# Molecular Docking

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## I. Preparing the protein

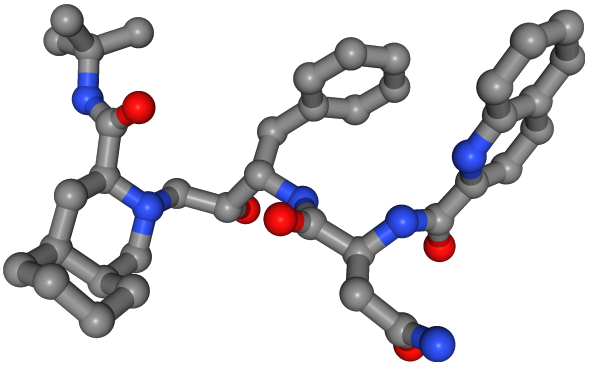

Figure 1: Saquinavir

## II. Selecting a ligand with the best fit

I used a `python` script to parse the `qvina` output files and extract the most negative binding affinity score for each ligand out of 2116 tested. This involved identifying lines containing the "REMARK VINA RESULT" and capturing the first numerical value (the binding affinity score).

I parsed the `qvina` output and found scores for all models tested for each ligand. I then selected a ligand with the minimal score The ligand with the lowest binding affinity score can be seen in Figure 2. It's structure is somewhat simmilar to Saquinavir which is not suprising.

| Ligand | Model | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | min |
| fda_553 | -11.4 | -10.4 | -10.4 | -9.7 | -9.6 | -9.5 | -9.3 | -9.3 | -8.9 | -11.4 |
| fda_554 | -11.4 | -10.8 | -10.4 | -10.1 | -10.0 | -9.9 | -9.9 | -9.5 | -9.0 | -11.4 |
| fda_1700 | -11.1 | -10.2 | -10.1 | -9.9 | -9.9 | -9.8 | -9.7 | -9.6 | -9.6 | -11.1 |
| fda_1755 | -11.0 | -10.8 | -10.7 | -10.4 | -10.1 | -10.0 | -10.0 | -10.0 | -9.9 | -11.0 |
| fda_871 | -11.0 | -11.0 | -10.8 | -10.7 | -10.6 | -10.1 | -9.9 | -9.8 | -9.8 | -11.0 |
| fda_872 | -11.0 | -11.0 | -10.8 | -10.6 | -10.5 | -10.5 | -10.1 | -9.6 | -9.5 | -11.0 |
| fda_1829 | -10.9 | -10.9 | -10.6 | -10.6 | -10.2 | -10.2 | -10.1 | -10.1 | -10.0 | -10.9 |
| fda_95 | -10.8 | -10.4 | -10.4 | -9.8 | -9.7 | -9.6 | -9.3 | -9.3 | -8.7 | -10.8 |
| fda_161 | -10.8 | -9.7 | -9.5 | -9.5 | -9.5 | -9.2 | -9.2 | -9.1 | -8.9 | -10.8 |
| fda_160 | -10.7 | -9.9 | -9.7 | -9.6 | -9.6 | -9.5 | -9.4 | -9.2 | -8.8 | -10.7 |

Table 1: Top 10 ligands with the lowest minimal (out of all models tested) binding affinity score

The ligand's binding affinity score was −11.4 kcal/mol which is less than Saquinavir's −10.7 kcal/mol.

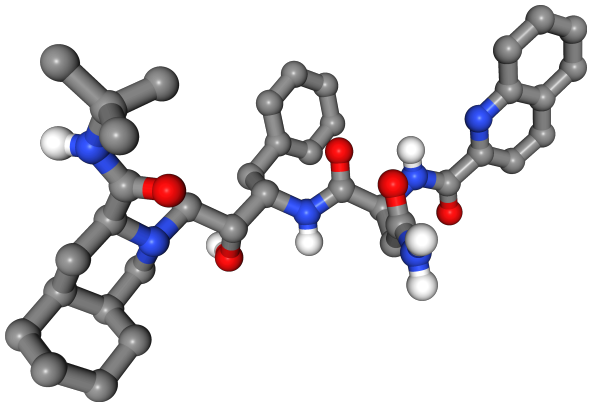

Figure 2: Ligand with name `fda_533` which reached the lowest binding affinity score of −11.4 kcal/mol out of 2116 ligands tested

Text text