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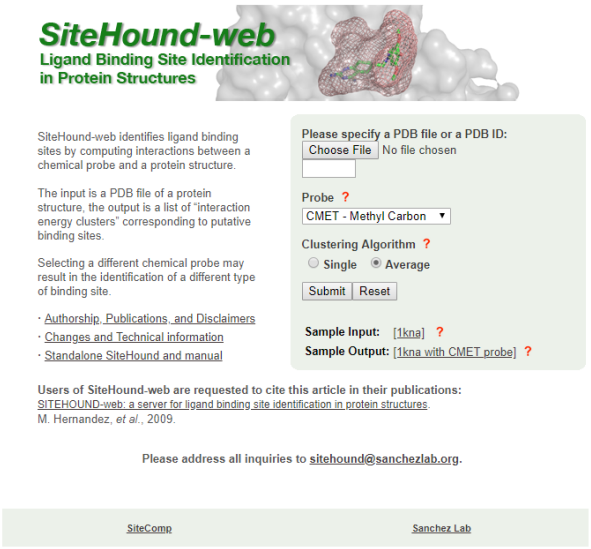
APPENDICES

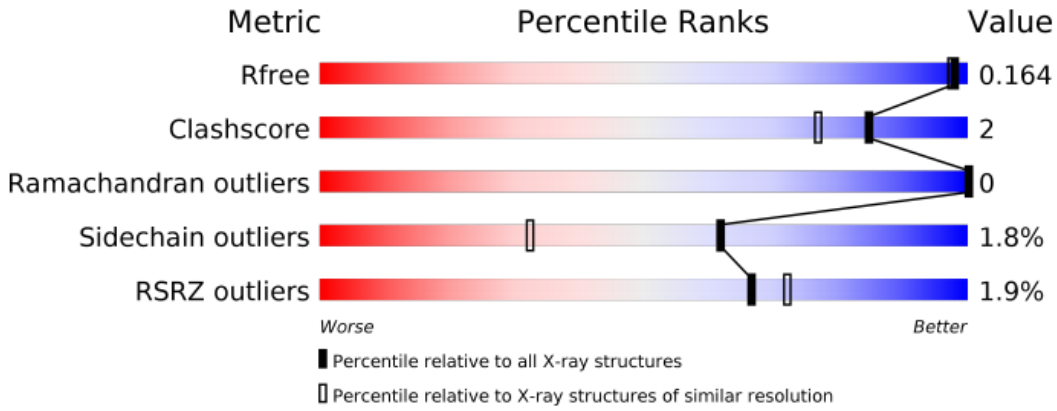
AutoDock Vina Usage Command Line

Correct Usage of AutoDock Vina:

```
Input:
  --receptor arg       rigid part of the receptor (PDBQT)
  --flex arg           flexible side chains, if any (PDBQT)
  --ligand arg         ligand (PDBQT)

Search space (required):
  --center_x arg       X coordinate of the center
  --center_y arg       Y coordinate of the center
  --center_z arg       Z coordinate of the center
  --size_x arg         size in the X dimension (Angstroms)
  --size_y arg         size in the Y dimension (Angstroms)
  --size_z arg         size in the Z dimension (Angstroms)

Output (optional):
  --out arg            output models (PDBQT), the default is chosen based on
                       the ligand file name
  --log arg            optionally, write log file

Misc (optional):
  --cpu arg            the number of CPUs to use (the default is to try to
                       detect the number of CPUs or, failing that, use 1)
  --seed arg           explicit random seed
  --exhaustiveness arg (=8) exhaustiveness of the global search (roughly
                       proportional to time): 1+
  --num_modes arg (=9)     maximum number of binding modes to generate
  --energy_range arg (=3)  maximum energy difference between the best binding
                       mode and the worst one displayed (kcal/mol)

Configuration file (optional):
  --config arg         the above options can be put here

Information (optional):
  --help               display usage summary
  --help_advanced      display usage summary with advanced options
  --version            display program version
```



A. 1 SiteHound-Web Interface



A. 2 Graphic Percentile Score of NAMPT Structure

config1lj - Notepad

File Edit Format View Help

```
receptor = namptfix.pdbqt
ligand = 1LJ.pdbqt

center_x = 12.951
center_y = 11.773
center_z = 9.485

size_x = 110
size_y = 114
size_z = 122
```

A. 3 AutoDock Vina Docking Configuration Files

CURCUMIN			
Mode	Affinity (kcal/mol)	Dist from best mode	
		RMSD Lower Bound	RMSD Upper Bound
1	-7.9	0.000	0.000
2	-7.8	1.269	2.465
3	-7.7	27.503	31.749
4	-7.7	26.155	30.504
5	-7.5	1.965	5.393
6	-7.4	28.075	32.316
7	-7.3	2.033	6.169
8	-7.1	1.947	5.738
9	-7.0	2.442	6.136

1QR			
Mode	Affinity (kcal/mol)	Dist from best mode	
		RMSD Lower Bound	RMSD Upper Bound
1	-11.5	0.000	0.000
2	-10.4	1.664	2.429
3	-10.4	43.457	47.947
4	-9.6	3.444	5.355
5	-9.2	44.814	48.793
6	-9.1	23.425	28.447
7	-8.9	5.052	7.891
8	-8.8	4.102	6.870
9	-8.7	25.192	30.006

GNE618			
Mode	Affinity (kcal/mol)	Dist from best mode	
		RMSD Lower Bound	RMSD Upper Bound
1	-10.9	0.000	0.000
2	-10.3	23.213	27.177
3	-10.3	28.297	33.162
4	-10.3	24.457	27.071
5	-10.2	3.196	4.475
6	-10.2	6.384	11.423
7	-10.0	24.987	27.733
8	-10.0	25.222	29.307
9	-9.9	24.643	28.573

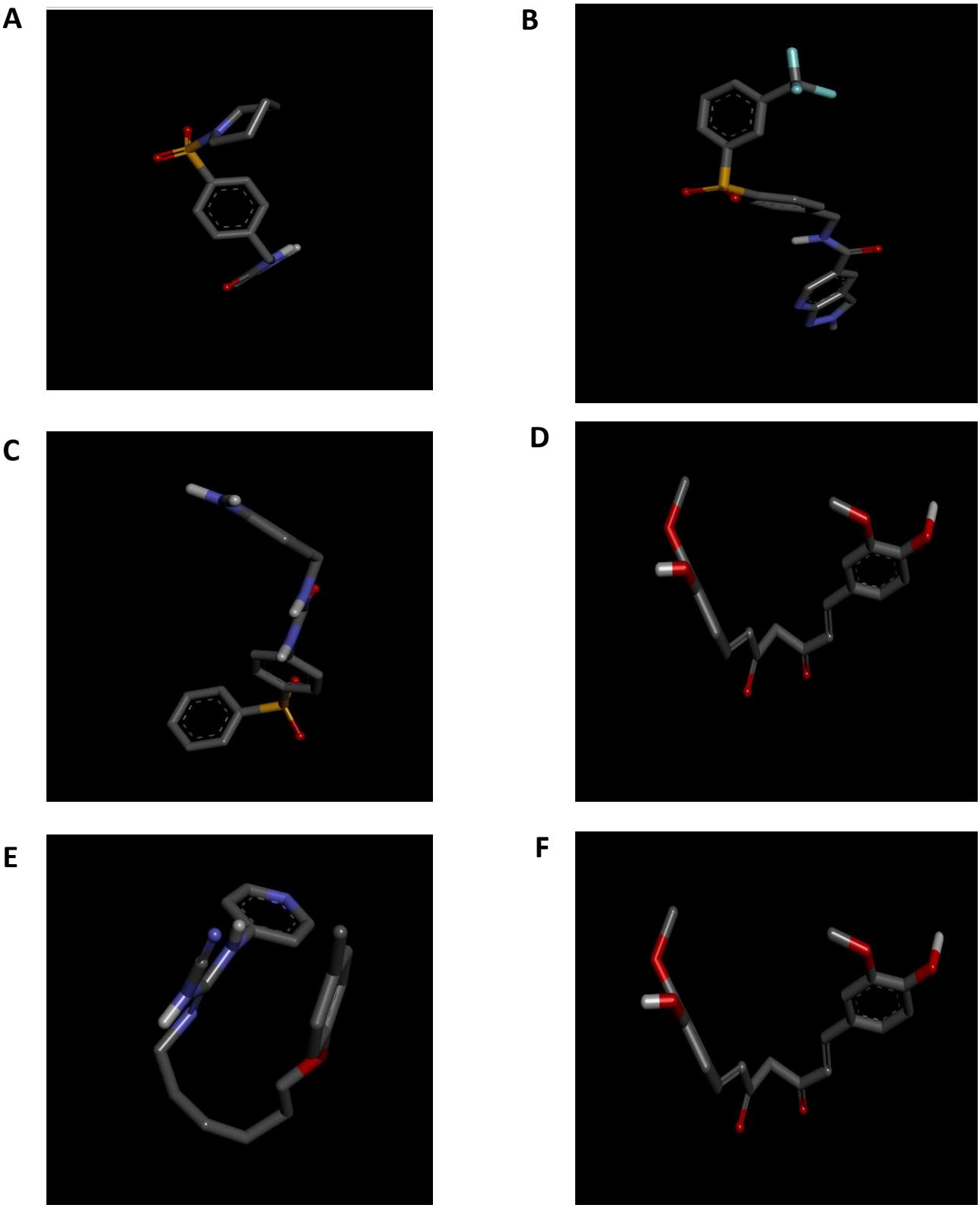
CHS-828			
Mode	Affinity (kcal/mol)	Dist from best mode	
		RMSD Lower Bound	RMSD Upper Bound
1	-6.9	0.000	0.000
2	-6.7	24.342	27.245
3	-6.7	4.654	6.087
4	-6.6	2.285	4.411
5	-6.3	25.312	28.321
6	-6.3	2.968	5.907
7	-6.3	5.889	9.427
8	-6.2	35.514	37.960
9	-6.1	6.952	9.003

FK866			
Mode	Affinity (kcal/mol)	Dist from best mode	
		RMSD Lower Bound	RMSD Upper Bound
1	-10.1	0.000	0.000
2	-9.7	1.901	2.160
3	-9.3	4.348	5.656
4	-8.9	47.548	51.837
5	-8.4	49.038	52.822
6	-8.3	3.034	4.669
7	-8.0	49.468	51.963
8	-8.0	3.418	5.108
9	-7.8	7.807	11.555

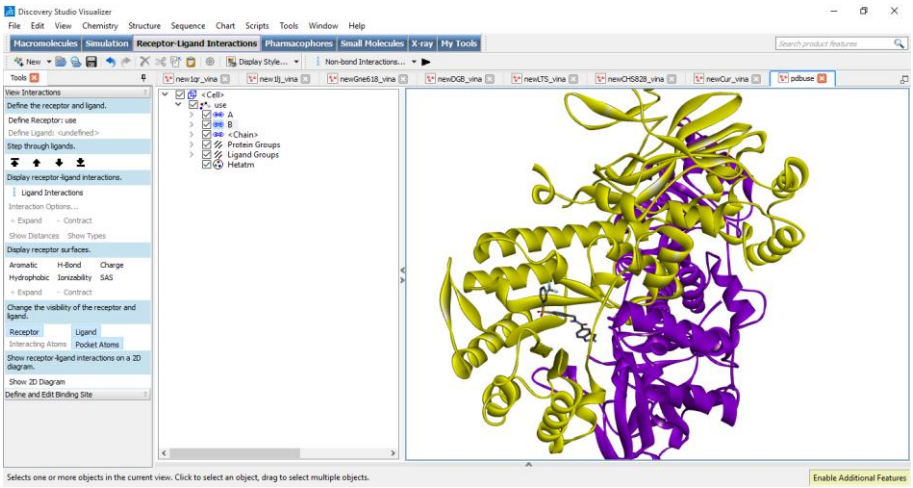
1LJ			
Mode	Affinity (kcal/mol)	Dist from best mode	
		RMSD Lower Bound	RMSD Upper Bound
1	-10.6	0.000	0.000
2	-10.3	1.521	1.940
3	-9.7	4.091	10.467
4	-9.2	22.361	26.121
5	-9.1	2.793	3.931
6	-9.1	27.027	31.680
7	-9.1	2.694	3.947
8	-9.0	45.138	48.877
9	-8.9	3.951	10.396

LTS			
Mode	Affinity (kcal/mol)	Dist from best mode	
		RMSD Lower Bound	RMSD Upper Bound
1	-7.2	0.000	0.000
2	-6.8	4.704	7.500
3	-6.2	32.383	34.798
4	-6.1	5.483	8.560
5	-6.0	57.795	60.024
6	-5.8	59.380	61.766
7	-5.5	16.755	19.161
8	-5.5	15.245	17.677
9	-5.4	56.654	58.961

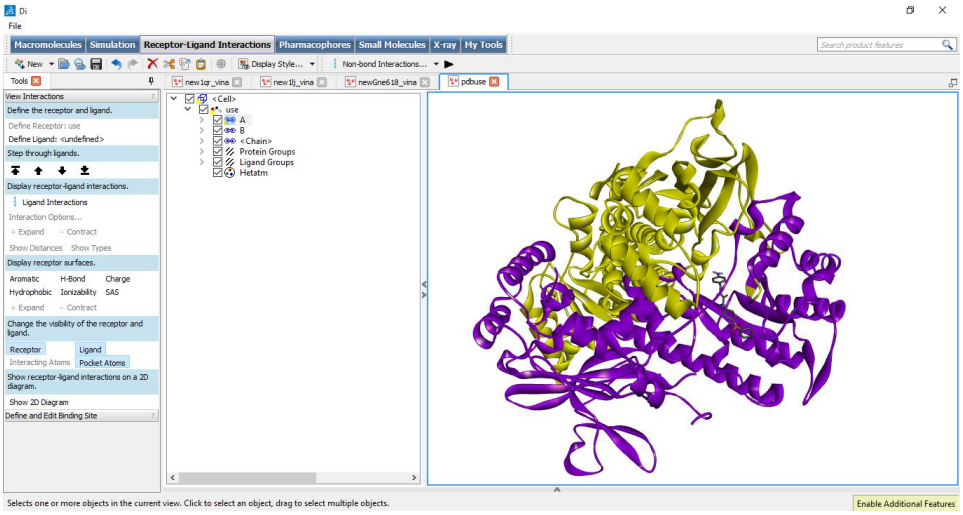
A. 4 Molecular docking result of 7 ligands. The binding affinity are all displayed for all 9 binding modes generated by AutoDock Vina.



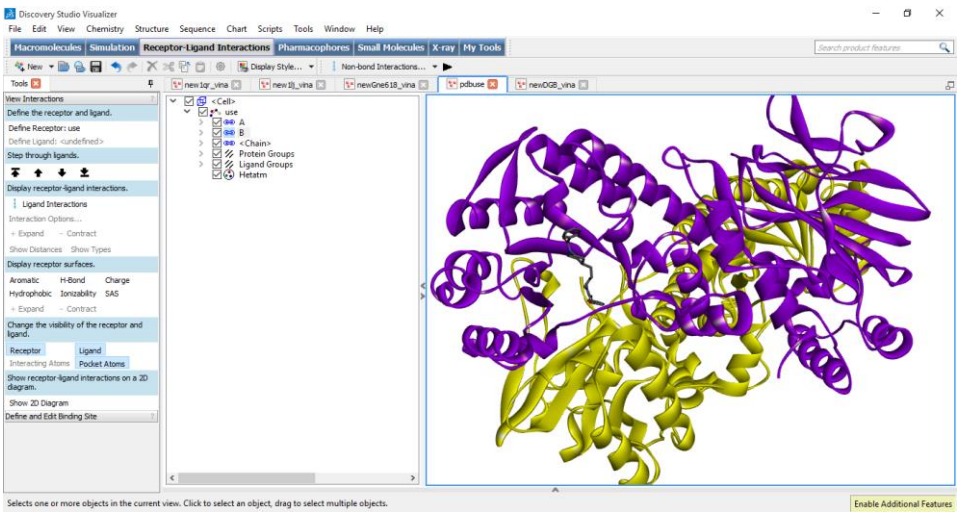
A. 5 Highest binding affinity ligand conformation. A) 1QR. B) GNE618. C) 1LJ. D) FK866. E) CHS88. F) Curcumin.



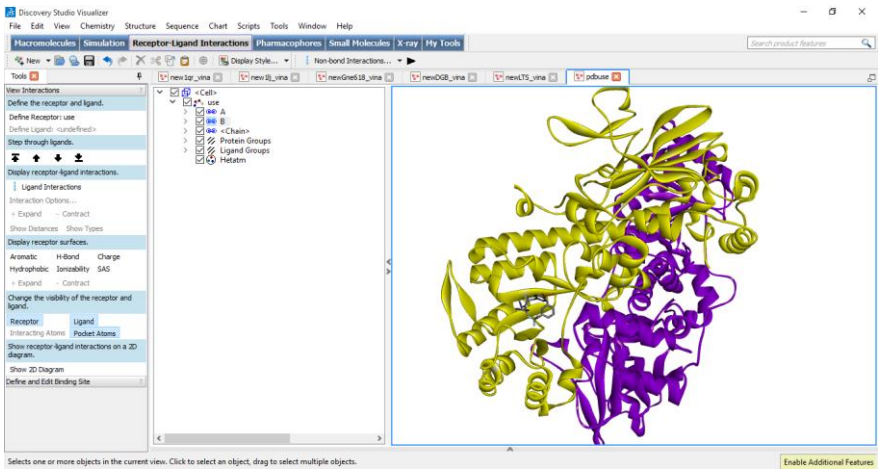
A. 6 NAMPT-GNE618 Visualization by Discovery Studio Two monomers included in NAMPT structure A (purple) and B (yellow), and GNE618 in between the dimer interface.



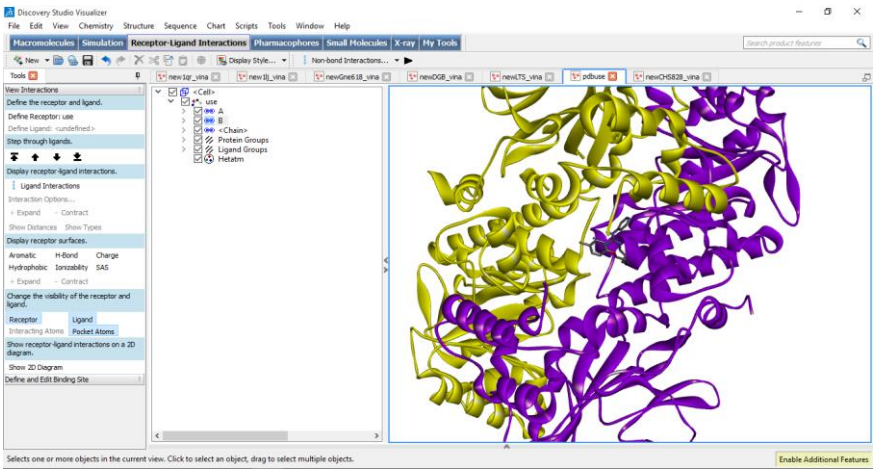
A. 7 NAMPT-1LJ Visualization by Discovery Studio Two monomers included in NAMPT structure A (purple) and B (yellow), and 1LJ in between the dimer interface.



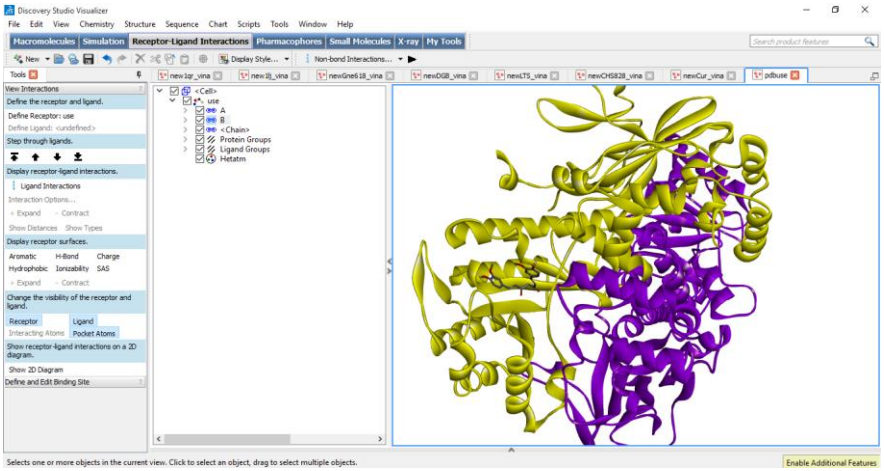
A. 8 NAMPT-FK866 Visualization by Discovery Studio Two monomers included in NAMPT structure A (purple) and B (yellow), and FK866 in between the dimer interface.



A. 9 NAMPT-LTS Visualization by Discovery Studio Two monomers included in NAMPT structure A (purple) and B (yellow), and LTS in between the dimer interface.



A. 10 NAMPT-CHS828 Visualization by Discovery Studio Two monomers included in NAMPT structure A (purple) and B (yellow), and CHS-828 in between the dimer interface.



A. 11 NAMPT-CURCUMIN Visualization by Discovery Studio Two monomers included in NAMPT structure A (purple) and B (yellow), and Curcumin in between the dimer interface.