

Supporting Information

Passive Sampling in Regulatory Chemical Monitoring of Nonpolar Organic Compounds in the Aquatic Environment

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Number of pages: 7

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Table S1. Types and configurations of passive samplers for nonpolar organic contaminants ($\log K_{ow} > 4$). The list of sampler types and target compounds is not exhaustive.

Sampler type	Configuration	Target contaminants ^a	references
Chemcatcher	1-octanol loaded C18 extraction disk covered with LDPE membrane	PCBs, PAHs	¹⁻⁵
Low-density polyethylene (LDPE)	25-200 μm polymer sheets	PCBs, PAHs, OCPs, PCDD/Fs, PBDEs, organophosphates, triclosan, alkylphenols, polycyclic musks	^{1,2,6-15}
Membrane-Enclosed Sorptive Coating (MESCO)	silicone rod enclosed within a water-filled LDPE membrane	PCBs, OCPs, PAHs	^{2,16-18}
Silicones	25-500 μm sheets, fibers, or wall coatings of poly(dimethylsiloxane) or related polymers	PCBs, PAHs, OCPs, PCDD/Fs, PBDEs, organophosphates, triclosan, pyrethroids, chlorobenzenes, alcohol ethoxylates, cyclyc methylsiloxanes, polycyclic musks, oxadiazon	^{1,2,7,10-12,15,19-27}
Poly(oxymethylene) (POM)	20-80 μm polymer sheets	PCBs, PAHs, OCPs, PCDD/Fs, PBDEs, triclosan, trifluralin	^{11,12,28-30}
Semi-permeable membrane device (SPMD)	triolein enclosed within an 75-90 μm LDPE membrane	PCBs, PAHs, OCPs, PCDD/Fs, PBDEs, organophosphates, trifluralin, pyrethroids, oxadiazon, alkylphenols, carbazoles	^{1,2,27,31-35}
Ceramic dosimeters	various sorbents enclosed within a ceramic membrane	PAHs, PCDD/Fs, PBDEs, organophosphates	³⁶⁻³⁹
Triolein-embedded cellulose acetate membrane	blend of cellulose acetate and triolein, 50 μm thickness	PAHs, OCPs	⁴⁰⁻⁴²
Poly(ethylene- <i>co</i> -vinylacetate) (EVA)	EVA impregnated glass fiber filter	PCBs, OCPs, organophosphates, trifluralin, pyrethroids, chlorobenzenes	⁴³⁻⁴⁵

^a PCBs = polychlorinated biphenyls, PAHs = polycyclic aromatic hydrocarbons, OCPs = organochlorine pesticides, PBDEs = polybrominated diphenyl ethers, PCDD/Fs = polychlorinated dibenz-p-dioxins and polychlorinated dibenzofurans

References

- (1) Jacquet, R.; Miege, C.; Smedes, F.; Tixier, C.; Tronczynski, J.; Togola, A.; Berho, C.; Valor, I.; Llorca, J.; Barillon, B.; Marchand, P.; Coquery, M. Comparison of five integrative samplers in laboratory for the monitoring of indicator and dioxin-like polychlorinated biphenyls in water. *Chemosphere* **2014**, *98*, 18-27.
- (2) Allan, I. J.; Booij, K.; Paschke, A.; Vrana, B.; Mills, G. A.; Greenwood, R. Field performance of seven passive sampling devices for monitoring of hydrophobic substances. *Environ. Sci. Technol.* **2009**, *43*, 5383-5390.
- (3) Lobpreis, T.; Vrana, B.; Dominiak, E.; Dercova, K.; Mills, G. A.; Greenwood, R. Effect of housing geometry on the performance of Chemcatcher (TM) passive sampler for the monitoring of hydrophobic organic pollutants in water. *Environ. Pollut.* **2008**, *153*, 706-710.
- (4) Vrana, B.; Mills, G. A.; Kotterman, M.; Leonards, P.; Booij, K.; Greenwood, R. Modelling and field application of the Chemcatcher passive sampler calibration data for the monitoring of hydrophobic organic pollutants in water. *Environ. Pollut.* **2007**, *145*, 895-904.
- (5) Vrana, B.; Mills, G.; Greenwood, R.; Knutsson, J.; Svensson, K.; Morrison, G. Performance optimisation of a passive sampler for monitoring hydrophobic organic pollutants in water. *J. Environ. Monit.* **2005**, *7*, 612-620.
- (6) Thompson, J. M.; Hsieh, C. H.; Luthy, R. G. Modeling uptake of hydrophobic organic contaminants into polyethylene passive samplers. *Environ. Sci. Technol.* **2015**, *49*, 2270-2277.
- (7) Estoppey, N.; Schopfer, A.; Omlin, J.; Esseiva, P.; Vermeirssen, E. L. M.; Delemont, O.; De Alencastro, L. F. Effect of water velocity on the uptake of polychlorinated biphenyls (PCBs) by silicone rubber (SR) and low-density polyethylene (LDPE) passive samplers: An assessment of the efficiency of performance reference compounds (PRCs) in river-like flow conditions. *Sci. Total Environ.* **2014**, *499*, 319-326.
- (8) Friedman, C. L.; Lohmann, R. Comparing sediment equilibrium partitioning and passive sampling techniques to estimate benthic biota PCDD/F concentrations in Newark Bay, New Jersey (USA). *Environ. Pollut.* **2014**, *186*, 172-179.
- (9) Khairy, M.; Muir, D.; Teixeira, C.; Lohmann, R. Spatial trends, sources, and air-water exchange of organochlorine pesticides in the great lakes basin using low density polyethylene passive samplers. *Environ. Sci. Technol.* **2014**, *48*, 9315-9324.
- (10) O'Connell, S. G.; McCartney, M. A.; Paulik, L. B.; Allan, S. E.; Tidwell, L. G.; Wilson, G.; Anderson, K. A. Improvements in pollutant monitoring: Optimizing silicone for co-deployment with polyethylene passive sampling devices. *Environ. Pollut.* **2014**, *193*, 71-78.
- (11) Perron, M. M.; Burgess, R. M.; Suuberg, E. M.; Cantwell, M. G.; Pennell, K. G. Performance of passive samplers for monitoring estuarine water column concentrations: 2. Emerging contaminants. *Environ. Toxicol. Chem.* **2013**, *32*, 2190-2196.
- (12) Perron, M. M.; Burgess, R. M.; Suuberg, E. M.; Cantwell, M. G.; Pennell, K. G. Performance of passive samplers for monitoring estuarine water column concentrations: 1. Contaminants of concern. *Environ. Toxicol. Chem.* **2013**, *32*, 2182-2189.
- (13) Lohmann, R. Critical review of low-density polyethylene's partitioning and diffusion coefficients for trace organic contaminants and implications for its use as a passive sampler. *Environ. Sci. Technol.* **2012**, *46*, 606-618.
- (14) Sacks, V. P.; Lohmann, R. Development and use of polyethylene passive samplers to detect triclosans and alkylphenols in an urban estuary. *Environ. Sci. Technol.* **2011**, *45*, 2270-2277.

- (15) Allan, I. J.; Harman, C.; Ranneklev, S. B.; Thomas, K. V.; Grung, M. Passive sampling for target and nontarget analyses of moderately polar and nonpolar substances in water. *Environ. Toxicol. Chem.* **2013**, *32*, 1718-1726.
- (16) Paschke, H.; Popp, P. New passive samplers for chlorinated semivolatile organic pollutants in ambient air. *Chemosphere* **2005**, *58*, 855-863.
- (17) Wennrich, L.; Vrana, B.; Popp, P.; Lorenz, W. Development of an integrative passive sampler for the monitoring of organic water pollutants. *J. Environ. Monit.* **2003**, *5*, 813-822.
- (18) Paschke, A.; Vrana, B.; Popp, P.; Wennrich, L.; Paschke, H.; Schuurmann, G. Membrane-enclosed sorptive coating for the monitoring of organic compounds in water. In *Passive Sampling Techniques in Environmental Monitoring*; Greenwood, R., Mills, G. A., Vrana, B., Eds.; Elsevier: Amsterdam, 2007; pp 231-249
- (19) Bruemmer, J.; Falcon, R.; Greenwood, R.; Mills, G. A.; Hastie, C.; Sparham, C.; van Egmond, R. Measurement of cyclic volatile methylsiloxanes in the aquatic environment using low-density polyethylene passive sampling devices using an in-field calibration study – Challenges and guidance *Chemosphere* **2015**, *122*, 38-44.
- (20) Bielska, L.; Smidova, K.; Hofman, J. Solid phase microextraction of organic pollutants from natural and artificial soils and comparison with bioaccumulation in earthworms. *Ecotox. Environ. Safe.* **2014**, *100*, 44-52.
- (21) Witt, G.; Lang, S. C.; Ullmann, D.; Schaffrath, G.; Schmidt, K.; Schulz-Bull, D.; Mayer, P. A passive sampler for in situ measurements of freely dissolved concentrations of hydrophobic organic chemicals in sediments. *Environ. Sci. Technol.* **2013**, *47*, 7830-7839.
- (22) Allan, I. J.; Nilsson, H. C.; Tjensvoll, I.; Bradshaw, C.; Naes, K. PCDD/F release during benthic trawler-induced sediment resuspension. *Environ. Toxicol. Chem.* **2012**, *31*, 2780-2787.
- (23) You, J.; Harwood, A. D.; Li, H. Z.; Lydy, M. J. Chemical techniques for assessing bioavailability of sediment-associated contaminants: SPME versus Tenax extraction. *J. Environ. Monit.* **2011**, *13*, 792-800.
- (24) Difilippo, E. L.; Eganhouse, R. P. Assessment of PDMS-water partition coefficients: implications for passive environmental sampling of hydrophobic organic compounds. *Environ. Sci. Technol.* **2010**, *44*, 6917-6925.
- (25) Droke, S. T. J.; Sinnige, T. L.; Hermens, J. L. M. Analysis of freely dissolved alcohol ethoxylate homologues in various seawater matrixes using solid-phase microextraction *Anal. Chem.* **2007**, *79*, 2885-2891.
- (26) Artola-Garicano, E.; Sinnige, T. L.; Van Holstein, I.; Vaes, W. H. J.; Hermens, J. L. M. Bioconcentration and acute toxicity of polycyclic musks in two benthic organisms (*Chironomus riparius*) and *Lumbriculus variegatus*). *Environ. Toxicol. Chem.* **2003**, *22*, 1086-1092.
- (27) O'Brien, D.; Komarova, T.; Mueller, J. F. Determination of deployment specific chemical uptake rates for SPMD and PDMS using a passive flow monitor. *Mar. Pollut. Bull.* **2012**, *64*, 1005-1011.
- (28) Arp, H. P.; Hale, S. E.; Elmquist Krusa, M.; Cornelissen, G.; Grabanski, C. B.; Miller, D. J.; Hawthorne, S. B. Review of polyoxymethylene passive sampling methods for quantifying freely dissolved porewater concentrations of hydrophobic organic contaminants. *Environ. Toxicol. Chem.* **2015**, *34*, 710-720.
- (29) Cornelissen, G.; Broman, D.; Naes, K. Freely dissolved PCDD/F concentrations in the Frierfjord, Norway: comparing equilibrium passive sampling with "active" water sampling. *J. Soils Sediments* **2010**, *10*, 162-171.

- (30) Jonker, M. T. O.; Koelmans, A. A. Polyoxyethylene solid phase extraction as a partitioning method for hydrophobic organic chemicals in sediment and soot. *Environ. Sci. Technol.* **2001**, *35*, 3742-3748.
- (31) Kim, U. J.; Kim, H. Y.; Alvarez, D.; Lee, I. S.; Oh, J. E. Using SPMDs for monitoring hydrophobic organic compounds in urban river water in Korea compared with using conventional water grab samples. *Sci. Total Environ.* **2014**, *470-471*, 1537-1544.
- (32) Harman, C.; Grung, M.; Djedjibegovic, J.; Marjanovic, A.; Sober, M.; Sinanovic, K.; Fjeld, E.; Rognerud, S.; Ranneklev, S. B.; Larssen, T. Screening for Stockholm Convention persistent organic pollutants in the Bosna River (Bosnia and Herzegovina). *Environ. Monit. Assess.* **2013**, *185*, 1671-1683.
- (33) Shaw, M.; Furnas, M. J.; Fabricius, K.; Haynes, D.; Carter, S.; Eaglesham, G.; Mueller, J. F. Monitoring pesticides in the Great Barrier Reef. *Mar. Pollut. Bull.* **2010**, *60*, 113-122.
- (34) Harman, C.; Tollesen, K. E.; Boyum, O.; Thomas, K.; Grung, M. Uptake rates of alkylphenols, PAHs and carbazoles in semipermeable membrane devices (SPMDs) and polar organic chemical integrative samplers (POCIS) *Chemosphere* **2008**, *72*, 1510-1516.
- (35) Lebo, J. A.; Gale, R. W.; Petty, J. D.; Tillitt, D. E.; Huckins, J. N.; Meadows, J. C.; Orazio, C. E.; Echols, K. R.; Schroeder, D. J.; Inmon, L. E. Use of the semipermeable membrane devices as an in situ sampler of waterborne bioavailable PCDD and PCDF residues at sub-partes-per-quadrillion concentrations. *Environ. Sci. Technol.* **1995**, *29*, 2886-2892.
- (36) Cristale, J.; Katsoyiannis, A.; Chen, C. E.; Jones, K. C.; Lacorte, S. Assessment of flame retardants in river water using a ceramic dosimeter passive sampler. *Environ. Pollut.* **2013**, *172*, 163-169.
- (37) Addeck, A.; Croes, K.; van Langenhove, K.; Denison, M. S.; Elhamalawy, A.; Iskens, M.; Baeyens, W. Time-integrated monitoring of polychlorinated dibenzo-p-dioxins and polychlorinated dibenzofurans (PCDD/Fs) in urban and industrial wastewaters using a ceramic toximeter and the CALUX bioassay. *Chemosphere* **2014**, *94*, 27-35.
- (38) Martin, H.; Patterson, B. M.; Davis, G. B. Field trial of contaminant groundwater monitoring: Comparing time-integrating ceramic dosimeters and conventional water sampling. *Environ. Sci. Technol.* **2003**, *37*, 1360-1364.
- (39) Weiss, H.; Schirmer, K.; Bopp, S.; Grathwohl, P. Use of ceramic dosimeters in water monitoring. In *Passive Sampling Techniques in Environmental Monitoring*; Greenwood, R., Mills, G. A., Vrana, B., Eds.; Elsevier: Amsterdam, 2007; pp 279-293
- (40) Tang, J. F.; Chen, S.; Xu, Y. P.; Zhong, W. J.; Ma, M.; Wang, Z. J. Calibration and field performance of triolein embedded acetate membranes for passive sampling persistent organic pollutants in water. *Environ. Pollut.* **2012**, *164*, 158-163.
- (41) Xu, Y. P.; Wang, Z. J.; Ke, R. H.; Khan, S. U. Accumulation of organochlorine pesticides from water using triolein embedded cellulose acetate membranes. *Environ. Sci. Technol.* **2005**, *39*, 1152-1157.
- (42) Ke, R. H.; Xu, Y. P.; Wang, Z. J.; Khan, S. U. Estimation of the uptake rate constants for polycyclic aromatic hydrocarbons accumulated by semipermeable membrane devices and triolein-embedded cellulose acetate membranes. *Environ. Sci. Technol.* **2006**, *40*, 3906-3911.
- (43) St George, T.; Vlahos, P.; Harner, T.; Helm, P.; Wilford, B. A rapidly equilibrating, thin film, passive water sampler for organic contaminants; characterization and field testing. *Environ. Pollut.* **2011**, *159*, 481-486.
- (44) Tucca, F.; Moya, H.; Barra, R. Ethylene vinyl acetate polymer as a tool for passive sampling monitoring of hydrophobic chemicals in the salmon farm industry. *Mar. Pollut. Bull.* **2014**, *88*, 174-179.

- (45) Meloche, L. M.; deBruyn, A. M. H.; Otton, S. V.; Ikonomou, M. G.; Gobas, F. A. P. C. Assessing exposure of sediment biota to organic contaminants by thin-film solid phase extraction. *Environ. Toxicol. Chem.* **2009**, 28, 247-253.