Supporting information for

PlayMolecule CrypticScoutt: Predicting Protein Cryptic Sites using Mixed-Solvent Molecular Simulations. Gerard Martinez-Rosell[†], Silvia Lovera[‡], Zara Sands[‡] and Gianni de Fabritiis*[†,¶,§]

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S1.1

RDF (radial distribution function) for benzene from 0.2M water+benzene simulations; calculated with VMD using a 0.1 Ang sphere resolution plus a moving average smoothing of 10; based on 4 x 80 ns long simulation of water+benzene; notice that the RDF flattens at a VDW cutoff of 9 Ang
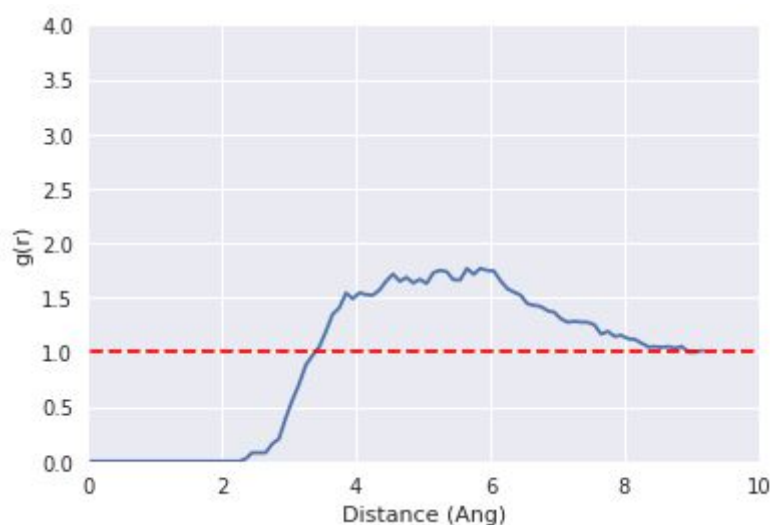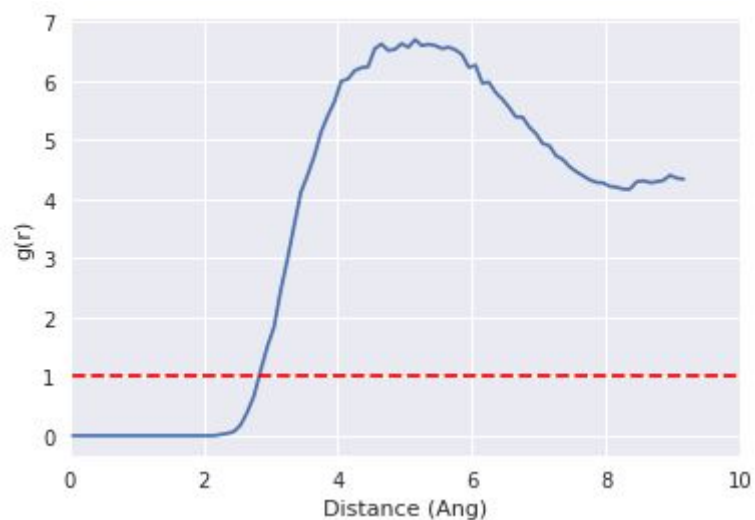

S1.2

RDF for benzene from an 80 ns-long simulation of 0.1M water+benzene using moving average of 10. Resolution was 0.1 Ang.
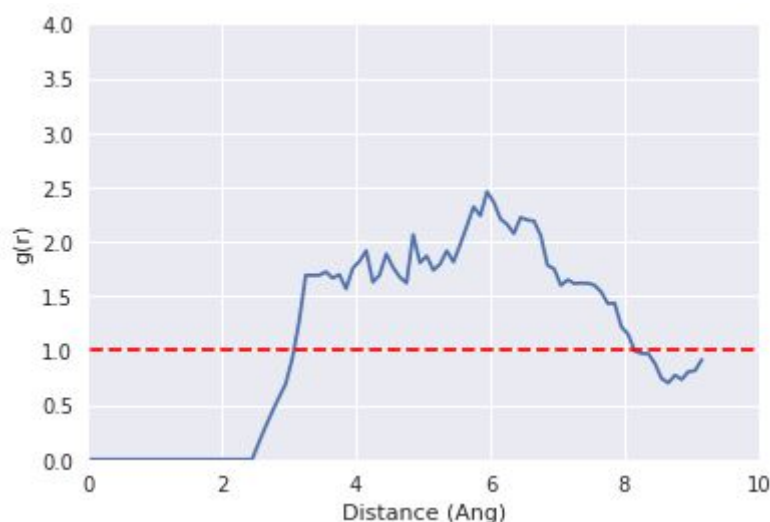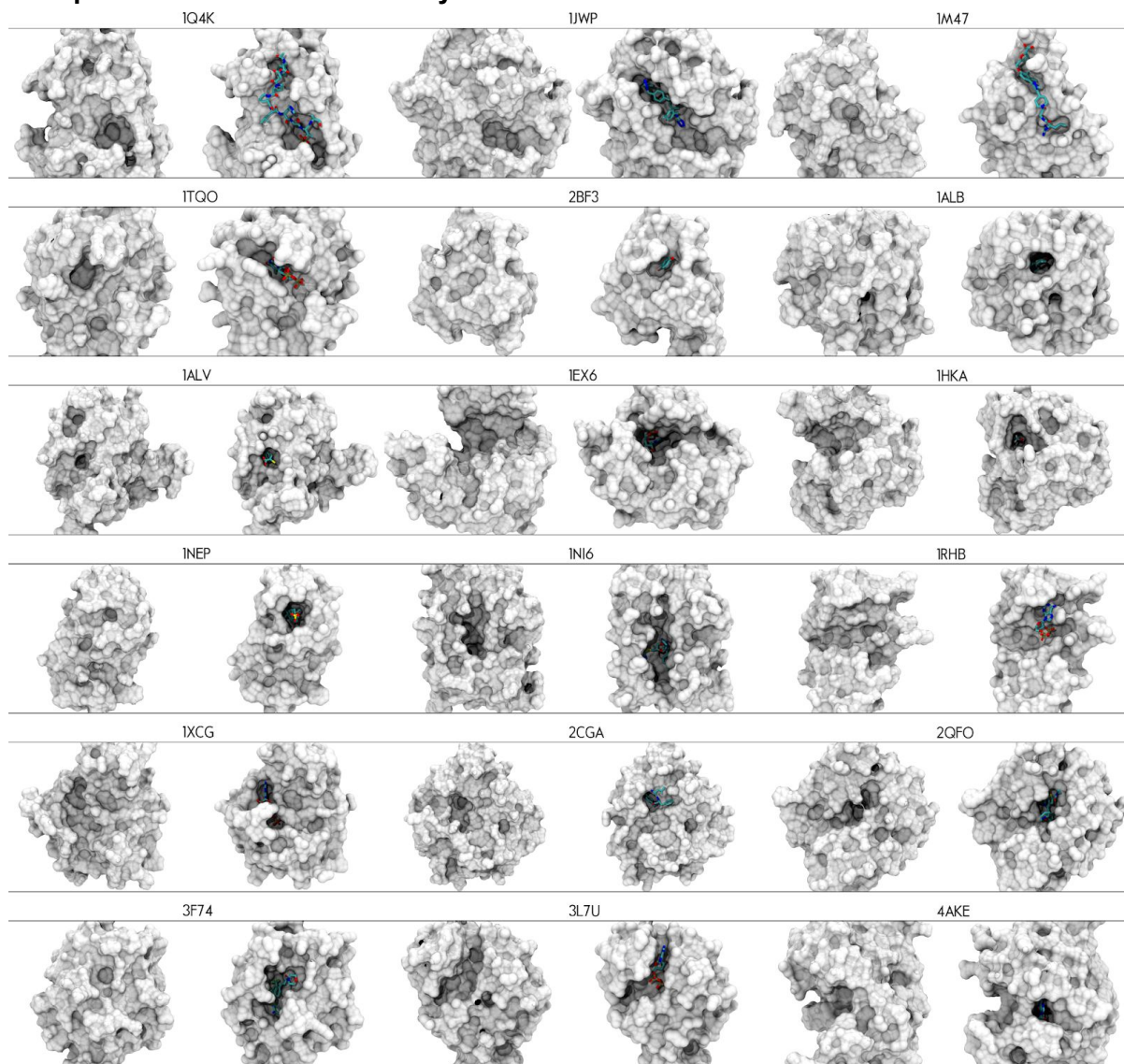
S1.3

RDF for benzene from an 80 ns-long 1M water+benzene simulation using a moving average of 10. Resolution was 0.1 Ang.
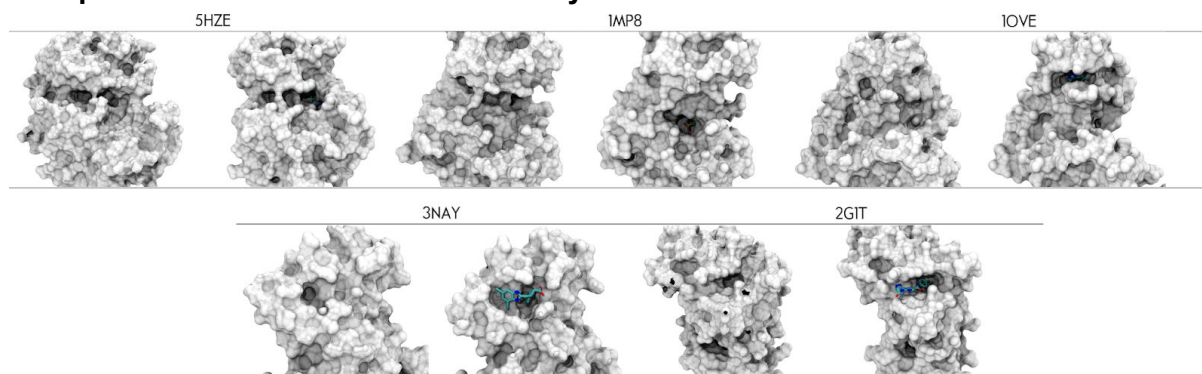

S.2 Apo and holo structures for systems 1-18

Snapshots of apo and holo structures for systems 1-18. For each protein ID, the apo structure is shown on the left and the holo structure on the right. The holo structure includes the ligand depicted in licorice. In both apo and holo structures, the protein surface is depicted in white.

S.3 Apo and holo structures for kinase systems 19-23

Snapshots of apo and holo structures for systems 19-23. For each protein ID, the apo structure is shown on the left and the holo structure on the right. The holo structure includes the ligand depicted in licorice. In both apo and holo structures, the protein surface is depicted in white.