

Supplementary information

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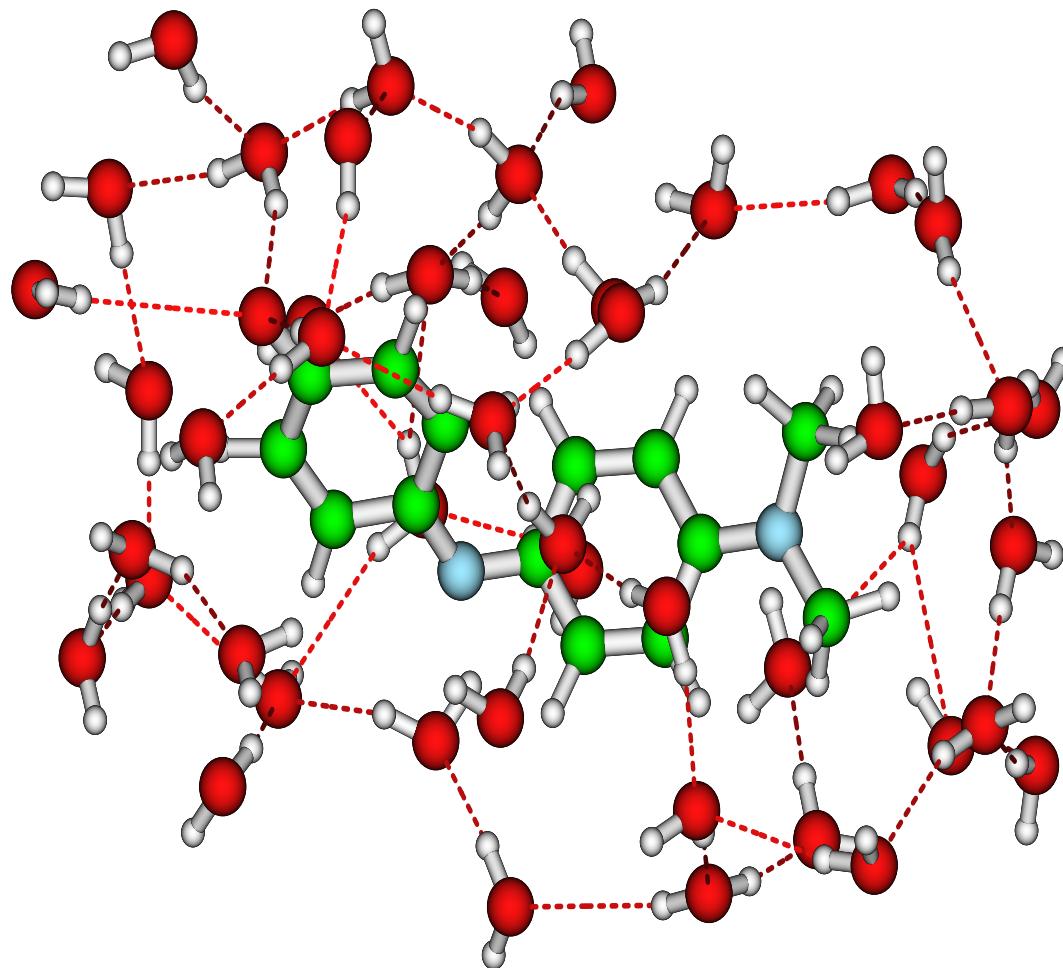


Figure 1 First and second solvation shell structure in PB-water system.

Table 1. Average atomic charges.

System	Gas phase	PB in chloroform	PB in water
C ₁	-0.21558	-0.02529	-0.01206
H ₂	0.08117	0.03706	0.06192
H ₃	0.07108	0.03661	0.05947
H ₄	0.09883	0.03578	0.06005
N ₅	0.07492	0.06932	0.09573
C ₆	-0.20442	-0.02492	-0.01235
H ₇	0.08792	0.03759	0.05575
H ₈	0.08992	0.03755	0.05955
H ₉	0.06542	0.03589	0.05925
C ₁₀	0.16392	0.02495	0.03308
C ₁₁	-0.26933	-0.05586	-0.04163
C ₁₂	-0.16158	-0.03216	-0.00892
H ₁₃	0.11508	0.04151	0.08938
H ₁₄	0.14142	0.03848	0.06878
C ₁₅	-0.20183	-0.06534	-0.03557
H ₁₆	0.12592	0.03484	0.10707
C ₁₇	-0.20442	-0.04613	-0.04281
H ₁₈	0.13608	0.00825	0.02668
C ₁₉	0.47958	-0.00830	-0.02915

Table 2. Average atomic charges (continued).

System	Gas phase	PB in chloroform	PB in water
N ₂₀	-0.60558	-0.08367	-0.23536
C ₂₁	0.51908	0.04639	0.01340
C ₂₂	-0.25633	-0.00519	0.00414
H ₂₃	0.13725	0.02133	0.02060
C ₂₄	-0.15800	-0.02229	-0.00609
H ₂₅	0.11508	0.03975	0.07609
C ₂₆	0.56067	0.03512	-0.01073
O ₂₇	-0.54983	-0.30053	-0.63012
C ₂₈	-0.22158	-0.01060	-0.01340
H ₂₉	0.13333	0.04229	0.04435
C ₃₀	-0.22242	0.00361	0.04000
H ₃₁	0.10875	0.05645	0.10419