

Molecular modelling studies to suggest novel scaffolds against SARS-CoV-2 target enzymes

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SUPPLEMENTARY MATERIALS

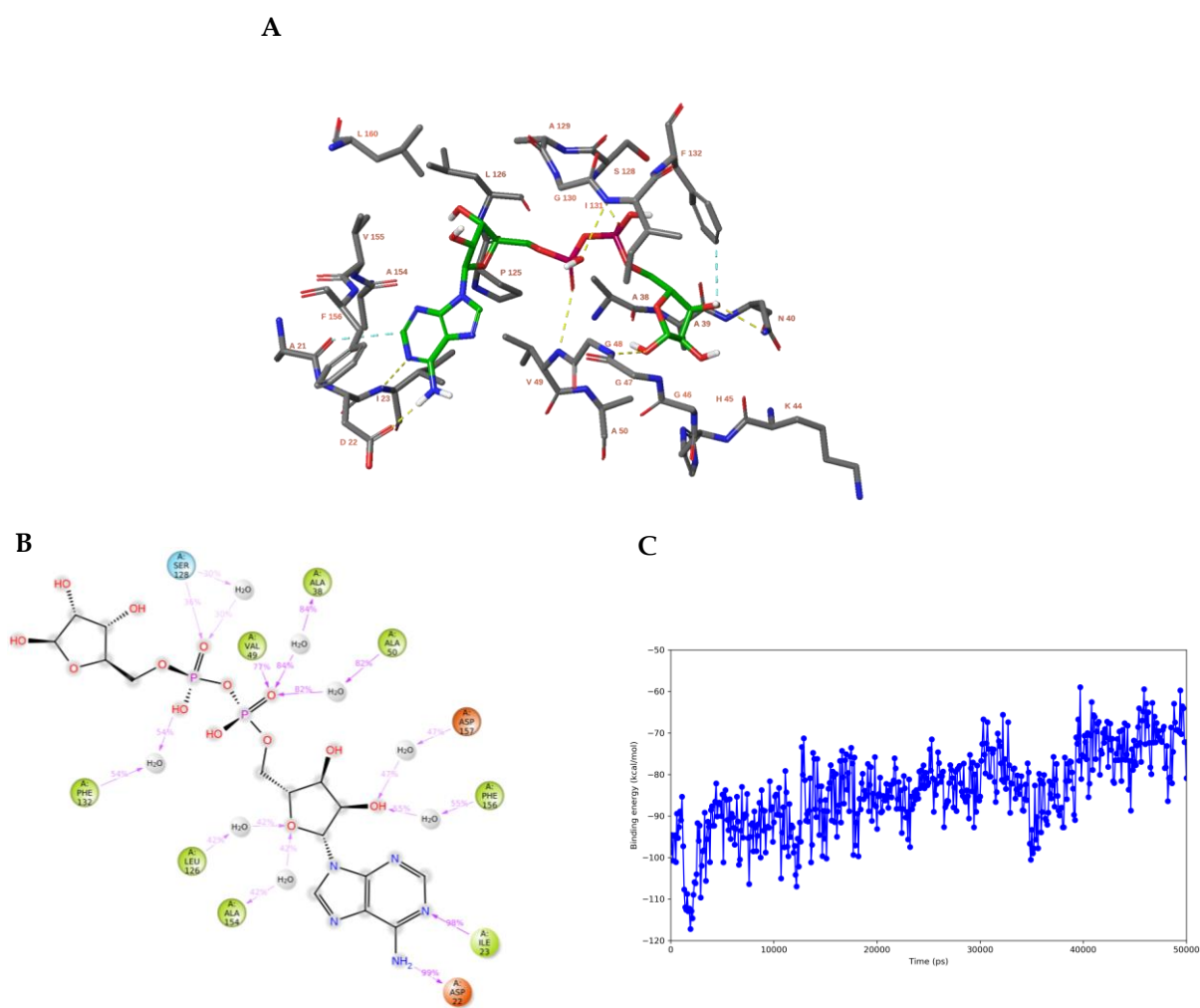


Figure S1. A) The cocrystal structure of adenosine-5-diphosphoribose (APR) in the active site of ADPR (pdb:6W02). B) The binding interactions of APR with the active site of ADPR during a 50ns MD simulation. C) The MM-GBSA binding energy. Hydrophobic amino acids are indicated in green, polar amino acids are indicated in blue, cationic amino acids are indicated in red. Hydrogen bonds are indicated in purple.

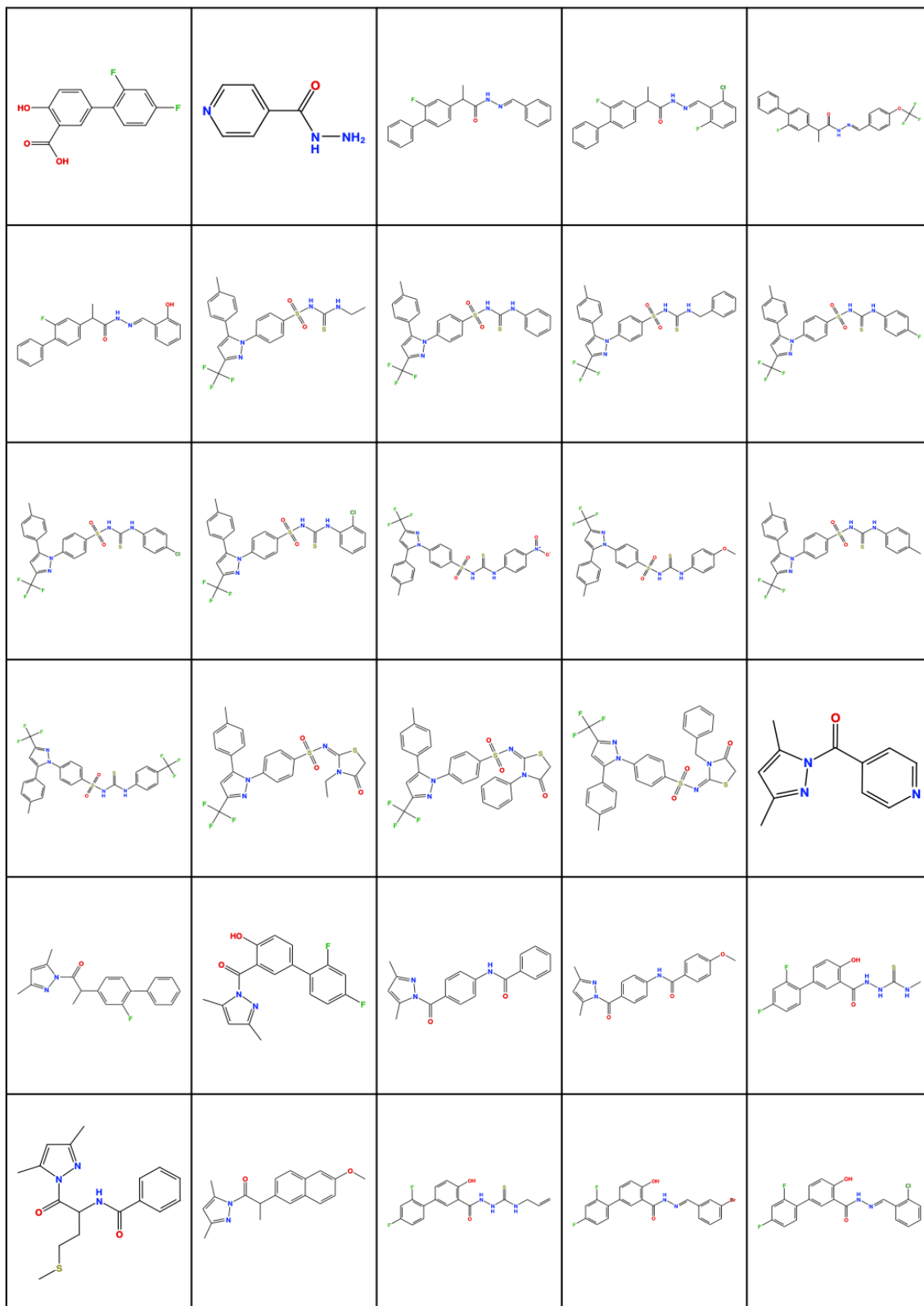


Figure S2. The 2D structures of the docked ligands.

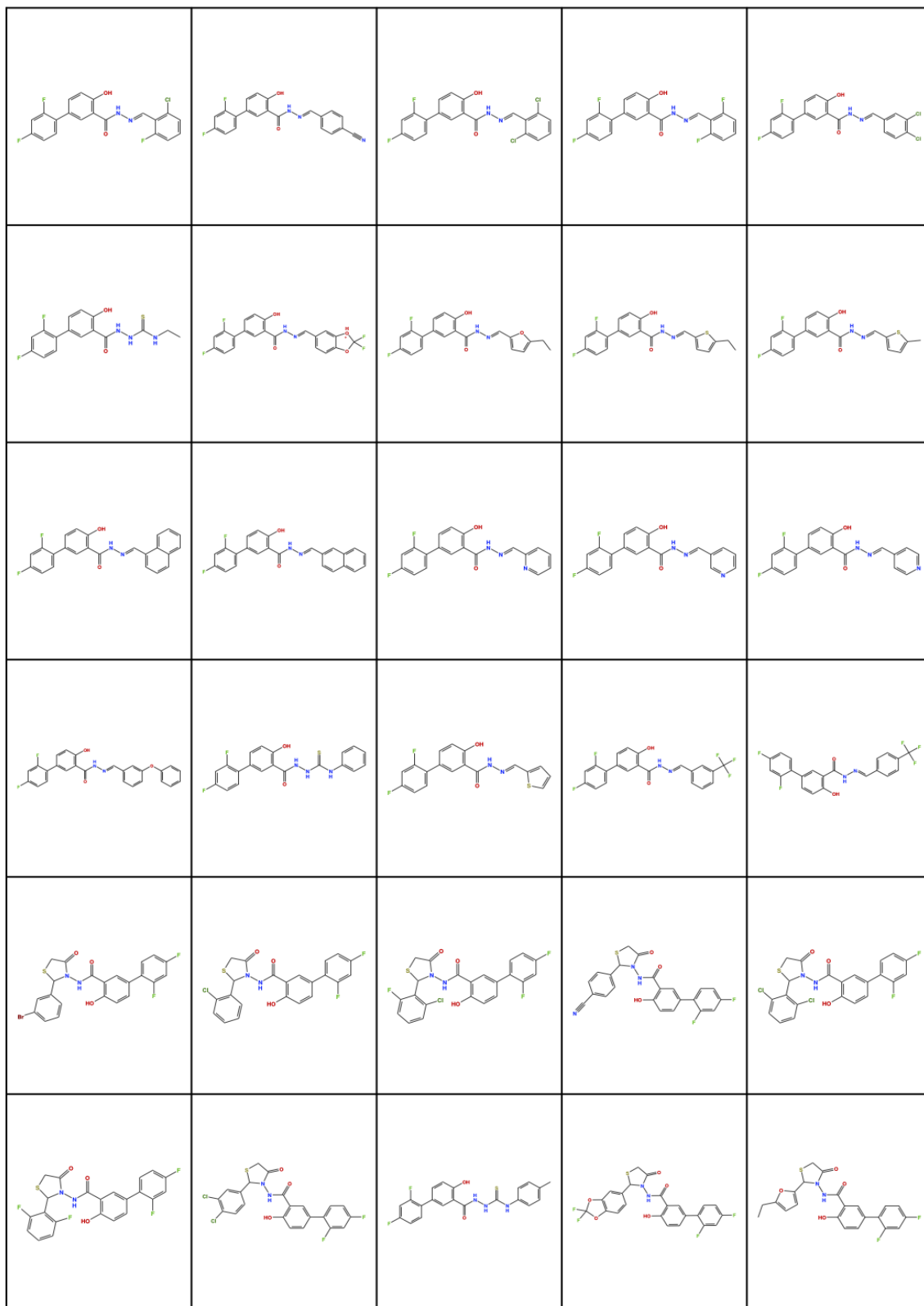


Figure S2 (continued). The 2D structures of the docked ligands.

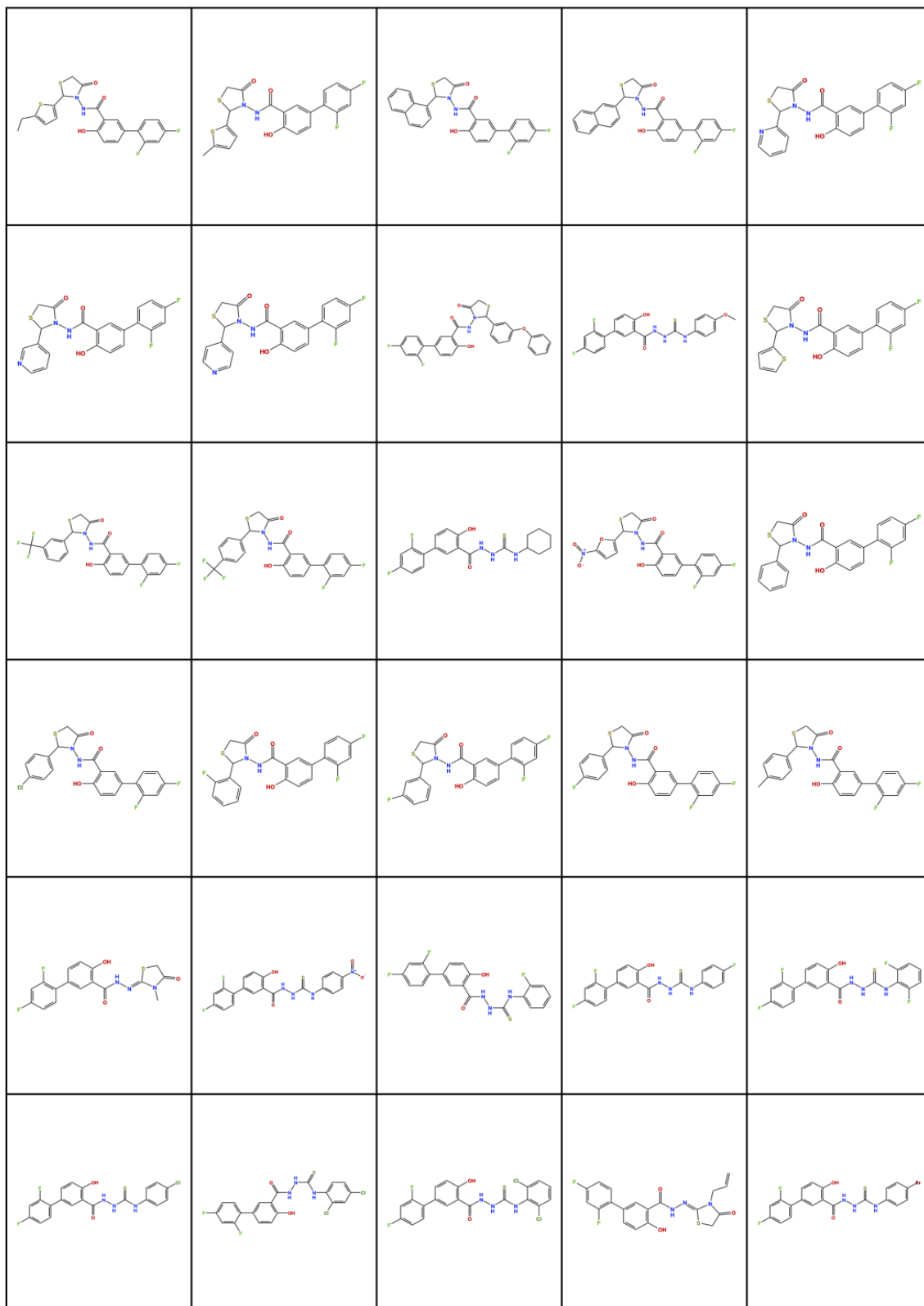


Figure S2 (continued). The 2D structures of the docked ligands.

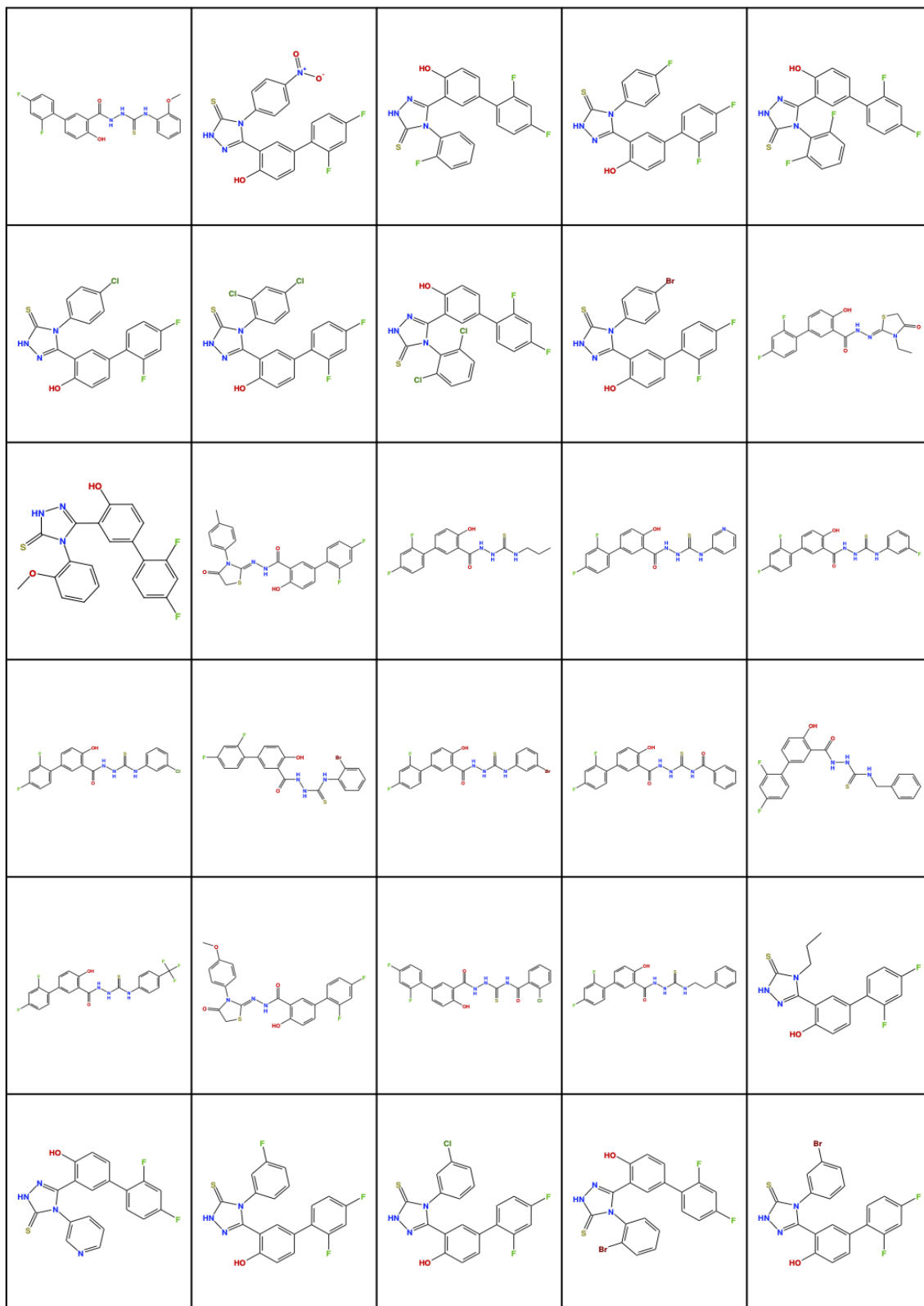


Figure S2 (continued). The 2D structures of the docked ligands.

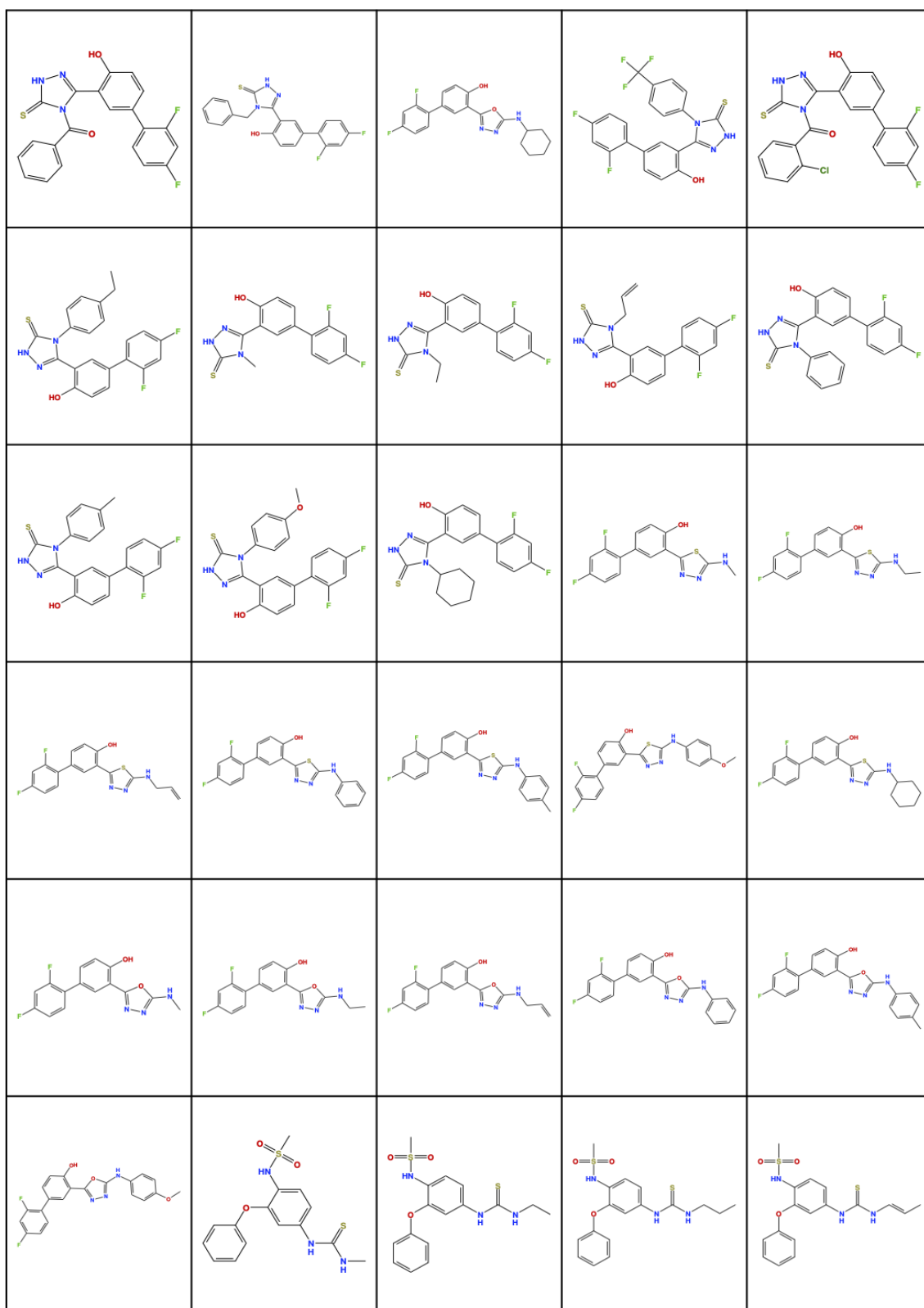


Figure S2 (continued). The 2D structures of the docked ligands.

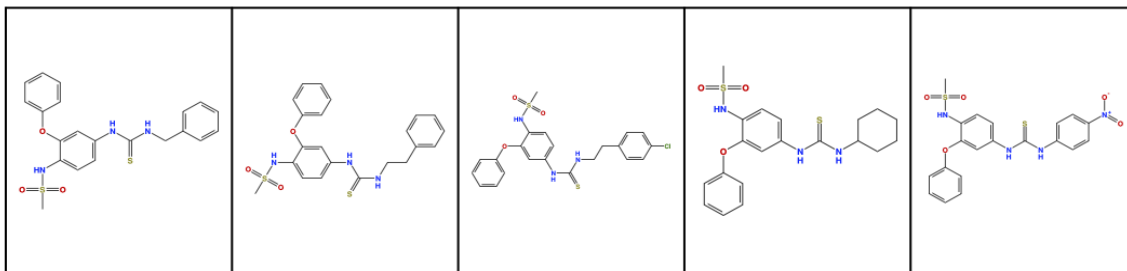


Figure S2 (continued). The 2D structures of the docked ligands.