Supplementary Information

Lung Cancer Targeting by Trimethoxy Flavans: A Molecular Simulation Study

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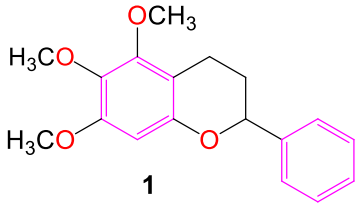
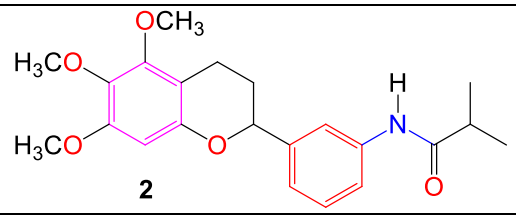
Table S1: Compound **1** Cartesian Z matrix

Compound 1		 **1**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	0.285651	-0.82322	-0.489776
2	C	0.098339	0.480122	-0.958676
3	C	1.52778	-1.135006	0.093685
4	C	1.109817	1.447018	-0.879689
5	C	2.333662	1.115416	-0.302433
6	C	2.549351	-0.185764	0.198474
7	H	0.903611	2.434625	-1.270774
8	O	1.681928	-2.401389	0.610052
9	C	2.700394	-3.208491	0.006389
10	H	3.690227	-2.767432	0.143021
11	H	2.651169	-4.178003	0.50676
12	H	2.504709	-3.346141	-1.064761
13	O	3.763179	-0.524583	0.758811
14	C	3.908953	-0.120774	2.122789
15	H	3.136959	-0.578353	2.753229
16	H	4.89312	-0.469052	2.444484
17	H	3.862829	0.969643	2.216951
18	O	3.379194	1.981278	-0.155323
19	C	3.221485	3.302009	-0.649061
20	H	2.403364	3.8301	-0.142573
21	H	4.162605	3.813927	-0.443003
22	H	3.035156	3.30904	-1.73031
23	O	-1.067462	0.910062	-1.547075
24	C	-1.783517	-1.422761	-1.726331
25	H	-2.669621	-2.064162	-1.740989
26	H	-1.298269	-1.511946	-2.7054
27	C	-2.21128	0.041216	-1.538791
28	H	-2.781518	0.358526	-2.419792
29	C	-3.082863	0.267546	-0.306725
30	C	-4.341134	-0.348291	-0.238001
31	C	-3.509962	1.279137	1.857415
32	C	-5.170494	-0.158666	0.865772
33	H	-4.68144	-0.9756	-1.058612
34	C	-4.754743	0.654828	1.922023
35	H	-3.179891	1.919567	2.670461
36	H	-6.142348	-0.642847	0.899491
37	H	-5.398901	0.803877	2.783606
38	C	-2.680686	1.091303	0.749113
39	H	-1.720747	1.591693	0.7009

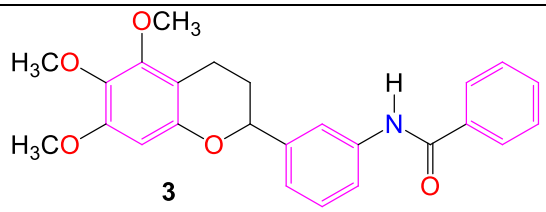
40	C	-0.814405	-1.848219	-0.620738
41	H	-0.387949	-2.832045	-0.835705
42	H	-1.355876	-1.952787	0.328664

Table S2: Compound **2** Cartesian Z matrix

Compound 2				
		2		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.948582	-0.717111	0.518654
2	C	-2.014887	0.611233	0.949156
3	C	-3.10238	-1.271911	-0.065348
4	C	-3.188316	1.368836	0.832086
5	C	-4.320666	0.797628	0.255537
6	C	-4.282224	-0.534518	-0.206884
7	H	-3.175826	2.388167	1.194985
8	O	-3.011509	-2.558951	-0.544999
9	C	-3.863009	-3.525219	0.082727
10	H	-4.91747	-3.281978	-0.066057
11	H	-3.63052	-4.482356	-0.389131
12	H	-3.650017	-3.592909	1.157257
13	O	-5.403893	-1.111426	-0.765347
14	C	-5.60306	-0.784127	-2.142695
15	H	-4.750463	-1.108558	-2.751574
16	H	-6.500391	-1.319778	-2.461064
17	H	-5.759728	0.292355	-2.272362
18	O	-5.5079	1.447946	0.073752
19	C	-5.607725	2.786525	0.532715
20	H	-4.896826	3.446521	0.019008
21	H	-6.625474	3.106986	0.305096
22	H	-5.440247	2.855719	1.614871
23	O	-0.958708	1.268545	1.533382
24	C	0.178854	-0.883341	1.791915
25	H	1.168743	-1.345947	1.834521
26	H	-0.295645	-1.03223	2.768936
27	C	0.327391	0.628368	1.56251
28	H	0.817531	1.072912	2.436201
29	C	1.157601	0.979076	0.329937
30	C	2.500675	0.5802	0.30448
31	C	1.429155	2.001646	-1.84123
32	C	3.305438	0.887819	-0.799004
33	H	2.940735	0.039038	1.131001

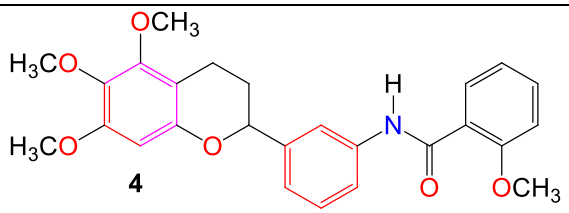
34	H	1.015441	2.55798	-2.677213
35	C	0.623659	1.698989	-0.741317
36	H	-0.408333	2.025728	-0.713859
37	C	-0.67857	-1.514148	0.692051
38	H	-0.917126	-2.55354	0.934427
39	H	-0.113482	-1.544483	-0.248861
40	C	5.436827	-0.192203	0.002581
41	O	5.025558	-0.62507	1.072614
42	C	6.889097	-0.415013	-0.439124
43	H	7.054645	0.052288	-1.419843
44	C	7.152615	-1.92497	-0.561168
45	C	7.833125	0.237619	0.584068
46	H	6.516759	-2.383787	-1.325253
47	H	8.196905	-2.111686	-0.830236
48	H	6.943877	-2.416224	0.392995
49	H	7.682514	1.320775	0.636423
50	H	7.647756	-0.178578	1.577909
51	H	8.877691	0.051674	0.315533
52	N	4.665365	0.51716	-0.889393
53	H	5.130028	0.813008	-1.735409
54	C	2.758965	1.600984	-1.878167
55	H	3.379083	1.842245	-2.738649

Table S3: Compound 3 Cartesian Z matrix

Compound 3		 **3**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	2.716119	-1.121481	0.04379
2	C	2.208615	-0.605835	-1.151617
3	C	3.69123	-0.363836	0.719877
4	C	2.660747	0.608267	-1.685557
5	C	3.631158	1.339196	-1.003183
6	C	4.149904	0.858298	0.218022
7	H	2.234902	0.945443	-2.621418
8	O	4.136793	-0.848241	1.927757
9	C	5.533404	-1.160193	2.00906
10	H	6.148704	-0.269535	1.865121
11	H	5.691848	-1.566549	3.010208
12	H	5.8066	-1.919245	1.264992
13	O	5.118914	1.570291	0.892194
14	C	4.610779	2.653692	1.676017
15	H	3.906671	2.293093	2.435584

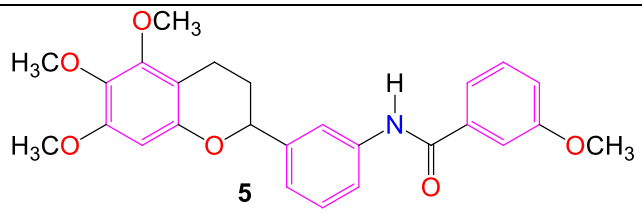
16	H	5.473039	3.108924	2.168277
17	H	4.119899	3.400477	1.042832
18	O	4.129694	2.539356	-1.419586
19	C	3.648531	3.07024	-2.644742
20	H	2.568557	3.262059	-2.607647
21	H	4.176896	4.013325	-2.790977
22	H	3.863992	2.40037	-3.486495
23	O	1.251144	-1.247726	-1.903776
24	C	1.609796	-3.262426	-0.564633
25	H	1.109372	-4.156602	-0.181675
26	H	2.390855	-3.595948	-1.257726
27	C	0.607931	-2.408596	-1.357317
28	H	0.28807	-2.968306	-2.243999
29	C	-0.640206	-2.039346	-0.559709
30	C	-1.492587	-3.055108	-0.103772
31	C	-2.129266	-0.386647	0.428186
32	C	-2.639423	-2.735541	0.619907
33	H	-1.263521	-4.095966	-0.315403
34	C	-2.956444	-1.408832	0.907957
35	H	-3.2884	-3.528112	0.980636
36	H	-3.832932	-1.169842	1.498385
37	C	-0.978023	-0.710093	-0.30472
38	H	-0.351372	0.087839	-0.686137
39	C	2.230739	-2.448952	0.573551
40	H	3.058968	-2.995486	1.033227
41	H	1.490119	-2.296714	1.369751
42	N	-2.37636	0.982638	0.698621
43	H	-1.572907	1.526704	0.990708
44	O	-3.519282	2.722473	1.571888
45	C	-4.841713	1.15736	0.369586
46	C	-4.917825	0.503048	-0.867932
47	C	-6.02154	1.45579	1.064752
48	C	-6.15782	0.139219	-1.391309
49	H	-4.012827	0.291964	-1.426893
50	C	-7.257555	1.072904	0.549384
51	H	-5.948527	1.996358	2.002362
52	C	-7.327643	0.41391	-0.680266
53	H	-6.210513	-0.357013	-2.355808
54	H	-8.166252	1.296951	1.100185
55	H	-8.291664	0.122467	-1.087143
56	C	-3.554434	1.669236	0.944819

Table S4: Compound 4 Cartesian Z matrix

Compound 4		 4		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.627084	-0.773007	0.532209
2	C	-2.361421	0.584019	0.735267
3	C	-3.948211	-1.139402	0.214262
4	C	-3.368228	1.55541	0.652208
5	C	-4.670421	1.17005	0.340734
6	C	-4.969312	-0.18943	0.110679
7	H	-3.097974	2.587811	0.830942
8	O	-4.188209	-2.468887	-0.046729
9	C	-5.100518	-3.131131	0.838075
10	H	-6.097966	-2.689441	0.784092
11	H	-5.134493	-4.17216	0.50986
12	H	-4.73721	-3.09179	1.87294
13	O	-6.258822	-0.578941	-0.184598
14	C	-6.61982	-0.408812	-1.557776
15	H	-5.961349	-0.992016	-2.212811
16	H	-7.644511	-0.7746	-1.655252
17	H	-6.584217	0.647572	-1.84556
18	O	-5.722418	2.031229	0.214273
19	C	-5.482988	3.410256	0.445854
20	H	-4.755116	3.82136	-0.265506
21	H	-6.443219	3.909156	0.307076
22	H	-5.125382	3.591771	1.467154
23	O	-1.113741	1.070268	1.048496
24	C	-0.391857	-1.221705	1.517297
25	H	0.482181	-1.879298	1.506207
26	H	-0.71885	-1.129275	2.559609
27	C	0.009532	0.17574	1.019981
28	H	0.711153	0.617841	1.736802
29	C	0.684305	0.164997	-0.349513
30	C	0.107249	0.77252	-1.468076
31	C	2.59683	-0.496119	-1.703123
32	C	0.762085	0.721096	-2.700679
33	H	-0.845302	1.279561	-1.376918
34	C	2.000048	0.099502	-2.823929
35	H	0.306759	1.183435	-3.571736
36	H	2.519176	0.083817	-3.778061
37	C	1.922464	-0.476759	-0.477597
38	H	2.371106	-0.963979	0.381118
39	C	-1.524418	-1.795169	0.662457

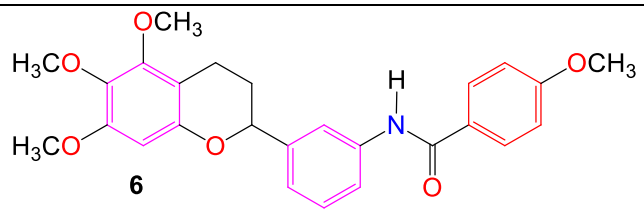
40	H	-1.915613	-2.716012	1.10385
41	H	-1.13978	-2.07287	-0.327743
42	N	3.83764	-1.149197	-1.871366
43	H	3.980265	-1.629758	-2.751194
44	O	5.785764	-2.138198	-1.322142
45	C	4.995379	-0.558516	0.263394
46	C	4.855436	0.844001	0.345891
47	C	5.340483	-1.273946	1.413863
48	C	5.00099	1.484843	1.582497
49	C	5.479763	-0.639913	2.647545
50	H	5.495007	-2.34388	1.319582
51	C	5.302897	0.740114	2.724221
52	H	4.89336	2.559799	1.659561
53	H	5.731198	-1.214642	3.532868
54	H	5.411274	1.25299	3.675593
55	C	4.911001	-1.332406	-1.022661
56	O	4.604626	1.496836	-0.821679
57	C	4.37186	2.897447	-0.786751
58	H	4.149883	3.186756	-1.81427
59	H	3.515632	3.146743	-0.14851
60	H	5.256642	3.444954	-0.439089

Table S5: Compound 5 Cartesian Z matrix

Compound 5		 **5**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	3.35641	1.023923	-0.215414
2	C	2.88979	0.664834	1.051787
3	C	4.242733	0.139926	-0.859479
4	C	3.29827	-0.517254	1.683868
5	C	4.180997	-1.375119	1.030909
6	C	4.655483	-1.053577	-0.258721
7	H	2.908388	-0.730618	2.670454
8	O	4.645743	0.470618	-2.132514
9	C	6.051243	0.683139	-2.316196
10	H	6.620877	-0.225631	-2.110522
11	H	6.176305	0.974486	-3.361196
12	H	6.409765	1.495049	-1.67067
13	O	5.538939	-1.891395	-0.905382
14	C	4.921431	-3.011455	-1.545969
15	H	4.197585	-2.682476	-2.301336
16	H	5.724441	-3.569628	-2.032478

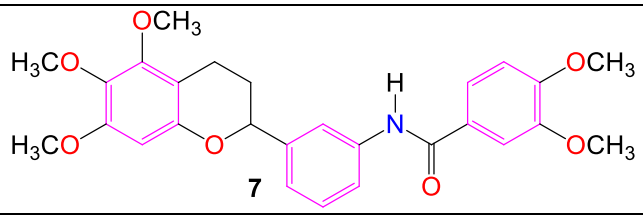
17	H	4.423716	-3.657225	-0.814632
18	O	4.629519	-2.558284	1.542157
19	C	4.189493	-2.931815	2.838782
20	H	3.099581	-3.05468	2.877779
21	H	4.667578	-3.888498	3.053657
22	H	4.493735	-2.197336	3.594872
23	O	2.018765	1.440342	1.782599
24	C	2.420362	3.283533	0.226215
25	H	1.953827	4.166644	-0.219941
26	H	3.260038	3.631407	0.839095
27	C	1.416673	2.58178	1.154132
28	H	1.184965	3.246872	1.99423
29	C	0.103122	2.219377	0.465802
30	C	-0.708608	3.238825	-0.051511
31	C	-1.543383	0.580215	-0.259969
32	C	-1.914247	2.925982	-0.67603
33	H	-0.402329	4.277729	0.035055
34	C	-2.331141	1.601898	-0.802888
35	H	-2.532129	3.71996	-1.085043
36	H	-3.25524	1.364161	-1.316137
37	C	-0.33265	0.897322	0.372654
38	H	0.263768	0.101918	0.804414
39	C	2.921983	2.321214	-0.853168
40	H	3.753132	2.762894	-1.410027
41	H	2.127451	2.140039	-1.589054
42	N	-1.890883	-0.789722	-0.370183
43	H	-1.140796	-1.413091	-0.645133
44	C	-3.120197	-1.417951	-0.483574
45	O	-3.183397	-2.527937	-1.002431
46	C	-4.340122	-0.768438	0.101201
47	C	-5.566268	-1.080647	-0.505903
48	C	-4.304001	0.02003	1.255087
49	C	-6.753926	-0.573837	0.024494
50	H	-5.553698	-1.731606	-1.370471
51	C	-5.500293	0.507784	1.787695
52	H	-3.361099	0.239421	1.741627
53	C	-6.716642	0.225958	1.177791
54	H	-5.482069	1.112488	2.689472
55	H	-7.652494	0.602944	1.576933
56	O	-7.99384	-0.802846	-0.496278
57	C	-8.094625	-1.630803	-1.64631
58	H	-7.716653	-2.641877	-1.450912
59	H	-9.157512	-1.683112	-1.885807
60	H	-7.552105	-1.205229	-2.499882

Table S6: Compound 6 Cartesian Z matrix

Compound 6				
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	3.165793	-1.146831	0.082608
2	C	2.577449	-0.714807	-1.108948
3	C	4.210703	-0.367852	0.614695
4	C	3.0161	0.436508	-1.7766
5	C	4.056083	1.18957	-1.235502
6	C	4.658631	0.793765	-0.022306
7	H	2.52523	0.709468	-2.701494
8	O	4.739575	-0.765338	1.820889
9	C	6.129203	-1.11604	1.817758
10	H	6.754171	-0.261936	1.548332
11	H	6.358637	-1.441183	2.834726
12	H	6.320123	-1.944181	1.12333
13	O	5.696221	1.527427	0.512385
14	C	5.279382	2.685546	1.24122
15	H	4.63074	2.409137	2.081218
16	H	6.189328	3.152677	1.624478
17	H	4.756689	3.393331	0.588952
18	O	4.549681	2.335507	-1.78849
19	C	3.984475	2.780207	-3.012043
20	H	2.916129	3.008258	-2.906489
21	H	4.522612	3.691258	-3.277372
22	H	4.114404	2.037928	-3.809455
23	O	1.547578	-1.385637	-1.72808
24	C	1.957976	-3.292913	-0.255167
25	H	1.467693	-4.136241	0.239755
26	H	2.670794	-3.707194	-0.97763
27	C	0.917967	-2.473455	-1.034573
28	H	0.510101	-3.092469	-1.842191
29	C	-0.248799	-1.994584	-0.174269
30	C	-1.075468	-2.936466	0.454549
31	C	-1.619139	-0.212365	0.758817
32	C	-2.149793	-2.515326	1.23532
33	H	-0.883874	-3.999042	0.333282
34	C	-2.418675	-1.158764	1.410037
35	H	-2.778355	-3.250239	1.729608
36	H	-3.236801	-0.838558	2.044058
37	C	-0.541044	-0.63813	-0.030581
38	H	0.063873	0.100199	-0.544184
39	C	2.690771	-2.410351	0.758247

40	H	3.539185	-2.944471	1.195236
41	H	2.02158	-2.169558	1.594788
42	N	-1.817285	1.1832	0.906056
43	H	-0.980193	1.734059	1.056445
44	C	-2.95345	1.924898	1.183689
45	O	-2.840493	3.039925	1.680831
46	C	-4.301049	1.387836	0.798167
47	C	-5.398075	1.762752	1.589998
48	C	-4.500966	0.636181	-0.359857
49	C	-6.674696	1.350685	1.228968
50	H	-5.228821	2.377968	2.466071
51	C	-5.794183	0.241891	-0.728907
52	H	-3.674909	0.352122	-1.001127
53	C	-6.886611	0.591415	0.073177
54	H	-7.892622	0.289374	-0.192166
55	O	-5.87919	-0.477613	-1.886408
56	C	-7.162428	-0.893246	-2.326224
57	H	-7.823098	-0.037582	-2.515864
58	H	-6.999797	-1.434238	-3.259391
59	H	-7.643053	-1.562855	-1.60131
60	H	-7.526692	1.626648	1.843349

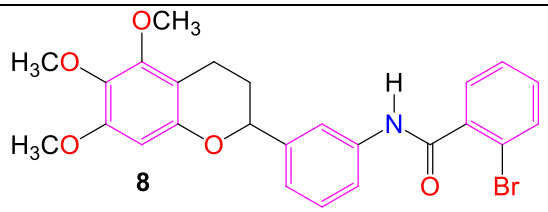
Table S7: Compound 7 Cartesian Z matrix

Compound 7		 7		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-4.218268	0.980755	0.379489
2	C	-3.64591	0.904953	-0.893164
3	C	-5.183806	0.014626	0.719712
4	C	-4.02589	-0.076503	-1.818502
5	C	-4.987913	-1.019658	-1.462998
6	C	-5.571228	-0.984822	-0.178532
7	H	-3.551791	-0.072599	-2.791179
8	O	-5.694398	0.057935	1.996579
9	C	-7.104181	0.291192	2.105942
10	H	-7.677544	-0.51506	1.643373
11	H	-7.318621	0.336303	3.175802
12	H	-7.377539	1.248165	1.643367
13	O	-6.533054	-1.907144	0.175533
14	C	-6.00706	-3.172073	0.58677
15	H	-5.349514	-3.060304	1.457349
16	H	-6.866058	-3.789727	0.858415

17	H	-5.458943	-3.654081	-0.229892
18	O	-5.41848	-2.028659	-2.275137
19	C	-4.87015	-2.109972	-3.581555
20	H	-3.78492	-2.271956	-3.557065
21	H	-5.351374	-2.966328	-4.056044
22	H	-5.083338	-1.205786	-4.165291
23	O	-2.690979	1.786591	-1.344373
24	C	-3.185689	3.233928	0.563547
25	H	-2.739583	3.965964	1.242983
26	H	-3.955953	3.753862	-0.017946
27	C	-2.118912	2.720644	-0.415987
28	H	-1.792745	3.550715	-1.053361
29	C	-0.885276	2.146072	0.275463
30	C	-0.099934	2.977321	1.086499
31	C	0.643966	0.307739	0.728838
32	C	1.033725	2.47117	1.718852
33	H	-0.369427	4.021184	1.221875
34	C	1.403032	1.13622	1.56329
35	H	1.631809	3.118149	2.353717
36	H	2.269646	0.742628	2.080832
37	C	-0.49399	0.820012	0.089232
38	H	-1.067383	0.176335	-0.567836
39	C	-3.809355	2.071389	1.339593
40	H	-4.675672	2.409657	1.914997
41	H	-3.089825	1.686067	2.074008
42	N	0.943349	-1.065151	0.540542
43	H	0.153186	-1.697383	0.591638
44	C	2.136853	-1.76419	0.615407
45	O	2.114919	-2.96597	0.864631
46	C	3.426804	-1.063631	0.315002
47	C	4.579651	-1.580234	0.924821
48	C	3.530259	-0.025946	-0.607293
49	C	5.8229	-1.023865	0.640542
50	H	4.468896	-2.411861	1.60744
51	C	4.781755	0.518509	-0.925375
52	H	2.663279	0.375436	-1.116733
53	C	5.942111	0.031588	-0.297211
54	O	4.755948	1.55989	-1.80861
55	C	5.795769	1.713122	-2.774256
56	H	6.064925	0.750021	-3.225094
57	H	5.382102	2.362567	-3.549281
58	H	6.686639	2.172561	-2.342283
59	O	7.146586	0.650168	-0.524083
60	C	8.186842	-0.143688	-1.108817
61	H	7.872691	-0.546341	-2.080235
62	H	9.031092	0.532678	-1.256115
63	H	8.480982	-0.963479	-0.451003
64	O	6.990318	-1.413614	1.234998
65	C	6.92915	-2.440291	2.216059

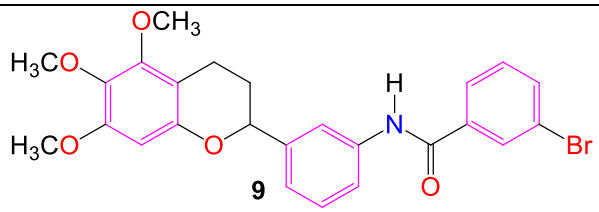
66	H	6.565319	-3.384227	1.792442
67	H	7.951564	-2.573637	2.572018
68	H	6.286246	-2.153237	3.056811

Table S8: Compound 8 Cartesian Z matrix

Compound 8				
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.49986	1.116121	0.171064
2	C	-3.096446	0.683884	-1.094936
3	C	-4.402427	0.302469	0.88196
4	C	-3.581771	-0.502038	-1.66214
5	C	-4.479257	-1.28943	-0.943667
6	C	-4.89139	-0.893448	0.346697
7	H	-3.238595	-0.773494	-2.651799
8	O	-4.742972	0.703712	2.152753
9	C	-6.129766	0.988745	2.37696
10	H	-6.747016	0.099849	2.230518
11	H	-6.202261	1.328101	3.412363
12	H	-6.475097	1.789411	1.710568
13	O	-5.788812	-1.661077	1.057759
14	C	-5.20122	-2.781514	1.725341
15	H	-4.437133	-2.455978	2.44154
16	H	-6.011444	-3.280399	2.261682
17	H	-4.759542	-3.479944	1.006496
18	O	-5.000467	-2.469421	-1.388818
19	C	-4.627294	-2.915047	-2.683572
20	H	-3.546537	-3.091952	-2.756093
21	H	-5.157316	-3.855316	-2.841436
22	H	-4.924895	-2.197357	-3.458202
23	O	-2.217164	1.386613	-1.8873
24	C	-2.477376	3.308909	-0.397471
25	H	-1.954717	4.186265	-0.005381
26	H	-3.321759	3.67112	-0.995365
27	C	-1.541332	2.52312	-1.328841
28	H	-1.309448	3.14172	-2.203677
29	C	-0.222379	2.126674	-0.670508
30	C	0.657759	3.126477	-0.231595
31	C	1.368045	0.448329	0.078337
32	C	1.86782	2.786099	0.368821
33	H	0.398617	4.174087	-0.359164
34	C	2.22359	1.449764	0.548475

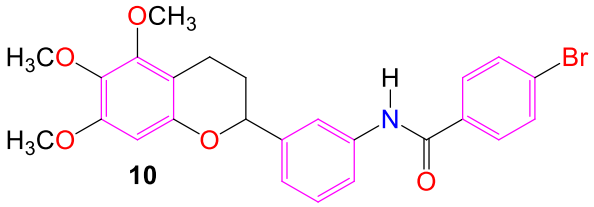
35	H	2.535554	3.567203	0.719876
36	H	3.141123	1.183704	1.060366
37	C	0.152101	0.79031	-0.528058
38	H	-0.495969	0.005314	-0.90017
39	C	-2.983292	2.41611	0.738144
40	H	-3.772542	2.919046	1.303891
41	H	-2.172061	2.227387	1.45362
42	N	1.674663	-0.928853	0.240144
43	H	0.943523	-1.527196	0.606865
44	O	3.015513	-2.735738	0.502333
45	C	3.983883	-0.881177	-0.63731
46	C	3.863479	-0.704847	-2.02196
47	C	5.187392	-0.515617	-0.02827
48	C	4.918721	-0.191043	-2.773202
49	H	2.932259	-0.980963	-2.507114
50	C	6.24668	0.011032	-0.763035
51	C	6.111822	0.163471	-2.143003
52	H	4.808766	-0.067543	-3.845929
53	H	7.161457	0.298061	-0.257338
54	H	6.93887	0.566431	-2.71954
55	C	2.876902	-1.586641	0.111698
56	Br	5.36767	-0.646359	1.870829

Table S9: Compound 9 Cartesian Z matrix

Compound 9		 **9**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.980358	1.004605	0.19529
2	C	-3.507154	0.614483	-1.060062
3	C	-4.85454	0.12744	0.865111
4	C	-3.897597	-0.591557	-1.657116
5	C	-4.768746	-1.442204	-0.979439
6	C	-5.248949	-1.089449	0.300005
7	H	-3.504119	-0.828453	-2.636881
8	O	-5.263043	0.490723	2.12714
9	C	-6.672069	0.684789	2.306111
10	H	-7.226241	-0.239283	2.128686
11	H	-6.801041	1.005448	3.341957
12	H	-7.0446	1.470628	1.636753
13	O	-6.120715	-1.920272	0.970589
14	C	-5.488521	-3.012937	1.643611
15	H	-4.769902	-2.65235	2.389463

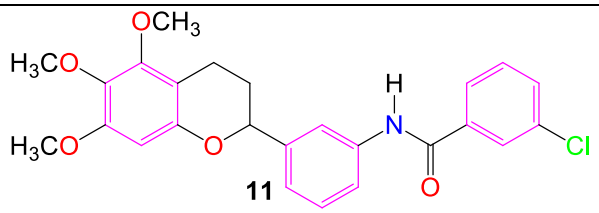
16	H	-6.284322	-3.567534	2.145688
17	H	-4.981604	-3.672802	0.931466
18	O	-5.199946	-2.645981	-1.455533
19	C	-4.755856	-3.050774	-2.741436
20	H	-3.664407	-3.15996	-2.778047
21	H	-5.221017	-4.019645	-2.928014
22	H	-5.070732	-2.342555	-3.517914
23	O	-2.645621	1.380555	-1.812982
24	C	-3.075926	3.263325	-0.312315
25	H	-2.622724	4.165963	0.107815
26	H	-3.918915	3.580917	-0.936856
27	C	-2.061161	2.548024	-1.217674
28	H	-1.835969	3.191359	-2.076296
29	C	-0.744484	2.223602	-0.516317
30	C	0.054143	3.268245	-0.029301
31	C	0.91956	0.629572	0.264394
32	C	1.26164	2.990994	0.608036
33	H	-0.264899	4.299989	-0.148791
34	C	1.693536	1.676285	0.777806
35	H	1.867892	3.805005	0.994207
36	H	2.616808	1.465361	1.304616
37	C	-0.292859	0.910396	-0.381214
38	H	-0.87814	0.094344	-0.788882
39	C	-3.566351	2.32674	0.794425
40	H	-4.405375	2.773	1.335553
41	H	-2.771754	2.179555	1.537804
42	N	1.289067	-0.731992	0.417252
43	H	0.558165	-1.357168	0.736676
44	O	2.642887	-2.426641	1.049214
45	C	3.717812	-0.671048	-0.135054
46	C	3.632478	0.074108	-1.318348
47	C	4.791304	0.574079	-1.910498
48	H	2.668738	0.251171	-1.781493
49	C	6.111387	-0.399192	-0.154923
50	C	6.03964	0.350412	-1.328532
51	H	4.726406	1.142269	-2.833339
52	H	6.943199	0.74413	-1.779781
53	C	2.531385	-1.332803	0.507886
54	B	r 7.81913500	-0.720268	0.645086
55	C	4.970279	-0.924938	0.439247
56	H	5.031301	-1.536347	1.331262

Table S10: Compound 10 Cartesian Z matrix

Compound 10		 10		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.906928	1.125557	-0.048333
2	C	-3.305947	0.600825	-1.195294
3	C	-4.937767	0.376092	0.549996
4	C	-3.718583	-0.614233	-1.758153
5	C	-4.745356	-1.336773	-1.153696
6	C	-5.359525	-0.846952	0.018882
7	H	-3.219799	-0.958472	-2.654578
8	O	-5.478068	0.869995	1.714345
9	C	-6.87568	1.186985	1.680377
10	H	-7.480562	0.297294	1.493179
11	H	-7.112854	1.600915	2.662652
12	H	-7.084806	1.941576	0.911474
13	O	-6.384191	-1.55028	0.615022
14	C	-5.948902	-2.63625	1.438233
15	H	-5.305195	-2.279727	2.251444
16	H	-6.851382	-3.08386	1.860305
17	H	-5.414765	-3.387845	0.847231
18	O	-5.214724	-2.536493	-1.603382
19	C	-4.641535	-3.074706	-2.785102
20	H	-3.569131	-3.273048	-2.662123
21	H	-5.162668	-4.015054	-2.969689
22	H	-4.785589	-2.406484	-3.643208
23	O	-2.286208	1.234183	-1.869693
24	C	-2.746179	3.258832	-0.576704
25	H	-2.275284	4.15381	-0.159663
26	H	-3.466501	3.590586	-1.333432
27	C	-1.686328	2.396587	-1.279785
28	H	-1.292272	2.949685	-2.140356
29	C	-0.509424	2.028068	-0.37997
30	C	0.308035	3.043132	0.137441
31	C	0.884765	0.377528	0.738954
32	C	1.389707	2.725074	0.955889
33	H	0.102423	4.083271	-0.100054
34	C	1.674489	1.399001	1.278829
35	H	2.010394	3.517738	1.362974
36	H	2.496813	1.160042	1.943016
37	C	-0.200371	0.699039	-0.088696
38	H	-0.797331	-0.099128	-0.514477
39	C	-3.461315	2.454603	0.511582

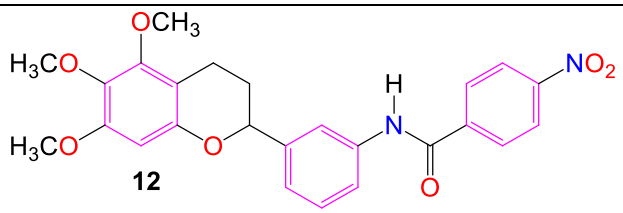
40	H	-4.322419	3.006815	0.898214
41	H	-2.789548	2.305215	1.367203
42	N	1.106525	-0.991379	1.039325
43	H	0.286307	-1.526756	1.299433
44	O	2.202354	-2.725327	1.98533
45	C	3.582891	-1.177235	0.832277
46	C	3.72548	-0.51348	-0.393781
47	C	4.988416	-0.160138	-0.864991
48	H	2.853095	-0.281146	-0.994058
49	C	6.109974	-0.465409	-0.0957
50	H	5.101495	0.343767	-1.817841
51	C	2.266692	-1.678667	1.34975
52	C	4.728205	-1.499418	1.572321
53	H	4.610981	-2.048484	2.500299
54	B	r 7.84225200	0.033793	-0.72904
55	C	5.993839	-1.134385	1.122241
56	H	6.878881	-1.372488	1.700803

Table S11: Compound 11 Cartesian Z matrix

Compound 11				
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.354247	1.050621	0.132829
2	C	-2.863197	0.609964	-1.098727
3	C	-4.269057	0.218996	0.806483
4	C	-3.274366	-0.601788	-1.669708
5	C	-4.185617	-1.406748	-0.988949
6	C	-4.685293	-1.002534	0.267608
7	H	-2.864987	-0.878838	-2.632268
8	O	-4.696045	0.631177	2.047175
9	C	-6.102733	0.869404	2.187059
10	H	-6.678661	-0.044063	2.024684
11	H	-6.245949	1.225293	3.209443
12	H	-6.43769	1.644199	1.485739
13	O	-5.596261	-1.788034	0.940672
14	C	-5.012011	-2.877591	1.660464
15	H	-4.300585	-2.515436	2.41243
16	H	-5.835093	-3.393887	2.159393
17	H	-4.508281	-3.572767	0.980371
18	O	-4.640388	-2.611425	-1.440173
19	C	-4.17834	-3.066667	-2.702667

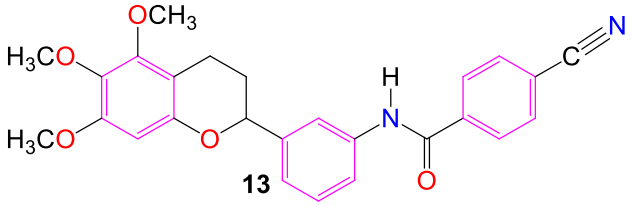
20	H	-3.089982	-3.20792	-2.709639
21	H	-4.667081	-4.027005	-2.87231
22	H	-4.45418	-2.37308	-3.506711
23	O	-1.962159	1.328388	-1.852361
24	C	-2.374153	3.266938	-0.418817
25	H	-1.905411	4.168949	-0.014674
26	H	-3.193312	3.588663	-1.072292
27	C	-1.359295	2.497098	-1.278235
28	H	-1.096383	3.107729	-2.149908
29	C	-0.068855	2.158626	-0.53603
30	C	0.74922	3.195825	-0.065701
31	C	1.528331	0.544805	0.337982
32	C	1.932975	2.905762	0.609334
33	H	0.463846	4.231644	-0.227663
34	C	2.321346	1.585691	0.833883
35	H	2.554329	3.714636	0.982064
36	H	3.225535	1.366397	1.389575
37	C	0.340051	0.838288	-0.345791
38	H	-0.259902	0.025992	-0.739441
39	C	-2.916084	2.377789	0.702933
40	H	-3.753924	2.863211	1.211158
41	H	-2.142929	2.230447	1.468585
42	N	1.852811	-0.82088	0.546242
43	H	1.09571	-1.412718	0.868161
44	O	3.138342	-2.530961	1.272029
45	C	4.29547	-0.851543	0.055358
46	C	4.262006	-0.146888	-1.154949
47	C	5.450259	0.295774	-1.734125
48	H	3.316012	0.042746	-1.648587
49	C	6.696543	-0.653957	0.087863
50	C	6.676376	0.055447	-1.113404
51	H	5.425641	0.832236	-2.677606
52	H	7.603657	0.404286	-1.553867
53	C	3.073656	-1.454259	0.690152
54	C	5.524293	-1.123173	0.670423
55	H	5.545243	-1.704648	1.584265
56	C	1 8.23783100	-0.971668	0.873826

Table S12: Compound S12 Cartesian Z matrix

Compound 12				
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	3.037136	-1.112718	0.035865
2	C	2.509773	-0.61768	-1.159802
3	C	4.015919	-0.338953	0.687636
4	C	2.946122	0.591989	-1.716663
5	C	3.92008	1.339379	-1.057687
6	C	4.459099	0.879106	0.162525
7	H	2.504712	0.913276	-2.650896
8	O	4.481796	-0.802759	1.89617
9	C	5.881143	-1.105075	1.961153
10	H	6.488787	-0.212937	1.795135
11	H	6.057109	-1.495788	2.965638
12	H	6.148174	-1.873295	1.224228
13	O	5.431602	1.607942	0.813685
14	C	4.924036	2.694141	1.593931
15	H	4.235317	2.334347	2.367818
16	H	5.788777	3.163667	2.068186
17	H	4.415599	3.429013	0.960585
18	O	4.403836	2.537671	-1.497155
19	C	3.899859	3.049128	-2.721177
20	H	2.819033	3.232865	-2.670056
21	H	4.418306	3.994453	-2.887416
22	H	4.107753	2.370452	-3.557833
23	O	1.547601	-1.276905	-1.889851
24	C	1.937822	-3.269469	-0.527196
25	H	1.449043	-4.161531	-0.124872
26	H	2.71242	-3.60728	-1.22556
27	C	0.919111	-2.434329	-1.318153
28	H	0.592374	-3.008639	-2.192955
29	C	-0.321154	-2.062872	-0.509381
30	C	-1.156162	-3.079078	-0.023257
31	C	-1.813118	-0.404836	0.469373
32	C	-2.295796	-2.756195	0.710403
33	H	-0.919966	-4.121433	-0.219203
34	C	-2.622807	-1.427837	0.978465
35	H	-2.932032	-3.54799	1.095068
36	H	-3.494659	-1.18714	1.574649
37	C	-0.668881	-0.732736	-0.273993
38	H	-0.055439	0.063932	-0.678894
39	C	2.567368	-2.435347	0.59112

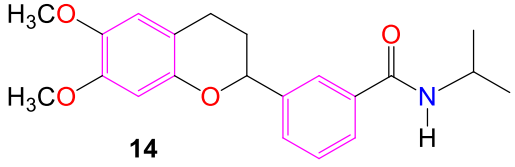
40	H	3.404836	-2.969496	1.048686
41	H	1.835263	-2.27586	1.393669
42	N	-2.065738	0.966073	0.715885
43	H	-1.256348	1.518313	0.973835
44	O	-3.165547	2.681744	1.684861
45	C	-4.542016	1.143585	0.511516
46	C	-4.681591	0.431577	-0.690035
47	C	-5.936346	0.081931	-1.170659
48	H	-3.803595	0.163983	-1.267463
49	C	-6.961726	1.14879	0.743923
50	C	-7.099617	0.425535	-0.456401
51	H	-6.025079	-0.461107	-2.108127
52	C	-3.238854	1.642674	1.034564
53	C	-5.705395	1.510308	1.205889
54	H	-5.600784	2.094679	2.113848
55	H	-7.849736	1.428921	1.304909
56	N	-8.350802	0.020868	-0.900965
57	H	-9.137487	0.551984	-0.555742
58	H	-8.424921	-0.19363	-1.88511

Table S13: Compound 13 Cartesian Z matrix

Compound 13		 13		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	3.168555	-1.127893	-0.030793
2	C	2.591708	-0.588359	-1.183106
3	C	4.18955	-0.388246	0.596291
4	C	3.018447	0.631647	-1.724132
5	C	4.035514	1.34407	-1.091784
6	C	4.624927	0.839473	0.087366
7	H	2.538844	0.987126	-2.626623
8	O	4.704927	-0.897255	1.765136
9	C	6.102722	-1.21627	1.75698
10	H	6.712689	-0.325318	1.594219
11	H	6.31798	-1.643221	2.738682
12	H	6.326955	-1.961237	0.983036
13	O	5.639991	1.53242	0.710988
14	C	5.193626	2.6142	1.533874
15	H	4.530977	2.254725	2.330423
16	H	6.089582	3.052857	1.978524
17	H	4.67647	3.373781	0.938059
18	O	4.517415	2.546742	-1.519063

19	C	3.972162	3.098216	-2.708027
20	H	2.898144	3.299899	-2.606434
21	H	4.500887	4.038023	-2.872445
22	H	4.132301	2.437237	-3.568829
23	O	1.582925	-1.210933	-1.884419
24	C	2.013479	-3.252035	-0.606499
25	H	1.532318	-4.150628	-0.209342
26	H	2.747424	-3.57693	-1.352947
27	C	0.969962	-2.378838	-1.320526
28	H	0.591159	-2.921134	-2.194702
29	C	-0.223598	-2.017769	-0.439797
30	C	-1.056922	-3.035779	0.045718
31	C	-1.632488	-0.378517	0.674582
32	C	-2.153815	-2.725575	0.846652
33	H	-0.851196	-4.07323	-0.203059
34	C	-2.438304	-1.402753	1.183475
35	H	-2.786113	-3.521353	1.228801
36	H	-3.271564	-1.168902	1.836158
37	C	-0.532036	-0.691454	-0.135082
38	H	0.07731	0.110036	-0.53627
39	C	2.709417	-2.462408	0.504693
40	H	3.561863	-3.021304	0.9007
41	H	2.022288	-2.321914	1.349624
42	N	-1.8591	0.987512	0.991294
43	H	-1.050359	1.515567	1.298555
44	O	-3.007753	2.721615	1.877578
45	C	-4.320372	1.172573	0.652363
46	C	-4.397211	0.539081	-0.595906
47	C	-5.632086	0.189113	-1.131108
48	H	-3.4939	0.328893	-1.156751
49	C	-6.736725	1.105561	0.833481
50	C	-6.808599	0.460836	-0.413287
51	H	-5.694501	-0.292194	-2.100957
52	C	-3.030152	1.674786	1.240379
53	C	-5.499386	1.469212	1.349746
54	H	-5.42589	1.996801	2.294151
55	H	-7.648562	1.323079	1.378869
56	C	-8.082001	0.085949	-0.956596
57	N	-9.114242	-0.220981	-1.396572

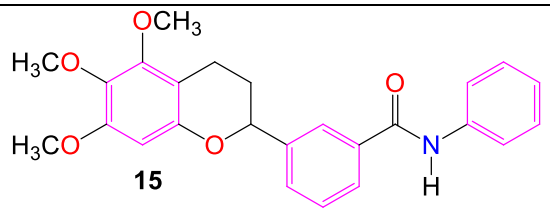
Table S14: Compound 14 Cartesian Z matrix

Compound 14		 **14**
Center	Atom	Standard orientation: Coordinates (Angstroms)

Number		X	Y	Z
1	C	-1.796776	-0.803285	0.408576
2	C	-1.723009	0.469421	0.982339
3	C	-3.021288	-1.190284	-0.166259
4	C	-2.827593	1.33175	1.011967
5	C	-4.031693	0.926497	0.440348
6	C	-4.135042	-0.344464	-0.162828
7	H	-2.70626	2.300005	1.479496
8	O	-3.06873	-2.41934	-0.784796
9	C	-3.977143	-3.372352	-0.220246
10	H	-5.010385	-3.024212	-0.286321
11	H	-3.85361	-4.287543	-0.803396
12	H	-3.725494	-3.577372	0.82827
13	O	-5.328417	-0.75755	-0.718182
14	C	-5.555857	-0.265584	-2.041223
15	H	-4.764693	-0.595679	-2.725282
16	H	-6.512492	-0.681716	-2.365576
17	H	-5.616395	0.82822	-2.048866
18	O	-5.16215	1.691701	0.393923
19	C	-5.117343	2.977525	0.99141
20	H	-4.372352	3.623843	0.509696
21	H	-6.110417	3.407699	0.853192
22	H	-4.895833	2.916696	2.06436
23	O	-0.587018	0.965038	1.575057
24	C	0.359481	-1.291435	1.540023
25	H	1.304653	-1.838508	1.479494
26	H	-0.086035	-1.511143	2.517526
27	C	0.636408	0.218406	1.470238
28	H	1.196994	0.516732	2.363841
29	C	1.448019	0.632201	0.245557
30	C	2.760305	0.148725	0.127332
31	C	1.722636	1.832575	-1.833604
32	C	3.536643	0.509451	-0.971454
33	H	3.193587	-0.500038	0.878443
34	H	1.319604	2.49168	-2.597285
35	C	0.932618	1.483024	-0.73386
36	H	-0.071896	1.87548	-0.637049
37	C	-0.595677	-1.716928	0.422301
38	H	-0.913883	-2.754599	0.556619
39	H	-0.0758	-1.680295	-0.544033
40	C	6.56916	-0.065353	0.410045
41	H	6.21341	0.874716	0.848439
42	C	7.632776	0.246091	-0.649252
43	C	7.108554	-0.960896	1.528968
44	H	7.211044	0.848931	-1.456158
45	H	8.469781	0.796578	-0.207362
46	H	8.032602	-0.679595	-1.082201
47	H	6.341697	-1.152735	2.28397
48	H	7.447977	-1.925614	1.132153

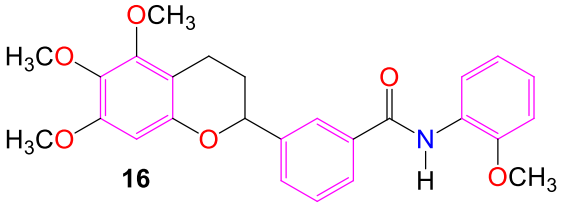
49	H	7.966063	-0.486013	2.014202
50	O	4.833266	0.090826	-1.187002
51	N	5.363353	-0.730378	-0.124289
52	H	5.659916	-1.567102	-0.632175
53	C	3.020449	1.35318	-1.963165
54	H	3.645372	1.619237	-2.809246

Table S15: Compound 15 Cartesian Z matrix

Compound 15				
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.402455	-0.779316	0.468646
2	C	-2.2932	0.529081	0.948148
3	C	-3.658031	-1.19641	-0.010658
4	C	-3.391463	1.39916	0.97932
5	C	-4.626685	0.963874	0.504218
6	C	-4.767032	-0.344485	-0.004547
7	H	-3.241749	2.39606	1.372522
8	O	-3.742212	-2.464491	-0.539374
9	C	-4.623709	-3.370482	0.135141
10	H	-5.657917	-3.021177	0.097318
11	H	-4.532404	-4.324479	-0.388668
12	H	-4.31962	-3.503954	1.18126
13	O	-5.990222	-0.786605	-0.463688
14	C	-6.293869	-0.377911	-1.799858
15	H	-5.543078	-0.752554	-2.50611
16	H	-7.267126	-0.811122	-2.041748
17	H	-6.355805	0.713355	-1.872602
18	O	-5.755642	1.731332	0.468513
19	C	-5.675233	3.053764	0.976033
20	H	-4.957034	3.662555	0.411852
21	H	-6.673638	3.479272	0.864738
22	H	-5.394525	3.062598	2.036695
23	O	-1.123882	1.056274	1.442242
24	C	-0.185042	-1.201843	1.505657
25	H	0.753449	-1.758387	1.429113
26	H	-0.571259	-1.348552	2.521163
27	C	0.089004	0.297815	1.313679
28	H	0.705581	0.65457	2.146909
29	C	0.821913	0.622855	0.014401
30	C	2.114996	0.10748	-0.16613
31	C	0.975446	1.708935	-2.140615

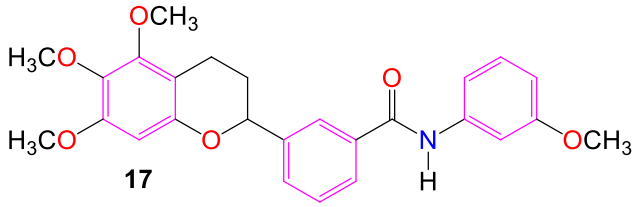
32	C	2.815682	0.394902	-1.333368
33	H	2.587171	-0.507816	0.590164
34	H	0.53191	2.335108	-2.90931
35	C	0.257352	1.432276	-0.973233
36	H	-0.731682	1.848988	-0.830236
37	C	-1.2063	-1.699573	0.48001
38	H	-1.520487	-2.721725	0.709296
39	H	-0.744521	-1.73958	-0.515344
40	O	4.099667	-0.049284	-1.608158
41	N	4.621774	-0.943182	-0.625419
42	H	4.724192	-1.832	-1.111132
43	C	2.252396	1.1947	-2.333376
44	H	2.822253	1.399706	-3.233426
45	C	5.866808	-0.492458	-0.115735
46	C	6.797314	-1.448295	0.314708
47	C	6.143028	0.869858	0.045647
48	C	7.987371	-1.041192	0.913453
49	H	6.585658	-2.507091	0.185
50	C	7.343083	1.262917	0.636652
51	H	5.427458	1.606102	-0.29971
52	C	8.269442	0.316317	1.076983
53	H	8.700647	-1.790973	1.243227
54	H	7.552876	2.322361	0.752667
55	H	9.200659	0.631397	1.536953

Table S16: Compound 16 Cartesian Z matrix

Compound 16		 **16**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.847886	-0.771046	0.454651
2	C	-2.840138	0.532783	0.958721
3	C	-4.066948	-1.273992	-0.036023
4	C	-4.002024	1.315473	1.001849
5	C	-5.199287	0.795917	0.51449
6	C	-5.238056	-0.509884	-0.017855
7	H	-3.929792	2.313551	1.413512
8	O	-4.053745	-2.534963	-0.5883
9	C	-4.861652	-3.517947	0.069995
10	H	-5.919652	-3.247978	0.039954
11	H	-4.69935	-4.452323	-0.471748
12	H	-4.545612	-3.647483	1.113095

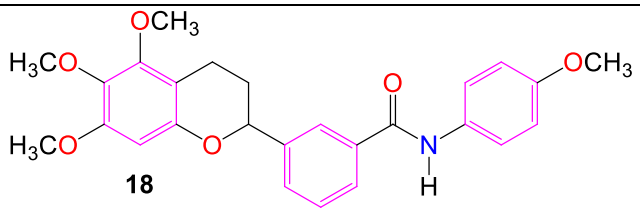
13	O	-6.423134	-1.035944	-0.488719
14	C	-6.75134	-0.632014	-1.82042
15	H	-5.97193	-0.939271	-2.528197
16	H	-7.688588	-1.13315	-2.073245
17	H	-6.894424	0.452551	-1.878241
18	O	-6.38365	1.475528	0.488306
19	C	-6.404794	2.791671	1.017381
20	H	-5.733253	3.462207	0.465855
21	H	-7.432257	3.142312	0.909278
22	H	-6.128202	2.80448	2.079114
23	O	-1.716041	1.138374	1.466672
24	C	-0.606973	-1.04215	1.491856
25	H	0.371522	-1.523584	1.408258
26	H	-0.983642	-1.237603	2.502782
27	C	-0.447789	0.477366	1.32913
28	H	0.136791	0.864375	2.171853
29	C	0.261945	0.881914	0.03943
30	C	1.590479	0.468438	-0.14505
31	C	0.339389	2.016488	-2.094121
32	C	2.27212	0.829502	-1.303558
33	H	2.106229	-0.124131	0.600861
34	H	-0.147644	2.622039	-2.853036
35	C	-0.359551	1.665	-0.935153
36	H	-1.377524	2.00351	-0.788622
37	C	-1.584414	-1.596477	0.452614
38	H	-1.819342	-2.644245	0.660187
39	H	-1.11835	-1.580355	-0.541347
40	O	3.58386	0.486369	-1.581439
41	N	4.174118	-0.370833	-0.601052
42	H	4.343278	-1.256671	-1.073978
43	C	1.651883	1.603514	-2.290773
44	H	2.207283	1.867956	-3.184359
45	C	5.391698	0.17012	-0.122247
46	C	6.424029	-0.732919	0.212802
47	C	5.578585	1.534169	0.091211
48	C	7.614473	-0.262105	0.762589
49	C	6.77632	2.0035	0.636715
50	H	4.786786	2.220646	-0.184511
51	C	7.788265	1.110452	0.97509
52	H	8.409549	-0.951925	1.019825
53	H	6.910536	3.068962	0.794476
54	H	8.719177	1.469377	1.402619
55	O	6.140269	-2.050107	-0.055193
56	C	7.153171	-3.015686	0.182848
57	H	6.7347	-3.975182	-0.123993
58	H	8.05483	-2.806876	-0.40638
59	H	7.420554	-3.06194	1.245707

Table S17: Compound 17 Cartesian Z matrix

Compound 17		 17		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.012923	-0.858695	0.367509
2	C	-2.944633	0.376109	1.019034
3	C	-4.267245	-1.272182	-0.118051
4	C	-4.080365	1.174677	1.210648
5	C	-5.313251	0.743816	0.725603
6	C	-5.413867	-0.488683	0.046642
7	H	-3.960716	2.115263	1.731992
8	O	-4.315118	-2.459089	-0.813597
9	C	-5.12176	-3.493657	-0.237675
10	H	-6.171779	-3.197119	-0.18663
11	H	-5.010141	-4.361067	-0.891869
12	H	-4.764461	-3.752728	0.767257
13	O	-6.633809	-0.927731	-0.424162
14	C	-7.011998	-0.359784	-1.680685
15	H	-6.275034	-0.597051	-2.457489
16	H	-7.973493	-0.806188	-1.944684
17	H	-7.127361	0.726757	-1.602104
18	O	-6.477565	1.448733	0.837449
19	C	-6.437117	2.692331	1.519039
20	H	-5.773356	3.40883	1.018227
21	H	-7.458226	3.076257	1.504117
22	H	-6.111274	2.571745	2.559801
23	O	-1.781133	0.892098	1.537583
24	C	-0.734968	-1.301331	1.254149
25	H	0.22455	-1.791833	1.066877
26	H	-1.069474	-1.605701	2.252873
27	C	-0.540313	0.222802	1.262011
28	H	0.093714	0.494368	2.114025
29	C	0.120341	0.759893	-0.005164
30	C	1.429437	0.346773	-0.297909
31	C	0.128478	2.130666	-1.997023
32	C	2.065747	0.826273	-1.438721
33	H	1.963604	-0.336195	0.351512
34	H	-0.377985	2.827879	-2.658189
35	C	-0.525583	1.66071	-0.854052
36	H	-1.527913	1.998102	-0.622147
37	C	-1.775221	-1.707293	0.207311
38	H	-2.030404	-2.766376	0.303747
39	H	-1.35578	-1.586184	-0.800123

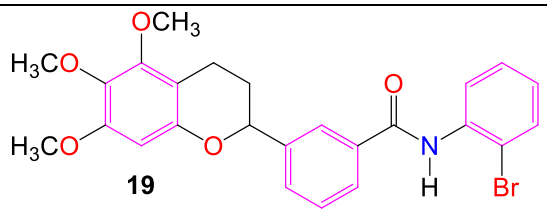
40	O	3.357798	0.495804	-1.814734
41	N	3.964927	-0.490533	-0.980009
42	H	4.093356	-1.299481	-1.584361
43	C	1.420987	1.719489	-2.301146
44	H	1.941931	2.074696	-3.183929
45	C	5.203876	-0.041455	-0.455581
46	C	6.200465	-0.988634	-0.217667
47	C	5.401732	1.299407	-0.09609
48	C	7.398356	-0.607936	0.398395
49	C	6.603488	1.661441	0.502141
50	H	4.631295	2.033295	-0.294719
51	C	7.610255	0.727229	0.761839
52	H	6.765729	2.699565	0.777618
53	H	8.533127	1.043595	1.231136
54	O	8.299497	-1.616826	0.587793
55	C	9.544615	-1.29865	1.189478
56	H	10.101938	-2.235121	1.240415
57	H	10.110874	-0.574005	0.590699
58	H	9.414924	-0.9009	2.203996
59	H	6.069311	-2.030481	-0.494866

Table S18: Compound 18 Cartesian Z matrix

Compound 18		 **18**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.10331	-0.679005	0.593609
2	C	-2.913918	0.679275	0.864154
3	C	-4.396122	-1.098024	0.228846
4	C	-3.969086	1.59962	0.80152
5	C	-5.24215	1.162211	0.442454
6	C	-5.463846	-0.198796	0.144736
7	H	-3.757218	2.635294	1.032439
8	O	-4.561276	-2.425136	-0.097296
9	C	-5.452021	-3.172577	0.739706
10	H	-6.469876	-2.779668	0.687967
11	H	-5.428074	-4.197838	0.364065
12	H	-5.107719	-3.163235	1.781836
13	O	-6.724696	-0.640979	-0.197869
14	C	-7.063847	-0.427997	-1.570472
15	H	-6.36181	-0.94688	-2.234349
16	H	-8.065892	-0.840587	-1.708768

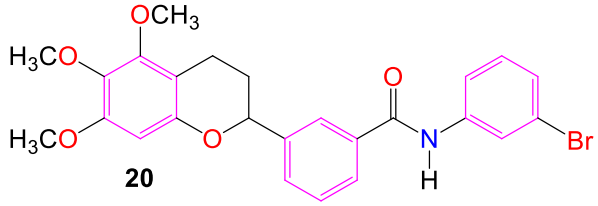
17	H	-7.076685	0.640683	-1.810963
18	O	-6.335378	1.972926	0.330008
19	C	-6.172451	3.35087	0.625581
20	H	-5.451952	3.829084	-0.050417
21	H	-7.154092	3.806041	0.485963
22	H	-5.846173	3.505596	1.661689
23	O	-1.701696	1.213768	1.229729
24	C	-0.865639	-1.054886	1.60438
25	H	0.042461	-1.664063	1.580652
26	H	-1.215544	-1.027717	2.643051
27	C	-0.531117	0.382742	1.177401
28	H	0.134761	0.828239	1.925618
29	C	0.162166	0.469889	-0.17992
30	C	1.42568	-0.12531	-0.319051
31	C	0.273051	1.197848	-2.482741
32	C	2.091888	-0.055807	-1.539157
33	H	1.902826	-0.636188	0.508478
34	H	-0.175361	1.715575	-3.325775
35	C	-0.408993	1.139985	-1.263441
36	H	-1.374385	1.618265	-1.155683
37	C	-1.950615	-1.64717	0.701785
38	H	-2.300719	-2.606466	1.093236
39	H	-1.533366	-1.858008	-0.291675
40	O	3.343909	-0.593872	-1.782216
41	N	3.876927	-1.335121	-0.677365
42	H	3.93325	-2.29178	-1.022582
43	C	1.520102	0.602849	-2.633585
44	H	2.061584	0.639168	-3.572938
45	C	5.171232	-0.858308	-0.323978
46	C	6.132522	-1.77315	0.129805
47	C	5.476979	0.50262	-0.328727
48	C	7.367303	-1.330544	0.584188
49	C	6.72455	0.950296	0.112605
50	H	4.744746	1.215372	-0.689276
51	C	7.675898	0.036643	0.577771
52	H	6.936948	2.012365	0.088355
53	H	5.9111	-2.837852	0.132342
54	O	8.922438	0.367938	1.034976
55	C	9.286195	1.738025	1.043007
56	H	10.302396	1.778675	1.438021
57	H	9.275582	2.167586	0.03264
58	H	8.625222	2.3306	1.68907
59	H	8.116384	-2.031388	0.937047

Table S19: Compound 19 Cartesian Z matrix

Compound 19		 19		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.170765	-0.715655	0.625139
2	C	-3.056189	0.669926	0.770788
3	C	-4.422668	-1.230563	0.241121
4	C	-4.146733	1.526839	0.568736
5	C	-5.378543	0.995103	0.193643
6	C	-5.523531	-0.397243	0.018933
7	H	-3.993549	2.588934	0.707785
8	O	-4.51132	-2.589414	0.038629
9	C	-5.411167	-3.296094	0.900733
10	H	-6.441283	-2.960749	0.761099
11	H	-5.321807	-4.350314	0.629528
12	H	-5.123683	-3.169687	1.952443
13	O	-6.743626	-0.932028	-0.339231
14	C	-7.023168	-0.859598	-1.739568
15	H	-6.26466	-1.398019	-2.320644
16	H	-7.996143	-1.334512	-1.885373
17	H	-7.074874	0.181376	-2.07675
18	O	-6.499551	1.736609	-0.048823
19	C	-6.413785	3.142738	0.119168
20	H	-5.681033	3.589799	-0.5649
21	H	-7.406115	3.533661	-0.110534
22	H	-6.149183	3.410703	1.149735
23	O	-1.890104	1.295363	1.14108
24	C	-0.972821	-0.882093	1.770816
25	H	-0.038732	-1.445582	1.849558
26	H	-1.374886	-0.771131	2.784733
27	C	-0.681869	0.521585	1.218251
28	H	-0.071622	1.069475	1.945643
29	C	0.067552	0.512034	-0.111883
30	C	1.348201	-0.060517	-0.149005
31	C	0.267102	1.063808	-2.457248
32	C	2.067588	-0.067228	-1.34043
33	H	1.80509	-0.477561	0.739578
34	H	-0.1535	1.50366	-3.356942
35	C	-0.468941	1.080768	-1.268683
36	H	-1.449215	1.539679	-1.2407
37	C	-1.983949	-1.611654	0.883079
38	H	-2.311581	-2.543939	1.3518
39	H	-1.507879	-1.897989	-0.064013

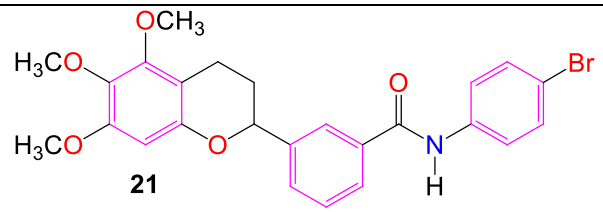
40	O	3.333368	-0.603614	-1.491792
41	N	3.800243	-1.325906	-0.328751
42	H	3.647175	-2.303236	-0.5758
43	C	1.532184	0.490064	-2.506658
44	H	2.115162	0.468471	-3.421211
45	C	5.191358	-1.104314	-0.157767
46	C	6.094281	-2.163509	-0.318196
47	C	5.693897	0.13807	0.262443
48	C	7.452871	-2.000698	-0.055727
49	C	7.054656	0.315213	0.495671
50	C	7.936633	-0.755397	0.341949
51	H	7.414518	1.287367	0.812696
52	H	5.718282	-3.125624	-0.657585
53	H	8.130202	-2.839389	-0.181326
54	H	8.994689	-0.610951	0.535829
55	Br	4.517417	1.606059	0.551596

Table S20: Compound 20 Cartesian Z matrix

Compound 20		 **20**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.565375	-0.708187	0.550693
2	C	-3.282666	0.619444	0.883699
3	C	-4.875342	-1.012895	0.136401
4	C	-4.26381	1.618943	0.835669
5	C	-5.555711	1.294293	0.427501
6	C	-5.870049	-0.032528	0.064924
7	H	-3.981842	2.625074	1.116774
8	O	-5.128725	-2.309286	-0.250225
9	C	-6.099872	-3.020461	0.527085
10	H	-7.083475	-2.550244	0.461279
11	H	-6.139137	-4.028723	0.109165
12	H	-5.79067	-3.078613	1.578573
13	O	-7.150161	-0.363697	-0.327248
14	C	-7.439566	-0.057726	-1.693809
15	H	-6.759815	-0.591542	-2.368964
16	H	-8.464483	-0.389923	-1.874196
17	H	-7.371008	1.019825	-1.878345
18	O	-6.581892	2.18907	0.324673
19	C	-6.325552	3.537343	0.684929
20	H	-5.553273	3.988054	0.048443

21	H	-7.266572	4.070395	0.541655
22	H	-6.017564	3.622924	1.73451
23	O	-2.043752	1.045083	1.301119
24	C	-1.388824	-1.293187	1.595543
25	H	-0.528644	-1.968286	1.566617
26	H	-1.761009	-1.28111	2.626645
27	C	-0.938068	0.131436	1.237188
28	H	-0.25788	0.494552	2.016426
29	C	-0.209284	0.222589	-0.101381
30	C	1.003008	-0.469907	-0.247873
31	C	0.015052	1.052501	-2.362037
32	C	1.697554	-0.395156	-1.450511
33	H	1.416075	-1.058699	0.562214
34	H	-0.369011	1.648112	-3.184983
35	C	-0.696477	0.991299	-1.160091
36	H	-1.620523	1.543743	-1.045363
37	C	-2.492371	-1.765261	0.64581
38	H	-2.92405	-2.709006	0.990904
39	H	-2.067557	-1.97023	-0.345746
40	O	2.909315	-1.02715	-1.698986
41	N	3.341191	-1.876662	-0.641972
42	H	3.308219	-2.818936	-1.025425
43	C	1.211089	0.361978	-2.520619
44	H	1.775303	0.398937	-3.446383
45	C	4.64166	-1.545363	-0.193
46	C	5.42954	-2.554365	0.379777
47	C	6.674082	-2.239408	0.917034
48	C	6.362707	0.051689	0.305405
49	C	7.159937	-0.930861	0.88677
50	H	5.064559	-3.577535	0.40809
51	H	7.28015	-3.024558	1.358835
52	H	8.130457	-0.681826	1.297996
53	B	r 7.00647600	1.853094	0.241382
54	C	5.110779	-0.227614	-0.234313
55	H	4.513826	0.552222	-0.686703

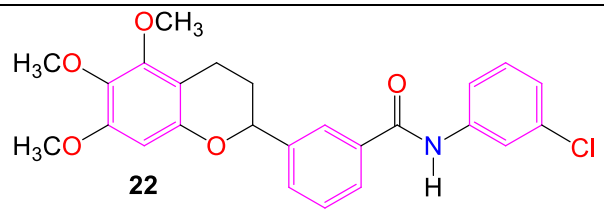
Table S21: Compound 21 Cartesian Z matrix

Compound 21		 **21**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.753061	-0.666887	0.621612

2	C	-3.553261	0.694643	0.865896
3	C	-5.058176	-1.089436	0.307591
4	C	-4.608783	1.615675	0.827114
5	C	-5.894027	1.174962	0.518944
6	C	-6.127173	-0.189835	0.247548
7	H	-4.388209	2.654129	1.036353
8	O	-5.234484	-2.420756	0.006448
9	C	-6.100267	-3.15542	0.880531
10	H	-7.119003	-2.762549	0.853463
11	H	-6.087629	-4.185959	0.519163
12	H	-5.724926	-3.131058	1.911603
13	O	-7.399247	-0.634967	-0.045165
14	C	-7.789062	-0.433835	-1.406209
15	H	-7.111641	-0.958222	-2.091006
16	H	-8.795156	-0.848091	-1.503658
17	H	-7.811565	0.632685	-1.6551
18	O	-6.989648	1.985229	0.43389
19	C	-6.816258	3.366799	0.706763
20	H	-6.119882	3.836193	0.000056
21	H	-7.802129	3.82065	0.596016
22	H	-6.453942	3.533743	1.728846
23	O	-2.327897	1.232689	1.181354
24	C	-1.480636	-1.03131	1.556606
25	H	-0.574579	-1.642288	1.509076
26	H	-1.791731	-0.987951	2.606925
27	C	-1.16153	0.399806	1.096886
28	H	-0.466882	0.855006	1.812429
29	C	-0.520497	0.467244	-0.287218
30	C	0.734321	-0.135149	-0.469295
31	C	-0.496074	1.170325	-2.60118
32	C	1.35037	-0.080765	-1.71525
33	H	1.240292	-0.638687	0.345583
34	H	-0.974959	1.681149	-3.431408
35	C	-1.12958	1.128393	-1.355508
36	H	-2.08781	1.612545	-1.215299
37	C	-2.598716	-1.63567	0.70383
38	H	-2.935944	-2.58747	1.123833
39	H	-2.218526	-1.864521	-0.300523
40	O	2.593804	-0.627866	-2.001853
41	N	3.158387	-1.368116	-0.923217
42	H	3.187858	-2.3317	-1.249989
43	C	0.741646	0.567658	-2.794414
44	H	1.246091	0.590745	-3.754527
45	C	4.449398	-0.896742	-0.582321
46	C	5.369697	-1.799333	-0.031515
47	C	6.614159	-1.356541	0.408153
48	C	6.943847	-0.008245	0.285714
49	H	5.112588	-2.851569	0.060137
50	H	7.324195	-2.056479	0.833398

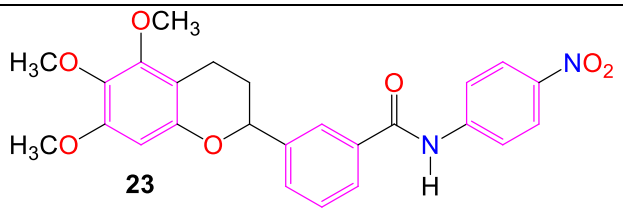
51	C	4.792793	0.454814	-0.70042
52	H	4.089057	1.152376	-1.137376
53	B	r 8.65709800	0.602568	0.878322
54	C	6.041929	0.896703	-0.268733
55	H	6.310703	1.942493	-0.36489

Table S22: Compound 22 Cartesian Z matrix

Compound 22		 22		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.985041	-0.738138	0.525863
2	C	-2.781552	0.591461	0.90555
3	C	-4.272627	-1.103386	0.09085
4	C	-3.818388	1.533989	0.883007
5	C	-5.086886	1.149623	0.453851
6	C	-5.321821	-0.179958	0.044277
7	H	-3.596678	2.544548	1.199926
8	O	-4.448307	-2.398303	-0.341134
9	C	-5.381664	-3.190171	0.403799
10	H	-6.390312	-2.775275	0.345701
11	H	-5.360023	-4.184207	-0.048098
12	H	-5.076248	-3.266216	1.455251
13	O	-6.578242	-0.570846	-0.36892
14	C	-6.877574	-0.234124	-1.726103
15	H	-6.163588	-0.702544	-2.41433
16	H	-7.879962	-0.61965	-1.92594
17	H	-6.871975	0.851463	-1.872124
18	O	-6.162426	1.986847	0.373087
19	C	-5.986745	3.334474	0.781031
20	H	-5.238436	3.850781	0.166109
21	H	-6.956307	3.816855	0.648947
22	H	-5.690039	3.401436	1.835199
23	O	-1.571896	1.073167	1.347294
24	C	-0.785397	-1.232266	1.569096
25	H	0.112359	-1.855632	1.525239
26	H	-1.164659	-1.276298	2.596739
27	C	-0.415068	0.227069	1.262152
28	H	0.238115	0.602133	2.058654
29	C	0.315778	0.404843	-0.066588
30	C	1.565633	-0.213879	-0.227014

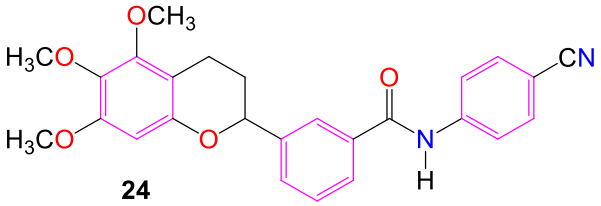
31	C	0.507483	1.323952	-2.295548
32	C	2.262326	-0.058968	-1.420731
33	H	2.005746	-0.8069	0.565554
34	H	0.095859	1.925508	-3.100652
35	C	-0.206911	1.181685	-1.102193
36	H	-1.161063	1.677571	-0.976041
37	C	-1.853424	-1.734414	0.594521
38	H	-2.232136	-2.712679	0.903773
39	H	-1.410788	-1.880412	-0.39967
40	O	3.509239	-0.613352	-1.680762
41	N	3.979672	-1.476585	-0.651631
42	H	3.998084	-2.404978	-1.068434
43	C	1.741072	0.706729	-2.46811
44	H	2.30797	0.806944	-3.387527
45	C	5.258723	-1.094273	-0.182092
46	C	6.09556	-2.081332	0.358448
47	C	7.318775	-1.720961	0.915556
48	H	5.785124	-3.122608	0.346533
49	H	7.963111	-2.489087	1.332259
50	C	5.65682	0.246882	-0.171601
51	H	5.022067	1.011088	-0.599018
52	C	6.890206	0.572628	0.38666
53	C	7.735253	-0.388804	0.937061
54	H	8.689235	-0.102982	1.363384
55	C	1 7.39310100	2.25948	0.391941

Table S23: Compound 23 Cartesian Z matrix

Compound 23		 **23**		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.781551	-0.72683	0.546262
2	C	-2.636723	0.619577	0.893292
3	C	-4.054088	-1.161005	0.131592
4	C	-3.716567	1.51238	0.856856
5	C	-4.968959	1.060047	0.447248
6	C	-5.145407	-0.288452	0.072565
7	H	-3.539205	2.539562	1.14714
8	O	-4.174534	-2.47264	- 0.268732
9	C	-5.05994	-3.288463	0.507635
10	H	-6.087546	-2.921923	0.454653

11	H	-4.998662	-4.291033	0.0787
12	H	-4.737379	-3.325593	1.556109
13	O	-6.385867	-0.746388	-0.320478
14	C	-6.703748	-0.467911	-1.686393
15	H	-5.973065	-0.928428	-2.36231
16	H	-7.689797	-0.901429	-1.868782
17	H	-6.744314	0.611589	-1.86839
18	O	-6.082597	1.845322	0.354486
19	C	-5.964736	3.209517	0.72535
20	H	-5.244454	3.742308	0.091235
21	H	-6.955823	3.644655	0.58849
22	H	-5.664034	3.317992	1.775002
23	O	-1.448426	1.16669	1.313537
24	C	-0.556193	-1.095453	1.586054
25	H	0.369442	-1.677006	1.550197
26	H	-0.929575	-1.135245	2.61617
27	C	-0.253301	0.371906	1.245347
28	H	0.381763	0.794019	2.032881
29	C	0.468653	0.551318	-0.08758
30	C	1.754244	0.004596	-0.223545
31	C	0.610663	1.397474	-2.347293
32	C	2.44858	0.156183	-1.421056
33	H	2.228166	-0.531891	0.589474
34	H	0.165994	1.942857	-3.1748
35	C	-0.098831	1.256396	-1.150437
36	H	-1.081951	1.697481	-1.044116
37	C	-1.603622	-1.666811	0.62737
38	H	-1.933783	-2.655964	0.956972
39	H	-1.158955	-1.809683	-0.366269
40	O	3.720042	-0.329326	-1.658824
41	N	4.258022	-1.101749	-0.565978
42	H	4.339554	-2.041033	-0.95243
43	C	1.879949	0.851319	-2.495349
44	H	2.442713	0.9536	-3.417147
45	C	5.547285	-0.611898	-0.206734
46	C	6.601827	-1.504565	0.003639
47	C	7.8338	-1.053165	0.471259
48	H	6.461896	-2.565665	-0.190505
49	H	8.64086	-1.764058	0.628733
50	C	5.75579	0.750678	0.035864
51	H	4.947137	1.45375	-0.130493
52	C	8.053573	0.311404	0.711448
53	C	6.9932	1.20418	0.476656
54	H	7.143336	2.267613	0.645425
55	N	9.31223	0.780465	1.107139
56	H	9.295675	1.666003	1.595312
57	H	9.877904	0.102716	1.600413

Table S24: Compound 24 Cartesian Z matrix

Compound 24				
		24		
Center Number	Atom	Standard orientation: Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.920754	-0.727289	0.546927
2	C	-2.761784	0.611343	0.915087
3	C	-4.206184	-1.150154	0.159729
4	C	-3.838341	1.508215	0.927702
5	C	-5.103701	1.067272	0.546114
6	C	-5.295271	-0.272985	0.14836
7	H	-3.649606	2.52869	1.233988
8	O	-4.339607	-2.453161	-0.261838
9	C	-5.214267	-3.281931	0.514117
10	H	-6.241474	-2.912145	0.485515
11	H	-5.162257	-4.276059	0.065028
12	H	-4.873825	-3.339318	1.555898
13	O	-6.54737	-0.719422	-0.21801
14	C	-6.912563	-0.397893	-1.562857
15	H	-6.205138	-0.835253	-2.277775
16	H	-7.903682	-0.82774	-1.724507
17	H	-6.960643	0.686644	-1.708501
18	O	-6.216714	1.85637	0.502733
19	C	-6.086472	3.211414	0.90362
20	H	-5.38479	3.759191	0.261577
21	H	-7.080693	3.649846	0.806714
22	H	-5.75497	3.293349	1.946254
23	O	-1.558199	1.147353	1.310592
24	C	-0.665983	-1.121734	1.511782
25	H	0.256015	-1.705823	1.437597
26	H	-1.005905	-1.177714	2.55245
27	C	-0.370577	0.351243	1.188437
28	H	0.293668	0.757173	1.960331
29	C	0.305634	0.554246	-0.165456
30	C	1.581424	0.002326	-0.362473
31	C	0.372438	1.45634	-2.409131
32	C	2.22702	0.181365	-1.580756
33	H	2.077969	-0.556843	0.421502
34	H	-0.098441	2.0248	-3.205665
35	C	-0.292207	1.289757	-1.190527
36	H	-1.267114	1.734831	-1.036895
37	C	-1.745526	-1.673679	0.577678
38	H	-2.0704	-2.665748	0.903615
39	H	-1.333214	-1.805715	-0.431455

40	O	3.496001	-0.306857	-1.877598
41	N	4.043696	-1.135151	-0.864366
42	H	4.082885	-2.072469	-1.258056
43	C	1.631393	0.904614	-2.61786
44	H	2.160349	1.023483	-3.557427
45	C	5.298616	-0.684482	-0.416261
46	C	6.189599	-1.622789	0.131495
47	C	7.398211	-1.206945	0.669111
48	H	5.929173	-2.677727	0.139186
49	H	8.084327	-1.933773	1.090251
50	C	5.639463	0.675524	-0.427662
51	H	4.956972	1.394865	-0.861814
52	C	7.746146	0.155511	0.662026
53	C	6.853731	1.08741	0.105525
54	H	7.119555	2.138997	0.092859
55	C	8.996429	0.585356	1.210581
56	N	10.01338	0.933418	1.657289

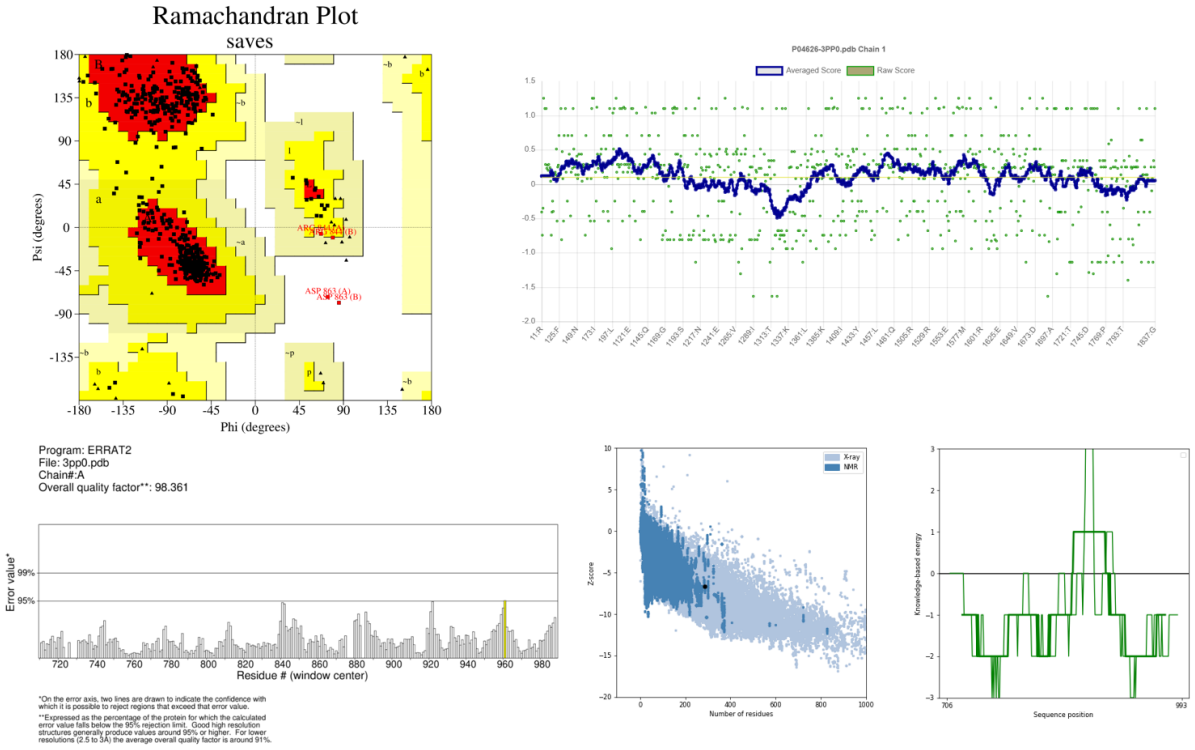


Figure A1: Protein verification of target protein 3PP0

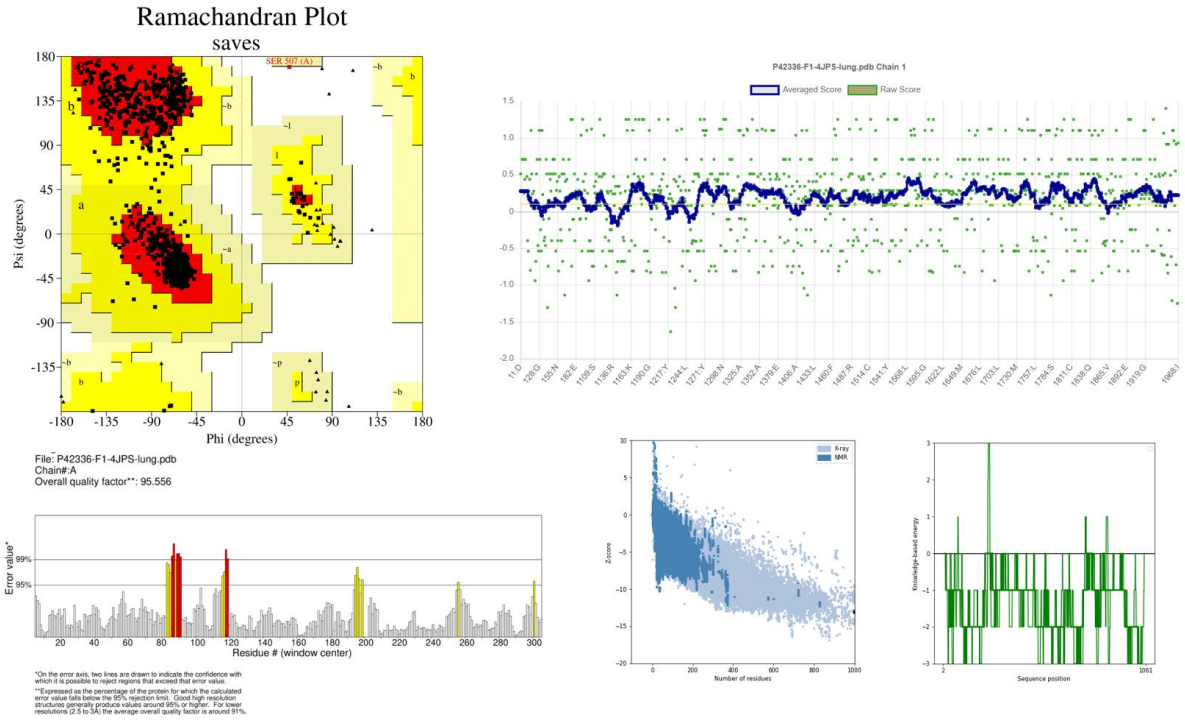


Figure A2: Protein verification of target protein 4JPS

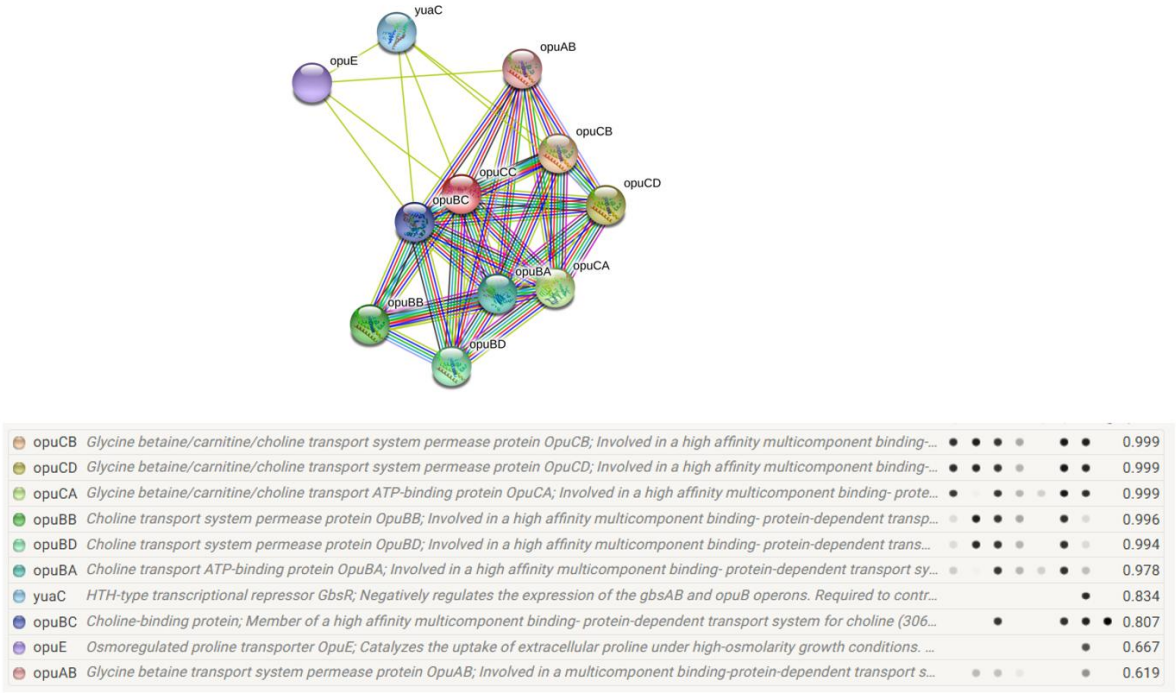
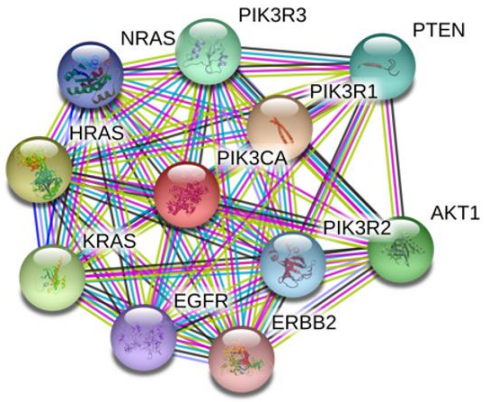


Figure A3: Protein-protein interaction of 3PP0 with its partners



PIK3R1	Phosphatidylinositol 3-kinase regulatory subunit alpha; Binds to activated (phosphorylated) protein-Tyr kinases, through its SH2...	0.999
HRAS	GTPase HRas; Involved in the activation of Ras protein signal transduction. Ras proteins bind GDP/GTP and possess intrinsic G...	0.999
KRAS	GTPase KRas; Ras proteins bind GDP/GTP and possess intrinsic GTPase activity. Plays an important role in the regulation of ce...	0.998
AKT1	RAC-alpha serine/threonine-protein kinase; AKT1 is one of 3 closely related serine/threonine- protein kinases (AKT1, AKT2 and ...	0.998
PIK3R3	Phosphatidylinositol 3-kinase regulatory subunit gamma; Binds to activated (phosphorylated) protein-tyrosine kinases through i...	0.997
PTEN	Phosphatase and tensin homolog; Tumor suppressor. Acts as a dual-specificity protein phosphatase, dephosphorylating tyrosi...	0.996
PIK3R2	Phosphatidylinositol 3-kinase regulatory subunit beta; Regulatory subunit of phosphoinositide-3-kinase (PI3K), a kinase that ph...	0.995
NRAS	GTPase NRas; Ras proteins bind GDP/GTP and possess intrinsic GTPase activity (189 aa)	0.995
EGFR	Epidermal growth factor receptor; Receptor tyrosine kinase binding ligands of the EGF family and activating several signaling c...	0.990
ERBB2	Receptor tyrosine-protein kinase erbB-2; Protein tyrosine kinase that is part of several cell surface receptor complexes, but that ...	0.986

Figure A4: Protein-protein interaction of 4JPS with its partners

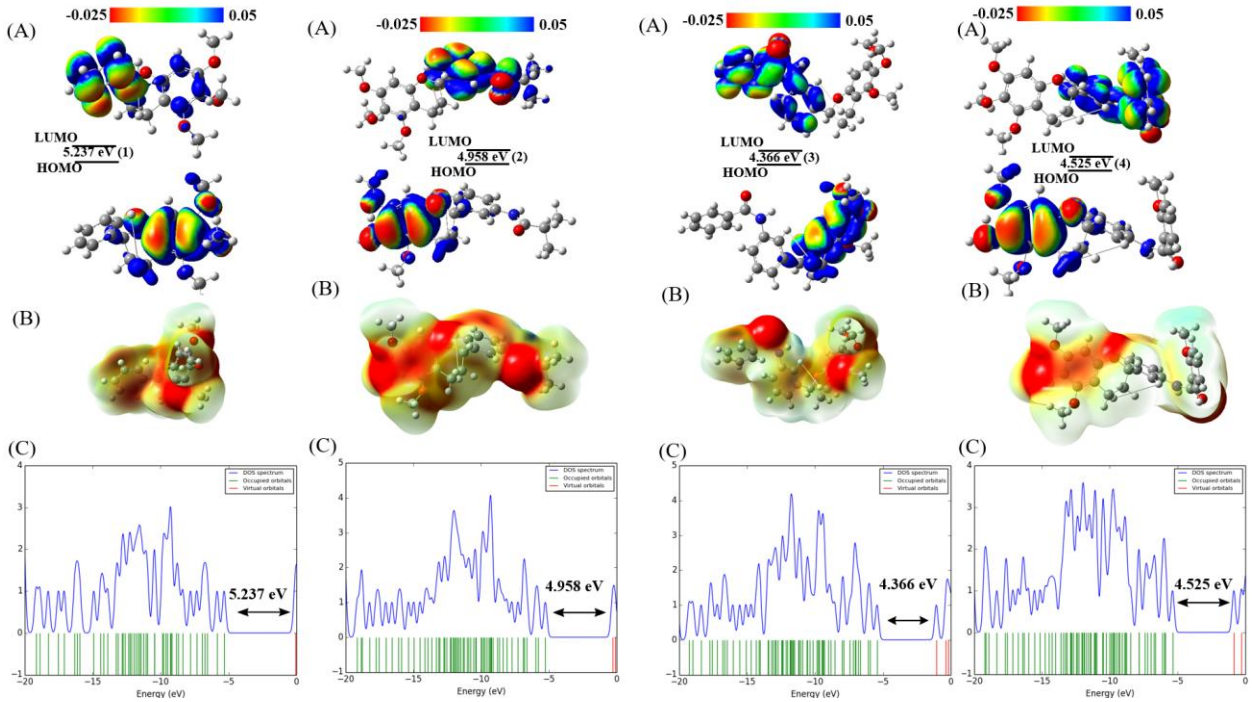


Figure A5: (A) Molecular orbitals of isodensity surfaces (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient) of HOMO and LUMO; (B) Maps of electrostatic potential (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient); and (C) DOS plot and HOMO-LUMO energy gap of compounds 1-4

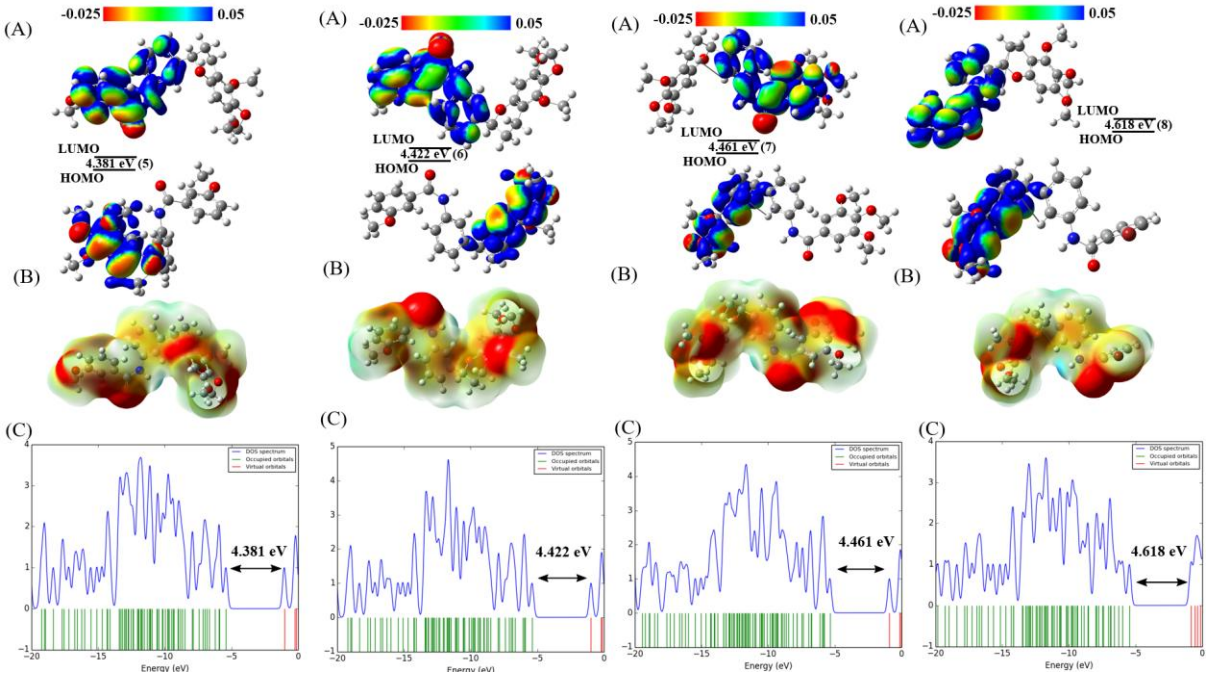


Figure A6: (A) Molecular orbitals of isodensity surfaces (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient) of HOMO and LUMO; (B) Maps of electrostatic potential (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient); and (C) DOS plot and HOMO-LUMO energy gap of compounds 5-8

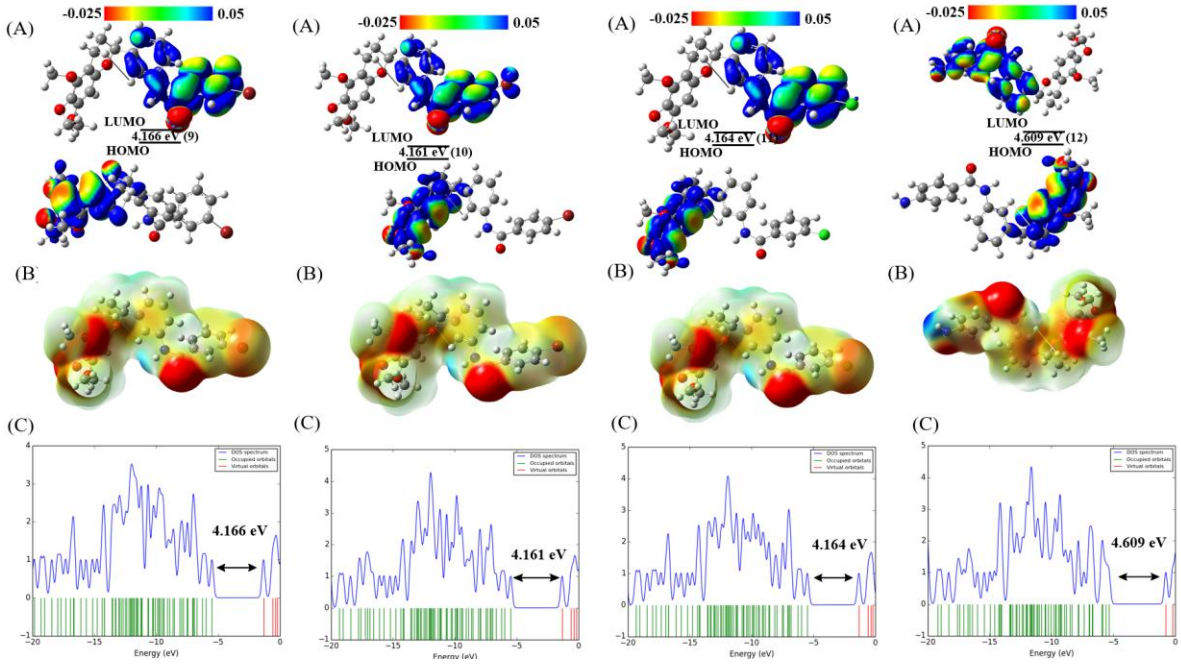


Figure A7: (A) Molecular orbitals of isodensity surfaces (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient) of HOMO and LUMO; (B) Maps of electrostatic potential (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient); and (C) DOS plot and HOMO-LUMO energy gap of compounds 9-12

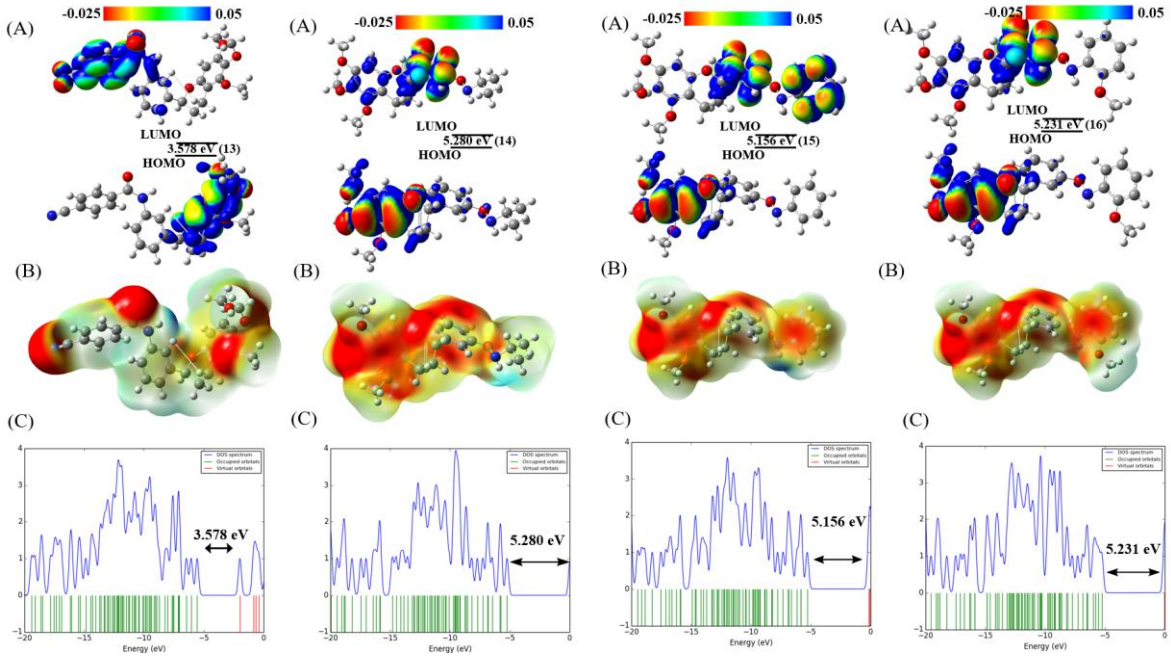


Figure A8: (A) Molecular orbitals of isodensity surfaces (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient) of HOMO and LUMO; (B) Maps of electrostatic potential (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient); and (C) DOS plot and HOMO-LUMO energy gap of compounds 13-16

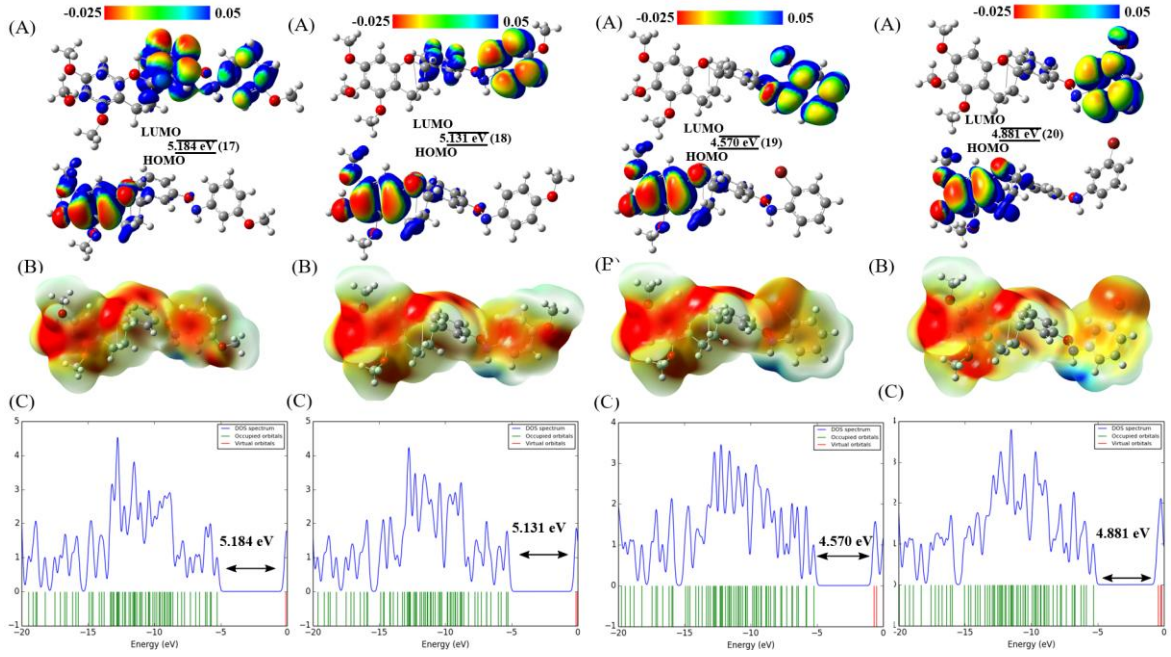


Figure A9: (A) Molecular orbitals of isodensity surfaces (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient) of HOMO and LUMO; (B) Maps of electrostatic potential (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient); and (C) DOS plot and HOMO-LUMO energy gap of compounds 17-20

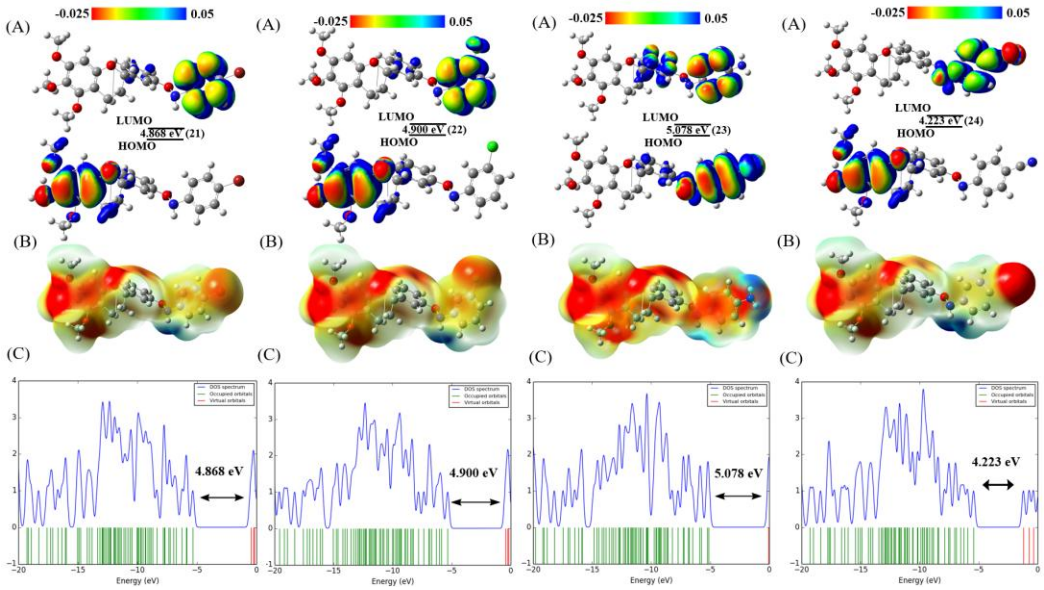


Figure A10: (A) Molecular orbitals of isodensity surfaces (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient) of HOMO and LUMO; (B) Maps of electrostatic potential (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient); and (C) DOS plot and HOMO-LUMO energy gap of compounds 21-24

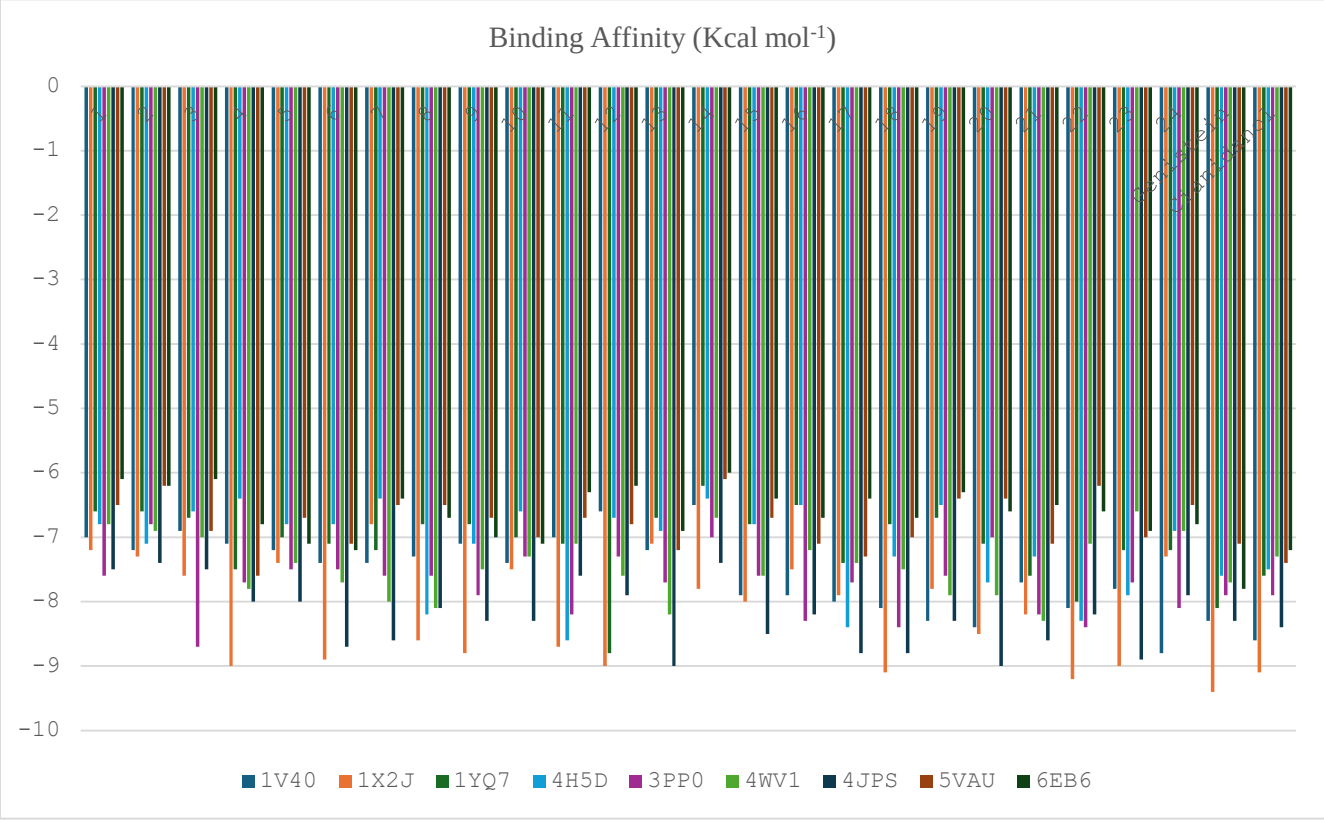


Figure A11: Binding affinity of compounds and reference drugs with respect to target proteins.

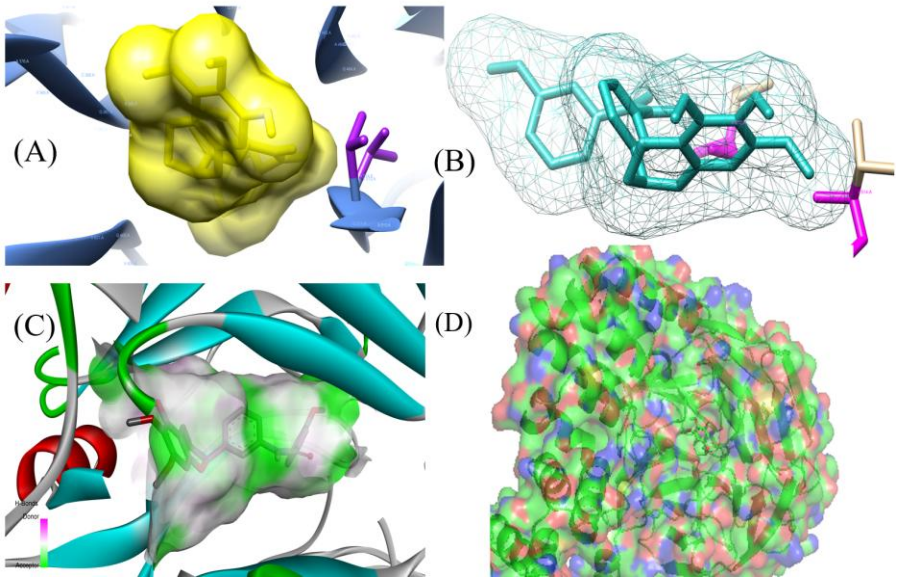


Figure A12: **Molecular Docking Configurations:** (A) Compound positioned within the protein pocket; (B) Active site visualization; (C) Hydrogen bonding in the solid state; (D) Protein-ligand binding cavity for compound 6 and receptor protein Keap1 on Nrf2 (1X2J).

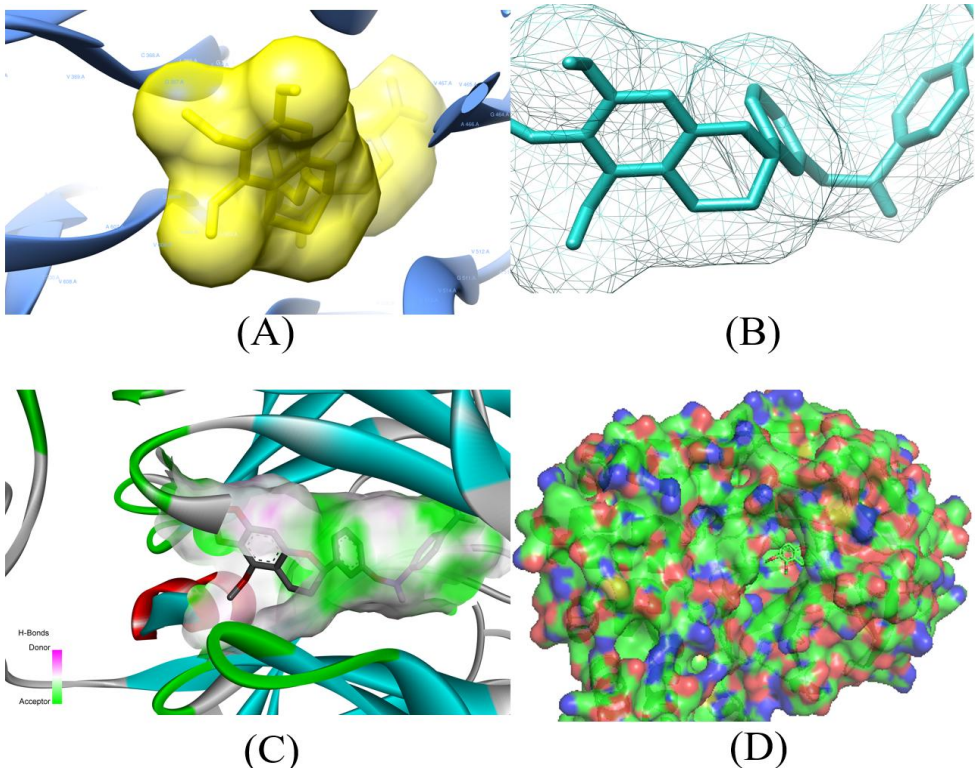


Figure A13: **Molecular Docking Configurations:** (A) Compound positioned within the protein pocket; (B) Active site visualization; (C) Hydrogen bonding in the solid state; (D) Protein-ligand binding cavity for compound 23 and receptor protein Keap1 on Nrf2 (1X2J).

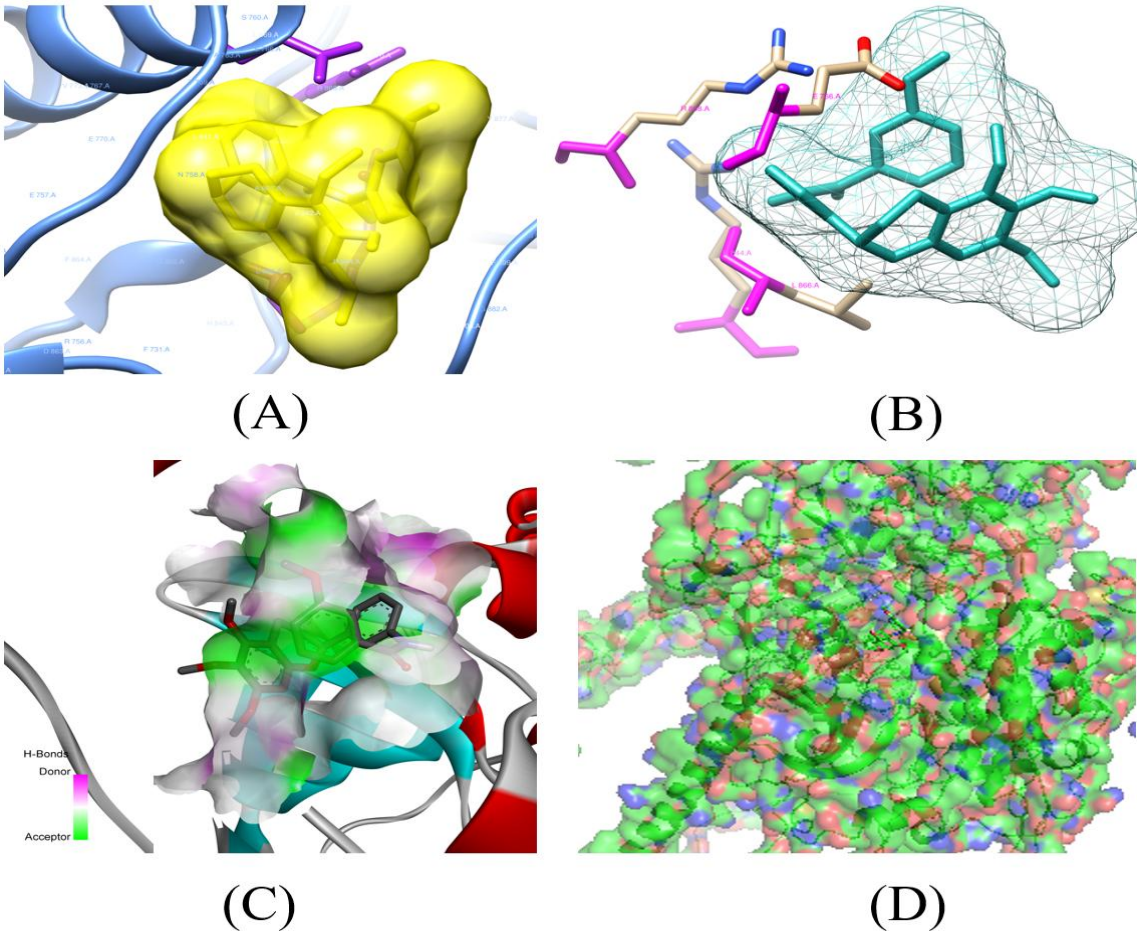


Figure A14: **Molecular Docking Configurations:** (A) Compound positioned within the protein pocket; (B) Active site visualization; (C) Hydrogen bonding in the solid state; (D) Protein-ligand binding cavity for compound 6 and receptor protein Kinase domain of HER2 (3PP0).

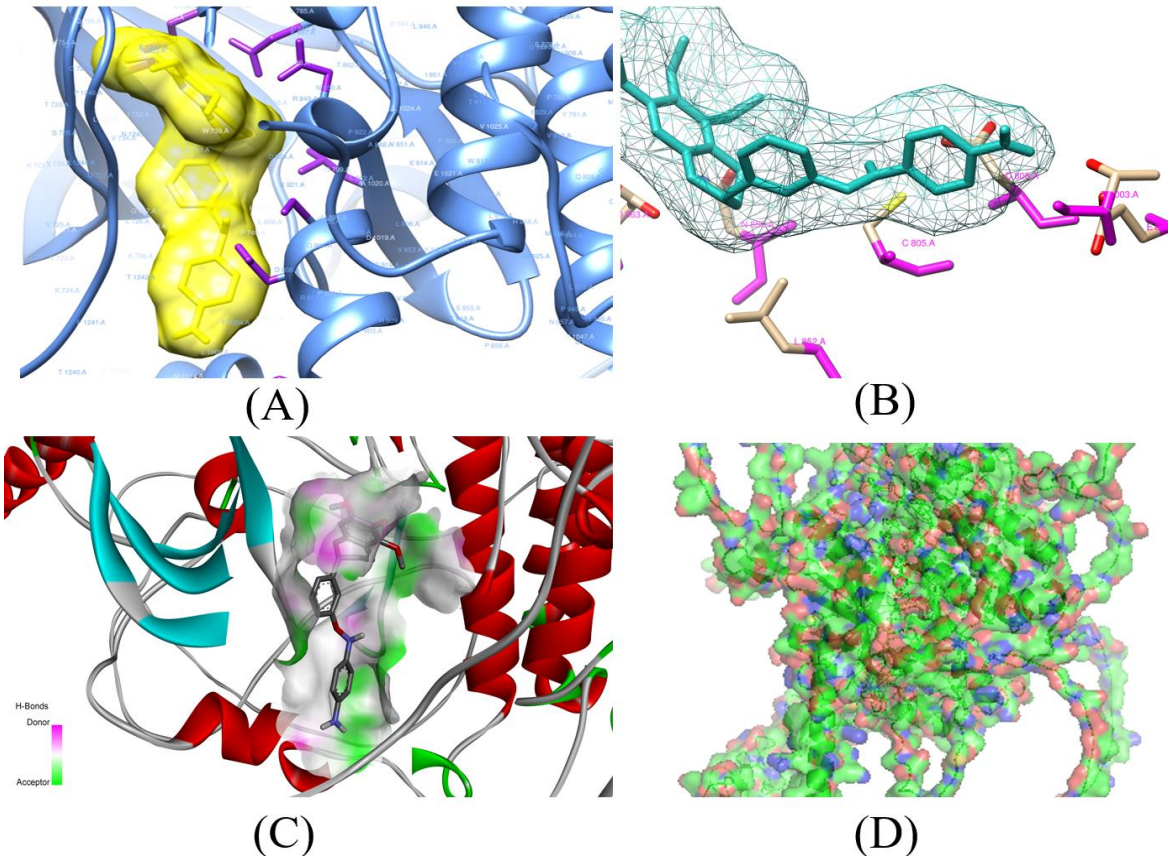


Figure A15: **Molecular Docking Configurations:** (A) Compound positioned within the protein pocket; (B) Active site visualization; (C) Hydrogen bonding in the solid state; (D) Protein-ligand binding cavity for compound 23 and receptor protein Kinase domain of HER2 (3PP0).

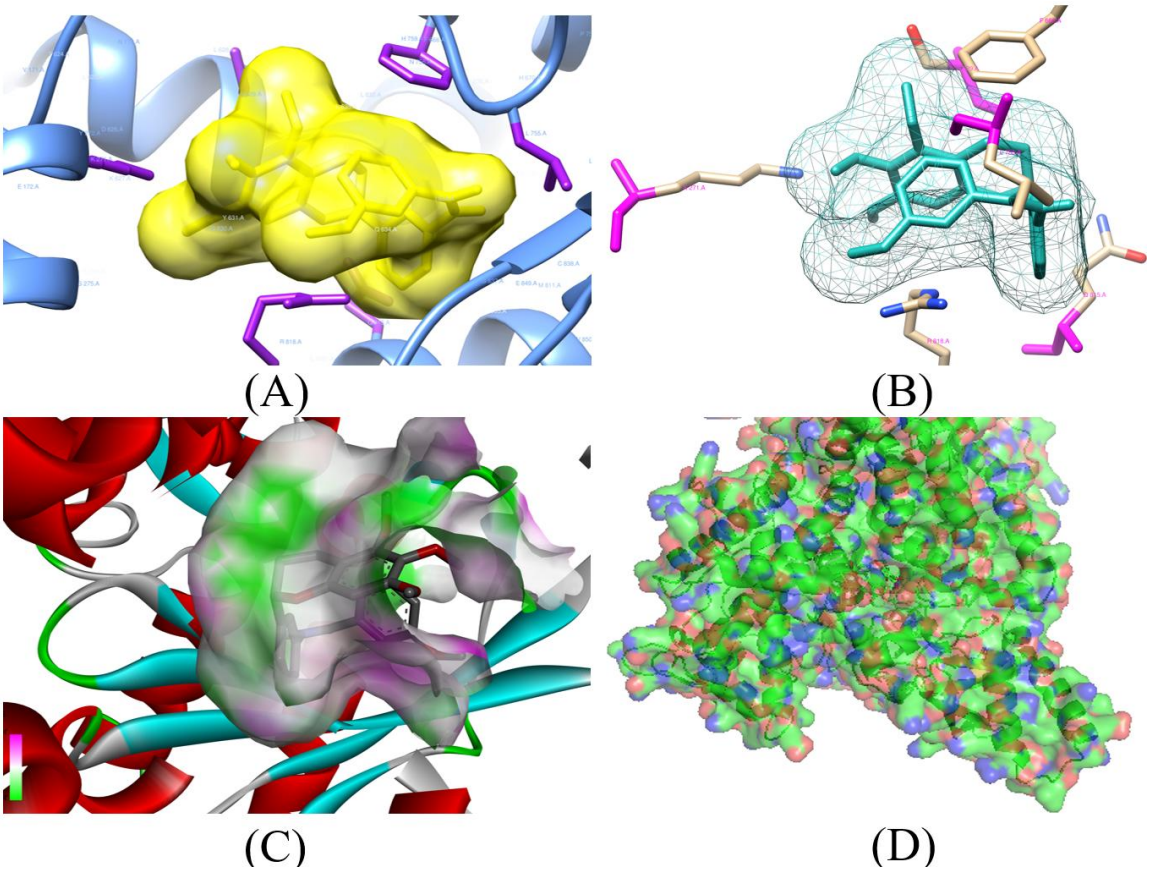


Figure A 16: **Molecular Docking Configurations:** (A) Compound positioned within the protein pocket; (B) Active site visualization; (C) Hydrogen bonding in the solid state; (D) Protein-ligand binding cavity for compound 6 and receptor lipid kinase PI3Kα (4JPS).

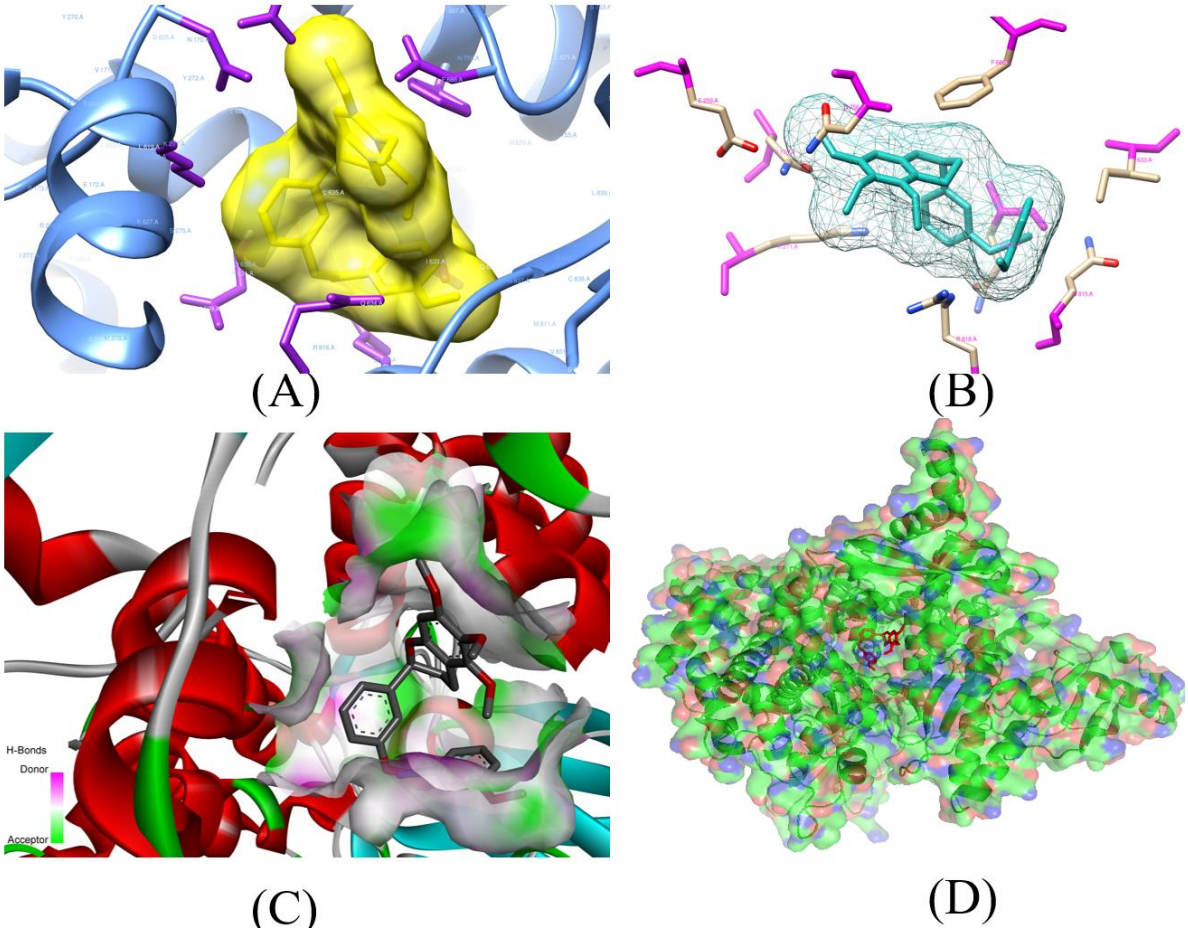


Figure A17: **Molecular Docking Configurations:** (A) Compound positioned within the protein pocket; (B) Active site visualization; (C) Hydrogen bonding in the solid state; (D) Protein-ligand binding cavity for compound 18 and receptor protein lipid kinase PI3Kα (4JPS).

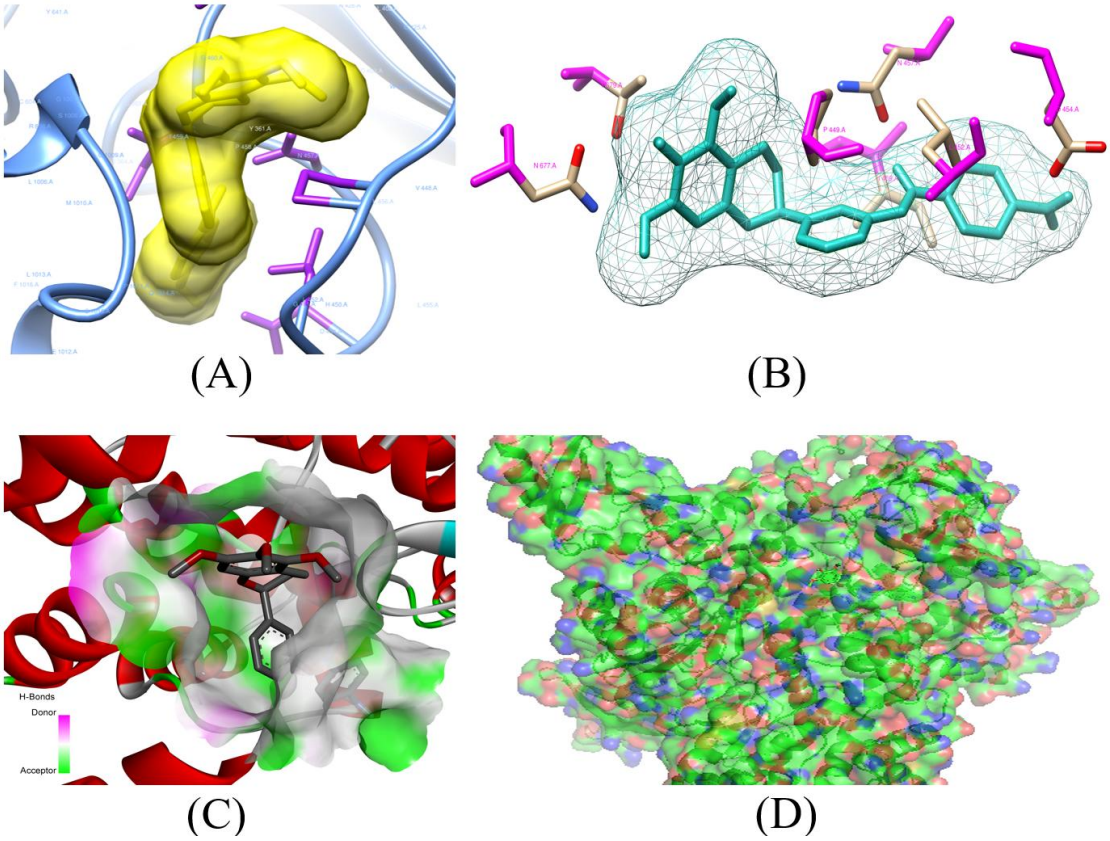


Figure A18: **Molecular Docking Configurations:** (A) Compound positioned within the protein pocket; (B) Active site visualization; (C) Hydrogen bonding in the solid state; (D) Protein-ligand binding cavity for compound 23 and receptor protein lipid kinase PI3Kα (4JPS).

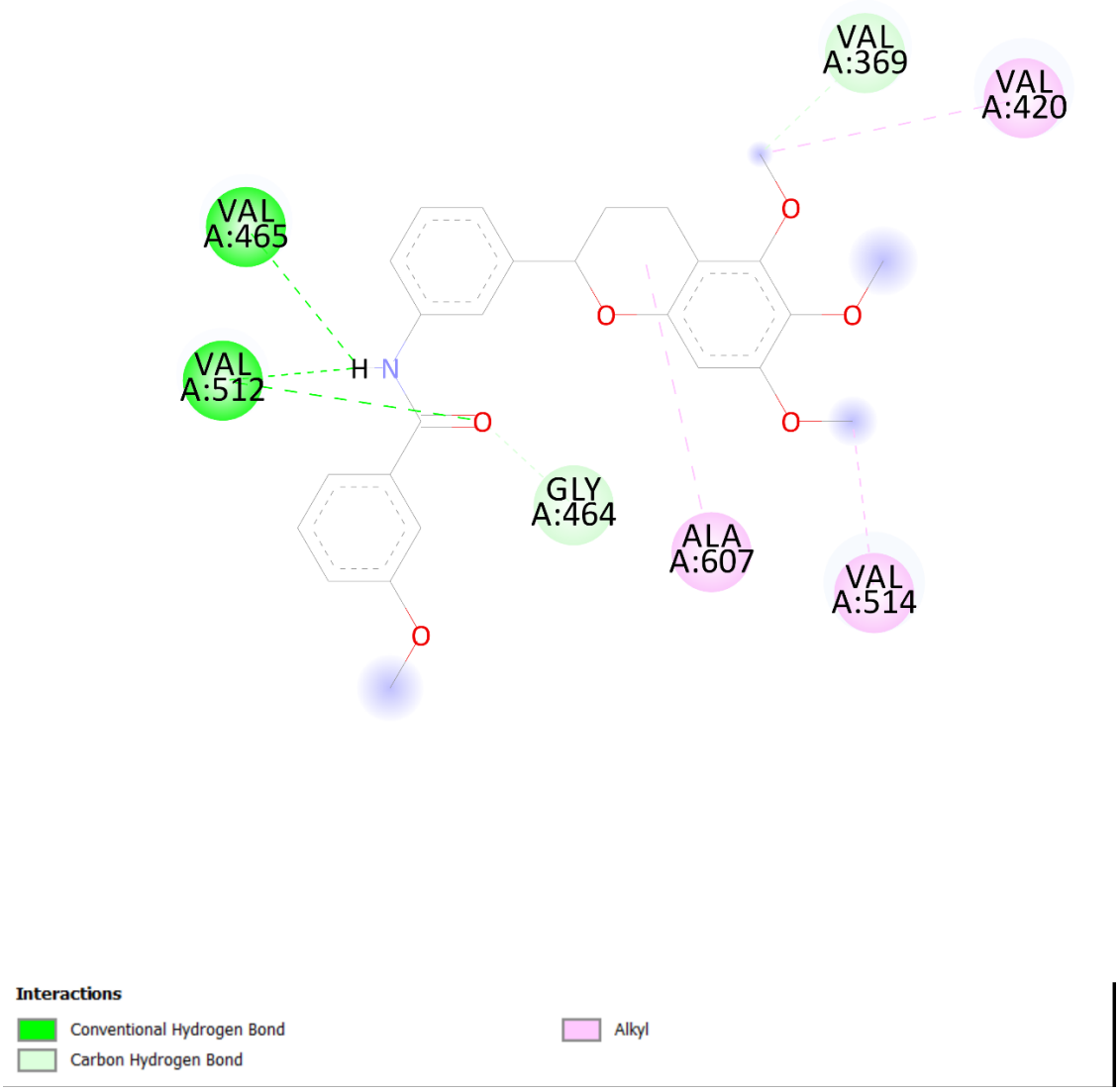


Figure A19: Ligand-protein interacting amino acid residues of ligand 6 against target proteins 1X2J.

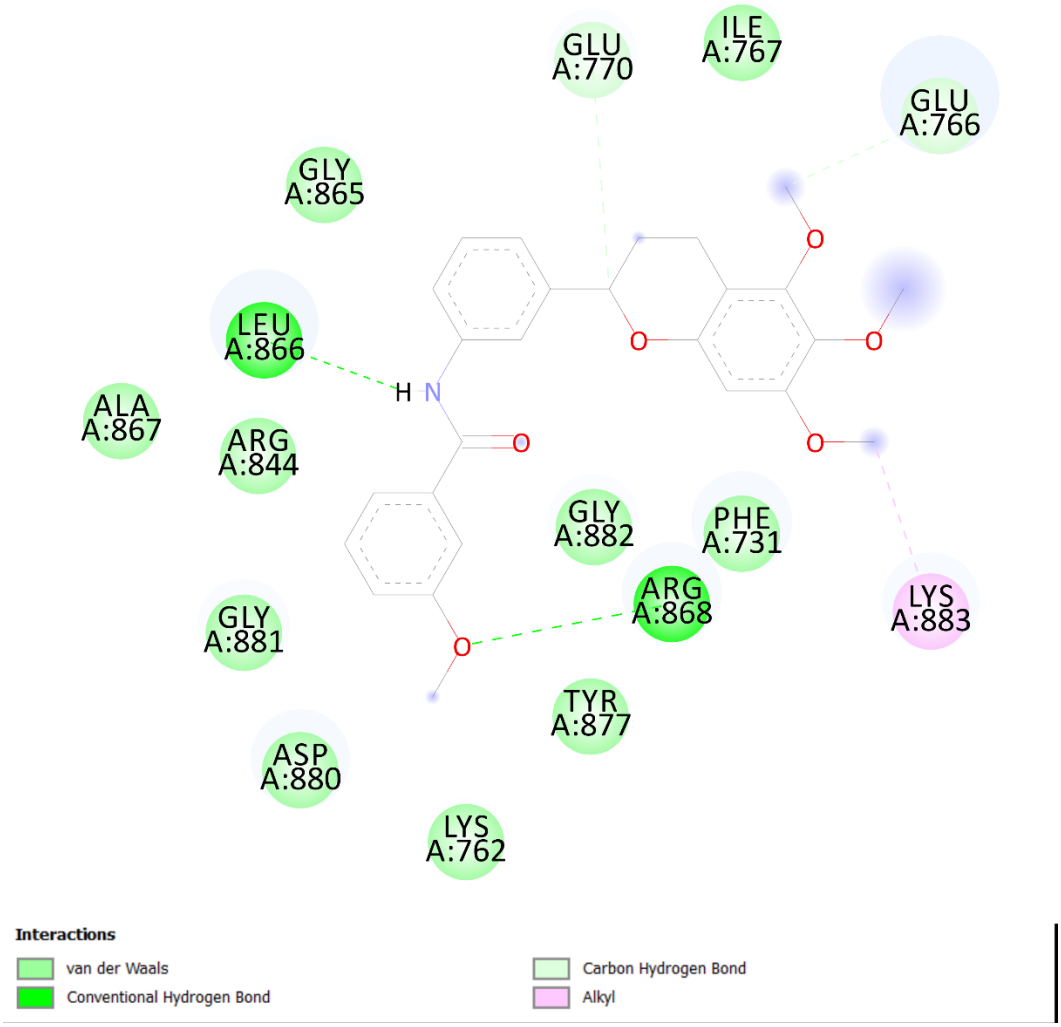


Figure A20: Ligand-protein interacting amino acid residues of ligand 6 against target proteins 3PP0.

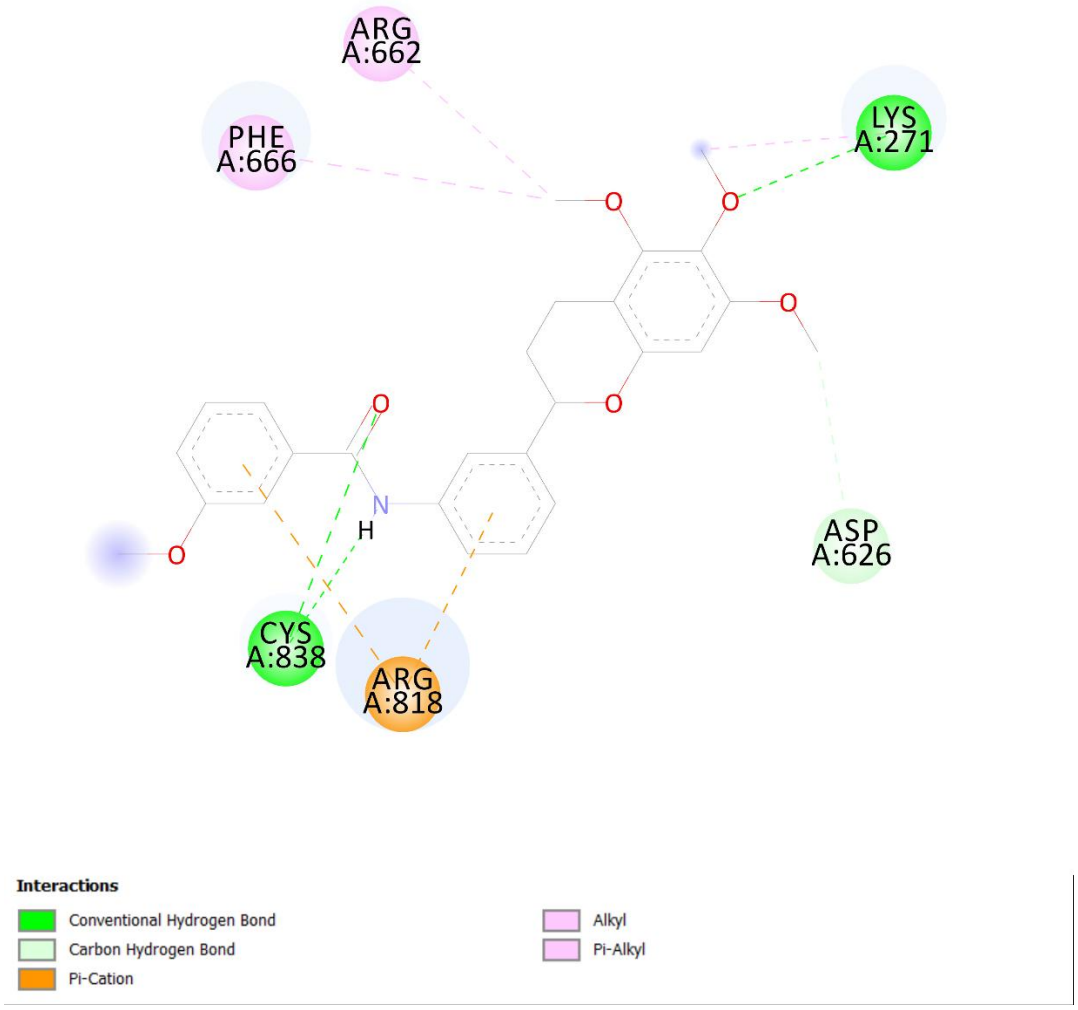


Figure 21: Ligand-protein interacting amino acid residues of ligand 6 against target proteins 4JPS.

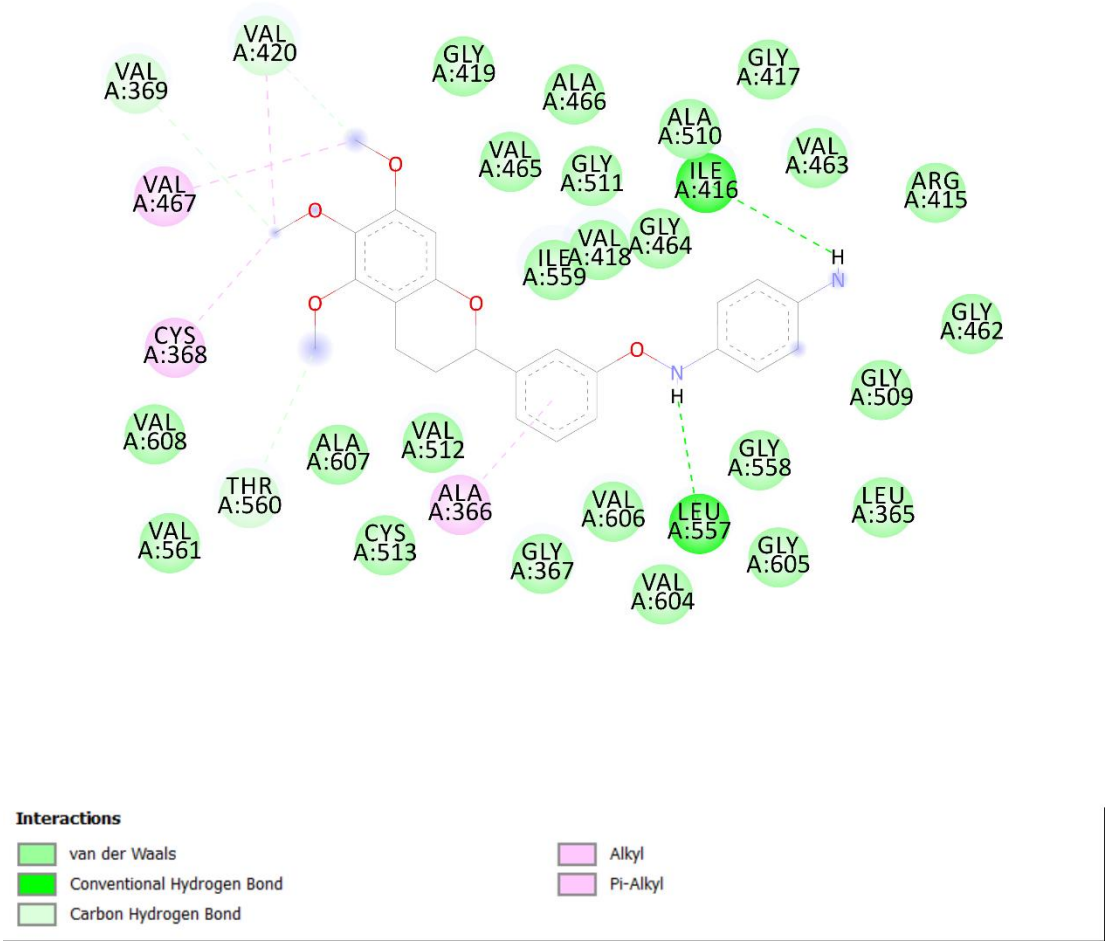


Figure A22: Ligand-protein interacting amino acid residues of ligand 23 against target proteins 1X2J.

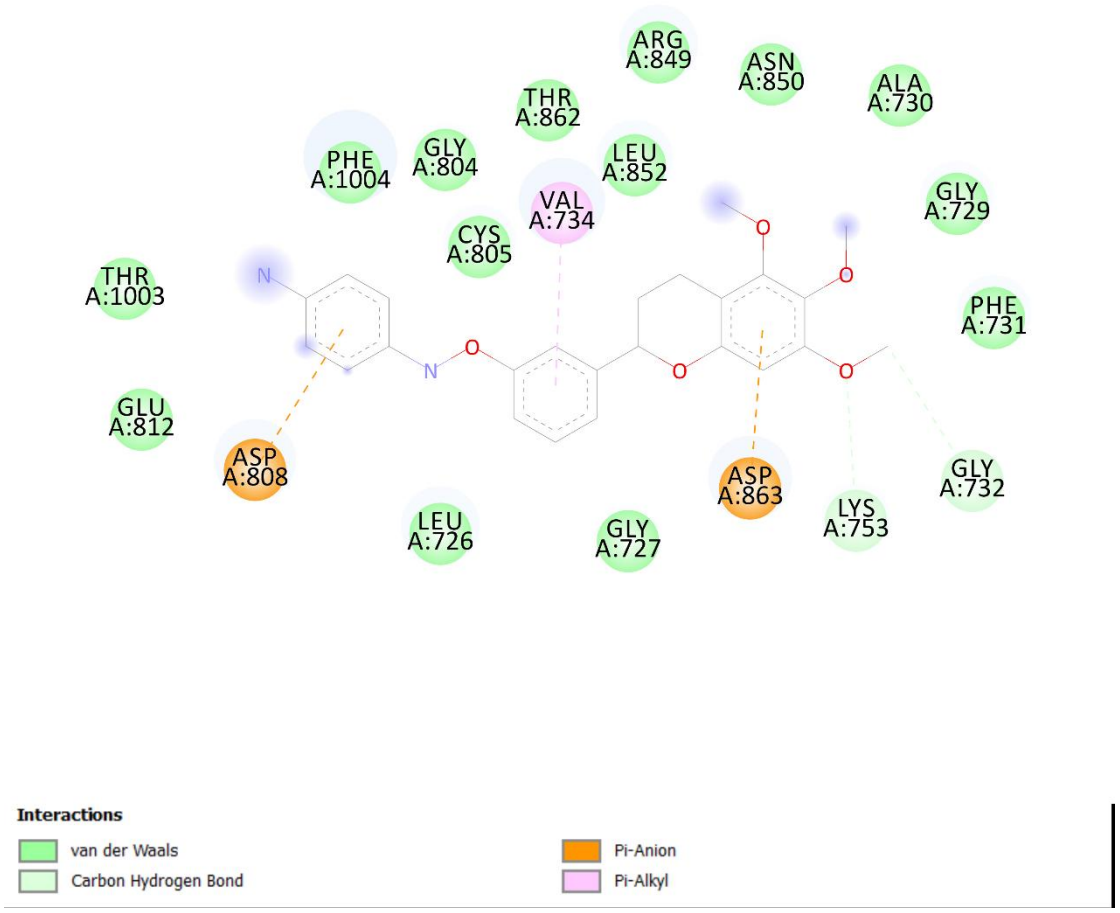


Figure A23: Ligand-protein interacting amino acid residues of ligand 23 against target proteins 3PP0.

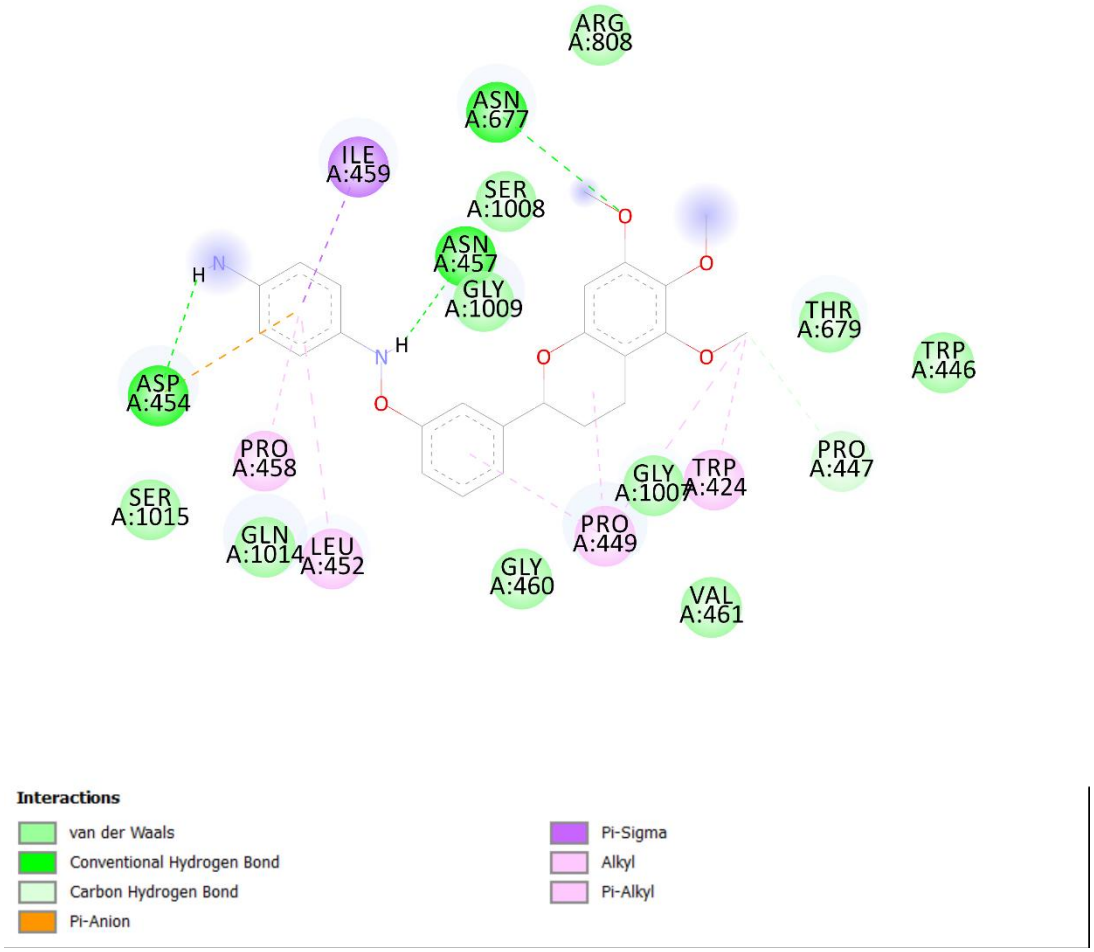


Figure A24: Ligand-protein interacting amino acid residues of ligand 23 against target proteins 4JPS.

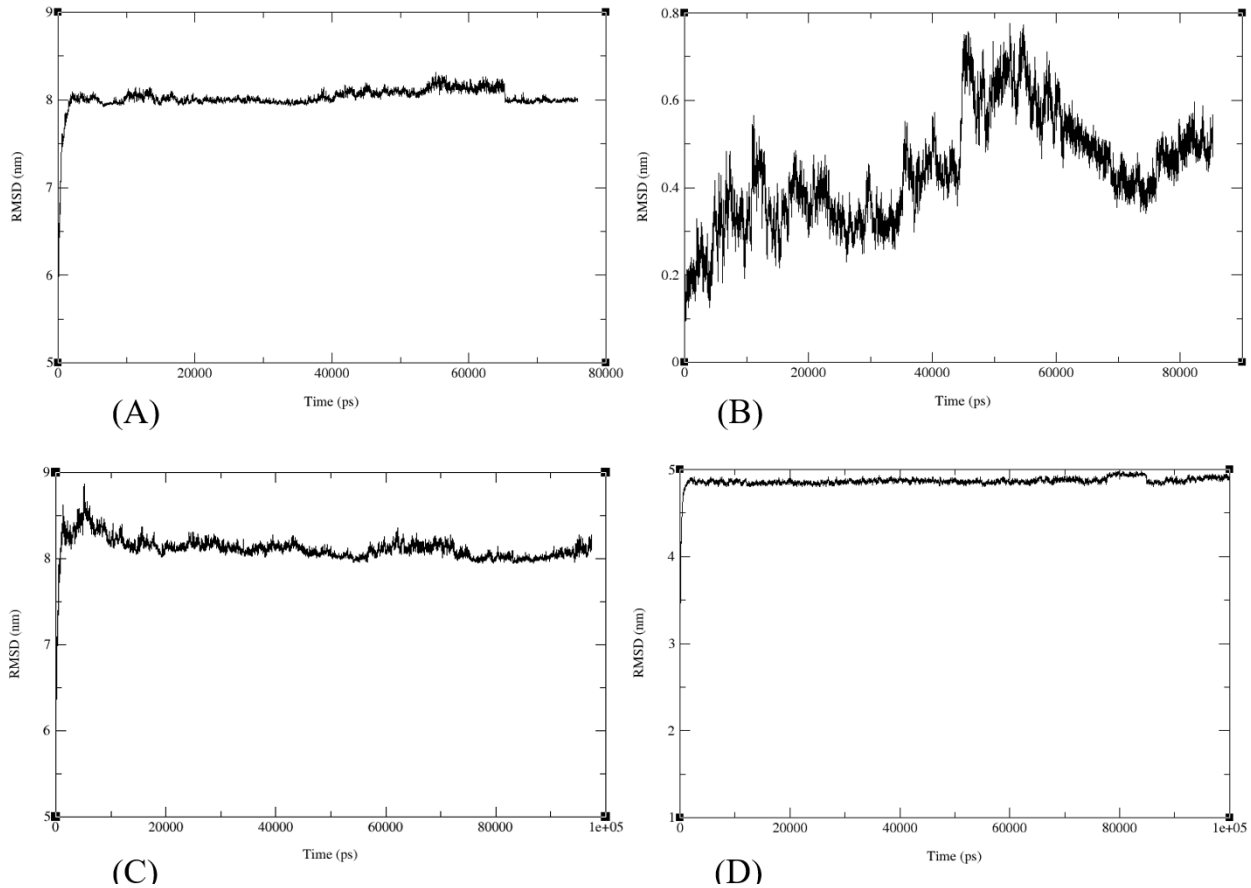


Figure A25: Root mean square deviation RMSD of compounds: (A) compound 6, (B) compound 18, (C) compound 23, and (D) reference drug Genistein.

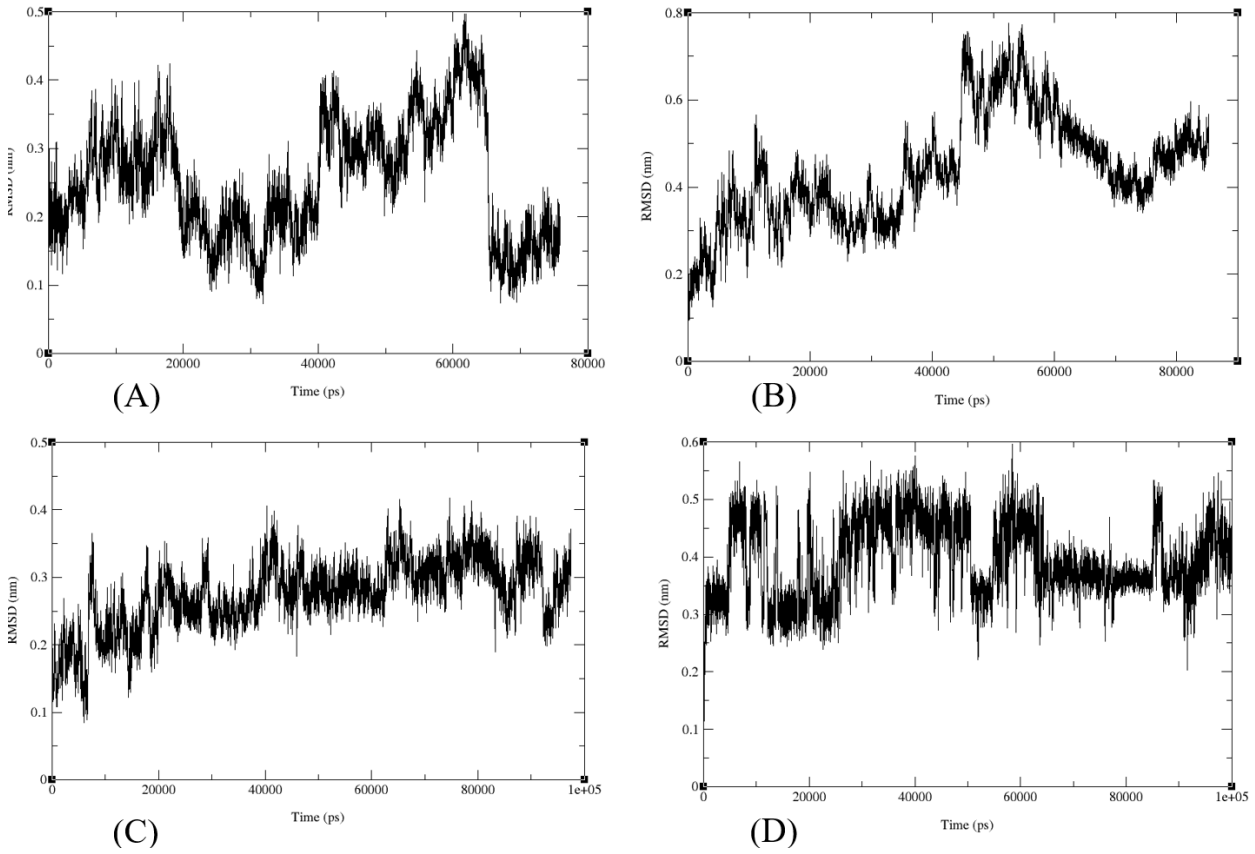


Figure A26: Root mean square deviation RMSD of compounds and target protein (1X2J) complex : (A) compound 6, (B) compound 18, (C) compound 23, and (D) reference drug Genistein.

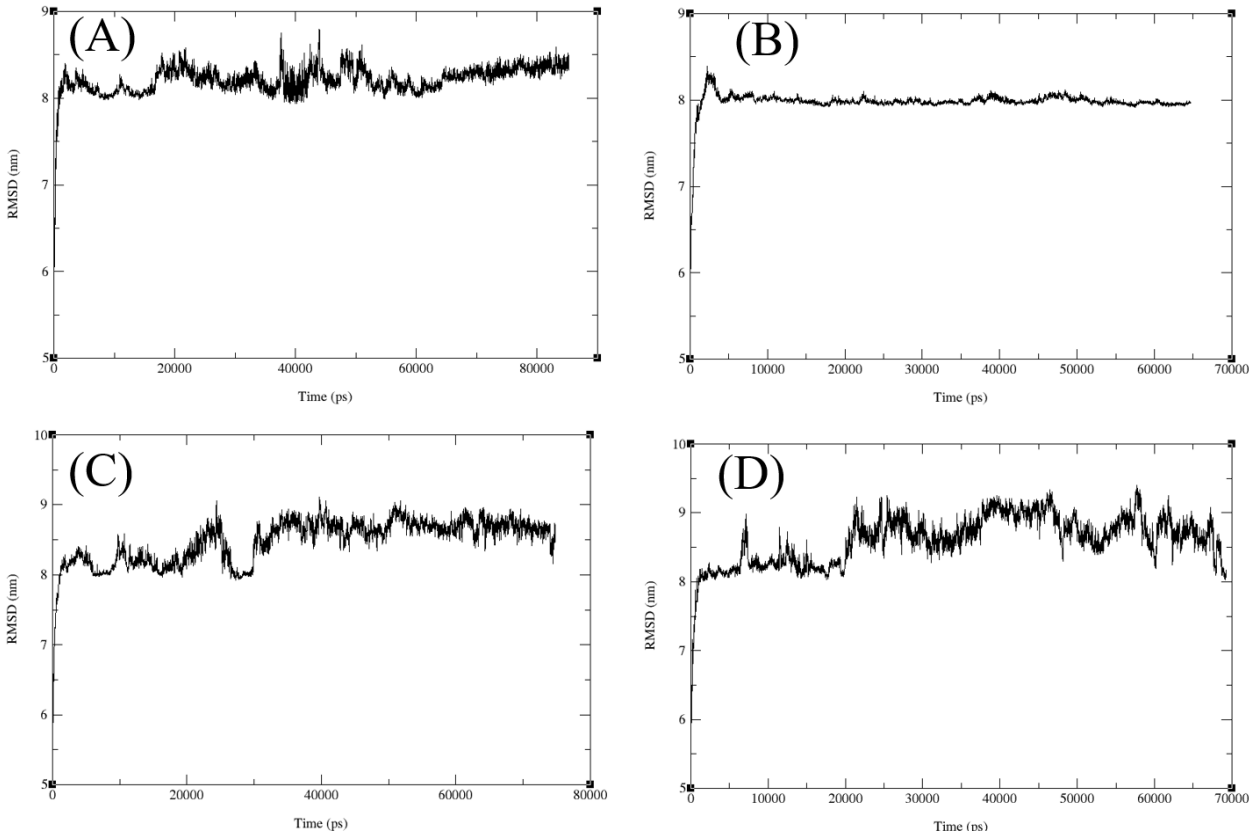


Figure A27: Root mean square deviation (RMSD) of compound 18 at (A) 300K (B) 305K (C) 310K and (D) 320K

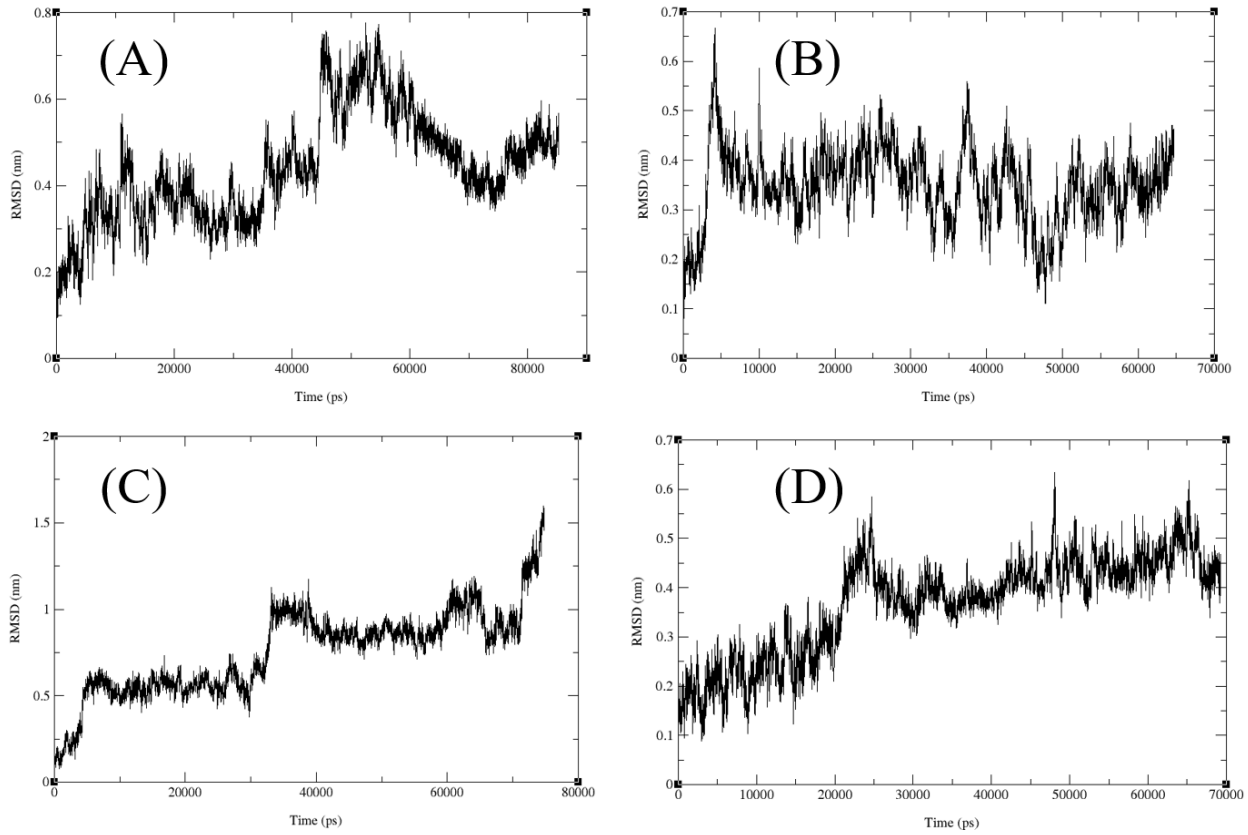


Figure A28: RMSD of compound 18 and target protein (1X2J) complex at (A) 300K (B) 305K (C) 310K and (D) 320K temperature.

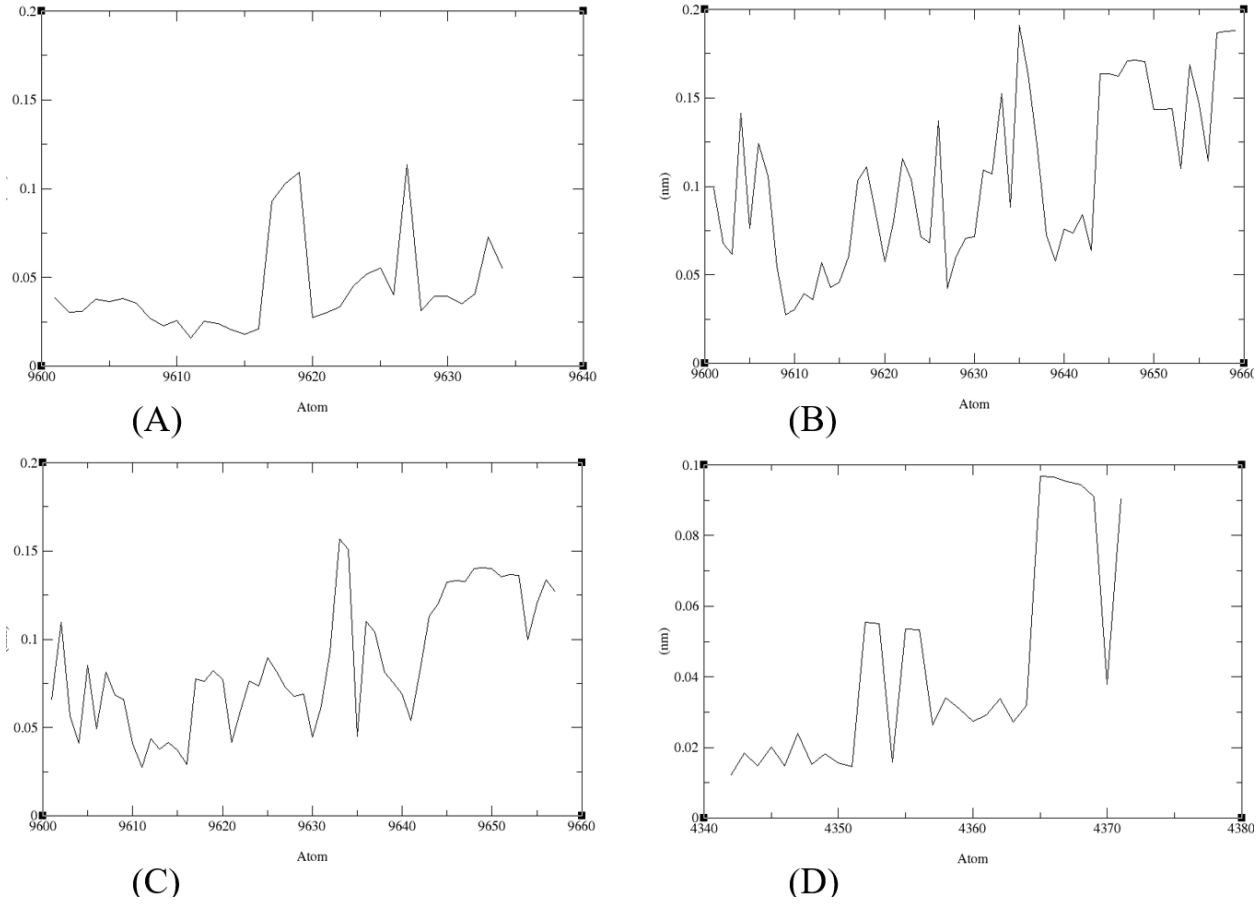


Figure A29: Root mean square fluctuation RMSF value of compounds: (A) compound 6, (B) compound 18, (C) compound 23, and (D) reference drug Genistein at 300k.

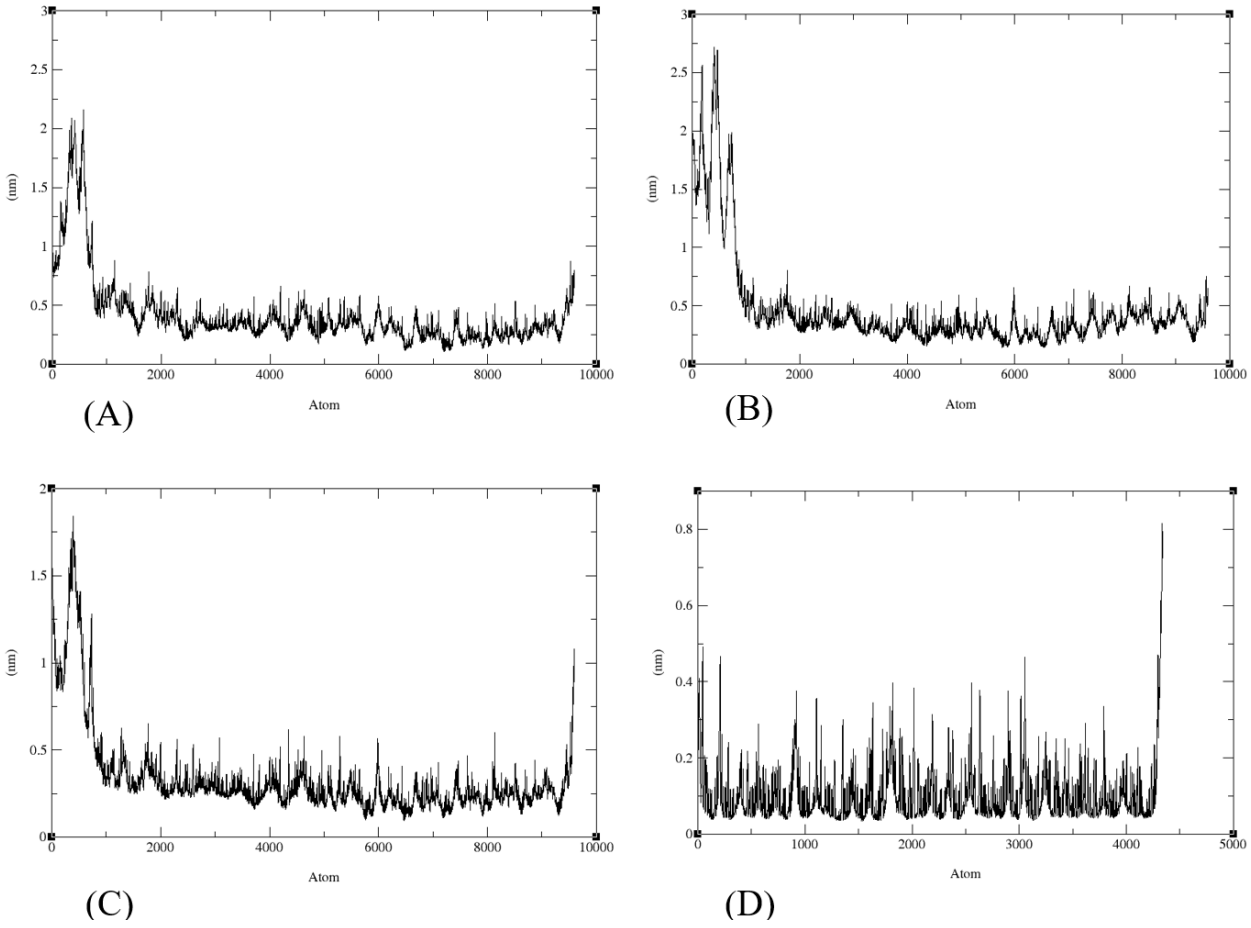


Figure A30: Root mean square fluctuation RMSF value of compounds and target protein (1X2J) complex: (A) compound 6, (B) compound 18, (C) compound 23, and (D) reference drug Genistein at 300k.

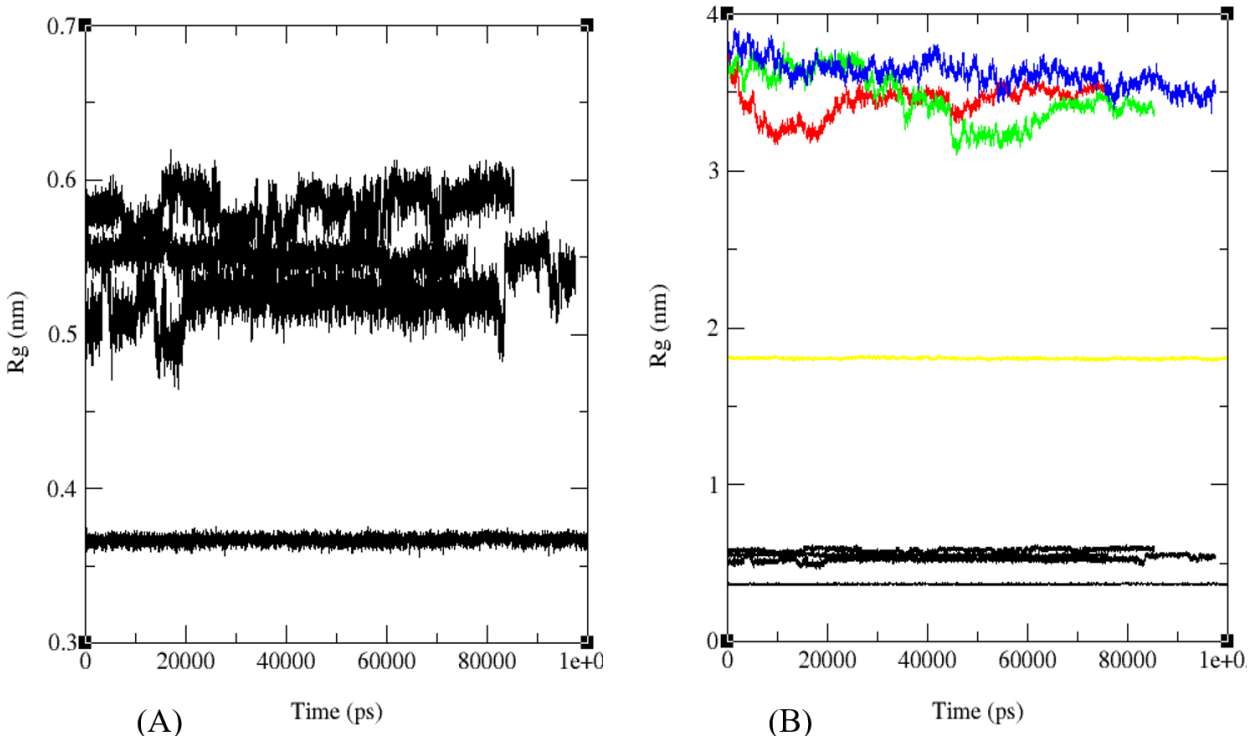


Figure A31: Merge of Radius of gyration Rg of (A) compounds and (B) compounds target protein (1X2J) complex.

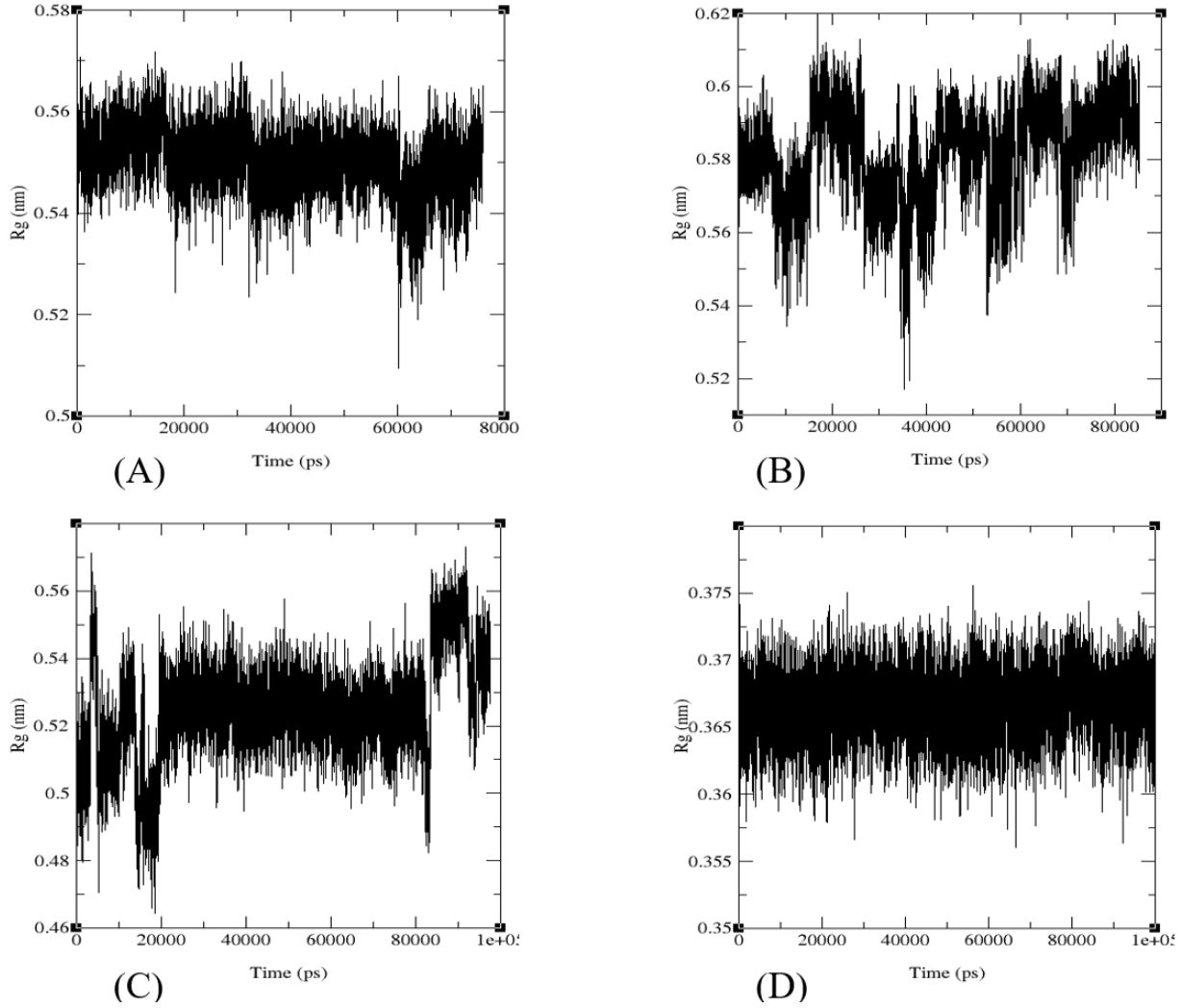


Figure A32: Radius of gyration Rg of compounds: (A) compound 6, (B) compound 18, (C) compound 23 and (D) reference drug Genistein.

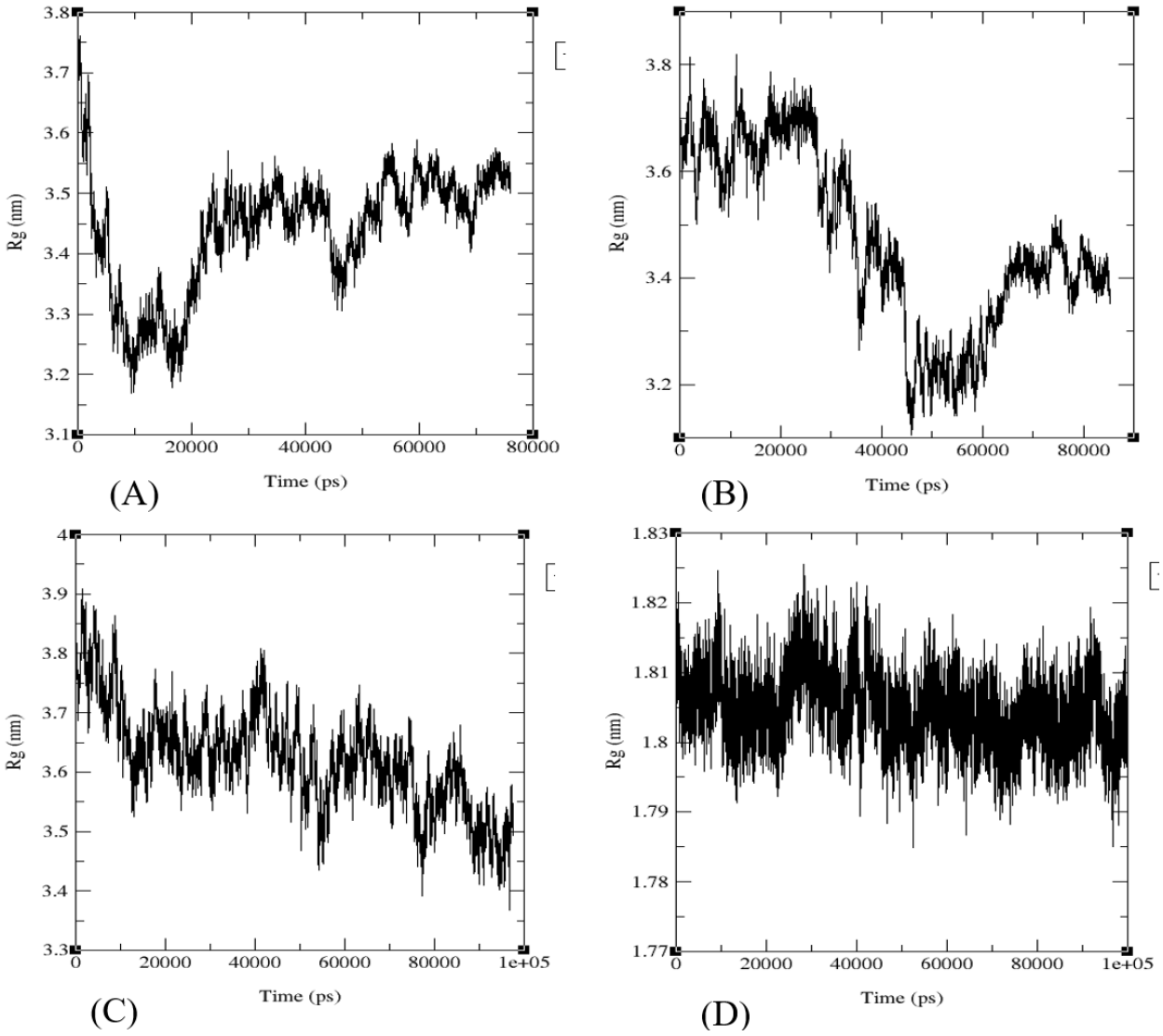


Figure A33: Radius of gyration Rg of compounds and target protein (1X2J) complex: (A) compound 6, (B) compound 18, (C) compound 23, and (D) reference drug Genistein.

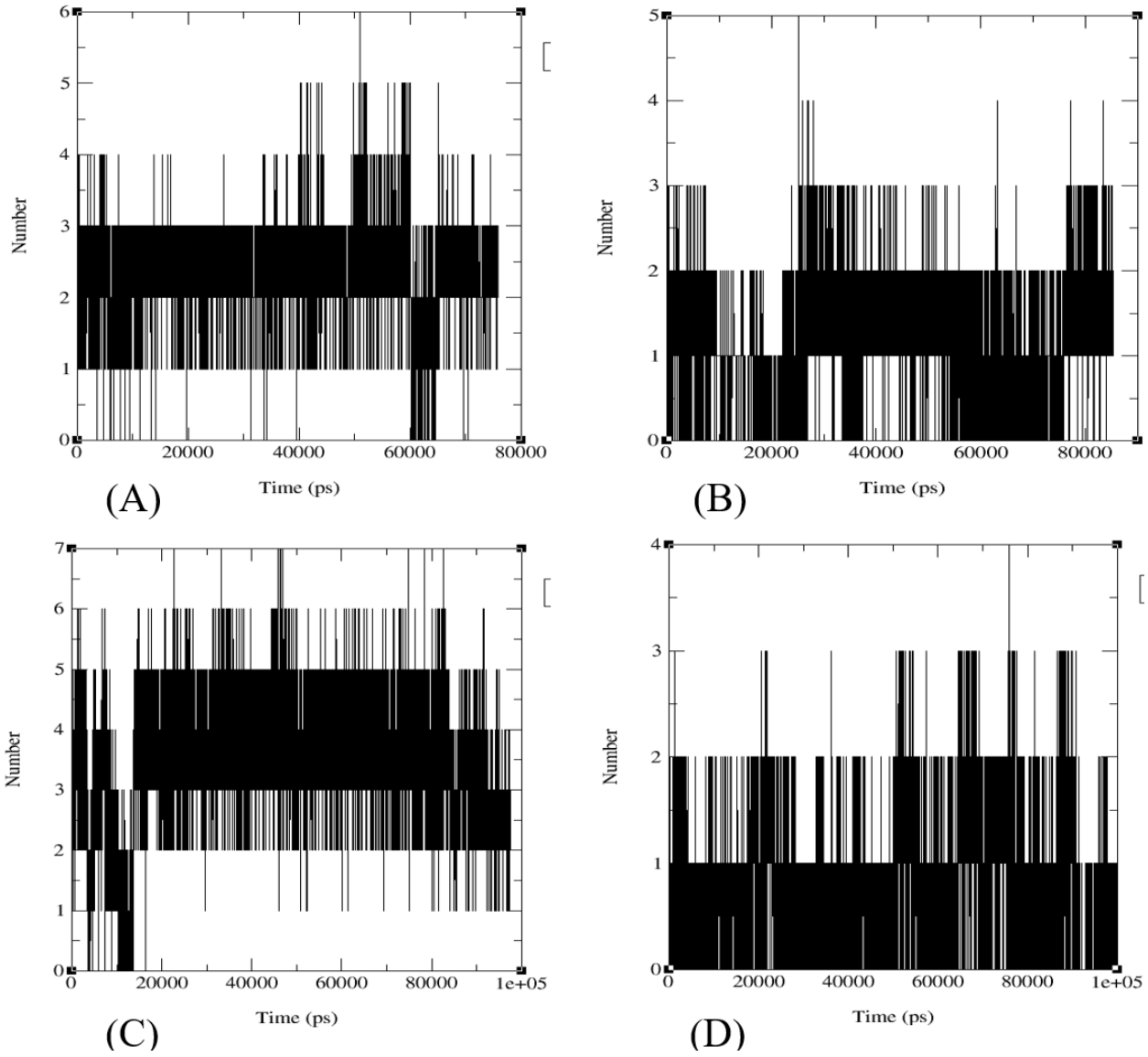


Figure A34: Count of hydrogen bond formation of compounds over time: (A) compound 6, (B) compound 18, (C) compound 23, and (D) reference drug Genistein.

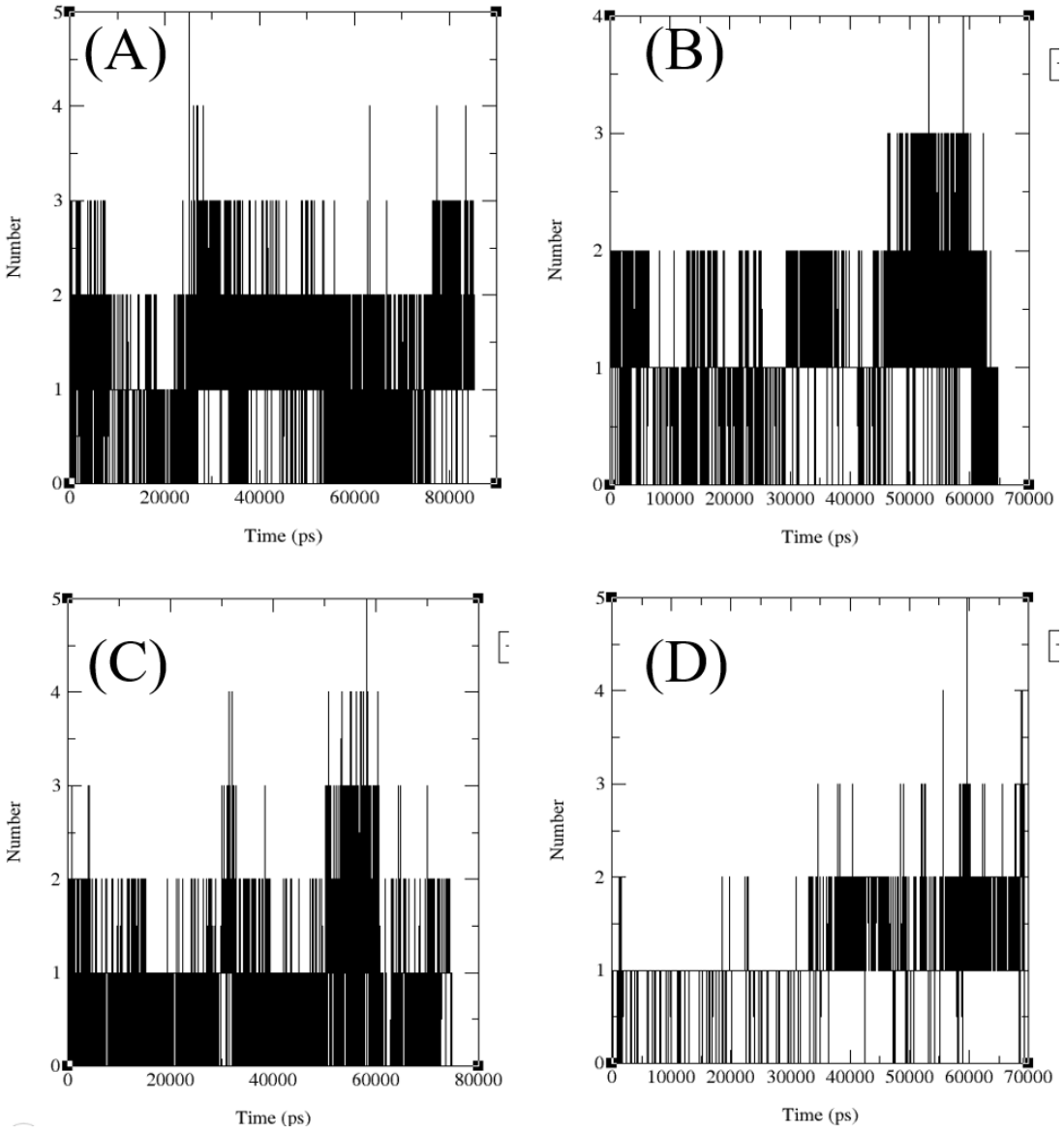


Figure A35: Count of hydrogen bond formation of compound **18** at (A) 300K (B) 305K (C) 310K and (D) 320K temperature.

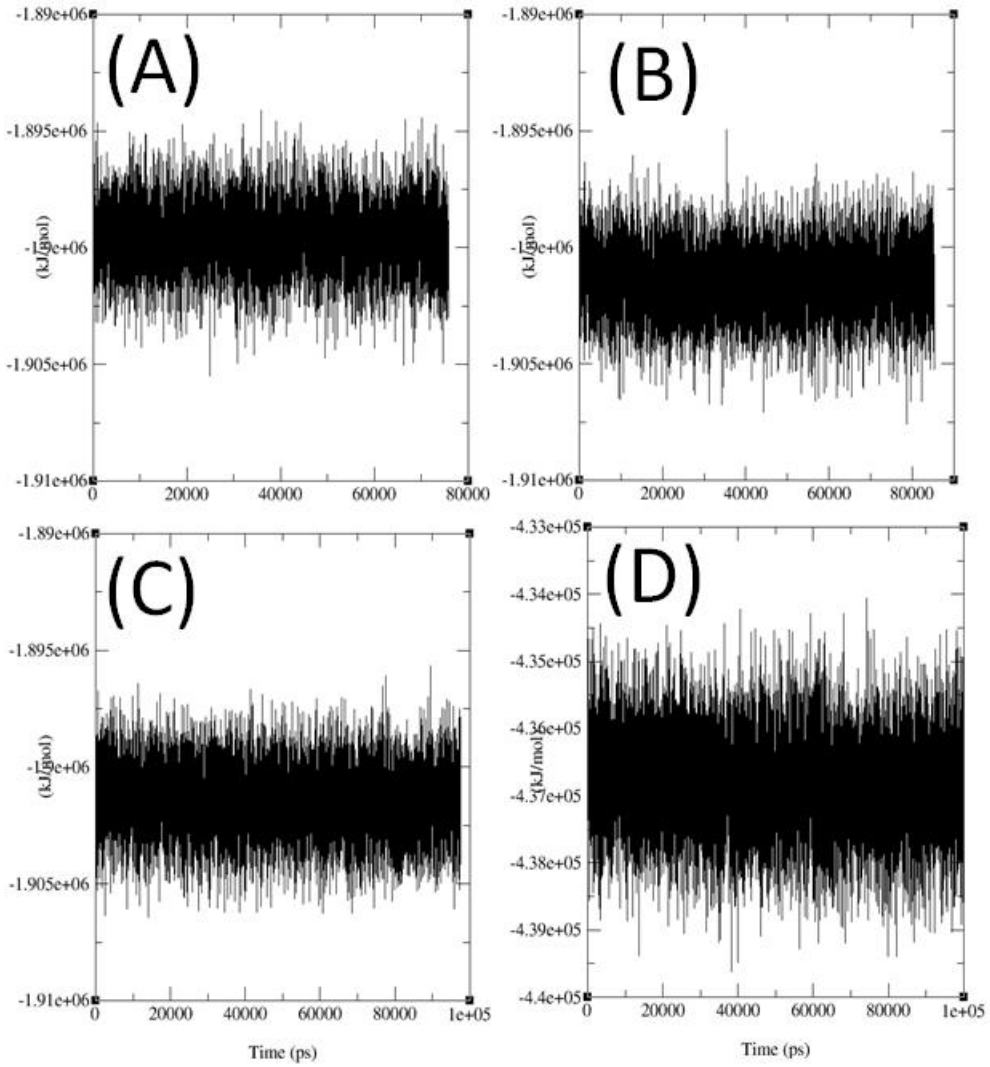


Figure A36. Potential energy curves of (A) compound **6**; (B) compound **18**; (C) compound **23**; and (D) Genistein over 100 ns MD simulation at 300 K.

Alanine Scanning Mutagenesis and Stability Analysis

Figures 37A–37C summarize the MMPBSA stability and alanine-scanning mutagenesis analysis for the wild-type ligand **18**–protein (1X2J) complex. The overall energetic components: G_{GAS}, G_{SOLV}, and G_{TOTAL} capture the global stability of the complex by incorporating van der Waals (EVDW), electrostatic (EEL), polar solvation (EGB), and nonpolar solvation (ESURF)

contributions. Figure 37A presents the energetic profile of the wild-type residues before alanine substitution. These values provide the baseline interaction strength and reflect the full side-chain contributions to ligand stabilization. Figure 37B displays the mutant–normal (ΔΔG) comparison, revealing how alanine substitution perturbs residue–ligand interactions. Changes across G_{GAS}, G_{SOLV}, and G_{TOTAL} energy terms indicate whether the native side chain contributed favorably or unfavorably to binding. Alterations in E_{EL}, E_{VDW}, and solvation terms reveal the specific energetic origin of these differences. Figure 37C shows the energetic contributions of the mutated (alanine) residues alone. Comparing Figures 37A and 37C reveals the energetic penalty or benefit resulting from the removal of the original residue's side chain. This analysis identifies hotspot residues that are critical contributors to ligand **18** binding affinity. Figure 37D provides the MMPBSA stability profile for the normal (wild-type) ligand–protein complex. Energetic components: G_{GAS}, G_{SOLV}, and E_{TOTAL} capture the global stability of the ligand **18**-1X2J interaction. The values reflect the combined effects of van der Waals forces, electrostatics, and solvation contributions that define the binding free energy and overall structural stability of the complex.

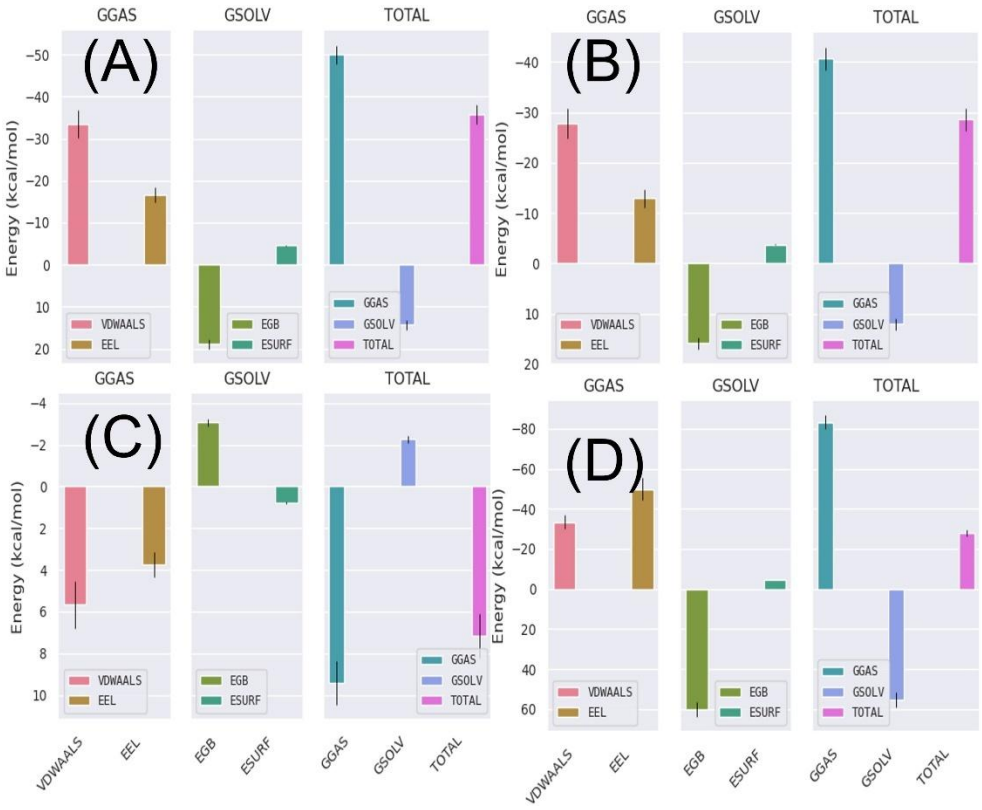


Figure A37. (A) Per-residue MMPBSA energetic components for the wild-type system during alanine scanning; (B) mutant–normal energy differences illustrating the effect of alanine substitution on ligand **18** binding; (C) energetic contributions of the alanine-mutated residues; and (D) Stability interaction map identifying key residues that stabilize compound **18** within the 1X2J complex.

Per-Residue Decomposition Analysis

Figures A38A–A38D provide detailed per-residue MMPBSA decomposition using both Total Decomposition Components (TDC) and Single Decomposition Components (SDC). Figures A38A and A38B illustrate the TDC results, which report total per-residue binding contributions. Figure A38A (TDC bar plot) highlights residues such as AHD-15, ATR-23, ASE-32, ATRP-34, BAL-4, BPRO-5, BLEU-7, BPRO-8, and BARG-9 as key contributors influencing ligand binding. Strongly negative ΔG values denote stabilizing interactions, while positive values indicate destabilizing residues. Figure A38B (TDC heatmap) visualizes binding contributions across simulation frames. Dark blue regions correspond to residues consistently stabilizing the ligand, while lighter regions represent weaker or fluctuating interactions. This

visualization confirms the temporal robustness of hotspot residues identified in Figure A38A. Figures A38C and A38D provide the SDC decomposition, which isolates contributions from individual energetic components. Figure A38C (SDC bar plot) reveals the specific interaction types (e.g., electrostatic vs van der Waals) responsible for residue stabilization or destabilization. Several residues retain strong stabilizing roles consistent with the TDC analysis, validating the reliability of the observed interaction patterns. Figure A38D (SDC heatmap) presents per-frame fluctuations of SDC terms. Residues showing consistently dark regions indicate stable energetic contributions, whereas mixed intensities reveal dynamic, frame-dependent interactions. Together, TDC and SDC analyses provide a comprehensive view of residue-level energetics within the binding interface.

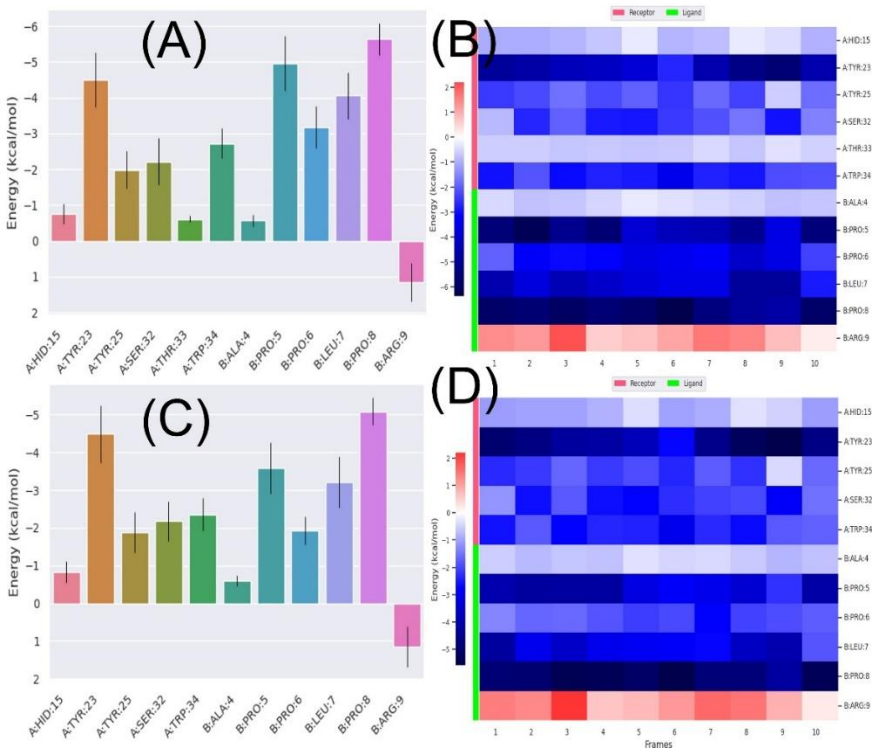


Figure A38. Per-residue MMPBSA analysis using Total Decomposition Components (TDC) and Single Decomposition Components (SDC) for the ligand **18**–1X2J complex: (A) TDC bar plot for the normal (wild-type) system; (B) TDC heatmap showing per-frame binding contributions across the simulation; (C) SDC bar plot illustrating specific energetic interaction types for key residues; and (D) SDC heatmap depicting temporal fluctuations in residue contributions that stabilize compound **18** within the 1X2J complex.

Interaction Entropy and Binding Energy Analysis

Figures A39A–A39C present the Interaction Entropy (IE) and total binding energy evaluation for ligand **18**–1X2J. Figure A39A reports the numerical Interaction Entropy (IE) value and its associated σ-fluctuation parameter. The slightly negative IE value indicates a mild but favorable entropic contribution to ligand binding, whereas the σ parameter represents the underlying fluctuation amplitude used in the IE calculation. Figure A39B provides the temporal evolution of IE for both the full trajectory and a refined selection of stable frames. The observed downward trend, yielding progressively negative IE values, reflects increasing entropic stabilization during the simulation. Figure A39C summarizes the binding thermodynamics combining MMPBSA enthalpic terms with Interaction Entropy: ΔH (Enthalpy): Strongly negative, driven by favorable gas-phase and solvation contributions. –TΔS (Entropy): IE-based entropic term contributing modestly to the total free energy. ΔG (GB+IE): The combined free energy (ΔG = ΔH – TΔS) remains strongly negative, confirming stable and favorable binding of ligand **18** to 1X2J. A comparative evaluation of MM-PBSA energy parameters for compounds **6**, **18**, **23**, and genistein is provided in Figures A41 to A43 of the Supporting Information. These results allow direct comparison of binding strengths and energetic signatures across the ligand series, supporting structure-activity relationship (SAR) interpretation and prioritization of lead compounds.

Table S25. (A) Numerical Interaction Entropy (IE) value and its corresponding σ-fluctuation parameter; (B) temporal evolution of IE across the full trajectory and a refined subset of stable frames; (C) combined binding free energy (ΔG = ΔH – TΔS), demonstrating a strongly negative value consistent with stable and favorable binding of ligand **18** to the 1X2J complex.

Complex:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	1932.28	29.48	29.48	4.17	4.17
ANGLE	4864.27	57.97	57.97	8.20	8.20
DIHED	6516.35	36.15	36.15	5.11	5.11
VDWAALS	-4733.66	30.41	30.41	4.30	4.30
EEL	-41676.40	102.78	102.78	14.53	14.53
1-4 VDW	2215.85	16.07	16.07	2.27	2.27
1-4 EEL	22202.27	74.49	74.49	10.53	10.53

EGB	-7261.35	55.77	55.77	7.89	7.89
ESURF	253.21	3.06	3.06	0.43	0.43
GGAS	-8679.05	151.10	113.58	21.37	16.06
GSOLV	-7008.15	55.86	54.88	7.90	7.76
TOTAL	-15687.20	161.09	84.91	22.78	12.01

Receptor:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	1921.78	29.18	29.18	4.13	4.13
ANGLE	4842.38	57.81	57.81	8.18	8.18
DIHED	6485.85	36.50	36.50	5.16	5.16
VDWAALS	-4678.79	30.16	30.16	4.27	4.27
EEL	-41628.47	103.31	103.31	14.61	14.61
1-4 VDW	2197.74	16.23	16.23	2.29	2.29
1-4 EEL	22223.39	74.32	74.32	10.51	10.51
EGB	-7275.05	55.56	55.56	7.86	7.86
ESURF	255.13	3.21	3.21	0.45	0.45
GGAS	-8636.13	151.31	114.36	21.40	16.17
GSOLV	-7019.92	55.65	54.58	7.87	7.72
TOTAL	-15656.05	161.22	85.50	22.80	12.09

Ligand:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	10.50	2.83	2.83	0.40	0.40
ANGLE	21.89	3.81	3.81	0.54	0.54
DIHED	30.50	2.61	2.61	0.37	0.37
VDWAALS	-5.19	1.10	1.10	0.16	0.16
EEL	-23.70	0.68	0.68	0.10	0.10
1-4 VDW	18.11	1.04	1.04	0.15	0.15
1-4 EEL	-21.13	0.91	0.91	0.13	0.13
EGB	-24.61	0.73	0.73	0.10	0.10
ESURF	3.91	0.03	0.03	0.00	0.00
GGAS	30.98	5.74	5.45	0.81	0.77
GSOLV	-20.71	0.73	0.72	0.10	0.10
TOTAL	10.28	5.79	5.35	0.82	0.76

Delta (Complex - Receptor - Ligand):

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
ΔBOND	0.00	2.54	0.00	0.36	0.00
ΔANGLE	-0.00	3.65	0.00	0.52	0.00
ΔDIHED	-0.00	2.26	0.00	0.32	0.00
ΔVDWAALS	-49.68	0.86	2.66	0.12	0.38
ΔEEL	-24.23	0.14	4.55	0.02	0.64

Δ1-4 VDW	0.00	0.88	0.00	0.12	0.00
Δ1-4 EEL	-0.00	0.74	0.00	0.10	0.00
ΔEGB	38.31	0.51	2.83	0.07	0.40
ΔESURF	-5.83	0.12	0.22	0.02	0.03
ΔGGAS	-73.91	0.87	4.87	0.12	0.69
ΔGSOLV	32.48	0.52	2.67	0.07	0.38
ΔTOTAL	-41.43	1.01	3.02	0.14	0.43

Table S26. (A) Numerical Interaction Entropy (IE) value and its corresponding σ-fluctuation parameter; (B) temporal evolution of IE across the full trajectory and a refined subset of stable frames; (C) combined binding free energy (ΔG = ΔH – TΔS), demonstrating a strongly negative value consistent with stable and favorable binding of ligands **6**, **23**, and Genistein to the 1X2J complex.

Data for ligand 6:

| Run on Thu Nov 20 12:47:32 2025

||gmx_MMPBSA Version=1.6.4 based on MMPBSA.py v.16.0

|Complex Structure file: md_0_5.tpr

|Complex (GROMACS) topology file: topol.top

|Complex (AMBER) topology file: COM.prmtop

|Receptor (AMBER) topology file: REC.prmtop

|Ligand (AMBER) topology file: LIG.prmtop

|Initial trajectories: COM_traj_0.xtc

||Receptor mask: ":1-624"

|Ligand mask: ":625"

|Ligand residue name is: "UNK"

||Calculations performed using 50 complex frames

|

|Generalized Born ESURF calculated using 'LCPO' surface areas

|

|Using temperature = 298.15 K

|All units are reported in kcal/mol

||SD - Sample standard deviation, SEM - Sample standard error of the mean

|SD(Prop.), SEM(Prop.) - SD and SEM obtained with propagation of uncertainty formula

|https://en.wikipedia.org/wiki/Propagation_of_uncertainty#Example_formulae

|GENERALIZED BORN:

Complex:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	1947.70	35.47	35.47	5.02	5.02
ANGLE	4891.71	50.93	50.93	7.20	7.20
DIHED	6517.39	35.83	35.83	5.07	5.07
VDWAALS	-4719.41	28.87	28.87	4.08	4.08
EEL	-41598.60	147.14	147.14	20.81	20.81
1-4 VDW	2210.21	15.79	15.79	2.23	2.23
1-4 EEL	22140.18	85.78	85.78	12.13	12.13
EGB	-7277.69	82.93	82.93	11.73	11.73
ESURF	255.18	2.61	2.61	0.37	0.37
GGAS	-8610.81	187.69	117.02	26.54	16.55
GSOLV	-7022.51	82.98	81.48	11.73	11.52
TOTAL	-15633.32	205.21	75.41	29.02	10.66

Receptor:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	1935.74	35.72	35.72	5.05	5.05
ANGLE	4868.48	50.22	50.22	7.10	7.10
DIHED	6487.49	36.38	36.38	5.14	5.14
VDWAALS	-4667.03	28.63	28.63	4.05	4.05
EEL	-41590.28	145.82	145.82	20.62	20.62
1-4 VDW	2192.20	15.98	15.98	2.26	2.26

1-4 EEL	22184.08	86.09	86.09	12.17	12.17
EGB	-7284.36	82.88	82.88	11.72	11.72
ESURF	256.84	2.56	2.56	0.36	0.36
GGAS	-8589.33	186.74	116.78	26.41	16.52
GSOLV	-7027.51	82.92	81.47	11.73	11.52
TOTAL	-15616.85	204.32	75.80	28.90	10.72

Ligand:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	11.96	2.50	2.50	0.35	0.35
ANGLE	23.23	4.14	4.14	0.59	0.59
DIHED	29.91	2.61	2.61	0.37	0.37
VDWAALS	-5.59	1.26	1.26	0.18	0.18
EEL	-4.94	0.98	0.98	0.14	0.14
1-4 VDW	18.02	1.35	1.35	0.19	0.19
1-4 EEL	-43.89	0.94	0.94	0.13	0.13
EGB	-18.83	0.76	0.76	0.11	0.11
ESURF	4.16	0.03	0.03	0.00	0.00
GGAS	28.69	5.95	4.93	0.84	0.70
GSOLV	-14.67	0.77	0.75	0.11	0.11
TOTAL	14.01	6.00	4.84	0.85	0.69

Delta (Complex - Receptor - Ligand):

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM

ΔBOND	-0.00	2.24	0.00	0.32	0.00
ΔANGLE	-0.00	3.43	0.00	0.49	0.00
ΔDIHED	-0.00	2.07	0.00	0.29	0.00
ΔVDWAALS	-46.79	1.01	2.12	0.14	0.30
ΔEEL	-3.37	0.34	2.86	0.05	0.40
Δ1-4 VDW	-0.00	1.17	0.00	0.17	0.00
Δ1-4 EEL	0.00	0.64	0.00	0.09	0.00
ΔEGB	25.50	0.71	1.75	0.10	0.25
ΔESURF	-5.82	0.02	0.16	0.00	0.02
ΔGGAS	-50.16	1.07	2.75	0.15	0.39
ΔGSOLV	19.67	0.71	1.75	0.10	0.25
ΔTOTAL	-30.48	1.28	2.35	0.18	0.33

Data for ligand 23:

gmx_MMPBSA Version=v.1.6.3 based on MMPBSA.py v.16.0

|Complex Structure file: md_0_5.tpr

|Complex (GROMACS) topology file: topol.top

|Complex (AMBER) topology file: COM.prmtop

|Receptor (AMBER) topology file: REC.prmtop

|Ligand (AMBER) topology file: LIG.prmtop

|Initial trajectories: COM_traj_0.xtc

||Receptor mask: ":1-624"

|Ligand mask: ":625"

|Ligand residue name is: "UNK"

|

|Calculations performed using 500 complex frames

|

|Generalized Born ESURF calculated using 'LCPO' surface areas

|

|Using temperature = 298.15 K

|All units are reported in kcal/mol

|

|SD - Sample standard deviation, SEM - Sample standard error of the mean

|SD(Prop.), SEM(Prop.) - SD and SEM obtained with propagation of uncertainty formula

|https://en.wikipedia.org/wiki/Propagation_of_uncertainty#Example_formulae

|

GENERALIZED BORN:

Complex:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	1962.82	37.77	37.77	1.69	1.69
ANGLE	5432.75	55.04	55.04	2.46	2.46
DIHED	6505.20	35.22	35.22	1.58	1.58
VDWAALS	-4779.86	41.86	41.86	1.87	1.87
EEL	-42021.10	214.63	214.63	9.60	9.60
1-4 VDW	2273.46	20.24	20.24	0.91	0.91
1-4 EEL	22241.47	78.39	78.39	3.51	3.51
EGB	-6955.79	177.25	177.25	7.93	7.93
ESURF	245.89	6.44	6.44	0.29	0.29
GGAS	-8385.25	245.10	207.97	10.96	9.30
GSOLV	-6709.90	177.36	171.68	7.93	7.68

TOTAL -15095.15 302.54 75.48 13.53 3.38

Receptor:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	1932.68	37.81	37.81	1.69	1.69
ANGLE	4866.94	54.47	54.47	2.44	2.44
DIHED	6477.39	35.00	35.00	1.57	1.57
VDWAALS	-4720.58	41.28	41.28	1.85	1.85
EEL	-42036.58	214.47	214.47	9.59	9.59
1-4 VDW	2189.35	19.61	19.61	0.88	0.88
1-4 EEL	22337.73	78.35	78.35	3.50	3.50
EGB	-6965.14	177.26	177.26	7.93	7.93
ESURF	246.95	6.42	6.42	0.29	0.29
GGAS	-8953.08	244.64	207.14	10.94	9.26
GSOLV	-6718.19	177.38	171.73	7.93	7.68
TOTAL	-15671.26	302.17	75.17	13.51	3.36

Ligand:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	30.14	5.15	5.15	0.23	0.23
ANGLE	565.82	5.26	5.26	0.24	0.24

DIHED	27.81	3.14	3.14	0.14	0.14
VDWAALS	-6.17	1.46	1.46	0.07	0.07
EEL	27.42	1.06	1.06	0.05	0.05
1-4 VDW	84.11	4.65	4.65	0.21	0.21
1-4 EEL	-96.26	1.65	1.65	0.07	0.07
EGB	-19.65	0.52	0.52	0.02	0.02
ESURF	4.06	0.03	0.03	0.00	0.00
GGAS	632.88	9.57	4.28	0.43	0.19
GSOLV	-15.59	0.52	0.52	0.02	0.02
TOTAL	617.29	9.59	4.26	0.43	0.19

Delta (Complex - Receptor - Ligand):

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
ΔBOND	0.00	5.11	0.00	0.23	0.00
ΔANGLE	0.00	4.69	0.00	0.21	0.00
ΔDIHED	-0.00	2.92	0.00	0.13	0.00
ΔVDWAALS	-53.11	0.88	2.55	0.04	0.11
ΔEEL	-11.94	0.90	3.11	0.04	0.14
Δ1-4 VDW	-0.00	4.02	0.00	0.18	0.00
Δ1-4 EEL	-0.00	1.60	0.00	0.07	0.00
ΔEGB	29.00	0.50	2.21	0.02	0.10
ΔESURF	-5.12	0.01	0.24	0.00	0.01
ΔGGAS	-65.06	1.25	4.04	0.06	0.18
ΔGSOLV	23.88	0.50	2.15	0.02	0.10

ΔTOTAL -41.17 1.35 2.99 0.06 0.13

Data for ref drug for Genistein:

| Run on Fri Nov 14 00:21:20 2025

||gmx_MMPBSA Version=1.6.4 based on MMPBSA.py v.16.0

|Complex Structure file: md_0_5.tpr

|Complex (GROMACS) topology file: topol.top

|Complex (AMBER) topology file: COM.prmtop

|Receptor (AMBER) topology file: REC.prmtop

|Ligand (AMBER) topology file: LIG.prmtop

|Initial trajectories: COM_traj_0.xtc

||Receptor mask: ":1-290"

|Ligand mask: ":291"

|Ligand residue name is: "UNK"

||Calculations performed using 50 complex frames

||Generalized Born ESURF calculated using 'LCPO' surface areas

||Using temperature = 298.15 K

|All units are reported in kcal/mol

||SD - Sample standard deviation, SEM - Sample standard error of the mean

|SD(Prop.), SEM(Prop.) - SD and SEM obtained with propagation of uncertainty formula

|https://en.wikipedia.org/wiki/Propagation_of_uncertainty#Example_formulae

GENERALIZED BORN:

Complex:

Energy Component Average SD(Prop.) SD SEM(Prop.) SEM

BOND 890.46 23.73 23.73 3.36 3.36

ANGLE 2214.24 33.00 33.00 4.67 4.67

DIHED 2879.66 23.60 23.60 3.34 3.34

VDWAALS -2305.99 27.59 27.59 3.90 3.90

EEL	-18693.80	64.54	64.54	9.13	9.13
1-4 VDW	978.89	13.65	13.65	1.93	1.93
1-4 EEL	9213.65	33.67	33.67	4.76	4.76
EGB	-3048.23	57.88	57.88	8.19	8.19
ESURF	89.71	2.39	2.39	0.34	0.34
GGAS	-4822.88	91.95	82.21	13.00	11.63
GSOLV	-2958.52	57.93	56.39	8.19	7.97
TOTAL	-7781.40	108.68	52.11	15.37	7.37

Receptor:

Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
BOND	883.91	23.78	23.78	3.36	3.36
ANGLE	2205.03	32.99	32.99	4.66	4.66
DIHED	2866.70	22.88	22.88	3.24	3.24
VDWAALS	-2273.26	26.70	26.70	3.78	3.78
EEL	-18823.16	63.42	63.42	8.97	8.97
1-4 VDW	966.84	13.74	13.74	1.94	1.94
1-4 EEL	9476.82	33.75	33.75	4.77	4.77
EGB	-3050.20	57.89	57.89	8.19	8.19
ESURF	91.21	2.32	2.32	0.33	0.33
GGAS	-4697.12	90.77	81.70	12.84	11.55
GSOLV	-2959.00	57.94	56.49	8.19	7.99
TOTAL	-7656.12	107.68	52.03	15.23	7.36

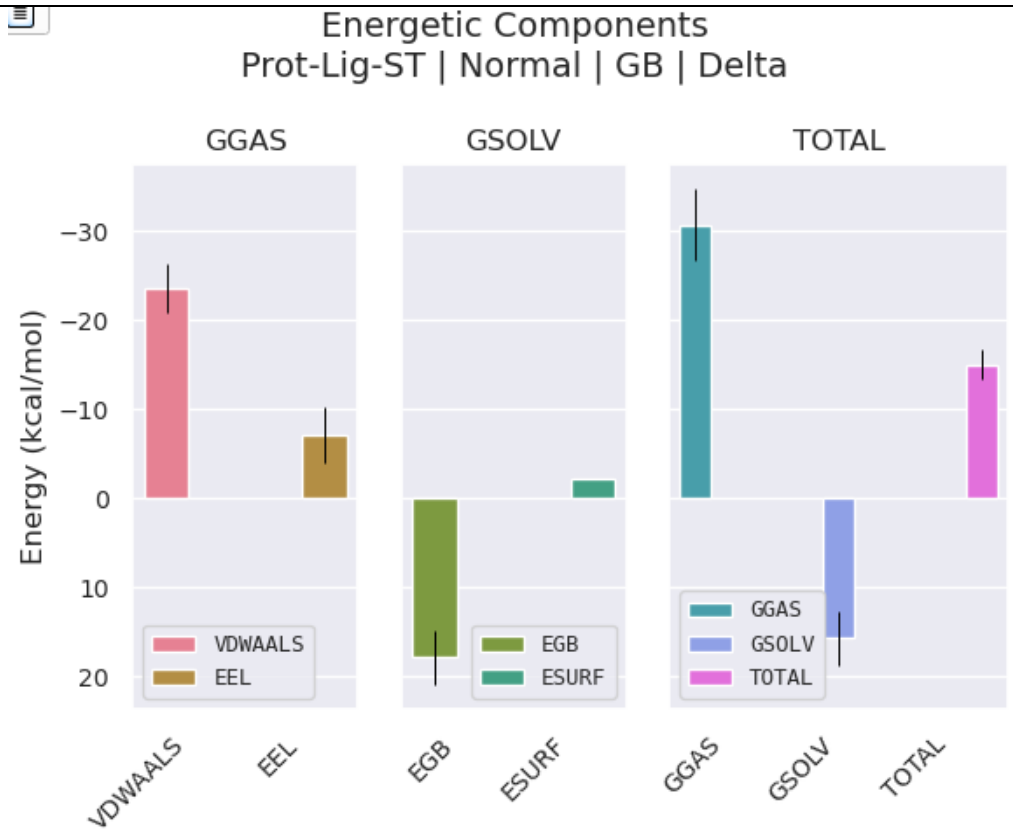
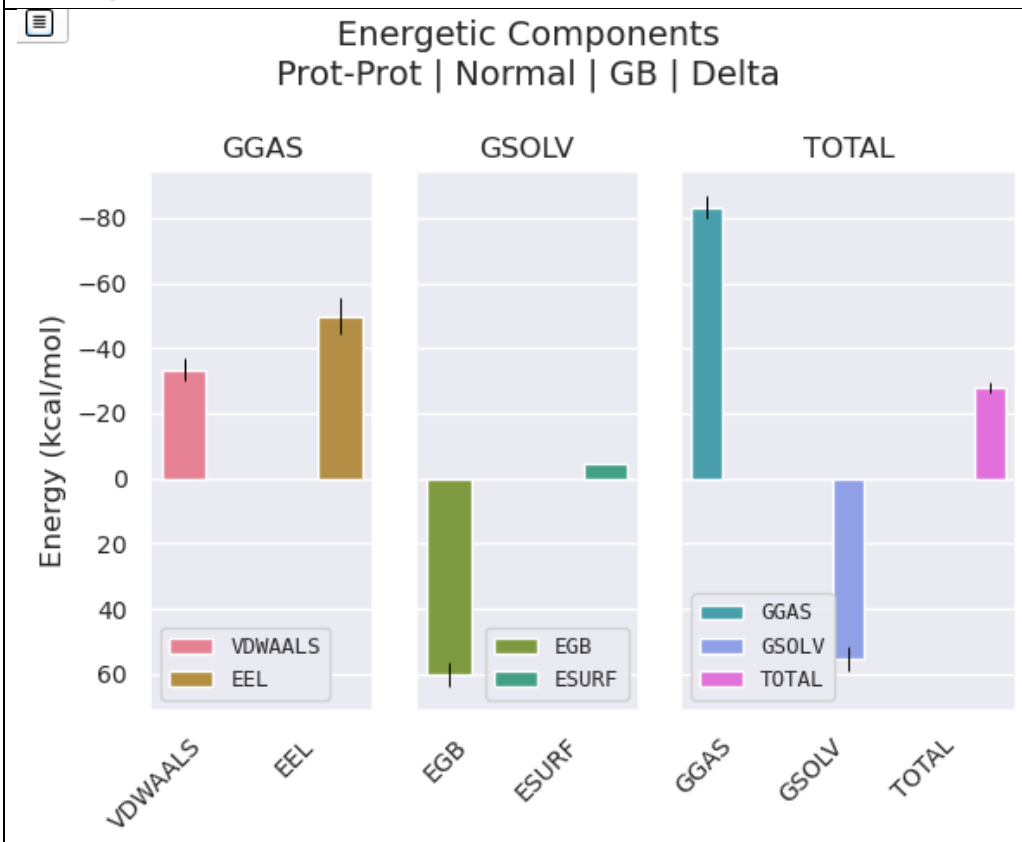
Ligand:

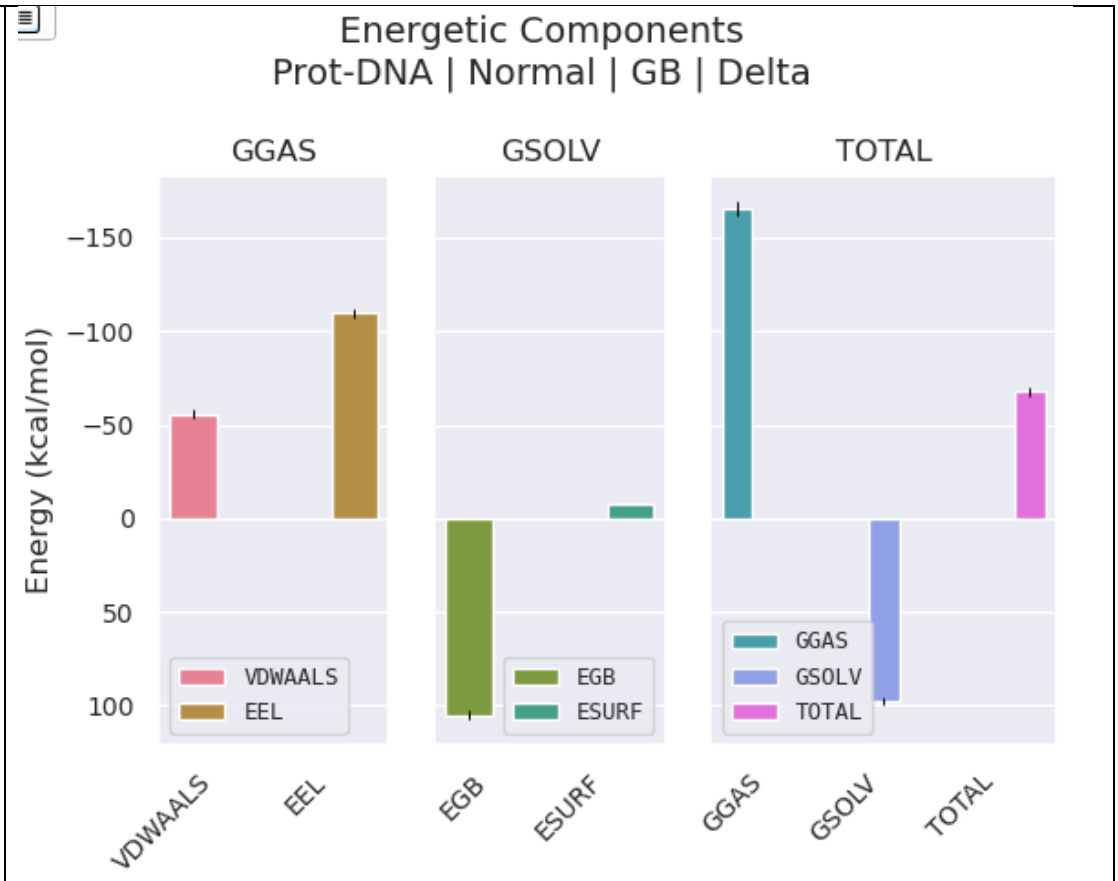
Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM

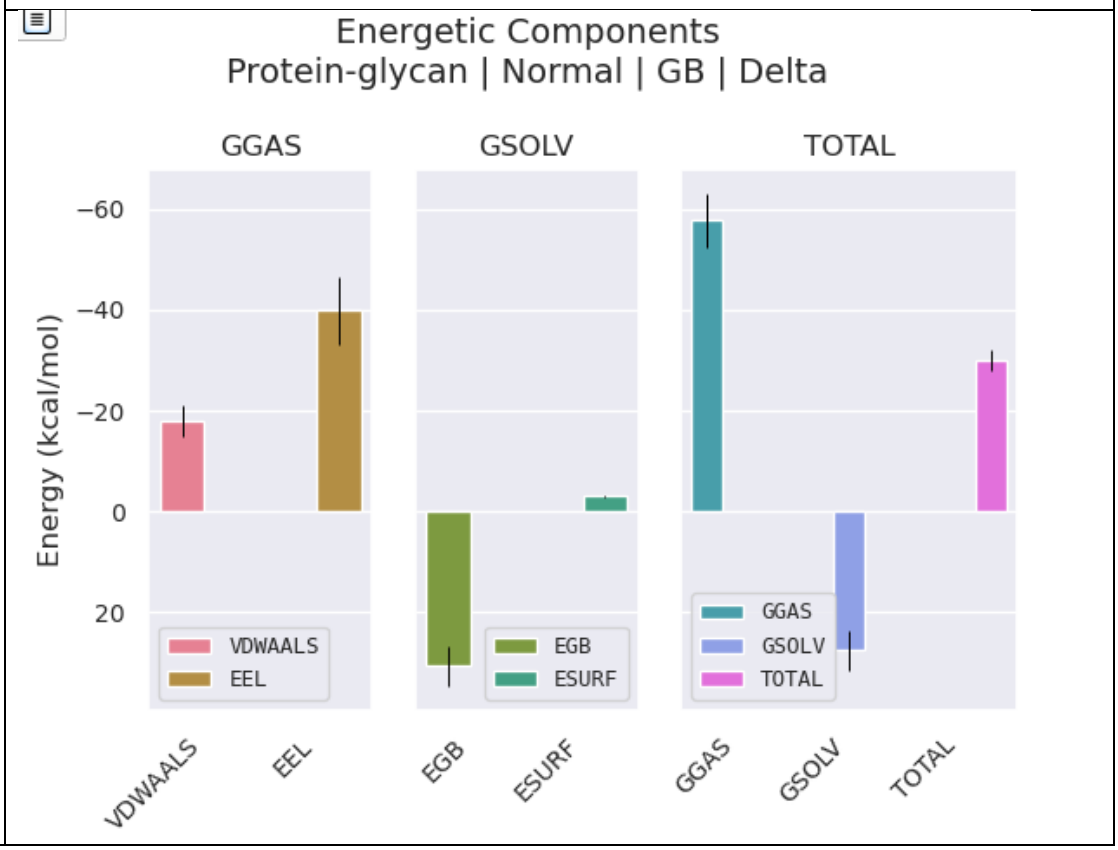
BOND	6.55	1.92	1.92	0.27	0.27
ANGLE	9.21	2.29	2.29	0.32	0.32
DIHED	12.96	2.30	2.30	0.32	0.32
VDWAALS	-0.53	1.05	1.05	0.15	0.15
EEL	137.21	1.68	1.68	0.24	0.24
1-4 VDW	12.05	0.78	0.78	0.11	0.11
1-4 EEL	-263.17	1.41	1.41	0.20	0.20
EGB	-20.50	0.78	0.78	0.11	0.11
ESURF	2.64	0.01	0.01	0.00	0.00
GGAS	-85.70	4.55	4.14	0.64	0.59
GSOLV	-17.86	0.78	0.78	0.11	0.11
TOTAL	-103.56	4.62	3.82	0.65	0.54

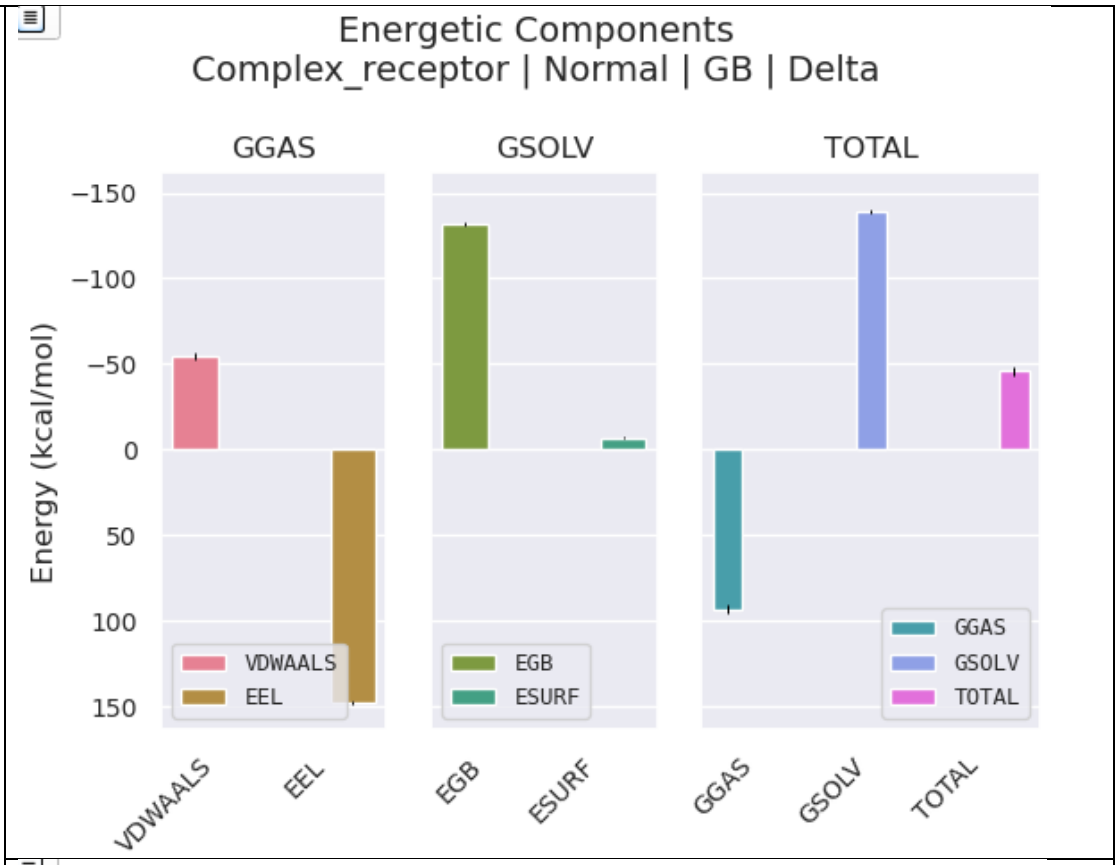
Delta (Complex - Receptor - Ligand):

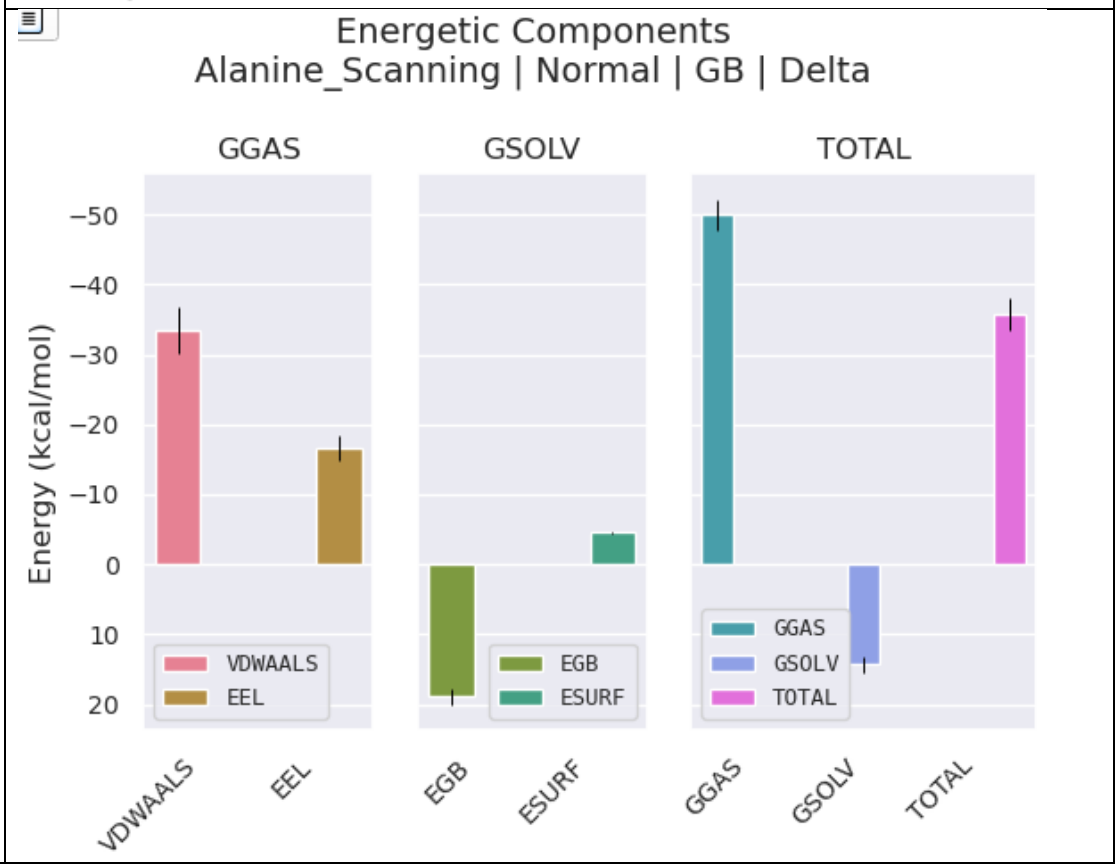
Energy Component	Average	SD(Prop.)	SD	SEM(Prop.)	SEM
ΔBOND	0.00	1.87	0.00	0.26	0.00
ΔANGLE	0.00	2.27	0.00	0.32	0.00
ΔDIHED	0.00	1.57	0.00	0.22	0.00
ΔVDWAALS	-32.20	0.16	2.57	0.02	0.36
ΔEEL	-7.85	0.56	3.70	0.08	0.52
Δ1-4 VDW	0.00	0.69	0.00	0.10	0.00
Δ1-4 EEL	-0.00	1.32	0.00	0.19	0.00
ΔEGB	22.47	0.77	2.51	0.11	0.36
ΔESURF	-4.14	0.06	0.17	0.01	0.02
ΔGGAS	-40.05	0.58	4.35	0.08	0.62
ΔGSOLV	18.34	0.77	2.50	0.11	0.35
ΔTOTAL	-21.71	0.96	3.20	0.14	0.45

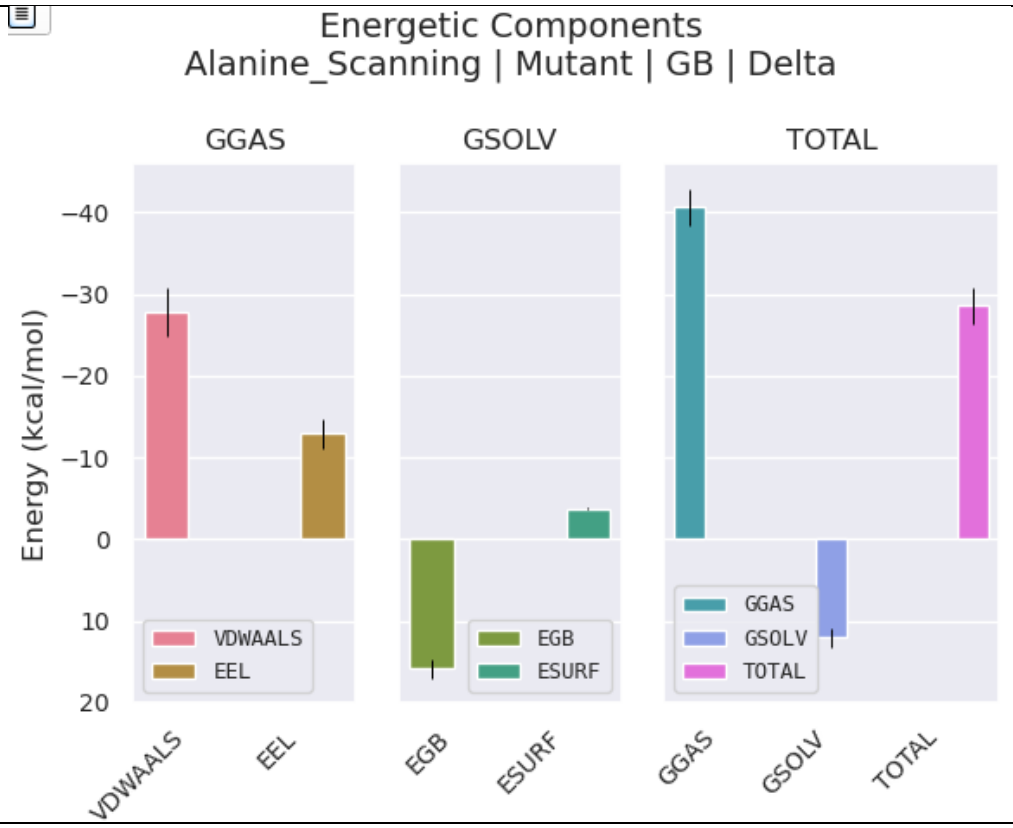
18	 Energetic Components Prot-Lig-ST | Normal | GB | Delta GGAS GSOLV TOTAL Energy (kcal/mol) −30 −20 −10 0 10 20 VDWAALS EEL EGB ESURF GGAS GSOLV TOTAL  Energetic Components Prot-Prot | Normal | GB | Delta GGAS GSOLV TOTAL Energy (kcal/mol) −80 −60 −40 −20 0 20 40 60 VDWAALS EEL EGB ESURF GGAS GSOLV TOTAL


Energetic Components
Prot-DNA | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

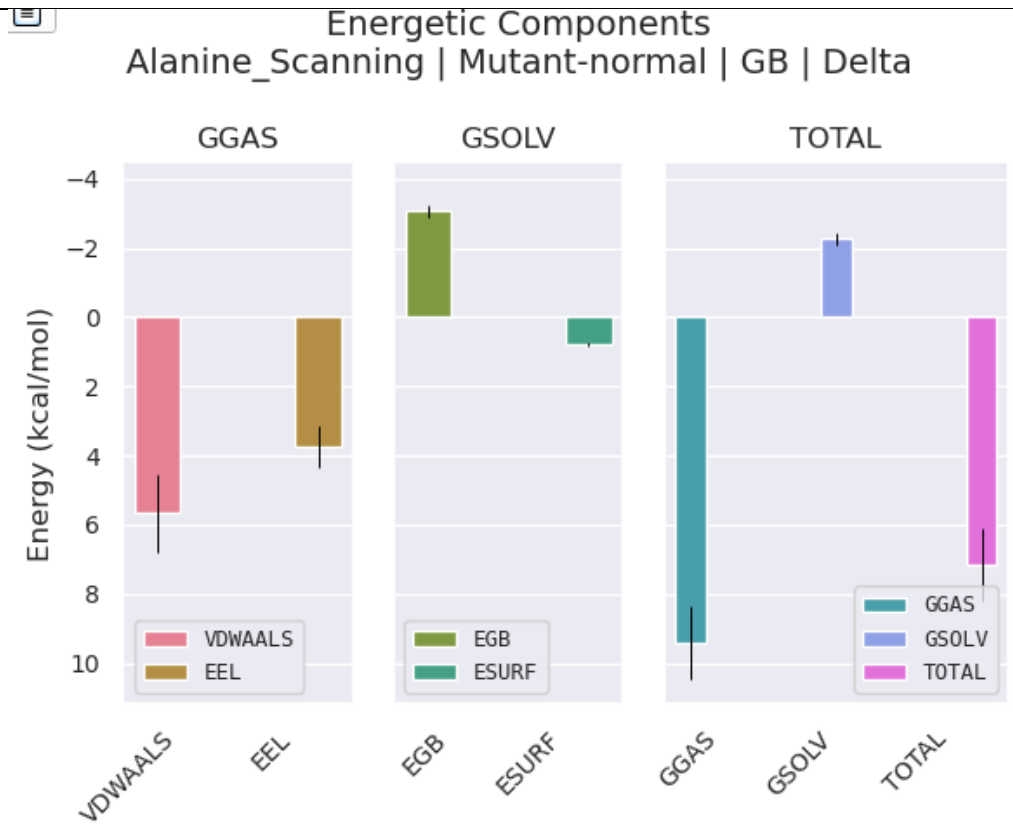

Energetic Components
Protein-glycan | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−60
−40
−20
0
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

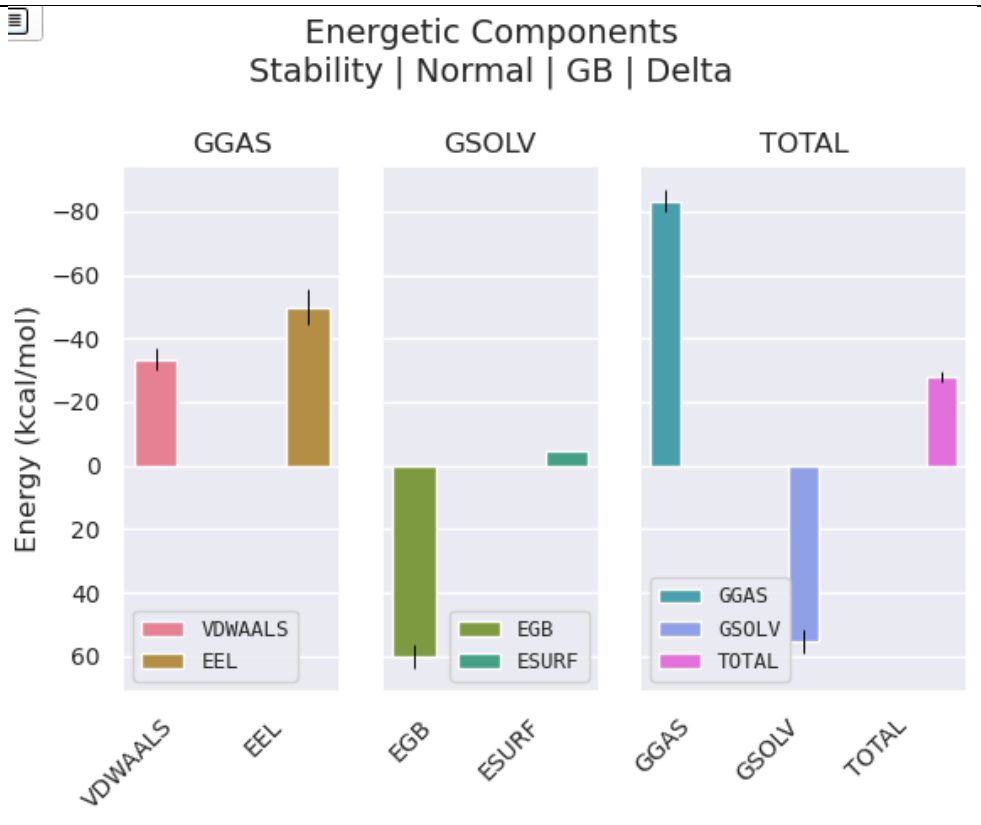

Energetic Components
Complex_receptor | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
150
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

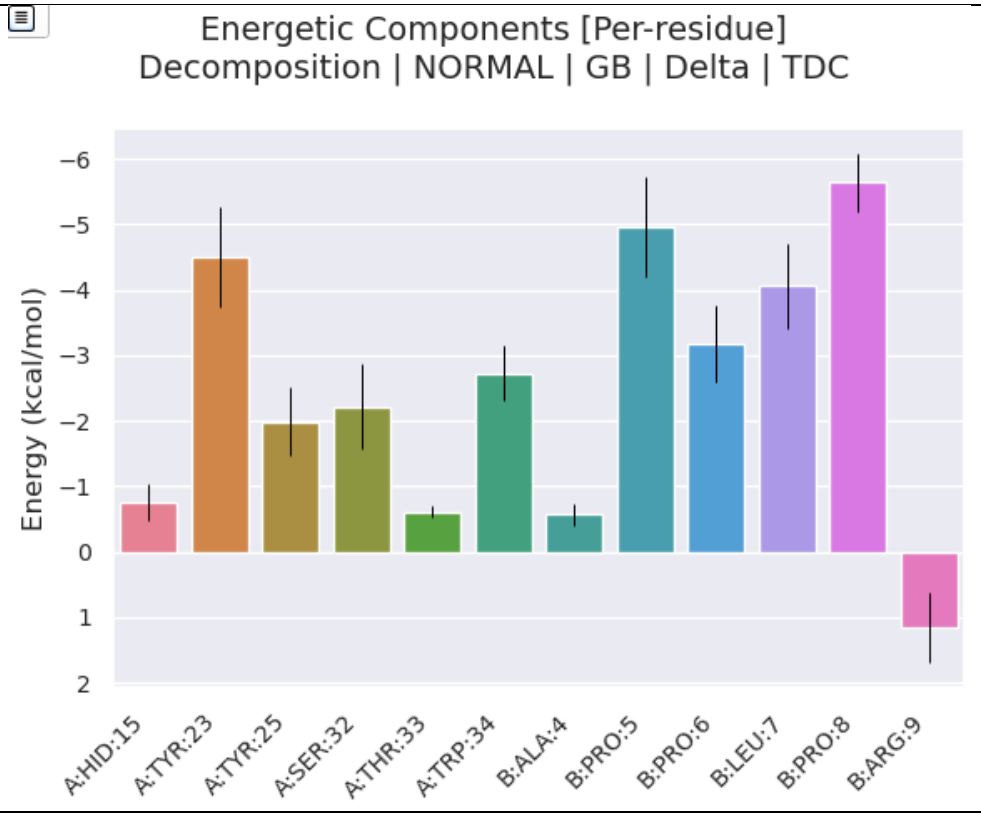

Energetic Components
Alanine_Scanning | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−50
−40
−30
−20
−10
0
10
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

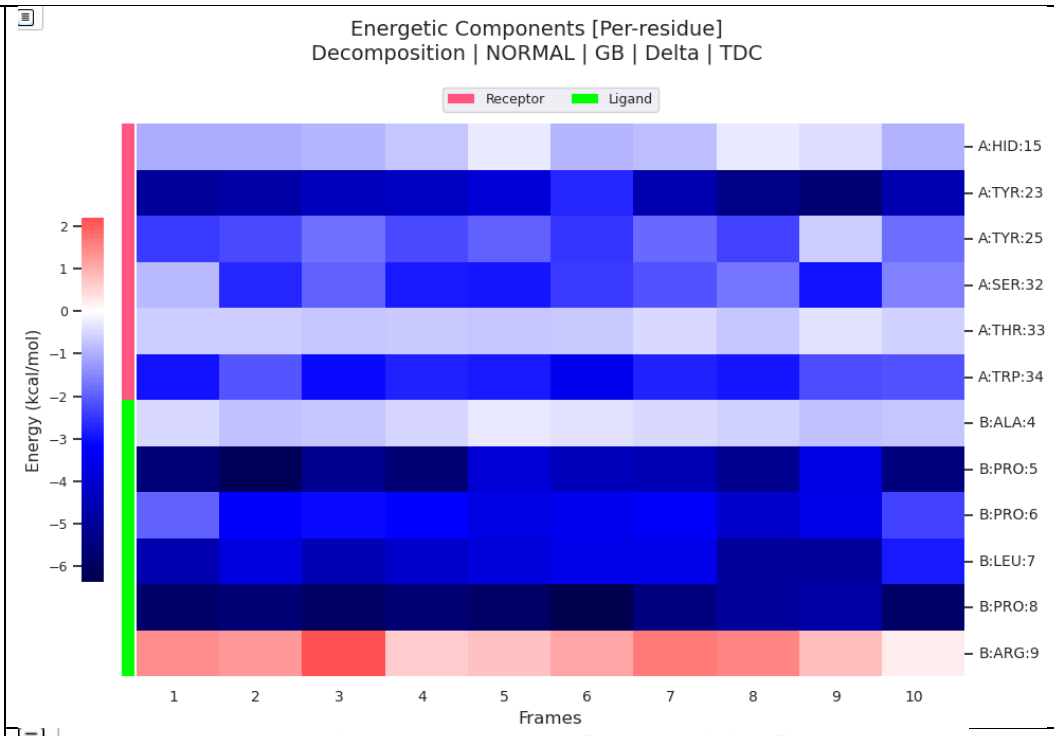

Energetic Components
Alanine_Scanning | Mutant | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−40
−30
−20
−10
0
10
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

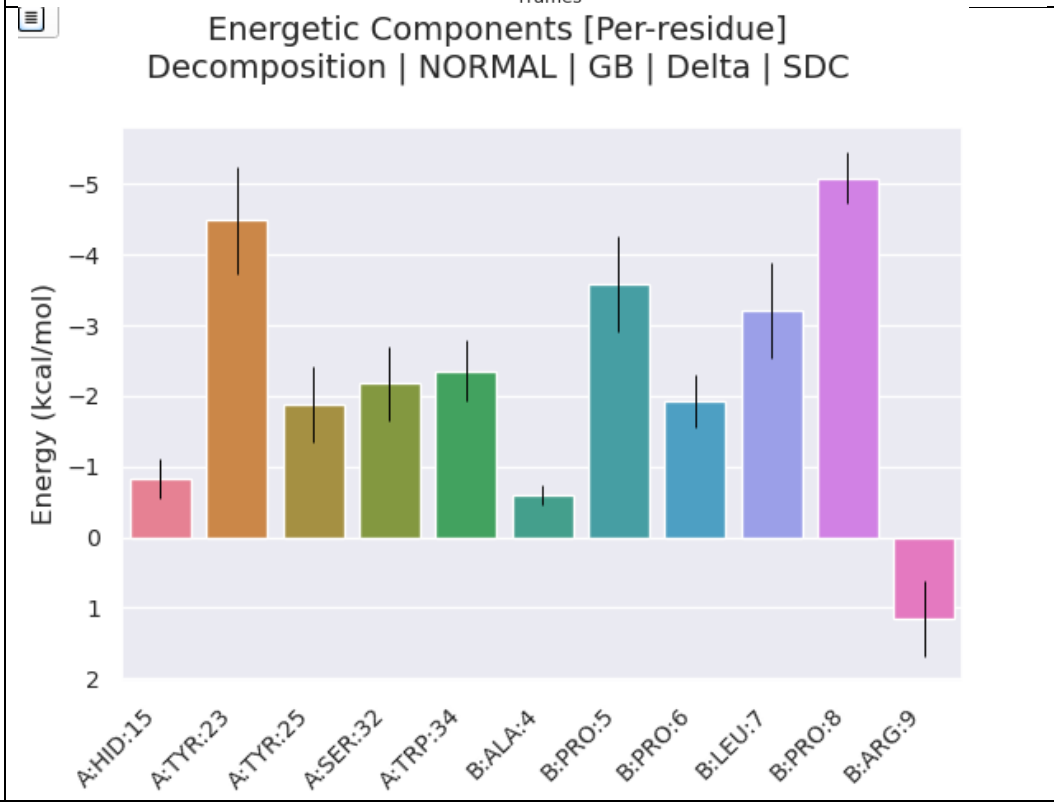
18

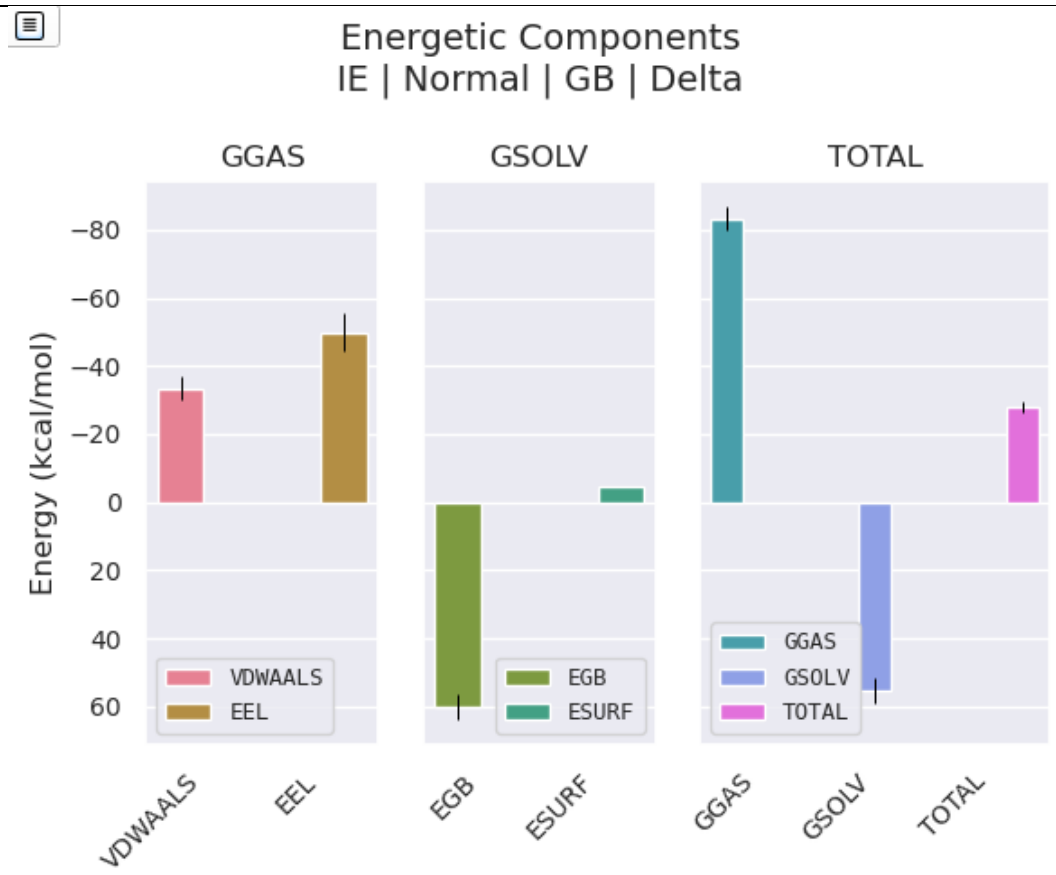

Energetic Components
Alanine_Scanning | Mutant-normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−4
−2
0
2
4
6
8
10
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Energetic Components
Stability | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

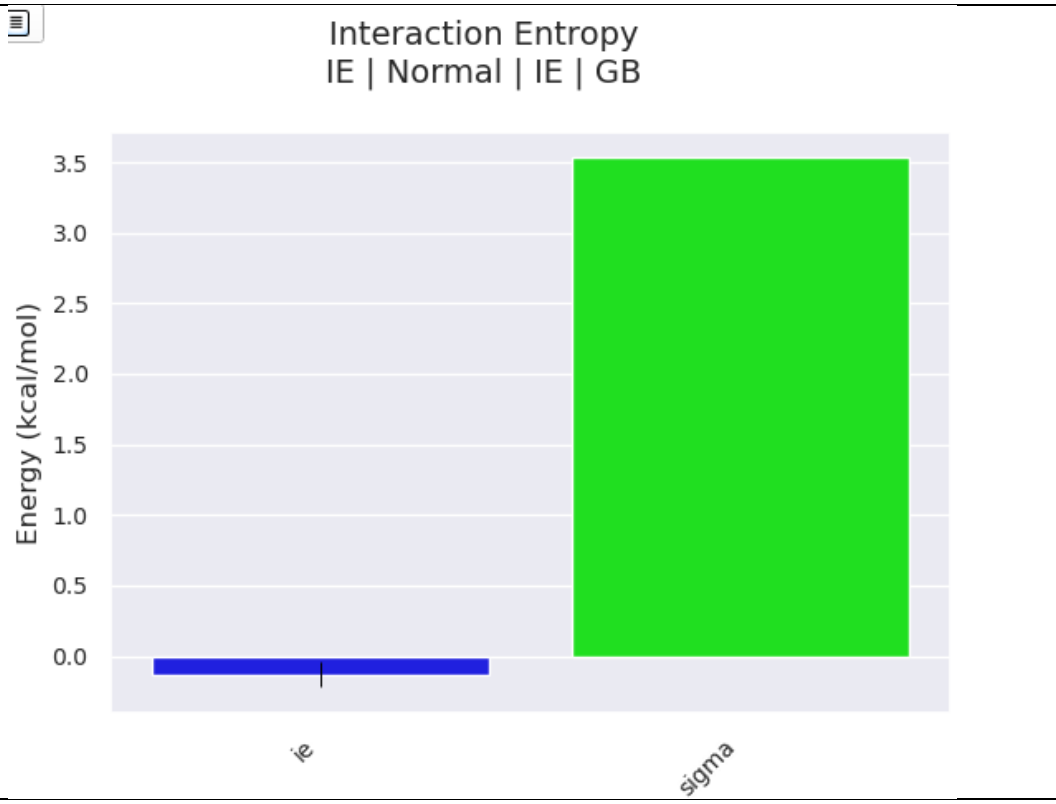

Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Energy (kcal/mol)
−6
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Receptor
Ligand
Energy (kcal/mol)
2
1
0
−1
−2
−3
−4
−5
−6
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9
1
2
3
4
5
6
7
8
9
10
Frames


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | SDC
Energy (kcal/mol)
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9


Energetic Components
IE | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

18


Interaction Entropy
IE | Normal | IE | GB
Energy (kcal/mol)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ie
sigma

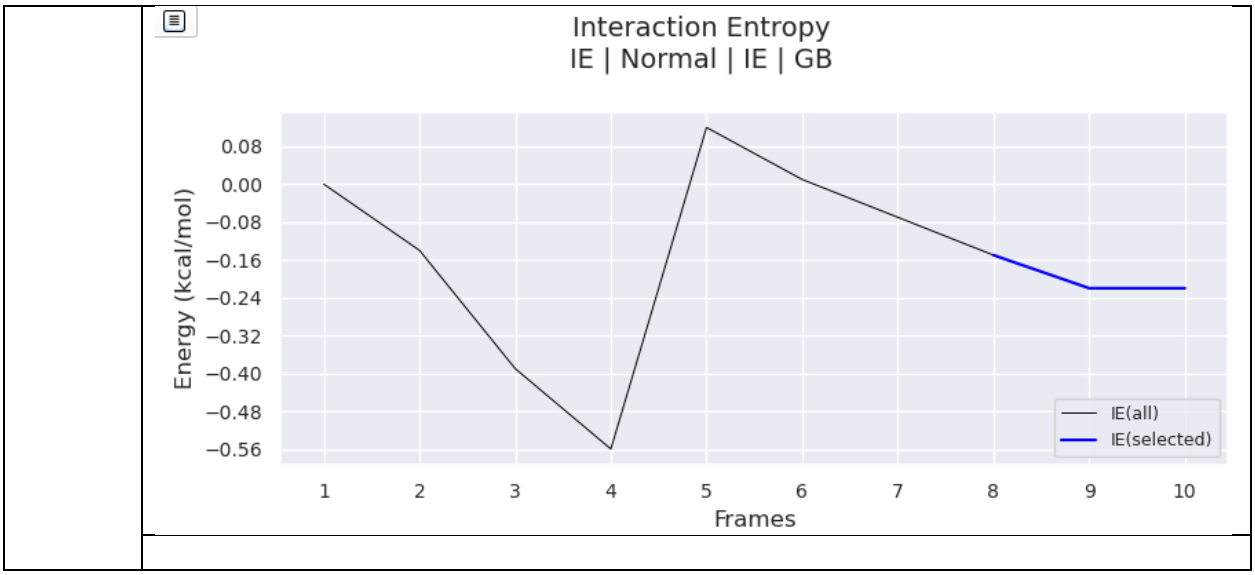
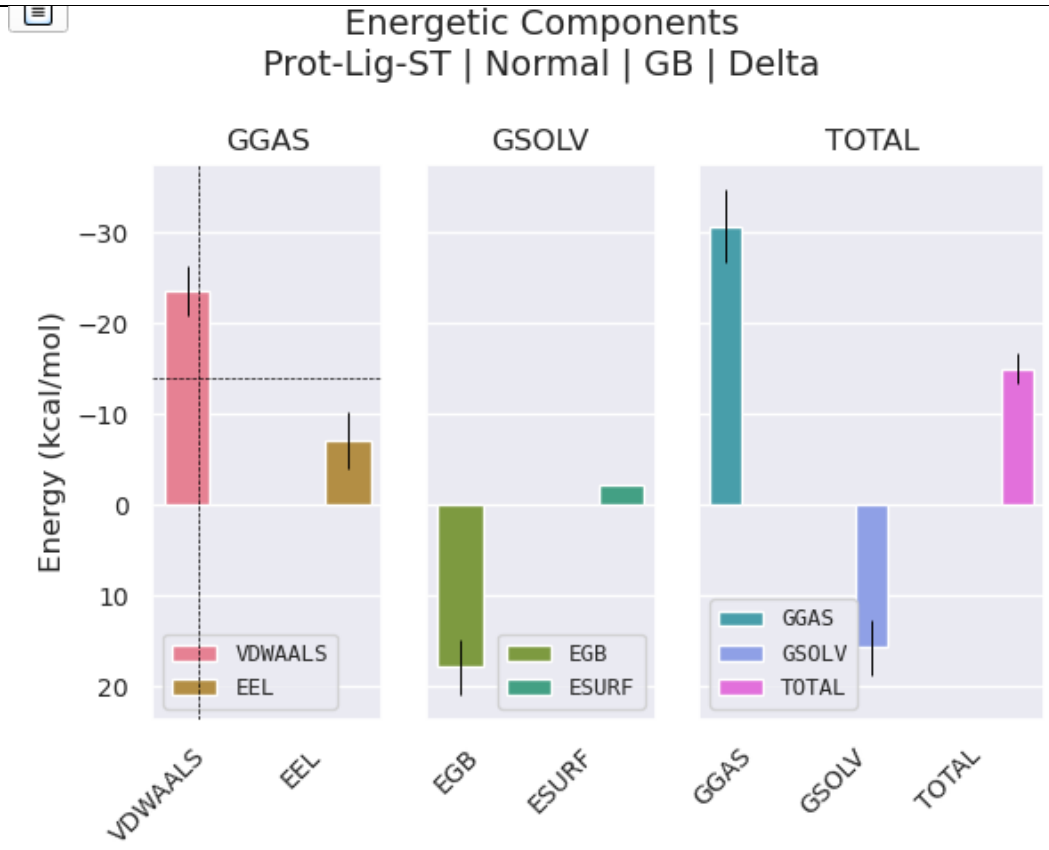
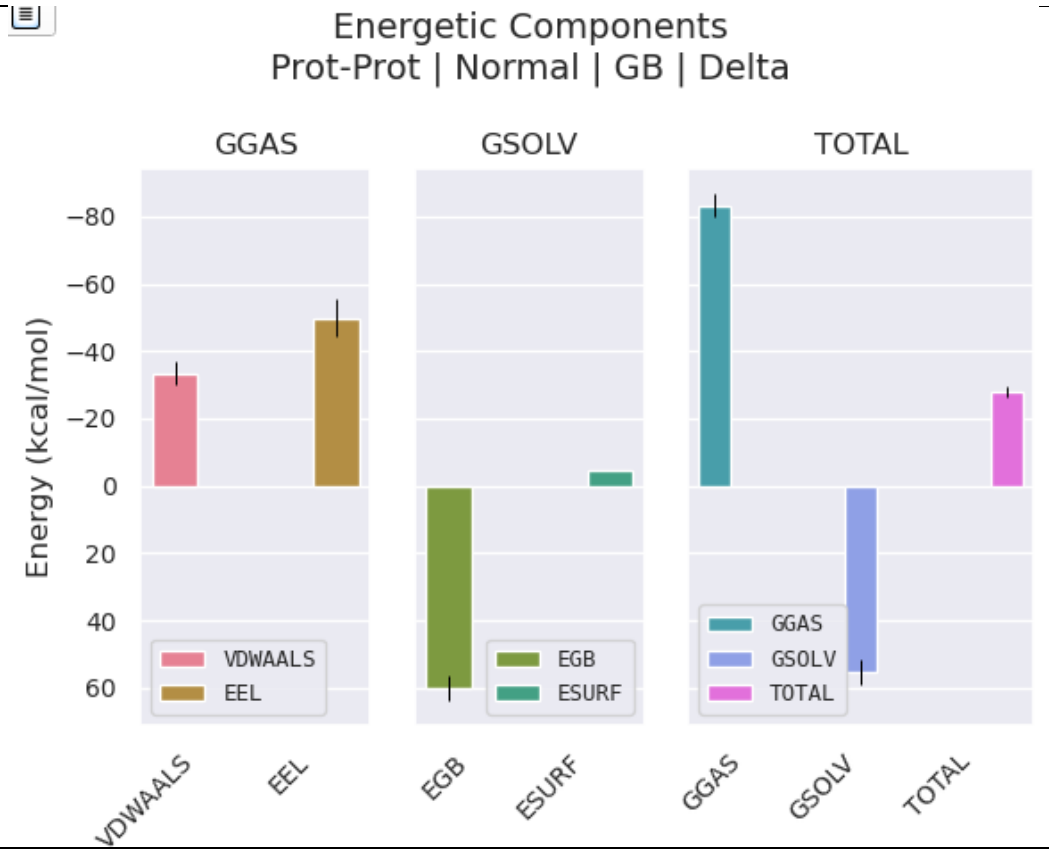
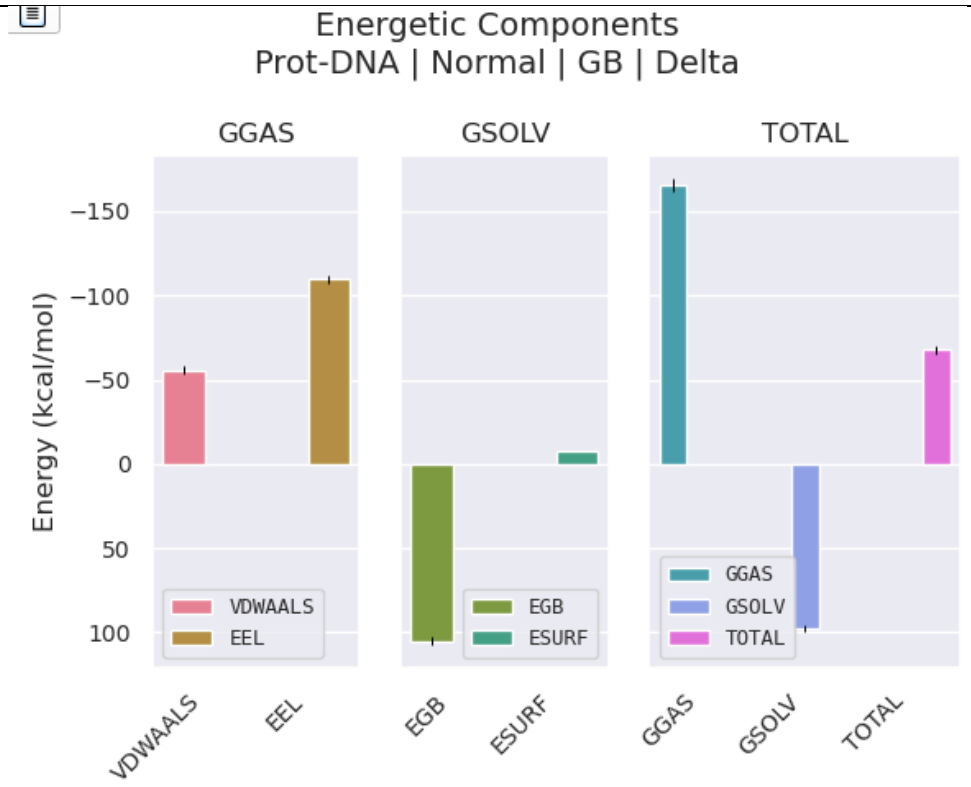
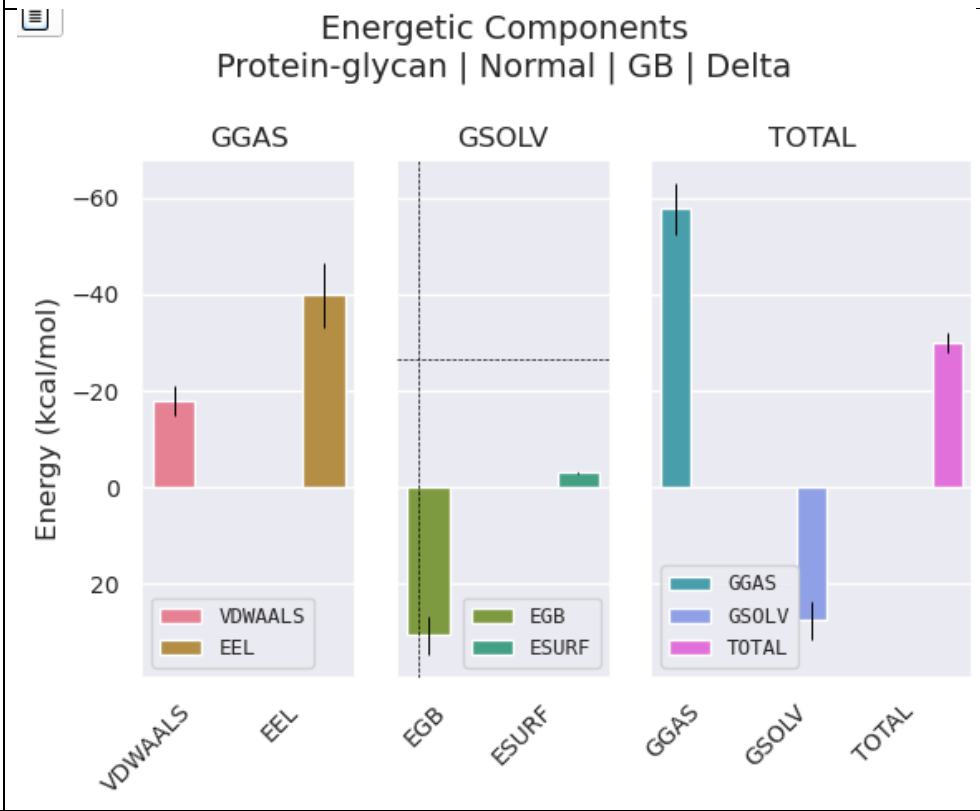
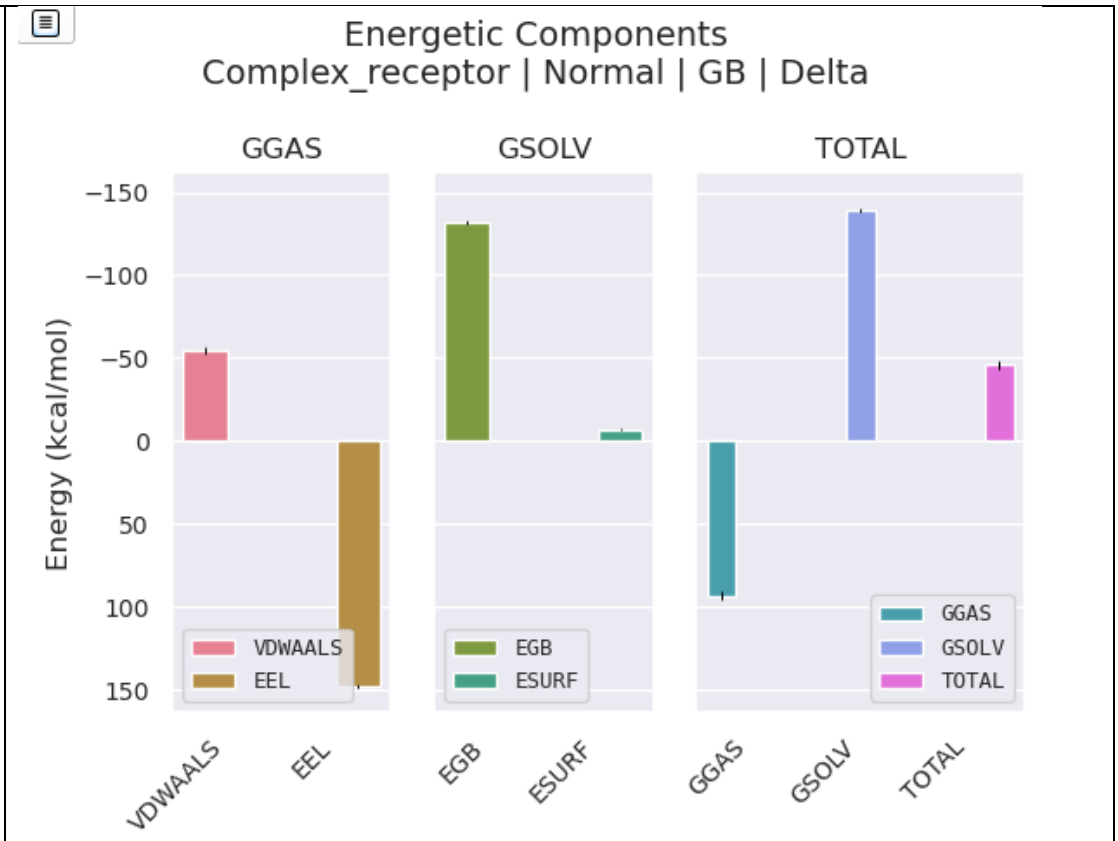


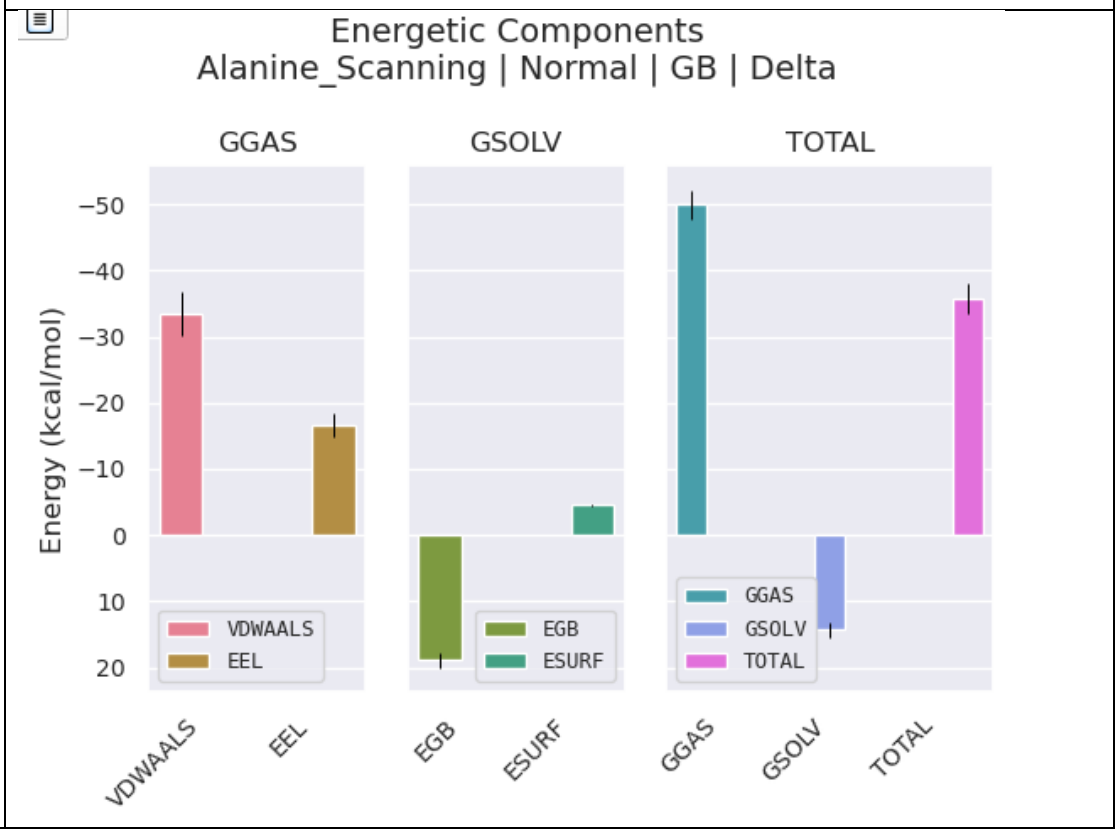
Figure A39. Residue-level MMPBSA energetic analysis showing the interaction map of key residues involved in stabilizing compound **18** within the 1X2J complex.

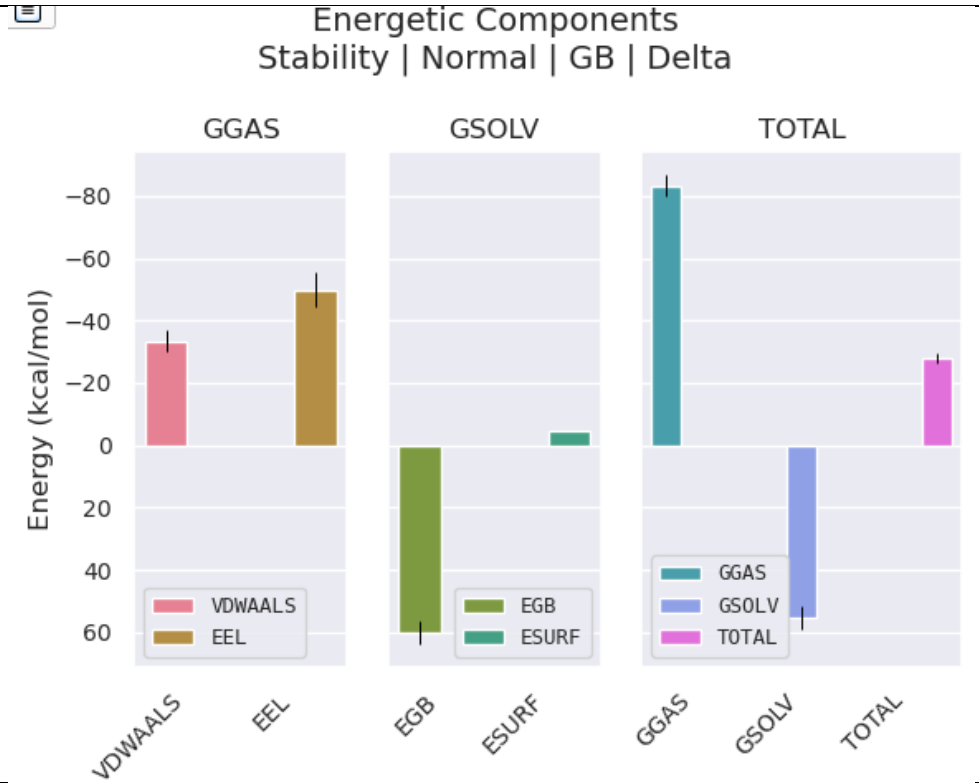
6	 Energetic Components Prot-Lig-ST | Normal | GB | Delta GGAS GSOLV TOTAL Energy (kcal/mol) −30 −20 −10 0 10 20 VDWAALS EEL EGB ESURF GGAS GSOLV TOTAL  Energetic Components Prot-Prot | Normal | GB | Delta GGAS GSOLV TOTAL Energy (kcal/mol) −80 −60 −40 −20 0 20 40 60 VDWAALS EEL EGB ESURF GGAS GSOLV TOTAL

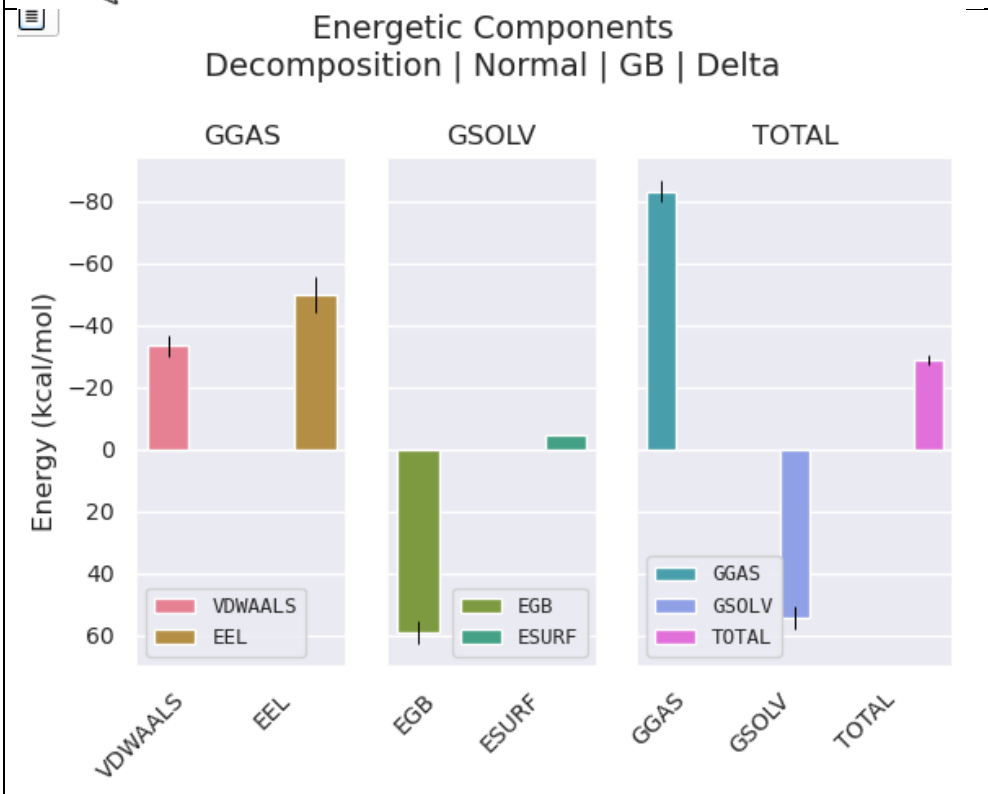

Energetic Components
Prot-DNA | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

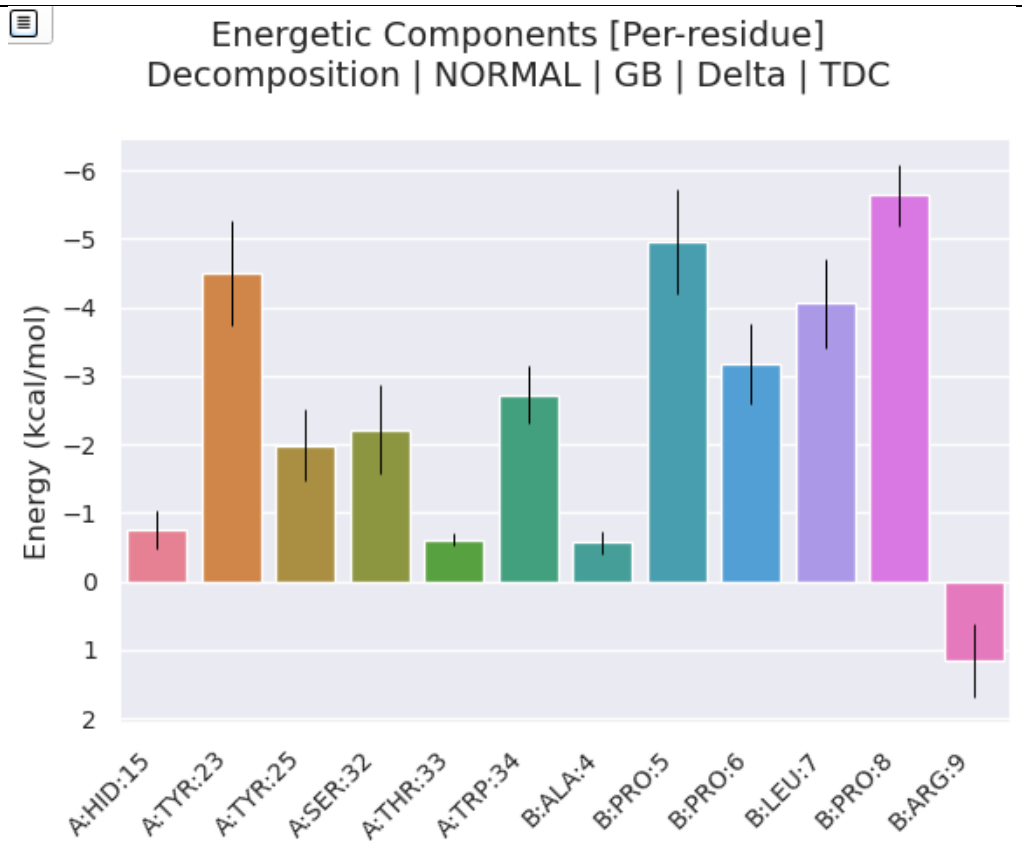

Energetic Components
Protein-glycan | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−60
−40
−20
0
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

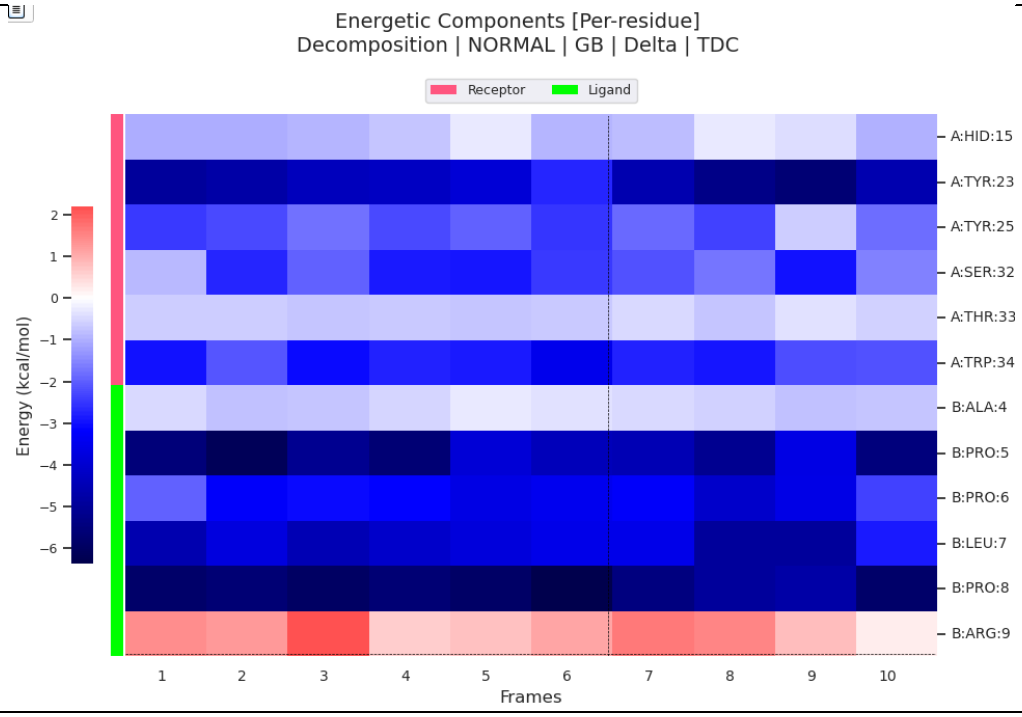

Energetic Components
Complex_receptor | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
150
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

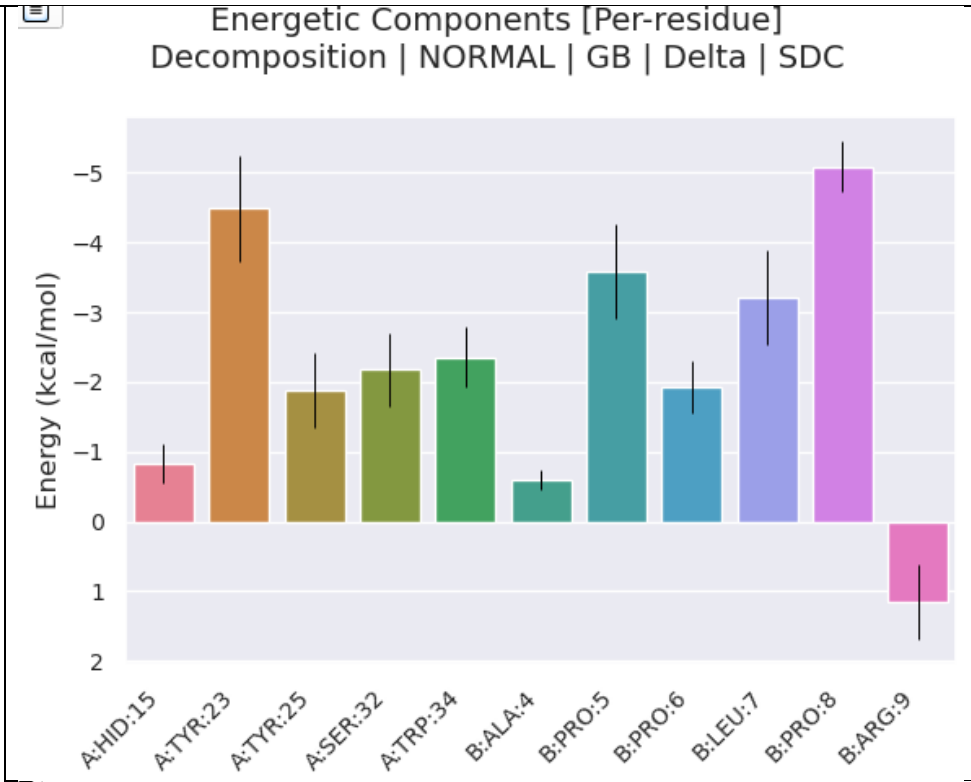

Energetic Components
Alanine_Scanning | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−50
−40
−30
−20
−10
0
10
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

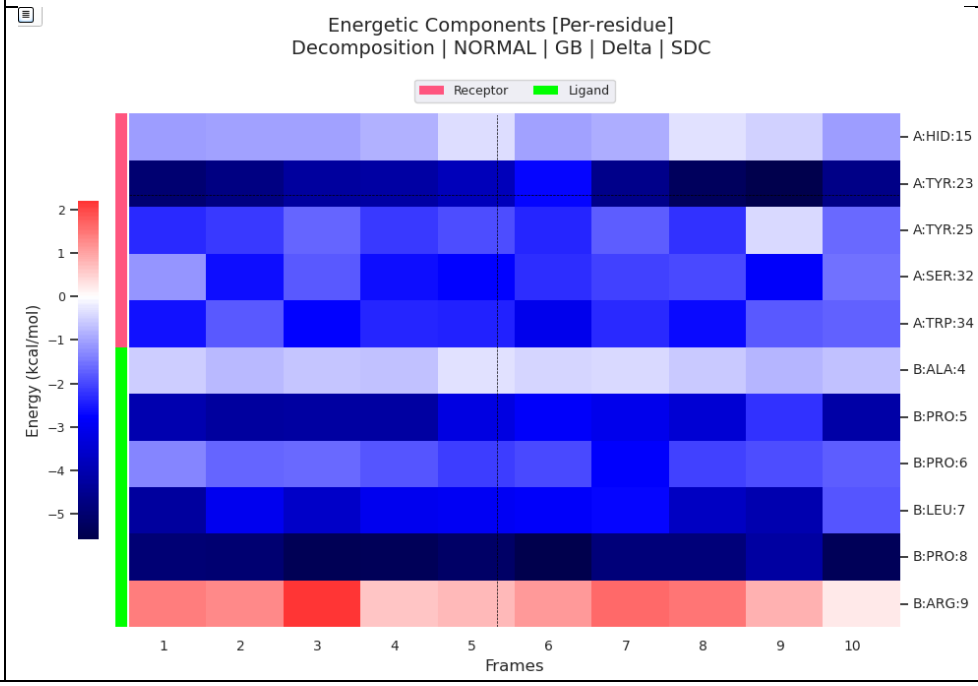

Energetic Components
Stability | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

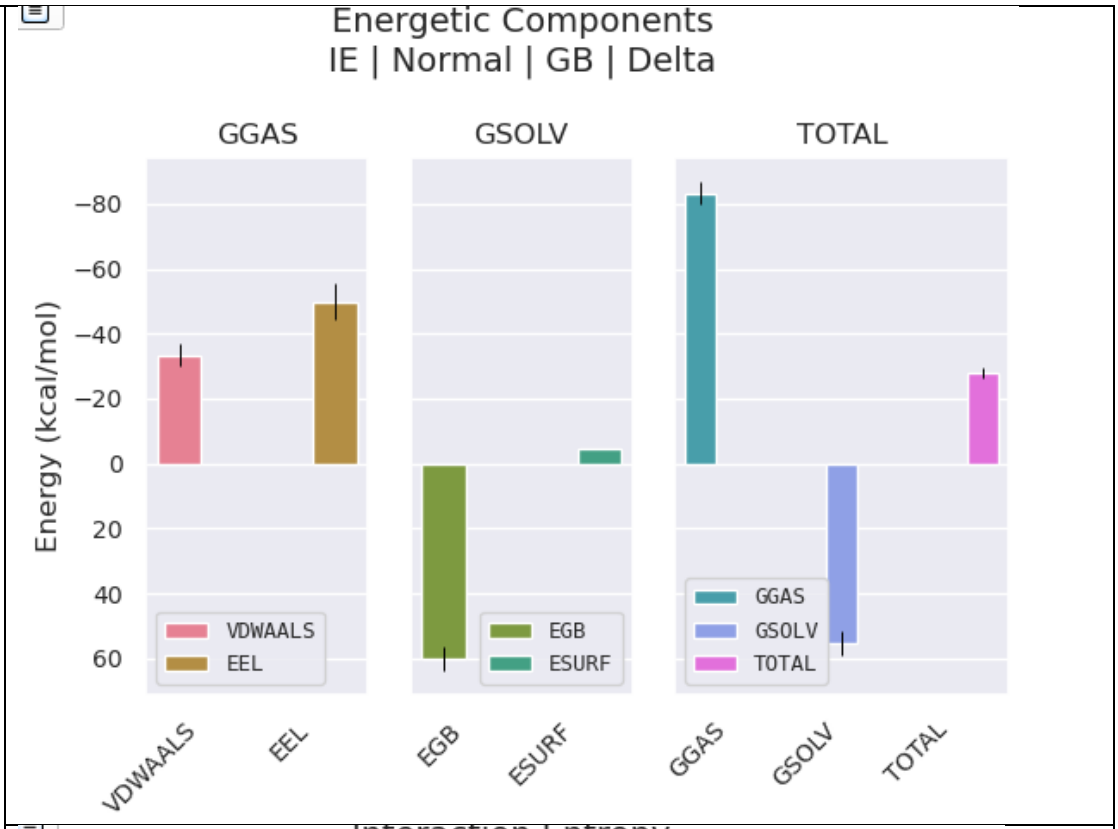

Energetic Components
Decomposition | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

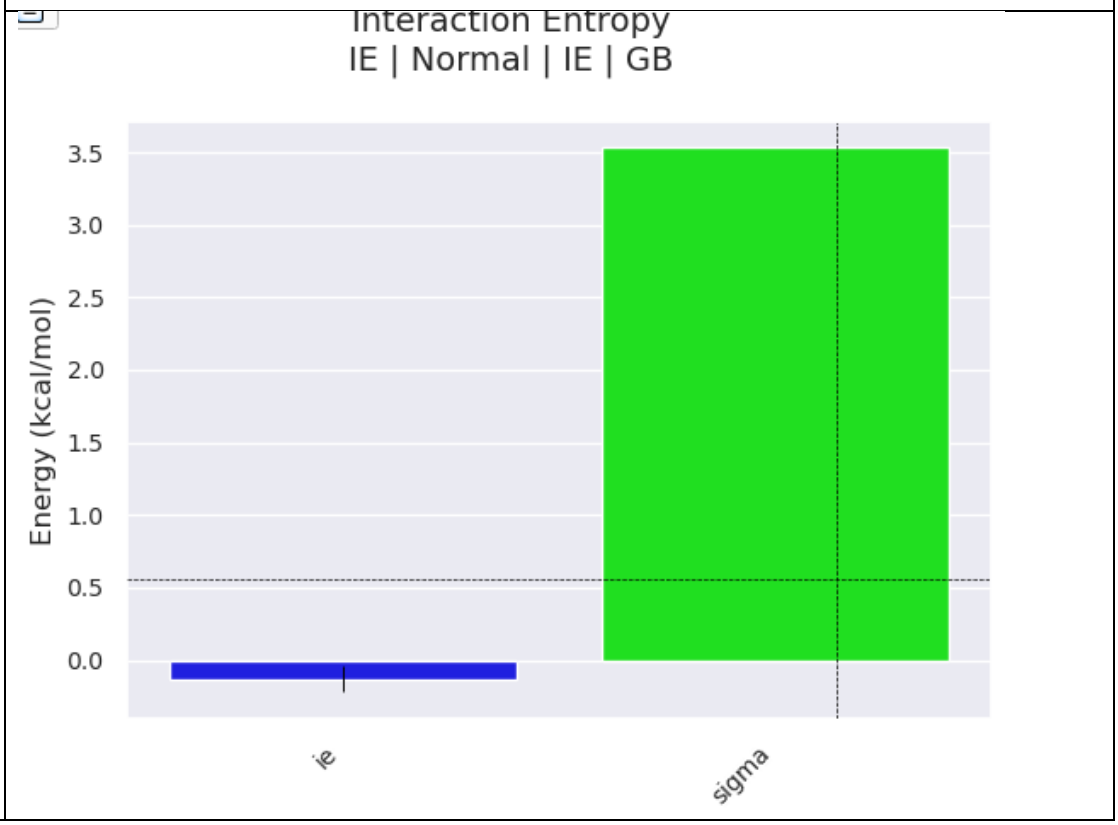

Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Energy (kcal/mol)
−6
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Receptor
Ligand
Energy (kcal/mol)
2
1
0
−1
−2
−3
−4
−5
−6
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9
1
2
3
4
5
6
7
8
9
10
Frames


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | SDC
Energy (kcal/mol)
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | SDC
Receptor
Ligand
Energy (kcal/mol)
2
1
0
−1
−2
−3
−4
−5
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9
1
2
3
4
5
6
7
8
9
10
Frames


Energetic Components
IE | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Interaction Entropy
IE | Normal | IE | GB
Energy (kcal/mol)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ie
sigma

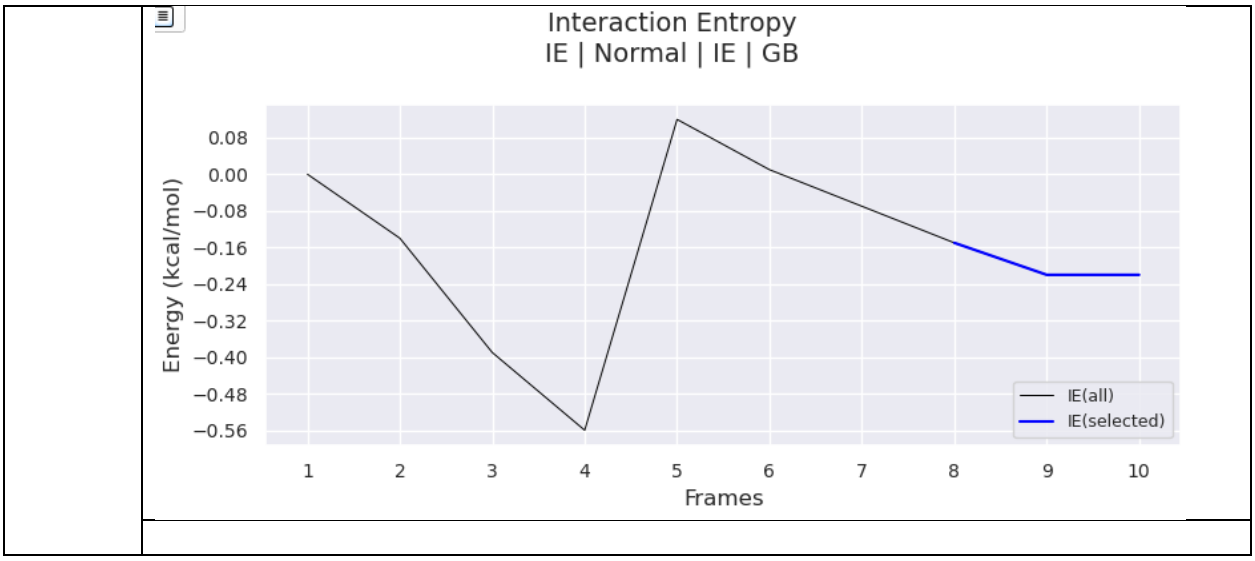
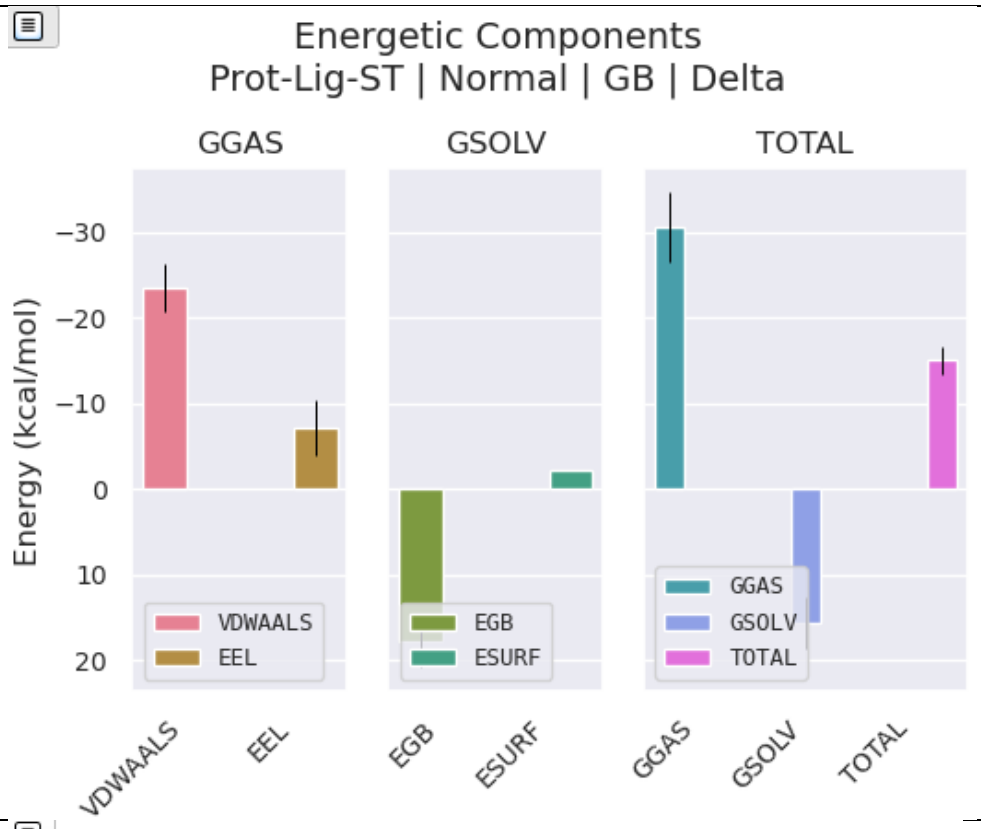
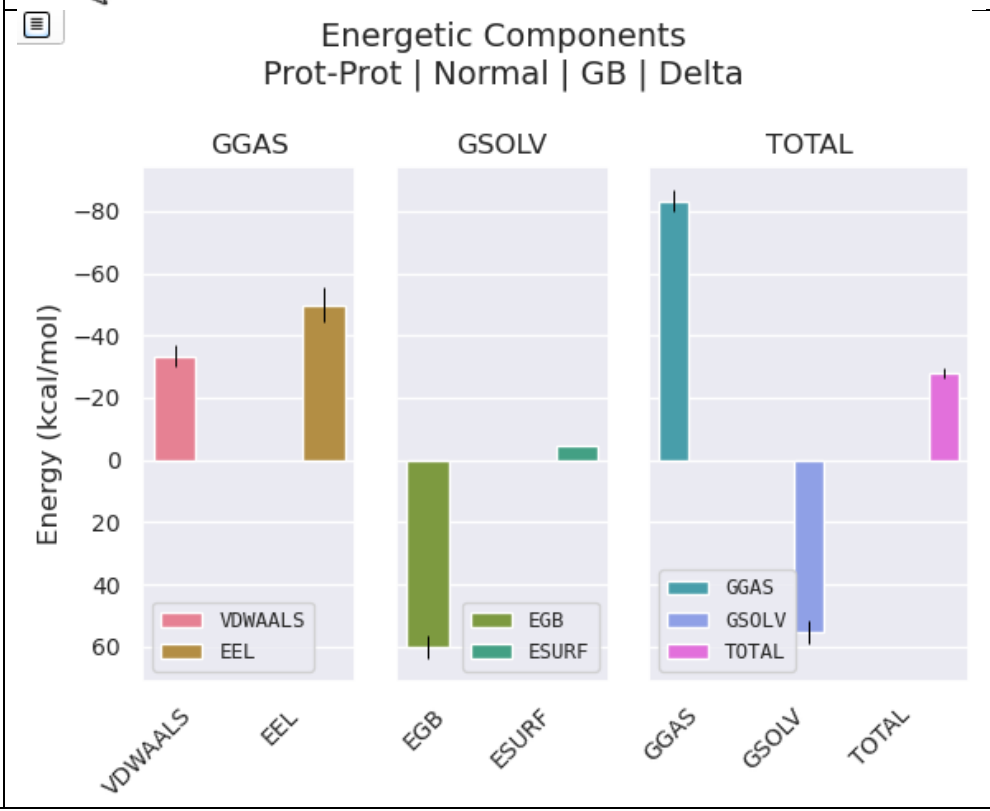
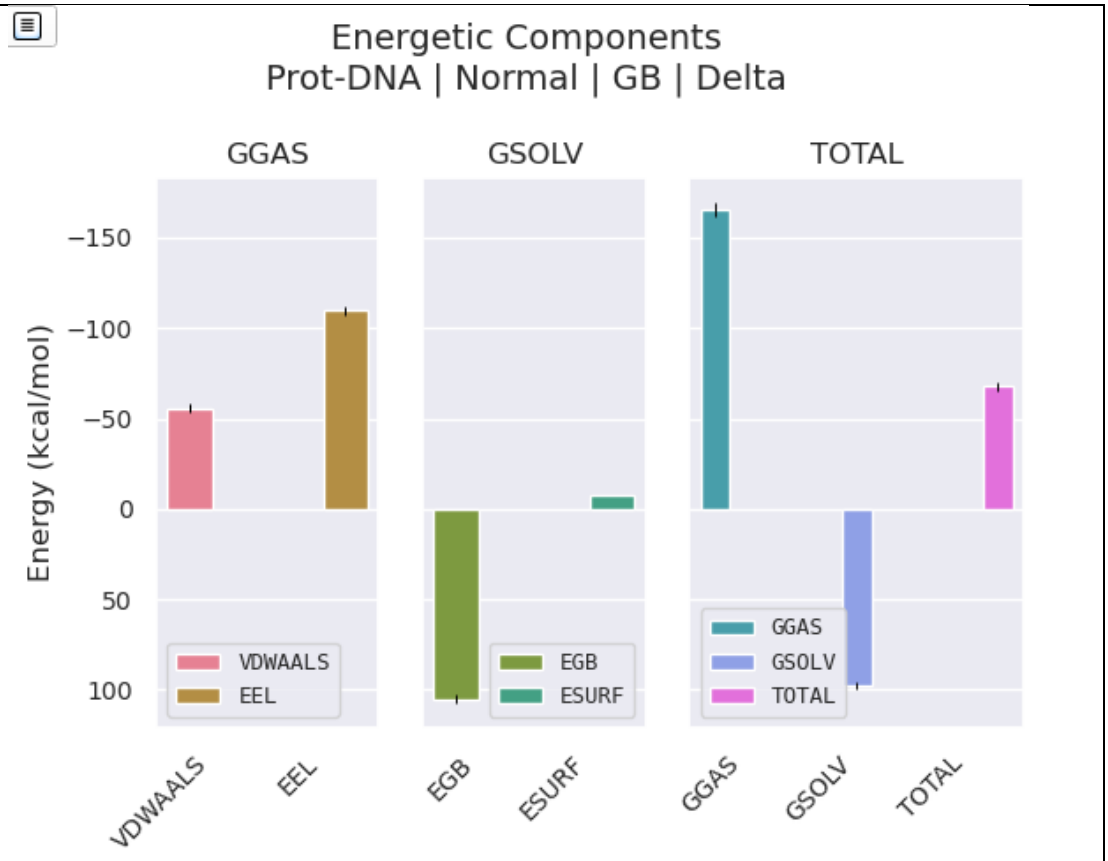
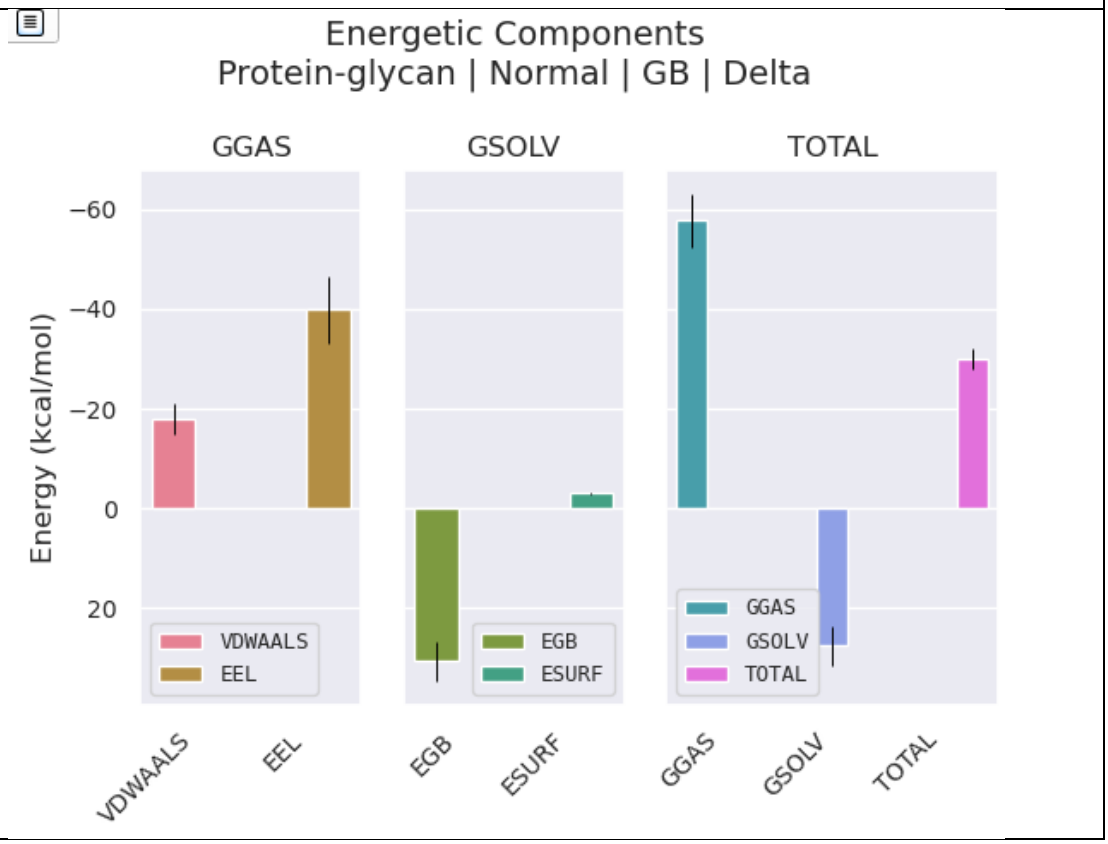
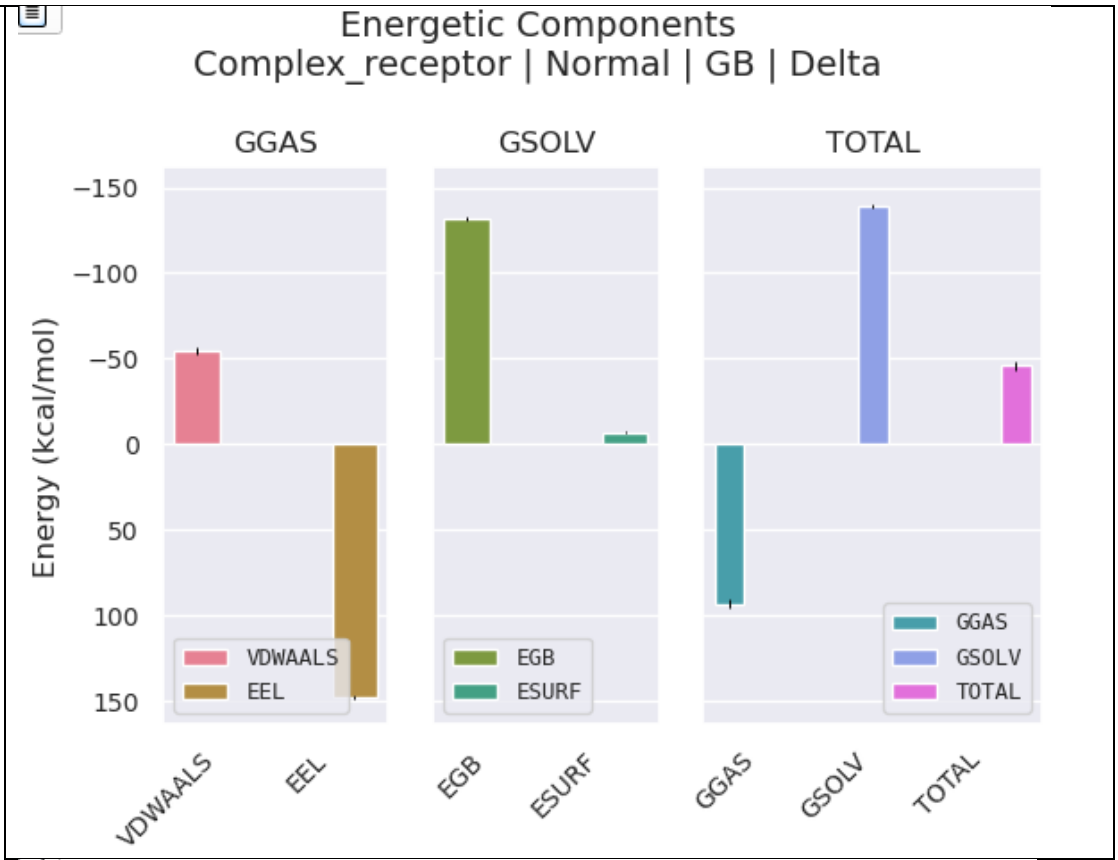


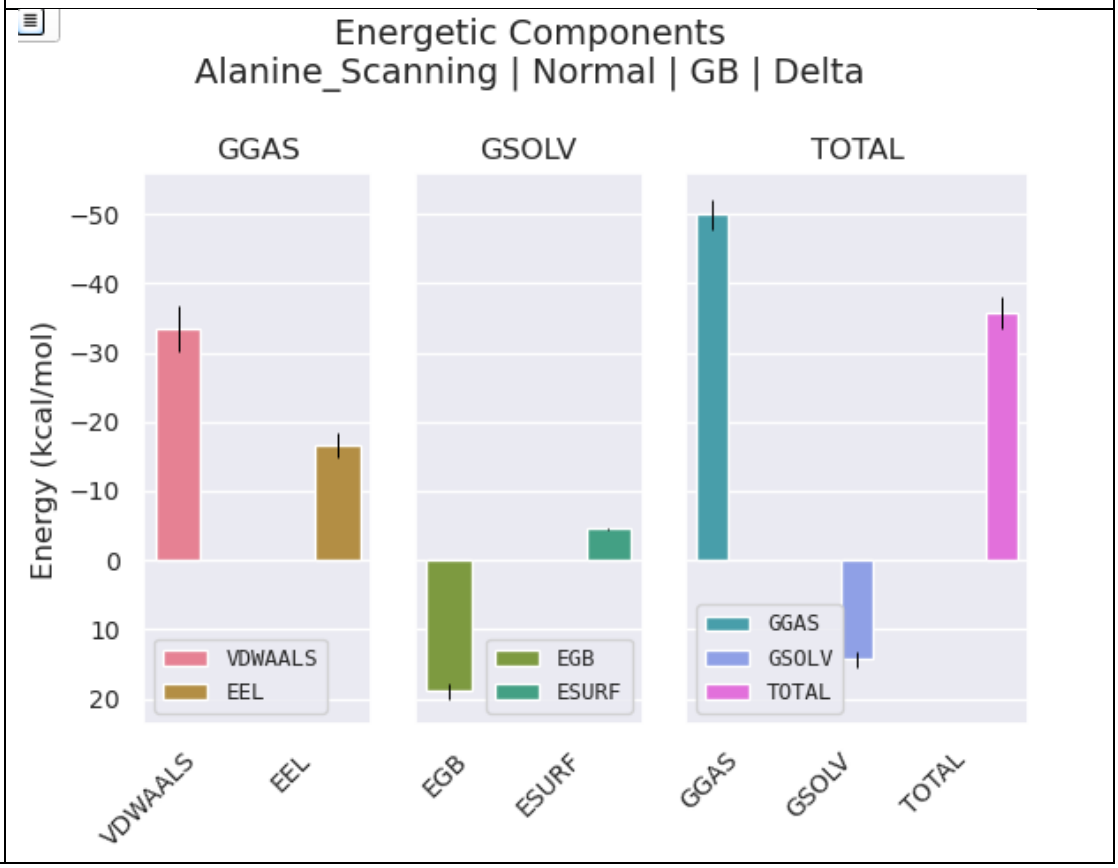
Figure A40. Residue-level MMPBSA energetic analysis showing the interaction map of key residues involved in stabilizing compound **6** within the 1X2J complex.

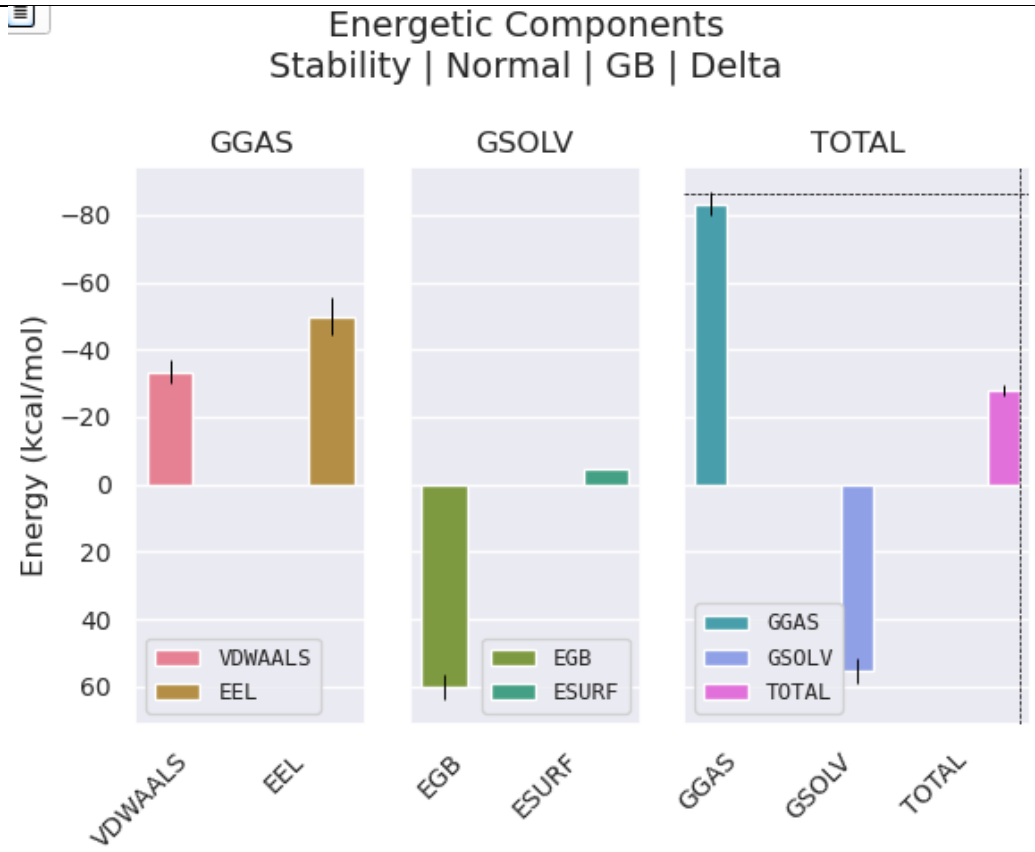
23	 Energetic Components Prot-Lig-ST | Normal | GB | Delta GGAS GSOLV TOTAL Energy (kcal/mol) −30 −20 −10 0 10 20 VDWAALS EEL EGB ESURF GGAS GSOLV TOTAL  Energetic Components Prot-Prot | Normal | GB | Delta GGAS GSOLV TOTAL Energy (kcal/mol) −80 −60 −40 −20 0 20 40 60 VDWAALS EEL EGB ESURF GGAS GSOLV TOTAL

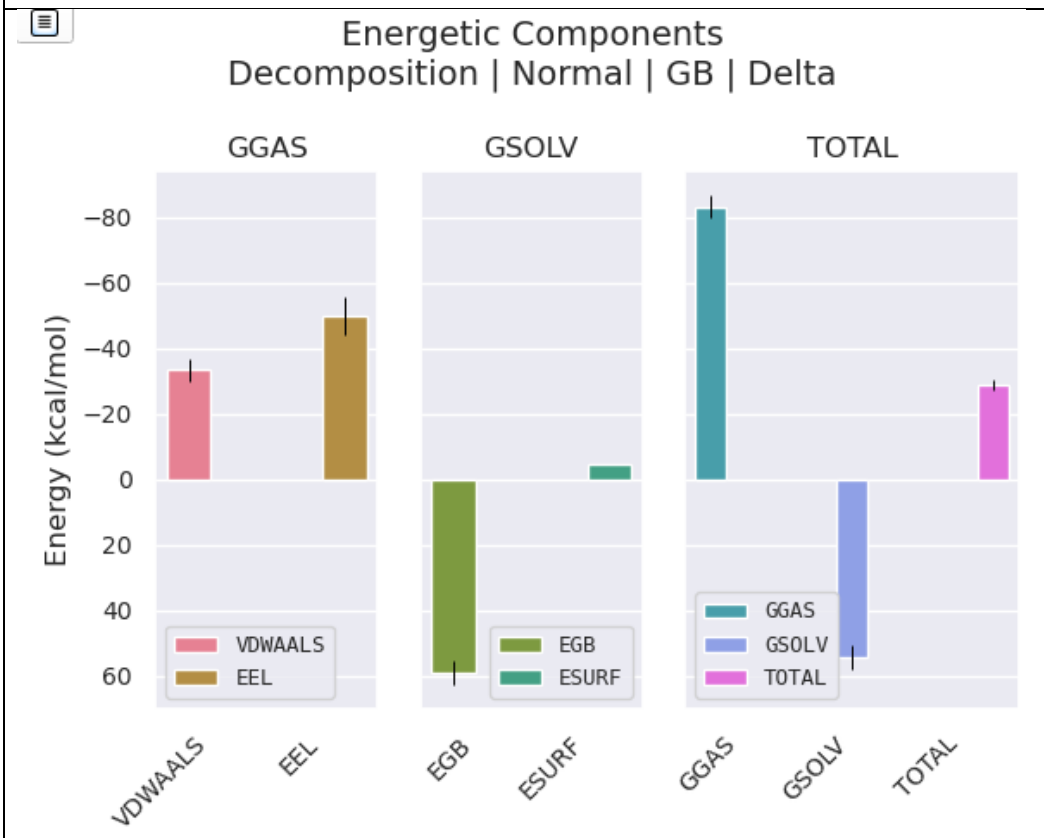

Energetic Components
Prot-DNA | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

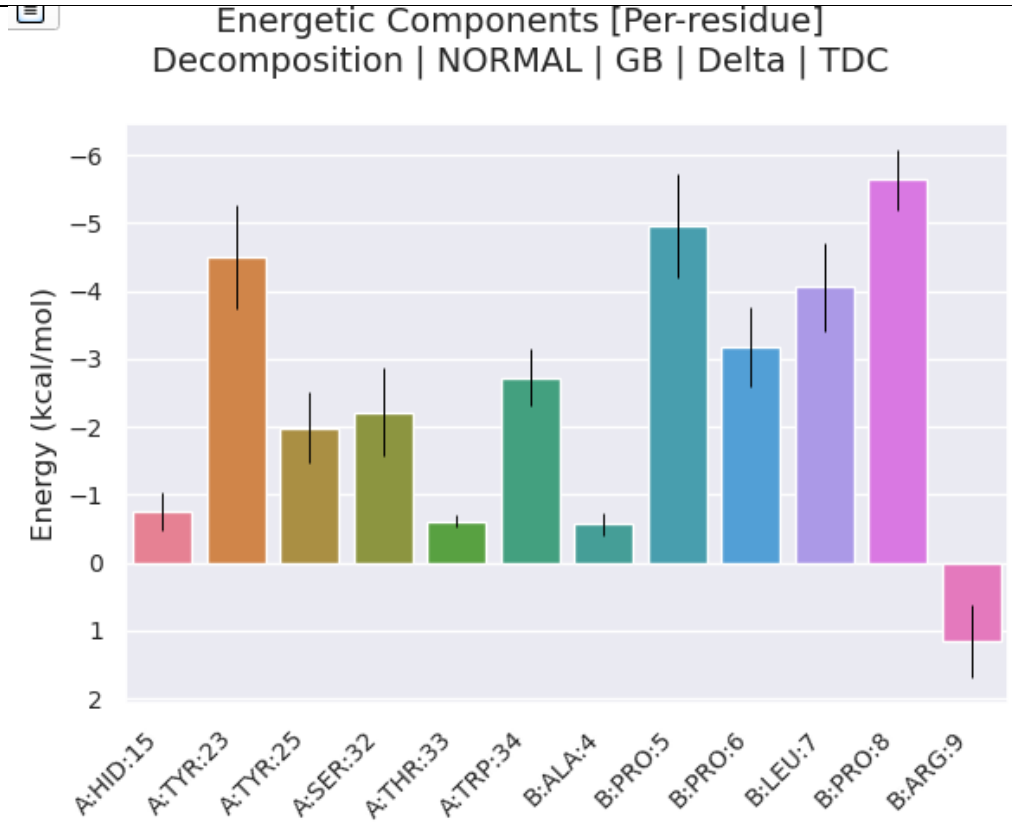

Energetic Components
Protein-glycan | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−60
−40
−20
0
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

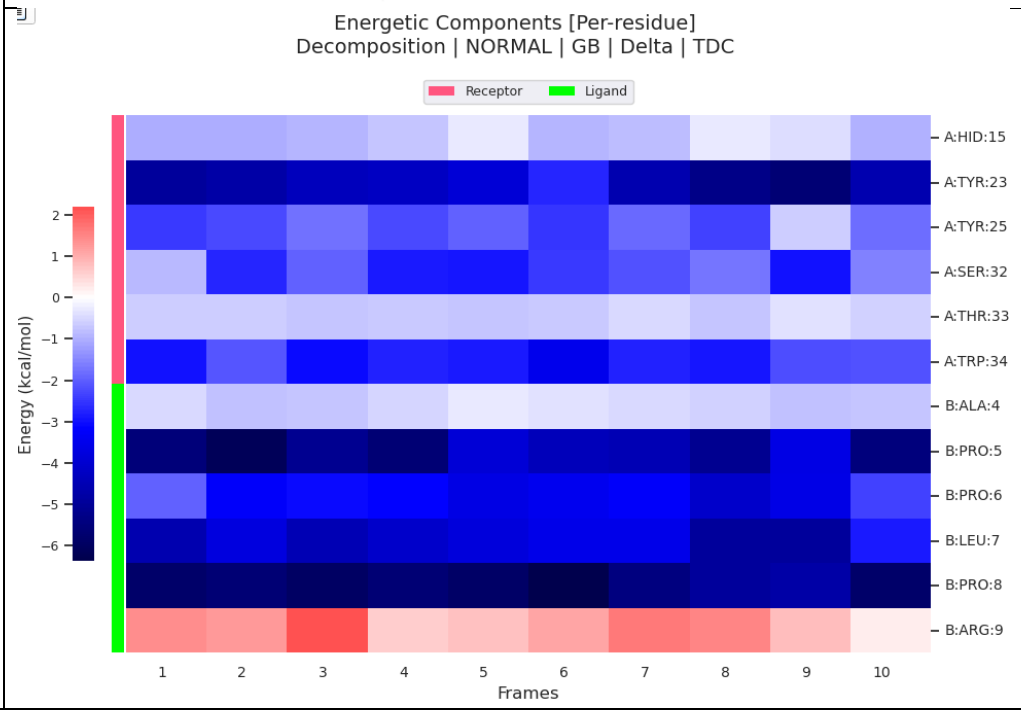

Energetic Components
Complex_receptor | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
150
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

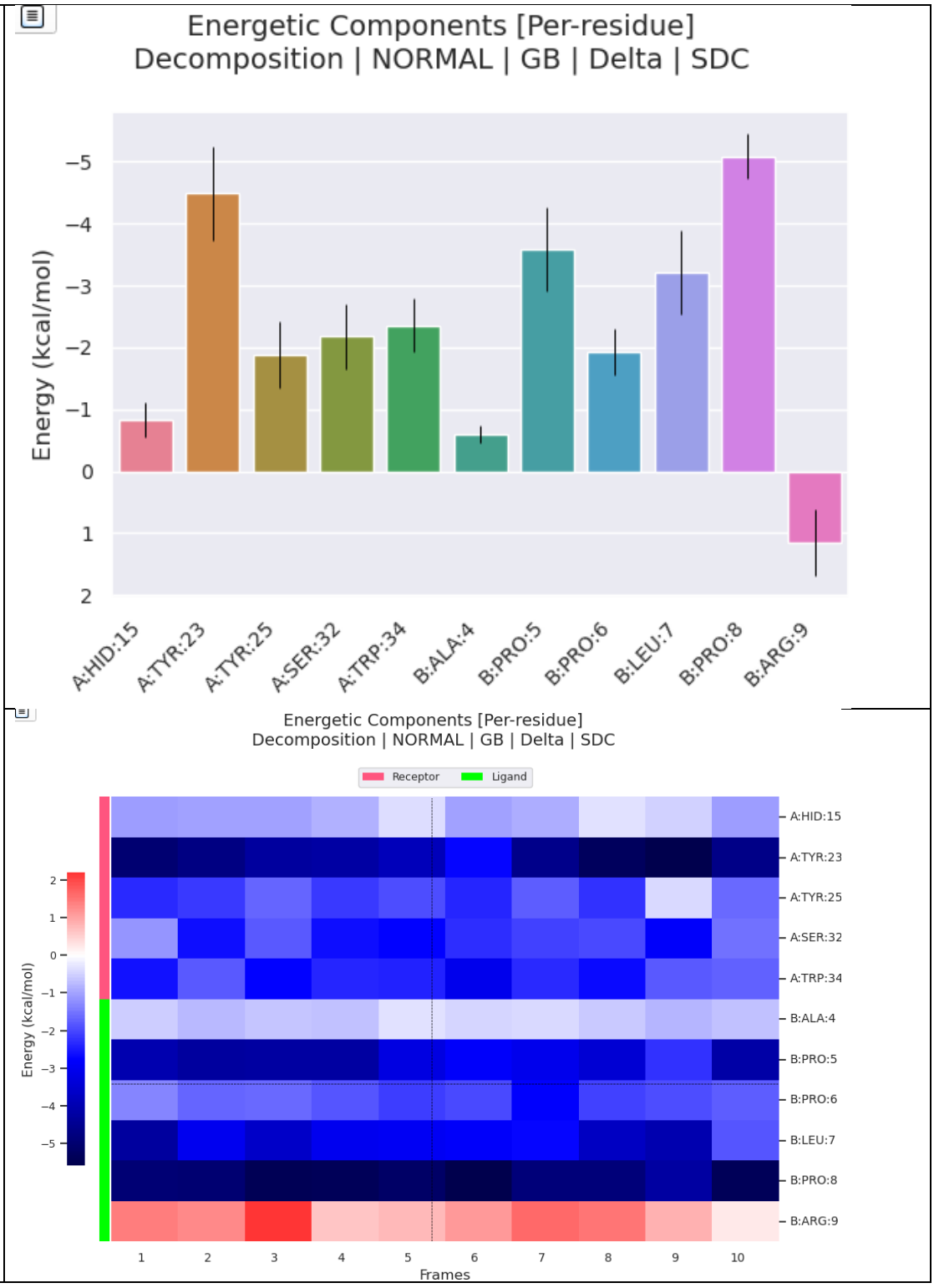

Energetic Components
Alanine_Scanning | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−50
−40
−30
−20
−10
0
10
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

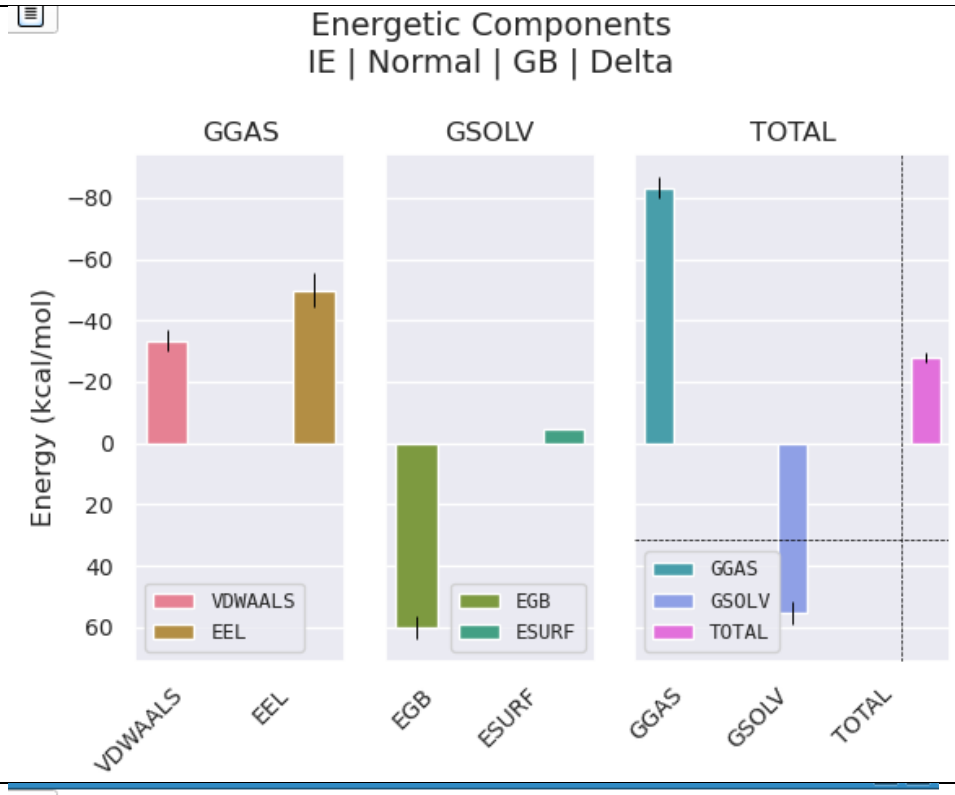

Energetic Components
Stability | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

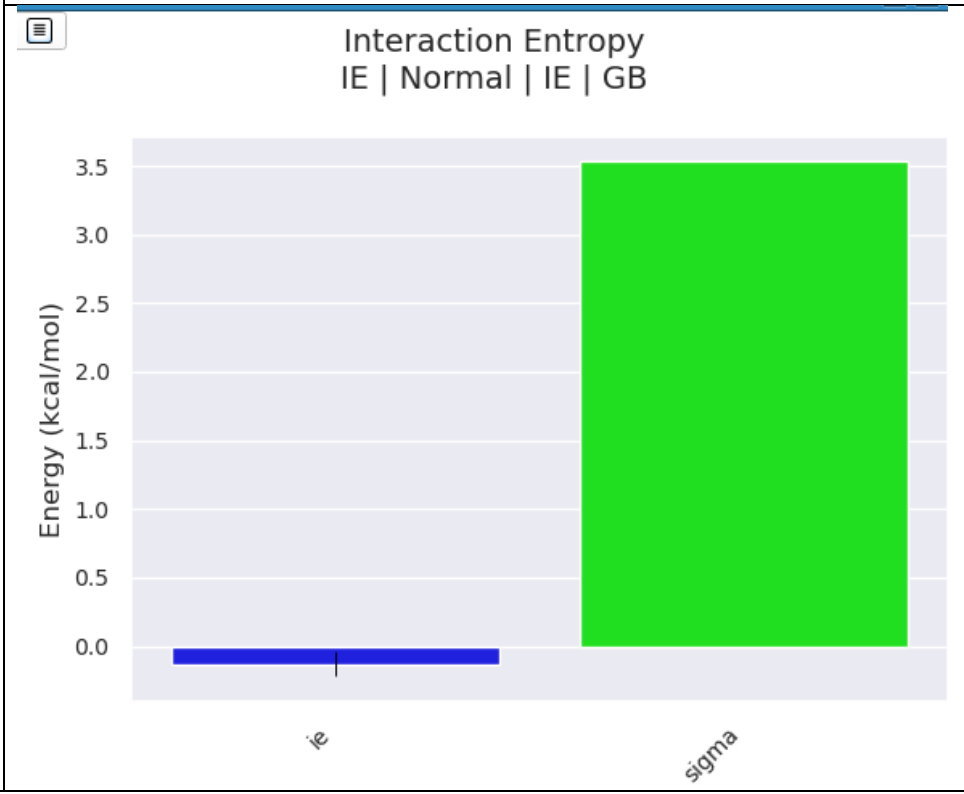

Energetic Components
Decomposition | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Energy (kcal/mol)
−6
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Receptor
Ligand
Energy (kcal/mol)
2
1
0
−1
−2
−3
−4
−5
−6
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9
1
2
3
4
5
6
7
8
9
10
Frames


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | SDC
Energy (kcal/mol)
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9
Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | SDC
Receptor
Ligand
Energy (kcal/mol)
Frames
1
2
3
4
5
6
7
8
9
10


Energetic Components
IE | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Interaction Entropy
IE | Normal | IE | GB
Energy (kcal/mol)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ie
sigma

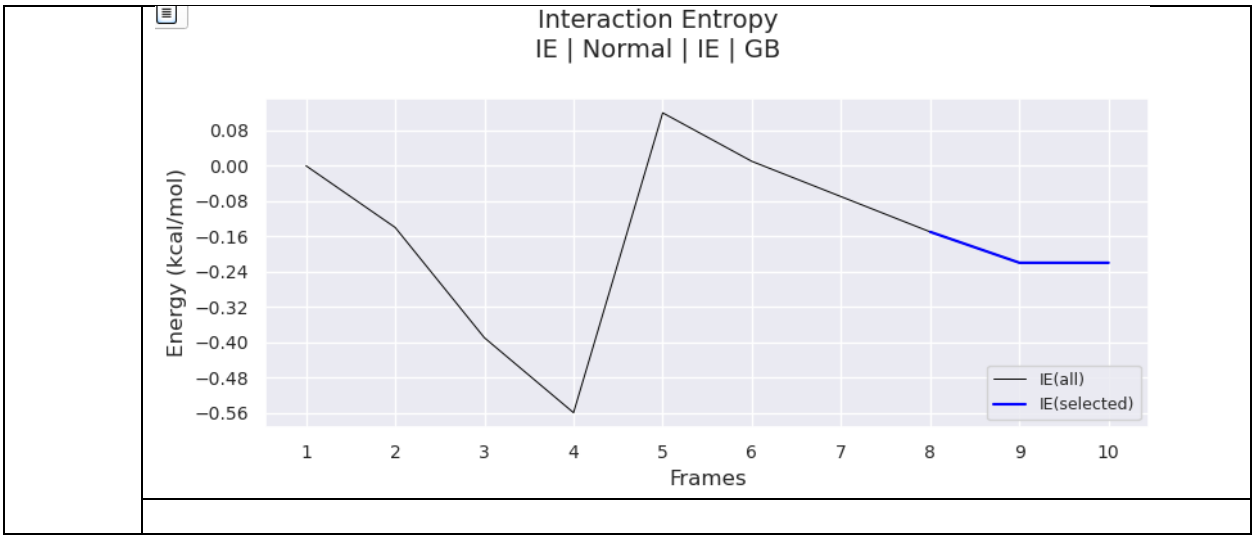
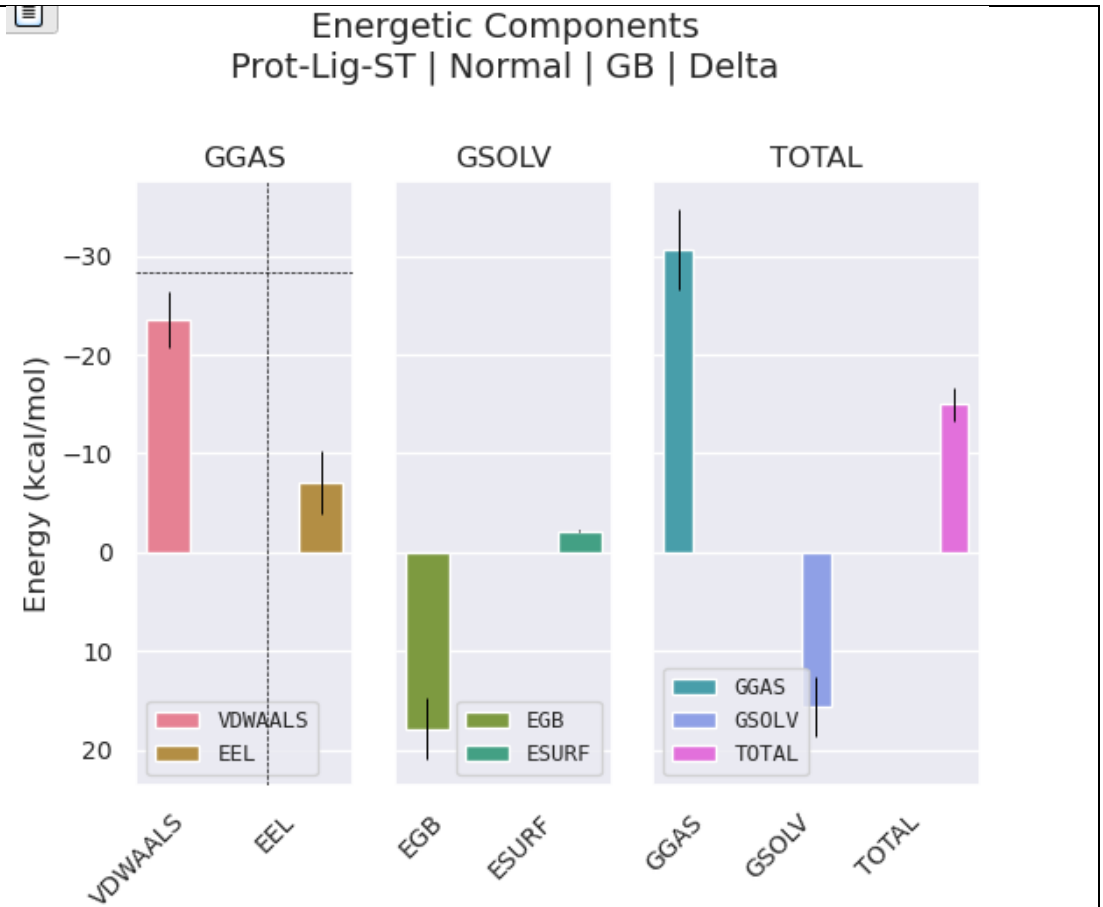
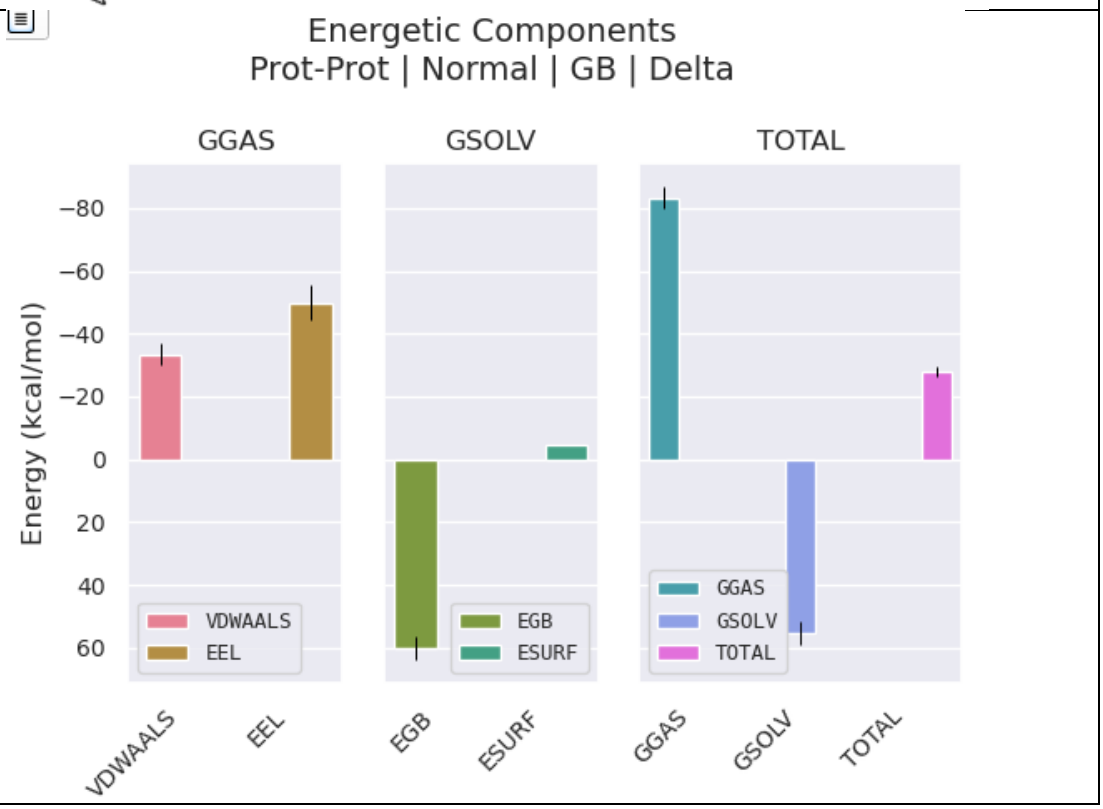
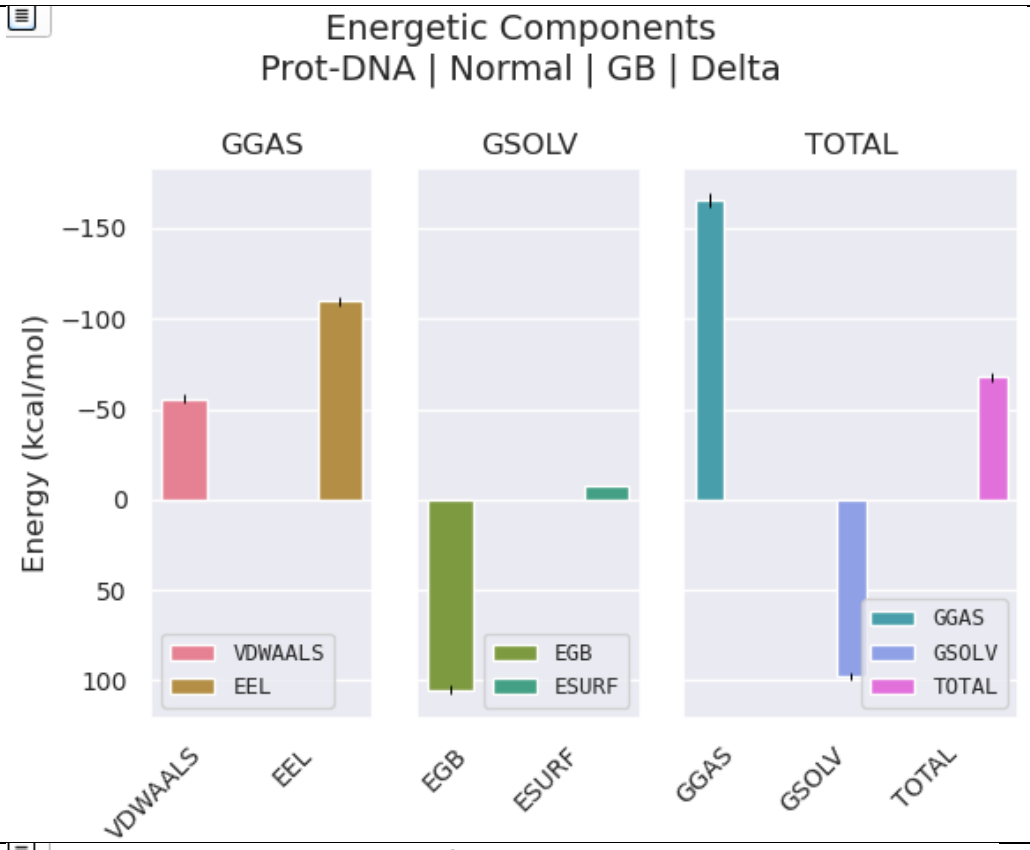
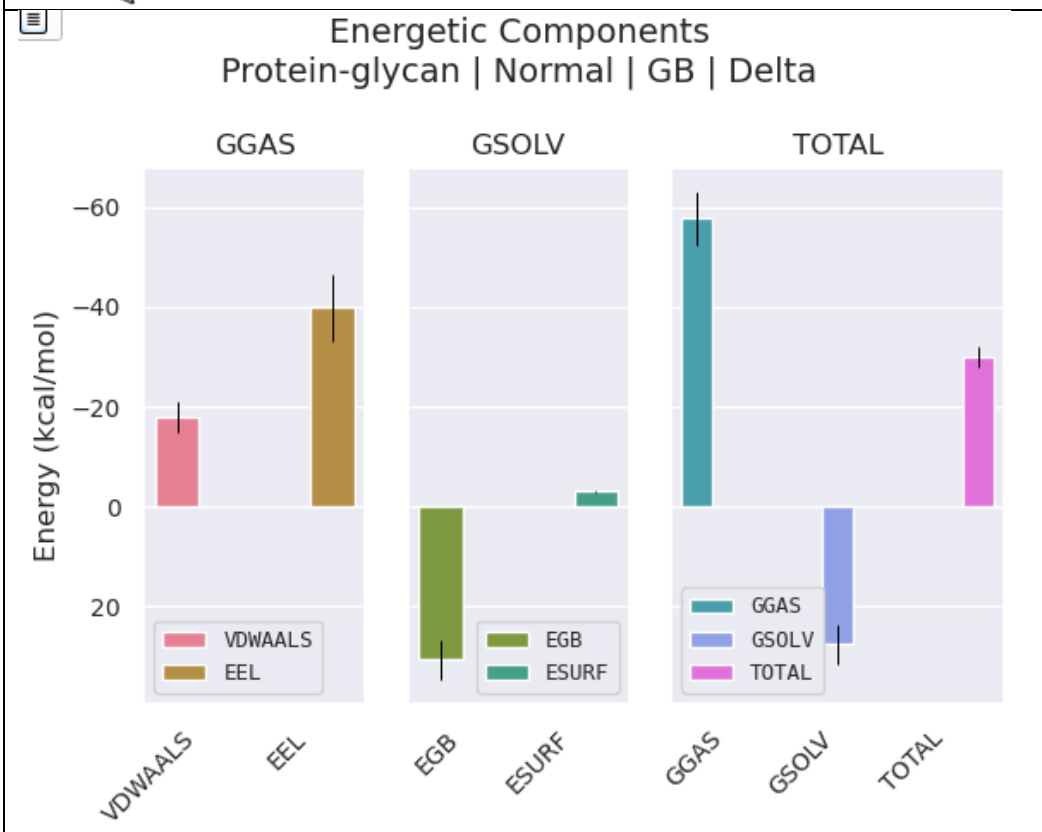
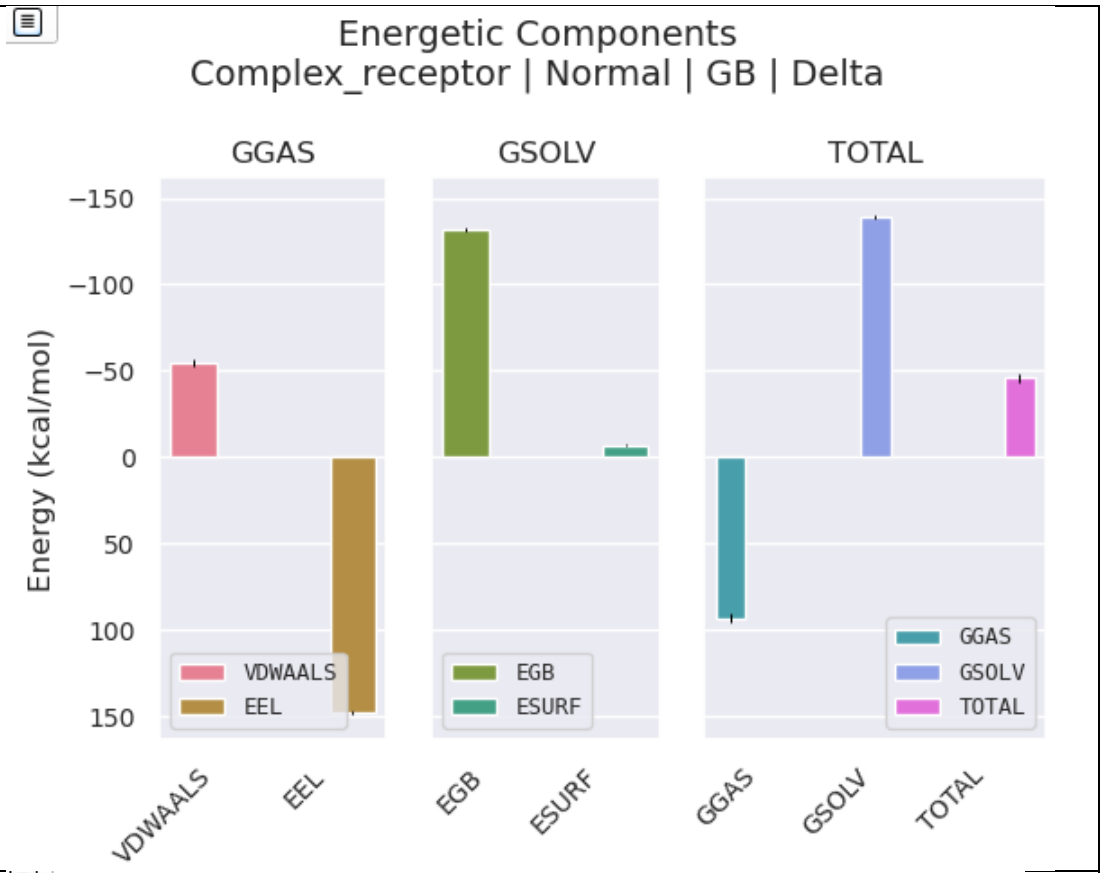


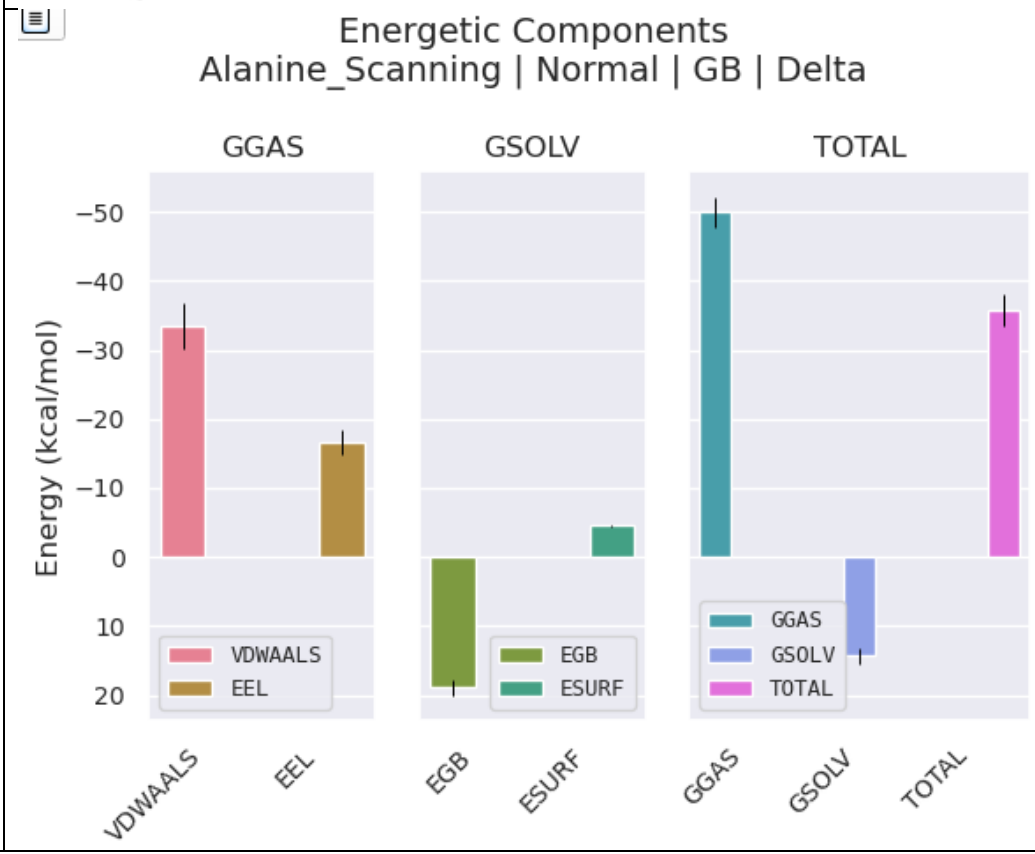
Figure A41. Residue-level MMPBSA energetic analysis showing the interaction map of key residues involved in stabilizing compound **23** within the 1X2J complex.

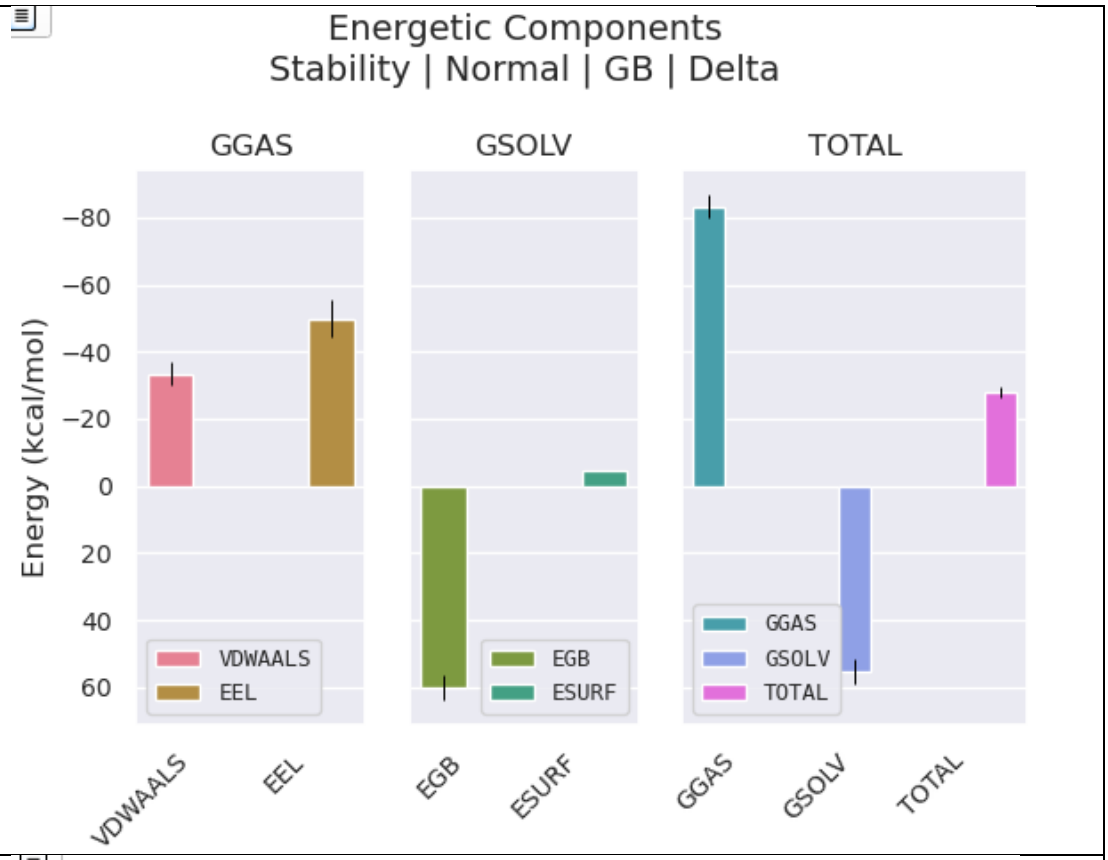
Genistein	 

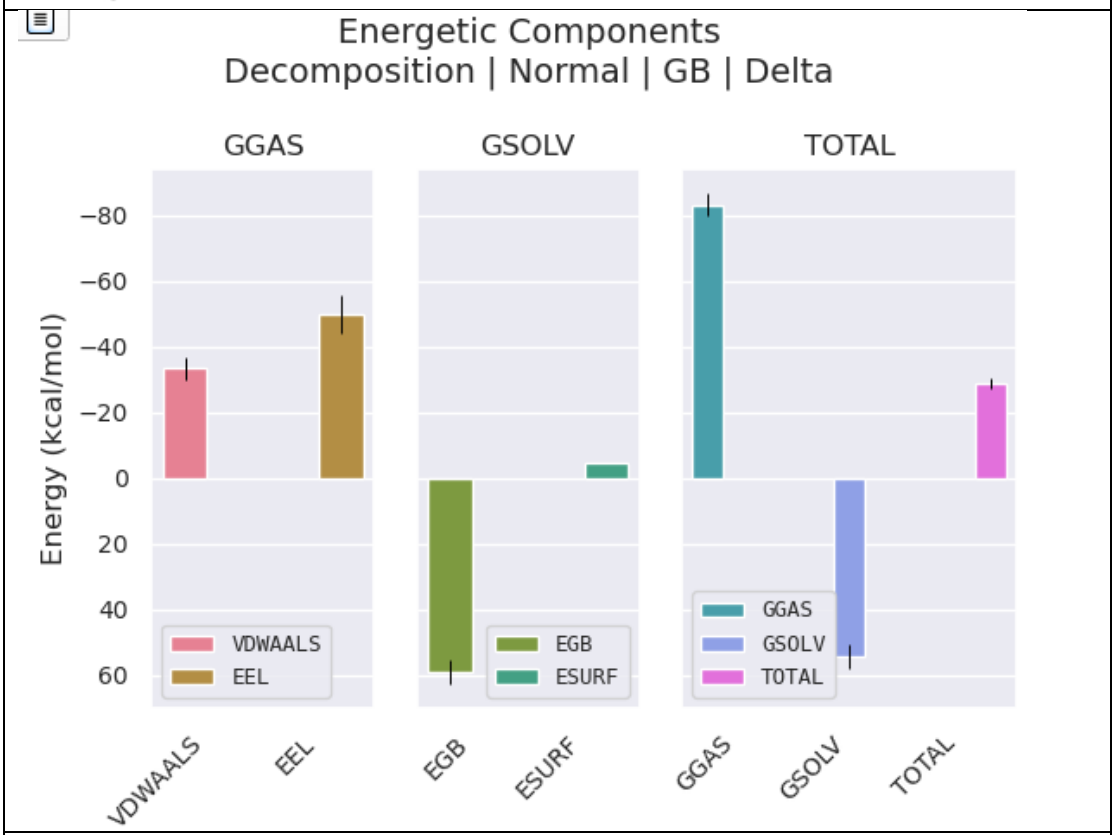

Energetic Components
Prot-DNA | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

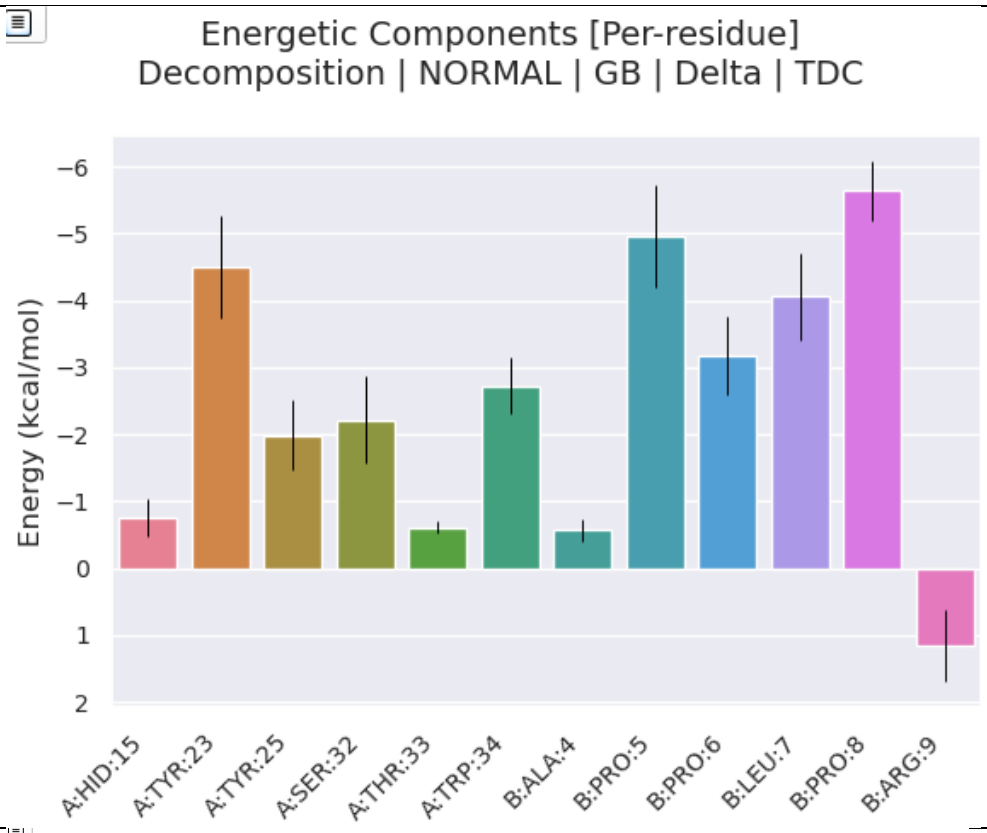

Energetic Components
Protein-glycan | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−60
−40
−20
0
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL

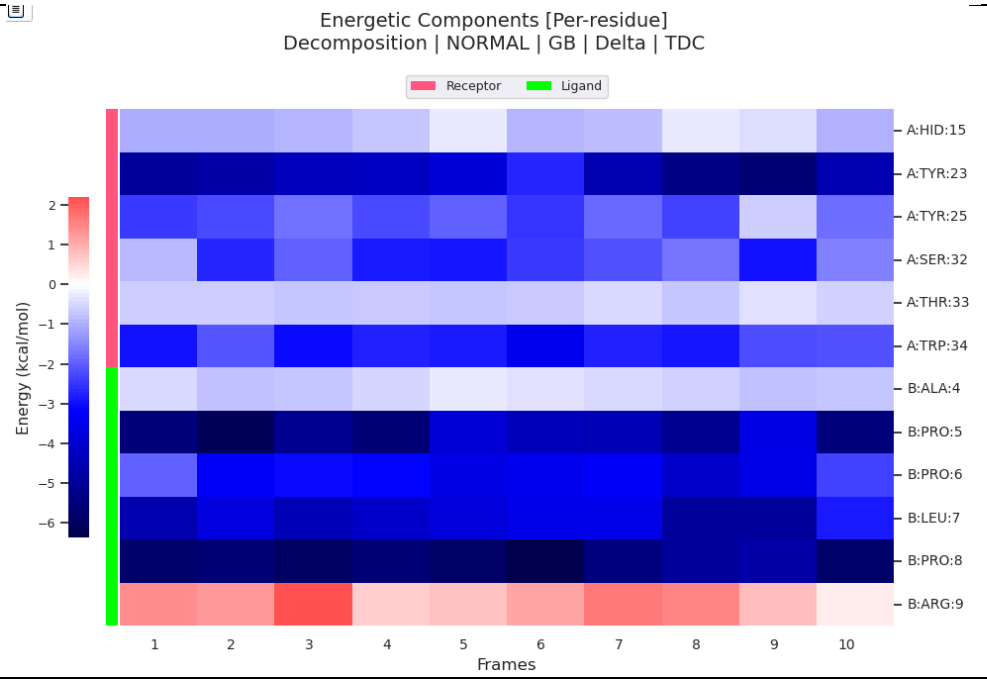

Energetic Components
Complex_receptor | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−150
−100
−50
0
50
100
150
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Energetic Components
Alanine_Scanning | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−50
−40
−30
−20
−10
0
10
20
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Energetic Components
Stability | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Energetic Components
Decomposition | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Energy (kcal/mol)
−6
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | TDC
Receptor
Ligand
Energy (kcal/mol)
2
1
0
−1
−2
−3
−4
−5
−6
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:THR:33
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9
1
2
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4
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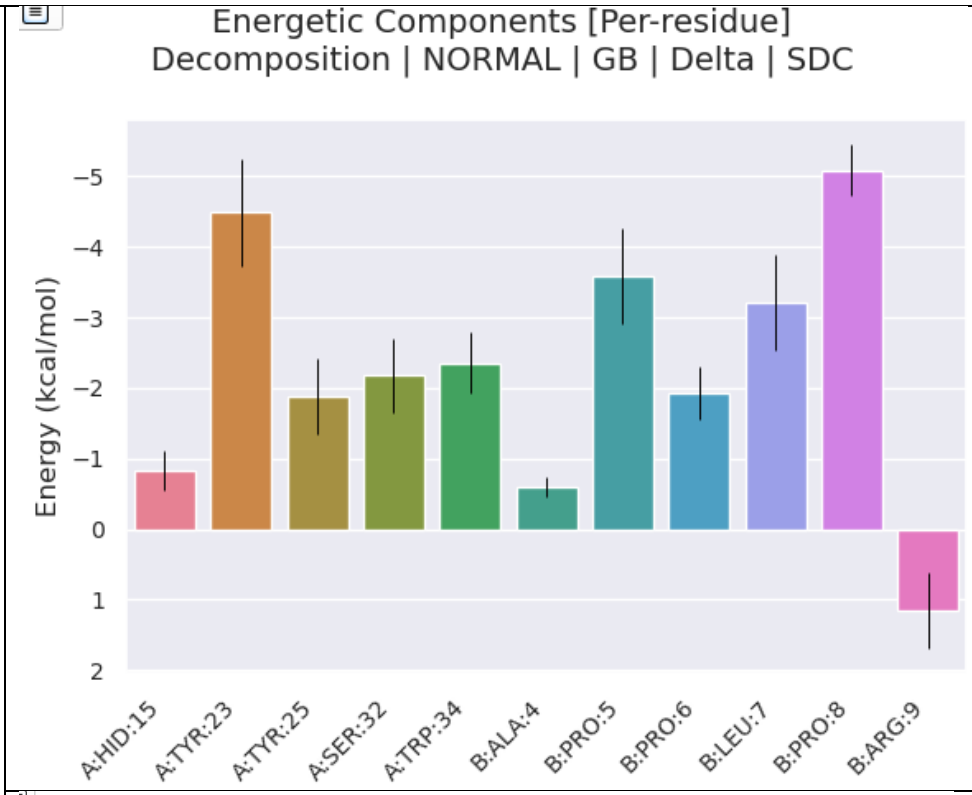
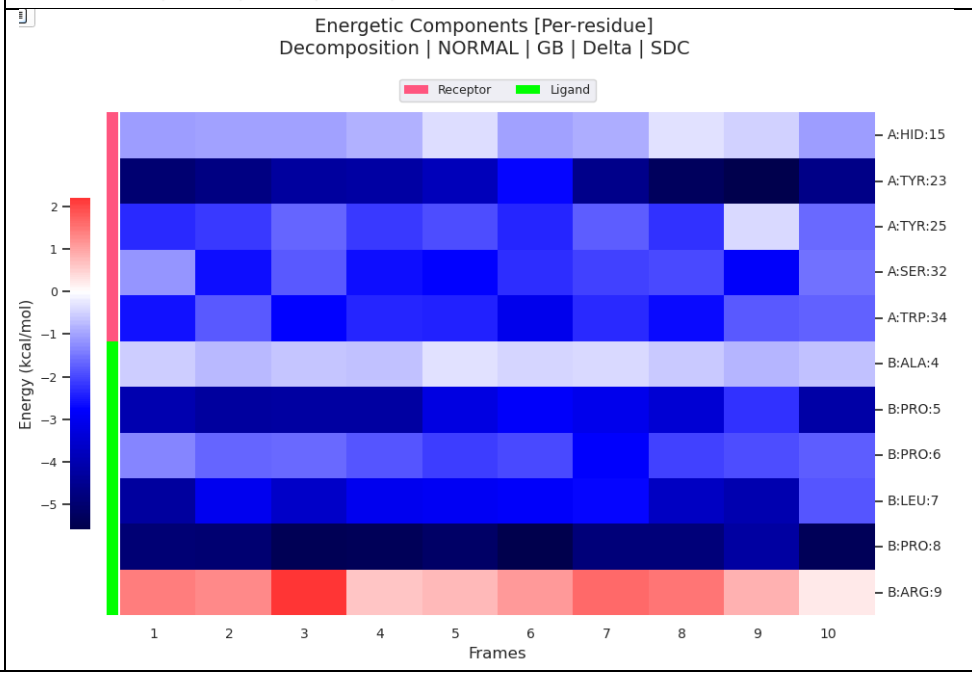
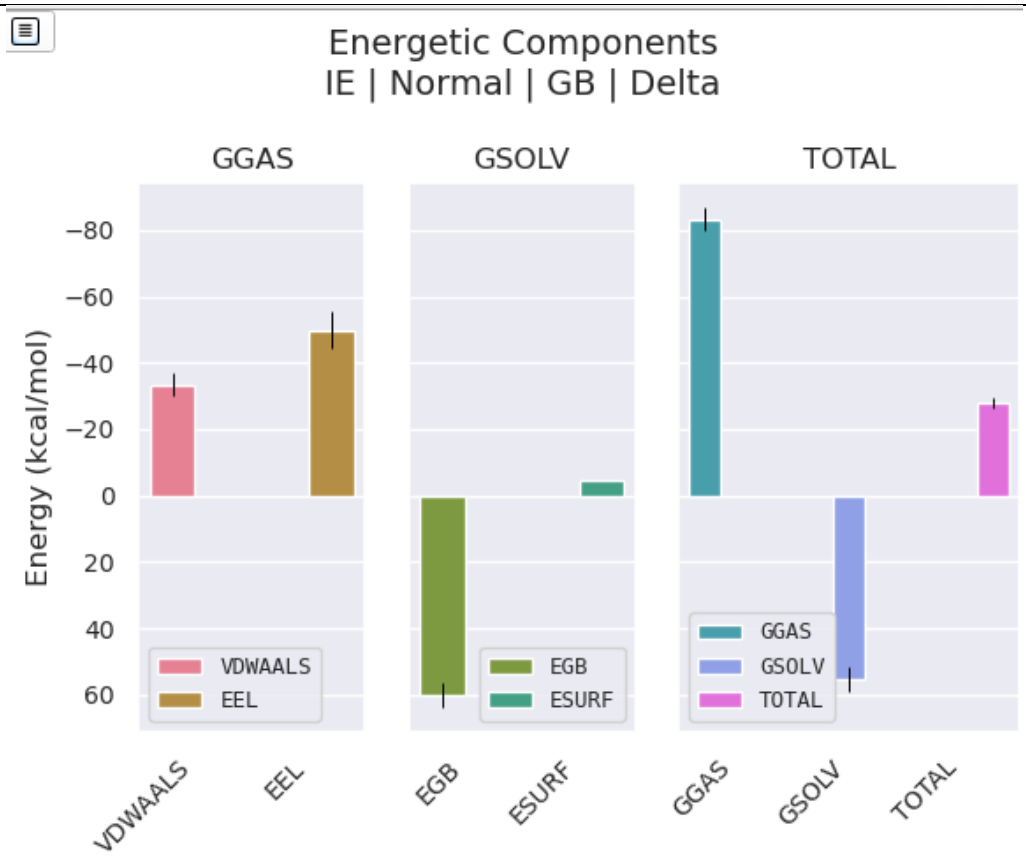
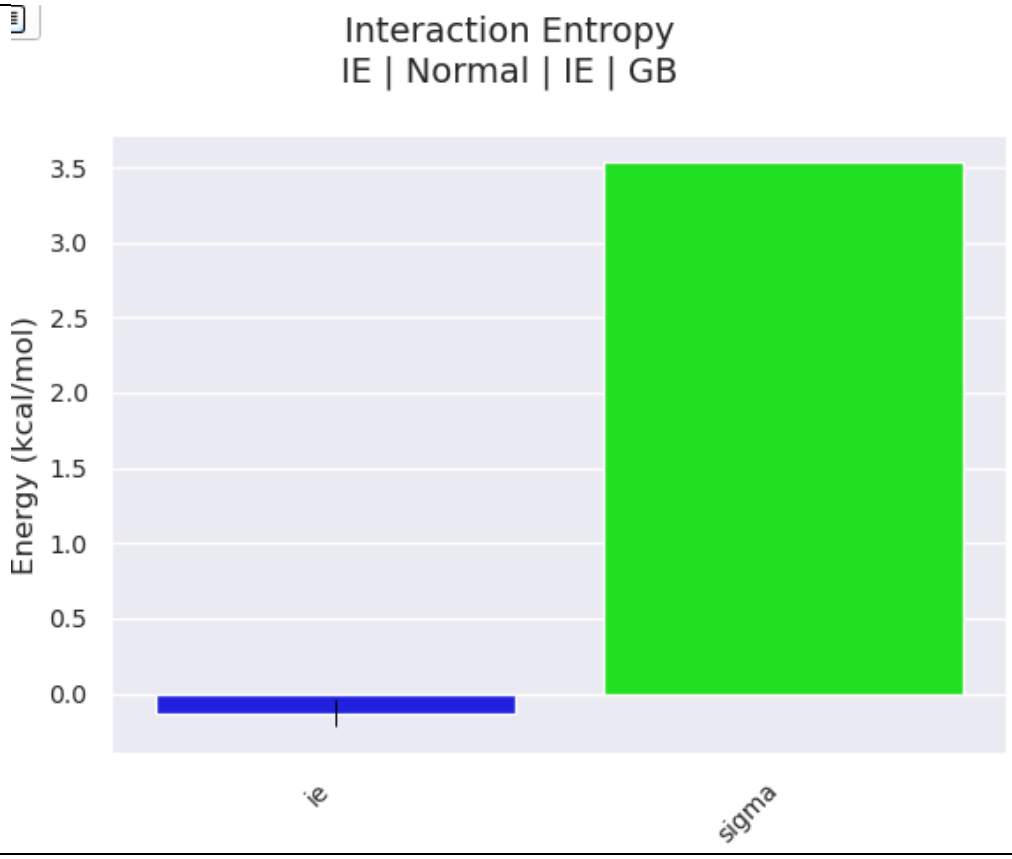
6
7
8
9
10
Frames


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | SDC
Energy (kcal/mol)
−5
−4
−3
−2
−1
0
1
2
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9


Energetic Components [Per-residue]
Decomposition | NORMAL | GB | Delta | SDC
Receptor
Ligand
Energy (kcal/mol)
2
1
0
−1
−2
−3
−4
−5
A:HID:15
A:TYR:23
A:TYR:25
A:SER:32
A:TRP:34
B:ALA:4
B:PRO:5
B:PRO:6
B:LEU:7
B:PRO:8
B:ARG:9
1
2
3
4
5
6
7
8
9
10
Frames


Energetic Components
IE | Normal | GB | Delta
GGAS
GSOLV
TOTAL
Energy (kcal/mol)
−80
−60
−40
−20
0
20
40
60
VDWAALS
EEL
EGB
ESURF
GGAS
GSOLV
TOTAL


Interaction Entropy
IE | Normal | IE | GB
Energy (kcal/mol)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ie
sigma

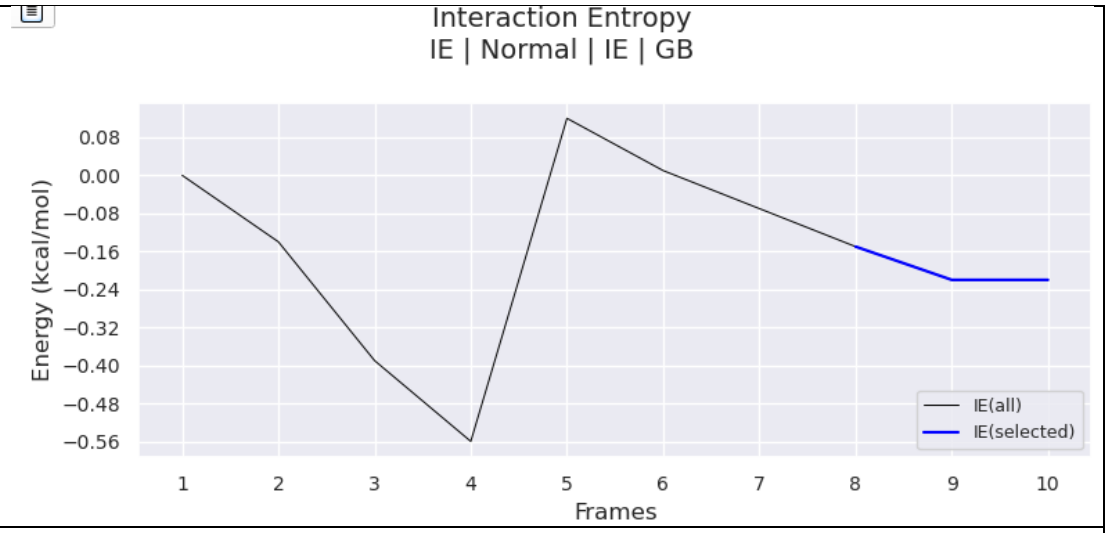


Figure A42. Residue-level MMPBSA energetic analysis showing the interaction map of key residues involved in stabilizing genistein within the 1X2J complex.