

Hygroline derivatives from *Schizanthus tricolor* and their anti-trypanosomatid and antiplasmodial activities.

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Fig. S1 IR spectrum of schizanthoside A1 (**1**).

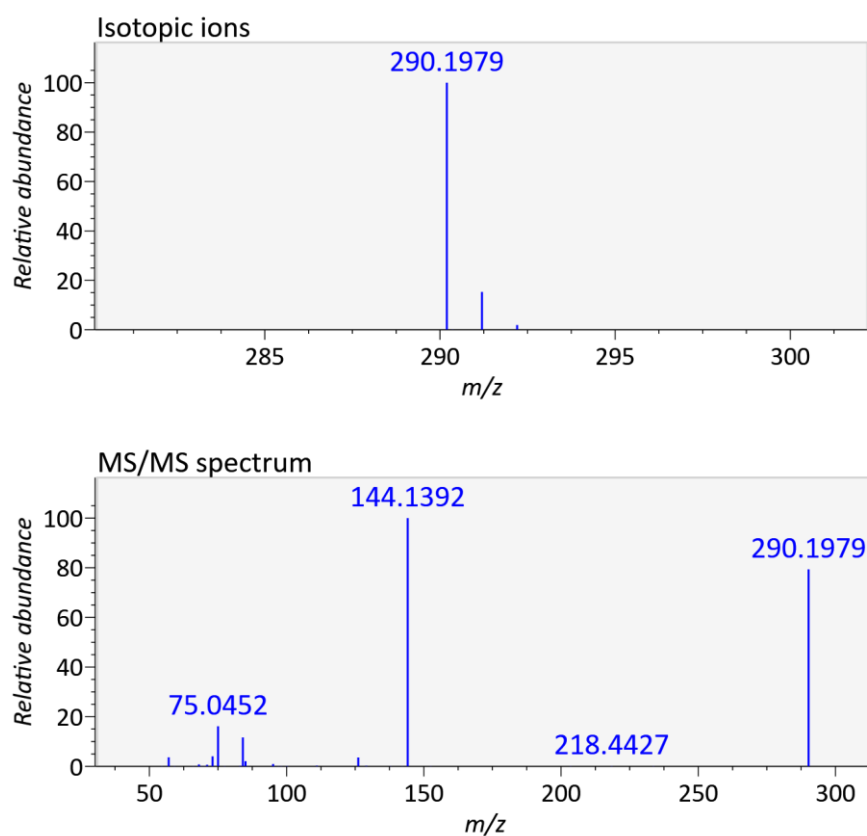


Fig. S2 HRESIMS and MS/MS spectra of schizanthoside A1 (**1**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

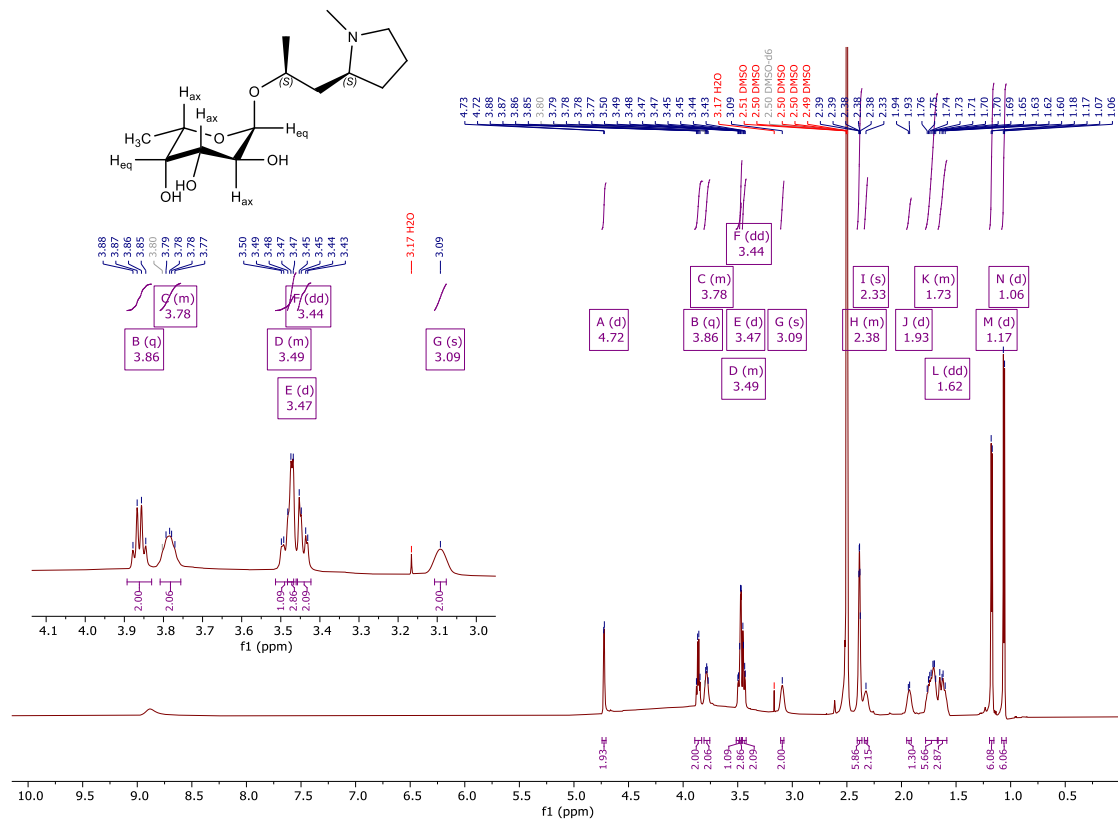


Fig. S3 ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A1 (1).

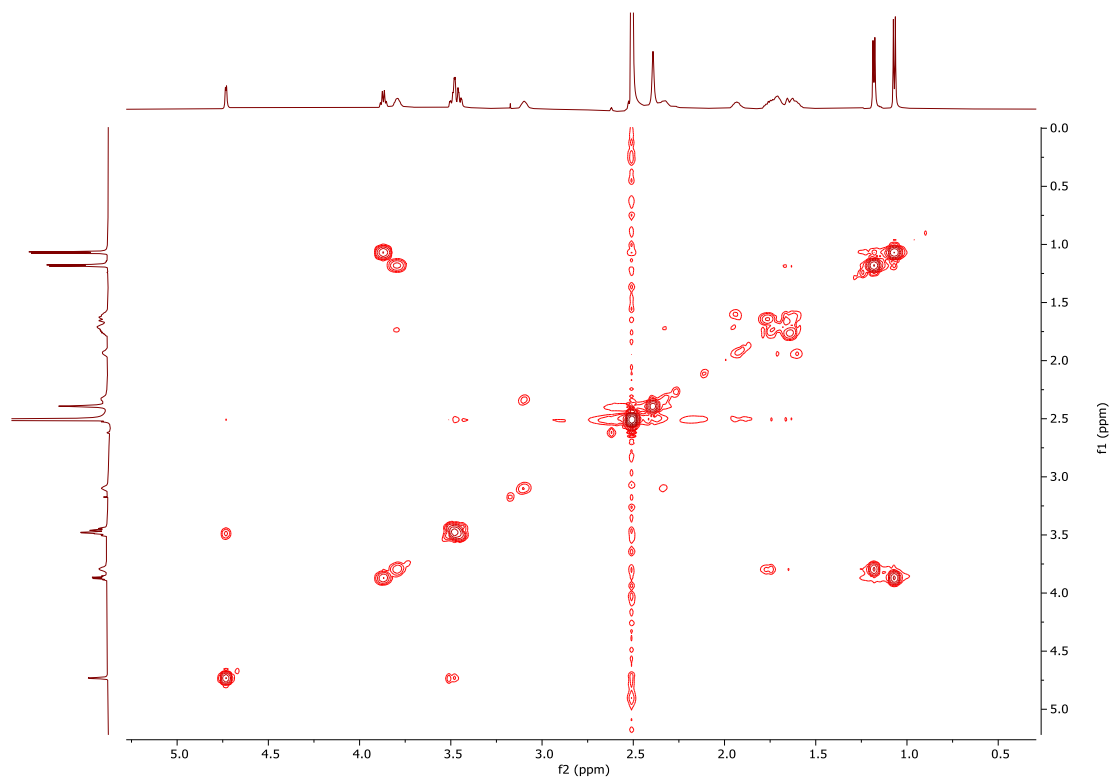


Fig. S4 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A1 (1).

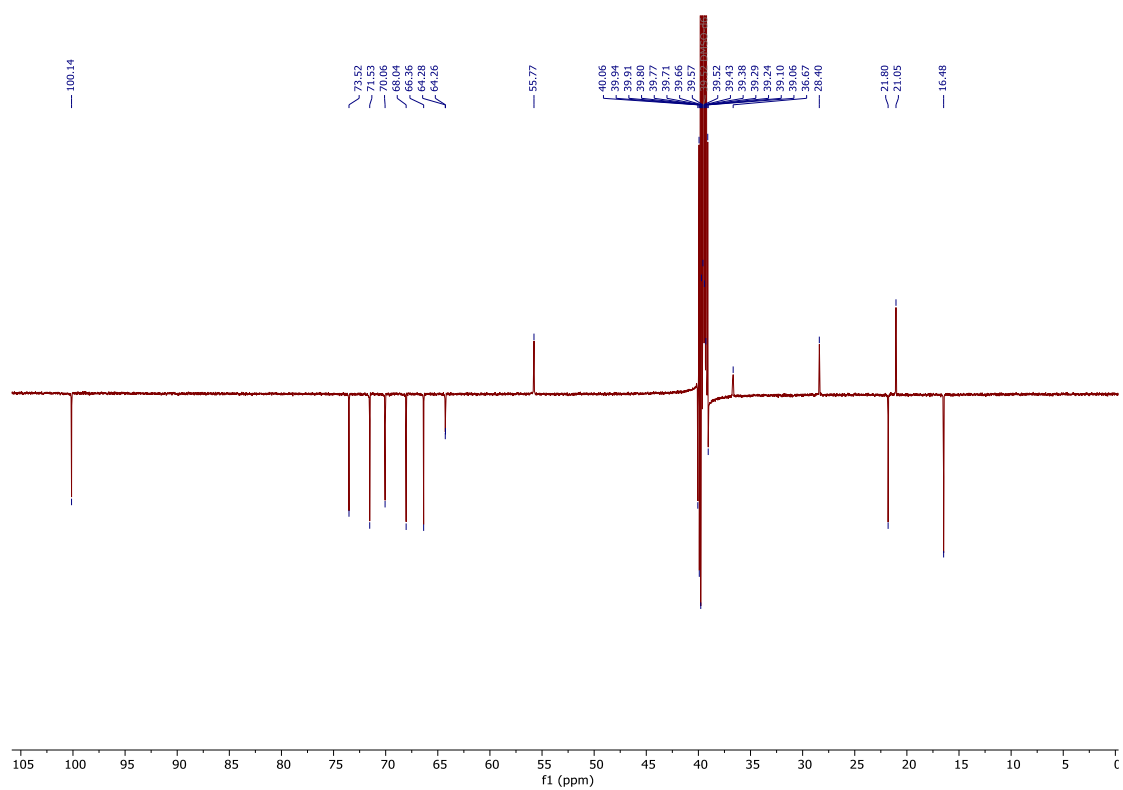


Fig. S5 DEPTQ (125 MHz, DMSO- d_6) spectrum of schizanthoside A1 (**1**).

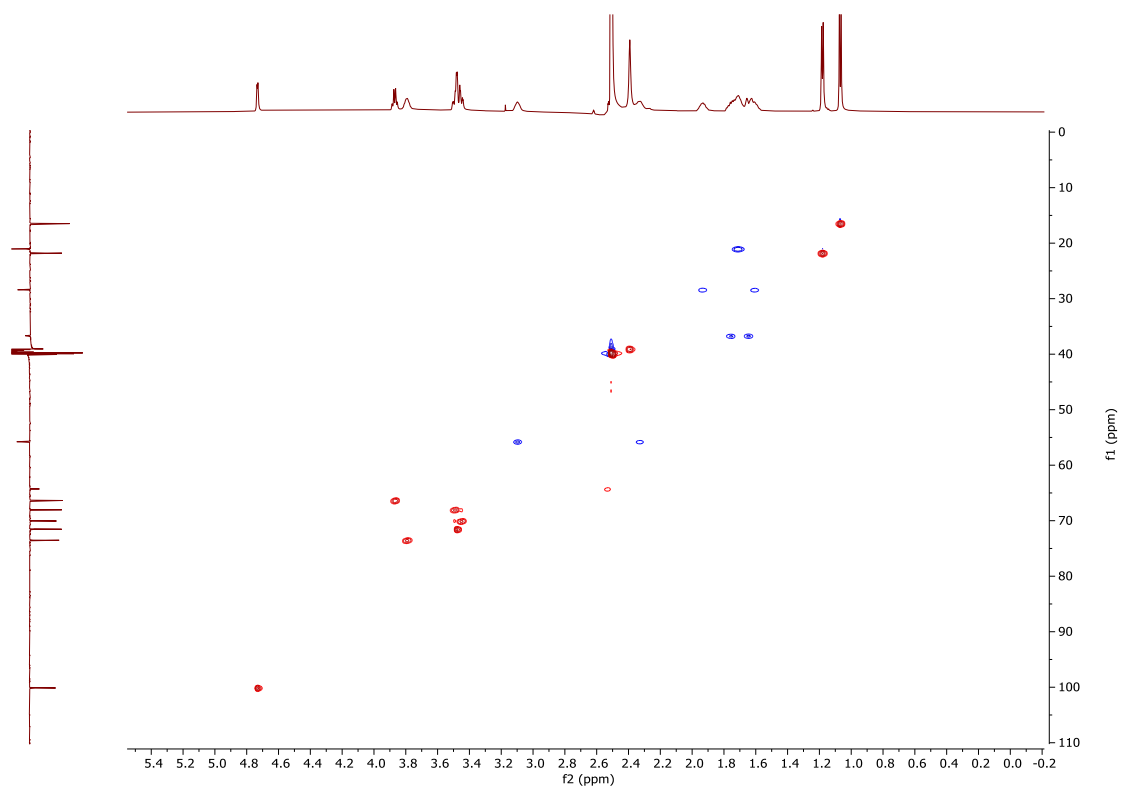


Fig. S6 HSQC (600 MHz, DMSO- d_6) spectrum of schizanthoside A1 (**1**).

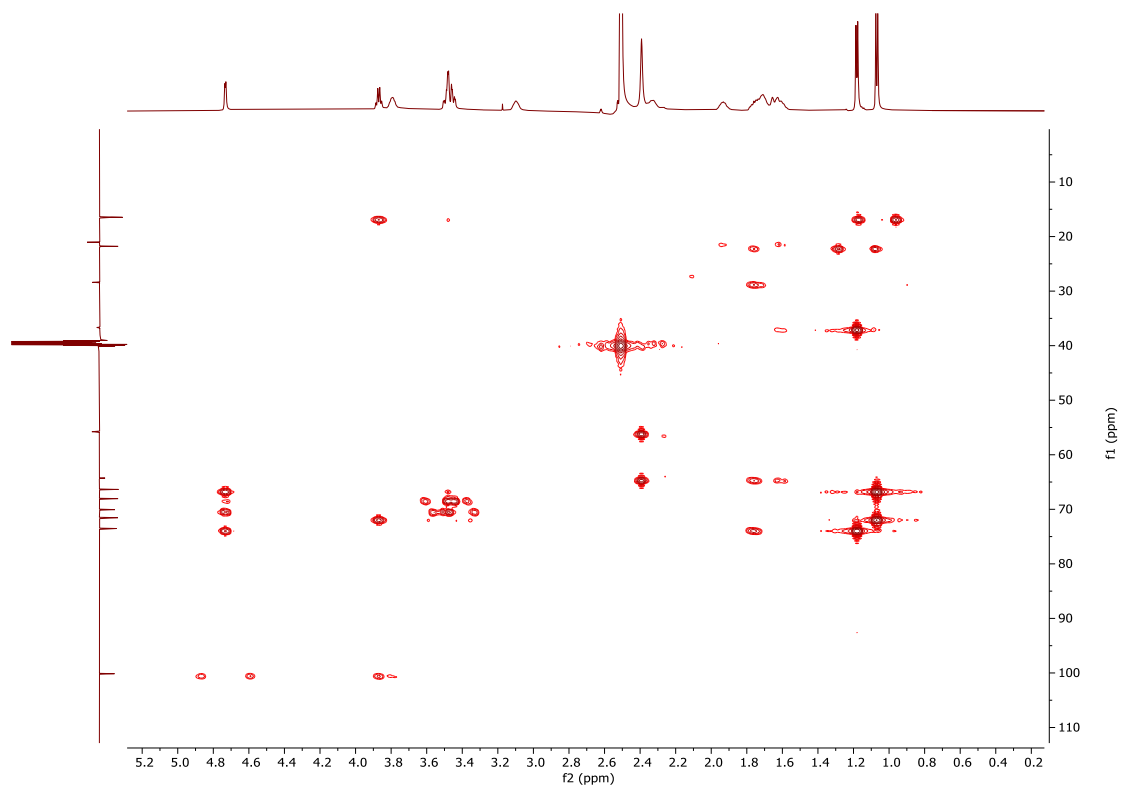


Fig. S7 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A1 (**1**).

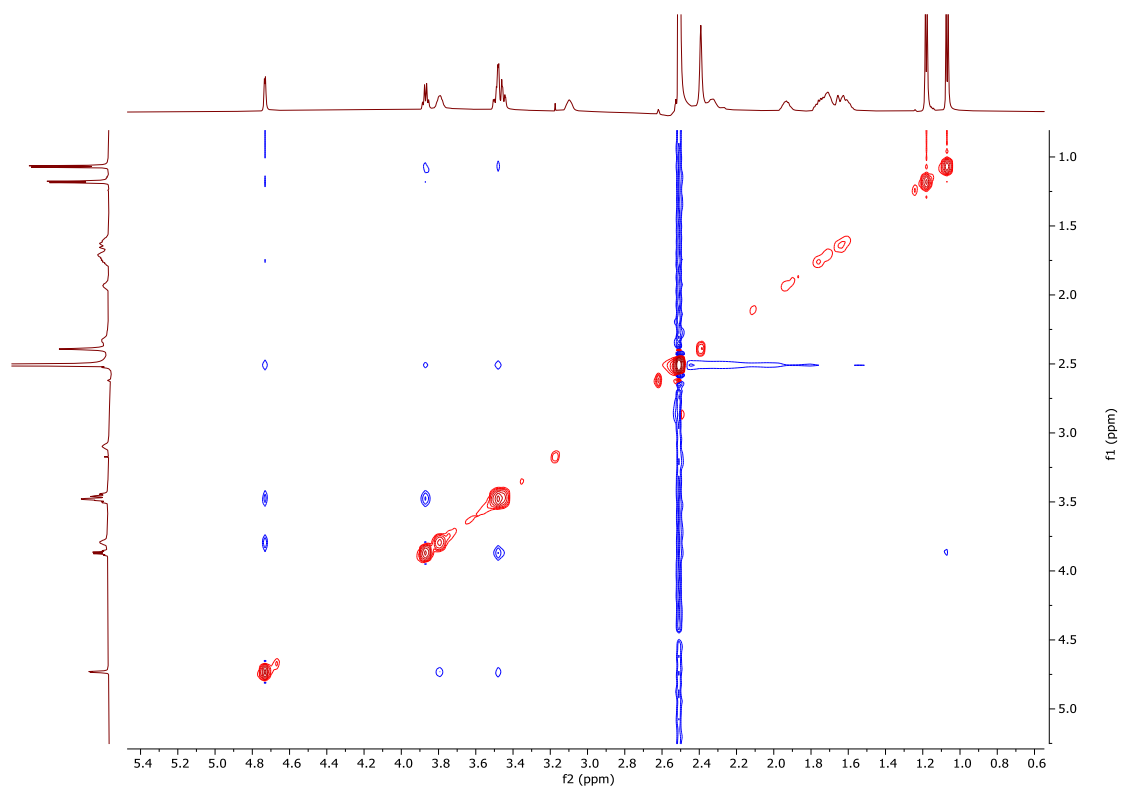


Fig. S8 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A1 (**1**).

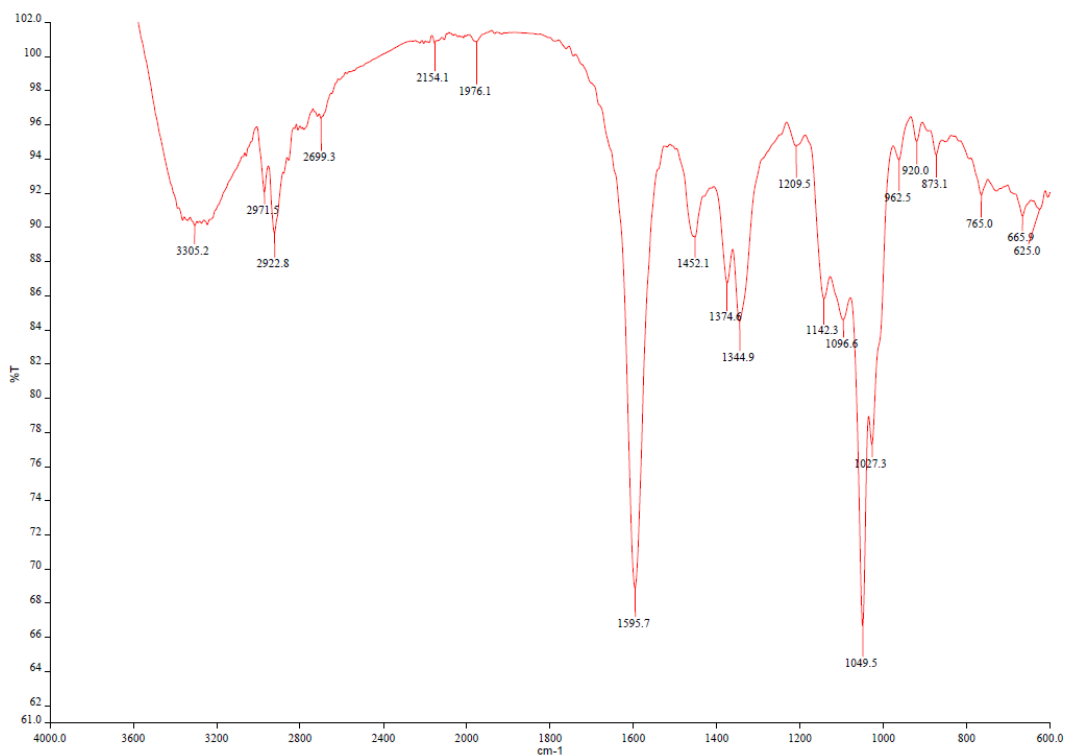


Fig. S9 IR spectrum of schizanthoside A2 (**2**).

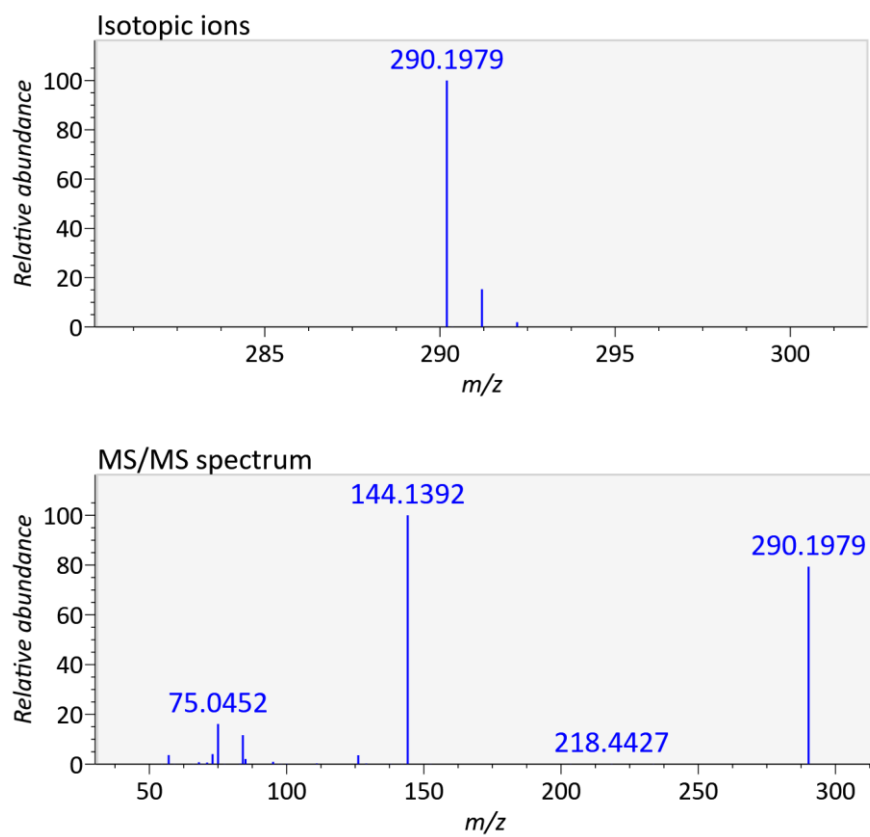


Fig. S10 HRESIMS and MS/MS spectra of schizanthoside A2 (**2**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

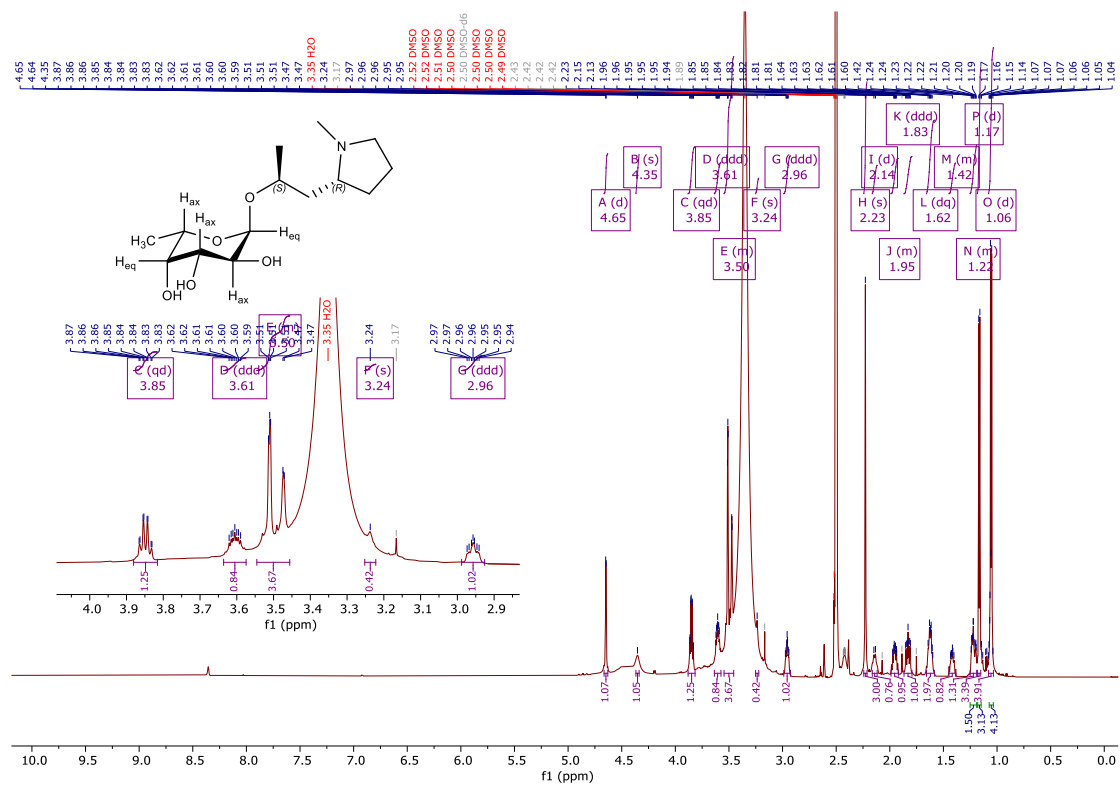


Fig. S11 ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A2 (2).

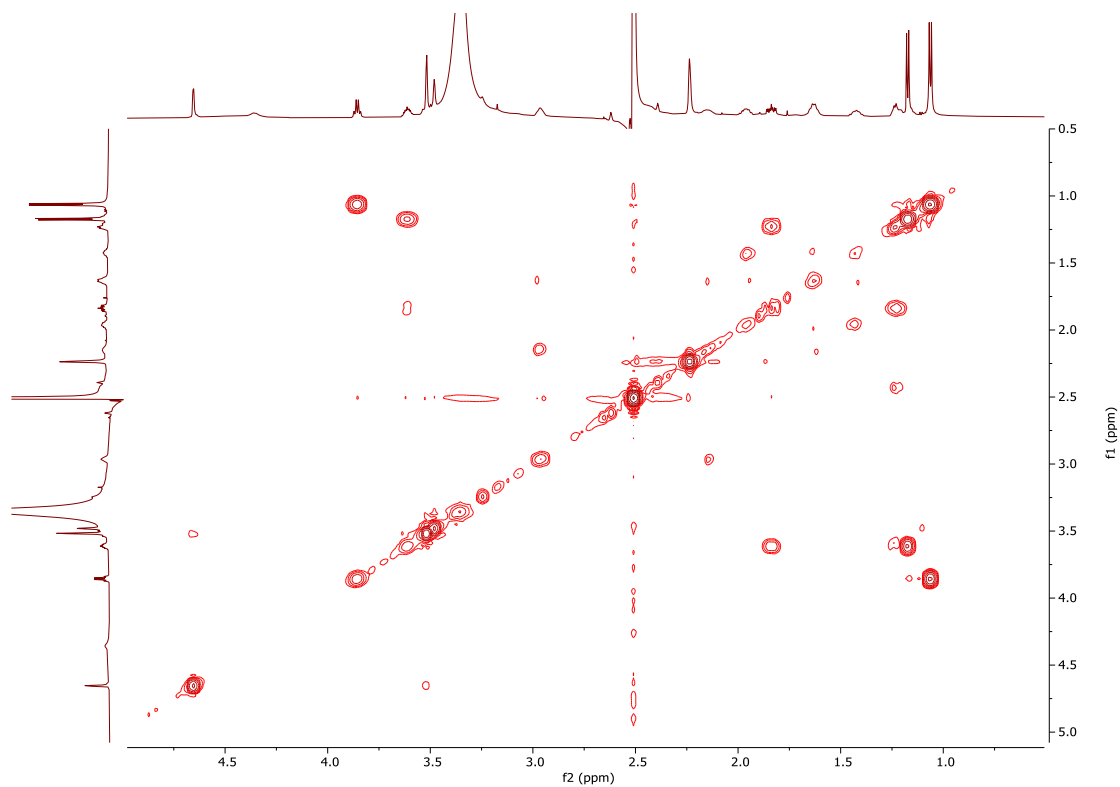


Fig. S12 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A2 (2).

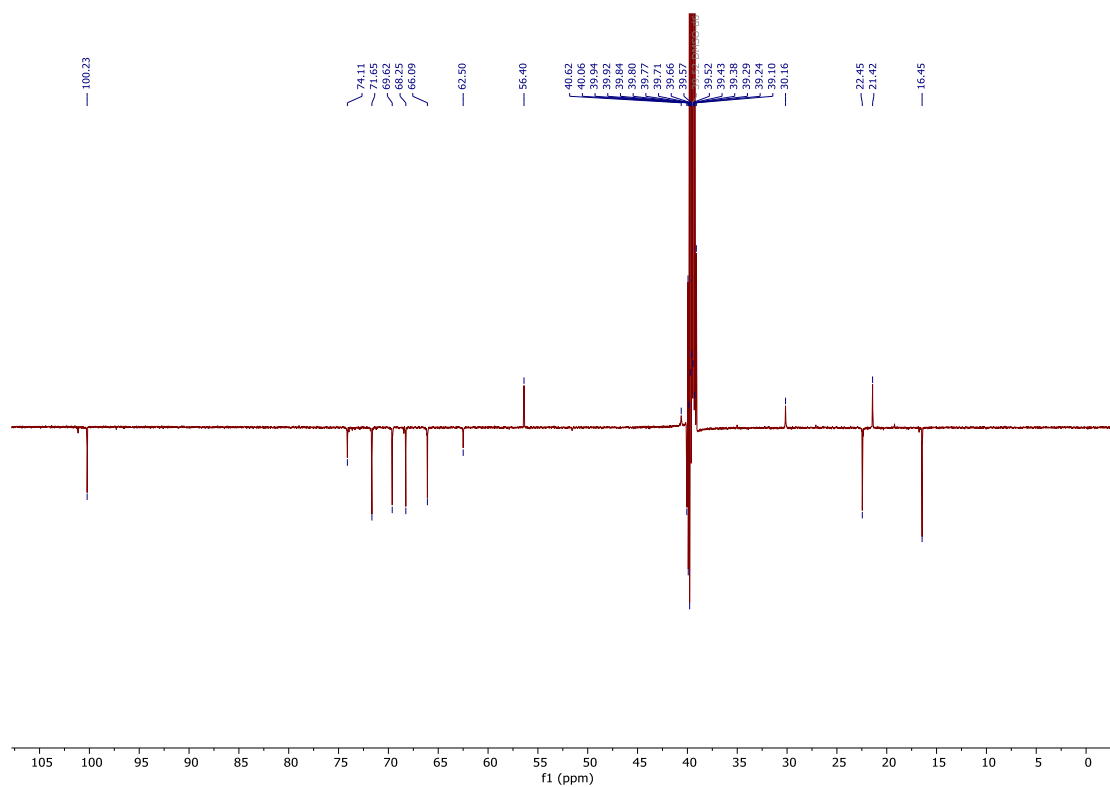


Fig. S13 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside A2 (**2**).

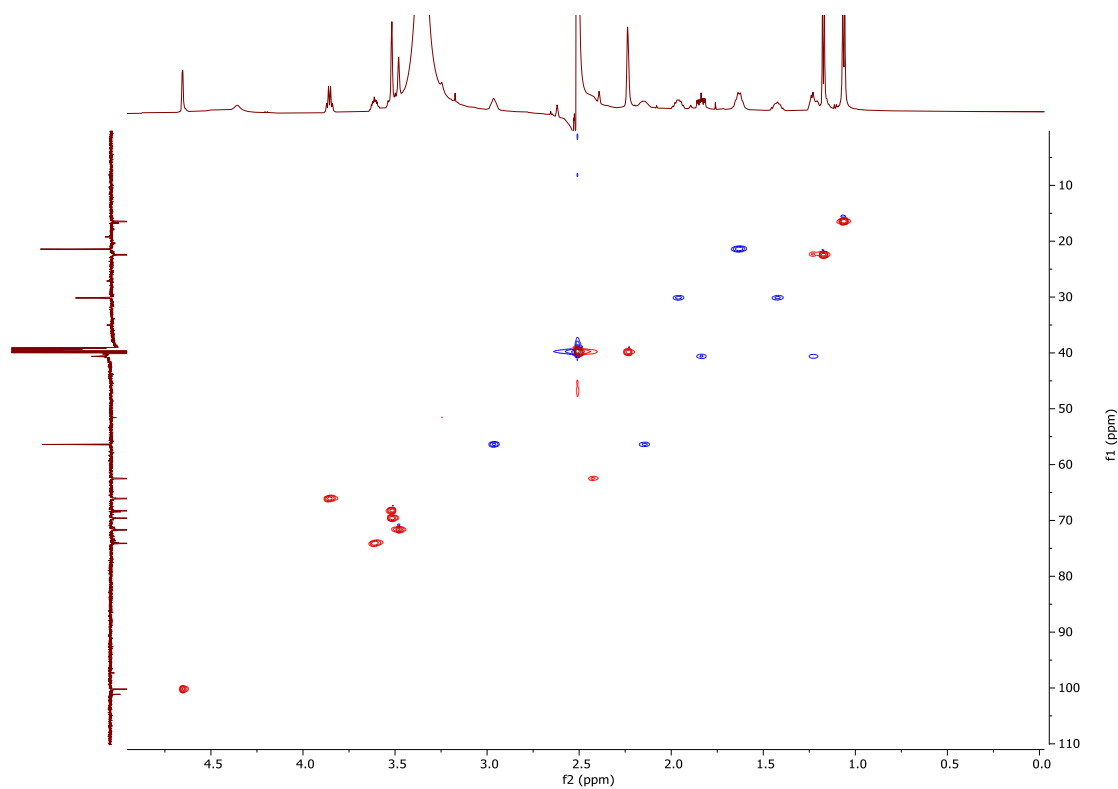


Fig. S14 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A2 (**2**).

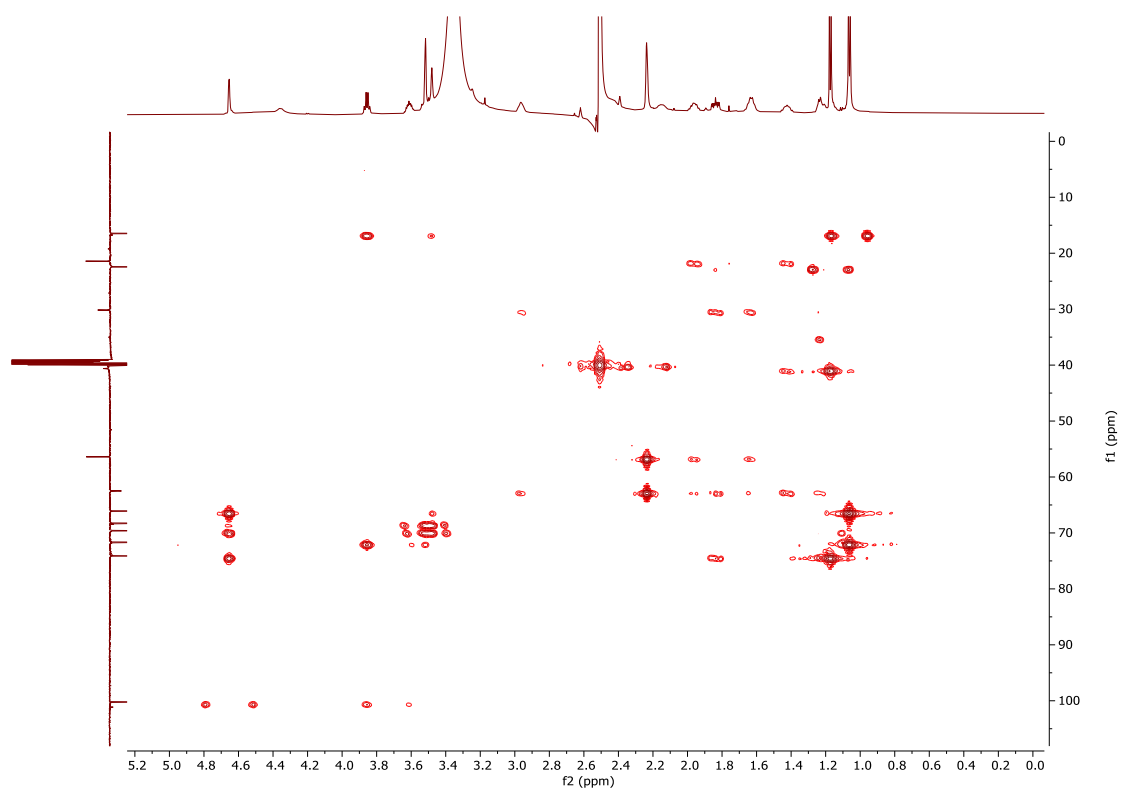


Fig. S15 HMBC (600 MHz, DMSO- d_6) spectrum of schizanthoside A2 (**2**).

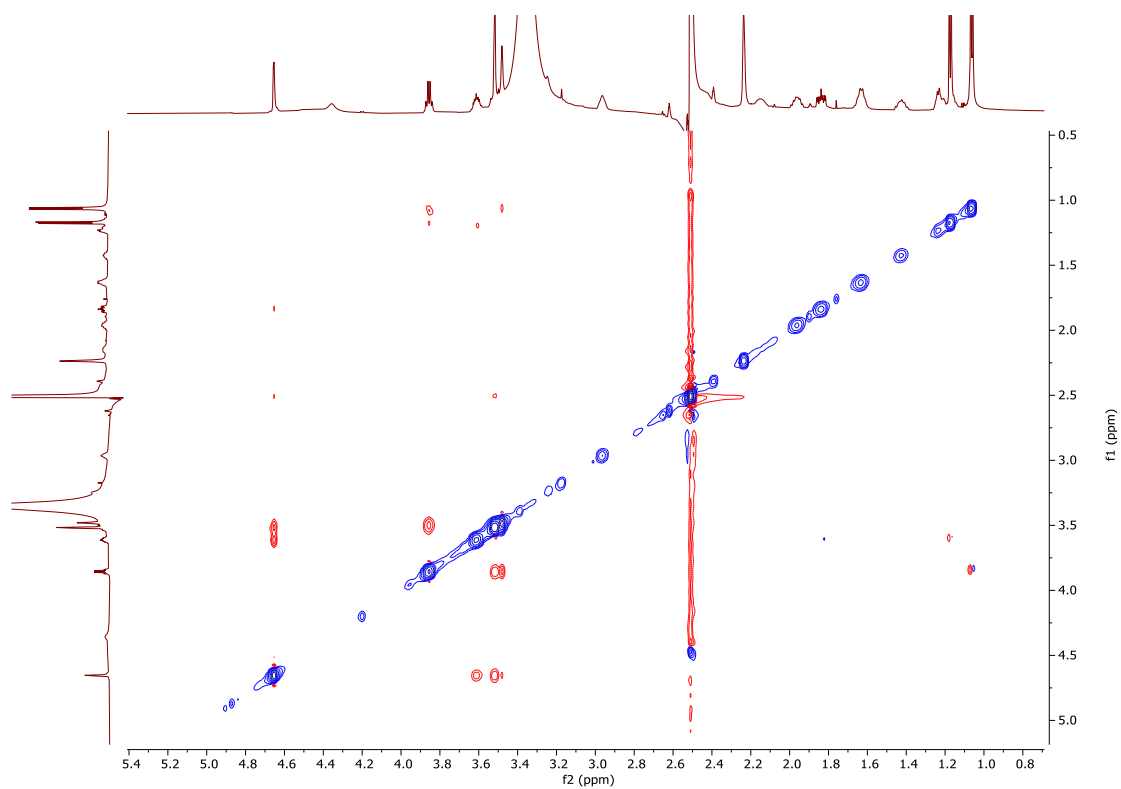


Fig. S16 ROESY (600 MHz, DMSO- d_6) spectrum of schizanthoside A2 (**2**).

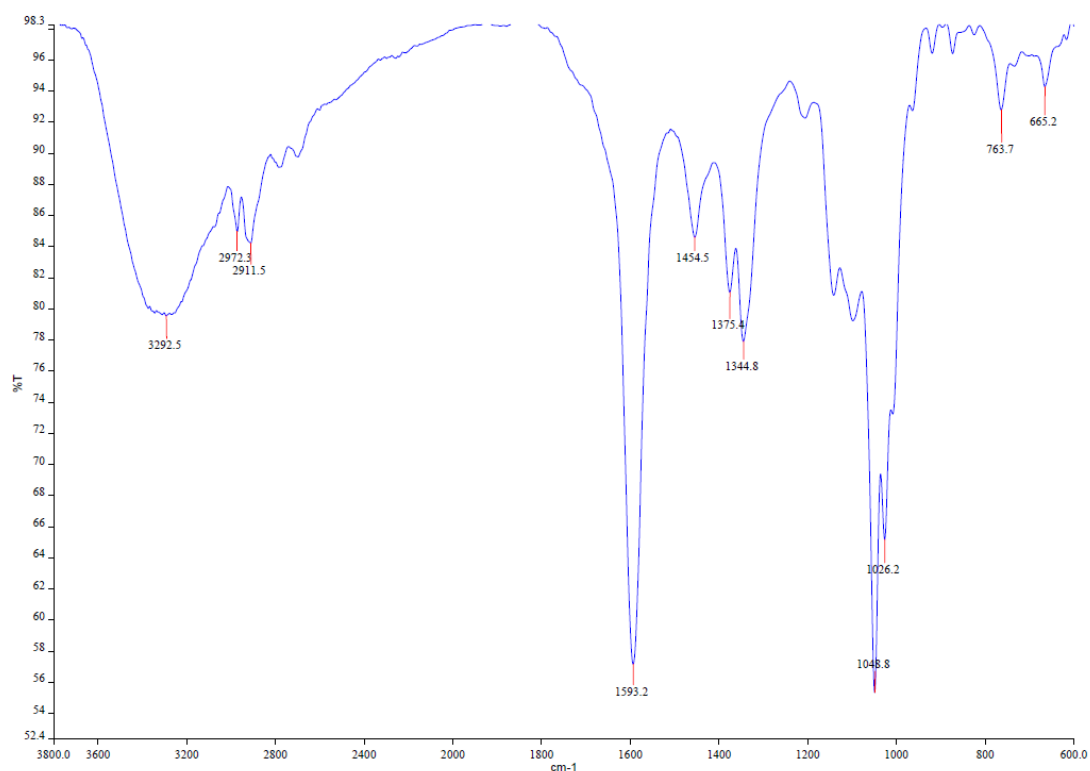


Fig. S17 IR spectrum of schizanthoside A3 (**3**).

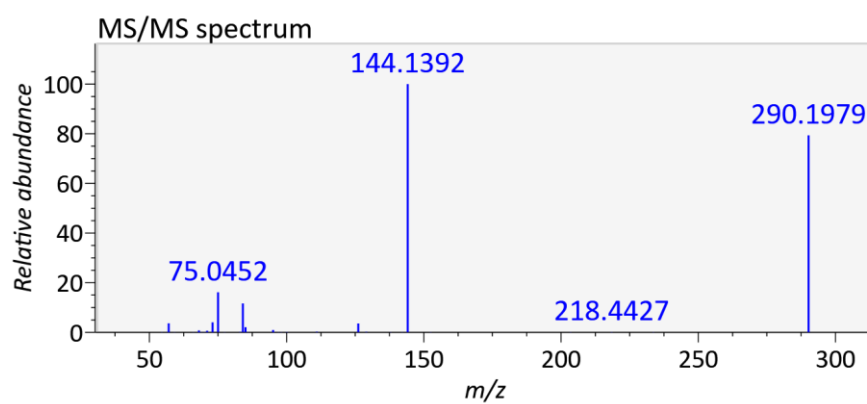
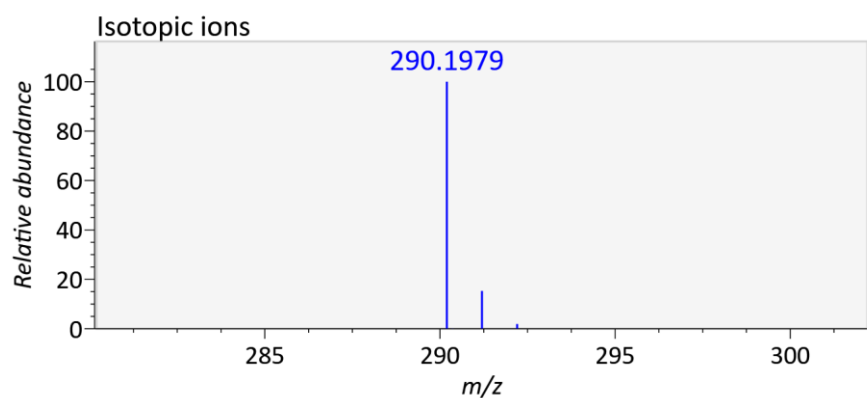


Fig. S18 HRESIMS and MS/MS spectra of schizanthoside A3 (**3**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

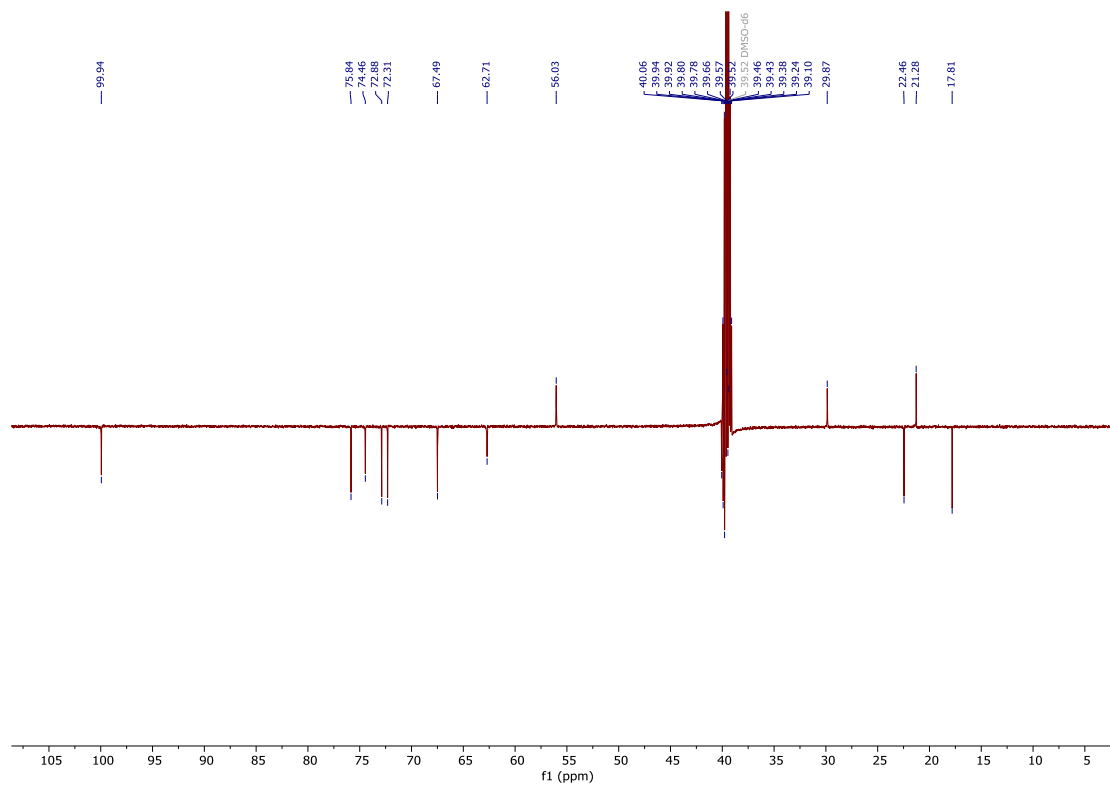


Fig. S21 DEPTQ (125 MHz, DMSO- d_6) spectrum of schizanthoside A3 (**3**).

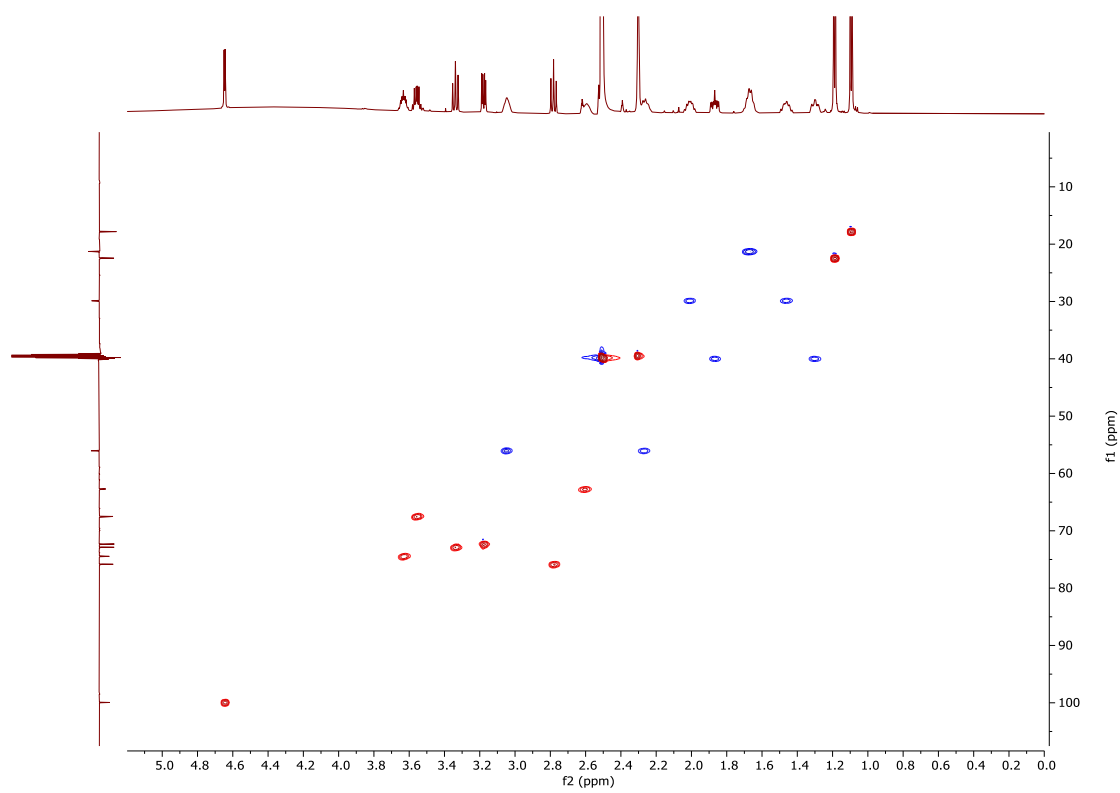


Fig. S22 HSQC (600 MHz, DMSO- d_6) spectrum of schizanthoside A3 (**3**).

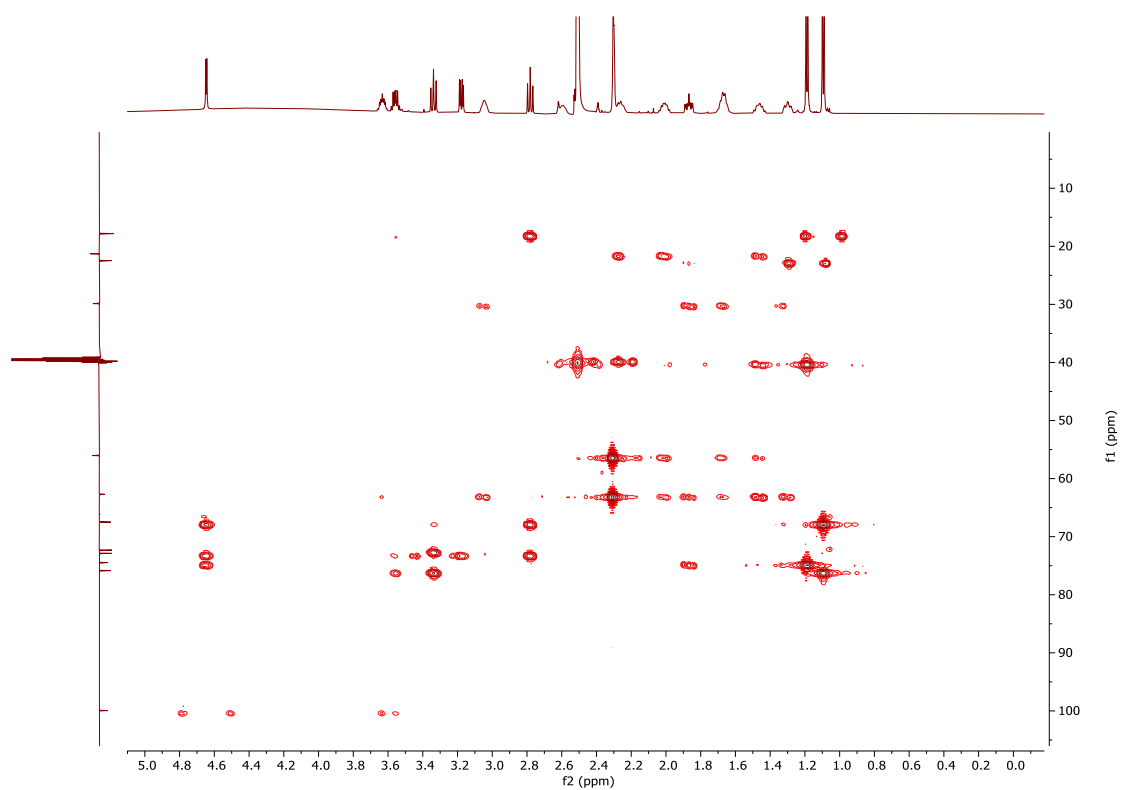


Fig. S23 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A3 (**3**).

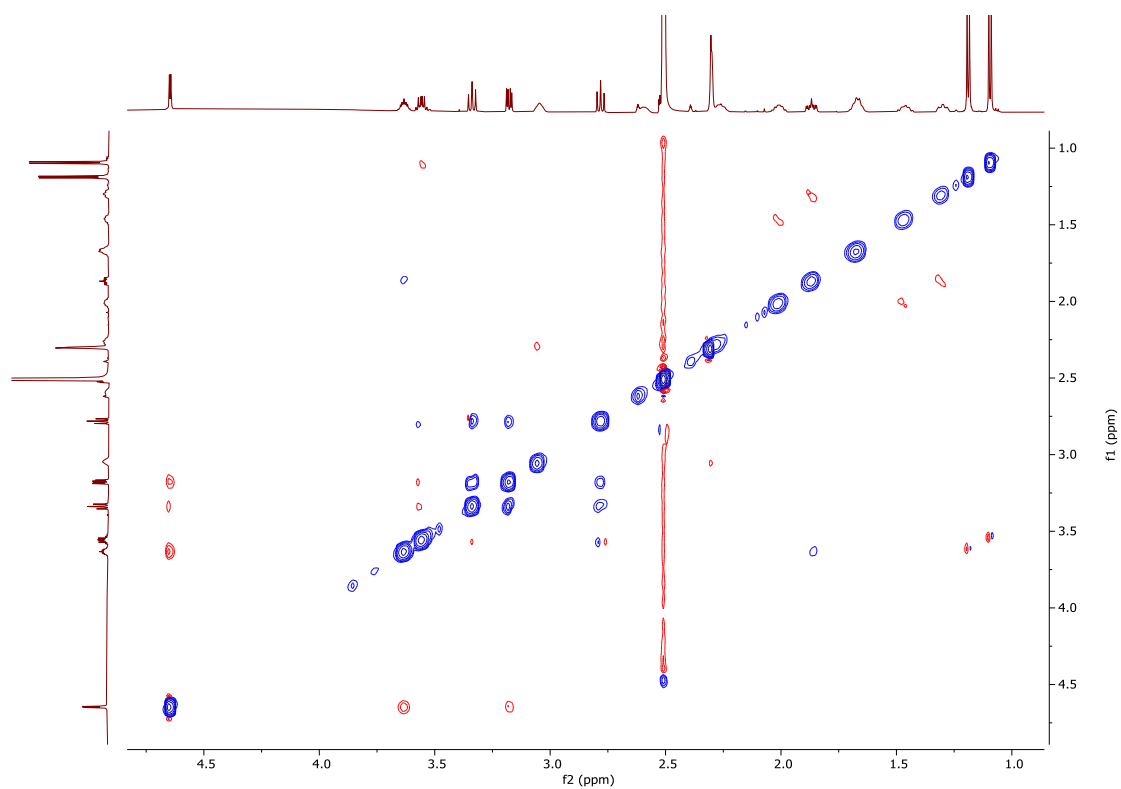


Fig. S24 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside A3 (**3**).

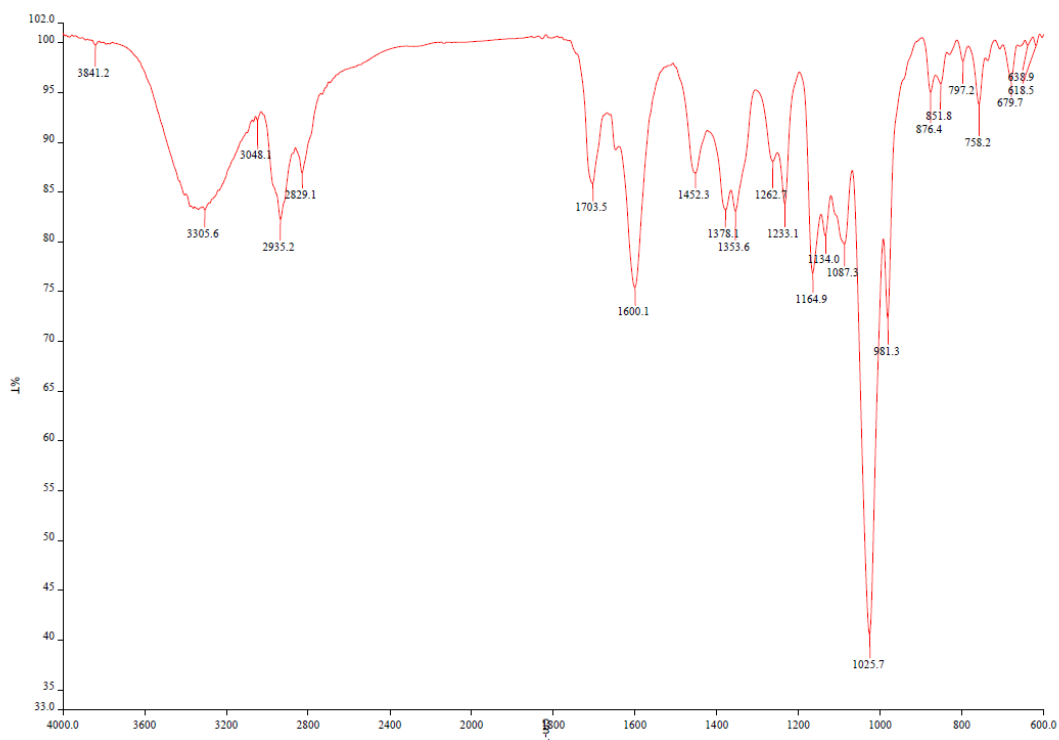


Fig. S25 IR spectrum of schizanthoside B1 (**4**).

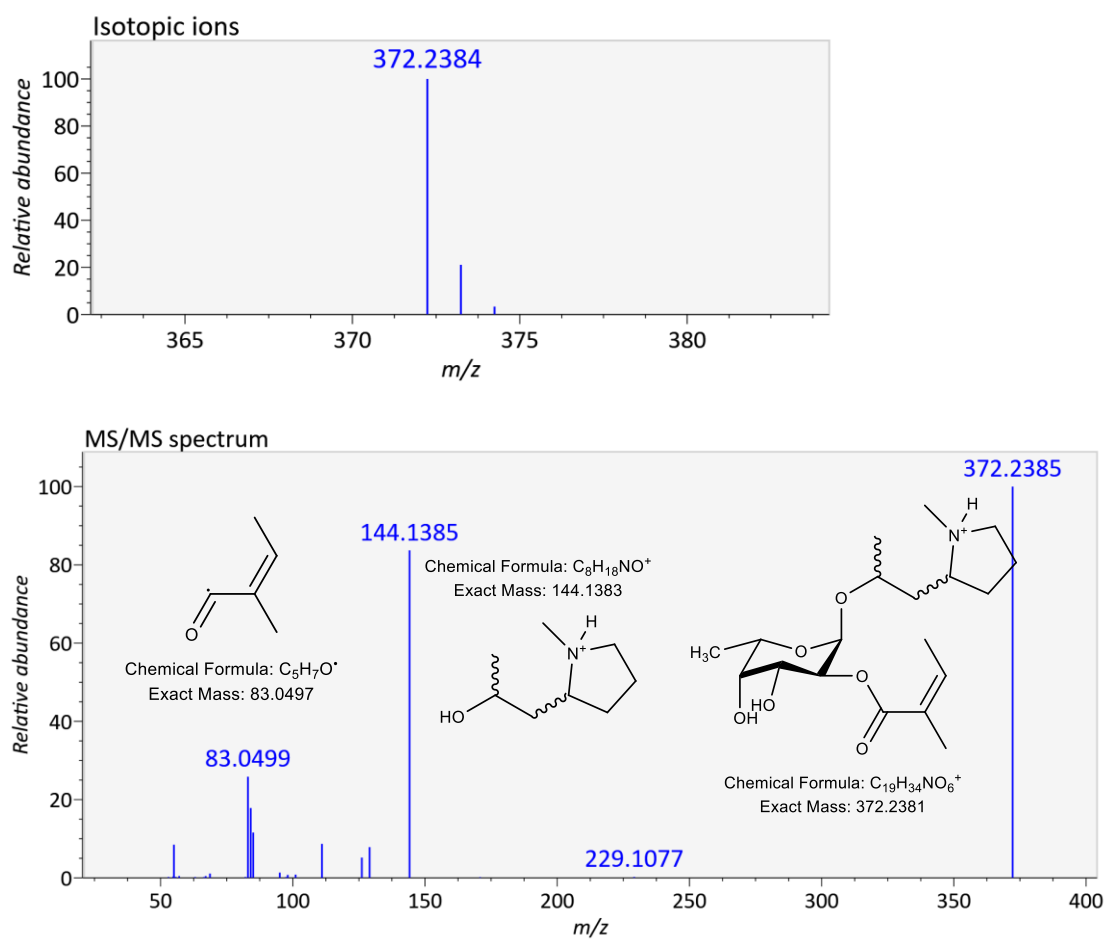


Fig. S26 HRESIMS and MS/MS spectra of schizanthoside B1 (**4**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

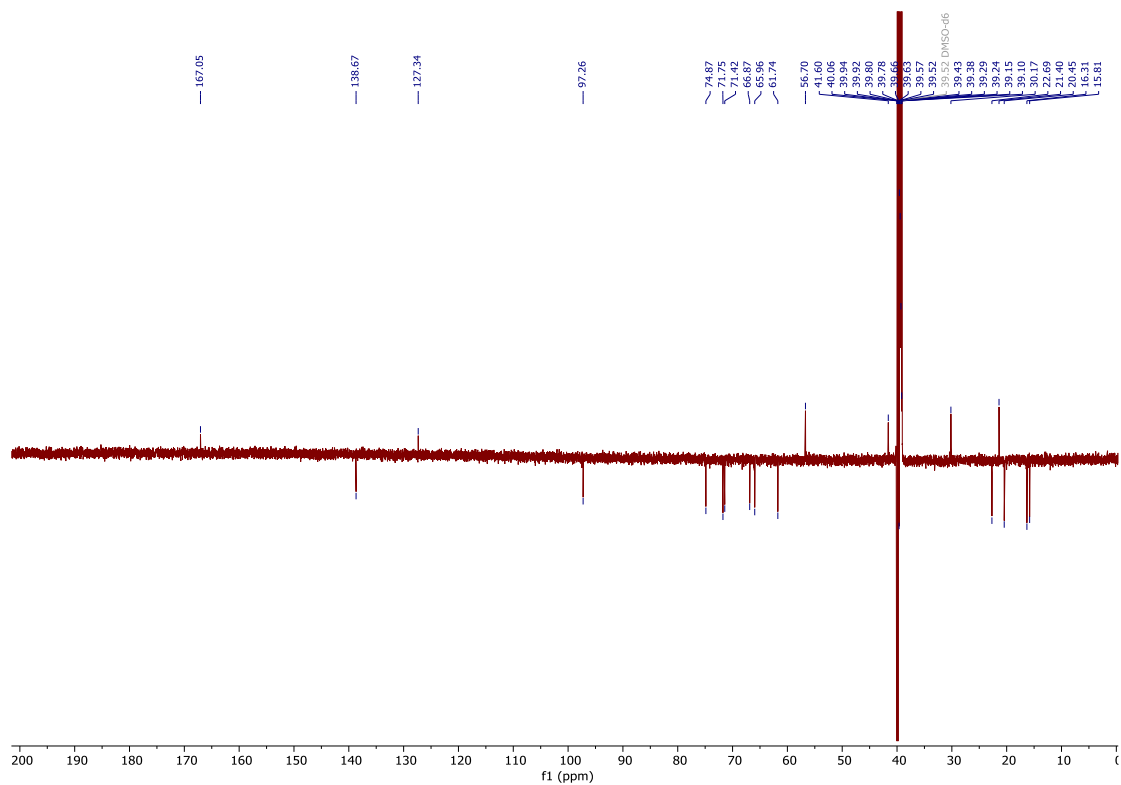


Fig. S29 DEPTQ (125 MHz, DMSO- d_6) spectrum of schizanthoside B1 (4).

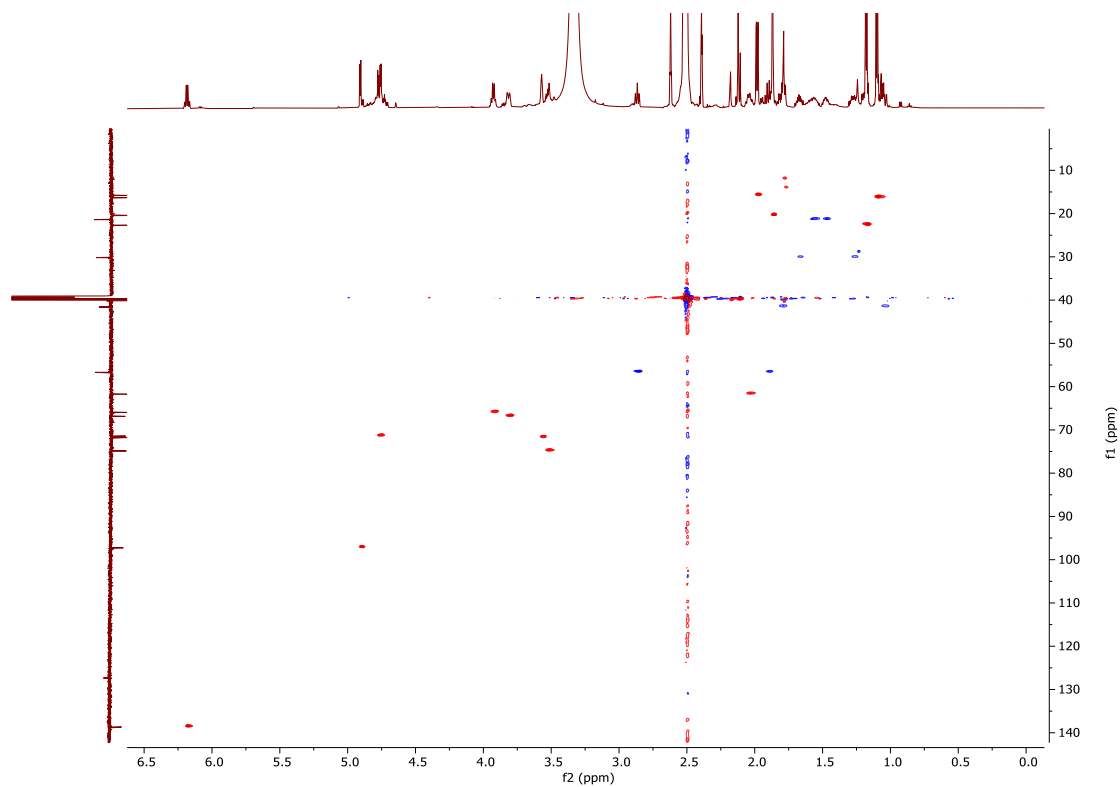


Fig. S30 HSQC (600 MHz, DMSO- d_6) spectrum of schizanthoside B1 (4).

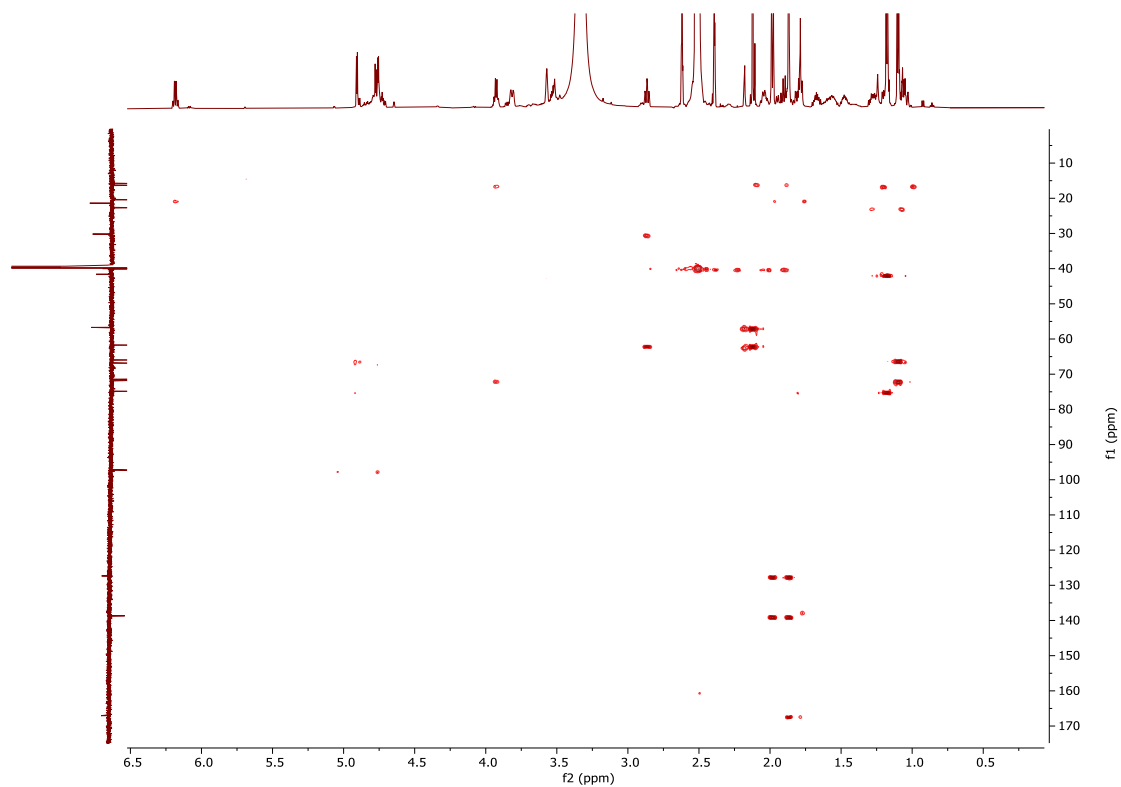


Fig. S31 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B1 (**4**).

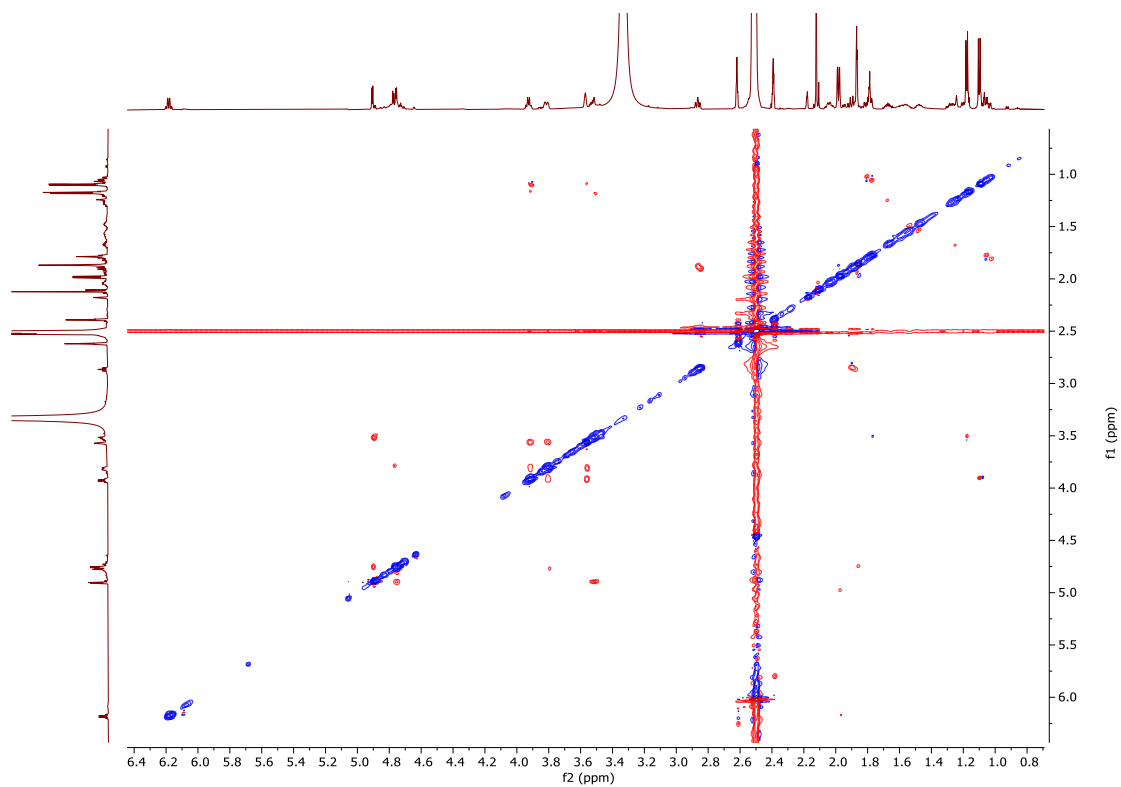


Fig. S32 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B1 (**4**).

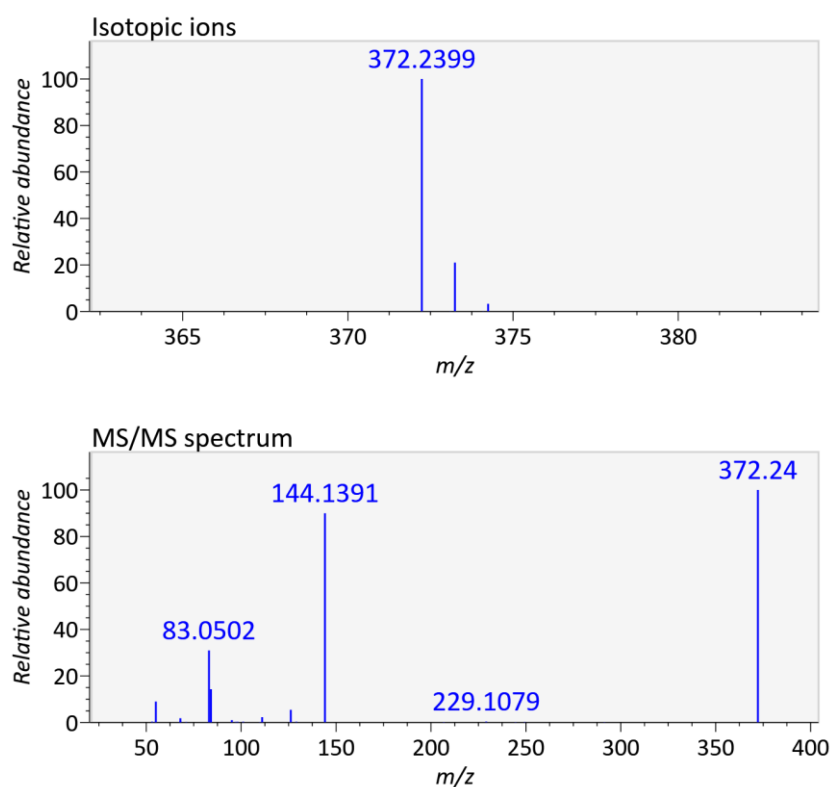


Fig. S33 HRESIMS and MS/MS spectra of schizanthoside B2 (**5**). (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

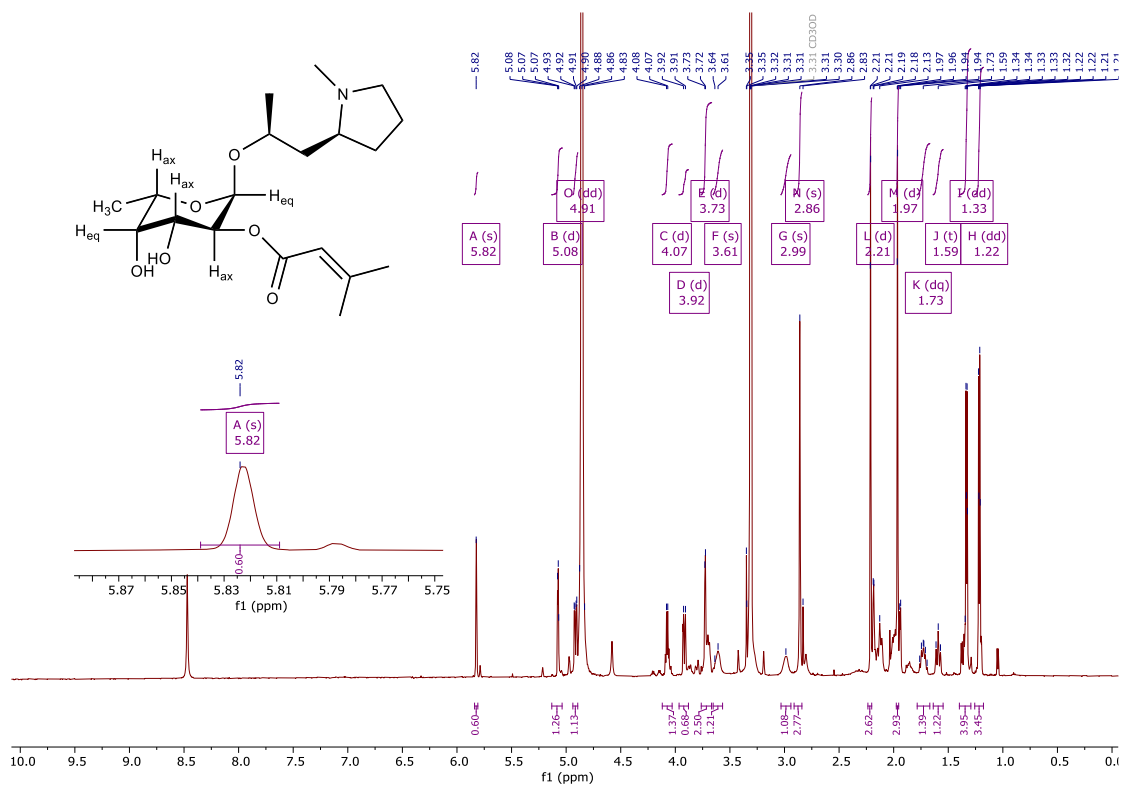


Fig. S34 ¹H NMR (600 MHz, CD₃OD) spectrum of schizanthoside B2 (**5**).

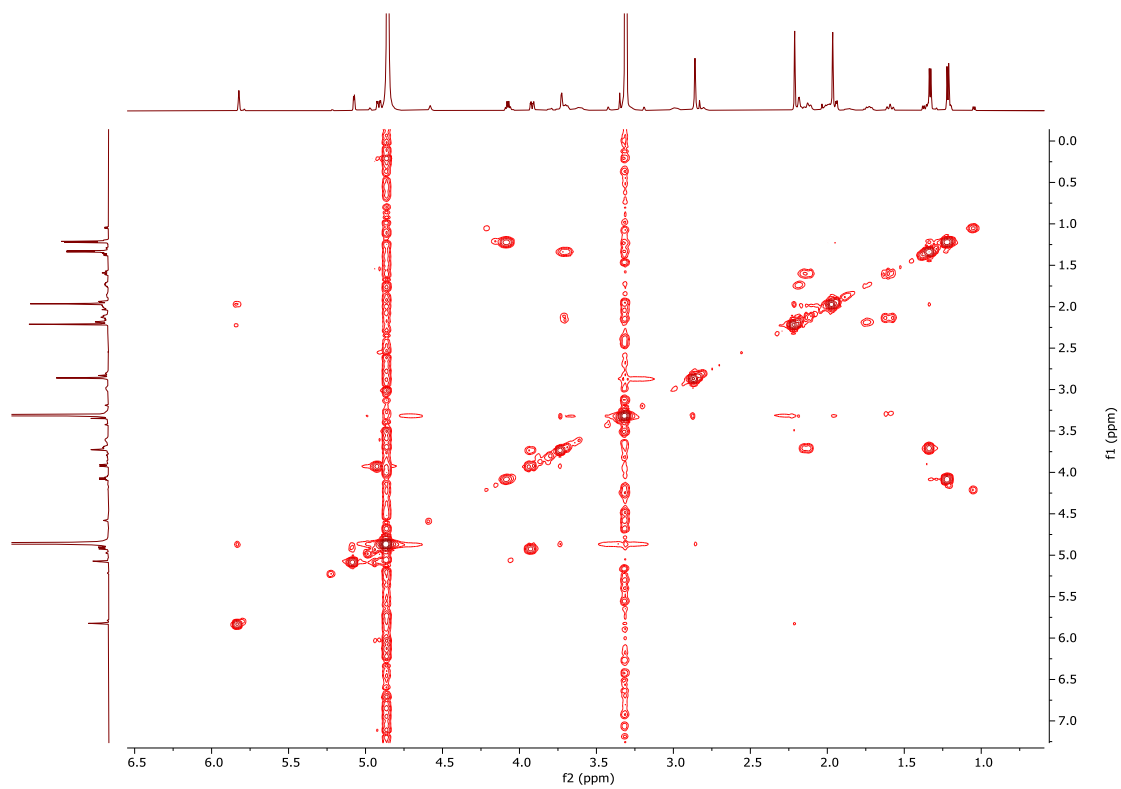


Fig. S35 COSY (600 MHz, CD₃OD) spectrum of schizanthoside B2 (**5**).

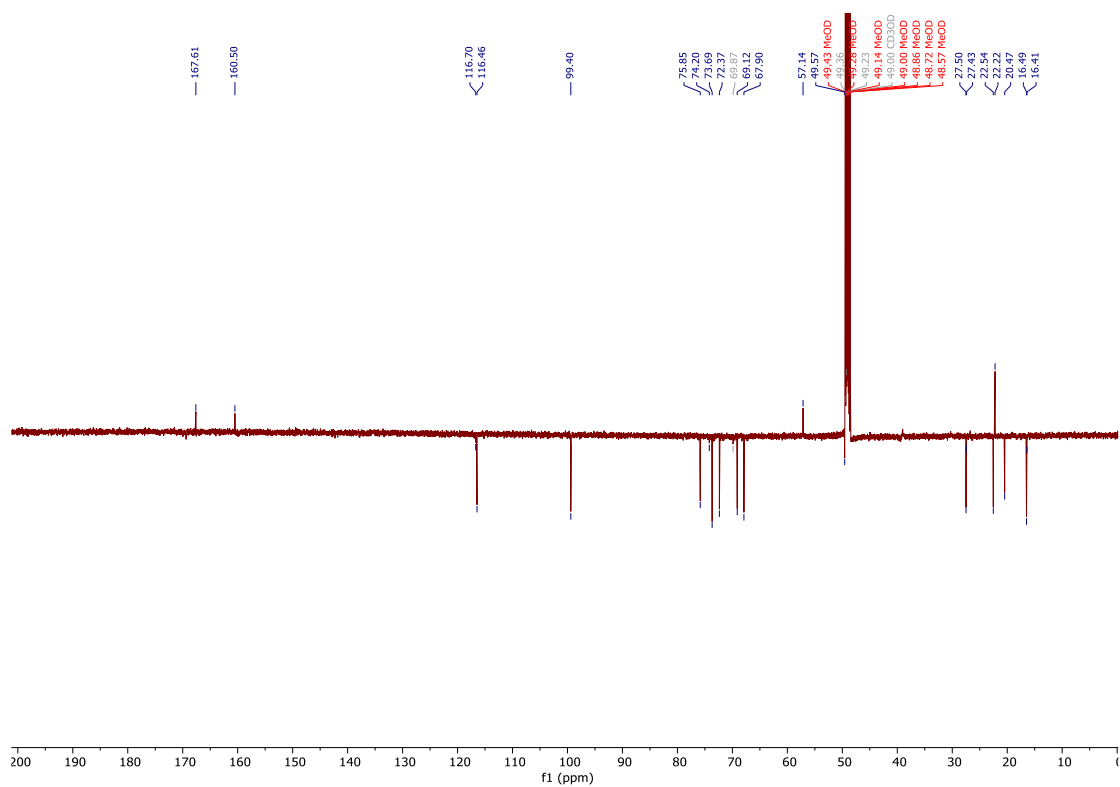


Fig. S36 DEPTQ (125 MHz, CD₃OD) spectrum of schizanthoside B2 (**5**).

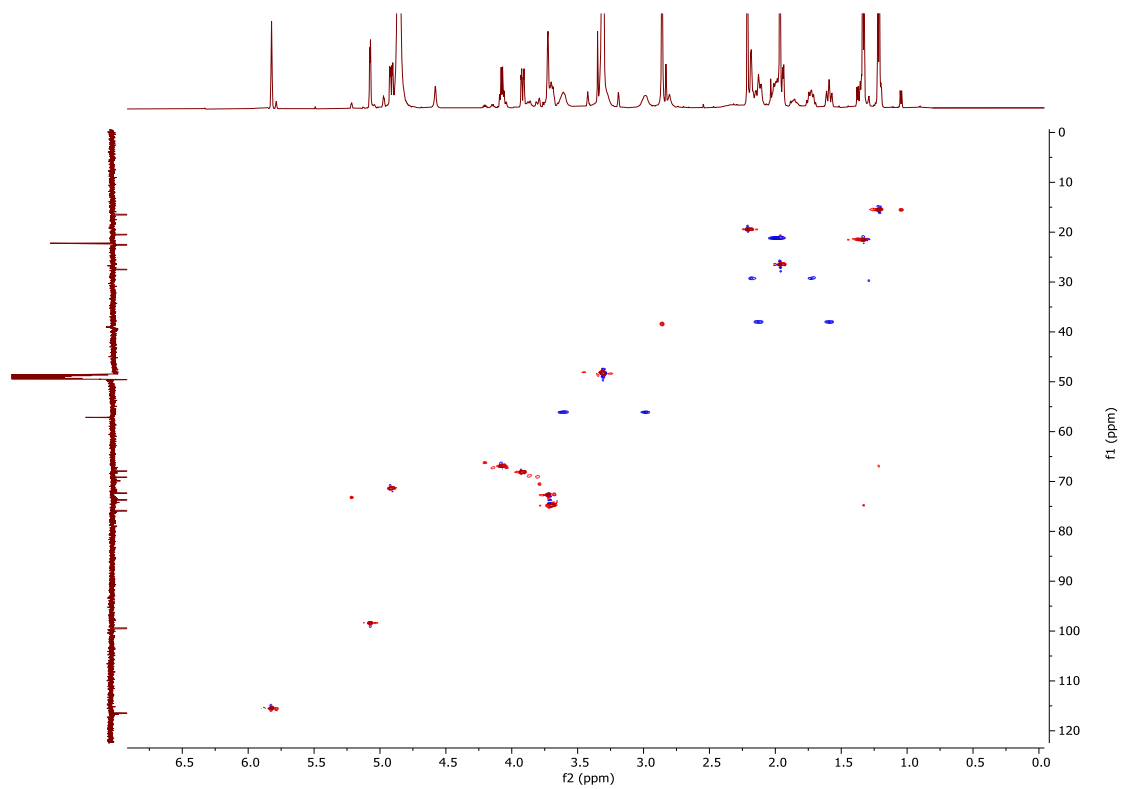


Fig. S37 HSQC (600 MHz, CD₃OD) spectrum of schizanthoside B2 (**5**).

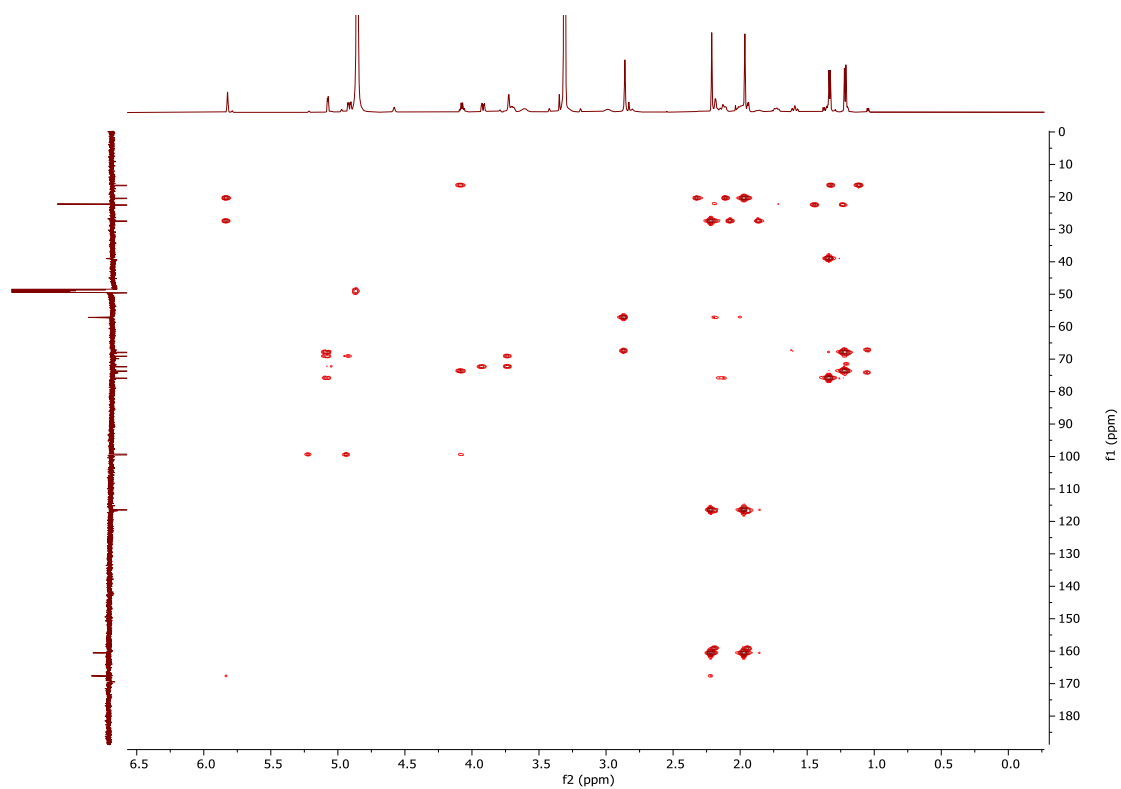


Fig. S38 HMBC (600 MHz, CD₃OD) spectrum of schizanthoside B2 (**5**).

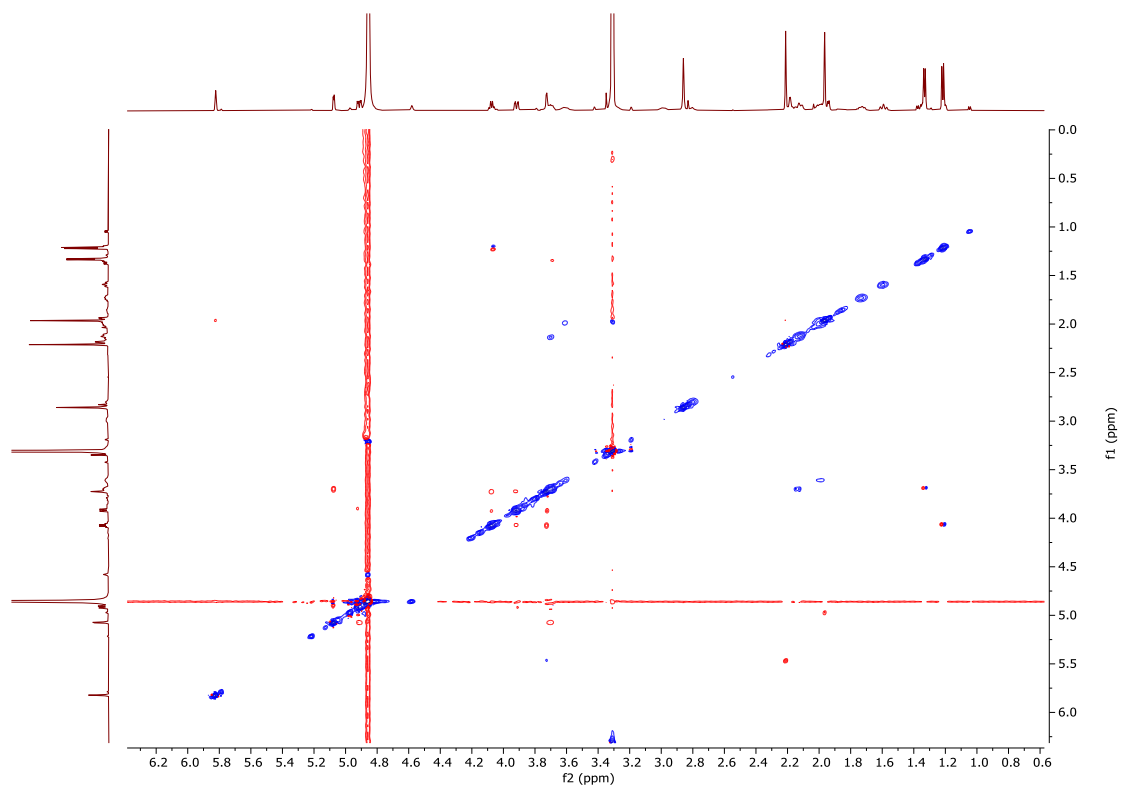


Fig. S39 ROESY (600 MHz, CD₃OD) spectrum of schizanthoside B2 (**5**).

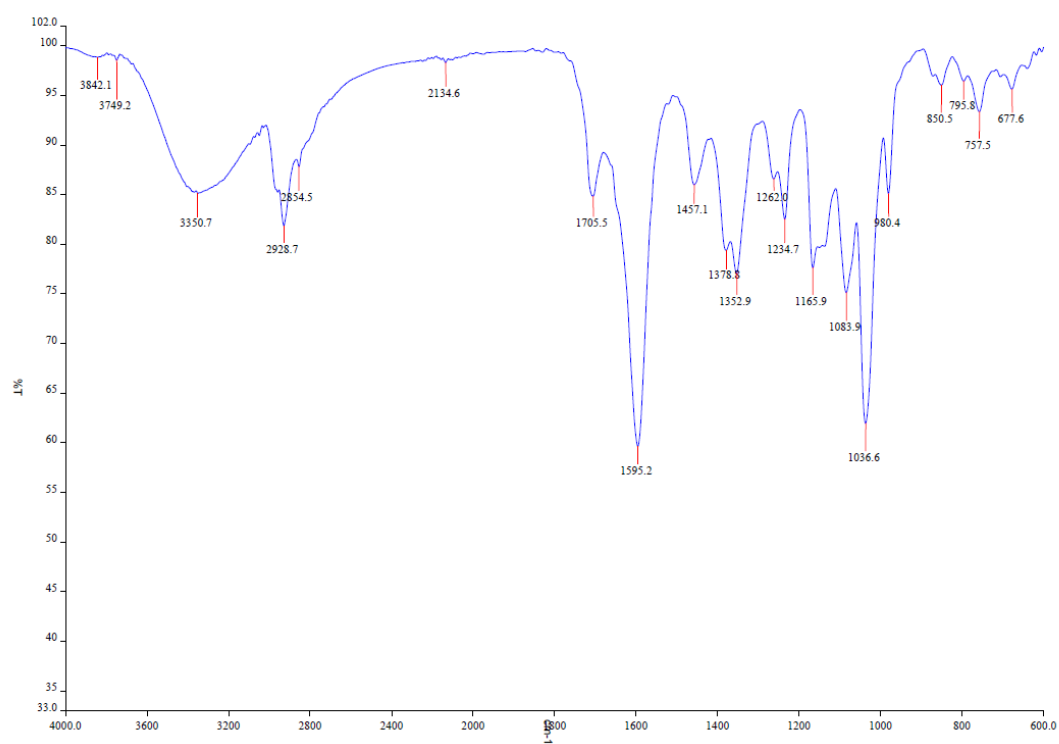


Fig. S40 IR spectrum of schizanthoside B3 (**6**).

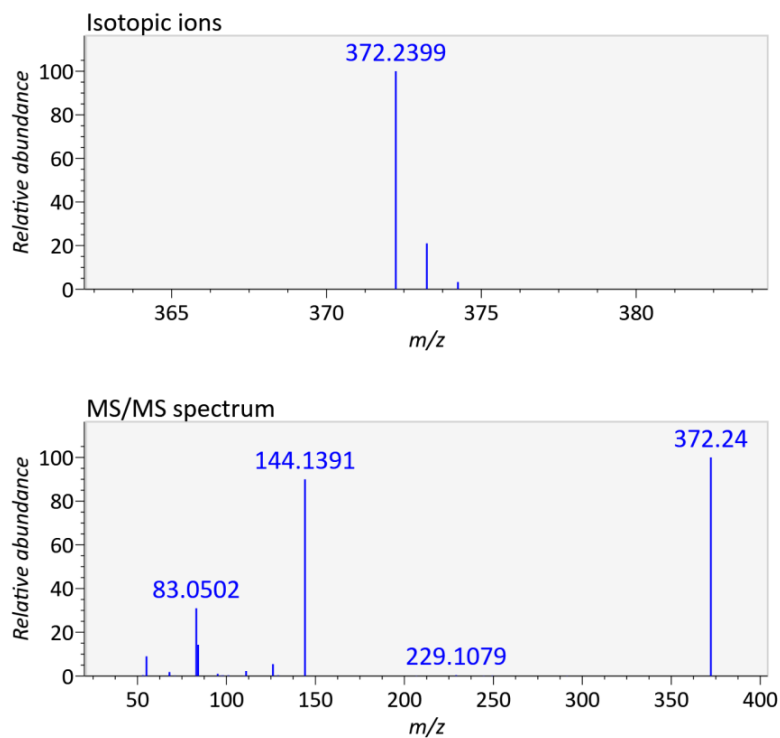


Fig. S41 HRESIMS and MS/MS spectra of schizanthoside B3 (**6**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

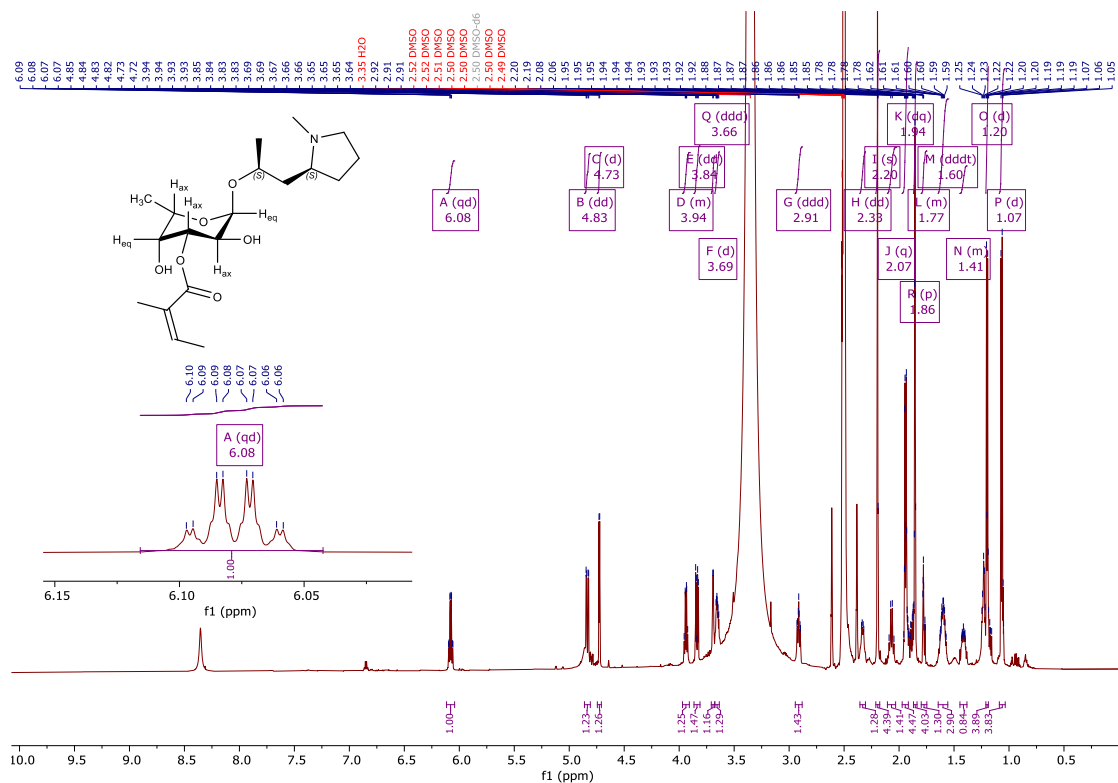


Fig. S42 ¹H NMR (600 MHz, DMSO-d₆) spectrum of schizanthoside B3 (**6**).

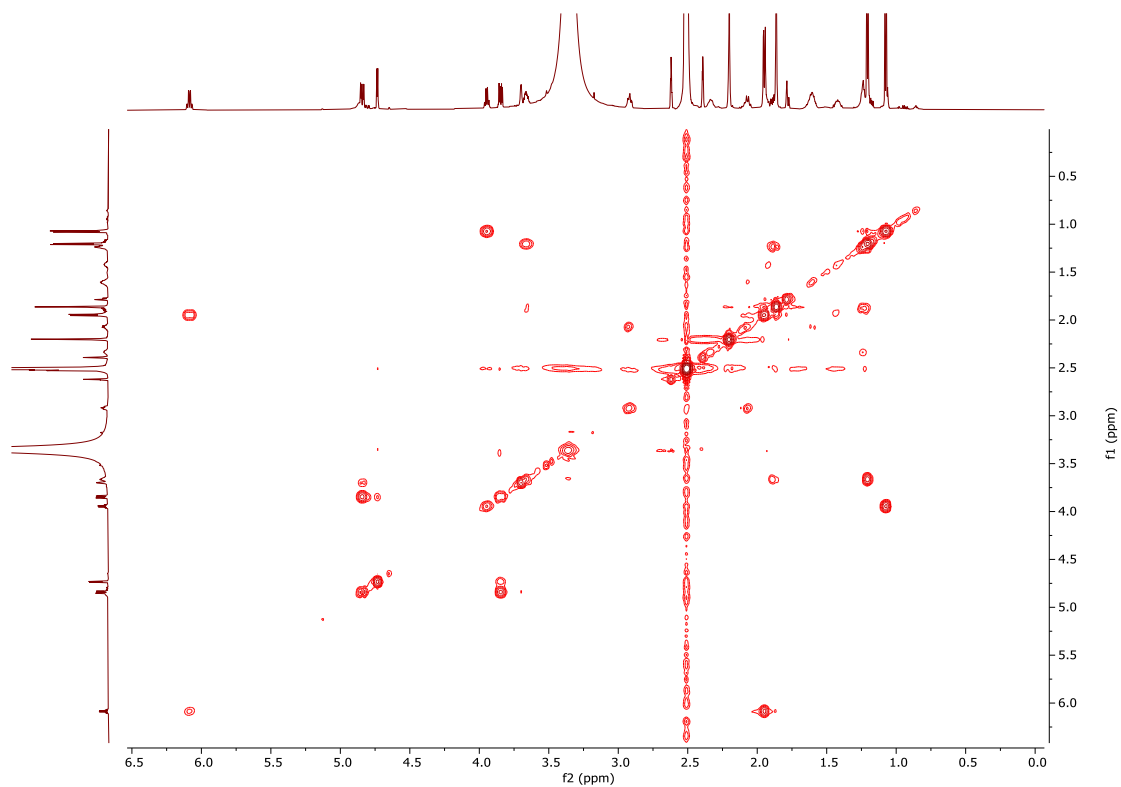


Fig. S43 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B3 (**6**).

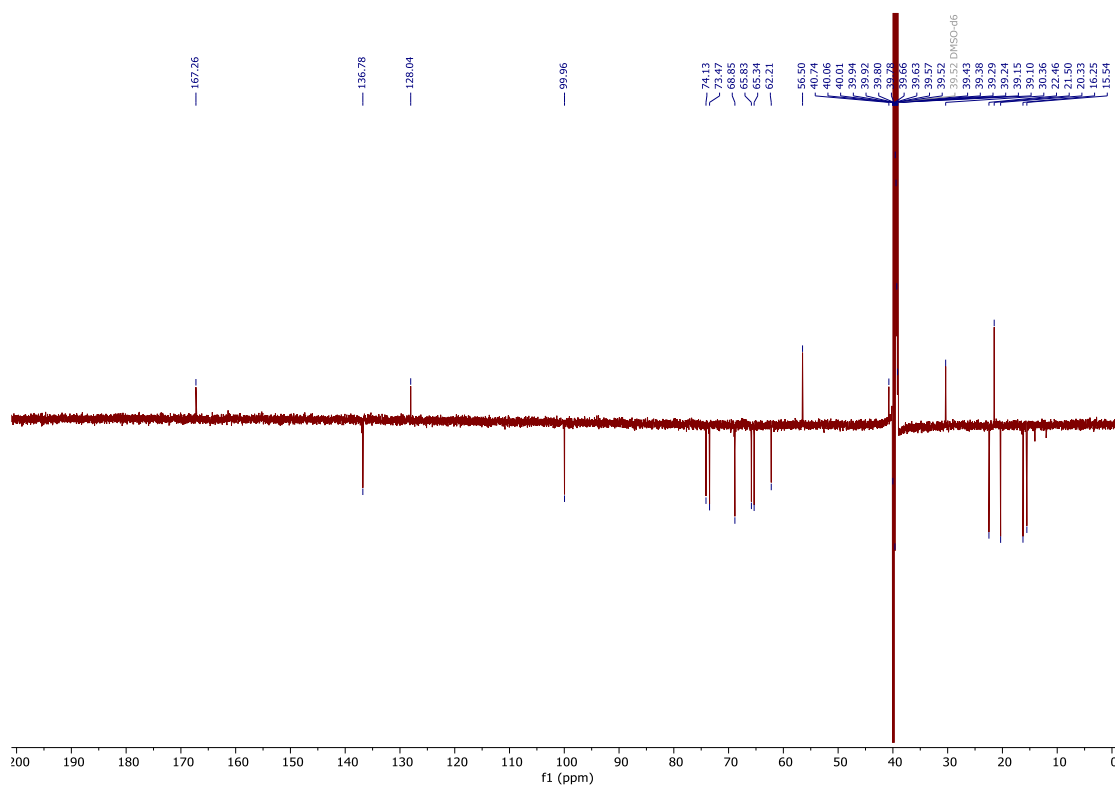


Fig. S44 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside B3 (**6**).

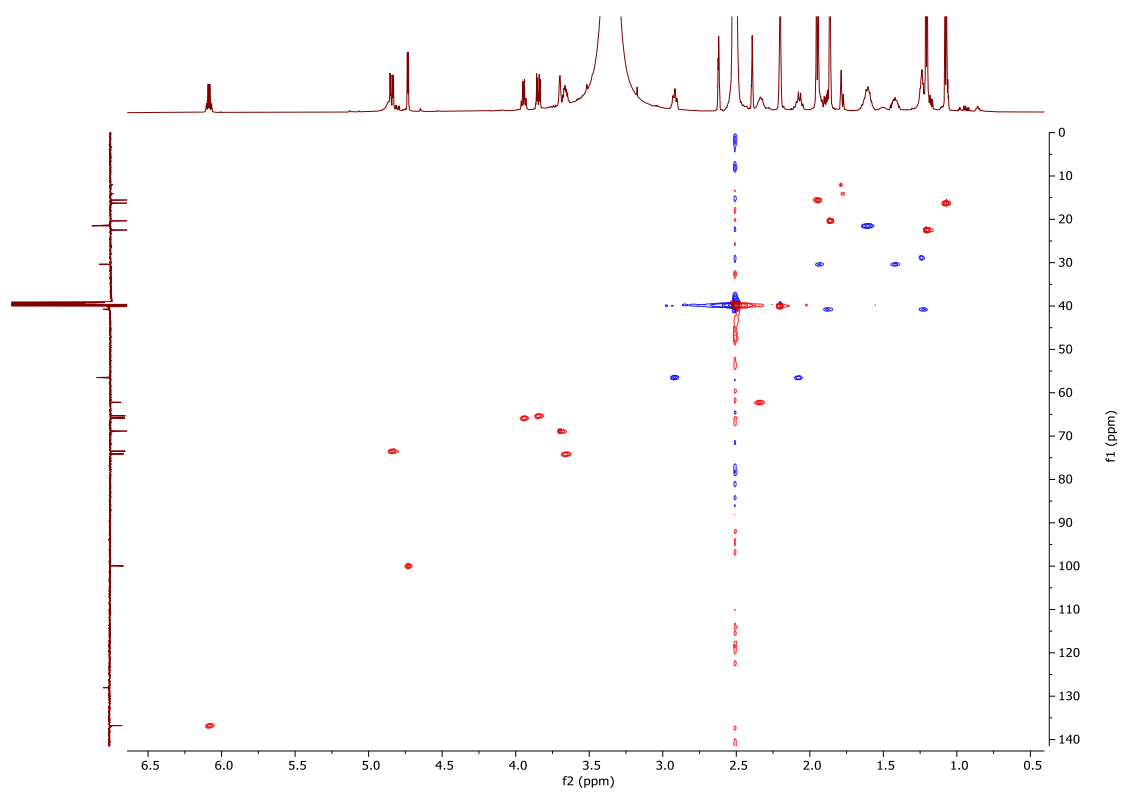


Fig. S45 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B3 (**6**).

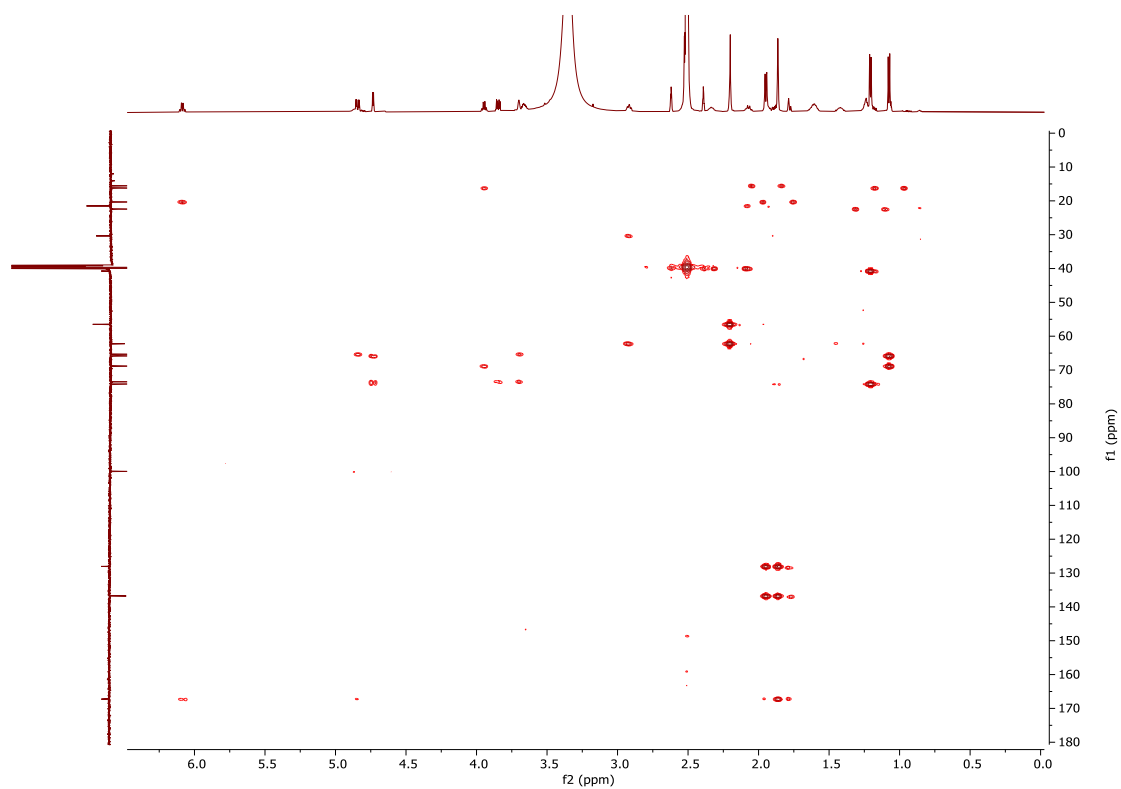


Fig. S46 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B3 (**6**).

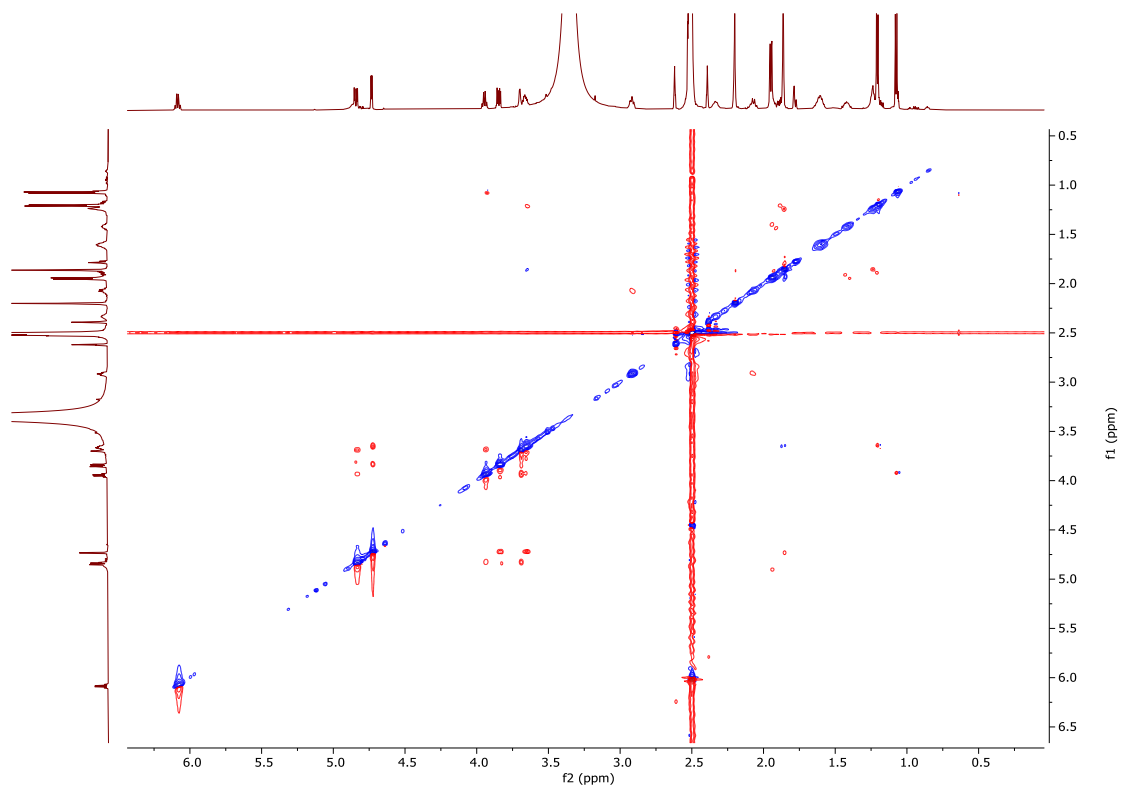


Fig. S47 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B3 (**6**).

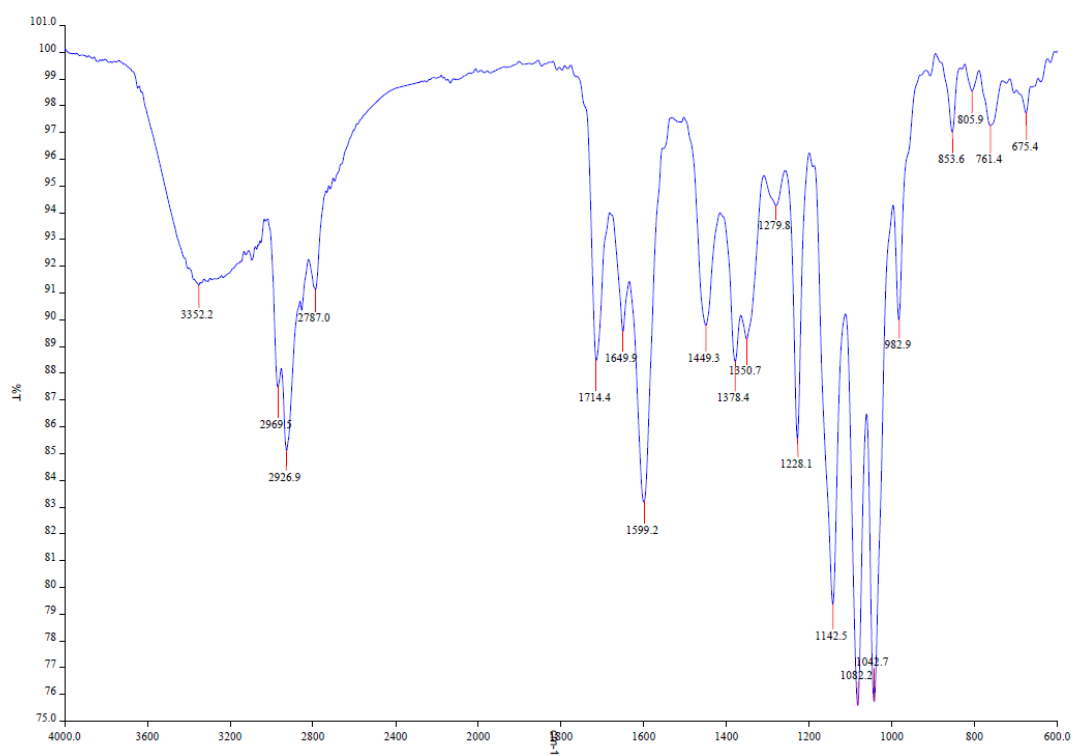


Fig. S48 IR spectrum of schizanthoside B4 (**7**).

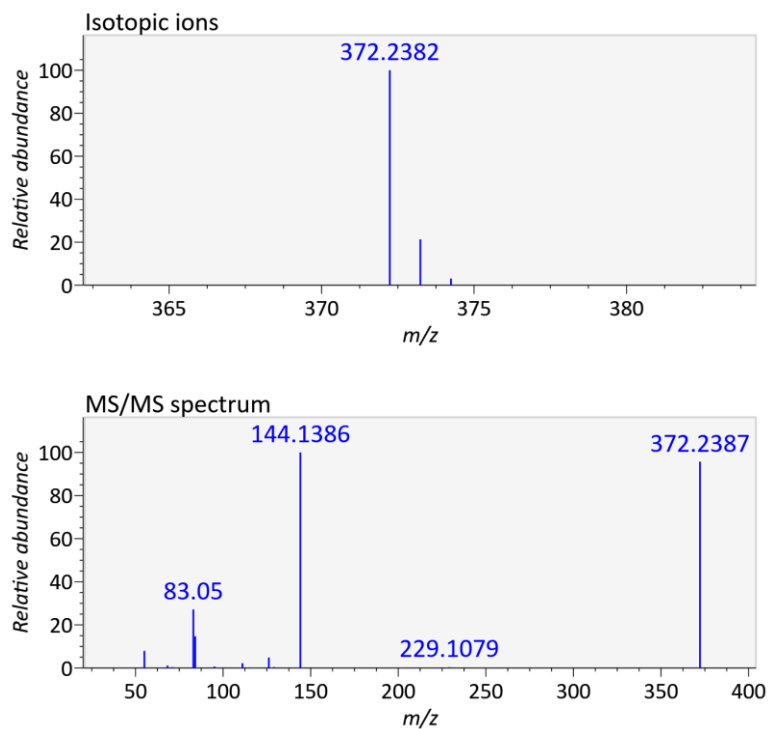


Fig. S49 HRESIMS and MS/MS spectra of schizanthoside B4 (**7**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

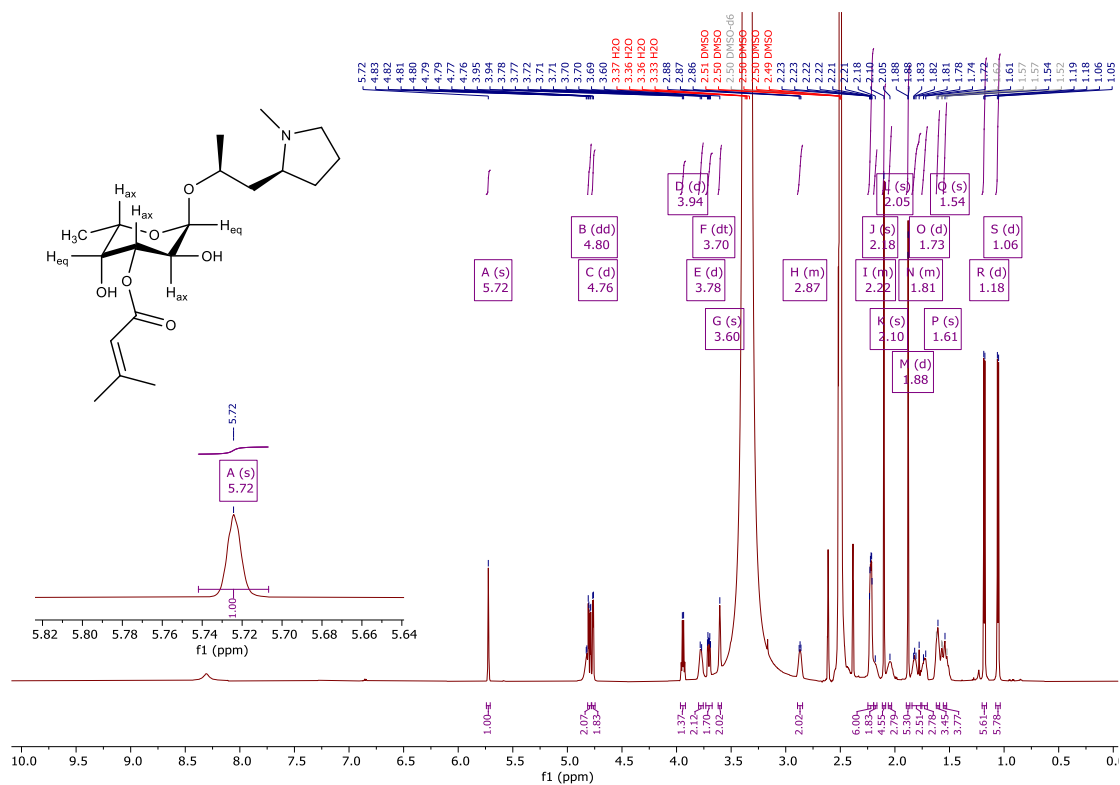


Fig. S50 ¹H NMR (600 MHz, DMSO-d₆) spectrum of schizanthoside B4 (**7**).

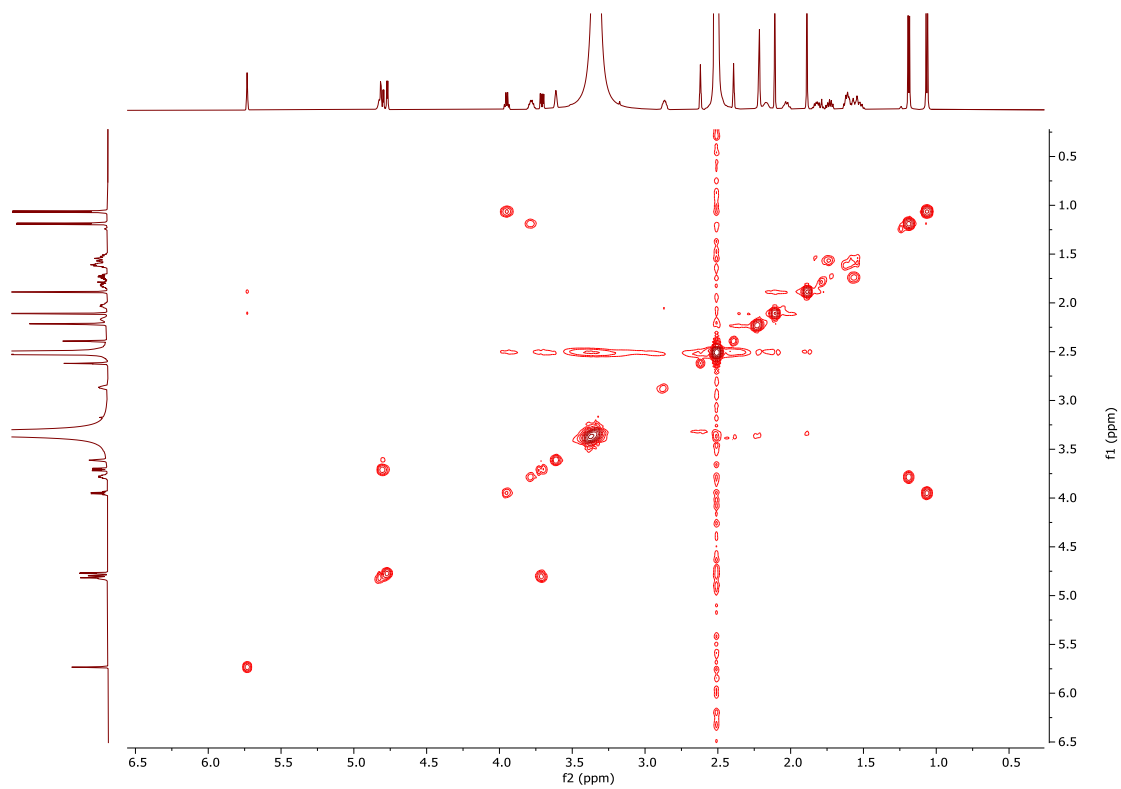


Fig. S51 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B4 (7).

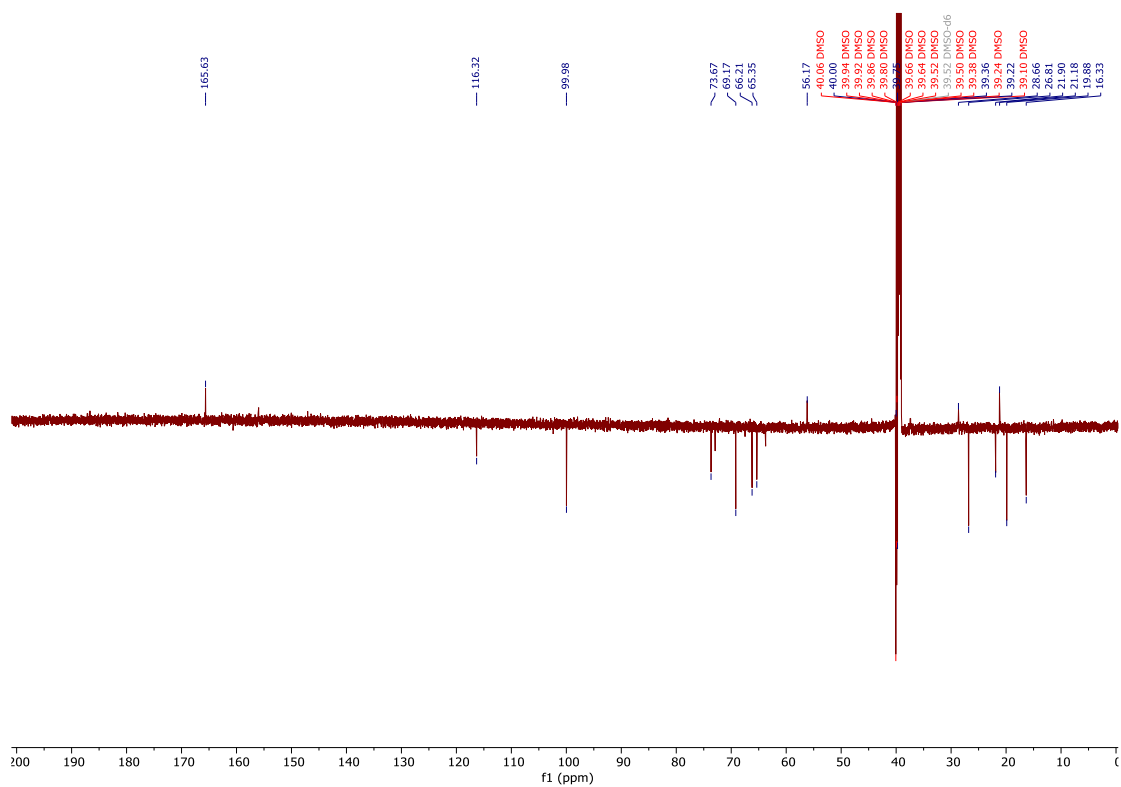


Fig. S52 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside B4 (7).

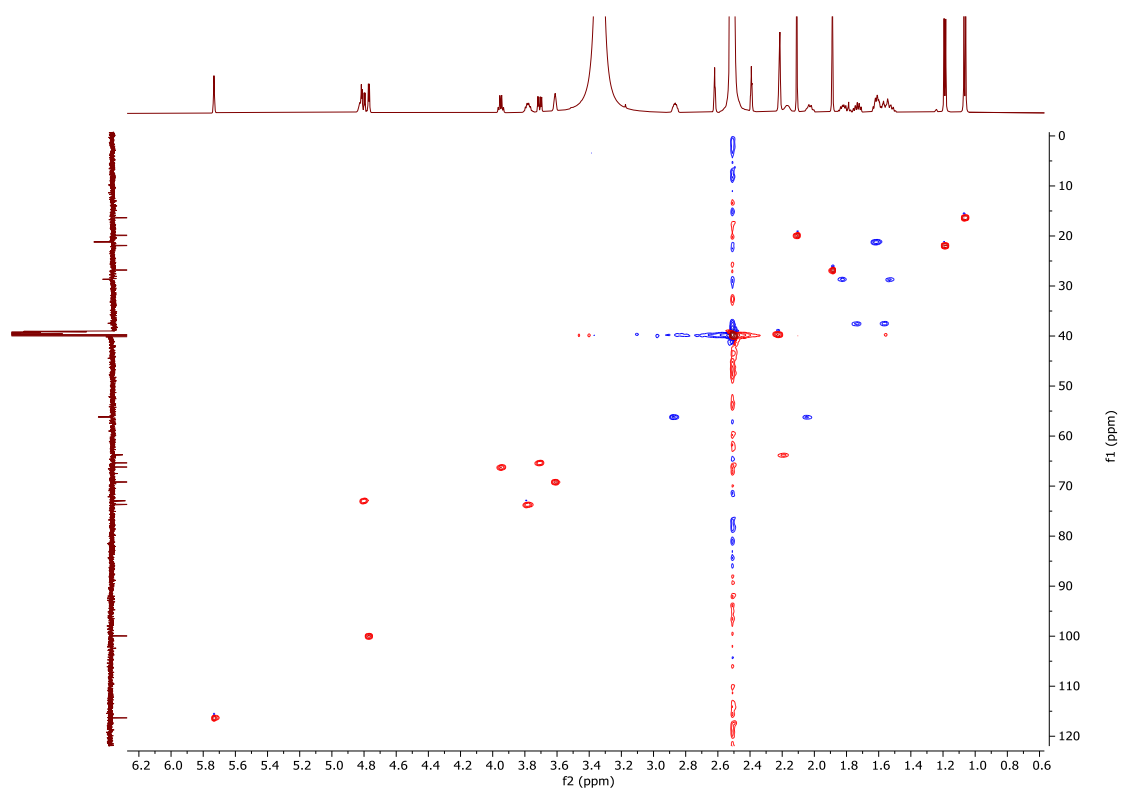


Fig. S53 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B4 (**7**).

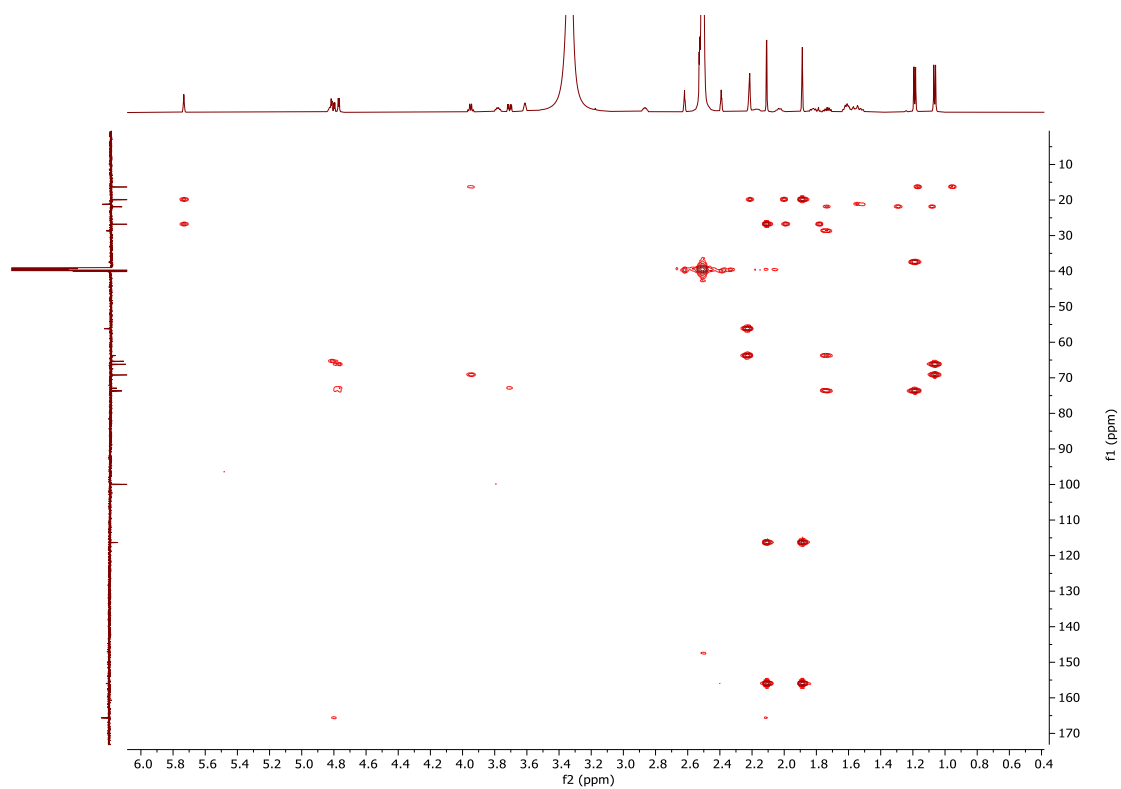


Fig. S54 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B4 (**7**).

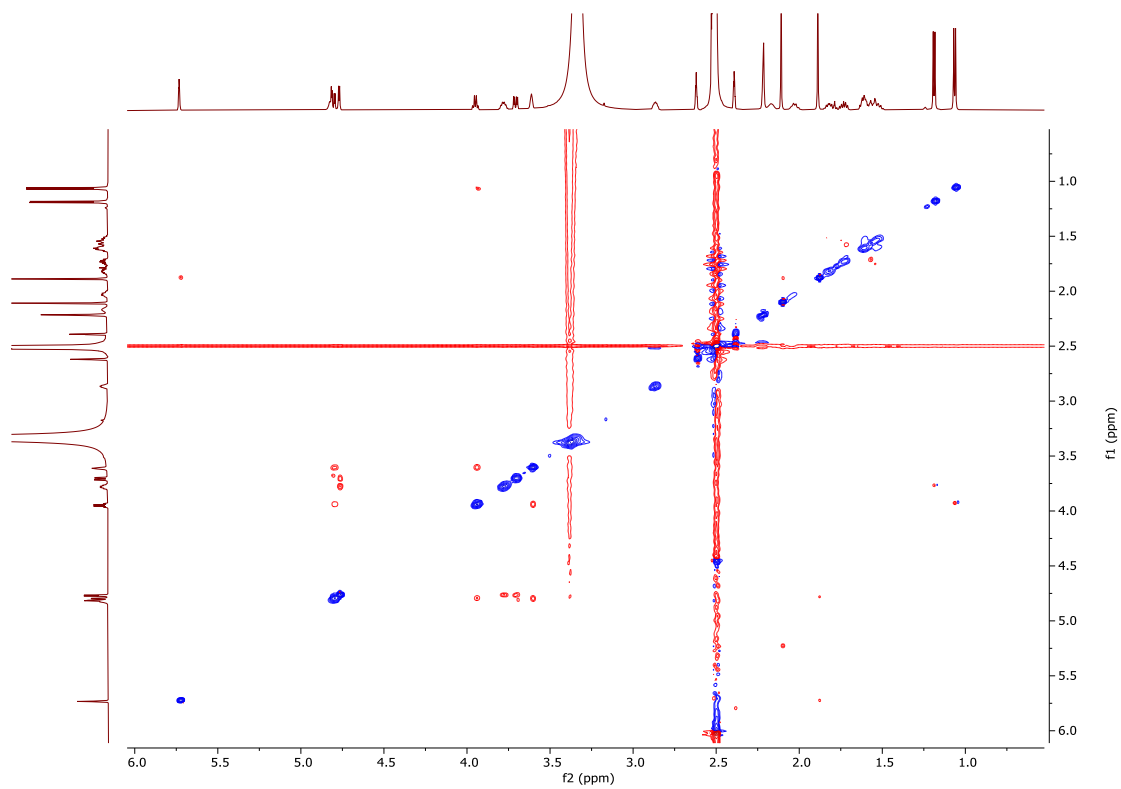


Fig. S55 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B4 (**7**).

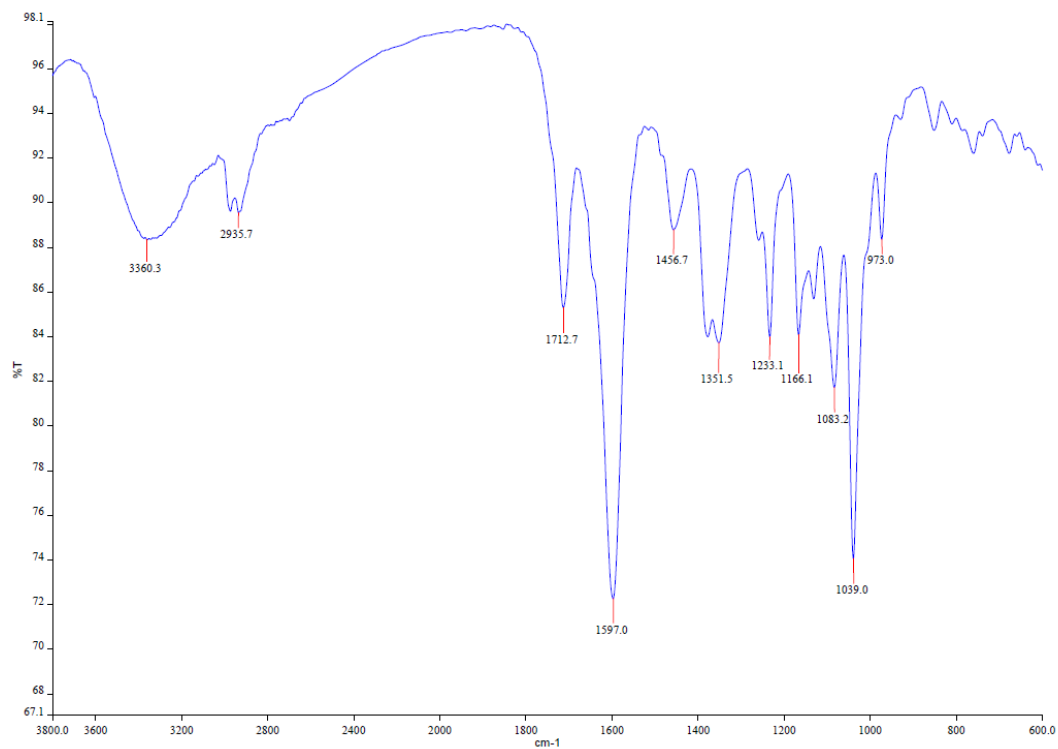


Fig. S56 IR spectrum of schizanthoside B5 (**8**).

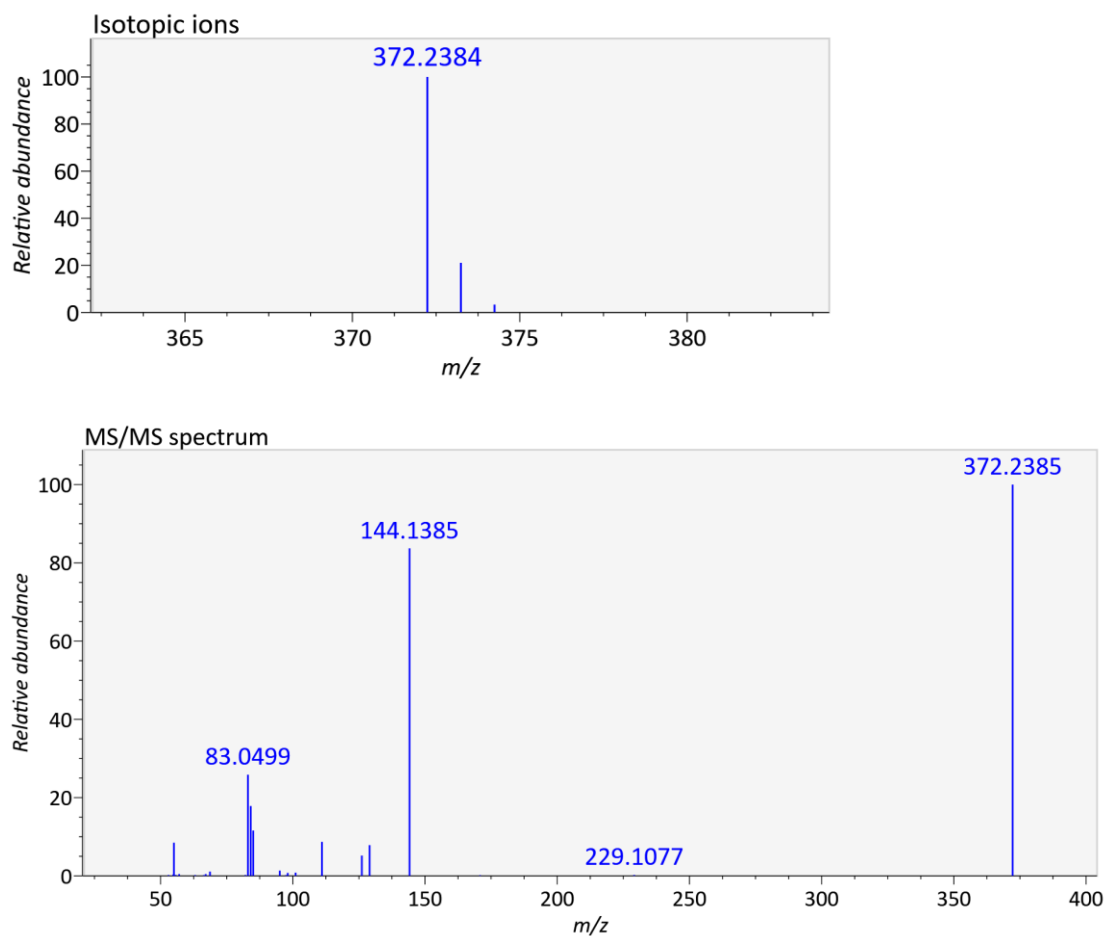


Fig. S57 HRESIMS and MS/MS spectra of schizanthoside B5 (**8**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

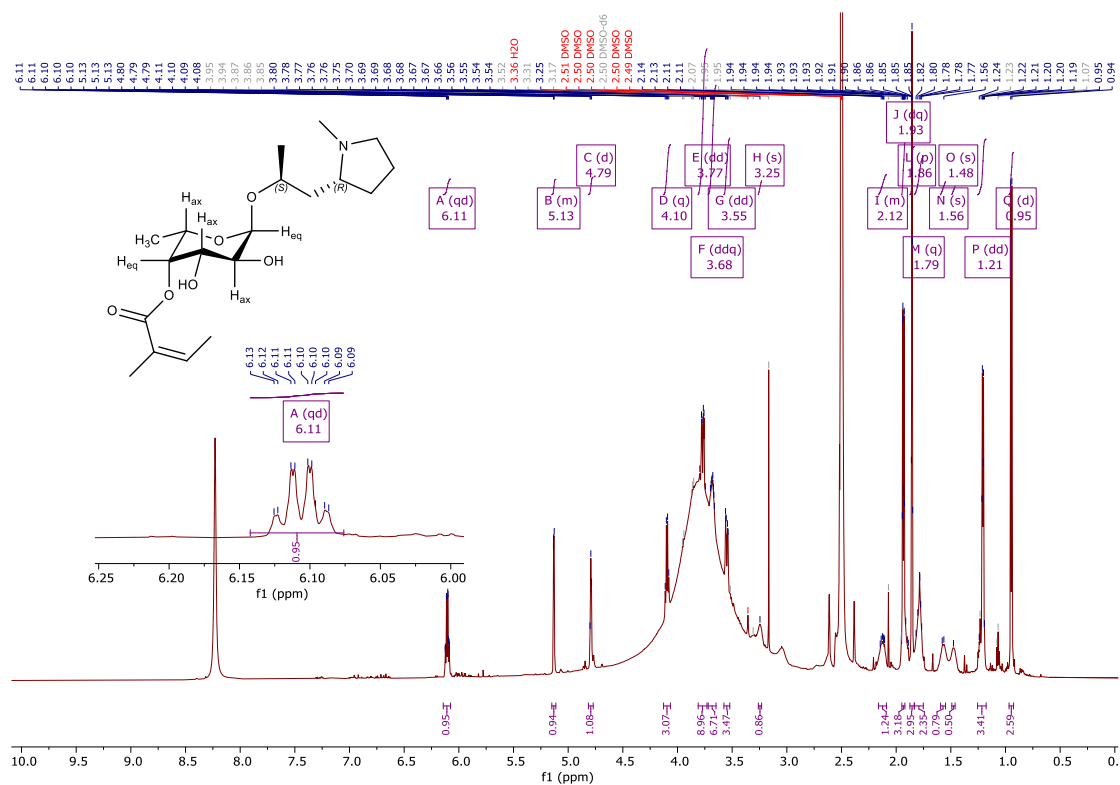


Fig. S58 ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of schizanthoside B5 (**8**).

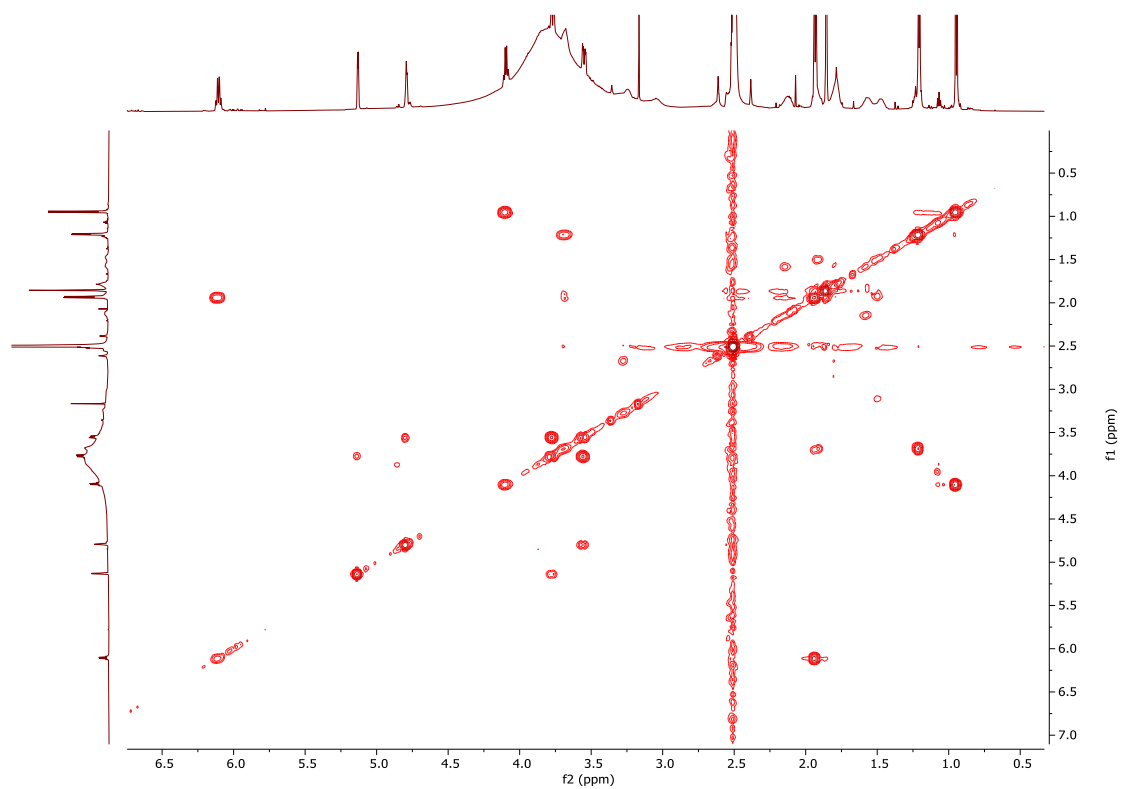


Fig. S59 COSY (600 MHz, $\text{DMSO-}d_6$) spectrum of schizanthoside B5 (**8**).

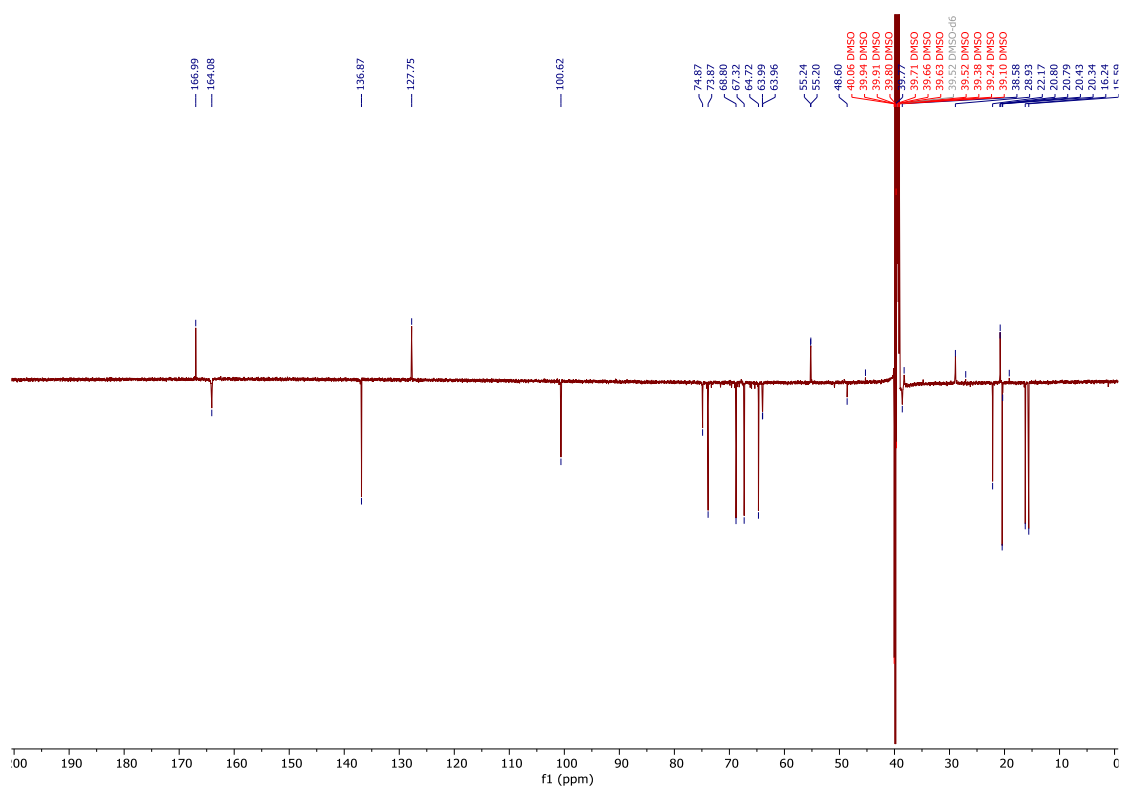


Fig. S60 DEPTQ (125 MHz, $\text{DMSO-}d_6$) spectrum of schizanthoside B5 (**8**).

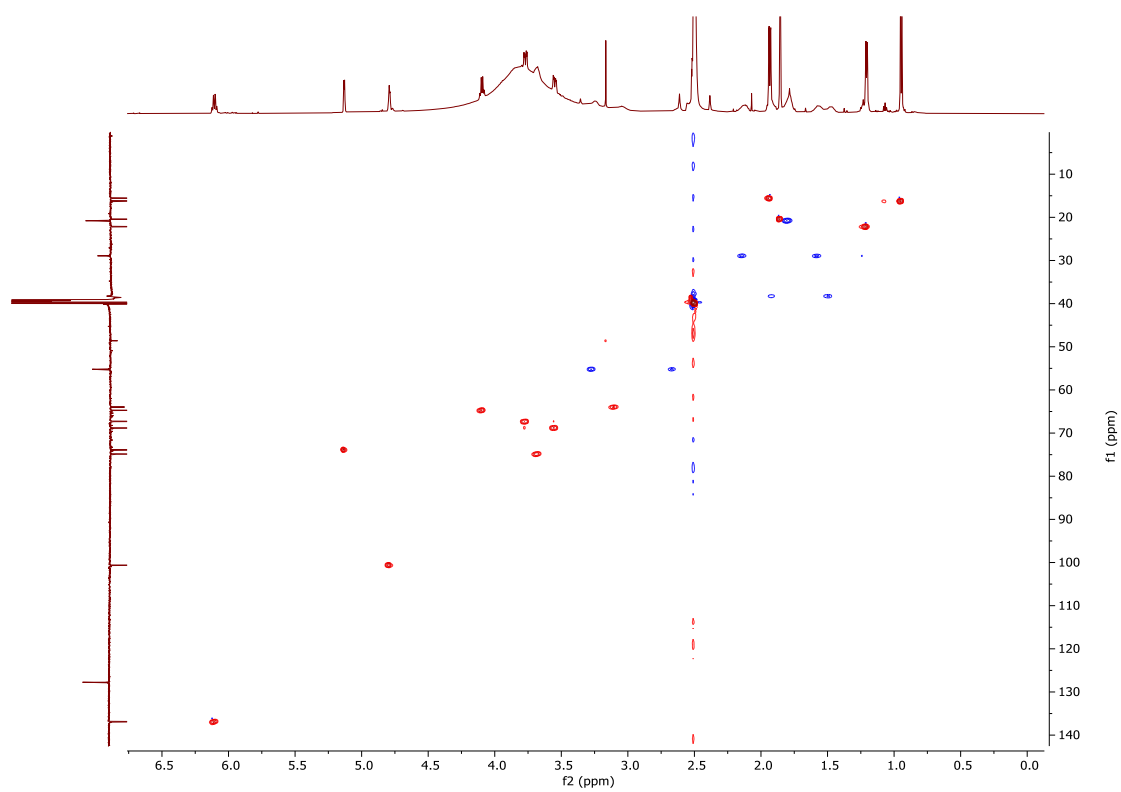


Fig. S61 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B5 (**8**).

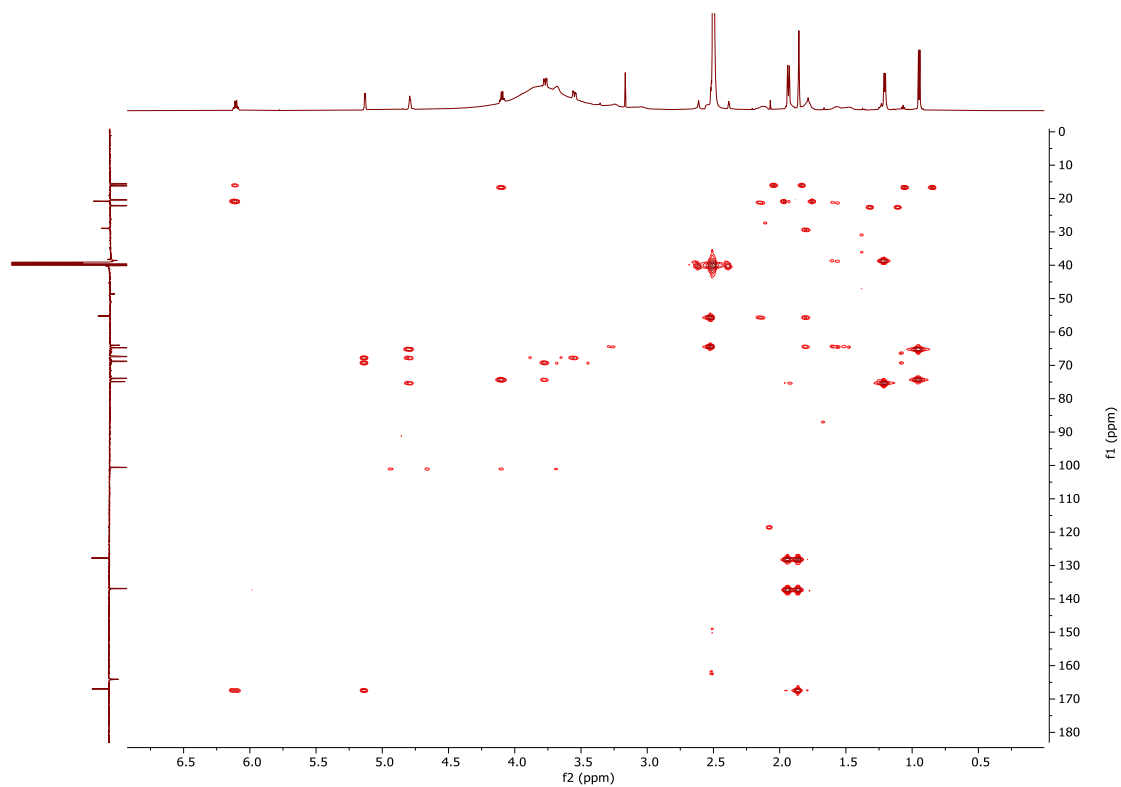


Fig. S62 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B5 (**8**).

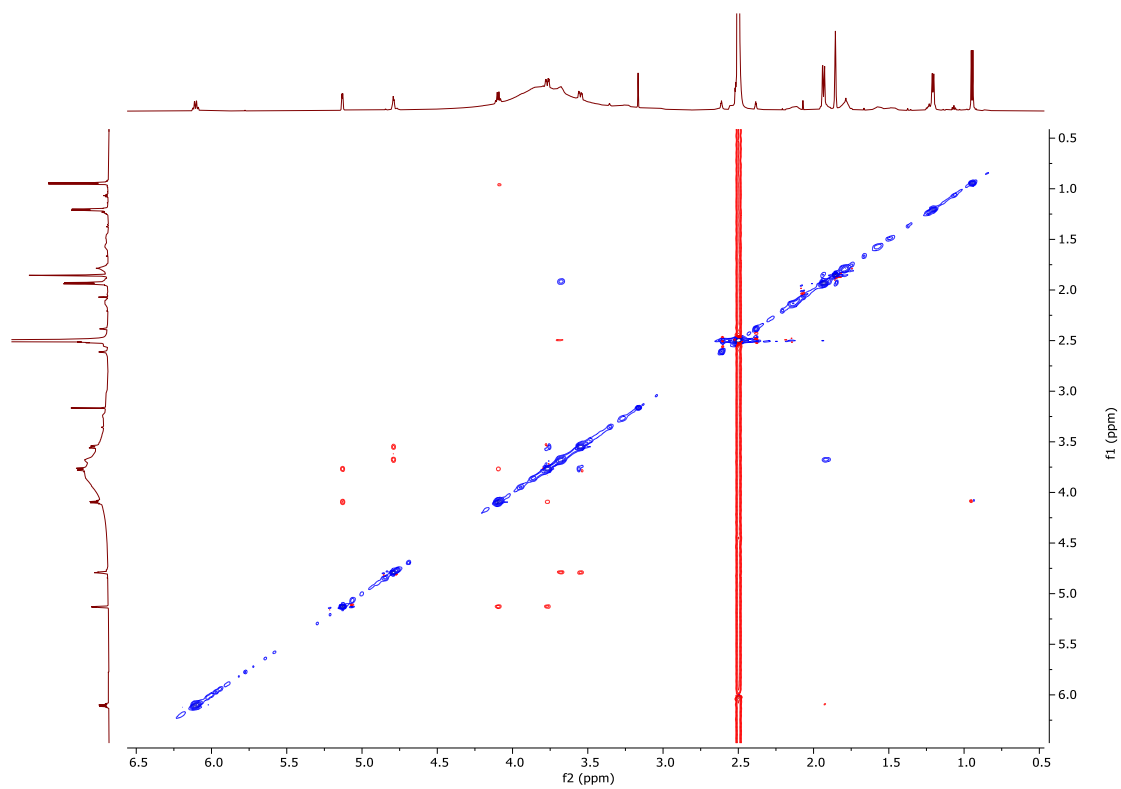


Fig. S63 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B5 (**8**).



Fig. S64 IR spectrum of schizanthoside B6 (**9**).

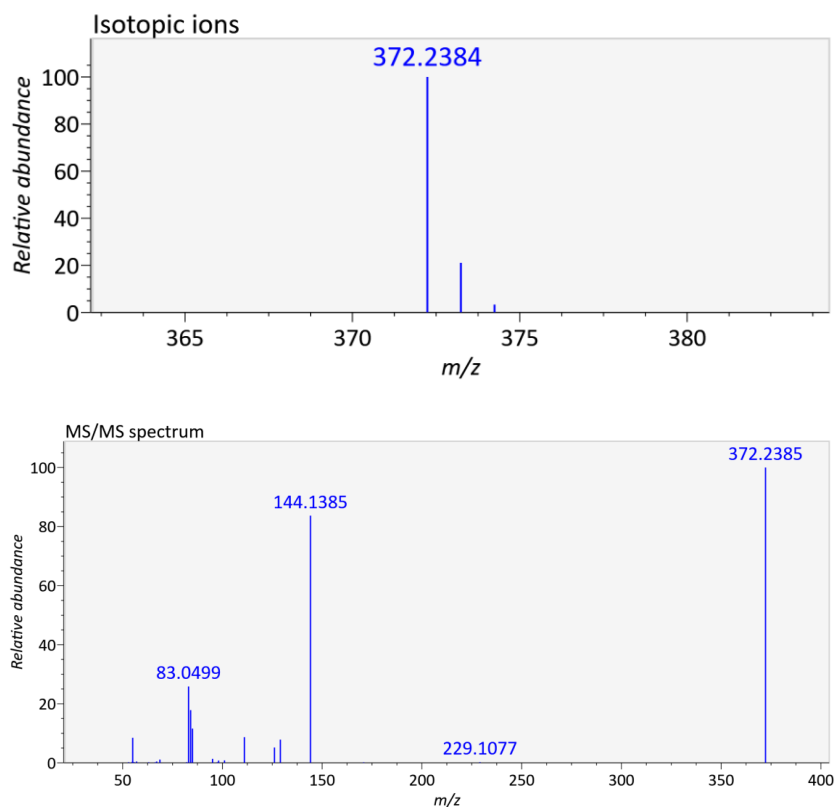


Fig. S65 HRESIMS and MS/MS spectra of schizanthoside B6 (**9**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

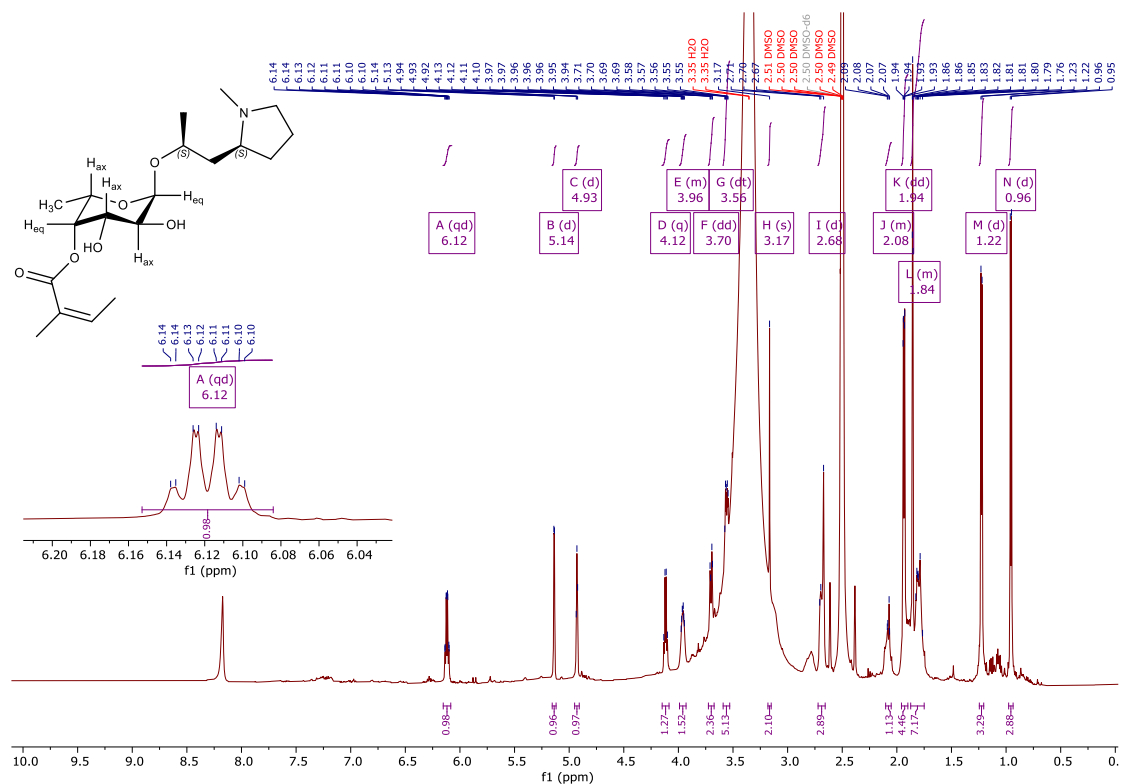


Fig. S66 ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B6 (**9**).

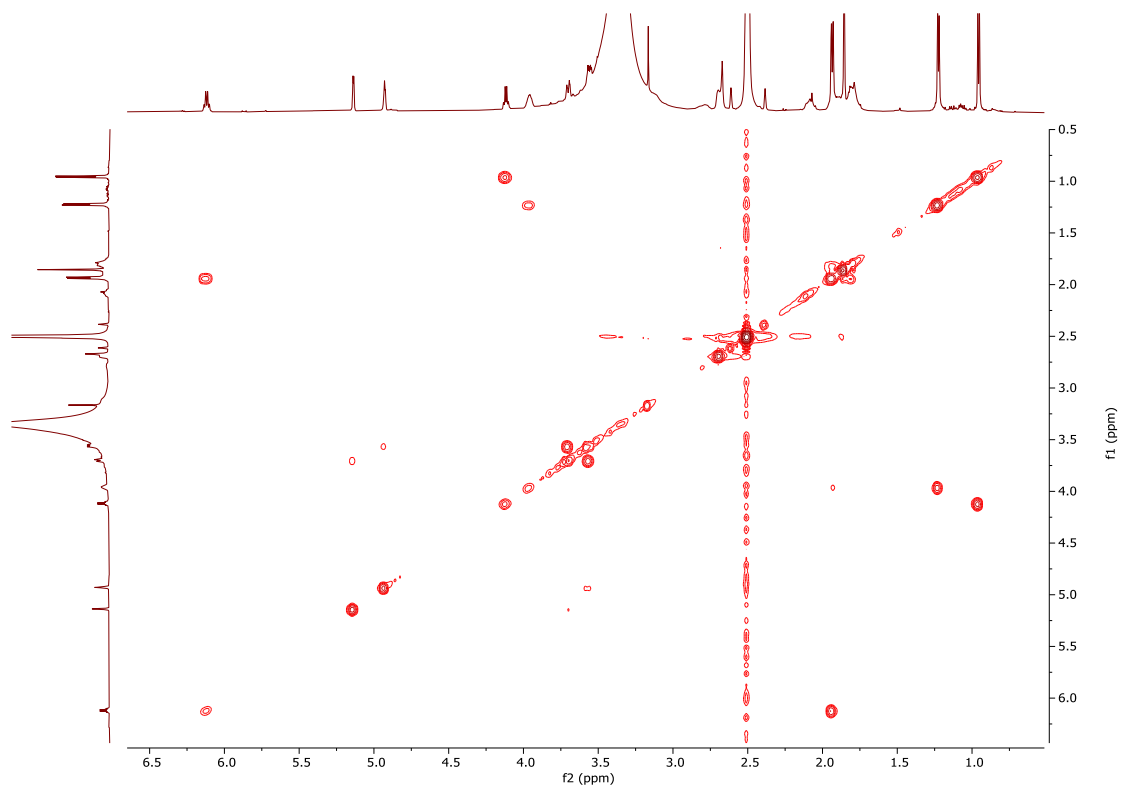


Fig. S67 COSY (600 MHz, DMSO- d_6) spectrum of schizanthoside B6 (**9**).

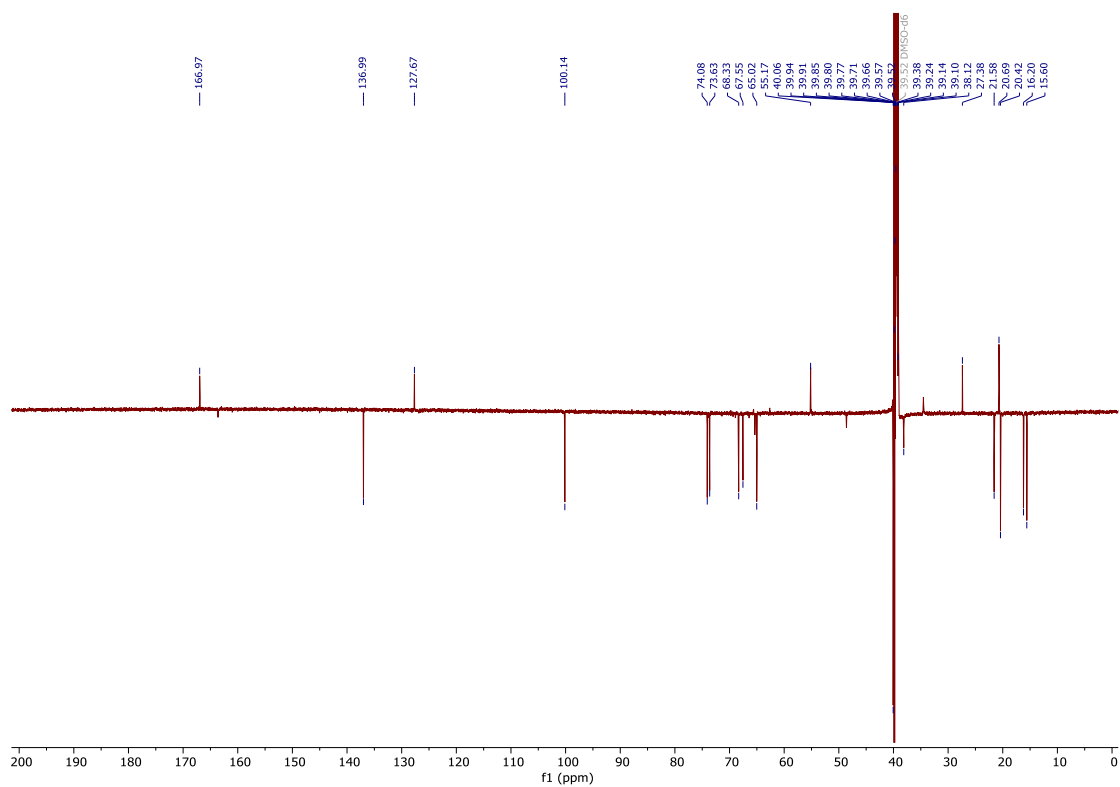


Fig. S68 DEPTQ (125 MHz, DMSO- d_6) spectrum of schizanthoside B6 (**9**).

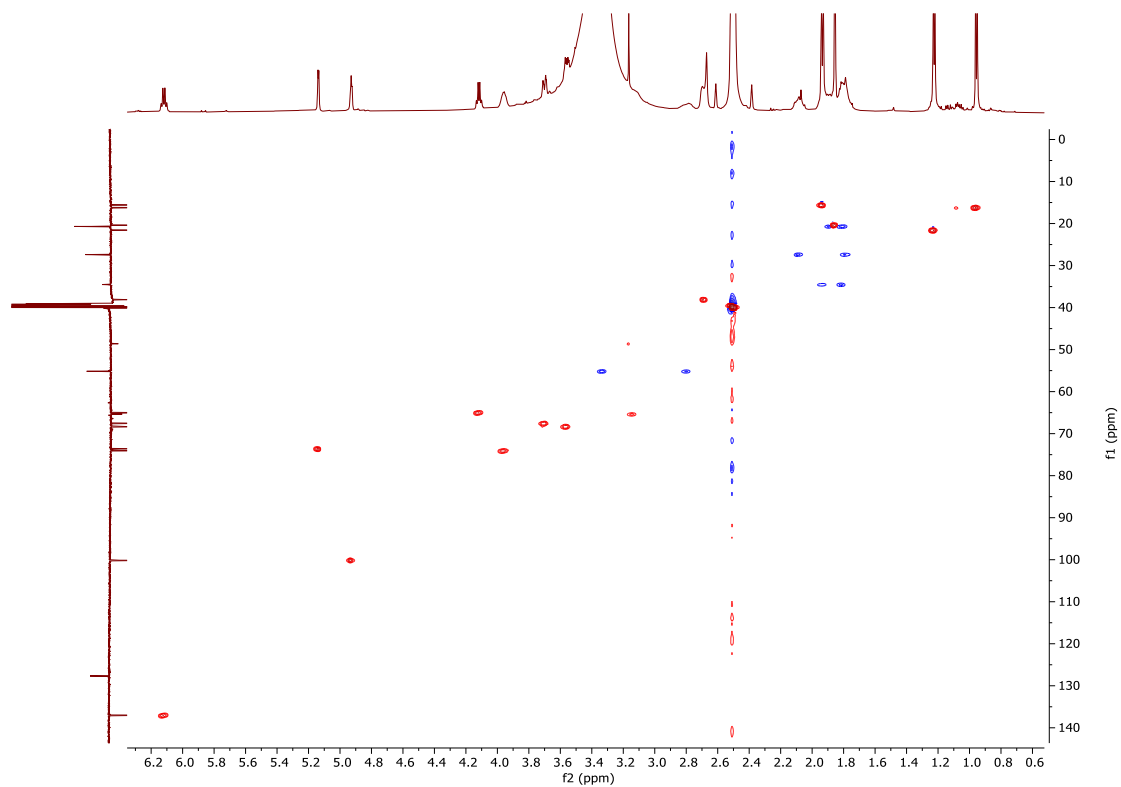


Fig. S69 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B6 (**9**).

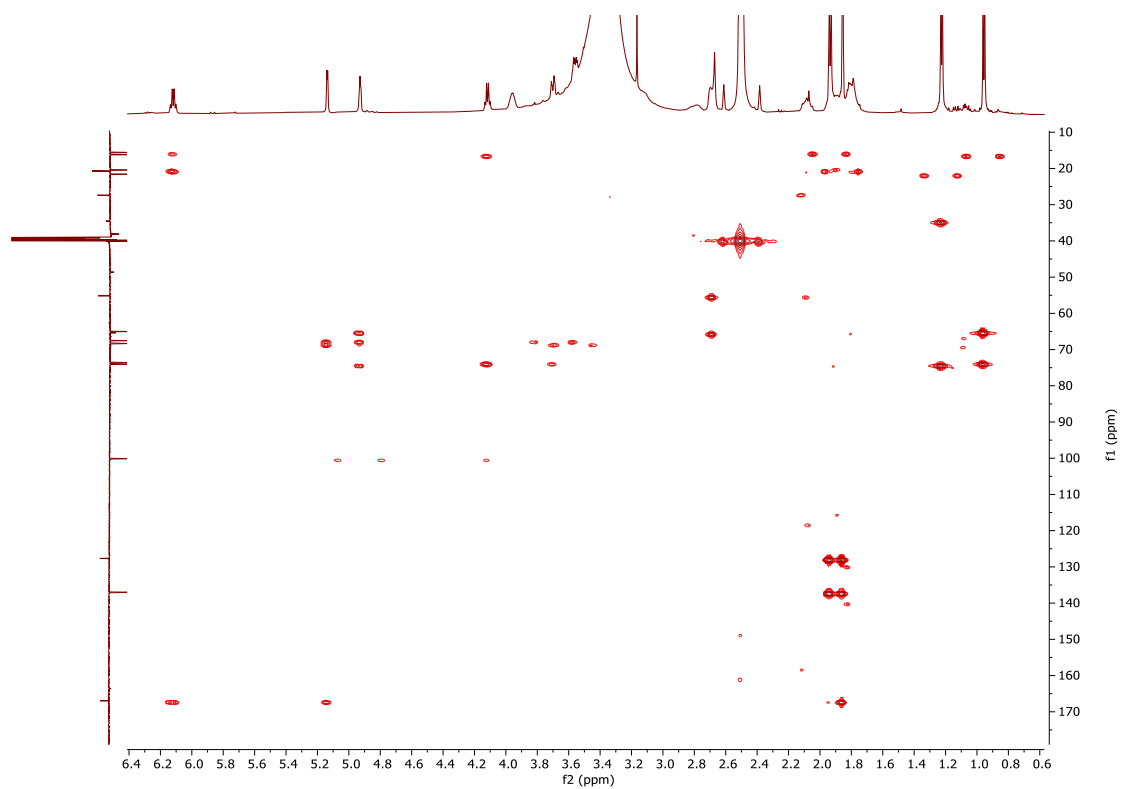


Fig. S70 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B6 (**9**).

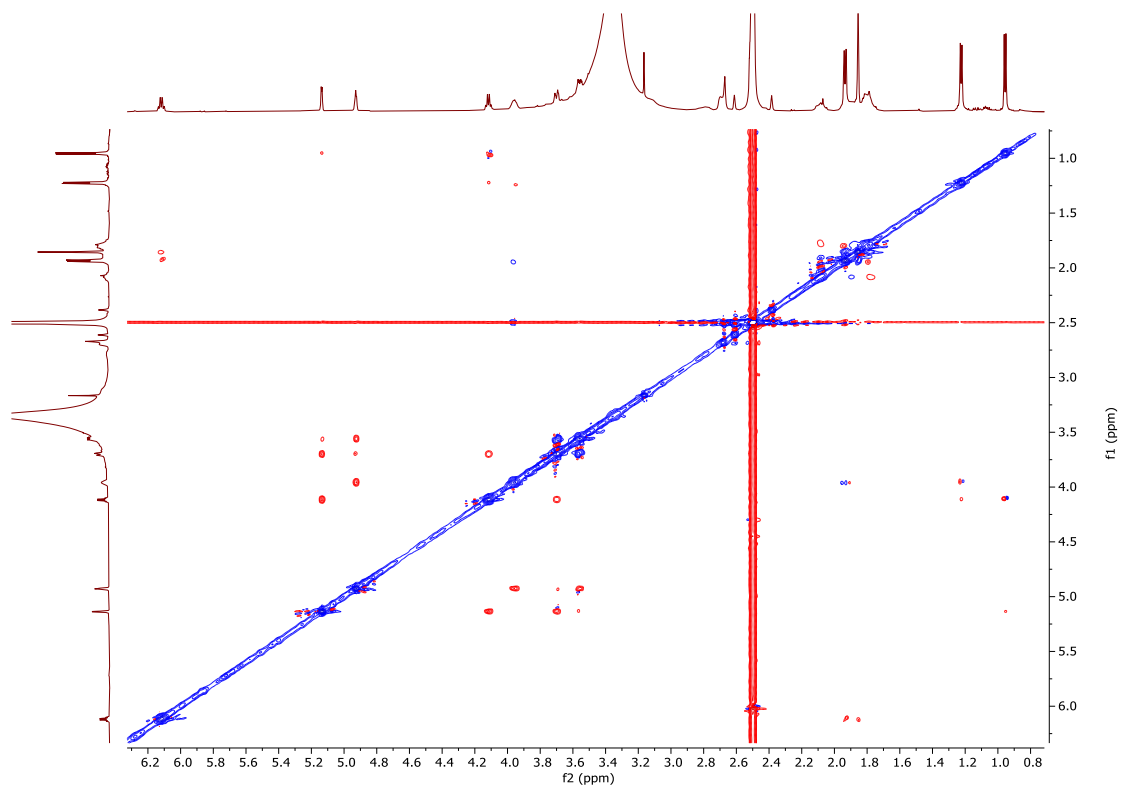


Fig. S71 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B6 (**9**).

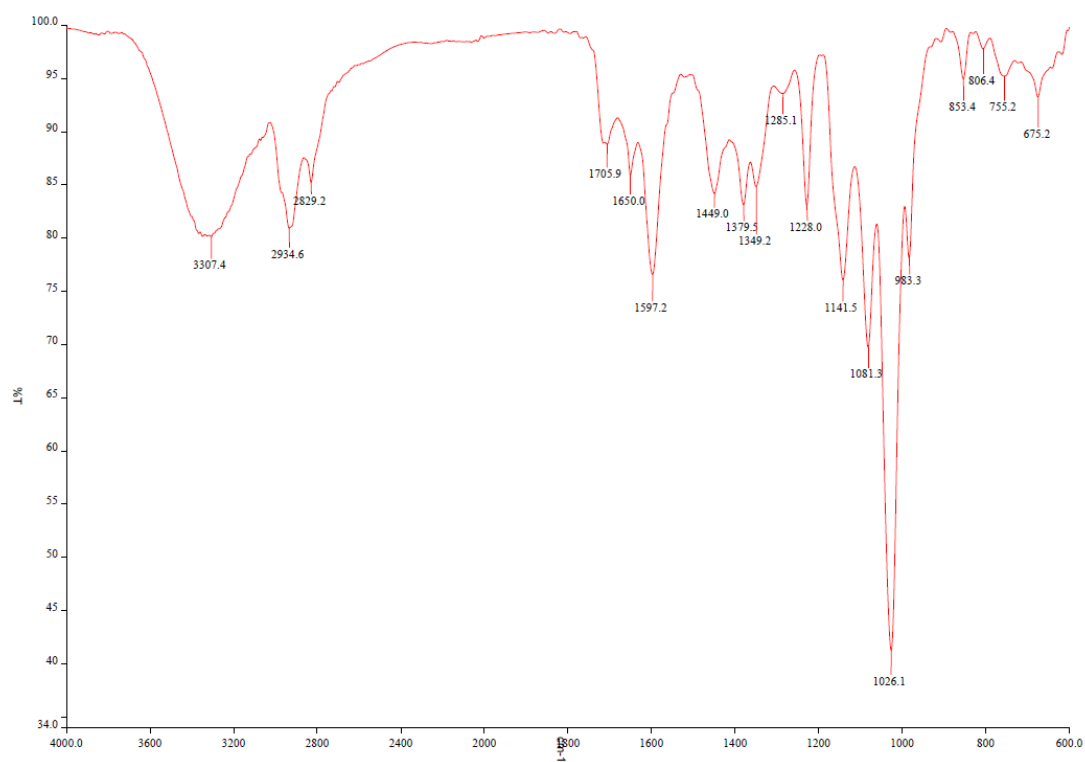


Fig. S72 IR spectrum of schizanthoside B7 (**10**).

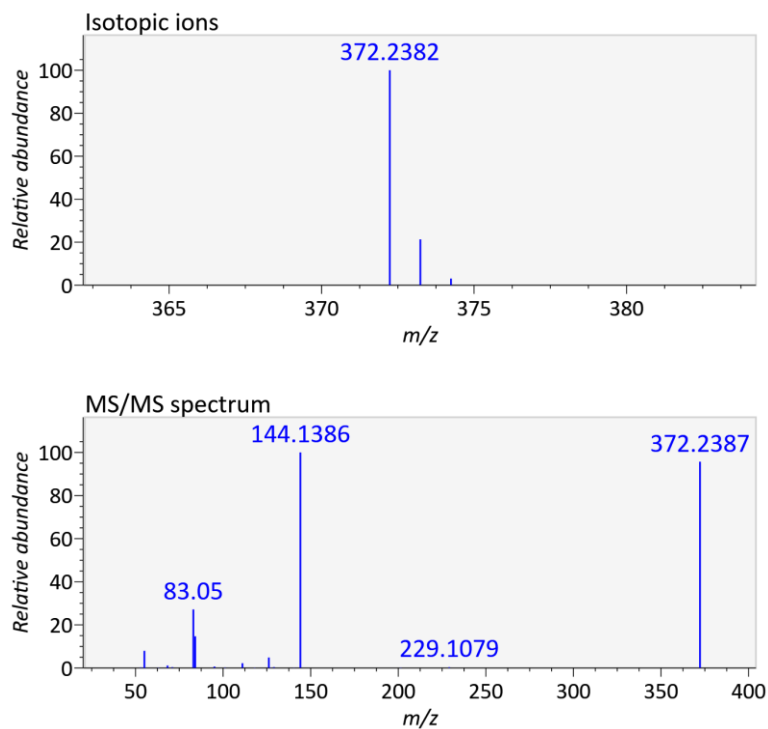


Fig. S73 HRESIMS and MS/MS spectra of schizanthoside B7 (**10**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

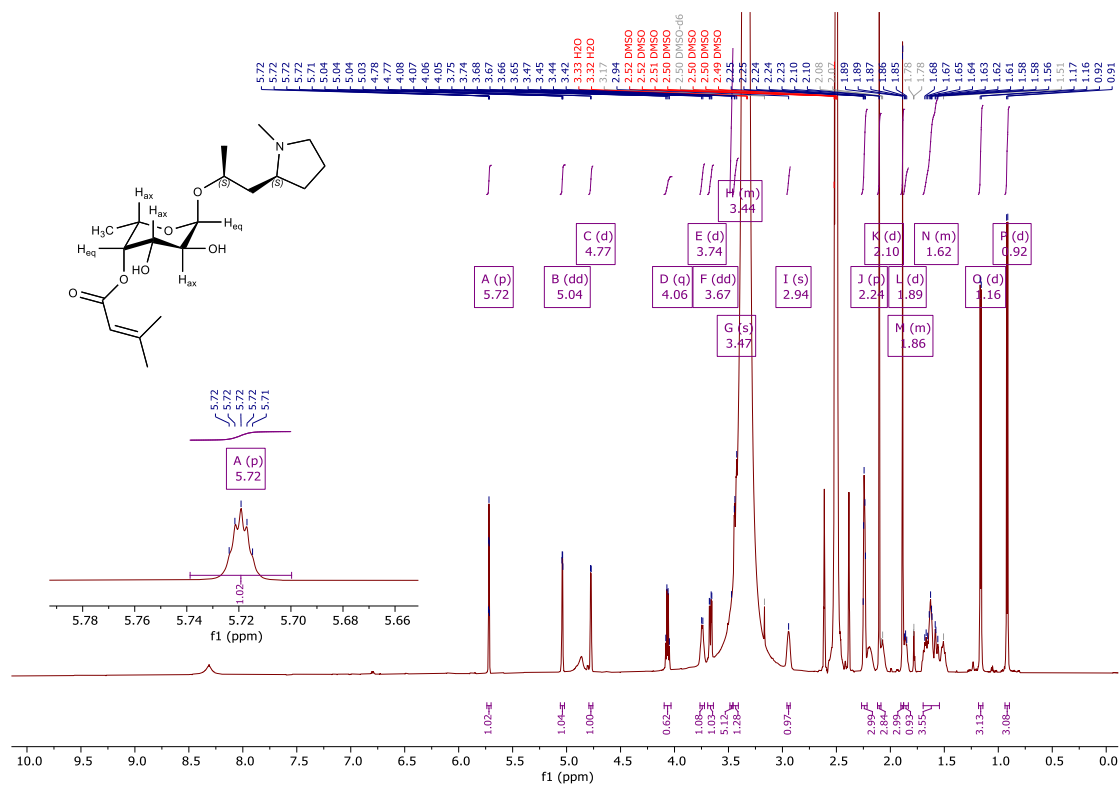


Fig. S74 ¹H NMR (600 MHz, DMSO-d₆) spectrum of schizanthoside B7 (**10**).

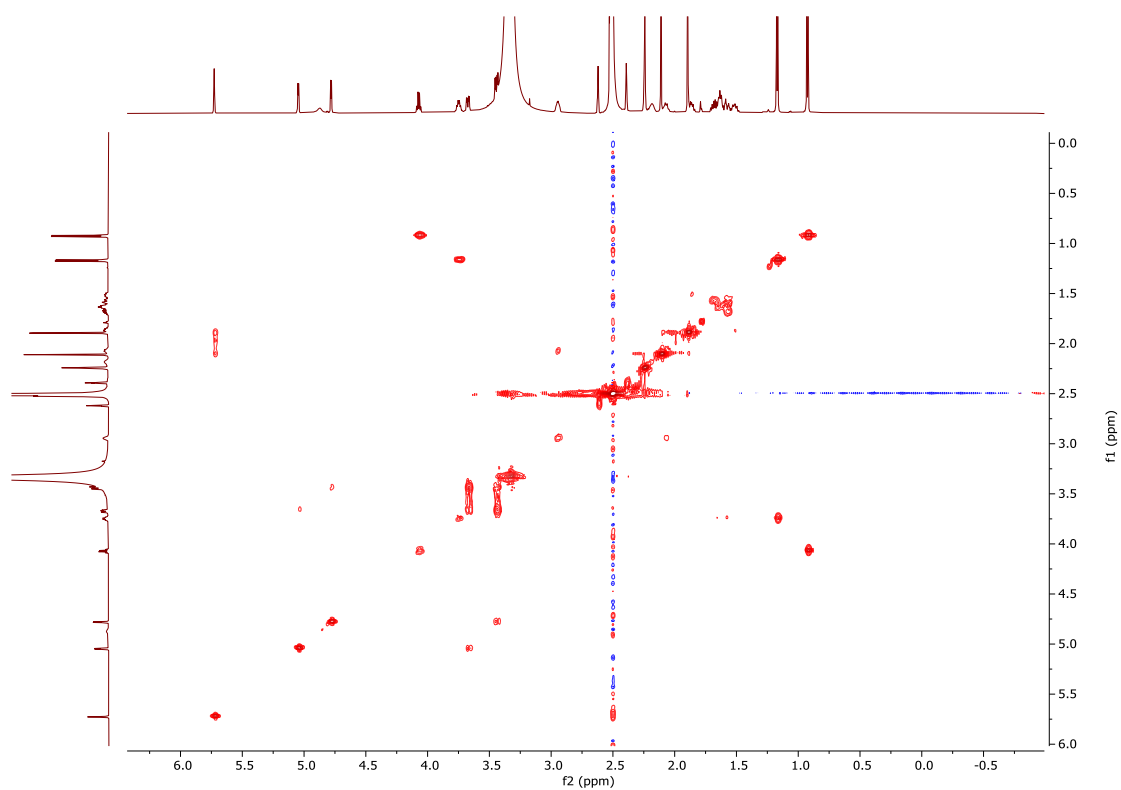


Fig. S75 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B7 (**10**).

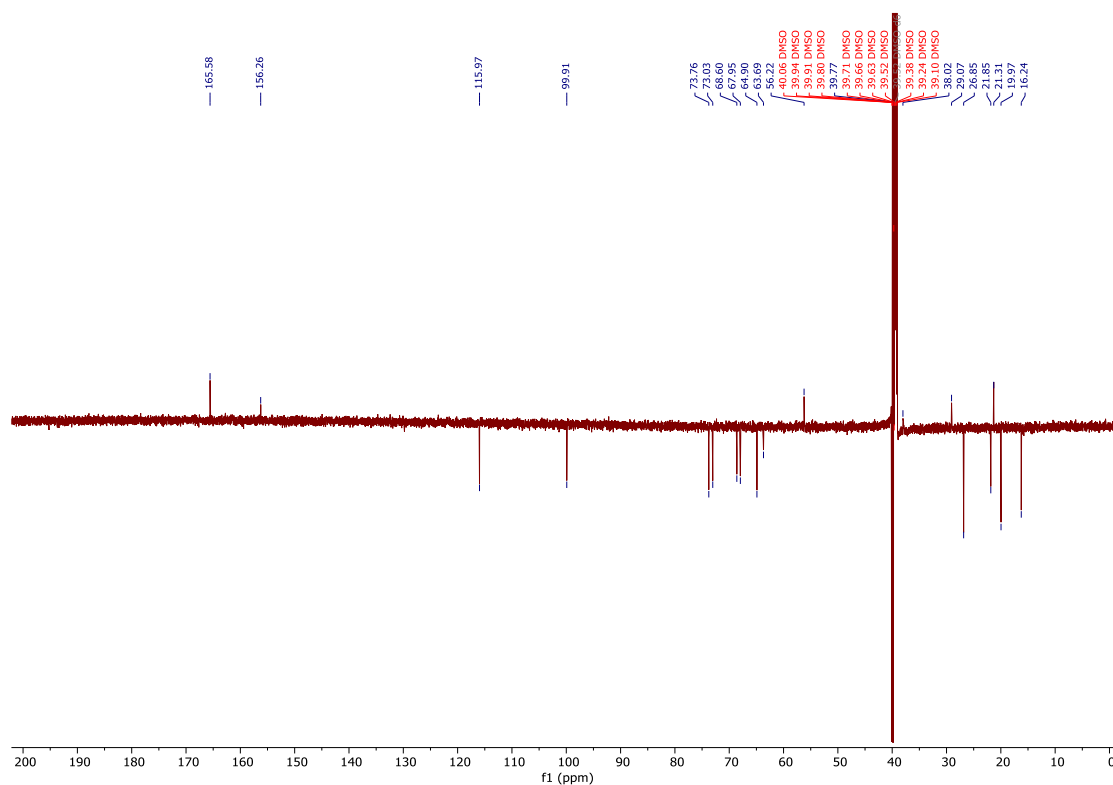


Fig. S76 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside B7 (**10**).

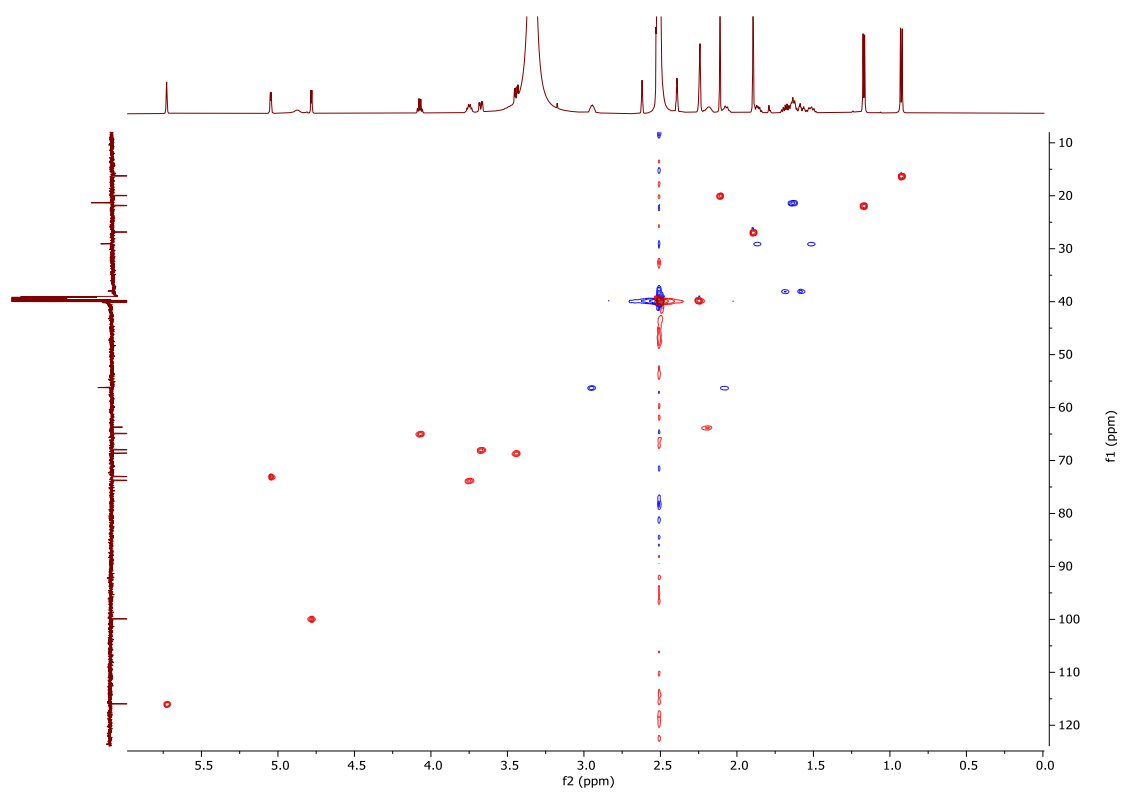


Fig. S77 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B7 (**10**).

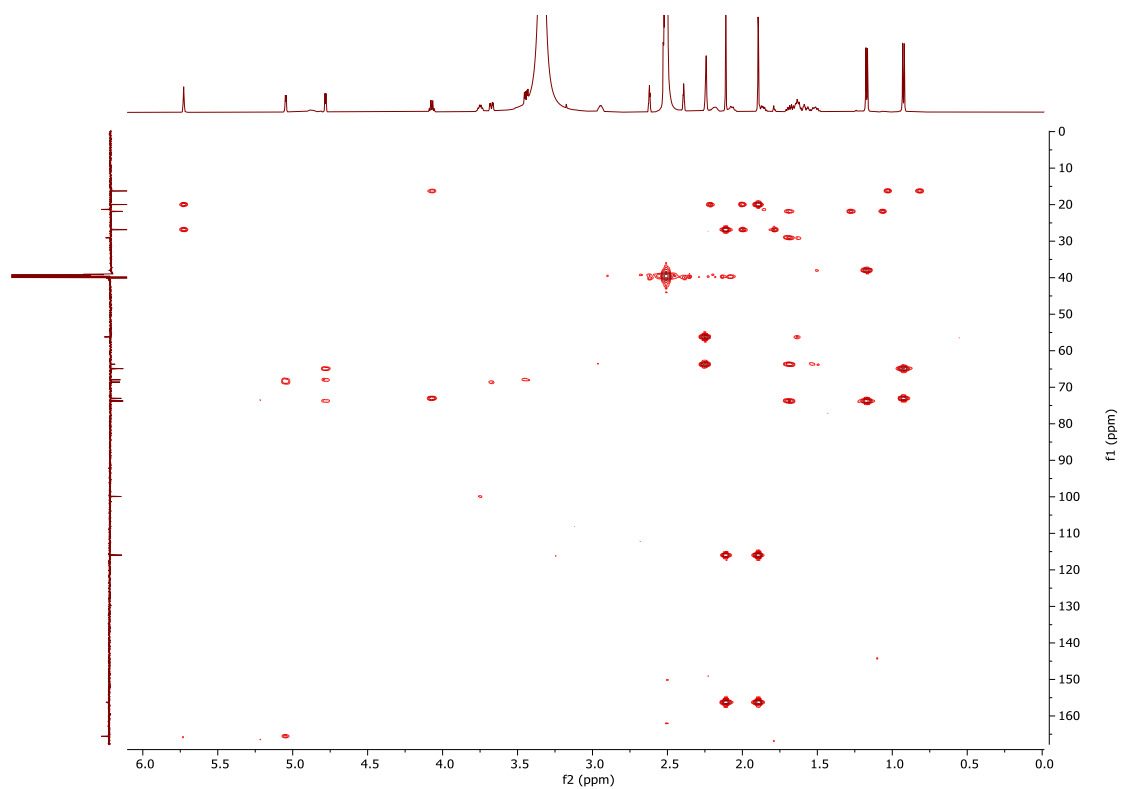


Fig. S78 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B7 (**10**).

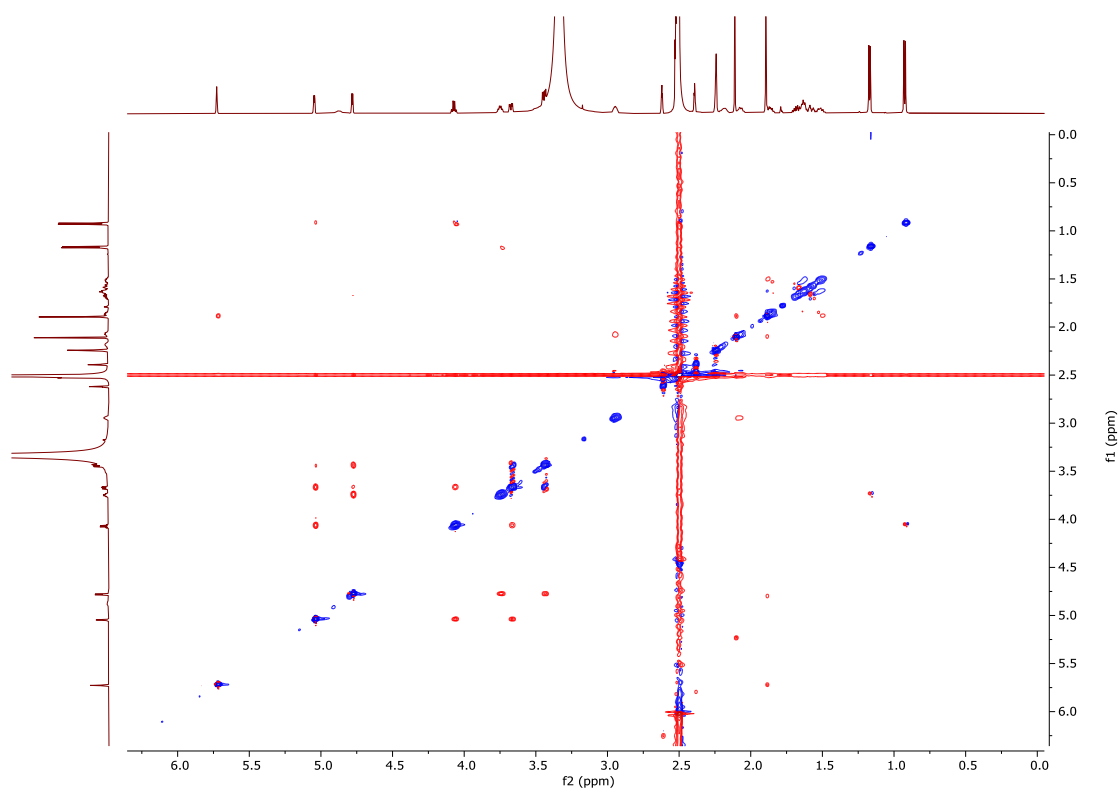


Fig. S79 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside B7 (**10**).

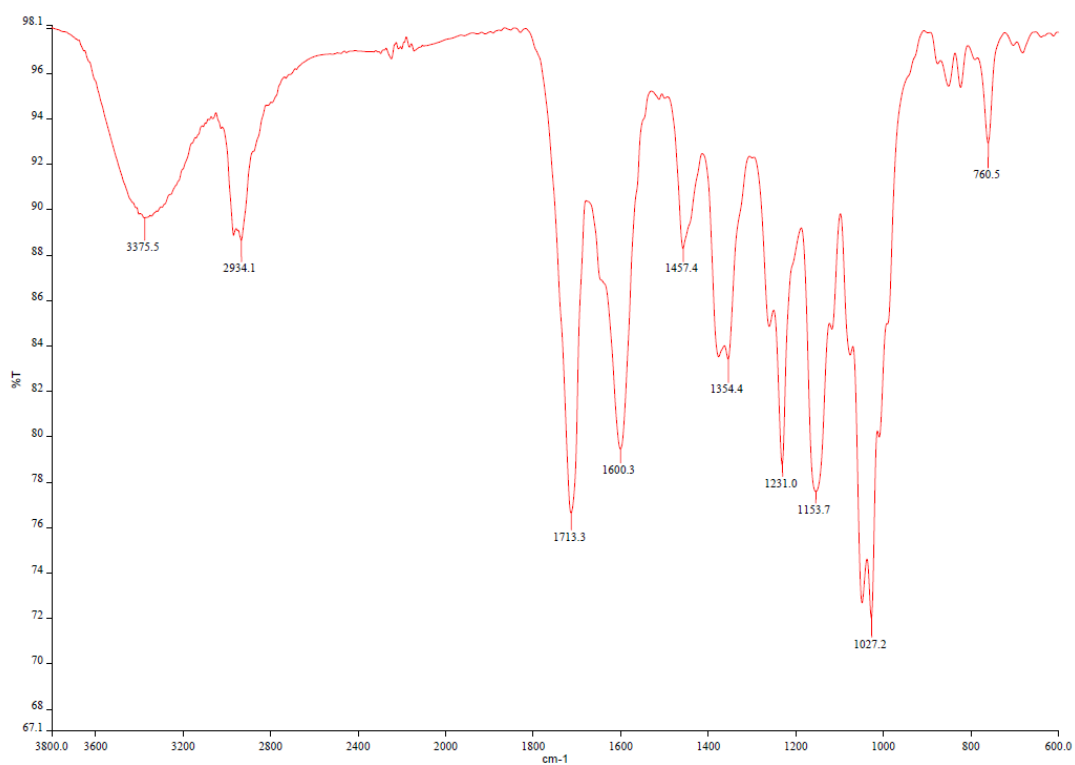


Fig. S80 IR spectrum of schizanthoside C1 (**11**).

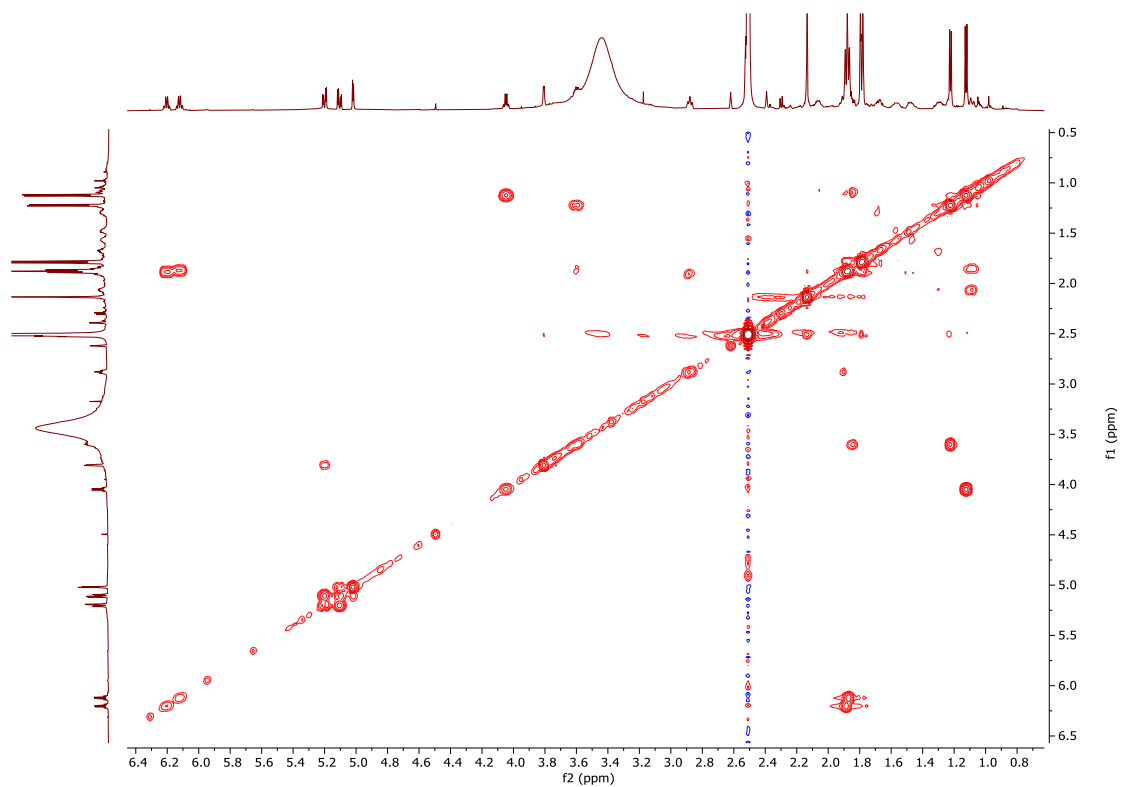


Fig. S83 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C1 (**11**).

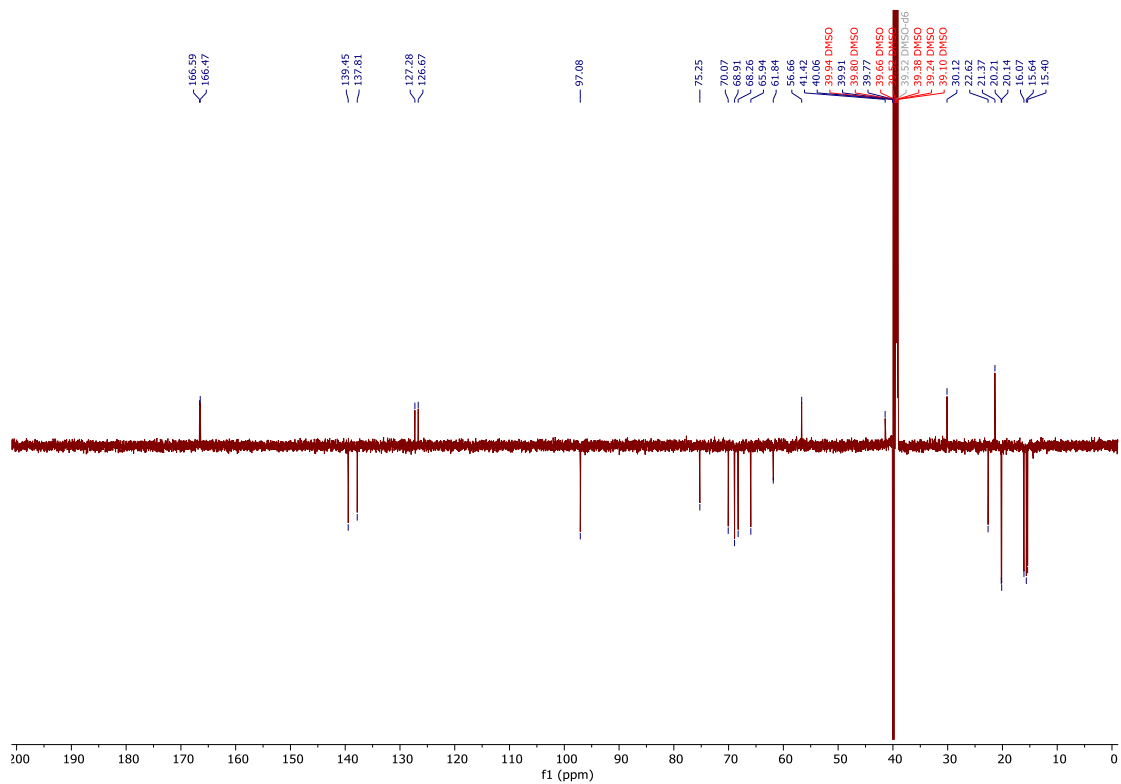


Fig. S84 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside C1 (**11**).

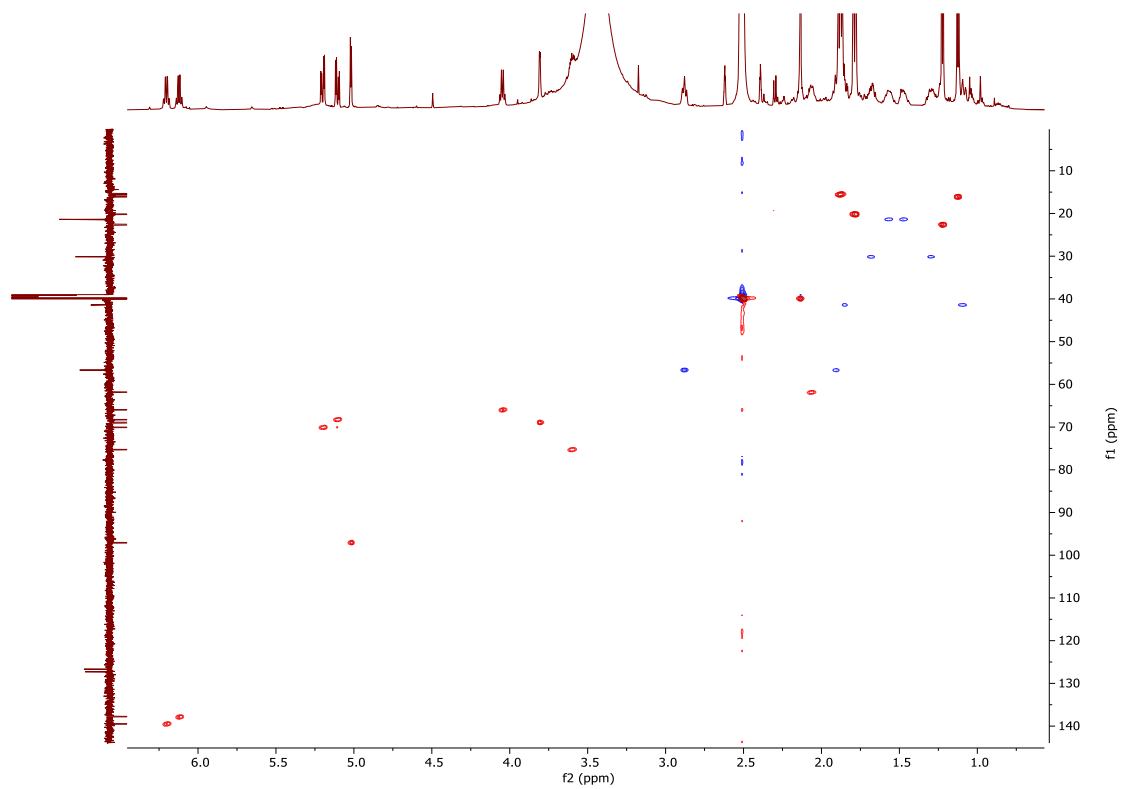


Fig. S85 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C1 (**11**).

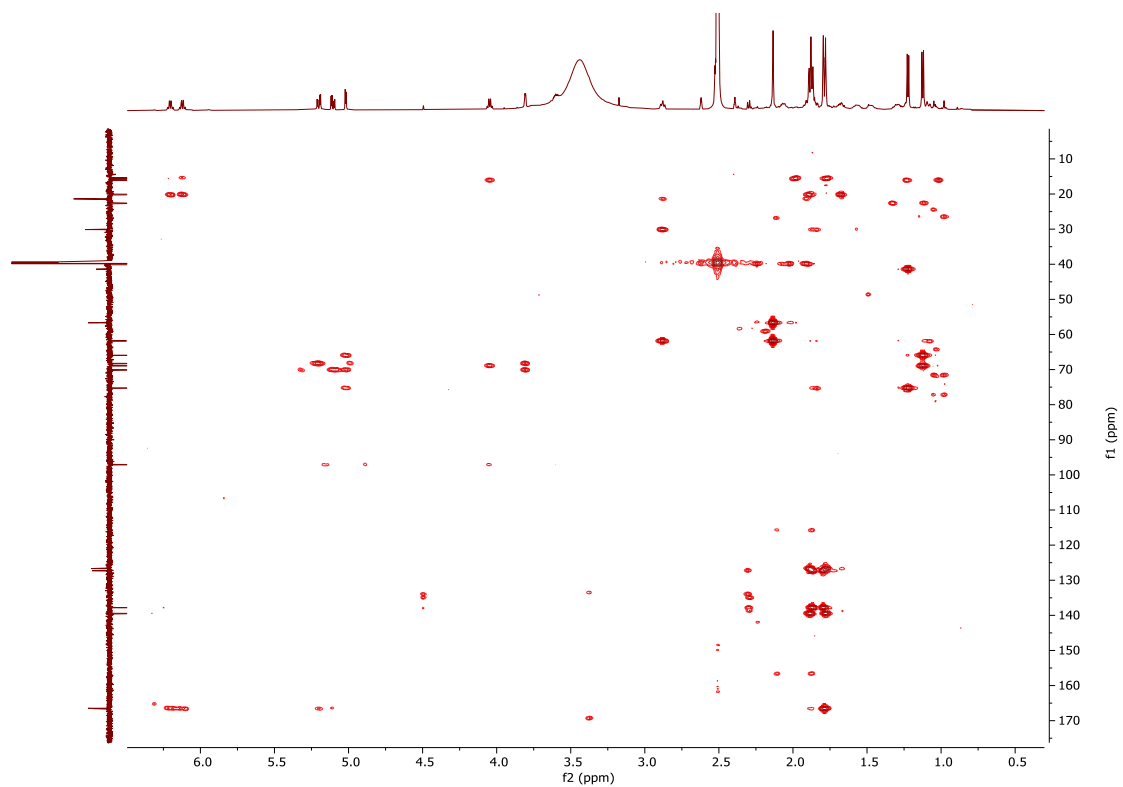


Fig. S86 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C1 (**11**).

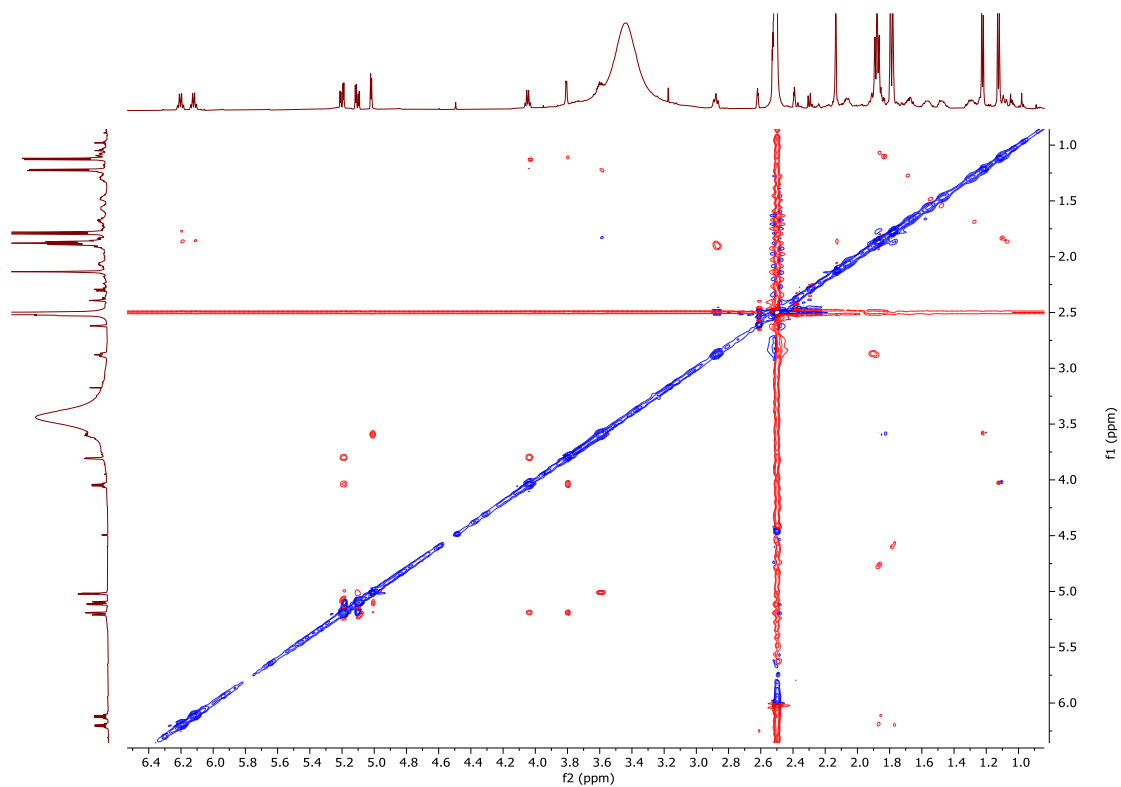


Fig. S87 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C1 (**11**).

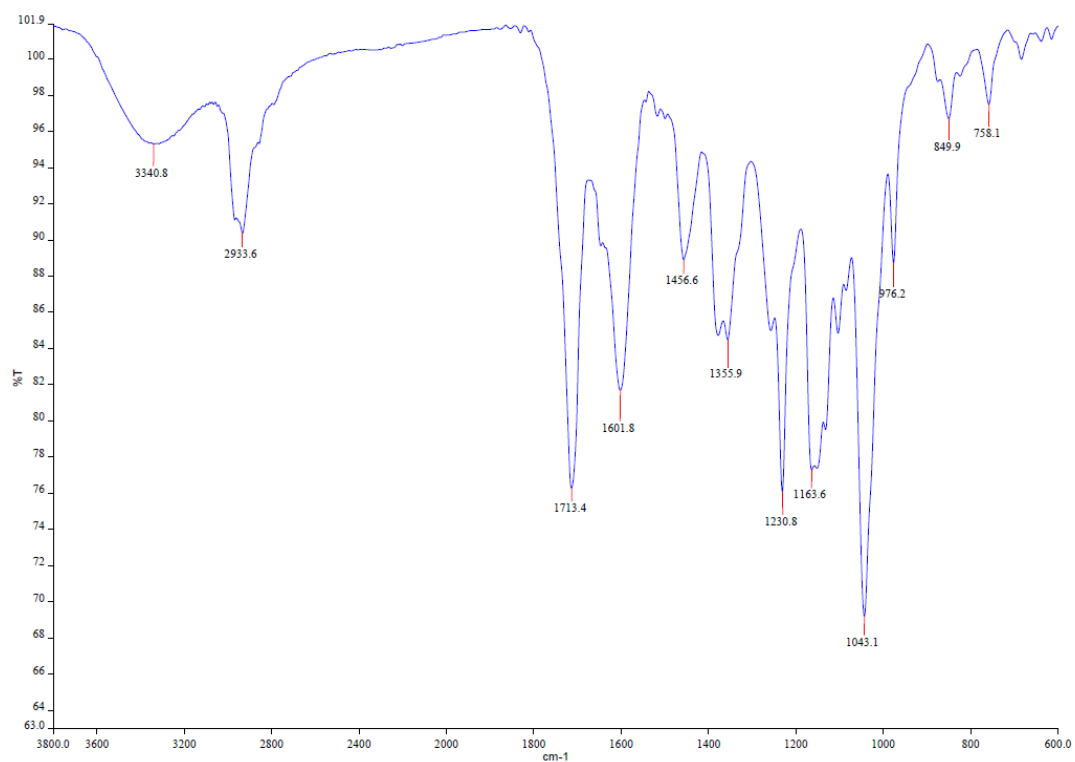


Fig. S88 IR spectrum of schizanthoside C2 (**12**).

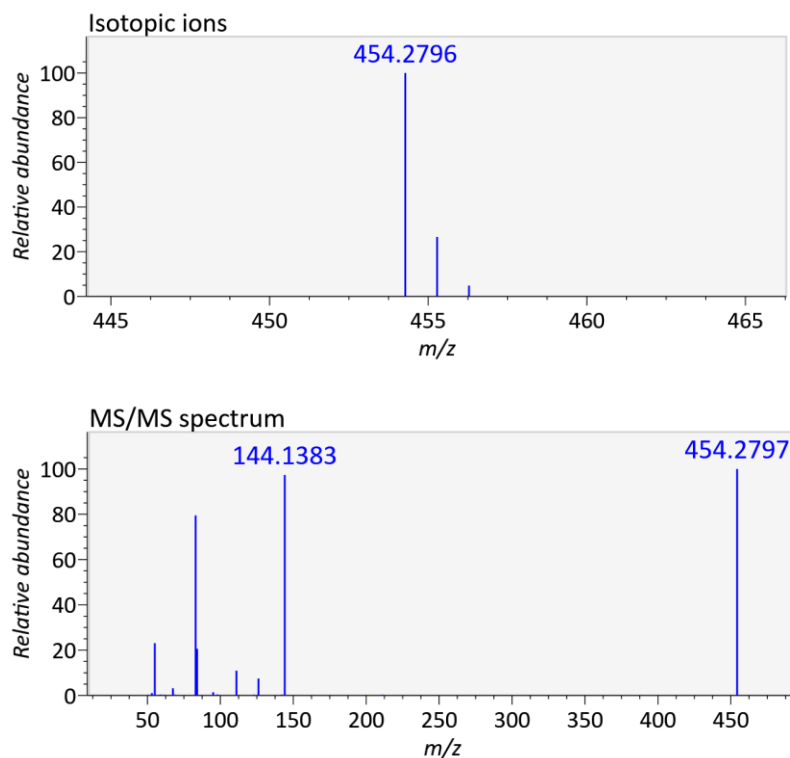


Fig. S89 HRESIMS and MS/MS spectra of schizanthoside C2 (**12**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

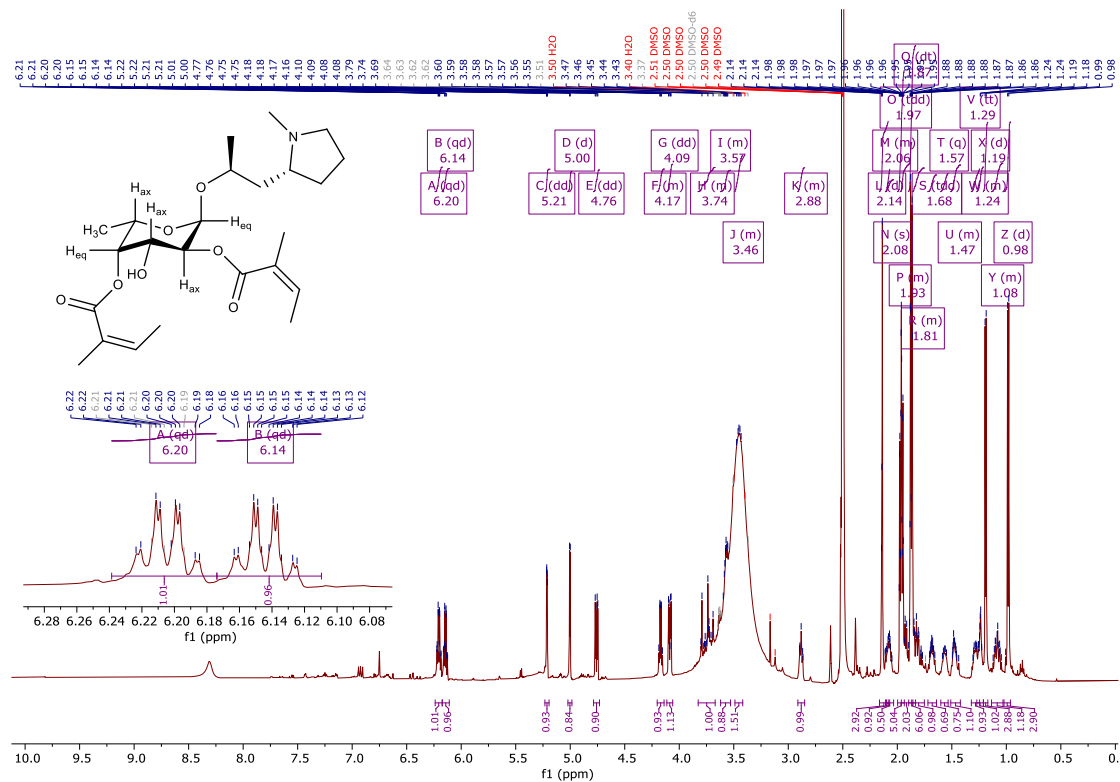


Fig. S90 ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C2 (**12**).

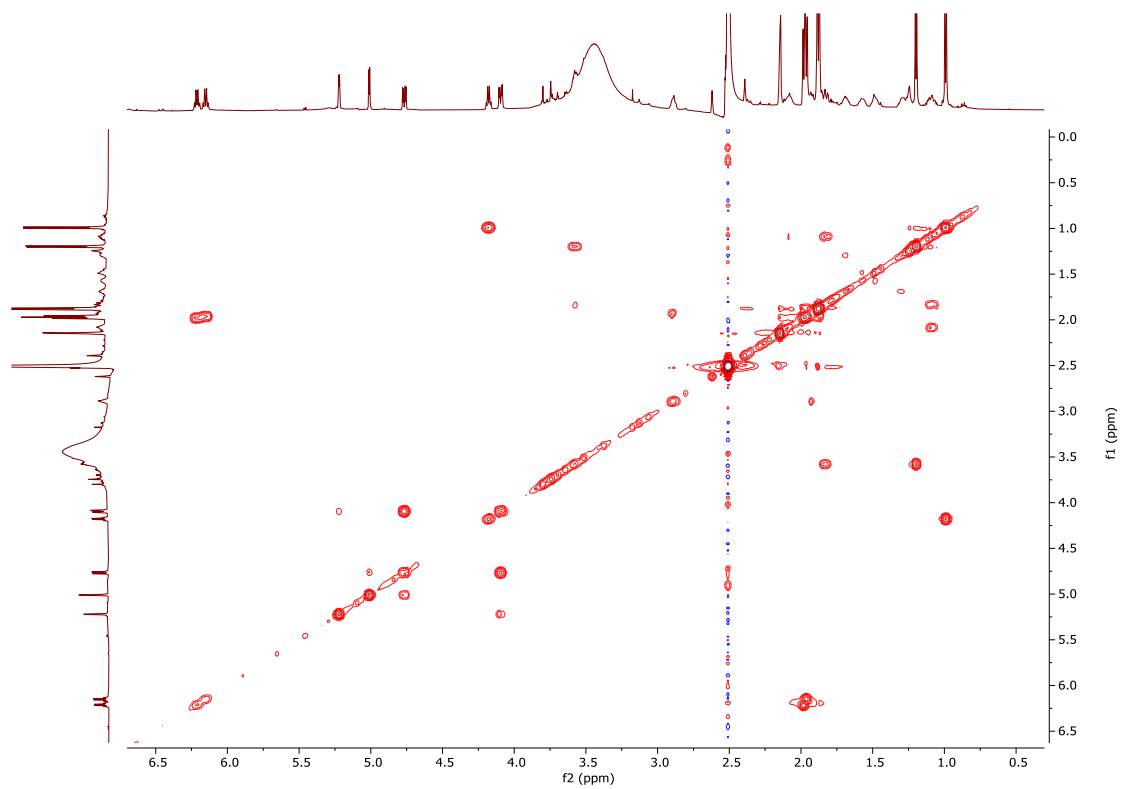


Fig. S91 COSY (600 MHz, DMSO- d_6) spectrum of schizanthoside C2 (**12**).

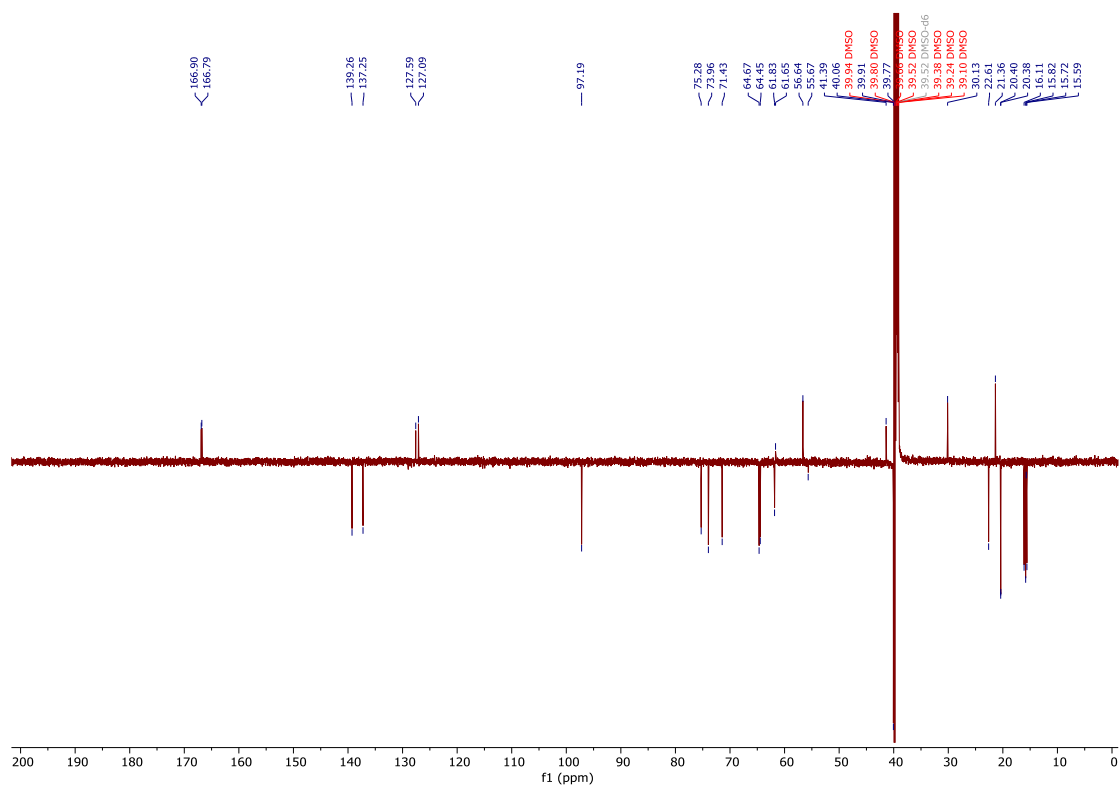


Fig. S92 DEPTQ (125 MHz, DMSO- d_6) spectrum of schizanthoside C2 (**12**).

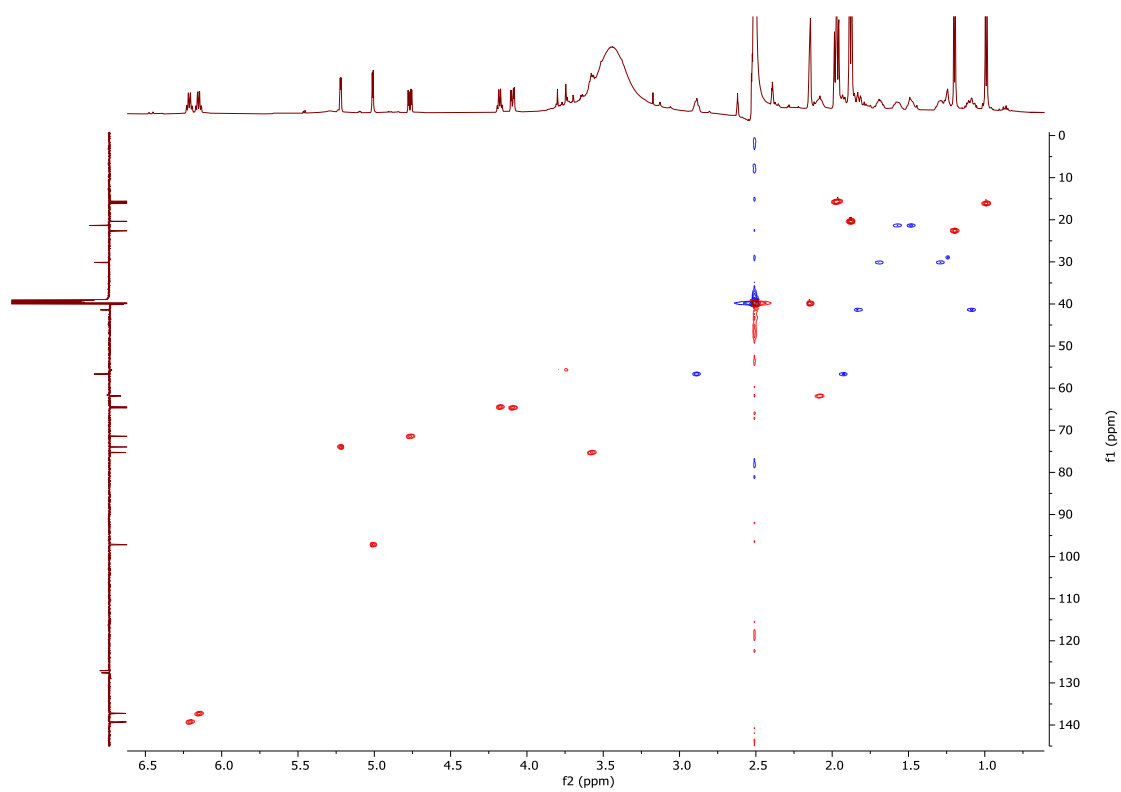


Fig. S93 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C2 (**12**).

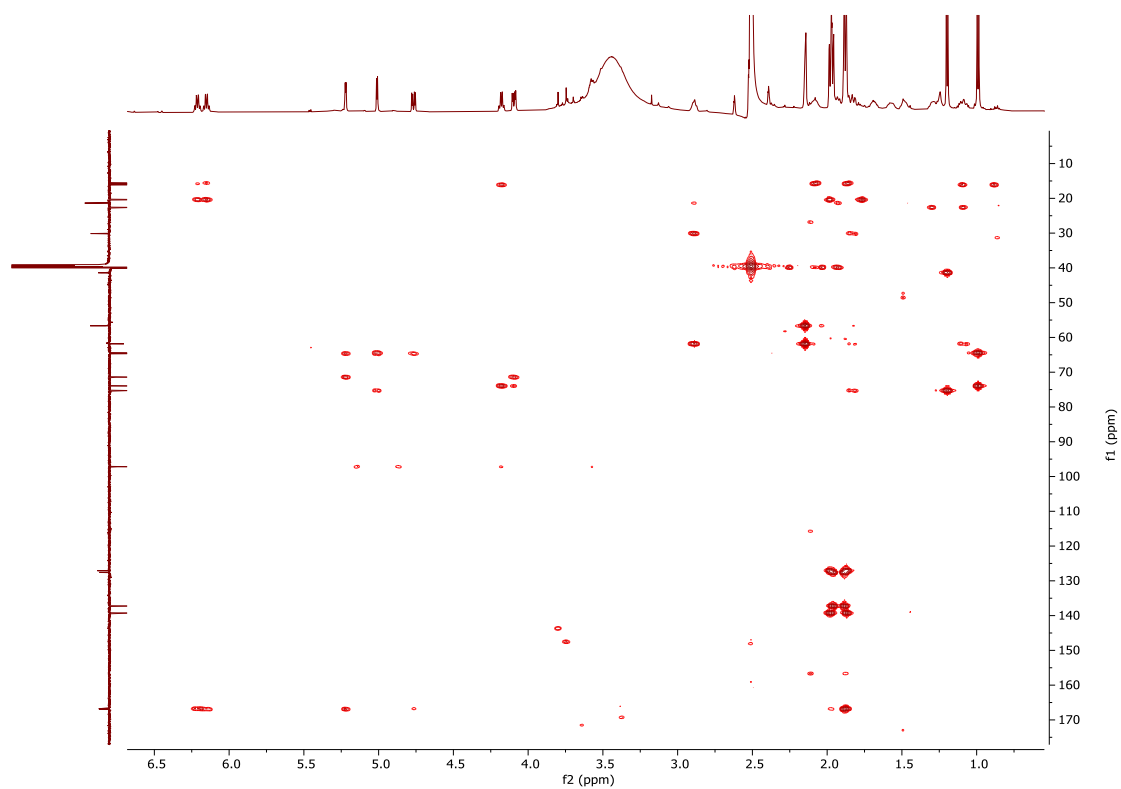


Fig. S94 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C2 (**12**).

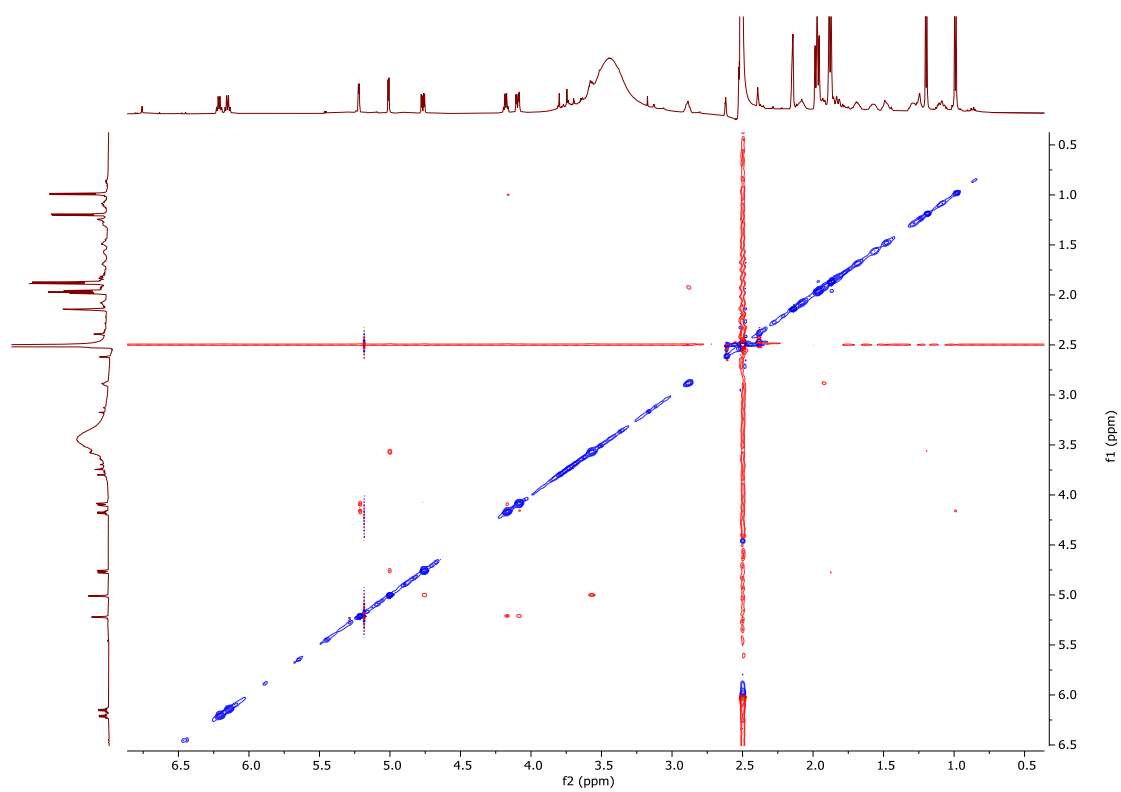


Fig. S95 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C2 (**12**).

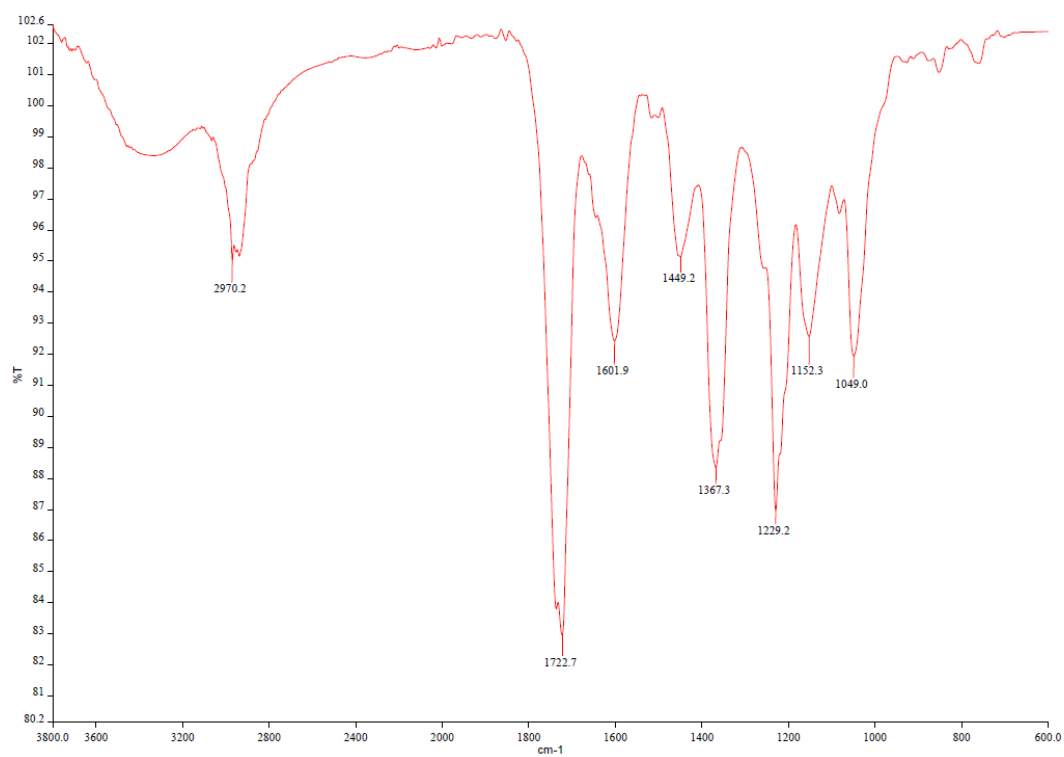


Fig. S96 IR spectrum of schizanthoside C3 (**13**).

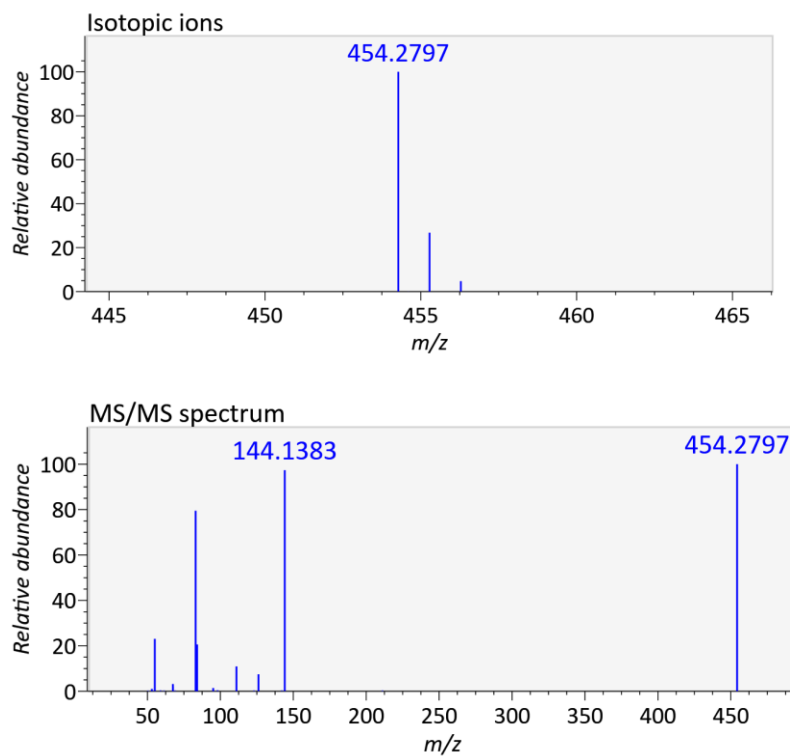


Fig. S97 HRESIMS and MS/MS spectra of schizanthoside C3 (**13**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

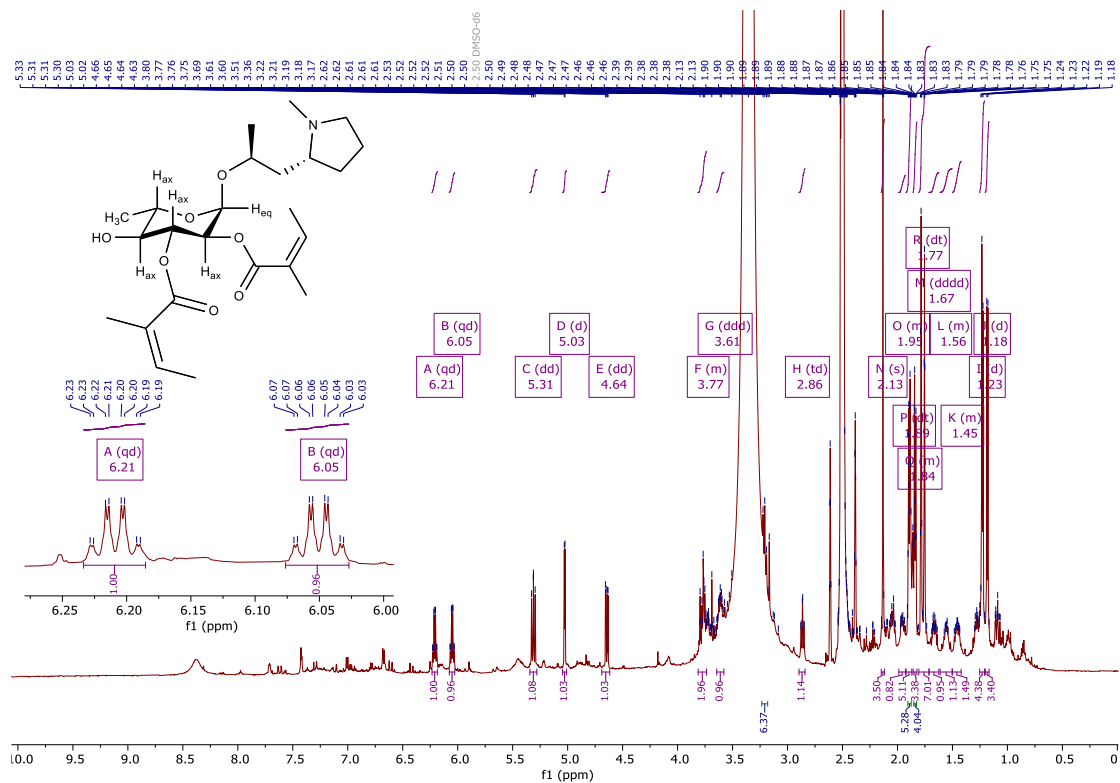


Fig. S98 ¹H NMR (600 MHz, DMSO-d₆) spectrum of schizanthoside C3 (**13**).

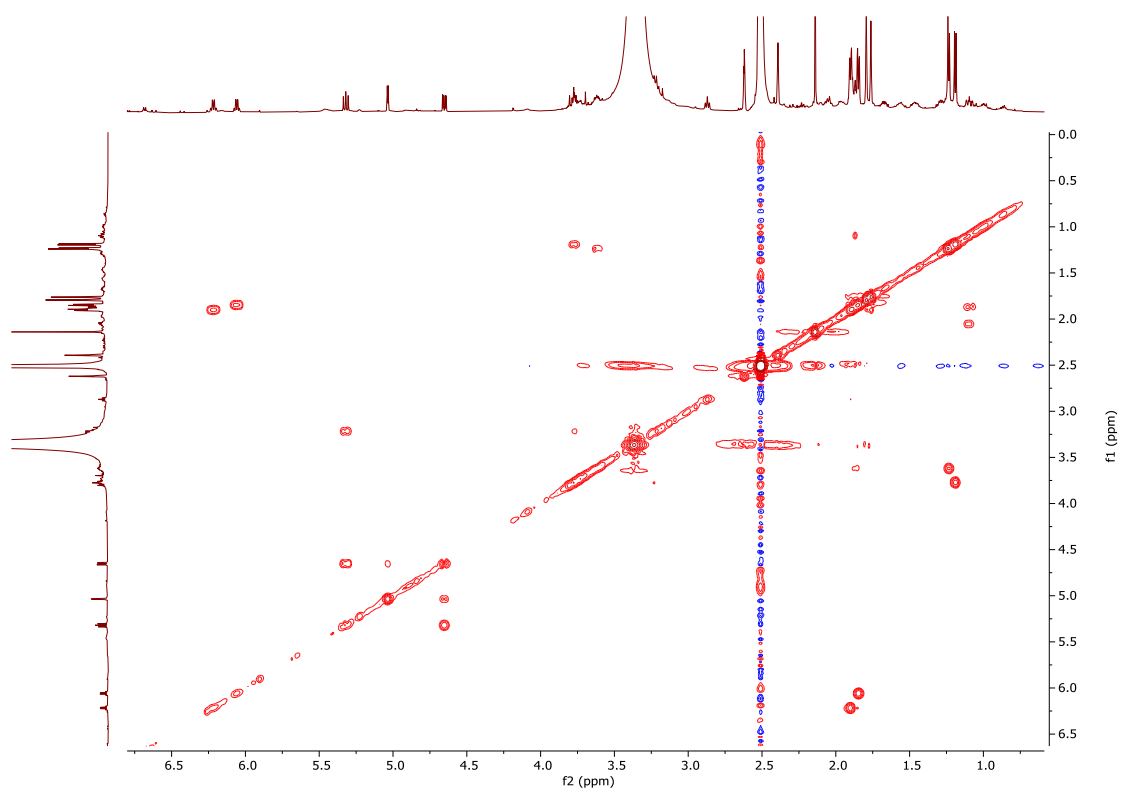


Fig. S99 COSY (600 MHz, DMSO- d_6) spectrum of schizanthoside C3 (**13**).

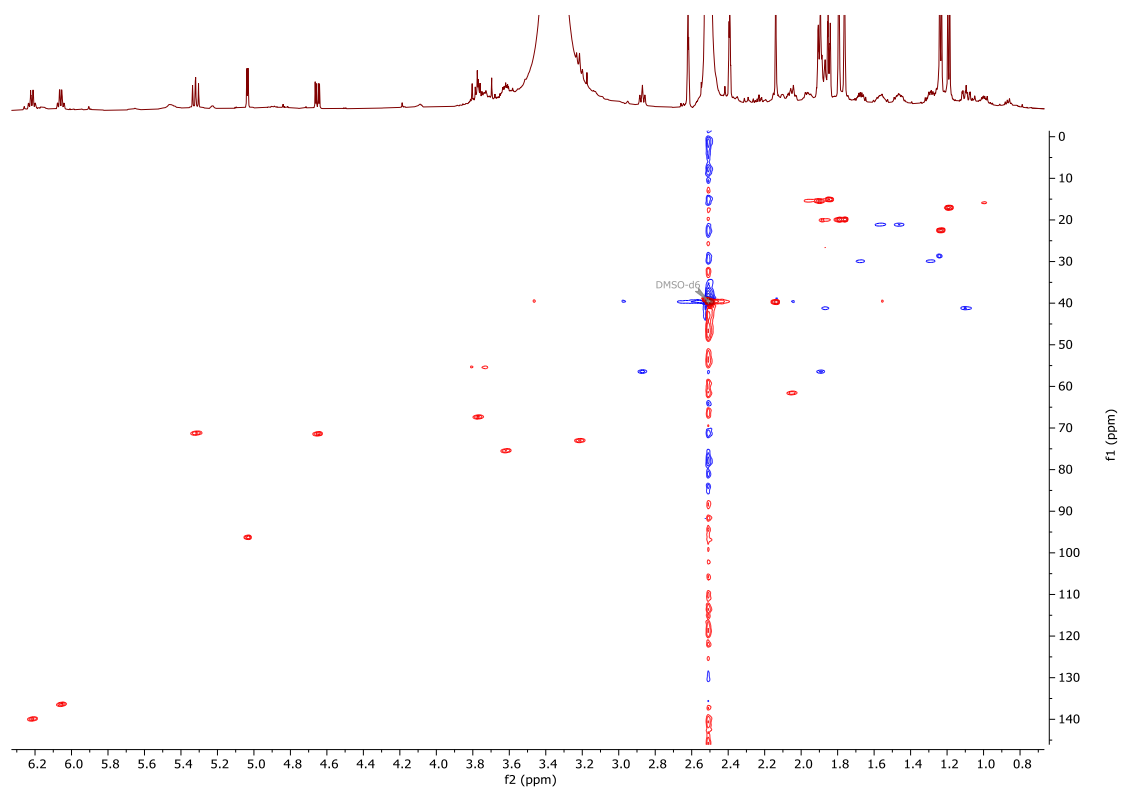


Fig. S100 HSQC (600 MHz, DMSO- d_6) spectrum of schizanthoside C3 (**13**).

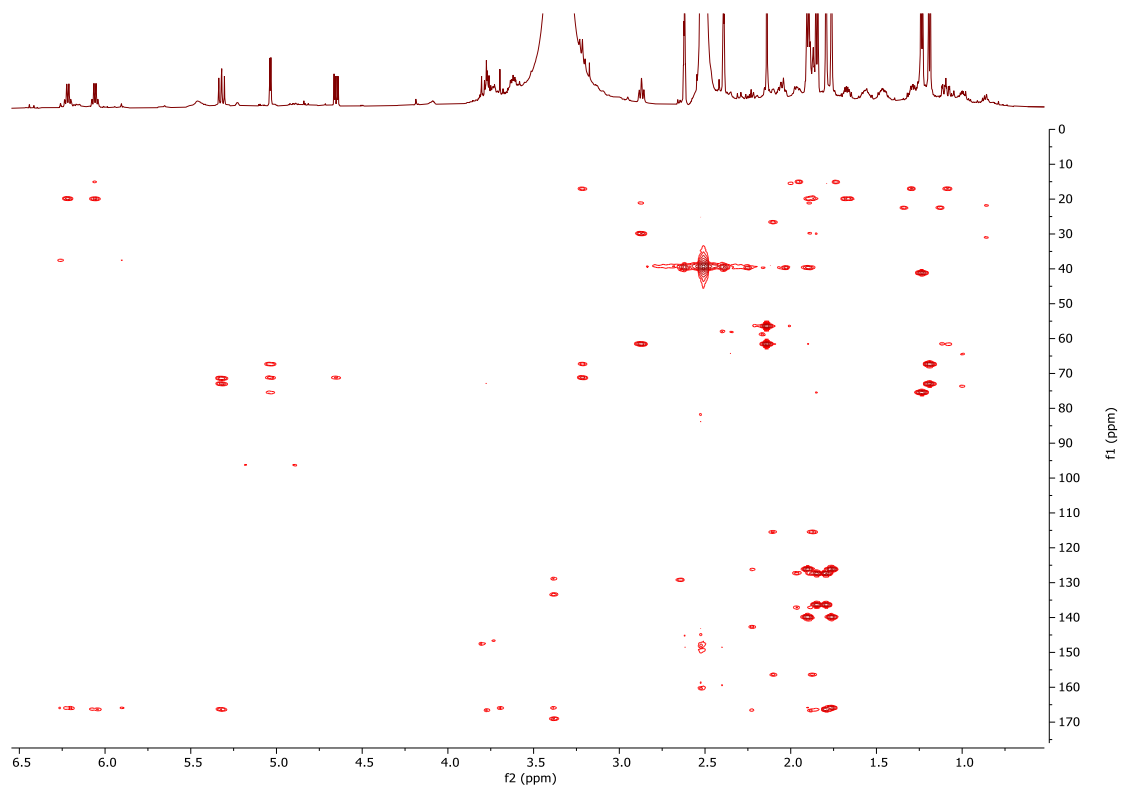


Fig. S101 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C3 (**13**).

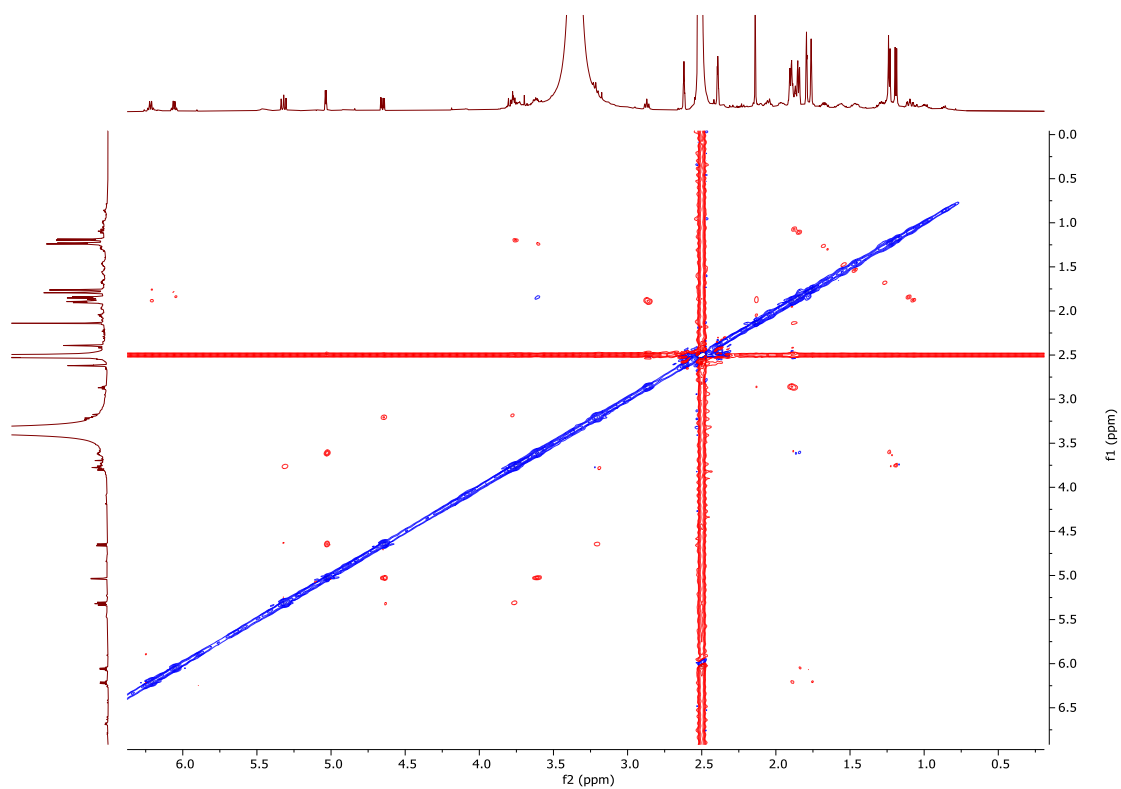


Fig. S102 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C3 (**13**).

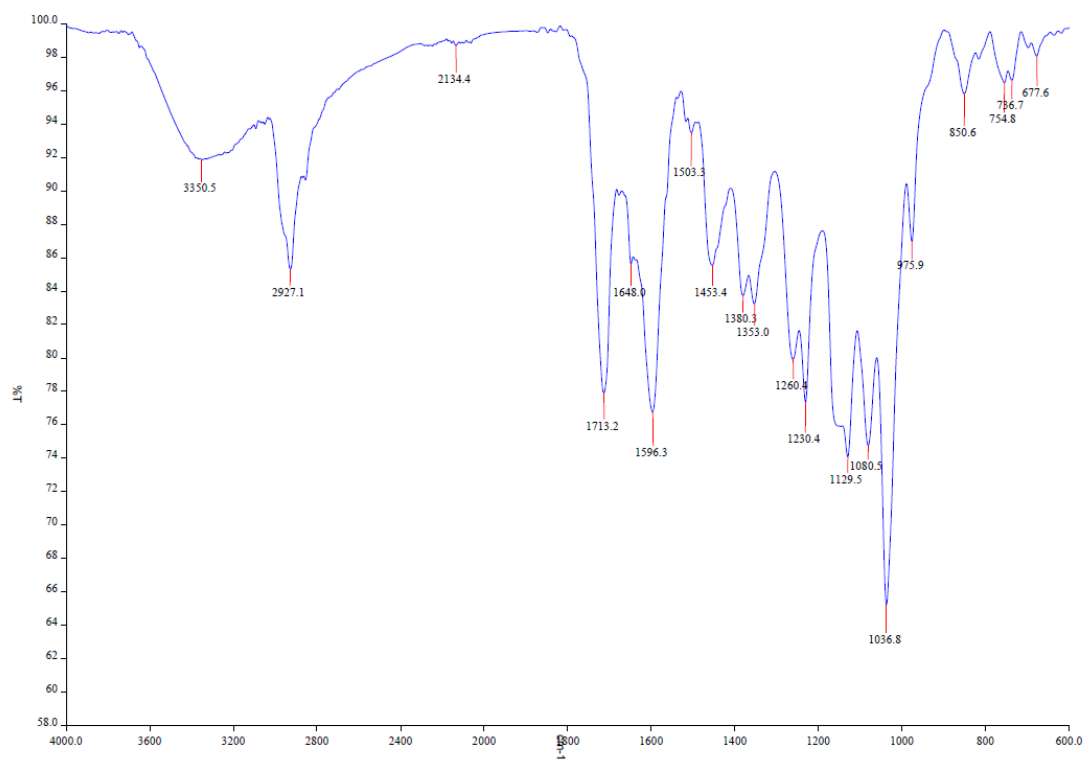


Fig. S103 IR spectrum of schizanthoside C4 (**14**).

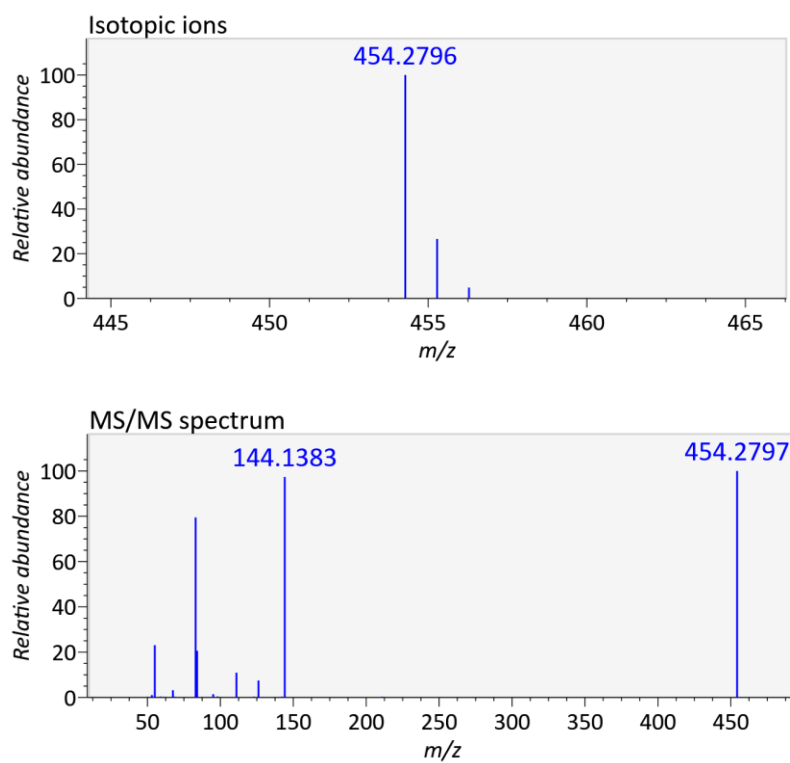


Fig. S104 HRESIMS and MS/MS spectra of schizanthoside C4 (**14**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

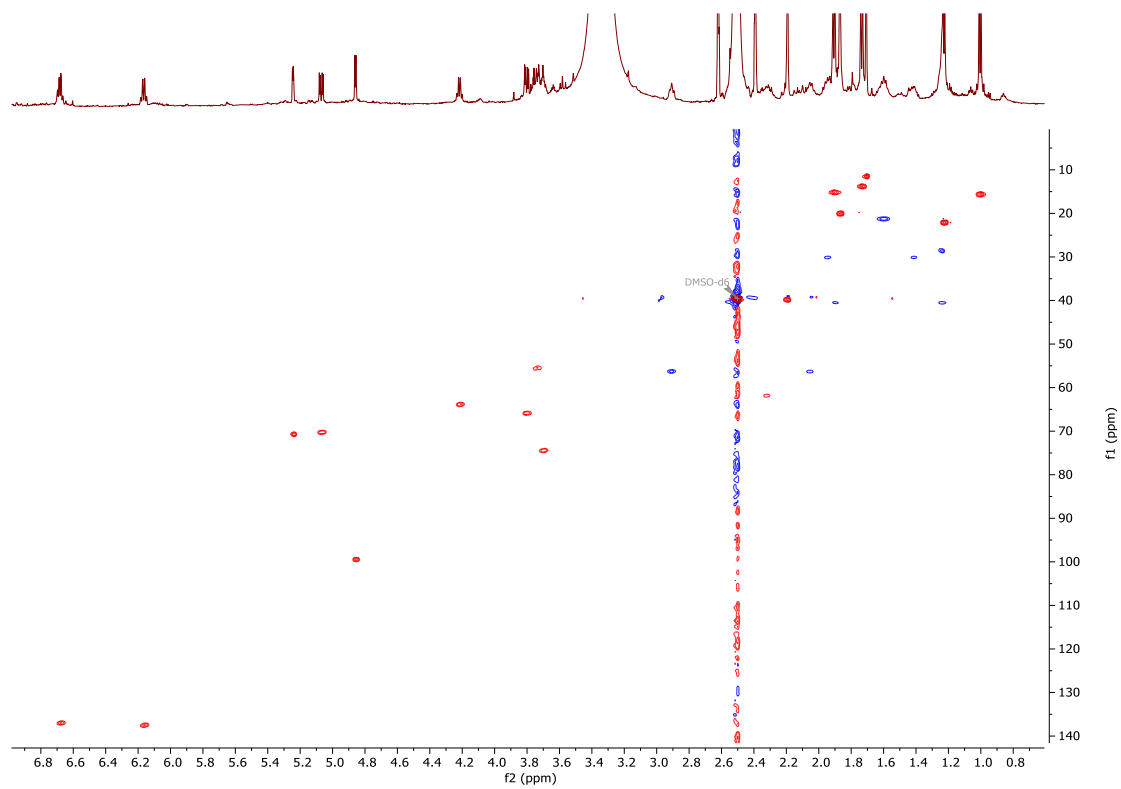


Fig. S107 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C4 (**14**).

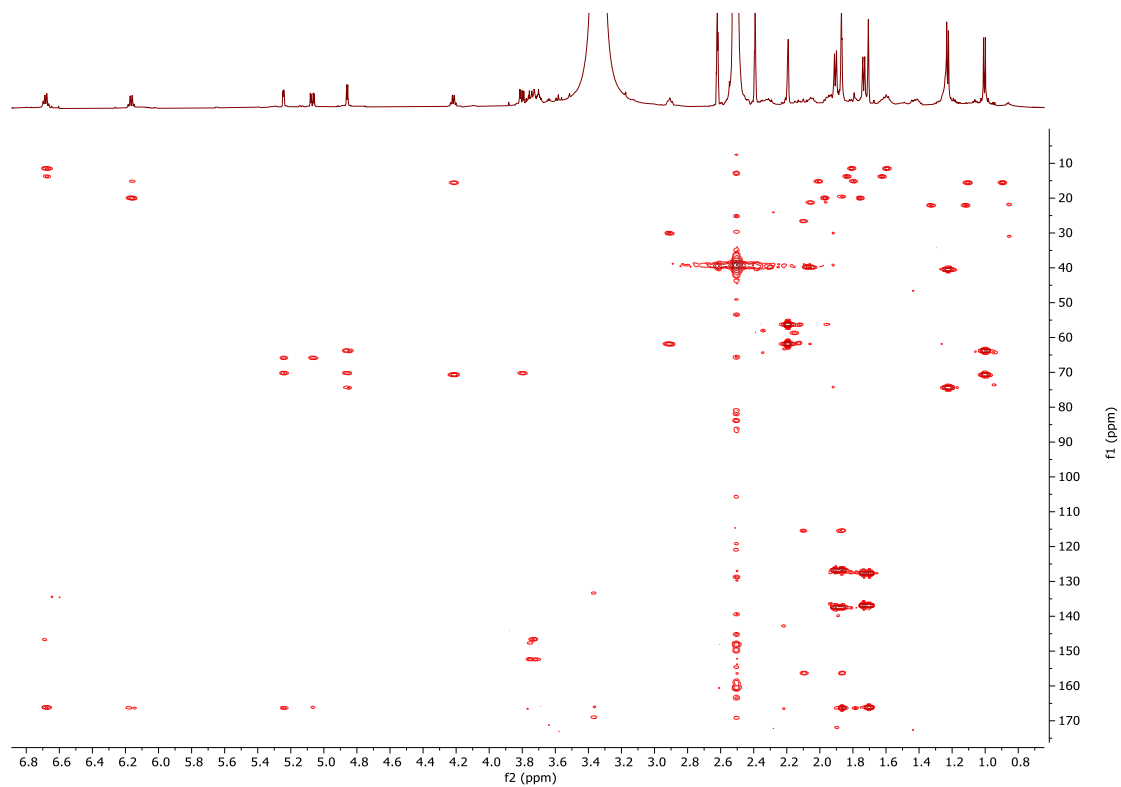


Fig. S108 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C4 (**14**).

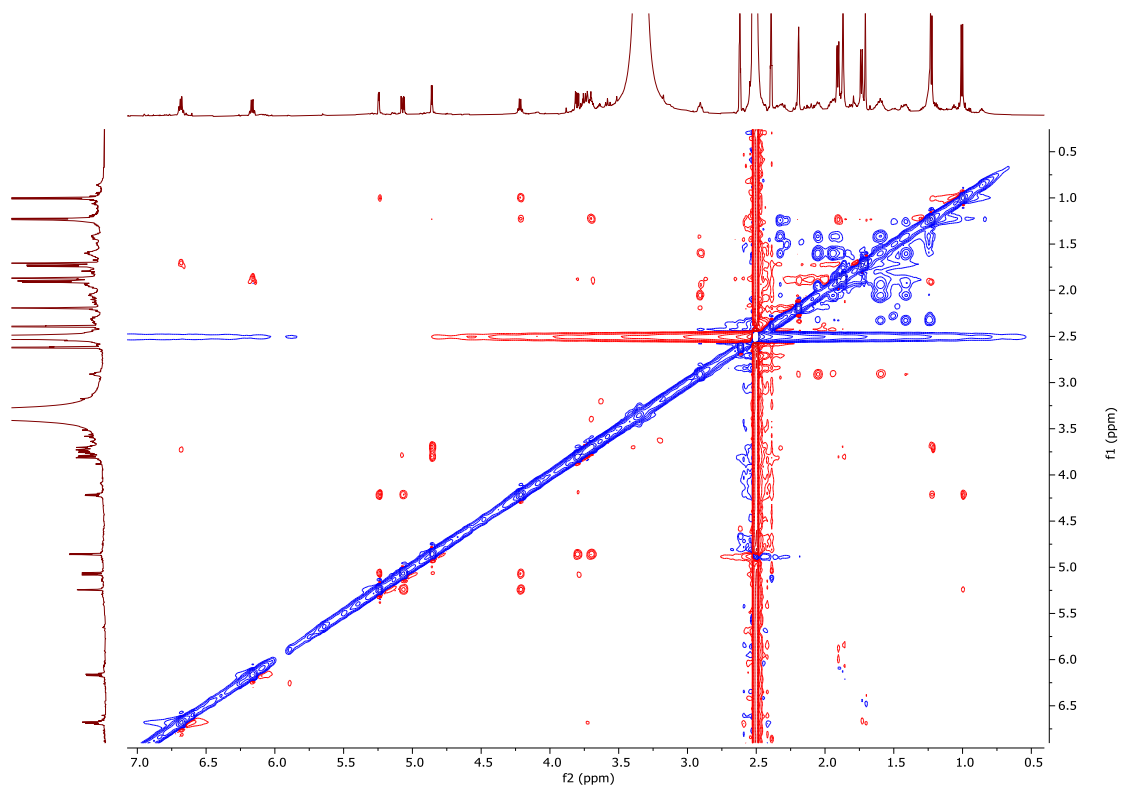


Fig. S109 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C4 (**14**).

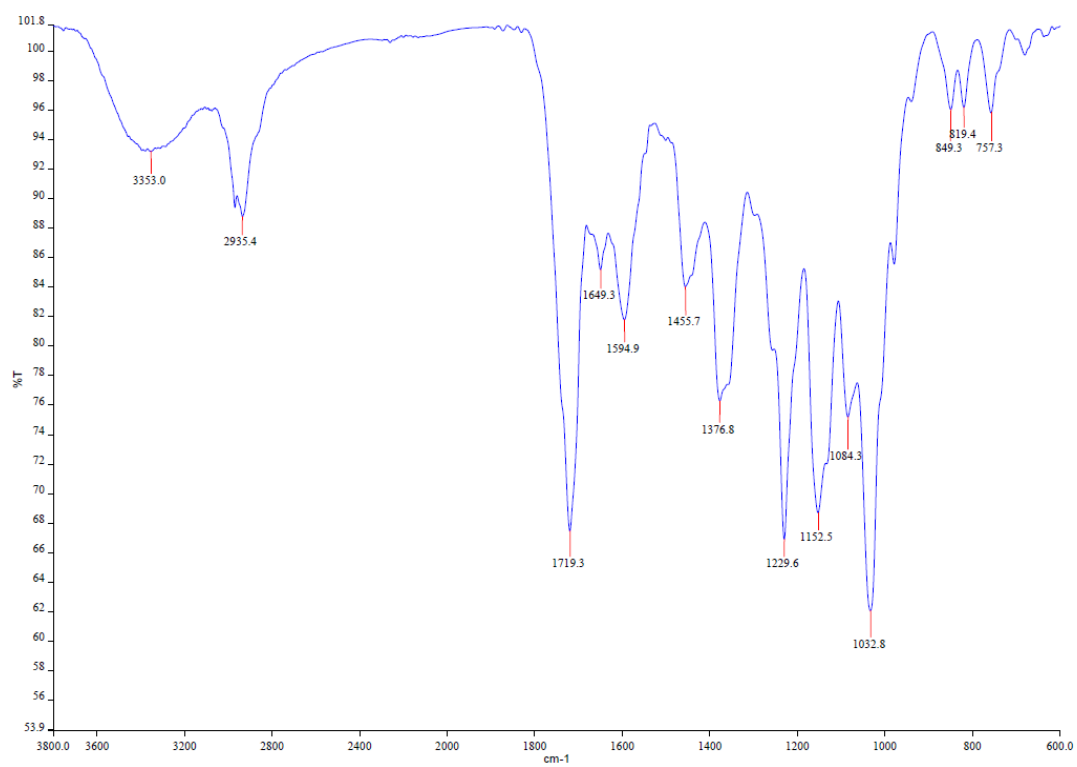


Fig. S110 IR spectrum of schizanthoside C5 (**15**).

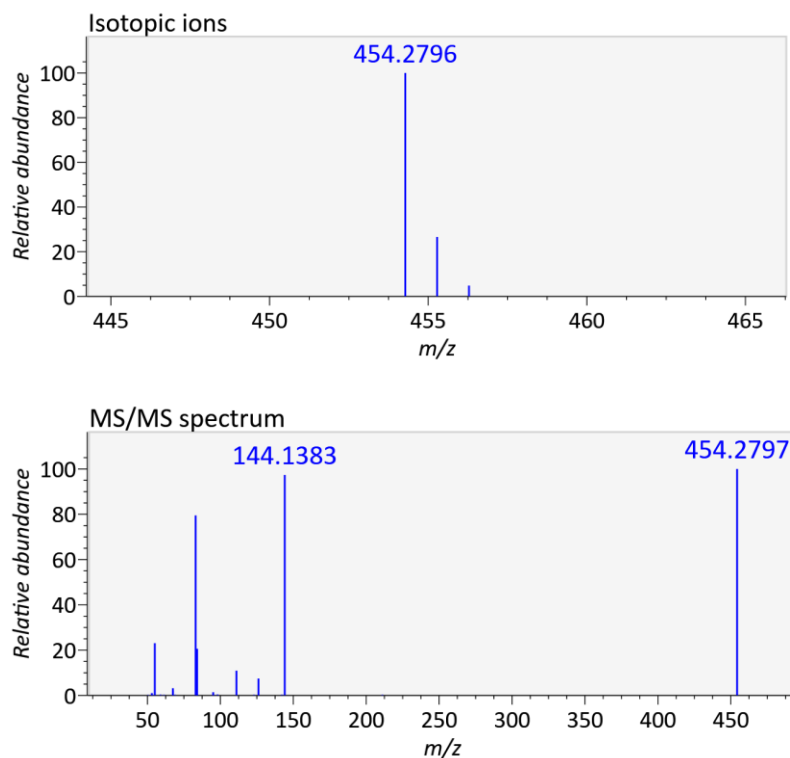


Fig. S111 HRESIMS and MS/MS spectra of schizanthoside C5 (**15**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

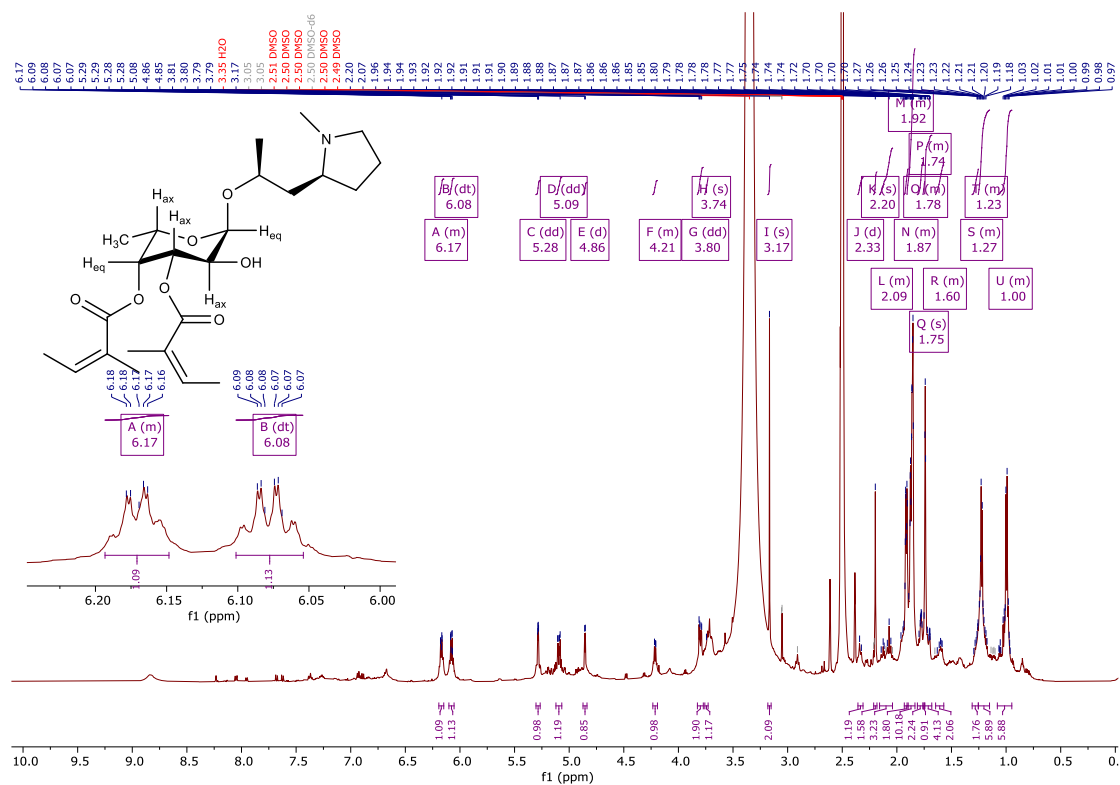


Fig. S112 ¹H NMR (600 MHz, DMSO-d₆) spectrum of schizanthoside C5 (**15**).

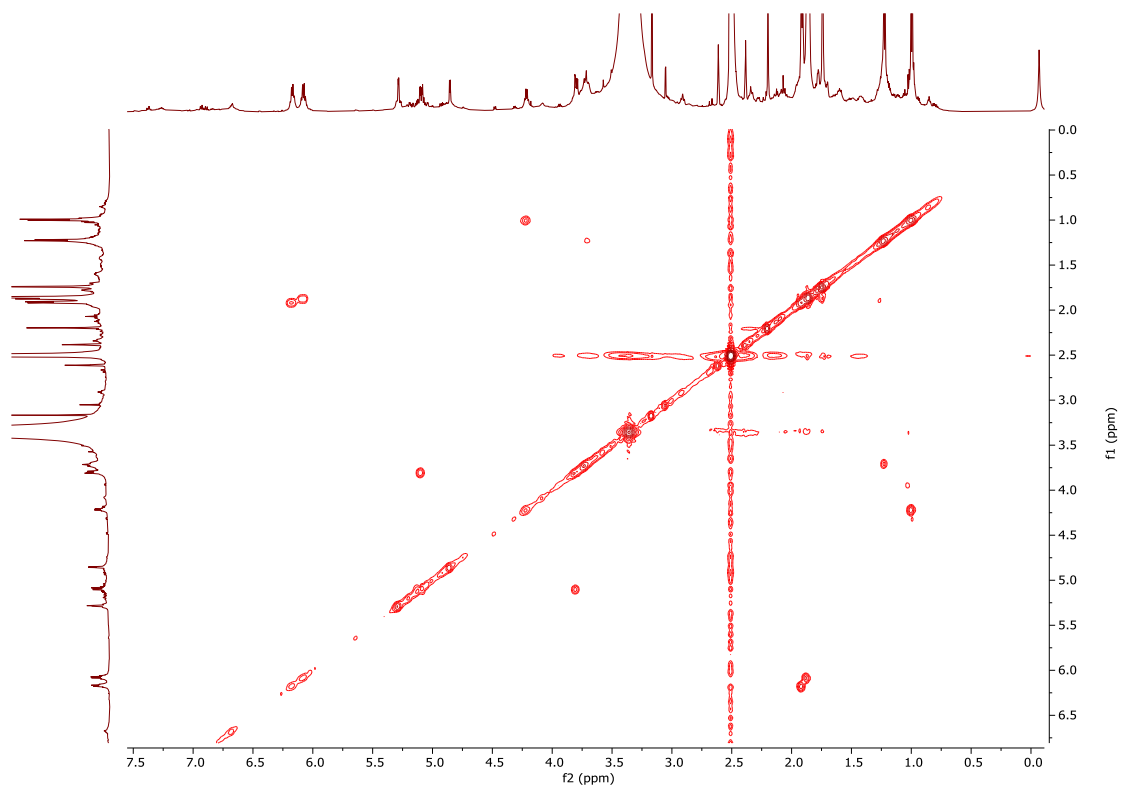


Fig. S113 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C5 (**15**).

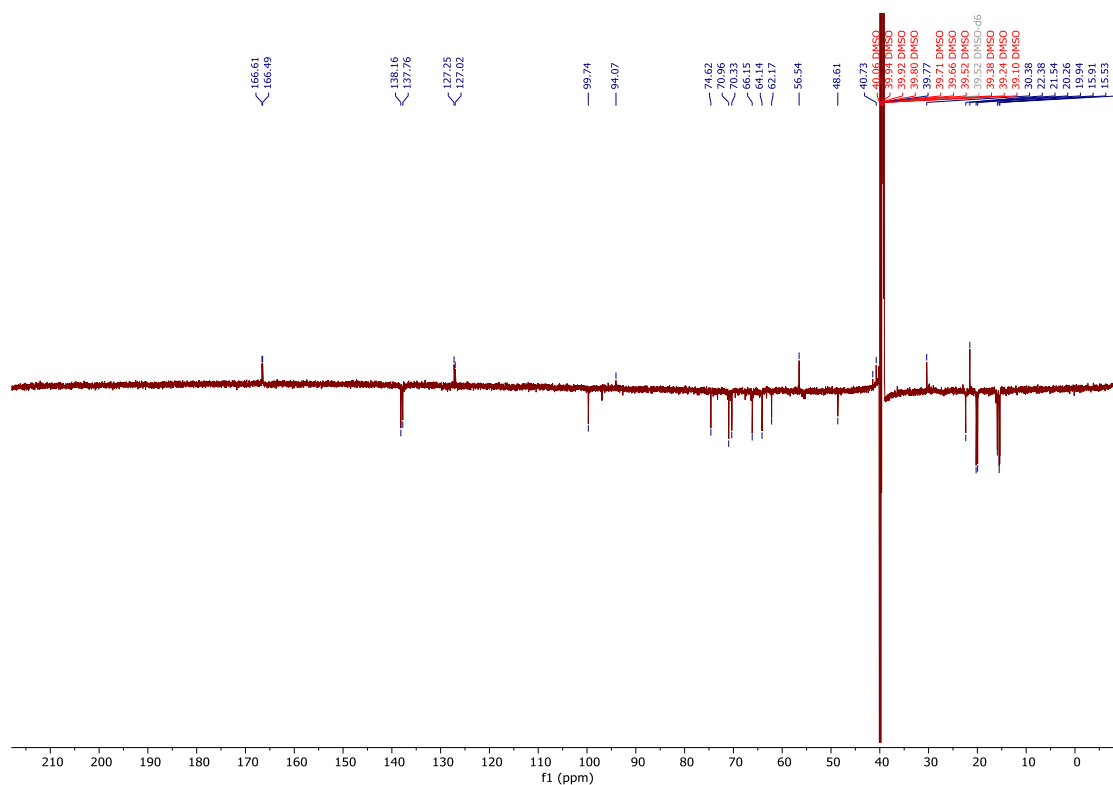


Fig. S114 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside C5 (**15**).

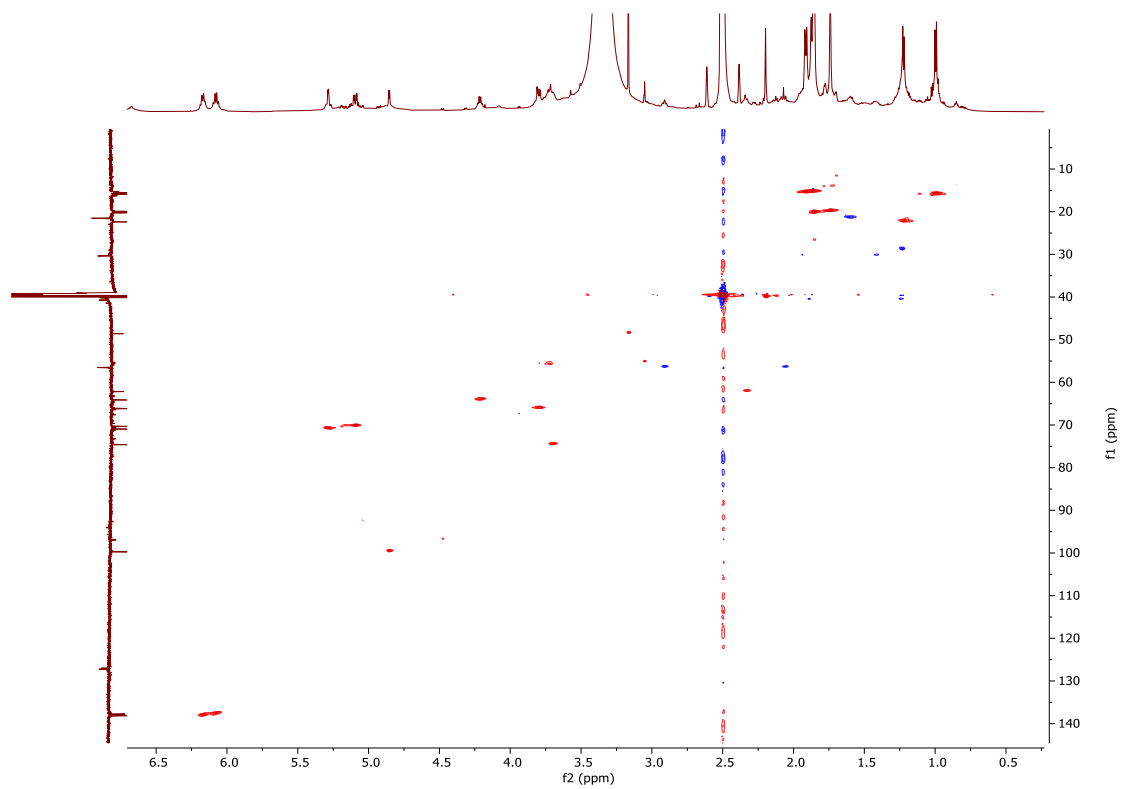


Fig. S115 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C5 (**15**).

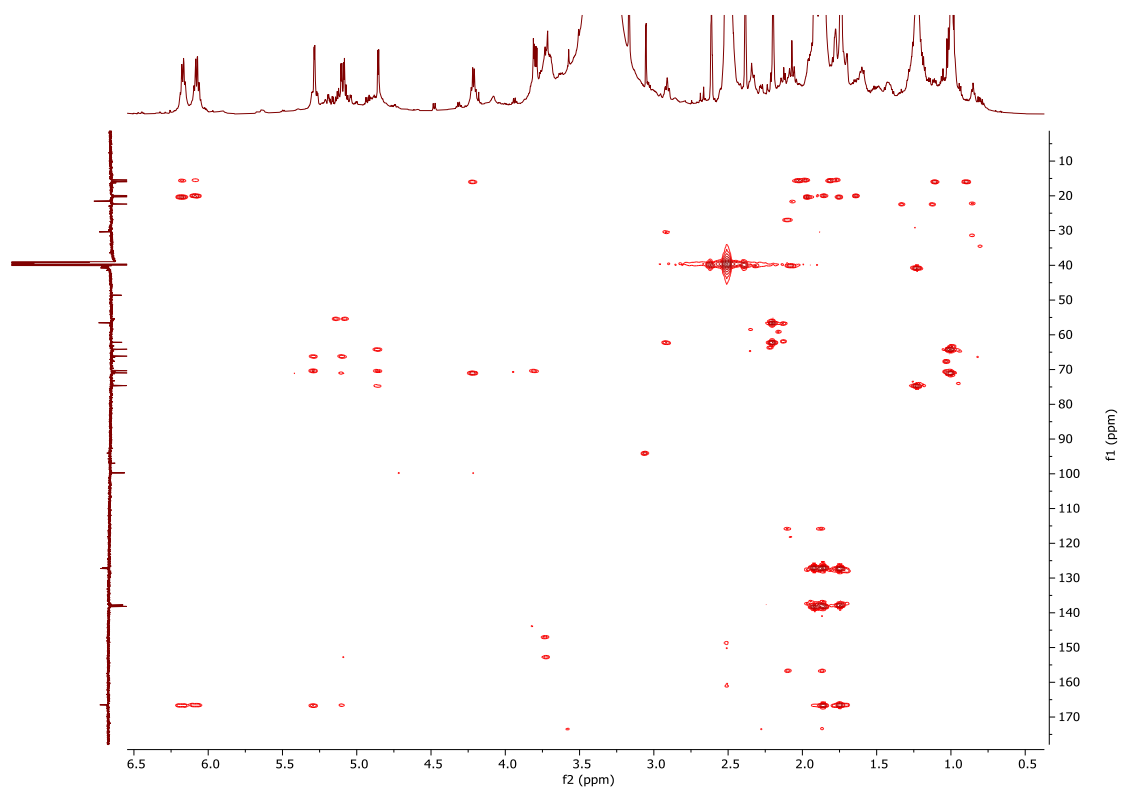


Fig. S116 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C5 (**15**).

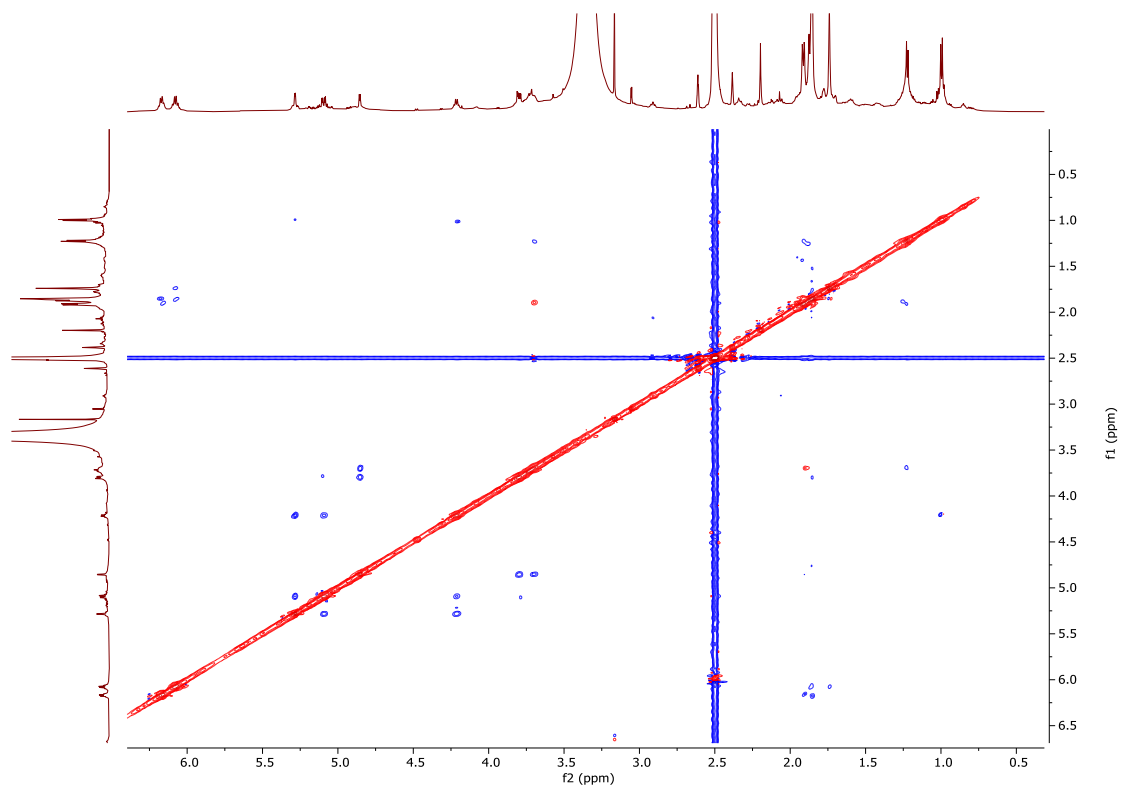


Fig. S117 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C5 (**15**).

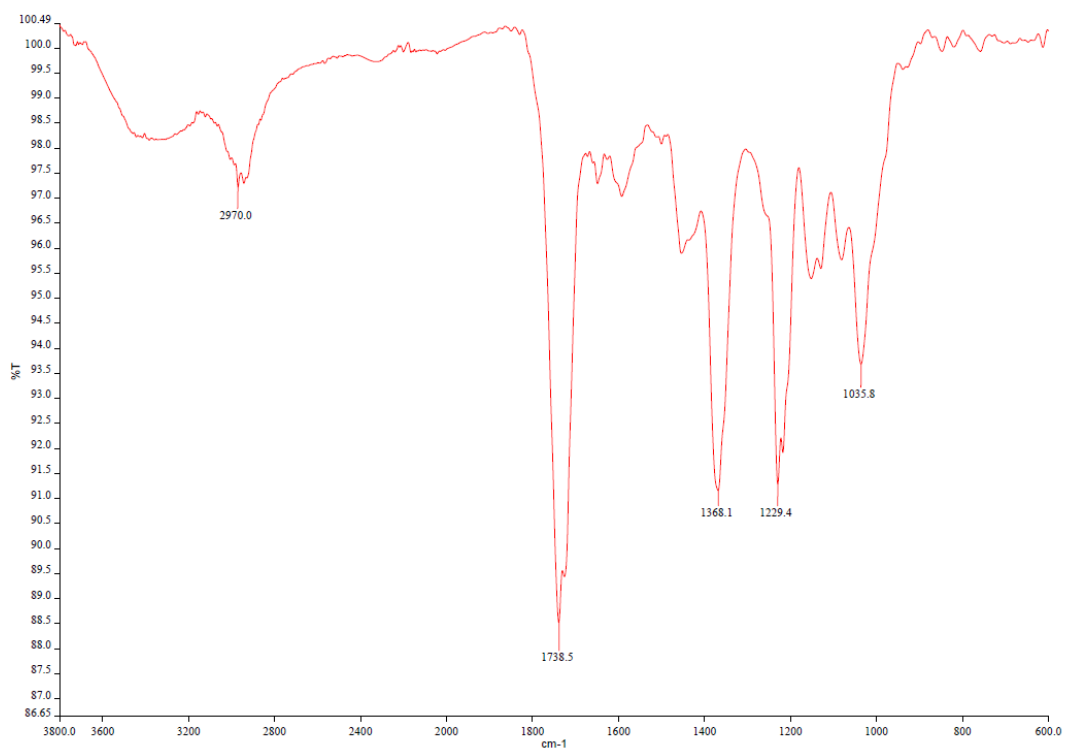


Fig. S118 IR spectrum of schizanthoside C6 (**16**).

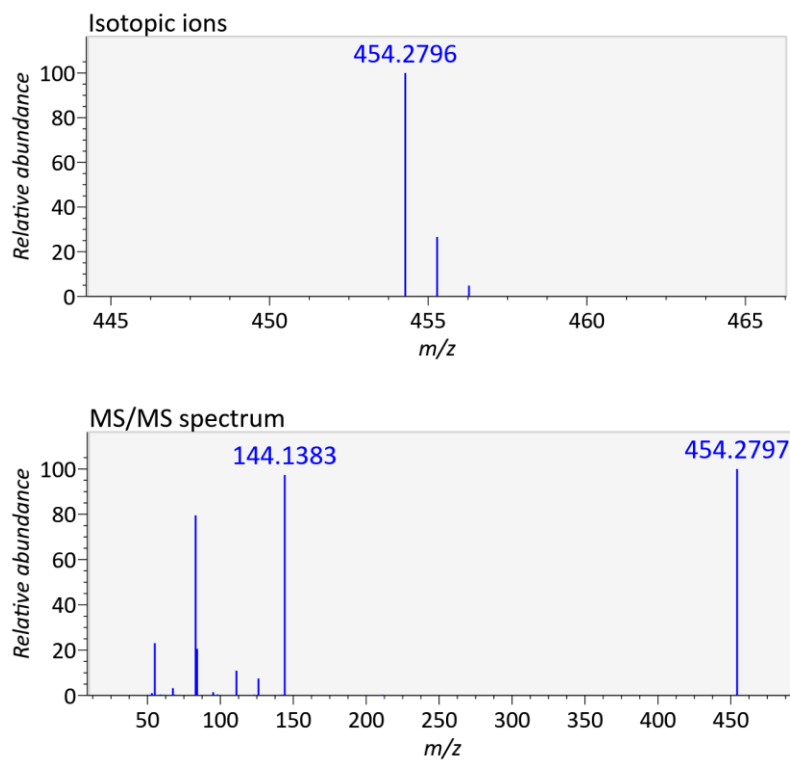


Fig. S119 HRESIMS and MS/MS spectra of schizanthoside C6 (**16**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

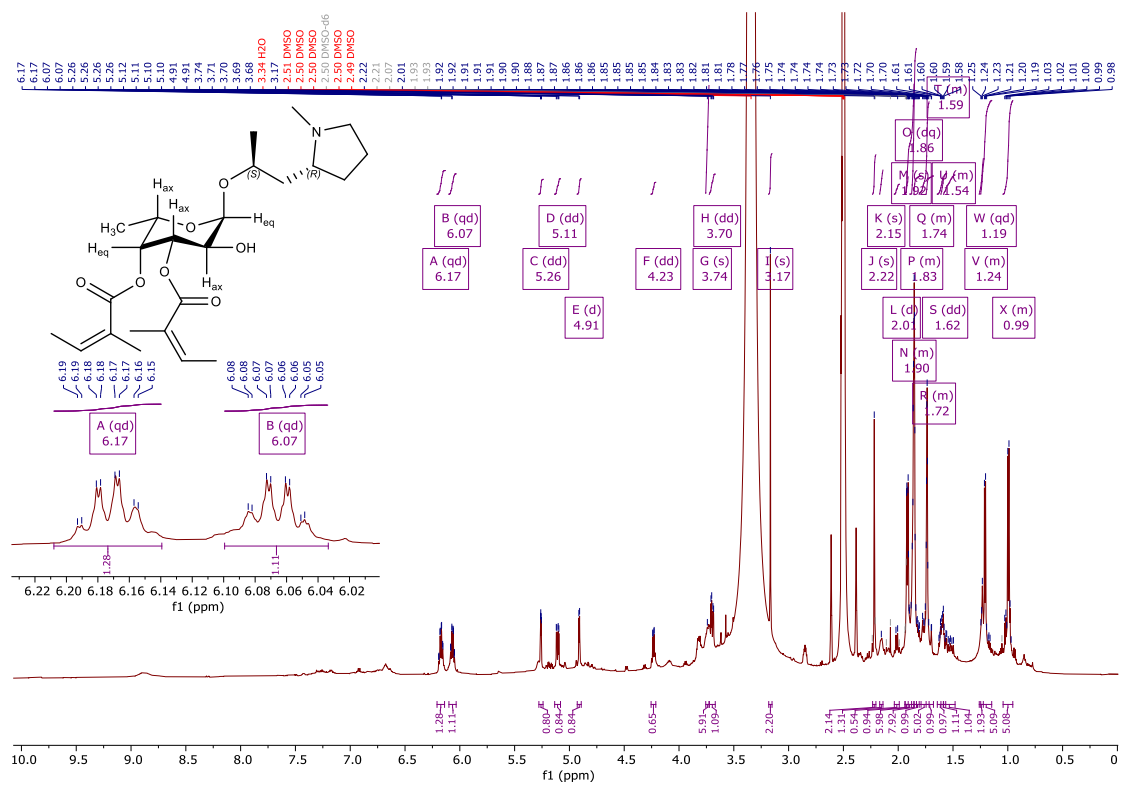


Fig. S120 ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C6 (**16**).

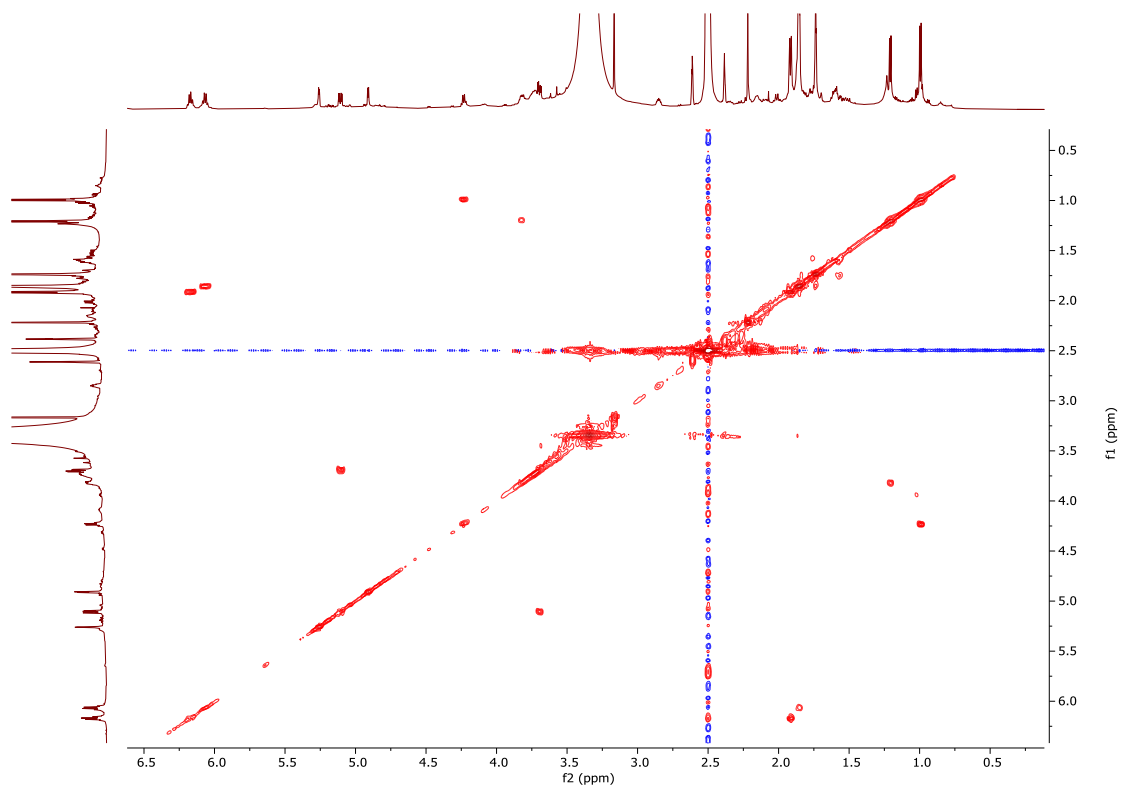


Fig. S121 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C6 (**16**).

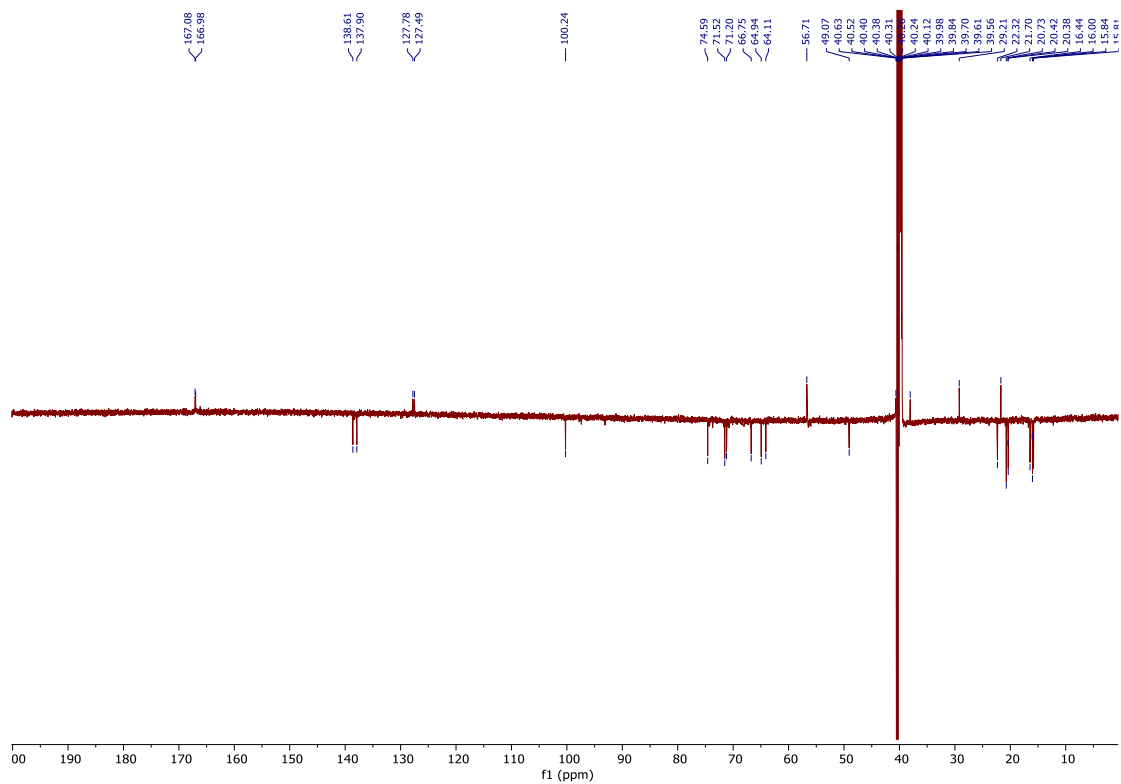


Fig. S122 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside C6 (**16**).

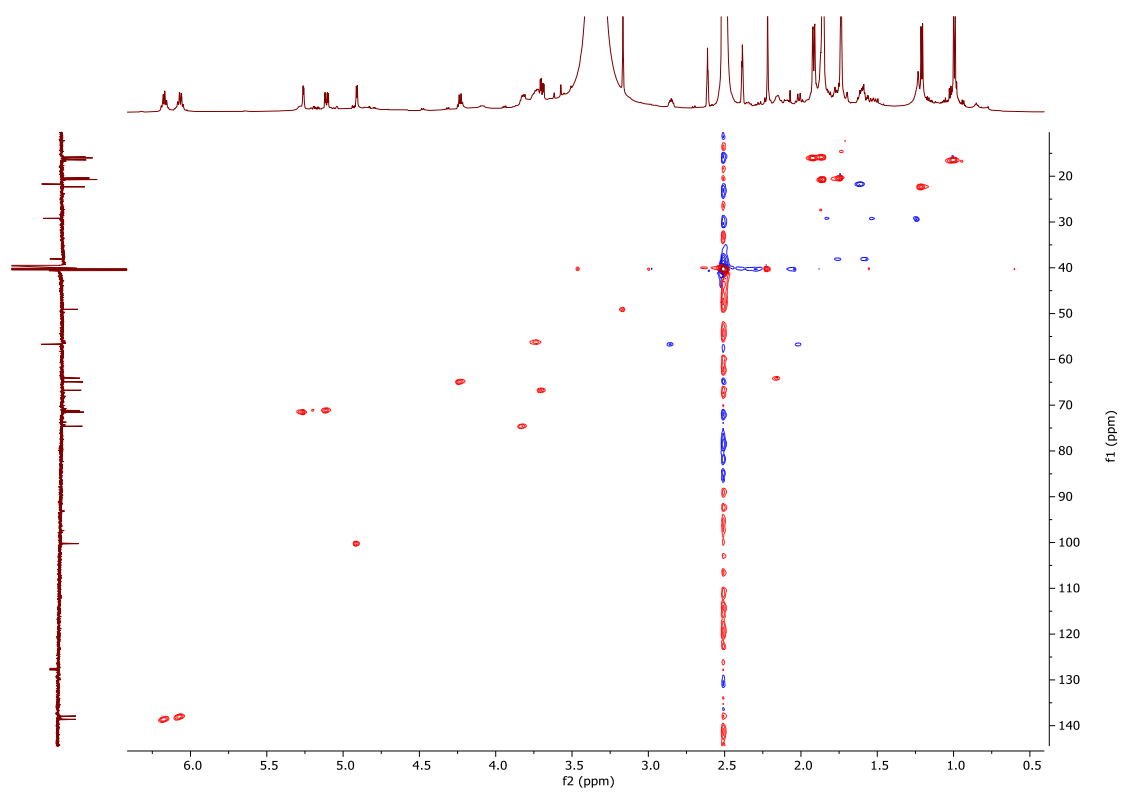


Fig. S123 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C6 (**16**).

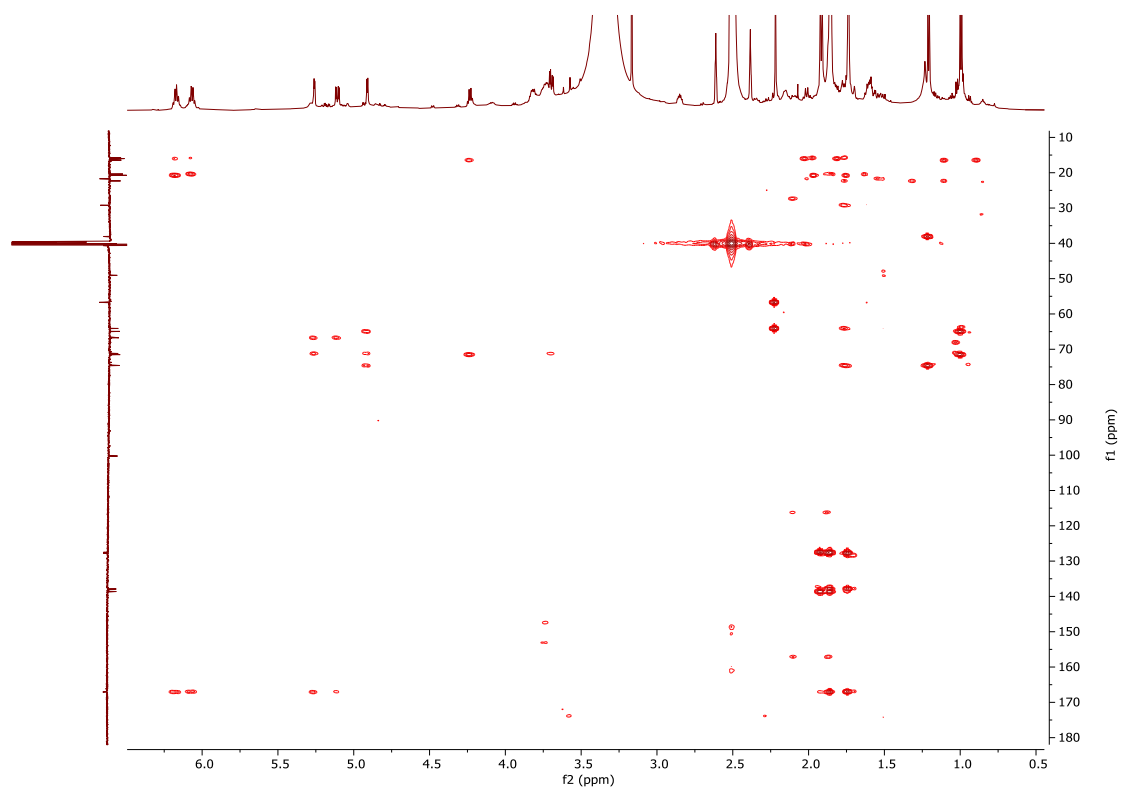


Fig. S124 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C6 (**16**).

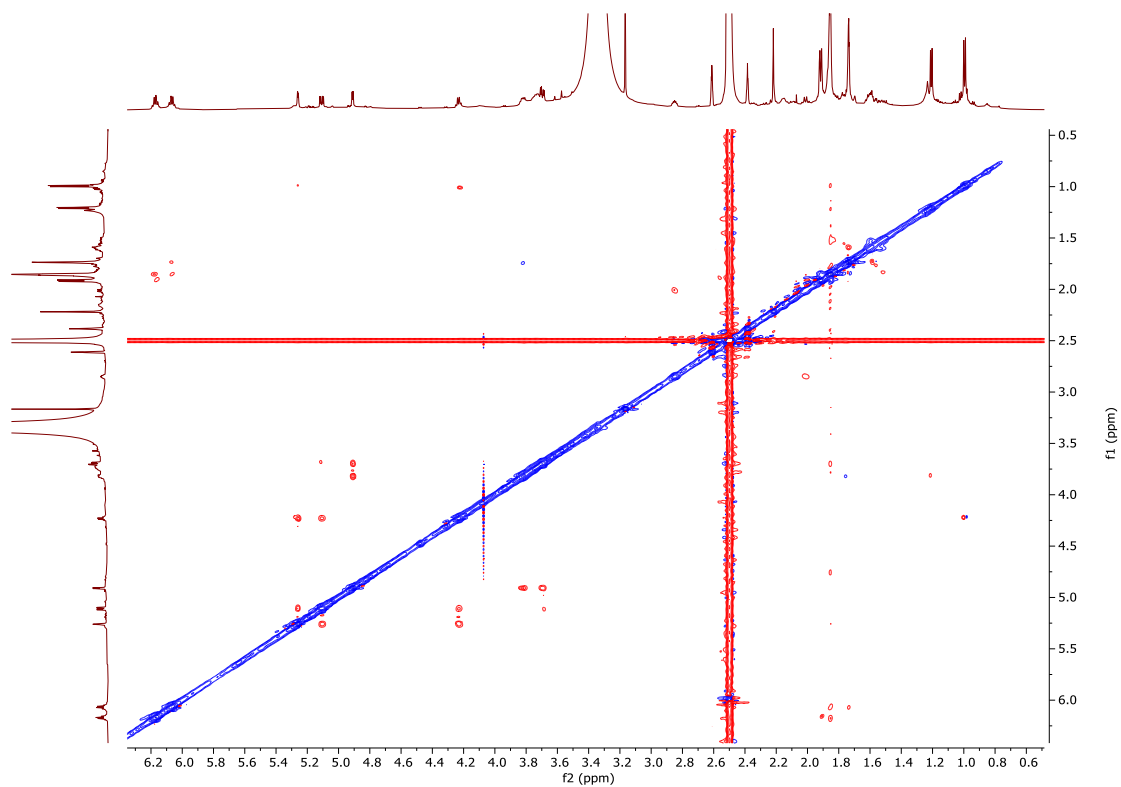


Fig. S125 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside C6 (**16**).

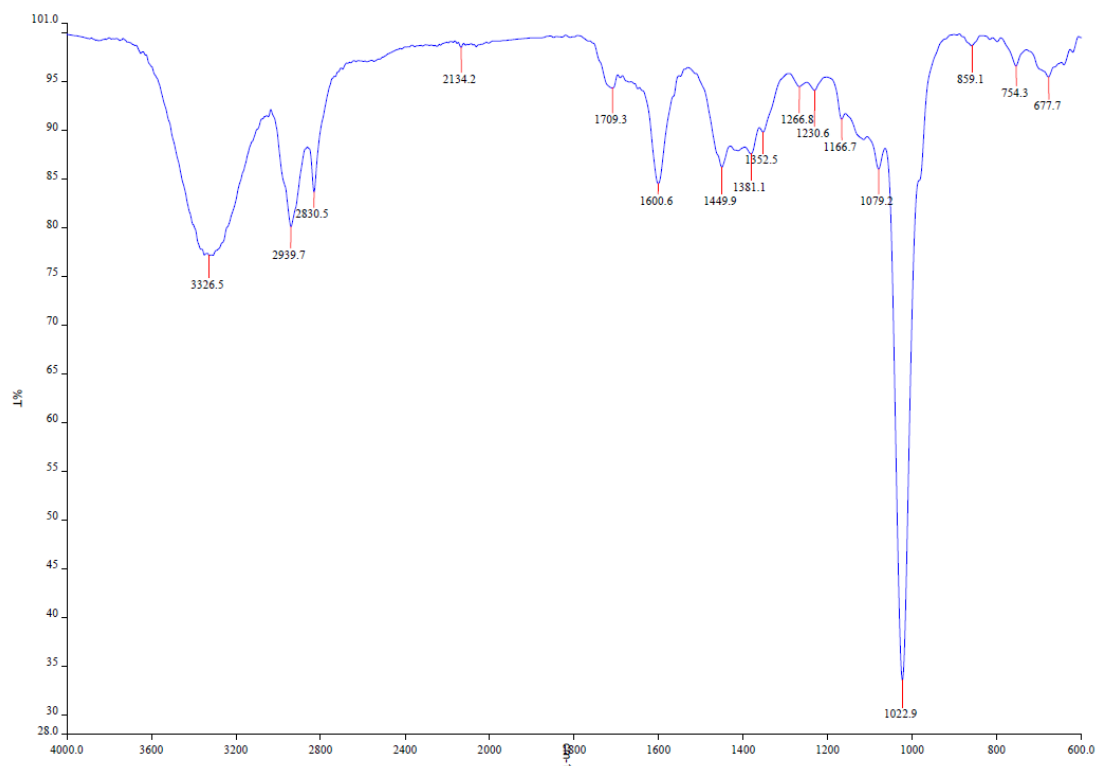


Fig. S126 IR spectrum of schizanthoside D1 (**17**).

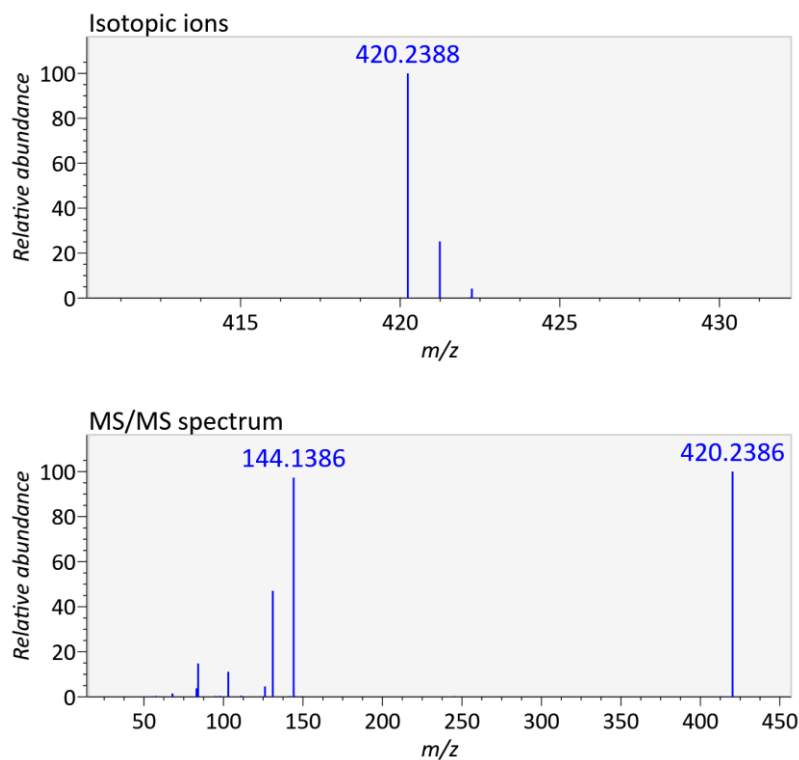


Fig. S127 HRESIMS and MS/MS spectra of schizanthoside D1 (**17**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

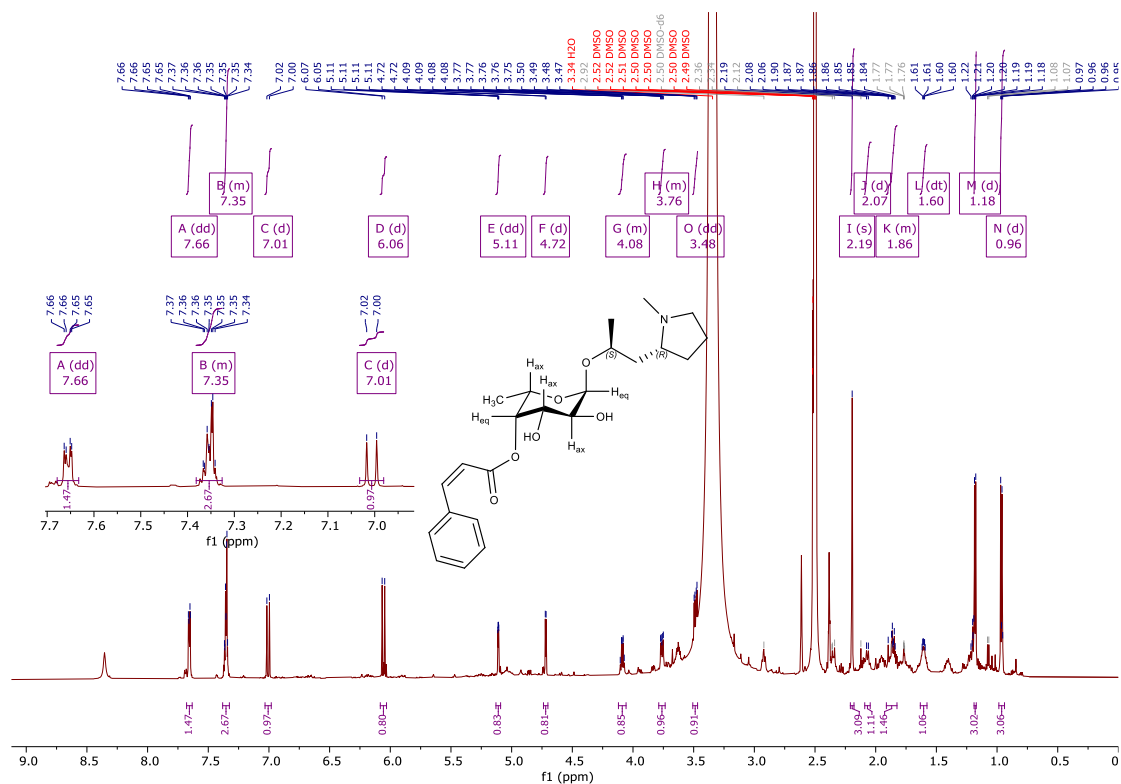


Fig. S128 ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of schizanthoside D1 (**17**).

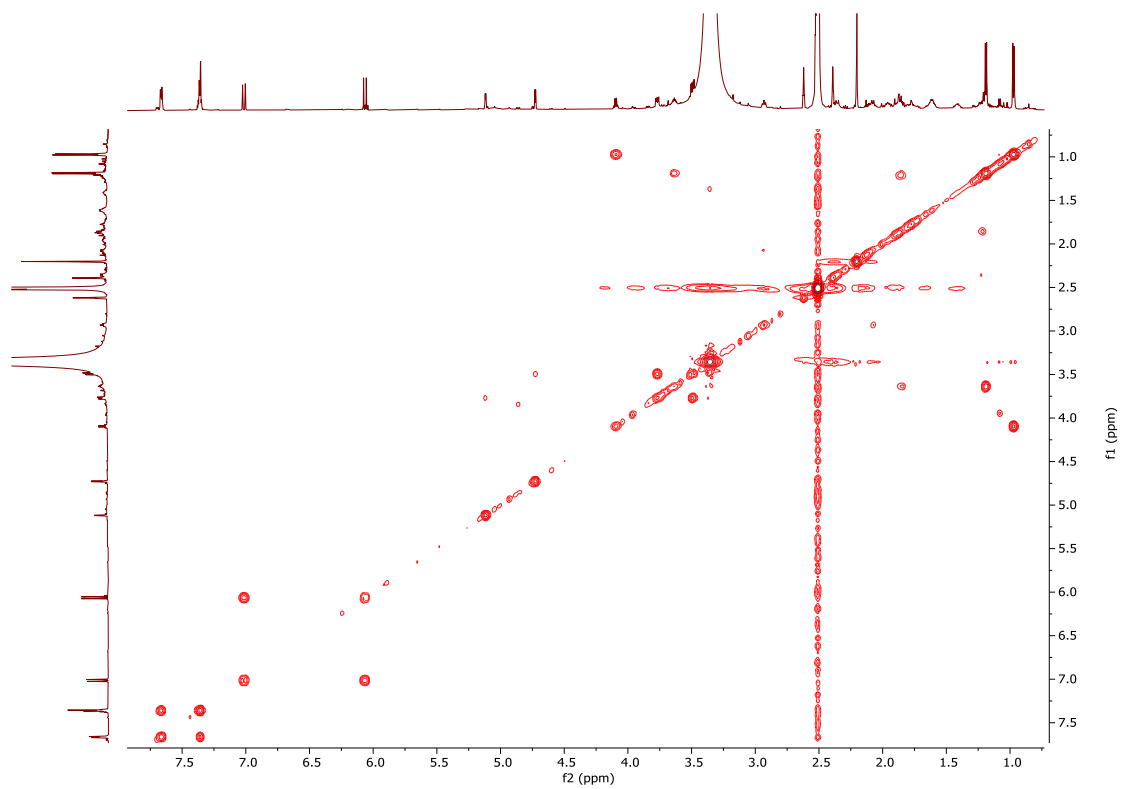


Fig. S129 COSY (600 MHz, DMSO- d_6) spectrum of schizanthoside D1 (**17**).

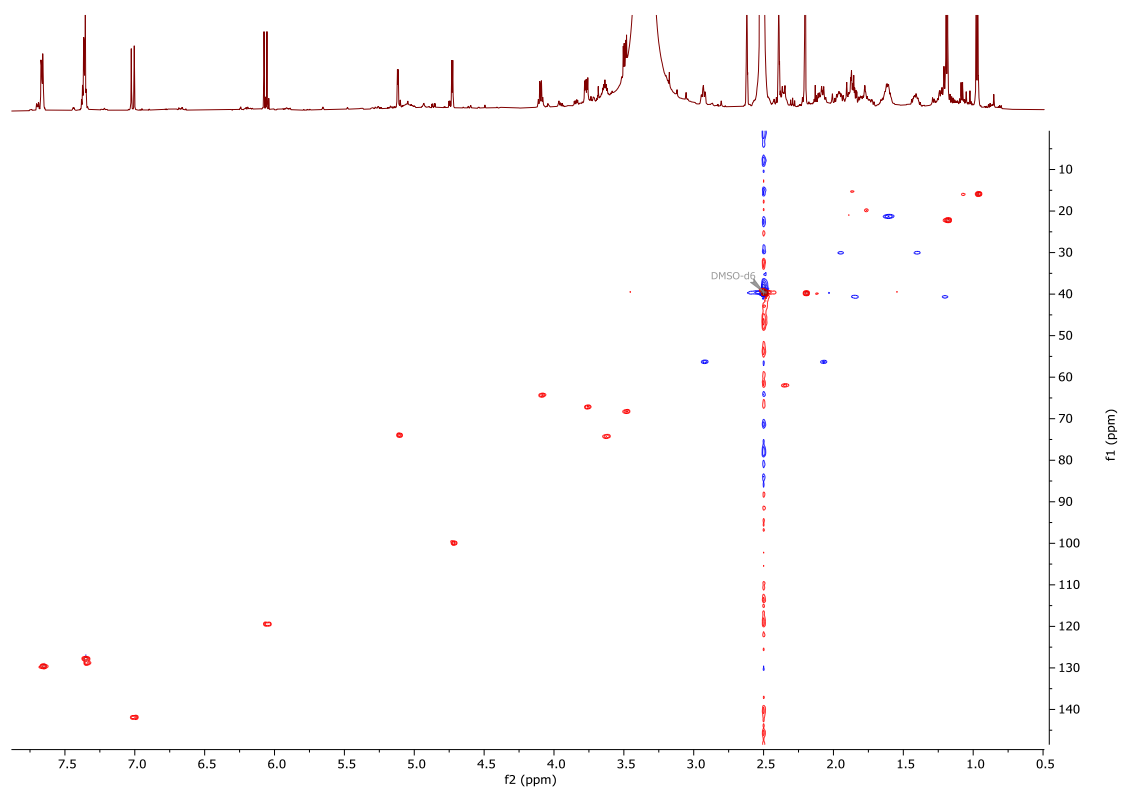


Fig. S130 HSQC (600 MHz, DMSO- d_6) spectrum of schizanthoside D1 (**17**).

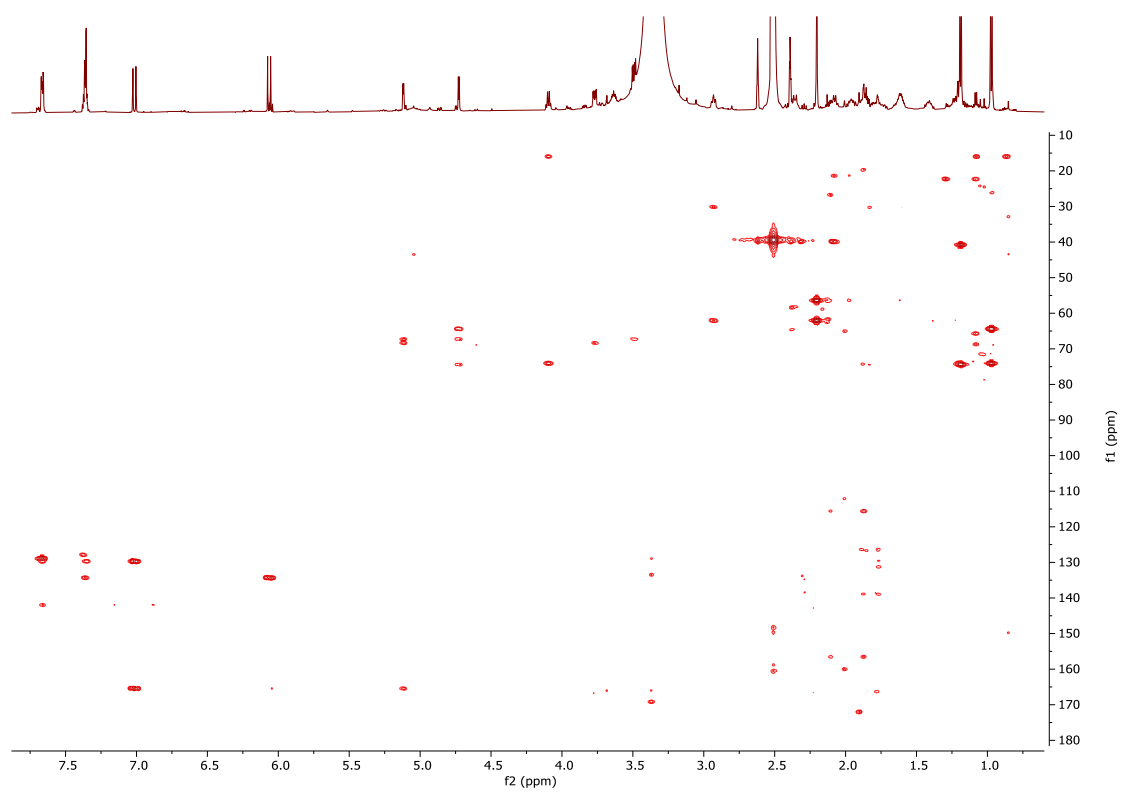


Fig. S131 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside D1 (**17**).

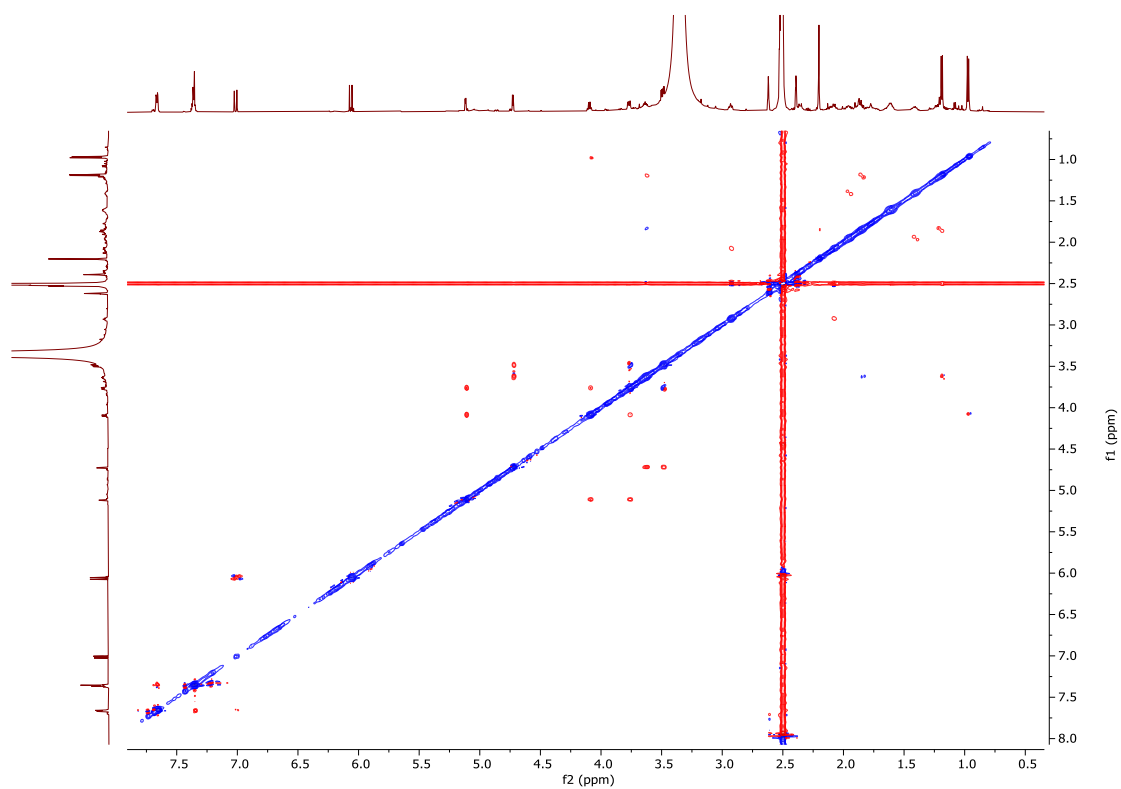


Fig. S132 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside D1 (**17**).

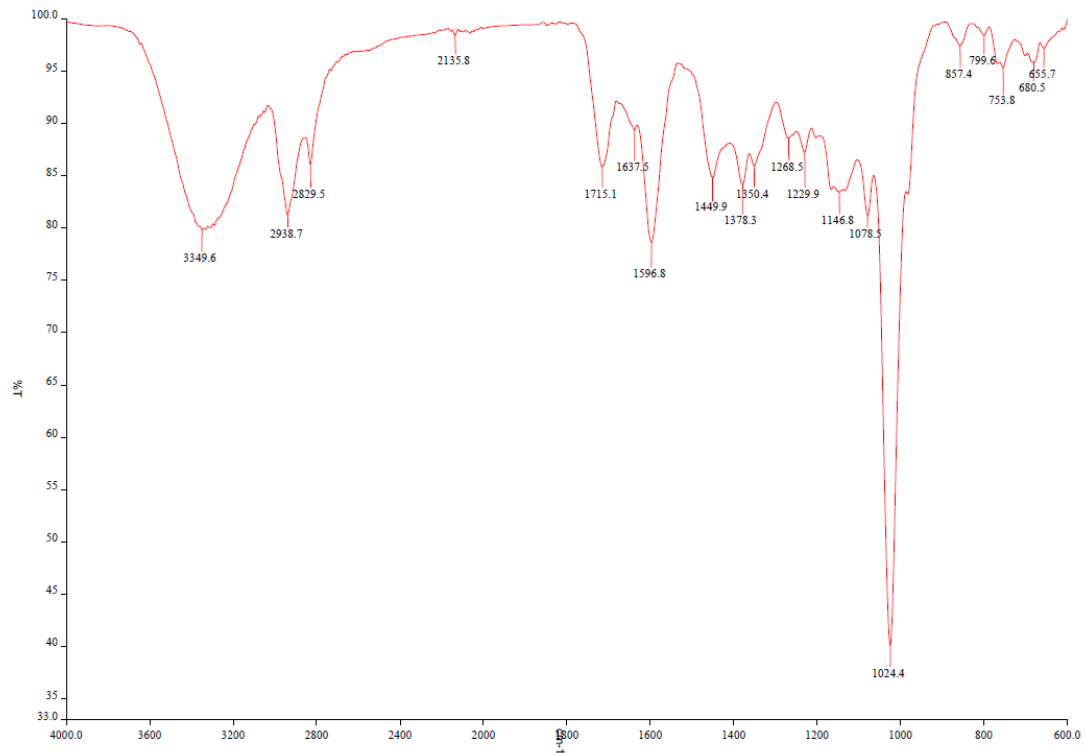


Fig. S133 IR spectrum of schizanthoside D2 (**18**).

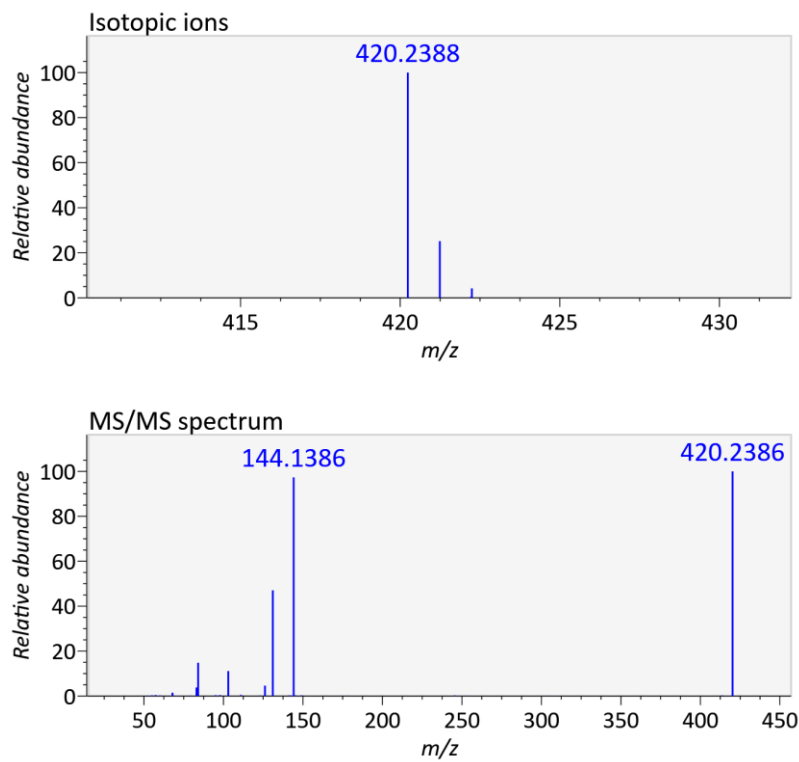


Fig. S134 HRESIMS and MS/MS spectra of schizanthoside D2 (**18**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

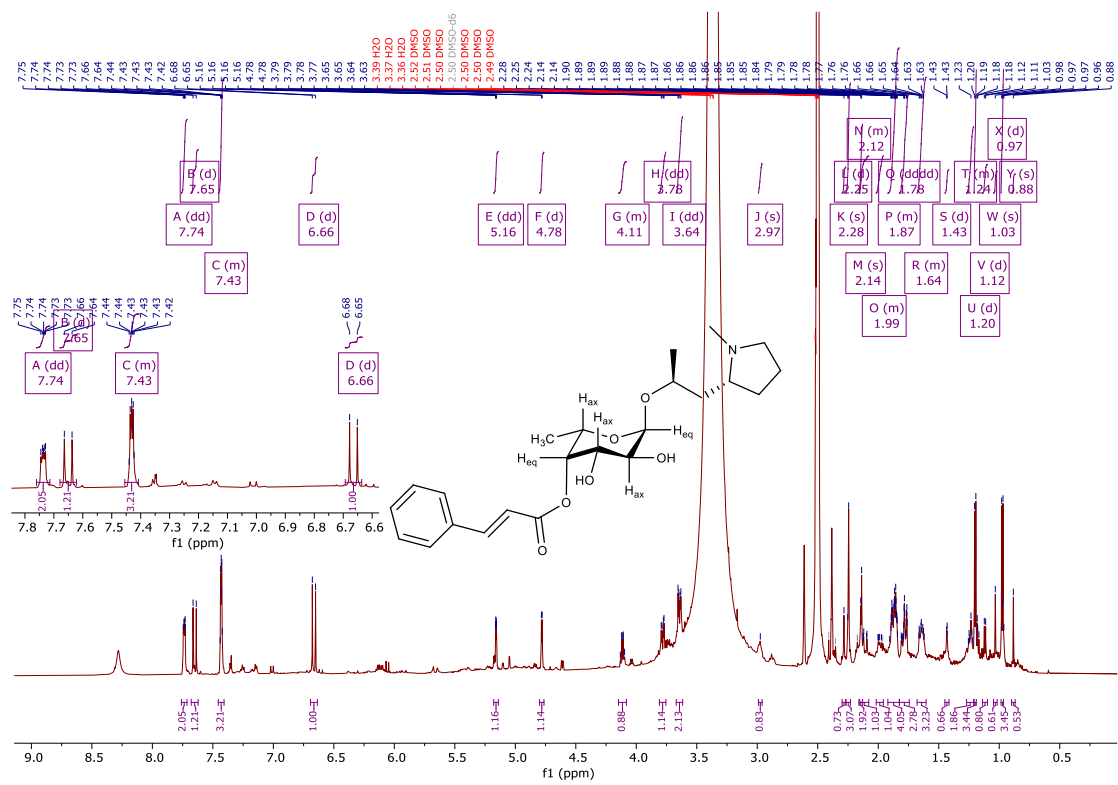


Fig. S135 ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of schizanthoside D2 (18).

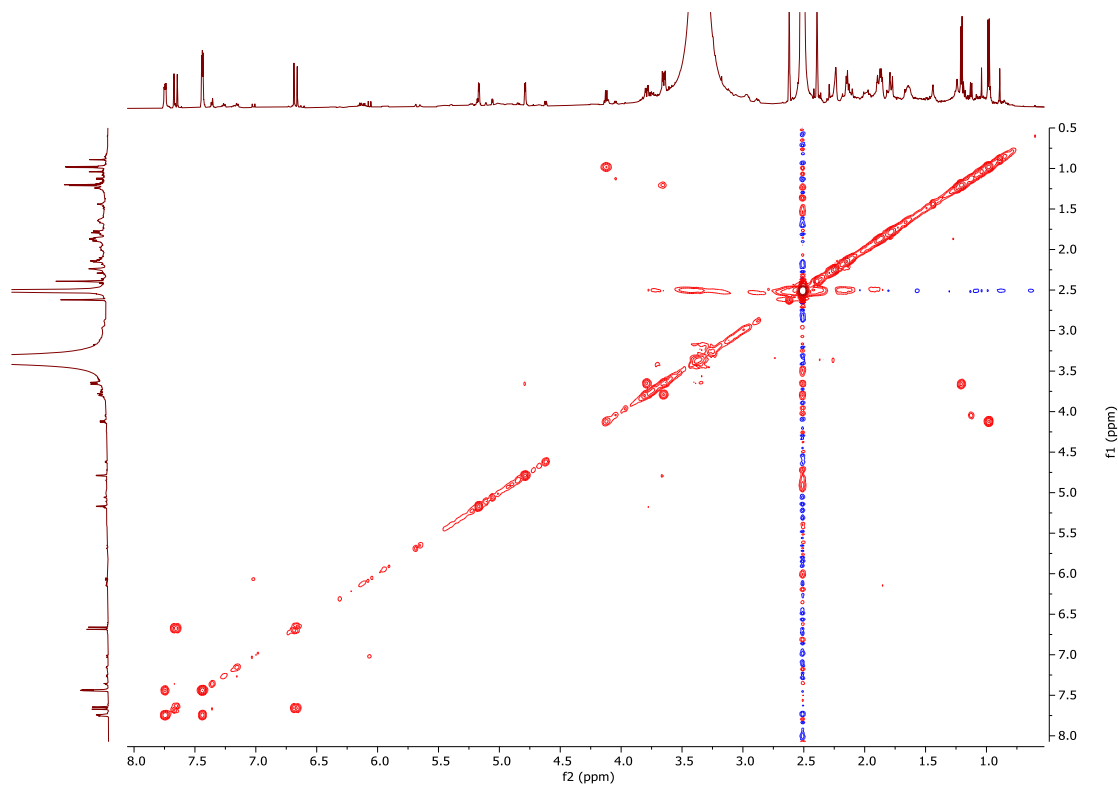


Fig. S136 COSY (600 MHz, $\text{DMSO-}d_6$) spectrum of schizanthoside D2 (18).

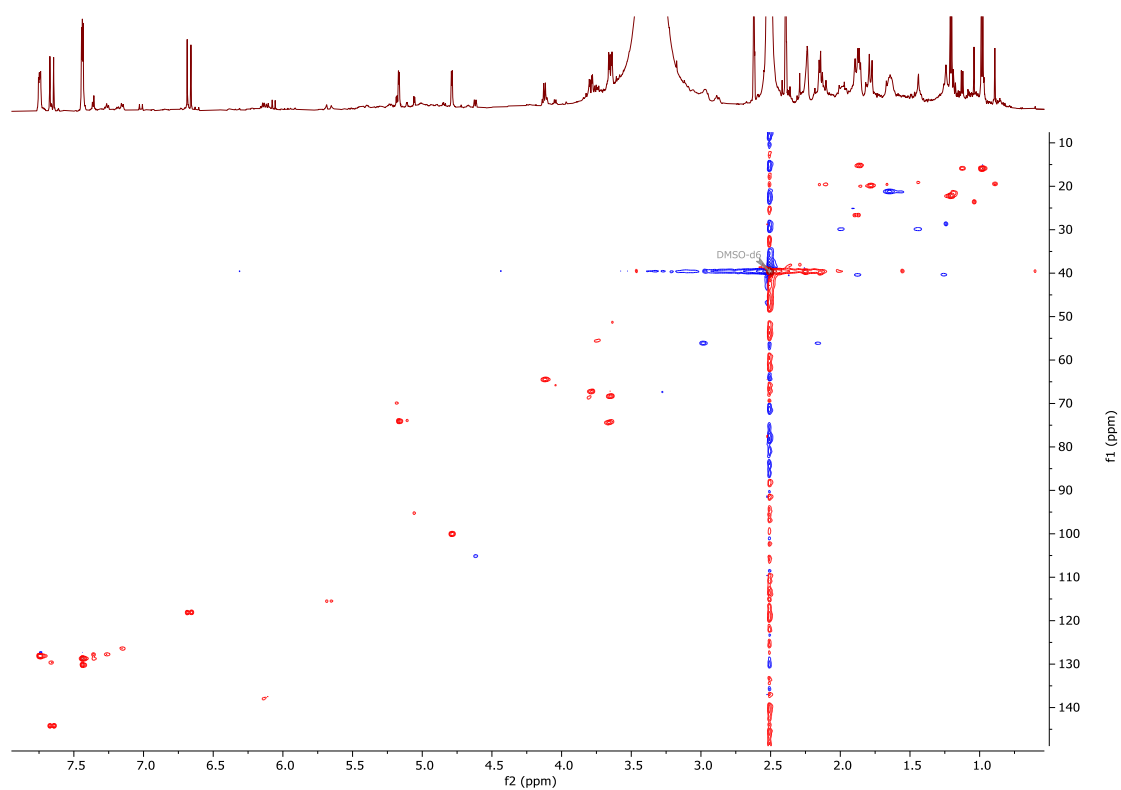


Fig. S137 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside D2 (**18**).

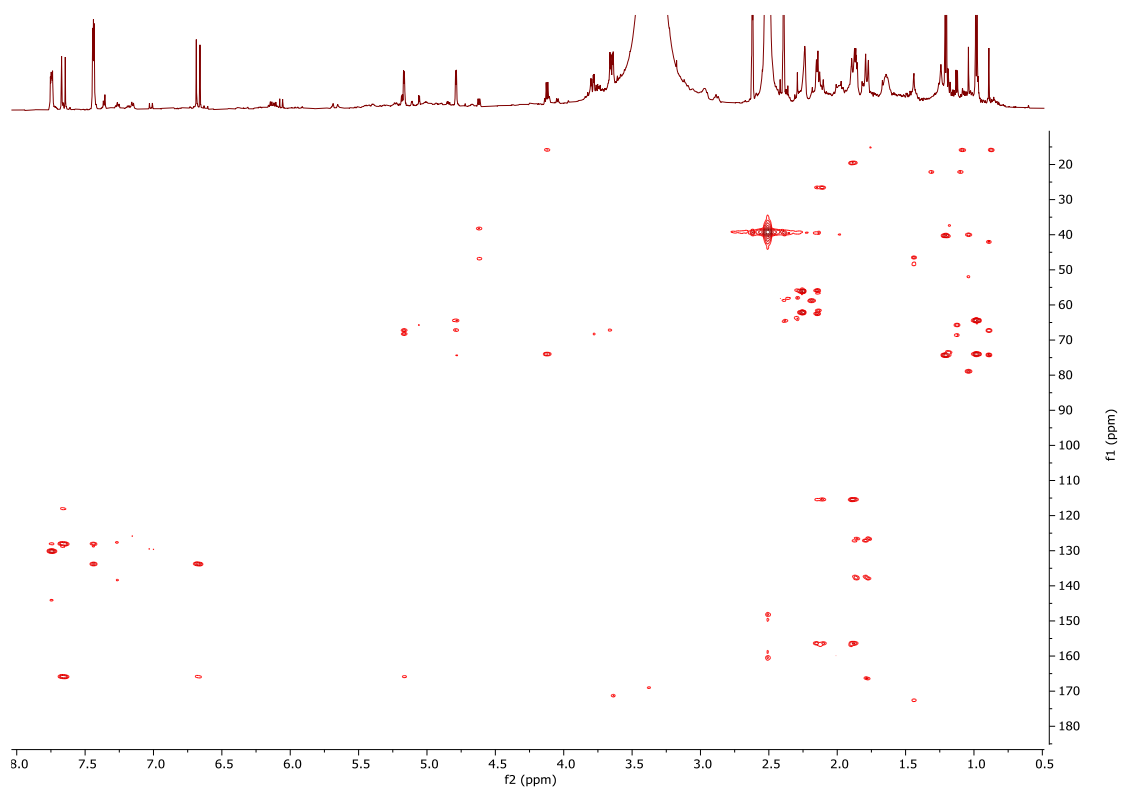


Fig. S138 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside D2 (**18**).

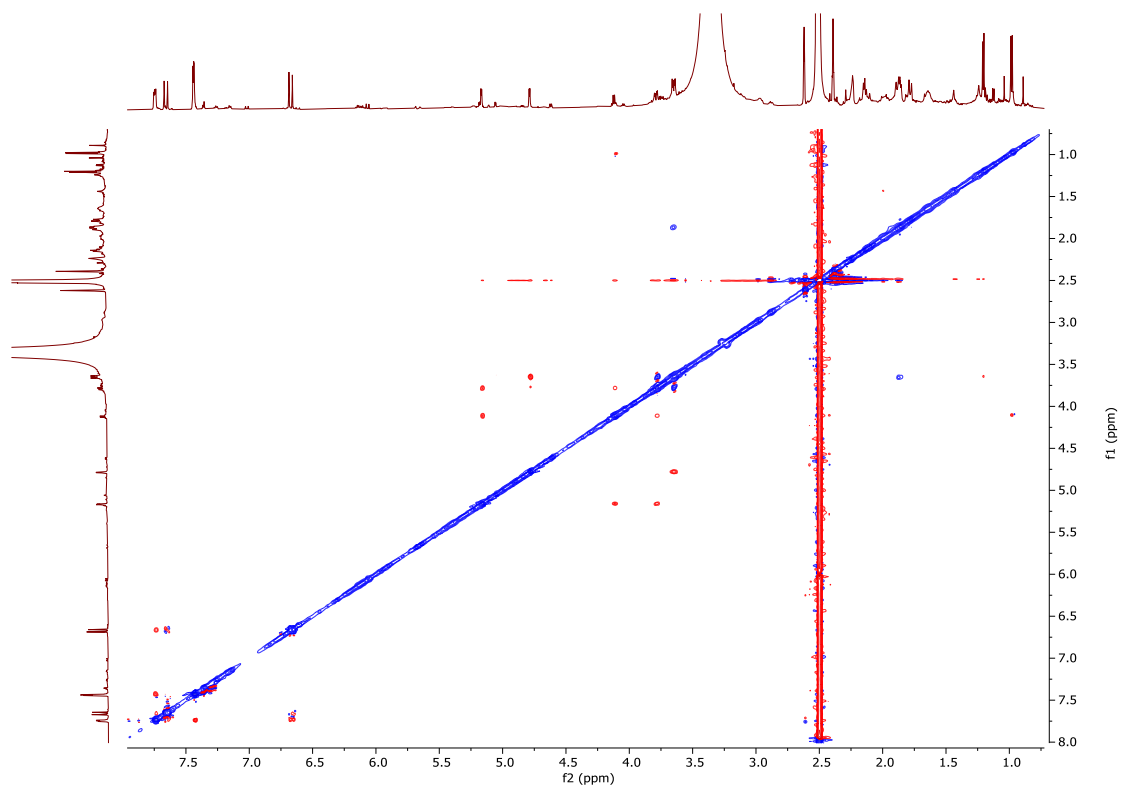


Fig. S139 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside D2 (**18**).

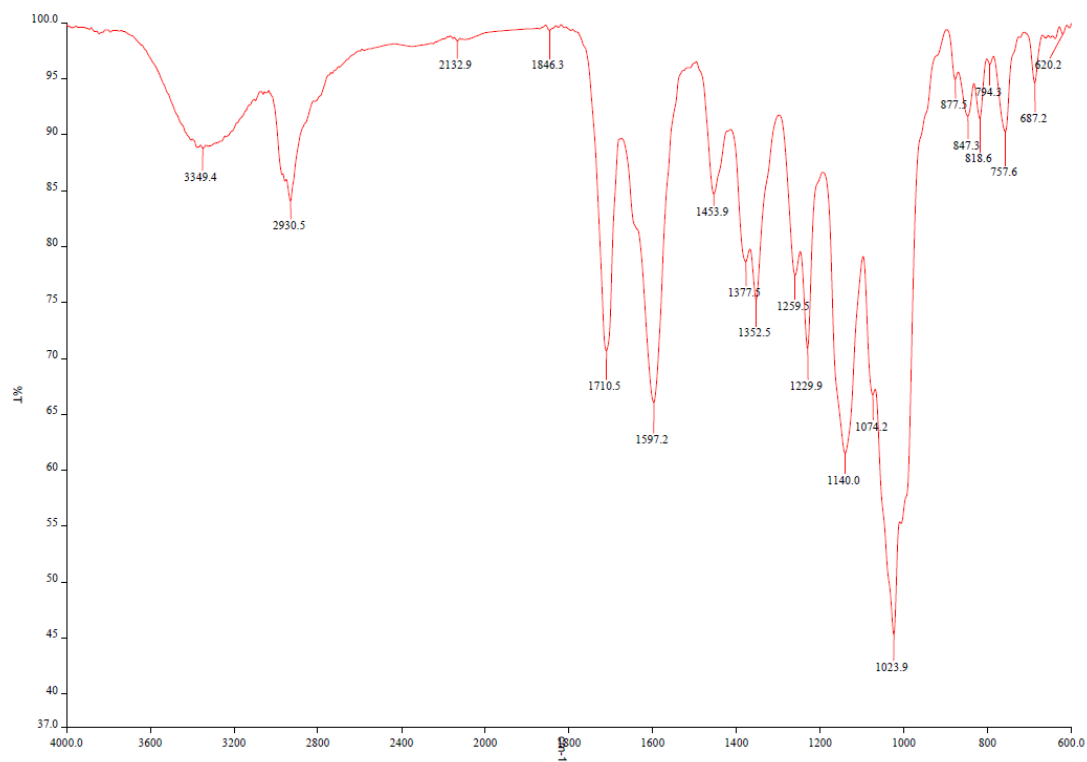


Fig. S140 IR spectrum of schizanthoside E1 (**19**).

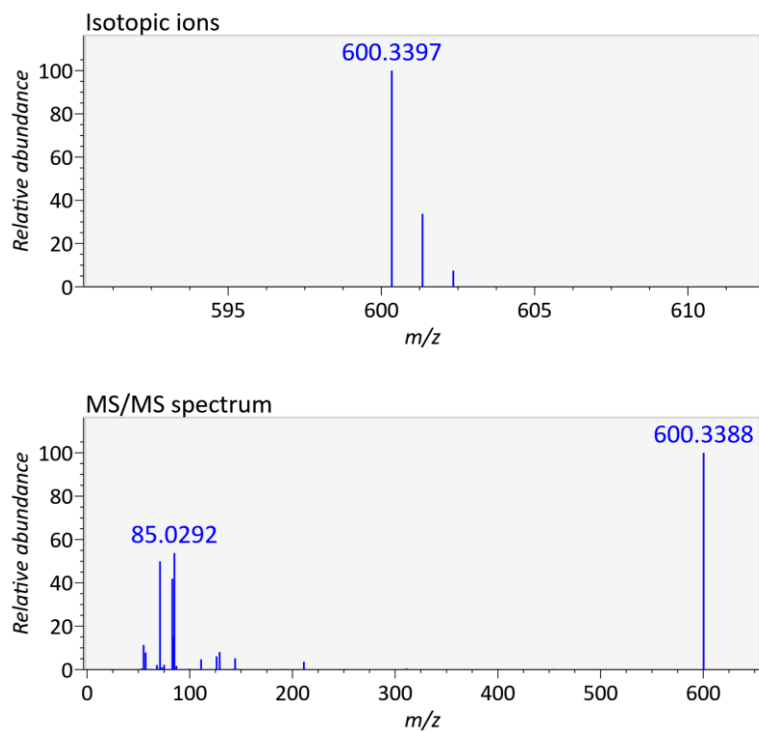


Fig. S141 HRESIMS and MS/MS spectra of schizanthoside E1 (**19**) (Q Exactive Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

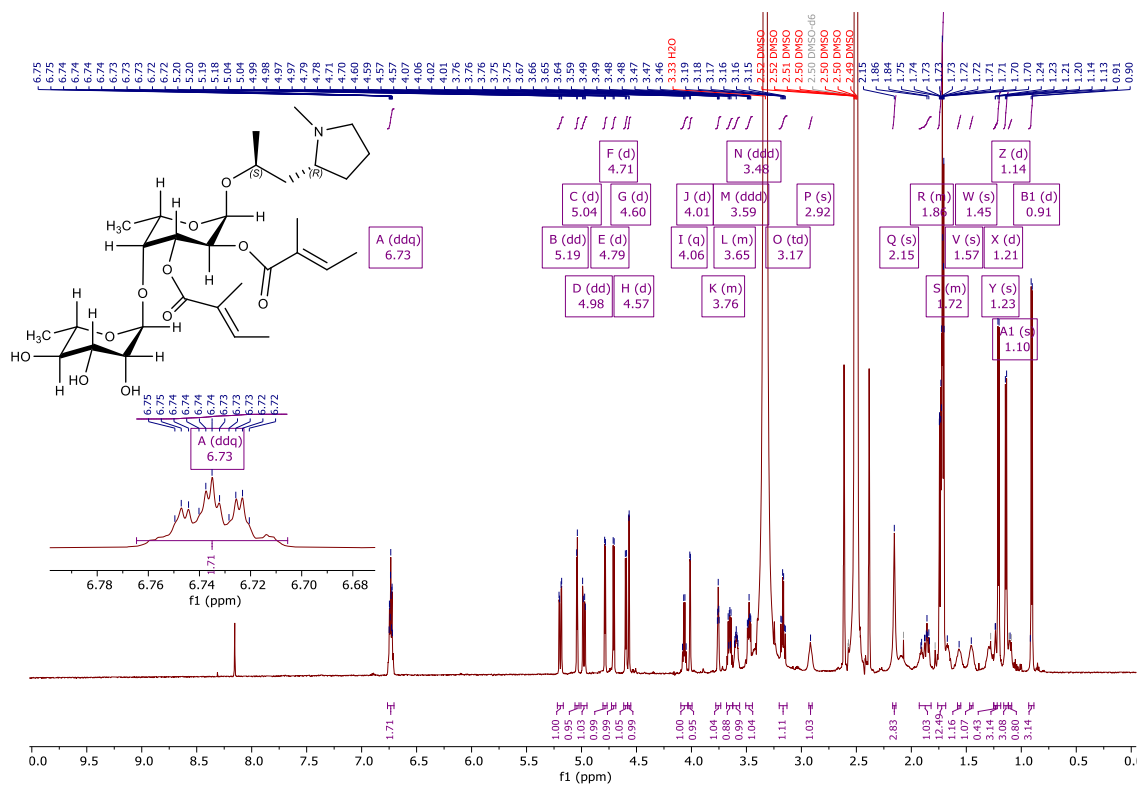


Fig. S142 ¹H NMR (600 MHz, DMSO-d₆) spectrum of schizanthoside E1 (**19**).

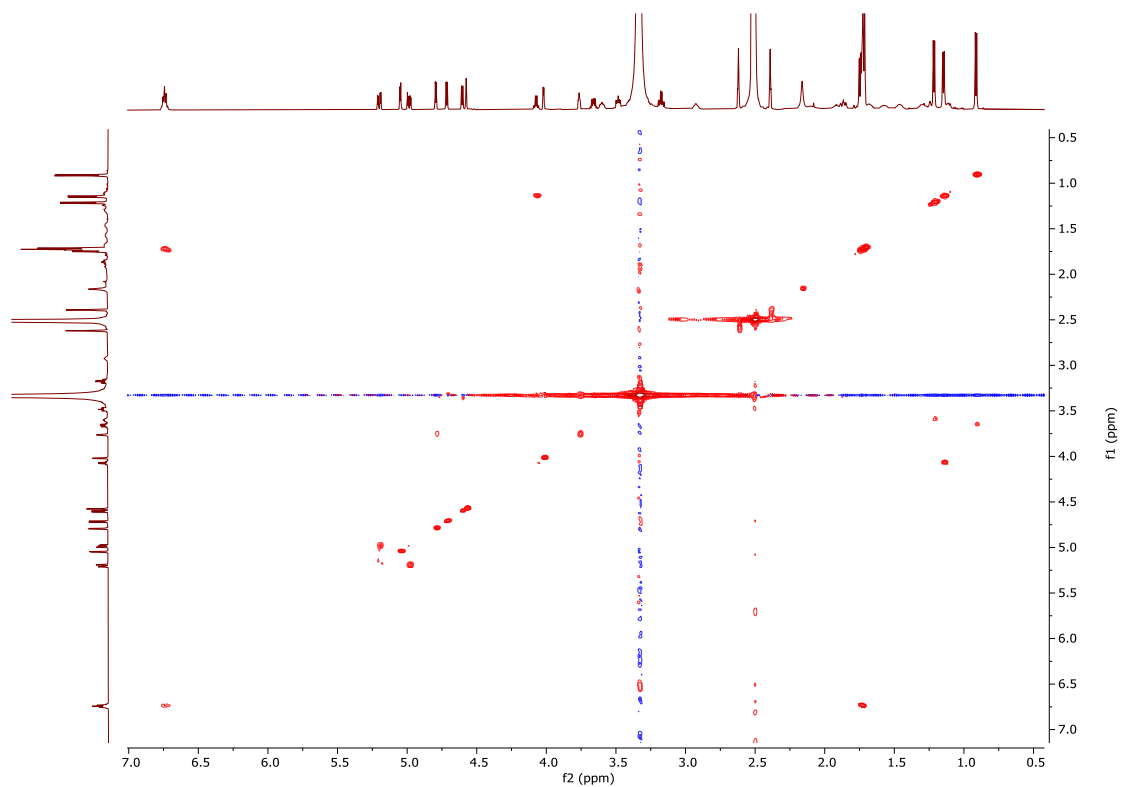


Fig. S143 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside E1 (**19**).

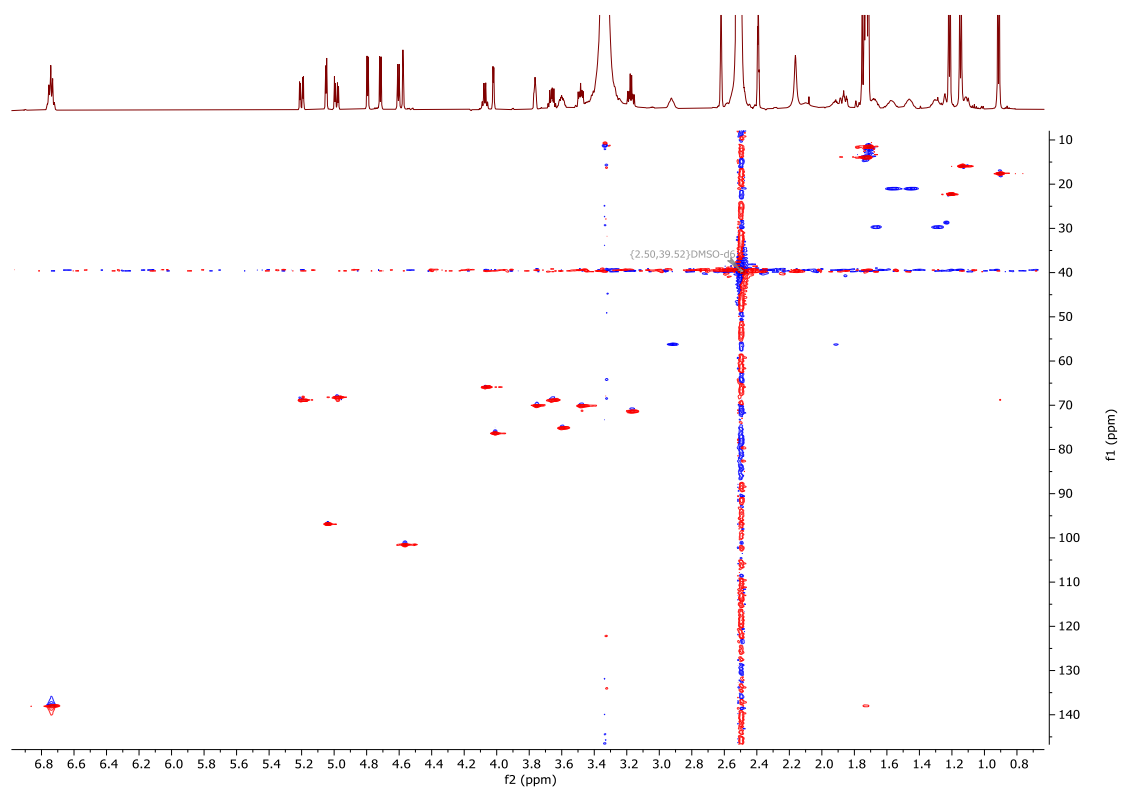


Fig. S144 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside E1 (**19**).

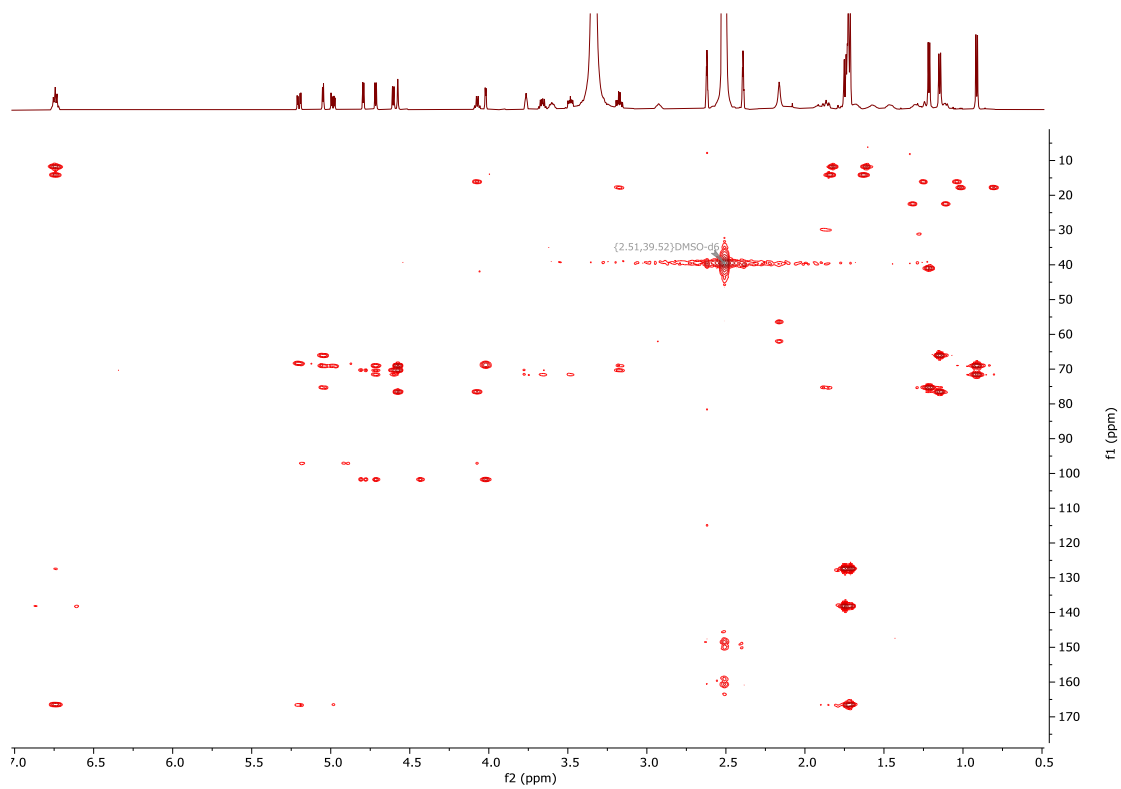


Fig. S145 HMBC (600 MHz, DMSO- d_6) spectrum of schizanthoside E1 (**19**).

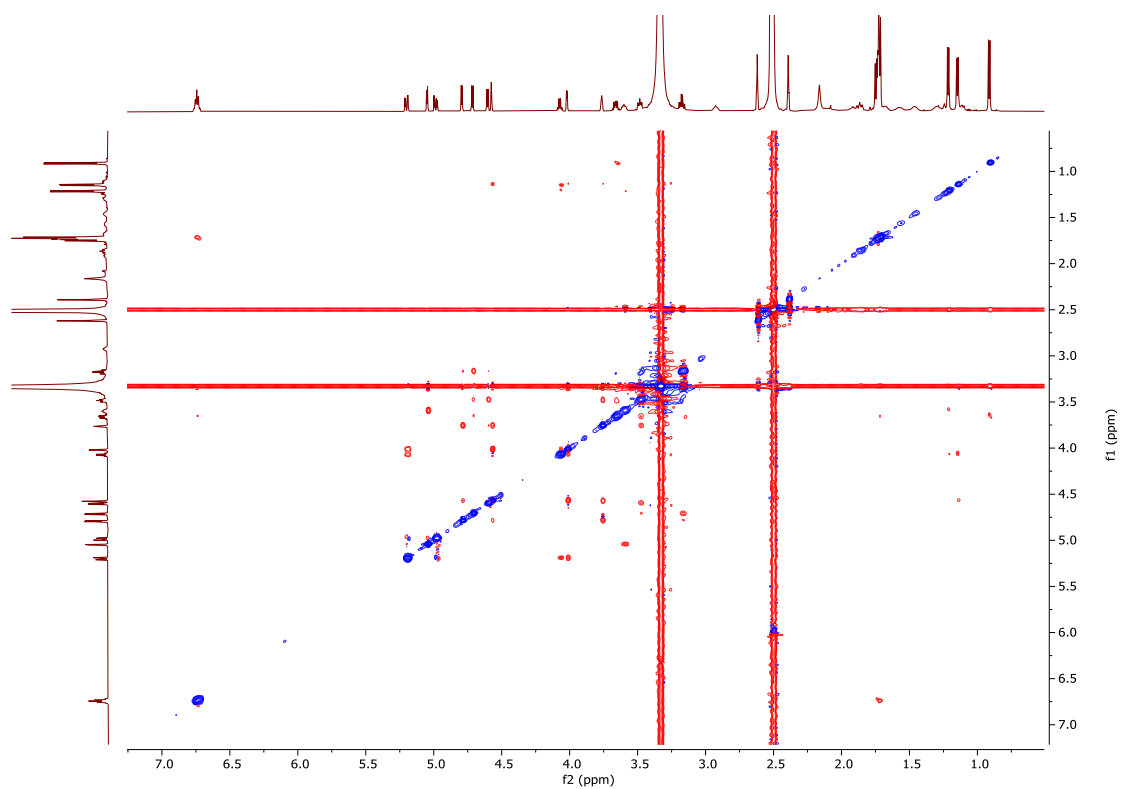


Fig. S146 ROESY (600 MHz, DMSO- d_6) spectrum of schizanthoside E1 (**19**).

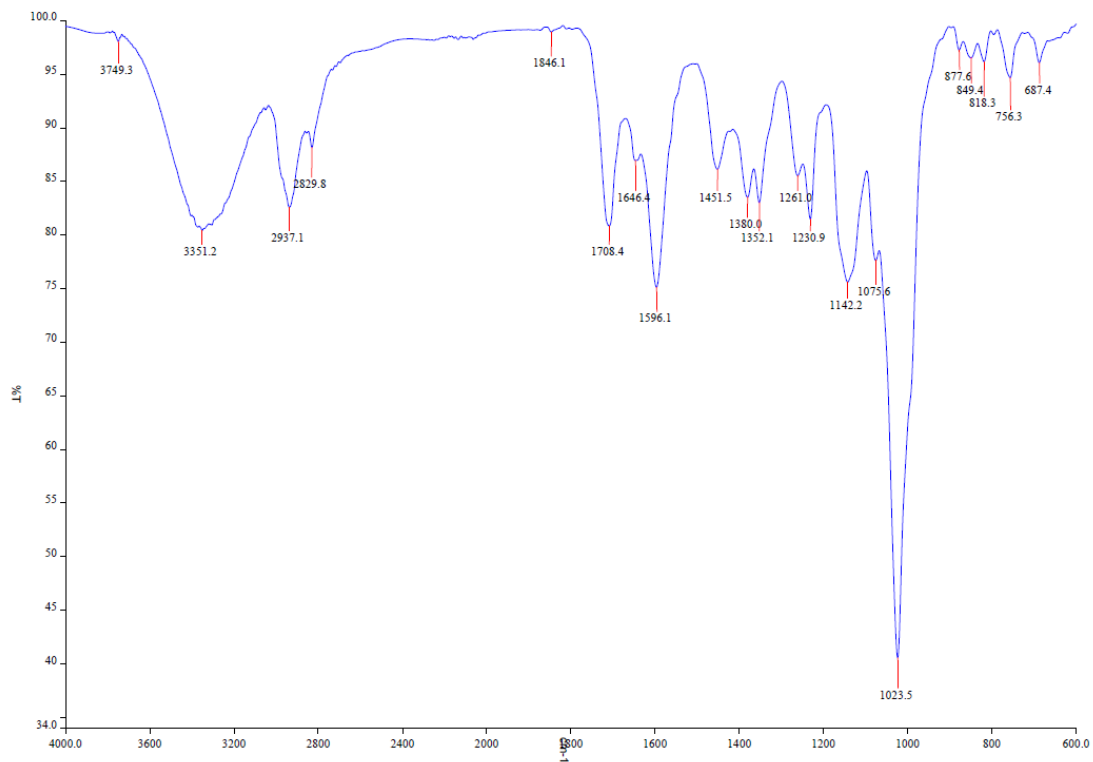


Fig. S147 IR spectrum of schizanthoside E2 (**20**).

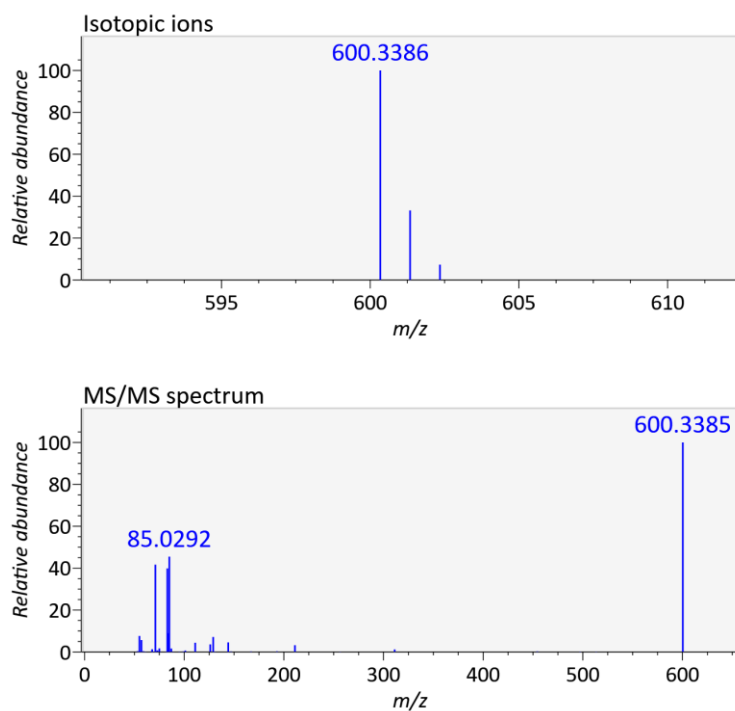


Fig. S148 HRESIMS and MS/MS spectra of schizanthoside E2 (**20**) (Q Exact Focus Hybrid quadrupole-orbitrap mass spectrometer, positive mode).

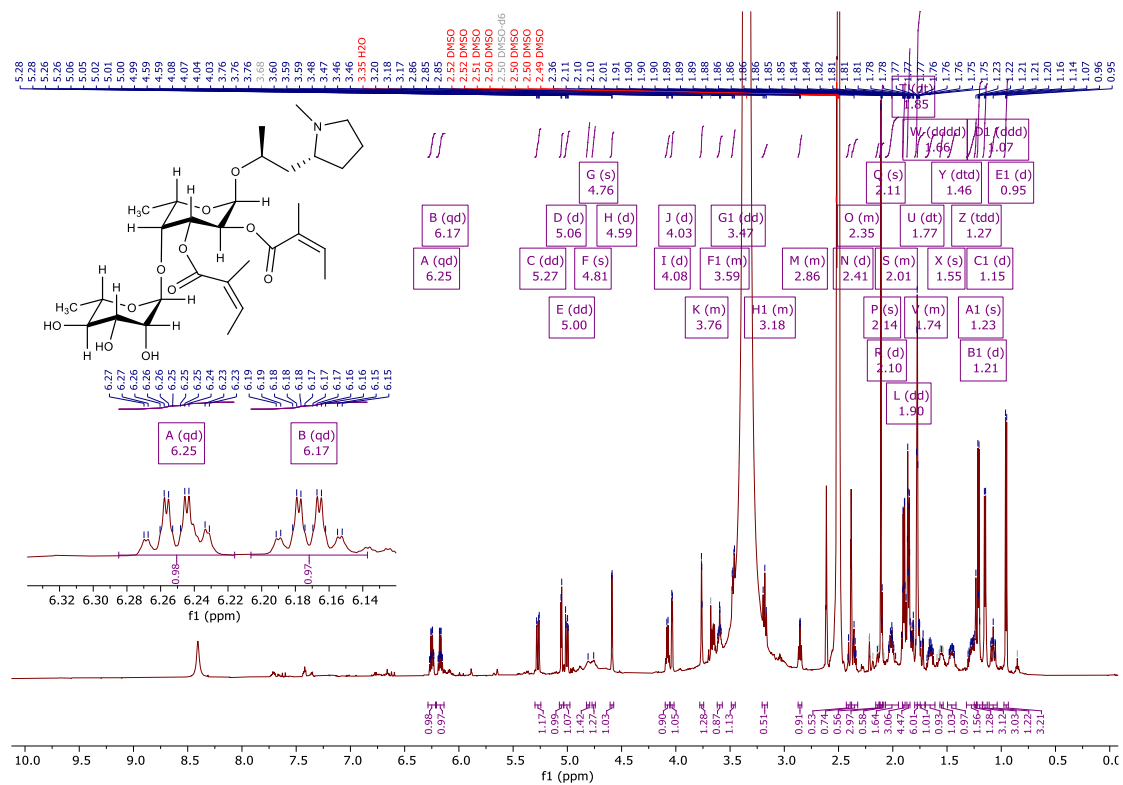


Fig. S149 ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of schizanthoside E2 (20).

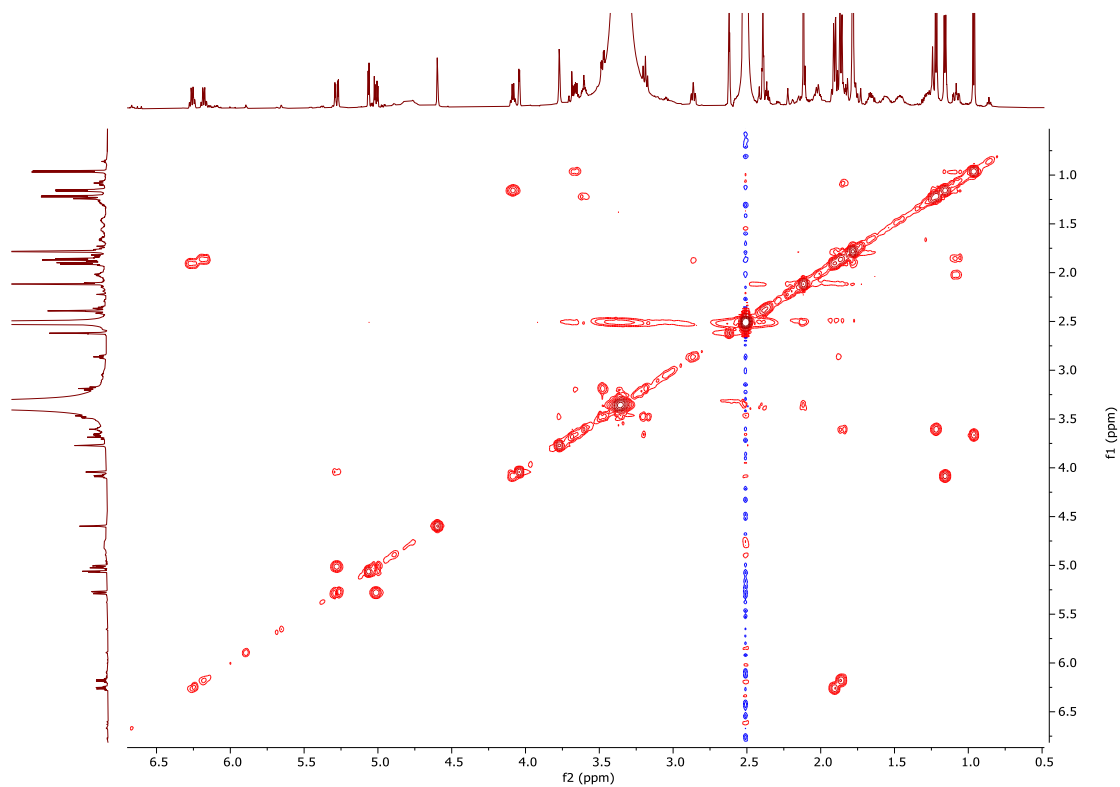


Fig. S150 COSY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside E2 (20).

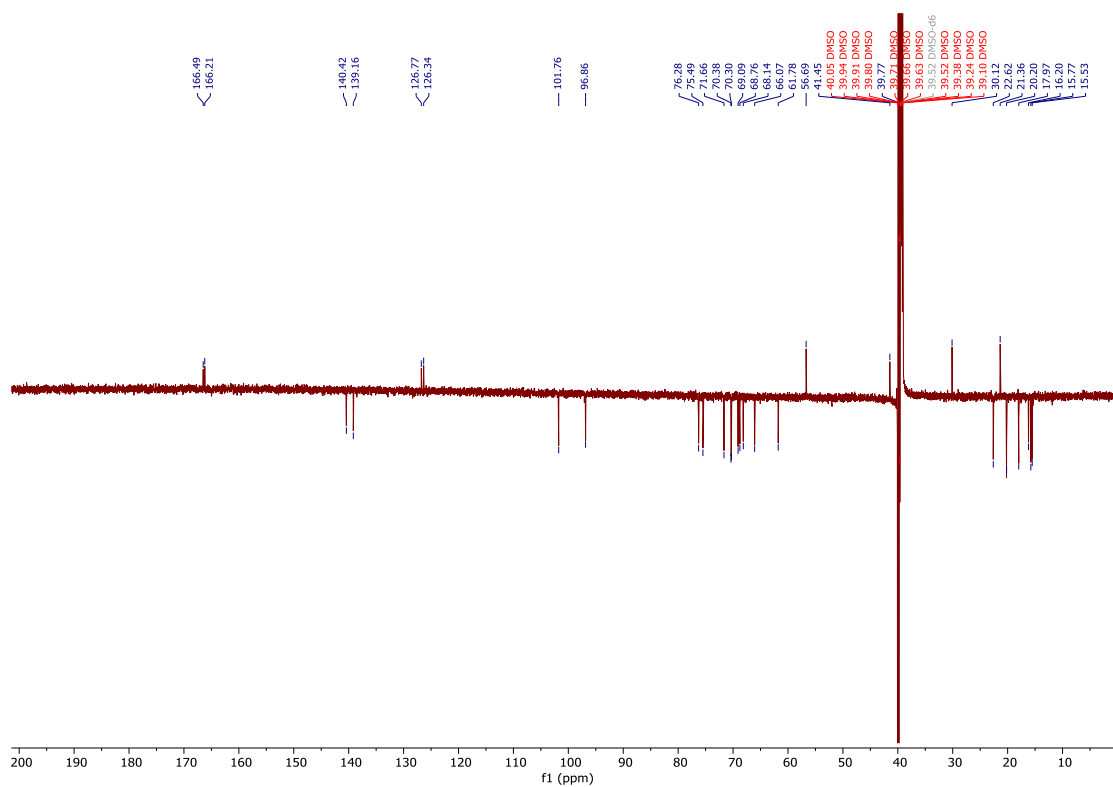


Fig. S151 DEPTQ (125 MHz, DMSO-*d*₆) spectrum of schizanthoside E2 (**20**).

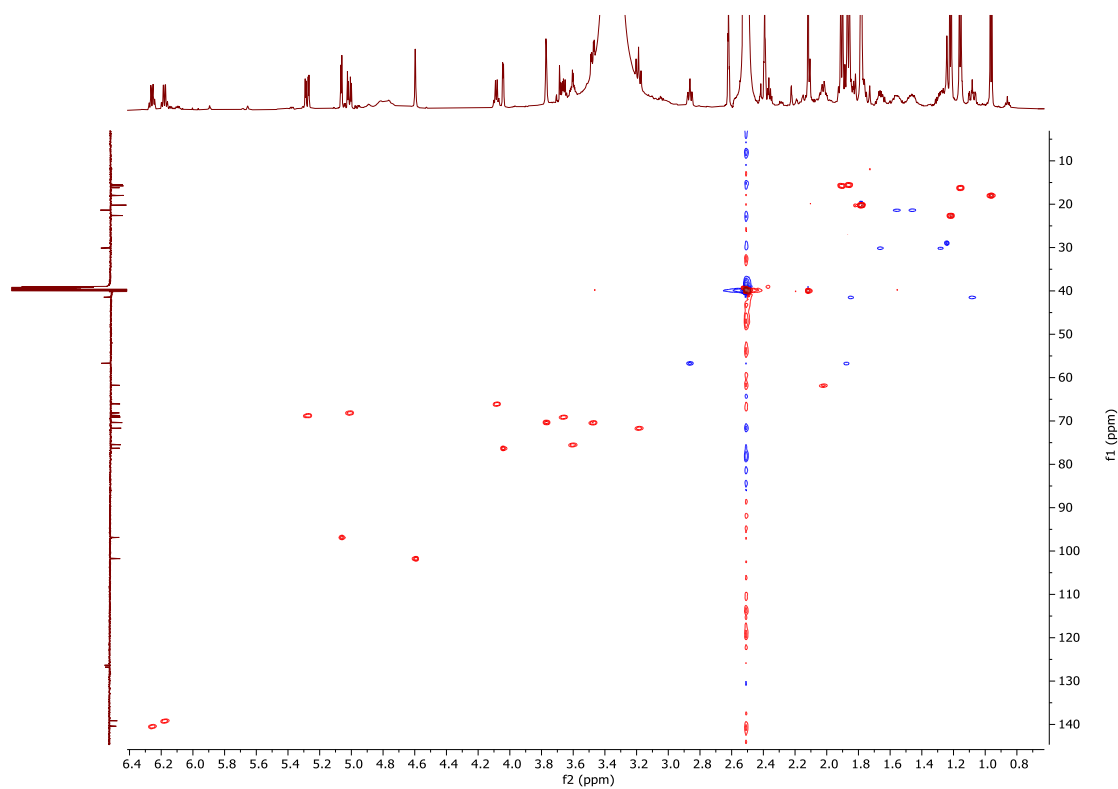


Fig. S152 HSQC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside E2 (**20**).

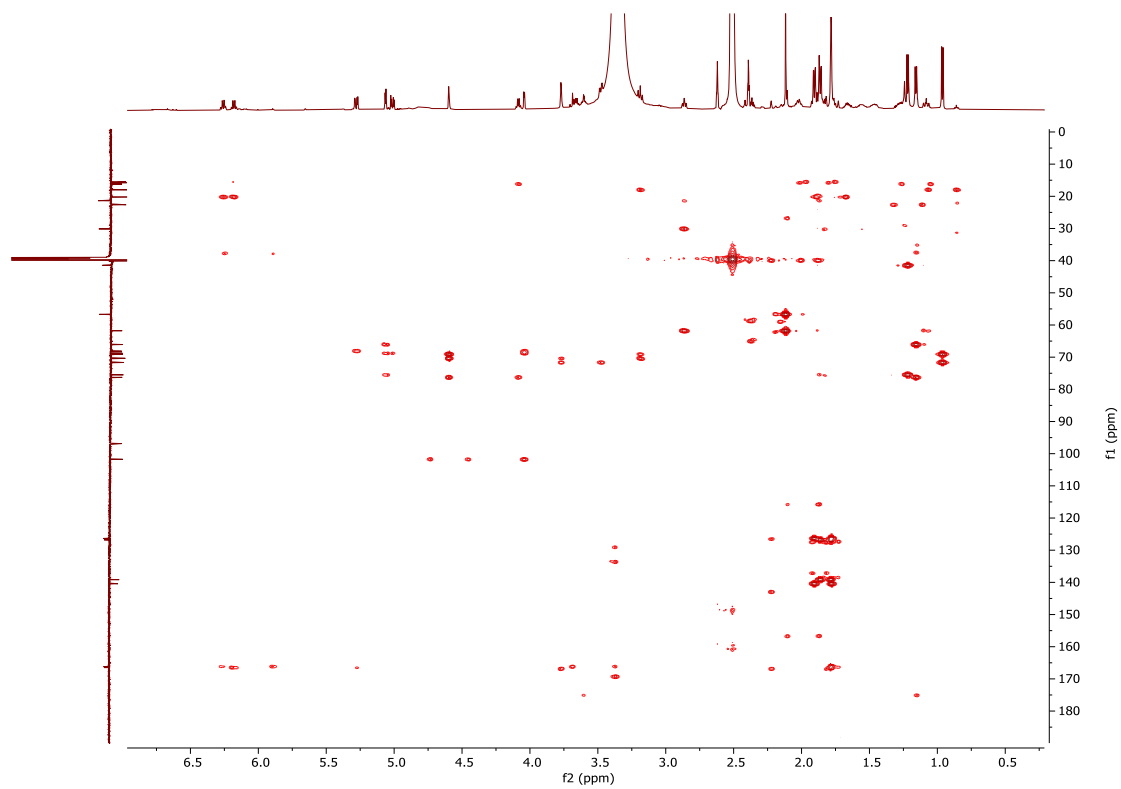


Fig. S153 HMBC (600 MHz, DMSO-*d*₆) spectrum of schizanthoside E2 (**20**).

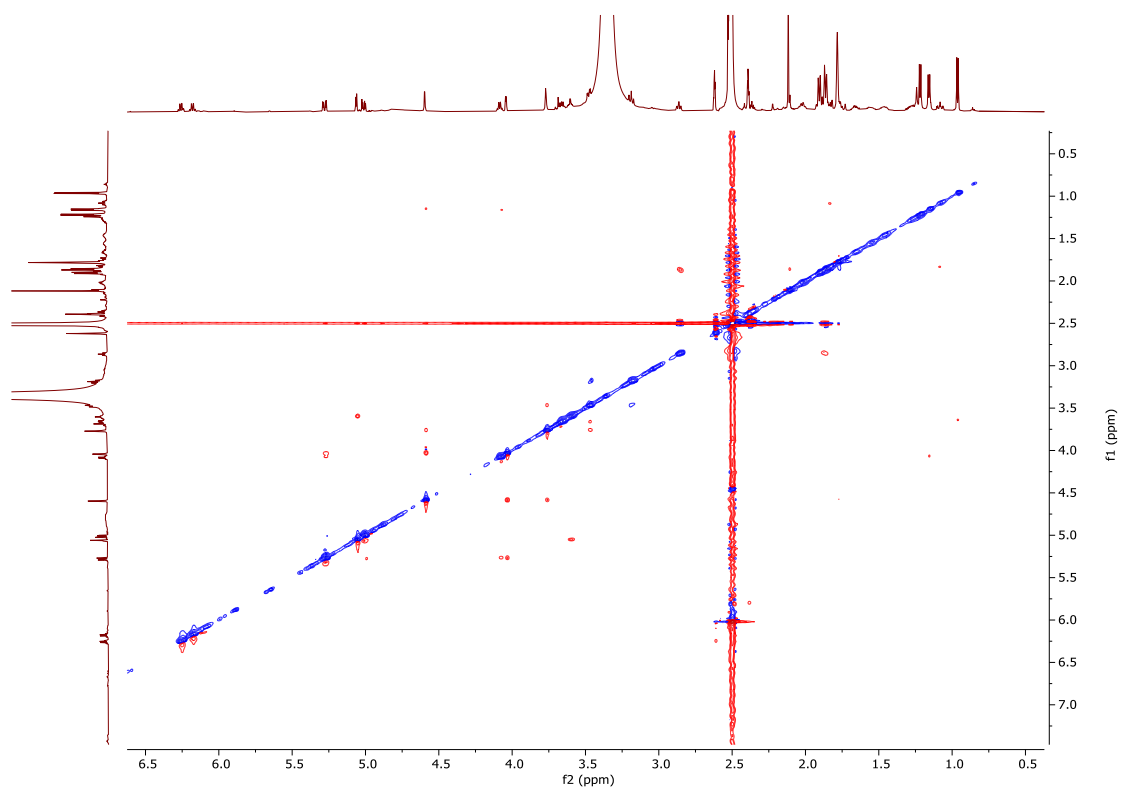


Fig. S154 ROESY (600 MHz, DMSO-*d*₆) spectrum of schizanthoside E2 (**20**).

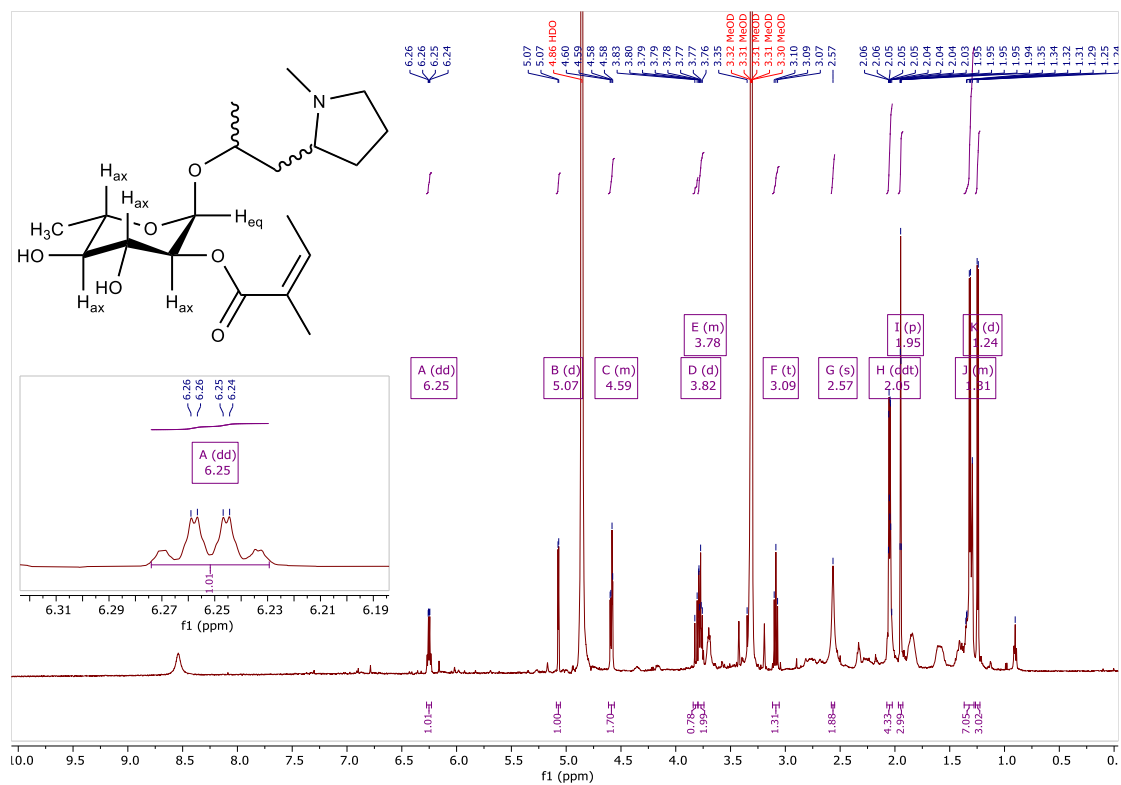


Fig. S155 ^1H NMR (600 MHz, CD_3OD) spectrum of compound 21.

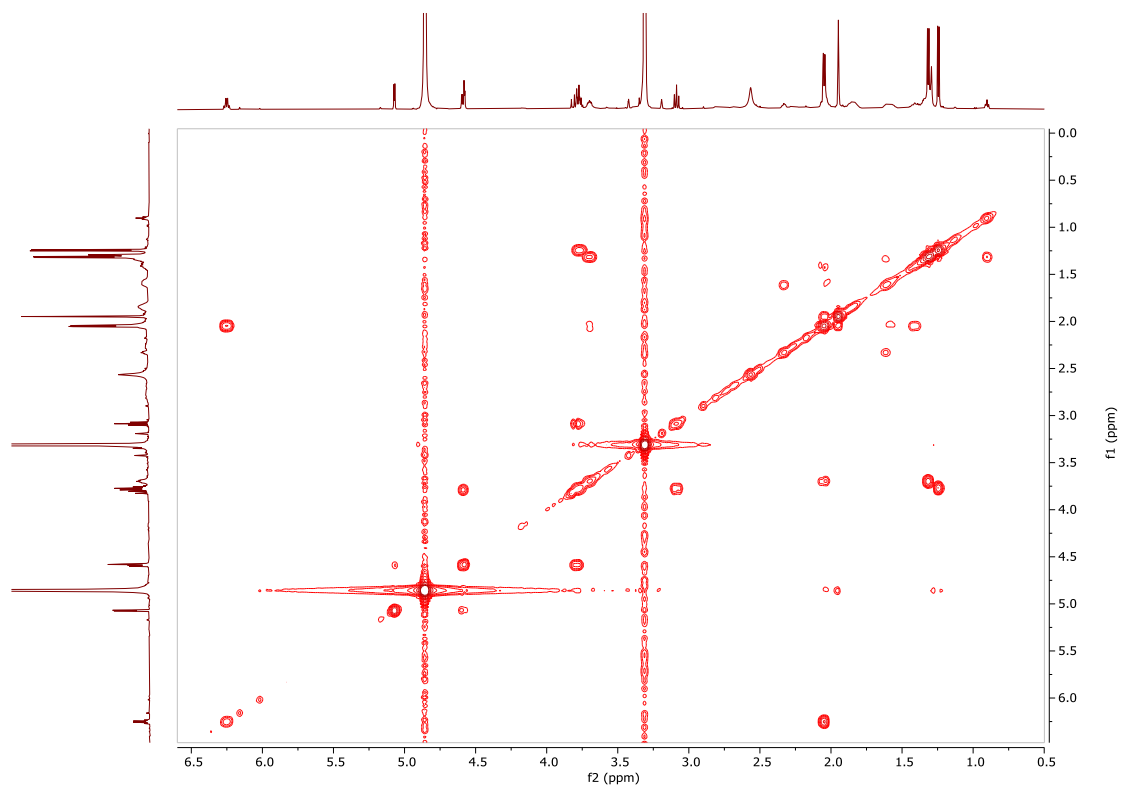


Fig. S156 COSY (600 MHz, $\text{DMSO}-d_6$) spectrum of compound 21.

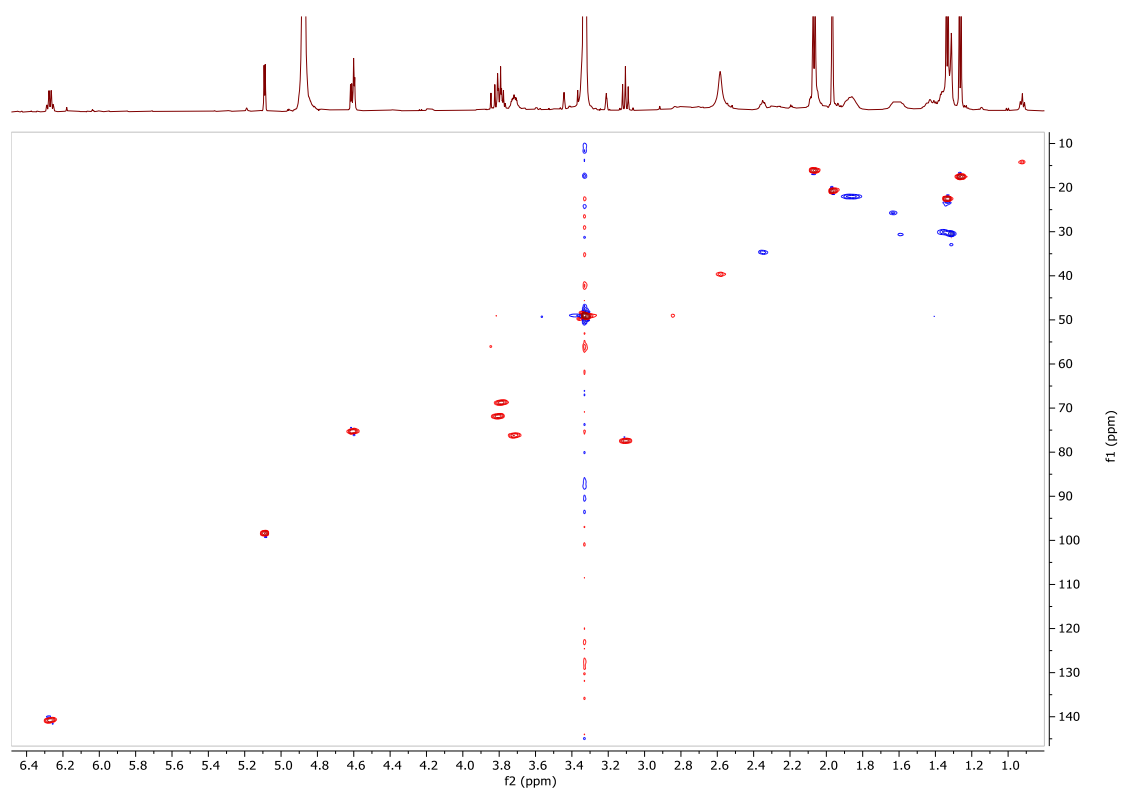


Fig. S157 HSQC (600 MHz, DMSO-*d*₆) spectrum of compound **21**.

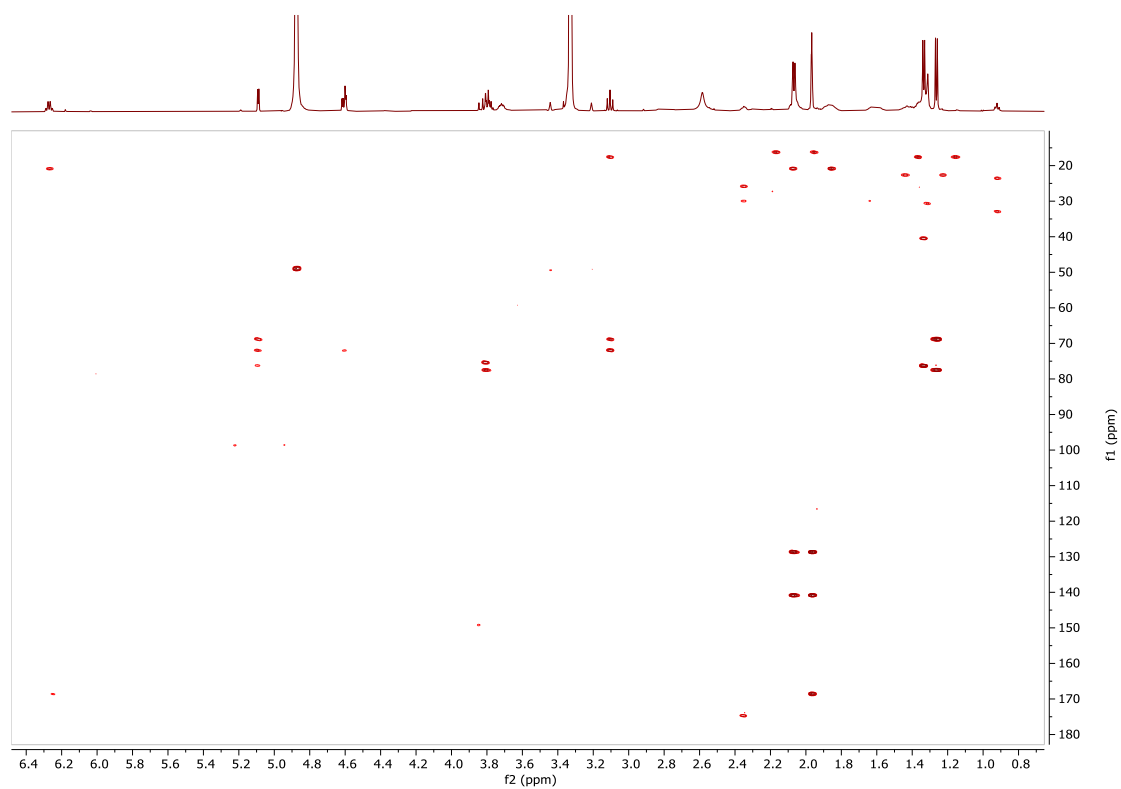


Fig. S158 HMBC (600 MHz, DMSO-*d*₆) spectrum of compound **21**.

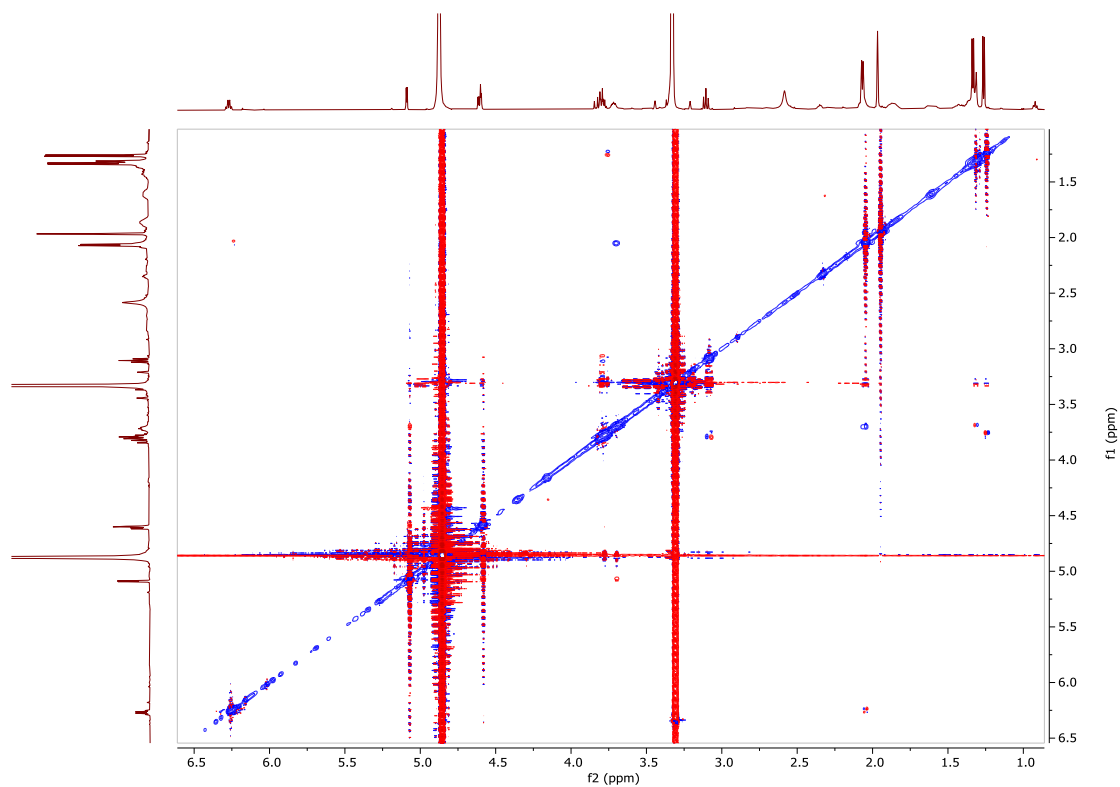


Fig. S159 ROESY (600 MHz, DMSO-*d*₆) spectrum of compound 21.

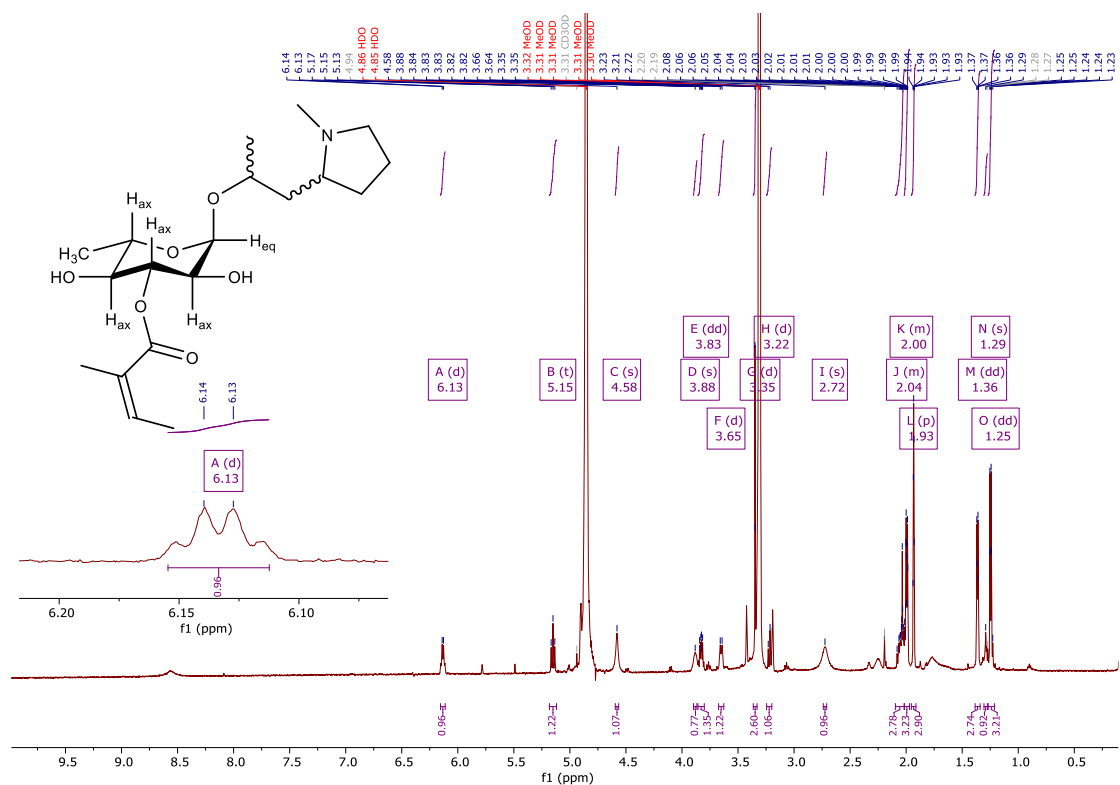


Fig. S160 ¹H NMR (600 MHz, CD₃OD) spectrum of compound 22.

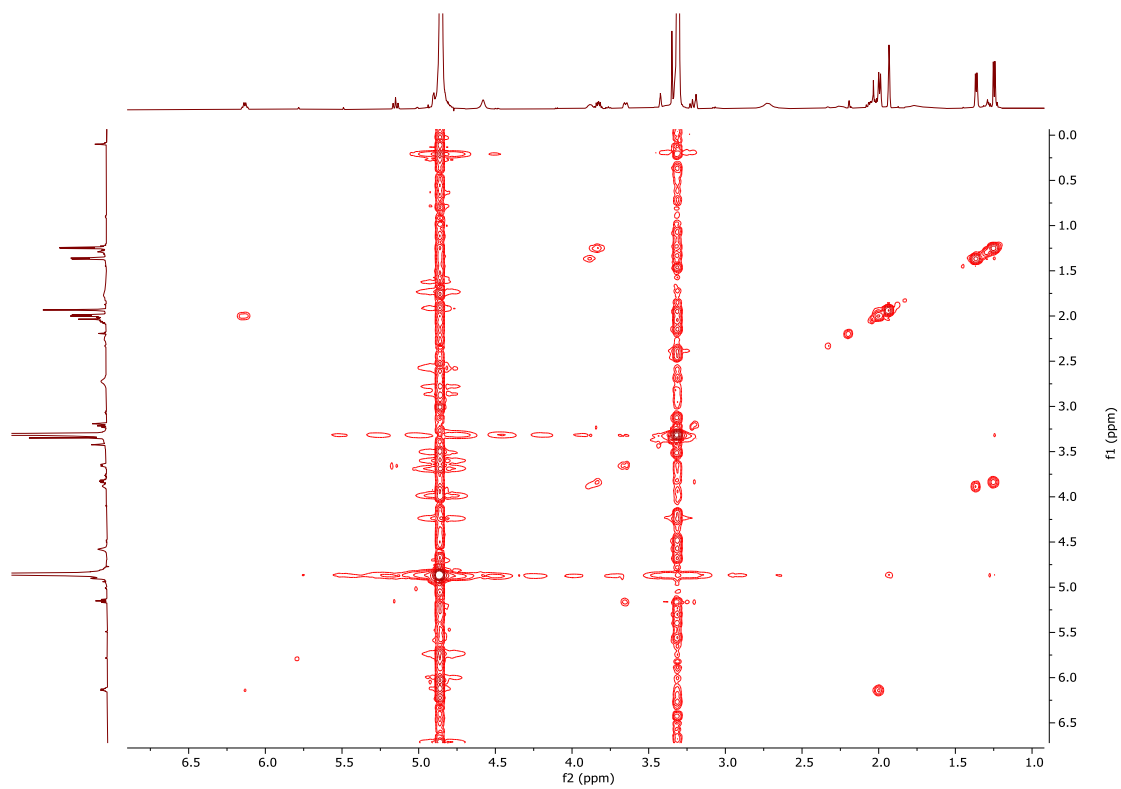


Fig. S161 COSY (600 MHz, DMSO-*d*₆) spectrum of compound **22**.

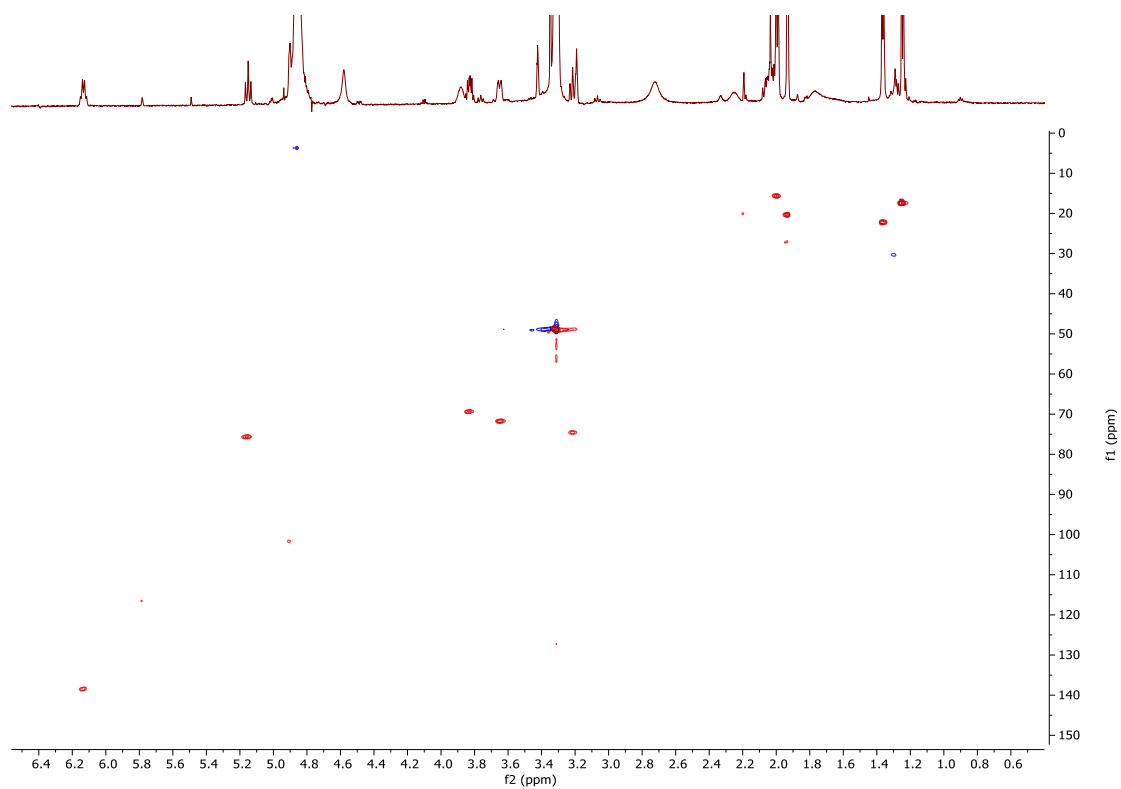


Fig. S162 HSQC (600 MHz, DMSO-*d*₆) spectrum of compound **22**.

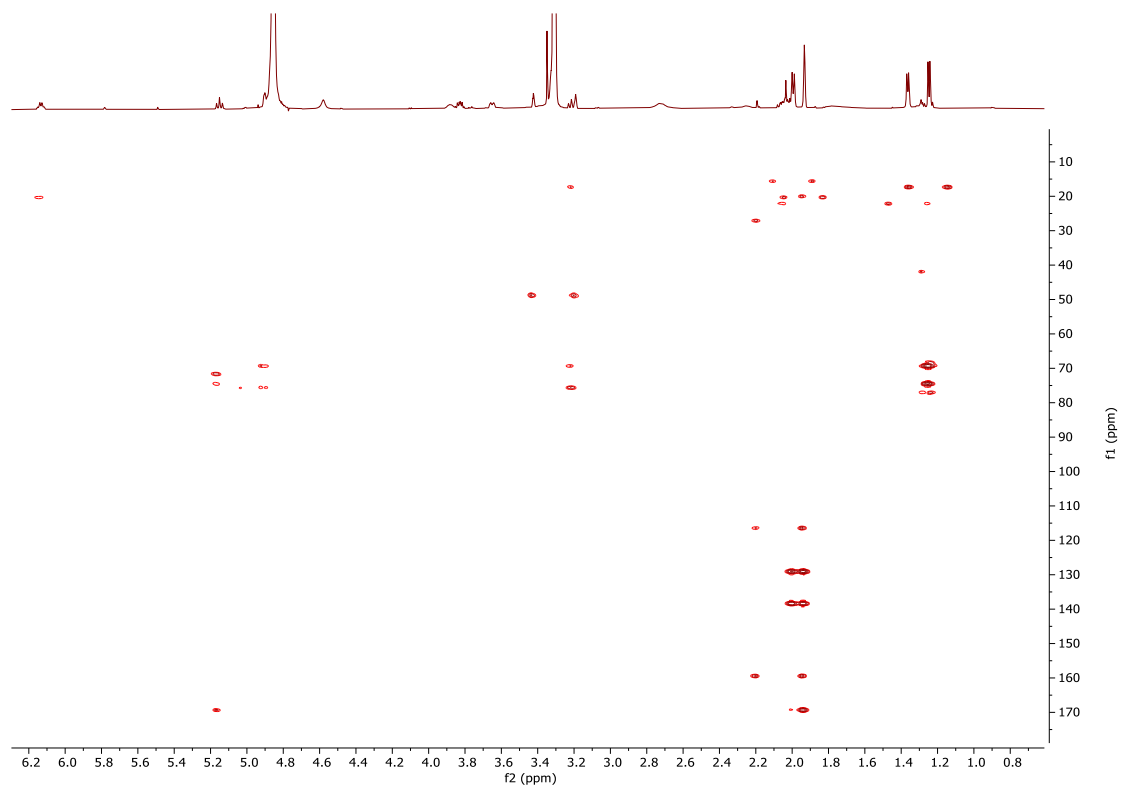


Fig. S163 HMBC (600 MHz, DMSO-*d*₆) spectrum of compound **22**.

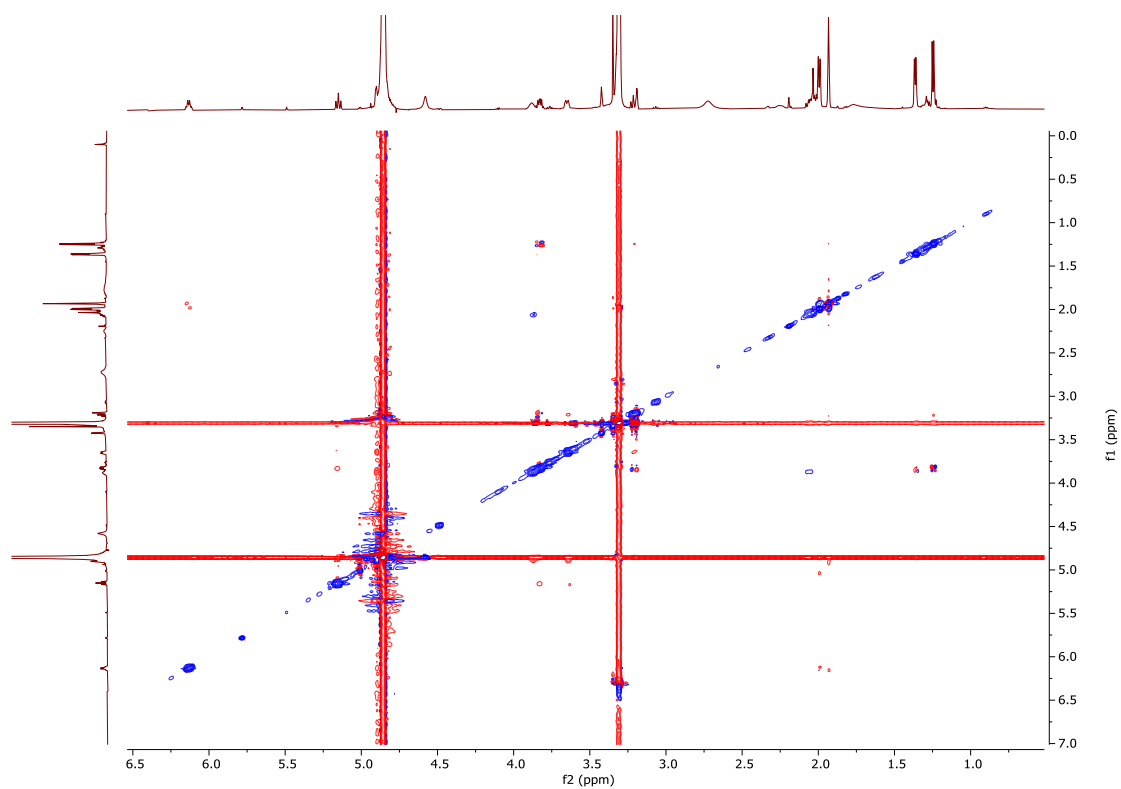


Fig. S164 ROESY (600 MHz, DMSO-*d*₆) spectrum of compound **22**.

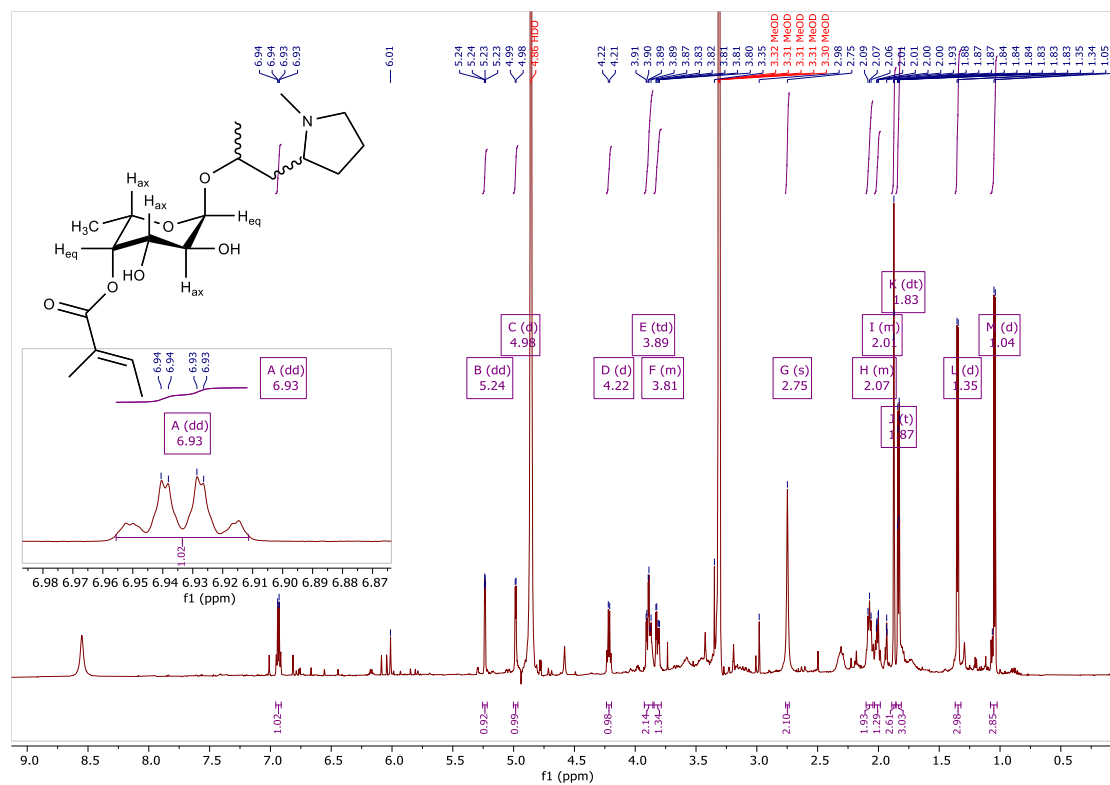


Fig. S165 ¹H NMR (600 MHz, CD₃OD) spectrum of compound 23.

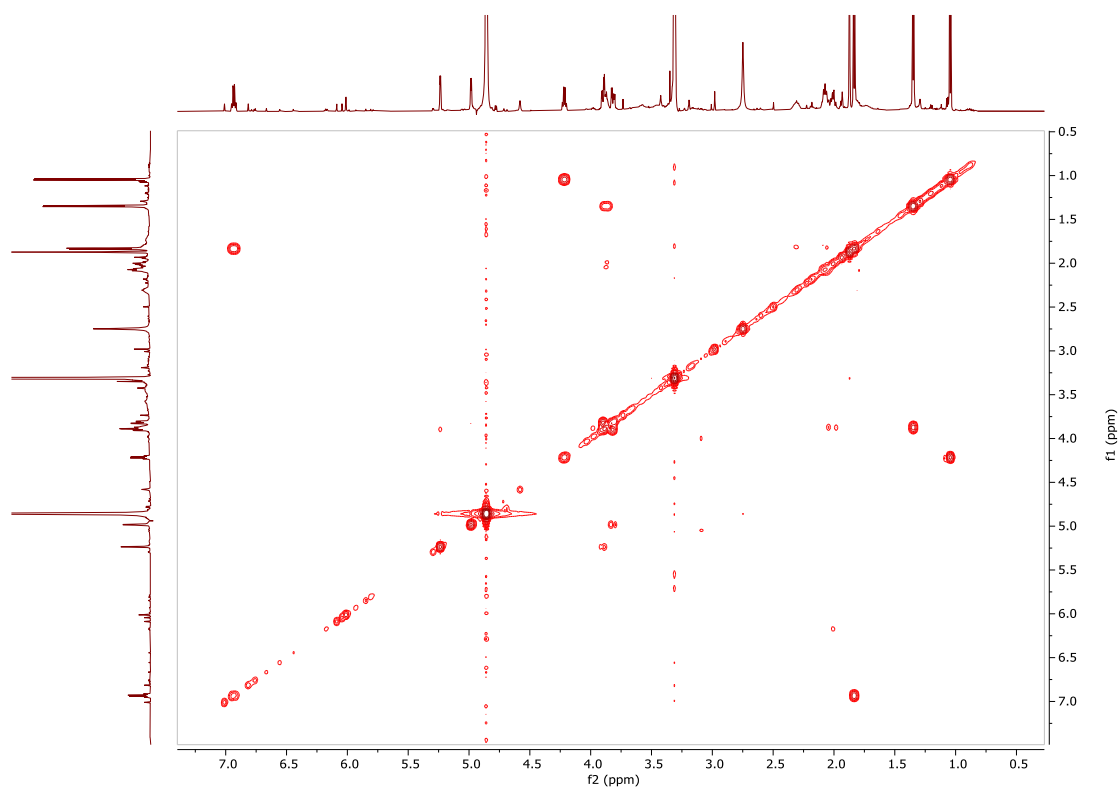


Fig. S166 COSY (600 MHz, DMSO-*d*₆) spectrum of compound 23.

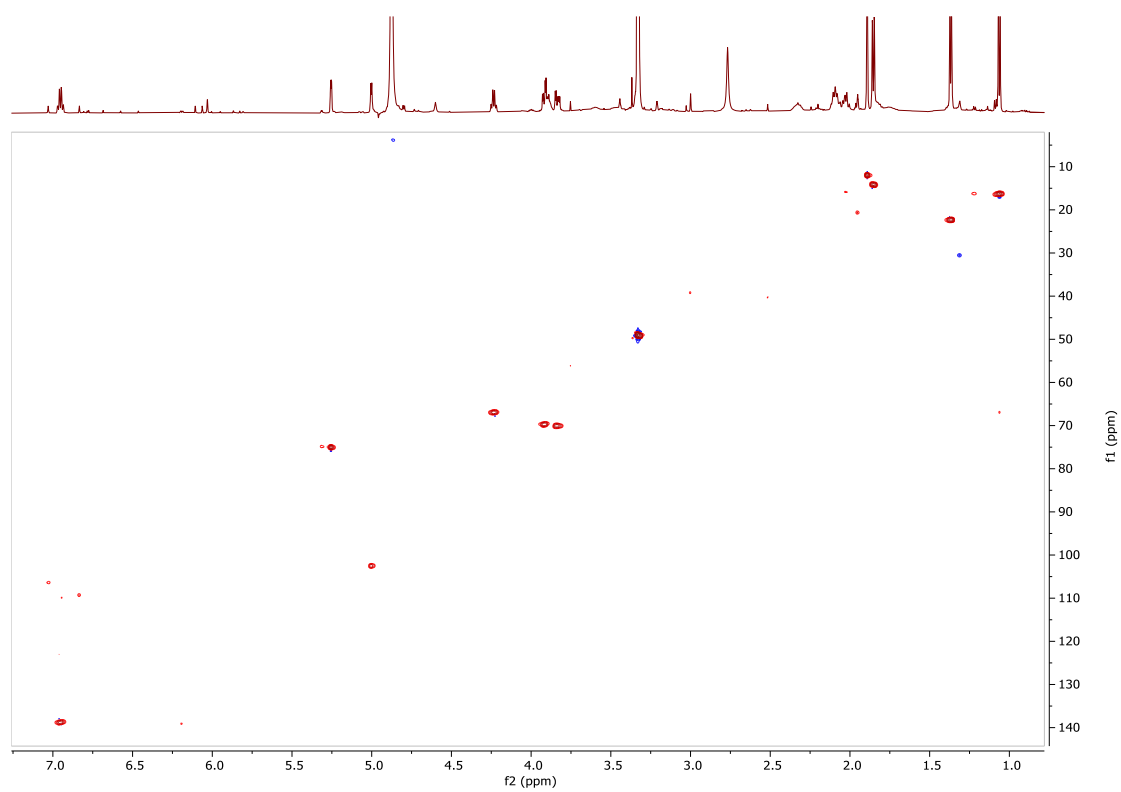


Fig. S167 HSQC (600 MHz, DMSO-*d*₆) spectrum of compound **23**.

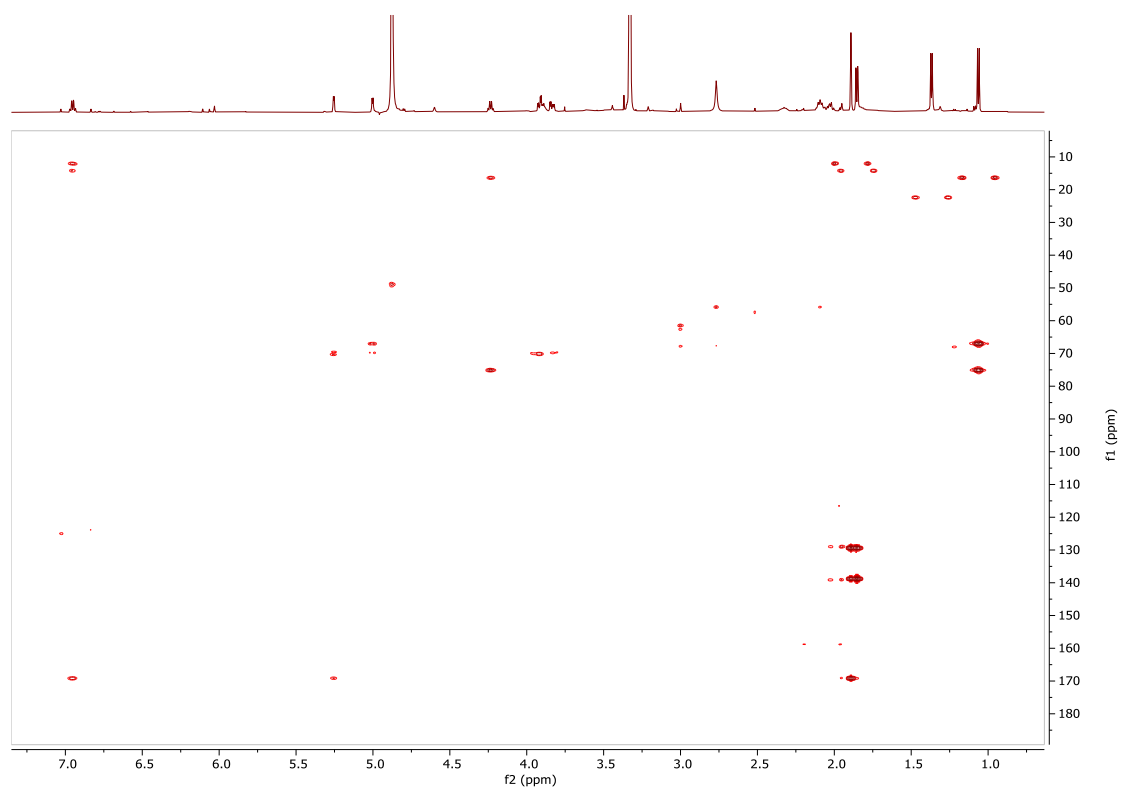


Fig. S168 HMBC (600 MHz, DMSO-*d*₆) spectrum of compound **23**.

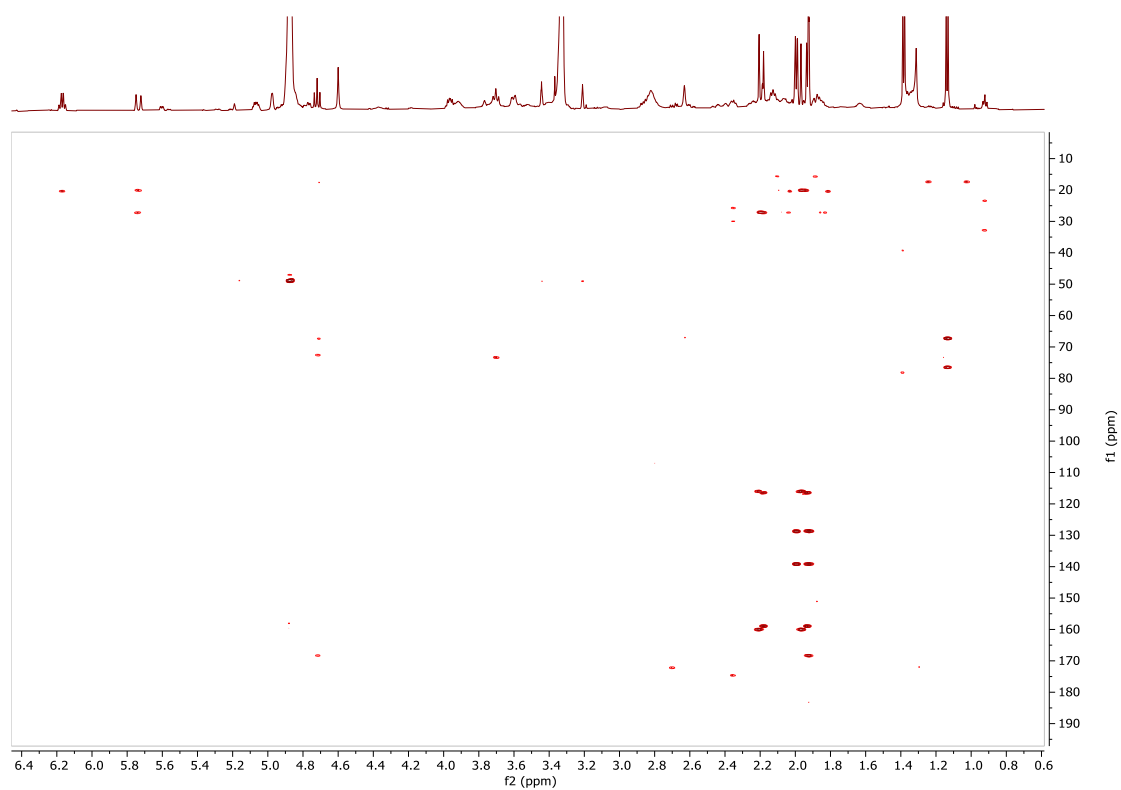


Fig. S173 HMBC (600 MHz, DMSO-*d*₆) spectrum of compound **24**.

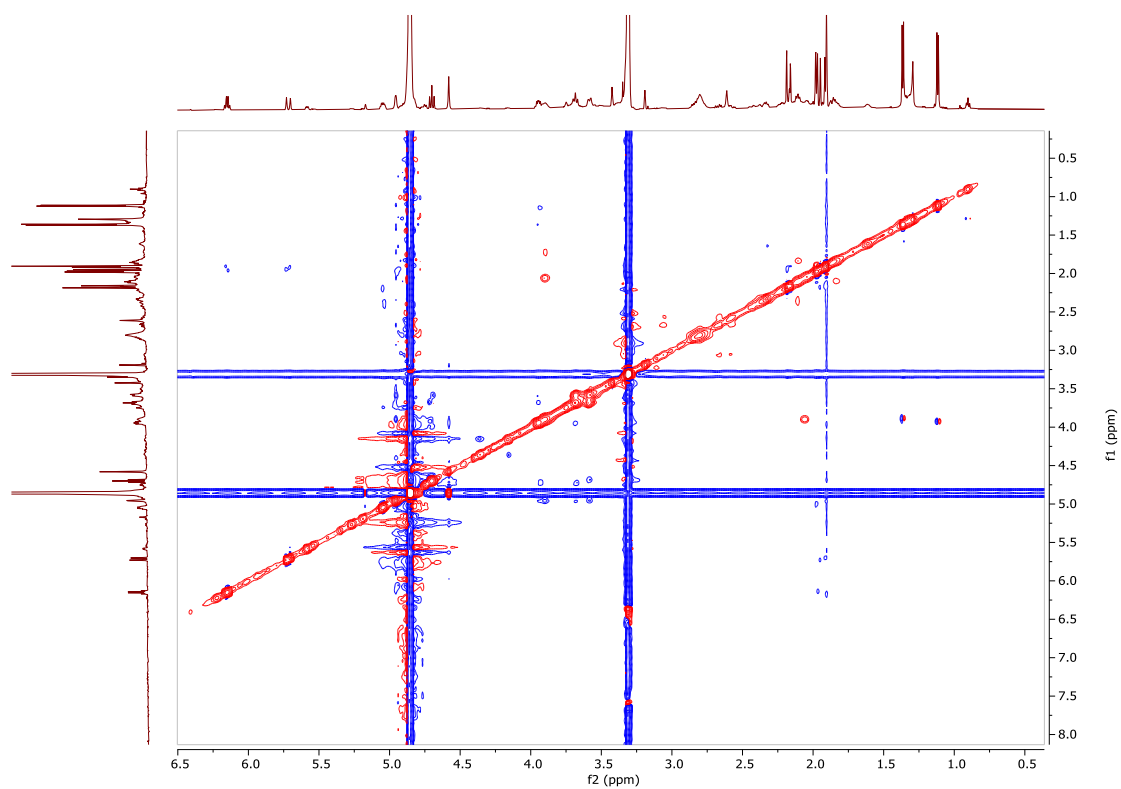


Fig. S174 ROESY (600 MHz, DMSO-*d*₆) spectrum of compound **24**.

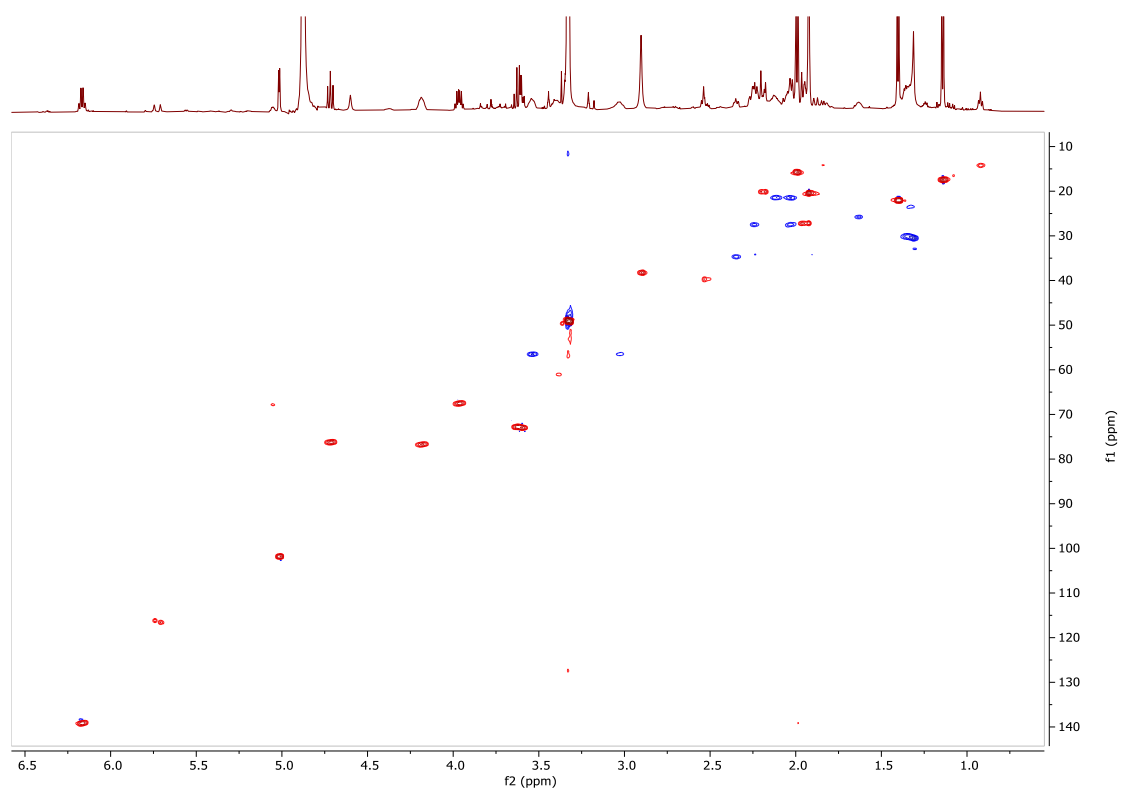


Fig. S177 HSQC (600 MHz, DMSO-*d*₆) spectrum of compound **25**.

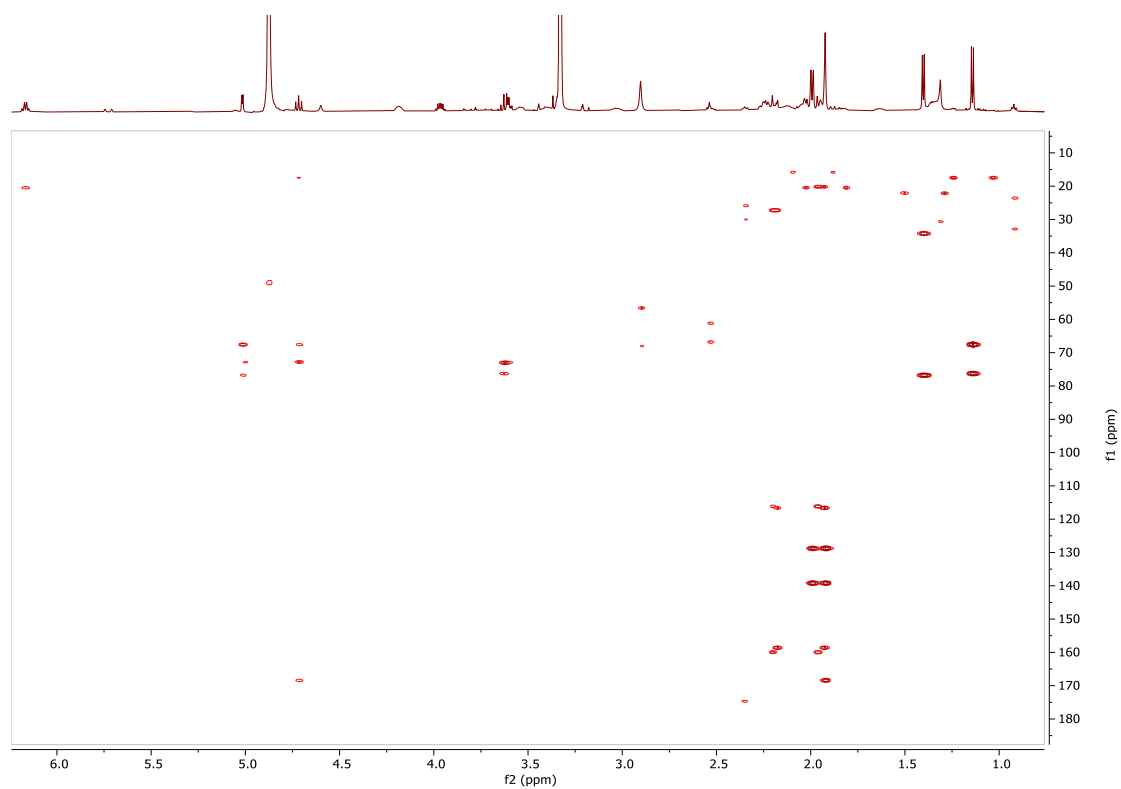


Fig. S178 HMBC (600 MHz, DMSO-*d*₆) spectrum of compound **25**.

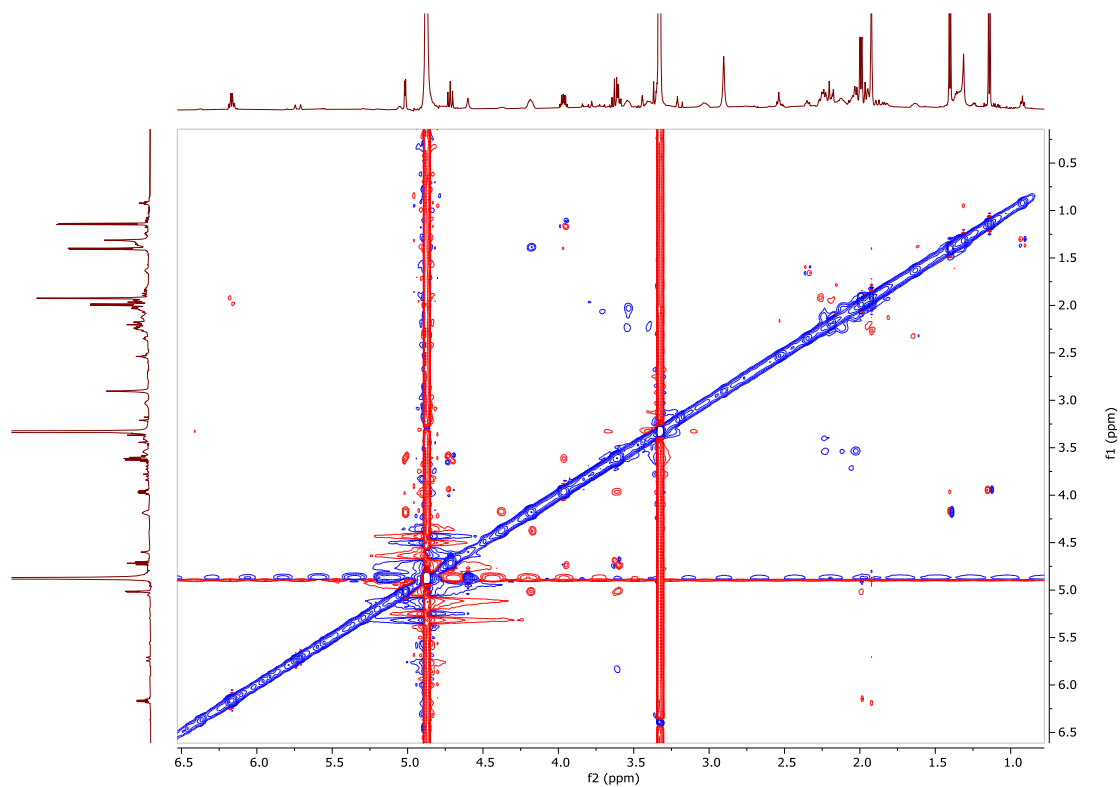


Fig. S179 ROESY (600 MHz, DMSO-*d*₆) spectrum of compound 25.

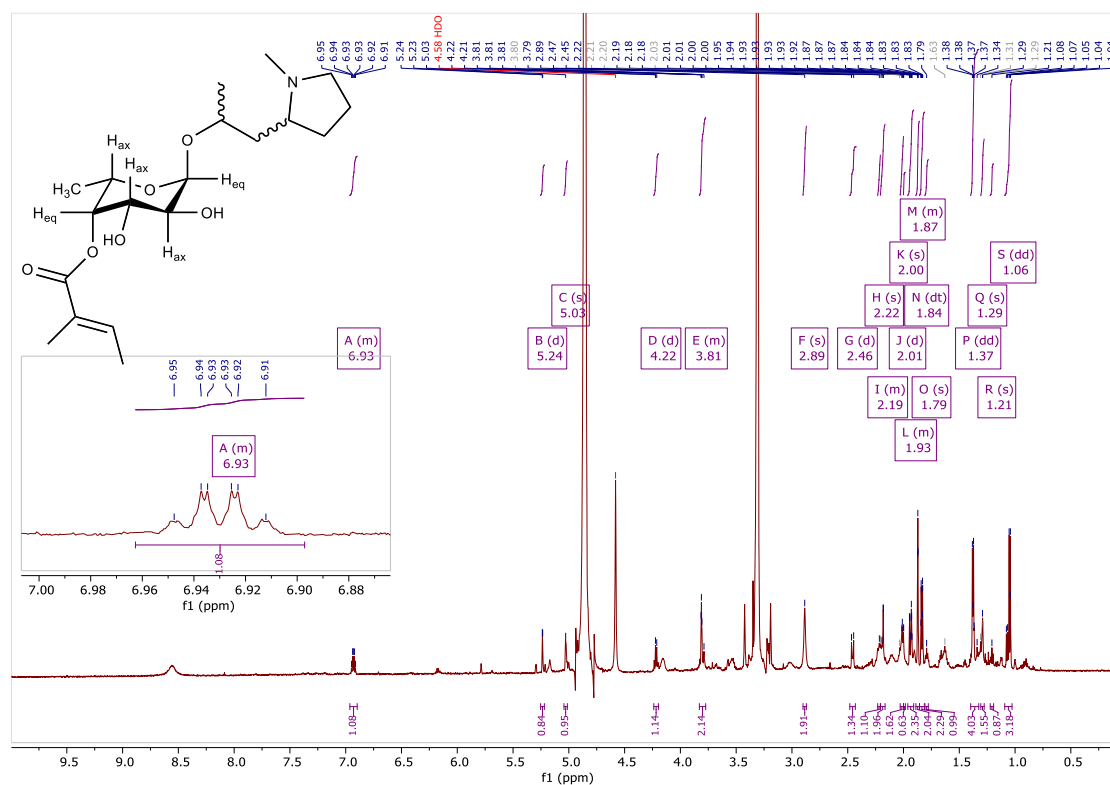


Fig. S180 ¹H NMR (600 MHz, CD₃OD) spectrum of compound 26.

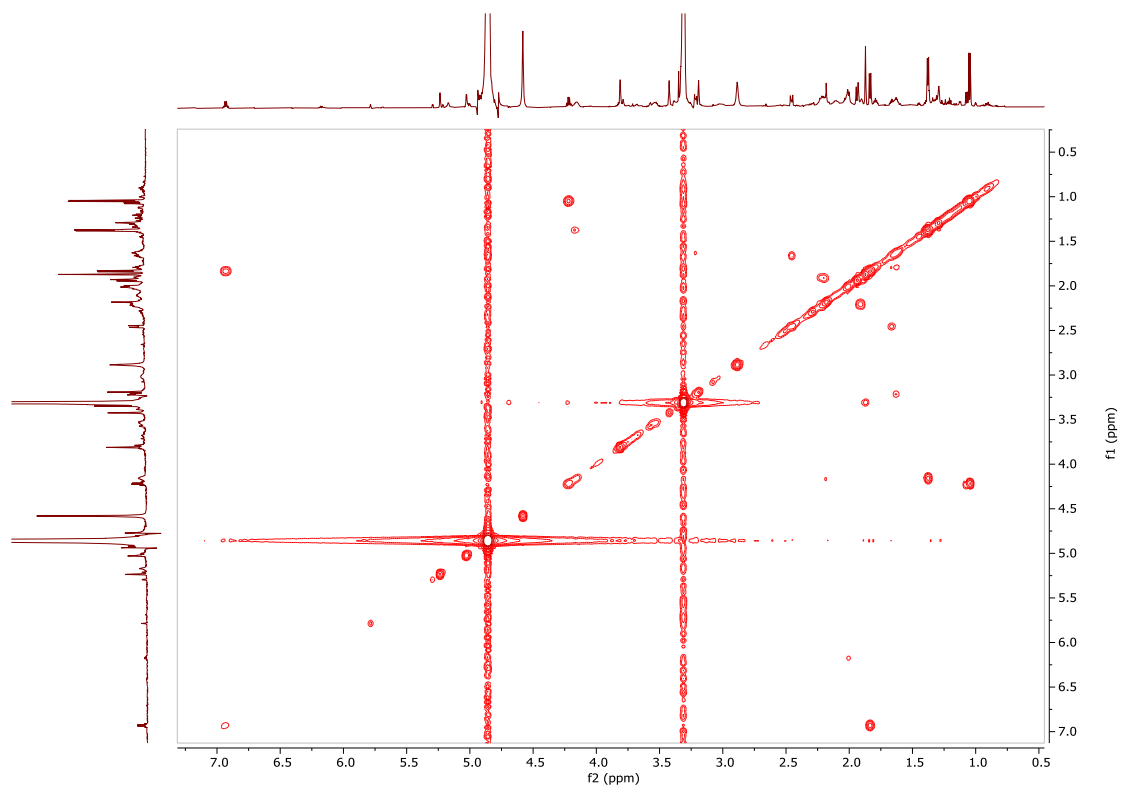


Fig. S181 COSY (600 MHz, DMSO- d_6) spectrum of compound **26**.

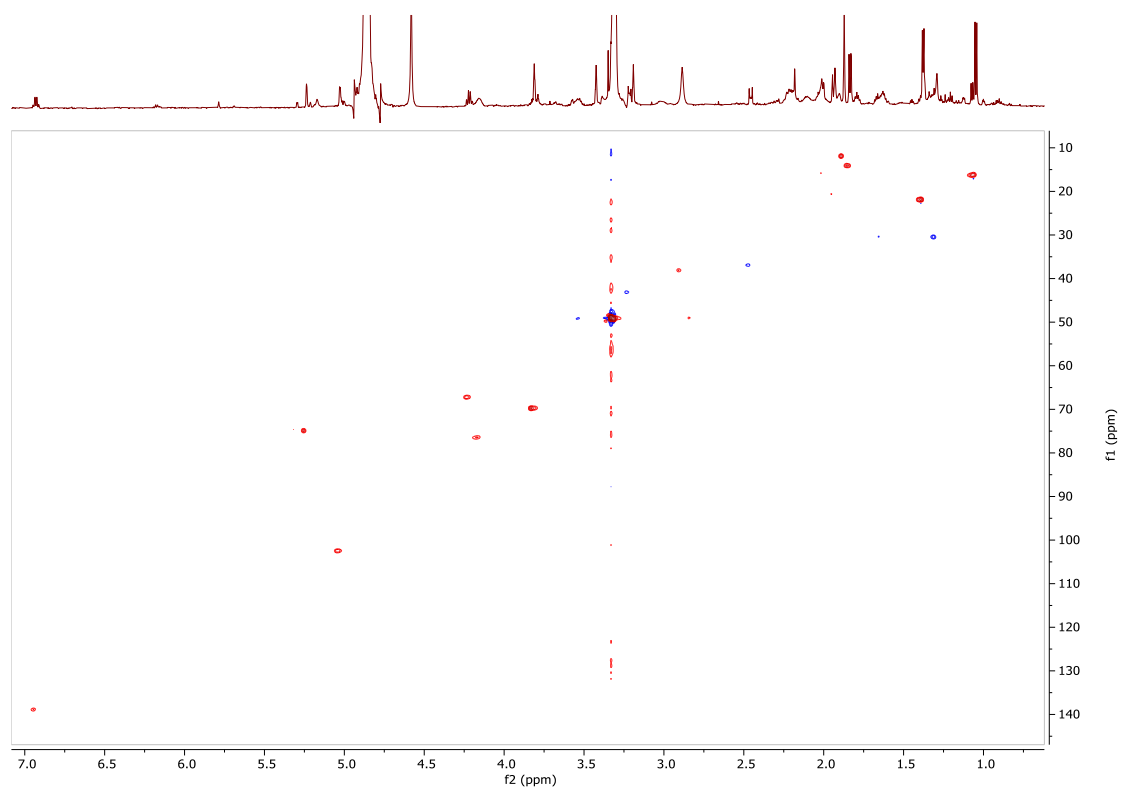


Fig. S182 HSQC (600 MHz, DMSO- d_6) spectrum of compound **26**.

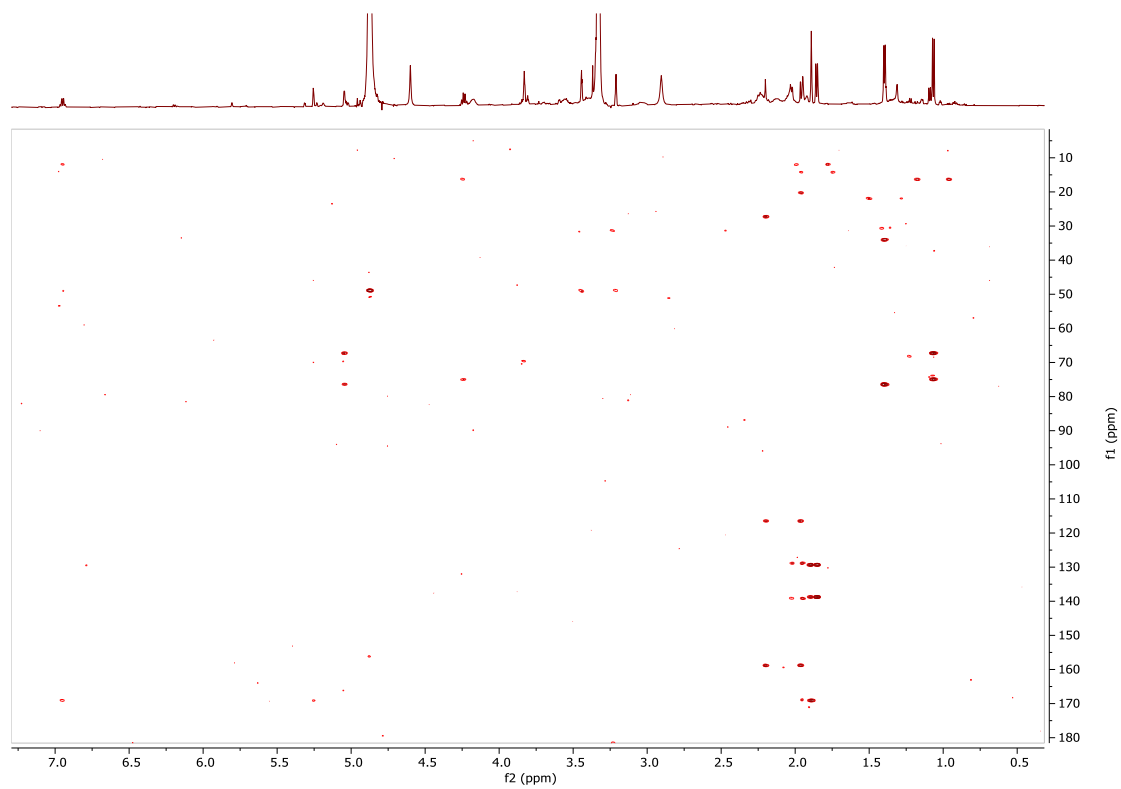


Fig. S183 HMBC (600 MHz, DMSO-*d*₆) spectrum of compound **26**.

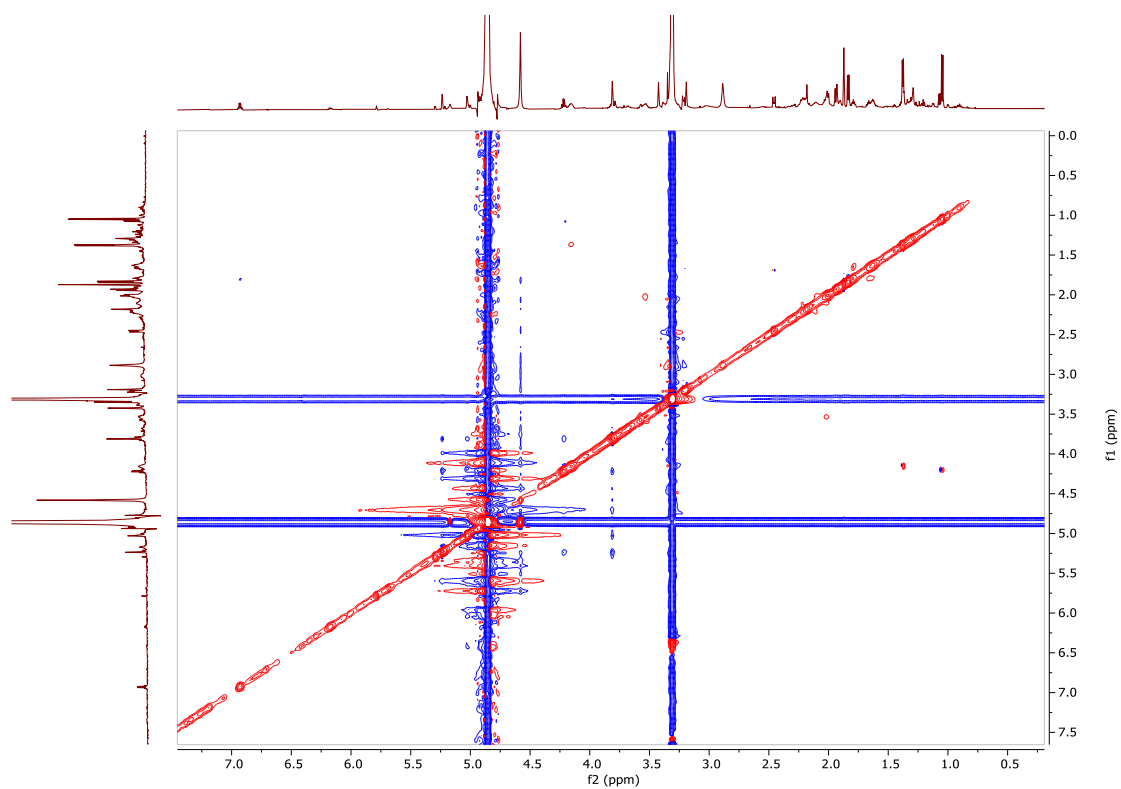


Fig. S184 ROESY (600 MHz, DMSO-*d*₆) spectrum of compound **26**.

Table S1. ¹H NMR data of compounds **21-26** (600 MHz, in CD₃OD, δ in ppm, *J* in Hz)

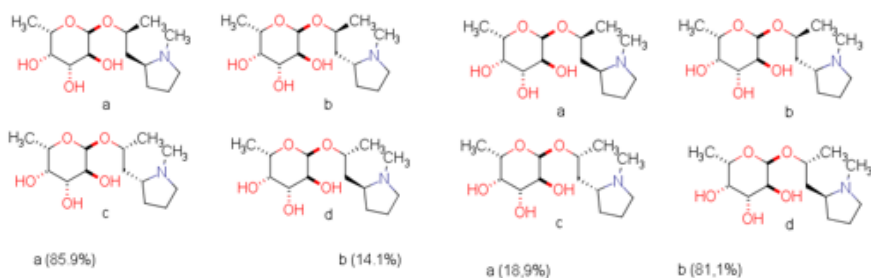
Position	21	22	23	24	25	26
1	5.07, d (3.8)	4.91, s	4.98, d (4.0)	4.96, s	5.00, d (3.8)	5.03, d (3.8)
2	4.59, m	3.65, d (9.8)	3.81, m	3.58, d (10.5)	3.58, dd (9.5, 3.8)	3.81, m
3	3.82, d (12.7)	5.15, t (9.8)	3.89, td (10.3, 3.7)	3.68, t (9.6)	3.61, d (9.0)	3.81, m
4	3.09, t (9.2)	3.22, d (9.8)	5.24, dd (3.4, 1.3)	4.70, t (9.6)	4.70, t (9.4)	5.24, d (2.1)
5	3.78, m	3.83, dd (9.5, 6.5)	4.22, q (6.7)	3.95, dd (10.0, 6.1)	3.95, dq (9.9, 6.3)	4.22, q (6.7)
6	1.24, d (6.3)	1.25, d (6.5)	1.04, d (6.7)	1.12, d (6.3)	1.12, d (6.3)	1.06, d (6.7)
2'	a	a	a	a	a	a
3'	a	2.24, m 2.04, m	a	a	2.24, m 2.02, d (8.5)	2.21, m 2.02, m
4'	a	a	a	a	2.11, m 2.02, d (8.5)	2.13, m 2.02, m
5'	a	a	a	a	3.52, brs 3.01, brs	a
6'	2.04, m 1.59, m	a	2.02, m a	a	2.24, m 1.92, m	2.20 a
7'	3.70, m	3.88, brs	3.87, m	3.88, m	4.17, brs	4.16, brs
8'	1.36, d (6.1)	1.36, d (6.3)	1.35, d (6.1)	1.36, d (6.1)	1.38, d (6.0)	1.37, d (6.2)
9'	2.57, s	2.72, s	2.75, s	2.61, s	2.88, s	2.89, s
2''	6.25, qd (7.3, 1.5)	6.13, q (7.4)	6.93, qd (7.1, 1.3)	6.15, dd (7.3, 1.6)	6.17, dd (7.2, 1.6)	6.93, qd (7.1, 1.3)
3''	2.05, dq (7.2, 1.5)	2.00, dq (7.3, 1.6)	1.83, dq (7.1, 1.3)	1.97, dq (7.3, 1.6)	1.97, dq (7.4, 1.6)	1.84, dq (7.1, 1.3)
4''	1.95, t (1.5)	1.93, t (1.6)	1.87, t (1.3)	1.91, t (1.6)	1.91, t (1.6)	1.87, t (1.3)
5''	5.07, d (3.8)	4.91, s	4.98, d (4.0)	4.96, s	5.00, d (3.8)	5.03, d (3.8)

^a Signal too weak to be observed

Table S2. ^{13}C NMR data of compounds **21-26** (150 MHz, in CD_3OD , δ in ppm, C type)

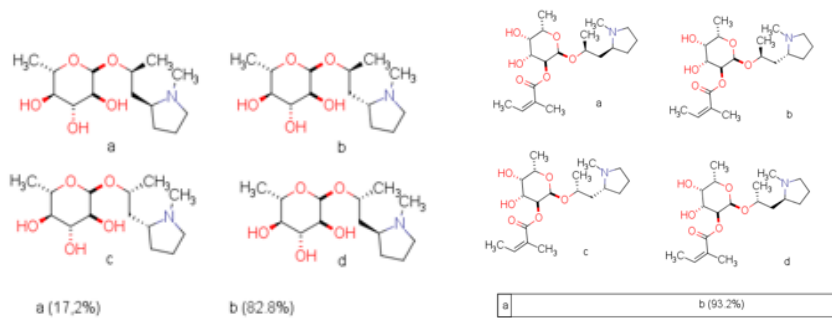
Position	21	22	23	24	25	26
1	98.4, CH	101.6, CH	102.5, CH	102.0, CH	101.8, CH	102.4, CH
2	75.3, CH	71.7, CH	70.0, CH	73.4, CH	72.9, CH	69.7, CH
3	71.8, CH	75.6, CH	69.7, CH	72.5, CH	72.9, CH	69.7, CH
4	77.5, CH	74.6, CH	75.0, CH	76.6, CH	76.2, CH	74.8, CH
5	68.7, CH	69.4, CH	66.9, CH	67.3, CH	67.5, CH	67.3, CH
6	17.5, CH_3	17.4, CH_3	16.3, CH_3	17.5, CH_3	17.4, CH_3	16.3, CH_3
2'	a	a	67.6, CH	67.0, CH	68.0, CH	a
3'	a	a	a	a	27.5, CH_2	27.4, CH_2
4'	a	a	a	a	21.5, CH_2	21.3, CH_2
5'	a	a	55.8, CH_2	a	56.6, CH_2	a
6'	30.6, CH_2	a	a	39.4, CH_2	34.2, CH_2	33.9, CH_2
7'	76.2, CH	a	a	78.2, CH	76.7, CH	76.4, CH
8'	22.6, CH_3	22.2, CH_3	22.3, CH_3	22.3, CH_3	22.0, CH_3	21.9, CH_3
9'	39.5, CH_3	a	a	39.5, CH_3	38.2, CH_3	38.1, CH_3
1''	168.5, C	169.3, C	169.1, C	168.3, C	168.4, C	169.0, C
2''	128.7, C	129.0, C	129.4, C	128.6, C	128.7, C	129.3, C
3''	140.8, CH	138.3, CH	138.8, CH	139.1, CH	139.2, CH	138.8, CH
4''	16.1, CH_3	15.6, CH_3	14.1, CH_3	15.7, CH_3	15.8, CH_3	14.2, CH_3
5''	20.7, CH_3	20.3, CH_3	12.0, CH_3	20.4, CH_3	20.5, CH_3	11.9, CH_3

^a Signal too weak to be observed



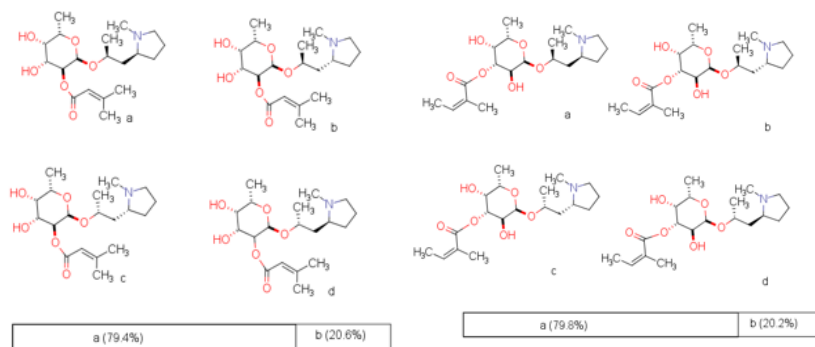
Compound 1

Compound 2



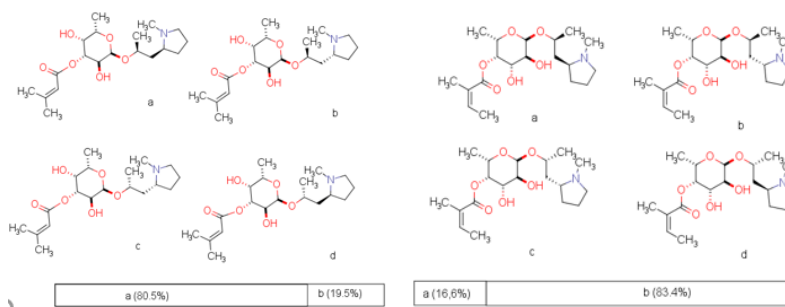
Compound 3

Compound 4



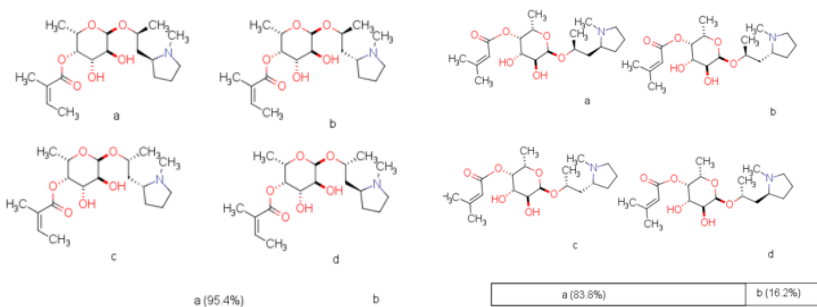
Compound 5

Compound 6



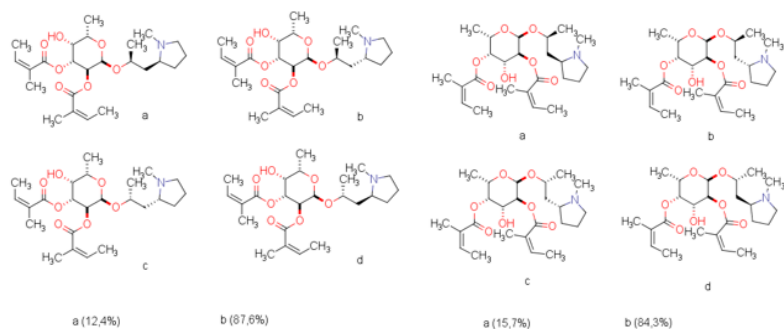
Compound 7

Compound 8



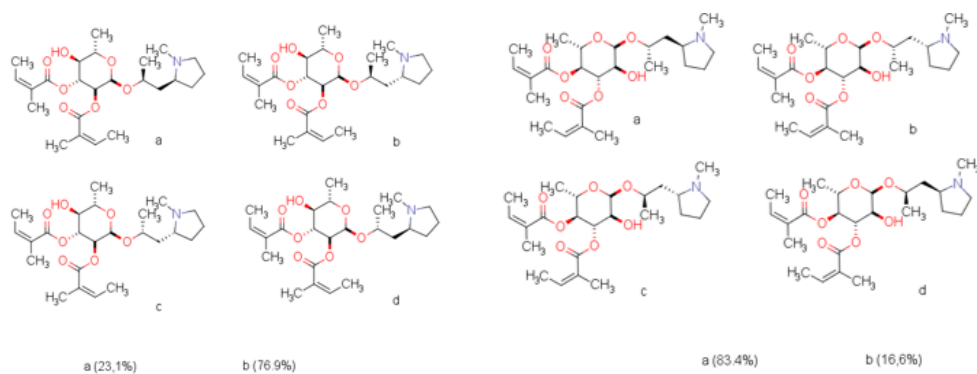
Compound 9

Compound 10



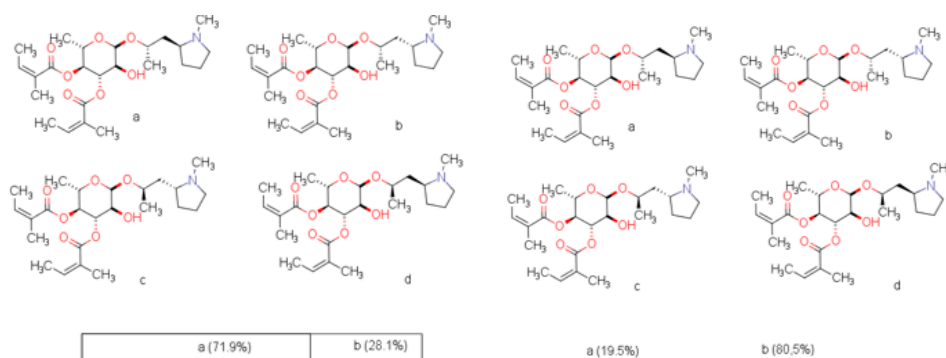
Compound 11

Compound 12



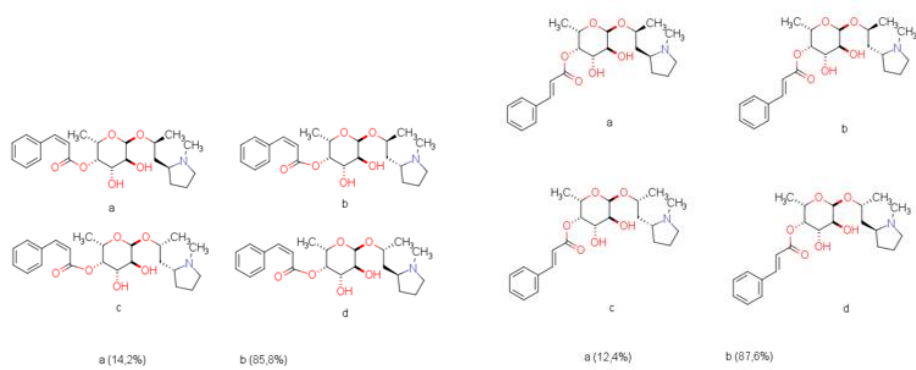
Compound 13

Compound 14



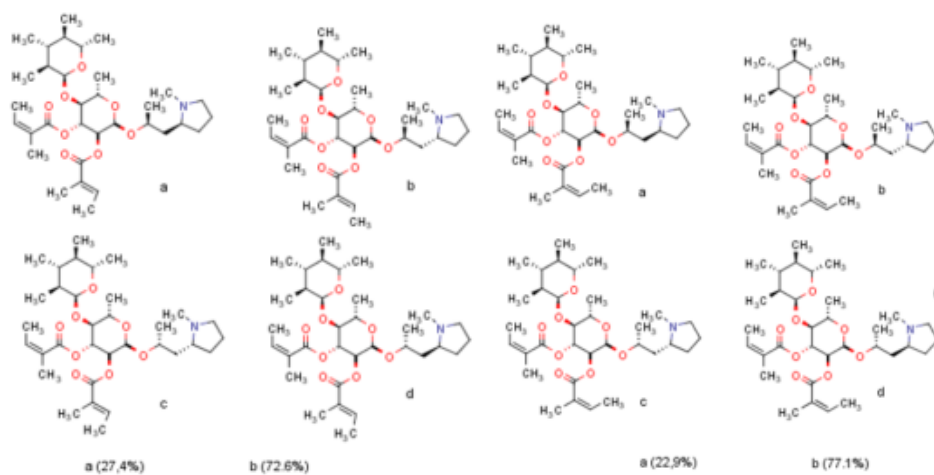
Compound 15

Compound 16



Compound 17

Compound 18



Compound 19

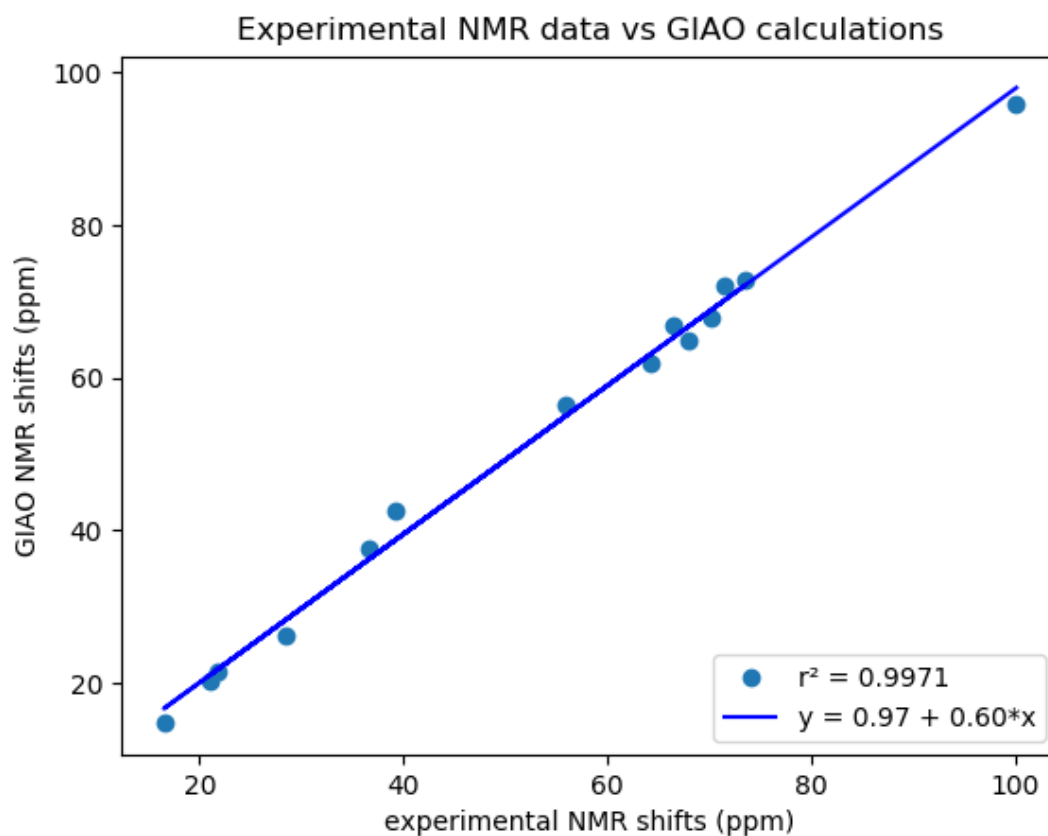
Compound 20

Fig. S185 DP4 calculation for compounds 1 to 20

Fig. S186 Experimental vs GIAO NMR shift of compounds **1** to **20**

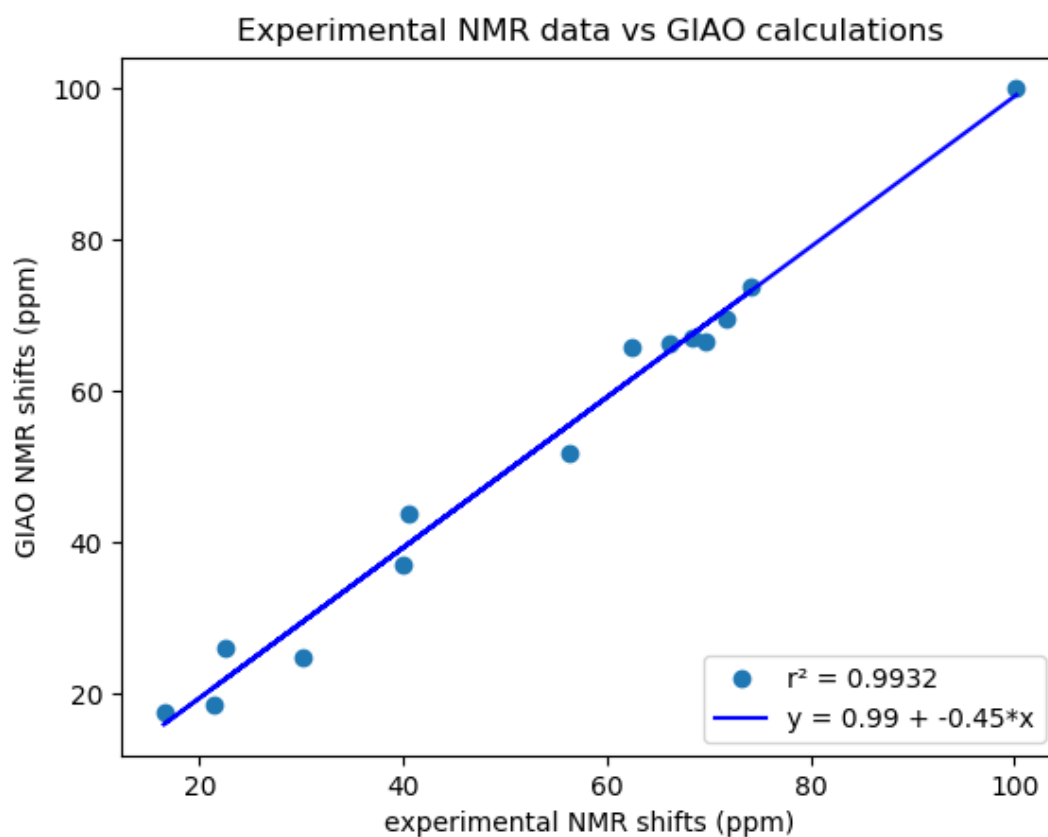
Compound **1**

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	100.10	95.88	99.16	103.50	98.01	4.22	0.94	-3.40	2.09
2	68.00	64.94	66.62	67.36	67.46	3.06	1.38	0.64	0.54
3	70.10	67.88	70.63	67.46	72.39	2.22	-0.53	2.64	-2.29
4	71.50	72.06	72.49	71.38	70.36	-0.56	-0.99	0.12	1.14
5	66.40	66.92	66.61	69.61	63.67	-0.52	-0.21	-3.21	2.73
6	16.50	14.72	12.30	16.69	14.61	1.78	4.20	-0.19	1.89
2'	64.30	62.03	66.09	67.02	63.40	2.27	-1.79	-2.72	0.90
3'	28.40	26.12	26.22	30.43	27.48	2.28	2.18	-2.03	0.92
4'	21.10	20.35	21.44	21.03	22.95	0.75	-0.34	0.07	-1.85
5'	55.80	56.53	48.06	59.48	56.32	-0.73	7.74	-3.68	-0.52
6'	36.70	37.70	35.85	34.21	37.06	-1.00	0.85	2.49	-0.36
7'	73.50	72.89	72.97	78.25	75.01	0.61	0.53	-4.75	-1.51
8'	21.80	21.62	20.60	18.84	23.51	0.18	1.20	2.96	-1.71
9'	39.20	42.51	37.43	37.12	44.29	-3.31	1.77	2.08	-5.09
					STD	1.90	2.31	2.54	2.04
					RMSD	1.38	1.52	1.59	1.43



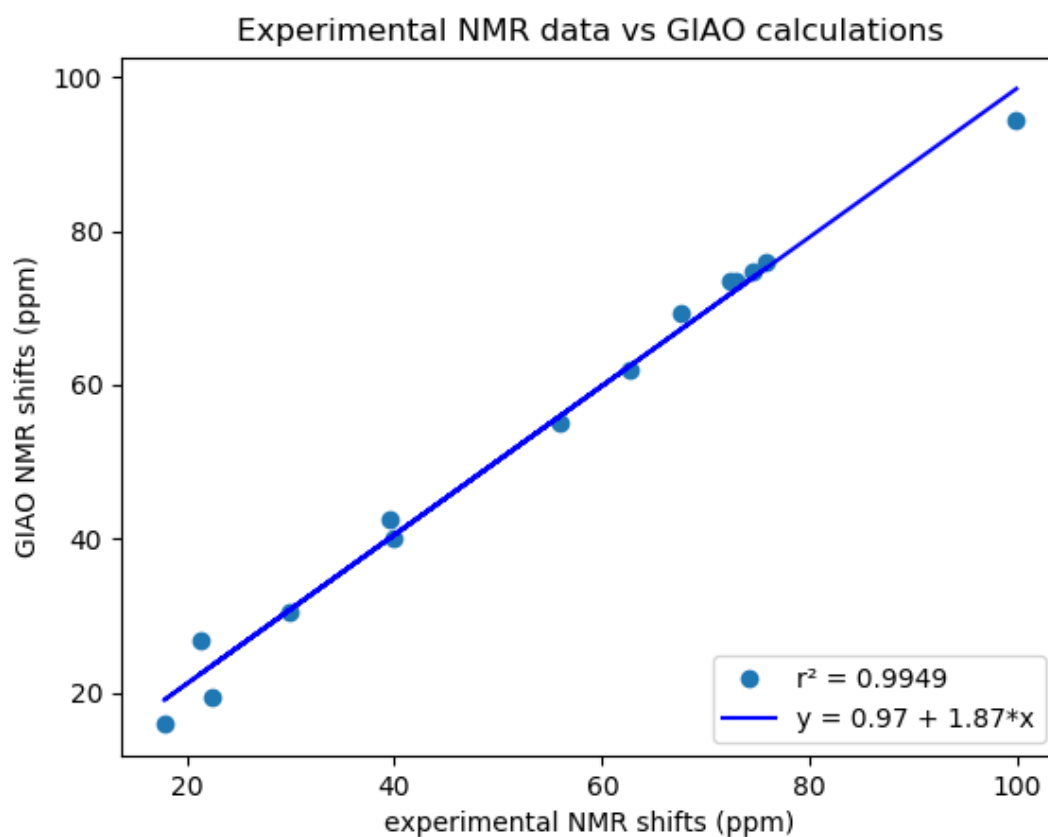
Compound 2

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm	
1	100.20	99.96	101.03	99.09	102.67	0.24	-0.83	1.11	-2.47	
2	68.30	67.17	66.01	66.34	68.86	1.13	2.29	1.96	-0.56	
3	69.60	66.65	71.99	72.18	68.36	2.95	-2.39	-2.58	1.24	
4	71.70	69.63	72.49	67.00	73.47	2.07	-0.79	4.70	-1.77	
5	66.10	66.31	62.30	62.86	59.17	-0.21	3.80	3.24	6.93	
6	16.50	17.67	16.17	18.97	19.59	-1.17	0.33	-2.47	-3.09	
2'	62.50	65.78	63.90	60.20	63.75	-3.28	-1.40	2.30	-1.25	
3'	30.20	24.82	29.92	31.18	29.74	5.38	0.28	-0.98	0.46	
4'	21.40	18.47	22.52	24.10	20.25	2.93	-1.12	-2.70	1.15	
5'	56.40	51.84	54.04	55.60	59.14	4.56	2.36	0.80	-2.74	
6'	40.60	43.83	39.66	43.58	40.86	-3.23	0.94	-2.98	-0.26	
7'	74.10	73.83	73.89	76.19	68.94	0.27	0.21	-2.09	5.16	
8'	22.50	26.17	23.41	19.68	24.03	-3.67	-0.91	2.82	-1.53	
9'	39.90	37.12	35.29	39.67	40.93	2.78	4.61	0.23	-1.03	
						STD	2.78	1.98	2.46	2.79
						RMSD	1.67	1.41	1.57	1.67



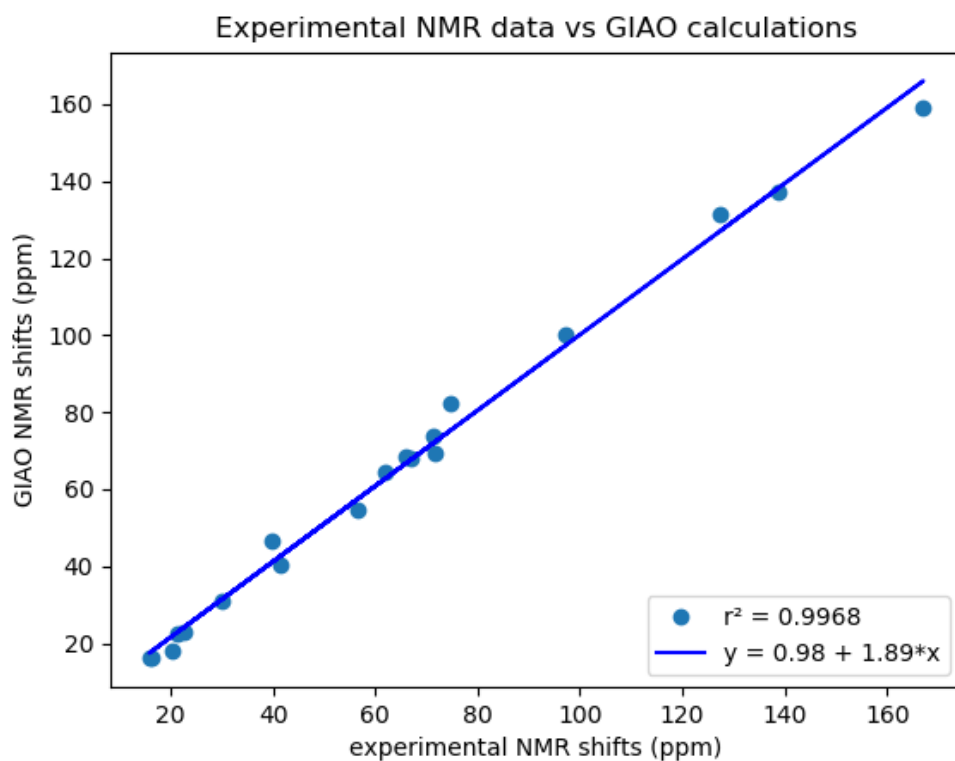
Compound 3

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	99.90	94.46	97.45	99.24	103.64	5.44	2.45	0.66	-3.74
2	72.30	73.42	71.84	70.97	73.84	-1.12	0.46	1.33	-1.54
3	72.90	73.49	73.29	72.68	75.37	-0.59	-0.39	0.22	-2.47
4	75.80	75.85	76.22	74.66	73.09	-0.05	-0.42	1.14	2.71
5	67.50	69.32	67.06	63.88	69.21	-1.82	0.44	3.62	-1.71
6	17.80	15.94	20.59	20.28	22.74	1.86	-2.79	-2.48	-4.94
2'	62.70	62.00	62.43	64.17	59.92	0.70	0.27	-1.47	2.78
3'	29.90	30.60	26.55	27.56	25.96	-0.70	3.35	2.34	3.94
4'	21.30	26.79	22.31	23.98	23.12	-5.49	-1.01	-2.68	-1.82
5'	56.00	55.01	53.49	51.75	54.73	0.99	2.51	4.25	1.27
6'	40.00	40.15	42.90	44.46	40.30	-0.15	-2.90	-4.46	-0.30
7'	74.50	74.65	78.30	73.39	73.00	-0.15	-3.80	1.11	1.50
8'	22.50	19.39	23.25	24.05	21.83	3.11	-0.75	-1.55	0.67
9'	39.50	42.67	38.09	37.51	38.17	-3.17	1.41	1.99	1.33
					STD	2.53	2.04	2.42	2.53
					RMSD	1.59	1.43	1.56	1.59



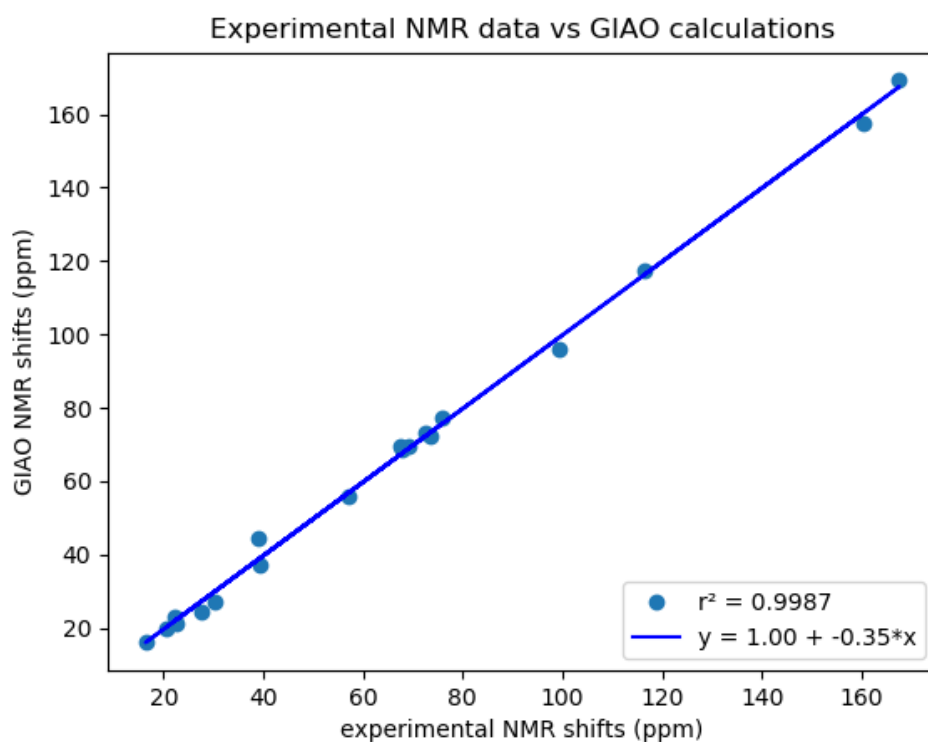
Compound 4

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	97.20	99.94	95.75	100.50	97.01	-2.74	1.45	-3.30	0.19
2	71.40	73.71	69.82	68.76	72.63	-2.31	1.58	2.64	-1.23
3	66.90	67.96	65.19	63.93	63.79	-1.06	1.71	2.97	3.11
4	71.80	69.33	70.70	71.22	73.71	2.47	1.10	0.58	-1.91
5	66.00	68.33	67.92	63.35	68.35	-2.33	-1.92	2.65	-2.35
6	16.30	16.05	18.77	11.76	18.79	0.25	-2.47	4.54	-2.49
2'	61.90	64.57	64.37	59.16	61.74	-2.67	-2.47	2.74	0.16
3'	30.10	31.07	26.83	29.81	32.17	-0.97	3.27	0.29	-2.07
4'	21.40	22.61	22.88	22.56	22.44	-1.21	-1.48	-1.16	-1.04
5'	56.60	54.42	55.27	57.83	54.82	2.18	1.33	-1.23	1.78
6'	41.30	40.23	44.23	46.19	38.79	1.07	-2.93	-4.89	2.51
7'	74.80	82.24	74.54	75.70	78.18	-7.44	0.26	-0.90	-3.38
8'	22.60	22.86	19.72	17.91	20.18	-0.26	2.88	4.69	2.42
9'	39.90	46.58	44.94	40.45	42.32	-6.68	-5.04	-0.55	-2.42
1''	167.10	159.06	166.58	171.52	164.95	8.04	0.52	-4.42	2.15
2''	127.30	131.60	128.28	127.43	127.17	-4.30	-0.98	-0.13	0.13
3''	138.70	137.31	139.88	137.19	140.72	1.39	-1.18	1.51	-2.02
4''	15.80	16.18	9.78	13.66	16.45	-0.38	6.02	2.14	-0.65
5''	20.40	17.95	25.33	16.64	15.15	2.45	-4.93	3.76	5.25
					STD	3.41	2.76	2.76	2.31
					RMSD	1.85	1.66	1.66	1.52



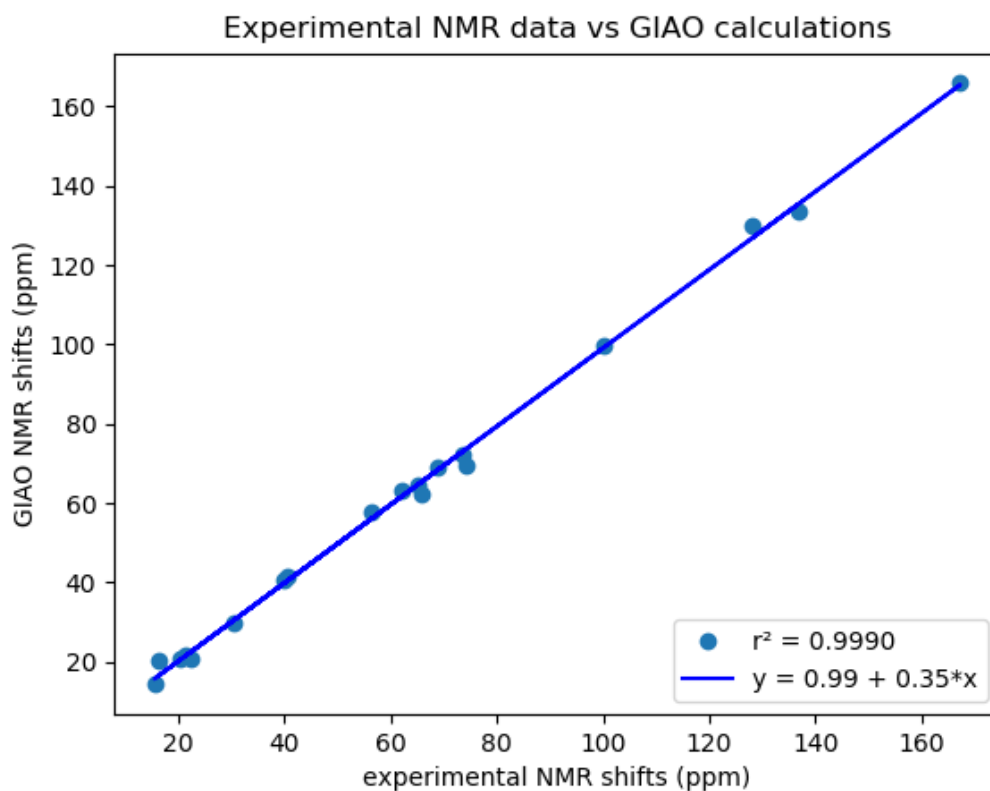
Compound 5

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	99.40	95.87	98.95	99.99	99.83	3.53	0.45	-0.59	-0.43
2	72.40	73.30	74.13	73.26	71.70	-0.90	-1.73	-0.86	0.70
3	69.10	69.75	68.95	67.78	65.18	-0.65	0.15	1.32	3.92
4	73.70	72.09	76.66	72.25	74.94	1.61	-2.96	1.45	-1.24
5	67.90	68.68	70.60	69.38	70.95	-0.78	-2.70	-1.48	-3.05
6	16.40	16.32	15.80	19.21	17.31	0.08	0.60	-2.81	-0.91
2'	67.40	69.75	68.74	68.43	70.04	-2.35	-1.34	-1.03	-2.64
3'	30.30	27.26	30.51	29.19	24.68	3.04	-0.21	1.11	5.62
4'	22.20	23.00	19.48	22.28	21.61	-0.80	2.72	-0.08	0.59
5'	57.10	55.75	57.16	60.63	53.04	1.35	-0.06	-3.53	4.06
6'	39.00	44.29	39.21	36.93	39.84	-5.29	-0.21	2.07	-0.84
7'	75.90	77.20	77.26	80.34	76.73	-1.30	-1.36	-4.44	-0.83
8'	22.50	21.18	22.68	19.17	21.73	1.32	-0.18	3.33	0.77
9'	39.40	37.43	42.54	36.66	37.93	1.97	-3.14	2.74	1.47
1''	167.60	169.18	167.91	166.59	173.87	-1.58	-0.31	1.01	-6.27
2''	116.50	117.49	120.34	118.01	113.41	-0.99	-3.84	-1.51	3.09
3''	160.50	157.66	158.84	161.16	154.25	2.84	1.66	-0.66	6.25
4''	27.50	24.26	27.08	23.20	26.56	3.24	0.42	4.30	0.94
5''	20.50	19.80	23.31	17.33	22.31	0.70	-2.81	3.17	-1.81
					STD	2.18	1.70	2.34	3.03
					RMSD	1.48	1.30	1.53	1.74



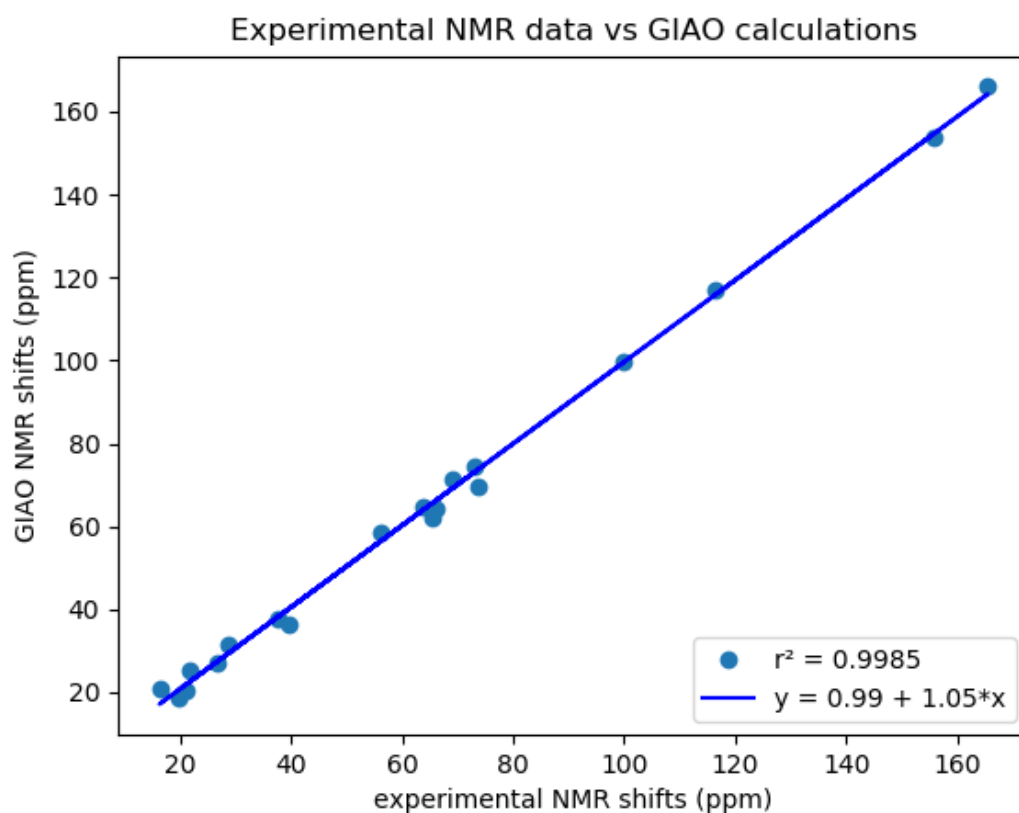
Compound 6

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm	
1	100.00	99.66	96.67	98.44	100.40	0.34	3.33	1.56	-0.40	
2	65.30	64.48	71.11	62.41	69.83	0.82	-5.81	2.89	-4.53	
3	73.50	72.14	68.41	72.32	74.12	1.36	5.09	1.18	-0.62	
4	68.90	69.13	71.71	60.71	70.26	-0.23	-2.81	8.19	-1.36	
5	65.80	62.27	67.83	63.71	62.96	3.53	-2.03	2.09	2.84	
6	16.30	20.10	15.38	18.96	16.55	-3.80	0.92	-2.66	-0.25	
2'	62.20	63.27	63.13	59.76	59.34	-1.07	-0.93	2.44	2.86	
3'	30.40	29.55	34.09	28.99	33.48	0.85	-3.69	1.41	-3.08	
4'	21.50	21.70	23.75	22.53	18.67	-0.20	-2.25	-1.03	2.83	
5'	56.50	57.89	59.00	56.06	58.89	-1.39	-2.50	0.44	-2.39	
6'	40.70	41.53	46.85	38.92	39.18	-0.83	-6.15	1.78	1.52	
7'	74.10	69.61	77.43	69.31	74.00	4.49	-3.33	4.79	0.10	
8'	22.50	20.64	27.59	23.14	19.99	1.86	-5.09	-0.64	2.51	
9'	40.00	40.41	42.46	42.99	41.05	-0.41	-2.46	-2.99	-1.05	
1''	167.30	165.87	164.78	166.89	166.70	1.43	2.52	0.41	0.60	
2''	128.00	129.99	130.44	131.35	126.33	-1.99	-2.44	-3.35	1.67	
3''	136.80	133.34	136.54	135.47	132.21	3.46	0.26	1.33	4.59	
4''	15.50	14.25	14.61	10.76	13.74	1.25	0.89	4.74	1.76	
5''	20.30	20.83	23.84	16.63	20.56	-0.53	-3.54	3.67	-0.26	
						STD	1.97	2.98	2.79	2.26
						RMSD	1.40	1.73	1.67	1.50



Compound 7

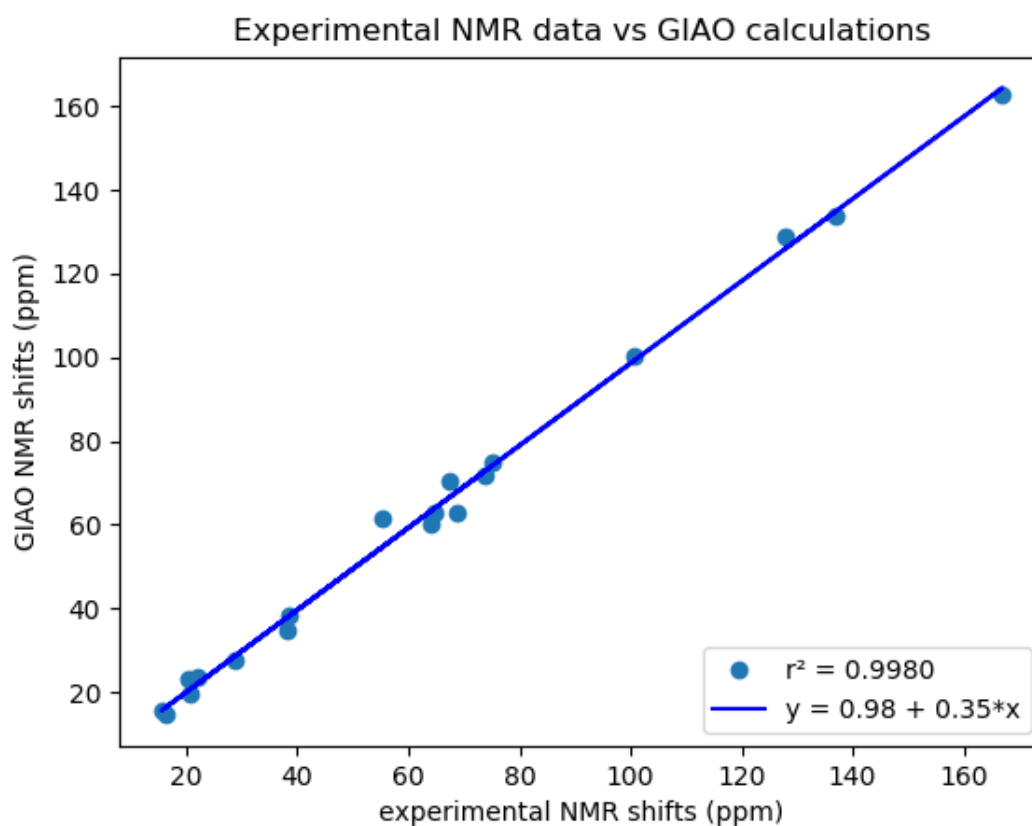
position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	100.00	99.74	99.92	99.21	97.80	0.26	0.08	0.79	2.20
2	65.40	61.86	63.18	64.93	62.89	3.54	2.22	0.47	2.51
3	73.00	74.54	75.46	70.95	68.30	-1.54	-2.46	2.05	4.70
4	69.20	71.52	71.21	73.52	69.84	-2.32	-2.01	-4.32	-0.64
5	66.20	64.28	66.28	67.58	66.43	1.92	-0.08	-1.38	-0.23
6	16.30	20.98	14.22	18.31	10.45	-4.68	2.08	-2.01	5.85
2'	63.80	64.61	62.81	62.47	63.40	-0.81	0.99	1.33	0.40
3'	28.70	31.50	32.25	30.49	25.95	-2.80	-3.55	-1.79	2.75
4'	21.20	20.61	20.85	16.97	18.18	0.59	0.35	4.23	3.02
5'	56.20	58.52	54.91	52.36	53.01	-2.32	1.29	3.84	3.19
6'	37.50	37.78	33.00	39.93	31.16	-0.28	4.50	-2.43	6.34
7'	73.70	69.46	70.18	65.19	78.48	4.24	3.52	8.51	-4.78
8'	21.90	25.19	16.44	19.84	23.83	-3.29	5.46	2.06	-1.93
9'	39.60	36.53	39.90	38.98	37.16	3.07	-0.30	0.62	2.44
1''	165.60	166.02	162.79	165.73	165.08	-0.42	2.81	-0.13	0.52
2''	116.30	117.19	114.99	110.40	111.75	-0.89	1.31	5.90	4.55
3''	155.90	153.62	154.65	159.54	161.70	2.28	1.25	-3.64	-5.80
4''	26.80	27.05	29.05	21.98	22.73	-0.25	-2.25	4.82	4.07
5''	19.90	18.75	17.22	18.78	14.99	1.15	2.68	1.12	4.91
					STD	2.36	2.34	3.26	3.26
					RMSD	1.54	1.53	1.81	1.81



Compound 8

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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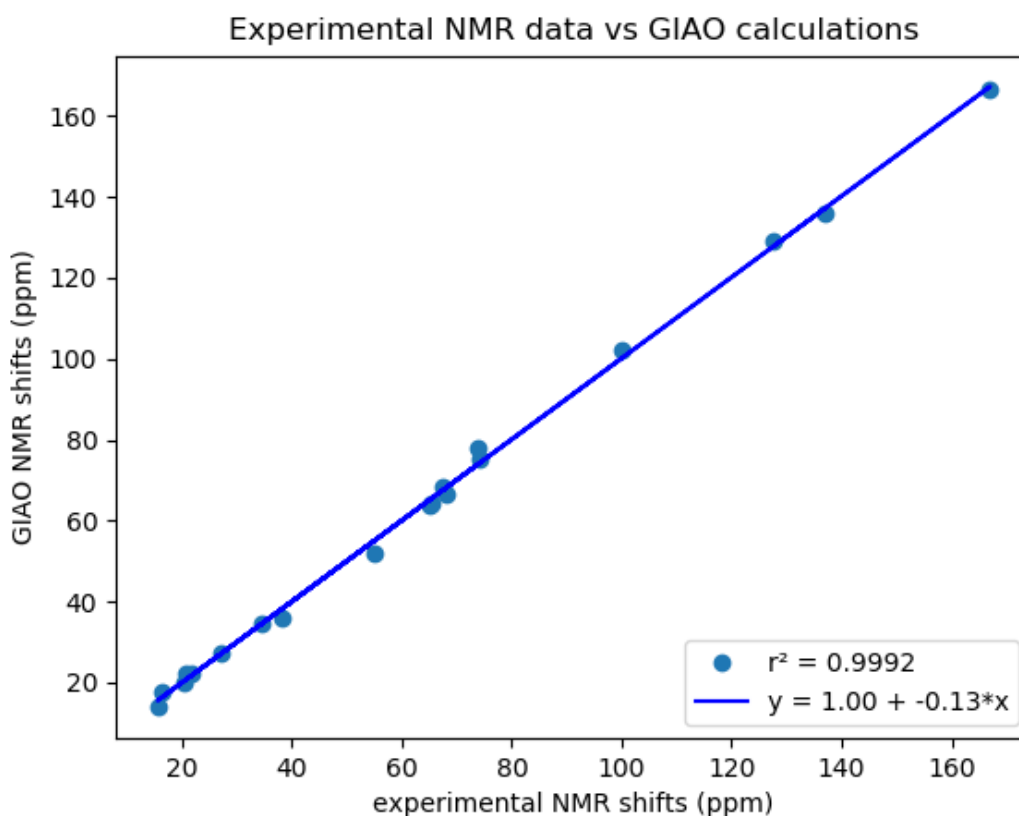
1	100.60	100.39	94.15	99.96	100.08	0.21	6.45	0.64	0.52	
2	68.80	62.93	70.57	68.39	71.63	5.87	-1.77	0.41	-2.83	
3	67.40	70.62	67.12	68.76	74.41	-3.22	0.28	-1.36	-7.01	
4	73.90	71.68	75.24	71.79	69.09	2.22	-1.34	2.11	4.81	
5	64.80	62.75	68.78	66.96	62.46	2.05	-3.98	-2.16	2.34	
6	16.20	14.52	18.63	13.42	14.44	1.68	-2.43	2.78	1.76	
2'	64.00	60.33	62.80	65.90	62.61	3.67	1.20	-1.90	1.39	
3'	28.90	27.67	28.88	27.17	28.47	1.23	0.02	1.73	0.43	
4'	20.80	19.81	22.27	20.49	20.03	0.99	-1.47	0.31	0.77	
5'	55.30	61.38	54.63	55.28	54.17	-6.08	0.67	0.02	1.13	
6'	38.20	34.80	33.00	40.98	33.62	3.40	5.20	-2.78	4.58	
7'	75.00	74.83	76.67	70.57	69.84	0.17	-1.67	4.43	5.16	
8'	22.20	23.54	19.27	19.39	18.72	-1.34	2.93	2.81	3.48	
9'	38.50	38.36	40.21	40.66	41.93	0.14	-1.71	-2.16	-3.43	
1''	167.00	162.93	164.30	173.03	171.31	4.07	2.70	-6.03	-4.31	
2''	127.80	128.80	125.78	128.23	125.68	-1.00	2.02	-0.43	2.12	
3''	136.80	133.86	140.78	136.18	138.10	2.94	-3.98	0.62	-1.30	
4''	15.50	15.49	17.79	22.29	18.82	0.01	-2.29	-6.79	-3.32	
5''	20.40	23.11	19.97	23.59	20.62	-2.71	0.43	-3.19	-0.22	
						STD	2.77	2.78	2.84	3.23
						RMSD	1.66	1.67	1.68	1.80



Compound 9

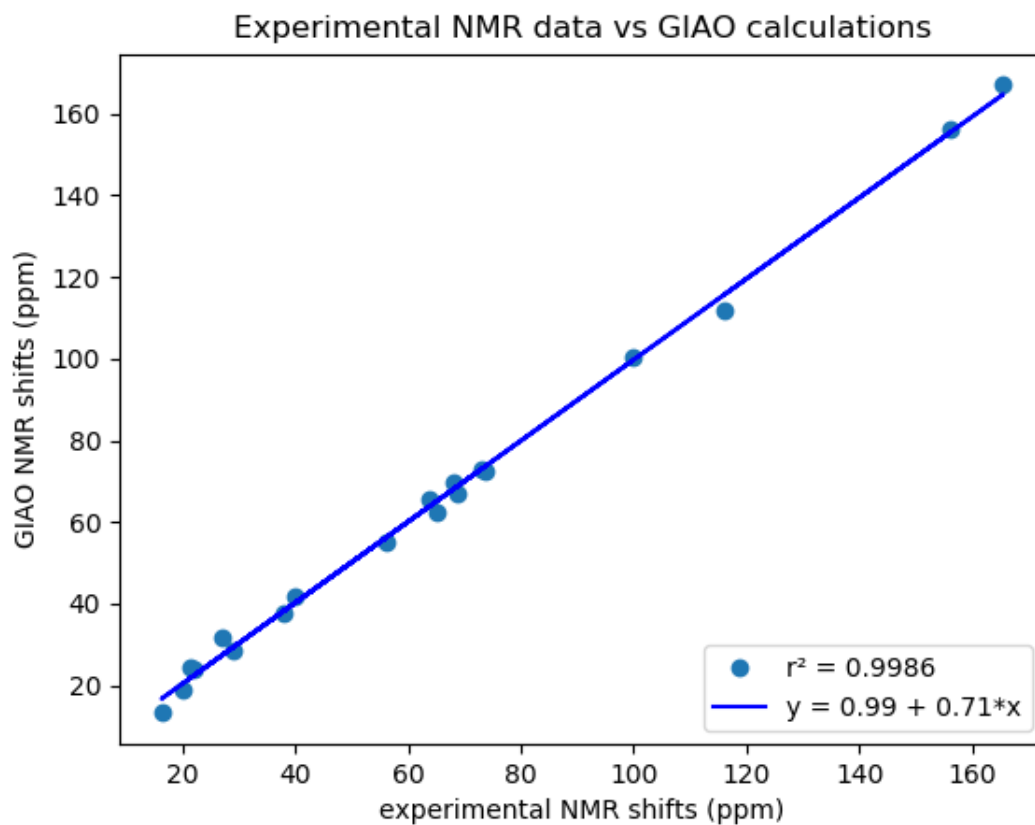
position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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1	100.10	102.34	101.02	101.88	104.57	-2.24	-0.92	-1.78	-4.47	
2	68.30	66.72	67.73	69.18	70.81	1.58	0.57	-0.88	-2.51	
3	67.60	68.27	73.69	65.33	70.34	-0.67	-6.09	2.27	-2.74	
4	73.80	78.08	74.00	73.97	77.25	-4.28	-0.20	-0.17	-3.45	
5	65.20	63.68	65.57	67.52	63.22	1.52	-0.37	-2.32	1.98	
6	16.30	17.82	15.72	21.10	14.65	-1.52	0.58	-4.80	1.65	
2'	65.50	64.35	69.45	71.68	72.45	1.15	-3.95	-6.18	-6.95	
3'	27.30	27.06	28.36	22.14	28.95	0.24	-1.06	5.16	-1.65	
4'	20.70	22.47	19.67	16.54	18.28	-1.77	1.03	4.16	2.42	
5'	55.20	52.15	52.26	55.45	54.19	3.05	2.94	-0.25	1.01	
6'	34.60	34.68	34.03	37.54	38.59	-0.08	0.57	-2.94	-3.99	
7'	74.10	75.44	72.49	74.52	70.62	-1.34	1.61	-0.42	3.48	
8'	21.70	22.46	21.60	26.24	19.50	-0.76	0.10	-4.54	2.20	
9'	38.10	36.00	33.67	38.28	33.48	2.10	4.43	-0.18	4.62	
1''	167.00	166.37	170.84	166.27	166.14	0.63	-3.84	0.73	0.86	
2''	127.70	129.27	128.23	120.79	125.98	-1.57	-0.53	6.91	1.72	
3''	137.10	135.97	134.80	140.69	136.26	1.13	2.30	-3.59	0.84	
4''	15.60	13.85	13.25	20.42	11.39	1.75	2.35	-4.82	4.21	
5''	20.50	20.05	19.99	14.76	20.15	0.45	0.51	5.74	0.35	
						STD	1.76	2.45	3.72	3.13
						RMSD	1.33	1.56	1.93	1.77



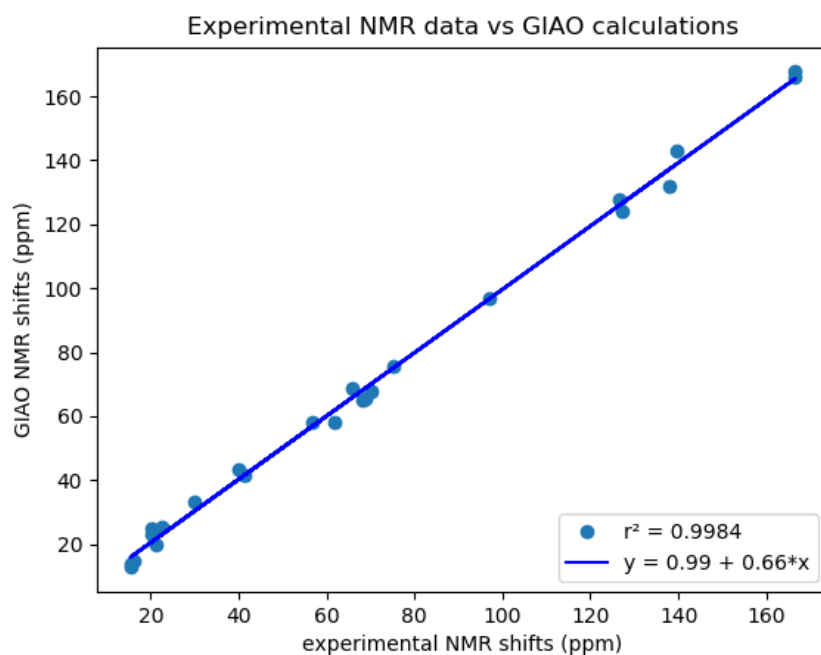
Compound **10**

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm	
1	99.90	100.13	100.79	96.57	97.66	-0.23	-0.89	3.33	2.24	
2	68.60	66.88	61.24	67.77	71.82	1.72	7.36	0.83	-3.22	
3	68.00	69.78	61.70	71.13	67.67	-1.78	6.30	-3.13	0.33	
4	73.00	73.01	71.08	68.21	71.92	-0.01	1.92	4.79	1.08	
5	64.90	62.21	58.34	63.98	61.29	2.69	6.56	0.92	3.61	
6	16.20	13.29	15.29	13.88	13.48	2.91	0.91	2.32	2.72	
2'	63.70	65.45	63.76	58.19	65.83	-1.75	-0.06	5.51	-2.13	
3'	29.10	28.35	27.21	33.14	30.30	0.75	1.89	-4.04	-1.20	
4'	21.30	24.49	24.09	25.52	20.35	-3.19	-2.79	-4.22	0.95	
5'	56.20	55.29	57.54	47.43	52.48	0.91	-1.34	8.77	3.72	
6'	38.00	37.91	36.43	35.35	41.21	0.09	1.57	2.65	-3.21	
7'	73.80	72.32	72.07	74.50	75.53	1.48	1.73	-0.70	-1.73	
8'	21.90	24.12	23.46	26.49	25.30	-2.22	-1.56	-4.59	-3.40	
9'	39.80	41.78	36.98	38.92	39.91	-1.98	2.82	0.88	-0.11	
1''	165.60	166.94	165.18	170.08	167.11	-1.34	0.42	-4.48	-1.51	
2''	116.00	111.62	115.41	120.72	116.67	4.38	0.59	-4.72	-0.67	
3''	156.30	156.33	157.15	153.61	160.04	-0.03	-0.85	2.69	-3.74	
4''	26.90	31.99	27.38	30.53	27.52	-5.09	-0.48	-3.63	-0.62	
5''	20.00	18.86	20.64	19.49	19.20	1.14	-0.64	0.51	0.80	
						STD	2.24	2.75	3.86	2.28
						RMSD	1.50	1.66	1.97	1.51



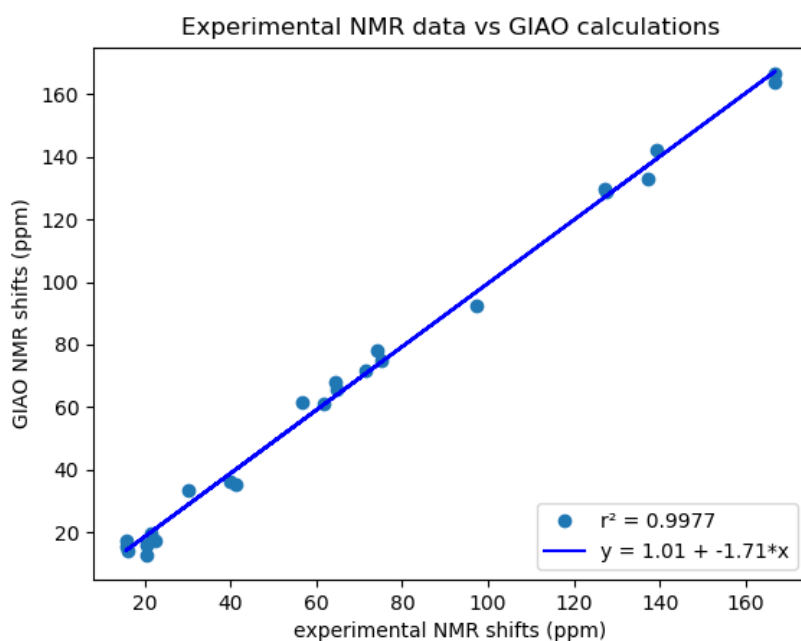
Compound 11

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	97.10	97.03	95.14	97.49	101.78	0.07	1.96	-0.39	-4.68
2	68.30	65.09	67.33	73.45	68.82	3.21	0.97	-5.15	-0.52
3	70.10	67.79	65.97	67.19	69.87	2.31	4.13	2.91	0.23
4	68.90	65.33	70.38	61.65	71.05	3.57	-1.48	7.25	-2.15
5	65.90	68.56	65.68	59.92	61.40	-2.66	0.22	5.98	4.50
6	16.10	15.03	16.13	12.70	14.86	1.07	-0.03	3.40	1.24
2'	61.80	58.32	63.12	64.50	53.94	3.48	-1.32	-2.70	7.86
3'	30.10	33.45	30.38	27.46	29.27	-3.35	-0.28	2.64	0.83
4'	21.40	19.88	20.13	19.38	23.16	1.52	1.27	2.02	-1.76
5'	56.70	57.96	58.34	56.06	56.68	-1.26	-1.64	0.64	0.02
6'	41.40	41.61	41.06	38.62	42.51	-0.21	0.34	2.78	-1.11
7'	75.30	75.58	78.71	76.49	75.16	-0.28	-3.41	-1.19	0.14
8'	22.70	25.48	23.81	21.34	26.63	-2.78	-1.11	1.36	-3.93
9'	39.90	43.54	42.15	35.63	42.08	-3.64	-2.25	4.27	-2.18
1''	166.50	166.10	164.13	164.42	168.27	0.40	2.37	2.08	-1.77
2''	127.30	124.01	124.64	131.61	127.57	3.29	2.66	-4.31	-0.27
3''	139.50	143.15	138.93	142.82	144.27	-3.65	0.57	-3.32	-4.77
4''	15.40	14.10	18.30	11.76	8.77	1.30	-2.90	3.64	6.63
5''	20.10	23.07	18.84	13.76	20.26	-2.97	1.26	6.34	-0.16
1'''	166.60	167.68	167.79	167.28	165.43	-1.08	-1.19	-0.68	1.17
2'''	126.70	127.91	125.48	131.28	127.94	-1.21	1.22	-4.58	-1.24
3'''	137.80	132.01	135.83	136.69	141.19	5.79	1.97	1.11	-3.39
4'''	15.60	12.78	13.15	17.91	15.51	2.82	2.45	-2.31	0.09
5'''	20.20	24.79	18.70	16.16	18.73	-4.59	1.50	4.04	1.47
					STD	2.78	1.87	3.46	3.04
					RMSD	1.67	1.37	1.86	1.74



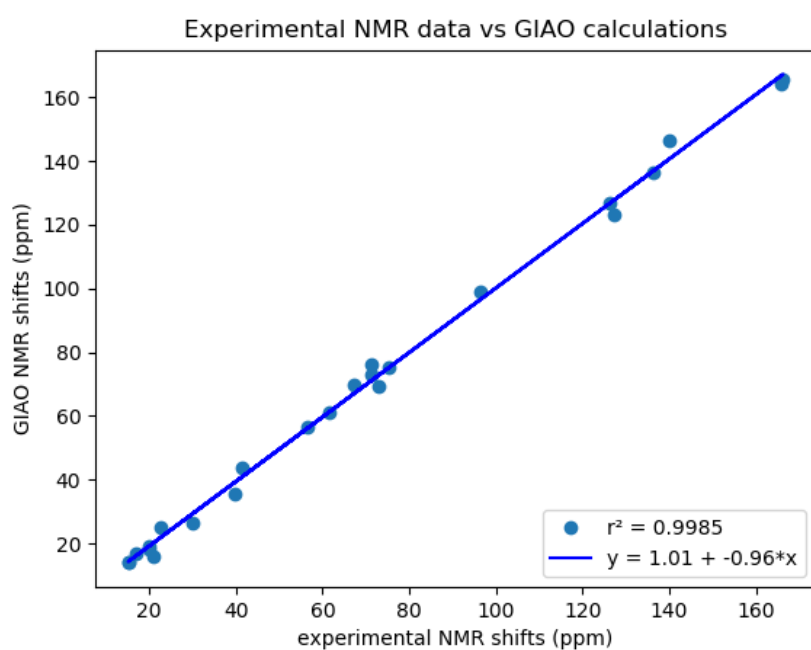
Compound 12

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	97.20	92.42	93.77	92.76	98.50	4.78	3.43	4.44	-1.30
2	71.40	71.47	75.44	72.41	78.61	-0.07	-4.04	-1.01	-7.21
3	64.70	65.79	64.16	65.52	62.66	-1.09	0.54	-0.82	2.04
4	74.00	77.92	74.10	81.52	74.44	-3.92	-0.10	-7.52	-0.44
5	64.50	67.96	65.65	69.09	62.35	-3.46	-1.15	-4.59	2.15
6	16.10	14.18	20.61	10.88	17.16	1.92	-4.51	5.22	-1.06
2'	61.80	61.09	62.43	56.88	68.76	0.71	-0.63	4.92	-6.96
3'	30.10	33.35	30.81	30.98	31.59	-3.25	-0.71	-0.88	-1.49
4'	21.30	19.51	23.89	22.51	24.36	1.79	-2.59	-1.21	-3.06
5'	56.60	61.43	57.49	55.84	55.04	-4.83	-0.89	0.76	1.56
6'	41.30	35.12	41.39	42.57	36.90	6.18	-0.09	-1.27	4.40
7'	75.30	75.00	74.96	70.76	70.18	0.30	0.34	4.54	5.12
8'	22.60	17.41	18.90	29.46	22.52	5.19	3.70	-6.86	0.08
9'	39.90	36.37	39.84	39.01	43.75	3.53	0.06	0.89	-3.85
1''	166.80	166.57	168.66	165.58	166.22	0.23	-1.86	1.22	0.58
2''	127.10	129.91	125.47	132.08	126.12	-2.81	1.63	-4.98	0.98
3''	139.30	142.00	136.26	134.41	142.36	-2.70	3.04	4.89	-3.06
4''	15.60	17.39	19.90	11.59	17.16	-1.79	-4.30	4.01	-1.56
5''	20.40	12.51	20.13	18.59	24.27	7.89	0.27	1.81	-3.87
1'''	166.90	163.83	165.12	169.96	167.82	3.07	1.78	-3.06	-0.92
2'''	127.60	128.69	125.24	123.13	121.52	-1.09	2.36	4.47	6.08
3'''	137.30	133.14	141.20	136.39	135.85	4.16	-3.90	0.91	1.45
4'''	15.70	15.36	13.61	11.79	12.94	0.34	2.09	3.91	2.76
5'''	20.40	15.88	22.05	18.40	23.99	4.52	-1.65	2.00	-3.59
STD						3.44	2.37	3.75	3.36
RMSD						1.85	1.54	1.94	1.83



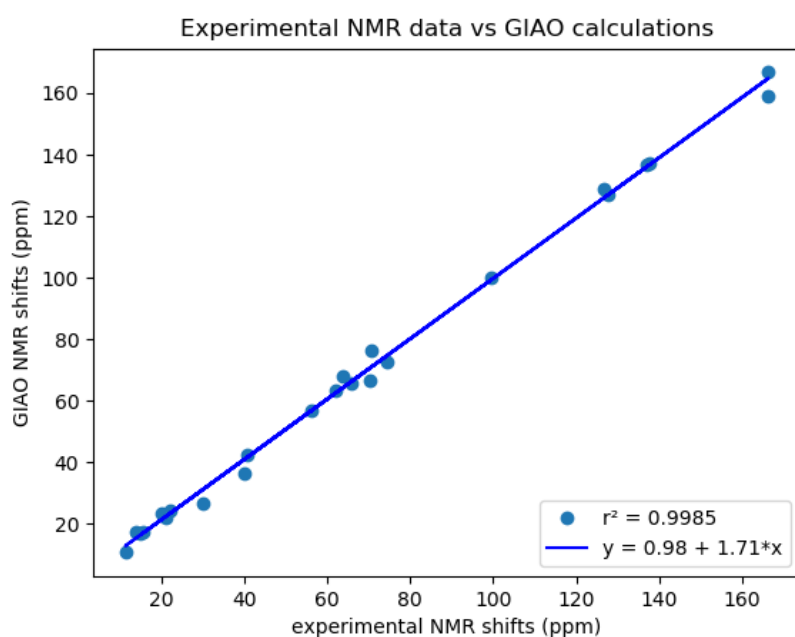
Compound 13

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	96.30	99.13	93.16	94.00	97.73	-2.83	3.14	2.30	-1.43
2	71.40	75.98	73.33	71.08	68.01	-4.58	-1.93	0.32	3.39
3	71.20	72.81	71.28	71.57	68.47	-1.61	-0.08	-0.37	2.73
4	72.90	69.34	80.45	77.58	69.50	3.56	-7.55	-4.68	3.40
5	67.30	69.79	69.48	68.69	72.39	-2.49	-2.18	-1.39	-5.09
6	17.00	17.07	16.32	21.16	15.04	-0.07	0.68	-4.16	1.96
2'	61.50	61.11	59.11	58.61	66.01	0.39	2.39	2.89	-4.51
3'	29.90	26.65	28.92	24.15	34.66	3.25	0.98	5.75	-4.76
4'	21.10	15.82	23.59	17.97	22.42	5.28	-2.49	3.13	-1.32
5'	56.40	56.59	51.88	54.71	63.12	-0.19	4.52	1.69	-6.72
6'	41.30	43.73	39.19	43.66	44.20	-2.43	2.11	-2.36	-2.90
7'	75.40	75.34	77.64	68.94	78.83	0.06	-2.24	6.46	-3.43
8'	22.50	24.94	25.21	20.71	22.71	-2.44	-2.71	1.79	-0.21
9'	39.70	35.47	42.24	42.70	44.41	4.23	-2.54	-3.00	-4.71
1''	165.90	164.14	167.03	163.34	167.19	1.76	-1.13	2.56	-1.29
2''	126.20	126.78	124.13	125.35	123.78	-0.58	2.07	0.85	2.42
3''	139.90	146.43	141.53	137.43	136.22	-6.53	-1.63	2.47	3.68
4''	15.40	14.26	14.77	16.24	11.11	1.14	0.63	-0.84	4.29
5''	19.80	19.33	16.67	22.66	15.78	0.47	3.13	-2.86	4.02
1'''	166.30	165.73	167.51	165.97	164.73	0.57	-1.21	0.33	1.57
2'''	127.20	123.01	131.44	129.82	127.62	4.19	-4.24	-2.62	-0.42
3'''	136.40	136.32	141.18	129.20	134.06	0.08	-4.78	7.20	2.34
4'''	15.10	13.98	13.53	10.87	14.92	1.12	1.57	4.23	0.18
5'''	20.00	18.27	20.81	15.37	16.96	1.73	-0.81	4.63	3.04
STD						2.80	2.80	3.27	3.33
RSMD						1.67	1.67	1.81	1.83



Compound **14**

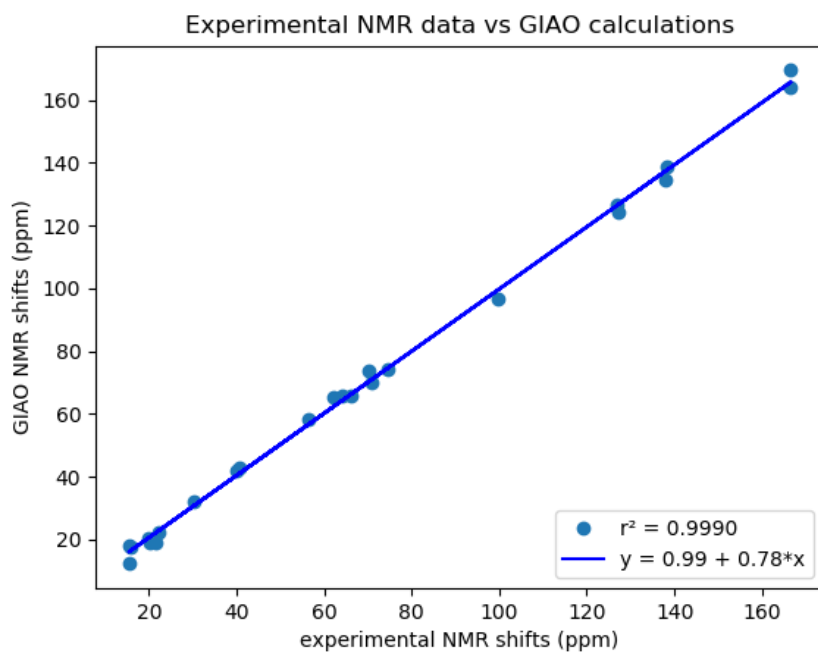
position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
1	99.50	99.87	106.18	98.22	100.03	-0.37	-6.68	1.28	-0.53
2	65.90	65.89	63.89	68.55	68.62	0.01	2.01	-2.65	-2.72
3	70.30	66.57	68.56	77.11	69.88	3.73	1.74	-6.81	0.42
4	70.60	76.40	68.39	65.40	66.99	-5.80	2.21	5.20	3.61
5	63.80	68.21	61.16	61.08	64.66	-4.41	2.64	2.72	-0.86
6	15.60	17.22	13.99	15.51	10.37	-1.62	1.61	0.09	5.23
2'	61.90	63.35	56.31	57.50	58.87	-1.45	5.59	4.40	3.03
3'	30.10	26.87	24.92	32.53	30.59	3.23	5.18	-2.43	-0.49
4'	21.20	21.87	20.75	21.58	26.33	-0.67	0.45	-0.38	-5.13
5'	56.20	56.73	58.32	59.53	53.97	-0.53	-2.12	-3.33	2.23
6'	40.60	42.59	42.19	36.27	36.41	-1.99	-1.59	4.33	4.19
7'	74.40	72.73	77.37	69.51	72.87	1.67	-2.97	4.89	1.53
8'	22.10	24.30	15.92	18.49	22.02	-2.20	6.18	3.61	0.08
9'	39.90	36.41	42.27	39.41	41.08	3.49	-2.37	0.49	-1.18
1''	166.10	166.78	161.09	169.09	167.67	-0.68	5.01	-2.99	-1.57
2''	127.60	126.93	129.85	126.24	131.19	0.67	-2.25	1.36	-3.59
3''	136.90	136.89	137.52	141.17	140.88	0.01	-0.62	-4.27	-3.98
4''	13.90	17.45	11.54	12.09	14.05	-3.55	2.36	1.81	-0.15
5''	11.40	10.75	5.44	11.62	13.25	0.65	5.96	-0.22	-1.85
1'''	166.30	159.18	166.28	167.27	161.16	7.12	0.02	-0.97	5.14
2'''	126.80	128.91	130.46	126.60	131.94	-2.11	-3.66	0.20	-5.14
3'''	137.50	137.10	141.90	139.02	137.66	0.40	-4.40	-1.52	-0.16
4'''	15.10	17.08	14.21	9.55	11.63	-1.98	0.89	5.55	3.47
5'''	20.00	23.57	26.81	20.19	22.65	-3.57	-6.81	-0.19	-2.65
STD						2.80	3.72	3.19	3.01
RMSD						1.67	1.93	1.79	1.73



Compound 15

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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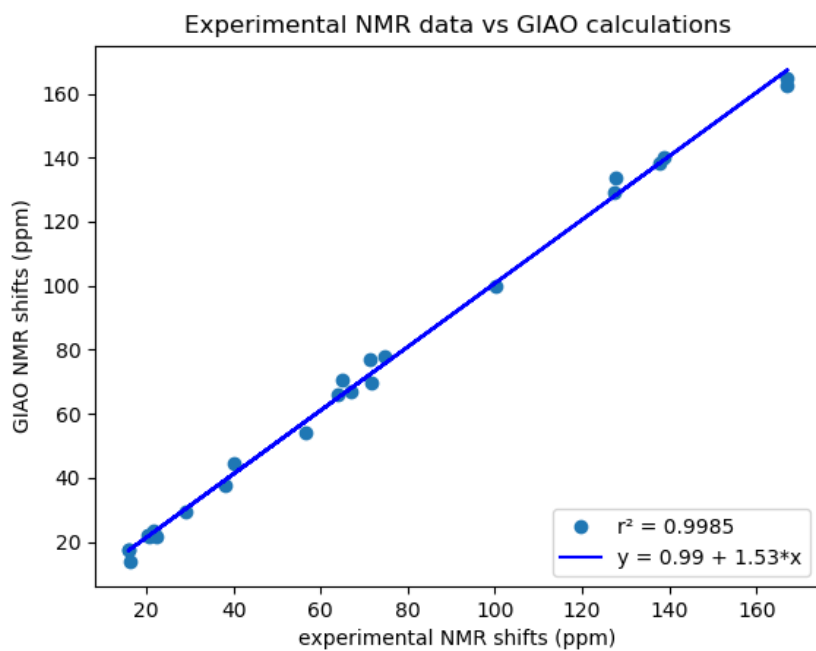
1	99.70	96.45	101.69	93.67	99.60	3.25	-1.99	6.03	0.10
2	66.20	65.65	71.15	68.31	70.74	0.55	-4.95	-2.11	-4.54
3	70.30	73.69	70.80	74.81	68.50	-3.39	-0.50	-4.51	1.80
4	71.00	69.87	69.82	69.60	72.36	1.13	1.18	1.40	-1.36
5	64.10	65.58	64.95	61.73	61.10	-1.48	-0.85	2.37	3.00
6	15.90	17.54	20.24	12.16	13.61	-1.64	-4.34	3.74	2.29
2'	62.20	65.22	60.32	60.58	55.85	-3.02	1.88	1.62	6.35
3'	30.40	32.13	28.47	30.41	30.47	-1.73	1.93	-0.01	-0.07
4'	21.50	18.81	26.23	29.36	26.64	2.69	-4.73	-7.86	-5.14
5'	56.50	58.19	49.22	58.79	57.12	-1.69	7.28	-2.29	-0.62
6'	40.70	42.92	39.12	44.04	43.64	-2.22	1.58	-3.34	-2.94
7'	74.60	74.35	78.12	81.22	72.70	0.25	-3.52	-6.62	1.90
8'	22.40	22.18	19.28	25.85	23.99	0.22	3.12	-3.45	-1.59
9'	40.00	41.85	39.12	43.50	44.28	-1.85	0.88	-3.50	-4.28
1''	166.50	164.14	167.12	166.80	166.25	2.36	-0.62	-0.30	0.25
2''	127.30	124.16	127.58	125.25	128.91	3.14	-0.28	2.05	-1.61
3''	137.80	134.34	136.48	137.22	132.56	3.46	1.32	0.58	5.24
4''	15.40	12.29	14.35	12.54	16.53	3.11	1.05	2.86	-1.13
5''	19.90	20.50	17.70	23.13	23.32	-0.60	2.20	-3.23	-3.42
1'''	166.60	169.42	162.75	167.58	168.44	-2.82	3.85	-0.98	-1.84
2'''	127.00	126.51	123.80	130.40	124.18	0.49	3.20	-3.40	2.82
3'''	138.20	138.67	136.34	143.71	143.69	-0.47	1.86	-5.51	-5.49
4'''	15.50	18.12	14.45	17.63	19.14	-2.62	1.05	-2.13	-3.64
5'''	20.30	18.99	16.52	17.54	23.39	1.31	3.78	2.76	-3.09
					STD	2.18	2.90	3.43	3.13
					RMSD	1.47	1.70	1.85	1.77



Compound 16

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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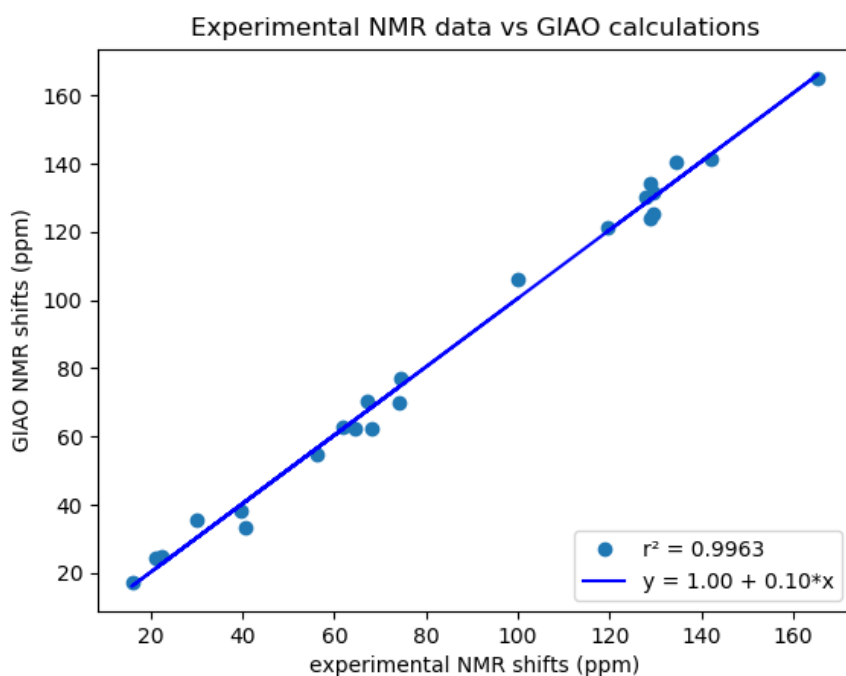
1	100.20	99.73	97.81	100.06	96.81	0.47	2.39	0.14	3.39
2	66.80	67.03	67.68	67.12	70.00	-0.23	-0.88	-0.32	-3.20
3	71.20	77.24	70.59	72.53	72.91	-6.04	0.61	-1.33	-1.71
4	71.50	69.65	73.08	72.04	69.12	1.85	-1.58	-0.54	2.38
5	64.90	70.51	65.36	66.19	68.71	-5.61	-0.46	-1.29	-3.81
6	16.40	13.73	18.47	15.68	14.64	2.67	-2.07	0.72	1.76
2'	64.10	66.21	65.80	67.78	62.40	-2.11	-1.70	-3.68	1.70
3'	29.20	29.54	26.47	30.70	25.91	-0.34	2.73	-1.50	3.29
4'	21.70	23.53	24.58	20.06	25.97	-1.83	-2.88	1.64	-4.27
5'	56.70	54.16	58.19	51.74	52.16	2.54	-1.49	4.96	4.54
6'	38.10	37.65	40.07	36.19	38.55	0.45	-1.97	1.91	-0.45
7'	74.60	77.95	69.15	73.77	75.94	-3.35	5.45	0.83	-1.34
8'	22.30	21.63	20.54	23.61	19.33	0.67	1.76	-1.31	2.97
9'	40.20	44.46	37.63	38.97	45.81	-4.26	2.57	1.23	-5.61
1''	167.00	164.87	164.90	169.42	166.72	2.13	2.10	-2.42	0.28
2''	127.80	133.86	126.52	130.38	124.62	-6.06	1.28	-2.58	3.18
3''	137.90	138.45	138.04	134.96	145.89	-0.55	-0.14	2.94	-7.99
4''	15.80	17.54	10.20	14.00	13.14	-1.74	5.60	1.80	2.66
5''	20.40	22.02	19.46	21.35	20.41	-1.62	0.94	-0.95	-0.01
1'''	167.10	162.30	166.86	167.78	167.36	4.80	0.24	-0.68	-0.26
2'''	127.50	129.15	126.64	128.95	128.39	-1.65	0.86	-1.45	-0.89
3'''	138.60	140.19	138.25	137.19	134.88	-1.59	0.35	1.41	3.72
4'''	16.00	17.72	16.11	14.30	16.60	-1.72	-0.11	1.70	-0.60
5'''	20.70	21.69	24.50	14.19	21.93	-0.99	-3.80	6.51	-1.23
					STD	2.73	2.31	2.31	3.16
					RMSD	1.65	1.52	1.52	1.78



Compound 17

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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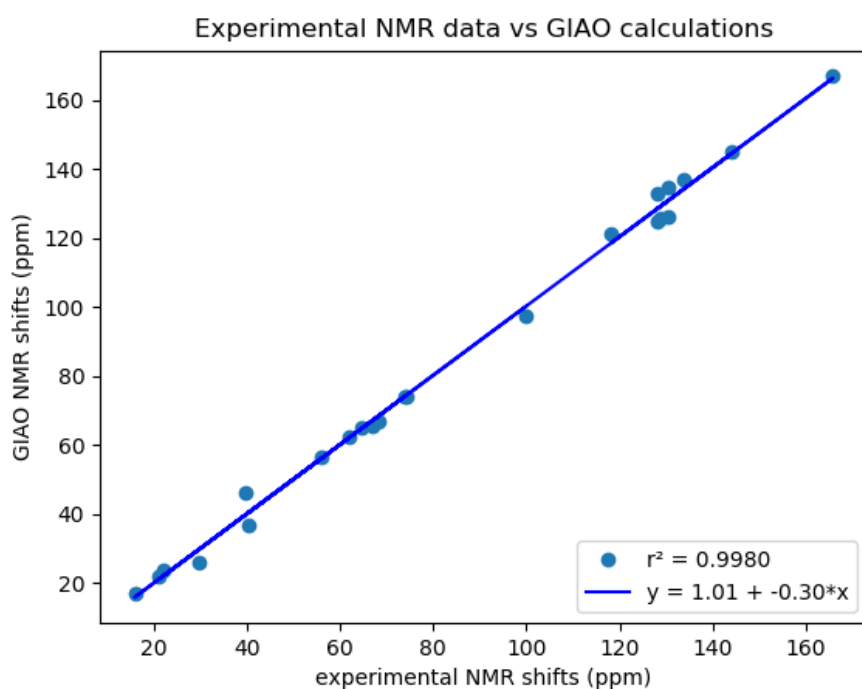
1	100.00	106.20	96.92	98.28	102.81	-6.20	3.08	1.72	-2.81
2	68.20	62.17	70.00	69.73	66.63	6.03	-1.80	-1.53	1.57
3	67.10	70.55	68.02	64.92	65.33	-3.45	-0.92	2.18	1.77
4	74.00	69.79	76.53	75.25	75.09	4.21	-2.53	-1.25	-1.09
5	64.40	62.23	63.92	61.16	70.04	2.17	0.48	3.24	-5.64
6	16.00	17.06	15.52	20.81	15.56	-1.06	0.48	-4.81	0.44
2'	62.00	62.87	60.88	63.55	62.78	-0.87	1.12	-1.55	-0.78
3'	30.00	35.56	30.35	31.90	28.96	-5.56	-0.35	-1.90	1.04
4'	21.20	24.39	23.83	22.99	15.62	-3.19	-2.63	-1.79	5.58
5'	56.20	54.97	56.92	57.14	54.92	1.23	-0.72	-0.94	1.28
6'	40.60	33.39	40.63	44.15	42.09	7.21	-0.03	-3.55	-1.49
7'	74.30	77.04	74.79	73.85	77.05	-2.74	-0.49	0.45	-2.75
8'	22.30	24.75	26.19	23.66	21.38	-2.45	-3.89	-1.36	0.92
9'	39.70	38.24	38.27	36.93	38.41	1.46	1.43	2.77	1.29
1''	165.40	165.15	165.15	167.40	163.67	0.25	0.25	-2.00	1.73
2''	119.40	121.28	122.14	123.73	122.21	-1.88	-2.74	-4.33	-2.81
3''	141.90	141.49	142.73	140.94	144.91	0.41	-0.83	0.96	-3.01
4''	134.50	140.71	132.28	135.54	133.03	-6.21	2.22	-1.04	1.47
5''	129.60	131.46	126.39	130.89	126.55	-1.86	3.21	-1.29	3.05
6''	128.90	134.16	133.35	128.67	134.01	-5.26	-4.45	0.23	-5.11
7''	127.80	130.23	127.17	122.92	128.16	-2.43	0.63	4.88	-0.36
8''	128.90	123.93	126.66	131.02	130.95	4.97	2.24	-2.12	-2.05
9''	129.60	125.16	128.99	131.86	130.13	4.44	0.61	-2.26	-0.53
					STD	3.84	2.03	2.35	2.58
					RMSD	1.96	1.42	1.53	1.61



Compound 18

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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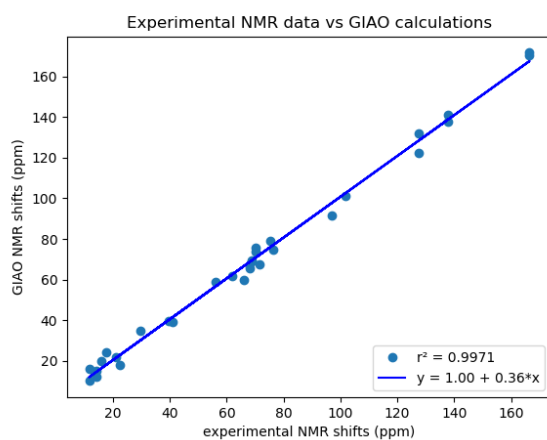
1	100.00	97.46	98.93	96.89	102.92	2.54	1.07	3.11	-2.92	
2	68.40	66.85	68.36	64.05	69.82	1.55	0.04	4.35	-1.42	
3	67.10	65.57	67.00	67.14	63.27	1.53	0.10	-0.04	3.83	
4	74.00	73.80	75.01	70.63	71.81	0.20	-1.01	3.37	2.19	
5	64.50	65.09	62.41	69.31	62.24	-0.59	2.09	-4.81	2.26	
6	16.00	16.79	19.40	15.76	14.33	-0.79	-3.40	0.24	1.67	
2'	62.10	62.16	60.43	60.63	68.06	-0.06	1.67	1.47	-5.96	
3'	29.90	25.92	30.11	27.03	28.55	3.98	-0.21	2.87	1.35	
4'	21.20	21.87	21.61	23.64	21.20	-0.67	-0.41	-2.44	-0.00	
5'	56.10	56.52	56.81	55.35	55.15	-0.42	-0.71	0.75	0.95	
6'	40.30	36.72	36.09	39.48	36.35	3.58	4.21	0.82	3.95	
7'	74.30	73.84	74.00	72.61	76.08	0.46	0.30	1.69	-1.78	
8'	22.10	23.48	23.86	23.83	22.18	-1.38	-1.76	-1.73	-0.08	
9'	39.60	46.23	36.20	33.90	36.41	-6.63	3.40	5.70	3.19	
1''	165.80	166.98	164.22	163.38	169.12	-1.18	1.58	2.42	-3.32	
2''	118.10	121.23	117.32	116.38	117.02	-3.13	0.78	1.72	1.08	
3''	144.20	145.11	147.69	149.10	142.24	-0.91	-3.49	-4.90	1.96	
4''	133.80	136.84	131.34	135.89	128.55	-3.04	2.46	-2.09	5.25	
5''	128.10	125.01	129.86	134.63	129.34	3.09	-1.76	-6.53	-1.24	
6''	130.30	134.81	130.32	134.07	131.93	-4.51	-0.02	-3.77	-1.63	
7''	128.70	125.91	121.21	129.12	132.24	2.79	7.49	-0.42	-3.54	
8''	130.30	126.23	130.65	129.50	129.84	4.07	-0.35	0.80	0.46	
9''	128.10	133.00	126.07	125.82	128.58	-4.90	2.03	2.28	-0.48	
						STD	2.85	2.38	3.08	2.67
						RMSD	1.69	1.54	1.76	1.64



Compound 19

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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1	96.80	91.39	95.14	94.10	93.23	5.41	1.66	2.70	3.57
2	68.20	65.64	70.39	63.56	67.52	2.56	-2.19	4.64	0.68
3	68.90	68.78	67.52	65.19	67.29	0.12	1.38	3.71	1.61
4	76.50	74.72	79.00	76.49	79.83	1.78	-2.50	0.01	-3.33
5	65.90	59.77	68.43	63.77	71.24	6.13	-2.53	2.13	-5.34
6	16.00	19.83	17.49	15.82	16.92	-3.83	-1.49	0.18	-0.92
2'	62.00	61.91	64.30	65.07	66.73	0.09	-2.30	-3.07	-4.73
3'	29.70	34.68	29.79	33.24	23.32	-4.98	-0.09	-3.54	6.38
4'	21.10	21.64	23.82	21.12	21.77	-0.54	-2.72	-0.02	-0.67
5'	56.20	58.81	56.39	54.02	56.79	-2.61	-0.19	2.18	-0.59
6'	40.80	39.20	40.00	35.91	40.38	1.60	0.80	4.89	0.42
7'	75.20	79.20	69.54	80.41	74.86	-4.00	5.66	-5.21	0.34
8'	22.30	17.95	23.37	21.56	19.78	4.35	-1.07	0.74	2.52
9'	39.60	39.70	36.83	38.83	35.54	-0.10	2.77	0.77	4.06
1''	166.50	170.57	169.16	167.81	169.81	-4.07	-2.66	-1.31	-3.31
2''	127.60	131.78	127.82	130.89	134.17	-4.18	-0.22	-3.29	-6.57
3''	138.00	137.54	131.70	140.72	137.65	0.46	6.30	-2.72	0.35
4''	14.00	12.18	9.65	10.70	12.68	1.82	4.35	3.30	1.32
5''	11.60	15.92	17.74	9.39	9.97	-4.32	-6.14	2.21	1.63
1'''	166.50	171.71	164.37	163.77	166.46	-5.21	2.13	2.73	0.04
2'''	127.60	122.58	126.72	126.42	119.01	5.02	0.88	1.18	8.59
3'''	138.00	141.32	144.15	139.20	136.27	-3.32	-6.15	-1.20	1.73
4'''	14.00	15.07	13.86	13.84	15.95	-1.07	0.14	0.16	-1.95
5'''	11.60	10.10	13.93	8.92	11.31	1.50	-2.33	2.68	0.29
1''''	101.60	101.26	101.36	101.22	103.94	0.34	0.24	0.38	-2.34
2''''	70.10	75.71	72.78	75.15	71.75	-5.61	-2.68	-5.05	-1.65
3''''	70.10	73.83	68.63	65.05	71.52	-3.73	1.47	5.05	-1.42
4''''	71.40	67.67	71.58	71.34	63.85	3.73	-0.18	0.06	7.55
5''''	68.90	69.40	68.89	71.69	76.35	-0.50	0.01	-2.79	-7.45
6''''	17.50	24.00	20.24	20.41	18.76	-6.50	-2.74	-2.91	-1.26
STD						3.52	2.85	2.85	3.68
RMSD						1.88	1.69	1.69	1.92



Compound 20

position	Exp	1a	1b	1c	1d	Δ ppm	Δ ppm	Δ ppm	Δ ppm
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1	96.90	101.72	92.00	97.09	97.08	-4.82	4.90	-0.19	-0.18
2	68.10	63.10	63.95	66.20	67.80	5.00	4.15	1.90	0.30
3	68.80	72.73	68.80	70.27	64.20	-3.93	-0.00	-1.47	4.60
4	76.30	76.65	75.57	70.91	84.34	-0.35	0.73	5.39	-8.04
5	66.10	69.02	64.19	62.96	67.37	-2.92	1.91	3.14	-1.27
6	16.20	16.52	14.42	11.02	16.84	-0.32	1.78	5.18	-0.64
2'	61.80	63.50	65.82	60.81	58.13	-1.70	-4.02	0.99	3.67
3'	30.10	34.48	31.68	24.88	33.30	-4.38	-1.58	5.22	-3.20
4'	21.40	21.28	18.14	25.40	20.06	0.12	3.26	-4.00	1.34
5'	56.70	53.20	54.59	58.69	55.57	3.50	2.11	-1.99	1.13
6'	41.50	43.70	38.66	42.02	41.49	-2.20	2.84	-0.52	0.01
7'	75.50	74.99	77.93	76.46	78.96	0.51	-2.43	-0.96	-3.46
8'	22.60	19.27	20.10	25.62	18.47	3.33	2.50	-3.02	4.13
9'	39.80	40.64	39.74	39.27	41.98	-0.84	0.06	0.53	-2.18
1''	166.20	170.54	168.39	170.41	163.14	-4.34	-2.19	-4.21	3.06
2''	126.30	125.21	123.43	122.05	127.25	1.09	2.87	4.25	-0.95
3''	140.40	144.16	137.69	140.72	140.43	-3.76	2.71	-0.32	-0.03
4''	15.80	16.28	18.31	19.34	21.09	-0.48	-2.51	-3.54	-5.29
5''	20.20	23.89	20.85	17.91	22.86	-3.69	-0.65	2.29	-2.66
1'''	166.50	167.98	170.02	166.44	167.34	-1.48	-3.52	0.06	-0.84
2'''	126.80	126.85	126.58	127.64	125.58	-0.05	0.22	-0.84	1.22
3'''	139.20	140.43	135.01	141.25	144.22	-1.23	4.19	-2.05	-5.02
4'''	15.80	11.19	17.98	12.71	11.88	4.61	-2.18	3.09	3.92
5'''	20.20	19.88	16.47	18.83	20.40	0.32	3.73	1.37	-0.20
1''''	101.80	102.74	102.94	106.96	103.49	-0.94	-1.14	-5.16	-1.69
2''''	70.30	71.43	67.62	67.04	72.05	-1.13	2.68	3.26	-1.75
3''''	70.40	68.87	71.45	73.58	71.94	1.53	-1.05	-3.18	-1.54
4''''	71.70	66.29	68.30	74.15	72.79	5.41	3.40	-2.45	-1.09
5''''	69.10	69.45	65.47	72.40	67.01	-0.35	3.63	-3.30	2.09
6''''	18.00	17.39	21.83	20.61	17.80	0.61	-3.83	-2.61	0.20
STD	2.74	2.65	3.01	2.85					
RMSD	1.66	1.63	1.73	1.69					

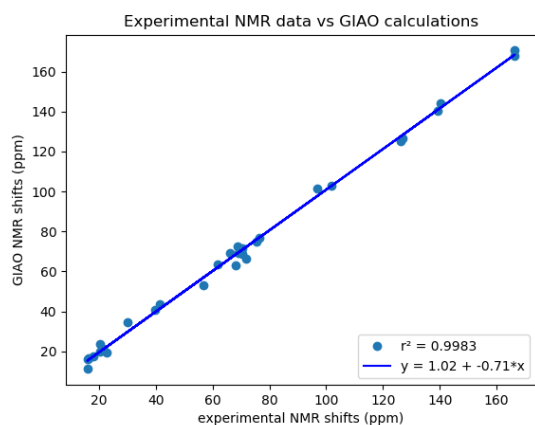


Table S3. ^1H and ^{13}C NMR data of compounds **1-3** (600 and 150 MHz, in CD_3OD , δ in ppm)

Position	1		2		3	
	δ_{H} , (<i>J</i> in Hz)	δ_{C} , type	δ_{H} , (<i>J</i> in Hz)	δ_{C} , type	δ_{H} , (<i>J</i> in Hz)	δ_{C} , type
1	4.94, d (4.2)	102.8, CH	4.91, d (4.2)	102.9, CH	4.81, d (4.0)	101.7, CH
2	3.80, dd (10.0, 4.2)	69.4, CH	3.81, dd (10.0, 4.2)	69.9, CH	3.40, dd (9.8, 3.9)	73.9, CH
3	3.58, dd (10.0, 3.6)	71.8, CH	3.67, dd (10.0, 3.7)	71.7, CH	3.53, t (9.3)	74.9, CH
4	3.68, dd (3.3, 1.2)	73.4, CH	3.69, m	73.5, CH	2.98, t (9.2)	77.4, CH
5	4.04, qd (6.6, 1.2)	68.5, CH	4.05, q (6.6)	68.2, CH	3.73, m	69.2, CH
6	1.20, d (6.6)	16.5, CH_3	1.20, d (6.6)	16.6, CH_3	1.21, d (6.3)	17.9, CH_3
2'	3.44, td (7.3, 3.9)	68.4, CH	3.72, m	68.2, CH	a	65.5, CH
3'	2.20, m	27.5, CH_2	2.33, dd (13.9, 7.2)	28.4, CH_2	a	
	2.04, m		1.83, m			
4'	2.11, dtd (8.4, 5.4, 2.7)	21.6, CH_2	2.10, p (7.8)	20.8, CH_2	a	
	2.04, m					
5'	3.58, d	56.6, CH_2	3.51, brs	55.8, CH_2	3.20, brs	57.1, CH_2
	3.05, dt (11.3, 8.6)		3.27, brs		2.60, brs	
	2.20, m		1.98, m			
6'	1.91, ddd (16.3, 4.1, 2.4)	34.0, CH_2	1.83, m	37.8, CH_2	a	
7'	4.13, ddd (10.6, 6.1, 2.5)	76.5, CH	3.85, m	79.0, CH	3.78, m	77.4, CH
8'	1.37, d (6.1)	22.2, CH_3	1.34, d (6.1)	22.6, CH_3	1.30, d (6.2)	22.9, CH_3
9'	2.90, s	38.3, CH_3	2.80, s	a	2.49, s	39.4, CH_3

^a Signal not observed

Table S4. ¹H NMR data of compounds **4-10** (600 MHz, in CD₃OD or * DMSO-*d*₆, δ in ppm, *J* in Hz)

Position	4	5*	6	7	8	9	10
1	5.12, d (3.9)	4.87, d (4.0)	4.97, d (4.0)	4.99, m	4.98, d (4.0)	5.02, d (3.8)	5.01, brs
2	4.95, dd (10.6, 3.9)	4.75, dd (10.0, 4.0)	4.10, dd (10.6, 4.0)	4.03, dd (10.4, 3.8)	3.81, dd (10.2, 4.0)	3.81, dd (10.1, 3.8)	3.79, s
3	3.98, dd (10.6, 3.4)	3.75, dd (10.0, 3.4)	5.12, brs	5.02, d (10.4)	3.91, dd (10.2, 3.4)	3.81, dd (10.1, 3.8)	3.79, s
4	3.72, d (3.4)	3.56, m	3.83, brs	3.76, d (3.1)	5.30, dd (3.5, 1.2)	5.29, dd (3.2, 1.3)	5.21, s
5	4.09, dd (6.6, 1.3)	3.90, q (6.6)	4.16, q (6.8)	4.15, m	4.23, dd (6.6, 1.2)	4.23, q (6.6)	4.20, m
6	1.22, d (6.6)	1.08, d (6.6)	1.21, d (6.6)	1.21, d (6.8)	1.07, d (6.6)	1.07, d (6.6)	1.05, d (6.3)
2'		a	a	3.42, brs	a	3.43, brs	3.44, brs
3'	2.08, m	1.82, m		2.21, m		2.22, m	2.23, m
	1.62, m	1.47, m	a	2.06, m	a	2.02, m	2.04, m
4'		1.72, m		2.10, m		2.13, m	2.12, m
		1.63, m	a	1.98, m	a	2.02, m	2.02, m
5'	3.40, brs			3.47, td (8.2, 4.0)		3.55, brs	3.56, brs
	2.68	a	a	3.03, d (10.0)	a	3.03, d (10.7)	3.06, d (9.8)
6'	2.08, m			2.26, m		2.22, m	2.23, m
	1.46, t	a	a	1.93, m	a	1.92, m	1.91, m
7'	3.70, m	3.58, m	3.90, brs	4.18, brs	3.88, m	4.16, d (7.5)	4.17, brs
8'	1.32, d (6.2)	1.19, d (6.1)	1.38, d (6.1)	1.40, d (6.3)	1.36, d (6.1)	1.38, d (6.1)	1.38, d (6.3)
9'	2.64, s	a	2.84, s	2.98, s	2.79, s	2.90, s	2.91, s
2''		5.74, s		5.82, s			5.79, s
3''	6.24, qd (7.3, 1.5)		6.17, qd (7.2, 1.5)		6.17, qd (7.3, 1.6)	6.18, qd (7.3, 1.6)	
4''	2.05, d	1.89, s	2.02, dq (7.2, 1.5)	1.94, s	2.01, dq (7.3, 1.6)	2.01, dq (7.3, 1.6)	1.94, s
5''	1.95, s	2.12, s	1.95, t (1.5)	2.19, s	1.95, t (1.6)	1.95, t (1.5)	2.18, s

^a Signal not observed

Table S5. ^{13}C NMR data of compounds **4-10** (150 MHz, in CD_3OD or * $\text{DMSO}-d_6$, δ in ppm, C type)

Position	4	5*	6	7	8	9	10
1	99.1, CH	97.5, CH	102.3, CH	102.8, CH	102.8, CH	102.4, CH	102.7, CH
2	73.0, CH	70.6, CH	67.3, CH	67.3, CH	70.4, CH	69.7, CH	69.8, CH
3	69.1, CH	66.8, CH	73.7, CH	73.1, CH	69.7, CH	69.7, CH	70.0, CH
4	73.9, CH	71.7, CH	71.0, CH	71.5, CH	74.9, CH	74.6, CH	74.1, CH
5	67.8, CH	66.1, CH	68.1, CH	68.5, CH	67.1, CH	67.1, CH	67.4, CH
6	16.5, CH_3	16.3, CH_3	16.1, CH_3	16.4, CH_3	16.7, CH_3	16.4, CH_3	16.6, CH_3
2'	66.3, CH	a	67.3, CH	68.5, CH	68.2, CH	68.0, CH	68.4, CH
3'	30.7, CH_2	29.2 CH_2	a	27.3, CH_2	a	27.3, CH_2	27.5, CH_2
4'	a	20.9 CH_2	a	21.5, CH_2	a	21.4, CH_2	21.6, CH_2
5'	57.5, CH_2	56.2 CH_2	55.5, CH_2	56.5, CH_2	55.9, CH_2	56.4, CH_2	56.6, CH_2
6'	40.2, CH_2	39.1 CH_2	a	33.9, CH_2	a	34.0, CH_2	34.1, CH_2
7'	76.0, CH	74.3, CH	a	76.9, CH	a	76.4, CH	76.7, CH
8'	22.7, CH_3	22.4 CH_3	22.1, CH_3	22.1, CH_3	22.6, CH_3	21.9, CH_3	22.2, CH_3
9'	39.7, CH_3	a	41.2, CH_3	38.5, CH_3	a	38.1, CH_3	38.3, CH_3
1''	169.0, C	165.6, C	169.0, C	167.7, C	169.1, C	168.8, C	167.8, C
2''	129.0, C	115.6, CH	129.0, C	116.9, CH	129.1, C	128.9, C	116.7, CH
3''	140.8, CH	157.7, C	139.3, CH	159.2, C	139.3, CH	139.1, CH	159.1, C
4''	16.4, CH_3	26.9 CH_3	15.9, CH_3	27.4, CH_3	16.1, CH_3	15.9, CH_3	27.5, CH_3
5''	21.0, CH_3	19.9 CH_3	20.5, CH_3	20.4, CH_3	20.9, CH_3	20.6, CH_3	20.5, CH_3

^a Signal not observed

Table S6. ¹H NMR data of compounds **11-16** (600 MHz, in CD₃OD, δ in ppm, *J* in Hz)

Position	11	12	13	14	15	16
1	5.20, d (3.8)	5.18, d (3.8)	5.16, d (3.9)	5.04, d (3.9)	5.05, d (4.0)	5.10, d (4.0)
2	5.28, dd (10.9, 3.8)	4.97, dd (10.6, 3.8)	4.82, m	4.03, dd (10.5, 3.9)	4.05, dd (10.5, 4.0)	4.03, dd (10.5, 4.0)
3	5.37, dd (11.0, 3.2)	4.23, dd (10.6, 3.5)	4.82, m	5.26, dd (10.6, 3.5)	5.33, brs	5.31, dd (10.5, 3.4)
4	3.93, d (3.4)	5.36, d (3.5)	5.46, t (9.3)	5.37, d (3.4)	5.42, d (3.3)	5.39, d (4.2)
5	4.21, q (6.5)	4.27, q (6.5)	3.92, m	4.35, q (6.6)	4.37, d (7.0)	4.37, q (6.6)
6	1.24, d (6.6)	1.10, d (6.5)	1.28, d (6.3)	1.11, d (6.5)	1.11, d (6.5)	1.11, d (6.6)
2'	3.19, m	3.19, m	a	a	a	3.47, m
3'	2.17, m	2.19, m				2.23, m
	1.72, m	1.75, m	a	a	a	2.07, m
4'	1.98, m	2.00, m	a	a	a	2.11, m
						1.98, m
5'	3.55, m	3.59, brs				3.48, m
	2.92, m	2.95, brs	a	a	a	3.06, m
6'	2.18, m	2.16, m				2.30, m
	1.60, t (11.5)	1.62, t (11.5)	a	a	a	1.96, m
7'	3.80, m	3.79, m	3.80, m	3.93, m	3.95, m	4.24, m
8'	1.37, d (6.1)	1.35, d (6.1)	1.38, d (6.1)	1.38, d (6.2)	1.40, d (6.1)	1.42, d (6.0)
9'	2.81, s	2.82, s	2.83, s	2.77, s	2.86, s	3.03, s
3''	6.24, qd (7.3, 1.9)	6.27, q (7.4)	6.23, qd (7.3, 1.7)	6.82, qd (6.9, 1.4)	6.22, q (7.4)	6.23, qd (7.2, 1.6)
4''	1.97, dd (7.3, 1.9)	2.04, m	1.96, m	1.79, dd (7.0, 1.4)	2.00, d (7.4)	2.00, d (7.2)
5''	1.86, t (1.5)	1.95, d (6.8)	1.83, t (1.6)	1.79, t (1.4)	1.93, m	1.93, m
3'''	6.18, qd (7.3, 1.9)	6.20, q (7.3)	6.14, qd (7.2, 1.6)	6.21, qd (7.2, 1.5)	6.16, q (7.3)	6.17, qd (7.3, 1.6)
4'''	1.97, dd (7.3, 1.9)	2.04, m	1.94, m	1.99, m	1.95, d (7.3)	1.95, d (7.3)
5'''	1.86, t (1.5)	1.95, d (6.8)	1.86, t (1.6)	1.86, m	1.82, m	1.82, m

^a Signal not observed

Table S7. ^{13}C NMR data of compounds **11-16** (150 MHz, in CD_3OD , δ in ppm, C type)

Position	11	12	13	14	15	16
1	99.0, CH	99.0, CH	98.3, CH	102.4, CH	102.6, CH	102.6, CH
2	70.2, CH	73.1, CH	73.3, CH	68.2, CH	68.3, CH	68.0, CH
3	71.6, CH	67.2, CH	71.2, CH	72.0, CH	71.3, CH	71.3, CH
4	71.3, CH	75.2, CH	72.9, CH	72.5, CH	72.4, CH	72.4, CH
5	67.8, CH	66.7, CH	69.3, CH	66.7, CH	66.9, CH	67.1, CH
6	16.4, CH_3	16.6, CH_3	17.6, CH_3	16.5, CH_3	16.4, CH_3	16.4, CH_3
2'	67.2, CH	67.2, CH	a	a	68.5, CH	68.6, CH
3'	30.4, CH_2	30.2, CH_2	a	a	a	27.4, CH_2
4'	22.2, CH_2	22.2, CH_2	a	a	a	21.5, CH_2
5'	57.2, CH_2	57.2, CH_2	a	a	55.5, CH_2	56.6, CH_2
6'	39.3, CH_2	39.0, CH_2	a	a	a	33.9, CH_2
7'	75.9, CH	75.8, CH	76.1, CH	a	a	77.2, CH
8'	22.4, CH_3	22.4, CH_3	22.3, CH_3	22.2, CH_3	22.4, CH_3	22.1, CH_3
9'	39.6, CH_3	39.5, CH_3	39.7, CH_3	a	a	38.6, CH_3
1''	168.3, C	168.8, C	167.7, C	168.5, C	168.5, C	168.3, C
2''	128.7, C	129.0, C	127.8, C	129.3, C	128.6, C	128.5, C
3''	141.0, CH	141.0, CH	141.2, CH	139.3, CH	140.4, CH	140.5, CH
4''	16.3, CH_3	16.3, CH_3	15.4, CH_3	12.0, CH_3	16.2, CH_3	16.2, CH_3
5''	20.9, CH_3	20.9, CH_3	19.8, CH_3	14.3, CH_3	20.8, CH_3	20.8, CH_3
1'''	168.6, C	169.0, C	168.4, C	168.4, C	168.5, C	168.3, C
2'''	128.5, C	128.8, C	128.6, C	128.5, C	128.6, C	128.5, C
3'''	140.3, CH	139.6, CH	139.0, CH	140.0, CH	140.4, CH	140.5, CH
4'''	16.1, CH_3	16.2, CH_3	15.9, CH_3	16.1, CH_3	16.1, CH_3	16.2, CH_3
5'''	20.7, CH_3	20.9, CH_3	20.6, CH_3	16.1, CH_3	20.7, CH_3	20.6, CH_3

^a Signal not observed