

Supplementary S 1: List of analyzed polycyclic aromatic hydrocarbons (PAHs) with according octanol-water partition coefficient log K_{OW} and soil organic carbon-water partition coefficient log K_{OC} (US environmental protection agency (EPA, 1996))

Compound	Acronym	Category	log K _{OW}	log K _{OC}
Naphthalene	Nap	2-ring PAH	3.38	3.30
Acenaphthylene	Acy	3-ring PAH	4.07	4.00
Acenaphthene	Ace		3.92	3.85
Fluorene	Fl		4.10	4.14
Phenanthrene	Phe		4.46	4.38
Anthracene	Ant	4-ring PAH	4.54	4.47
Fluoranthene	Flu		4.84	5.03
Pyrene	Pyr		5.18	5.02
Benzo(a)anthracene	BaA		5.60	5.60
Chrysene	Chr	5-ring PAH	5.84	5.60
Benzo(b)fluoranthene	BbF		6.44	6.09
Benzo(k)fluoranthene	BkF		6.44	6.09
Benzo(a)pyrene	BaP	6-ring PAH	6.42	6.01
Indeno(1,2,3-c,d)pyrene	InP		6.42	6.54
Benzo(g,h,i)perylene	BgP		6.63	6.52
Dibenzo(a,h)anthracene	DBA		6.50	6.58

Supplementary S 2: List of investigated polychlorinated biphenyls (PCBs) with according octanol-water partition coefficient log K_{OW} predicted by algorithm (ChemAxon) and soil organic carbon-water partition coefficient log K_{OC} calculated from log K_{OW}-value (US environmental protection agency (EPA, 1996))

Compound	Acronym	Category	log K _{OW}	log K _{OC}
2,4,4'/2,5,4'-Trichlorobiphenyl	PCB #28	indicator PCB	5.43	4.38
2,2',5,5'-Tetrachlorobiphenyl	PCB #52		6.04	4.86
2,2',4,5,5'-Pentachlorobiphenyl	PCB #101		6.64	5.34
2,2',3,4,4',5'-Hexachlorobiphenyl	PCB #138		7.24	5.81
2,2',4,4',5,5'-Hexachlorobiphenyl	PCB #153		7.24	5.81
2,2',3,4,4',5,5'-Heptachlorobiphenyl	PCB #180	non-ortho PCB	7.85	6.29
3,3',4,4'-Tetrachlorobiphenyl	PCB #77		6.04	4.86
3,4,4',5-Tetrachlorobiphenyl	PCB #81		6.04	4.86
3,3',4,4',5-Pentachlorobiphenyl	PCB #126		6.64	5.34
3,3',4,4',5,5'-Hexachlorobiphenyl	PCB #169		7.24	5.81
2,3,3',4,4'-Pentachlorobiphenyl	PCB #105	mono- ortho PCB	6.64	5.34
2,3,4,4',5-Pentachlorobiphenyl	PCB #114		6.64	5.34
2,3',4,4',5-Pentachlorobiphenyl	PCB #118		6.64	5.34
2',3,4,4',5-Pentachlorobiphenyl	PCB #123		6.64	5.34
2,3,3',4,4',5-Hexachlorobiphenyl	PCB #156		7.24	5.81
2,3,3',4,4',5'-Hexachlorobiphenyl	PCB #157		7.24	5.81
2,3',4,4',5,5'-Hexachlorobiphenyl	PCB #167		7.24	5.81
2,3,3',4,4',5,5'-Heptachlorobiphenyl	PCB #189		7.85	6.29

Supplementary S 3: List of analyzed organochlorine pesticides (OCPs) with according octanol-water partition coefficient log K_{OW} and soil organic carbon-water partition coefficient log K_{OC} (US environmental protection agency (EPA, 1996)) and predicted by algorithm (ChemAxon) where no values were available

Compound	Acronym	Category	log K _{OW}	log K _{OC}
α-Hexachlorocyclohexane	α-HCH	Hexachloro-cyclohexanes	3.80	3.09
β-Hexachlorocyclohexane	β-HCH		3.81	3.10
γ-Hexachlorocyclohexane	γ-HCH		3.73	3.03
δ-Hexachlorocyclohexane	δ-HCH		4.14	3.36
ε-Hexachlorocyclohexane	ε-HCH		4.14	3.36
Pentachlorobenzene			4.99	4.03
Hexachlorobenzene			5.89	4.74
Pentachloroanisole			4.84	3.91
Octachlorostyrene			6.64	5.34
4,4'-Dichlorodiphenyltrichloroethane	4,4'-DDT	DDT-related pesticides	6.53	6.42
2,4'-Dichlorodiphenyltrichloroethane	2,4'-DDT		6.53	6.42
4,4'-Dichlorodiphenyldichloroethane	4,4'-DDD		6.10	6.00
2,4'-Dichlorodiphenyldichloroethane	2,4'-DDD		6.10	6.00
4,4'-Dichlorodiphenyldichloroethene	4,4'-DDE		6.76	6.65
2,4'-Dichlorodiphenyldichloroethene	2,4'-DDE		6.76	6.65
trans-Chlordane		Chlordane-related pesticides	6.32	5.08
cis-Chlordane			6.32	5.08
oxy-Chlordane			5.05	4.08
Heptachlor			6.26	6.15
cis-Heptachloroepoxide			4.04	3.28
trans-Heptachloroepoxide			4.04	3.28
Aldrin			6.50	6.39
Dieldrin			5.37	4.33
Endrin			5.06	4.03
Endosulfan-I			4.10	3.33
Endosulfan-II			4.10	3.33
Endosulfan-sulfate			4.10	3.33
Methoxychlor			5.08	4.90
Mirex			7.63	6.12

Supplementary S 4: List of analyzed perfluoroalkylic acids (PFAAs) with their corresponding octanol-water partition coefficient log K_{OW} predicted by algorithm (ChemAxon)

Compound	Acronym	log K _{OW}
Perfluorobutanoic acid	PFBA	2.31
Perfluoropentanoic acid	PFPeA	3.01
Perfluorohexanoic acid	PFHxA	3.71
Perfluoroheptanoic acid	PFHpA	4.41
Perfluorooctanoic acid	PFOA	5.11
Perfluorononanoic acid	PFNA	5.81
Perfluorodecanoic acid	PFDA	6.51
Perfluoroundecanoic acid	PFUdA	7.21
Perfluorododecanoic acid	PFDoA	7.92
Perfluorotridecanoic acid	PFTTrDA	8.62
Perfluorotetradecanoic acid	PFTeDA	9.32
Perfluorobutanesulfonate	PFBS	2.63
Perfluorohexanesulfonate	PFHxS	4.03
Perfluorooctanesulfonate	PFOS	5.43
Perfluorodecanesulfonate	PFDS	-

Supplementary S 5: List of analyzed pharmaceutical residues and polar pesticides with their corresponding octanol-water partition coefficient log K_{OW} predicted by algorithm (ChemAxon)

Compound	Class	log K _{OW}
Sulfamethoxazole	antibiotic	0.89
Simazine	herbicide	2.18
Carbamazepine	anticonvulsant; mood stabilizer	2.45
Atrazine	herbicide	2.61
Naproxen	nonsteroidal anti-inflammatory drug	3.18
Linuron	herbicide	3.20
Diclofenac	nonsteroidal anti-inflammatory drug	4.26
Ibuprofen	nonsteroidal anti-inflammatory drug	3.84

Supplementary S 6: Binary chromatographic gradient; flushing of the sample loop during the isocratic hold at the start, re-equilibration of the separation column for 5 min at the end of each injection

Time [min]	Solvent A [%]	Solvent B [%]
00.0	100	0
01.5	100	0
25.0	0	100
30.0	0	100
30.1	100	0
35.0	100	0

Supplementary S 7: Blank corrected minimum PAH concentration values determined in glass cartridges with XAD2-resin and glass wool filter cartridges in pg L⁻¹; estimated maximum concentration boundary shown at the bottom

values in pg L ⁻¹	11 m water depth		31 m water depth		61 m water depth	
Compound	XAD	Glass Wool Filter	XAD	Glass Wool Filter	XAD	Glass Wool Filter
Naphthalene	n.d.	183	n.d.	183	n.d.	2270
Acenaphthylene	n.d.	30	n.d.	30	n.d.	162
Acenaphthene	26	81	32	82	n.d.	105
Fluorene	n.d.	228	n.d.	228	n.d.	1034
Phenanthrene	342	1328	286	1329	241	2401
Anthracene	40	311	23	311	33	381
Fluoranthene	426	2488	343	2488	147	2226
Pyrene	1437	1836	693	1836	266	1595
Benzo(a)anthracene	129	927	67	927	42	823
Chrysene	361	1339	140	1339	89	1070
Benzo(b)fluoranthene	205	1536	87	1536	71	1005
Benzo(k)fluoranthene	58	386	34	386	28	335
Benzo(a)pyrene	96	920	46	920	34	706
Indeno(1,2,3-c,d)pyrene	78	675	36	675	39	544
Benzo(g,h,i)perylene	124	970	53	970	52	709
Dibenzo(a,h)anthracene	24	171	10	171	11	129
Sum PAH	3346	13407	1850	13412	1053	15494
Sum minimum total PAH	16753		15262		16547	
Est. maximum total PAH	17333		15539		n/a*	

*no valid separation between master/backup sample

Supplementary S 8: Blank corrected minimum PCB concentration values determined in glass cartridges with XAD2-resin and glass wool filter cartridges in pg L⁻¹; estimated maximum concentration boundary shown at the bottom

values in pg L ⁻¹	11 m water depth		31 m water depth		61 m water depth	
Compound	XAD	Glass Wool Filter	XAD	Glass Wool Filter	XAD	Glass Wool Filter
2,4,4'/2,5,4'-Trichlorobiphenyl	0.6	1.0	0.4	1.5	0.8	0.3
2,2',5,5'-Tetrachlorobiphenyl	0.7	1.4	0.6	1.4	1.2	0.4
2,2',4,5,5'-Pentachlorobiphenyl	0.6	1.1	0.4	1.4	0.8	0.5
2,2',3,4,4',5'-Hexachlorobiphenyl	0.2	0.2	0.1	0.3	0.5	0.4
2,2',4,4',5,5'-Hexachlorobiphenyl	0.5	0.5	0.3	0.8	0.4	0.3
2,2',3,4,4',5,5'-Heptachlorobiphenyl	0.3	0.1	0.2	0.3	0.2	0.2
3,3',4,4'-Tetrachlorobiphenyl	0.0	0.1	0.1	0.1	0.1	0.0
3,4,4',5-Tetrachlorobiphenyl	0.0	0.0	0.0	0.0	0.0	0.0
3,3',4,4',5-Pentachlorobiphenyl	0.0	0.0	0.0	0.0	0.0	0.0
3,3',4,4',5,5'-Hexachlorobiphenyl	0.0	0.0	0.0	0.0	0.0	0.0
2,3,3',4,4'-Pentachlorobiphenyl	0.2	0.2	0.2	0.2	0.1	0.1
2,3,4,4',5-Pentachlorobiphenyl	n.d.	0.0	0.0	0.0	n.d.	0.0
2,3',4,4',5-Pentachlorobiphenyl	0.4	0.4	0.2	0.6	0.4	0.2
2',3,4,4',5-Pentachlorobiphenyl	0.0	0.0	0.0	0.0	0.0	0.0
2,3,3',4,4',5-Hexachlorobiphenyl	0.1	0.0	0.0	0.1	0.1	n.d.
2,3,3',4,4',5'-Hexachlorobiphenyl	0.0	0.0	0.0	0.0	0.0	0.0
2,3',4,4',5,5'-Hexachlorobiphenyl	0.0	0.0	0.0	0.0	0.0	0.0
2,3,3',4,4',5,5'-Heptachlorobiphenyl	0.0	0.0	0.0	0.0	0.0	0.0
Sum PCB	3.5	4.9	2.5	6.6	4.5	2.3
Sum minimum total PCB	8.4		9.1		6.8	
Est maximum total PCB	n/a*		13.4		n/a*	

* no valid separation between master/backup sample

Supplementary S 9: Blank corrected minimum OCP concentration values determined in glass cartridges with XAD2-resin and glass wool filter cartridges in pg L⁻¹; estimated maximum concentration boundary shown at the bottom

values in pg L ⁻¹	11 m water depth		31 m water depth		61 m water depth	
Compound	XAD	Glass Wool Filter	XAD	Glass Wool Filter	XAD	Glass Wool Filter
α-Hexachlorocyclohexane	97	1	80	1	35	1
β-Hexachlorocyclohexane	103	2	84	2	39	1
γ-Hexachlorocyclohexane	20	1	16	1	8	1
δ-Hexachlorocyclohexane	9	2	7	1	3	2
ε-Hexachlorocyclohexane	6	2	5	0	3	0
Pentachlorobenzene	38	6	29	5	14	5
Hexachlorobenzene	104	29	101	23	38	17
Pentachloroanisole	41	2	38	2	15	2
Octachlorostyrene	2	1	2	2	1	1
4,4'-Dichlorodiphenyltrichloroethane	11	8	6	5	3	3
2,4'-Dichlorodiphenyltrichloroethane	4	2	2	1	1	1
4,4'-Dichlorodiphenyldichloroethane	7	3	5	2	1	2
2,4'-Dichlorodiphenyldichloroethane	5	1	3	1	1	1
4,4'-Dichlorodiphenyldichloroethene	9	9	6	6	2	5
2,4'-Dichlorodiphenyldichloroethene	1	1	1	0	0	0
trans-Chlordane	1	0	0	0	0	0
cis-Chlordane	0	0	0	0	n.d.	0
oxy-Chlordane	0	0	0	0	0	0
Heptachlor	0	0	0	0	0	0
cis-Heptachloroepoxide	0	0	0	0	0	0
trans-Heptachloroepoxide	0	0	0	0	0	0
Aldrin	0	0	0	0	2	1
Dieldrin	0	n.d.	0	0	1	0
Endrin	0	0	0	0	0	0
Endosulfan-I	2	0	2	0	0	0
Endosulfan-II	0	0	0	0	0	0
Endosulfan-sulfate	81	1	61	1	31	n.d.
Methoxychlor	n.d.	0	n.d.	0	0	1
Mirex	0	0	0	0	0	0
Sum OCP	541	71	448	54	197	43

Sum minimum total OCP	612	502	240
Est. maximum total OCP	1551	695	984

Supplementary S 10: Blank corrected minimum PFAA concentration values determined in glass cartridges with XAD7/16-resin and glass wool filter cartridges in pg L⁻¹; estimated maximum concentration boundary shown at the bottom

values in pg L ⁻¹	31 m water depth		50 m water depth	
Compound	XAD	Glass Wool Filter	XAD	Glass Wool Filter
Perfluorobutanoic acid	0	0	0	0
Perfluoropentanoic acid	11	0	1	0
Perfluorohexanoic acid	20	16	15	10
Perfluoroheptanoic acid	0	0	31	0
Perfluorooctanoic acid	902	1	1119	0
Perfluorononanoic acid	17	0	20	0
Perfluorodecanoic acid	9	0	7	1
Perfluoroundecanoic acid	3	0	4	0
Perfluorododecanoic acid	0	0	1	0
Perfluorotridecanoic acid	0	0	0	0
Perfluorotetradecanoic acid	0	0	0	0
Perfluorobutanesulfonate	n. d.	0	n. d.	0
Perfluorohexanesulfonate	13	0	3	0
Perfluorooctanesulfonate	54	0	61	0
Perfluorodecanesuflonate	0	0	0	0
Sum PFAA	1028	17	1263	13
Sum minimum total PFAA	1045		1276	
Est. maximum total PFAA	2100		2833	

Supplementary S 11: Blank corrected minimum concentration values of selected pharmaceuticals and polar pesticides determined in glass cartridges with XAD7/16-resin and glass wool filter cartridges in pg L⁻¹; estimated maximum concentration boundary shown at the bottom

values in pg L ⁻¹	11m water depth		31m water depth		61m water depth	
Compound	XAD	Glass Wool Filter	XAD	Glass Wool Filter	XAD	Glass Wool Filter
Sulfamethoxazole	0	6	1	59	0	56
Simazine	33	0	9	0	9	0
Carbamazepine	116	0	52	0	47	0
Atrazine	4644	1	1631	1	1249	2
Naproxen	0	33	n. d.	114	n. d.	37
Linuron	107	0	22	0	0	0
Diclofenac	n. d.	4	31	158	26	2
Ibuprofen	n. d.	0	n. d.	28	n. d.	0
Sum Pharm+Pesticide	4900	56	2841	377	2659	110
Sum minimum total Pharm+Pesticide	4956		3218		2769	
Est. maximum total Pharm+Pesticide	9032		10289		4649	