

Using model-based screening to help discover unknown environmental contaminants

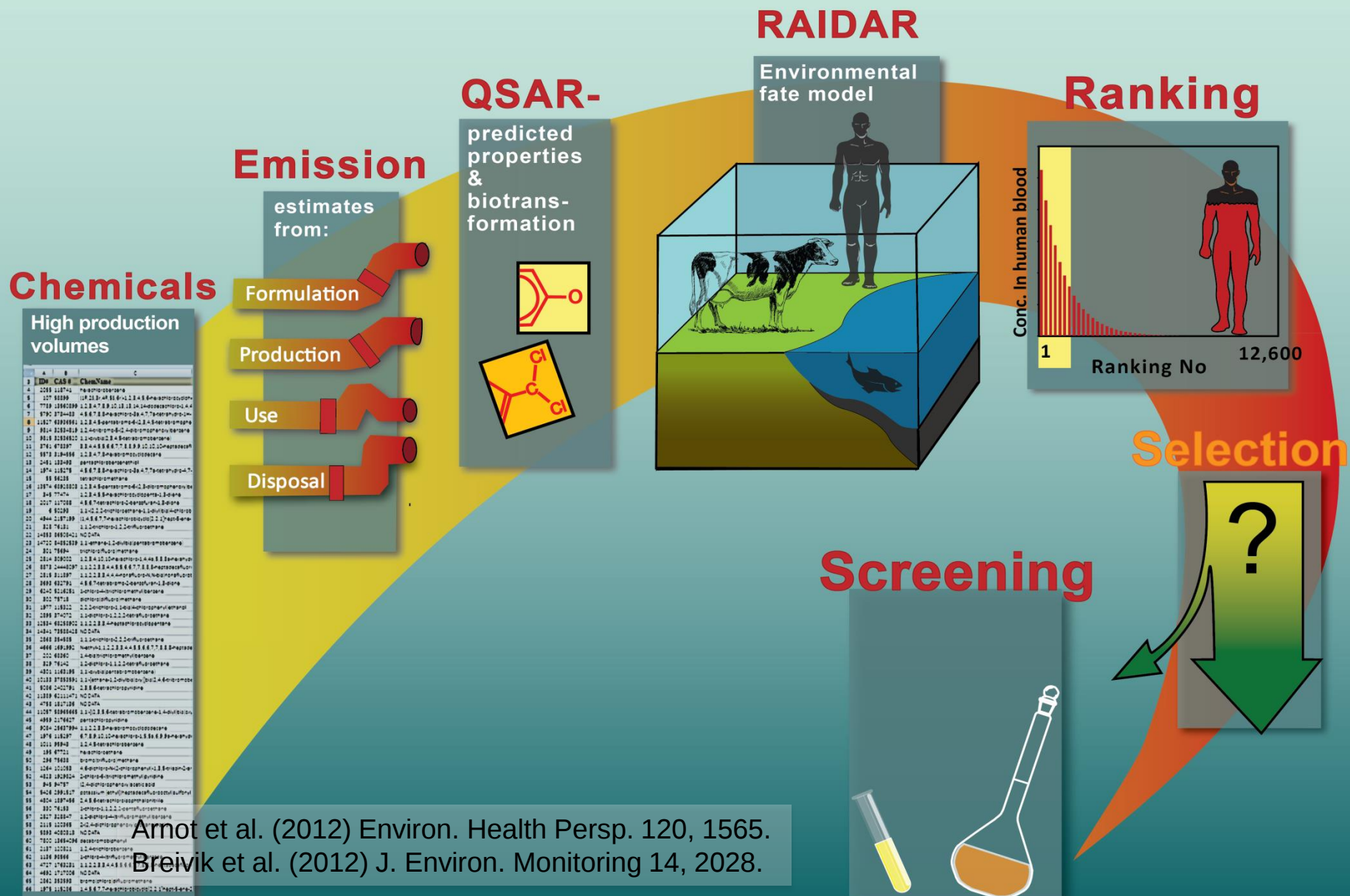


How 215 chemicals were boiled down to 3!

The other SCREEN-POPers

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Procedure



REVISED Ch ranking	CAS #	ChemName	TBB_human	TBB_Cf	Upper 97.5%ile	Ranking	A
NEW			ng/g - ww	ifidence fac	ng/g - ww		(mol
Revised emissions estimates and biotransformation half-lives					"Actual" concentration in Human		
	540976	dodecamethylcyclhexa	1.05E+00	63.4	6.69E+01	1	4.70
	556672	2,2,4,4,6,6,8,8-octameth	1.10E-01	44.7	4.92E+00	2	1.16
	68440711	NO DATA	2.40E-02	52.8	1.27E+00	3	3.33
	541026	2,2,4,4,6,6,8,8,10,10-de	1.87E-02	68.4	1.28E+00	4	9.51
	68607772	NO DATA	1.16E-02	48.2	5.61E-01	5	3.22
	13573154	calcium dimagnesium di	1.01E-02	87.2	8.79E-01	6	2.75
	67762907	NO DATA	4.04E-03	211.4	8.55E-01	7	3.32
	90552593	NO DATA	1.93E-03	634.3	1.02E+00	8	2.15
	2116849	1,1,1,5,5,5-hexamethyl-	1.90E-03	290.4	5.51E-01	9	6.25
	10026047	tetrachlorosilane	1.30E-03	15.5	2.02E-02	10	6.36
	68083192	NO DATA	9.16E-04	537.8	4.93E-01	11	1.61
	107712674	NO DATA	4.08E-04	575.2	2.34E-01	12	2.19
	78137	tetrakis(2-ethylbutyl) orth	2.72E-04	209.9	5.71E-02	13	3.58
	15901403	N,N,N"-tricyclohexyl-1-n	2.62E-04	93.6	2.45E-02	14	1.38
	67763002	NO DATA	2.38E-04	573.5	1.37E-01	15	3.55
	107460	hexamethyldisiloxane	2.14E-04	20.6	4.41E-03	16	4.43
	68037763	NO DATA	1.76E-04	743.8	1.31E-01	17	2.15
	75785	dichloro(dimethyl)silane	1.58E-04	88.6	1.40E-02	18	2.84
	68440700	NO DATA	1.50E-04	211.1	3.16E-02	19	4.09
	68083147	NO DATA	1.44E-04	867.0	1.25E-01	20	7.30
	2374143	2,4,6-trimethyl-2,4,6-tris	1.42E-04	486.5	6.60E-02	21	1.20
	141628	decamethyltetrasiloxane	1.32E-04	86.5	1.14E-02	22	2.83
	40372723	4,4,15,15-tetraethoxy-3,	1.15E-04	100.0	1.15E-02	23	6.30
	68952012	NO DATA	1.03E-04	755.1	7.76E-02	24	5.54
	33434638	trichloro(2,3,4,5-tetrachl	1.02E-04	147.3	1.51E-02	25	2.00
	546565	2,2,4,4,6,6,8,8-octaphen	9.92E-05	1025.8	1.02E-01	26	2.78
	68952023	NO DATA	9.32E-05	191.2	1.78E-02	27	2.42
	63148527	NO DATA	9.06E-05	449.1	4.07E-02	28	3.09
	68951940	NO DATA	8.50E-05	479.2	4.07E-02	29	2.27
	5283669	trichloro(octyl)silane	7.76E-05	129.2	1.00E-02	30	2.21
	80104	dichloro(diphenyl)silane	7.48E-05	184.9	1.38E-02	31	4.88
	68037774	NO DATA	7.37E-05	761.7	5.62E-02	32	9.69
	2943751	triethoxy(octyl)silane	5.68E-05	77.5	4.40E-03	33	5.84
	17704222	2,4,6,8,10-pentaethenyl-	4.86E-05	205.9	1.00E-02	34	1.17
	3982829	1,3,3,5-tetramethyl-1,1,5	4.61E-05	350.4	1.61E-02	35	4.63
	2554065	2,4,6,8-tetraethenyl-2,4,	3.94E-05	652.5	2.57E-02	36	3.12
	2652133	icosamethylmonasiloxane	3.66E-05	206.7	7.58E-03	37	4.78
	68440904	NO DATA	3.43E-05	483.0	1.66E-02	38	3.20
	429674	2,4,6,8-tetramethyl-2,4,6	3.06E-05	440.6	1.35E-02	39	6.15
	16415126	hexadecyl(trimethoxy)sil	3.04E-05	103.4	3.14E-03	40	2.20
	68909013	NO DATA	2.84E-05	484.1	1.38E-02	41	1.66
	27668526	N,N-dimethyl-N-(3-trime	2.03E-05	100.4	2.04E-03	42	6.46

Sub-group organosilicon compounds

A total of 215 Si-compounds

Selection priorities

Abundancy in sediment and air

	Air	Sediment
Abundancy	52	24

Ranking "Actual" concentration in Human	Air (mol / m3)
10	6.36E-10
75	4.08E-11
18	2.84E-11
56	2.72E-12
69	2.55E-12
2	1.16E-12
74	9.64E-13
95	8.57E-13
16	4.43E-13
64	3.73E-13
165	3.06E-13
77	2.64E-13
82	2.16E-13
57	2.12E-13
49	1.88E-13
96	1.12E-13
107	1.08E-13
4	9.51E-14
92	7.34E-14
68	5.93E-14
67	5.64E-14
113	5.21E-14
55	4.94E-14
58	4.37E-14
116	3.04E-14
22	2.83E-14
62	2.07E-14
79	1.94E-14
90	1.66E-14
117	1.44E-14
170	1.03E-14
140	9.49E-15
258	7.60E-15
131	6.96E-15
91	6.79E-15
155	5.82E-15
178	5.69E-15
138	5.44E-15
31	4.88E-15
166	4.77E-15
1	4.70E-15
112	3.74E-15
160	3.46E-15
192	2.97E-15
106	2.65E-15
171	2.50E-15
161	2.49E-15
30	2.21E-15
121	1.88E-15
184	1.65E-15
118	1.54E-15
260	1.28E-15
194	1.24E-15
188	1.21E-15
21	1.20E-15
43	8.79E-16
85	7.22E-16
276	7.04E-16
125	6.78E-16

Ranking "Actual" conc. in Human	Sediment mole/cm ³
2	3.76E-13
21	3.67E-13
4	1.08E-13
1	9.06E-14
11	6.55E-14
51	4.90E-14
22	3.48E-14
54	1.99E-14
31	1.08E-14
23	8.65E-15
16	7.65E-15
30	7.35E-15
39	5.36E-15
9	4.88E-15
67	4.72E-15
58	4.40E-15
49	3.79E-15
184	3.45E-15
36	2.94E-15
35	2.64E-15
18	2.43E-15
8	1.64E-15
33	1.44E-15
14	1.36E-15
72	1.32E-15
13	1.09E-15
20	6.84E-16
92	6.24E-16
73	5.49E-16
100	5.13E-16
62	5.04E-16
12	4.85E-16
65	4.78E-16
81	4.71E-16
10	4.56E-16
82	4.47E-16
26	4.00E-16
5	3.70E-16
40	3.69E-16
87	3.66E-16
53	3.65E-16
55	3.02E-16
25	2.79E-16
77	2.72E-16
3	2.67E-16
165	2.44E-16
274	2.39E-16
79	2.39E-16
104	2.39E-16
80	2.38E-16
75	2.24E-16
15	2.18E-16
46	2.11E-16
32	2.10E-16
63	1.82E-16
128	1.80E-16
64	1.76E-16
43	1.75E-16
27	1.74E-16
48	1.73E-16
28	1.73E-16
70	1.73E-16
29	1.71E-16
59	1.68E-16
122	1.65E-16
60	1.59E-16

Ranking "Actual" concentration in Human	Air (mol / m3)
10	6.36E-10
75	4.08E-11
18	2.84E-11
56	2.72E-12
69	2.55E-12
2	1.16E-12
74	9.64E-13
95	8.57E-13
16	4.43E-13
64	3.73E-13
165	3.06E-13
77	2.64E-13
82	2.16E-13
57	2.12E-13
49	1.88E-13
96	1.12E-13
107	1.08E-13
4	9.51E-14
92	7.34E-14
68	5.93E-14
67	5.64E-14
113	5.21E-14
55	4.94E-14
58	4.37E-14
116	3.04E-14
22	2.83E-14
62	2.07E-14
79	1.94E-14
90	1.66E-14
117	1.44E-14
170	1.03E-14
140	9.49E-15
258	7.60E-15
131	6.96E-15
91	6.79E-15
155	5.82E-15
178	5.69E-15
138	5.44E-15
31	4.88E-15
166	4.77E-15
1	4.70E-15
112	3.74E-15
160	3.46E-15
192	2.97E-15
106	2.65E-15
171	2.50E-15
161	2.49E-15
30	2.21E-15
121	1.88E-15
184	1.65E-15
118	1.54E-15
260	1.28E-15
194	1.24E-15
188	1.21E-15
21	1.20E-15
43	8.79E-16
85	7.22E-16
276	7.04E-16
125	6.78E-16
33	5.84E-16
66	5.78E-16
97	5.42E-16
220	5.17E-16
191	5.05E-16
185	4.28E-16
227	4.02E-16
126	3.86E-16

Selection priorities

Abundancy in sediment and air

C_{human} ranking < 65

	Air	Sediment
Abundancy	52	24
C _{human}	29	23

Ranking "Actual" conc. in Human	Sediment mole/cm ³
2	3.76E-13
21	3.67E-13
4	1.08E-13
1	9.06E-14
11	6.55E-14
51	4.90E-14
22	3.48E-14
54	1.99E-14
31	1.08E-14
23	8.65E-15
16	7.65E-15
30	7.35E-15
39	5.36E-15
9	4.88E-15
67	4.72E-15
58	4.40E-15
49	3.79E-15
184	3.45E-15
36	2.94E-15
35	2.64E-15
18	2.43E-15
8	1.64E-15
33	1.44E-15
14	1.36E-15
72	1.32E-15
13	1.09E-15
20	6.84E-16
92	6.24E-16
73	5.49E-16
100	5.13E-16
62	5.04E-16
12	4.85E-16
65	4.78E-16
81	4.71E-16
10	4.56E-16
82	4.47E-16
26	4.00E-16
5	3.70E-16
40	3.69E-16
87	3.66E-16
53	3.65E-16
55	3.02E-16
25	2.79E-16
77	2.72E-16
3	2.67E-16
165	2.44E-16
274	2.39E-16
79	2.39E-16
104	2.39E-16
80	2.38E-16
75	2.24E-16
15	2.18E-16
46	2.11E-16
32	2.10E-16
63	1.82E-16
128	1.80E-16
64	1.76E-16
43	1.75E-16
27	1.74E-16
48	1.73E-16
28	1.73E-16
70	1.73E-16
29	1.71E-16
59	1.68E-16
122	1.65E-16
60	1.59E-16
50	1.59E-16

Ranking	Air
"Actual" concentration in Human	(mol / m ³)
10	1.1E-10
75	1.1E-11
18	1.1E-11
56	2.72E-12
69	2.55E-12
2	1.16E-12
74	9.64E-13
95	8.57E-13
16	1.1E-13
21	1.1E-13
165	1.1E-13
77	1.1E-13
82	1.1E-13
37	1.1E-13
49	1.1E-13
96	1.1E-13
107	1.1E-13
4	1.1E-14
92	7.34E-14
68	5.93E-14
67	5.64E-14
113	5.21E-14
55	4.94E-14
58	4.37E-14
100	3.04E-14
22	8.3E-14
62	1.07E-14
79	1.94E-14
90	1.66E-14
117	1.44E-14
170	1.03E-14
140	9.49E-15
258	7.60E-15
131	6.96E-15
91	6.79E-15
155	5.82E-15
178	1.1E-15
138	1.1E-15
31	1.1E-15
100	1.1E-15
1	1.1E-15
112	3.74E-15
160	3.46E-15
192	2.97E-15
106	2.65E-15
171	2.50E-15
161	2.49E-15
30	2.21E-15
121	1.88E-15
184	1.65E-15
118	1.54E-15
260	1.28E-15
194	1.24E-15
188	1.21E-15
21	1.20E-15
43	8.79E-16
85	7.22E-16
276	7.04E-16
125	6.78E-16
33	5.84E-16
66	5.78E-16
97	5.42E-16
220	5.17E-16
191	5.05E-16
185	4.28E-16
227	4.02E-16
126	3.86E-16

Selection priorities

- Abundancy in sediment and air
- C_{human} ranking < 65
- Excluding wellknowns, cVMS and IVMS

	Air	Sediment
Abundancy	52	24
C _{human}	29	23
- cVMS/IVMS	22	16

Ranking	Sediment
"Actual" conc. in Human	mole/cm ³
2	1.1E-13
21	1.1E-13
4	1.1E-13
1	9.06E-14
11	6.55E-14
51	1.1E-14
22	1.1E-14
34	1.1E-14
31	1.1E-14
23	8.65E-15
16	1.1E-15
30	1.1E-15
39	1.1E-15
9	1.1E-15
37	4.72E-15
58	4.40E-15
49	1.1E-15
36	1.1E-15
35	1.1E-15
18	2.43E-15
8	1.64E-15
33	1.44E-15
14	1.36E-15
72	1.32E-15
13	1.09E-15
20	6.84E-16
92	6.24E-16
73	5.49E-16
100	5.13E-16
62	5.04E-16
12	4.85E-16
65	4.78E-16
81	4.71E-16
10	4.56E-16
82	4.47E-16
26	4.00E-16
5	3.70E-16
40	3.69E-16
87	3.66E-16
53	3.65E-16
55	3.02E-16
25	2.79E-16
77	2.72E-16
3	2.67E-16
165	2.44E-16
274	2.39E-16
79	2.39E-16
104	2.39E-16
80	2.38E-16
75	2.24E-16
15	2.18E-16
46	2.11E-16
32	2.10E-16
63	1.82E-16
128	1.80E-16
64	1.76E-16
43	1.75E-16
27	1.74E-16
48	1.73E-16
28	1.73E-16
70	1.73E-16
29	1.71E-16
59	1.68E-16
122	1.65E-16
60	1.59E-16
50	1.59E-16

Ranking "Actual" concentration in Human	Air mole/m ³
10	6.36E-10
75	4.08E-11
18	2.84E-11
56	2.72E-12
69	2.55E-12
2	1.16E-12
74	9.64E-13
95	8.57E-13
16	4.43E-13
64	3.73E-13
165	3.06E-13
77	2.64E-13
82	2.16E-13
57	2.12E-13
49	1.88E-13
96	1.12E-13
107	1.08E-13
4	9.51E-14
92	7.34E-14
68	5.93E-14
67	5.64E-14
113	5.21E-14
55	4.94E-14
58	4.37E-14
116	3.04E-14
22	2.83E-14
62	2.07E-14
79	1.94E-14
90	1.66E-14
117	1.44E-14
170	1.03E-14
140	9.49E-15
258	7.60E-15
131	6.96E-15
91	6.79E-15
155	5.82E-15
178	5.69E-15
138	5.44E-15
31	4.88E-15
166	4.77E-15
1	4.70E-15
112	3.74E-15
160	3.46E-15
192	2.97E-15
106	2.65E-15
171	2.50E-15
161	2.49E-15
30	2.21E-15
121	1.88E-15
184	1.65E-15
118	1.54E-15
260	1.28E-15
194	1.24E-15
188	1.21E-15
21	1.20E-15
43	8.79E-16
85	7.22E-16
276	7.04E-16
125	6.78E-16
33	5.84E-16
66	5.78E-16
97	5.42E-16
220	5.17E-16
191	5.05E-16
185	4.28E-16
227	4.02E-16
126	3.86E-16

Selection priorities

- Abundancy in sediment and air
- C_{human} ranking < 65
- Excluding wellknowns, cVMS and IVMS
- Reactivity (hydrolysis)

	Air	Sediment
Abundancy	52	24
C_{human}	29	23
- cVMS/IVMS	22	16
Reactivity	4	11

Ranking "Actual" conc. in Human	Sediment mole/cm ³
2	3.76E-13
21	3.67E-13
4	1.08E-13
1	9.06E-14
11	6.55E-14
51	4.90E-14
22	3.48E-14
54	1.99E-14
31	1.08E-14
23	8.65E-15
16	7.65E-15
30	7.35E-15
39	5.36E-15
9	4.88E-15
67	4.72E-15
58	4.40E-15
49	3.79E-15
184	3.45E-15
36	2.94E-15
35	2.64E-15
18	2.43E-15
8	1.64E-15
33	1.44E-15
14	1.36E-15
72	1.32E-15
13	1.09E-15
20	6.84E-16
92	6.24E-16
73	5.49E-16
100	5.13E-16
62	5.04E-16
12	4.85E-16
65	4.78E-16
81	4.71E-16
10	4.56E-16
82	4.47E-16
26	4.00E-16
5	3.70E-16
40	3.69E-16
87	3.66E-16
53	3.65E-16
55	3.02E-16
25	2.79E-16
77	2.72E-16
3	2.67E-16
165	2.44E-16
274	2.39E-16
79	2.39E-16
104	2.39E-16
80	2.38E-16
75	2.24E-16
15	2.18E-16
46	2.11E-16
32	2.10E-16
63	1.82E-16
128	1.80E-16
64	1.76E-16
43	1.75E-16
27	1.74E-16
48	1.73E-16
28	1.73E-16
70	1.73E-16
29	1.71E-16
59	1.68E-16
122	1.65E-16
60	1.59E-16
50	1.59E-16

Chemicals selected by model-based screening

(○ = not prioritized for method development)

Name	Air Conc. Rank	Sediment Conc. Rank	Human Conc. Rank	Hydrolysis	Result [#]
1,1,1,5,5,5-hexamethyl-3-phenyl-3-[(trimethylsilyl)oxy]trisiloxane	92	13	4	slow	
tetrakis(2-ethylbutyl) orthosilicate	171	24	5	medium	
N,N',N''-tricyclohexyl-1-methylsilanetriamine	143	22	6	medium	
2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)-1,3,5,2,4,6-trioxatrisilinane	52	2	9	slow	
4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	119	9	11	medium	○
triethoxy(octyl)silane	57	21	16	medium	○
1,3,3,5-tetramethyl-1,1,5,5-tetraphenyltrisiloxane	123	19	17	slow	
2,4,6,8-tetraethenyl-2,4,6,8-tetramethyl-1,3,5,7,2,4,6,8-tetroxatetrasilocane	132	18	19	slow	○
2,4,6,8-tetramethyl-2,4,6,8-tetrakis(3,3,3-trifluoropropyl)-1,3,5,7,2,4,6,8-tetroxatetrasilocane	121	12	21	slow	
(2Z)-N-[[[(3E,8E)-3,6,9-trimethyl-5,7-dioxa-4,8-diaza-6-silaundeca-3,8-dien-6-yl]oxy]butan-2-imine	68	7	30	medium	
1,1,1-trimethyl-N-(trimethylsilyl)silanamine	12	85	33	medium	
trimethyl[(2-methylbut-3-yn-2-yl)oxy]silane	27	48	56	medium	○
1,1,1,3,5,5,5-heptamethyltrisiloxane	19	14	39	slow	○

Chemicals selected by model-based screening

(**NDM** = detection method attempted but unsuccessful)

Name	Air Conc. Rank	Sediment Conc. Rank	Human Conc. Rank	Hydrolysis	Result [#]
1,1,1,5,5,5-hexamethyl-3-phenyl-3-[(trimethylsilyl)oxy]trisiloxane	92	13	4	slow	
tetrakis(2-ethylbutyl) orthosilicate	171	24	5	medium	
N,N',N''-tricyclohexyl-1-methylsilanetriamine	143	22	6	medium	NDM
2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)-1,3,5,2,4,6-trioxatrisilinane	52	2	9	slow	
4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	119	9	11	medium	O
triethoxy(octyl)silane	57	21	16	medium	O
1,3,3,5-tetramethyl-1,1,5,5-tetraphenyltrisiloxane	123	19	17	slow	
2,4,6,8-tetraethenyl-2,4,6,8-tetramethyl-1,3,5,7,2,4,6,8-tetroxatetrasilocane	132	18	19	slow	O
2,4,6,8-tetramethyl-2,4,6,8-tetrakis(3,3,3-trifluoropropyl)-1,3,5,7,2,4,6,8-tetroxatetrasilocane	121	12	21	slow	
(2Z)-N-[[[(3E,8E)-3,6,9-trimethyl-5,7-dioxa-4,8-diaza-6-silaundeca-3,8-dien-6-yl]oxy]butan-2-imine	68	7	30	medium	NDM
1,1,1-trimethyl-N-(trimethylsilyl)silanamine	12	85	33	medium	NDM
trimethyl[(2-methylbut-3-yn-2-yl)oxy]silane	27	48	56	medium	O
1,1,1,3,5,5,5-heptamethyltrisiloxane	19	14	39	slow	O

Chemicals selected by model-based screening

(**R** = detection method successful but reactive in solution)

Name	Air Conc. Rank	Sediment Conc. Rank	Human Conc. Rank	Hydrolysis	Result [#]
1,1,1,5,5,5-hexamethyl-3-phenyl-3-[(trimethylsilyl)oxy]trisiloxane	92	13	4	slow	
tetrakis(2-ethylbutyl) orthosilicate	171	24	5	medium	R
N,N',N''-tricyclohexyl-1-methylsilanetriamine	143	22	6	medium	NDM
2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)-1,3,5,2,4,6-trioxatrisilinane	52	2	9	slow	
4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	119	9	11	medium	O
triethoxy(octyl)silane	57	21	16	medium	O
1,3,3,5-tetramethyl-1,1,5,5-tetraphenyltrisiloxane	123	19	17	slow	
2,4,6,8-tetraethenyl-2,4,6,8-tetramethyl-1,3,5,7,2,4,6,8-tetroxatetrasilocane	132	18	19	slow	O
2,4,6,8-tetramethyl-2,4,6,8-tetrakis(3,3,3-trifluoropropyl)-1,3,5,7,2,4,6,8-tetroxatetrasilocane	121	12	21	slow	
(2Z)-N-[[[(3E,8E)-3,6,9-trimethyl-5,7-dioxa-4,8-diaza-6-silaundeca-3,8-dien-6-yl]oxy]butan-2-imine	68	7	30	medium	NDM
1,1,1-trimethyl-N-(trimethylsilyl)silanamine	12	85	33	medium	NDM
trimethyl[(2-methylbut-3-yn-2-yl)oxy]silane	27	48	56	medium	O
1,1,1,3,5,5,5-heptamethyltrisiloxane	19	14	39	slow	O

Chemicals selected by model-based screening

(**NXM** = detection method successful but sample prep. not optimized)

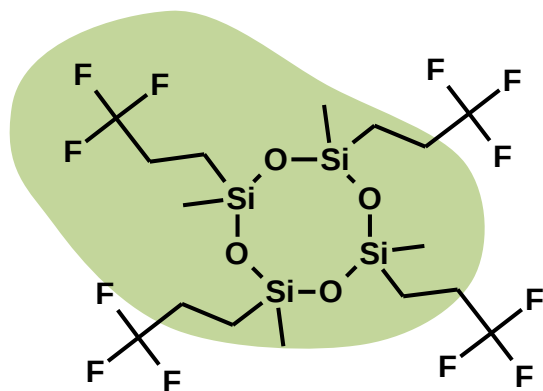
Name	Air Conc. Rank	Sediment Conc. Rank	Human Conc. Rank	Hydrolysis	Result [#]
1,1,1,5,5,5-hexamethyl-3-phenyl-3-[(trimethylsilyl)oxy]trisiloxane	92	13	4	slow	
tetrakis(2-ethylbutyl) orthosilicate	171	24	5	medium	R
N,N',N''-tricyclohexyl-1-methylsilanetriamine	143	22	6	medium	NDM
2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)-1,3,5,2,4,6-trioxatrisilinane	52	2	9	slow	
4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	119	9	11	medium	O
triethoxy(octyl)silane	57	21	16	medium	O
1,3,3,5-tetramethyl-1,1,5,5-tetraphenyltrisiloxane	123	19	17	slow	NXM
2,4,6,8-tetraethenyl-2,4,6,8-tetramethyl-1,3,5,7,2,4,6,8-tetroxatetrasilocane	132	18	19	slow	O
2,4,6,8-tetramethyl-2,4,6,8-tetrakis(3,3,3-trifluoropropyl)-1,3,5,7,2,4,6,8-tetroxatetrasilocane	121	12	21	slow	
(2Z)-N-[[[(3E,8E)-3,6,9-trimethyl-5,7-dioxa-4,8-diaza-6-silaundeca-3,8-dien-6-yl]oxy]butan-2-imine	68	7	30	medium	NDM
1,1,1-trimethyl-N-(trimethylsilyl)silanamine	12	85	33	medium	NDM
trimethyl[(2-methylbut-3-yn-2-yl)oxy]silane	27	48	56	medium	O
1,1,1,3,5,5,5-heptamethyltrisiloxane	19	14	39	slow	O

Chemicals selected by model-based screening

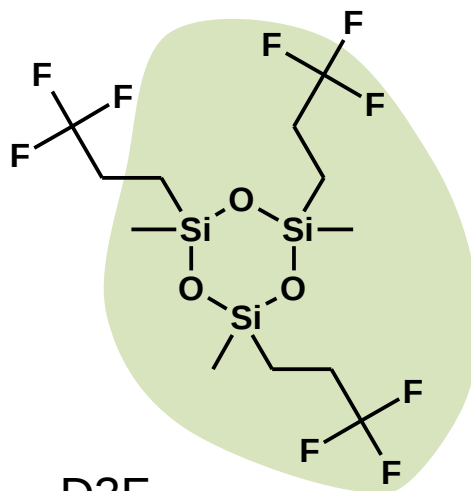
(**S** = screening in environmental samples)

Name	Air Conc. Rank	Sediment Conc. Rank	Human Conc. Rank	Hydrolysis	Result [#]
1,1,1,5,5,5-hexamethyl-3-phenyl-3-[(trimethylsilyl)oxy]trisiloxane	92	13	4	slow	S
tetrakis(2-ethylbutyl) orthosilicate	171	24	5	medium	R
N,N',N''-tricyclohexyl-1-methylsilanetriamine	143	22	6	medium	NDM
2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)-1,3,5,2,4,6-trioxatrisilinane	52	2	9	slow	S
4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	119	9	11	medium	O
triethoxy(octyl)silane	57	21	16	medium	O
1,3,3,5-tetramethyl-1,1,5,5-tetraphenyltrisiloxane	123	19	17	slow	NXM
2,4,6,8-tetraethenyl-2,4,6,8-tetramethyl-1,3,5,7,2,4,6,8-tetroxatetrasilocane	132	18	19	slow	O
2,4,6,8-tetramethyl-2,4,6,8-tetrakis(3,3,3-trifluoropropyl)-1,3,5,7,2,4,6,8-tetroxatetrasilocane	121	12	21	slow	S
(2Z)-N-[[[(3E,8E)-3,6,9-trimethyl-5,7-dioxa-4,8-diaza-6-silaundeca-3,8-dien-6-yl]oxy]butan-2-imine	68	7	30	medium	NDM
1,1,1-trimethyl-N-(trimethylsilyl)silanamine	12	85	33	medium	NDM
trimethyl[(2-methylbut-3-yn-2-yl)oxy]silane	27	48	56	medium	O
1,1,1,3,5,5,5-heptamethyltrisiloxane	19	14	39	slow	O

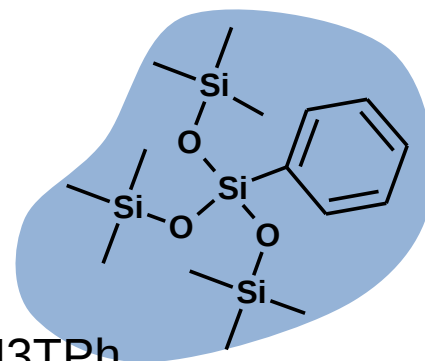
Substances Analyzed



D4F
Trifluoropropylmethyl-
cyclotetrasiloxane



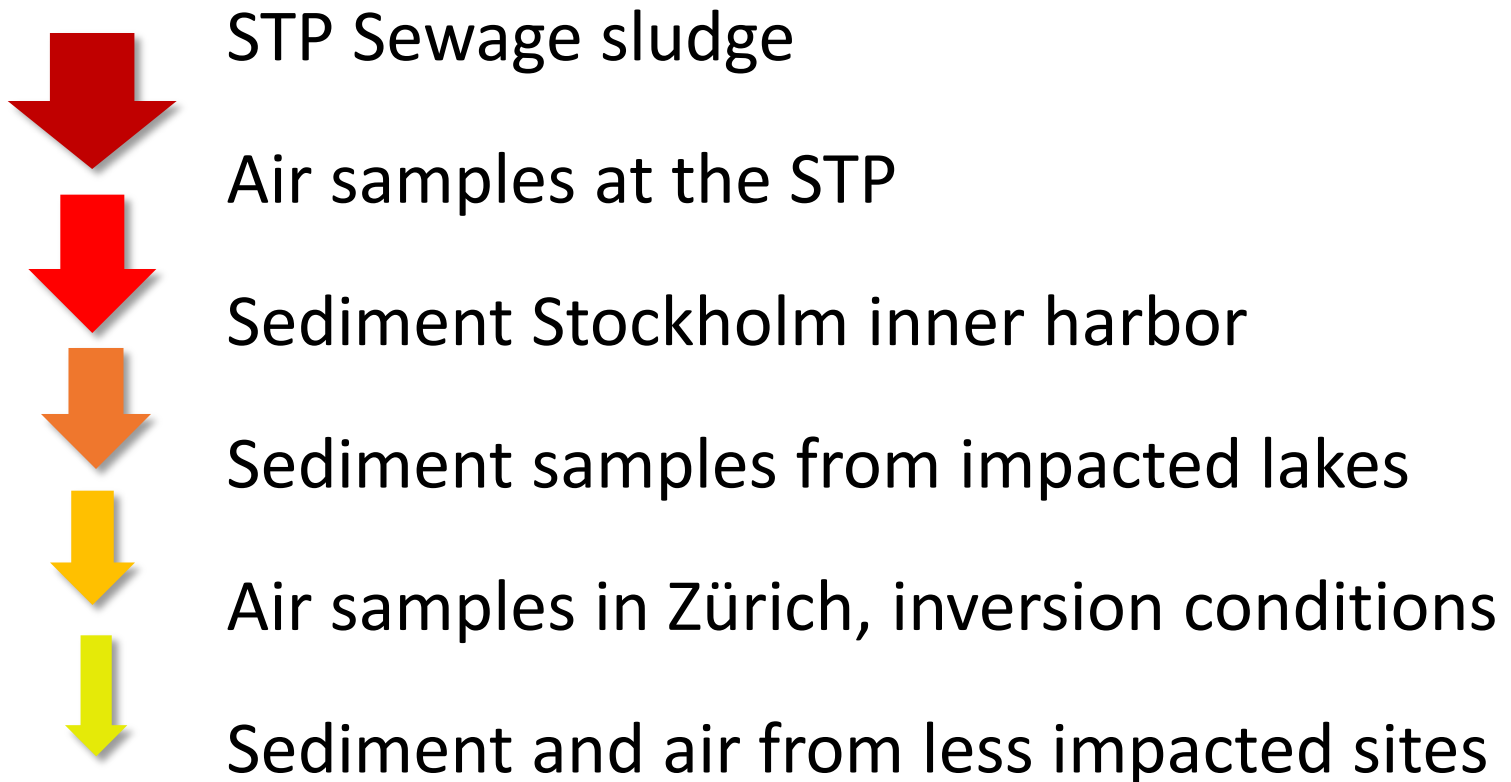
D3F
Trifluoropropylmethyl-
cyclotrisiloxane



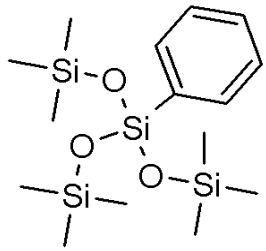
M3TPh
Phenyl-tris(trimethylsiloxy)-
silane

Environmental screening

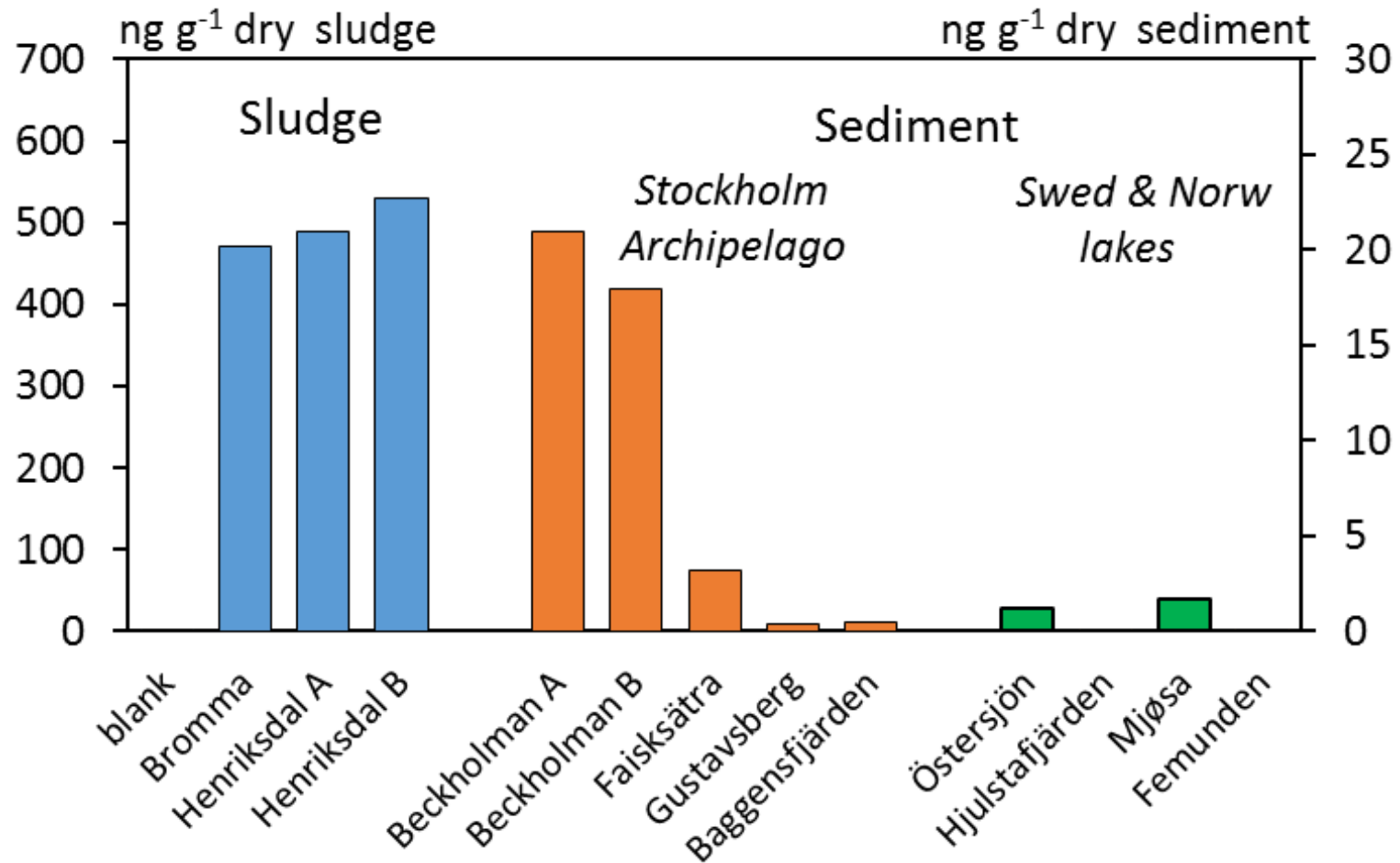
Tiered approach







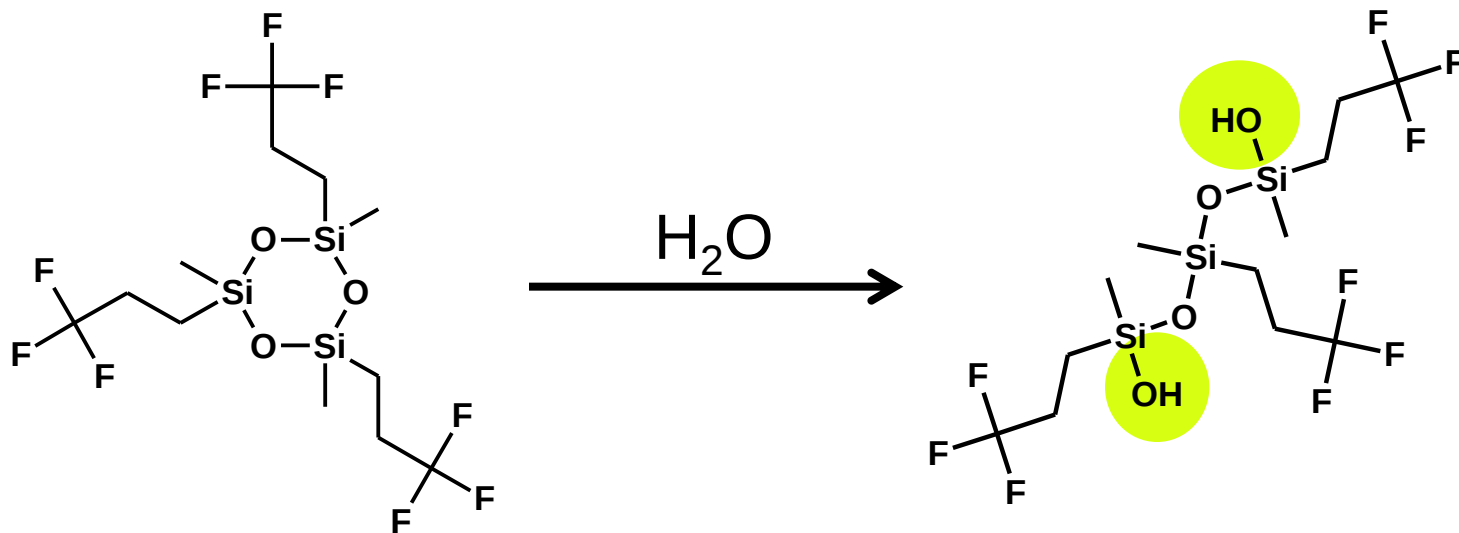
Screening for M3TPh Sludge & sediment



D3F

Trifluoropropylmethylcyclotrisiloxane

Not possible to analyze on GCMS, although hydrophobic
ESI- : Ionized after hydrolysis to a linear silanediol
 $[M+H_2O-H]^-$

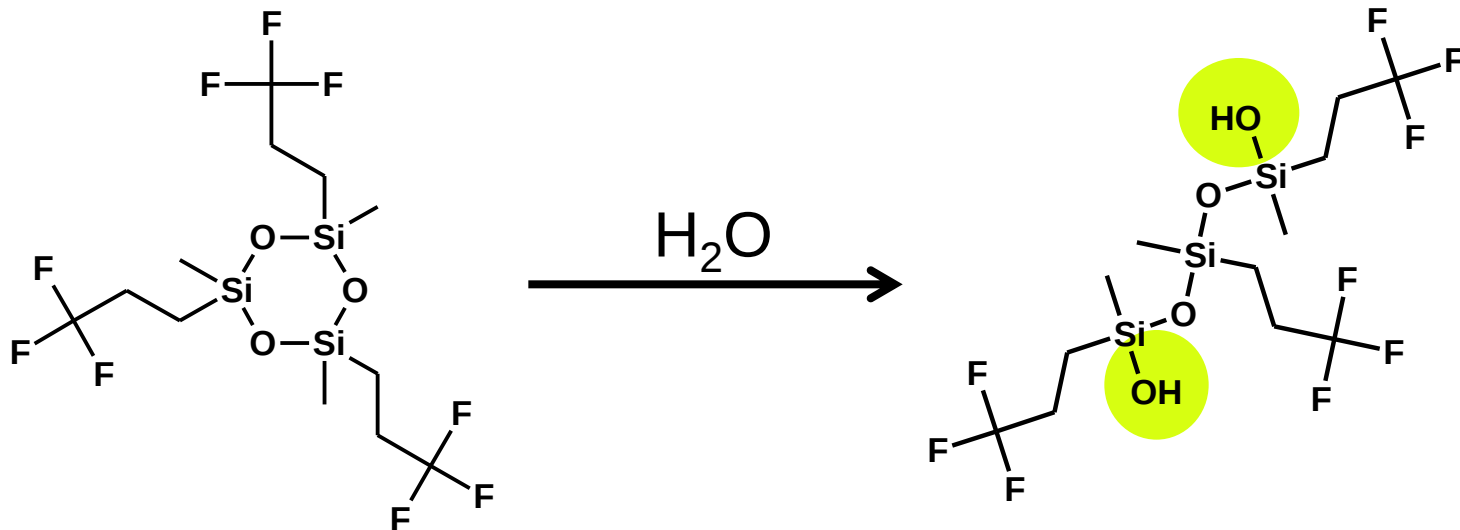


D3F

Trifluoropropylmethylcyclotrisiloxane

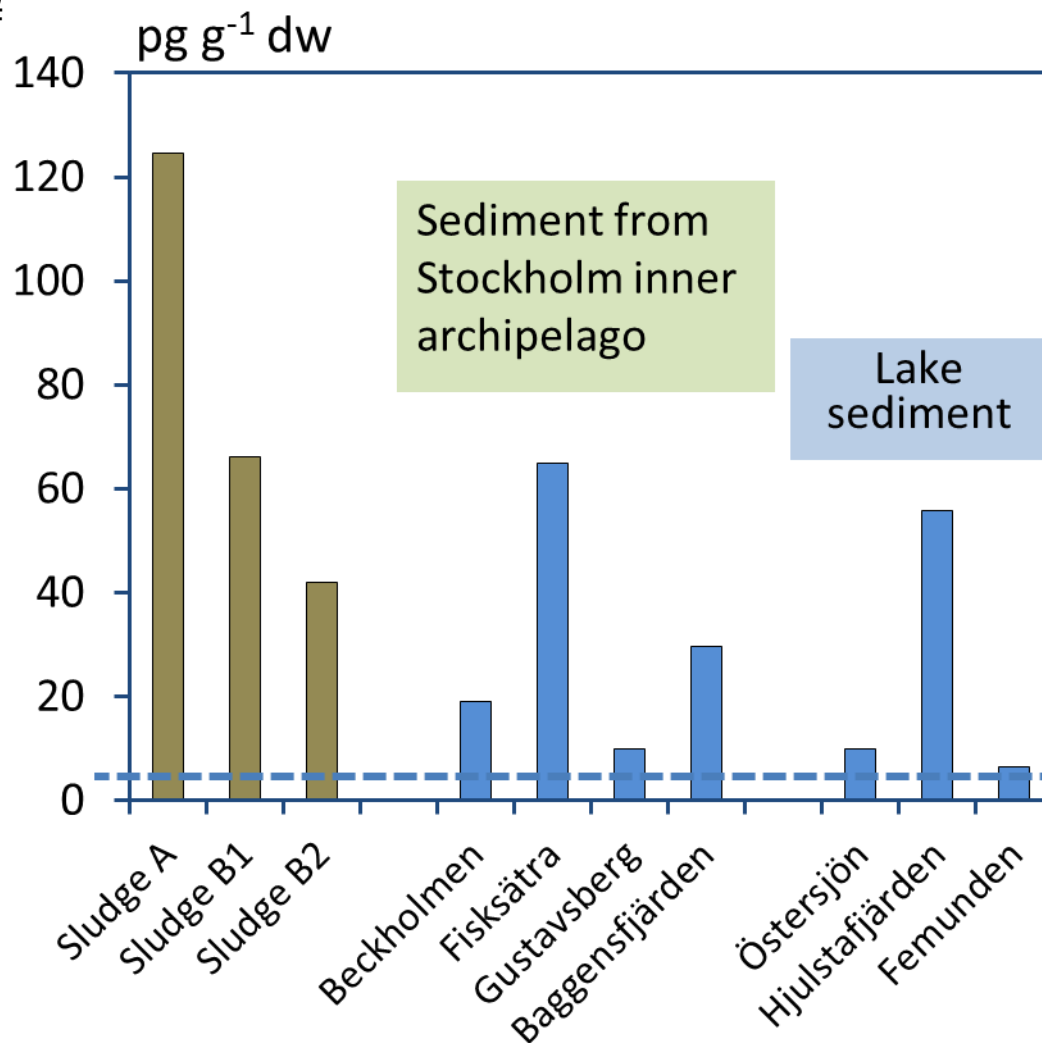
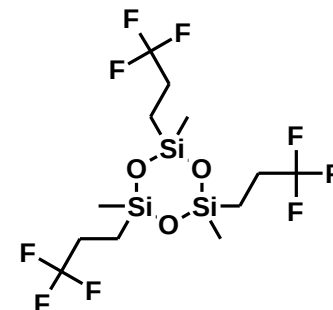
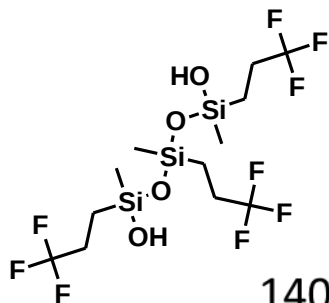
Both forms present in the environment

→ we quantified both: sum of D3F and D3FOH



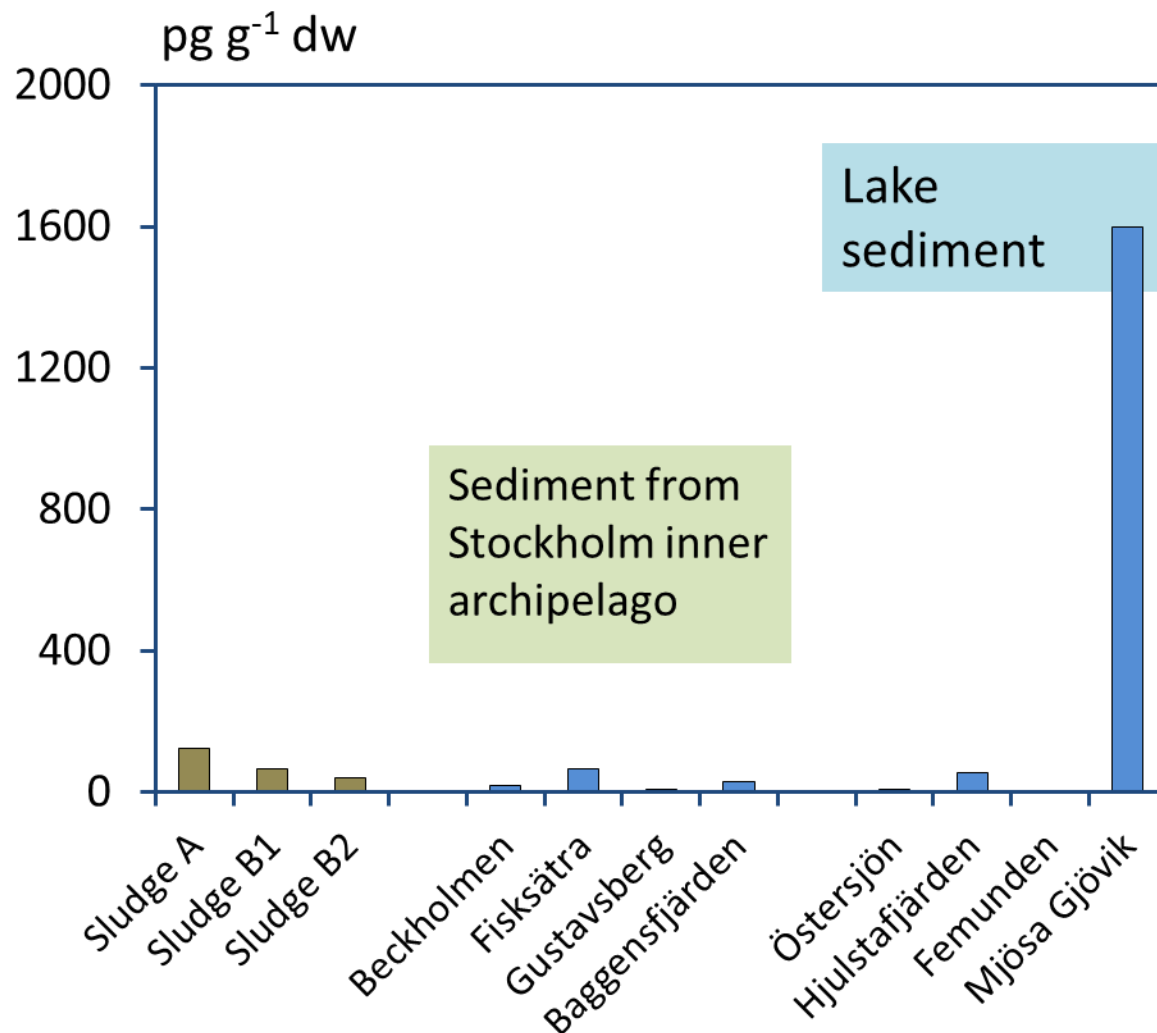
Environmental conc.

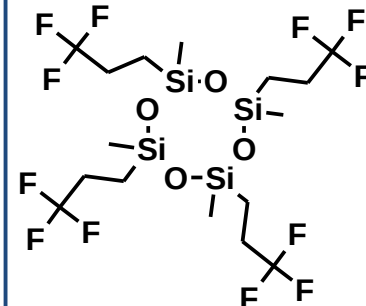
Sum of D3FOH and D3F



Environmental conc.

Sum of D3FOH and D3F



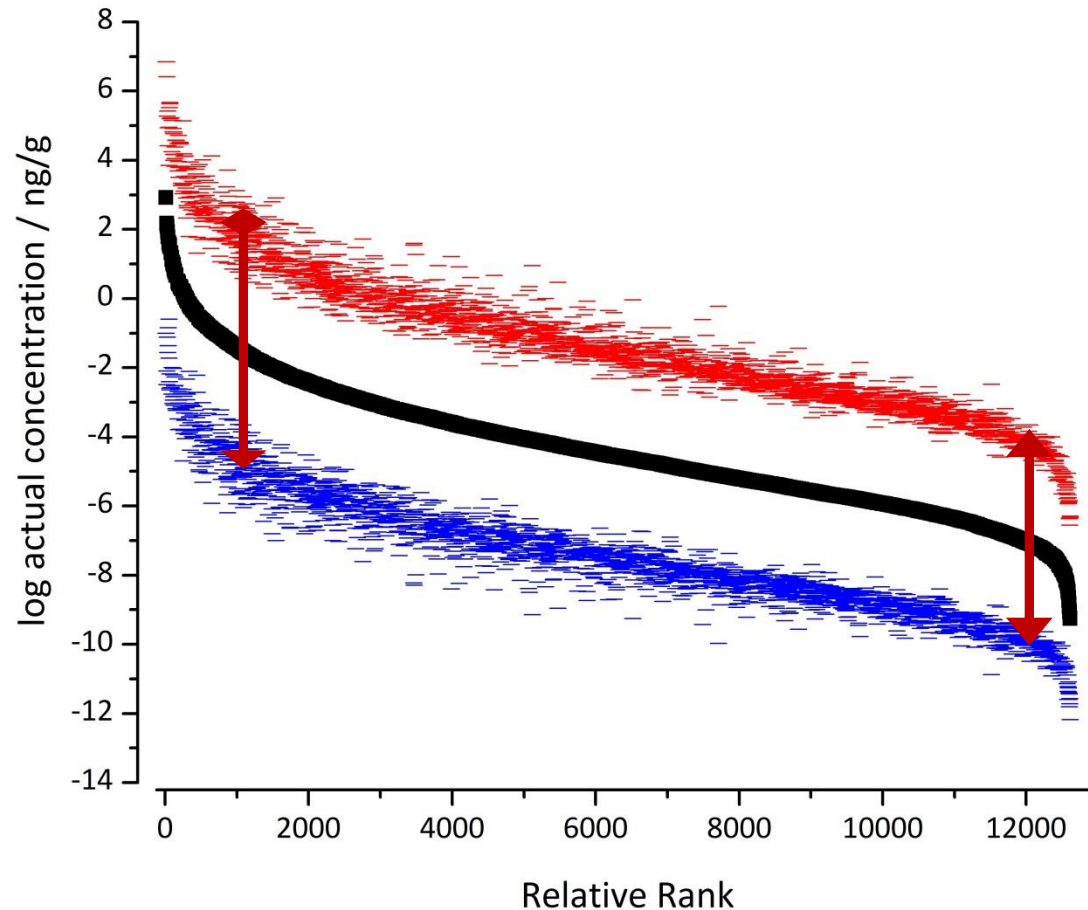


Conc < LOD
(Lake Femunden)

Conclusions

- Models can help to “find” environmental contaminants

Some self-criticism



Conclusions

- Models can help to “find” environmental contaminants
- Better information on chemical production and use is needed to make this approach useful

Acknowledgements

Cefic LRI

Research Council of Norway

Monitoring team

Katrine Borgå & Eirik Fjeld

Andreas Buser

Markus Meili Per Jonsson

Cajsa Wahlberg