

Supporting Information

Advancing the use of passive sampling in risk assessment and management of sediments contaminated with hydrophobic organic chemicals: Results of an international ex situ passive sampling inter-laboratory comparison

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Material and Methods: Supplementary Tests

Participants using polymer sheets ($n = 10$) received 6 or 9 (i.e., 2 or 3 triplicate) pieces of POM, having a weight similar to the polymer weights prescribed in their standardized protocol (2.5, 6, 10, and/or 30 mg). All pieces had been cut, coded and weighed on two different, recently serviced/calibrated analytical balances by the coordinating laboratory. Participants reported back the weights of their pieces and the results were used to evaluate any contribution of sampler mass determination to the variability in C_{free} . Likewise, the accuracy of nominal coating volumes, as applied by participants using SPME fibers, was evaluated by determining the actual coating thickness of all fibers by microscopic measurements (methods described under Table S5).

To investigate the possible contribution of sediment heterogeneity to the overall C_{free} variability, 10 batches of each sediment were randomly sampled from the concrete mixers directly after completing the mixing. C_{free} in all batches was determined by the coordinating laboratory, according to the standardized protocol with POM as the sampler.

Because it was impossible to synchronize the measurements by all participants, sediments were stored in refrigerators in different laboratories for different lengths of time. The time between starting the first and the last measurement was 4 months. The coordinating laboratory investigated any effects of sediment storage time by performing the measurements first and last (two time points, 4.5 months apart). Measurements were performed according to the standardized protocol with POM and SPME (S30-1) as the samplers.

Table S1. Passive sampling formats applied during the inter-laboratory comparison study: codes, polymer types, thicknesses, and suppliers.

Code	Polymer type	Polymer thickness	Supplier
<i>Sheets</i>			
PE-1	Polyethylene	25 µm	Ace Hardware Corporation, Oak Brook, IL, USA
PE-2	Polyethylene	25 µm	Berry Plastics Corporation, Evansville, IN, USA
PE-3	Polyethylene	51 µm	Brentwood Plastics, St. Louis, MO, USA
PE-4	Polyethylene	25 µm	Covalence Plastics, Minneapolis, MN, USA
PE-5	Polyethylene	25 µm	Berry Plastics Corporation (Film Gard sheeting)
PE-6	Polyethylene	26 µm	VWR International Ltd., Leicestershire, UK
POM	Polyoxymethylene	77 µm	CS Hyde Company, Lake Villa, IL, USA
SR	Silicone rubber	100 µm	Shielding Solutions Ltd., Great Notley Essex, UK
<i>SPME fibers</i> ^{a,b}			
S10-1	Polydimethylsiloxane	10 µm	Poly Micro Industries, Phoenix, AZ, USA
S10-2	Polydimethylsiloxane	10 µm	Fiberguide, Stirling, NJ, USA
S30-1	Polydimethylsiloxane	30 µm	Poly Micro Industries, Phoenix, AZ, USA
S30-2	Polydimethylsiloxane	30 µm	Poly Micro Industries, Phoenix, AZ, USA
S100	Polydimethylsiloxane	100 µm	Fiberguide, Stirling, NJ, USA
PAc	Polyacrylate	30 µm	Poly Micro Industries, Phoenix, AZ, USA

^a Actual (measured) polymer coating volumes are listed in Table S5.

^b Core thickness of the S30-1 and PAc fiber was about 100 µm. Core thickness of the S30-2 fiber was about 500 µm. The other fibers had a core thickness of about 200 µm.

Table S2. Physico-chemical characteristics of the test sediments. ^a

	BB sediment	FD sediment	SP sediment
Dry weight (%)	53.5 ± 0.03	52.2 ± 0.05	55.0 ± 0.18
<i>f</i> _{oc} (fraction organic carbon) ^b	4.29 ± 0.07	2.31 ± 0.14	1.40 ± 0.10
Phenanthrene	1507 ± 68	590 ± 213	505 ± 10
Anthracene	918 ± 9	204 ± 32	333 ± 4
Fluoranthene	2888 ± 139	1821 ± 493	812 ± 32
Pyrene	2236 ± 118	1338 ± 330	698 ± 24
Benz[a]anthracene	1884 ± 87	1006 ± 133	654 ± 21
Chrysene	1474 ± 67	803 ± 97	605 ± 21
Benzo[e]pyrene	1286 ± 41	835 ± 88	636 ± 9
Benzo[b]fluoranthene	1579 ± 58	1044 ± 102	642 ± 10
Benzo[k]fluoranthene	747 ± 33	507 ± 54	536 ± 6
Benzo[a]pyrene	1399 ± 65	1004 ± 126	579 ± 19
Benzo[g,h,i]perylene	1079 ± 35	837 ± 113	591 ± 8
Dibenz[a,h]anthracene	142 ± 6	105 ± 8	443 ± 6
Indeno[123-cd]pyrene	996 ± 67	687 ± 75	560 ± 8
PCB-18	34 ± 1	10 ± 1	266 ± 5
PCB-28	61 ± 4	44 ± 4	265 ± 6
PCB-52	66 ± 1	489 ± 28	276 ± 6
PCB-66	<i>n.d.</i>	<i>n.d.</i>	290 ± 12
PCB-77	<i>n.d.</i>	<i>n.d.</i>	277 ± 12
PCB-101	66 ± 1	1902 ± 115	301 ± 12
PCB-118	37 ± 0	678 ± 55	294 ± 14
PCB-138	58 ± 0	5913 ± 895	279 ± 14
PCB-153	64 ± 1	6274 ± 966	271 ± 13
PCB-170	19 ± 0	2315 ± 558	281 ± 14
PCB-180	26 ± 1	4204 ± 915	275 ± 14
PCB-187	21 ± 0	1454 ± 282	271 ± 13

^a Concentrations of target chemicals are in $\mu\text{g}/\text{kg}$; ^b Values are multiplied by 100; *n.d.*: not detected.

Table S3. Materials and methods applied by the 11 participants of the inter-laboratory comparison study *in the first experiment* (C_{free} determinations according to own procedures); presented in an anonymous way (“participant A-K”) and in the second, *standardized experiment* (last table; “standardized protocol”).

Participant A	
Equilibration:	
Equilibration system	Jar, amber, 250 mL, Teflon-lined stopper
Mass of sediment per system (g)	100
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	1 g/L NaN ₃ solution (100 mL per sample)
Pre-cleaning procedure sampler	Wash the samplers by rolling in a bottle (@ 2 rpm) with hexanes (mixture of isomers) – 24 hr, then acetone – 30 min, then water – 30 min. Remove moisture using Kimwipes and further dry at 60°C for 4 hr.
Mass (or length for SPME; cm) of sampler (mg) for each sediment	two pieces of approx. 30 mg PE per jar (ca. 60 mg per jar)
Equilibration: static or dynamic	Dynamic
If dynamic: type of ‘shaker’ (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	1D shaker
Speed of shaker (rpm)	150
Equilibration time (days)	125
PRCs added (Y/N). If yes, which ones	Y; For PCBs: PCB 29, 69, 103, 155, 192. For PAHs: d10-fluorene, d10-fluoranthene, d12-perylene.
Time series to confirm equilibration (Y/N). If yes: which time points	N
Equilibration temperature (°C ± ..)	20±2
Precautions taken against exposure to light	Used amber glassware throughout the experiment for PAH samples
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	In a 40 mL amber vial, added 40 mL hexane (mixture of isomers) & rolled @ 2 rpm for 24 hrs. Repeated the procedure once and combined the extracts. The remaining vial and PSM were rinsed twice with hexane.
Clean-up (Y/N)	Y
If clean-up: brief description (sorbent material, solvent, etc)	i) For PAHs (EPA Method 3630C) – the extract in hexane was concentrated and exchanged to cyclohexane (~ 2 mL). The cyclohexane extract was introduced to an activated silica gel column, and after flushing the column with pentane, the PAHs attached to the silica gel were eluted using 3:2 pentane/methylene chloride. ii) For PCBs (EPA Method 3660B & 3630C) – the extract in hexane was concentrated to ~2 mL. Activated copper was added to each sample to remove sulfur species. The extract was introduced to a 3% deactivated silica gel column and hexane was used to elute the PCBs from the column.
If clean-up: recoveries and blanks determined	Y

(Y/N) and how	Spiked surrogate standards at the beginning of the extraction procedure. The recoveries were checked for all samples. Data were accepted when the surrogate recovery was 50-120%. Surrogate standards used: 2-fluorobiphenyl & d-terphenyl for PAHs; PCB 14 & 65 for PCBs.
Data corrected for blanks and recoveries (Y/N)	N
Final solvent after clean-up (injection solvent)	PAHs: methylene chloride PCBs: hexane (mixture of isomers)
Volume of final extract (solvent) (mL)	1
Type of autosampler vial (volume; clear, amber)	2 mL; amber for PAHs & clear for PCBs
Analysis/calculation:	
Internal standard(s) used (Y/N)	Y
If internal standard(s): specify	PAHs: d8-naphthalene, d10-acenaphthene, d10-anthracene, d10-pyrene, d12-chrysene, d12-benzo[a]pyrene; PCBs: PCB 30 & 204
Analysis technique used for PAHs (+ detection)	GC-MS (selective ion monitoring mode)
Brief description of column, injection technique, temperature program/gradient, length of run, etc	Column: HP-5MS, 30 m x 0.25 mm ID, 0.25 µm film thickness. Injection: splitless, 1.0 µL. Temperature: Hold @ 60°C for 2 min, ramp @ 6°C/min to 258°C, ramp @ 2°C/min to 300°C, hold @ 300°C for 4 min. Length of run: 60 min.
Analysis technique used for PCBs (+ detection)	GC (+ µECD)
Brief description of column, injection technique, temperature program, length of run, etc	Column: DB-5MS, 60 m x 0.25 mm ID, 0.25 µm film thickness. Injection: splitless, 2.0 µL. Temperature: Start @ 100°C, ramp @ 1.5°C/min to 270°C, ramp @ 15°C to 280°C, Hold @ 280°C for 15 min. Length of run: 129 min.
Automatic or manual integration of chromatograms	PAHs – manual PCBs – automatic with full review of the chromatograms (manual integration if needed)
PRC data used for calculation of C_{free} (Y/N)	N
Reference for PRC calculation method	NA

Participant B	
Equilibration:	
Equilibration system	Jar, amber, 120 mL, aluminum foil lined cap
Mass of sediment per system (g)	Approximately 90 mL (~80 g)
Aqueous solution added (Y/N)	N
Composition of aqueous solution (biocide, salts)	-
Pre-cleaning procedure sampler	Samplers were rinsed in DCM twice, Methanol twice, and Milli-Q water twice for at least 24 hours in each rinse. The samplers were stored in Milli-Q water afterward.
Mass (or length for SPME; cm) of sampler (mg) for each sediment	~25 mg PE; ~100 mg POM
Equilibration: static or dynamic	Static
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	-
Speed of shaker (rpm)	-

Equilibration time (days)	42 days
PRCs added (Y/N). If yes, which ones	Y (PCBs – 28, 52, 118, 128; PAHs – d10 pyrene, d10 phenanthrene, d12 chrysene).
Time series to confirm equilibration (Y/N). If yes: which time points	N
Equilibration temperature (°C ± ..)	20.6°C
Precautions taken against exposure to light	Stored in dark (cardboard boxes); hood light left off.
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Samplers were removed from sediment with DCM-cleaned tweezers and rinsed with Millipore water. Then they were wiped with a Kimwipe and place in a cleaned (DCM and methanol rinsed x3) foiled amber vial. Recovery compounds (100 ng of d10-anthracene, d10-fluoranthene, and d12-benz(a)anthracene in 100 µL of DCM) we added to the PE in the vial and allowed to dry. High purity DCM was then added to cover sampler (~15 mL). Samplers were placed on an orbital shaker (80 rpm) for 3 days. Vials were removed and DCM was transferred to cleaned and foiled amber vials. The original sampler vials were filled again with high purity DCM to cover sampler and returned to the shaker. The combined extracts were blown down with ultra high purity nitrogen. The process was repeated twice more with at least a 24 hour wait time in between. The vials with DCM were blown down to approximately 1 mL. The solution was then transferred to amber 2 mL autosampler vial using glass pipettes. The autosampler vials were labelled and placed in the freezer.
Clean-up (Y/N)	N
If clean-up: brief description (sorbent material, solvent, etc)	-
If clean-up: recoveries and blanks determined (Y/N) and how	-
Data corrected for blanks and recoveries (Y/N)	Y; Surrogate Standards (PCBs 8, 77, 153; PAHs d10 anthracene, d12 fluoranthene, d12 benz[a]anthracene).
Final solvent after clean-up (injection solvent)	DCM
Volume of final extract (solvent) (mL)	1 mL nominally
Type of autosampler vial (volume; clear, amber)	Amber, 2 mL, PTFE Septum
Analysis/calculation:	
Internal standard(s) used (Y/N)	Y
If internal standard(s): specify	p-terphenyl-d14
Analysis technique used for PAHs (+ detection)	GC/MS/MS
Brief description of column, injection technique, temperature program/gradient, length of run, etc	Column – Thermo Scientific TG – 5MS, L 30M, ID 0.25 mM, Film 0.25 um; Splitless, PTV injector; Oven temperature program: initial temp: 70°C, raised 20°C/min to 180°C, then 6°C/min to 300°C and held for 7.5 min.
Analysis technique used for PCBs (+ detection)	GC/MS/MS

Brief description of column, injection technique, temperature program, length of run, etc	Column – Thermo Scientific TG – 5MS, L 30M, ID 0.25 mm, Film 0.25 um; Splitless, PTV injector; Oven temperature program: initial temp: 70°C, raised 20°C/min to 180°C, then 6°C/min to 300°C and held for 7.5 min.
Automatic or manual integration of chromatograms	Manual
PRC data used for calculation of C_{free} (Y/N)	Y
Reference for PRC calculation method	Fernandez et al., <i>ES&T</i> , 43, 8888-8894.

Participant C	
Equilibration:	
Equilibration system	Jar, amber, 250 mL, PTFE-lined lid
Mass of sediment per system (g)	100
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	Sodium azide
Pre-cleaning procedure sampler	Soaking in hexane-acetone over night
Mass (or length for SPME; cm) of sampler (mg) for each sediment	40 mg POM
Equilibration: static or dynamic	dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	TCLP
Speed of shaker (rpm)	28
Equilibration time (days)	32 days
PRCs added (Y/N). If yes, which ones	Y. pyrene-d10
Time series to confirm equilibration (Y/N). If yes: which time points	N
Equilibration temperature (°C ± ..)	25°C
Precautions taken against exposure to light	Dark room. Amber glass.
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Passive samplers were extracted with 1:1 hexane and acetone mixtures (3 × 24 h, with sequential extracts pooled). Prior to extraction phenanthrene-d10 surrogate was added to assess the effectiveness of sample processing. The final extraction volume was concentrated to 10mL. 1mL of this volume was analyzed for PCBs. The rest was concentrated to 1mL and analyzed for PAHs
Clean-up (Y/N)	N
If clean-up: brief description (sorbent material, solvent, etc)	-
If clean-up: recoveries and blanks determined (Y/N) and how	-
Data corrected for blanks and recoveries (Y/N)	Y
Final solvent after clean-up (injection solvent)	Hexane-acetone
Volume of final extract (solvent) (mL)	1 mL
Type of autosampler vial (volume; clear, amber)	clear
Analysis/calculation:	
Internal standard(s) used (Y/N)	Y

If internal standard(s): specify	Fluoronaphthalene, p-terphenyl-d14, Benzo(a)pyrene-d12, Dibenz(a,h)anthracene-d14.
Analysis technique used for PAHs (+ detection)	gas chromatography with mass detection (Agilent 6890 gas chromatograph coupled to an Agilent 5973N MS detector)
Brief description of column, injection technique, temperature program/gradient, length of run, etc	GC-MS is equipped with a fused silica capillary column (HP-5, 60m x 250µm x 0.25µm). Oven temperature remains at 35 °C for 1 minute. Then it increases from 35 °C to 300 °C at 6°C /min, and maintains at 300°C for 20 minutes. The MS temperature is 300 ° C. Sample total run time is 65 minutes.
Analysis technique used for PCBs (+ detection)	gas chromatography with electron capture detection (an Agilent 6890N).
Brief description of column, injection technique, temperature program, length of run, etc	GC-ECD is equipped with a fused silica capillary column (HP-5, 60m x 250µm x 0.25µm). Oven temperature remains at 100 °C for 1 minute. Then it increases from 100 °C to 280 °C at 2°C /min, and then rises from 280 °C to 300°C at 10°C /min. The temperature is maintained at 300°C for 6 minutes. The detector temperature is 300 ° C. Sample total run time is 98 minutes.
Automatic or manual integration of chromatograms	manual
PRC data used for calculation of C_{free} (Y/N)	N
Reference for PRC calculation method	Although only %50 loss of PRCs was observed in samplers, no PRC correction was performed to calculate C_{free} . This is because the values of K_{POM} from Hawthorne et al., 2011 were obtained by shaking 76µm POM strips in contaminated sediments for 28 days (very similar condition to own experiment). Thus, K_{POM} values that are used here already account for the possible non-equilibration.

Participant D	
Equilibration:	
Equilibration system	Jar, amber, 125 mL, aluminum foil-lined Teflon
Mass of sediment per system (g)	mass sent by coordinating lab split into 5
Aqueous solution added (Y/N)	N
Composition of aqueous solution (biocide, salts)	n/a
Pre-cleaning procedure sampler	Soak (24 h) twice with DCM, twice with methanol, soaked (>2 weeks) in methanol:water PRC solution, and soaked (24 h) twice with pure water
Mass (or length for SPME; cm) of sampler (mg) for each sediment	~20 mg PE for PCBs and ~15 mg for PAHs
Equilibration: static or dynamic	static
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	n/a
Speed of shaker (rpm)	n/a

Equilibration time (days)	56 days
PRCs added (Y/N). If yes, which ones	Yes, labelled PCBs (13C 28, 47, 54, 97, 111, 153, and 178) or PAHs (phenanthrene-d10, pyrene-d10, chrysene-d12)
Time series to confirm equilibration (Y/N). If yes: which time points	no
Equilibration temperature (°C ± ..)	Room temperature, usually about 21 °C
Precautions taken against exposure to light	In amber jars, placed in container covered with foil while experiment was going on
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Wipe PE with Kimwipe, place in amber vial, spike with surrogate standard, extract 3 times with DCM, combine extract in combusted round bottom flask, evaporate to 1 mL by heating solvent and allowing vapor go through a chilled condenser column while under vacuum, quantitative transfer to 4 mL vial, evaporate under N2 line to 0.1 mL and solvent exchange to hexane, quantitative transfer to small volume insert of autosampler, spike with injection standards
Clean-up (Y/N)	no
If clean-up: brief description (sorbent material, solvent, etc)	n/a
If clean-up: recoveries and blanks determined (Y/N) and how	n/a
Data corrected for blanks and recoveries (Y/N)	yes
Final solvent after clean-up (injection solvent)	hexane
Volume of final extract (solvent) (mL)	~ 0.05-0.3 mL, calculated using injection standards
Type of autosampler vial (volume; clear, amber)	2 mL amber, Agilent brand with Teflon septa screw caps
Analysis/calculation:	
Internal standard(s) used (Y/N)	yes
If internal standard(s): specify	PCBs (non-labelled 39, 55, 104, 150, 188) and PAHs (acenaphthene-d10, m-terphenyl, perylene-d12)
Analysis technique used for PAHs (+ detection)	High res GC, low res MS
Brief description of column, injection technique, temperature program/gradient, length of run, etc	60 m DB-5MS, splitless; operated in 'selected ion monitoring'. Injection port: 305 C; Program: 67C, ramp at 15C to 180C, ramp at 4C to 315C, hold for 5.7 min; total run time 47 min. Flow: 2 mL/min.
Analysis technique used for PCBs (+ detection)	Same as above
Brief description of column, injection technique, temperature program, length of run, etc	Injection port: 280 C; Program: 67C, ramp at 25C to 188C, ramp at 1.5C to 276C, ramp at 25C to 300C, hold for 1 min. Flow: 1 mL/min
Automatic or manual integration of chromatograms	Automatic integration by program, manual selection of peak area to integrate
PRC data used for calculation of C _{free} (Y/N)	Yes. Only PRCs with 10-90% remaining in the PE were used. Generally, 5 PCB congeners could be used – except for the SP samples that went dry during nitrogen blowdown (PCB 28 could not be used). There were only 3 PRCs for

	the PAHs (imitating earlier work like Fernandez & Gschwend 2009). Phenanthrene always had <10% remaining, so only 2 PRCs were used to correct PAHs – this leads to more variability in PRC corrections than were seen for the PCBs.
Reference for PRC calculation method	Apell and Gschwend 2014 (ES&T) – used the GUI for PRC-based corrections available at: https://www.serdp-estcp.org/Tools-and-Training/Tools/PRC-Correction-Calculator .

Participant E	
Equilibration:	
Equilibration system	Vial, amber, 15 mL for SPME; bottle, amber, 120 mL for sheets
Mass of sediment per system (g)	Approx. 8 for SPME and 60 for sheets (ww)
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	100 mg/L NaN ₃
Pre-cleaning procedure sampler	Shake with different solvents (depending on polymer) successively and store in water (fibers) or air-dry (sheets)
Mass (or length for SPME; cm) of sampler (mg) for each sediment	2-30 cm fiber (depending on sediment and coating); 2.5-30 mg sheet (depending on sediment and polymer)
Equilibration: static or dynamic	Dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	Rock & Roller for SPME, 1-D shaker for sheets
Speed of shaker (rpm)	60 for SPME; 150 for sheets
Equilibration time (days)	42
PRCs added (Y/N). If yes, which ones	N
Time series to confirm equilibration (Y/N). If yes: which time points	2, 4, 6, 9, 12 weeks
Equilibration temperature (°C ± ..)	20 ± 1 °C
Precautions taken against exposure to light	Amber glassware, dark room, covered box
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Samplers were removed from the sediment slurry, cleaned with wet tissue, cut, and placed in autosampler vials containing acetonitrile. Internal standards were added and the vials were placed in the freezer. Prior to analysis, they were left at room temperature for several hours and vortexed for 1-4 min (depending on the sampler)
Clean-up (Y/N)	N
If clean-up: brief description (sorbent material, solvent, etc)	-
If clean-up: recoveries and blanks determined (Y/N) and how	-
Data corrected for blanks and recoveries (Y/N)	Y (blanks)
Final solvent after clean-up (injection solvent)	Acetonitrile
Volume of final extract (solvent) (mL)	0.2-0.5 (SPME), 1.0 for sheets
Type of autosampler vial (volume; clear, amber)	Amber, 1.8 mL (with 200 µL insert for SPME if necessary)

Analysis/calculation:	
Internal standard(s) used (Y/N)	Y
If internal standard(s): specify	PCB-209 and 2-methylchrysene
Analysis technique used for PAHs (+ detection)	HPLC-FLD
Brief description of column, injection technique, temperature program/gradient, length of run, etc	Twenty μL of sample were injected by a Varian Prostar 420 autosampler on a Vydac 201TP54 C_{18} column (25 cm; d.i. 4.2 mm; d.f. 5 μm ; kept at 27.0 $^{\circ}\text{C}$). The mobile phase consisted of methanol and water (mixture changing from 30:70 to 100:0; degassed by a Grace 590 degasser), and was pumped at a flow increasing from 0.7 to 1.5 mL/min by a Gynkotec P680HPG HPLC pump. Detection was performed by a Jasco FP-2020 Plus fluorescence detector (programmed to measure at different excitation/emission wavelength combinations and detector gain for different PAHs)
Analysis technique used for PCBs (+ detection)	GC-ECD
Brief description of column, injection technique, temperature program, length of run, etc	One μL of sample was injected in the split mode (split ratio 12) by a TriPlus autosampler on a Zebtron ZB-5MSi column (Phenomenex; 30 m, 0.25 mm i.d., 0.25 μm f.t.). Temperature program of the Thermo Trace GC Ultra: 185 $^{\circ}\text{C}$ (0 min); 2.5 $^{\circ}/\text{min}$ to 240 (0 min); 15 $^{\circ}/\text{min}$ to 300 (3 min). Carrier gas: He, at a rate of 1.2 mL/min. Detector temp of the ECD: 365 $^{\circ}\text{C}$.
Automatic or manual integration of chromatograms	Manual
PRC data used for calculation of C_{free} (Y/N)	N
Reference for PRC calculation method	-

Participant F	
Equilibration:	
Equilibration system	Jar, tin foil wrapped, 500 mL, Teflon lid
Mass of sediment per system (g)	50 g dry weight basis
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	NaN3
Pre-cleaning procedure sampler	In acetone and n-hexane for 24 hours each
Mass (or length for SPME; cm) of sampler (mg) for each sediment	400-1200 mg PE
Equilibration: static or dynamic	dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	Orbital table shaker
Speed of shaker (rpm)	120
Equilibration time (days)	90 days
PRCs added (Y/N). If yes, which ones	Y. Fluorene-d10, pyrene-d10, benzo(a)pyrene-d12, dibromobiphenyl, tetrabromobiphenyl, pentabromobiphenyl, octachloronaphthalene
Time series to confirm equilibration (Y/N). If yes: which time points	no
Equilibration temperature ($^{\circ}\text{C} \pm \dots$)	20

Precautions taken against exposure to light	Jars covered with tin foil
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Cold extraction using n-hexane for 24 hours, then solvent reduction using a turbovap (set at 30 °C and the nitrogen at 5 psi)
Clean-up (Y/N)	yes
If clean-up: brief description (sorbent material, solvent, etc)	SPE cartridge (1 g silica gel), elution with n-hexane/DCM (70:30)
If clean-up: recoveries and blanks determined (Y/N) and how	yes
Data corrected for blanks and recoveries (Y/N)	yes
Final solvent after clean-up (injection solvent)	n-hexane/nonane
Volume of final extract (solvent) (mL)	0.05
Type of autosampler vial (volume; clear, amber)	(2.0 mL amber vials and samples were in glass inserts 50 uL volume)
Analysis/calculation:	
Internal standard(s) used (Y/N)	Y
If internal standard(s): specify	Internal standards for PCBs: ¹³ C ₁₂ PCB 8, ¹³ C ₁₂ PCB 18, ¹³ C ₁₂ PCB 52, ¹³ C ₁₂ PCB 118, ¹³ C ₁₂ PCB 138, ¹³ C ₁₂ PCB 180 & ¹³ C ₁₂ PCB 209. For PAHs: acenaphthene-d10; phenanthrene-d10; chrysene-d12 and perylene-d12. Injection standards used were p-terphenyl-d14 for PAHs and 2,4,6-tribromobiphenyl for PCBs. The labeled PCBs and deuterated PAHs were used as surrogates in the own experiment only.
Analysis technique used for <u>PAHs</u> (+ detection)	GC/MS in the SIM mode
Brief description of column, injection technique, temperature program/gradient, length of run, etc	DB5-MS 30 m x 0.25 x 0.25, autoinjection of 1 uL in the splitless mode
Analysis technique used for <u>PCBs</u> (+ detection)	Same as PAHs
Brief description of column, injection technique, temperature program, length of run, etc	Same as PAHs but with a different temperature program
Automatic or manual integration of chromatograms	Manual integration
PRC data used for calculation of C _{free} (Y/N)	Y
Reference for PRC calculation method	An improved method for estimating in situ sampling rates of nonpolar passive samplers. ES&T 44, 2010, 6789-6794.

Participant G	
Equilibration:	
Equilibration system	Scintillation vial, clear, 20 mL, plastic-lined cap
Mass of sediment per system (g)	~10 g (wet weight)
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	10 mL moderately hard water, 3 mL, 3 mg/mL HgCl ₂
Pre-cleaning procedure sampler	none
Mass (or length for SPME; cm) of sampler (mg) for each sediment	30 cm fiber

Equilibration: static or dynamic	Dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	Rock & Roller
Speed of shaker (rpm)	100 rpm
Equilibration time (days)	42 d
PRCs added (Y/N). If yes, which ones	N
Time series to confirm equilibration (Y/N). If yes: which time points	Y, 21, 28, 42 d
Equilibration temperature (°C ± ..)	25 ± 1°C
Precautions taken against exposure to light	Covered the vials in foil
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Fibers were held in 4 mL of hexane for 48 h, the hexane was removed, concentrated to 0.75 mL, transferred to GC vials for analysis
Clean-up (Y/N)	Y
If clean-up: brief description (sorbent material, solvent, etc)	Hexane
If clean-up: recoveries and blanks determined (Y/N) and how	Surrogates, 50 ng of 4,4'-dibromooctafluorobiphenyl (DBOFB) and decachlorobiphenyl (DCBP) were added prior to concentration of hexane used to extract SPME fibers
Data corrected for blanks and recoveries (Y/N)	N
Final solvent after clean-up (injection solvent)	Hexane
Volume of final extract (solvent) (mL)	1 mL
Type of autosampler vial (volume; clear, amber)	1.5 mL amber GC vial
Analysis/calculation:	
Internal standard(s) used (Y/N)	Y
If internal standard(s): specify	Chrysene d12, Perylene d12
Analysis technique used for PAHs (+ detection)	GC-MS
Brief description of column, injection technique, temperature program/gradient, length of run, etc	HP-5MS 5% Phenyl Methyl Siloxane 30 m Column, 0.25 µm film thickness, pulsed splitless injection, 100°C (hold 1 min) to 205°C at 10°C/min, 205°C to 230°C at 2°C/min, 230°C to 270°C 5°C/min (hold 13.5 min); 45.50 minute run
Analysis technique used for PCBs (+ detection)	GC-MS
Brief description of column, injection technique, temperature program, length of run, etc	Same as PAHs
Automatic or manual integration of chromatograms	Manual
PRC data used for calculation of C _{free} (Y/N)	N
Reference for PRC calculation method	N/A

Participant H	
Equilibration:	
Equilibration system	Scintillation vial, amber, 20 mL, Teflon-lined cap
Mass of sediment per system (g)	20 wet weight
Aqueous solution added (Y/N)	N
Composition of aqueous solution (biocide, salts)	N

Pre-cleaning procedure sampler	pre-cleaned by sonication with methylene chloride, methanol, and deionized water for 15 min in each solvent.
Mass (or length for SPME; cm) of sampler (mg) for each sediment	5 mg PE
Equilibration: static or dynamic	dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	Barnstead Thermolyne M49235 Bigger Bill orbital platform shaker
Speed of shaker (rpm)	175
Equilibration time (days)	15
PRCs added (Y/N). If yes, which ones	Y. 13C PCB28, 13C PCB52, 13C PCB118, 13C PCB128, 13C p,p'-DDE, 13C p,p'-DDD
Time series to confirm equilibration (Y/N). If yes: which time points	Y. 3, 12, and 15 d
Equilibration temperature (°C ± ..)	22°C ±1
Precautions taken against exposure to light	No, due to the amber vial.
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	The PED is extracted by dichloromethane (DCM). Before extraction, spike surrogate solution on each piece of PED. The PED is extracted three times in DCM by sonication for 15 min. Combine the extracts, concentrate and exchange solvent into hexane. The volume of the extract was blown down to 0.2mL, add internal standard for GC/EI-MS analysis.
Clean-up (Y/N)	N
If clean-up: brief description (sorbent material, solvent, etc)	NA
If clean-up: recoveries and blanks determined (Y/N) and how	NA
Data corrected for blanks and recoveries (Y/N)	N
Final solvent after clean-up (injection solvent)	Hexane
Volume of final extract (solvent) (mL)	0.2
Type of autosampler vial (volume; clear, amber)	1.5 mL clear vial with 200 uL insert
Analysis/calculation:	
Internal standard(s) used (Y/N)	Y
If internal standard(s): specify	2-Fluorobiphenyl-d14(PAH2 IS 1) p-Terphenyl-d14 (PAHs IS2) PCB30 (IS1-PCB) PCB205 (IS2-PCB)
Analysis technique used for <u>PAHs</u> (+ detection)	GC/EI-MS. PAHs and PCBs are analyzed together in one injection.
Brief description of column, injection technique, temperature program/gradient, length of run, etc	DB-XLB column (30m × 0.25mm × 0.25 μm, Agilent J&W Scientific, Santa Clara, CA, USA); The split/splitless inlet is operated isothermally at 300°C in 1-min splitless mode for the PE analysis. Injection volume is 1 uL. The oven temperature is programmed from 80°C held for 1 min to 190°C at 5°C/min, to 260 °C at 4°C/min, to 290°C at 20°C/min, and to 300°C at 50°C/min held for 20 min. The running time is 67 min.
Analysis technique used for <u>PCBs</u> (+ detection)	See above

Brief description of column, injection technique, temperature program, length of run, etc	See above
Automatic or manual integration of chromatograms	manual integration
PRC data used for calculation of C_{free} (Y/N)	Y
Reference for PRC calculation method	Own method (to be published).

Participant I	
Equilibration:	
Equilibration system	Glass flask, clear, 50 mL, glass stopper
Mass of sediment per system (g)	5
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	40 ml water spiked with sodium azide, amount of sodium azide added 1% by water volume from a 20 g/L stock
Pre-cleaning procedure sampler	Submerging the materials 24 h in each solvent (hexane, methanol, deionized water) and then allowed to dry at 20 °C for 12 h between each solvent rinse. After last 24 h rinse in deionized water, 4 x rinse in smaller volumes of deionized water.
Mass (or length for SPME; cm) of sampler (mg) for each sediment	100 mg
Equilibration: static or dynamic	Dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	End-over-end
Speed of shaker (rpm)	7-10 rpm
Equilibration time (days)	28
PRCs added (Y/N). If yes, which ones	N
Time series to confirm equilibration (Y/N). If yes: which time points	N
Equilibration temperature (°C ± ..)	22-23 °C
Precautions taken against exposure to light	Flasks wrapped and packed in box during equilibration
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Place the clean PE or POM in a 50 ml glass flask with glass stopper for extraction, add 20 ml of an 80:20 mixture of heptane:acetone. Add surrogate standard, shake for 2 days (orbital shaker at 100 rpm). Remove sampler from the solvent. Reduce the volume of solvent with evaporation until approximately 1 ml.
Clean-up (Y/N)	Y
If clean-up: brief description (sorbent material, solvent, etc)	Silica gel clean up (modified Silica gel clean-up method 3630C (USEPA)). Preclean the silica column with heptane. After the sample has completely entered the silica column (achieved by pipetting the approximately 1 ml from the above extraction method), elute the column with 10 ml heptane. Rinse the glass vial that contained the sample with a few ml of heptane in order that the entire sample is transferred to

	the column
If clean-up: recoveries and blanks determined (Y/N) and how	Y, using blank samples and by spiking internal standard (PCB77) in order to look at the recovery of the process.
Data corrected for blanks and recoveries (Y/N)	Y
Final solvent after clean-up (injection solvent)	heptane
Volume of final extract (solvent) (mL)	0.7 ml
Type of autosampler vial (volume; clear, amber)	1.5 ml clear glass
Analysis/calculation:	
Internal standard(s) used (Y/N)	Y
If internal standard(s): specify	PCB77
Analysis technique used for PAHs (+ detection)	GCMS to 0,001 ug/ml
Brief description of column, injection technique, temperature program/gradient, length of run, etc	Agilent 6850 Gas Chromatograph equipped with a Agilent DB-XLB Column (length 30 m, 0.25 mm id and 0.1 lm film thickness, TeknoLab, Kolbotn, Norway) with a flow of 1 mL min ⁻¹ and the following temperature program: 2 min at 50 °C, to 150 °C at 10 °C min ⁻¹ , to 280 °C at 5°C min ⁻¹ , 9 min at 280 °C, to 310 °C with 40°C min ⁻¹ , at 310 °C for 8 min. Detection was performed with an Agilent 5973 mass spectrometer in the electron impact mode with a 70 eV ionisation energy and a dwelling time of 25 ms. Identification of the PAH was assured by using two compound-specific ions: a quantifier ion corresponding to the respective molecular weight (m/z=M+) and a qualifier ion ([M ₂ H] ⁺ for analytes and [M ₂ D] ⁺ for internal standards) with a mass ratio similar to the one determined in the calibration
Analysis technique used for PCBs (+ detection)	GCMS 0,0001 ug/ml
Brief description of column, injection technique, temperature program, length of run, etc	As above
Automatic or manual integration of chromatograms	Manual
PRC data used for calculation of C _{free} (Y/N)	N
Reference for PRC calculation method	-

Participant J	
Equilibration:	
Equilibration system	Jar, amber, 20 or 40 mL, Teflon-lined cap
Mass of sediment per system (g)	Approx 20 (SPME) or 10 (POM) g
Aqueous solution added (Y/N)	N for SPME; Y for POM
Composition of aqueous solution (biocide, salts)	POM: Sodium azide 100 mg/L + 0.01 M calcium chloride
Pre-cleaning procedure sampler	SPME: Soak in hexane for 1 hour, soak in acetonitrile for 1 hour, soak in Millipore water for 1 hour, blot dry with lint free tissue. POM: 1× n-hexane + 3 × methanol wash
Mass (or length for SPME; cm) of sampler (mg) for each sediment	2 cm fibers; 5 mg POM for PAH and 40 mg for PCBs

Equilibration: static or dynamic	Dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	2D Shaker
Speed of shaker (rpm)	60 rpm for SPME; 160 for POM
Equilibration time (days)	20 days for SPME; 32 days for POM
PRCs added (Y/N). If yes, which ones	Y (fluoranthene-d10, chrysene-d12, benzo(b)fluoranthene-d12, dibenz(a,h)anthracene-d14, PCB 209)
Time series to confirm equilibration (Y/N). If yes: which time points	N
Equilibration temperature (°C ± ..)	Approx 25°C for SPME, 20 °C for POM
Precautions taken against exposure to light	Amber vials and aluminum foil on top of batch box for POM
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	<p>Fibers were removed from sediment and wiped with a damp lint free tissue, cut with a ceramic column cutter into 1 cm segments, and placed in 150 µL of solvent (acetonitrile for PAH analysis/hexane for PCB analysis). The fibers were left in the solvent for 1 day (previous time series shows that desorption of the compounds from the PDMS layer occurs in less than a minute) before analysis.</p> <p>POM strips approx. 5 mg each for PAH analysis were removed from sediment, rinsed with MiliQ water and wiped with a damp lint free tissue, and placed in 250 µL of acetonitrile (in inserts). The samples were placed on a 2D shaker and mixed @ 160 rpm for 3 h. The POM strips were withdrawn from the inserts and the extracts were analyzed for PAHs using HPLC. POM strips for PCB analysis (40 mg) were removed from sediment, rinsed with MiliQ water and wiped with a damp lint free tissue. The samplers were placed in 40 mL vials containing 20 mL of hexane/acetone (1:1) and mixed @ 160 rpm for 3 h using the 2D shaker. Following this procedure the extracts were transferred to small volumetric flasks and reduced to 200 µL under gentle flow of nitrogen. The final extracts were transferred to 2 ml amber vials with 250 µL glass inserts and analyzed for PCB-12 using GC- µECD.</p>
Clean-up (Y/N)	N
If clean-up: brief description (sorbent material, solvent, etc)	-
If clean-up: recoveries and blanks determined (Y/N) and how	-
Data corrected for blanks and recoveries (Y/N)	N
Final solvent after clean-up (injection solvent)	Acetonitrile for PAHs, hexane for PCBs
Volume of final extract (solvent) (mL)	0.15- 0.25 mL
Type of autosampler vial (volume; clear, amber)	2 ml amber vial with 250 µL glass insert
Analysis/calculation:	
Internal standard(s) used (Y/N)	N

If internal standard(s): specify	-
Analysis technique used for PAHs (+ detection)	LC with fluorescence
Brief description of column, injection technique, temperature program/gradient, length of run, etc	Column: Phenomenex; Temperature: Constant 40°C; Length of run: 42 min; Solvent: 70% Acetonitrile 30% Water @ 1 ml/min
Analysis technique used for PCBs (+ detection)	GC μ ECD
Brief description of column, injection technique, temperature program, length of run, etc	Agilent Technologies, HP-5, 30m x 0.320 mm x 0.25 micron, injection volume = 2 μ L, mode: splitless, run time = 48 min, He@ 100 °C oven. Analysis of standards in hexane
Automatic or manual integration of chromatograms	Manual
PRC data used for calculation of C_{free} (Y/N)	Y
Reference for PRC calculation method	Lampert, D.J., Thomas, C., Reible, D.D., 2015. Internal and external transport significance for predicting contaminant uptake rates in passive samplers. Chemosphere 119, 910-916.

Participant K	
Equilibration:	
Equilibration system	Bottles, amber, 30-250 mL, alu foil-lined caps
Mass of sediment per system (g)	30-40 dw.
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	1ml per g dry sediment of 1g NaN ₃ /L (1mg NaN ₃ per gram sediment)
Pre-cleaning procedure sampler	Wet tissue
Mass (or length for SPME; cm) of sampler (mg) for each sediment	25-30 mg
Equilibration: static or dynamic	dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	2D shaker
Speed of shaker (rpm)	130
Equilibration time (days)	90
PRCs added (Y/N). If yes, which ones	Yes
Time series to confirm equilibration (Y/N). If yes: which time points	N
Equilibration temperature (°C \pm ..)	Ambient ~20°C
Precautions taken against exposure to light	Placed in box
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	First extraction overnight with 10 methanol , second with 30mL 30% acetone/methanol
Clean-up (Y/N)	Y
If clean-up: brief description (sorbent material, solvent, etc)	Florisil and elution with 15 mL 20 diethylether/hexane
If clean-up: recoveries and blanks determined (Y/N) and how	Blanks and recovery standards
Data corrected for blanks and recoveries (Y/N)	Not for blanks (except solvent blank) but yes for recovery standards
Final solvent after clean-up (injection solvent)	hexane
Volume of final extract (solvent) (mL)	1 or 5 or 10mL
Type of autosampler vial (volume; clear, amber)	amber

Analysis/calculation:	
Internal standard(s) used (Y/N)	Yes
If internal standard(s): specify	C13-PCBs and
Analysis technique used for PAHs (+ detection)	GCMS-EI
Brief description of column, injection technique, temperature program/gradient, length of run, etc	2 µL, splitless injection at 300°C, AT-5MS column, 30 m length, 0.25 mm internal diameter and 0.25 µm film thickness (Grace, USA). The PAH temperature program applied starts with 60°C (1 min hold), 10 °C/min to 100 °C, 20°C/min to 320°C for 9 minutes hold
Analysis technique used for PCBs (+ detection)	GC MSMS
Brief description of column, injection technique, temperature program, length of run, etc	Two µL were splitless injected at 280°C on an AT-5MS column of 30 m length, 0.25 mm internal diameter and 0.25 µm film thickness (Grace, USA).
Automatic or manual integration of chromatograms	Automatic with manual inspection
PRC data used for calculation of C _{free} (Y/N)	No, only for quality assurance, i.e. confirm non depletion and indication of equilibrium.
Reference for PRC calculation method	-

Standardized experiment	
Equilibration:	
Equilibration system	Vial, amber, 15 mL for SPME; bottle, amber, 120 mL for sheets
Mass of sediment per system (g)	Approx. 8 for SPME and 60 for sheets (ww)
Aqueous solution added (Y/N)	Y
Composition of aqueous solution (biocide, salts)	100 mg/L NaN ₃
Pre-cleaning procedure sampler	Shake with different solvents (depending on polymer) successively and store in water (fibers) or air-dry (sheets)
Mass (or length for SPME; cm) of sampler (mg) for each sediment	2-30 cm fiber (depending on sediment and coating); 2.5-30 mg sheet (depending on sediment and polymer)
Equilibration: static or dynamic	Dynamic
If dynamic: type of 'shaker' (e.g. tumbler/1D shaker/2D shaker/Rock&Roller)	Rock & Roller for SPME, 1-D shaker for sheets
Speed of shaker (rpm)	60 for SPME; 150 for sheets
Equilibration time (days)	42
PRCs added (Y/N). If yes, which ones	N
Time series to confirm equilibration (Y/N). If yes: which time points	N
Equilibration temperature (°C ± ..)	20 ± 2 °C
Precautions taken against exposure to light	Amber glassware, dark room/covered box
Extraction/clean-up:	
Brief extraction procedure (extraction method, equipment, solvent, time, etc)	Samplers were removed from the sediment slurry, cleaned with wet tissue, cut, and placed in autosampler vials containing the appropriate solvent. Internal standards were added and the vials were placed in the freezer. Prior to analysis, they were left at room temperature for several hours and vortexed for 1-4 min

	(depending on the sampler)
Clean-up (Y/N)	N
Data corrected for blanks and recoveries (Y/N)	Y (blanks)
Final solvent after clean-up (injection solvent)	Depending on participant and sampler
Volume of final extract (solvent) (mL)	0.2-0.5 (SPME), 1.0 for sheets
Type of autosampler vial (volume; clear, amber)	Amber, 1.8 mL (with 200 μ L insert for SPME if necessary)

Table S4. Concentration ranges (expressed as factors) in C_{free} values in the first experiment (measurements based on own procedures). More specifically: the highest (averaged) C_{free} for the respective chemical measured by a specific participant / lowest (averaged) C_{free} for that chemical (measured by another participant).

	BB sediment	FD sediment	SP sediment
Phenanthrene	32	15	15
Anthracene	6	8	9
Fluoranthene	10	10	10
Pyrene	10	7	9
Benz[a]anthracene	24	15	21
Chrysene	11	11	11
Benzo[e]pyrene	13	8	14
Benzo[b]fluoranthene	11	14	13
Benzo[k]fluoranthene	10	5	9
Benzo[a]pyrene	18	10	34
Benzo[g,h,i]perylene	13	21	20
Dibenz[a,h]anthracene	22	32	19
Indeno[123-cd]pyrene	10	14	13
PCB-18	7	14	67
PCB-28	26	16	68
PCB-52	9	9	14
PCB-66	32	53	20
PCB-77	98	2371	20
PCB-101	7	11	10
PCB-118	15	19	31
PCB-138	12	20	35
PCB-153	16	27	41
PCB-170	16	45	120
PCB-180	9	57	204
PCB-187	13	56	59

Table S5. Determination of the actual coating thickness/volume of SPME fibers.

Fiber	Manufacturer provided (nominal) volume (L/cm)	Actual (measured) volume (L/cm)	% deviation
S10-1 (10 μm)	$6.912 \cdot 10^{-8}$	$7.821 \cdot 10^{-8}$	11.6
S10-2 (10 μm)	$6.912 \cdot 10^{-8}$	$6.654 \cdot 10^{-8}$	3.9
S30-1 (30 μm)	$1.329 \cdot 10^{-7}$	$1.142 \cdot 10^{-7}$	16.4
S30-2 (30 μm)	$5.904 \cdot 10^{-7}$	$5.704 \cdot 10^{-7}$	3.5
S100 (100 μm)	$9.425 \cdot 10^{-7}$	$9.421 \cdot 10^{-7}$	0.04
PAC (30 μm)	$1.536 \cdot 10^{-7}$	$1.408 \cdot 10^{-7}$	9.1

The accuracy of the nominal coating volume of the fiber-bound polymers (PDMS on the S10-1, S10-2, S30-1, S30-2, and S100 fibers and polyacrylate on the PAc fiber) was evaluated by determining the exact coating thickness of all fibers by microscopic measurements. Five pieces of 3 cm were cut from different positions of the stock fibers. They were sampled from either end and, if possible, from the middle. The pieces were cleaned with solvents and water according to the methods prescribed in the standardized protocol. Next, the coating of one half of each fiber piece was stripped with a razorblade. Here, it should be noted that the razor stripping did not affect the glass core, as thorough scraping was found to have no effect on its thickness. Subsequently, the pieces were examined at the largest magnification possible (100 - 400 x). After pulling the maximal width of the object into focus, the diameter of the coated and stripped parts were measured at 10 positions each with the assistance of microscopy software. After subtraction of the core diameter from the total diameter, the coating thickness was derived. The error of the measurements is estimated to be about 0.5 μm (based on full width of the fibers) (i.e., < 0.5%).

Table S6. Variation Factors (*VFs*) calculated for the sediment heterogeneity experiment.

	BB sediment	FD sediment	SP sediment
Phenanthrene	1.1	1.2	1.2
Anthracene	1.1	1.2	1.2
Fluoranthene	1.2	1.2	1.5
Pyrene	1.2	1.2	1.6
Benz[a]anthracene	1.2	1.2	1.8
Chrysene	1.2	1.2	1.9
Benzo[e]pyrene	1.2	1.2	1.9
Benzo[b]fluoranthene	1.2	1.2	2.1
Benzo[k]fluoranthene	1.2	1.2	2.1
Benzo[a]pyrene	1.2	1.2	2.1
Benzo[g,h,i]perylene	1.2	1.3	2.1
Dibenz[a,h]anthracene	1.4	1.4	2.4
Indeno[123-cd]pyrene	1.2	1.2	2.4
PCB-18	1.2	1.2	1.6
PCB-28	1.2	1.2	1.7
PCB-52	1.2	1.2	1.8
PCB-66	-	-	1.9
PCB-77	-	-	2.0
PCB-101	1.2	1.3	2.0
PCB-118	1.2	1.3	2.1
PCB-138	1.2	1.3	2.2
PCB-153	1.2	1.3	2.2
PCB-170	1.2	1.3	2.1
PCB-180	1.3	1.4	2.4
PCB-187	1.2	1.3	2.4

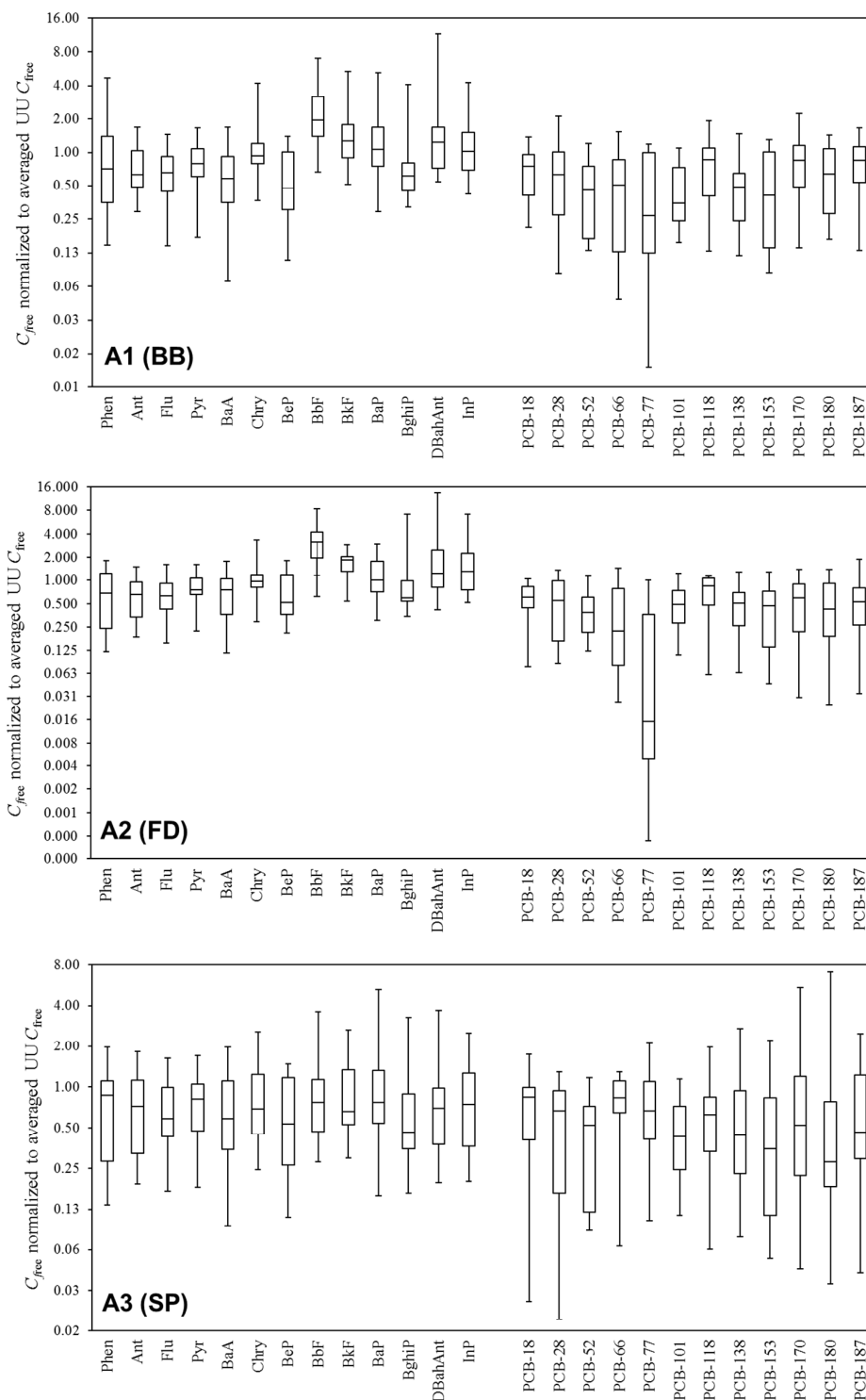
Table S7. Averaged relative standard deviations (RSDs; %) calculated for replicated ($n = 5$) measurements by the coordinating laboratory, with different samplers, according to the standardized protocols (intra-method variability).

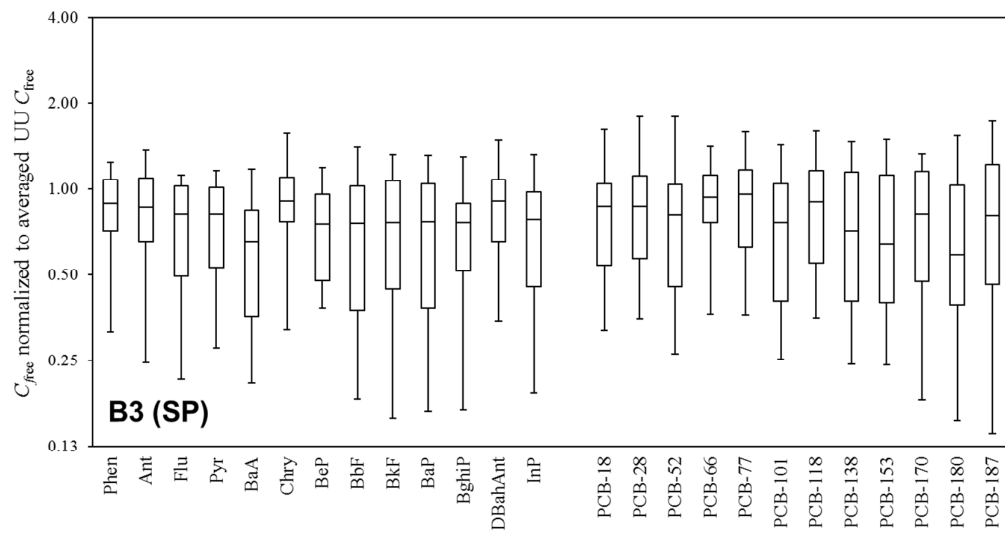
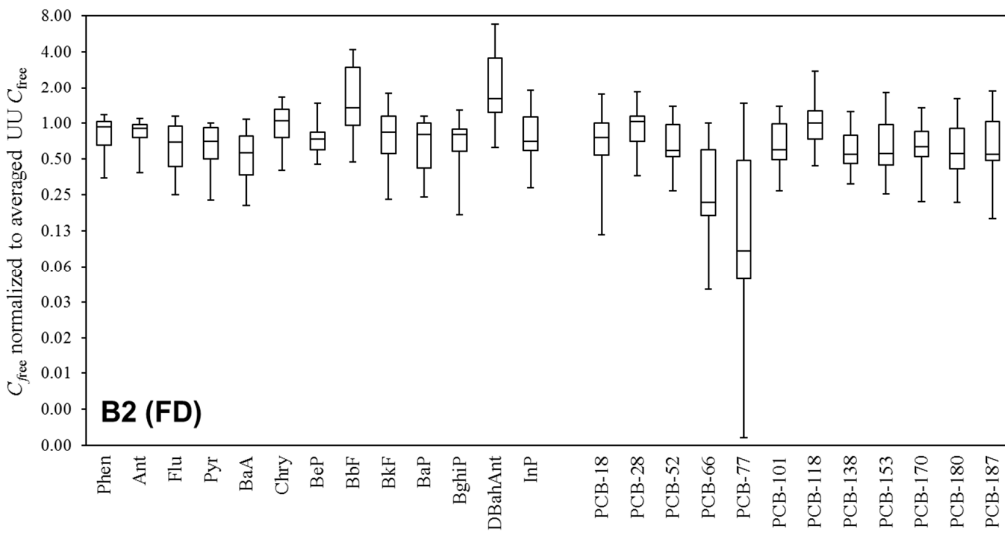
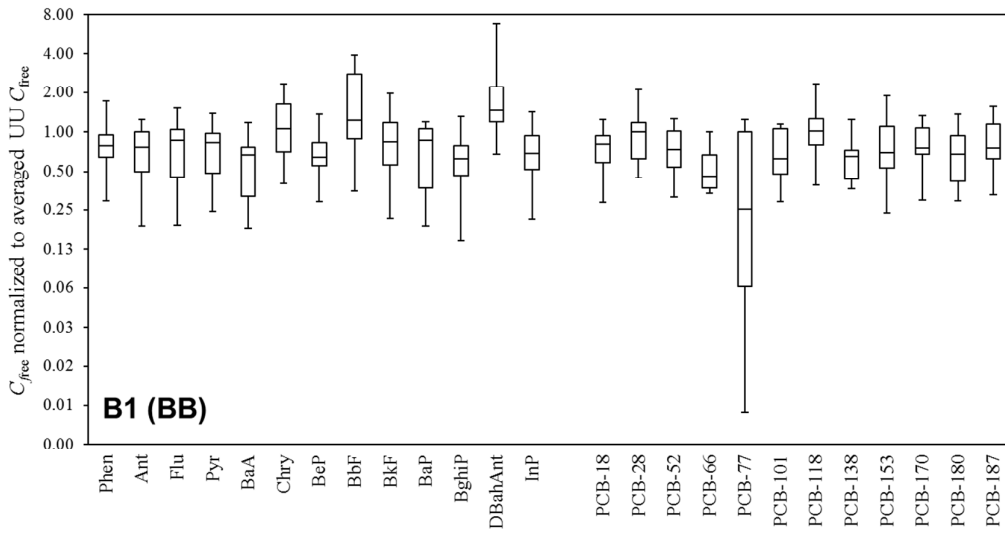
	BB sediment	FD sediment	SP sediment
<i>Sheets</i>			
PE-1	1.5	3.1	2.2
PE-2	2.3	4.8	7.6
PE-3	1.8	3.1	6.0
PE-4	2.4	4.8	1.5
PE-5	2.0	3.5	2.5
PE-6	2.2	4.7	4.3
POM	2.3	3.4	3.2
SSP	1.7	5.0	2.0
<i>SPME fibers</i>			
S10-1 (10 μm)	7.6	9.9	6.2
S10-2 (10 μm)	5.8	9.9	3.6
S30-1 (30 μm)	5.0	10.3	4.3
S30-2 (30 μm)	4.1	7.6	5.2
S100 (100 μm)	3.0	6.7	1.7
PAC (30 μm)	4.9	7.2	3.6

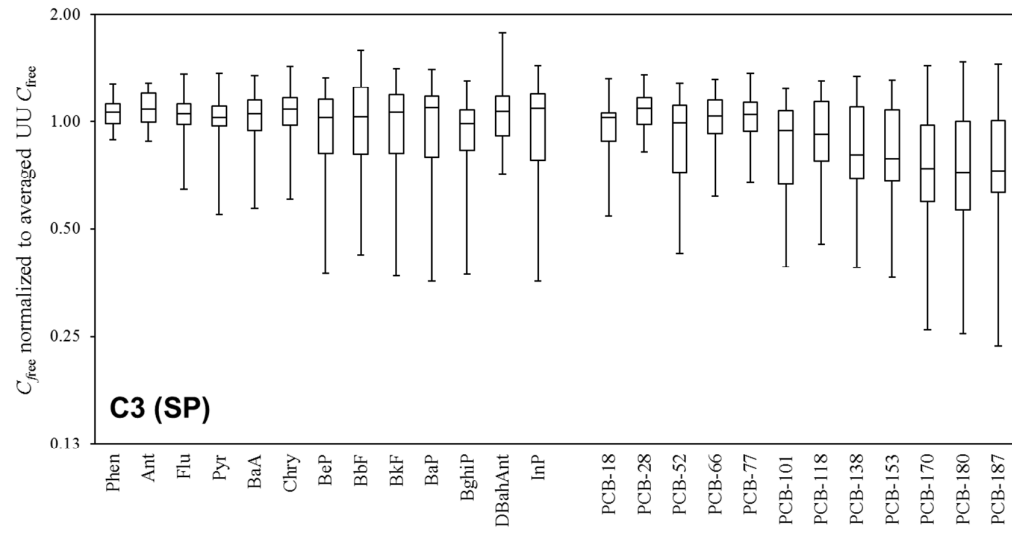
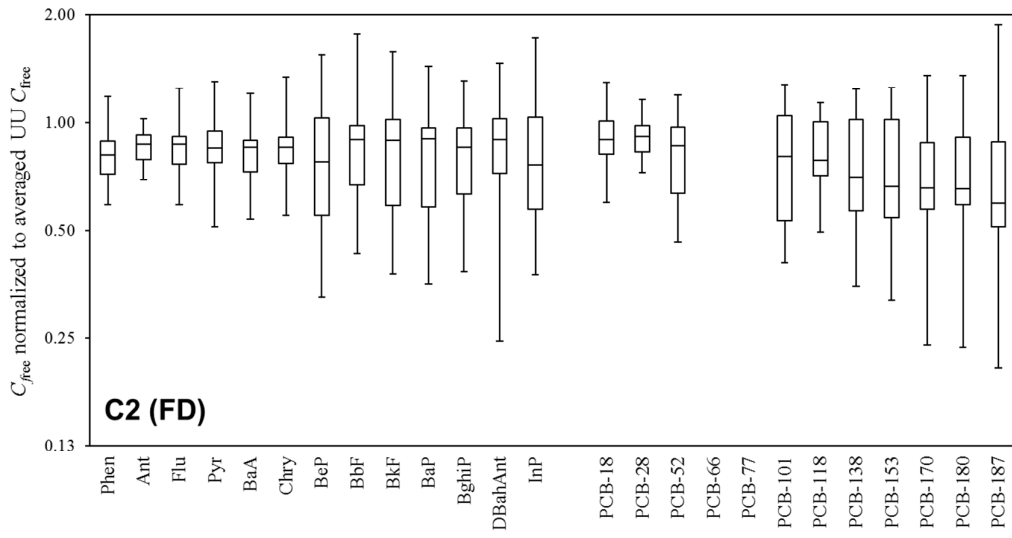
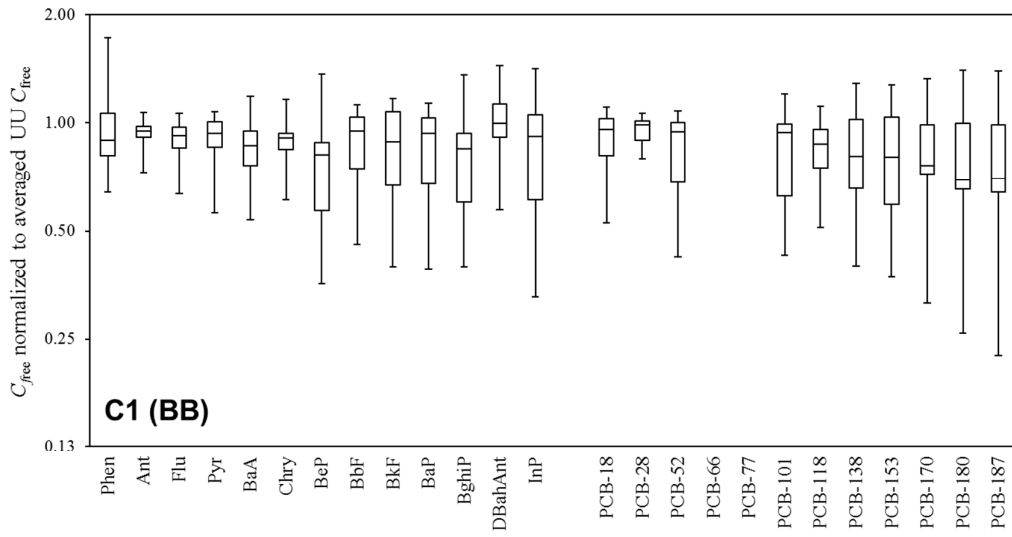
Table S8. Variation Factors (*VFs*) calculated based on the (range of) concentrations obtained with all the different sampling formats (inter-method variability).

	BB sediment	FD sediment	SP sediment
Phenanthrene	1.7	1.4	1.4
Anthracene	1.2	1.3	1.5
Fluoranthene	1.2	1.3	1.3
Pyrene	1.3	1.3	1.3
Benz[a]anthracene	1.5	1.4	1.5
Chrysene	1.3	1.4	1.5
Benzo[e]pyrene	2.0	2.4	1.6
Benzo[b]fluoranthene	1.4	1.6	1.6
Benzo[k]fluoranthene	1.6	1.6	1.7
Benzo[a]pyrene	1.5	1.5	1.6
Benzo[g,h,i]perylene	2.1	2.1	1.8
Dibenz[a,h]anthracene	1.7	2.2	1.9
Indeno[123-cd]pyrene	2.1	2.1	1.9
PCB-18	1.3	1.3	1.3
PCB-28	1.2	1.4	1.5
PCB-52	1.4	1.5	1.4
PCB-66	-	-	1.4
PCB-77	-	-	1.6
PCB-101	1.4	1.6	1.6
PCB-118	1.5	1.4	1.6
PCB-138	1.8	1.9	1.9
PCB-153	1.9	1.9	1.9
PCB-170	2.0	2.1	2.3
PCB-180	2.3	2.2	2.4
PCB-187	2.2	2.7	2.3

Figure S1. Box Plots corresponding to Figure 1 in the main text (codes here refer to the panel codes in Figure 1). All C_{free} values were divided (normalized) to the averaged C_{free} values from the coordinating laboratory (lab UU). Note that (i) y-axis scales are different for the different plots; (ii) data for PCBs 66 and 77 in plots A1, A2, B1, and B2 were normalized to the C_{free} value of another lab, as lab UU did not report a value in these cases (compounds were actually not present in the BB and FD sediment). For this reason, no data are given for these chemicals in plots C1, C2, D1, and D2 (extracts analyzed by lab UU).







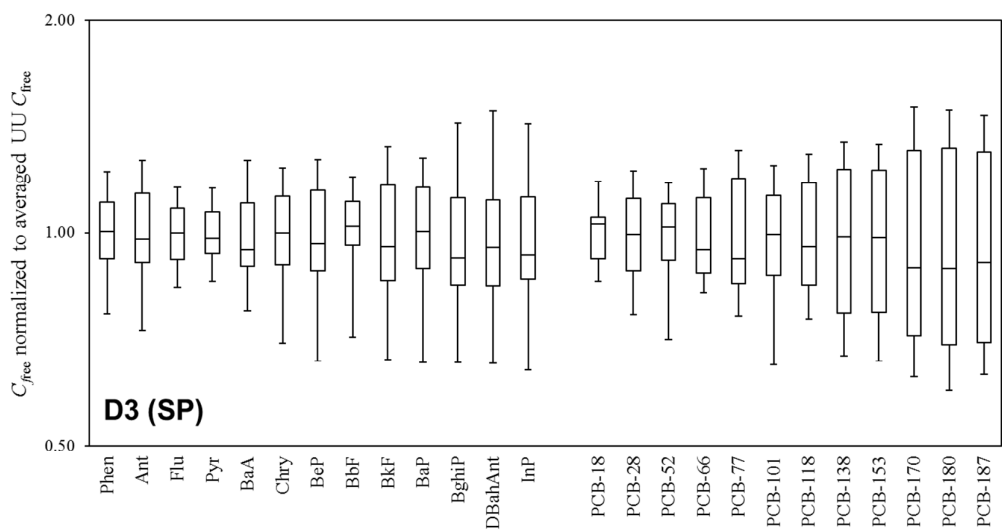
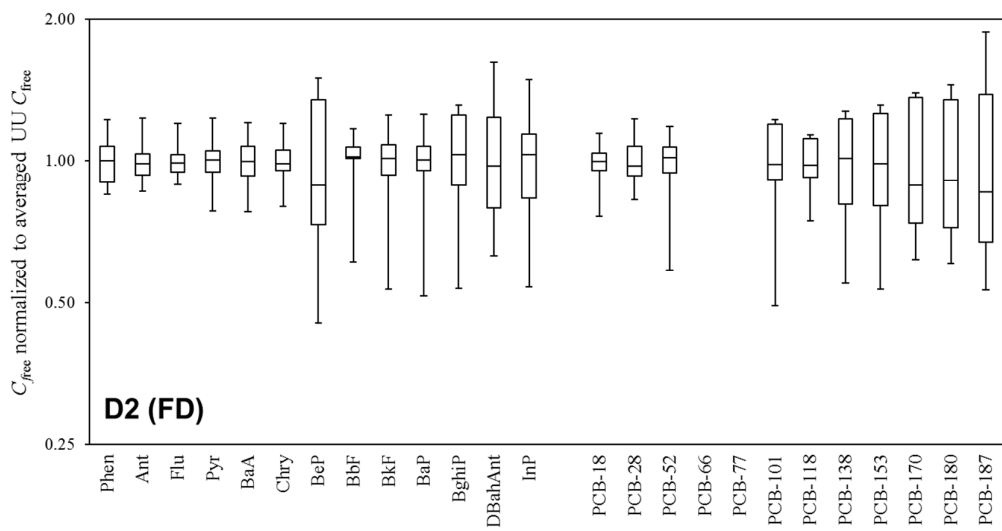
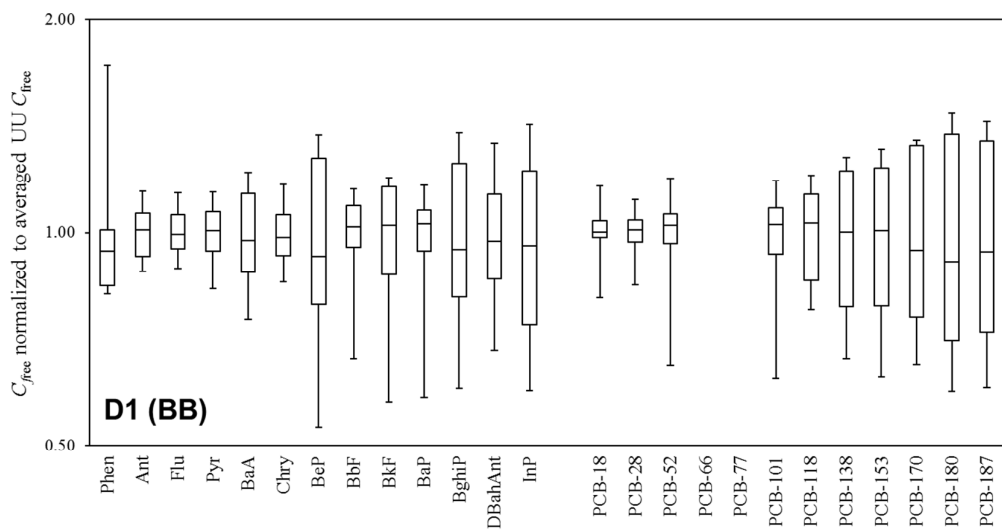


Figure S2. Effect of standardizing K_{pw} values on the inter-laboratory variability.

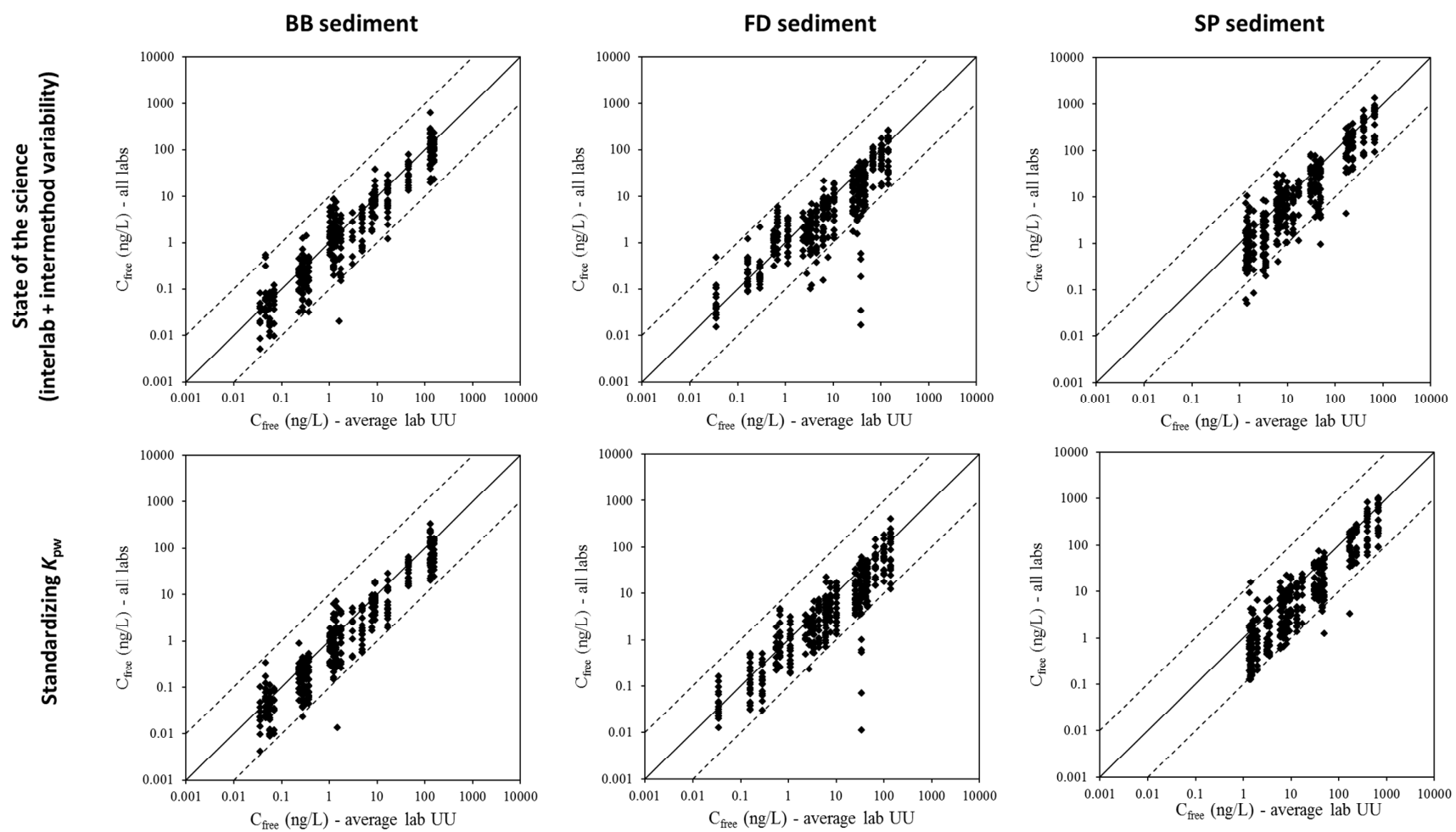


Figure S3. C_{free} (ng/L) as determined with SR as the sampler, by applying an increasing sampler–sediment mass ratio (ca. $1/1000$, $1/100$, $1/20$, $1/5$, and $1/1$) plotted against the “sampler–extracted” concentration from the sediment ($\mu\text{g}/\text{kg}$; i.e., the amount in the sampler expressed on a sediment mass basis). The downward arrows indicate the total concentrations in the sediments. Data for PCB153 show a linear decrease, with C_{free} approaching zero when the sediment is fully depleted (extracted). The C_{free} values for benzo[*a*]pyrene decrease with a factor of about 4 going from the lowest to the highest sampler–sediment ratio ($1/1$), but for this chemical, only about 5% max is extracted from the sediment.

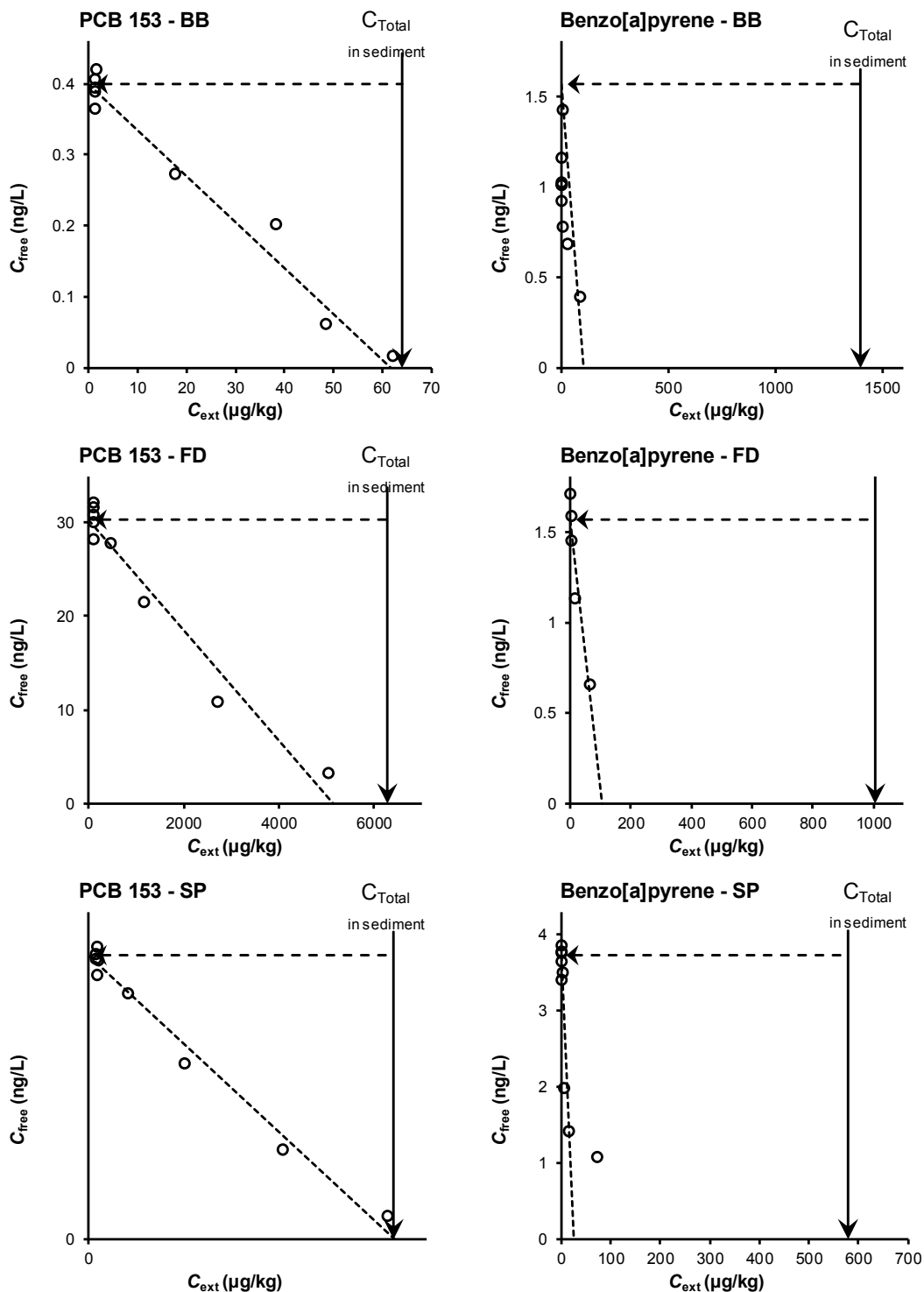
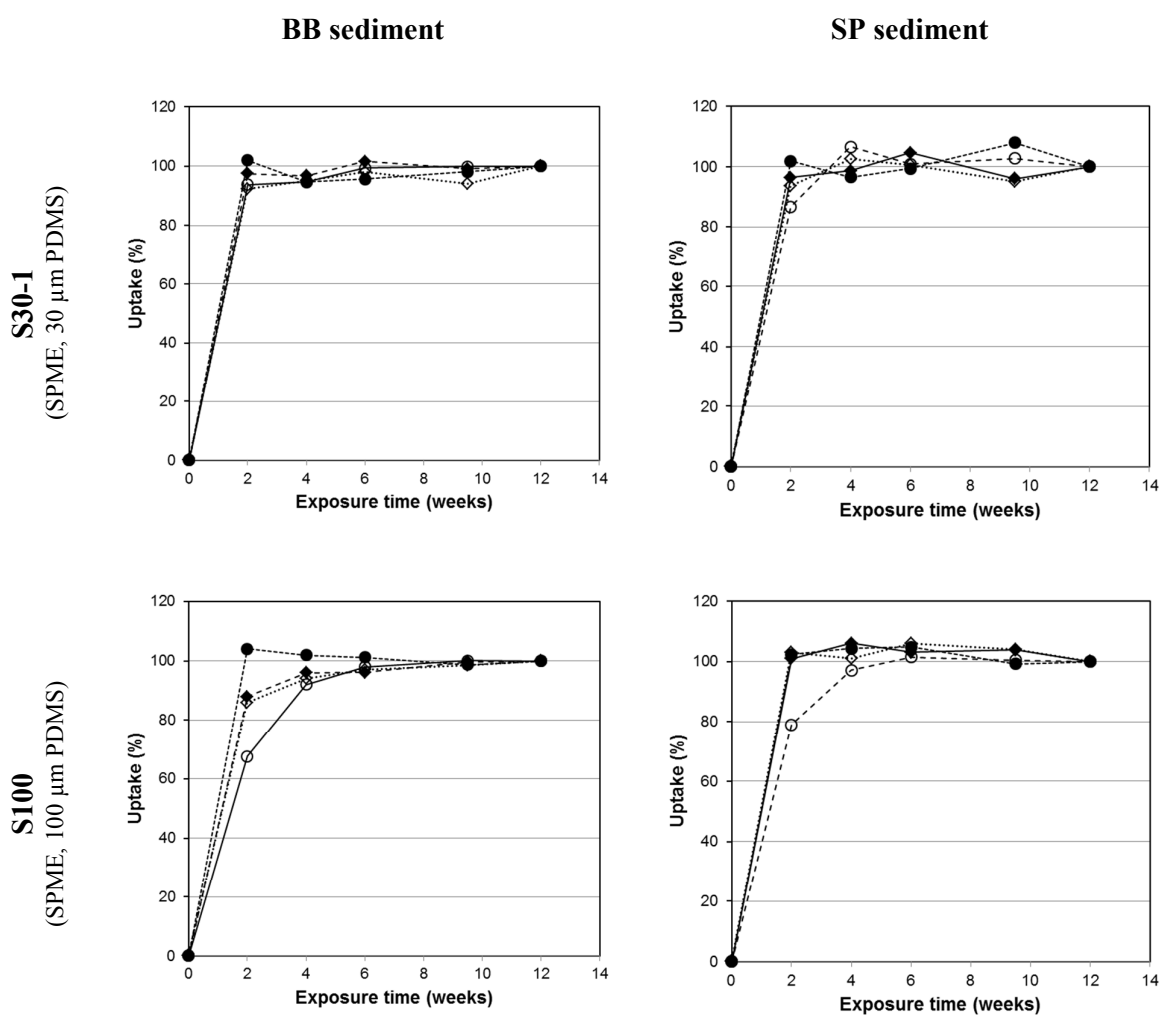


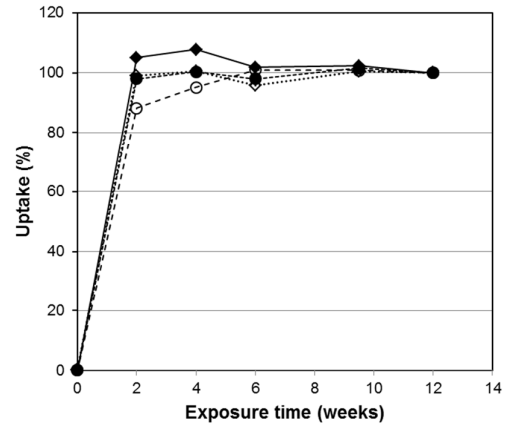
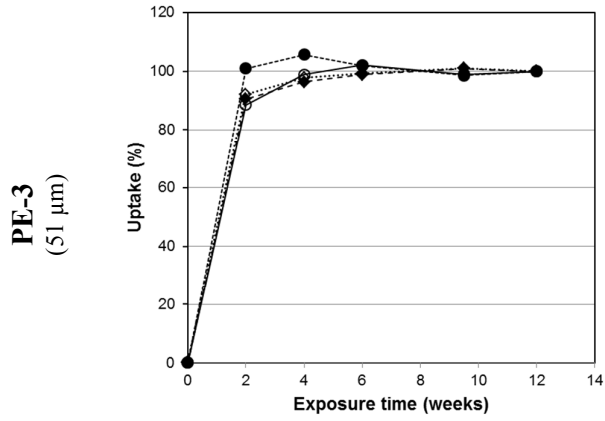
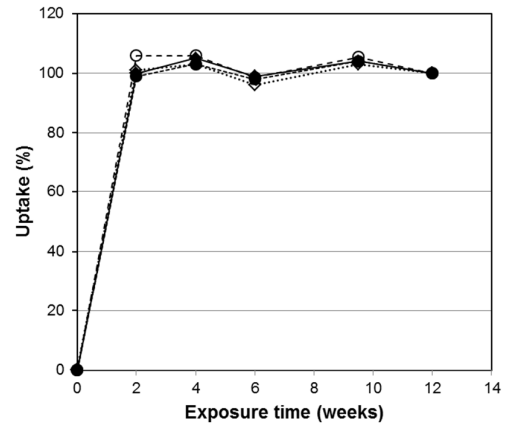
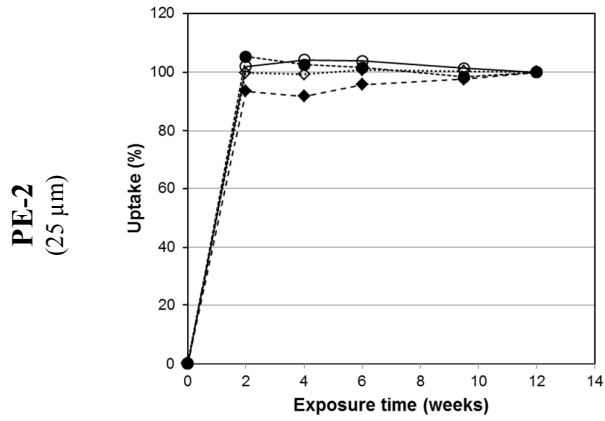
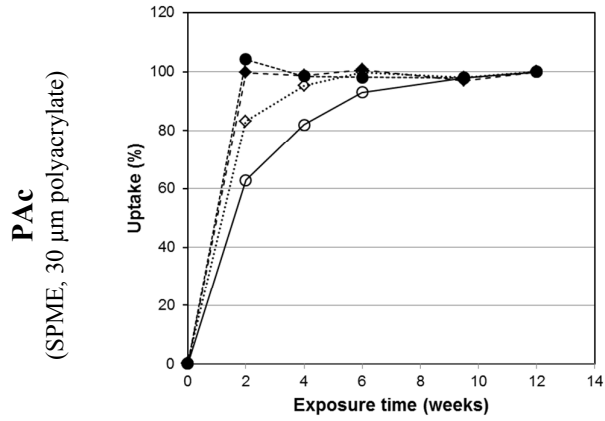
Figure S4. Uptake kinetics in different passive samplers.

Uptake kinetics from sediment-water slurries with continuous shaking were determined for seven samplers, according to the standardized protocol: S30-1, S100, PAc, PE-2, PE-3, POM, and SR (see Table S1 for explanation of abbreviations). Kinetics in the other PE samplers was assumed to be similar to uptake in PE-2. Likewise, S30-2 kinetics were assumed to be represented by kinetics in S30-1. Kinetics in S10-1 and S10-2 will be faster than for S30 and were therefore not quantified. Uptake was determined after exposure for 2, 4, 6, 9.5, and 12 weeks to the BB and the SP sediment. Uptake of chemicals in PAc from the SP sediment was not determined due to logistic reasons. Each measurement was performed in three-fold. For the graphical presentation below, four chemicals were selected (a moderately and very hydrophobic PAH and a moderately and very hydrophobic PCB): fluoranthene (\blacklozenge), benzo[*g,h,i*]perylene (\diamond), PCB-52 (\bullet), and PCB-180 (\circ).



BB sediment

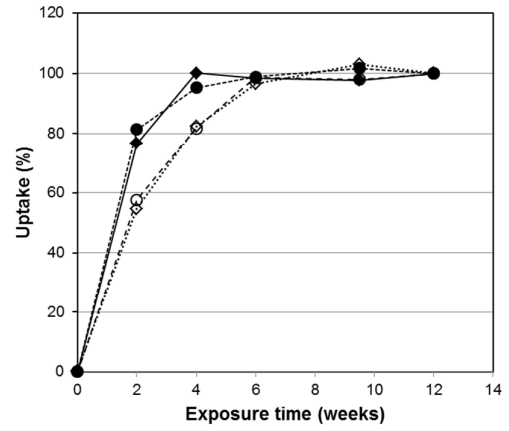
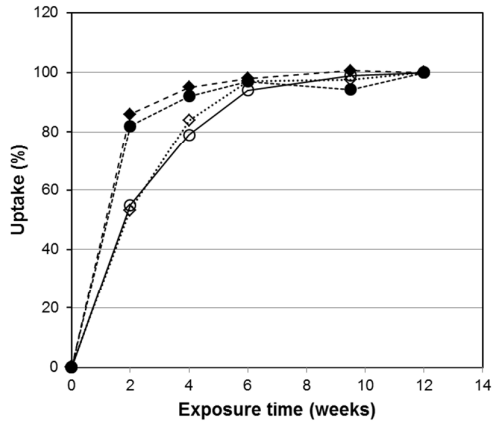
SP sediment



BB sediment

SP sediment

POM
(77 μm)



SR
(100 μm silicone rubber)

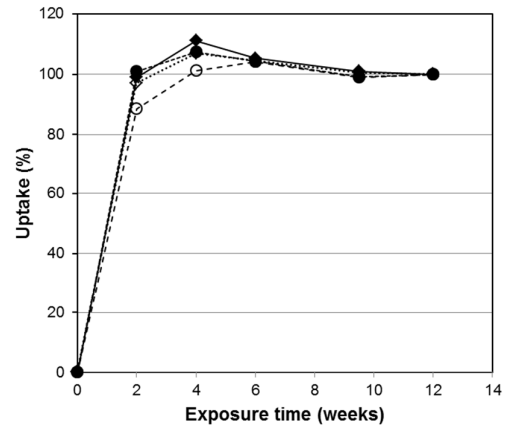
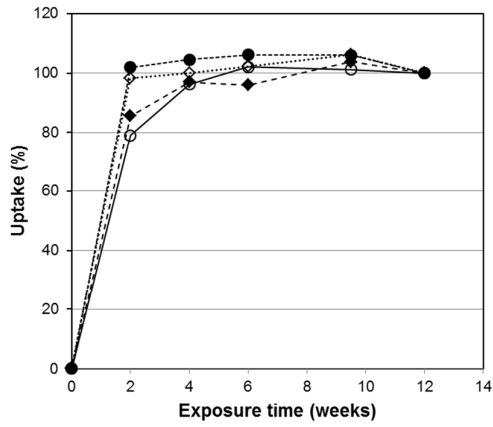


Figure S5. Relationship between C_{free} determined statically (with PRC correction to calculate equilibrium concentrations in the sampler) and in well-mixed (dynamic) systems. Results were obtained with 25 μm -thick PE by one of the participants. The solid line represents the 1:1 relationship; the dashed lines the 1:2 and 2:1 relationships. Data are for C_{free} values determined in all three sediments.

