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Performance of Semipermeable Membrane Devices for Sampling of Organic Contaminants in Groundwater

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Electronic Supplementary information

8 Tables with detailed information on the contaminants identified in the SPMD extracts.

Table 1 Selected physicochemical properties of organic chemicals identified by GC/MS in SPMD extracts. Samplers were deployed for 20 days in groundwater monitoring wells in Bitterfeld, Saxony-Anhalt, Germany.

no.	Compound	Component Type[a]	RT[b] [min]	LRI[c] Calc.	LRI[d] Lit.	BP[e] [°C]	MW[f] [g/mol]	log Kow[g]
1	Nonane	MI	7.62	146		151	128	
2		INC						
3	Methylpropylcyclopentane	INC	7.72	146				
4	Tetrachloroethane	IC	7.74	147		146	168	2.2
5	Tetrachloroethane	IC	7.8	147		146	168	2.2
6	Tetrachloroethane	IC	7.85	147		146	168	2.2
7	Tetrachloroethane	IC	7.9	148		146	168	2.2
9	Dimethyloctane	IC	8.08	149		160		5.1
10	Ethylmethylcyclohexane	IC	8.16	149		152	126	4.5
11	Propylcyclohexane	IC	8.2	149		157	126	4.6
12	Butylcyclopentane	MI	8.32	150		157	126	4.6
13	Trichloropropene	IC	8.72	152		142	145	2.8
14	2-Chlorotoluene	IC	8.87	153		159	127	3.2
15	4-Chlorotoluene	IC	9.06	155		162	127	3.2
16	1,3,5-Trimethylbenzene	IC	9.26	156		165	120	3.6
17	Dimethyltrisulfide	IC	9.46	157		177	126	1.9
18	Pentachloroethane	IC	9.67	158		162	202	3.1
19	Ethyltoluene	IC	9.88	159		162	120	3.6
20	1,2,4-Trimethylbenzene	IC	10.4	163		169	120	3.6
21	1,3-Dichlorbenzene	IC	10.75	165		173	147	3.3
22	1,4-Dichlorobenzene	MI	11.18	167		173	147	3.3
23	1,2,3-Trimethylbenzene	IC	11.42	169		175		
24	1,2-Dichlorobenzene	MI	11.95	172		181	147	3.3
25	Brommethylbenzene	IC	12.06	173		199	171	2.9
26	Chlorodimethylbenzene	IC	12.55	176		222	140	3.7
27	Chlorodimethylbenzene	IC	12.62	176		222	140	3.7

28	Methylpropylcyclohexane	INC	12.82					
29	Trichloropropene	INC	12.93					
30	Ethyl-dimethyl-bicycloheptane	INC	12.98					
31	Methyl (methylethyl)-benzene	INC	13.28					
32	Methylthiobenzene	IC	13.42	181		188	124	2.6
33	Butenylbenzene	IC	13.49	181		176	132	3.9
34	Chlorodimethylbenzene	IC	13.56	182		222	140	3.7
35	Chloromethylphenol	INC	13.61					
36	Bromochlorobenzene	IC	13.7	182		204	191	3.5
37	Bromochlorobenzene	IC	13.87	183		196	191	3.5
38	Bromochlorobenzene	IC	13.93	184		196	191	3.5
39	Undecane	MI	13.98	184	183	195	156	
40	Methylbenzofurane	IC	14.18	185		198	132	3.1
41	Dichlorotoluene	IC	14.76	189		204	161	3.8
42	Dichlorotoluene	IC	14.79	189		204	161	3.8
43	Dichlorotoluene	IC	14.96	190		204	161	3.8
44	1,3,5-Trichlorobenzene	IC	14.97	190		208	181	3.9
45	Dihydromethylindene	IC	15.19	191		191	132	3.9
46	Dihydromethylindene	IC	15.23	192		191	132	3.9
47	Methylindane	IC	15.47	193		191		
48	Dichlortoluene	IC	15.53	193		204	161	3.8
49	Methylethyltoluene	IC	15.69	194		192	134	4.1
50	Chlorobenzofuran	INC	15.76	195				
51	Tetrahydronaphthalene	IC	15.84	195		207	132	4
52	Chloronitrobenzene	INC	15.9	195	246			
53	Decahydrodimethylnaphthalene	MI	15.93	196		208	166	
54	Pentachlorobutadiene	IC	16	196		191	202	4.2
55	1,2,4-Trichlorobenzene	IC	16.53	199		214	181	3.9
56	Naphthalene	MI	16.62	200	200	218	128	3.2
57	Chloroxylenol	IC	16.7	201		246	157	3.3
58	Benzo(b)thiophene	IC	16.74	201	201	221	134	3
59	Bromodichlorothiophene	IC	16.86	202			231	
60	Bromodichlorothiophene	IC	17	203				
61	Dodecane	MI	17.12	203	204	216	170	6.1
62	Trimethylphenol	IC	17.17	204	204- 225	227	136	3.2
63	Dimethylnaphthalene	INC	17.26	204	204- 225	227	136	
64	Bromochloromethylbenzene	INC	17.34	205	241 - 250	267	156	4.1
65	1,2,3-Trichlorobenzene	IC	17.47	206		219	181	3.9
66	Dimethyltetrasulfide	IC	17.56	206		234	158	1.9
67	Chloromethylphenol	IC	17.65	207		205	143	2.7
68	Cyclopentylbenzene	IC	17.76	208		219	146	4.3
69	Dichlorodimethylbenzene	IC	17.94	209		253	175	3.6
70	Trimethylphenol	IC	17.96	209		225	136	3.2
71	Ethenylthiobenzene	IC	18.6	213		206	136	3
72	Trichloropropene	INC	18.63	213		142		

73	Tetrachlorothiophene	IC	19.13	217		233	222	4.4
74	Chloromethylphenol	IC	19.16	217		205	143	2.7
75	Bromodichlorobenzene	IC	19.17	217		235	226	4.2
76	Dichlorostyrene	IC	19.44	219		214	173	4.2
77	(Methylthio) thiophenol	INC	19.56	220				
78	Methylbenzenamine	INC	19.68	221	177	196	107	1.6
79	Methylnaphthalene	IC	19.71	221		242	142	3.7
80	Trichlortoluene	IC	19.83	221		238	195	4.5
81	Dimethylethylphenol	INC	19.84	221				
82	Tridecane	MI	19.92	222	223	235	184	6.7
83	Chlorodimethylpyridine	INC	19.96	223				
84	Trichlortoluene	IC	20.12	223		238	195	4.5
85	Methylnaphthalene	IC	20.22	224		242	142	3.7
86	Dichlortetramethylcyclobutene	INC	20.42	225				
87	Diethylphenol	IC	20.42	225		248	150	3.6
88	Tetrachlorobenzene	IC	20.81	228		246	216	4.6
89	Trichlorotoluene	IC	20.92	229		238	195	4.5
90	Tetrachloropropene	INC	21.27	232		180		
91	Chloromethylphenol	INC	21.45	233	242	143	2	0
92	Chlorobenside	INC	21.65	234	352	269.2	5.6	0
93	Tetrahydroisoquinolin-6,7-diol	INC	21.92	235				
94	Chloronaphthalene	IC	21.93	236		260	162	4.5
95	Dimethylpropylphenol	INC	22.06	237				
96	1,2,3,4-Tetrachlorobenzene	IC	22.09	237		238	215.89	4.6
97	Tetrachloropropene	IC	22.18	237			180	
98	Benzylmethyldisulfide	IC	22.28	238		260	170	3.6
99	Tetradecane	MI	22.57	240	240	254	198	7.2
100	Methylbiphenyl	IC	22.63	240		267	168	4.3
101	Bromotrichlorbenzene	IC	23.15	244		256	260	4.8
102	Diphenylmethan	IC	23.42	245		264	168	4
103	Tetrachloroheptene	INC	23.58	248				
104	Chloroquinoline	INC	23.84	249	262	164	3	0
106	Dimethylphthalate	MI	24.01	249		284	194	1.6
107	Dimethyltrisulfide	INC	24.09	251	177	126	2	0.1
108	Tetrachloroheptene	INC	24.25	251				
109	Tetrachloroheptene	INC	24.29	251				
110	Chloroquinoline	INC	24.29	248	262	164	3	0
111	Bromotrichlorobenzene	IC	24.4	244		256	260	4.8
112	Butylated Hydroxyanisol	MI	24.42	252		264	180	3.5
113	Bromtrichlorobenzene	IC	24.58	244		256	260	4.8
115	Dichlorobenzenamine	IC	24.62	254		258	162	2.4
116	Pentadecane	MI	25.07	257	257	271	212	7.7
117	Chlorobiphenyl	IC	25.1	257		284	188	4.4
118	Bis-(Dimethylethyl)phenol	IC	25.45	259		263	206	5.2
119	Butylated Hydroxytoluene	MI	25.48	259		265	220	5.1
120	Methyl-(phenylmethyl)-benzene	IC	25.88	262		286	182	4.6

121	Methyl-(phenylmethyl)-benzene	IC	26.07	263		286	182	4.6
122	Dichlortoluene	INC	26.61	267	204	161	4	0.1
123	Chlorobiphenyl	IC	26.76	268		284	188	4.4
124	Bromofluorobenzene	INC	26.88		151	175	3	0.1
125	Chlorobiphenyl	IC	26.91	269		284	188	4.4
126	Diphenylsulfide	IC	27.17	271		296	186	4.3
127	Hexadecane	MI	27.46	272	272	287	226	8.3
128	Methylnitrobenzene	INC	28.32	278	222	137	2	0
129	Bis-(chlormethyl)-benzene	IC	28.47	279		254	175	3.6
130	N-(1,1-Dimethylethyl)benzamide	INC	28.77	281	328	177	3	0
131	Dichloromethylquinoline	INC	29.51	286				
132	alpha-HCH	IC	29.68	287		288	291	4.3
133	Tetramethylbutylphenol	IC	29.83	288		310	220	5.5
134	Nonylphenol	IC	30.05	290		295	220	6
135	Diisopropylnaphthalene	IC	30.22	291		309	212	6.1
137	Dimethylpropylphenol	IC	30.83	295		262	164	3.9
138	beta-HCH	IC	30.85	295		304	291	4.3
139	(4-Methylphenyl)-phenylmethanone	IC	30.95	296		326	196	3.7
140	gamma-HCH	IC	31.05	296		323	291	4.3
141	Benzylbenzoate	IC	31.17	297		323	212	3.5
142	Anthracene- d10	IC	31.28	298	300	340	188	4.5
143	Phenanthrene-d10	IC	31.57	300	301	340	188	4.5
144	Trichlorbenzenamine	INC	31.87	300	275	196	3	0
146	delta-HCH	IC	32.09	304		323	291	4.3
147	Trichlorbenzenamine	INC	32.18	302	275	196	3	0
148	Trichlorobenzenamine	INC	32.27	303	275	196	3	0
149	Trichlorobenzenamine	IC	32.5	308		275	196	3
150	Trichlorobenzenamine	INC	32.6	306	275	196	3	0
151	Trichlorobenzenamine	INC	32.81	307	275	196	3	0
152	N-Butyldecanamine	IC	33.48	316				
153	Thiophenone	INC	33.48	312	172	100	1	0
154	Chloro-(trichloromethyl)-benzene	INC	33.92	316	264	230	5	0
155	Tetrachlorobenzenamine	IC	33.93	320		298	231	3.7
156	Tetrachlorobenzenamine	IC	34.01	321		298	231	3.7
157	Tetrachlorobenzenamine	INC	34.76	322	298	231	4	0
158	Dibutylphthalate	IC	35.09	330		340	278	4.6
159	Dichlorophenylsulfide	INC	35.21	325				
160	Sulphur	INC	36.27	333	440	256	0	0.4
161	(1,1-Biphenyl)-4,4-diamine,3,3-dimethyl	IC	36.78	344		339	212	3
162	Octadecenoic acid, methylester	MI	37.65	351	351	352	296	7.5
163	(1,1-Biphenyl)-4,4-diamine,3,3-dimethyl	IC	37.74	352		339	212	3
164	Octadecanoic acid	MI	38.73	360		361	284	8.2
165	Octadecenamid	INC	42.16	378				
166	benzanthracene-d12	PRC	43.42	400	399	437		
167	Bis(2-ethylhexyl)phthalate	MI	45.08	414		386	391	7.6

[a] MI – SPMD matrix impurity; IC – identified contaminant; INC – identity not confirmed; PRC – performance reference compound;

[b]GC retention time
[c]Lee retention index calculated using equation 1 from GC retention time
[d]Lee retention index from reference 17
[e]Boiling point
[f]Molar weight
[g]Octanol/water partition coefficient

Table 2. Molar concentrations of semi-volatile compounds (boiling point > 200°C) identified in extracts from SPMDs deployed for 20 days in groundwater monitoring well SafBit 30/98 in Bitterfeld.

Sample	Component	*SafBit 30/98 A*		*SafBit 30/98 B*		
	Type[a]	Match quality[b]	Concentration[c]	Match quality[b]	Concentration[c]	RPD[d]
no. Compound		[%]	[µmol/SPMD]	[%]	[µmol/SPMD]	[%]
1 Nonane	MI	95	NQ[f]	91	NQ	175%
22 1,4-Dichlorobenzene	MI	97	NQ	91	NQ	77%
24 1,2-Dichlorobenzene	MI	93	NQ	91	NQ	42%
39 Undecane	MI	83	NQ	87	NQ	111%
55 1,2,4-Trichlorobenzene	IC	87	0.001	87	0.001	27%
61 Dodecane	MI	96	0.007	94	0.002	87%
73 Tetrachlorothiophene	IC	#[e]		95	0.001	
82 Tridecane	MI	94	0.004	97	0.001	90%
99 Tetradecane	MI	97	0.007	98	0.001	119%
106 Dimethylphthalate	MI	91	0.004	90	0.001	84%
116 Pentadecane	MI	94	0.004	90	0.001	126%
118 Bis-(Dimethylethyl)phenol	IC	94	0.013	64	0.004	62%
127 Hexadecane	MI	93	0.010	90	0.002	111%
142 Anthracene- d10	PRC	95	0.020	94	0.020	42%
143 Phenanthrene-d10	PRC	94	0.020	94	0.019	42%
158 Dibutylphthalate	IC	94	0.011	41	NQ	85%
161 (1,1-Biphenyl)-4,4-diamine,3,3-dimethyl	IC	85	0.018	58	NQ	115%
162 Octadecenoic acid, methylester	MI	86	25.560	98	0.292	193%
164 Octadecanoic acid	MI	99	8.110	99	2.746	61%
165 Octadecenamid	INC	96	0.139	96	0.009	164%
166 benzanthracene-d12	PRC	95	0.043	90	0.043	45%
167 Bis(2-ethylhexyl)phthalate	MI	96	1.957	37	NQ	199%

[a]MI – SPMD matrix impurity; IC – identified contaminant; INC – identity not confirmed; PRC – performance reference compound
[b]Match quality of the found mass spectrum with the mass spectrum library search
[c]Concentrations of analytes identified in sample quantified using RMRF approach. Only concentrations of analytes with normal boiling point higher than 200°C are reported
[d]Relative percent difference of peak areas in duplicate samples
[e]# - not found in the sample
[f]Compound was not quantified because its normal boiling point was lower than 200°C or the match quality was lower than 80%.

Table 3. Molar concentrations of semi-volatile compounds (boiling point > 200°C) identified in extracts from SPMDs deployed for 20 days in groundwater monitoring well SafBit 31/98 in Bitterfeld.

Sample	*Component*	*SafBit 31/98 A*		*SafBit 31/98 B*		
no. Compound	**Type[a]**	**Match quality[b]** [%]	**Concentration[c]** [µmol/SPMD]	**Match quality[b]** [%]	**Concentration[c]** [µmol/SPMD]	**RPD[d]** [%]
1 Nonane	MI	95	NQ[f]	91	NQ	85%
22 1,4-Dichlorobenzene	MI	93	NQ	94	NQ	19%
24 1,2-Dichlorobenzene	MI	95	NQ	87	NQ	31%
55 1,2,4-Trichlorobenzene	IC	81	0.000	87	0.000	14%
56 Naphthalene	MI	84	0.000	#[e]		
61 Dodecane	MI	96	0.001	94	0.000	94%
73 Tetrachlorothiophene	IC	87	0.000	#		
82 Tridecane	MI	97	0.001	91	0.000	46%
99 Tetradecane	MI	97	0.001	97	0.001	25%
106 Dimethylphthalate	MI	81	0.001	91	0.001	52%
116 Pentadecane	MI	96	0.001	93	0.000	37%
119 Butylated Hydroxytoluene	MI	96	0.001	94	0.001	14%
127 Hexadecane	MI	96	0.001	52	NQ	17%
142 Anthracene- d10	PRC	94	0.021	93	0.020	11%
143 Phenanthrene-d10	PRC	90	0.020	87	0.019	10%
162 Octadecenoic acid, methylester	MI	86	0.210	99	0.286	27%
164 Octadecanoic acid	MI	99	2.929	99	3.067	1%
165 Octadecenamid	INC	95	0.009	98	0.011	13%
166 benzanthracene-d12	PRC	90	0.018	90	0.020	1%
167 Bis(2-ethylhexyl)phthalate	MI	64	NQ	83	0.003	31%

[a]MI – SPMD matrix impurity; IC – identified contaminant; INC – identity not confirmed; PRC – performance reference compound
[b]Match quality of the found mass spectrum with the mass spectrum library search
[c]Concentrations of analytes identified in sample quantified using RMRF approach. Only concentrations of analytes with normal boiling point higher than 200°C are reported
[d]Relative percent difference of duplicate samples
[e]# - not found in the sample
[f]Compound was not quantified because its normal boiling point was lower than 200°C or the match quality was lower than 80%.

Table 4. Molar concentrations of semi-volatile compounds (boiling point > 200°C) identified in extracts from SPMDs deployed for 20 days in groundwater monitoring well SafBit 2/96U in Bitterfeld.

Sample	*Component*	*SafBit 2/96U A*		*SafBit 2/96U B*		
no. Compound	Type[a]	Match quality[b] [%]	Concentration[c] [µmol/SPMD]	Match quality[b] [%]	Concentration[c] [µmol/SPMD]	RPD[d] [%]
1 Nonane	MI	96	NQ[f]	95	2	101%
3 Methylpropylcyclopentane	INC	81	NQ	#[e]		
10 Ethylmethylcyclohexane	IC	86	NQ	64	NQ	126%
12 Butylcyclopentane	MI	94	NQ	90	NQ	153%
14 2-Chlorotoluene	IC	97	NQ	68	NQ	161%
21 1,3-Dichlorbenzene	IC	90	NQ	50	NQ	101%
22 1,4-Dichlorobenzene	MI	97	NQ	98	NQ	121%
24 1,2-Dichlorobenzene	MI	95	NQ	92	NQ	111%
39 Undecane	MI	95	NQ	94	NQ	106%
55 1,2,4-Trichlorobenzene	IC	70	NQ	94	0.001	65%
61 Dodecane	MI	97	0.002	95	0.003	41%
82 Tridecane	MI	96	0.001	97	0.001	11%
99 Tetradecane	MI	96	0.003	96	0.002	13%
106 Dimethylphthalate	MI	94	0.001	90	0.001	21%
116 Pentadecane	MI	97	0.001	96	0.001	2%
118 Bis-(Dimethylethyl)phenol	IC	96	0.002	94	0.003	44%
119 Butylated Hydroxytoluene	MI	95	0.001	95	0.001	10%
127 Hexadecane	MI	86	0.002	66	NQ	4%
135 Diisopropylnaphthalene	IC	64	NQ	86	0.002	6%
142 Anthracene- d10	PRC	94	0.029	94	0.031	10%
143 Phenanthrene-d10	PRC	87	0.028	94	0.031	11%
162 Octadecenoic acid, methylester	MI	99	0.204	99	0.160	21%
164 Octadecanoic acid	MI	99	0.000	99	3.939	100%
165 Octadecenamid	MI	96	0.009	96	0.011	22%
166 benzanthracene-d12	PRC	90	0.022	90	0.024	20%
167 Bis(2-ethylhexyl)phthalate	MI	80	0.003	72	NQ	3%

[a]MI – SPMD matrix impurity; IC – identified contaminant; INC – identity not confirmed; PRC – performance reference compound
[b]Match quality of the found mass spectrum with the mass spectrum library search
[c]Concentrations of analytes identified in sample quantified using RMRF approach. Only concentrations of analytes with normal boiling point higher than 200°C are reported
[d]Relative percent difference of duplicate samples
[e]# - not found in the sample
[f]Compound was not quantified because its normal boiling point was lower than 200°C or the match quality was lower than 80%.

Table 5. Molar concentrations of semi-volatile compounds (boiling point > 200°C) identified in extracts from SPMDs deployed for 20 days in groundwater monitoring well SafBit 2/96O in Bitterfeld.

Sample	*Component*	*SafBit 2/96O A*		*SafBit 2/96O B*		
	Type[a]	Match quality[b]	Concentration[c]	Match quality[b]	Concentration[c]	RPD[d]
no. Compound		[%]	[µmol/SPMD]	[%]	[µmol/SPMD]	[%]
1 Nonane	MI	90	NQ[f]	91	NQ	189%
12 Butylcyclopentane	MI	91	NQ	#[e]	NQ	
22 1,4-Dichlorobenzene	MI	96	NQ	75	NQ	117%
24 1,2-Dichlorobenzene	MI	97	NQ	74	NQ	107%
39 Undecane	MI	94	NQ	95	NQ	114%
53 Decahydrodimethylnaphthalene	MI	91	0.001	70	NQ	78%
55 1,2,4-Trichlorobenzene	IC	93	0.000	56	NQ	15%
61 Dodecane	MI	87	0.002	95	0.001	54%
82 Tridecane	MI	87	0.001	93	0.001	43%
99 Tetradecane	MI	95	0.001	97	0.001	3%
106 Dimethylphthalate	MI	91	0.001	85	0.001	8%
116 Pentadecane	MI	90	0.000	94	0.000	18%
119 Butylated Hydroxytoluene	MI	97	0.011	95	0.012	14%
127 Hexadecane	MI	93	0.001	72	NQ	3%
142 Anthracene- d10	PRC	94	0.027	90	0.022	18%
143 Phenanthrene-d10	PRC	93	0.027	90	0.022	17%
162 Octadecenoic acid, methylester	MI	99	0.098	99	0.117	20%
164 Octadecanoic acid	MI	99	2.557	99	2.486	0%
165 Octadecenamid	INC	94	0.004	93	0.005	20%
166 benzanthracene-d12	PRC	90	0.024	92	0.019	21%
167 Bis(2-ethylhexyl)phthalate	MI	80	0.003	87	0.002	12%

[a]MI – SPMD matrix impurity; IC – identified contaminant; INC – identity not confirmed; PRC – performance reference compound
[b]Match quality of the found mass spectrum with the mass spectrum library search
[c]Concentrations of analytes identified in sample quantified using RMRF approach. Only concentrations of analytes with normal boiling point higher than 200°C are reported
[d]Relative percent difference of duplicate samples
[e]# - not found in the sample
[f]Compound was not quantified because its normal boiling point was lower than 200°C or the match quality was lower than 80%.

Table 6. Molar concentrations of semi-volatile compounds (boiling point > 200°C) identified in extracts from SPMDs deployed for 20 days in groundwater monitoring well SafBit 16/97 in Bitterfeld.

Sample	*Component*	*SafBit 16/97 A*		*SafBit 16/97 B*		
	Type[a]	Match quality[b]	Concentration[c]	Match quality[b]	Concentration[c]	RPD[d]
no. Compound		[%]	[µmol/SPMD]	[%]	[µmol/SPMD]	[%]
1 Nonane	MI	90	NQ[e]	90	NQ	
9 Dimethyloctane	IC	81	NQ	87	NQ	
11 Propylcyclohexane	IC	87	NQ	93	NQ	
12 Butylcyclopentane	MI	91	NQ	94	NQ	
14 2-Chlorotoluene	IC	96	NQ	96	NQ	
19 Ethyltoluene	IC	87	NQ	59	NQ	
20 1,2,4-Trimethylbenzene	IC	90	NQ	90	NQ	
21 1,3-Dichlorbenzene	IC	92	NQ	91	NQ	
22 1,4-Dichlorobenzene	MI	93	NQ	91	NQ	
23 1,2,3-Trimethylbenzene	IC	43	NQ	91	NQ	
24 1,2-Dichlorobenzene	MI	91	NQ	95	NQ	
39 Undecane	MI	93	NQ	94	NQ	
40 Methylbenzofurane	IC	93	NQ	93	NQ	
41 Dichlorotoluene	IC	94	0.001	96	0.002	46%
51 Tetrahydronaphthalene	IC	92	0.000	46	NQ	71%
56 Naphthalene	MI	91	0.003	91	0.005	40%
58 Benzo(b)thiophene	IC	93	0.002	87	0.003	20%
61 Dodecane	MI	93	0.004	97	0.005	
70 Trimethylphenol	IC	93	0.001	90	0.001	36%
74 Chloromethylphenol	IC	90	0.002	95	0.002	5%
82 Tridecane	MI	94	0.001	96	0.002	
99 Tetradecane	MI	96	0.002	97	0.002	32%
106 Dimethylphthalate	MI	96	0.001	92	0.001	37%
116 Pentadecane	MI	93	0.001	97	0.001	26%
118 Bis-(Dimethylethyl)phenol	IC	70	NQ	92	0.001	6%
134 Nonylphenol	IC	94	0.002	46	NQ	51%
142 Anthracene- d10	PRC	92	0.0225	94	0.026	13%
143 Phenanthrene-d10	PRC	93	0.0225	95	0.025	12%
162 Octadecenoic acid, methylester	MI	99	0.001	99	0.259	
164 Octadecanoic acid	MI	99	34.319	99	5.195	
165 Octadecenamid	INC	92	0.004	76	NQ	
166 benzanthracene-d12	PRC	97	0.017	95	0.022	27%
167 Bis(2-ethylhexyl)phthalate	MI	80	0.002	87	0.005	

[a]MI – SPMD matrix impurity; IC – identified contaminant; INC – identity not confirmed; PRC – performance reference compound
[b]Match quality of the found mass spectrum with the mass spectrum library search
[c]Concentrations of analytes identified in sample quantified using RMRF approach. Only concentrations of analytes with normal boiling point higher than 200°C are reported
[d]Relative percent difference of duplicate samples
[e]Compound was not quantified because its normal boiling point was lower than 200°C or the match quality was lower than 80%.

Table 7. Molar concentrations of semi-volatile compounds (boiling point > 200°C) identified in extracts from SPMDs deployed for 20 days in groundwater monitoring well GWM 19/91 in Bitterfeld.

Sample	*Component*	*GWM 19/91 A*		*GWM 19/91 B*		
	Type[a]	Match quality[b]	Concentration[c]	Match quality[b]	Concentration[c]	RPD[d]
no. Compound		[%]	[µmol/SPMD]	[%]	[µmol/SPMD]	[%]
1 Nonane	MI	95	NQ[f]	99	NQ	23%
4 Tetrachloroethane	IC	#[e]	NQ	95	NQ	
5 Tetrachloroethane	IC	94	NQ	96	NQ	125%
6 Tetrachloroethane	IC	96	NQ	91	NQ	179%
7 Tetrachloroethane	IC	97	NQ	72	NQ	96%
10 Ethylmethylcyclohexane	IC	87	NQ	87	NQ	97%
11 Propylcyclohexane	IC	94	NQ	90	NQ	59%
12 Butylcyclopentane	MI	96	NQ	94	NQ	38%
14 2-Chlorotoluene	IC	92	NQ	97	NQ	44%
15 4-Chlorotoluene	IC	87	NQ	95	NQ	53%
16 1,3,5-Trimethylbenzene	IC	72	NQ	80	NQ	113%
17 Dimethyltrisulfide	IC	97	NQ	97	NQ	55%
18 Pentachloroethane	IC	98	NQ	99	NQ	38%
20 1,2,4-Trimethylbenzene	IC	94	NQ	94	NQ	52%
21 1,3-Dichlorbenzene	IC	93	NQ	95	NQ	42%
22 1,4-Dichlorobenzene	MI	95	NQ	95	NQ	25%
23 1,2,3-Trimethylbenzene	IC	95	NQ	95	NQ	54%
24 1,2-Dichlorobenzene	MI	94	NQ	95	NQ	25%
25 Brommethylbenzene	IC	96	NQ	96	NQ	46%
26 Chlorodimethylbenzene	IC	95	0.018	96	0.017	72%
27 Chlorodimethylbenzene	IC	95	0.019	96	0.012	101%
32 Methylthiobenzene	IC	91	NQ	95	NQ	76%
36 Bromochlorobenzene	IC	95	0.003	89	0.003	61%
37 Bromochlorobenzene	IC	95	NQ	95	NQ	174%
41 Dichlorotoluene	IC	97	1.958	96	0.715	138%
42 Dichlorotoluene	IC	97	0.775	97	0.283	138%
43 Dichlorotoluene	IC	97	0.156	96	2.914	161%
44 1,3,5-Trichlorobenzene	IC	97	0.000	97	0.006	155%
45 Dihydromethylindene	IC	86	NQ	86	NQ	103%
48 Dichlortoluene	IC	97	0.922	97	1.304	35%
54 Pentachlorobutadiene	IC	99	NQ	99	NQ	88%
55 1,2,4-Trichlorobenzene	IC	95	2.688	97	3.930	31%
56 Naphthalene	MI	91	0.123	91	0.176	33%
59 Bromodichlorothiophene	IC	70	NQ	91	0.000	52%
60 Bromodichlorothiophene	IC	93	0.000	90	0.000	49%
61 Dodecane	MI	90	0.004	62	NQ	45%
64 Bromochloromethylbenzene	INC	99	0.043	97	0.098	13%
65 1,2,3-Trichlorobenzene	IC	97	0.626	97	0.873	36%
66 Dimethyltetrasulfide	IC	87	0.149	87	0.184	47%
68 Cyclopentylbenzene	IC	91	0.052	96	0.064	47%
69 Dichlorodimethylbenzene	IC	94	0.020	97	0.024	49%
73 Tetrachlorothiophene	IC	98	3.582	99	5.314	30%
75 Bromodichlorobenzene	IC	98	0.037	98	0.062	18%
76 Dichlorostyrene	IC	83	0.103	87	0.155	28%
80 Trichlortoluene	IC	98	0.502	98	0.718	33%
84 Trichlortoluene	IC	98	0.274	98	0.378	37%

85	Methylnaphthalene	IC	94	0.016	91	0.015	74%
88	Tetrachlorobenzene	IC	98	1.090	?	NQ	31%
89	Trichlorotoluene	IC	97	0.216	97	0.300	36%
96	1,2,3,4-Tetrachlorobenzene	IC	98	1.136	98	1.550	38%
98	Benzylmethyldisulfide	IC	43	NQ	81	0.081	27%
101	Bromotrichlorbenzene	IC	95	0.027	64	NQ	83%
117	Chlorobiphenyl	IC	96	0.047	94	0.066	35%
119	Butylated Hydroxytoluene	MI	95	0.023	#		
120	Methyl-(phenylmethyl)-benzene	IC	97	0.244	98	0.263	60%
121	Methyl-(phenylmethyl)-benzene	IC	94	0.149	97	0.163	59%
123	Chlorobiphenyl	IC	91	0.013	62	NQ	42%
125	Chlorobiphenyl	IC	59	NQ	91	0.048	39%
126	Diphenylsulfide	IC	95	0.095	75	NQ	35%
132	alpha-HCH	IC	96	0.132	95	0.172	42%
134	Nonylphenol	IC	38	NQ	87	0.006	97%
138	beta-HCH	IC	91	0.014	87	0.020	34%
139	(4-Methylphenyl)-phenylmethanone	IC	87	0.002	60	NQ	70%
140	gamma-HCH	IC	95	0.003	97	0.050	152%
142	Anthracene- d10	PRC	93	0.021	95	0.0290	39%
143	Phenanthrene-d10	PRC	?	0.0212	?	NQ	
146	delta-HCH	IC	93	0.009	93	0.013	36%
158	Dibutylphthalate	IC	25	NQ	86	0.041	176%
160	Sulphur	INC	#	NQ	81	0.004	
162	Octadecenoic acid, methylester	MI	99	0.121	99	0.105	79%
164	Octadecanoic acid	MI	99	2.717	99	2.894	61%
165	Octadecenamid	MI	96	0.005	98	0.005	67%
166	benzanthracene-d12	PRC	74	0.018	87	0.024	43%
167	Bis(2-ethylhexyl)phthalate	MI	91	0.003	80	0.003	85%

[a]MI – SPMD matrix impurity; IC – identified contaminant; INC – identity not confirmed; PRC – performance reference compound
[b]Match quality of the found mass spectrum with the mass spectrum library search
[c]Concentrations of analytes identified in sample quantified using RMRF approach. Only concentrations of analytes with normal boiling point higher than 200°C are reported
[d]Relative percent difference of duplicate samples
[e]# - not found in the sample
[f]Compound was not quantified because its normal boiling point was lower than 200°C or the match quality was lower than 80%.

Table 8. Molar concentrations of semi-volatile compounds (boiling point > 200°C) identified in extracts from SPMD blanks.

Sample	*Component*	*Procedural blank*		*Field blank*	
	Type[a]	Match quality[b]	Concentration[c]	Match quality[b]	Concentration[c]
no. Compound		[%]	[µmol/SPMD]	[%]	[µmol/SPMD]
1 Nonane	MI	94	NQ[e]	94	NQ
22 1,4-Dichlorobenzene	MI	95	NQ	95	NQ
24 1,2-Dichlorobenzene	MI	85	NQ	94	NQ
39 Undecane	MI	95	NQ	95	NQ
53 Decahydrodimethylnaphthalene	MI	*53*	NQ	90	NQ
61 Dodecane	MI	96	0.002	96	0.003
82 Tridecane	MI	95	0.000	96	0.001
99 Tetradecane	MI	98	0.002	98	0.001
106 Dimethylphthalate	MI	94	0.000	65	0.000
112 Butylated Hydroxyanisol	MI	86	0.000	*38*	0.000
116 Pentadecane	MI	95	0.001	95	0.001
119 Butylated Hydroxytoluene	MI	58	NQ	98	0.004
127 Hexadecane	MI	98	0.002	96	0.003
162 Octadecenoic acid, methylester	MI	99	2.141	99	22.411
164 Octadecanoic acid	MI	99	2.329	99	2.891
165 Octadecenamid	MI	98	0.020	98	0.021
167 Bis(2-ethylhexyl)phthalate	MI	91	0.020	91	

[a]MI – SPMD matrix impurity
[b]Match quality of the found mass spectrum with the mass spectrum library search
[c]Concentrations of analytes identified in sample quantified using RMRF approach. Only concentrations of analytes with normal boiling point higher than 200°C are reported
[d]Relative percent difference of duplicate samples
[e]Compound was not quantified because its normal boiling point was lower than 200°C or the match quality was lower than 80%.