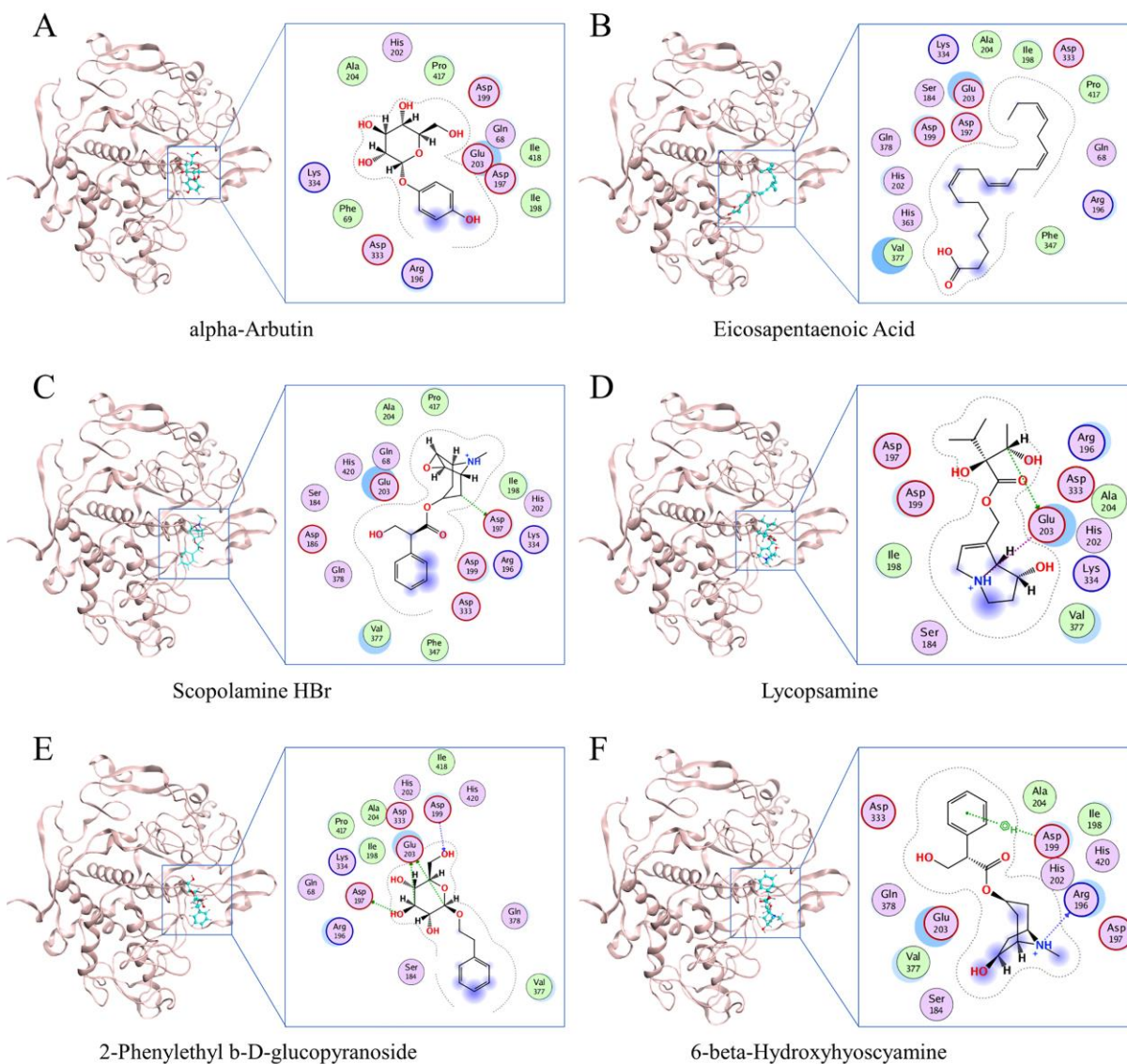


Supplementary Figure 2. Molecular docking pattern of TYR with natural product library active compounds



- | | | | |
|---------------------|----------------------|---------------------|-----------------|
| ○ polar | → sidechain acceptor | ○ solvent residue | ⊗ arene-arene |
| ● acidic | ← sidechain donor | ⊙ metal complex | ⊗H arene-H |
| ○ basic | → backbone acceptor | ⋯ solvent contact | ⊗+ arene-cation |
| ● greasy | ← backbone donor | ⋯ metal/ion contact | |
| ○ proximity contour | ● ligand exposure | ○ receptor exposure | |