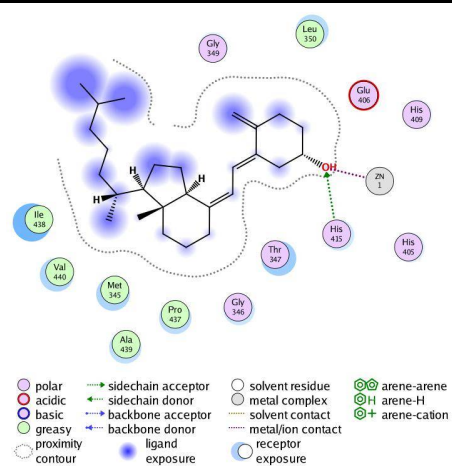


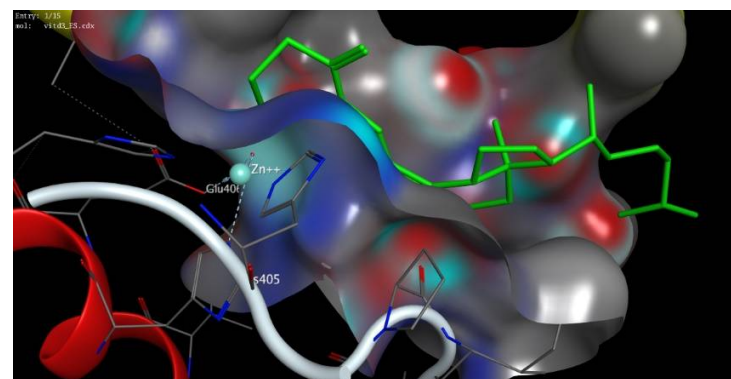
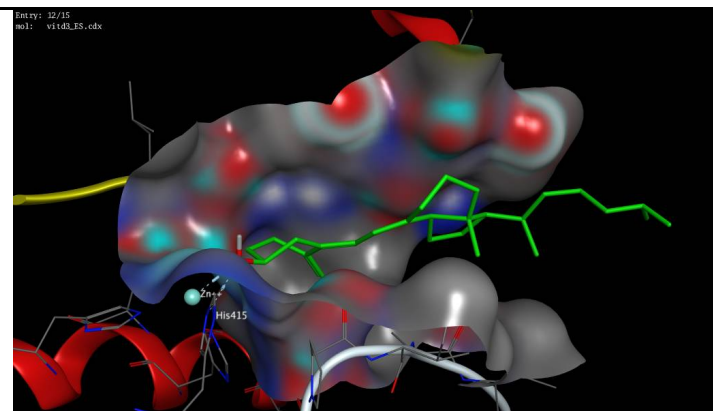
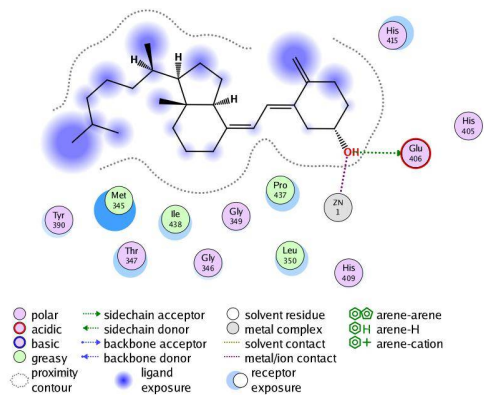
Table S1. The 2D and 3D molecular docking interactions of the docked vitamin D3 with ADAM17 binding site.

PDB	2D interactions	3D interactions
2ddf	<p> polar acidic basic greasy proximity contour </p> <p> sidechain acceptor sidechain donor backbone acceptor backbone donor ligand exposure </p> <p> solvent residue metal complex solvent contact metal/ion contact receptor exposure </p> <p> arene-arene arene-H arene-cation </p>	
3l0v	<p> polar acidic basic greasy proximity contour </p> <p> sidechain acceptor sidechain donor backbone acceptor backbone donor ligand exposure </p> <p> solvent residue metal complex solvent contact metal/ion contact receptor exposure </p> <p> arene-arene arene-H arene-cation </p>	

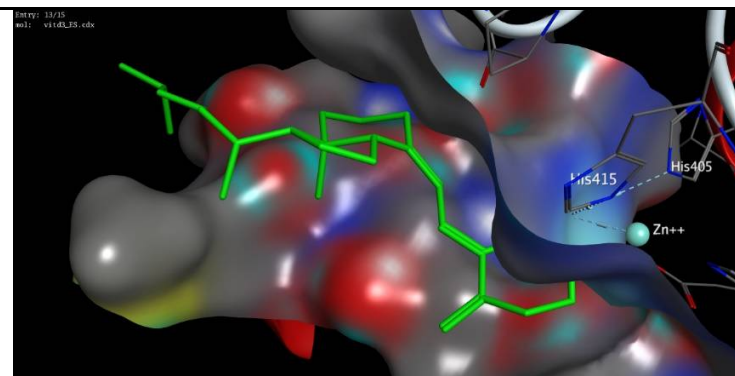
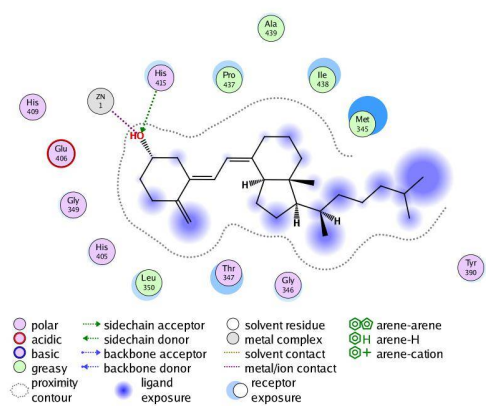
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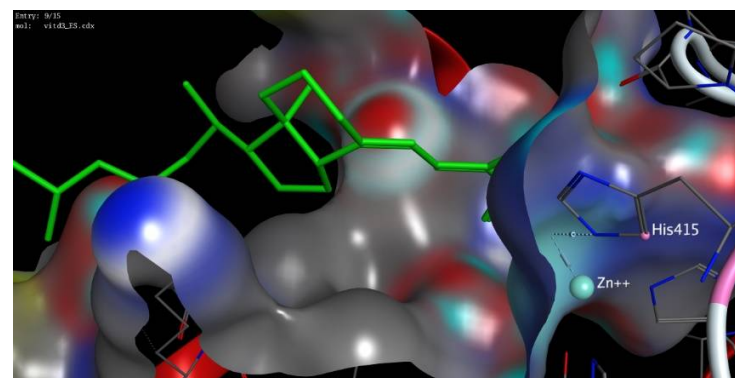
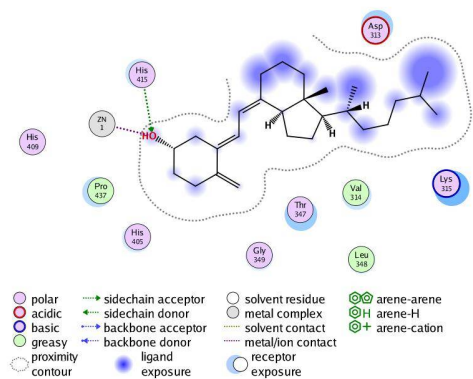
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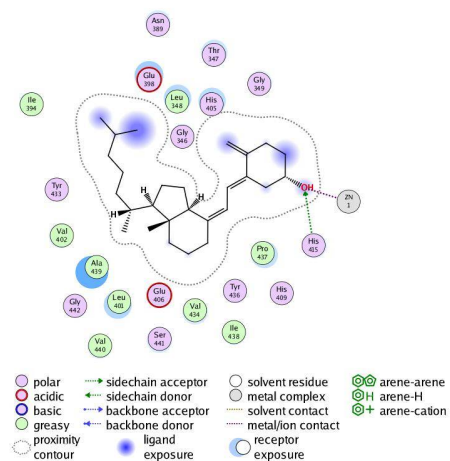
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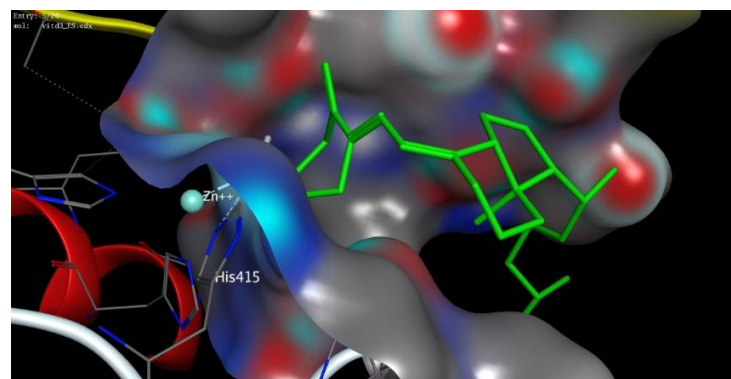
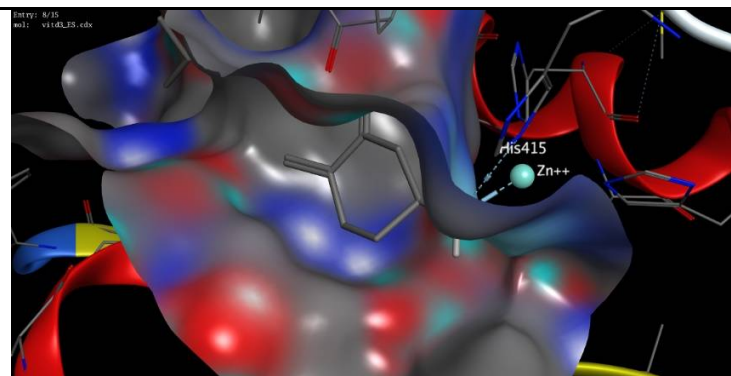
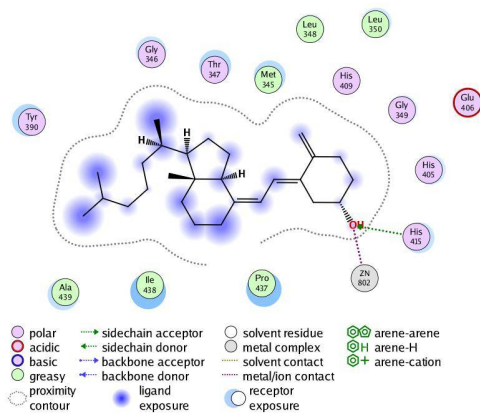
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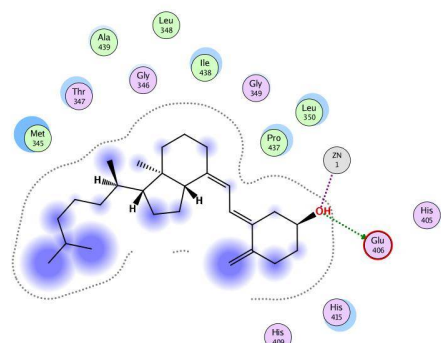
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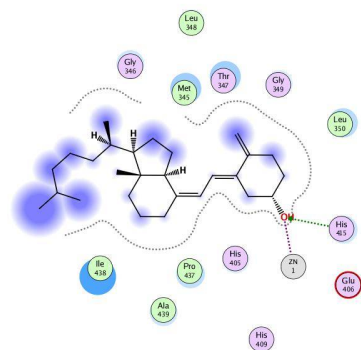
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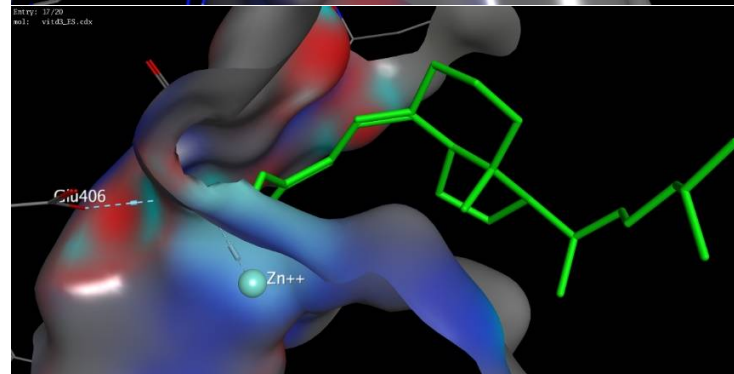
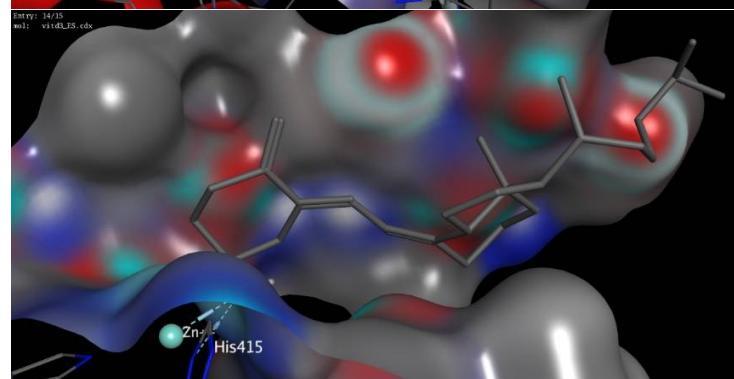
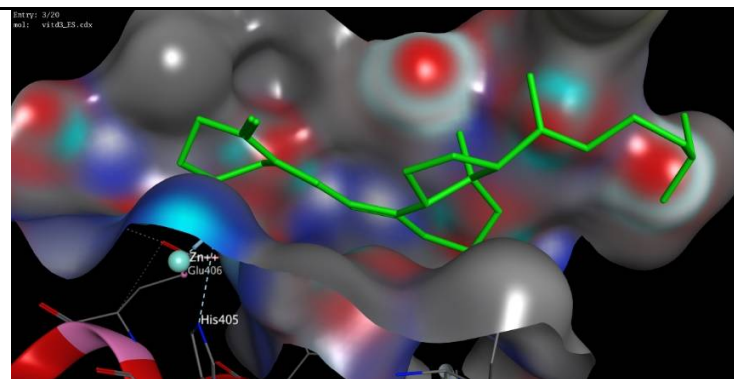
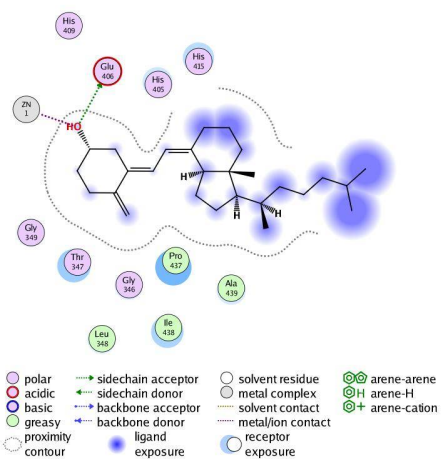
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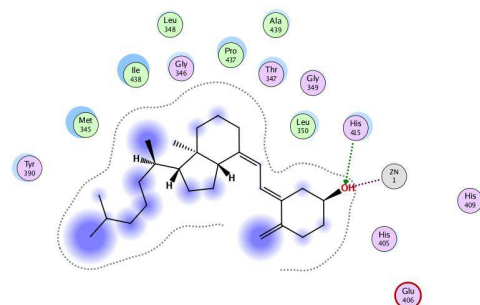
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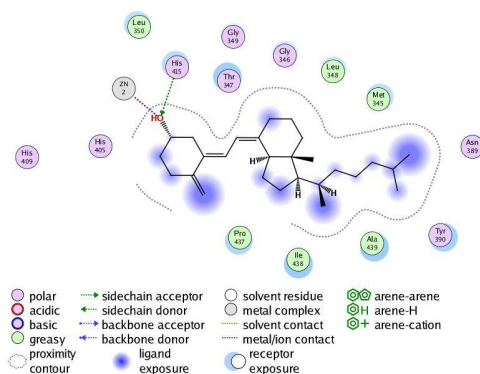
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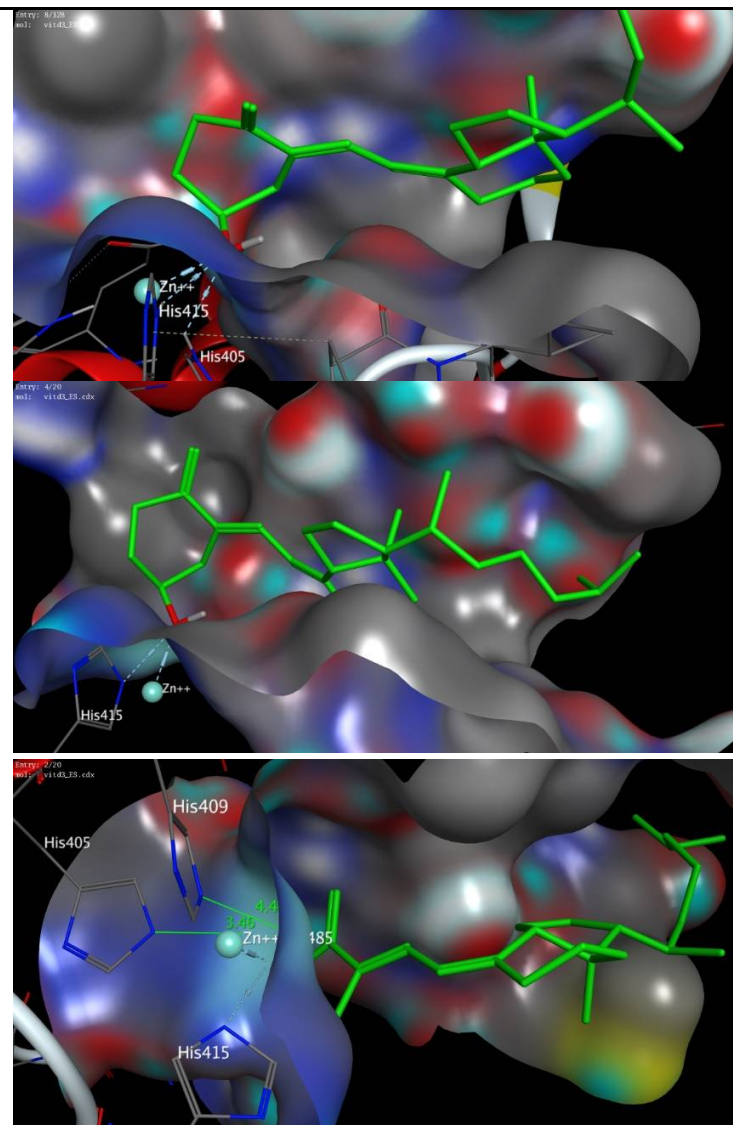
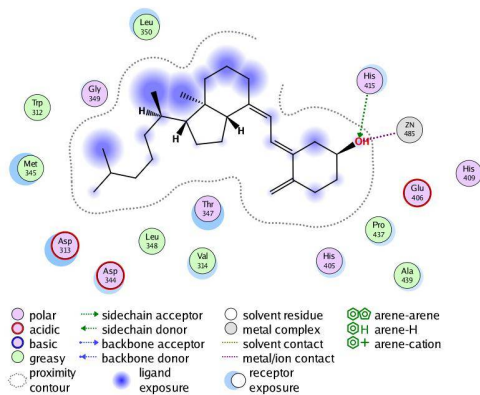
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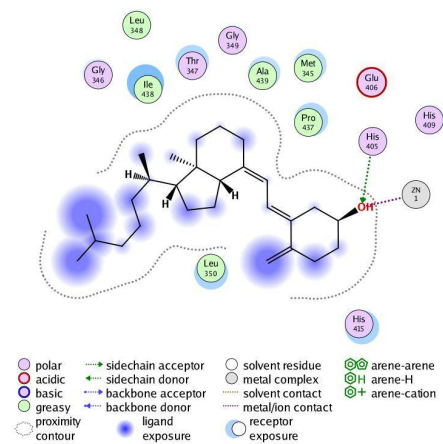
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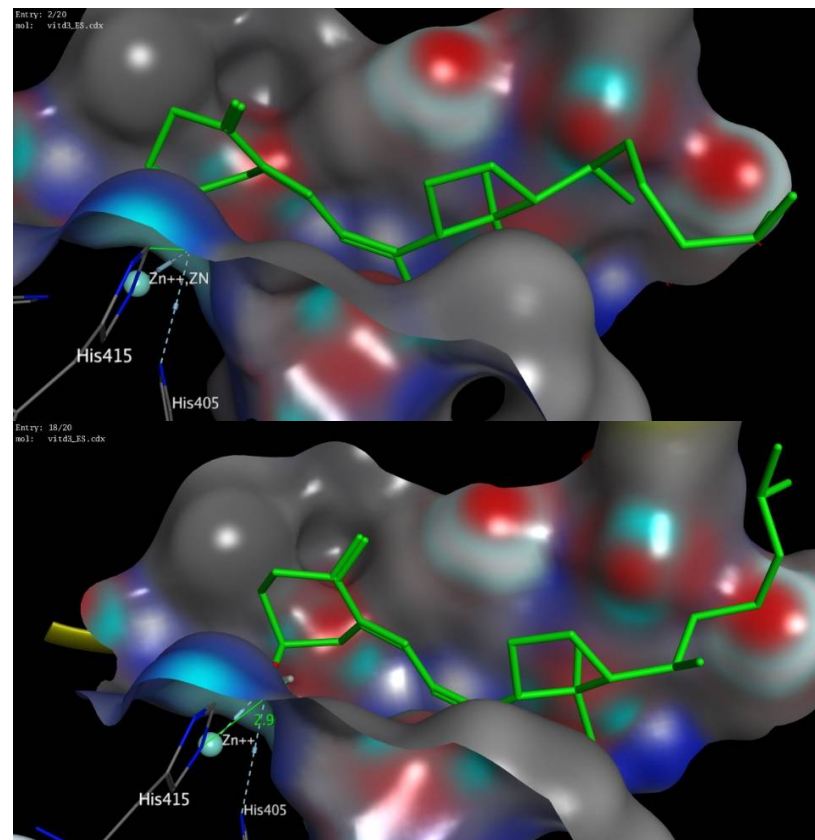
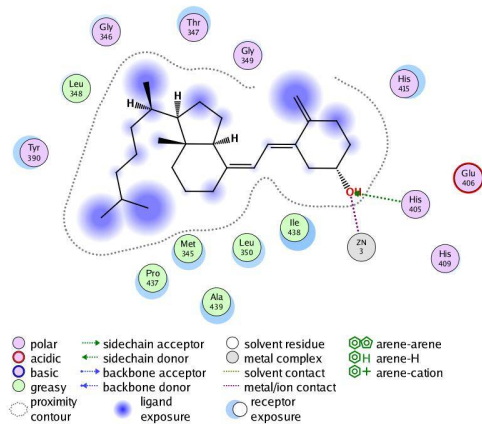
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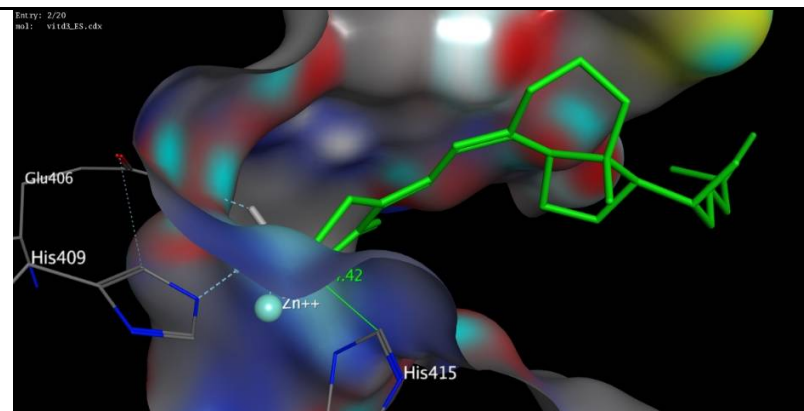
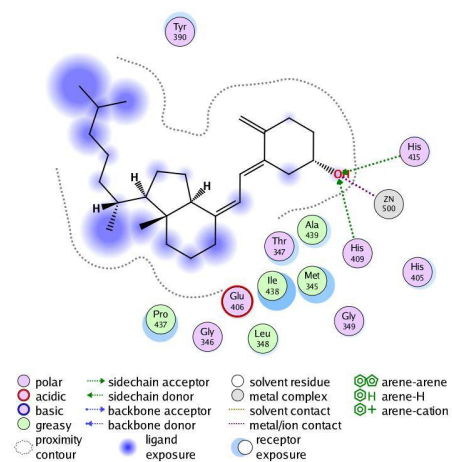
2fv9



2fv5



3g42



2a8h

