Supplementary Materials

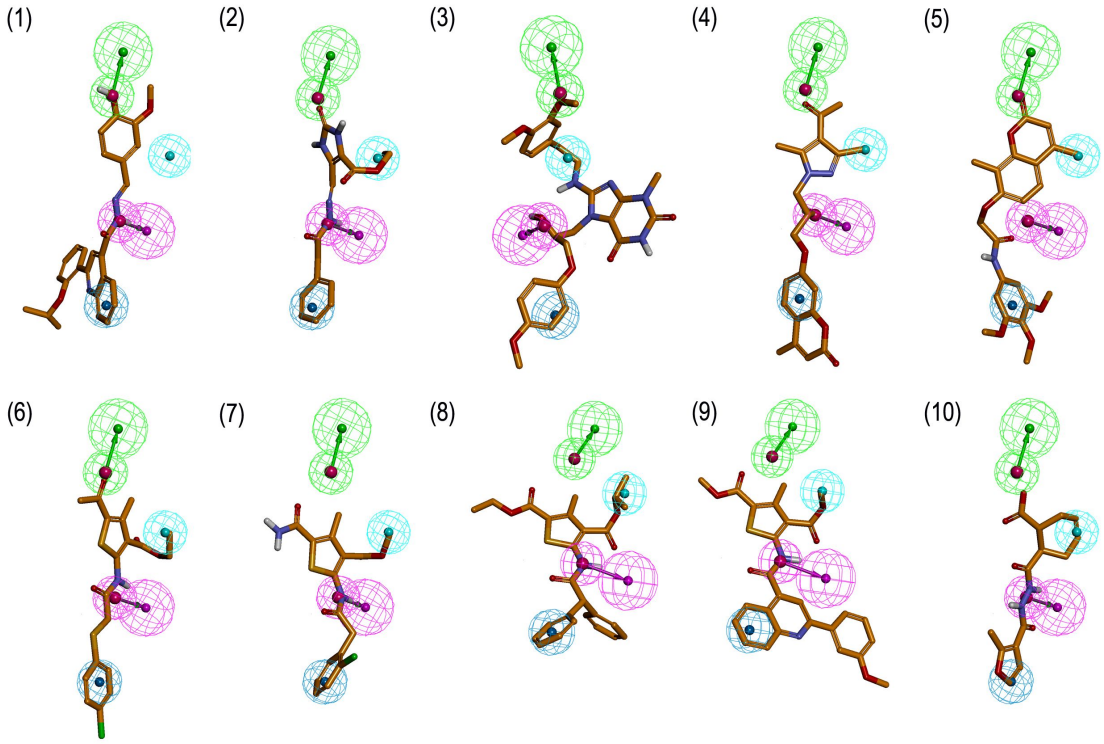

Figure S1. 3D structures of all ten proposed inhibitors mapping onto the ligand-based pharmacophore model.

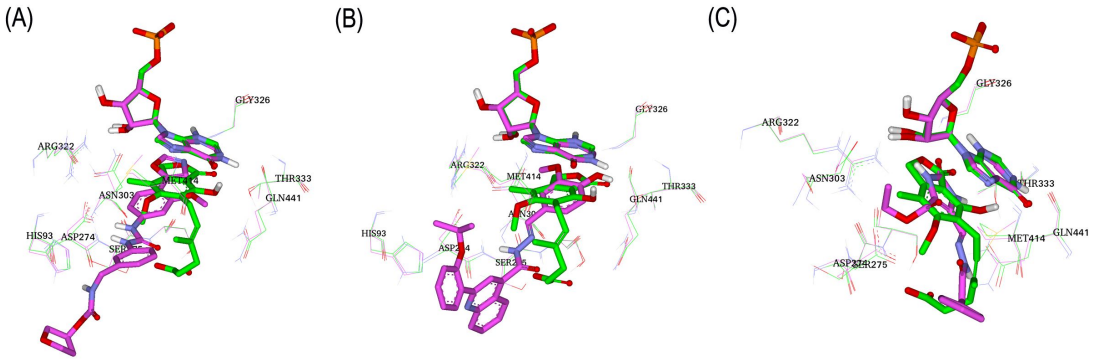

Figure S2. Close-up of superimposition between 1JR1 crystal structure (green) and docked structures of IMPDH in complex with inhibitors (magenta). For clarity, side chains that form this position of the inhibitor-binding pocket have been labeled. (A) A superimposition of MAP and VX-497. (B) A superimposition of MAP and

ZINC02090792. (C) A superimposition of MAP and ZINC00048033.