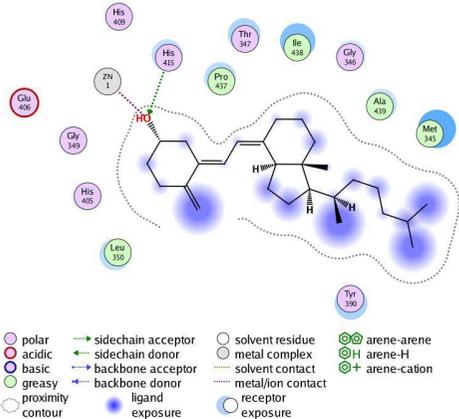
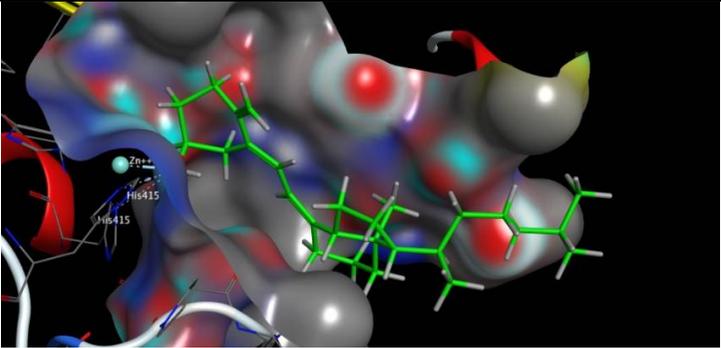
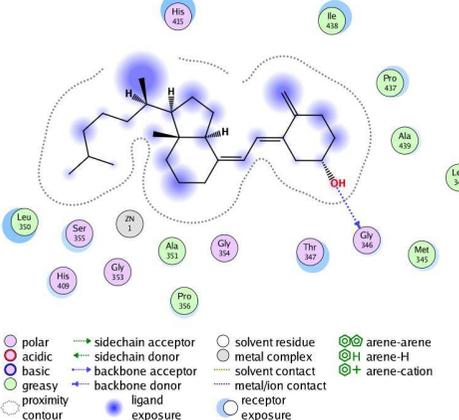
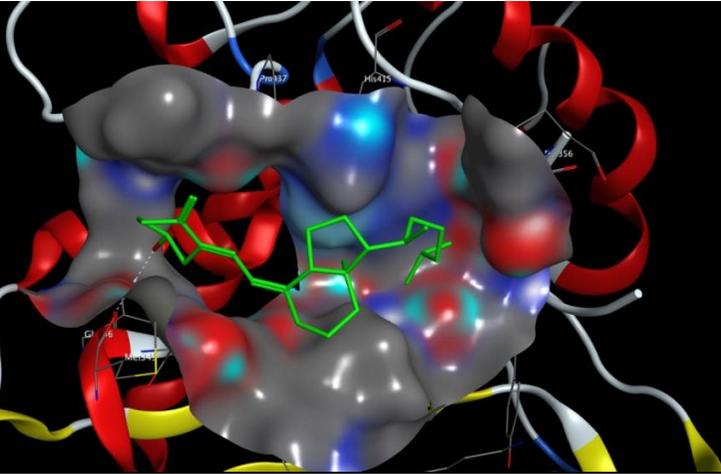
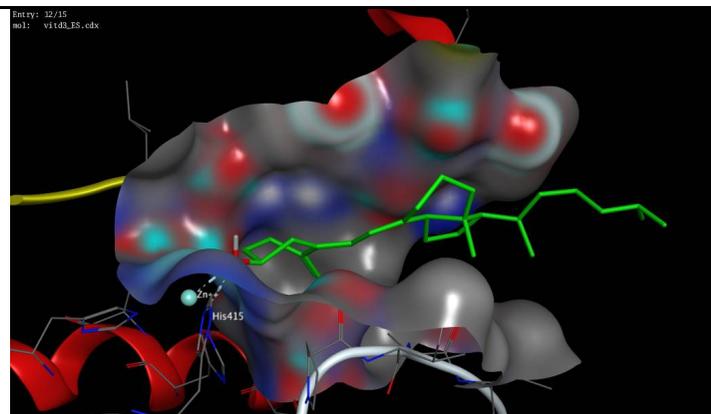
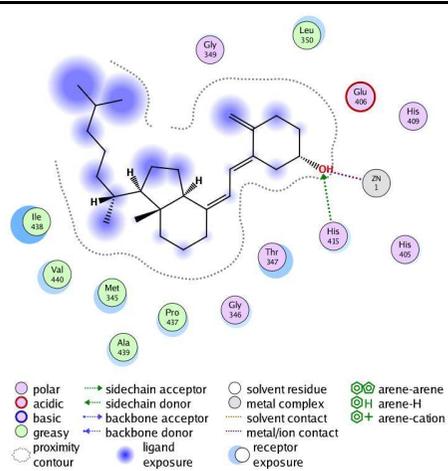


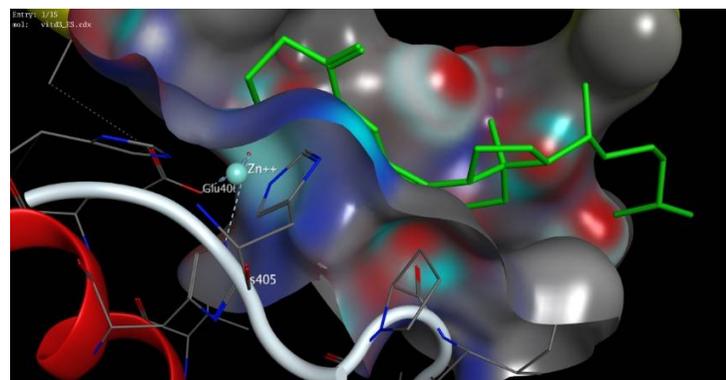
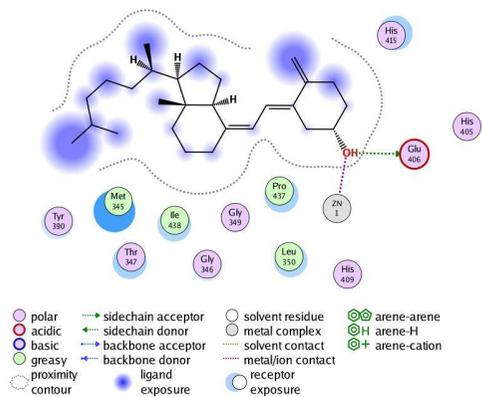
Table S1. The 2D and 3D molecular docking interactions of the docked vitamin D3 with ADAM17 binding site.

PDB	2D interactions	3D interactions
<i>2ddf</i>		
<i>310v</i>		

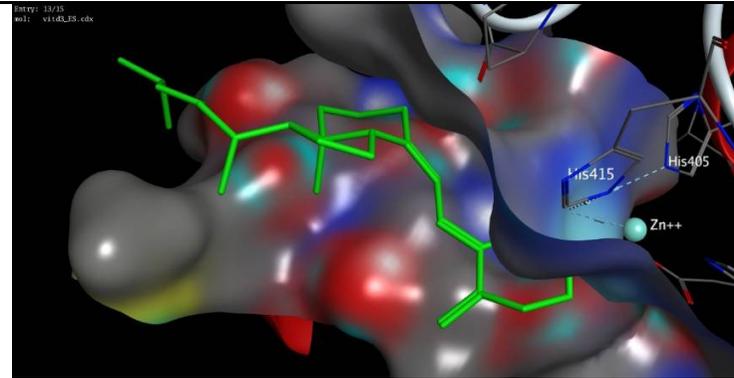
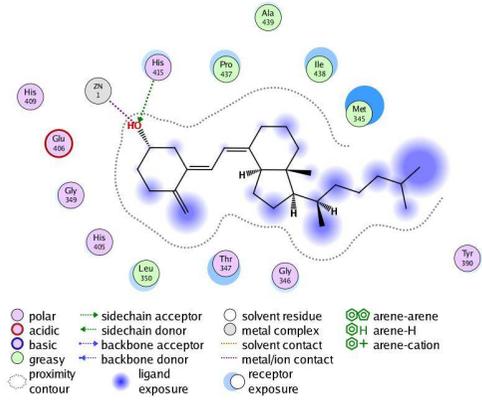
3ewl



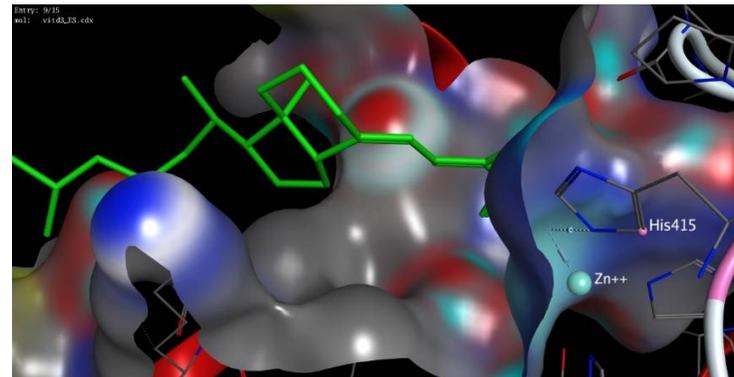
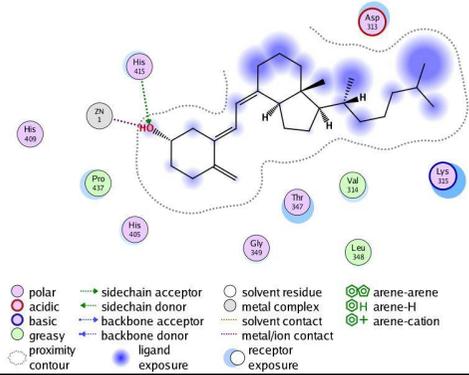
3kmc



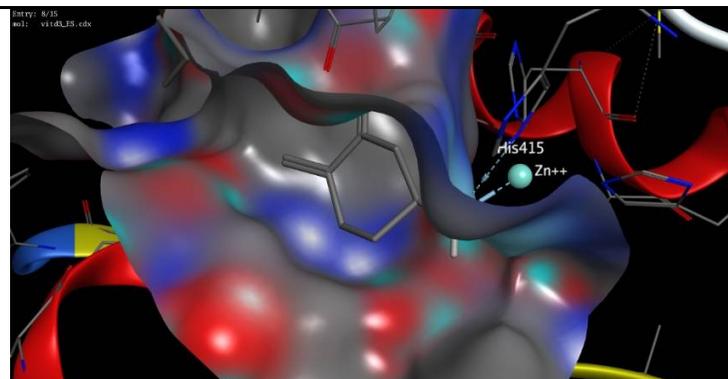
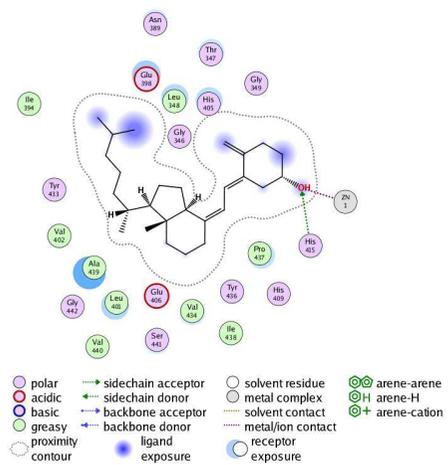
3kme



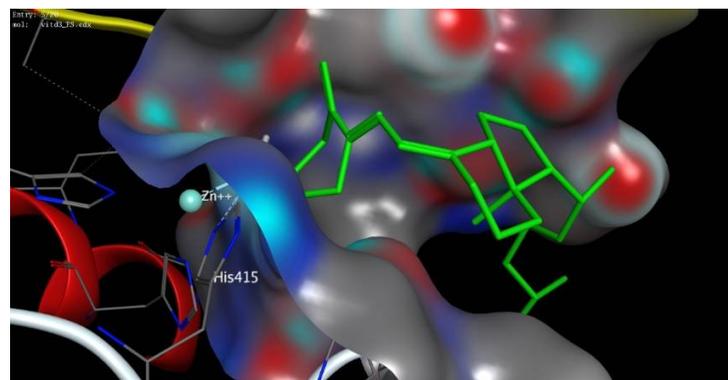
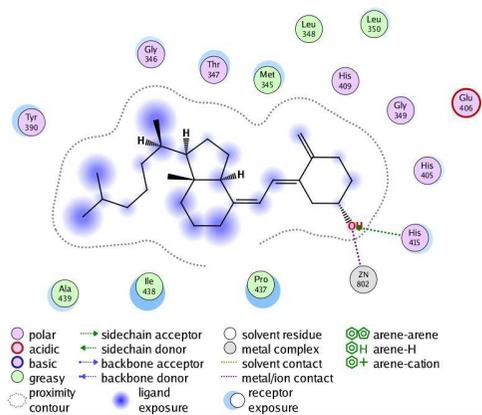
3le9



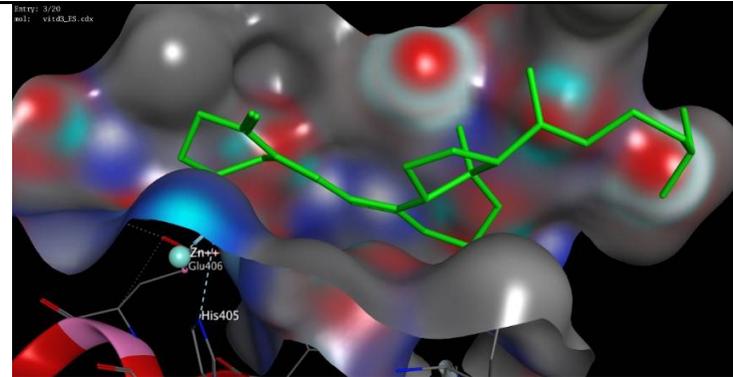
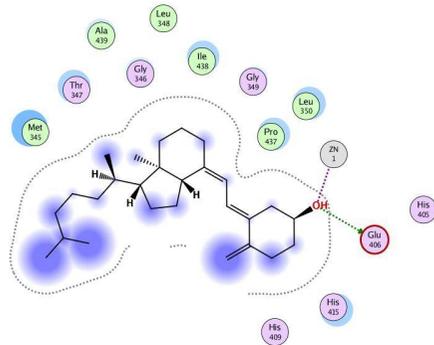
3o64



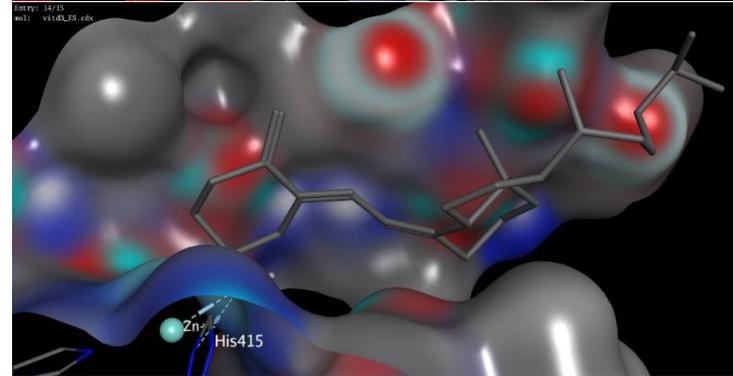
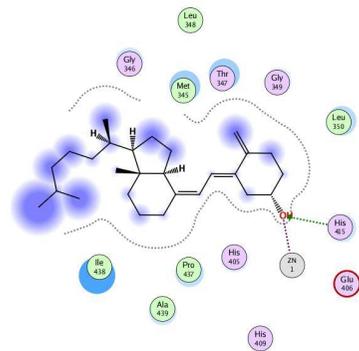
2i47



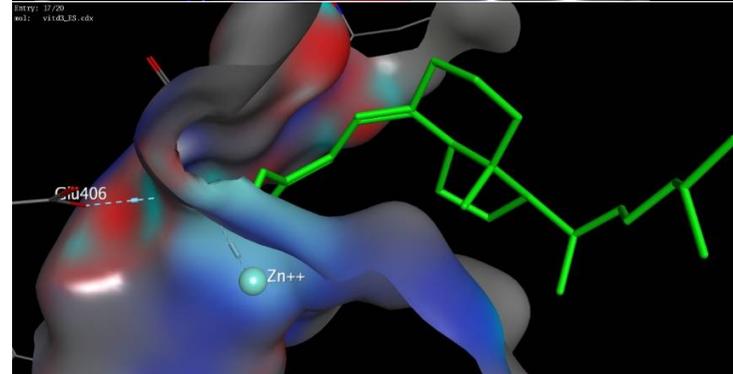
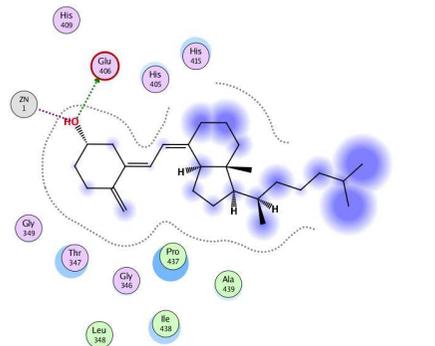
3e8r



3edz

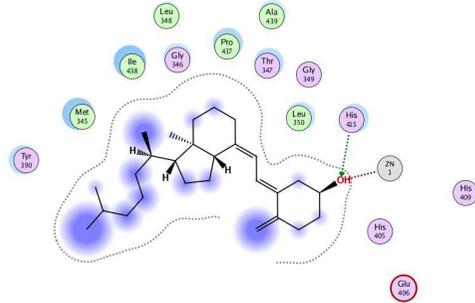


3lgp

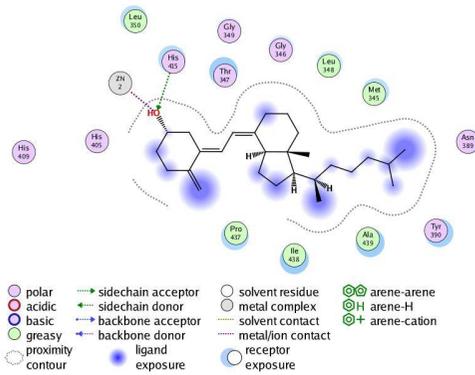


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|---------------------|----------------------|---------------------|-----------------|
| ○ polar | → sidechain acceptor | ○ solvent residue | ⊗⊗ arene-arene |
| ○ acidic | ← sidechain donor | ○ metal complex | ⊗ H arene-H |
| ○ basic | → backbone acceptor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

1bkc

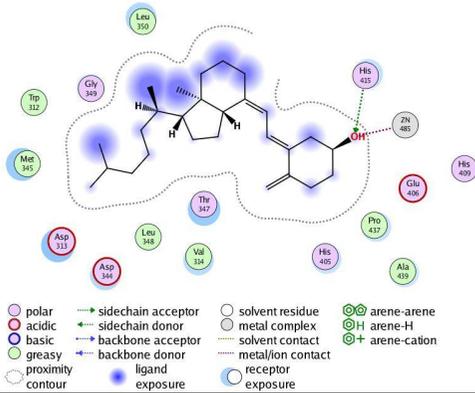


2oi0

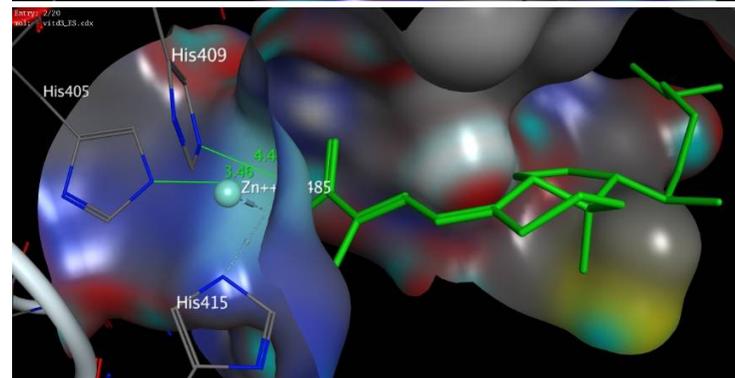
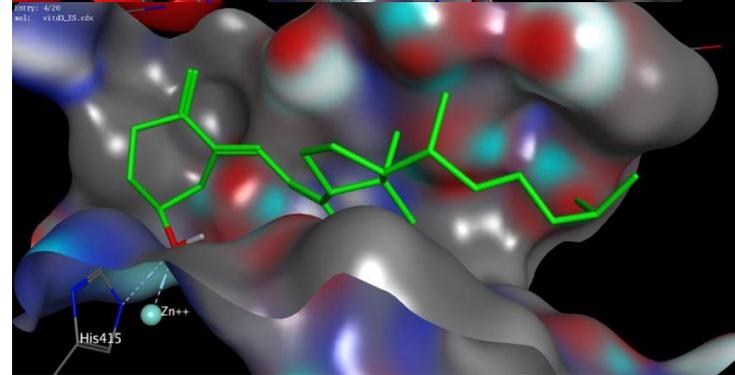
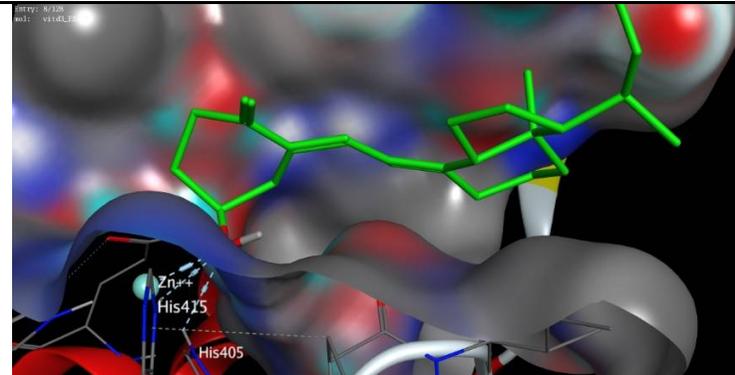


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|-------------|----------------------|---------------------|------------------|
| ● polar | → sidechain acceptor | ○ solvent residue | ⊗ arene-arene |
| ● acidic | ← sidechain donor | ○ metal complex | ⊗ H arene-H |
| ● basic | → backbone acceptor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

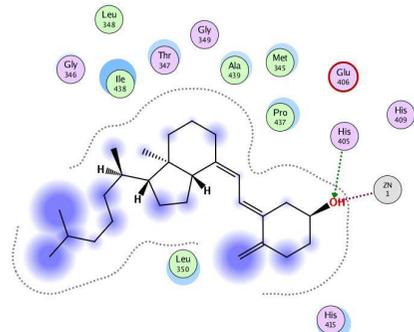
3lea



- | | | | |
|-------------|----------------------|---------------------|------------------|
| ● 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 | → ligand exposure | ○ receptor | |
| ○ contour | | ○ exposure | |

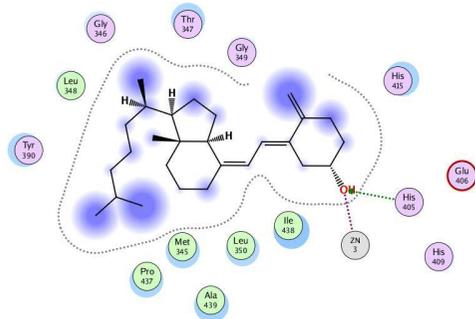


2fv9

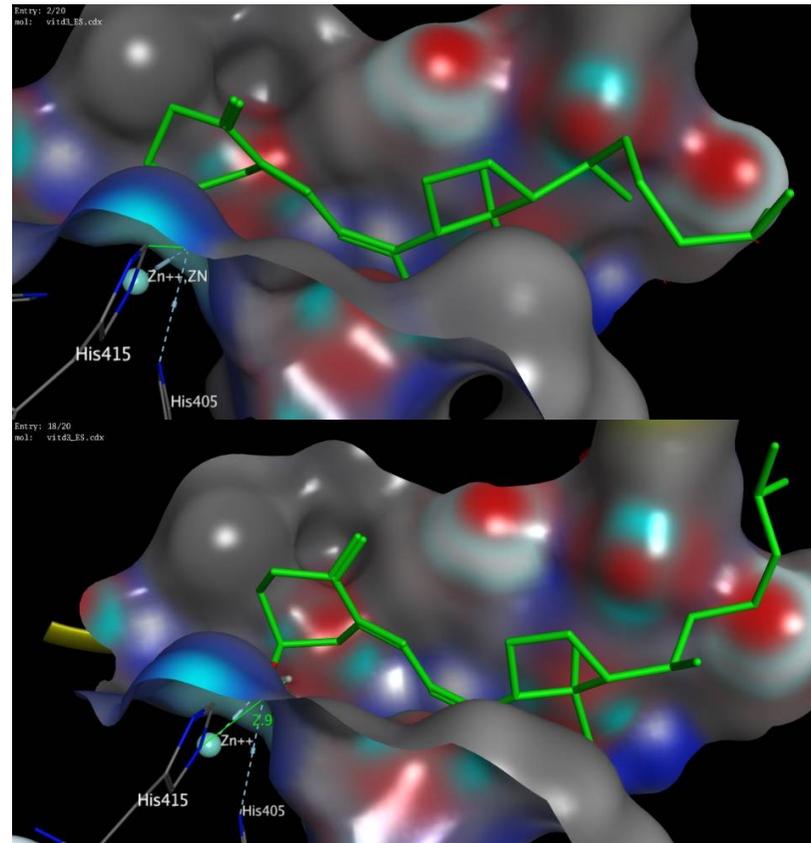


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|-------------|----------------------|---------------------|------------------|
| ○ polar | → sidechain acceptor | ○ solvent residue | ⊗⊗ arene-arene |
| ○ acidic | ← sidechain donor | ⊗ metal complex | ⊗⊗ arene-H |
| ○ basic | → backbone acceptor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

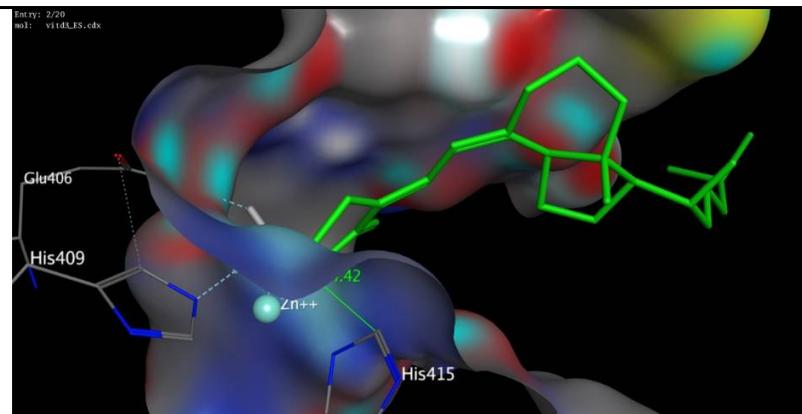
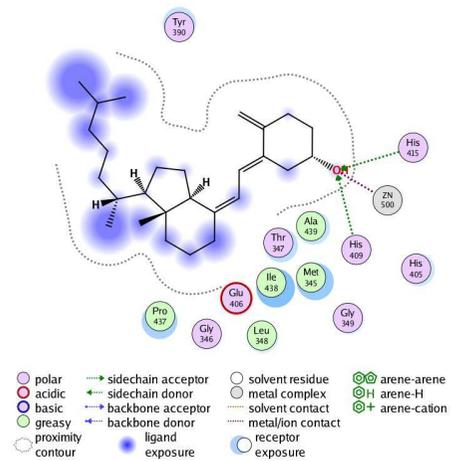
2fv5



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



3g42



2a8h

