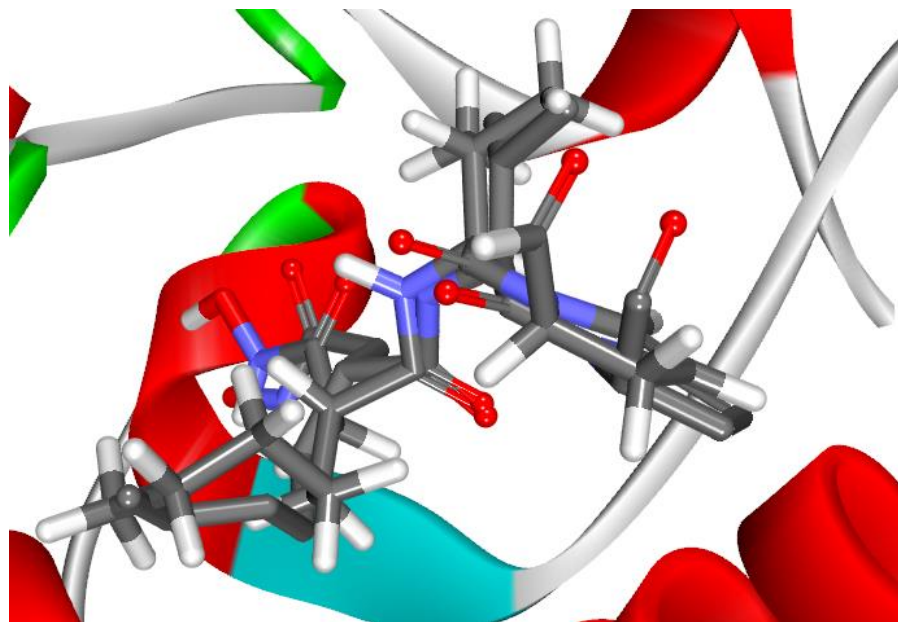
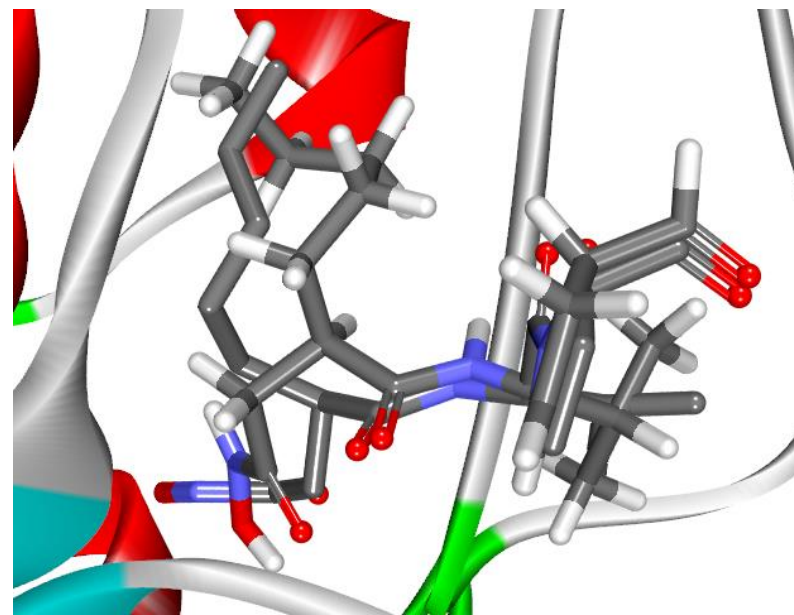


A

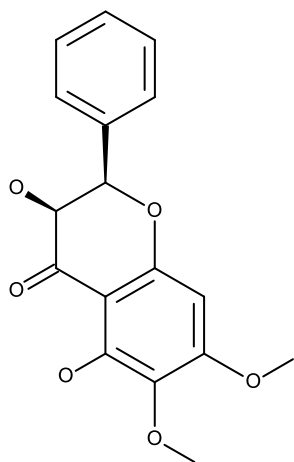
Docking of cocrystal into the proteins  
active site employing CDOCKER



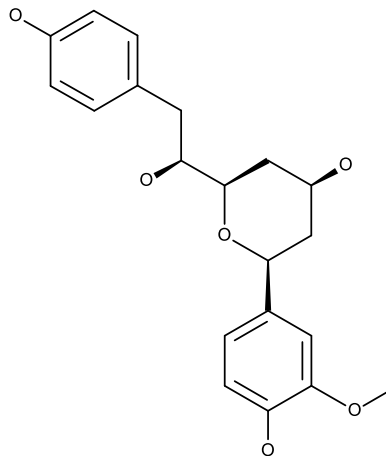
Docking of cocrystal into the proteins  
active site employing GOLD



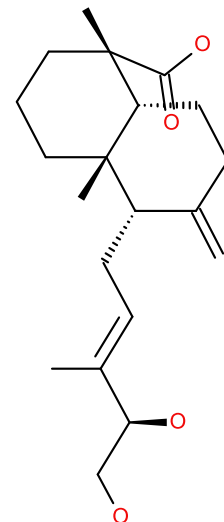
**Supplementary Figure 1.** Evaluation of the docking parameters



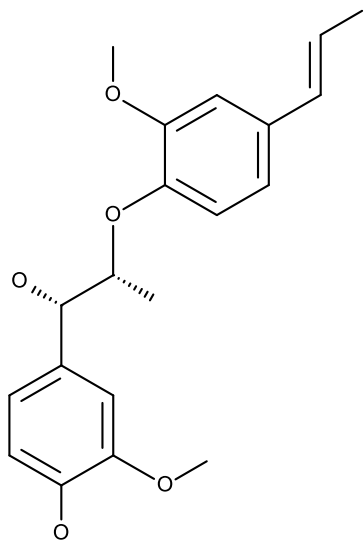
**Compound 1**



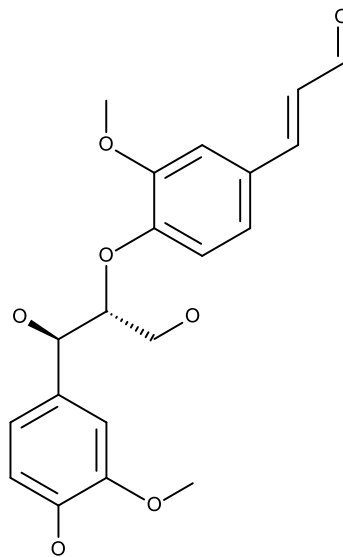
**Compound 2**



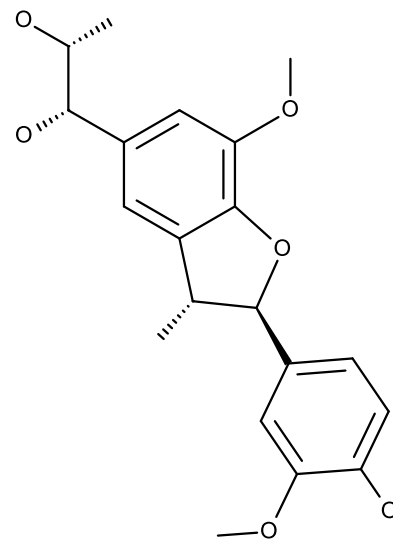
**Compound 3**



**Compound 4**



**Compound 5**



**Compound 6**

**Supplementary Figure 2. 2D structures of six compounds**

Diagram illustrating the interaction of a protein-ligand complex. The protein structure is shown in blue, with three specific residues highlighted in yellow and labeled A, B, and C. The ligand is shown in red and orange. Surrounding the protein are 15 circles, each representing a different amino acid residue, color-coded by type: green for polar/charged, yellow for non-polar, and pink for aromatic. Dashed lines indicate interactions between the protein residues and the ligand.

Residue	Type	Color
VAL A:59	Non-polar	Yellow
VAL A:151	Non-polar	Yellow
HIS A:154	Aromatic	Pink
GLU A:155	Polar/charged	Green
GLY A:60	Polar/charged	Green
LEU A:112	Non-polar	Yellow
CSD A:111	Polar/charged	Green
GLY A:58	Polar/charged	Green
SER A:57	Polar/charged	Green
TYR A:147	Aromatic	Pink
ASN A:117	Polar/charged	Green
ARG A:56	Polar/charged	Green
GLY A:110	Polar/charged	Green
GLU A:109	Polar/charged	Green
GLY A:108	Polar/charged	Green
GLU A:185	Polar/charged	Green
LEU A:105	Non-polar	Yellow

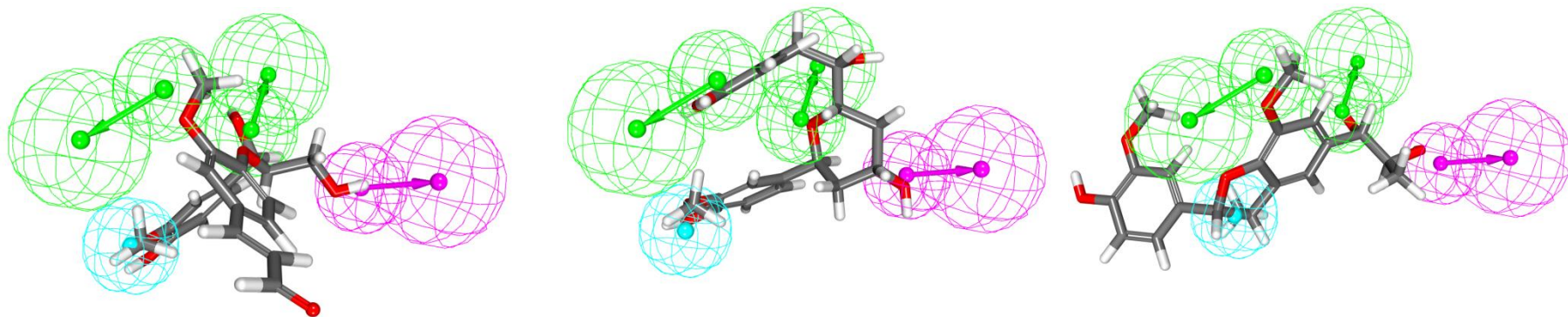
**Hit3**

Residues shown in green circles:

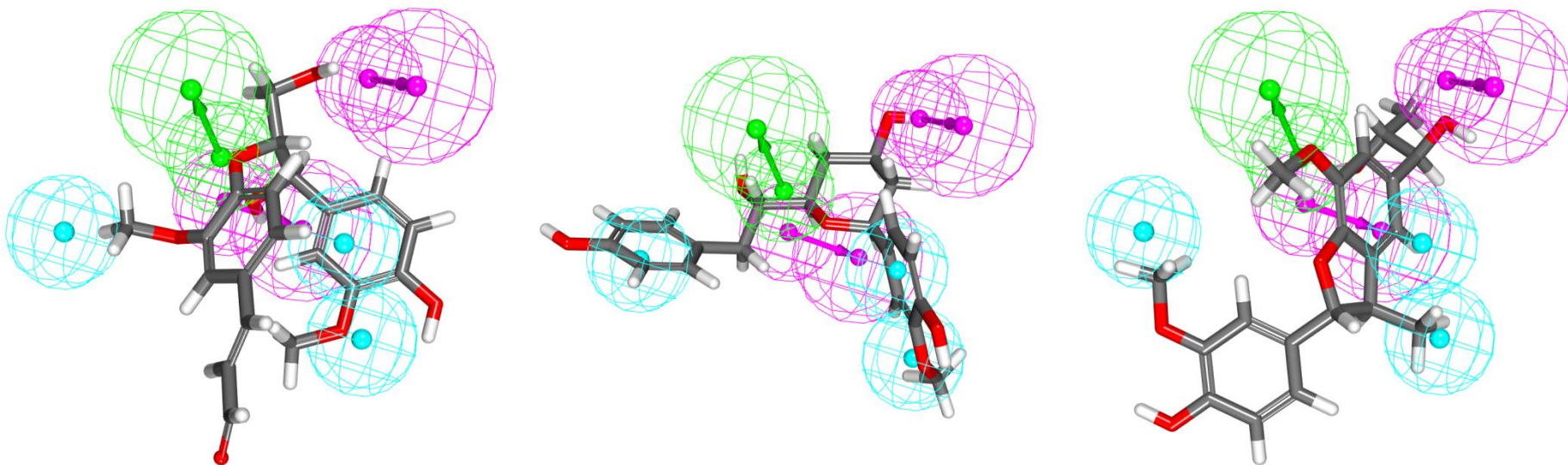
- ILE A:150
- GLU A:109
- LEU A:105
- VAL A:151
- GLU A:185
- ILE A:77
- HIS A:186
- PRO A:78
- SER A:57
- VAL A:59
- GLY A:58
- GLY A:60
- LEU A:41
- ARG A:56
- HIS A:158
- GLU A:155
- LEU A:112
- GLN A:65
- HIS A:61
- HIS A:154
- CSD A:111
- GLY A:110
- TYR A:147

### 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**