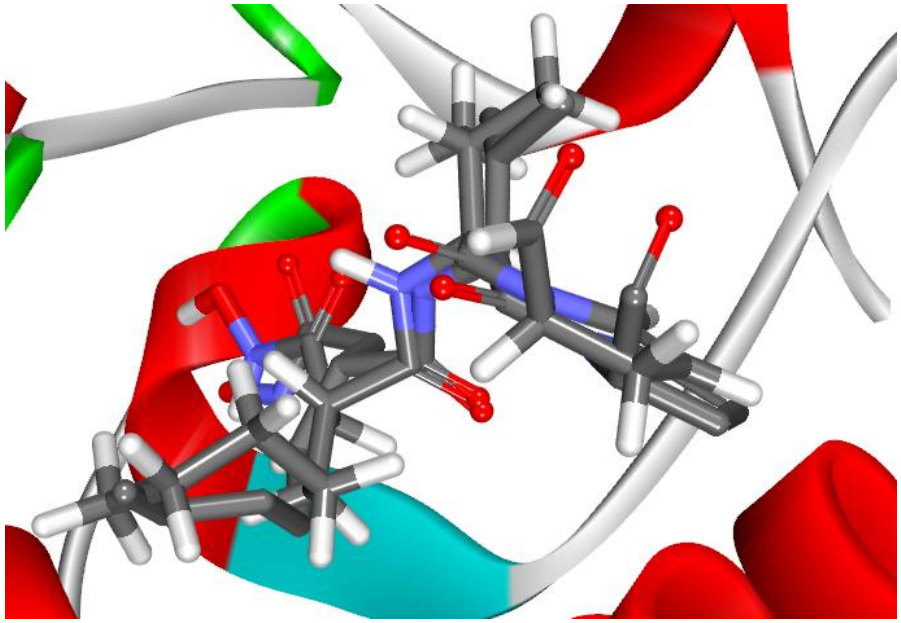
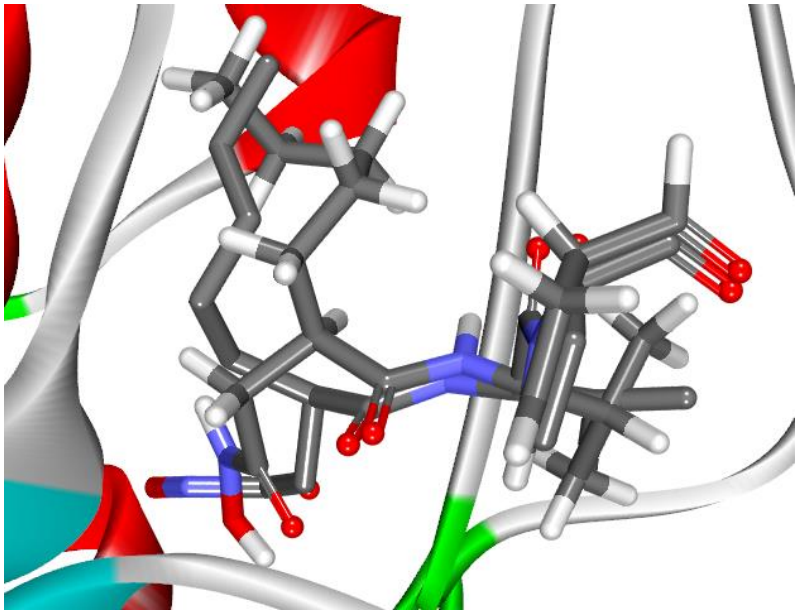
A

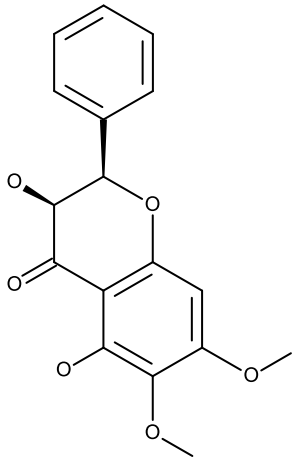
Docking of cocrystal into the proteins active site employing CDOCKER

Docking of cocrystal into the proteins active site employing GOLD

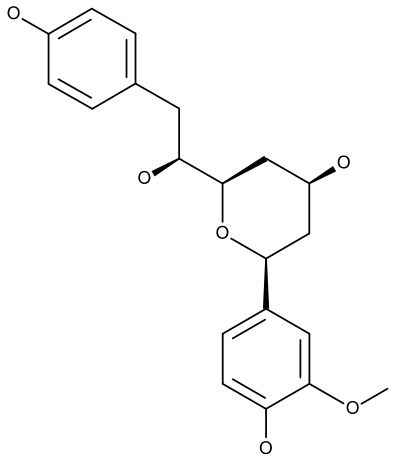




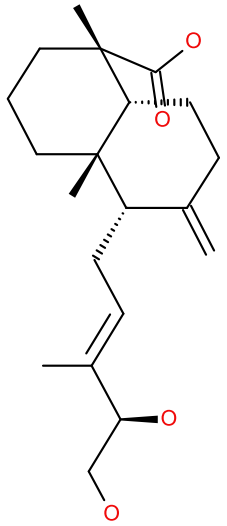
Supplementary Figure 1. Evaluation of the docking parameters



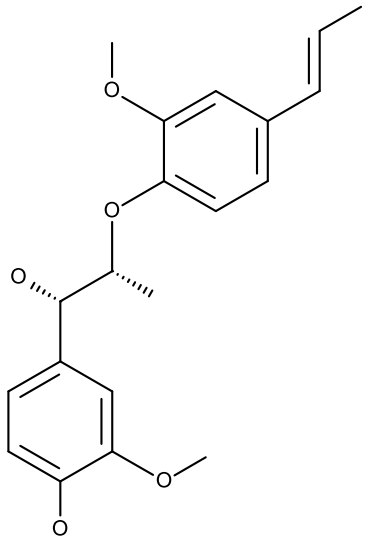
Compound 1



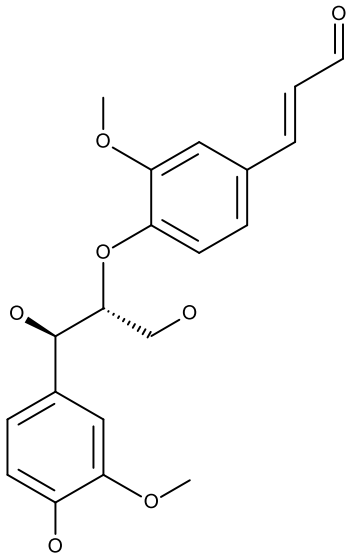
Compound 2



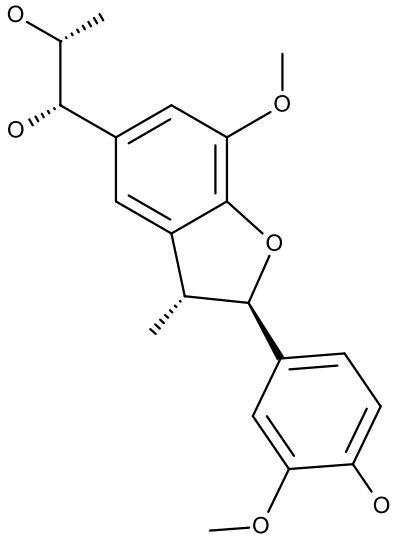
Compound 3



Compound 4

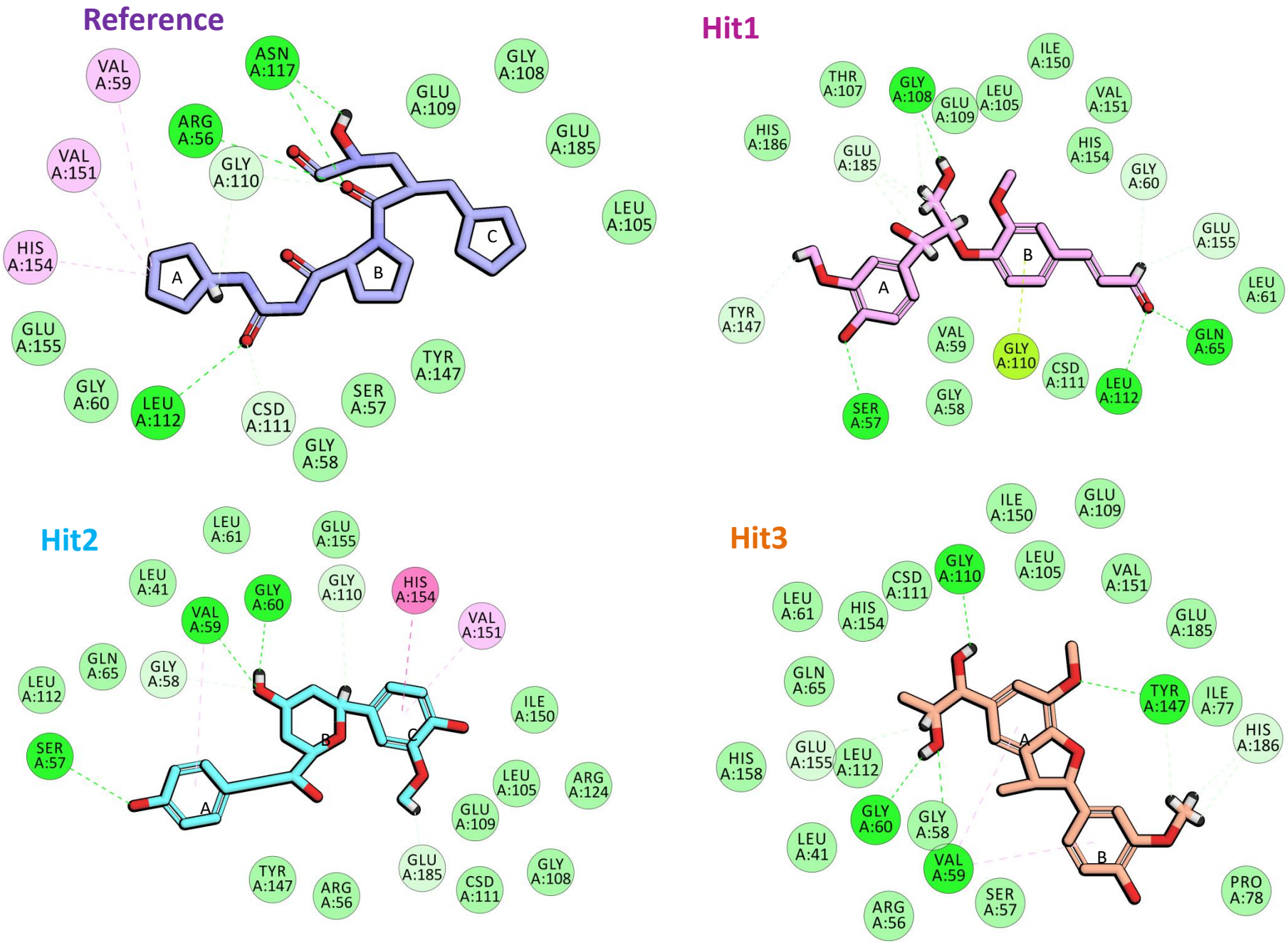


Compound 5



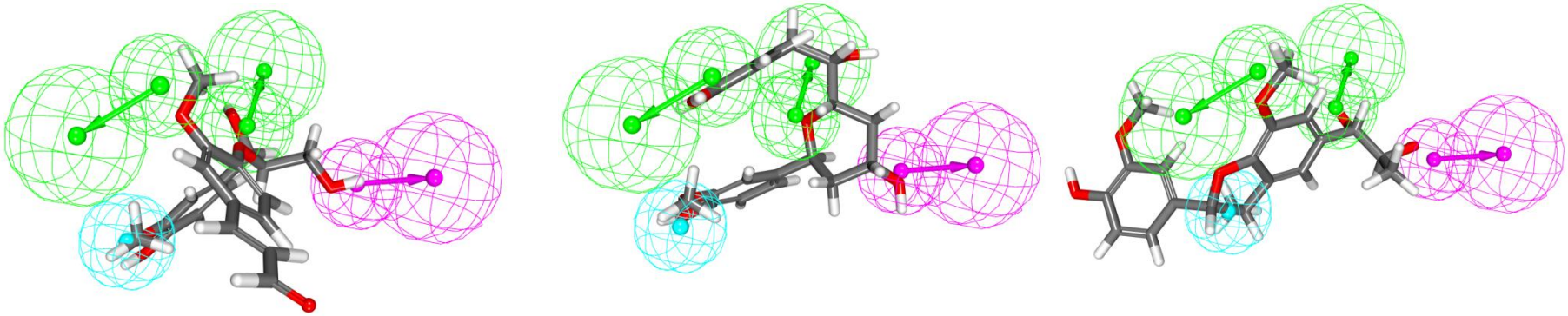
Compound 6

Supplementary Figure 2. 2D structures of six compounds

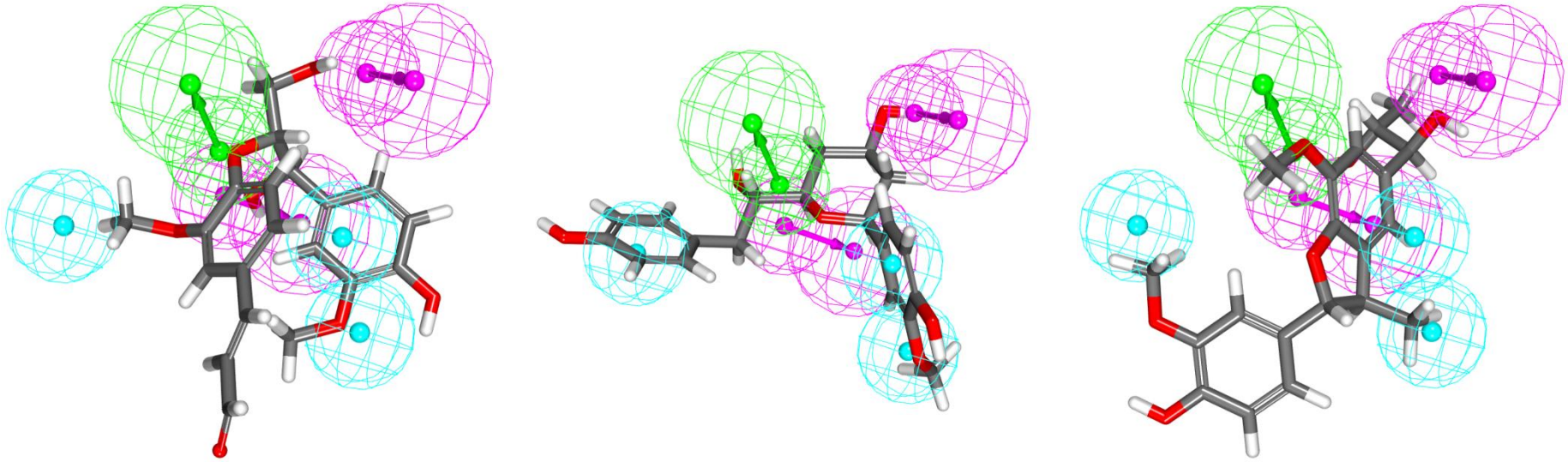


Supplementary Figure 3. Intermolecular interactions

Ligand-based pharmacophore mapping to the compounds



Structure-based pharmacophore mapping to the compounds



Supplementary Figure 4. Pharmacophore models and hits alignment