

AKT1-baicalein

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-7.3	0
2	-7.2	1.041
3	-6.8	2.674
4	-6.7	2.623
5	-6.7	3.115
6	-6.6	10.512
7	-6.4	24
8	-6.3	10.385
9	-6.3	1.901
10	-6.3	1.63
11	-6.2	28.275
12	-6.1	18.641
13	-5.7	25.874
14	-5.6	21.896
15	-5.4	23.252
16	-5.4	19.621
17	-5.3	25.372
18	-5.3	28.741
19	-5.1	11.59
20	-5.1	10.351

AKT1-kaempferol

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-6.7	0
2	-6.6	2.876
3	-6.6	1.525
4	-6.5	3.773
5	-6.5	3.325
6	-6.1	3.394
7	-6.1	1.684
8	-6	26.605
9	-6	17.48
10	-5.9	22.62
11	-5.8	23.467
12	-5.7	24.194
13	-5.7	3.203
14	-5.6	26.36
15	-5.6	24.202
16	-5.6	17.49
17	-5.6	26.571
18	-5.6	22.325
19	-5.6	24.821
20	-5.5	24.2

AKT1-quercetin

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-6.9	0
2	-6.8	1.536
3	-6.7	2.891
4	-6.5	2.385
5	-6.4	9.906
6	-6.3	16.784
7	-6.1	2.231
8	-6	26.61
9	-6	22.319
10	-5.9	22.686

11	-5.9	2.735
12	-5.8	24.921
13	-5.7	21.217
14	-5.7	26.72
15	-5.7	18.136
16	-5.7	20.703
17	-5.6	24.245
18	-5.6	24.174
19	-5.4	18.536
20	-5.3	24.419

AKT1-wogonin  
mode

	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-7.3	0
2	-6.8	2.057
3	-6.7	1.268
4	-6.6	2.676
5	-6.1	10.281
6	-5.9	26.089
7	-5.9	20.786
8	-5.9	18.168
9	-5.8	28.225
10	-5.8	28.708
11	-5.4	20.425
12	-5.4	25.571
13	-5.3	23.052
14	-5.3	28.654
15	-5.2	19.216
16	-5.2	24.422
17	-5.2	18.987
18	-5.1	25.42
19	-5.1	25.322
20	-5.1	18.642

JUN-beta-sitostero  
mode

	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-6.9	0
2	-6.8	2.188
3	-6.8	15.638
4	-6.7	13.929
5	-6.6	13.927
6	-6.5	3.488
7	-6.5	13.397
8	-6.3	14.011
9	-6.3	13.563
10	-6.2	5.598
11	-6.1	13.846
12	-6.1	13.568
13	-5.9	13.694
14	-5.9	15.252
15	-5.8	6.48
16	-5.7	14.968
17	-5.6	14.286
18	-5.6	35.943
19	-5.5	7.896
20	-5.4	4.75

JUN-kaempferol

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-8.1	0
2	-8	13.267
3	-7.9	23.7
4	-7.9	24.012
5	-7.8	10.793
6	-7.8	24.424
7	-7.7	5.769
8	-7.7	27.715
9	-7.6	25.357
10	-7.5	8.045
11	-7.5	18.545
12	-7.4	29.246
13	-7.4	14.139
14	-7.4	26.102
15	-7.3	21.982
16	-7.3	5.955
17	-7.2	1.561
18	-7.2	1.616
19	-7.2	26.649
20	-7.2	14.816

JUN-quercetin

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-8.6	0
2	-8.5	23.601
3	-8.5	25.423
4	-8.3	10.894
5	-8.2	23.974
6	-8.1	25.671
7	-8	5.92
8	-8	1.669
9	-8	5.743
10	-7.9	24.435
11	-7.9	29.058
12	-7.7	26.353
13	-7.7	30.953
14	-7.6	1.799
15	-7.6	1.8
16	-7.5	4.397
17	-7.5	2.399
18	-7.5	3.849
19	-7.4	1.728
20	-7.2	10.996

JUN-wogonin

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-7.5	0
2	-7.2	14.141
3	-7.1	13.969
4	-6.9	28.399
5	-6.9	31.786
6	-6.9	13.666
7	-6.8	13.679
8	-6.7	13.449
9	-6.6	32.281
10	-6.5	13.844
11	-6.5	33.369

12	-6.5	14.037
13	-6.4	31.305
14	-6.4	14.276
15	-6.2	13.833
16	-6.2	9.722
17	-6.1	13.06
18	-5.9	14.376
19	-5.8	14.969
20	-5.7	9.697

MAPK1-quercetin

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-8.7	0
2	-8.5	20.693
3	-8.5	17.348
4	-8.3	27.892
5	-8.3	1.504
6	-8.2	4.042
7	-8.1	3.448
8	-8	21.13
9	-8	25.074
10	-8	21.405
11	-7.9	24.65
12	-7.9	19.37
13	-7.8	28.246
14	-7.7	19.288
15	-7.6	23.782
16	-7.4	22.866
17	-7.4	4.48
18	-7.3	28.042
19	-7.2	22.611
20	-7.1	28.406

MAPK8-kaempferol

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-8.7	0
2	-8.5	39.353
3	-8.4	36.843
4	-8.3	51.938
5	-8.3	59.526
6	-8.1	59.906
7	-8	60.521
8	-8	65.102
9	-7.9	20.735
10	-7.8	60.368
11	-7.8	63.855
12	-7.8	21.387
13	-7.6	65.348
14	-7.6	32.16
15	-7.5	60.262
16	-7.5	65.551
17	-7.4	53.465
18	-7.4	51.454
19	-7.4	21.232
20	-7.3	21.193

TP53-acacetin

mode	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
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1	-8.6	0
2	-8.3	3.093
3	-8.2	33.399
4	-8.2	59.862
5	-8.2	60.809
6	-8	51.92
7	-7.9	3.976
8	-7.7	99.405
9	-7.6	2.01
10	-7.5	17.693
11	-7.5	100.592
12	-7.3	64.589
13	-7.3	48.659
14	-7.3	54.169
15	-7.2	18.23
16	-7.2	95.197
17	-7.1	60.215
18	-7	41.456
19	-6.9	2.152
20	-6.9	22.353

TP53-baicalein  
mode

	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-8.5	0
2	-8.5	70.024
3	-8.4	33.178
4	-8.2	23.665
5	-8.2	74.457
6	-8.1	52.113
7	-8	70.282
8	-7.9	70.553
9	-7.9	51.947
10	-7.9	74.52
11	-7.9	75.991
12	-7.8	74.032
13	-7.7	55.672
14	-7.7	23.307
15	-7.6	59.773
16	-7.5	57.265
17	-7.5	50.658
18	-7.4	49.578
19	-7.3	31.57
20	-7.3	30.853

TP53-queracetin  
mode

	affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-8.9	0
2	-8.5	74.875
3	-8.4	113.018
4	-8.3	3.173
5	-8	26.093
6	-8	25.546
7	-8	75.845
8	-8	110.861
9	-8	25.102
10	-8	51.699
11	-7.9	50.184
12	-7.9	113.803

13	-7.9	3.773
14	-7.8	108.292
15	-7.5	103.603
16	-7.4	50.964
17	-7.3	24.537
18	-7.3	22.349
19	-7.2	103.073
20	-7.1	104.204

TP53-wogonin

mode		affinity(kcal/mol)	dist from best mode (rmsd l.b.)
1	-8.8	0.000	0.000
2	-8.4	33.622	36.969
3	-7.8	29.434	32.483
4	-7.7	21.954	25.289
5	-7.6	32.867	34.065
6	-7.6	22.487	25.179
7	-7.4	1.594	1.889
8	-7.3	81.258	84.607
9	-7.3	22.939	25.711
10	-7.3	80.945	84.244
11	-7.2	32.048	35.004
12	-7.2	24.870	26.223
13	-7.2	6.008	9.455
14	-7.2	24.798	25.808
15	-7.2	72.797	75.730
16	-7.1	31.872	34.353
17	-7.0	7.893	11.267
18	-6.8	22.496	24.781
19	-6.6	12.148	14.275
20	-6.5	32.303	34.805

dist from best mode ( rmsd u.b.)

0  
2.622  
4.553  
4.452  
4.198  
10.768  
25.493  
10.897  
2.815  
3.304  
30.614  
20.326  
27.221  
23.24  
25.071  
22.629  
26.303  
31.031  
11.833  
10.833

dist from best mode ( rmsd u.b.)

0  
6.529  
3.297  
6.439  
6.788  
6.886  
6.471  
27.955  
18.97  
24.574  
24.87  
26.382  
6.881  
27.522  
25.834  
19.107  
28.196  
24.373  
26.184  
26.834

dist from best mode ( rmsd u.b.)

0  
2.983  
6.903  
6.646  
12.783  
18.767  
2.982  
28.658  
24.454  
24.732

6.576  
26.465  
23.553  
28.42  
20.024  
23.151  
26.354  
25.841  
20.525  
26.861

dist from best mode ( rmsd u.b.)

0  
4.86  
3.393  
4.759  
11.328  
27.227  
23.063  
19.869  
30.672  
30.378  
22.745  
26.66  
25.443  
29.684  
20.523  
26.824  
21.163  
25.924  
27.023  
19.977

dist from best mode ( rmsd u.b.)

0  
4.495  
17.334  
17.629  
16.81  
6.707  
15.26  
17.562  
16.578  
10.05  
18.163  
15.494  
16.077  
19.151  
13.358  
16.937  
16.849  
39.051  
14.256  
8.158



dist from best mode ( rmsd u.b.)

0  
16.578  
25.729  
26.03  
14.941  
25.542  
11.072  
29.316  
27.163  
11.934  
21.761  
31.938  
16.033  
28.295  
24.755  
10.788  
3.24  
6.335  
27.949  
17.781

dist from best mode ( rmsd u.b.)

0  
25.601  
27.441  
14.954  
26.046  
28.031  
10.95  
2.001  
9.449  
25.597  
31.743  
27.74  
34.243  
6.699  
3.691  
9.43  
4.724  
7.032  
6.435  
15.432

dist from best mode ( rmsd u.b.)

0  
16.543  
15.854  
31.034  
34.681  
15.786  
16.118  
15.386  
35.157  
16.291  
36.212

16.62  
32.68  
16.552  
16.087  
12.816  
14.769  
16.162  
16.913  
13.191

dist from best mode ( rmsd u.b.)

0  
21.618  
22.12  
29.259  
6.483  
6.98  
6.447  
22.199  
26.323  
22.46  
25.449  
23.955  
30.045  
24.409  
24.842  
23.878  
6.913  
29.88  
23.572  
29.444

dist from best mode ( rmsd u.b.)

0  
41.583  
38.936  
54.608  
61.524  
61.782  
62.517  
66.364  
22.697  
62.187  
65.951  
22.323  
66.997  
33.772  
62.259  
67.564  
54.961  
54.524  
22.97  
22.155

dist from best mode ( rmsd u.b.)

0  
4.257  
37.293  
61.431  
62.846  
53.394  
6.03  
101.278  
2.539  
19.782  
102.862  
66.348  
50.506  
56.122  
21.218  
96.06  
61.644  
43.484  
8.854  
23.107

dist from best mode ( rmsd u.b.)

0  
71.809  
35.04  
25.776  
75.845  
53.344  
70.568  
71.618  
53.465  
76.635  
78.142  
76.562  
57.681  
25.54  
61.797  
59.194  
52.757  
51.602  
33.69  
33.821

dist from best mode ( rmsd u.b.)

0  
76.793  
116.243  
6.417  
27.443  
27.171  
76.544  
113.5  
26.691  
53.228  
52.061  
117.842

6.412  
111.952  
107.706  
52.781  
27.216  
26.224  
106.84  
107.765

dist from best mode ( rmsd u.b.)