International Journal of
Molecular Sciences

MDPI

Supplementary Materials

Inverse Mixed-Solvent Molecular Dynamics for Visualization of Residue Interaction Profile of Molecular Probes

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Supplementary Figures

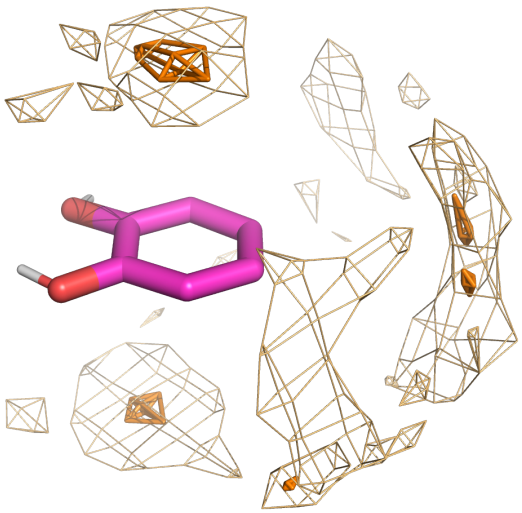

Figure S1. Interaction profile of aromatic rings of Phe, Tyr, and Trp, around catechol (purple). light and dark orange meshes indicate the profile with different thresholds.

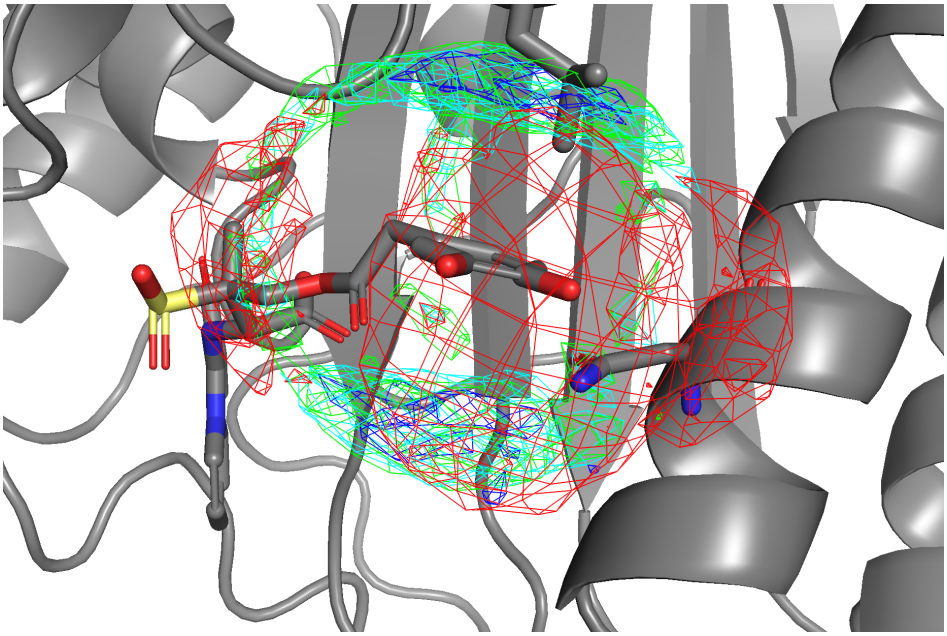

Figure S2. A superimposition of residue interaction profile of catechol to a β-Lactamase Inhibitor, LN-1-255 (PDBID: 3D4F). LN-1-255 has a catechol substituent and the profile was superimposed to it in accordance with the 3D structure of catechol. Green, cyan, gray, blue, and red meshes indicate profiles of hydrophobic, hydrophilic, aromatic, basic, and acidic residues, respectively.