

Supplementary Material to:

Accurate prediction of hydration free energies and solvation structures using molecular density functional theory with a simple bridge functional

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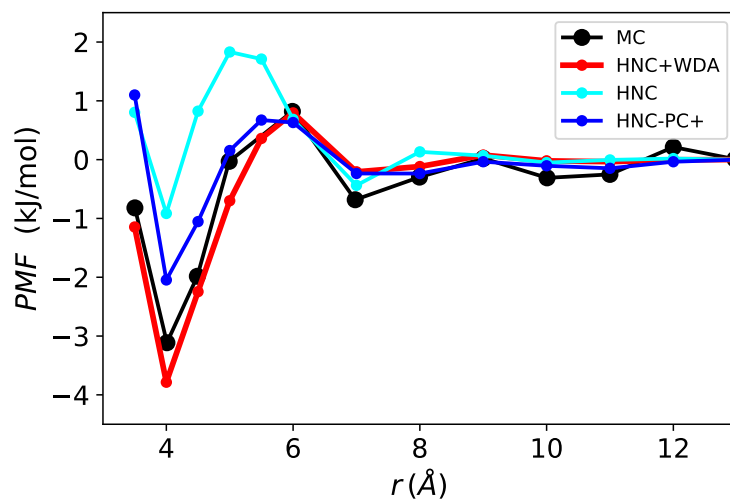


Figure 1. Potential of mean force (PMF) between two methane in TIP3P water computed by MDFT in different approximations and for the same distances as reference Monte-Carlo simulations.

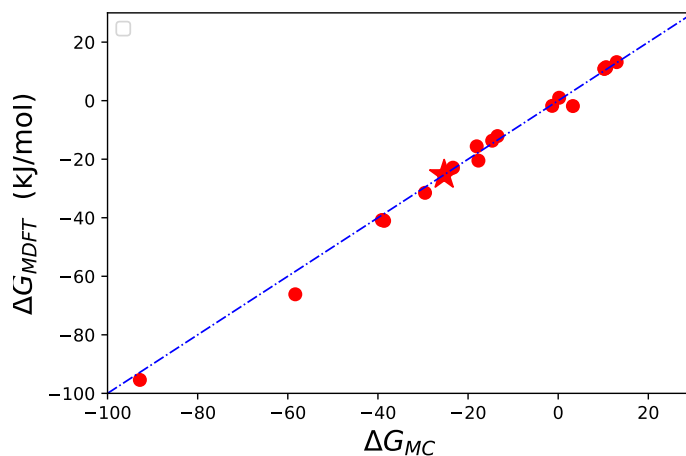


Figure 2. Correlation between HNC-WDA* and H4D-MC simulations for a reduced dataset of 19 organic molecules, in addition to water marked by a star. The dataset includes 14 amino-acid side chain analogs (methane, butane, isobutane, isopropane, butan-1-amine, methanethiol, methanol, ethanol, toluene, pyrrolidine, p-cresol, acetamide, propionic acid, acetic acid) + quinoline + cyanuric acid and 1,2-dinitroxyethane (the two molecules having the smallest, negative hydrophobic free-energy in the Mobley database) + octafluorocyclobutane and ethion (the ones with the largest hydrophobic, positive free-energies). In Fig. 11 of the manuscript, those molecules are sorted by decreasing hydration free energies, thus from hydrophobic ($\Delta G_{solv} > 0$) to hydrophilic ($\Delta G_{solv} < 0$) solutes (see Fig 3 below).

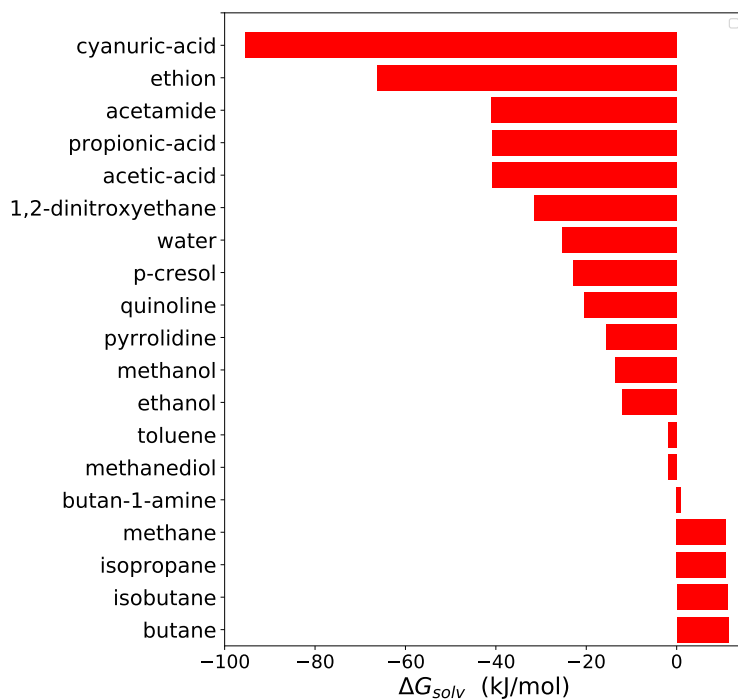


Figure 3. The 20 molecules of the reduced dataset classified according to their MDFT hydration free energies. This classification corresponds to that displayed in Fig. 11 of the manuscript.