Supplementary Information

In Silico Docking Studies of *Yucca gloriosa* L. Phytoconstituents with TNF-α, IL-6 and IL-13 Receptor Against Asthma

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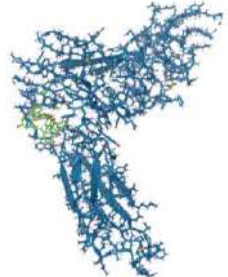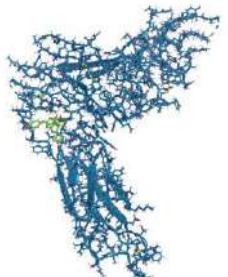E-mail: ajmergrewal2007@gmail.com; Mobile: +91-9416700430
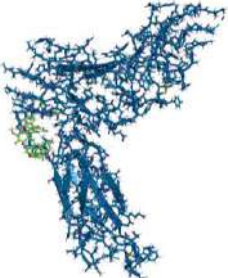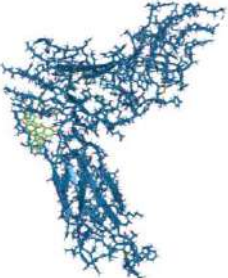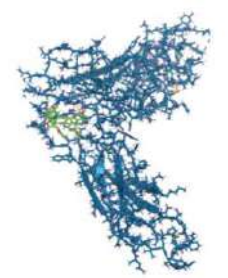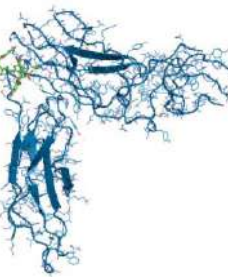
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The ligand-protein target complexes

IL-13 (PDB ID: 3LB6)

Gol A		**Yul A**	
Gol B		**Yul B**	
Gol C		**Yul C**	
Gol D		**Yul D**	
Gol E		**Yul E**	
Mlt			

Grid coordinates (X, Y and Z)

IL-13 (PDB ID: 3LB6)

gridbox x cent	gridbox y cent	gridbox z cent	gridbox x range	gridbox y range	gridbox z range	gridbox lig x range	gridbox lig y range	gridbox lig z range
56.16	-12.7121	28.39036	26.23765	26.23765	26.23765	10	10	10

IL-6 (PDB ID: 1N26)

gridbox x cent	gridbox y cent	gridbox z cent	gridbox x range	gridbox y range	gridbox z range	gridbox lig x range	gridbox lig y range	gridbox lig z range
35.99769	57.63538	55.87539	28.4	28.4	28.4	10	10	10

TNF-α (PDB ID: 2AZ5)

gridbox x cent	gridbox y cent	gridbox z cent	gridbox x range	gridbox y range	gridbox z range	gridbox lig x range	gridbox lig y range	gridbox lig z range
-19.7858	74.92655	33.56477	23.86427	23.86427	23.86427	10	10	10

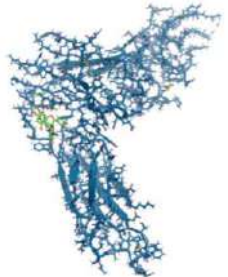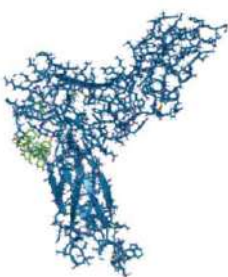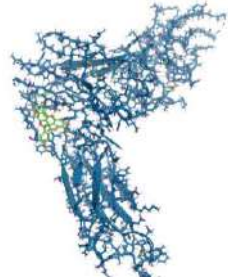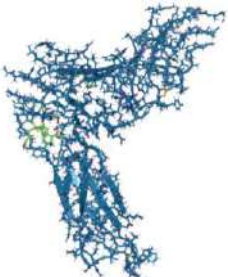## RMSD and RMSF results (raw data for all docking poses of all the ligands)

IL-13 (PDB ID: 3LB6)

Title	RMS Derivative-OPLS-2005	XP rmscomp	glide rmsd to input
gloriosaol C	0.041559	0	51.991222
yuccarol D	0.024402	0	54.56502
yuccarol D	0.038944	0	53.8797
yuccarol A	0.004517	0	52.89355
yuccarol C	0.006004	0	55.358463
yuccarol D	0.017377	0	54.91104
yuccarol E	0.004219	0	55.213079
gloriosaol C	0.016309	0	51.986171
gloriosaol C	0.037306	0	52.203671
gloriosaol A	0.034731	0	52.99957
gloriosaol C	0.024466	0	53.900561
yuccarol C	0.001193	0	55.104916
yuccarol B	0.029803	0	54.845193
gloriosaol A	0.040265	0	52.752902
gloriosaol D	0.034987	0	59.366208
yuccarol E	0.024643	0	55.176125
gloriosaol A	0.035829	0	52.667549

yuccarol B	0.037703	0	54.898422
gloriosaol B	0.015299	0	53.219734
yuccarol D	0.0339	0	54.113973
gloriosaol A	0.038502	0	53.057539
yuccarol A	0.016447	0	56.103014
gloriosaol B	0.00162	0	59.203782
gloriosaol C	0.021212	0	52.97952
yuccarol B	0.010534	0	55.68438
yuccarol C	0.049458	0	54.734096
gloriosaol D	0.011526	0	56.212438
yuccarol C	0.025429	0	55.338568
gloriosaol A	0.02323	0	54.913342
gloriosaol A	0.023091	0	51.638054
yuccarol E	0.03736	0	55.685514
gloriosaol A	0.018903	0	52.972864
gloriosaol D	0.005817	0	65.474974
gloriosaol B	0.007581	0	54.256822
gloriosaol D	0.003556	0	51.430084
yuccarol A	0.011757	0	53.726962
gloriosaol E	0.036436	0	50.249255
yuccarol E	0.012308	0	55.154308
montelukast Na	0.044953	0	52.974562
yuccarol B	0.003853	0	55.643367
gloriosaol D	0.007956	0	53.449101
yuccarol C	0.019035	0	54.170909
gloriosaol B	0.03719	0	54.706911
gloriosaol E	0.021635	0	54.261267
gloriosaol B	0.021944	0	58.354432
gloriosaol E	0.022525	0	57.639152
yuccarol A	0.013203	0	54.792958
gloriosaol E	0.038616	0	52.863458
gloriosaol E	0.011222	0	55.628557
gloriosaol E	0.006935	0	29.544151
gloriosaol B	0.005039	0	53.989518
yuccarol D	0.014029	0	53.606606
gloriosaol B	0.035615	0	54.282721
gloriosaol D	0.044038	0	48.276702
gloriosaol C	0.001208	0	58.496706
gloriosaol D	0.009486	0	60.861597
gloriosaol D	0.004486	0	47.44927
gloriosaol A	0.025519	0	52.352505
gloriosaol A	0.048886	0	52.188037
yuccarol A	0.017845	0	54.805832
gloriosaol E	0.017767	0	50.724505
gloriosaol A	0.017006	0	52.97584
gloriosaol B	0.017369	0	28.524777

gloriosaol E	0.014565	0	52.745914
gloriosaol E	0.016524	0	51.571814
yuccarol B	0.034225	0	55.014971
gloriosaol C	0.030147	0	52.021564
gloriosaol D	0.048511	0	56.310882
gloriosaol C	0.026637	0	51.589347
gloriosaol E	0.042578	0	51.2498
gloriosaol D	0.009586	0	46.718638
gloriosaol B	0.006271	0	60.208439
gloriosaol B	0.006701	0	60.483195
gloriosaol C	0.030695	0	52.288804
gloriosaol C	0.048503	0	51.991967
yuccarol E	0.027878	0	55.310601

IL-6 (PDB ID: 1N26)

Title	RMS Derivative-OPLS-2005	glide rmsd to input
montelukast Na	0.007069	95.165545
montelukast Na	0.039036	94.657152
gloriosaol B	0.010913	97.93652
yuccarol E	0.047419	100.382323
gloriosaol B	0.011575	103.867163
yuccarol C	0.045714	99.434089
gloriosaol B	0.00458	97.478122
yuccarol C	0.001841	99.492501
yuccarol C	0.007958	99.988968
yuccarol E	0.027672	101.21612
gloriosaol C	0.037793	103.600321
yuccarol D	0.005151	100.641159
gloriosaol C	0.036757	101.563152
yuccarol C	0.044336	99.385037
gloriosaol E	0.040926	101.704232
yuccarol A	0.005503	100.805614
gloriosaol D	0.03162	103.601182
gloriosaol B	0.047472	100.329679
yuccarol D	0.022038	100.483477
yuccarol D	0.018805	100.87014
yuccarol E	0.038806	100.210694
yuccarol B	0.026947	100.691059
yuccarol D	0.030999	100.159325
yuccarol B	0.007544	101.580757
yuccarol C	0.017309	98.989989
gloriosaol A	0.023317	100.999643
gloriosaol C	0.002201	89.916762
gloriosaol A	0.00798	101.207442
yuccarol C	0.005018	99.284165

yuccarol D	0.014001	100.816648
gloriosaol D	0.024667	101.028759
gloriosaol D	0.014177	109.665683
gloriosaol B	0.014725	100.400254
yuccarol D	0.036543	99.870493
gloriosaol C	0.025341	103.420461
yuccarol C	0.028414	99.340543
yuccarol A	0.007875	100.297772
gloriosaol D	0.043672	104.810398
gloriosaol D	0.017285	95.145999
yuccarol A	0.042209	100.366167
yuccarol E	0.00395	100.989761
gloriosaol E	0.00767	101.146222
yuccarol B	0.009114	101.893329
yuccarol C	0.035143	100.012944
yuccarol D	0.009958	100.497572
gloriosaol B	0.024592	97.600579
gloriosaol D	0.006847	103.618018
gloriosaol D	0.001144	87.326403
yuccarol E	0.045799	100.195317
yuccarol A	0.007517	100.901367
gloriosaol B	0.020117	101.858975
gloriosaol A	0.025718	99.888448
yuccarol A	0.011247	100.794885
yuccarol E	0.040583	100.604568
gloriosaol D	0.049705	105.103334
gloriosaol A	0.025999	101.093222
gloriosaol A	0.027313	101.238773
gloriosaol B	0.027011	119.412638
gloriosaol C	0.017327	103.041982
gloriosaol B	0.038259	100.285047
gloriosaol D	0.019106	102.14283
gloriosaol E	0.028666	101.60701
gloriosaol B	0.018921	99.384188
yuccarol D	0.035553	100.519623
yuccarol B	0.049885	101.136459
yuccarol D	0.01643	101.68144
gloriosaol C	0.017318	103.843209
gloriosaol E	0.002103	100.959935
gloriosaol A	0.037902	100.445858
yuccarol E	0.046485	101.007952
yuccarol E	0.034864	100.910802
yuccarol C	0.020481	100.393235
gloriosaol E	0.019336	101.220694
gloriosaol C	0.002185	104.055054
yuccarol A	0.001142	101.789095

gloriosaol A	0.0112	100.2057
gloriosaol D	0.049728	105.023912
gloriosaol C	0.004979	111.444807
gloriosaol C	0.005062	87.532301
yuccarol D	0.037824	101.990817
gloriosaol E	0.016662	101.7929
gloriosaol A	0.014736	100.867639
gloriosaol A	0.030721	101.067167
gloriosaol A	0.046961	100.674321
gloriosaol D	0.048	105.015656
gloriosaol C	0.009598	87.867926
gloriosaol D	0.033065	101.778036
gloriosaol D	0.009192	104.895226
gloriosaol B	0.014284	102.208347
gloriosaol B	0.0334	96.764735
gloriosaol A	0.046185	101.097381
gloriosaol E	0.015954	102.951898
gloriosaol C	0.015459	113.427011
gloriosaol E	0.012601	100.97061
gloriosaol B	0.017291	100.267211
yuccarol B	0.049535	101.661768
gloriosaol D	0.004207	100.260724
yuccarol A	0.012983	101.191713
yuccarol A	0.027851	100.380866
gloriosaol A	0.03939	101.737559
gloriosaol B	0.038024	101.852042
gloriosaol C	0.034885	103.41138
gloriosaol E	0.032191	101.828647
gloriosaol C	0.04334	102.727404
gloriosaol A	0.038428	101.346764
yuccarol B	0.012116	101.557647
yuccarol B	0.020371	101.221688
gloriosaol C	0.025169	103.37508
gloriosaol C	0.028162	103.513468
gloriosaol C	0.019565	110.63965
gloriosaol D	0.018182	101.992426
gloriosaol B	0.0263	106.699723
yuccarol B	0.022421	101.475067
gloriosaol E	0.00732	104.592964
gloriosaol B	0.040673	100.369043
gloriosaol D	0.041486	104.468056
gloriosaol A	0.025097	101.127032
gloriosaol D	0.025894	105.991918
gloriosaol B	0.016974	103.438746
gloriosaol B	0.016098	107.446455
gloriosaol D	0.012736	106.577388

gloriosaol A	0.036596	101.227068
gloriosaol C	0.021573	103.554977
gloriosaol D	0.006421	106.035084
yuccarol E	0.044103	100.289203
gloriosaol E	0.028309	101.453191
gloriosaol E	0.008711	102.429872
gloriosaol A	0.026137	101.531964
gloriosaol E	0.037602	105.398537
gloriosaol B	0.004721	93.452451
gloriosaol E	0.041863	101.308474
yuccarol C	0.045166	100.231702
gloriosaol E	0.022697	112.225291
gloriosaol B	0.007359	103.011955
gloriosaol C	0.015568	103.401431
yuccarol B	0.019804	101.725337
gloriosaol C	0.007227	102.790294
yuccarol B	0.030127	101.604737
yuccarol A	0.014944	101.529457
gloriosaol E	0.038616	101.154118
gloriosaol D	0.016073	99.491033
yuccarol A	0.00363	101.265935
yuccarol E	0.018721	101.003924
gloriosaol C	0.008787	102.90021
gloriosaol E	0.031005	101.941799
gloriosaol A	0.049475	101.176242
gloriosaol A	0.009091	100.959017
gloriosaol E	0.006734	100.442409
gloriosaol A	0.039298	101.079056
gloriosaol A	0.020742	101.14859
gloriosaol E	0.00643	101.989391

TNF-α (PDB ID: 2AZ5)

Title	RMS Derivative-OPLS-2005	XP rmscomp	glide rmsd to input
montelukast Na	0.033478	0	102.600244
yuccarol B	0.031171	0	101.265133
yuccarol A	0.001142	0	100.171529
yuccarol C	0.01979	0	97.37389
yuccarol A	0.005855	0	98.472973
montelukast Na	0.006173	0	98.938546
gloriosaol B	0.049878	0	102.282654
yuccarol A	0.004767	0	98.516901
gloriosaol E	0.016662	0	108.724663
yuccarol D	0.035708	0	102.542545
yuccarol C	0.019826	0	97.58126

yuccarol B	0.030586	0	99.250211
gloriosaol B	0.029408	0	93.877702
yuccarol A	0.021946	0	102.947304
yuccarol B	0.009114	0	104.636989
yuccarol D	0.003597	0	107.161931
yuccarol B	0.039507	0	99.45561
yuccarol C	0.025246	0	104.088685
yuccarol D	0.014001	0	98.170728
yuccarol B	0.006918	0	99.365615
gloriosaol C	0.017327	0	108.275752
yuccarol D	0.04139	0	105.334808
yuccarol C	0.043212	0	101.884221
yuccarol C	0.008885	0	101.776733
yuccarol E	0.008486	0	103.641375
yuccarol B	0.006268	0	110.781676
yuccarol A	0.01824	0	100.344801
yuccarol D	0.006159	0	106.254711
gloriosaol C	0.020585	0	109.384565
gloriosaol A	0.002172	0	99.285505
yuccarol B	0.026947	0	103.555473
gloriosaol C	0.002185	0	102.162503
gloriosaol B	0.029123	0	108.072039
yuccarol C	0.047557	0	97.252294
gloriosaol B	0.010761	0	109.836831
gloriosaol D	0.0304	0	108.688488
yuccarol E	0.02604	0	99.250945
gloriosaol C	0.012624	0	107.026521
gloriosaol D	0.03306	0	100.187726
yuccarol D	0.015587	0	97.922438
yuccarol A	0.045243	0	98.745778
gloriosaol C	0.027109	0	101.565659
gloriosaol E	0.017235	0	108.102108
yuccarol D	0.02091	0	99.455622
gloriosaol D	0.026511	0	103.049694
yuccarol D	0.028268	0	97.978223
gloriosaol B	0.021621	0	92.874635
yuccarol E	0.014043	0	98.307843
gloriosaol C	0.003178	0	105.190379
gloriosaol A	0.00079	0	99.926017
gloriosaol A	0.039109	0	100.213521
yuccarol E	0.005362	0	109.28625
yuccarol A	0.006923	0	100.479287
yuccarol E	0.00395	0	108.065038
gloriosaol D	0.021479	0	107.110878
yuccarol D	0.009933	0	103.235335
yuccarol E	0.040583	0	103.409287

yuccarol C	0.030262	0	102.845191
gloriosaol D	0.00795	0	110.518152
gloriosaol E	0.041863	0	103.156665
gloriosaol E	0.030007	0	105.654266
yuccarol D	0.01021	0	98.243231
gloriosaol B	0.036748	0	94.361569
gloriosaol D	0.028253	0	99.461199
gloriosaol D	0.005744	0	110.28883
yuccarol A	0.008027	0	99.483495
yuccarol B	0.020663	0	106.450209
yuccarol E	0.046272	0	103.787385
yuccarol C	0.015919	0	104.844025
yuccarol B	0.009552	0	99.916133
gloriosaol C	0.017318	0	108.902657
yuccarol A	0.012983	0	104.566783
yuccarol E	0.014649	0	100.682657
yuccarol D	0.048814	0	104.168777
yuccarol E	0.015116	0	99.032571
yuccarol B	0.007544	0	100.105621
yuccarol D	0.016744	0	98.506538
yuccarol E	0.011864	0	98.294032
yuccarol E	0.045799	0	98.521854
yuccarol A	0.038652	0	99.543961
gloriosaol C	0.010795	0	110.231266
gloriosaol B	0.034845	0	110.809523
yuccarol D	0.021696	0	105.646039
yuccarol C	0.037237	0	102.56108
gloriosaol B	0.018355	0	106.695535
yuccarol C	0.038849	0	97.610033
yuccarol E	0.012821	0	101.099038
gloriosaol B	0.037816	0	106.578225
yuccarol A	0.002446	0	104.003925
yuccarol B	0.015305	0	103.663953
yuccarol A	0.034498	0	106.013265
yuccarol A	0.014841	0	98.697116
yuccarol C	0.028414	0	103.104935
yuccarol C	0.045784	0	97.740797
yuccarol A	0.028377	0	100.034566
gloriosaol B	0.019597	0	112.613604
gloriosaol B	0.000721	0	102.616287
gloriosaol B	0.008603	0	104.240377

Energies of docking (raw data for all docking poses of all the ligands)

IL-13 (PDB ID: 3LB6)

Title	glide energy	glide einternal	glide emodel
gloriosaol C	-47.830057	3.847742	-65.795144
yuccarol D	-35.518446	6.983872	-44.42386
yuccarol D	-39.912793	6.199408	-45.471236
yuccarol A	-38.760744	5.099175	-48.855014
yuccarol C	-39.727782	2.334171	-54.374663
yuccarol D	-41.851848	10.607025	-39.709503
yuccarol E	-45.579893	4.250886	-59.596861
gloriosaol C	-42.752757	9.540369	-51.744557
gloriosaol C	-53.408792	6.223657	-68.937117
gloriosaol A	-35.955372	9.508076	-41.954628
gloriosaol C	-37.551477	6.189549	-38.603279
yuccarol C	-39.646314	2.635975	-42.731862
yuccarol B	-36.366099	2.904071	-50.326236
gloriosaol A	-24.497985	11.968476	-35.462135
gloriosaol D	-35.783937	15.045412	-27.70636
yuccarol E	-41.789588	4.647333	-55.661651
gloriosaol A	-37.523485	2.95184	-48.328997
yuccarol B	-36.295363	4.486757	-51.075145
gloriosaol B	-38.26185	7.708173	-45.637223
yuccarol D	-36.083351	6.041239	-45.547333
gloriosaol A	-34.076393	10.275298	-44.277657
yuccarol A	-31.958054	1.043358	-41.664504
gloriosaol B	-28.044451	11.128315	-34.665985
gloriosaol C	-37.08206	9.547755	-49.370778
yuccarol B	-33.833458	0.132075	-35.372966
yuccarol C	-37.613433	1.927594	-51.093084
gloriosaol D	-40.602964	3.884795	-49.372964
yuccarol C	-31.106348	3.619407	-42.251927
gloriosaol A	-32.683272	1.911892	-46.656567
gloriosaol A	-42.519292	2.838679	-51.857213
yuccarol E	-39.362883	1.187113	-44.994682
gloriosaol A	-40.786965	12.587261	-42.869821
gloriosaol D	-32.02602	5.203156	-35.514908
gloriosaol B	-33.356563	2.425962	-39.796701
gloriosaol D	-42.657215	9.226548	-48.539768
yuccarol A	-34.112367	0.612244	-45.593366
gloriosaol E	-47.644578	14.934	-50.945909
yuccarol E	-43.814596	8.118791	-56.544902
montelukast Na	-47.296857	11.745018	-70.937602
yuccarol B	-36.241267	1.877447	-40.869974
gloriosaol D	-37.287031	2.818697	-46.486268
yuccarol C	-39.637492	8.158802	-46.452185
gloriosaol B	-26.570545	0.565257	-33.83728
gloriosaol E	-29.770698	0.443671	-43.429472
gloriosaol B	-33.57051	16.101673	-37.060489

gloriosaol E	-38.780591	5.291747	-42.213205
yuccarol A	-39.274152	1.597287	-53.83586
gloriosaol E	-27.732248	3.251156	-39.577886
gloriosaol E	-29.486371	1.128966	-30.655641
gloriosaol E	-45.161695	5.754282	-42.994586
gloriosaol B	-32.861064	11.305589	-32.422282
yuccarol D	-41.52029	8.300401	-51.993888
gloriosaol B	-36.597136	10.855862	-36.919648
gloriosaol D	-48.304438	9.166431	-44.457806
gloriosaol C	-31.864396	1.202121	-36.682737
gloriosaol D	-35.750513	7.53166	-39.762071
gloriosaol D	-40.957294	1.570248	-50.678761
gloriosaol A	-39.627323	10.170596	-44.247413
gloriosaol A	-31.708683	1.843504	-39.049384
yuccarol A	-40.478685	1.021783	-52.678927
gloriosaol E	-41.75248	8.200768	-36.679563
gloriosaol A	-41.225814	3.231949	-51.883744
gloriosaol B	-25.462579	1.398692	-30.762141
gloriosaol E	-35.147532	10.201187	-35.362536
gloriosaol E	-39.720472	9.694171	-33.561576
yuccarol B	-34.522215	7.586243	-44.801636
gloriosaol C	-41.693326	14.425492	-48.456399
gloriosaol D	-33.245698	1.419523	-43.290359
gloriosaol C	-41.545272	8.006799	-41.213112
gloriosaol E	-43.089914	15.356148	-44.486701
gloriosaol D	-28.870718	2.768782	-27.339869
gloriosaol B	-34.649745	8.53052	-41.126764
gloriosaol B	-35.976833	7.745214	-38.712425
gloriosaol C	-49.798902	7.586304	-62.267067
gloriosaol C	-49.335332	13.599216	-62.960363
yuccarol E	-40.071869	3.00552	-45.917198

IL-6 (PDB ID: 1N26)

Title	glide energy	glide einternal	glide emodel
montelukast Na	-56.0778	7.239724	-87.7704
montelukast Na	-50.3891	10.08124	-74.6441
gloriosaol B	-45.2098	10.08294	-64.0494
yuccarol E	-42.6998	1.576955	-64.0624
gloriosaol B	-37.299	2.894474	-53.8222
yuccarol C	-43.4126	8.833568	-48.6926
gloriosaol B	-52.5838	12.523	-52.4561
yuccarol C	-42.3028	9.873615	-58.692
yuccarol C	-52.0571	6.335784	-57.5495
yuccarol E	-43.1622	6.299595	-53.7167
gloriosaol C	-42.9651	4.206898	-54.8084

yuccarol D	-47.0163	0.987211	-71.3616
gloriosaol C	-36.1469	10.89892	-53.6418
yuccarol C	-45.4505	1.447486	-58.2827
gloriosaol E	-43.4803	4.940523	-56.5684
yuccarol A	-46.9267	3.403886	-61.4088
gloriosaol D	-39.1177	12.63658	-59.2153
gloriosaol B	-52.5197	9.770594	-64.9185
yuccarol D	-45.0655	3.295342	-54.9431
yuccarol D	-46.2388	0.908651	-68.4843
yuccarol E	-37.2415	1.443168	-53.9612
yuccarol B	-45.7556	7.108507	-58.5827
yuccarol D	-46.2196	0.286088	-56.6345
yuccarol B	-50.5136	2.158123	-65.0858
yuccarol C	-40.2581	3.088689	-52.6127
gloriosaol A	-53.6836	5.41782	-67.1131
gloriosaol C	-40.8828	2.54543	-51.7079
gloriosaol A	-49.0287	1.217506	-61.0829
yuccarol C	-43.9318	0.957092	-55.75
yuccarol D	-48.5738	1.030853	-71.8595
gloriosaol D	-43.4596	8.833676	-61.2031
gloriosaol D	-44.8887	8.87631	-65.0914
gloriosaol B	-50.5055	4.56331	-58.506
yuccarol D	-49.5755	0.519506	-66.7956
gloriosaol C	-50.4311	7.241063	-64.2109
yuccarol C	-43.58	0.943212	-59.1563
yuccarol A	-43.2507	2.953432	-62.6565
gloriosaol D	-41.8504	14.60817	-45.3346
gloriosaol D	-41.0914	9.656169	-58.3636
yuccarol A	-43.6881	1.201478	-64.3665
yuccarol E	-47.4919	5.889288	-63.3129
gloriosaol E	-42.9513	1.744717	-60.9524
yuccarol B	-42.7075	3.071826	-56.6697
yuccarol C	-51.0097	0.376475	-60.512
yuccarol D	-39.5725	2.237543	-53.2897
gloriosaol B	-51.6435	14.26078	-54.871
gloriosaol D	-47.8701	7.086343	-64.1301
gloriosaol D	-46.9597	2.181561	-57.9266
yuccarol E	-38.0929	1.60682	-45.377
yuccarol A	-46.3177	1.70304	-62.33
gloriosaol B	-50.3606	12.22042	-61.9982
gloriosaol A	-47.6473	9.32932	-62.8762
yuccarol A	-47.4412	1.767315	-63.6795
yuccarol E	-41.8314	1.230064	-60.9777
gloriosaol D	-39.4284	7.111075	-57.5229
gloriosaol A	-49.3224	3.408216	-62.1136
gloriosaol A	-46.9524	0.880389	-63.9991

gloriosaol B	-41.6421	9.20797	-37.7953
gloriosaol C	-43.5969	5.143847	-50.4716
gloriosaol B	-48.245	9.453151	-59.2118
gloriosaol D	-47.8332	6.385351	-64.2817
gloriosaol E	-48.1731	9.51378	-58.1295
gloriosaol B	-45.238	11.37171	-58.407
yuccarol D	-43.211	6.985825	-56.0476
yuccarol B	-47.4843	2.684976	-58.6108
yuccarol D	-42.2818	7.892298	-58.4429
gloriosaol C	-45.027	2.417475	-57.8388
gloriosaol E	-42.0039	12.11805	-47.6299
gloriosaol A	-46.2182	5.483679	-64.0986
yuccarol E	-48.1758	2.529789	-57.6361
yuccarol E	-48.3538	2.168027	-65.3416
yuccarol C	-38.8427	2.262846	-61.2556
gloriosaol E	-50.1891	4.595771	-54.2457
gloriosaol C	-47.0956	2.549208	-62.1515
yuccarol A	-41.9139	0.296055	-52.867
gloriosaol A	-45.975	8.193759	-57.5428
gloriosaol D	-39.1819	10.94106	-51.46
gloriosaol C	-45.2211	1.121468	-69.5435
gloriosaol C	-45.8446	5.43694	-58.2737
yuccarol D	-44.4966	3.325305	-63.4973
gloriosaol E	-45.8903	10.45989	-47.7854
gloriosaol A	-49.283	9.812132	-63.0562
gloriosaol A	-43.2046	2.269267	-61.1243
gloriosaol A	-47.0092	3.301427	-60.0623
gloriosaol D	-32.5546	11.99888	-41.7122
gloriosaol C	-47.1297	7.321368	-51.3115
gloriosaol D	-43.495	11.31578	-57.9322
gloriosaol D	-49.2067	0.761434	-60.9343
gloriosaol B	-48.9863	9.057932	-59.7775
gloriosaol B	-42.7624	4.453605	-57.3835
gloriosaol A	-46.4711	3.206808	-57.0302
gloriosaol E	-39.8529	6.158118	-51.9298
gloriosaol C	-38.3256	1.024772	-55.4019
gloriosaol E	-42.9228	1.488212	-56.8844
gloriosaol B	-42.0714	1.075976	-61.3218
yuccarol B	-42.4006	5.368453	-54.741
gloriosaol D	-46.5723	2.476824	-53.3297
yuccarol A	-38.6948	8.128881	-48.7768
yuccarol A	-44.0305	6.050776	-61.6574
gloriosaol A	-46.013	4.979729	-61.4647
gloriosaol B	-44.9721	0.538198	-58.8968
gloriosaol C	-48.0634	4.814164	-67.8699
gloriosaol E	-45.2411	7.038802	-57.0887

gloriosaol C	-43.9526	3.530161	-51.5267
gloriosaol A	-47.4996	5.473004	-50.0094
yuccarol B	-42.4603	4.465275	-56.9603
yuccarol B	-42.3942	0.651483	-55.6573
gloriosaol C	-46.395	5.116021	-63.0997
gloriosaol C	-43.369	2.730776	-60.651
gloriosaol C	-41.2623	8.670175	-54.3611
gloriosaol D	-44.0333	4.011833	-58.0527
gloriosaol B	-41.9682	0.746207	-56.0723
yuccarol B	-35.2808	0.418128	-52.6691
gloriosaol E	-45.1536	8.489405	-51.4345
gloriosaol B	-43.2207	1.052049	-59.6643
gloriosaol D	-38.3139	5.661915	-46.7576
gloriosaol A	-47.3393	3.488853	-61.1525
gloriosaol D	-46.4912	9.65339	-58.3736
gloriosaol B	-41.147	2.989008	-49.5678
gloriosaol B	-38.6654	1.629802	-52.7214
gloriosaol D	-46.4106	6.615666	-59.8942
gloriosaol A	-45.6539	1.169605	-63.2151
gloriosaol C	-42.2374	5.173017	-56.317
gloriosaol D	-38.1665	0.579392	-47.1209
yuccarol E	-41.038	1.676407	-54.728
gloriosaol E	-42.9601	1.2822	-59.9219
gloriosaol E	-43.9428	8.317873	-55.8213
gloriosaol A	-48.5309	6.873689	-64.3625
gloriosaol E	-28.5201	10.18678	-42.0353
gloriosaol B	-42.7347	1.637771	-48.3427
gloriosaol E	-39.8198	1.893761	-55.4314
yuccarol C	-45.0634	2.241043	-59.5784
gloriosaol E	-43.7917	0.94723	-54.0314
gloriosaol B	-44.178	11.49442	-59.2542
gloriosaol C	-44.6049	6.53164	-45.023
yuccarol B	-46.8598	2.252193	-61.8503
gloriosaol C	-45.6982	1.796272	-63.8031
yuccarol B	-45.1933	1.680959	-65.7639
yuccarol A	-45.2656	5.350368	-56.717
gloriosaol E	-40.4979	4.71639	-58.7294
gloriosaol D	-49.6138	1.570827	-55.7949
yuccarol A	-45.3094	1.388921	-69.441
yuccarol E	-46.66	2.447021	-58.5051
gloriosaol C	-45.7778	2.564734	-47.2168
gloriosaol E	-47.596	5.725535	-59.8004
gloriosaol A	-51.8421	5.401415	-70.2458
gloriosaol A	-50.0759	1.885808	-64.4214
gloriosaol E	-46.1388	1.22232	-67.8805
gloriosaol A	-52.2407	3.543412	-63.6245

| gloriosaol A | -51.3782 | 5.757458 | -70.0331 |
| gloriosaol E | -47.8849 | 0.982058 | -62.8262 |

TNF-α (PDB ID: 2AZ5)

Title	glide energy	glide einternal	glide emodel
montelukast Na	-43.6844	4.865219	-58.51
yuccarol B	-27.7297	3.768461	-36.0728
yuccarol A	-24.3463	5.117326	-32.2554
yuccarol C	-26.6506	7.232219	-36.3764
yuccarol A	-28.7693	3.617506	-40.3279
montelukast Na	-38.5913	4.41171	-52.3995
gloriosaol B	-20.8437	1.104717	-3105.56
yuccarol A	-28.5184	4.531583	-39.7011
gloriosaol E	-43.6494	0.877265	-49.0101
yuccarol D	-28.7887	0.051969	-41.4279
yuccarol C	-25.4108	0.547121	-33.6825
yuccarol B	-27.5057	4.364279	-38.619
gloriosaol B	-27.4428	8.477933	-33.4005
yuccarol A	-24.4407	1.381857	-33.6958
yuccarol B	-22.8066	0.481427	-31.7574
yuccarol D	-30.1182	3.579647	-37.0727
yuccarol B	-24.6025	3.924225	-32.6545
yuccarol C	-32.1647	3.938087	-41.2579
yuccarol D	-27.318	10.3212	-34.8076
yuccarol B	-28.7172	4.001814	-40.1159
gloriosaol C	-26.8092	0.296571	-37.153
yuccarol D	-34.1474	1.299959	-46.7303
yuccarol C	-26.6298	4.934205	-33.189
yuccarol C	-30.1158	2.35824	-40.7413
yuccarol E	-25.4561	12.85015	-27.6886
yuccarol B	-29.2813	3.406495	-35.1849
yuccarol A	-28.2748	3.414767	-37.1999
yuccarol D	-29.5627	1.267073	-43.578
gloriosaol C	-42.3786	0.609912	-52.1588
gloriosaol A	-31.2992	5.120471	-3430.51
yuccarol B	-26.3613	4.153176	-33.9309
gloriosaol C	-35.2933	12.32624	-39.9204
gloriosaol B	-28.6614	12.0843	-32.2564
yuccarol C	-28.6043	13.62771	-35.2191
gloriosaol B	-30.6945	10.01225	-3419.15
gloriosaol D	-37.5198	0.129291	-46.8237
yuccarol E	-28.2795	3.355916	-33.4217
gloriosaol C	-32.2021	1.579023	-42.193
gloriosaol D	-31.6174	0.205484	-36.8934
yuccarol D	-28.6072	0.238831	-38.4084

yuccarol A	-30.6905	1.78253	-40.7808
gloriosaol C	-40.1672	6.050853	-49.2131
gloriosaol E	-25.7477	0.385425	-2471.91
yuccarol D	-29.4579	0.815685	-36.8941
gloriosaol D	-32.307	0.983111	-42.6289
yuccarol D	-30.035	0.157554	-39.4061
gloriosaol B	-33.3414	10.14306	-45.3665
yuccarol E	-31.4453	6.81746	-38.5074
gloriosaol C	-24.2029	7.929821	-3208.58
gloriosaol A	-29.0091	3.225156	-36.7503
gloriosaol A	-28.2655	2.439959	-3760.38
yuccarol E	-28.7863	2.774247	-35.0417
yuccarol A	-23.0904	0.357977	-30.8849
yuccarol E	-25.1747	7.960192	-31.4051
gloriosaol D	-37.1894	2.168061	-53.3268
yuccarol D	-23.2235	1.269007	-27.4085
yuccarol E	-28.1231	2.501232	-38.4691
yuccarol C	-27.3213	10.01374	-32.5052
gloriosaol D	-28.0649	0.666628	-36.1722
gloriosaol E	-26.0082	8.909509	-31.6219
gloriosaol E	-33.3045	0.144061	-43.6996
yuccarol D	-30.3178	6.703156	-37.9775
gloriosaol B	-18.5904	11.10448	-3337.46
gloriosaol D	-32.6702	0.591545	-39.8587
gloriosaol D	-39.0808	1.896587	-50.673
yuccarol A	-26.7805	6.162511	-33.1147
yuccarol B	-30.5548	0.941045	-41.5903
yuccarol E	-32.1355	4.339731	-35.871
yuccarol C	-30.1935	5.876821	-38.7102
yuccarol B	-25.7467	4.764282	-35.548
gloriosaol C	-33.5731	6.50371	-35.614
yuccarol A	-26.9011	0.172254	-34.9329
yuccarol E	-26.2612	0.610642	-34.2548
yuccarol D	-28.4578	0.666769	-35.5787
yuccarol E	-24.7633	4.918478	-31.6908
yuccarol B	-25.7863	4.422193	-32.9883
yuccarol D	-26.2158	0.381545	-36.0746
yuccarol E	-21.5813	5.669405	-28.2696
yuccarol E	-27.1576	1.690488	-33.0733
yuccarol A	-24.9082	3.657704	-31.2633
gloriosaol C	-31.6108	0.910206	-32.0333
gloriosaol B	-29.2653	1.78662	-34.1879
yuccarol D	-24.9227	1.345553	-33.7198
yuccarol C	-30.1826	0.975695	-39.4418
gloriosaol B	-34.5148	1.584683	-43.6449
yuccarol C	-26.8768	8.198062	-32.7965

yuccarol E	-19.2667	1.189552	-23.114
gloriosaol B	-34.5993	7.606232	-42.6509
yuccarol A	-24.089	3.966136	-31.5797
yuccarol B	-25.3119	0.895703	-35.2154
yuccarol A	-32.8637	3.037384	-42.782
yuccarol A	-23.3787	3.865674	-31.545
yuccarol C	-26.0568	1.029084	-35.9638
yuccarol C	-26.1807	0.701996	-36.1907
yuccarol A	-24.9269	5.188844	-31.3025
gloriosaol B	-30.3303	11.4674	-33.802
gloriosaol B	-29.485	8.069066	-33.4538
gloriosaol B	-25.7304	1.582213	-28.1633