isopropyl-5-oxohexanal | CC(C)C(CCC(C)=O)C=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-Methyl-3-propan-2-yloxan-2-one | CC1CCC(C(=O)O1)C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclohexanecarboxylic acid, 3-methyl-, methyl ester, (1R,3S)-rel- | COC(=O)C1CCCC(C)C1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(cyclohexyloxy)acetone | O=C(C)COC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Allyl hexanoate | CCCCCC(=O)OCC=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclohexanepropionic acid | OC(=O)CCC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methylcyclohexyl acetate | CC1CCCCC1OC(C)=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methylcyclohexylacetate | COC(=O)CC1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| gamma-Nonanolactone | [C@H]1(OC(CC1)=O)CCCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (2Z)-3-Methyl-4-methylideneoct-2-ene | CCCCOC(=O)C(/C)=CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (Z)-Hept-3-enyl Acetate. | CCC/C=C/CCOC(C)=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (3Z)-Hex-3-en-1-yl propanoate | CCC=C/CCOC(=O)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclohexanecarboxylic acid, ethyl ester | CCOC(=O)C1CCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Octenoic acid, methyl ester | CCCCC/C=C/C(=O)OC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Hexen-1-ol, 1-propanoate, (2E)- | CCC/C=C/COC(=O)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Methylbutyl 2-Butenoate. | C/C=C/C(=O)OCCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Butenoic acid, 2-methyl-, 2-methylpropyl ester, (2E)- | CC=C(/C)C(=O)OCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2(3H)-Furanone, 5-butyldihydro-4-methyl- | CCCCC1OC(=O)CC1C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2H-Pyran-2-one, 6-butyltetrahydro- | CCCCC1CCCC(=O)O1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (4R,6R)-4-Hydroxy-2,2,6-trimethylcyclohexanone / 60046-50-6 | CC1CC(O)CC(C)(C)C1=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| g-Nonalactone | CCCCCC1CCC(O1)=O | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dihydro-3-(3-methylbutyl)furan-2(3H)-one | O=C1OCCC1CCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hept-1-enyl acetate | O=C(OC=CCCCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methyl-1,4-dioxaspiro[4.5]decane | O1CC(OC12CCCCC2)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| trans-2-pentylcyclopropanecarboxylic acid | O=C(O)C1CC1CCCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4,6,6-trimethyloxepan-2-one | O=C1OCC(C)(C)CC(C)C1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Allyl 2-ethylbutyrate | O=C(OCC=C)C(CC)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methylpentyl acrylate | O=C(OCC(C)CCC)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-methyloctan-4-olide | O=C1OC(C)(CC1)CCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [(cyclohexyloxy)methyl]oxirane | O1CC1COC2CCCCC2 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-ethylbutyl acrylate | O=C(OCC(CC)CC)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl 5-methylhex-2-enoate | O=C(OCC)C=CCC(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methylcyclohexyl acetate | O=C(OC1(C)CCCCC1)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Pentyl 2-butenoate | O=C(OCCCCC)C=CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl (Z)-oct-4-enoate | O=C(OC)CCC=CCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(tetrahydro-4-methyl-2H-pyran-2-yl)acetone | O=C(C)CC1OCCC(C)C1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hexyl acrylate | CCCCCCOC(=O)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-vinylpentyl acetate | O=C(OC(C=C)CCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclooctyl formate | O=COC1CCCCCCC1 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-dimethylbutyl acrylate | O=C(OC(C)CC(C)C)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bicyclo[2.2.1]heptane-2,2-dimethanol | OCC1(CO)CC2CCC1C2 | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Propyl (E)-hex-2-enoate | O=C(OCCC)C=CCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(1-ethoxyethoxy)pent-1-yne | C#CCCCOC(OCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (E)-hept-2-enyl acetate | O=C(OCC=CCCCC)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 7,7-dimethoxyhept-3-yne | C(#CCCC(OC)OC)CC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methylbutyl methacrylate | O=C(OCC(C)CC)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,3,5-trimethyloxepan-2-one | O=C1OCCC(C)CC1(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl (E)oct-3-enoate | O=C(OC)CC=CCCCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-methyl-2-(2-methyl-1-propenyl)-1,3-dioxane | O1CCC(OC1C=C(C)C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-methylpentyl acrylate | O=C(OC(C)CCCC)C=C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (Z)-pent-2-enyl butyrate | O=C(OCC=CCC)CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (Z)-non-6-enoic acid | O=C(O)CCCCC=CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl (E)-hept-4-enoate | O=C(OCC)CCC=CCC | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-dimethylheptane-3,5-dione | O=C(CC(=O)C(C)C)C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Pentenoic acid, 2,4-dimethyl-, ethyl ester, (2E)- | CCOC(=O)/C(=C/C(C)C)/C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Pentyl methacrylate | CCCCCOC(=O)C(=C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isobutyl 3-methyl-2-butenoate | CC(C)COC(=O)C=C(C)C | 156.11503 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2'-Bipyrimidine | c1cnc(nc1)c1ncccn1 | 158.05925 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Chlorophthalic anhydride | Clc1ccc2C(=O)OC(=O)c2c1 | 181.97707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Chlorophthalic anhydride | Clc1cccc2C(=O)OC(=O)c12 | 181.97707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-(3-hydroxypropyl)stearamide | O=C(NCCCO)CCCCCCCCCCCCCCCCC | 341.32938 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Sodium N-octadecyl-ß-alaninate | [Na+].O=C([O-])CCNCCCCCCCCCCCCCCCCCC | 341.32938 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Octadecanamide, N-(2-hydroxypropyl)- | CCCCCCCCCCCCCCCCCC(=O)NCC(C)O | 341.32938 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dioleoyl phthalate | O=C(OC(=O)CCCCCCCC=CCCCCCCCC)C=1C=CC=CC1C(=O)OC(=O)CCCCCCCC=CCCCCCCCC | 694.51724 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N,N-dimethyladenosine | OCC1OC(N2C=NC=3C2=NC=NC3N(C)C)C(O)C1O | 295.12805 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-D-Gluconoyl-L-valine | CC(C)[C@H](NC(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO)C(O)=O | 295.12672 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| p-amino-DL-phenylalanine hydrate | O=C(O)C(N)CC1=CC=C(N)C=C1.O | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-diisocyanato-2-methylcyclohexane | O=C=NC1CCCC(N=C=O)C1C | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-hydroxy-N-propylpyridine-2-carboxamide | O=C(NCCC)C1=NC=CC=C1O | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Acetanilide, mono(aminomethoxy) derivative | O=C(NC=1C=CC=CC1)COCN | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-hydroxy-N-isopropylpyridine-2-carboxamide | O=C(NC(C)C)C1=NC=CC=C1O | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dulcin | CCOc1ccc(NC(=O)N)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-(2-aminoethyl)-4-hydroxybenzamide monohydrochloride | Cl.O=C(NCCN)C1=CC=C(O)C=C1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tyrosinamide | NC(=O)[C@@H](N)Cc1ccc(O)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methoxy-4,6-dimethylpyridine-3-carboxamide | CC1=CC(=NC(=C1C(=O)N)OC)C | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-methyl-2-(4-nitrophenyl)ethanamine | CNCCC1=CC=C(C=C1)[N+](=O)[O-] | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Methoxy-1-methyl-3-phenylurea | CON(C)C(=O)Nc1ccccc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Carbamic acid, [[3-(aminomethyl)phenyl]methyl]- | NCc1cccc(CNC(=O)O)c1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,4-diisocyanato-1-methylcyclohexane | O=C=NC1CCC(C)C(N=C=O)C1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(((2-Hydroxyphenyl)methyl)amino)acetamide | NC(=O)CNCc1ccccc1O | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzenamine, N-ethyl-2-methyl-5-nitro- | CCNc1c(C)ccc(c1)[N+](=O)[O-] | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl 3,5-diaminobenzoate | CCOC(=O)c1cc(N)cc(N)c1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzenamine, N-(1-methylethyl)-4-nitro- | CC(C)Nc1ccc(cc1)[N+](=O)[O-] | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Amino-N-(2-hydroxyethyl)benzamide | Nc1c(cccc1)C(=O)NCCO | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2-Furoyl)piperazine | O=C(N1CC[NH2+]CC1)c1ccco1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(1H-Imidazol-1-yl)ethyl methacrylate | CC(=C)C(=O)OCCn1ccnc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-(3-Amino-4-methoxyphenyl)acetamide | COc1c(N)cc(NC(=O)C)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-((3-Hydroxy-4-methylphenyl)amino)acetamide | Cc1c(O)cc(NCC(=O)N)cc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(2-Hydroxyphenyl)-1,1-dimethylurea | CN(C)C(=O)Nc1c(O)cccc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2-Hydroxyethyl)-3-phenylurea | OCCNC(=O)Nc1ccccc1 | 180.08988 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Dicyclopentyl-3,5-xylenol | Cc1cc(C)c(C2CCCC2)c(O)c1C1CCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Dicyclohexylphenol | Oc1c(cccc1C1CCCCC1)C1CCCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-cyclohexylidene-6-(1-cyclohexen-1-yl)cyclohexan-1-one | O=C1C(=C2CCCCC2)CCCC1C3=CCCCC3 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-bis(1-cyclohexen-1-yl)cyclohexan-1-one | O=C1C(C2=CCCCC2)CCCC1C3=CCCCC3 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Oestr-4-en-17-one | O=C1CCC2C3CCC4=CCCCC4C3CCC12C | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Di(cyclohexylidene)cyclohexan-1-one | O=C1C(=C2CCCCC2)CCCC1=C1CCCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Acetylethyltetramethyltetralin | CCc1c(cc2c(c1)C(C)(C)CCC2(C)C)C(=O)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-Cyclopentyl-1,1,3,3-tetramethylindan-5-ol | CC1(C)CC(C)(C)c2cc(C3CCCC3)c(O)cc12 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[2,3-Dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-inden-5-yl]ethan-1-one | CC(C)C1C(C)C(C)(C)c2cc(C)c(cc12)C(C)=O | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Xibornol | CC1=CC(=C(C=C1C)O)C2CC3CCC2(C3(C)C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-ethyl-1,3,4,6,7,8-hexahydro-4,6,8,8-tetramethylcyclopenta[g]-2-benzopyran | O1CC=2C=C3C(=CC2C(C)C1)C(C)(CC)CC3(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[1,3,3,6-Tetramethyl-1-(propan-2-yl)-2,3-dihydro-1H-inden-5-yl]ethan-1-one | CC(C)C1(C)CC(C)(C)c2cc(C(C)=O)c(C)cc12 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(4-(trans-4-butylcyclohexyl)phenyl)ethanone | CCCC[C@H]1CCC(CC1)c1ccc(cc1)C(C)=O | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1H-Naphtho[2,3-c]pyran, 3,4,6,7,8,9-hexahydro-4,6,6,9,9-pentamethyl- | CC1COCc2cc3c(cc12)C(C)(C)CCC3(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 8-ethyl-1,3,4,6,7,8-hexahydro-4,6,6,8-tetramethylcyclopenta[g]-2-benzopyran | O1CC=2C=C3C(=CC2C(C)C1)C(C)(C)CC3(C)CC | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1'-Biphenyl, 4-cyclohexyl- | OC1CCC(CC1)c1cccc(c1)C1CCCCC1 | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl- | CC1C(C)(C)c2cc3COCC(C)c3cc2C1(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-Acetyl-1,1,2,4,4,7-hexamethyltetralin | CC1CC(C)(C)c2cc(C(C)=O)c(C)cc2C1(C)C | 258.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Choline chloride | [Cl-].C[N+](C)(C)CCO | 139.07639 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Arachidoyl glycine | CCCCCCCCCCCCCCCCCCCC(=O)NCC(=O)O | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Oxiranylmethyl octadecylcarbamate | O=C(OCC1OC1)NCCCCCCCCCCCCCCCCCC | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(15-methylhexadecyl)-2-oxazoline-4,4-dimethanol | OCC1(N=C(OC1)CCCCCCCCCCCCCCC(C)C)CO | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-[(2-hydroxyethyl)amino]ethyl oleate | O=C(OCCNCCO)CCCCCCCC=CCCCCCCCC | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Heptadecyl-4,4(5H)-oxazoledimethanol | CCCCCCCCCCCCCCCCCC1=NC(CO)(CO)CO1 | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Stearoyl methyl beta-alanine | CCCCCCCCCCCCCCCCCC(=O)N(C)CCC(=O)O | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9-Octadecenamide, N-[2-(2-hydroxyethoxy)ethyl]-, (9Z)- | CCCCCCCCC=C/CCCCCCCC(=O)NCCOCCO | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (9Z)-N,N-Bis(2-hydroxyethyl)octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N(CCO)CCO | 369.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2-dimethylpropane-1,3-diyl dinonanoate | O=C(OCC(C)(C)COC(=O)CCCCCCCC)CCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Propylene didecanoate | O=C(OCC(OC(=O)CCCCCCCCC)C)CCCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [isopropylidenedicyclohexane-4,1-diyl]bis(tert-butyl) peroxide | O(OC(C)(C)C)C1CCC(CC1)C(C)(C)C2CCC(OOC(C)(C)C)CC2 | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-dihydroxypropan-2-yl (Z)-icos-11-enoate | CCCCCCCCC=CCCCCCCCCCC(=O)OC(CO)CO | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tetradecyl hydrogen azelate | CCCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)O | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diethyl cetylmalonate | CCCCCCCCCCCCCCCCC(C(=O)OCC)C(=O)OCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [2-(1-ethylpentyl)-1,3-dioxolan-4-yl]methyl laurate | O=C(OCC1OC(OC1)C(CC)CCCC)CCCCCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(1-ethylpentyl)-1,3-dioxan-5-yl laurate | O=C(OC1COC(OC1)C(CC)CCCC)CCCCCCCCCCC | 384.32396 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| trans-4-(4-propylcyclohexyl)phenyl trans-4-pentylcyclohexanecarboxylate | O=C(OC1=CC=C(C=C1)C2CCC(CCC)CC2)C3CCC(CCCCC)CC3 | 398.31848 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| trans-4-propylcyclohexyl trans-p-(4-pentylcyclohexyl)benzoate | O=C(OC1CCC(CCC)CC1)C2=CC=C(C=C2)C3CCC(CCCCC)CC3 | 398.31848 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| C12 Fatty acid methyl ester (MEE), 1 EO | CCCCCCCCCCCCOCCC(OC)=O | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 8-(2,2-diethoxyethoxy)-2,6-dimethyloct-2-ene | O(CCC(C)CCC=C(C)C)CC(OCC)OCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-hydroxyethyl myristate | O=C(OCCO)CCCCCCCCCCCCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-hydroxypalmitic acid | O=C(O)C(O)CCCCCCCCCCCCCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 16-Hydroxypalmitic acid | C(CCCCCCCC(=O)O)CCCCCCCO | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,4,4-Trimethylpentan-2-yl 2-ethylhexaneperoxoate | CCCCC(CC)C(=O)OOC(C)(C)CC(C)(C)C | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dodecanoic acid, 2-ethoxyethyl ester | CCCCCCCCCCCC(=O)OCCOCC | 272.23514 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| a,a'-dimethylpiperazine-1,4-diethanol | OC(C)CN1CCN(CC1)CC(O)C | 202.16813 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,5-dimethylpiperazine-1,4-diethanol | OCCN1CC(N(CCO)CC1C)C | 202.16813 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (3s)-3-Amino-1-(cyclopropylamino)heptane-2,2-Diol | CCCC[C@H](N)C(O)(O)CNC1CC1 | 202.16813 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Doxercalciferol | C=C1/C(=C/C=C2CCC[C@@]3(C)[C@H]2CC[C@@H]3[C@H](C)/C=C/[C@H](C)C(C)C)C[C@@H](O)C[C@@H]1O | 412.33413 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-{2-[1-(5,6-dimethylhept-3-en-2-yl)-7a-methyl-octahydro-1h-inden-4-ylidene]ethylidene}-4-methylidenecyclohexane-1,3-diol | C=C1/C(=C/C=C2CCC[C@@]3(C)[C@H]2CC[C@@H]3[C@H](C)/C=C[C@H](C)C(C)C)C[C@@H](O)C[C@@H]1O | 412.33413 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(3,3,5-trimethylcyclohexyl) hydrogen 2-octadecenylsuccinate | O=C(OC1CC(C)CC(C)(C)C1)CC(C(=O)[O-])CC=CCCCCCCCCCCCCCCC | 492.41786 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-phenyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-one | O=C(C=CCC1CC=C(C)C1(C)C)C=2C=CC=CC2 | 254.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Estra-1(10),2,4,16-tetraen-3-ol | CC12CCC3C(C1CC=C2)CCC4=C3C=CC(=C4)O | 254.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Enzacamene | Cc1ccc(C=C2/C3CCC(C)(C2=O)C3(C)C)cc1 | 254.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-methylbenzylidene camphor | CC12C(/C(C(C(C)2C)CC1)=CC3=CC=C(C)C=C3)=O | 254.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(1-methylpropyl)-2-(1-phenylethyl)phenol | OC1=CC=C(C=C1C(C=2C=CC=CC2)C)C(C)CC | 254.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Enzacamene | Cc1ccc(/C=C2/C(=O)[C@@]3(C)CC[C@H]2C3(C)C)cc1 | 254.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [4-[[4-(dimethylamino)phenyl]imino]cyclohexa-2,5-dien-1-ylidene]dimethylammonium chloride | CN(C)c1ccc(cc1)N=C2C=CC(=[N+](C)C)C=C2.[Cl-] | 254.16572 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethanone, 1-[(3R,3aR,7R,8aS)-2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl]- | C[C@@H]1CC[C@H]2C(C)(C)[C@H]3C[C@@]12CC(C(C)=O)=C3C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [3R-(3Î±,3aÎ²,7Î²,8aÎ±)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)ethan-1-one | CC1CCC2C(C)(C)C3CC12CC(C(C)=O)=C3C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethanone, 1-(1,3,4,4a,5,6,7-hexahydro-2,5,5-trimethyl-2H-2,4a-ethanonaphthalen-8-yl)- | CC(=O)C1=C2CC3(C)CCC2(CC3)C(C)(C)CC1 | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1H-Indene-5-ethanol, 2,3-dihydro-beta,1,1,2,3,3-hexamethyl- | CC(CO)c1ccc2c(c1)C(C)(C)C(C)C2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 2,6,10-trimethylcyclododeca-2,5,9-trien-1-yl ketone | CC(=O)C1CCC(=CCCC(=C/C/C=C1/C)C)/C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2,4,6-Tris(1-methylethyl)phenyl)ethan-1-one | CC(C)c1cc(C(C)C)c(C(=O)C)c(c1)C(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4,6-Bis(isopropyl)-3,3-dimethylindan-5-ol | CC(C)c1cc2c(c(C(C)C)c1O)C(C)(C)CC2 | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Phenylundecanone | CCCCCCCCCCC(=O)c1ccccc1 | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-(tert-Butyl)-1,1,3,3-tetramethylindan-5-ol | CC(C)(C)c1cc2c(cc1O)C(C)(C)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Cyclohexyl-6-isobutyl-p-cresol | CC(C)Cc1cc(C)cc(C2CCCCC2)c1O | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-Isobutyl-1,1,3,3-tetramethylindan-5-ol | CC(C)Cc1c(O)cc2c(c1)C(C)(C)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (3R-(3alpha,3abeta,7beta,8aalpha))-1-(2,3,4,7,8,8a-Hexahydro-3,8,8-trimethyl-1H-3a,7-methanoazulen-6-yl)acetone | C[C@H]1CC[C@@H]2C(C)(C)[C@@H]3C[C@]12CC=C3CC(C)=O | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[10,10-dimethyl-2,6-bis(methylene)bicyclo[7.2.0]undec-5-yl]ethan-1-one | O=C(C)C1C(=C)CCC2C(C(=C)CC1)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-2H-2,4a-methanonaphthalen-8-yl)ethan-1-one | O=C(C1=C2C(C)(C)C3CCC2(C3)C(C)(C)CC1)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(octahydro-7,7,8,8-tetramethyl-2,3b-methano-3bH-cyclopenta[1,3]cyclopropa[1,2]benzen-4-yl)ethanone | O=C(C)C1CCC(C)(C)C23CC4CC2C13C4(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| trans-p-(4-propylcyclohexyl)phenetole | O(C1=CC=C(C=C1)C2CCC(CCC)CC2)CC | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-[7-isopropyl-3,5-dimethylbicyclo[2.2.2]oct-5-en-2-yl]-3-buten-2-one | O=C(C=CC1C2C=C(C)C(CC2C(C)C)C1C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Di-tert-butyl-4-(prop-2-en-1-yl)phenol | CC(C)(C)C1=CC(CC=C)=CC(=C1O)C(C)(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethanone, 1-(2,6,10-trimethyl-2,5,9-cyclododecatrien-1-yl)- | CC(=O)C1CCC(C)=CCCC(C)=CCC=C1C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1,3,3-tetramethyl-6-(1-methylpropyl)indan-5-ol | OC=1C=C2C(=CC1C(C)CC)C(C)(C)CC2(C)C | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(6,6,9-trimethyl-2-methylenecycloundeca-4,8-dien-1-yl)ethan-1-one | O=C(C)C1C(=C)CC=CC(C)(C)CC=C(C)CC1 | 246.19837 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diazidodimethylsilane | [N-]=[N+]=N[Si](N=[N+]=[N-])(C)C | 144.05797 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Naphthalenol | Oc1ccc2ccccc2c1 | 144.05751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Phenyl-3-butyn-2-one | CC(=O)C#Cc1ccccc1 | 144.05751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Naphthol | Oc1cccc2ccccc12 | 144.05751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Acetylgalactosamine 4-sulfate | CC(=O)NC1C(C(C(OC1O)CO)OS(=O)(=O)O)O | 301.04675 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Acetyl-D-galactosamine 6-sulfate | CC(=O)N[C@H]1[C@H](O)O[C@H](COS(=O)(=O)O)[C@H](O)[C@@H]1O | 301.04675 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [5-acetamido-4,6-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxidanesulfonic acid | CC(=O)N[C@H]1[C@@H](O)O[C@H](CO)[C@H](OS(=O)(=O)O)[C@@H]1O | 301.04675 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Amino-5,6-dimethyl-1,2,4-triazine | Cc1c(C)nc(N)nn1 | 124.07490 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isooctyl nonyl phthalate | CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCC(C)C | 404.29266 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-ethylhexyl nonyl phthalate | O=C(OCCCCCCCCC)C=1C=CC=CC1C(=O)OCC(CC)CCCC | 404.29266 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (20S)-5a-pregnane-3ß,20-diol diacetate | O=C(OC(C)C1CCC2C3CCC4CC(OC(=O)C)CCC4(C)C3CCC12C)C | 404.29266 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 12a-hydroxy-3-oxo-5ß-cholan-24-oate | O=C(OC)CCC(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CC(O)C12C | 404.29266 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2(3H)-Benzothiazolethione, 3-methyl- | Cn1c(=S)sc2c1cccc2 | 181.00199 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(Methylthio)benzothiazole | CSc1nc2ccccc2s1 | 181.00199 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2-dimethoxy-1-methylethylamine | O(C)C(OC)C(N)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[(2-hydroxyethyl)amino]propan-2-ol | OCCNCC(O)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-((Hydroxymethyl)amino)-2-methyl-1-propanol | CC(C)(CO)NCO | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(ethylamino)propane-1,2-diol | OCC(O)CNCC | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-dimethylaminopropane-1,2-diol | OCC(O)CN(C)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-((2-Hydroxyethyl)amino)propanol | OCCCNCCO | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2-Dimethoxyethyl(methyl)amine | CNCC(OC)OC | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(dimethylamino)propane-1,3-diol | OCCC(O)N(C)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-amino-2-methylbutane-2,3-diol | C[C@@H](O)[C@@](C)(O)CN | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Amino-2-ethyl-1,3-propanediol | CCC(N)(CO)CO | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methanamine, 1,1-dimethoxy-N,N-dimethyl- | COC(OC)N(C)C | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Methyldiethanolamine | CN(CCO)CCO | 119.09463 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,3'-((1-Methylethylidene)bis(4,1-phenyleneoxy))dipropionodihydrazide | CC(C)(c1ccc(OCCC(=O)NN)cc1)c1ccc(OCCC(=O)NN)cc1 | 400.21106 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Pieristoxin G | C[C@@]1(O)CC23[C@@H](O)[C@@H]1CC[C@@]2(O)[C@@](C)(O)[C@@H]1[C@@H]2O[C@@H]2C(C)(C)[C@@]1(O)[C@H](O)[C@H]3O | 400.20972 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Hydroxy-2,4,6-triiodobenzoic acid | OC(=O)c1c(I)c(O)c(I)cc1I | 515.72162 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-Bis(((3-(aminomethyl)phenyl)methyl)amino)propan-2-ol | NCc1cc(CNCC(O)CNCc2cc(CN)ccc2)ccc1 | 328.22631 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,4:3,6-Dianhydro-D-glucitol monolaurate | CCCCCCCCCCCC(=O)OC1COC2C(O)COC12 | 328.22497 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Corchorifatty acid F | CC/C=CCC(C(/C=C/C(CCCCCCCC(=O)O)O)O)O | 328.22497 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(3,5-di-sec-butylcyclopent-1-enyl)-2,3,5-trihydroxyvaleric acid | O=C(O)C(O)C(O)CC(O)C1=CC(CC1C(C)CC)C(C)CC | 328.22497 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethanol, 2-decylthio- | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-mercaptododecan-2-ol | OC(CS)CCCCCCCCCC | 218.17044 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-methoxyundecane-3-thiol | SC(CCOC)CCCCCCCC | 218.17044 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dimethoxymethyloctylsilane | O(C)C(OC)[SiH2]CCCCCCCC | 218.17021 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-[(2-hydroxyethyl)[4-[(6-methoxybenzothiazol-2-yl)azo]-3-methylphenyl]amino]propiononitrile | N#CCCN(C1=CC=C(N=NC2=NC=3C=CC(OC)=CC3S2)C(=C1)C)CCO | 395.14160 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-[(1R,2R)-2-(Dimethylamino)cyclohexyl]-N-methyl-1,3-benzodioxole-5-carboxamide hydrochloride (1:1) | CN(C)[C@@H]1CCCC[C@H]1N(C)C(=O)c2ccc3c(c2)OCO3.Cl | 340.15537 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(hydroxymethyl)-2-[[(2-methyl-1-oxoallyl)oxy]methyl]-1,3-propanediyl bismethacrylate | O=C(OCC(CO)(COC(=O)C(=C)C)COC(=O)C(=C)C)C(=C)C | 340.15220 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Deacetylneosolaniol | CC1=C[C@@H]2[C@](C[C@@H]1O)([C@]3([C@@H]([C@H]([C@H]([C@@]34CO4)O2)O)O)C)COC(=O)C | 340.15220 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2'-Thiobisethanol | OCCSCCO | 122.04015 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-methylthiopropane-1,2-diol | OCC(O)CSC | 122.04015 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diethyl sulphone | O=S(=O)(CC)CC | 122.04015 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Trimethoxysilane | O(C)[SiH](OC)OC | 122.03992 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tripotassium propylsilanetriolate | [K+].[K+].[K+].[O-][Si]([O-])([O-])CCC | 122.03992 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| MEGESTROL | CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C=C(C)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6,7-DIHYDROCANRENONE | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@]21CCC(=O)O1 | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Endrisone | O=C1C=CC2(C(=C1)C(C)CC3C4CCC(C(=O)C)C4(C)CC(O)C32)C | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17Î²-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CCC2(O)C#CCO | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-oxopregna-1,4-diene-20-carboxylic acid | O=C1C=CC2(C(=C1)CCC3C2CCC4(C)C(CCC34)C(C(=O)O)C)C | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| retinol acetate;retinol, acetate;retinyl acetate;o~15~-acetylretinoic acid;[(2e,4e,6e,8e)-3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)nona-2,4,6,8-tetraenyl] acetate;retinol acetate retinol, acetate retinyl acetate o~15~-acetylretinoic acid [(2e,4e,6e,8e)-3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)nona-2,4,6,8-tetraenyl] acetate | CC1CCCC(C)(C)C=1C=CC(C)=CC=CC(C)=CC(=O)OC(C)=O | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 16a-ethyl-21-hydroxy-19-norpregna-4,9-diene-3,20-dione | O=C1C=C2C(=C3CCC4(C)C(C(=O)CO)C(CC)CC4C3CC2)CC1 | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Trimegestone | C[C@H](O)C(=O)[C@@]1(C)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3CC[C@@]21C | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Estra-1,3,5(10)-triene-3,17ß-diol 17-butyrate | O=C(OC1CCC2C3CCC4=CC(O)=CC=C4C3CCC12C)CCC | 342.21949 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methylene dibutyldithiocarbamate | CCCCN(CCCC)C(=S)SCSC(=S)N(CCCC)CCCC | 422.19178 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5'-Methylthioadenosine | CSC[C@H]1O[C@@H](n2cnc3c2ncnc3N)[C@H](O)[C@@H]1O | 297.08956 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-Benzodioxol-2-one | O=c1oc2c(o1)cccc2 | 136.01604 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Ethyl-2-benzothiazolamine | C1=CC=CC2=C1SC(=N2)NCC | 178.05647 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Amino-5,6-dimethylbenzothiazole | Cc1cc2c(cc1C)nc(N)s2 | 178.05647 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Amino-4,5,6,7-tetrahydrobenzo(b)thiophene-3-carbonitrile | Nc1c(C#N)c2c(CCCC2)s1 | 178.05647 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isothiocyanic acid, p-dimethylaminophenyl ester | CN(C)c1ccc(cc1)N=C=S | 178.05647 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Etisazole | C1=CC=CC2=C1C(=NS2)NCC | 178.05647 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Picolinic acid | C1=CC=NC(=C1)C(=O)O | 123.03203 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Nitrosophenol | Oc1ccc(cc1)N=O | 123.03203 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isonicotinic acid | OC(=O)c1ccncc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isonicotinaldehyde 1-oxide | [O-][n+]1ccc(C=O)cc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Nicotinic acid | OC(=O)c1cccnc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Nitrobenzene | O=N(=O)c1ccccc1 | 123.03203 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(Hydroxymethyl)furan-2-carbonitrile | OCc1ccc(o1)C#N | 123.03203 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hexadecanamide, N,N-dimethyl- | CCCCCCCCCCCCCCCC(=O)N(C)C | 283.28751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isooctadecanoic acid, monoamide with 2-[(2-aminoethyl)amino]ethanol | O=C(N)CCCCCCCCCCCCCCC(C)C.OCCNCCN | 283.28751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Octadecanamide | CCCCCCCCCCCCCCCCCC(N)=O | 283.28751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Amines, C14-18; C16-18-unsaturated, alkyl, ethoxylated | CCOCCCCCCC=CCCCCCCCCN | 283.28751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Morpholine, 4-tetradecyl- | CCCCCCCCCCCCCCN1CCOCC1 | 283.28751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Aldimorph | C(N1CC(OC(C1)C)C)CCCCCCCCCCC | 283.28751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(Hexadecyl((1-hydroxy-2-naphthyl)carbonyl)amino)isophthalic acid | CCCCCCCCCCCCCCCCN(C(=O)c1ccc2ccccc2c1O)c1cc(cc(c1)C(=O)O)C(=O)O | 575.32469 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-Diphenylguanidine | N=C(Nc1ccccc1)Nc2ccccc2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Varenicline | c1cnc2cc3c(cc2n1)[C@H]1CNC[C@@H]3C1 | 211.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Anthranilaldehyde phenylhydrazone | N(=CC=1C=CC=CC1N)NC=2C=CC=CC2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Varenicline | C1C2CNCC1C3=CC4=NC=CN=C4C=C23 | 211.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Methyl-4-aminoazobenzene | CNc1ccc(cc1)N=Nc1ccccc1 | 211.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(p-tolylazo)aniline | N(=NC1=CC=C(C=C1)C)C2=CC=C(N)C=C2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9-Methyl-9H-carbazole-3,6-diamine | Cn1c2c(cc(N)cc2)c2c1ccc(N)c2 | 211.11095 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Fosinopril | CCC(=O)O[C@@H](C(C)C)O[P@](=O)(CCCCc1ccccc1)CC(=O)N2C[C@@H](C[C@H]2C(=O)O)C3CCCCC3 | 563.30119 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methyl-1-o-tolylpent-1-en-3-one | O=C(C(=CC=1C=CC=CC1C)C)CC | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2,3,6-trimethylphenyl)-2-buten-1-one | O=C(C=CC)C=1C(=CC=C(C1C)C)C | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-phenylcycloheptan-1-one | O=C1CCCCCC1C=2C=CC=CC2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| a,a-dicyclopropylbenzyl alcohol | OC(C=1C=CC=CC1)(C2CC2)C3CC3 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-benzylcyclohexan-1-one | O=C1CCCCC1CC=2C=CC=CC2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4,4-dimethyl-1-phenylpent-1-en-3-one | O=C(C=CC=1C=CC=CC1)C(C)(C)C | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Hexen-3-one, 5-methyl-1-phenyl- | CC(C)CC(=O)C=Cc1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzenepropanal, .beta.-methyl-3-(1-methylethenyl)- | CC(CC=O)c1cccc(c1)C(C)=C | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| p-Cumenyl cyclopropyl ketone | CC(C)c1ccc(cc1)C(=O)C1CC1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2,5,7-Tetramethylindan-1-one | Cc1cc2c(C(=O)C(C)(C)C2)c(C)c1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Propenal, 2-methyl-3-[2-(1-methylethyl)phenyl]- | CC(C)c1c(/C=C(C)/C=O)cccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| p-Cyclohexylbenzaldehyde | O=Cc1ccc(cc1)C1CCCCC1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Methyl-4-methylidene-6-phenyltetrahydro-2H-pyran | CC1CC(=C)CC(O1)c2ccccc2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| p-tert-butylcinnamaldehyde | CC(C)(C)c1ccc(C=CC=O)cc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| alpha-Butylcinnamaldehyde | CCCCC(C=O)=C/c1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Octahydro-8,8-dimethylnaphthalene-2-carbaldehyde | CC1(C)CCCc2ccc(C=O)cc12 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Propenal, 2-methyl-3-[4-(1-methylethyl)phenyl]- | CC(C)c1ccc(cc1)C=C(/C)C=O | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2H-Pyran, 3,6-dihydro-2,4-dimethyl-6-phenyl- | CC1CC(=CC(O1)c2ccccc2)C | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2H-Pyran, 3,6-dihydro-4,6-dimethyl-2-phenyl- | CC1OC(CC(=C1)C)c2ccccc2 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-Methyl-2-phenyl-2-hexenal | CC(C)CC=C(C=O)/c1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclohexylphenylketone | O=C(C1CCCCC1)c1ccccc1 | 188.12012 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tetrahydrofurfuryl oleate | O=C(OCC1OCCC1)CCCCCCCC=CCCCCCCCC | 366.31340 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (tetrahydro-3-furyl)methyl oleate | O=C(OCC1COCC1)CCCCCCCC=CCCCCCCCC | 366.31340 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[[1-(isopropyl)cyclohexyl]carbonyl]pyrrolidine | O=C(N1CCCC1)C2(CCCCC2)C(C)C | 223.19361 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(3,7-dimethylocta-1,6-dien-1-yl)morpholine | O1CCN(C=CC(C)CCC=C(C)C)CC1 | 223.19361 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Propanenitrile, 3-(10-undecenyloxy)- | C=CCCCCCCCCCOCCC#N | 223.19361 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-hydroxy-1,2,3,4-tetrahydropyrimidin-2-one | O=C1NC=C[C@H](O)N1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,5-Piperazinedione | C1C(=O)NCC(=O)N1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dimethyl cyanoimidocarbonate | N#CN=C(OC)OC | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Maleamide | O=C(N)C=CC(=O)N | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,4(1H,3H)-Pyrimidinedione, dihydro- | O=C1CCNC(=O)N1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Muscimol | NCc1cc(=O)[nH]o1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Methylhydantoin | O=C1NC(=O)N(C)C1 | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,4-imidazolidinedione, 5-methyl- | CC1NC(=O)NC1=O | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Sodium ethyl cyanocarbamate | [Na+].N#CNC(=O)OCC | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (3S)-3-Aminopyrrolidine-2,5-dione | N[C@H]1CC(=O)NC1=O | 114.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Decanedioic acid, di-2-propenyl ester | C=CCOC(=O)CCCCCCCCC(=O)OCC=C | 282.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethylene bis(cyclohexanecarboxylate) | O=C(OCCOC(=O)C1CCCCC1)C1CCCCC1 | 282.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,10-Decanediyl diacrylate | C=CC(=O)OCCCCCCCCCCOC(=O)C=C | 282.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dibutyl cyclohex-4-ene-1,2-dicarboxylate | O=C(OCCCC)C1CC=CCC1C(=O)OCCCC | 282.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-ethyl-1-propyl-1,3-propanediyl bismethacrylate | O=C(OCC(CC)C(OC(=O)C(=C)C)CCC)C(=C)C | 282.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2-bis(allyloxymethyl)butyl methacrylate | O=C(OCC(COCC=C)(COCC=C)CC)C(=C)C | 282.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-isopropyl-2,2-dimethylpropane-1,3-diyl bismethacrylate | O=C(OCC(C)(C)C(OC(=O)C(=C)C)C(C)C)C(=C)C | 282.18311 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 11-nor-delta(9)-tetrahydrocannabinol-9-carboxylicacid | CCCCCc1cc(O)c2[C@@H]3CC(=CC[C@H]3C(C)(C)Oc2c1)C(O)=O | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6H-Dibenzo[b,d]pyran-9-carboxylic acid,6a,7,8,10a-tetrahydro-1-hydroxy-6,6-dimethyl-3-pentyl- | CCCCCc1cc(O)c2C3C=C(CCC3C(C)(C)Oc2c1)C(O)=O | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bisphenol A bis(2-hydroxypropyl) ether | CC(O)COc1ccc(cc1)C(C)(C)c1ccc(OCC(C)O)cc1 | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 21-hydroxypregn-4-ene-3,11,20-trione | O=C1C=C2CCC3C(C(=O)CC4(C)C(C(=O)CO)CCC34)C2(C)CC1 | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 16a,17-epoxy-11a-hydroxypregn-4-ene-3,20-dione | O=C1C=C2CCC3C4CC5OC5(C(=O)C)C4(C)CC(O)C3C2(C)CC1 | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Anecortave | C[C@]12CCC(=O)C=C1CC[C@@H]1C2=CC[C@@]2(C)[C@H]1CC[C@]2(O)C(=O)CO | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,3'-[isopropylidenebis(p-phenyleneoxy)]dipropanol | OCCCOC1=CC=C(C=C1)C(C2=CC=C(OCCCO)C=C2)(C)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Deprodone | O=C1C=CC2(C(=C1)CCC3C4CCC(O)(C(=O)C)C4(C)CC(O)C32)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Formebolone | O=CC1=CC2(C(=CC1=O)CCC3C4CCC(O)(C)C4(C)CC(O)C32)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 21-Deoxycortisone | CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3C(=O)C[C@]12C | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (isopropylidene)bis(1-methyl-1-phenylethyl) peroxide | O(OC(C=1C=CC=CC1)(C)C)C(OOC(C=2C=CC=CC2)(C)C)(C)C | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [isopropylidenebis(p-phenyleneoxy)]dipropanol | OC(OC1=CC=C(C=C1)C(C2=CC=C(OC(O)CC)C=C2)(C)C)CC | 344.19876 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| EPTC | CCCN(CCC)C(=O)SCC | 189.11873 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dromostanolone proprionate | CCC(=O)O[C@H]1CC[C@H]2[C@@H]3CC[C@H]4CC(=O)[C@H](C)C[C@]4(C)[C@H]3CC[C@]12C | 360.26644 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (3ß,17ß)-17-hydroxy-17-methylandrost-5-ene-3-ol propionate | O=C(OC1CC2=CCC3C(CCC4(C)C3CCC4(O)C)C2(C)CC1)CC | 360.26644 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cholan-24-oic acid, 3,6-dihydroxy-, methyl ester, (3alpha,5beta,6alpha)- | COC(=O)CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3C[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C | 406.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Irisoquin | CCCCCCCCCCCCCCCCCCC1=C(O)C(=O)C=C(OC)C1=O | 406.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 3-a,12-a-dihydroxy-5-ß-cholan-24-oate | O=C(OC)CCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CC(O)C12C | 406.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,3,5,6,8,9,11,12,14,15-Decahydro-4,13-(ethanoxyethanoxyethano)-4H,13H-1,7,10,16,4,13-benzotetraoxadiazacyclooctadecine | C1COCCN2CCOCCOCCN(CCO1)CCOc1ccccc1OCC2 | 424.25734 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ppi-2458 | CO[C@H]1[C@H]([C@@]2(C)O[C@@H]2CC=C(C)C)[C@]2(CC[C@H]1OC(=O)N[C@@H](C(N)=O)C(C)C)CO2 | 424.25734 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| ruscogenin | C[C@H]1[C@H]2[C@H](C[C@H]3[C@@H]4CC=C5C[C@@H](O)C[C@@H](O)[C@]5(C)[C@H]4CC[C@]23C)O[C@]11CC[C@@H](C)CO1 | 430.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3beta,17-Dihydroxypregn-5-en-20-one 17-hexanoate | CCCCCC(=O)O[C@@]1(CC[C@H]2[C@@H]3CC=C4CC(O)CC[C@]4(C)[C@H]3CC[C@]12C)C(=O)C | 430.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hecogenin | C[C@H]1[C@H]2[C@H](C[C@H]3[C@@H]4CC[C@H]5C[C@@H](O)CC[C@]5(C)[C@H]4CC(=O)[C@]23C)O[C@@]21CC[C@@H](C)CO2 | 430.30831 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [2-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl]ethylamino]ethyl](2-hydroxyethyl)dimethylammonium acetate | O=C([O-])C.O=[N+]([O-])C1=CC=C(N=NC2=CC=C(C=C2)N(CC)CC[N+](C)(C)CCO)C(Cl)=C1 | 421.18807 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(benzoylamino)-2-[(ethoxycarbonyl)methylamino]-5-methoxybenzenediazonium tetrachlorozincate (2:1) | N#[N+]C=1C=C(OC)C(=CC1N(C(=O)OCC)C)NC(=O)C=2C=CC=CC2.N#[N+]C=1C=C(OC)C(=CC1N(C(=O)OCC)C)NC(=O)C=2C=CC=CC2.Cl[Zn-2](Cl)(Cl)Cl | 355.14063 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-(p-tolyl)butyramide | O=C(NC1=CC=C(C=C1)C)C(N=NC2=CC=C(C=C2[N+](=O)[O-])C)C(=O)C | 355.14063 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Testosterone isocaproate | CC(C)CCC(=O)OC1CCC2C1(CCC3C2CCC4=CC(=O)CCC34C)C | 386.28209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| HU-210 | CCCCCCC(C)(C)C1=CC2=C(C3CC(=CCC3C(O2)(C)C)CO)C(=C1)O | 386.28209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dexanabinol | CCCCCCC(C)(C)c1cc(O)c2c(c1)OC(C)(C)[C@H]1CC=C(CO)C[C@H]21 | 386.28209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| HU 210 | CCCCCCC(C)(C)c1cc(c2c(c1)OC([C@H]3[C@H]2CC(=CC3)CO)(C)C)O | 386.28209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17beta-Hydroxyandrost-4-en-3-one 3,3-dimethylbutyrate | CC(C)(C)CC(=O)OC1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C | 386.28209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17ß-hydroxyandrost-4-en-3-one hexanoate | O=C(OC1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C)CCCCC | 386.28209 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-amino-6-hydroxy-2-pyridone hydrochloride | Cl.O=C1NC(O)=CC=C1N | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-methylisoxazole-3-carboxamide | O=C(N)C1=NOC(=C1)C | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-Methyluracil | Cc1cc(=O)[nH]c(=O)[nH]1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,6-Pyridazinedione, 1,2-dihydro-1-methyl- (8CI)(9CI) | CN1C(=O)C=CC(=O)N1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Furoic acid hydrazide | NNC(=O)c1ccco1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Imidazole-1-acetic acid | OC(=O)Cn1ccnc1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-Methyl-1H-4-carboxylic acid | Cc1c(nc[nH]1)C(=O)O | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Methyl-1H-imidazole-4-carboxylic acid | Cc1ncc([nH]1)C(=O)O | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Methyl-1H,5H-pyrimidine-4,5-dione | Cc1nc(O)cc(=O)[nH]1 | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Imidazole-4-acetic acid | C1=C(N=CN1)CC(=O)O | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Methyloxazole-5-carboxamide | Cc1ncoc1C(N)=O | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Methylpyridazine-3,6-diol | Cc1cc(=O)[nH][nH]c1=O | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Thymine | Cc1c[nH]c(=O)[nH]c1=O | 126.04293 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Triisobutylphosphine sulphide | S=P(CC(C)C)(CC(C)C)CC(C)C | 234.15711 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tributylphosphine sulphide | S=P(CCCC)(CCCC)CCCC | 234.15711 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Chlorodecyldimethylsilane | Cl[Si](C)(C)CCCCCCCCCC | 234.15706 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tributylchlorosilane | Cl[Si](CCCC)(CCCC)CCCC | 234.15706 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(methylsulphinyl)decane | O=S(C)CCCCCCCCCC | 204.15479 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dibutoxy(dimethyl)silane | O(CCCC)[Si](OCCCC)(C)C | 204.15456 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bis(1,1-dimethylethoxy)dimethylsilane | O(C(C)(C)C)[Si](OC(C)(C)C)(C)C | 204.15456 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Arachidonoyl glycerol | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OC(CO)CO | 378.27701 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| GLYCERYL ARACHIDO- NATE | CCCCC/C=CCC=C/C/C=CCC=C/CCCC(=O)OCC(O)CO | 378.27701 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bolenol | OC1(CC)CCC2C3CC=C4CCCCC4C3CCC21C | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethylestrenol | CC[C@]1(O)CC[C@H]2[C@@H]3CCC4=CCCC[C@@H]4[C@H]3CC[C@]12C | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Abietyl alcohol | CC(C)C1=CC2=CCC3C(C)(CO)CCCC3(C)C2CC1 | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(p-cumenyl)-2-octylpropionaldehyde | O=CC(CC1=CC=C(C=C1)C(C)C)CCCCCCCC | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tetradecanophenone | O=C(C=1C=CC=CC1)CCCCCCCCCCCCC | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-methyl-5-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthyl)pent-2-en-1-al | O=CC=C(C)CCC1=C(C)CCC2C1(C)CCCC2(C)C | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [1R-(1a,4aß,10aa)]-1,2,3,4,4a,5,6,9,10,10a-decahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol | OCC1(C)CCCC2(C3=C(C=C(CC3)C(C)C)CCC21)C | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1,3-trimethyl-6-(1,1,3,3-tetramethylbutyl)indan-5-ol | OC=1C=C2C(=CC1C(C)(C)CC(C)(C)C)C(C)(C)CC2C | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Desoxymethyltestosterone | [H][C@@]12CC[C@](C)(O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])CC[C@@]2([H])CC=CC[C@]12C | 288.24532 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (1-methylethylidene)di-4,1-cyclohexanediyl bismethacrylate | O=C(OC1CCC(CC1)C(C)(C)C2CCC(OC(=O)C(=C)C)CC2)C(=C)C | 376.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (5ß)-3ß,14-dihydroxycardanolide | O=C1OCC(C1)C2CCC3(O)C4CCC5CC(O)CCC5(C)C4CCC23C | 376.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hexyl nonyl phthalte | O=C(OCCCCCCCCC)C1=CC=CC=C1C(OCCCCCC)=O | 376.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2,6-diisopropyl-3,5-dimethyl- | CC(C)c1c(O)c(C(C)C)c(C)cc1C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Diisopropyl-3,4-xylenol | CC(C)c1c(O)c(C(C)C)c(C)c(C)c1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[3-methyl-2-(3-methyl-2-butenyl)-3-cyclohexen-1-yl]ethan-1-one | O=C(C)C1CCC=C(C)C1CC=C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(tert-butyl)-2,3,4,5,6,7-hexahydro-2-methyl-1H-inden-1-one | O=C1C2=C(CC1C)CC(CC2)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(4-isopropyl-1-cyclohexen-1-yl)pent-4-enal | O=CCCC=CC1=CCC(CC1)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(5-isopropyl-2-methyl-1-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1=C(C)CCC(C1)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-ethyl-5,9-dimethyldeca-2,4,8-trienal | O=CC(=CC=C(C)CCC=C(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Octahydro-a-methyl-4,7-methano-1H-indene-5-propionaldehyde | O=CC(C)CC1CC2CC1C3CCCC23 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Decahydro-5-methylspiro[furan-2(3H),5'-[4,7]methano[5H]indene] | O1C(C)CCC12CC3CC2C4CCCC34 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2-ethyl-4,4-dimethyl-2-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1C(=CC(C)(C)CC1)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-(4-methyl-3-cyclohexen-1-yl)hept-4-enal | O=CCCC=CC(C)C1CC=C(C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Penten-2-one, 3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)- | CC(C=C/C1CC=C(C)C1(C)C)C(C)=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2-(1-ethylhexyl)- | CCCCCC(CC)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 4-(1-ethylhexyl)- | CCCCCC(CC)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Penten-2-one, 3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)- | CC(=O)C(C)=CCC1CC=C(C)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2-(1-propylpentyl)- | CCCCC(CCC)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(1,1,3,3-Tetramethylbutyl)phenol | CC(C)(C)CC(C)(C)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methyl-1-(1-methylbicyclo[2.2.1]hept-5-en-2-yl)pent-1-en-3-ol | OC(C(=CC1CC2C=CC1(C)C2)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-bicyclo[2.2.1]hept-2-yl-2,4-dimethylpent-2-en-1-al | O=CC(=CC(C)CC1CC2CCC1C2)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1,2,3,5,6,7,8,8a-octahydro-8,8-dimethyl-2-naphthyl)ethan-1-one | O=C(C)C1CC=C2CCCC(C)(C)C2C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-(1,1-dimethylethyl)-3,4,5,6,7,8-hexahydronaphthalen-2(1H)-one | O=C1CC2=C(CC1)CC(CC2)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,4,4a,5,6,7-hexahydro-3,3,5,5-tetramethylnaphthalene-2(1H)-one | O=C1CC2=CCCC(C)(C)C2CC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-(2,2,3-trimethylcyclopent-3-en-1-yl)hex-5-en-3-one | O=C(CC=CC1CC=C(C)C1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[4-methyl-5-(3-methyl-2-butenyl)-3-cyclohexen-1-yl]ethan-1-one | O=C(C)C1CC=C(C)C(CC=C(C)C)C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,4-Di-tert-butylphenol | Oc(c(cc(c1)C(C)(C)C)C(C)(C)C)c1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,4,5,6,7,8-hexahydro-3,3,5,5-tetramethylnaphthalene-2(1H)-one | O=C1CC2=C(CC1(C)C)C(C)(C)CCC2 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,3,4,5,6,7-hexahydro-4-isopropyl-2,7-dimethyl-1H-inden-1-one | O=C1C2=C(CC1C)C(CCC2C)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hexahydro-2,5,5-trimethyl-2H-2,4a-methanonaphthalen-1(5H)-one | O=C1C2CCCC(C)(C)C32CCC1(C)C3 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- | CC(=O)C(C)=CC1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Buten-2-one, 4-(1,2,6,6-tetramethyl-2-cyclohexen-1-yl)- | CC1=CCCC(C)(C)C1(C)/C=C/C(=O)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Di-tert-butylphenol | CC(C)(C)C1=C(C(=CC=C1)C(C)(C)C)O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 4-(1-propylpentyl)- | CCCCC(CCC)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one | CCC(=O)C=CC1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-tert-butyl-2-sec-butylphenol | CCC(C)c1cc(ccc1O)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Octylphenol | CCCCCCCCc1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(1,1,3,3-Tetramethylbutyl)phenol | CC(C)(C)CC(C)(C)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| o-(1-methylheptyl)phenol | CCCCCCC(C)c1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6,9,10-trimethylundeca-3,5,9-trien-2-one | CC(C)=C(C)CCC(C)=CC=CC(C)=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, (1-methylheptyl)- | CCCCCCC(C)c1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, (2-ethylhexyl)- | CCCCC(CC)Cc1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2-octyl- | CCCCCCCCc1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methylionone | CCC(=O)C=CC1C(C)=CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzenepropanol, 4-(1,1-dimethylethyl)-.beta.-methyl- | CC(CO)Cc1ccc(cc1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dihydro-1,1,2,3,3-pentamethyl-4(5H)-indanone | CC1C(C)(C)C2=C(C(=O)CCC2)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Di(butan-2-yl)phenol | CC[C@H](C)c1cccc([C@H](C)CC)c1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Butenal, 2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)- | CCC(C=O)=CCC1CC=C(C)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| alpha-Isomethylionone | CC(=O)C(C)=CC1C(C)=CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, isooctyl- | CC(C)CCCCCc1ccccc1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Methyl-4-(2,6,6-trimethyl-1-cyclohexenyl)-3-buten-2-one; | CC(=O)C(C)=C/C1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(5(or 6)-Methyl-7(or 8)-(1-methylethyl) bicyclo[2.2.2]oct-5-en-2-yl)ethan-1-one. | CC(C)C1CC2=C(C)CC1C(C2)C(C)=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)- | CC1CCC(=C(C=CC(C)=O)C1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| alpha-Irone | C[C@@H]1CC=C(C)[C@H](C=CC(C)=O)C1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-tert-Octylphenol | OC1=CC=C(C(C)(C)CCCCC)C=C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)- | CC(=O)C=C(C)C1C(C)=CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2,3,3a,4,5,6-hexahydro-1,1,3-trimethyl-1H-inden-5-yl)ethan-1-one | O=C(C)C1CC=C2C(C1)C(C)CC2(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzenepropanol, .beta.-pentyl- | CCCCCC(CO)Cc1ccccc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[4-(4-methyl-3-pentenyl)-3-cyclohexen-1-yl]ethan-1-one | O=C(C)C1CC=C(CCC=C(C)C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | O=CC1CC=C(CCC=C(C)C)CC1C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 8-isopropyl-6-methylbicyclo[2.2.2]oct-5-en-2-yl methyl ketone | O=C(C)C1CC2C=C(C)C1CC2C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-(2,2,3-trimethylcyclopent-3-en-1-yl)hex-4-en-3-one | O=C(C=CCC1CC=C(C)C1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (E)-1-(2-ethyl-6,6-dimethyl-1-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1=C(CC)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(5,5-dimethylcyclohex-1-en-1-yl)hex-4-en-1-one | O=C(C1=CCCC(C)(C)C1)CCC=CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,5-diisobutylphenol | OC=1C=C(C=C(C1)CC(C)C)CC(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(5,5-dimethyl-1-cyclohexen-1-yl)-3-methylpent-4-en-1-one | O=C(C1=CCCC(C)(C)C1)CC(C=C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(3,3,5-trimethyl-1-cyclohexen-1-yl)pent-4-en-1-one | O=C(C1=CC(C)(C)CC(C)C1)CCC=C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(3,5,5-trimethyl-1-cyclohexen-1-yl)pent-4-en-1-one | O=C(C1=CC(C)CC(C)(C)C1)CCC=C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (E,E)-1-(6-ethylidene-2,2-dimethylcyclohexyl)-2-buten-1-one | O=C(C=CC)C1C(=CC)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2,2-dimethyl-6-methylenecyclohexyl)pent-1-en-3-one | O=C(C=CC1C(=C)CCCC1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (E)-1-(2-ethyl-6,6-dimethyl-2-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1C(=CCCC1(C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diisobutylphenol | OC1=CC=CC(=C1CC(C)C)CC(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Di-sec-butylphenol | OC1=CC=CC(=C1C(C)CC)C(C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-methyl-4-(2,2-dimethyl-6-methylenecyclohexyl)-3-buten-2-one | O=C(C(=CC1C(=C)CCCC1(C)C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methyl-2-phenylheptan-4-ol | OC(CCC)CC(C=1C=CC=CC1)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,6,10-trimethylundeca-3,5,9-trien-2-one | O=C(C(=CC=C(C)CCC=C(C)C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)pent-1-en-3-one | O=C(C=CC1C(C=CCC1(C)C)C)CC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(3,3-dimethylbicyclo[2.2.1]hept-2-ylidene)-2-methyl-2-buten-1-ol | OCC(=CC=C1C2CCC(C2)C1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(2,2,3-trimethyl-6-methylenecyclohexyl)-3-buten-2-one | O=C(C=CC1C(=C)CCC(C)C1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Methyl-1-(2,4,4-trimethylcyclohexen-1-yl)-2-buten-1-one | CC(=CC(=O)C1=C(C)CC(C)(C)CC1)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Penten-3-ol, 2-methyl-1-(methylbicyclo[2.2.1]hept-5-en-2-yl)- | C[C@@]1([C@@H]2C=C[C@@H](C1)C2)C=C([C@@H](O)CC)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2,4-bis(2-methylpropyl)- | CC(C)Cc1cc(CC(C)C)c(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,2,3,4,5,6,7,8-octahydro-2,5,5-trimethylnaphthalene-2-carbaldehyde | O=CC1(C)CC2=C(CC1)C(C)(C)CCC2 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,5-Diisopropyl-3,4-xylenol | CC(C)c1c(C)c(C)c(C(C)C)c(O)c1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-butenal | O=CC(C=CC1=C(C)CCCC1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| alpha,alpha-Diisopropylphenethyl alcohol | CC(C)C(O)(Cc1ccccc1)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)-2,2-dimethylpropanal | CC(C)(CC1=CCC2CC1C2(C)C)C=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Buten-2-one, 3-methyl-4-(3,5,6-trimethyl-3-cyclohexen-1-yl)- | CC1C=C(C)CC(C=C(/C)C(C)=O)C1C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Buten-2-one, 3-methyl-4-(2,4,6-trimethyl-3-cyclohexen-1-yl)- | CC1CC(=CC(C)C1C=C(/C)C(C)=O)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Butenal, 2-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- | CC(C=O)C=C/C1C(=CCCC1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Butenal, 2-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- | CC(C=O)=C/CC1C(=CCCC1(C)C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-butenal | CC(C=O)=C/CC1=C(C)CCCC1(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Penten-3-one, 1-(2,4,6-trimethyl-3-cyclohexen-1-yl)- | CCC(=O)/C=C/C1C(C)CC(=CC1C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | CC(C)=CCCC1=CCC(C)(CC1)C=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1,2,3,4,5,6,7,8-octahydro-8,8-dimethyl-2-naphthyl)ethan-1-one | O=C(C)C1CC2=C(CCCC2(C)C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,2,3,4,5,6,7,8-octahydro-2,8,8-trimethylnaphthalene-2-carbaldehyde | O=CC1(C)CC2=C(CCCC2(C)C)CC1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-methyl-3-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | O=CC1CC(=CCC1C)CCC=C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(p-tert-butylphenyl)butan-2-ol | OC(C)CCC1=CC=C(C=C1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1,2,3,4,6,7,8,8a-octahydro-8,8-dimethyl-2-naphthyl)ethan-1-one | O=C(C)C1CCC2=CCCC(C)(C)C2C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hexahydro-3,5,5-trimethyl-2H-2,4a-methanonaphthalen-1(5H)-one | O=C1C2CC3(CC2C)C1CCCC3(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Cyclohexene-1-carboxaldehyde, 1-methyl-3-(4-methyl-3-penten-1-yl)- | CC(C)=CCCC1=CCCC(C)(C1)C=O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2,6-bis(2-methylpropyl)- | CC(C)Cc1cccc(CC(C)C)c1O | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Penten-3-one, 1-(3,5,6-trimethyl-3-cyclohexen-1-yl)- | CCC(=O)/C=C/C1CC(=CC(C)C1C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Oxaspiro[4.5]deca-3,6-diene, 2,7-dimethyl-10-(1-methylethyl)- | CC(C)C1CCC(C)=CC11OC(C)C=C1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,5-Di-tert-butylphenol | CC(C)(C)c1cc(cc(O)c1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (1S-(1alpha(E),5beta))-1-(5-Isopropyl-2-methyl-2-cyclohexen-1-yl)-2-buten-1-one | CC=CC(=O)C1CC(CC=C1C)C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, p-isooctyl- | CC(C)CCCCCc1ccc(O)cc1 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dibutylphenol | CCCCc1cccc(O)c1CCCC | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 7,11-dimethyldodeca-4,6,10-trien-3-one | CCC(=O)/C=C/C=C(C)/CCC=C(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Oxaspiro[4,5]deca-3,6-diene,6-ethyl-2,10,10-trimethyl- | CCC1=CCCC(C)(C)C21OC(C)C=C2 | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2,5-bis(1,1-dimethylethyl)- | CC(C)(C)c1cc(O)c(cc1)C(C)(C)C | 206.16707 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4,7-Dimethylindan | CC1=CC=C(C)C2=C1CCC2 | 146.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1-Dimethylindan | CC1(C)CCc2ccccc12 | 146.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| p-Isopropylstyrene | CC(C)c1ccc(C=C)cc1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,4,6-Trimethylstyrene | Cc1cc(C)c(C=C)c(C)c1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Phenyl-1-pentene | CC(CC=C)C1=CC=CC=C1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-pentenylbenzene | C=1C=CC(=CC1)C=CCCC | 146.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1H-Indene, 2,3-dihydro-4,6-dimethyl- | CC1=CC2=C(CCC2)C(C)=C1 | 146.10955 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4,4a,5,6,7,8-hexahydro-6-(1-methylethyl)naphthalen-2(3H)-one | O=C1C=C2CCC(CC2CC1)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-3-en-2-one | O=C(C=CCC1CC=C(C)C1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| a-ethyl-5-isopropyl-2-methylbenzyl alcohol | OC(C1=CC(=CC=C1C)C(C)C)CC | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-[1-(1-methylethyl)allyl]cyclohex-2-ene-1-carbaldehyde | O=CC1C=CCCC1C(C=C)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| a,2-dimethyl-5-(1-methylvinyl)cyclohex-2-en-1-acetaldehyde | O=CC(C)C1C(=CCC(C(=C)C)C1)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)-2-butenal | O=CC=C(C)C1C2CCC(C2)C1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| a-methyl-4-(1-methylvinyl)cyclohexene-1-propan-1-al | O=CC(C)CC1=CCC(C(=C)C)CC1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| a,3,3-trimethyl-a-vinylbicyclo[2.2.1]hept-5-ene-2-methanol | OC(C=C)(C)C1C2C=CC(C2)C1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (1a,2ß,5ß)-4,5-dimethyl-2-(2-methylpropen-1-yl)cyclohex-3-ene-1-carbaldehyde | O=CC1CC(C(=CC1C=C(C)C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Butanone, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- | CC(=O)CCC1=C(C)C=CCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(2,4,4-Trimethyl-2-cyclohexenyl)-2-buten-1-one. | C/C=C/C(=O)C1CCC(C)(C)C=C1C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (Z)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one | CC=C/C(=O)C1C(=CCCC1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(4,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one | O=C(C=CC)C1CC=C(C)CC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Naphthalenecarboxaldehyde, 1,2,3,4,5,6,7,8-octahydro-5,5-dimethyl- | CC1(C)CCCC2=C1CCC(C2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,2,3,4,5,6,7,8-Octahydro-8,8-dimethyl-2-naphthaldehyde | CC1(C)CCCC2=C1CC(CC2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(4-Methyl-3-penten-1-yl)-3-cyclohexene-1-carbaldehyde | CC(C)=CCCC1=CCCC(C1)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 6-methyl-8-(1-methylethyl)- | CC(C)C1CC2C(CC1C=C2C)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 4-methyl-1-(1-methylethyl)- | CC(C)C12CCC(C)(CC1C=O)C=C2 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 1-methyl-4-(1-methylethyl)- | CC(C)C12CCC(C)(C=C1)C(C2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5(or 6)-Methyl-7(or 8)-(1-methylethyl)bicyclo[2.2.2]oct-5-ene-2-carbaldehyde | CC(C)C1CC2=C(C)CC1C(C2)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(4-Methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde | CC(C)=CCCC1=CCC(CC1)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Methylbutyl 2-phenylethyl ether | CC(C)CCOCCc1ccccc1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Octahydro-5,5-dimethylnaphthalene-2-carbaldehyde | CC1(C)CCC=C2CC(CCC12)C=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methyl-1-(4-methyl-3-cyclohexen-1-yl)pent-1-en-3-one | O=C(C(=CC1CC=C(C)CC1)C)CC | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3a,4,5,6,7,7a-hexahydro-6-methoxydimethyl-4,7-methano-1H-indene | O(C)C1CC2CC1C3C2C=CC3(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 7-isopropyl-5-methylbicyclo[2.2.2]oct-5-ene-2-carbaldehyde | O=CC1CC2C(=CC1C(C2)C(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6,10,10-tetramethyl-1-oxaspiro[4.5]deca-3,6-diene | O1C(C=CC12C(=CCCC2(C)C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-methyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-butenal | O=CC(=CCC1CC=C(C)C1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one | O=C(C)CC=CC1CC=C(C)C1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-allyl-octahydro-4,7-methano-1H-inden-5-ol | OC1(CC=C)CC2CC1C3CCCC23 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6,9,10-Tetramethyl-1-oxaspiro[4.5]deca-3,6-diene | CC1OC2(C=C1)C(C)C(C)CC=C2C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Heptylphenol | CCCCCCCC1=CC=C(C=C1)O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Buten-2-one, 4-(3,5,6-trimethyl-3-cyclohexen-1-yl)- | CC1C=C(C)CC(C=CC(C)=O)C1C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| α-Damascone | CC1=CCCC(C)(C)C1C(=O)CC=C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Methyl-9-(1-methylethylidene)bicyclo[3.3.1]nonan-2-one | [H]C12CCCC(C)(C(=O)CC1)C2=C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (4r,s)-4-(2-butyl)-cis-bicyclo[4.3.0]-2-nonen-8-one | CCC(C)C1CC2CC(=O)CC2C=C1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)- | CC=CC(=O)C1C(C)C=CCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (2E)- | CC=CC(=O)C1C(C)=CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (2Z)- | CC=C/C(=O)C1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- | CC(=O)C=CC1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [2-(2-methylbutoxy)ethyl]benzene | O(CCC=1C=CC=CC1)CC(C)CC | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3a,4,5,6-tetrahydro-1,3,3-trimethylindancarbaldehyde | O=CC1(C2=CCCCC2C(C)(C)C1)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3a,4,5,6-tetrahydro-2,2,3a-trimethylindancarbaldehyde | O=CC1C2=CCCCC2(C)CC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3a,4,5,6,7,7a-hexahydromethoxydimethyl-4,7-methano-1H-indene | O(C)C1(C(=CC2C3CCC(C3)C21)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,2-dimethyl-1-phenylpentan-3-ol | OC(CC)C(C)(C)CC=1C=CC=CC1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(2,4,6-Trimethyl-3-cyclohexen-1-yl)-3-buten-2-one | CC1CC(=CC(C)C1C=CC(C)=O)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| alpha-Ionone | CC(=O)/C=C/C1C(=CCCC1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-allyl-2,4,6-trimethylcyclohex-3-ene-1-carbaldehyde | O=CC1(CC=C)C(C=C(C)CC1C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Decahydrospiro[furan-2(3H),5'-[4,7]methano[5H]indene] | C1COC2(C1)CC3CC2C4CCCC34 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (2-(Pentyloxy)ethyl)benzene | CCCCCOCCc1ccccc1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 2-tert-butyl-4-isopropyl- | CC(C)c1cc(c(O)cc1)C(C)(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,6-Diisopropyl-3-methylphenol | CC(C)c1ccc(C)c(C(C)C)c1O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-Azulenemethanol, 1,2,3,3a,4,5,6,7(or 1,2,3,4,5,6,7,8)-octahydro-.alpha.,.alpha.,3,8-tetramethyl- | C[C@@H]1CC=C2[C@@H]1C[C@H](CO)CC=C2C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(3-Butenyl)-2,4,4-trimethylcyclohex-2-en-1-one | CC1=C(CCC=C)C(C)(C)CCC1=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(2,2-Dimethyl-6-methylenecyclohexyl)-3-buten-2-one | CC(=O)/C=C/C1C(=C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (4-methyl-3-pentenyl)cyclohexenecarbaldehyde | O=CC1=C(CCC=C(C)C)CCCC1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-butyraldehyde | O=CCCCC1=CCC2CC1C2(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(3,3-dimethyl-2-norbornyl)-3-buten-2-one | O=C(C=CC1C2CCC(C2)C1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(5,5-Dimethyl-1-cyclohexen-1-yl)pent-4-en-1-one | CC1(C)CCC=C(C1)C(=O)CCC=C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Isobutyl-2-isopropylphenol | CC(C)Cc1cc(C(C)C)c(O)cc1 | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ibuprofenol | CC(C)Cc1ccc(cc1)C(C)CO | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| beta-Ionone | CC(=O)C=CC1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6,7,8,8a-tetrahydro-2,5,5,8a-tetramethyl-5H-1-benzopyran | O1C(=CC=C2C1(C)CCCC2(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Pseudoionone | CC(C)=CCCC(C)=CC=CC(C)=O | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (2E)-1-[(1R,2S)-2,6,6-Trimethylcyclohex-3-en-1-yl]but-2-en-1-one | CC=CC(=O)C1C(C)C=CCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(2,2-dimethyl-6-methylenecyclohexyl)methacrylaldehyde | O=CC(=CC1C(=C)CCCC1(C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(2,6,6-trimethyl-2-cyclohexen-1-yl)methacrylaldehyde | O=CC(=CC1C(=CCCC1(C)C)C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Damascone | CC=CC(=O)C1=C(C)CCCC1(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (E,Z,Z)-trideca-2,4,7-trienal | O=CC=CC=CCC=CCCCCC | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (E)-3-(2-butenyl)-2,4,4-trimethylcyclohex-2-en-1-one | O=C1C(=C(CC=CC)C(C)(C)CC1)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diisopropyl-m-cresol | OC1=CC=C(C(=C1C(C)C)C)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-methyl-5-phenylhexan-3-ol | OC(CC)CC(C=1C=CC=CC1)(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(p-cumenyl)-2-methylpropanol | OCC(C)CC1=CC=C(C=C1)C(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| TP\_2690 | Cc1cc(c(O)c(C)c1C)C(C)(C)C | 192.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Chlorpheniramine,Â Desmethyl | CNCCC(c1ccc(Cl)cc1)c1ccccn1 | 260.10803 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1,3,3,5,5-hexamethyl-1,5-divinyltrisiloxane | O([Si](O[Si](C=C)(C)C)(C)C)[Si](C=C)(C)C | 260.10841 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Buturon | CC(C#C)N(C)C(=O)Nc1ccc(Cl)cc1 | 236.07164 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diacetoxydiethoxysilane | O=C(O[Si](OC(=O)C)(OCC)OCC)C | 236.07161 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(2-chloroethyl)-2,8-dimethyl-4H-pyrido[1,2-a]pyrimidin-4-one | O=C1C(=C(N=C2C=C(C=CN12)C)C)CCCl | 236.07164 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| oxybis(methyl-2,1-ethanediyl) diacrylate | CC(COCC(C)OC(=O)C=C)OC(=O)C=C | 242.11542 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Di(ethylene glycol) dimethacrylate | C(OC(C(C)=C)=O)COCCOC(C(C)=C)=O | 242.11542 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Propenoic acid, 2-ethyl-2-(hydroxymethyl)-1,3-propanediyl ester | CCC(CO)(COC(=O)C=C)COC(=O)C=C | 242.11542 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (4aalpha,5abeta,9aalpha,10abeta)-Octahydro-5aH,10aH-4a,9a-epoxydibenzo(b,e)(1,4)dioxin-5a,10a-diol | OC12CCCCC31OC1(O)CCCCC1(O2)O3 | 242.11542 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-hydroxy-1,6-hexanediyl diacrylate | O=C(OCCCCC(O)COC(=O)C=C)C=C | 242.11542 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tributyl citrate | CCCCOC(=O)CC(O)(CC(=O)OCCCC)C(=O)OCCCC | 360.21480 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Triisobutyl citrate | CC(C)COC(=O)CC(O)(CC(=O)OCC(C)C)C(=O)OCC(C)C | 360.21480 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dodecyl dihydrogen 2-hydroxypropane-1,2,3-tricarboxylate | O=C(O)CC(O)(C(=O)O)CC(=O)OCCCCCCCCCCCC | 360.21480 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tetracosahydrodibenz[b,n][1,4,7,10,13,16,19,22]octaoxacyclotetracosin | O1CCOCCOC2CCCCC2OCCOCCOCCOC3CCCCC3OCC1 | 460.30362 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 7-chloro-5-cyclohexyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one | O=C1NC=2C=CC(Cl)=CC2C(=NC1)C3CCCCC3 | 276.10294 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [3-(2,3-epoxypropoxy)propyl]triethoxysilane | O(CCC[Si](OCC)(OCC)OCC)CC1OC1 | 278.15495 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isooctyl [(2,3-dihydroxypropyl)thio]acetate | O=C(OCCCCCC(C)C)CSCC(O)CO | 278.15518 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 13,20,22-trihydroxy-8,14-dimethoxy-4,10,12,16-tetramethyl-3-oxo-19-[(prop-2-en-1-yl)amino]-2-azabicyclo[16.3.1]docosa-1(21),4,6,10,18(22),19-hexaen-9-yl carbamate | C=CCNc1c(O)cc2c(O)c1C[C@@H](C)C[C@H](OC)[C@H](O)[C@@H](C)C=C(C)[C@H](OC(N)=O)[C@@H](OC)C=CC=C(C)C(=O)N2 | 587.32067 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Merphos | CCCCSP(SCCCC)SCCCC | 298.10125 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(acryloyloxy)-1-propanesulfonic acid | OS(=O)(=O)CCCOC(=O)C=C | 194.02489 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Acetamide, N-(4-chlorophenyl)-2-cyano- | Clc1ccc(NC(=O)CC#N)cc1 | 194.02469 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Propenoic acid, 2-methyl-, 2-sulfoethyl ester, sodium salt | [Na+].CC(=C)C(=O)OCCS(=O)(=O)[O-] | 194.02489 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-chloro-2-(1H-pyrazol-3-yl)phenol | ClC=1C=CC(O)=C(C1)C2=NNC=C2 | 194.02469 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Sulphoethyl methacrylate | O=C(OC(C)S(=O)(=O)O)C(=C)C | 194.02489 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| sulphoethyl methacrylate | CC(=C)C(=O)OCCS(O)(=O)=O | 194.02489 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Perfluorooctanesulfonic acid | C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isooctanesulfonic acid, heptadecafluoro-, lithium salt | [Li+].[O-][S](=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tetrakis[(phosphonooxy)methyl]urea | OP(=O)(O)OCN(COP(=O)(O)O)C(=O)N(COP(=O)(O)O)COP(=O)(O)O | 499.93994 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Heptadecafluorooctane-2-sulfonic acid | OS(=O)(=O)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| D-Glucitol monoacetate monopalmitate | CCCCCCCCCCCCCCCC(=O)O[C@@H](COC(C)=O)[C@@H](O)[C@H](O)[C@H](O)CO | 462.31927 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| D-glucitol mono(12-hydroxyoleate) | O=C(OCC(O)C(O)C(O)C(O)CO)CCCCCCCC=CCC(O)CCCCCC | 462.31927 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| ST50987637 | O=C(NC1CCCCC1)Nc1ccc(Cc2ccc(NC(=O)NC3CCCCC3)cc2)cc1 | 448.28383 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| alpha-Amylcinnamyl alcohol | CCCCCC(CO)=Cc1ccccc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(4-Tert-Butylbenzyl)propionaldehyde | CC(Cc1ccc(cc1)C(C)(C)C)C=O | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4'-tert-Butyl-2',6'-dimethylacetophenone | CC(=O)c1c(C)cc(cc1C)C(C)(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(3-tert-Butylphenyl)-2-methylpropanal | CC(Cc1cccc(c1)C(C)(C)C)C=O | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Methyl-3-[4-(2-methylpropyl)phenyl]propanal | CC(C)Cc1ccc(CC(C)C=O)cc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzene, [2-(cyclohexyloxy)ethyl]- | C1CCC(CC1)OCCc2ccccc2 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,2,3,4,5,6,7,8,9,10-Decahydro-5,9-methanobenzocycloocten-11-one | CC1C2CCCC(C2=O)C3=C1CCCC3 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,4,4a,5,8,8a-Hexahydro-3',6-dimethylspiro[1,4-methanonaphthalene-2(1H),2'-oxirane] | CC1OC12CC3CC2C4CC=C(C)CC34 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,4,4a,5,8,8a-Hexahydro-3',7'-dimethylspiro[1,4-methanonaphthalene-2(1H),2'-oxirane] | CC1OC12CC3CC2C4CC(=CCC34)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Butanone, 3-methyl-2-(1-methylethyl)-1-phenyl- | CC(C)C(C(C)C)C(=O)c1ccccc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(Octahydro-5H-4,7-methanoinden-5-ylidene)butanal | O=CCCC=C1/CC2CC1C3CCCC23 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Cyclohexyl-2,6-xylenol | Cc1cc(cc(C)c1O)C1CCCCC1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Phenol, 4-methyl-2-(1-methylcyclohexyl)- | Cc1cc(c(O)cc1)C1(C)CCCCC1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Octanophenone | CCCCCCCC(=O)c1ccccc1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-Benzylcycloheptan-1-ol | OC1(Cc2ccccc2)CCCCCC1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(Dipropylamino)benzenediazonium tetrafluoroborate | [B+++].[F-].[F-].[F-].[F-].CCCN(CCC)c1ccc(cc1)[N+]#N | 204.15007 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1,3,3,6-Pentamethylindan-4-ol | Cc1cc2c(c(O)c1)C(C)(C)CC2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1,3,3,7-Pentamethylindan-5-ol | Cc1cc(O)cc2c1C(C)(C)CC2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cyclomenol [INN:DCF] | Cc1cc(O)c(C2CCCCC2)c(C)c1 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(1,1-Dimethylethyl)-5,6,7,8-tetrahydro-2-naphthol | CC(C)(C)c1c(O)ccc2c1CCCC2 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethanone, 1-[2-(1,1-dimethylethyl)-4,6-dimethylphenyl]- | CC(=O)c1c(cc(C)cc1C)C(C)(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Cyclopentyl-6-isopropylphenol | CC(C)c1cccc(C2CCCC2)c1O | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(3,4-Bis(1-methylethyl)phenyl)ethan-1-one | CC(C)c1c(cc(cc1)C(=O)C)C(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-(phenylmethyl)heptan-4-one | O=C(CCC)C(CC=1C=CC=CC1)CC | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bornelone | O=C(C=CC=C1C2CCC(C2)C1(C)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-methyl-4-(4-isopropylphenyl)butan-2-one | O=C(C)C(C)CC1=CC=C(C=C1)C(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tetraallyloxirane | O1C(CC=C)(CC=C)C1(CC=C)CC=C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,2,3,3',3a,4,4',6,7,7a-decahydrospiro[4,7-methano-5H-indene-5,2'-[2H]pyran] | O1C=CCCC12CC3CC2C4CCCC34 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(bicyclo[2.2.1]hept-5-en-2-ylmethylene)hexenal | O=CC(=CC1CC2C=CC1C2)CCCC | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-ethyl-1,3,3-trimethylindan-5-ol | OC1=CC=C2C(=C1)C(C)(C)CC2(C)CC | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(3,7,7-trimethylbicyclo[4.1.0]hept-3-en-2-yl)-2-buten-1-one | O=C(C=CC)C1C(=CCC2C1C2(C)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[2,4-bis(1-methylethyl)phenyl]ethan-1-one | O=C(C1=CC=C(C=C1C(C)C)C(C)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-tert-butyl-a-cyclopropylbenzyl alcohol | OC(C1=CC=C(C=C1)C(C)(C)C)C2CC2 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,1,2,3,3-pentamethylindan-5-ol | OC1=CC=C2C(=C1)C(C)(C)C(C)C2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3'a,4,4',5,6',7',7'a-octahydro-4-methylspiro[furan-2(3H),5'-[4,7]methano[5H]indene] | O1CC(C)CC12CC3CC2C4C=CCC43 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-2-naphthol | OC1CC2=CC=C(C=C2CC1)C(C)(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(4,7,7-trimethylbicyclo[4.1.0]hept-3-en-3-yl)-2-buten-1-one | O=C(C=CC)C1=C(C)CC2C(C1)C2(C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Butyl-1,2,3,4-tetrahydro-1-naphthol | OC1(C=2C=CC=CC2CCC1)CCCC | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(3a,4,5,6,7,7a-hexahydrodimethyl-4,7-methano-1H-indenyl)ethanone | O=C(C)C1(C(=CC2C3CCC(C3)C21)C)C | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-(4-methylphenyl)heptanal | O=CCCCC(C1=CC=C(C=C1)C)CC | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,3,3a,4,7,7a-hexahydro-a-methyl-4,7-methano-1H-indene-5-propionaldehyde | O=CC(C)CC1=CC2CC1C3CCCC23 | 204.15142 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Rimexolone | CCC(=O)[C@@]1(C)[C@H](C)CC2C3CCC4=CC(=O)C=C[C@]4(C)C3[C@@H](O)C[C@]12C | 370.25080 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-ethoxypregna-3,5-diene-21,17a-carbolactone | CCOC1=CC2=CC[C@H]3[C@@H]4CC[C@@]5(CCC(=O)O5)[C@@]4(C)CC[C@@H]3[C@@]2(C)CC1 | 370.25080 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 16-methyl-20-oxopregna-5,16-dien-3-ß-yl acetate | O=C(OC1CC2=CCC3C4CC(=C(C(=O)C)C4(C)CCC3C2(C)CC1)C)C | 370.25079 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3ß-hydroxypregna-5,16-dien-20-one 3-propionate | O=C(OC1CC2=CCC3C4CC=C(C(=O)C)C4(C)CCC3C2(C)CC1)CC | 370.25079 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-methyl-20-oxopregna-5,16-dien-3-ß-yl acetate | O=C(OC1CC2=C(C)CC3C4CC=C(C(=O)C)C4(C)CCC3C2(C)CC1)C | 370.25079 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Rimexolone | Vexol | CCC(=O)[C@@]1(C)[C@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C | 370.25079 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-Cyanopurine | N#Cc1ncnc2c1[nH]cn2 | 145.03885 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-[formyl(6-methoxyquinolin-8-yl)amino]pentanoic acid | COC1=CC2=CC=CN=C2C(=C1)N(C=O)C(C)CCC(O)=O | 302.12666 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-[(benzoyl-5-oxopyrrolidin-2-yl)carbonyl]morpholine | O=C(C=1C=CC=CC1)N2C(=O)CCC2C(=O)N3CCOCC3 | 302.12666 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dnc008126 | CC[C@@H](C)Nc1ncc(C(=O)Nc2cc(C(=O)NC)ccc2C)s1 | 346.14635 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dicofol | OC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl | 367.90960 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| o,p'-Dicofol | OC(c1ccc(Cl)cc1)(c1ccccc1Cl)C(Cl)(Cl)Cl | 367.90960 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Viminol | CCC(C)N(CC(O)c1cccn1Cc1ccccc1Cl)C(C)CC | 362.21249 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (9Z)-17-carboxy-9-heptadecene-1-sulfonic acid | OC(=O)CCCCCCCC=CCCCCCCCCS(O)(=O)=O | 362.21270 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-Fluoro ADB-PINACA | CC(C)(C)C(C(=O)N)NC(=O)C1=NN(C2=CC=CC=C21)CCCCCF | 362.21180 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-Fluoro ADB-PINACA isomer 2 | O=C(N[C@H](C(N)=O)[C@H](CC)C)C1=NN(CCCCCF)C2=C1C=CC=C2 | 362.21180 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-Fluoro-2-ADB-PINACA isomer 2 | CC[C@H](C)[C@@H](C(=O)N)NC(=O)c1c2ccccc2nn1CCCCCF | 362.21180 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Sodium hydrogen sulphonatooleate | [Na+].O=C([O-])C(CCCCCCC=CCCCCCCCC)S(=O)(=O)[O-] | 362.21270 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9-sulpho-9-octadecenoic acid | O=C(O)CCCCCCCC(=CCCCCCCCC)S(=O)(=O)O | 362.21270 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Sodium hydrogen 9-sulphonatooctadecenoate | [H+].[Na+].O=C([O-])C=CCCCCCC(CCCCCCCCC)S(=O)(=O)[O-] | 362.21270 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,4-Dioxaspiro[4.5]decane-2-methanol, 9-methyl-6-(1-methylethyl)- | CC(C)C1CCC(C)CC11OCC(CO)O1 | 228.17255 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Glycidyl neodecanoate | CCC(C)(CCC(C)C)C(=O)OCC1CO1 | 228.17255 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Propanoic acid, 2-hydroxy-, 5-methyl-2-(1-methylethyl)cyclohexyl ester | CC(C)C1CCC(C)CC1OC(=O)C(C)O | 228.17255 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-tert-Butylcyclohexyl ethyl carbonate | CCOC(=O)OC1CCCCC1C(C)(C)C | 228.17255 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-Methylbutyl 1-hydroxycyclohexaneacetate | CC(C)CCOC(=O)CC1(O)CCCCC1 | 228.17255 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 12-oxotridecanoic acid | O=C(O)CCCCCCCCCCC(=O)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dihydro-5-(5-methoxy-1,5-dimethylhexyl)furan-2(3H)-one | O=C1OC(CC1)C(C)CCCC(OC)(C)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl menthyl carbonate | O=C(OCC)OC1CC(C)CCC1C(C)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl 2-hydroxycyclopentanehexanoate | O=C(OCC)CCCCCC1CCCC1O | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl 2-acetylnonan-1-oate | O=C(OCC)C(C(=O)C)CCCCCCC | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 3-oxododecanoate | O=C(OC)CC(=O)CCCCCCCCC | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-dioxacyclopentadecan-2-one | O=C1OCCCCCCCCCCCCO1 | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-hydroxyethyl 2-(isopropyl)-5-methylcyclohexanecarboxylate | O=C(OCCO)C1CC(C)CCC1C(C)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl 1-hydroxy-3,3,5-trimethylcyclohexaneacetate | O=C(OCC)CC1(O)CC(C)CC(C)(C)C1 | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-ethylhexyl 4-oxovalerate | O=C(OCC(CC)CCCC)CCC(=O)C | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| neodecanoic acid, oxiranylmethyl ester;oxiran-2-ylmethyl 2,2-dimethyloctanoate;neodecanoic acid, oxiranylmethyl ester oxiran-2-ylmethyl 2,2-dimethyloctanoate | CCCCCCC(C)(C)C(=O)OCC1CO1 | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4s,6R-Dimethyl-7R-acetoxy-3-nonanone | CCC([C@@H](C)C[C@@H](C)[C@H](OC(C)=O)CC)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4s,6s-Dimethyl-7R-acetoxy-3-nonanone | CCC([C@@H](C)C[C@H](C)[C@H](OC(C)=O)CC)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4s,6s-Dimethyl-7s-acetoxy-3-nonanone | CCC([C@@H](C)C[C@H](C)[C@@H](OC(C)=O)CC)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| trans-5-Isopropyl-6,7-epoxy-8-hydroxy-8-methylnonan-2-one | CC(CCC(C(C)C)[C@H](O1)[C@@H]1C(C)(O)C)=O | 228.17254 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9,10-Anthracenedione, 1-amino-2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]-4-[(2,4,6-trimethylphenyl)amino]- | Cc1cc(C)c(Nc2cc(Oc3ccc(cc3)C(C)(C)CC(C)(C)C)c(N)c3c2C(=O)c2c(cccc2)C3=O)c(C)c1 | 560.30389 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzenediazonium, 4-(ethylamino)-3-methyl-, tetrafluoroborate(1-) | F[B-](F)(F)F.CCNc1c(C)cc(cc1)[N+]#N | 162.10312 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(ethylamino)-m-toluenediazonium trichlorozincate | N#[N+]C1=CC(=CC=C1NCC)C.Cl[Zn-](Cl)Cl | 162.10312 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(ethylamino)-2-methylbenzenediazonium hexafluoroarsenate | N#[N+]C1=CC=C(C=C1C)NCC.F[As-](F)(F)(F)(F)F | 162.10312 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Xanthurenic acid | C1=CC2=C(C(=C1)O)NC(=CC2=O)C(=O)O | 205.03751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Phthalylglycine | OC(=O)CN1C(=O)c2c(cccc2)C1=O | 205.03751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1H-Indole-2,7-dicarboxylic acid | OC(=O)c1cc2c([nH]1)c(ccc2)C(=O)O | 205.03751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Norverapamil | COc1ccc(CCNCCCC(C#N)(C(C)C)c2ccc(OC)c(OC)c2)cc1OC | 440.26751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-(3,4-dimethoxyphenyl)-5-{[2-(4-hydroxy-3-methoxyphenyl)ethyl](methyl)amino}-2-(propan-2-yl)pentanenitrile | COc1cc(CCN(C)CCCC(C#N)(C(C)C)c2ccc(OC)c(OC)c2)ccc1O | 440.26751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| M3 | COc1ccc(CCN(C)CCCC(C#N)(C(C)C)c2ccc(OC)c(OC)c2)cc1O | 440.26751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (+)-[3-cyano-3-(3,4-dimethoxyphenyl)hex-6-yl](5,6-dimethoxyphenethyl)methylammonium chloride | [Cl-].N#CC(C1=CC=C(OC)C(OC)=C1)(CC)CCC[NH+](C)CCC=2C=CC=C(OC)C2OC | 440.26751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (-)-[3-cyano-3-(3,4-dimethoxyphenyl)hex-6-yl][2-(3,4-dimethoxyphenyl)ethyl]methylammonium chloride | [Cl-].N#CC(C1=CC=C(OC)C(OC)=C1)(CC)CCC[NH+](C)CCC2=CC=C(OC)C(OC)=C2 | 440.26751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 6-{4-[(4-ethylpiperazin-1-yl)methyl]phenyl}-n-(1-phenylethyl)-7h-pyrrolo[2,3-d]pyrimidin-4-amine | CCN1CCN(Cc2ccc(-c3cc4c(N[C@H](C)c5ccccc5)ncnc4[nH]3)cc2)CC1 | 440.26885 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Norverapamil | COc1ccc(CCNCCC[C@](C#N)(c2ccc(OC)c(OC)c2)C(C)C)cc1OC | 440.26751 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diethyl 4,4'-[hexamethylenebis(oxy)]dibenzimidate | N=C(OCC)C1=CC=C(OCCCCCCOC2=CC=C(C=C2)C(=N)OCC)C=C1 | 412.23621 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-[2-(diethylamino)ethyl]-a-[(2,4,5-trimethoxyphenyl)methylene]phenylacetamide monohydrochloride | Cl.O=C(NCCN(CC)CC)C(=CC1=CC(OC)=C(OC)C=C1OC)C=2C=CC=CC2 | 412.23621 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tribufos | CCCCSP(=O)(SCCCC)SCCCC | 314.09616 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Tris(trimethylsilyl) phosphate | O=P(O[Si](C)(C)C)(O[Si](C)(C)C)O[Si](C)(C)C | 314.09548 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-(2,4-dichlorophenyl)-ß-methylpiperidin-1-propionamide monohydrochloride | Cl.O=C(NC1=CC=C(Cl)C=C1Cl)CC(N2CCCCC2)C | 314.09527 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Clibucaine | CC(CC(=O)Nc1ccc(cc1Cl)Cl)N2CCCCC2 | 314.09527 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-[(4-Cyclopropyl-5-hydroxy-4H-1,2,4-triazol-3-yl)sulfanyl]-1-(4-morpholinophenyl)-1-ethanone | C1CC1N2C(=O)NN=C2SCC(=O)C3=CC=C(C=C3)N4CCOCC4 | 360.12561 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-ethylhexyl 4-(2,4-dichlorophenoxy)butyrate | O=C(OCC(CC)CCCC)CCCOC1=CC=C(Cl)C=C1Cl | 360.12590 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isooctyl 4-(2,4-dichlorophenoxy)butyrate | O=C(OCCCCCC(C)C)CCCOC1=CC=C(Cl)C=C1Cl | 360.12590 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Nonyl 2-(2,4-dichlorophenoxy)propionate | O=C(OCCCCCCCCC)C(OC1=CC=C(Cl)C=C1Cl)C | 360.12590 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,4-Dioxane-2,3-diol | OC1OCCOC1O | 120.04226 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| L-Erythrose | OCC(O)C(O)C=O | 120.04226 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Trimethyl(methylthio)silane | S(C)[Si](C)(C)C | 120.04290 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Acetic acid, 2-hydroxy-2-methoxy-, methyl ester | O=C(OC)C(O)OC | 120.04226 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Digitoxigenin | C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@@]1(O)CC[C@@H]2C1=CC(=O)OC1 | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-ß,21-dihydroxypregn-5-en-20-one 21-acetate | O=C(OCC(=O)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Androst-5-ene-(3ß,17ß)-diyl diacetate | O=C(OC1CC2=CCC3C(CCC4(C)C(OC(=O)C)CCC34)C2(C)CC1)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-ß,17-a-dihydroxypregn-5-en-20-one 3-acetate | O=C(OC1CC2=CCC3C(CCC4(C)C3CCC4(O)C(=O)C)C2(C)CC1)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 11,20-dioxo-5-ß-pregnan-3-a-yl acetate | O=C(OC1CCC2(C)C3C(=O)CC4(C)C(C(=O)C)CCC4C3CCC2C1)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-hydroxy-20-oxo-5-pregnen-17a-yl acetate | O=C(OC1(C(=O)C)CCC2C3CC=C4CC(O)CCC4(C)C3CCC21C)C | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [3-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy]propyl](2-hydroxyethyl)dimethylammonium chloride | [Cl-].N#CC(=CC1=CC=C(C=C1)N(CC)CC)C(=O)OCCC[N+](C)(C)CCO | 374.24437 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [2-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy]ethyl](3-hydroxypropyl)dimethylammonium chloride | [Cl-].N#CC(=CC1=CC=C(C=C1)N(CC)CC)C(=O)OCC[N+](C)(C)CCCO | 374.24437 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-benzyl hydrogen 2-dodecenylsuccinate | O=C(OCC=1C=CC=CC1)CC(C(=O)[O-])CC=CCCCCCCCCC | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Rostafuroxin | C[C@]12CC[C@H](O)C[C@H]1CC[C@@H]1[C@@H]2CC[C@@]2(C)[C@]1(O)CC[C@]2(O)c1ccoc1 | 374.24571 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (5ß)-3ß,14-dihydroxycardanolide | O=C1OCC(C1)C2CCC3(O)C4CCC5CC(O)CCC5(C)C4CCC23C | 376.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (1-methylethylidene)di-4,1-cyclohexanediyl bismethacrylate | O=C(OC1CCC(CC1)C(C)(C)C2CCC(OC(=O)C(=C)C)CC2)C(=C)C | 376.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Hexyl nonyl phthalte | O=C(OCCCCCCCCC)C1=CC=CC=C1C(OCCCCCC)=O | 376.26140 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-{2-[(4-fluorophenyl)methyl]-1,3-dioxo-decahydropyrrolo[3,4-a]pyrrolizin-4-yl}benzene-1-carboximidamide | N=C(N)c1ccc([C@H]2[C@H]3C(=O)N(Cc4ccc(F)cc4)C(=O)[C@H]3[C@@H]3CCCN32)cc1 | 406.18050 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dicyclohexyl sulfosuccinic acid | OS(=O)(=O)C(CC(=O)OC1CCCCC1)C(=O)OC1CCCCC1 | 362.13992 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Marbofloxacin | Fc4cc1c2N(/C=C(C1=O)C(=O)O)N(COc2c4N3CCN(C)CC3)C | 362.13903 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-[2-(1-amino-2-hydroxypropyl)-4-[(4-fluoro-1h-indol-3-yl)methyl]-5-hydroxy-1h-imidazol-1-yl]acetic acid | C[C@H](O)[C@H](N)c1nc(Cc2c[nH]c3cccc(F)c23)c(O)n1CC(=O)O | 362.13903 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3'H-Cycloprop[15,16]androsta-6,15-dien-17-one, 3-(2,2-dimethyl-1-oxopropoxy)-15,16-dihydro-5-hydroxy-, (3ÃŸ,5ÃŸ,15a,16a)- | CC(C)(C)C(=O)O[C@H]1CC[C@]2(C)[C@H]3CC[C@@]4(C)[C@@H]([C@@H]5C[C@@H]5C4=O)[C@@H]3C=C[C@]2(O)C1 | 400.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (2S,4aR,4bS,6aS,7aS,8aS,8bS)-9-Hydroxy-4a,6a-dimethyl-7-oxo-1,2,3,4,4a,4b,5,6,6a,7,7a,8,8a,8b,8c,9-hexadecahydrocyclopropa[4,5]cyclopenta[1,2-a]phenanthren-2-yl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OC1CCC2(C)C3CCC4(C)C(C5CC5C4=O)C3C(O)C=C2C1 | 400.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,20-bis(ethylenedioxy)pregna-5,7-diene | CC12CCC3C(=CC=C4CC5(CCC34C)OCCO5)C1CCC2C1(C)OCCO1 | 400.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Heliotrope B | [Cl-].CCN(CC)C1=C[CH+]c2nc3ccc(cc3n(c3ccccc3)c2=C1)N(CC)CC | 400.26270 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 17-hydroxy-3-methoxy-6-methylpregna-3,5-dien-20-one acetate | O=C(OC1(C(=O)C)CCC2C3CC(=C4C=C(OC)CCC4(C)C3CCC21C)C)C | 400.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-ethoxy-17-hydroxypregna-3,5-dien-20-one 17-acetate | O=C(OC1(C(=O)C)CCC2C3CC=C4C=C(OCC)CCC4(C)C3CCC21C)C | 400.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Lenabasum | CCCCCCC(C)(C)c1cc(O)c2c(c1)OC(C)(C)[C@@H]1CC=C(C(=O)O)C[C@@H]21 | 400.26136 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-(4-Butyl-2-methylphenyl)-N&#39;-(2-chlorobenzoyl)urea | CCCCC1=CC(=C(C=C1)NC(=O)NC(=O)C2=CC=CC=C2Cl)C | 344.12916 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-(3-amino-2h-indazol-5-yl)-n-tert-butylbenzene-1-sulfonamide | CC(C)(C)NS(=O)(=O)c1ccc(-c2ccc3n[nH]c(N)c3c2)cc1 | 344.13070 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Fluprednidene acetate | CC(=O)OCC(=O)[C@@]1(O)C(=C)CC2C3CCC4=CC(=O)C=CC4(C)[C@@]3(F)C(O)CC12C | 432.19482 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9ß,11ß-epoxy-6a-fluoro-17,21-dihydroxy-16a-methylpregna-1,4-diene-3,20-dione 21-acetate | O=C1C=CC2(C(=C1)C(F)CC3C4CC(C)C(O)(C(=O)COC(=O)C)C4(C)CC5OC532)C | 432.19482 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[[4-[(dimethylphenyl)azo]dimethylphenyl]azo]-2-naphthol | OC=1C=CC=2C=CC=CC2C1N=NC3=CC=C(N=NC4=CC=CC(=C4C)C)C(=C3C)C | 408.19501 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[2,5-dimethyl-4-(2,5-dimethylphenylazo)phenylazo]-2-naphthol | OC=1C=CC=2C=CC=CC2C1N=NC3=CC(=C(N=NC4=CC(=CC=C4C)C)C=C3C)C | 408.19501 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-[[2,5-dimethyl-4-[(dimethylphenyl)azo]phenyl]azo]-2-naphthol | OC=1C=CC=2C=CC=CC2C1N=NC3=CC(=C(N=NC4=CC=CC(=C4C)C)C=C3C)C | 408.19501 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzoic acid, 2-[(octadecylamino)carbonyl]-, monosodium salt | [Na+].CCCCCCCCCCCCCCCCCCNC(=O)c1ccccc1C([O-])=O | 417.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (9E)-N-[2-(3,4-Dihydroxyphenyl)ethyl]octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)NCCC1=CC(=C(C=C1)O)O | 417.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| CB-52 | CCCCCCC1=C(C=C(C=C1)O)OCCCCCCCCCCC(=O)NC2CC2 | 417.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Cyclopropyl-8-[3-hydroxy-5-(2-methylheptan-2-yl)phenoxy]octanamide | CCCCCCC(C)(C)C1=CC(=CC(=C1)OCCCCCCCC(=O)NC2CC2)O | 417.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzoic acid, 4-[(octadecylamino)carbonyl]-, monosodium salt | [Na+].CCCCCCCCCCCCCCCCCCNC(=O)c1ccc(cc1)C(=O)[O-] | 417.32429 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,4-Benzenediol, 2,5-dioctyl- | CCCCCCCCc1cc(O)c(CCCCCCCC)cc1O | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-Benzenediol, 4-methyl-5-pentadecyl- | CCCCCCCCCCCCCCCc1c(C)c(O)cc(O)c1 | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diisooctylhydroquinone | CC(C)CCCCCc1c(CCCCCC(C)C)c(O)ccc1O | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,5-Bis(1,1,3,3-tetramethylbutyl)hydroquinone | CC(C)(C)CC(C)(C)c1cc(O)c(cc1O)C(C)(C)CC(C)(C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,5-diisooctylhydroquinone | OC=1C=C(C(O)=C(C1)CCCCCC(C)C)CCCCCC(C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bis(1,1,3,3-tetramethylbutyl)hydroquinone | OC1=CC=C(O)C(=C1C(C)(C)CC(C)(C)C)C(C)(C)CC(C)(C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Butyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate | O=C(OCCCC)CCCCCCCC=CCC=CCC=CCC | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9,12-octadecadienyl methacrylate | O=C(OCCCCCCCCC=CCC=CCCCCC)C(=C)C | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 8,11,14-Eicosatrienoic acid ethyl ester | CCCCC/C=CC/C=CC/C=CCCCCCCC(=O)OCC | 334.28718 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Elmustine | OCCNC(=O)N(CCCl)N=O | 195.04107 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,3-Dihydroxypropyl 3-(hexylthio)propionate | CCCCCCSCCC(=O)OCC(O)CO | 264.13953 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Carbamic acid, (hydroxymethyl)-, 2-hydroxyethyl ester | OCCOC(=O)NCO | 135.05316 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl dimethylolcarbamate | COC(=O)N(CO)CO | 135.05316 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzenamine, 2,4-dinitro-N-phenyl- | [O-][N+](=O)c1cc(c(Nc2ccccc2)cc1)[N+](=O)[O-] | 259.05931 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cloethocarb | CNC(=O)Oc1c(OC(CCl)OC)cccc1 | 259.06114 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Pyridine, 2-[(2,4-dinitrophenyl)methyl]- | [O-][N+](=O)c1cc(c(Cc2ncccc2)cc1)[N+](=O)[O-] | 259.05931 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Nitro-N-(4-nitrophenyl)aniline | [O-][N+](=O)c1ccc(Nc2ccc(cc2)[N+](=O)[O-])cc1 | 259.05931 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Nitro-N-(2-nitrophenyl)aniline | [O-][N+](=O)c1c(Nc2c(cccc2)[N+](=O)[O-])cccc1 | 259.05931 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4,4'-Dinitro-2-biphenylamine | Nc1cc(ccc1c1ccc(cc1)[N+](=O)[O-])[N+](=O)[O-] | 259.05931 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-Nitro-N-(4-nitrophenyl)aniline | [O-][N+](=O)c1ccc(Nc2c(cccc2)[N+](=O)[O-])cc1 | 259.05931 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-(4,6-Dichloro-1,3,5-triazin-2-yl)benzenesulphonamide | Clc1nc(NS(=O)(=O)c2ccccc2)nc(Cl)n1 | 303.95885 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (isopropylidene)bis(4,1-phenyleneoxyethylene) dilaurate | O=C(OCCOC1=CC=C(C=C1)C(C2=CC=C(OCCOC(=O)CCCCCCCCCCC)C=C2)(C)C)CCCCCCCCCCC | 680.50159 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Thioinosine | OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1cnc2c1[nH]cnc2=S | 284.05793 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3,9-diethoxy-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane | O(P1OCC2(CO1)COP(OCC)OC2)CC | 284.05786 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Testosterone enanthate | CCCCCCC(=O)OC1CCC2C1(CCC3C2CCC4=CC(=O)CCC34C)C | 400.29775 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3ß-hydroxyandrost-5-en-17-one heptanoate | O=C(OC1CC2=CCC3C4CCC(=O)C4(C)CCC3C2(C)CC1)CCCCCC | 400.29775 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Inecalcitol | C[C@H](CC#CC(C)(C)O)[C@H]1CC[C@@H]2/C(=C/C=C3C[C@@H](O)C[C@H](O)C3)CCC[C@@]21C | 400.29775 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Retinyl propionate | CCC(=O)OCC=C(/C)C=CC=C(/C)C=CC1=C(C)CCCC1(C)C | 342.25588 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (17ß)-17-allyl-3-methoxyandrosta-3,5-dien-17-ol | OC1(CC=C)CCC2C3CC=C4C=C(OC)CCC4(C)C3CCC21C | 342.25588 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Docosahexaenoic acid methyl ester | CC/C=CC/C=CC/C=CC/C=CC/C=CC/C=CCCC(=O)OC | 342.25588 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Toreforant | Cc1cc(C)c2nc(-c3cnc(NCCCC4CCN(C)CC4)nc3C)[nH]c2c1 | 392.26885 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Atenolol met 4 - 223 | O(c1ccc(CC(N)=O)cc1)CC(C=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bendiocarb | CNC(=O)Oc1cccc2OC(C)(C)Oc12 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2,4-Pyridinedicarboxylic acid, diethyl ester | CCOC(=O)c1ccnc(c1)C(=O)OCC | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dioxacarb | CNC(=O)Oc1ccccc1C1OCCO1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Acetyl-L-tyrosine | CC(=O)NC(Cc1ccc(O)cc1)C(O)=O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| L-Aspartic acid &#946;-benzyl ester | N[C@H](C(=O)O)CC(=O)OCc1ccccc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Benzyloxycarbonyl-beta-alanine | C1=CC=C(C=C1)COC(=O)NCCC(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-[3-(Dimethylamino)acryloyl]-4-hydroxy-6-methyl-2H-pyran-2-one | Cc1cc(c(c(=O)o1)C(=O)/C=C/N(C)C)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Mephenoxalone | COC1=CC=CC=C1OCC2CNC(=O)O2 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Benzyloxycarbonyl-L-alanine | C[C@H](NC(=O)OCc1ccccc1)C(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Butyl 4-nitrobenzoate | CCCCOC(=O)c1ccc(cc1)[N+](=O)[O-] | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl N-benzyloxycarbonylglycinate | COC(=O)CNC(=O)OCc1ccccc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diethyl dipicolinate | CCOC(=O)c1cccc(n1)C(=O)OCC | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzene, 1,4-dimethoxy-2-(2-nitro-1-propenyl)- | COc1cc(/C=C(C)/[N+](=O)[O-])c(OC)cc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Isopropyl 3-nitro-p-toluate | CC(C)OC(=O)c1cc(c(C)cc1)[N+](=O)[O-] | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Dimethyl 2,6-dimethylpyridine-3,5-dicarboxylate | COC(=O)c1cc(C(=O)OC)c(C)nc1C | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Benzylaminodiacetic acid | OC(=O)CN(CC(=O)O)Cc1ccccc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 4-acetamido-o-anisate | COC(=O)c1ccc(NC(=O)C)cc1OC | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Nitrophenyl trimethylacetate | CC(C)(C)C(=O)Oc1ccc(cc1)[N+](=O)[O-] | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Diethyl pyridine-3,5-dicarboxylate | CCOC(=O)c1cc(cnc1)C(=O)OCC | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 2-((ethoxycarbonyl)amino)benzoate | CCOC(=O)Nc1ccccc1C(=O)OC | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 3-((4-methoxyphenyl)amino)-3-oxopropionate | COC(=O)CC(=O)Nc1ccc(OC)cc1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-benzyl-DL-aspartic acid | O=C(O)CC(NCC=1C=CC=CC1)C(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-benzoyl-DL-threonine | O=C(O)C(NC(=O)C=1C=CC=CC1)C(O)C | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-aminobenzylsuccinic acid | O=C(O)CC(C(=O)O)CC1=CC=C(N)C=C1 | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Methyl 5-(acetylamino)-o-anisate | O=C(OC)C1=CC(=CC=C1OC)NC(=O)C | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| [2-(2,5-dimethoxyphenyl)-1-methyl-2-oxoethylidene]hydroxyammonium chloride | [Cl-].O=C(C1=CC(OC)=CC=C1OC)C(=[NH+]O)C | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-({[(1z)-(2-methoxyphenyl)methylidene]amino}oxy)propanoic acid | COc1ccccc1/C=NOCCC(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N-Acetyl-L-tyrosine | CC(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)O | 223.08446 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (+)-Taxifolin | C1=CC(=C(C=C1C2C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O | 304.05830 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Sodium 2,4-dihydroxy-5-[(4-nitrophenyl)azo]benzoate | [Na+].O=C([O-])C1=CC(N=NC2=CC=C(C=C2)[N+](=O)[O-])=C(O)C=C1O | 304.05696 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| (2R-trans)-2,3-dihydro-3,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4-benzopyrone | O=C1C2=CC=C(O)C=C2OC(C3=CC(O)=C(O)C(O)=C3)C1O | 304.05830 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 2-[(2-methyl-1-oxoallyl)oxy]ethyl 1,3-dihydro-1,3-dioxoisobenzofuran-5-carboxylate | O=C1OC(=O)C2=CC(=CC=C12)C(=O)OCCOC(=O)C(=C)C | 304.05830 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4H-1-Benzopyran-4-one, 2-(2,6-dihydroxyphenyl)-2,3-dihydro-3,5,7-trihydroxy-, (2R,3R)- | C1=CC(=C(C(=C1)O)[C@@H]2[C@H](C(=O)C3=C(C=C(C=C3O2)O)O)O)O | 304.05830 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| n:1:2 fluorotelomer betaine-related, n=3 | C[N+](CC(O)=O)(C)CCC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 532.07690 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 9,10-bis(acetoxy)octadecanoic acid | O=C(OC(CCCCCCCC(=O)O)C(OC(=O)C)CCCCCCCC)C | 400.28249 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-amino-N-(2,5-dichloropentyl)-5-(ethylsulphonyl)-2-methoxybenzamide | O=C(NCC(Cl)CCCCl)C=1C=C(C(N)=CC1OC)S(=O)(=O)CC | 396.06773 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,2-Benzenedicarboxamide, 4-nitro- | NC(=O)c1ccc(cc1C(=O)N)[N+](=O)[O-] | 209.04366 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,3-Benzenedicarboxamide, 5-nitro- | NC(=O)c1cc(cc(c1)C(=O)N)[N+](=O)[O-] | 209.04366 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3-{[(E)-(nitromethylidene)amino]amino}benzoic acid | OC(=O)C1=CC(NN=C[N+]([O-])=O)=CC=C1 | 209.04366 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 3beta,5alpha,6beta,17-Tetrahydroxy-16alpha-methylpregnan-20-one 3-acetate | C[C@@H]1C[C@H]2[C@@H]3C[C@@H](O)[C@@]4(O)C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@@]1(O)C(=O)C)OC(=O)C | 422.26684 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Mevinolinic Acid | CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H](O)C[C@@H](O)CC(=O)O)[C@H]21 | 422.26684 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 7-{2,6-Dimethyl-8-[(2-methylbutanoyl)oxy]-1,2,6,7,8,8a-hexahydro-1-naphthalenyl}-3,5-dihydroxyheptanoic acid | CCC(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 422.26684 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Docosahexaenoic acid ethyl ester | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)OCC | 356.27153 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-Hydroxyphenobarbital | CCC1(C(=O)NC(=O)NC1=O)c1ccc(O)cc1 | 248.07971 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 5-methyl-5-piperonylhydantoin | O=C1NC(=O)C(N1)(C)CC2=CC=C3OCOC3=C2 | 248.07971 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,2-dihydro-3-oxo-2-phenyl-3H-pyrazol-1-yl ethyl carbonate | O=C(ON1C=CC(=O)N1C=2C=CC=CC2)OCC | 248.07971 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Censavudine | C#C[C@@]1(CO)C=C[C@H](n2cc(C)c(=O)[nH]c2=O)O1 | 248.07971 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Topiroxostat | N#Cc1cc(-c2n[nH]c(-c3ccncc3)n2)ccn1 | 248.08104 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Ethyl (2E)-2-(3-acetyloxy-1H-pyridin-2-ylidene)-2-cyanoacetate | CCOC(=O)/C(=C/1C(=CC=CN1)OC(=O)C)/C#N | 248.07971 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1-(propan-2-yl)-3-(quinolin-6-yl)-1h-pyrazolo[3,4-d]pyrimidin-4-amine | CC(C)n1nc(-c2ccc3ncccc3c2)c2c(N)ncnc21 | 304.14364 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| CETETH-8 PHOSPHATE | CCCCCCCCCCCCCCCCOCCO[P](O)(O)=O | 366.25351 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| N,N,N',N',N'',N''-hexaallyl-1,3,5-triazine-2,4,6-triamine | N=1C(=NC(=NC1N(CC=C)CC=C)N(CC=C)CC=C)N(CC=C)CC=C | 366.25320 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| Bis(2-ethylhexyl) 2-hydroxyethyl phosphate | O=P(OCCO)(OCC(CC)CCCC)OCC(CC)CCCC | 366.25351 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 1,12-Octadecanediol, phosphate | O=P([O-])([O-])OCCCCCCCCCCCC(O)CCCCCC | 366.25351 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | L |
| 20-hydroxy LTB4 | C(CCC=CCC(C=CC=CC=CC(CCCC(=O)O)O)O)CCO | 352.22160 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 5(S)-HEPE | CCC=CCC=CCC=CCC=CC=CC(CCCC(=O)O)O | 318.21670 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| Eicosapentaenoic Acid | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O | 302.22220 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 9,10-Epoxystearic acid | CCCCCCCCC1C(O1)CCCCCCCC(=O)O | 298.24800 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 13(R)-HODE | CCCCCC(C=CC=CCCCCCCCC(=O)O)O | 296.23210 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| Inosine | C1=NC2=C(C(=O)N1)N=CN2C3C(C(C(O3)CO)O)O | 268.07820 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| Stearidonic Acid | CCC=CCC=CCC=CCC=CCCCCC(=O)O | 276.20600 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 12(R)HETE | CCCCCC=CCC(C=CC=CCC=CCCCC(=O)[O-])O | 320.23210 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 5(Z),11(Z),14(Z)-Eicosatrienoic acid | CCCCCC=CCC=CCCCCC=CCCCC(=O)O | 306.25300 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 13-OXOode | CCCCCC(=O)C=CC=CCCCCCCCC(=O)O | 294.21660 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| DL-b-Hydrosycaprylic acid |  | 160.10740 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 2-Hydroxyhexadecanoic acid | CCCCCCCCCCCCCCC(C(=O)O)O | 272.23240 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 11(S)-HEPE | CCC=CCC=CC=CC(CC=CCC=CCCCC(=O)O)O | 318.21670 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 7Z,10Z, 13Z,19z-Docosapentaenoic acid | CCC=CCC=CCC=CCC=CCC=CCCCCCC(=O)O | 330.25270 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| PGD2 | CCCCCC(C=CC1C(C(CC1=O)O)CC=CCCCC(=O)O)O | 352.22160 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| Methyl N-(a-methylbutyryl)glycine |  | 188.10210 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| Sorbic acid | CC=CC=CC(=O)O | 112.05190 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| lyso-PAF C16 | CCCCCCCCCCCCCCCCOCC(COP(=O)([O-])OCC[N+](C)(C)C)O | 482.35850 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| Choline | C[N+](C)(C)CCO | 104.10710 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 1-Palmitoyllysophosphatidylcholine | CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O | 496.33580 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| 1-O-Palmtoyl-2-O-acetyl-sn-glycero-3-phosphocholine |  | 538.34670 | Suspect screening | Canal | LC-HRMS | Repeated\_reference | N |
| CB52 | C1=CC(=C(C=C1Cl)C2=C(C=CC(=C2)Cl)Cl)Cl | 291.91886 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB49 | C1=CC(=C(C=C1Cl)Cl)C2=C(C=CC(=C2)Cl)Cl | 291.91886 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB66 | C1=CC(=C(C=C1C2=C(C=C(C=C2)Cl)Cl)Cl)Cl | 291.91886 | Suspect screening | Canal | GC-HRMS | In house | G |
| pentaCB |  | 325.87994 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB101 | C1=CC(=C(C=C1Cl)C2=CC(=C(C=C2Cl)Cl)Cl)Cl | 325.87994 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB87 | C1=CC(=C(C=C1Cl)C2=C(C(=C(C=C2)Cl)Cl)Cl)Cl | 325.87994 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB118 | C1=CC(=C(C=C1C2=CC(=C(C=C2Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| hexaCB a |  | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| hexaCB b |  | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB105 | C1=CC(=C(C=C1C2=C(C(=C(C=C2)Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| hexaCB c |  | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB156 | C1=CC(=C(C=C1C2=CC(=C(C(=C2Cl)Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| hexaCB d |  | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB153 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C=C2Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | In house | G |
| heptaCB a |  | 393.80198 | Suspect screening | Canal | GC-HRMS | In house | G |
| heptaCB b |  | 393.80198 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB180 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl | 393.80198 | Suspect screening | Canal | GC-HRMS | In house | G |
| heptaCB c |  | 393.80198 | Suspect screening | Canal | GC-HRMS | In house | G |
| octaCB a |  | 429.76009 | Suspect screening | Canal | GC-HRMS | In house | G |
| octaCB b |  | 429.76009 | Suspect screening | Canal | GC-HRMS | In house | G |
| CB194 | C1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl | 429.76009 | Suspect screening | Canal | GC-HRMS | In house | G |
| hexaBDE |  | 643.52961 | Suspect screening | Canal | GC-HRMS | In house | G |
| BDE154 | C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br | 643.52961 | Suspect screening | Canal | GC-HRMS | In house | G |
| BDE153 | C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 643.52961 | Suspect screening | Canal | GC-HRMS | In house | G |
| BDE100 | C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br | 563.62113 | Suspect screening | Canal | GC-HRMS | In house | G |
| BDE47 | C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br | 485.71063 | Suspect screening | Canal | GC-HRMS | In house | G |
| BDE49 | C1=CC(=C(C=C1Br)Br)OC2=C(C=CC(=C2)Br)Br | 485.71063 | Suspect screening | Canal | GC-HRMS | In house | G |
| BDE28 | C1=CC(=CC=C1OC2=C(C=C(C=C2)Br)Br)Br | 405.80214 | Suspect screening | Canal | GC-HRMS | In house | G |
| pp'DDE | C1=CC(=CC=C1C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 317.93459 | Suspect screening | Canal | GC-HRMS | In house | G |
| op'DDD | C1=CC=C(C(=C1)C(C2=CC=C(C=C2)Cl)C(Cl)Cl)Cl | 235.00758 | Suspect screening | Canal | GC-HRMS | In house | G |
| methyltriclosan | COC1=C(C=CC(=C1)Cl)OC2=C(C=C(C=C2)Cl)Cl | 301.96626 | Suspect screening | Canal | GC-HRMS | In house | G |
| fragment of HBCDD | C1CC(C(CCC(C(CCC(C1Br)Br)Br)Br)Br)Br | 398.87762 | Suspect screening | Canal | GC-HRMS | In house | G |
| Benzothiazole | C1=CC=CC2=C1N=CS2 |  | Suspect screening | Canal | GC-HRMS | Reference | G |
| Diphenyl sulfone | C2=C([S](=O)(=O)C1=CC=CC=C1)C=CC=C2 |  | Suspect screening | Canal | GC-HRMS | Reference | G |
| 3,5-di-tert-Butyl-4-hydroxybenzaldehyde | C1=C(C=O)C=C(C(=C1C(C)(C)C)O)C(C)(C)C |  | Suspect screening | Canal | GC-HRMS | Reference | G |
| Squalene | C(\C(=C\CC/C=C(/CC/C=C(/CCC=C(C)C)C)C)C)C/C=C(/CCC=C(C)C)C |  | Suspect screening | Canal | GC-HRMS | Reference | G |
| Benzenesulfonamide, N-butyl- | C1=CC(=CC=C1)[S](=O)(=O)NCCCC |  | Suspect screening | Canal | GC-HRMS | Reference | G |
| 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)- | CC(C1=CC(=O)C=C(C1=O)C(C)(C)C)(C)C |  | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB52 | C1=CC(=C(C=C1Cl)C2=C(C=CC(=C2)Cl)Cl)Cl | 291.91886 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB49 | C1=CC(=C(C=C1Cl)Cl)C2=C(C=CC(=C2)Cl)Cl | 291.91886 | Suspect screening | Canal | GC-HRMS | Reference | G |
| pentaCB |  | 325.87994 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB101 | C1=CC(=C(C=C1Cl)C2=CC(=C(C=C2Cl)Cl)Cl)Cl | 325.87994 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB87 | C1=CC(=C(C=C1Cl)C2=C(C(=C(C=C2)Cl)Cl)Cl)Cl | 325.87994 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB118 | C1=CC(=C(C=C1C2=CC(=C(C=C2Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | Reference | G |
| hexaCB a |  | 359.84096 | Suspect screening | Canal | GC-HRMS | Reference | G |
| hexaCB b |  | 359.84096 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB105 | C1=CC(=C(C=C1C2=C(C(=C(C=C2)Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | Reference | G |
| hexaCB c |  | 359.84096 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB156 | C1=CC(=C(C=C1C2=CC(=C(C(=C2Cl)Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB153 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C=C2Cl)Cl)Cl | 359.84096 | Suspect screening | Canal | GC-HRMS | Reference | G |
| heptaCB b |  | 393.80198 | Suspect screening | Canal | GC-HRMS | Reference | G |
| heptaCB c |  | 393.80198 | Suspect screening | Canal | GC-HRMS | Reference | G |
| octaCB a |  | 429.76009 | Suspect screening | Canal | GC-HRMS | Reference | G |
| octaCB b |  | 429.76009 | Suspect screening | Canal | GC-HRMS | Reference | G |
| CB194 | C1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl | 429.76009 | Suspect screening | Canal | GC-HRMS | Reference | G |
| BDE47 | C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br | 485.71063 | Suspect screening | Canal | GC-HRMS | Reference | G |
| pp'DDE | C1=CC(=CC=C1C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 317.93459 | Suspect screening | Canal | GC-HRMS | Reference | G |
| op'DDD | C1=CC=C(C(=C1)C(C2=CC=C(C=C2)Cl)C(Cl)Cl)Cl | 235.00758 | Suspect screening | Canal | GC-HRMS | Reference | G |
| methyltriclosan | COC1=C(C=CC(=C1)Cl)OC2=C(C=C(C=C2)Cl)Cl | 301.96626 | Suspect screening | Canal | GC-HRMS | Reference | G |
| 2,4-DDT | c1ccc(c(c1)C(c2ccc(cc2)Cl)C(Cl)(Cl)Cl)Cl | 351.91470 | Suspect screening | Canal | GC-HRMS | Reference | H |
| 4,4'-Dichlorobenzophenone | c1cc(ccc1C(=O)c2ccc(cc2)Cl)Cl | 249.99520 | Suspect screening | Canal | GC-HRMS | Reference | H |
| BDE 47 | C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br | 485.71110 | Suspect screening | Canal | GC-HRMS | Reference | H |
| Dicofol | OC(C1=CC=C(Cl)C=C1)(C1=CC=C(Cl)C=C1)C(Cl)(Cl)Cl | 367.90960 | Suspect screening | Canal | GC-HRMS | Reference | H |
| Hexachlorobenzene | ClC1=C(Cl)C(Cl)=C(Cl)C(Cl)=C1Cl | 281.81312 | Suspect screening | Canal | GC-HRMS | Reference | H |
| PCB 101 | ClC1=CC(=C(Cl)C=C1)C1=C(Cl)C=C(Cl)C(Cl)=C1 | 323.88339 | Suspect screening | Canal | GC-HRMS | Reference | H |
| PCB 138 | ClC1=CC(Cl)=C(C=C1Cl)C1=C(Cl)C(Cl)=C(Cl)C=C1 | 357.84442 | Suspect screening | Canal | GC-HRMS | Reference | H |
| PCB 153 | ClC1=CC(Cl)=C(C=C1Cl)C1=CC(Cl)=C(Cl)C=C1Cl | 357.84442 | Suspect screening | Canal | GC-HRMS | Reference | H |
| PCB 180 | ClC1=CC(Cl)=C(C=C1Cl)C1=C(Cl)C(Cl)=C(Cl)C(Cl)=C1 | 391.80544 | Suspect screening | Canal | GC-HRMS | Reference | H |
| PCB 52 | ClC1=CC(=C(Cl)C=C1)C1=C(Cl)C=CC(Cl)=C1 | 289.92236 | Suspect screening | Canal | GC-HRMS | Reference | H |
| 4-Androsten-9à-fluoro-17à-methyl-3à,6á,11á,17á-tetra-ol, tetra-trimethylsilyl |  | 207.1200 | Suspect screening | Canal | GC-HRMS | Reference | O |
| (22R)-21-Acetoxy-6à,11á-dihydroxy-16à,17à-propylmethylenedioxypregna-1,4-diene-3,20-dione |  | 253.2500 | Suspect screening | Canal | GC-HRMS | Reference | O |
| 17á-Acetoxy-1',1'-dicarboethoxy-1á,2á-dihydro-17à-methyl-3'H-cycloprop[1,2]-5à-androst-1-en-3-one |  | 103.0391 | Suspect screening | Canal | GC-HRMS | Reference | O |
| Cyclopropane, 1,1,2,3-tetramethyl- | CC1C(C)C1(C)C | 83.0491 | Suspect screening | Canal | GC-HRMS | Reference | O |
| (2,6,6-Trimethylcyclohex-1-enylmethanesulfonyl)benzene | O=S(C1=CC=CC=C1)(CC2=C(C)CCCC2(C)C)=O | 137.0963 | Suspect screening | Canal | GC-HRMS | Reference | O |
| Androst-8-en-3-ol, 4,4,14à-trimethyl-17-(2-bromo-1-methylethyl)- | C[C@@]12C(C(C)CBr)CC[C@@]1(C)C(CCC3C(C)(C)C(O)CC[C@]43C)=C4CC2 | 221.1319 | Suspect screening | Canal | GC-HRMS | Reference | O |
| Pregn-5-ene-3,8,11,12,14,20-hexol, (3á,11à,12á,14á,20R)- | C[C@@H](O)[C@H]1CC[C@@]2(O)[C@]3(O)CC=C4C[C@H](O)CC[C@]4(C)[C@@]3([H])[C@H](O)[C@H](O)[C@]12C | 112.0518 | Suspect screening | Canal | GC-HRMS | Reference | O |
| à-D-Galactopyranose, 6-O-(trimethylsilyl)-, cyclic 1,2:3,4-bis(butylboronate) | B1(OC2C(OC3C(C2O1)OB(O3)CCCC)CO[Si](C)(C)C)CCCC | 103.0388 | Suspect screening | Canal | GC-HRMS | Reference | O |
| D:A-Friedooleanan-7-one, 3-hydroxy- | CC1C(CCC2C1(CC(=O)C3C2(CCC4(C3(CCC5(C4CC(CC5)(C)C)C)C)C)C)C)O | 219.1745 | Suspect screening | Canal | GC-HRMS | Reference | O |
| 9-Hydroxy-2,2-dimethyl-dec-5-en-3-one | CC(C)(C)C(CC=CCCC(O)C)=O | 95.0493 | Suspect screening | Canal | GC-HRMS | Reference | O |
| L-Valine | O=C(O)C(N)C(C)C | 117.07919 | Suspect screening | Lake | LC-HRMS | In house | C |
| Allopurinol | O=C1NC=NC=2NN=CC12 | 136.03867 | Suspect screening | Lake | LC-HRMS | In house | C |
| Niacinamide | O=C(N)C=1C=NC=CC1 | 122.04832 | Suspect screening | Lake | LC-HRMS | In house | C |
| Creatinine | O=C1NC=NC2=C1C=NN2C3OC(CO)C(O)C3O | 113.05928 | Suspect screening | Lake | LC-HRMS | In house | C |
| Allopurinol | O=C1N=C(N)N(C)C1 | 136.03867 | Suspect screening | Lake | LC-HRMS | In house | C |
| 4H-3a,7-Methanoazulen-4-one, 1,2,3,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, (3R,3aR,7S,8aS)- | O=C1NC=NC=2NN=CC12 | 218.16722 | Suspect screening | Lake | LC-HRMS | In house | C |
| Exo-(+/-)-1-methyl-4-(1-methylethyl)-2-[(2-methylphenyl)methoxy]-7-oxabicyclo[2.2.1]heptane | O=C(O)CC1(CN)CCCCC1 | 274.19335 | Suspect screening | Lake | LC-HRMS | In house | C |
| Dehydroepiandrosterone | O=C(NC=1C=CC=CC1)N(C)C | 288.20906 | Suspect screening | Lake | LC-HRMS | In house | C |
| 4,4'-(2-Ethylhexane-1,1-diyl)diphenol | OC1(CCCCC1)C(C2=CC=C(OC)C=C2)CN(C)C | 298.19339 | Suspect screening | Lake | LC-HRMS | In house | C |
| Drofenine | OCC12CCC(=CC2OC3CC(O)C1(C)C43OC4)C | 317.23552 | Suspect screening | Lake | LC-HRMS | In house | C |
| Spiroxamine | O=C1C=C(C)C2CC13C(C)CCC3C2(C)C | 297.26671 | Suspect screening | Lake | LC-HRMS | In house | C |
| Linoleic acid | CCCCCC=CCC=CCCCCCCCC(=O)O | 280.24041 | Suspect screening | Lake | LC-HRMS | In house | C |
| Docosahexaenoic acid | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O | 328.24020 | Suspect screening | Lake | LC-HRMS | In house | D |
| Eicosapentaenoic acid | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O | 302.22460 | Suspect screening | Lake | LC-HRMS | In house | D |
| 2-Ethylhexanoic anhydride | CCCCC(CC)C(=O)OC(=O)C(CC)CCCC | 270.21950 | Suspect screening | Lake | LC-HRMS | In house | D |
| 12,13-epoxy-9Z-octadecenoic acid | CCCCCC1C(O1)CC=CCCCCCCCC(=O)O | 296.23510 | Suspect screening | Lake | LC-HRMS | In house | D |
| 9-Oxononanoic acid | C(CCCC=O)CCCC(=O)O | 172.10990 | Suspect screening | Lake | LC-HRMS | In house | D |
| Docosa-4,8,12,15,19-pentaenoic acid | CCC=CCCC=CCC=CCCC=CCCC=CCCC(=O)O | 330.25590 | Suspect screening | Lake | LC-HRMS | In house | D |
| 11-Aoctadecenoic acid | CCCCCCC=CCCCCCCCCCC(=O)O | 282.25590 | Suspect screening | Lake | LC-HRMS | In house | D |
| Azelaic acid | C(CCCC(=O)O)CCCC(=O)O | 188.10490 | Suspect screening | Lake | LC-HRMS | In house | D |
| 4-oxonon-2-enoic Acid | CCCCCC(=O)C=CC(=O)O | 170.09430 | Suspect screening | Lake | LC-HRMS | In house | D |
| 7-Ketooctanoic acid | CC(=O)CCCCCC(=O)O | 158.09430 | Suspect screening | Lake | LC-HRMS | In house | D |
| Propanoic acid, 3-(2-butoxyethoxy)- | CCCCOCCOCCC(=O)O | 190.12050 | Suspect screening | Lake | LC-HRMS | In house | D |
| Butyl 3-hydroxy-3-4-dimethyl-5-(2-6-6-trimethyl-2-cyclohexen-1-yl)pent-4-en-1-oate | CCCCOC(=O)CC(C)(/C(=C/C1C(=CCCC1(C)C)C)/C)O | 322.25080 | Suspect screening | Lake | LC-HRMS | In house | D |
| Methoxydienone | CCC12CCC3C(C1CCC2=O)CCC4=C3CC=C(C4)OC | 300.20890 | Suspect screening | Lake | LC-HRMS | In house | D |
| 1-2-dimethyl-3-(2-6-6-trimethyl-2-cyclohexen-1-yl)propen-1-yl acetate | CC1=CCCC(C1/C=C(\C)/C(C)OC(=O)C)(C)C | 250.19330 | Suspect screening | Lake | LC-HRMS | In house | D |
| Linolenic acid | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O | 278.22460 | Suspect screening | Lake | LC-HRMS | In house | D |
| Dihydro-3-(tetrapropenyl)-2,5-furandione | CC(C)CC(C)CC(C)C=C(C)C1CC(=O)OC1=O | 266.18820 | Suspect screening | Lake | LC-HRMS | In house | D |
| Cyclopropanecarboxylic acid- 2-[1-(3-3-dimethylcyclohexyl)ethoxy]-2-methylpropyl ester | CC(C1CCCC(C1)(C)C)OC(C)(C)COC(=O)C2CC2 | 296.23510 | Suspect screening | Lake | LC-HRMS | In house | D |
| Methoprene | CC(C)OC(=O)C=C(C)C=CCC(C)CCCC(C)(C)OC | 310.25080 | Suspect screening | Lake | LC-HRMS | In house | D |
| 13-keto-9Z,11E-octadecadienoic acid | CCCCCC(=O)C=CC=CCCCCCCCC(=O)O | 294.21950 | Suspect screening | Lake | LC-HRMS | In house | D |
| Prednienic acid | CC12CC(C3C(C1CCC2(C(=O)O)O)CCC4=CC(=O)C=CC34C)O | 346.17800 | Suspect screening | Lake | LC-HRMS | In house | D |
| Leucylproline | CC(C)CC(C(=O)N1CCCC1C(=O)O)N | 228.14740 | Suspect screening | Lake | LC-HRMS | In house | D |
| (R)-1-phenylpropylamine  BMPEA  3-Phenylpropylamine  N-Methylphenethylamine  N-Ethylbenzylamin  benzyldimethylamine  N-Ethyl-4-methylaniline | CCC(C1=CC=CC=C1)N  CC(CN)C1=CC=CC=C1  NCCCC1=CC=CC=C1  CNCCC1=CC=CC=C1  CCNCC1=CC=CC=C1  CN(C)CC1=CC=CC=C1 | 135.10480 | Suspect screening | Lake | LC-HRMS | In house | I |
| N-Allylcyclohexylamine | C=CCNC1CCCCC1 | 139.13610 | Suspect screening | Lake | LC-HRMS | In house | I |
| 1-Naphthol | OC1=CC=CC2=CC=CC=C12 | 144.05751 | Suspect screening | Lake | LC-HRMS | In house | I |
| N,N,3,5-Tetramethylaniline | CN(C)C1=CC(C)=CC(C)=C1 | 149.12045 | Suspect screening | Lake | LC-HRMS | In house | I |
| Tetrahydro-1,3,5,5-tetramethyl-1H-pyrimidin-2-one | CN1CC(C)(C)CN(C)C1=O | 156.12626 | Suspect screening | Lake | LC-HRMS | In house | I |
| 1-[(1R,2S)-2,6,6-trimethylcyclohex-3-en-1-yl]ethanone | CC1C=CCC(C1C(=O)C)(C)C | 166.13577 | Suspect screening | Lake | LC-HRMS | In house | I |
| Levetiracetam | CC[C@H](N1CCCC1=O)C(N)=O | 170.10553 | Suspect screening | Lake | LC-HRMS | In house | I |
| 3-[(4R)-4-(propan-2-yl)cyclohex-1-en-1-yl]propanal | CC(C)C1CCC(=CC1)CCC=O | 180.15142 | Suspect screening | Lake | LC-HRMS | In house | I |
| methyprylon | CCC1(CC)C(=O)NCC(C)C1=O | 183.12593 | Suspect screening | Lake | LC-HRMS | In house | I |
| 1-(1H-Indol-3-yl)butan-1-one 3-(3-Oxobutyl)-1H-indole | CCCC(=O)C1=CNC2=CC=CC=C12 CC(=O)CCc1c[nH]c2c1cccc2 | 187.09971 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2,2,5,7-Tetramethylindan-1-one | CC1=CC(C)=C2C(CC(C)(C)C2=O)=C1 | 188.12012 | Suspect screening | Lake | LC-HRMS | In house | I |
| Benzamide, N,N-diethyl-4-methyl- or DEET | CCN(CC)C(=O)C1=CC=C(C=C1)C | 191.13101 | Suspect screening | Lake | LC-HRMS | In house | I |
| Benzyl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OCC1=CC=CC=C1 | 192.11503 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-[(3-aminopyrazolo[1,5-a]pyridin-2-yl)oxy]ethanol, hydrochloride | C1=CC2=C(C(=NN2C=C1)OCCO)N | 193.08513 | Suspect screening | Lake | LC-HRMS | In house | I |
| Gabapentin | NCC1(CC(O)=O)CCCCC1 | 171.12593 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-Amino-5-isopentyl-6-methylpyrimidin-4-ol | CC1=C(C(=O)NC(=N1)N)CCC(C)C | 195.13716 | Suspect screening | Lake | LC-HRMS | In house | I |
| Methyl 2-acetyl-2-allylpent-4-ene-1-oate | COC(=O)C(CC=C)(CC=C)C(C)=O | 196.10994 | Suspect screening | Lake | LC-HRMS | In house | I |
| 4-Octylmorpholine | CCCCCCCCN1CCOCC1 | 199.19361 | Suspect screening | Lake | LC-HRMS | In house | I |
| alpha,alpha-Dicyclopropyl-4-methylbenzyl alcohol | CC1=CC=C(C=C1)C(O)(C1CC1)C1CC1 | 202.13577 | Suspect screening | Lake | LC-HRMS | In house | I |
| N-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Lake | LC-HRMS | In house | I |
| 3,3'-[butane-1,4-diylbis(oxy)]bispropanamine | C(CCOCCCN)COCCCN | 204.18378 | Suspect screening | Lake | LC-HRMS | In house | I |
| N,N-Dibutylaniline | CCCCN(CCCC)C1=CC=CC=C1 | 205.18305 | Suspect screening | Lake | LC-HRMS | In house | I |
| Ibuprofen | CC(C)CC1=CC=C(C=C1)C(C)C(O)=O | 206.13068 | Suspect screening | Lake | LC-HRMS | In house | I |
| 4-tert-octylphenol | CC(C)(C)CC(C)(C)c1ccc(cc1)O | 206.16707 | Suspect screening | Lake | LC-HRMS | In house | I |
| MDEA / 3,4-Methylenedioxyethamphetamine | CCNC(C)CC1=CC2=C(C=C1)OCO2 | 207.12593 | Suspect screening | Lake | LC-HRMS | In house | I |
| 3-Ethyl-3-phenylpentane-1,5-diol | CCC(CCO)(CCO)C1=CC=CC=C1 | 208.14633 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2,4,4,7-Tetramethylnona-6,8-dien-3-one oxime | CC(C)C(=NO)C(C)(C)CC=C(C)C=C | 209.17796 | Suspect screening | Lake | LC-HRMS | In house | I |
| 3-(Decyloxy)propionitrile 3-(isodecyloxy)propiononitrile | CCCCCCCCCCOCCC#N CC(C)CCCCCCCOCCC#N | 211.19361 | Suspect screening | Lake | LC-HRMS | In house | I |
| hexaminolevulinic acid | CCCCCCOC(=O)CCC(=O)CN | 215.15214 | Suspect screening | Lake | LC-HRMS | In house | I |
| 4-tert-butyl-3-hydroxy-2,6-xylylacetonitrile | CC1=CC(=C(C(=C1CC#N)C)O)C(C)(C)C | 217.14666 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Lake | LC-HRMS | In house | I |
| Ritalinic acid | OC(=O)C(C1CCCCN1)C1=CC=CC=C1 | 219.12593 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-(3,4-dimethoxyphenyl)-3-methylbutyronitrile | COC1=CC=C(C=C1OC)C(C#N)C(C)C | 219.12593 | Suspect screening | Lake | LC-HRMS | In house | I |
| Precocene II | COC1=CC2=C(C=CC(C)(C)O2)C=C1OC | 220.10994 | Suspect screening | Lake | LC-HRMS | In house | I |
| Benzoic acid, 2-amino-, hexyl ester | CCCCCCOC(=O)C1=CC=CC=C1N | 221.14158 | Suspect screening | Lake | LC-HRMS | In house | I |
| 3,4-methylenedioxypropylamphetamine | CCCNC(C)CC1=CC2=C(C=C1)OCO2 | 221.14158 | Suspect screening | Lake | LC-HRMS | In house | I |
| ethyl 2-allyl-2-cyano-3-methylhexanoate | CCCC(C)C(CC=C)(C#N)C(=O)OCC | 223.15723 | Suspect screening | Lake | LC-HRMS | In house | I |
| 7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole | CCC12COC(N1C(OC2)C(C)C)C(C)C | 227.18853 | Suspect screening | Lake | LC-HRMS | In house | I |
| (2S)-1-(tert-butoxycarbonyl)-4-oxopyrrolidine-2-carboxylic acid | CC(C)(C)OC(=O)N1CC(=O)CC1C(=O)O | 229.09502 | Suspect screening | Lake | LC-HRMS | In house | I |
| diethyl 4-oxopentane-1,2-dicarboxylate | CCOC(=O)CC(CC(=O)C)C(=O)OCC | 230.11542 | Suspect screening | Lake | LC-HRMS | In house | I |
| (Acetylazanediyl)di(ethane-2,1-diyl) diacetate | CC(=O)OCCN(CCOC(C)=O)C(C)=O | 231.11067 | Suspect screening | Lake | LC-HRMS | In house | I |
| 5,6,7,8-Tetrahydro-gamma-oxonaphthalene-2-butyric acid | OC(=O)CCC(=O)C1=CC2=C(CCCC2)C=C1 | 232.10994 | Suspect screening | Lake | LC-HRMS | In house | I |
| Pentylone Dibutylone | CCCC(NC)C(=O)C1=CC=C2OCOC2=C1 CCC(N(C)C)C(=O)C1=CC=C2OCOC2=C1 | 235.12084 | Suspect screening | Lake | LC-HRMS | In house | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Lake | LC-HRMS | In house | I |
| viloxazine | CCOC1=C(OCC2CNCCO2)C=CC=C1 | 237.13649 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate | CC1(COC(=O)C2CC=CCC2C(=O)OC1)C | 238.12051 | Suspect screening | Lake | LC-HRMS | In house | I |
| N-Dodecylacrylamide | CCCCCCCCCCCCNC(=O)C=C | 239.22491 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-((2-Methyl-1-oxoallyl)oxy)ethyl 6-hydroxyhexanoate | CC(=C)C(=O)OCCOC(=O)CCCCCO | 244.13107 | Suspect screening | Lake | LC-HRMS | In house | I |
| Celestolide | CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C | 244.18272 | Suspect screening | Lake | LC-HRMS | In house | I |
| Bisnortilidin | CCOC(=O)C1(CCC=CC1N)C2=CC=CC=C2 | 245.14158 | Suspect screening | Lake | LC-HRMS | In house | I |
| Ethyl 1-benzylpiperidine-4-carboxylate | CCOC(=O)C1CCN(CC2=CC=CC=C2)CC1 | 247.15723 | Suspect screening | Lake | LC-HRMS | In house | I |
| alprenolol | CC(C)NCC(O)COC1=C(CC=C)C=CC=C1 | 249.17288 | Suspect screening | Lake | LC-HRMS | In house | I |
| (Z)-9-Cycloheptadecen-1-one. | O=C1CCCCCCC\C=C/CCCCCCC1 | 250.22967 | Suspect screening | Lake | LC-HRMS | In house | I |
| Tricyclo(3.3.1.13,7)dec-1,3-diyldi(acetic acid) | [H]C12CC3([H])CC(CC(O)=O)(C1)CC(CC(O)=O)(C2)C3 | 252.13616 | Suspect screening | Lake | LC-HRMS | In house | I |
| Ifosfamide | ClCCNP1(=O)OCCCN1CCCl | 260.02482 | Suspect screening | Lake | LC-HRMS | In house | I |
| N-(3-Acetyl-4-hydroxyphenyl)heptan-1-amide | CCCCCCC(=O)NC1=CC(C(C)=O)=C(O)C=C1 | 263.15214 | Suspect screening | Lake | LC-HRMS | In house | I |
| 7-Aminonimetazepam | CN1C(=O)CN=C(C2=C1C=CC(=C2)N)C3=CC=CC=C3 | 265.12151 | Suspect screening | Lake | LC-HRMS | In house | I |
| N-Tetradecylacrylamide | CCCCCCCCCCCCCCNC(=O)C=C | 267.25621 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-(3,5-dimethylhex-3-en-2-yloxy)-2-methylpropyl cyclopropanecarboxylate | CC(C)C=C(C)C(C)OC(C)(C)COC(=O)C1CC1 | 268.20384 | Suspect screening | Lake | LC-HRMS | In house | I |
| Tridecyl methacrylate Isotridecyl methacrylate tetradecyl acrylate | CCCCCCCCCCCCCOC(=O)C(C)=C CC(C)CCCCCCCCCCOC(=O)C(C)=C CCCCCCCCCCCCCCOC(=O)C=C | 268.24023 | Suspect screening | Lake | LC-HRMS | In house | I |
| N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine | COCCCNCC1=CC(OC)=C(OC)C(OC)=C1 | 269.16271 | Suspect screening | Lake | LC-HRMS | In house | I |
| Decyl 5-oxo-L-prolinate | CCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 269.19909 | Suspect screening | Lake | LC-HRMS | In house | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Lake | LC-HRMS | In house | I |
| Octanoic anhydride | CCCCCCCC(=O)OC(=O)CCCCCCC | 270.21949 | Suspect screening | Lake | LC-HRMS | In house | I |
| Alphameprodine [INN:BAN:DCF] | CC[C@H]1CN(C)CC[C@]1(OC(=O)CC)C1=CC=CC=C1 | 275.18853 | Suspect screening | Lake | LC-HRMS | In house | I |
| Venlafaxine | COC1=CC=C(C=C1)C(CN(C)C)C1(O)CCCCC1 | 277.20418 | Suspect screening | Lake | LC-HRMS | In house | I |
| Terbucarb | CNC(=O)OC1=C(C=C(C)C=C1C(C)(C)C)C(C)(C)C | 277.20418 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-(Decanoylamino)ethanesulfonic acid | CCCCCCCCCC(=O)NCCS(O)(=O)=O | 279.15043 | Suspect screening | Lake | LC-HRMS | In house | I |
| Brefeldin A | [H][C@@]12C[C@H](O)C[C@@]1([H])[C@H](O)\C=C\C(=O)O[C@@H](C)CCC\C=C\2 | 280.16746 | Suspect screening | Lake | LC-HRMS | In house | I |
| p-(1-(p-Pentylphenyl)vinyl)anisole | CCCCCC1=CC=C(C=C1)C(=C)C1=CC=C(OC)C=C1 | 280.18272 | Suspect screening | Lake | LC-HRMS | In house | I |
| Methyl 3-oxohexadecanoate | CCCCCCCCCCCCCC(=O)CC(=O)OC | 284.23514 | Suspect screening | Lake | LC-HRMS | In house | I |
| Sodium N-methyl-N-(1-oxododecyl)-ß-alaninate | CCCCCCCCCCCC(=O)N(O)CCC(=O)[O-]·[Na+] | 285.23039 | Suspect screening | Lake | LC-HRMS | In house | I |
| norethisterone | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C | 298.19328 | Suspect screening | Lake | LC-HRMS | In house | I |
| Sodium decyl phthalate diisopentyl phthalate CROMOPHTAL DPP RED TFP | [Na+].CCCCCCCCCCOC(=O)C1=CC=CC=C1C([O-])=O CC(C)CCOC(=O)C1=CC=CC=C1C(=O)OCCC(C)C CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCC | 306.18311 | Suspect screening | Lake | LC-HRMS | In house | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Lake | LC-HRMS | In house | I |
| Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate | COC(C)(C)CCCC(C)C\C=C\C(\C)=C\C(=O)OC(C)C | 310.25079 | Suspect screening | Lake | LC-HRMS | In house | I |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Lake | LC-HRMS | In house | I |
| homodihydrocapsaicin-I | CC(C)CCCCCCCC(=O)NCC1=CC(=C(C=C1)O)OC | 321.23039 | Suspect screening | Lake | LC-HRMS | In house | I |
| 15-(tert-Butyl)-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecine | CC(C)(C)C1=CC2=C(C=C1)OCCOCCOCCOCCO2 | 324.19367 | Suspect screening | Lake | LC-HRMS | In house | I |
| hydrogen N-(1-oxododecyl)-L-glutamic acid | CCCCCCCCCCCC(=O)NC(CCC(=O)O)C(=O)O | 329.22022 | Suspect screening | Lake | LC-HRMS | In house | I |
| ETHYL ARACHIDONATE | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OCC | 332.27153 | Suspect screening | Lake | LC-HRMS | In house | I |
| Pentadecyl 5-oxo-L-prolinate | CCCCCCCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 339.27734 | Suspect screening | Lake | LC-HRMS | In house | I |
| MEGESTROL | [H][C@@]12CC[C@](O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(C)C2=CC(=O)CC[C@]12C | 342.21949 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-Hydroxypropane-1,3-diyl bis(2-propylvalerate) | CCCC(CCC)C(=O)OCC(O)COC(=O)C(CCC)CCC | 344.25627 | Suspect screening | Lake | LC-HRMS | In house | I |
| Bis(tert-butyl) 1,4-dihydro-2,6-dimethyl-4-propylpyridine-3,5-dicarboxylate | CCCC1C(C(=O)OC(C)(C)C)=C(C)NC(C)=C1C(=O)OC(C)(C)C | 351.24096 | Suspect screening | Lake | LC-HRMS | In house | I |
| GLYCERYL LINOLENATE | CCC=CCC=CCC=CCCCCCCCC(=O)OCC(O)CO | 352.26136 | Suspect screening | Lake | LC-HRMS | In house | I |
| Diflufenican | FC1=CC=C(NC(=O)C2=C(OC3=CC(=CC=C3)C(F)(F)F)N=CC=C2)C(F)=C1 | 394.07407 | Suspect screening | Lake | LC-HRMS | In house | I |
| eplerenone | COC(=O)[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@@]23O[C@@H]2C[C@@]2(C)[C@@H](CC[C@@]22CCC(=O)O2)[C@H]13 | 414.20424 | Suspect screening | Lake | LC-HRMS | In house | I |
| Budesonide | CCCC1O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)C=C[C@]5(C)[C@H]4[C@@H](O)C[C@]3(C)[C@@]2(O1)C(=O)CO | 430.23554 | Suspect screening | Lake | LC-HRMS | In house | I |
| Isodecyl isononyl phthalate Decyl nonyl phthalate | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC© CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC | 432.32396 | Suspect screening | Lake | LC-HRMS | In house | I |
| LAURETH-12 | CCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO | 714.51294 | Suspect screening | Lake | LC-HRMS | In house | I |
| Glyceryl phosphate | OCC(O)COP(O)(O)=O | 172.01367 | Suspect screening | Lake | LC-HRMS | In house | I |
| Acamprosate | CC(=O)NCCCS(O)(=O)=O | 181.04088 | Suspect screening | Lake | LC-HRMS | In house | I |
| Sulfuric acid, monohexyl ester, sodium salt | [Na+].CCCCCCOS([O-])(=O)=O | 182.06128 | Suspect screening | Lake | LC-HRMS | In house | I |
| 4-morpholineethanesulfonic acid | OS(=O)(=O)CCN1CCOCC1 | 195.05653 | Suspect screening | Lake | LC-HRMS | In house | I |
| 3-Amino-4-methoxybenzenesulfonic acid 2-Amino-5-methoxybenzenesulfonic acid 5-Amino-6-hydroxytoluene-3-sulphonic acid | COC1=CC=C(C=C1N)S(O)(=O)=O COC1=CC(=C(N)C=C1)S(O)(=O)=O CC1=CC(=CC(N)=C1O)S(O)(=O)=O | 203.02523 | Suspect screening | Lake | LC-HRMS | In house | I |
| 3-morpholin-4-ylpropane-1-sulfonic acid | C1COCCN1CCCS(=O)(=O)O | 209.07218 | Suspect screening | Lake | LC-HRMS | In house | I |
| Icaridine | CCC(C)OC(=O)N1CCCCC1CCO | 229.16779 | Suspect screening | Lake | LC-HRMS | In house | I |
| 1-(2,5-Dihydroxyphenyl)octan-1-one | CCCCCCCC(=O)C1=C(O)C=CC(O)=C1 | 236.14124 | Suspect screening | Lake | LC-HRMS | In house | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Lake | LC-HRMS | In house | I |
| Loxoprofen alcohol | CC(C1=CC=C(C=C1)CC2CCCC2O)C(=O)O | 248.14124 | Suspect screening | Lake | LC-HRMS | In house | I |
| Propachlor ESA | CC(C)N(C(=O)CS(O)(=O)=O)C1=CC=CC=C1 | 257.07218 | Suspect screening | Lake | LC-HRMS | In house | I |
| Hydroxypethidine | CCOC(=O)C1(CCN(C)CC1)C1=CC(O)=CC=C1 | 263.15214 | Suspect screening | Lake | LC-HRMS | In house | I |
| Ethyl 3-(3,4,5-trimethoxyphenyl)propionate Butyl 3,4,5-trimethoxybenzoate | CCOC(=O)CCC1=CC(OC)=C(OC)C(OC)=C1 CCCCOC(=O)C1=CC(OC)=C(OC)C(OC)=C1 | 268.13107 | Suspect screening | Lake | LC-HRMS | In house | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Lake | LC-HRMS | In house | I |
| Triadimefon | CC(C)(C)C(=O)C(OC1=CC=C(Cl)C=C1)N1C=NC=N1 | 293.09310 | Suspect screening | Lake | LC-HRMS | In house | I |
| tetradecyl sulfonic acid Myristyl sulfate | CCCCC(CC)CCC(CC(C)C)OS(O)(=O)=O CCCCCCCCCCCCCCOS(O)(=O)=O | 294.18648 | Suspect screening | Lake | LC-HRMS | In house | I |
| Efavirenz | FC(F)(F)[C@]1(OC(=O)NC2=CC=C(Cl)C=C12)C#CC1CC1 | 315.02739 | Suspect screening | Lake | LC-HRMS | In house | I |
| Triaziflam | CC(COC1=CC(C)=CC(C)=C1)N=C1NC(=N)N=C(N1)C(C)(C)F | 333.19649 | Suspect screening | Lake | LC-HRMS | In house | I |
| cefaloram | CC(=O)OCC1=C(N2[C@H](SC1)[C@H](NC(=O)CC1=CC=CC=C1)C2=O)C(O)=O | 390.08856 | Suspect screening | Lake | LC-HRMS | In house | I |
| NONOXYNOL-4 | CCCCCCCCCC1=CC=CC=C1OCCOCCOCCOCCO | 396.28757 | Suspect screening | Lake | LC-HRMS | In house | I |
| simvastatin hydroxyl acid | CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 436.28249 | Suspect screening | Lake | LC-HRMS | In house | I |
| Bis(p-(1,1,3,3-tetramethylbutyl)phenyl) hydrogen phosphate | CC(C)(C)CC(C)(C)C1=CC=C(OP(O)(=O)OC2=CC=C(C=C2)C(C)(C)CC(C)(C)C)C=C1 | 474.28990 | Suspect screening | Lake | LC-HRMS | In house | I |
| GLIMEPIRIDE | CCC1=C(C)CN(C(=O)NCCC2=CC=C(C=C2)S(=O)(=O)NC(=O)N[C@H]2CC[C@H](C)CC2)C1=O | 490.22499 | Suspect screening | Lake | LC-HRMS | In house | I |
| Perfluorooctanesulfonic acid | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Lake | LC-HRMS | In house | I |
| N-Ethylperfluorooctane-1-sulfonamide | CCNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 526.98478 | Suspect screening | Lake | LC-HRMS | In house | I |
| Isodecyl undecyl phthalate Decyl isoundecyl phthalate Decyl undecyl phthalate | CCCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCC(C)C CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C CCCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCCC | 460.35526 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-Methylene-3-butyn-1-ol 1-Methoxybut-1-en-3-yne | OCC(=C)C#C COC=CC#C | 82.04186 | Suspect screening | Lake | LC-HRMS | In house | I |
| 2-(1,1-Dimethylethyl)-4-(1-methyl-1-phenylethyl)phenol | CC(C)(C)C1=C(O)C=CC(=C1)C(C)(C)C1=CC=CC=C1 | 268.18272 | Suspect screening | Lake | LC-HRMS | In house | I |
| 4-O-Desmethyl 4-O-Ethyl Trimethoprim | CCOC1=C(OC)C=C(CC2=CNC(=N)NC2=N)C=C1OC | 304.15354 | Suspect screening | Lake | LC-HRMS | In house | I |
| L-Valine | O=C(O)C(N)C(C)C | 117.07919 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Allopurinol | O=C1NC=NC=2NN=CC12 | 136.03867 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Niacinamide | O=C(N)C=1C=NC=CC1 | 122.04832 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Allopurinol riboside | O=C1NC=NC2=C1C=NN2C3OC(CO)C(O)C3O | 268.08074 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Creatinine | O=C1N=C(N)N(C)C1 | 113.05928 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Allopurinol | O=C1NC=NC=2NN=CC12 | 136.03867 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Gabapentin | O=C(O)CC1(CN)CCCCC1 | 171.12599 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Fenuron | O=C(NC=1C=CC=CC1)N(C)C | 164.09508 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Venlafaxine met 2-248 | OC1(CCCCC1)C(C2=CC=C(OC)C=C2)CN(C)C | 248.14129 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Verrucarol | OCC12CCC(=CC2OC3CC(O)C1(C)C43OC4)C | 266.15185 | Suspect screening | Lake | LC-HRMS | Reference | C |
| 4H-3a,7-Methanoazulen-4-one, 1,2,3,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, (3R,3aR,7S,8aS)- | O=C1C=C(C)C2CC13C(C)CCC3C2(C)C | 218.16722 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Dehydroepiandrosterone | O=C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C | 288.20906 | Suspect screening | Lake | LC-HRMS | Reference | C |
| 4,4'-(2-Ethylhexane-1,1-diyl)diphenol | OC1=CC=C(C=C1)C(C2=CC=C(O)C=C2)C(CC)CCCC | 298.19339 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Drofenine | CCN(CC)CCOC(=O)C(C1CCCCC1)C2=CC=CC=C2 | 317.23552 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Linoleic acid | CCCCCC=CCC=CCCCCCCCC(=O)O | 280.24041 | Suspect screening | Lake | LC-HRMS | Reference | C |
| Docosahexaenoic acid | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O | 328.24020 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Eicosapentaenoic acid | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O | 302.22460 | Suspect screening | Lake | LC-HRMS | Reference | D |
| 2-Ethylhexanoic anhydride | CCCCC(CC)C(=O)OC(=O)C(CC)CCCC | 270.21950 | Suspect screening | Lake | LC-HRMS | Reference | D |
| 12,13-epoxy-9Z-octadecenoic acid | CCCCCC1C(O1)CC=CCCCCCCCC(=O)O | 296.23510 | Suspect screening | Lake | LC-HRMS | Reference | D |
| 9-Oxononanoic acid | C(CCCC=O)CCCC(=O)O | 172.10990 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Docosa-4,8,12,15,19-pentaenoic acid | CCC=CCCC=CCC=CCCC=CCCC=CCCC(=O)O | 330.25590 | Suspect screening | Lake | LC-HRMS | Reference | D |
| 11-Aoctadecenoic acid | CCCCCCC=CCCCCCCCCCC(=O)O | 282.25590 | Suspect screening | Lake | LC-HRMS | Reference | D |
| 4-oxonon-2-enoic Acid | CCCCCC(=O)C=CC(=O)O | 170.09430 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Propanoic acid, 3-(2-butoxyethoxy)- | CCCCOCCOCCC(=O)O | 190.12050 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Butyl 3-hydroxy-3-4-dimethyl-5-(2-6-6-trimethyl-2-cyclohexen-1-yl)pent-4-en-1-oate | CCCCOC(=O)CC(C)(/C(=C/C1C(=CCCC1(C)C)C)/C)O | 322.25080 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Methoxydienone | CCC12CCC3C(C1CCC2=O)CCC4=C3CC=C(C4)OC | 300.20890 | Suspect screening | Lake | LC-HRMS | Reference | D |
| 1-2-dimethyl-3-(2-6-6-trimethyl-2-cyclohexen-1-yl)propen-1-yl acetate | CC1=CCCC(C1/C=C(\C)/C(C)OC(=O)C)(C)C | 250.19330 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Linolenic acid | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O | 278.22460 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Mibolerone | CC1=C(C=C(C=C1)C(C)(C)OOC(C)(C)C2=CC=CC=C2)C(C)C | 326.22460 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Cyclopropanecarboxylic acid- 2-[1-(3-3-dimethylcyclohexyl)ethoxy]-2-methylpropyl ester | CC(C1CCCC(C1)(C)C)OC(C)(C)COC(=O)C2CC2 | 296.23510 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Laurocapram | CCCCCCCCCCCCN1CCCCCC1=O | 281.27190 | Suspect screening | Lake | LC-HRMS | Reference | D |
| Ethyl thiocyanate | CCSC#N | 87.01427 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 6-Methylhepta-3,5-dien-2-one. | CC(C)=CC=CC(C)=O | 124.08881 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 1-Naphthol | OC1=CC=CC2=CC=CC=C12 | 144.05751 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Fenuron | CN(C)C(=O)NC1=CC=CC=C1 | 164.09496 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 1-[(1R,2S)-2,6,6-trimethylcyclohex-3-en-1-yl]ethanone | CC1C=CCC(C1C(=O)C)(C)C | 166.13577 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Octyl thiocyanate | CCCCCCCCSC#N | 171.10817 | Suspect screening | Lake | LC-HRMS | Reference | I |
| methyprylon | CCC1(CC)C(=O)NCC(C)C1=O | 183.12593 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 1-(1H-Indol-3-yl)butan-1-one 3-(3-Oxobutyl)-1H-indole | CCCC(=O)C1=CNC2=CC=CC=C12 CC(=O)CCc1c[nH]c2c1cccc2 | 187.09971 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Benzyl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OCC1=CC=CC=C1 | 192.11503 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Methyl 2-acetyl-2-allylpent-4-ene-1-oate | COC(=O)C(CC=C)(CC=C)C(C)=O | 196.10994 | Suspect screening | Lake | LC-HRMS | Reference | I |
| alpha,alpha-Dicyclopropyl-4-methylbenzyl alcohol | CC1=CC=C(C=C1)C(O)(C1CC1)C1CC1 | 202.13577 | Suspect screening | Lake | LC-HRMS | Reference | I |
| N-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 3,3'-[butane-1,4-diylbis(oxy)]bispropanamine | C(CCOCCCN)COCCCN | 204.18378 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Ibuprofen | CC(C)CC1=CC=C(C=C1)C(C)C(O)=O | 206.13068 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 4-tert-octylphenol | CC(C)(C)CC(C)(C)c1ccc(cc1)O | 206.16707 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 4-tert-butyl-3-hydroxy-2,6-xylylacetonitrile | CC1=CC(=C(C(=C1CC#N)C)O)C(C)(C)C | 217.14666 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-(3,4-dimethoxyphenyl)-3-methylbutyronitrile | COC1=CC=C(C=C1OC)C(C#N)C(C)C | 219.12593 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Precocene II | COC1=CC2=C(C=CC(C)(C)O2)C=C1OC | 220.10994 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 3,4-methylenedioxypropylamphetamine | CCCNC(C)CC1=CC2=C(C=C1)OCO2 | 221.14158 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 3-Phenyl-2,3-dihydro-1,3-benzothiazol-2-imine | C1=CC=C(C=C1)N2C3=CC=CC=C3SC2=N | 226.05647 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Tetradecanamide N,N-dimethyldodecanamide | CCCCCCCCCCCC(=O)N(C)C CCCCCCCCCCCC(=O)N(C)C | 227.22491 | Suspect screening | Lake | LC-HRMS | Reference | I |
| (2S)-1-(tert-butoxycarbonyl)-4-oxopyrrolidine-2-carboxylic acid | CC(C)(C)OC(=O)N1CC(=O)CC1C(=O)O | 229.09502 | Suspect screening | Lake | LC-HRMS | Reference | I |
| diethyl 4-oxopentane-1,2-dicarboxylate | CCOC(=O)CC(CC(=O)C)C(=O)OCC | 230.11542 | Suspect screening | Lake | LC-HRMS | Reference | I |
| (Acetylazanediyl)di(ethane-2,1-diyl) diacetate | CC(=O)OCCN(CCOC(C)=O)C(C)=O | 231.11067 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 5,6,7,8-Tetrahydro-gamma-oxonaphthalene-2-butyric acid | OC(=O)CCC(=O)C1=CC2=C(CCCC2)C=C1 | 232.10994 | Suspect screening | Lake | LC-HRMS | Reference | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Suspect screening | Lake | LC-HRMS | Reference | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Lake | LC-HRMS | Reference | I |
| viloxazine | CCOC1=C(OCC2CNCCO2)C=CC=C1 | 237.13649 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate | CC1(COC(=O)C2CC=CCC2C(=O)OC1)C | 238.12051 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-((2-Methyl-1-oxoallyl)oxy)ethyl 6-hydroxyhexanoate | CC(=C)C(=O)OCCOC(=O)CCCCCO | 244.13107 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Celestolide | CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C | 244.18272 | Suspect screening | Lake | LC-HRMS | Reference | I |
| (Z)-9-Cycloheptadecen-1-one. | O=C1CCCCCCC\C=C/CCCCCCC1 | 250.22967 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Tricyclo(3.3.1.13,7)dec-1,3-diyldi(acetic acid) | [H]C12CC3([H])CC(CC(O)=O)(C1)CC(CC(O)=O)(C2)C3 | 252.13616 | Suspect screening | Lake | LC-HRMS | Reference | I |
| N-(dodecyl)pyrrolidinone | CCCCCCCCCCCCN1CCCC1=O | 253.24056 | Suspect screening | Lake | LC-HRMS | Reference | I |
| LAURYL HYDROXYETHYL IMIDAZOLINE | CCCCCCCCCCCC1=NCCN1CCO | 268.25146 | Suspect screening | Lake | LC-HRMS | Reference | I |
| N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine | COCCCNCC1=CC(OC)=C(OC)C(OC)=C1 | 269.16271 | Suspect screening | Lake | LC-HRMS | Reference | I |
| N-(2-ethylhexyl)isononan-1-amide | CCCCC(CC)CNC(=O)CCCCCC(C)C | 269.27186 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Alphameprodine [INN:BAN:DCF] | CC[C@H]1CN(C)CC[C@]1(OC(=O)CC)C1=CC=CC=C1 | 275.18853 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Terbucarb | CNC(=O)OC1=C(C=C(C)C=C1C(C)(C)C)C(C)(C)C | 277.20418 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-((Dimethylamino)methyl)-4-isononylphenol | CC(C)CCCCCCC1=CC(CN(C)C)=C(O)C=C1 | 277.24056 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Brefeldin A | [H][C@@]12C[C@H](O)C[C@@]1([H])[C@H](O)\C=C\C(=O)O[C@@H](C)CCC\C=C\2 | 280.16746 | Suspect screening | Lake | LC-HRMS | Reference | I |
| p-(1-(p-Pentylphenyl)vinyl)anisole | CCCCCC1=CC=C(C=C1)C(=C)C1=CC=C(OC)C=C1 | 280.18272 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2,5-bis(tert-butylperoxy)-2,5-dimethylhexane | CC(C)(C)OOC(C)(C)CCC(C)(C)OOC(C)(C)C | 290.24571 | Suspect screening | Lake | LC-HRMS | Reference | I |
| norethisterone | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C | 298.19328 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Sodium decyl phthalate diisopentyl phthalate CROMOPHTAL DPP RED TFP | [Na+].CCCCCCCCCCOC(=O)C1=CC=CC=C1C([O-])=O CC(C)CCOC(=O)C1=CC=CC=C1C(=O)OCCC(C)C CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCC | 306.18311 | Suspect screening | Lake | LC-HRMS | Reference | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate | COC(C)(C)CCCC(C)C\C=C\C(\C)=C\C(=O)OC(C)C | 310.25079 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 15-(tert-Butyl)-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecine | CC(C)(C)C1=CC2=C(C=C1)OCCOCCOCCOCCO2 | 324.19367 | Suspect screening | Lake | LC-HRMS | Reference | I |
| hydrogen N-(1-oxododecyl)-L-glutamic acid | CCCCCCCCCCCC(=O)NC(CCC(=O)O)C(=O)O | 329.22022 | Suspect screening | Lake | LC-HRMS | Reference | I |
| ETHYL ARACHIDONATE | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OCC | 332.27153 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Pentadecyl 5-oxo-L-prolinate | CCCCCCCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 339.27734 | Suspect screening | Lake | LC-HRMS | Reference | I |
| MEGESTROL | [H][C@@]12CC[C@](O)(C(C)=O)[C@@]1(C)CC[C@@]1([H])[C@@]2([H])C=C(C)C2=CC(=O)CC[C@]12C | 342.21949 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-Hydroxypropane-1,3-diyl bis(2-propylvalerate) | CCCC(CCC)C(=O)OCC(O)COC(=O)C(CCC)CCC | 344.25627 | Suspect screening | Lake | LC-HRMS | Reference | I |
| GLYCERYL LINOLENATE | CCC=CCC=CCC=CCCCCCCCC(=O)OCC(O)CO | 352.26136 | Suspect screening | Lake | LC-HRMS | Reference | I |
| (Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine | CCCCCCCCC=CCCCCCCCC(=O)N(C)CC(=O)O | 353.29299 | Suspect screening | Lake | LC-HRMS | Reference | I |
| N-Phenyloctadecanamide | CCCCCCCCCCCCCCCCCC(=O)NC1=CC=CC=C1 | 359.31881 | Suspect screening | Lake | LC-HRMS | Reference | I |
| N-Stearylbenzylamine | CCCCCCCCCCCCCCCCCCNCC1=CC=CC=C1 | 359.35520 | Suspect screening | Lake | LC-HRMS | Reference | I |
| PALMITOYL GLUTAMIC ACID | CCCCCCCCCCCCCCCC(=O)N[C@@H](CCC(O)=O)C(O)=O | 385.28282 | Suspect screening | Lake | LC-HRMS | Reference | I |
| eplerenone | COC(=O)[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@@]23O[C@@H]2C[C@@]2(C)[C@@H](CC[C@@]22CCC(=O)O2)[C@H]13 | 414.20424 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Isodecyl isononyl phthalate Decyl nonyl phthalate | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC© CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC | 432.32396 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Glyceryl phosphate | OCC(O)COP(O)(O)=O | 172.01367 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Acamprosate | CC(=O)NCCCS(O)(=O)=O | 181.04088 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 3-Hydroxyphthalic acid 4-Hydroxybenzene-1,2-dicarboxylic acid | OC(=O)C1=C(C(O)=O)C(O)=CC=C1 OC(=O)C1=C(C=C(O)C=C1)C(O)=O | 182.02152 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 4-morpholineethanesulfonic acid | OS(=O)(=O)CCN1CCOCC1 | 195.05653 | Suspect screening | Lake | LC-HRMS | Reference | I |
| benzothiazole sulfonic acid | C1=CC=C2C(=C1)N=C(S2)S(=O)(=O)O | 214.97108 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Icaridine | CCC(C)OC(=O)N1CCCCC1CCO | 229.16779 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 1-(2,5-Dihydroxyphenyl)octan-1-one | CCCCCCCC(=O)C1=C(O)C=CC(O)=C1 | 236.14124 | Suspect screening | Lake | LC-HRMS | Reference | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Loxoprofen alcohol | CC(C1=CC=C(C=C1)CC2CCCC2O)C(=O)O | 248.14124 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Propachlor ESA | CC(C)N(C(=O)CS(O)(=O)=O)C1=CC=CC=C1 | 257.07218 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Hydroxypethidine | CCOC(=O)C1(CCN(C)CC1)C1=CC(O)=CC=C1 | 263.15214 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Ethyl 3-(3,4,5-trimethoxyphenyl)propionate Butyl 3,4,5-trimethoxybenzoate | CCOC(=O)CCC1=CC(OC)=C(OC)C(OC)=C1 CCCCOC(=O)C1=CC(OC)=C(OC)C(OC)=C1 | 268.13107 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Triaziflam | CC(COC1=CC(C)=CC(C)=C1)N=C1NC(=N)N=C(N1)C(C)(C)F | 333.19649 | Suspect screening | Lake | LC-HRMS | Reference | I |
| NONOXYNOL-4 | CCCCCCCCCC1=CC=CC=C1OCCOCCOCCOCCO | 396.28757 | Suspect screening | Lake | LC-HRMS | Reference | I |
| simvastatin hydroxyl acid | CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 436.28249 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Bis(p-(1,1,3,3-tetramethylbutyl)phenyl) hydrogen phosphate | CC(C)(C)CC(C)(C)C1=CC=C(OP(O)(=O)OC2=CC=C(C=C2)C(C)(C)CC(C)(C)C)C=C1 | 474.28990 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Perfluorooctanesulfonic acid | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Lake | LC-HRMS | Reference | I |
| Octyl thiocyanate | CCCCCCCCSC#N | 171.10817 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-Methylene-3-butyn-1-ol 1-Methoxybut-1-en-3-yne | OCC(=C)C#C COC=CC#C | 82.04186 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-(1,1-Dimethylethyl)-4-(1-methyl-1-phenylethyl)phenol | CC(C)(C)C1=C(O)C=CC(=C1)C(C)(C)C1=CC=CC=C1 | 268.18272 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 2-((2-Hydroxyethyl)(3-methoxypropyl)amino)ethyl methacrylate | COCCCN(CCO)CCOC(=O)C(C)=C | 245.16271 | Suspect screening | Lake | LC-HRMS | Reference | I |
| 4-O-Desmethyl 4-O-Ethyl Trimethoprim | CCOC1=C(OC)C=C(CC2=CNC(=N)NC2=N)C=C1OC | 304.15354 | Suspect screening | Lake | LC-HRMS | Reference | I |
| PGE3 | CCC=CCC(C=CC1C(CC(=O)C1CC=CCCCC(=O)O)O)O | 350.21040 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Methyl N-(a-methylbutyryl)glycine | C(CCCC(=O)O)CCCC(=O)O | 188.10530 | Suspect screening | Lake | LC-HRMS | Reference | N |
| DL-b-Hydrosycaprylic acid |  | 160.10990 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 8-iso-15keto-PGE2 | CCCCCC(=O)C=CC1C(CC(=O)C1CC=CCCCC(=O)O)O | 350.21040 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 20-hydroxy LTB4 | C(CCC=CCC(C=CC=CC=CC(CCCC(=O)O)O)O)CCO | 352.22570 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 13-OxoODE | CCCCCC(=O)C=CC=CCCCCCCCC(=O)O | 294.22150 | Suspect screening | Lake | LC-HRMS | Reference | N |
| (±)20-HDoHE | CCC(C=CC=CCC=CCC=CCC=CCC=CCCC(=O)O)O | 344.23720 | Suspect screening | Lake | LC-HRMS | Reference | N |
| (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,1 6,19-Docosahexaenoic acid | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O | 328.24210 | Suspect screening | Lake | LC-HRMS | Reference | N |
| (±)15-HETE | CCCCCC(C=CC=CCC=CCC=CCCCC(=O)O)O | 320.23700 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 11(S)-HEPE | CCC=CCC=CC=CC(CC=CCC=CCCCC(=O)O)O | 318.22160 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 5(S)-HEPE | CCC=CCC=CCC=CCC=CC=CC(CCCC(=O)O)O | 318.22160 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 5-Oxo-ETE | CCCCCC=CCC=CCC=CC=CC(=O)CCCC(=O)O | 318.22160 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 15(S)-HEPE | CCC=CCC(C=CC=CCC=CCC=CCCCC(=O)O)O | 318.22160 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 12(R)HETE | CCCCCC=CCC(C=CC=CCC=CCCCC(=O)[O-])O | 320.23700 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 9,10-Epoxystearic acid | CCCCCCCCC1C(O1)CCCCCCCC(=O)O | 298.25270 | Suspect screening | Lake | LC-HRMS | Reference | N |
| cis-9,10-Epoxystearic acid | CCCCCCCCC1C(O1)CCCCCCCC(=O)O | 298.25270 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 13(S)-HODE | CCCCCC(C=CC=CCCCCCCCC(=O)O)O | 296.23700 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 12(S)-HEPE | CCC=CCC=CCC(C=CC=CCC=CCCCC(=O)O)O | 318.22160 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 17(R)-HDoHE | CCC=CCC(C=CC=CCC=CCC=CCC=CCCC(=O)O)O | 344.23720 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Stearidonic Acid | CCC=CCC=CCC=CCC=CCCCCC(=O)O | 276.21070 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Sorbic acid | CC=CC=CC(=O)O | 112.05160 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Niacinamide | C1=CC(=CN=C1)C(=O)N | 122.04750 | Suspect screening | Lake | LC-HRMS | Reference | N |
| lyso-PAF C16 | CCCCCCCCCCCCCCCCOCC(COP(=O)([O-])OCC[N+](C)(C)C)O | 482.35600 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Glycerol monopalmitate | CCCCCCCCCCCCCCCC(=O)OCC(CO)O | 330.27460 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Fenuron | CN(C)C(=O)NC1=CC=CC=C1 | 164.09350 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Choline | C[N+](C)(C)CCO | 104.10680 | Suspect screening | Lake | LC-HRMS | Reference | N |
| Oleamide | CCCCCCCCC=CCCCCCCCC(=O)N | 281.27020 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 5,8,11-Eicosatriynoic acid | CCCCCCCCC#CCC#CCC#CCCCC(=O)O | 300.20660 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 4-oxo-2-Nonenal | CCCCCC(=O)C=CC=O | 154.09820 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 1-Palmitoyllysophosphatidylcholine | CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O | 496.33580 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 1,2-dipalmitoyl-sn-glycero-3PC | CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC | 734.56160 | Suspect screening | Lake | LC-HRMS | Reference | N |
| 6-Methylhepta-3,5-dien-2-one. | CC(C)=CC=CC(C)=O | 124.08881 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| N,N,3,5-Tetramethylaniline | CN(C)C1=CC(C)=CC(C)=C1 | 149.12045 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 1-[(1R,2S)-2,6,6-trimethylcyclohex-3-en-1-yl]ethanone | CC1C=CCC(C1C(=O)C)(C)C | 166.13577 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| methyprylon | CCC1(CC)C(=O)NCC(C)C1=O | 183.12593 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| (3-Carbamoyl-2,2,5,5-tetramethyl-2,5-dihydro-1H-pyrrol-1-yl)oxidanyl | CC1(C)C=C(C(N)=O)C(C)(C)N1[O] | 184.12118 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 1-(1H-Indol-3-yl)butan-1-one 3-(3-Oxobutyl)-1H-indole | CCCC(=O)C1=CNC2=CC=CC=C12 CC(=O)CCc1c[nH]c2c1cccc2 | 187.09971 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2,2,5,7-Tetramethylindan-1-one | CC1=CC(C)=C2C(CC(C)(C)C2=O)=C1 | 188.12012 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Benzyl 2,2-dimethylpropanoate | CC(C)(C)C(=O)OCC1=CC=CC=C1 | 192.11503 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Methyl 2-acetyl-2-allylpent-4-ene-1-oate | COC(=O)C(CC=C)(CC=C)C(C)=O | 196.10994 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| alpha,alpha-Dicyclopropyl-4-methylbenzyl alcohol | CC1=CC=C(C=C1)C(O)(C1CC1)C1CC1 | 202.13577 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| N-(6-Aminohexyl)-4-hydroxybutyramide | NCCCCCCNC(=O)CCCO | 202.16813 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Ibuprofen | CC(C)CC1=CC=C(C=C1)C(C)C(O)=O | 206.13068 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 4-tert-octylphenol | CC(C)(C)CC(C)(C)c1ccc(cc1)O | 206.16707 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 3-Ethyl-3-phenylpentane-1,5-diol | CCC(CCO)(CCO)C1=CC=CC=C1 | 208.14633 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2,4,4,7-Tetramethylnona-6,8-dien-3-one oxime | CC(C)C(=NO)C(C)(C)CC=C(C)C=C | 209.17796 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 3-(Decyloxy)propionitrile 3-(isodecyloxy)propiononitrile | CCCCCCCCCCOCCC#N CC(C)CCCCCCCOCCC#N | 211.19361 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 4-tert-butyl-3-hydroxy-2,6-xylylacetonitrile | CC1=CC(=C(C(=C1CC#N)C)O)C(C)(C)C | 217.14666 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-(Decylsulfanyl)ethan-1-ol | CCCCCCCCCCSCCO | 218.17044 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-(3,4-dimethoxyphenyl)-3-methylbutyronitrile | COC1=CC=C(C=C1OC)C(C#N)C(C)C | 219.12593 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Precocene II | COC1=CC2=C(C=CC(C)(C)O2)C=C1OC | 220.10994 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Benzoic acid, 2-amino-, hexyl ester | CCCCCCOC(=O)C1=CC=CC=C1N | 221.14158 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 3,4-methylenedioxypropylamphetamine | CCCNC(C)CC1=CC2=C(C=C1)OCO2 | 221.14158 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| ethyl 2-allyl-2-cyano-3-methylhexanoate | CCCC(C)C(CC=C)(C#N)C(=O)OCC | 223.15723 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| diethyl 4-oxopentane-1,2-dicarboxylate | CCOC(=O)CC(CC(=O)C)C(=O)OCC | 230.11542 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| (Acetylazanediyl)di(ethane-2,1-diyl) diacetate | CC(=O)OCCN(CCOC(C)=O)C(C)=O | 231.11067 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 5,6,7,8-Tetrahydro-gamma-oxonaphthalene-2-butyric acid | OC(=O)CCC(=O)C1=CC2=C(CCCC2)C=C1 | 232.10994 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Pentylone Dibutylone | CCCC(NC)C(=O)C1=CC=C2OCOC2=C1 CCC(N(C)C)C(=O)C1=CC=C2OCOC2=C1 | 235.12084 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| viloxazine | CCOC1=C(OCC2CNCCO2)C=CC=C1 | 237.13649 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate | CC1(COC(=O)C2CC=CCC2C(=O)OC1)C | 238.12051 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| N-Dodecylacrylamide | CCCCCCCCCCCCNC(=O)C=C | 239.22491 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-((2-Methyl-1-oxoallyl)oxy)ethyl 6-hydroxyhexanoate | CC(=C)C(=O)OCCOC(=O)CCCCCO | 244.13107 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-((2-Methyl-1-oxoallyl)oxy)ethyl 6-hydroxyhexanoate | CC(=C)C(=O)OCCOC(=O)CCCCCO | 244.13107 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Celestolide | CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C | 244.18272 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Bisnortilidin | CCOC(=O)C1(CCC=CC1N)C2=CC=CC=C2 | 245.14158 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2,2'-[oxybis(methylene)]bis[2-ethylpropane-1,3-diol] | CCC(CO)(CO)COCC(CC)(CO)CO | 250.17802 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| (Z)-9-Cycloheptadecen-1-one. | O=C1CCCCCCC\C=C/CCCCCCC1 | 250.22967 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Tricyclo(3.3.1.13,7)dec-1,3-diyldi(acetic acid) | [H]C12CC3([H])CC(CC(O)=O)(C1)CC(CC(O)=O)(C2)C3 | 252.13616 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| N-(dodecyl)pyrrolidinone | CCCCCCCCCCCCN1CCCC1=O | 253.24056 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| N-(3-Acetyl-4-hydroxyphenyl)heptan-1-amide | CCCCCCC(=O)NC1=CC(C(C)=O)=C(O)C=C1 | 263.15214 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-(3,5-dimethylhex-3-en-2-yloxy)-2-methylpropyl cyclopropanecarboxylate | CC(C)C=C(C)C(C)OC(C)(C)COC(=O)C1CC1 | 268.20384 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine | COCCCNCC1=CC(OC)=C(OC)C(OC)=C1 | 269.16271 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Decyl 5-oxo-L-prolinate | CCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 269.19909 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Octanoic anhydride | CCCCCCCC(=O)OC(=O)CCCCCCC | 270.21949 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Alphameprodine [INN:BAN:DCF] | CC[C@H]1CN(C)CC[C@]1(OC(=O)CC)C1=CC=CC=C1 | 275.18853 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Brefeldin A | [H][C@@]12C[C@H](O)C[C@@]1([H])[C@H](O)\C=C\C(=O)O[C@@H](C)CCC\C=C\2 | 280.16746 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| p-(1-(p-Pentylphenyl)vinyl)anisole | CCCCCC1=CC=C(C=C1)C(=C)C1=CC=C(OC)C=C1 | 280.18272 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Methyl 3-oxohexadecanoate | CCCCCCCCCCCCCC(=O)CC(=O)OC | 284.23514 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Sodium N-methyl-N-(1-oxododecyl)-ß-alaninate | CCCCCCCCCCCC(=O)N(O)CCC(=O)[O-]·[Na+] | 285.23039 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| norethisterone | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C | 298.19328 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Sodium decyl phthalate diisopentyl phthalate CROMOPHTAL DPP RED TFP | [Na+].CCCCCCCCCCOC(=O)C1=CC=CC=C1C([O-])=O CC(C)CCOC(=O)C1=CC=CC=C1C(=O)OCCC(C)C CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCC | 306.18311 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Sodium decyl phthalate diisopentyl phthalate CROMOPHTAL DPP RED TFP | [Na+].CCCCCCCCCCOC(=O)C1=CC=CC=C1C([O-])=O CC(C)CCOC(=O)C1=CC=CC=C1C(=O)OCCC(C)C CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCC | 306.18311 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| NONOXYNOL-2 4-nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group) | CCCCCCCCCC1=CC=C(OCCOCCO)C=C1 CCCCCCCCCC1=CC=C(C=C1)OCCOCCO | 308.23514 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Amorolfine | CCC(C)(C)C1=CC=C(CC(C)CN2C[C@H](C)O[C@H](C)C2)C=C1 | 317.27186 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| homodihydrocapsaicin-I | CC(C)CCCCCCCC(=O)NCC1=CC(=C(C=C1)O)OC | 321.23039 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 15-(tert-Butyl)-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecine | CC(C)(C)C1=CC2=C(C=C1)OCCOCCOCCOCCO2 | 324.19367 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| hydrogen N-(1-oxododecyl)-L-glutamic acid | CCCCCCCCCCCC(=O)NC(CCC(=O)O)C(=O)O | 329.22022 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| ETHYL ARACHIDONATE | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OCC | 332.27153 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Pentadecyl 5-oxo-L-prolinate | CCCCCCCCCCCCCCCOC(=O)[C@@H]1CCC(=O)N1 | 339.27734 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-Hydroxypropane-1,3-diyl bis(2-propylvalerate) | CCCC(CCC)C(=O)OCC(O)COC(=O)C(CCC)CCC | 344.25627 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Bis(tert-butyl) 1,4-dihydro-2,6-dimethyl-4-propylpyridine-3,5-dicarboxylate | CCCC1C(C(=O)OC(C)(C)C)=C(C)NC(C)=C1C(=O)OC(C)(C)C | 351.24096 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| GLYCERYL LINOLENATE | CCC=CCC=CCC=CCCCCCCCC(=O)OCC(O)CO | 352.26136 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| (Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine | CCCCCCCCC=CCCCCCCCC(=O)N(C)CC(=O)O | 353.29299 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Isodecyl isononyl phthalate Decyl nonyl phthalate | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCC© CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC | 432.32396 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| LAURETH-12 | CCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO | 714.51294 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Glyceryl phosphate | OCC(O)COP(O)(O)=O | 172.01367 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Acamprosate | CC(=O)NCCCS(O)(=O)=O | 181.04088 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 3-Hydroxyphthalic acid 4-Hydroxybenzene-1,2-dicarboxylic acid | OC(=O)C1=C(C(O)=O)C(O)=CC=C1 OC(=O)C1=C(C=C(O)C=C1)C(O)=O | 182.02152 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 4-morpholineethanesulfonic acid | OS(=O)(=O)CCN1CCOCC1 | 195.05653 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 3-Amino-4-methoxybenzenesulfonic acid 2-Amino-5-methoxybenzenesulfonic acid 5-Amino-6-hydroxytoluene-3-sulphonic acid | COC1=CC=C(C=C1N)S(O)(=O)=O COC1=CC(=C(N)C=C1)S(O)(=O)=O CC1=CC(=CC(N)=C1O)S(O)(=O)=O | 203.02523 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 3-morpholin-4-ylpropane-1-sulfonic acid | C1COCCN1CCCS(=O)(=O)O | 209.07218 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Icaridine | CCC(C)OC(=O)N1CCCCC1CCO | 229.16779 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 1-(2,5-Dihydroxyphenyl)octan-1-one | CCCCCCCC(=O)C1=C(O)C=CC(O)=C1 | 236.14124 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| CAPSO | C1CCC(CC1)NCC(CS(=O)(=O)O)O | 237.10348 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Loxoprofen alcohol | CC(C1=CC=C(C=C1)CC2CCCC2O)C(=O)O | 248.14124 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Hydroxypethidine | CCOC(=O)C1(CCN(C)CC1)C1=CC(O)=CC=C1 | 263.15214 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Ethyl 3-(3,4,5-trimethoxyphenyl)propionate Butyl 3,4,5-trimethoxybenzoate | CCOC(=O)CCC1=CC(OC)=C(OC)C(OC)=C1 CCCCOC(=O)C1=CC(OC)=C(OC)C(OC)=C1 | 268.13107 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Ethylene brassylate | O=C1CCCCCCCCCCCC(=O)OCCO1 | 270.18311 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Triaziflam | CC(COC1=CC(C)=CC(C)=C1)N=C1NC(=N)N=C(N1)C(C)(C)F | 333.19649 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| cefaloram | CC(=O)OCC1=C(N2[C@H](SC1)[C@H](NC(=O)CC1=CC=CC=C1)C2=O)C(O)=O | 390.08856 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| NONOXYNOL-4 | CCCCCCCCCC1=CC=CC=C1OCCOCCOCCOCCO | 396.28757 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| simvastatin hydroxyl acid | CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)O)O)O)C | 436.28249 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| Perfluorooctanesulfonic acid | OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 499.93749 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-(1,1-Dimethylethyl)-4-(1-methyl-1-phenylethyl)phenol | CC(C)(C)C1=C(O)C=CC(=C1)C(C)(C)C1=CC=CC=C1 | 268.18272 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 2-((2-Hydroxyethyl)(3-methoxypropyl)amino)ethyl methacrylate | COCCCN(CCO)CCOC(=O)C(C)=C | 245.16271 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 4-O-Desmethyl 4-O-Ethyl Trimethoprim | CCOC1=C(OC)C=C(CC2=CNC(=N)NC2=N)C=C1OC | 304.15354 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | I |
| 20-hydroxy LTB4 | C(CCC=CCC(C=CC=CC=CC(CCCC(=O)O)O)O)CCO | 352.22230 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| Eicosapentaenoic Acid | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O | 302.22200 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 9,10-Epoxystearic acid | CCCCCCCCC1C(O1)CCCCCCCC(=O)O | 298.24780 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 13(R)-HODE | CCCCCC(C=CC=CCCCCCCCC(=O)O)O | 296.23200 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| Inosine | C1=NC2=C(C(=O)N1)N=CN2C3C(C(C(O3)CO)O)O | 268.07950 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 12(R)HETE | CCCCCC=CCC(C=CC=CCC=CCCCC(=O)[O-])O | 320.23200 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| DL-b-Hydrosycaprylic acid |  | 160.10910 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 2-Hydroxyhexadecanoic acid | CCCCCCCCCCCCCCC(C(=O)O)O | 272.23210 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 15(S)-HEPE | CCC=CCC(C=CC=CCC=CCC=CCCCC(=O)O)O | 318.21630 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 7Z,10Z,13Z,19z-Docosapentaenoic acid | CCC=CCC=CCC=CCC=CCC=CCCCCCC(=O)O | 330.25270 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| Methyl N-(a-methylbutyryl)glycine |  | 188.10350 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| trans-EKODE-(E)-lb | CCCCCC1C(O1)C=CC(=O)CCCCCCCC(=O)O | 310.21190 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| Sebacic acid | C(CCCCC(=O)O)CCCC(=O)O | 202.11930 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| LTB4 | CCCCCC=CCC(C=CC=CC=CC(CCCC(=O)O)O)O | 336.22680 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| Arachidonic Acid | CCCCCC=CCC=CCC=CCC=CCCCC(=O)O | 304.23750 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| Stearidonic Acid | CCC=CCC=CCC=CCC=CCCCCC(=O)O | 276.20590 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| PGD2 | CCCCCC(C=CC1C(C(CC1=O)O)CC=CCCCC(=O)O)O | 352.22160 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 12(S)-HEPE | CCC=CCC=CCC(C=CC=CCC=CCCCC(=O)O)O | 318.21630 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,1 6,19-Docosahexaenoic acid | CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O | 328.23790 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| (±)17-HDoHE | CCC=CCC(C=CC=CCC=CCC=CCC=CCCC(=O)O)O | 344.23170 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| (R)15-HETE | CCCCCC(C=CC=CCC=CCC=CCCCC(=O)O)O | 320.23200 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| Sorbic acid | CC=CC=CC(=O)O | 112.05210 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 3-Methyl-4-pentenoic acid | CC(CC(=O)O)C=C | 114.06770 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| lyso-PAF C16 | CCCCCCCCCCCCCCCCOCC(COP(=O)([O-])OCC[N+](C)(C)C)O | 482.36260 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 1-Palmitoyllysophosphatidylcholine | CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O | 496.34180 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| 1-heptadecanoyl-sn-glycero-3-phosphocholine | CCCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O | | CCCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O | Lake | LC-HRMS | Repeated\_reference | 22 |
| Choline | C[N+](C)(C)CCO | 104.10740 | Suspect screening | Lake | LC-HRMS | Repeated\_reference | N |
| CB49 | C1=CC(=C(C=C1Cl)Cl)C2=C(C=CC(=C2)Cl)Cl | 291.91886 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB66 | C1=CC(=C(C=C1C2=C(C=C(C=C2)Cl)Cl)Cl)Cl | 291.91886 | Suspect screening | Lake | GC-HRMS | In house | G |
| pentaCB |  | 325.87994 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB101 | C1=CC(=C(C=C1Cl)C2=CC(=C(C=C2Cl)Cl)Cl)Cl | 325.87994 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB87 | C1=CC(=C(C=C1Cl)C2=C(C(=C(C=C2)Cl)Cl)Cl)Cl | 325.87994 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB118 | C1=CC(=C(C=C1C2=CC(=C(C=C2Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Lake | GC-HRMS | In house | G |
| hexaCB b |  | 359.84096 | Suspect screening | Lake | GC-HRMS | In house | G |
| hexaCB c |  | 359.84096 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB156 | C1=CC(=C(C=C1C2=CC(=C(C(=C2Cl)Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB153 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C=C2Cl)Cl)Cl | 359.84096 | Suspect screening | Lake | GC-HRMS | In house | G |
| heptaCB a |  | 393.80198 | Suspect screening | Lake | GC-HRMS | In house | G |
| heptaCB b |  | 393.80198 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB180 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl | 393.80198 | Suspect screening | Lake | GC-HRMS | In house | G |
| heptaCB c |  | 393.80198 | Suspect screening | Lake | GC-HRMS | In house | G |
| octaCB a |  | 429.76009 | Suspect screening | Lake | GC-HRMS | In house | G |
| octaCB b |  | 429.76009 | Suspect screening | Lake | GC-HRMS | In house | G |
| CB194 | C1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl | 429.76009 | Suspect screening | Lake | GC-HRMS | In house | G |
| BDE154 | C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br | 643.52961 | Suspect screening | Lake | GC-HRMS | In house | G |
| BDE153 | C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 643.52961 | Suspect screening | Lake | GC-HRMS | In house | G |
| BDE100 | C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br | 563.62113 | Suspect screening | Lake | GC-HRMS | In house | G |
| BDE47 | C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br | 485.71063 | Suspect screening | Lake | GC-HRMS | In house | G |
| BDE49 | C1=CC(=C(C=C1Br)Br)OC2=C(C=CC(=C2)Br)Br | 485.71063 | Suspect screening | Lake | GC-HRMS | In house | G |
| BDE28 | C1=CC(=CC=C1OC2=C(C=C(C=C2)Br)Br)Br | 405.80214 | Suspect screening | Lake | GC-HRMS | In house | G |
| pp'DDE | C1=CC(=CC=C1C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 317.93459 | Suspect screening | Lake | GC-HRMS | In house | G |
| op'DDD | C1=CC=C(C(=C1)C(C2=CC=C(C=C2)Cl)C(Cl)Cl)Cl | 235.00758 | Suspect screening | Lake | GC-HRMS | In house | G |
| Butylated Hydroxytoluene | C1=C(C=C(C(=C1C(C)(C)C)O)C(C)(C)C)C |  | Suspect screening | Lake | GC-HRMS | Reference | E |
| Benzoic acid, 4-ethoxy-, ethyl ester | C1=C(C=CC(=C1)OCC)C(=O)OCC |  | Suspect screening | Lake | GC-HRMS | Reference | E |
| Benzenesulfonamide, N-butyl- | C1=CC(=CC=C1)[S](=O)(=O)NCCCC |  | Suspect screening | Lake | GC-HRMS | Reference | E |
| Diphenyl sulfone | C2=C([S](=O)(=O)C1=CC=CC=C1)C=CC=C2 |  | Suspect screening | Lake | GC-HRMS | Reference | E |
| 3,5-di-tert-Butyl-4-hydroxybenzaldehyde | C1=C(C=O)C=C(C(=C1C(C)(C)C)O)C(C)(C)C |  | Suspect screening | Lake | GC-HRMS | Reference | E |
| Dibutyl phthalate | O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1 |  | Suspect screening | Lake | GC-HRMS | Reference | E |
| Squalene | C(\C(=C\CC/C=C(/CC/C=C(/CCC=C(C)C)C)C)C)C/C=C(/CCC=C(C)C)C |  | Suspect screening | Lake | GC-HRMS | Reference | E |
| pentaCB |  | 325.87994 | Suspect screening | Lake | GC-HRMS | Reference | G |
| CB118 | C1=CC(=C(C=C1C2=CC(=C(C=C2Cl)Cl)Cl)Cl)Cl | 359.84096 | Suspect screening | Lake | GC-HRMS | Reference | G |
| hexaCB a |  | 359.84096 | Suspect screening | Lake | GC-HRMS | Reference | G |
| hexaCB c |  | 359.84096 | Suspect screening | Lake | GC-HRMS | Reference | G |
| CB153 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C=C2Cl)Cl)Cl | 359.84096 | Suspect screening | Lake | GC-HRMS | Reference | G |
| octaCB a |  | 429.76009 | Suspect screening | Lake | GC-HRMS | Reference | G |
| octaCB b |  | 429.76009 | Suspect screening | Lake | GC-HRMS | Reference | G |
| CB194 | C1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl | 429.76009 | Suspect screening | Lake | GC-HRMS | Reference | G |
| BDE47 | C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br | 485.71063 | Suspect screening | Lake | GC-HRMS | Reference | G |
| pp'DDE | C1=CC(=CC=C1C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 317.93459 | Suspect screening | Lake | GC-HRMS | Reference | G |
| 2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol | COC1=C(C=CC(=C1)CCCO)OC(CO)CO | 278.11270 | Non-target screening | Canal | LC-HRMS | In house | B |
| 1-Dodecyl-5-oxopyrrolidine-3-carboxylic acid | CCCCCCCCCCCCN1CC(CC1=O)C(=O)O | 297.23040 | Non-target screening | Canal | LC-HRMS | In house | B |
| N-(2-(2-Hydroxyphenyl)-2H-benzotriazol-5-yl)methacrylamide | CC(=C)C(=O)NC1=CC2=NN(N=C2C=C1)C3=CC=CC=C3O | 294.11370 | Non-target screening | Canal | LC-HRMS | In house | B |
| (7R,8S,9S,14S,16S)-8-Hydroxy-5,5,9,13,13,14-hexamethyl-16-(2-methyl-1,3-benzothiazol-5-yl)-7-prop-2-enyl-oxacyclohexadecane-2,6-dione | | 542,3298 | 542.32980 | Canal | LC-HRMS | In house | 2 |
| 1-(Methylsulfanyl)-3-undecanone | CCCCCCCCC(=O)CCSC | 216.15479 | Non-target screening | Canal | LC-HRMS | In house | C |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Canal | LC-HRMS | In house | I |
| 1H-Benzimidazole, 2-(octylthio)- | CCCCCCCCSc1[nH]c2ccccc2n1 | 262.15037 | Non-target screening | Canal | LC-HRMS | In house | I |
| Linoleamide | CCCCC/C=C\C/C=C\CCCCCCCC(=O)N | 279.25621 | Non-target screening | Canal | LC-HRMS | In house | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Non-target screening | Canal | LC-HRMS | In house | I |
| Glycol ether sulfates n=2 (2 GES) | OCCOCCOCCOS(O)(=O)=O | 230.04600 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=3 (3 GES) | OCCOCCOCCOCCOS(O)(=O)=O | 274.07220 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=4 (4 GES) | OCCOCCOCCOCCOCCOS(O)(=O)=O | 318.09850 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=5 (5 GES) | OCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 362.12470 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=6 (6 GES) | OCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 406.15090 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=7 (7 GES) | OCCOCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 450.17710 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=8 (8 GES) | OCCOCCOCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 494.20330 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=9 (9 GES) | OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 506.25750 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=10 (10 GES) | OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 582.25570 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=11 (11 GES) | OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 626.28200 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=12 (12 GES) | OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 670.30820 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Glycol ether sulfates n=13 (13 GES) | OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOS(O)(=O)=O | 714.33440 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C9-LAS | O=S(=O)(O)C1=CC=C(C=C1)C(CCC)CCCCC | 284.14460 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C10-LAS | O=S(=O)(O)C1=CC=C(C=C1)C(CCC)CCCCCC | 298.16030 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C11-LAS | O=S(=O)(O)C1=CC=C(C=C1)C(CCCC)CCCCCC | 312.17590 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C2DEA | CCC(=O)N(CCO)CCO | 161.10519 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C3DEA | CCCC(=O)N(CCO)CCO | 175.12084 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C4DEA | CCCCC(=O)N(CCO)CCO | 189.13649 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C5DEA | CCCCCC(=O)N(CCO)CCO | 203.15214 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C7DEA | CCCCCCCC(=O)N(CCO)CCO | 231.18344 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C9DEA | CCCCCCCCC(=O)N(CCO)CCO | 245.19909 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C11DEA | CCCCCCCCCCCC(=O)N(CCO)CCO | 287.24604 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C13DEA | CCCCCCCCCCCCCC(=O)N(CCO)CCO | 315.27734 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C15DEA | CCCCCCCCCCCCCCCC(=O)N(CCO)CCO | 343.30864 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| C17DEA | CCCCCCCCCCCCCCCCCC(=O)N(CCO)CCO | 371.33994 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| NP-2EC | CCCCCCCCCC1=CC=C(OCCOCC(O)=O)C=C1 | 322.21441 | Non-target screening | Canal | LC-HRMS | In house | H\_2 |
| Metolachlor OA | CCC1=CC=CC(=C1N(C(C)COC)C(=O)C(=O)O)C | 279.14706 | Non-target screening | Canal | LC-HRMS | In house | H\_1 |
| Didecyldimethylammonium bromide (DADMAC-10:10) | CCCCCCCCCC[N+](C)(C)CCCCCCCCCC | 326.37868 | Non-target screening | Canal | LC-HRMS | In house | H\_1 |
| Eicosyltrimethylammonium | C[N+](C)(C)CCCCCCCCCCCCCCCCCCCC | 340.39370 | Non-target screening | Canal | LC-HRMS | Reference | A |
| Trimethyldocosenylammonium | C[N+](C)(C)CCCCCCCCC\C=C\CCCCCCCCCCC | 366.40940 | Non-target screening | Canal | LC-HRMS | Reference | A |
| 1-(Methylsulfanyl)-3-undecanone | CCCCCCCCC(=O)CCSC | 216.15479 | Non-target screening | Canal | LC-HRMS | Reference | C |
| 1,3-Diphenylguanidine | C1=CC=C(C=C1)NC(=NC2=CC=CC=C2)N | 211.11090 | Non-target screening | Canal | LC-HRMS | Reference | D |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Canal | LC-HRMS | Reference | I |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Canal | LC-HRMS | Reference | I |
| 1H-Benzimidazole, 2-(octylthio)- | CCCCCCCCSc1[nH]c2ccccc2n1 | 262.15037 | Non-target screening | Canal | LC-HRMS | Reference | I |
| Linoleamide | CCCCC/C=C\C/C=C\CCCCCCCC(=O)N | 279.25621 | Non-target screening | Canal | LC-HRMS | Reference | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Non-target screening | Canal | LC-HRMS | Reference | I |
| Thymine | CC1=CNC(=O)NC1=O | 126.04293 | Non-target screening | Canal | LC-HRMS | Reference | L |
| Stearamide | CCCCCCCCCCCCCCCCCC(=O)N | 283.28752 | Non-target screening | Canal | LC-HRMS | Reference | L |
| 2-Arachidonoyl glycerol | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OC(CO)CO | 378.27701 | Non-target screening | Canal | LC-HRMS | Reference | L |
| Eicosapentaenoic acid methyl ester | CCC=CCC=CCC=CCC=CCC=CCCCC(=O)OC | 316.24023 | Non-target screening | Canal | LC-HRMS | Reference | L |
| N,N'-Diphenylguanidine | C1=CC=C(C=C1)N(C2=CC=CC=C2)C(=N)N | 211.11095 | Non-target screening | Canal | LC-HRMS | Reference | L |
| 2-Arachidonoyl glycerol | CCCCCC=CCC=CCC=CCC=CCCCC(=O)OC(CO)CO | 378.27701 | Non-target screening | Canal | LC-HRMS | Reference | L |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17763 | Non-target screening | Canal | LC-HRMS | Reference | L |
| LPC 16:0 | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCCCCCCCCC |  | Non-target screening | Canal | LC-HRMS | Reference | L |
| Terpestacin |  | 402.27682 | Non-target screening | Canal | LC-HRMS | Reference | P |
| Benzaldehyde, 5-dodecyl-2-hydroxy-, oxime |  | 305.23538 | Non-target screening | Canal | LC-HRMS | Reference | P |
| 2-(3-Phenylpropyl)tetrahydrofuran |  | 190.13575 | Non-target screening | Canal | LC-HRMS | Reference | P |
| NONOXYNOL-5 |  | 440.31393 | Non-target screening | Canal | LC-HRMS | Reference | P |
| 4-(trans-4-propylcyclohexyl)acetophenone |  | 244.18272 | Non-target screening | Canal | LC-HRMS | Reference | P |
| N,N'-bis(2,2,6,6-tetramethyl-4-piperidyl)isophthalamide |  | 442.32963 | Non-target screening | Canal | LC-HRMS | Reference | P |
| N,N'-bis(2,2,6,6-tetramethyl-4-piperidyl)isophthalamide |  | 442.32961 | Non-target screening | Canal | LC-HRMS | Reference | P |
| simvastatin hydroxyl acid |  | 436.28254 | Non-target screening | Canal | LC-HRMS | Reference | P |
| Phenol, 4-octyl- |  | 206.16707 | Non-target screening | Canal | LC-HRMS | Reference | P |
| METHYL HYDROXY- METHYL OLEYL OXAZO- LINE |  | 351.31373 | Non-target screening | Canal | LC-HRMS | Reference | P |
| Octanophenone |  | 204.15145 | Non-target screening | Canal | LC-HRMS | Reference | P |
| Trihexyl benzene-1,2,4-tricarboxylate |  | 462.29830 | Non-target screening | Canal | LC-HRMS | Reference | P |
| Trimethyldocosenylammonium | C[N+](C)(C)CCCCCCCCC\C=C\CCCCCCCCCCC | 366.40940 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | A |
| 2-Ethoxyethyl 3-(4-methoxyphenyl)prop-2-enoate (previously co-reported with Cinoxate) | CCOCCOC(=O)C=CC1=CC=C(C=C1)OC | 250.12000 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | B |
| 2-Phenylethyl 2-ethylbutyrate | CCC(CC)C(=O)OCCC1=CC=CC=C1 | 220.14630 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | B |
| Phenethyl acetate (previously co-reported with 2-Phenylethyl 2-ethylbutyrate) | CC(=O)OCCC1=CC=CC=C1 | 164.08320 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | B |
| Glycidyl neodecanoate | CCCCCCC(C)(C)C(=O)OCC1CO1 | 228.17250 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | B |
| (z)-4-(2-((e)-7a-methyl-1-(6-methylheptan-2-yl)octahydro-4h-inden-4-ylidene)ethylidene)-5-methylenecyclohexane-1,2-diol | CC(C)CCCC(C)C1CCC2C(/CCCC12C)=C/C=C3/CC(O)C(O)CC3=C | 400.33410 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | B |
| Lauryl aspartic acid | CCCCCCCCCCCCNC(CC(=O)O)C(=O)O | 301.22530 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | B |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | I |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | I |
| 1H-Benzimidazole, 2-(octylthio)- | CCCCCCCCSc1[nH]c2ccccc2n1 | 262.15037 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | I |
| Linoleamide | CCCCC/C=C\C/C=C\CCCCCCCC(=O)N | 279.25621 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | I |
| 1-Naphthol | C1=CC=C2C(=C1)C=CC=C2O | 144.05752 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | L |
| Butyl benzoate | CCCCOC(=O)C1=CC=CC=C1 | 178.09938 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | L |
| Benzothiazole | C1=CC=C2C(=C1)N=CS2 | 135.01427 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | L |
| Cholecalciferol | CC(C)CCCC(C)C1CCC2C1(CCCC2=CC=C3CC(CCC3=C)O)C | 384.33922 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | L |
| Galaxolidone | CC1COC(=O)C2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 272.17763 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | L |
| LPC 16:0 | O=C(OCC(O)COP(=O)([O-])OCC[N+](C)(C)C)CCCCCCCCCCCCCCC |  | Non-target screening | Canal | LC-HRMS | Repeated\_reference | L |
| Perfluoro-1-octanesulfonic acid (PFOS) | C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F | 499.93749 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | L |
| 4-hydroxy Nonenal | CCCCCC(C=CC=O)O | 156.11580 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | N |
| 13-oxoODE |  | 294.22000 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | N |
| Methyl N-(a-methylbutyryl)glycine |  | 188.10500 | Non-target screening | Canal | LC-HRMS | Repeated\_reference | N |
| DDT-related |  | 235.00549 | Non-target screening | Canal | GC-HRMS | In house | G |
| hexachloroterphenyl |  | 435.87222 | Non-target screening | Canal | GC-HRMS | In house | G |
| heptachloroterphenyl |  | 469.83325 | Non-target screening | Canal | GC-HRMS | In house | G |
| pentachloroterphenyl |  | 401.91119 | Non-target screening | Canal | GC-HRMS | In house | G |
| tetrachloroterphenyl |  | 367.95016 | Non-target screening | Canal | GC-HRMS | In house | G |
| pentachloroterphenyl |  | 367.95016 | Non-target screening | Canal | GC-HRMS | In house | G |
| trichloroterphenyl |  | 331.99208 | Non-target screening | Canal | GC-HRMS | In house | G |
| op'-DDE | C1=CC=C(C(=C1)C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 317.93459 | Non-target screening | Canal | GC-HRMS | In house | G |
| pp'-DDMU | C1=CC(=CC=C1C(=CCl)C2=CC=C(C=C2)Cl)Cl | 281.97643 | Non-target screening | Canal | GC-HRMS | In house | G |
| op'-DDMU | C1=CC=C(C(=C1)C(=CCl)C2=CC=C(C=C2)Cl)Cl | 281.97643 | Non-target screening | Canal | GC-HRMS | In house | G |
| Dichlorophenoxybenzaldehyde | C1=CC(=CC=C1C=O)OC2=CC(=CC(=C2)Cl)Cl | 266.99741 | Non-target screening | Canal | GC-HRMS | In house | G |
| Triphenylmethyl chloride | C1=CC=C(C=C1)C(C2=CC=CC=C2)(C3=CC=CC=C3)Cl | 278.08568 | Non-target screening | Canal | GC-HRMS | In house | G |
| pentachloroanisole | COC1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl | 279.85915 | Non-target screening | Canal | GC-HRMS | In house | G |
| nonachlorophenoxy anisole |  | 509.72662 | Non-target screening | Canal | GC-HRMS | In house | G |
| hexachlorobromostyrene |  | 389.73333 | Non-target screening | Canal | GC-HRMS | In house | G |
| pentachlorothioanisole | CSC1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl | 296.84410 | Non-target screening | Canal | GC-HRMS | In house | G |
| tetrachlorothioanisole | CSC1=CC(=C(C(=C1Cl)Cl)Cl)Cl | 262.88307 | Non-target screening | Canal | GC-HRMS | In house | G |
| 5-Chloro-2-(2,4-dichlorophenoxy)aniline | C1=CC(=C(C=C1Cl)N)OC2=C(C=C(C=C2)Cl)Cl | 357.89353 | Non-target screening | Canal | GC-HRMS | In house | G |
| isomer of tris(chlorophenyl)methane (de-Cl fragment) | C1=CC=C(C(=C1)C(C2=CC=CC=C2Cl)C3=CC=CC=C3Cl)Cl | 311.03888 | Non-target screening | Canal | GC-HRMS | In house | G |
| pp'-DDCN | C1=CC(=CC=C1C(C#N)C2=CC=C(C=C2)Cl)Cl | 261.01066 | Non-target screening | Canal | GC-HRMS | In house | G |
| op'-DDCN |  | 261.01066 | Non-target screening | Canal | GC-HRMS | In house | G |
| pp'-DBP | C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)Cl)Cl | 251.00250 | Non-target screening | Canal | GC-HRMS | In house | G |
| op'-DBP |  | 251.00250 | Non-target screening | Canal | GC-HRMS | In house | G |
| fragment of TCPMOH | C1=CC=C(C(=C1)C(C2=CC=CC=C2Cl)(C3=CC=CC=C3Cl)O)Cl | 344.99991 | Non-target screening | Canal | GC-HRMS | In house | G |
| amino dibromobenzaldehyde | C1=C(C=C(C(=C1C=O)N)Br)Br | 279.87902 | Non-target screening | Canal | GC-HRMS | In house | G |
| trichlorostyrene | C1=CC=C(C=C1)C(=C(Cl)Cl)Cl | 208.95001 | Non-target screening | Canal | GC-HRMS | In house | G |
| pp'-DDCN | C1=CC(=CC=C1C(C#N)C2=CC=C(C=C2)Cl)Cl | 261.01066 | Non-target screening | Canal | GC-HRMS | Reference | G |
| op'-DDCN |  | 261.01066 | Non-target screening | Canal | GC-HRMS | Reference | G |
| pp'-DBP | C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)Cl)Cl | 251.00250 | Non-target screening | Canal | GC-HRMS | Reference | G |
| op'-DDE | C1=CC=C(C(=C1)C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 317.93459 | Non-target screening | Canal | GC-HRMS | Reference | G |
| pp'-DDMU | C1=CC(=CC=C1C(=CCl)C2=CC=C(C=C2)Cl)Cl | 281.97643 | Non-target screening | Canal | GC-HRMS | Reference | G |
| op'-DDMU | C1=CC=C(C(=C1)C(=CCl)C2=CC=C(C=C2)Cl)Cl | 281.97643 | Non-target screening | Canal | GC-HRMS | Reference | G |
| fragment of Dichlorophenoxybenzaldehyde |  | 266.99741 | Non-target screening | Canal | GC-HRMS | Reference | G |
| Triphenylmethyl chloride | C1=CC=C(C=C1)C(C2=CC=CC=C2)(C3=CC=CC=C3)Cl | 278.08568 | Non-target screening | Canal | GC-HRMS | Reference | G |
| Fipronil Sulfone | C1=C(C=C(C(=C1Cl)N2C(=C(C(=N2)C#N)S(=O)(=O)C(F)(F)F)N)Cl)C(F)(F)F | 452.94090 | Non-target screening | Canal | GC-HRMS | Reference | G |
| pentachloroanisole | COC1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl | 279.85915 | Non-target screening | Canal | GC-HRMS | Reference | G |
| hexachlorobromostyrene |  | 389.73333 | Non-target screening | Canal | GC-HRMS | Reference | G |
| isomer of tris(chlorophenyl)methane (de-Cl fragment) | C1=CC=C(C(=C1)C(C2=CC=CC=C2Cl)C3=CC=CC=C3Cl)Cl | 311.03888 | Non-target screening | Canal | GC-HRMS | Reference | G |
| fragment of TCPMOH | C1=CC=C(C(=C1)C(C2=CC=CC=C2Cl)(C3=CC=CC=C3Cl)O)Cl | 344.99991 | Non-target screening | Canal | GC-HRMS | Reference | G |
| amino dibromobenzaldehyde | C1=C(C=C(C(=C1C=O)N)Br)Br | 279.87902 | Non-target screening | Canal | GC-HRMS | Reference | G |
| 1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl- | O=C(C(C=C)=C1C)NC1=O | 137.04770 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 5,7-Dimethyltetralin | CC1=CC(C)=C2CCCCC2=C1 | 160.12520 | Non-target screening | Canal | GC-HRMS | Reference | J |
| alpha-Cedrene | CC1(C)[C@]2([H])C(C)=CC[C@]3(C2)[C@H](C)CC[C@@]13[H] | 204.18780 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans- | CC1(C)CCC(C)(C)[C@]2([H])CC(C)(C)C[C@@]12[H] | 208.21910 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 1H-Indene, 2,4,5,6,7,7a-hexahydro-7a-methyl-3-(2-methylpropyl)- | CC(C)CC1=C2CCCCC2(C)CC1 | 192.18780 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Hexanophenone | CCCCCC(=O)C1=CC=CC=C1 | 176.12010 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene | CC1=CC2=C(C(C)=C1C)CCC2(C)C | 188.15650 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Naphthalene, decahydro-1,6-bis(methylene)-4-(1-methylethyl)-, (4alpha,4aalpha,8aalpha)- | CC([C@@H]([C@]1([H])CC(CC[C@]21[H])=C)CCC2=C)C | 204.18780 | Non-target screening | Canal | GC-HRMS | Reference | J |
| alpha-Muurolene | CC(C)[C@@H]1CC=C(C)[C@H]2CCC(C)=C[C@@H]12 | 204.18780 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)- | CC(C1CC=C(C)C2CCC(C)=CC12)C | 204.18780 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 1S-cis-Calamenene | CC([C@@H]1CC[C@H](C)C2=C1C=C(C)C=C2)C | 202.17220 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Dihydroactinolide | O=C1O[C@@]2(C)C(C(C)(C)CCC2)=C1 | 180.11500 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-butylhexyl)- | CCCCCC(C1=CC=CC=C1)CCCC | 218.20350 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 2,6,10-trimethyltetradecane | CCCCC(C)CCCC(C)CCCC(C)C | 240.28170 | Non-target screening | Canal | GC-HRMS | Reference | J |
| trans-Calamenene | CC1CCC(C2=C1C=CC(=C2)C)C(C)C | 202.17220 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Cedran-8-ol | O[C@@]1(C)CC[C@]23[C@H](C)CCC2C(C)(C)[C@@]1([H])C3 | 222.19840 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-pentylhexyl)- | CCCCCC(C1=CC=CC=C1)CCCCC | 232.21910 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-butylheptyl)- | CCCCCCC(C1=CC=CC=C1)CCCC | 232.21910 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Hexylresorcinol | CCCCCCC1=C(O)C=C(O)C=C1 | 194.13070 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-propyloctyl)- | CCCCCCCC(C1=CC=CC=C1)CCC | 232.21910 | Non-target screening | Canal | GC-HRMS | Reference | J |
| (7a-Isopropenyl-4,5-dimethyloctahydroinden-4-yl)methanol | OCC1(C)C2CCCC2(C(C)=C)CCC1C | 222.19840 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl- | CC1(C2=CC=CC=C2)CC(C)(C)C3=C1C=CC=C3 | 236.15650 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Celestolide | CC(=O)C1=CC(=CC2=C1CCC2(C)C)C(C)(C)C | 244.18270 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-pentylheptyl)- | CCCCCCC(C1=CC=CC=C1)CCCCC | 246.23480 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-butyloctyl)- | CCCCCCCC(C1=CC=CC=C1)CCCC | 246.23480 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-propylnonyl)- | CCCCCCCCC(C1=CC=CC=C1)CCC | 246.23480 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Acetyl-alpha-cedrene | [H][C@]12C[C@@]3(CC(C(C)=O)=C1C)[C@H](C)CC[C@@]3([H])C2(C)C | 246.19840 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 8-Ethyl-4,6,6,8-tetramethyl-3,4,6,7-tetrahydro-1H-cyclopenta(G)-2-benzopyran (Galaxolide isomer 1) | CCC1(CC(C2=C1C=C3C(COCC3=C2)C)(C)C)C | 258.19840 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-hexylheptyl)- | CCCCCCC(C1=CC=CC=C1)CCCCCC | 260.25040 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, (1-butylnonyl)- | CCCCCCCCC(C1=CC=CC=C1)CCCC | 260.25040 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Benzene, 4-chloro-1-methoxy-2-(phenylmethyl)- | COC1=CC=C(Cl)C=C1CC2=CC=CC=C2 | 232.06550 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Galaxolide (main isomer) | CC1COCC2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C | 258.19840 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 1,3,4,7,8,9-hexahydro-4,7,7,8,9,9-hexamethylcyclopenta [H]-2-benzopyran (Galaxolide isomer 3) | CC1(C)C(C)C(C)(C)C(C=C2)=C1C3=C2C(C)COC3 | 258.19840 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 1,2,4,7,8,9-hexahydro-1,7,7,8,9,9-hexamethylcyclopenta[F]-2-benzopyran (Galaxolide isomer 4) | CC1(C)C(C)C(C)(C)C2=C1C3=C(C=C2)COCC3C | 258.19840 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Dehydroabietine | CC1CCCC2(C1CCC3=C2C=CC(=C3)C(C)C)C | 256.21910 | Non-target screening | Canal | GC-HRMS | Reference | J |
| p,p'-DDMU | ClC=C(C1=CC=C(Cl)C=C1)C1=CC=C(Cl)C=C1 | 281.97700 | Non-target screening | Canal | GC-HRMS | Reference | J |
| PCB 101 | ClC1=CC(=C(Cl)C=C1)C1=C(Cl)C=C(Cl)C(Cl)=C1 | 323.88340 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Methyl triclosan | COC1=C(OC2=CC=C(Cl)C=C2Cl)C=CC(Cl)=C1 | 301.96680 | Non-target screening | Canal | GC-HRMS | Reference | J |
| p,p'-DDMS | ClCC(C1=CC=C(Cl)C=C1)C1=CC=C(Cl)C=C1 | 283.99260 | Non-target screening | Canal | GC-HRMS | Reference | J |
| PCB 110 | ClC1=CC=C(Cl)C(=C1Cl)C1=CC(Cl)=C(Cl)C=C1 | 323.88340 | Non-target screening | Canal | GC-HRMS | Reference | J |
| o,p'-DDD | ClC(Cl)C(C1=CC=C(Cl)C=C1)C1=C(Cl)C=CC=C1 | 317.95370 | Non-target screening | Canal | GC-HRMS | Reference | J |
| m,p'-DDD | C1=CC(=CC(=C1)Cl)C(C2=CC=C(C=C2)Cl)C(Cl)Cl | 317.95370 | Non-target screening | Canal | GC-HRMS | Reference | J |
| PCB-138 | ClC1=CC(Cl)=C(C=C1Cl)C1=C(Cl)C(Cl)=C(Cl)C=C1 | 357.84440 | Non-target screening | Canal | GC-HRMS | Reference | J |
| p,p'-DDD | ClC(Cl)C(C1=CC=C(Cl)C=C1)C1=CC=C(Cl)C=C1 | 317.95370 | Non-target screening | Canal | GC-HRMS | Reference | J |
| Squalene | CC(C)=CCCC(C)=CCCC(C)=CCCC=C(C)CCC=C(C)CCC=C(C)C | 410.39130 | Non-target screening | Canal | GC-HRMS | Reference | J |
| 2-Cyano-2-methyl-1-cyclobutanone | CC1(CCC1=O)C#N |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 1,6-Bis(2-propyn-1-yloxy)hexane | C#CCOCCCCCCOCC#C |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 2,4-Diethyl-2-methyl-2,5-dihydro-1H-imidazole |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Octyl chloroacetate | CCCCCCCCOC(=O)CCl |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Cyclohexene, 3-methyl-6-(1-methylethyl)- |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| P- 1,2-epoxy-1-phenyl-2-phenylsulfinylbutane |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 1-Methoxy-1-(trichloromethyl)ethyl Cyclopentyl Ether |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 2,4 DECADIENAL | CCCCCC=CC=CC=O |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Isopentylacetylene |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Pentane, 3-bromo- | CCC(CC)Br |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Disulfide, dihexyl | CCCCCCSSCCCCCC |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Di-n-octyl disulfide | CCCCCCCCSSCCCCCCCC |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 3-Amino-1,2,4-triazole-5-carboxylic acid | C1(=NC(=NN1)N)C(=O)O |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| (E/Z)-o-Isocyano-.beta.methoxy-.alpha.-phenylstrene |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 1-Cyclopropyl-6-fluoro-1,4-dihydro-7-(3-methyl-1-piperazinyl)-4-oxo-8-(trifluoro |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 3,3-Dibutoxycarbonyl-1,2,3,9-tetrahydropyrrolo[2,1-b]quinazolin-9-one |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 1,3-Bis(2-methoxy-3-nitrophenyl)tetrahydro-2-pyrimidinone |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Diimidazo[1',2':1,8: 2'',1'':4,5][1,5]diazocino[3,2-b:7,6-b']diquinoline |  |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| 3.beta.-Acetoxy-5,6.alpha.-epoxycholestane | CC(C)CCCC(C)C1CCC2C1(CCC3C2CC4C5(C3(CCC(C5)OC(=O)C)C)O4)C |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| Cholest-5-en-3-ol (3.beta.)-, acetate | CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)OC(=O)C)C)C |  | Non-target screening | Canal | GC-HRMS | Reference | N |
| (Z,Z)-1(S)-Hydroxy-5,6-epoxycyclododeca-2,9-diene |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| (Bistrifluoromethylamino-oxy)cyclohexane |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| Benzene, 1-ethyl-2-methyl- | CCC1=CC=CC=C1C |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| (E)-1-((1'S,2'S)-trans-Methylcyclopentyl)-2-butylethylene |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| Disulfide, dipentyl | CCCCCSSCCCCC |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| Cyclohexene, 3-(bromomethyl)- | C1CC=CC(C1)CBr |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 1,1,1,2-tetrafluoro-2-tridecene |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 1-Nitro-2-(prop-2-enyl)cyclohexane |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 5-Methyl-2-(1'-methylenepropyl)cyclohexanol |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 2-Pyridyl acetate |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 1H-Imidazole | C1=CN=CN1 |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| Bicyclo[2.2.1]heptane, 2-(1-methylpropyl)- |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 1-Chloro-1-methylenespiro[2.4]hept-4-ene |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| Sabinene | CC(C)C12CCC(=C)C1C2 |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 2-Chloro-2-cyanospiro[6.2]nonan-1-methanol |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| Di-n-octyl disulfide | CCCCCCCCSSCCCCCCCC |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| DDMU | C1=CC(=CC=C1C(=CCl)C2=CC=C(C=C2)Cl)Cl |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 3-[2-[2-(Dimethylamino)ethoxy]ethenyl]thiophene |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 2-(1,2,3,3,4,4,5,5-octafluorocyclopentyl)oxepane |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| Squalene | CC(=CCCC(=CCCC(=CCCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 3.beta.-Cholesterol Methylsulfinate |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| (1Z)-1-(2-Oxo-5-phenyldihydrofuran-3-ylidene)ethyl trifluoromethanesulfonate |  |  | Non-target screening | Canal | GC-HRMS | Repeated\_reference | N |
| 1-(Methylsulfanyl)-3-undecanone | CCCCCCCCC(=O)CCSC | 216.15479 | Non-target screening | Lake | LC-HRMS | In house | C |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Lake | LC-HRMS | In house | I |
| 1H-Benzimidazole, 2-(octylthio)- | CCCCCCCCSc1[nH]c2ccccc2n1 | 262.15037 | Non-target screening | Lake | LC-HRMS | In house | I |
| Linoleamide | CCCCC/C=C\C/C=C\CCCCCCCC(=O)N | 279.25621 | Non-target screening | Lake | LC-HRMS | In house | I |
| 1-(Methylsulfanyl)-3-undecanone | CCCCCCCCC(=O)CCSC | 216.15479 | Non-target screening | Lake | LC-HRMS | Reference | C |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Lake | LC-HRMS | Reference | I |
| 1H-Benzimidazole, 2-(octylthio)- | CCCCCCCCSc1[nH]c2ccccc2n1 | 262.15037 | Non-target screening | Lake | LC-HRMS | Reference | I |
| Linoleamide | CCCCC/C=C\C/C=C\CCCCCCCC(=O)N | 279.25621 | Non-target screening | Lake | LC-HRMS | Reference | I |
| panthenyl ethyl ether | CCOCCCNC(=O)[C@H](O)C(C)(C)CO | 233.16271 | Non-target screening | Lake | LC-HRMS | Reference | I |
| S-Decyl ethanethioate | CCCCCCCCCCSC(=O)C | 216.15479 | Non-target screening | Lake | LC-HRMS | Repeated\_reference | I |
| 1H-Benzimidazole, 2-(octylthio)- | CCCCCCCCSc1[nH]c2ccccc2n1 | 262.15037 | Non-target screening | Lake | LC-HRMS | Repeated\_reference | I |
| Linoleamide | CCCCC/C=C\C/C=C\CCCCCCCC(=O)N | 279.25621 | Non-target screening | Lake | LC-HRMS | Repeated\_reference | I |
| 1-(Methylsulfanyl)-3-undecanone | CCCCCCCCC(=O)CCSC | 216.15479 | Non-target screening | Lake | GC-HRMS | In house | C |
| pp'-DDMU | C1=CC(=CC=C1C(=CCl)C2=CC=C(C=C2)Cl)Cl | 281.97643 | Non-target screening | Lake | GC-HRMS | In house | G |
| isomer of tris(chlorophenyl)methane (de-Cl fragment) | C1=CC=C(C(=C1)C(C2=CC=CC=C2Cl)C3=CC=CC=C3Cl)Cl | 311.03888 | Non-target screening | Lake | GC-HRMS | In house | G |
| pp'-DDCN | C1=CC(=CC=C1C(C#N)C2=CC=C(C=C2)Cl)Cl | 261.01066 | Non-target screening | Lake | GC-HRMS | In house | G |
| fragment of TCPMOH | C1=CC=C(C(=C1)C(C2=CC=CC=C2Cl)(C3=CC=CC=C3Cl)O)Cl | 344.99991 | Non-target screening | Lake | GC-HRMS | In house | G |
| 1-(Methylsulfanyl)-3-undecanone | CCCCCCCCC(=O)CCSC | 216.15479 | Non-target screening | Lake | GC-HRMS | Reference | C |
| pp'-DDMU | C1=CC(=CC=C1C(=CCl)C2=CC=C(C=C2)Cl)Cl | 281.97643 | Non-target screening | Lake | GC-HRMS | Reference | G |
| isomer of tris(chlorophenyl)methane (de-Cl fragment) | C1=CC=C(C(=C1)C(C2=CC=CC=C2Cl)C3=CC=CC=C3Cl)Cl | 311.03888 | Non-target screening | Lake | GC-HRMS | Reference | G |