

# Supplementary Material

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## **Polychlorinated biphenyls interactions with water – characterization based on the analysis of non-covalent interactions and energy partitioning**

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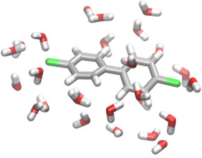
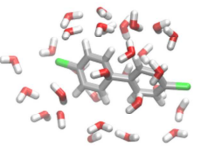
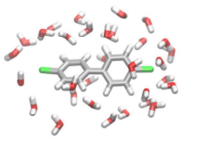
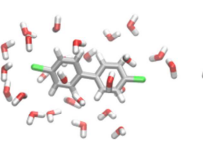
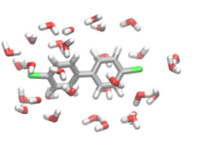
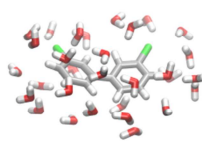
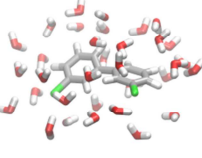
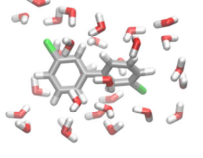
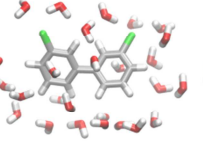
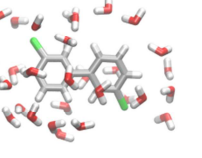
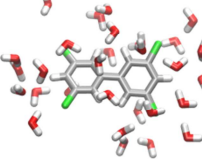
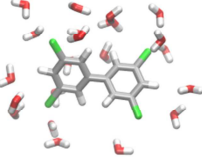
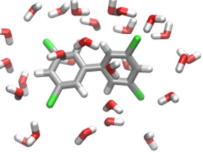
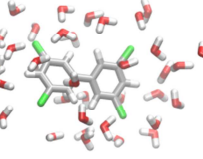
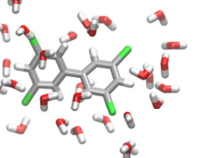
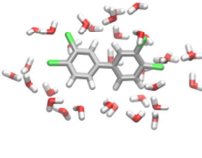
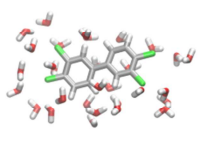
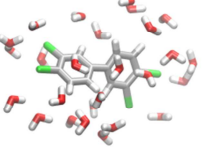
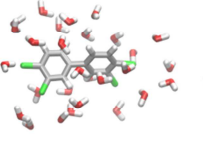
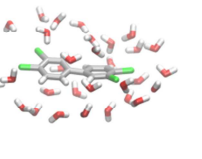
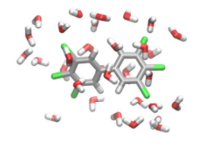
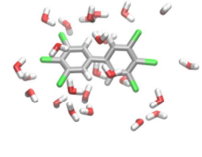
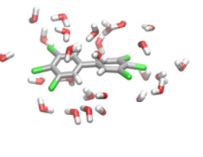
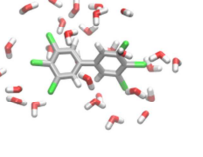
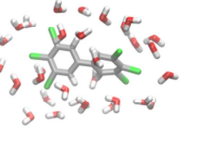
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**Table S1.** Binding or interaction energies in kcal mol<sup>-1</sup> between PCBs and water or chlorine in the studied 1:1 complexes. Results of supermolecular MP2 (binding energy) and perturbational SAPT2 (interaction energy) approaches with def2-TZVP basis set. The contributions summing up to the total SAPT2 energy are: Elst = electrostatics; Exch = Exchange; Ind = Induction; Disp = Dispersion.

System	RI-MP2/def2-TZVP	SAPT2/def2-TZVP	Elst	Exch	Ind	Disp
<b>Water complexes</b>						
<b>a1</b>	2.602	-2.914	-4.012	5.868	-1.001	-3.769
<b>a2</b>	3.283	-3.398	-4.799	6.175	-1.428	-3.345
<b>b1</b>	2.485	-2.835	-3.773	5.863	-1.064	-3.861
<b>b2</b>	2.526	-2.811	-3.834	6.211	-1.349	-3.839
<b>c1</b>	0.913	-1.053	-1.679	2.298	-0.623	-1.049
<b>c2</b>	2.567	-2.942	-4.523	5.831	-1.055	-3.195
<b>d1</b>	1.542	-1.655	-2.235	2.724	-0.689	-1.455
<b>d2</b>	3.847	-4.253	-5.474	5.737	-1.518	-2.999
<b>e1</b>	1.047	-1.299	-2.102	2.705	-0.498	-1.404
<b>e2</b>	2.124	-2.453	-3.665	6.018	-1.093	-3.713
<b>Chlorine complexes</b>						
<b>a1</b>	4.004	-4.123	-5.027	11.806	-2.508	-8.394
<b>a2</b>	3.858	-3.976	-5.009	11.401	-2.44	-7.928
<b>b1</b>	2.617	-2.855	-2.969	6.091	-0.885	-5.093
<b>b2</b>	3.883	-3.969	-5.216	11.844	-2.563	-8.034
<b>c1</b>	3.987	-4.109	-5.025	12.162	-2.563	-8.683
<b>c2</b>	3.994	-4.113	-5.003	12.097	-2.557	-8.65
<b>d1</b>	3.166	-3.691	-3.602	9.008	-1.537	-7.561
<b>d2</b>	4.000	-4.173	-5.050	12.185	-2.586	-8.723
<b>e1</b>	1.550	-1.610	-1.751	3.105	-0.409	-2.555
<b>e2</b>	4.278	-4.721	-3.961	9.291	-0.635	-9.416

Solute	Snapshot taken at the following time of production run:				
	0.5 ns	1.5 ns	2.5 ns	3.5 ns	4.5 ns
PCB15 (a)					
PCB11 (b)					
PCB80 (c)					
PCB77 (d)					
PCB169 (e)					

**Figure S1.** Microsolvation shells – snapshots from the classical MD runs of the studied PCBs in water, used in the solvation shell interaction energy study at the RI-MP2/def2-TZVP level.