

Supplementary materials

Development and validation of robust single extraction method for analysis of PAHs, HBCD, BDE, and PCBs in the coastal environment

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SF1 Location of sampling site

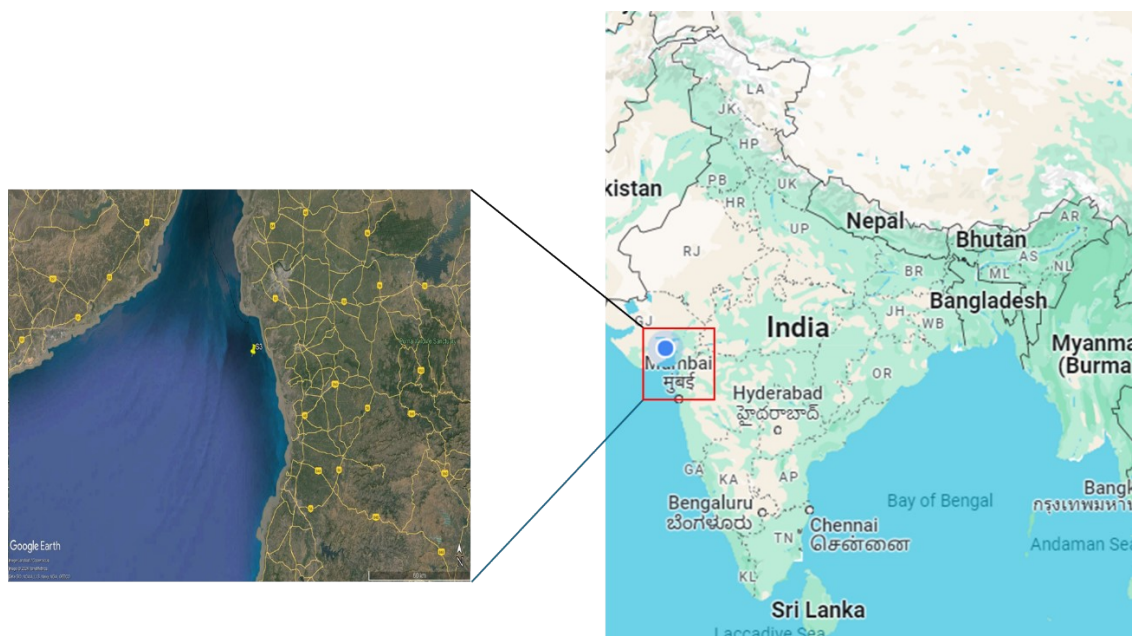


Table TS1 Physicochemical properties of target POPs.

Compounds Name	Chemical formula	logP	Melting Point (°C)	Boiling Point (°C)	Molar mass (g/mol)
Naphthalene	C ₁₀ H ₈	3.34	80.26	218	128.17
Acenaphthylene	C ₁₂ H ₈	5	277.5	280	154.21
Acenaphthene	C ₁₂ H ₁₀	3.39	93.4	279	154.2
Fluorene	C ₁₃ H ₁₀	4.18	114	295	166.22
Phenanthrene	C ₁₄ H ₁₀	4.52	101	340	178.23
Anthracene	C ₁₄ H ₁₀	4.5	215	340	178.23
Fluoranthene	C ₁₆ H ₁₀	5.2	110.8	375	202.26
Pyrene	C ₁₆ H ₁₀	5	150.62	404	202.25
Benz (a) anthracene	C ₁₈ H ₁₂	5.91	158	438	228.28
Chrysene	C ₁₈ H ₁₂	5.86	254	448	228.28
Benzo(b)fluoranthene	C ₂₀ H ₁₂	5.78	168.4	481	252.3
Benzo(a)pyrene	C ₂₀ H ₁₂	6.35	179.3	312	252.31
Benzo(ghi)perylene	C ₂₂ H ₁₂	6.9	278	550	276.3307
Indeno(1,2,3-cd) pyrene	C ₂₂ H ₁₂	7.66	164	536	276.3307
Dibenz(a,h)anthracene	C ₂₂ H ₁₄	6.75	262	524	278.35
2,4,4'-Tribromodiphenyl ether	C ₁₂ H ₇ Br ₃ O	5.5	66	370	406.89
α-Hexabromocyclododecane	C ₁₂ H ₁₈ Br ₆	8.6	185.9	505	641.7
2,4,4'-Trichlorobiphenyl	C ₁₂ H ₇ Cl ₃	5.8	55	99.2	257.7

2,2',5,5'-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	6.1	87	374.95	291.99
2,2',4,5,5'-Pentachlorobiphenyl	C ₁₂ H ₅ Cl ₅	6.5	78	412.3	326.4
2,2',3,4,4',5'-Hexachlorobiphenyl	C ₁₂ H ₄ Cl ₆	7.2	78	446.99	360.88
2,2',4,4',5,5'-Hexachlorobiphenyl	C ₁₂ H ₄ Cl ₆	7.2	138	446.99	360.9

Table TS2 Detection of target ion and qualifier ions using GCMS.

Name	Pollutants	Retention time (min)	Ions for selected ion monitoring
PAHs	Naphthalene	12.45	128*, 102, 64, 50
	Acenaphthene	20.936	153*, 76, 63, 50
	Acenaphthylene	20.258	152*, 76, 63, 50
	Fluorene	23.464	166*, 82, 69, 50
	Phenanthrene	30.132	178*, 76, 89, 152
	Anthracene	30.521	178*, 89, 76, 63
	Fluoranthene	37.215	202*, 203, 200, 199
	Pyrene	38.476	203*, 101, 88, 75
	Benz (a) anthracene	45.106	228*, 113, 101, 88
	Chrysene	44.755	228*, 114, 101, 88
	Benzo(b)fluoranthene	50.058	252*, 250, 126, 125
	Benzo(a)pyrene	51.772	252*, 250, 125, 110
	Benzo(ghi)perylene	56.128	276*, 138, 124, 111
	Indeno(1,2,3-cd) pyrene	57.383	276*, 138, 125, 91
	Dibenz(a,h)anthracene	56.189	278*, 139, 125, 100
BDE	2,4,4'-Tribromodiphenyl ether	16.973	73*, 221, 147, 355
HBOD	α-Hexabromocyclododecane	28.557	157*, 239, 319, 401
PCB	2,4,4'-Trichlorobiphenyl	10.485	290*, 256, 220, 288
	2,2',5,5'-Tetrachlorobiphenyl	11.585	326*, 256, 290, 220
	2,2',4,5,5'-Pentachlorobiphenyl	12.975	290*, 360, 290, 220
	2,2',3,4,4',5'-Hexachlorobiphenyl	13.825	290*, 292, 360, 220
	2,2',4,4',5,5'-Hexachlorobiphenyl	15.145	326*, 324, 254, 394

ST3 Analytical figures of merit and validation parameters of the method

	Analyte	Linearity (mg/L)	Coefficient of Determination	Mean Recovery (%)	Limit of Quantification (water) (mg/L)	Limit of Quantification (Sediment) (mg/Kg)	RSD %
PAHs	Naphthalene	0.97-0.99	0.995	99.8	0.069	0.057	15
	Acenaphthene	0.98-0.99	0.996	98.96	0.069	0.057	15
	Acenaphthylene	0.97-0.99	0.998	97.65	0.069	0.057	16
	Fluorene	0.98-0.99	0.998	99.65	0.069	0.057	14
	Phenanthrene	0.98-0.99	0.9999	99.89	0.069	0.057	13
	Anthracene	0.97-0.99	0.9994	99.65	0.069	0.057	17
	Fluoranthene	0.97-0.99	0.997	98.23	0.069	0.057	18
	Pyrene	0.98-0.99	0.996	99.85	0.069	0.065	19
	Benz(a)anthracene	0.98-0.99	0.9992	97.23	0.069	0.046	20
	Chrysene	0.98-0.99	0.998	99.85	0.069	0.057	14
	Benzo[b]fluoranthene	0.98-0.99	0.999	99.96	0.076	0.046	12
	Benzo[a]pyrene	0.98-0.99	0.9992	99.96	0.067	0.057	16
	Benzo[ghi]perylene	0.98-0.99	0.994	99.15	0.066	0.046	8
	Indeno[1,2,3-cd]pyrene	0.98-0.99	0.9992	99.113	0.069	0.057	4
	Dibenz[a,h]anthracene	0.98-0.99	0.9993	99.02	0.069	0.057	20
BDE	2,4,4'-Tribromodiphenyl ether	0.98-0.99	0.9991	99.89	0.069	0.057	16
HB CD	alpha-Hexabromocyclododecane	0.97-0.99	0.9992	99.089	0.065	0.045	7
PCB	2,4,4'-Trichlorobiphenyl	0.98-0.99	0.999	99.23	0.045	0.035	6
	2,2",5,5"-Trichlorobiphenyl	0.98-0.99	0.998	99.54	0.045	0.035	8
	2,2",4,5,5"-Trichlorobiphenyl	0.96-0.99	0.9991	99.68	0.045	0.035	16

	yl						
	2,2",3,4,4",5-Trichlorobiphenyl	0.98-0.99	0.997	99.06	0.045	0.035	14
	2,2",4,4",5,5"-Trichlorobiphenyl	0.98-0.99	0.996	99.23	0.045	0.035	17

ST4. Effect of the different methanol concentrations on the extraction efficiency and matrix effect for all the POPs

Group s	MeOH (%)	Compounds	Elution Efficiency	Matrix Effects (%)
PAHs	0	Naphthalene	0.203832	2.527536232
	10	Naphthalene	0.657877814	3.086021505
	20	Naphthalene	1.021007503	1.891454965
	30	Naphthalene	0.999785638	2.035377358
	40	Naphthalene	0.992711683	2.06888361
	50	Naphthalene	1.098821008	2.135193133
	60	Naphthalene	1.049303323	1.795505618
	70	Naphthalene	1.200214362	1.750491159
	80	Naphthalene	1.105456	3.867595819
	90	Naphthalene	1.431296892	1.248764415
	100	Naphthalene	1.058735263	1.926503341
	0	Acenaphthene	0.392365457	0.380952381
	10	Acenaphthene	0.443500805	0.436807095
	20	Acenaphthene	0.362864295	0.348238482
	30	Acenaphthene	0.993205793	0.101980198
	40	Acenaphthene	1.010101	0.477777778
	50	Acenaphthene	1.02558	0.578787879
	60	Acenaphthene	1.12021	0.285714286
	70	Acenaphthene	1.102023	0.692660551
	80	Acenaphthene	1.189880207	0.123140496
	90	Acenaphthene	1.740568568	0.706214689
	100	Acenaphthene	0.940103701	0.242259414
	0	Acenaphthylene	0.793103448	0.979405034
	10	Acenaphthylene	0.936479129	0.808139535
	20	Acenaphthylene	0.79491833	0.936073059
	30	Acenaphthylene	0.952813067	0.601904762
	40	Acenaphthylene	1.063520871	0.907849829
	50	Acenaphthylene	1.229945554	0.507710558
	60	Acenaphthylene	0.965517241	0.526315789
	70	Acenaphthylene	1.021778584	1.028419183
	80	Acenaphthylene	0.834845735	0.873913043
	90	Acenaphthylene	1.515970962	0.605970149
	100	Acenaphthylene	0.891107078	0.904276986
	0	Fluorene	1.005616225	0.61774744
	10	Fluorene	1.057098284	0.516233766

20	Fluorene	0.803120125	0.568376068
30	Fluorene	1.105148206	0.434782609
40	Fluorene	1.136037441	0.383685801
50	Fluorene	1.043369735	0.273355263
60	Fluorene	0.954134165	0.343884892
70	Fluorene	1.067394696	0.363344051
80	Fluorene	0.895787832	0.277777778
90	Fluorene	1.964430577	0.34911032
100	Fluorene	0.967862715	0.338297872
0	Phenanthrene	0.174316041	0.749883019
10	Phenanthrene	0.432501121	1.216258555
20	Phenanthrene	0.197338915	1.06823
30	Phenanthrene	0.383166393	0.892171674
40	Phenanthrene	0.891314098	0.844789668
50	Phenanthrene	1.015595	0.592526984
60	Phenanthrene	0.491702796	1.05309699
70	Phenanthrene	0.769621767	0.991188034
80	Phenanthrene	1.387950366	1.056725118
90	Phenanthrene	1.46356	0.624332824
100	Phenanthrene	1.009717447	1.082859935
0	Anthracene	1.077362805	0.245136187
10	Anthracene	1.087842988	0.271676301
20	Anthracene	0.821646341	0.37244898
30	Anthracene	1.008193598	0.272349272
40	Anthracene	1.092035061	0.238003839
50	Anthracene	1.010289634	0.2593361
60	Anthracene	1.029153963	0.234215886
70	Anthracene	0.968368902	0.246753247
80	Anthracene	1.027057927	0.22244898
90	Anthracene	1.888719512	0.242924528
100	Anthracene	0.989329268	0.230932203
0	Fluoranthene	1.047885889	0.356684492
10	Fluoranthene	1.036678553	0.315675676
20	Fluoranthene	0.83494651	0.404026846
30	Fluoranthene	1.07030056	0.296335079
40	Fluoranthene	1.003056546	0.296648045
50	Fluoranthene	1.031074885	0.34076087
60	Fluoranthene	1.031074885	0.35326087
70	Fluoranthene	0.986245543	0.276704545
80	Fluoranthene	1.01986755	0.291208791
90	Fluoranthene	1.924605196	0.327272727
100	Fluoranthene	1.014263882	0.261325967
0	Pyrene	0.999586948	0.868181818
10	Pyrene	1.108632796	0.848360656
20	Pyrene	0.817843866	1.111111111
30	Pyrene	0.967781908	0.915492958
40	Pyrene	1.11771995	0.760162602

50	Pyrene	1.02684841	0.880530973
60	Pyrene	1.022304833	0.893333333
70	Pyrene	1.113176373	0.648979592
80	Pyrene	0.931433292	0.868292683
90	Pyrene	1.404130525	0.755656109
100	Pyrene	0.890541099	0.790816327
0	Benz (a)anthrancene	0.795077403	1.439137134
10	Benz (a)anthrancene	1.223855663	1.071071071
20	Benz (a)anthrancene	0.885733378	1.410788382
30	Benz (a)anthrancene	0.984964918	1.233830846
40	Benz (a)anthrancene	1.087871701	1.082207207
50	Benz (a)anthrancene	1.060919924	1.140877598
60	Benz (a)anthrancene	0.949437577	1.287741935
70	Benz (a)anthrancene	1.116048558	0.912184413
80	Benz (a)anthrancene	0.931061365	1.178947368
90	Benz (a)anthrancene	1.93997104	1.109742441
100	Benz (a)anthrancene	0.871032409	1.161744023
0	Chrysene	0.508529048	0.79144385
10	Chrysene	0.845735476	0.553054662
20	Chrysene	0.769592089	0.989399293
30	Chrysene	0.987144623	0.564738292
40	Chrysene	1.131273177	0.629807692
50	Chrysene	1.036093943	0.664041995
60	Chrysene	1.19381953	0.312072893
70	Chrysene	1.172064277	0.197215777
80	Chrysene	1.14487021	0.382422803
90	Chrysene	1.19381953	0.366059226
100	Chrysene	1.017058096	0.326203209
0	Benzo[b]fluoranthene	0.454878311	0.588541667
10	Benzo[b]fluoranthene	0.741546414	0.495207668
20	Benzo[b]fluoranthene	0.326943786	1.108695652
30	Benzo[b]fluoranthene	0.506999785	0.700934579
40	Benzo[b]fluoranthene	1.186948094	0.295409182
50	Benzo[b]fluoranthene	0.978462201	0.404358354
60	Benzo[b]fluoranthene	1.21300883	0.310546875
70	Benzo[b]fluoranthene	1.449924618	0.222222222
80	Benzo[b]fluoranthene	1.281714409	0.256931608
90	Benzo[b]fluoranthene	1.542321775	0.204301075
100	Benzo[b]fluoranthene	1.317251777	0.214028777
0	Benzo[a]pyrene	0.894232815	0.731675393
10	Benzo[a]pyrene	1.056927006	0.880398671
20	Benzo[a]pyrene	0.828686955	1.103107345
30	Benzo[a]pyrene	0.990210683	0.871158392
40	Benzo[a]pyrene	1.103745478	0.808059385
50	Benzo[a]pyrene	1.075654395	0.842219804
60	Benzo[a]pyrene	1.0662907	0.840834248
70	Benzo[a]pyrene	1.075654395	0.750816104

	80	Benzo[a]pyrene	0.982017451	0.827175209
	90	Benzo[a]pyrene	1.993722069	0.784452297
	100	Benzo[a]pyrene	0.932858055	0.757841907
	0	Benzo[ghi]perylene	1.133680208	1.066019417
	10	Benzo[ghi]perylene	0.862917751	1.147959184
	20	Benzo[ghi]perylene	0.72203322	1.156097561
	30	Benzo[ghi]perylene	0.977386432	1.063063063
	40	Benzo[ghi]perylene	0.99939964	0.907488987
	50	Benzo[ghi]perylene	1.188713228	0.755555556
	60	Benzo[ghi]perylene	1.098459075	0.879759519
	70	Benzo[ghi]perylene	0.997198319	0.823399558
	80	Benzo[ghi]perylene	0.994996998	0.876106195
	90	Benzo[ghi]perylene	1.843426056	0.837552743
	100	Benzo[ghi]perylene	0.981789073	0.858744395
	0	Indeno[1,2,3-cd]pyrene	0.830679862	0.495726496
	10	Indeno[1,2,3-cd]pyrene	0.766781411	0.604938272
	20	Indeno[1,2,3-cd]pyrene	0.911144578	0.636363636
	30	Indeno[1,2,3-cd]pyrene	1.055507745	0.538116592
	40	Indeno[1,2,3-cd]pyrene	1.143072289	0.459627329
	50	Indeno[1,2,3-cd]pyrene	1.062607573	0.4922049
	60	Indeno[1,2,3-cd]pyrene	1.109939759	0.543710021
	70	Indeno[1,2,3-cd]pyrene	1.100473322	0.4
	80	Indeno[1,2,3-cd]pyrene	0.989242685	0.492822967
	90	Indeno[1,2,3-cd]pyrene	1.869707401	0.442477876
	100	Indeno[1,2,3-cd]pyrene	0.960843373	0.477832512
	0	Dibenz[a,h]anthracene	0.876487663	1.030965392
	10	Dibenz[a,h]anthracene	0.983454282	1.160714286
	20	Dibenz[a,h]anthracene	0.812626996	1.347740668
	30	Dibenz[a,h]anthracene	0.945137881	1.126689189
	40	Dibenz[a,h]anthracene	1.144702467	0.959553696
	50	Dibenz[a,h]anthracene	1.08563135	1.197058824
	60	Dibenz[a,h]anthracene	1.039332366	1.024577573
	70	Dibenz[a,h]anthracene	1.103193033	0.84081042
	80	Dibenz[a,h]anthracene	1.028156749	1.010869565
	90	Dibenz[a,h]anthracene	1.308998549	1.006329114
	100	Dibenz[a,h]anthracene	0.972278665	0.742200328
BDE	0	2,4,4'-Tribromodiphenyl ether	0.68554	1.176470588
	10	2,4,4'-Tribromodiphenyl ether	0.825251	1.029829172
	20	2,4,4'-Tribromodiphenyl ether	0.789831166	1
	30	2,4,4'-Tribromodiphenyl ether	1.23811372	1.055172414
	40	2,4,4'-Tribromodiphenyl ether	1.380425642	1.061340206
	50	2,4,4'-Tribromodiphenyl ether	1.060223818	1.134228188
	60	2,4,4'-Tribromodiphenyl ether	1.323500873	1.071505376
	70	2,4,4'-Tribromodiphenyl ether	1.302154085	1.03989071
	80	2,4,4'-Tribromodiphenyl ether	1.010414645	1.063380282
	90	2,4,4'-Tribromodiphenyl ether	1.996183453	0.95
	100	2,4,4'-Tribromodiphenyl ether	1.188304548	1.05508982

HBCD	0	α -Hexabromocyclododecane	0.947408537	0.838053097
	10	α -Hexabromocyclododecane	1.073170732	0.70390625
	20	α -Hexabromocyclododecane	0.84679878	0.825742574
	30	α -Hexabromocyclododecane	0.997713415	0.678151261
	40	α -Hexabromocyclododecane	1.073170732	0.62578125
	50	α -Hexabromocyclododecane	1.022865854	0.632786885
	60	α -Hexabromocyclododecane	1.056402439	0.637301587
	70	α -Hexabromocyclododecane	1.115091463	0.571428571
	80	α -Hexabromocyclododecane	0.93902439	0.605357143
	90	α -Hexabromocyclododecane	1.006097561	0.629166667
	100	α -Hexabromocyclododecane	0.922256098	0.547272727
PCBs	0	2,4,4'-Trichlorobiphenyl	1.187451286	1.026173285
	10	2,4,4'-Trichlorobiphenyl	0.900233827	1.076904762
	20	2,4,4'-Trichlorobiphenyl	0.726617303	1.061946903
	30	2,4,4'-Trichlorobiphenyl	1.011691348	1.049152542
	40	2,4,4'-Trichlorobiphenyl	1.024551832	1.044142259
	50	2,4,4'-Trichlorobiphenyl	1.069563523	1.041282565
	60	2,4,4'-Trichlorobiphenyl	1.063133281	1.044153226
	70	2,4,4'-Trichlorobiphenyl	1.050272798	1.026326531
	80	2,4,4'-Trichlorobiphenyl	0.988113796	1.039045553
	90	2,4,4'-Trichlorobiphenyl	1.1812159	1.028842105
	100	2,4,4'-Trichlorobiphenyl	0.960249415	1.025
	0	2,2',5,5'-Tetrachlorobiphenyl	0.722022956	1.019125683
	10	2,2',5,5'-Tetrachlorobiphenyl	1.116571019	0.961130742
	20	2,2',5,5'-Tetrachlorobiphenyl	0.840387374	1.211267606
	30	2,2',5,5'-Tetrachlorobiphenyl	0.879842181	1.253233831
	40	2,2',5,5'-Tetrachlorobiphenyl	1.191535151	0.90397351
	50	2,2',5,5'-Tetrachlorobiphenyl	1.073170732	1.176470588
	60	2,2',5,5'-Tetrachlorobiphenyl	1.06527977	1.018518519
	70	2,2',5,5'-Tetrachlorobiphenyl	1.12446198	0.81754386
	80	2,2',5,5'-Tetrachlorobiphenyl	0.9982066	0.944664032
	90	2,2',5,5'-Tetrachlorobiphenyl	1.17934003	0.891472868
	100	2,2',5,5'-Tetrachlorobiphenyl	0.970588235	0.817073171
	0	2,2',4,5,5'-Pentachlorobiphenyl	1.019940179	0.713261649
	10	2,2',4,5,5'-Pentachlorobiphenyl	1.063808574	0.762886598
	20	2,2',4,5,5'-Pentachlorobiphenyl	0.840810901	0.973913043
	30	2,2',4,5,5'-Pentachlorobiphenyl	0.93220339	0.843137255
	40	2,2',4,5,5'-Pentachlorobiphenyl	1.107676969	0.722772277
	50	2,2',4,5,5'-Pentachlorobiphenyl	1.319707544	0.656509695
	60	2,2',4,5,5'-Pentachlorobiphenyl	0.935859089	0.88671875
	70	2,2',4,5,5'-Pentachlorobiphenyl	1.023595879	0.732142857

80	2,2',4,5,5'- Pentachlorobiphenyl	0.957793287	0.812977099
90	2,2',4,5,5'- Pentachlorobiphenyl	1.924891991	0.806324111
100	2,2',4,5,5'- Pentachlorobiphenyl	0.873712197	0.811715481
0	2,2',3,4,4',5'- Hexachlorobiphenyl	0.621356291	1.052673797
10	2,2',3,4,4',5'- Hexachlorobiphenyl	1.043346926	1.071656051
20	2,2',3,4,4',5'- Hexachlorobiphenyl	0.935357197	1.031971581
30	2,2',3,4,4',5'- Hexachlorobiphenyl	1.016764839	1.04248366
40	2,2',3,4,4',5'- Hexachlorobiphenyl	1.09152696	0.919330289
50	2,2',3,4,4',5'- Hexachlorobiphenyl	1.059960731	1.089341693
60	2,2',3,4,4',5'- Hexachlorobiphenyl	1.073251775	1.241486068
70	2,2',3,4,4',5'- Hexachlorobiphenyl	1.071590394	0.905426357
80	2,2',3,4,4',5'- Hexachlorobiphenyl	1.035040024	0.913322632
90	2,2',3,4,4',5'- Hexachlorobiphenyl	1.101495242	0.819004525
100	2,2',3,4,4',5'- Hexachlorobiphenyl	0.950309621	0.842657343
0	2,2',4,4',5,5'- Hexachlorobiphenyl	1.285994508	0.365100671
10	2,2',4,4',5,5'- Hexachlorobiphenyl	1.337779521	0.403870968
20	2,2',4,4',5,5'- Hexachlorobiphenyl	0.657669674	0.719160105
30	2,2',4,4',5,5'- Hexachlorobiphenyl	0.649038839	0.857712766
40	2,2',4,4',5,5'- Hexachlorobiphenyl	0.84323264	0.57727738
50	2,2',4,4',5,5'- Hexachlorobiphenyl	0.819155	0.248089172
60	2,2',4,4',5,5'- Hexachlorobiphenyl	0.739662613	0.698949825
70	2,2',4,4',5,5'- Hexachlorobiphenyl	0.673205179	0.679487179
80	2,2',4,4',5,5'- Hexachlorobiphenyl	0.631777168	0.709016393
90	2,2',4,4',5,5'- Hexachlorobiphenyl	1.773322872	0.547991071
100	2,2',4,4',5,5'- Hexachlorobiphenyl	0.698234602	0.360939431