

Compound 1				Compound 2			
Rank	PDB_ID	Energy Score	TARGET NAME	Rank	PDB_ID	Energy Score	TARGET NAME
1	1C9C	-47.33	Aspartate Aminotransferase, Cytoplasmic	1	1HVR	-29.6	HIV Protease
2	1BMN	-46.48	Serine Proteinase alpha-thrombin	2	1LBV	-28.04	Inositol 1 phosphatase
3	1TCO	-46.02	FKBP,tacrolimus binding protein,FK506 binding prote	3	1Y79	-27.67	Peptidyl dipeptidase
4	1IYH	-45.33	Hematopoietic Prostaglandin D Synthase	4	1JTV	-27.57	Hydroxysteroid-Dehydrogenase Type 1
5	1IX6	-43.8	Aspartate Aminotransferase, Cytoplasmic	5	1D2V	-27.36	Myeloperoxidase
6	1DWD	-43.62	Serine Proteinase alpha-thrombin	6	1FNO	-27.36	Peptidase
7	1DIE	-43.52	D-Xylose Isomerase	7	2E9W	-27.23	Mast/stem cell growth factor receptor
8	1EFR	-43.35	Bovine Mitochondrial F1-ATPase	8	1DHF	-26.71	Dihydrofolate Reductase
9	1JR1	-43.24	Inosine-5'-monophosphate Dehydrogenase2;	9	1FT2	-26.69	Protein farnesyl transferase
10	1DFF	-43.1	Peptide deformylase	10	1HA3	-26.4	Elongation Factor Tu
11	1IG3	-43.08	Thiamin Pyrophosphokinase	11	1OJN	-26.33	Hyaluronate Lyase
12	1OJN	-42.87	Hyaluronate Lyase	12	1XIG	-26.1	D-Xylose Isomerase
13	1COY	-42.8	Cholesterol Oxidase	13	1JKL	-25.97	Death-Associated Protein Kinase
14	1BVY	-42.76	Unspecific Monooxygenase	14	1H82	-25.97	Polyamine oxidase
15	2ANH	-42.38	Alkaline phosphatase	15	2FJP	-25.95	Dipeptidyl Peptidase IV (DPP4)
16	1ED5	-42.21	Nitric Oxide Synthase	16	1BGV	-25.9	Glutamate Dehydrogenase
17	1FOI	-41.87	Phospholipase D	17	1DXJ	-25.8	Chitinase
18	1WOH	-41.68	Agmatinase	18	1DBK	-25.74	Fab' Fragment Of Monoclonal Antibody Db3
19	1ZYJ	-41.65	Map Kinase P38	19	1NNC	-25.67	Neuraminidase subtype N9 (TERN)(NA)
20	1IIC	-41.6	Peptide N-myristoyltransferase	20	1JJC	-25.62	Phenylalanyl-tRNA Synthetase
21	9AAT	-41.54	Aspartate Aminotransferase	21	1B74	-25.58	Glutamate racemase
22	1TCO	-41.52	FKBP,tacrolimus binding protein,FK506 binding prote	22	2DDH	-25.51	Acyl CoA oxidase-2
23	1AED	-41.52	Peroxidase	23	1KAE	-25.37	Histidinol Dehydrogenase
24	1ZZE	-41.45	Carbonyl reductase	24	1OPM	-25.28	Peptidylglycine Alpha-Hydroxylating Monooxyg
25	2B3K	-41.42	Methionine aminopeptidase	25	1VJT	-25.25	Alpha glucosidase;Glucosidase alpha 1
26	1I9C	-41.33	Glutamate Mutase	26	1YMJ	-25.22	Adenine nucleotide translocator
27	1F2A	-41.29	n/a	27	1QHG	-25.21	ATP-Dependent Helicase PcrA
28	1AXN	-41.26	Annexin A3	28	1BUQ	-25.19	Delta 5-3-ketosteroid isomerase
29	1SZ2	-41.17	Glucokinase	29	1ENT	-25.16	Endothiapepsin
30	1I7B	-40.99	Methionine decarboxylase	30	1K7Y	-25.07	5-methyltetrahydrofolate--homocysteine Mferase;
31	1AEV	-40.99	Peroxidase	31	1NM8	-24.94	Carnitine acyltransferase
32	1DBK	-40.93	Fab' Fragment Of Monoclonal Antibody Db3	32	1DIE	-24.85	D-Xylose Isomerase

33	1P8V	-40.91	Thrombin	33	1IIC	-24.78	Peptide N-myristoyltransferase
34	1DWC	-40.8	Serine Proteinase alpha-thrombin	34	2C0H	-24.77	Beta-mannosidase
35	1HKV	-40.78	Mycobacterium Diaminopimelate Decarboxylase	35	1YVB	-24.76	falcipain-2
36	2BH9	-40.74	Glucose-6-phosphate dehydrogenase	36	1ED5	-24.73	Nitric Oxide Synthase
37	1ETS	-40.58	Thrombin(inhibitor)	37	1DID	-24.72	D-Xylose Isomerase
38	1QHG	-40.58	ATP-Dependent Helicase PcrA	38	1IMB	-24.72	Inositol-1(or 4)-monophosphatase
39	1FT2	-40.55	Protein farnesyl transferase	39	1U4O	-24.53	Lactate dehydrogenase
40	1ZKK	-40.51	Histone lysine methyltransferase	40	1IG3	-24.51	Thiamin Pyrophosphokinase
41	1YMJ	-40.5	Adenine nucleotide translocator	41	1DKF	-24.47	Retinoid X Receptor
42	1OXO	-40.41	Aspartate Aminotransferase, Cytoplasmic	42	1Q0N	-24.44	HPPK
43	1LP4	-40.33	Casein Kinase II, Protein Kinase Ck2	43	1IN4	-24.35	Holliday Junction DNA Helicase Ruvb
44	1DHT	-40.3	Estrogenic 17-Beta Hydroxysteroid Dehydrogenase	44	2ANH	-24.3	Alkaline phosphatase
45	1BGV	-40.27	Glutamate Dehydrogenase	45	1F2A	-24.26	n/a
46	1PTG	-40.26	1-phosphatidylinositol-4,5-bisphosphate Phosphodiesterase beta 1	46	1J99	-24.09	Alcohol Sulfotransferase
47	1DMW	-40.24	Phenylalanine Hydroxylase	47	1DBB	-24.02	Fab' Fragment Of The Db3 Anti-Steroid M A
48	1BMM	-40.23	Serine Proteinase alpha-thrombin	48	1K3Y	-24.01	Glutathione Transferase A1-1
49	1Q0N	-39.9	HPPK	49	1HVB	-24.01	D-alanyl-D-alanine Carboxypeptidase
50	1NNB	-39.81	Neuramidase	50	1CLY	-23.99	n/a
51	1AEN	-39.74	Peroxidase	51	1IGJ	-23.96	Fab (Igg2A, )
52	2CG5	-39.67	Other phosphate group transferase	52	1W50	-23.91	Beta-secretase-1
53	1CGH	-39.63	Cathepsin G	53	1DGM	-23.85	Adenosine kinase

### Compound 3

Rank	PDB_ID	Energy Scor	TARGET NAME
1	1FT2	-46.97	Protein farnesyl transferase
2	1OOQ	-46.71	Dihydropteridine Reductase
3	2C6C	-45.75	Glutamate carboxypeptidase II
4	1AEC	-44.97	Actinidin
5	1F2A	-44.83	n/a
6	1Q0N	-44.53	HPPK
7	1HVR	-44.1	HIV Protease
8	1JCN	-43.73	IMP-1 dehydrogenase
9	1H7X	-43.66	Dihydropyrimidine dehydrogenase
10	1CY1	-43.4	DNA Topoisomerase

### Compound 4

Rank	PDB_ID	Energy Scor	TARGET NAME
1	2C6C	-47.98	Glutamate carboxypeptidase II
2	1BBP	-44.19	bilin binding protein (BBP)
3	1Q5M	-42.46	Alpha hydroxysteroid dehydrogenase
4	1Y79	-42.29	Peptidyl dipeptidase
5	1E1F	-41.78	beta-Glucosidase
6	1D2V	-41.73	Myeloperoxidase
7	1K4M	-41.61	Nicotinate-nucleotide Adenylyltransferase
8	1H7X	-40.63	Dihydropyrimidine dehydrogenase
9	1AEM	-40.33	Peroxidase
10	2CG5	-38.72	Other phosphate group transferase

11	2G63	-43.13	Dipeptidyl Peptidase IV (DPP4)	11	1EJB	-38.53	Lumazine Synthase
12	2FJP	-43.1	Dipeptidyl Peptidase IV (DPP4)	12	1HKV	-38.32	Mycobacterium Diaminopimelate Decarboxylase
13	1HKV	-43.09	Mycobacterium Diaminopimelate Decarboxylase	13	1X07	-38.24	Undecaprenyl diphosphate synthetase
14	1L1E	-43	Mycolic Acid Synthase	14	2B3K	-38.23	Methionine aminopeptidase
15	1STC	-42.76	Camp-dependent Protein Kinase A Type I	15	1XOS	-38.13	PDE 4b
16	2G5T	-42.73	Dipeptidyl peptidase IV	16	1IG0	-38.04	Thiamin Pyrophosphokinase
17	1ICP	-42.71	12-Oxophytodienoate Reductase 1	17	1QIP	-37.94	Lactoylglutathione lyase
18	1I9C	-42.64	Glutamate Mutase	18	1E55	-37.93	beta-Glucosidase
19	1AL8	-42.62	Oxidase	19	1FT2	-37.61	Protein farnesyl transferase
20	1FAX	-42.55	Coagulation Factor Xa	20	1EAP	-37.49	UNDEFINED
21	1PPL	-42.18	Penicillopepsin	21	1HS6	-37.4	Leukotriene A4 hydrolase
22	1IMB	-42.1	Inositol-1(or 4)-monophosphatase	22	1BOZ	-37.31	Dihydrofolate Reductase
23	1YMJ	-42.05	Adenine nucleotide translocator	23	1I7B	-37.26	Methionine decarboxylase
24	1QHG	-42.03	ATP-Dependent Helicase PcrA	24	1IA9	-37.23	Transient Receptor Potential-Related Protein;
25	1E7W	-41.95	Flavo-hemoglobin	25	1BVY	-37.23	Unspecific Monooxygenase
26	1LGR	-41.9	Glutamine Synthetase	26	1BU5	-37.16	Flavodoxin
27	1TCO	-41.76	FKBP,tacrolimus binding protein,FK506 binding	27	1XID	-37.12	D-Xylose Isomerase
28	1HDT	-41.41	Serine Proteinase alpha-thrombin	28	1HKV	-37.1	Mycobacterium Diaminopimelate Decarboxylase
29	1DWD	-41.07	Serine Proteinase alpha-thrombin	29	1ZKK	-37.02	Histone lysine methyltransferase
30	1TYP	-40.94	Trypanothione Reductase	30	1JCN	-36.99	IMP-1 dehydrogenase
31	1HDT	-40.91	Serine Proteinase alpha-thrombin	31	1E8W	-36.9	n/a
32	1CGH	-40.85	Cathepsin G	32	1PFX	-36.8	Coagulation Factor IX
33	1HA3	-40.79	Elongation Factor Tu	33	1OEC	-36.8	Fibroblast Growth Factor Receptor 2
34	2C6Q	-40.77	GMP reductase	34	1OOQ	-36.6	Dihydropteridine Reductase
35	1XMC	-40.72	Peroxisomal carnitine O-octanoyltransferase	35	1AEF	-36.44	Peroxidase
36	1UHL	-40.62	Liver X receptor alpha	36	1C9C	-36.39	Aspartate Aminotransferase, Cytoplasmic
37	1GAI	-40.61	Glucan 1,4-alpha-glucosidase	37	1COY	-36.37	Cholesterol Oxidase
38	1PPI	-40.57	alpha-Amylase	38	1LP4	-36.35	Casein Kinase II, Protein Kinase Ck2
39	1OEC	-40.55	Fibroblast Growth Factor Receptor 2	39	1HDT	-36.28	Serine Proteinase alpha-thrombin
40	1XOQ	-40.51	PDE 4d	40	1YTV	-36.21	Vasopressin V1a receptor
41	1HDC	-40.46	3-alpha-hydroxysteroid Dehydrogenase	41	1DBJ	-36.19	Fab' Fragment Of Monoclonal Antibody Db3
42	1BGV	-40.42	Glutamate Dehydrogenase	42	1OS0	-36.17	Thermolysin
43	1FIW	-40.38	Acrosin	43	1DBM	-36.13	Fab' Fragment Of Monoclonal Antibody Db3
44	1PPM	-40.37	Penicillopepsin	44	2ER6	-36.13	Endothiapepsin
45	1XIE	-40.34	D-Xylose Isomerase	45	1ICR	-36.11	Nitroreductase

46	1VKG	-40.33	Histone deacetylase-8	46	2BZ1	-36.1	GTP cyclohydrolase-II
47	1ZZE	-40.15	Carbonyl reductase	47	1FAX	-36.07	Coagulation Factor Xa
48	1VJT	-40.12	Alpha glucosidase	48	1Q0N	-36.06	HPPK
49	1O6L	-39.96	Activated Akt/Protein Kinase B	49	2G5P	-35.9	Dipeptidyl Peptidase IV (DPP4)
50	1JQH	-39.94	Insulin-like Growth Factor I Receptor	50	1HDT	-35.75	Serine Proteinase alpha-thrombin
51	1EED	-39.93	Endothiapepsin	51	1ZFJ	-35.73	Inosine-5'-monophosphate Dehydrogenase
52	1MCR	-39.9	Immunoglobulin lambda Light Chain Dimer (Mcg)	52	1PS9	-35.69	2,4-Dienoyl-Coa Reductase
53	2AGT	-39.74	Aldehyde Reductase	53	1TG7	-35.62	Beta-galactosidase

#### Compound 5

Rank	PDB_ID	Energy Score	TARGET NAME
1	1W6K	-38.12	Oxidosqualene cyclase
2	1GOX	-37.79	Spinach glycolate oxidase
3	1EFA	-37.59	Lac Repressor
4	1GOS	-37.48	Amine Oxidase [Flavin-containing] A
5	1DWC	-36.51	Serine Proteinase alpha-thrombin
6	1I76	-36.42	Neutrophil Collagenase, MMP8
7	1J96	-36.32	Aldo-Keto Reductase Family 1 Member C3
8	1OYA	-36.08	NADPH Dehydrogenase
9	1HS6	-35.2	Leukotriene A4 hydrolase
10	1HS6	-35.18	Histamine N-methyltransferase
11	1Q0N	-35	HPPK
12	1YTV	-34.94	Vasopressin V1a receptor
13	1DBJ	-34.88	Fab' Fragment Of Monoclonal Antibody Db3
14	1GAI	-34.72	Glucan 1,4-alpha-glucosidase
15	1VXR	-34.69	Acetylcholinesterase
16	2ADA	-34.68	Adenosine Deaminase
17	1PPM	-34.67	Penicillopepsin
18	2AGT	-34.59	Aldehyde Reductase
19	1LVG	-34.58	ZC protein kinase
20	1JJC	-34.44	Phenylalanyl-tRNA Synthetase
21	1HKV	-34.31	Mycobacterium Diaminopimelate Decarboxylase
22	1HP5	-34.26	Beta-N-acetylhexosaminidase
23	1NR5	-34.25	3-dehydroquinate Synthase
24	1ZKK	-34.18	Histone lysine methyltransferase
25	1C0K	-34.18	D-Amino acid oxidase
26	1K4M	-34.13	Nicotinate-nucleotide Adenylyltransferase

#### Compound 6

Rank	PDB_ID	Energy Score	TARGET NAME
1	1Y79	-47.44	Peptidyl dipeptidase
2	1HVK	-47.38	HIV Protease
3	1P38	-47.34	p38 MAP kinase
4	1UEA	-46.95	Metalloprotease 3
5	1ETT	-46.92	Thrombin(inhibitor)
6	1ICR	-46.71	Nitroreductase
7	1OS0	-46.57	Thermolysin
8	1HS6	-46.26	Leukotriene A4 hydrolase
9	1FT2	-46.25	Protein farnesyl transferase
10	1JS3	-45.88	Aromatic-L-amino-acid Decarboxylase
11	1OJN	-45.66	Hyaluronate Lyase
12	1XIG	-45.41	D-Xylose Isomerase
13	1DHT	-45.08	Estrogenic 17-Beta Hydroxysteroid Dehydrogenase
14	2DDH	-44.84	Acyl CoA oxidase-2
15	1DIF	-44.82	HIV Protease
16	1EFR	-44.09	Bovine Mitochondrial F1-ATPase
17	1HYT	-44.09	Thermolysin
18	1IG3	-43.68	Thiamin Pyrophosphokinase
19	1HVI	-43.67	HIV Protease
20	1W07	-43.59	Acyl CoA oxidase-1
21	1NSC	-43.57	Neuramidase
22	1JJC	-43.54	Phenylalanyl-tRNA Synthetase
23	1TYP	-43.11	Trypanothione Reductase
24	1PS9	-43.08	2,4-Dienoyl-Coa Reductase
25	2C6C	-42.9	Glutamate carboxypeptidase II
26	2G5T	-42.78	Dipeptidyl peptidase IV

27	1BBP	-34.12	bilin binding protein (BBP)	27	1E8W	-42.74	n/a
28	1DMW	-34.05	Phenylalanine Hydroxylase	28	2B3K	-42.48	Methionine aminopeptidase
29	2G5T	-34.02	Dipeptidyl peptidase IV	29	1PPK	-42.47	Penicillopepsin
30	2ACS	-33.99	Aldose Reductase	30	1P42	-42.4	N-acetylglucosamine deacetylase
31	1IUU	-33.95	Plasma retinol-binding protein	31	1TG7	-42.26	Beta-galactosidase
32	1BZS	-33.91	Neutrophil Collagenase, MMP8;Neutrophil Collagenase, MMP	32	1AJX	-42.22	HIV Protease
33	1ZSX	-33.86	Voltage gated potassium channel	33	1IN4	-42.21	Holliday Junction DNA Helicase Ruvb
34	1W07	-33.85	Acyl CoA oxidase-1	34	2BCE	-42.13	Cholesterol esterase
35	1CVW	-33.78	Coagulation Factor VIIa	35	1APU	-42.12	Penicillopepsin
36	1HKV	-33.7	Mycobacterium Diaminopimelate Decarboxylase	36	1DHF	-42	Dihydrofolate Reductase
37	1R1K	-33.68	Ecdysone Hormone Receptor	37	1JAP	-41.7	Metalloprotease 8
38	1AEO	-33.65	Peroxidase	38	1DMW	-41.57	Phenylalanine Hydroxylase
39	1BMT	-33.44	5-methyltetrahydrofolate--homocysteine Methyltransferase	39	1VKG	-41.56	Histone deacetylase-8
40	1ADD	-33.35	Adenosine Deaminase	40	1HTG	-41.39	HIV Protease
41	1EJB	-33.31	Lumazine Synthase	41	1APT	-41.31	Penicillopepsin
42	1ZFJ	-33.18	Inosine-5'-monophosphate Dehydrogenase;	42	1H8D	-41.29	Serine Proteinase alpha-thrombin
43	1PY5	-33.09	TGF-beta receptor type I	43	1PTG	-41.26	1-phosphatidylinositol-4,5-bisphosphate P beta 1
44	1ICR	-33.08	Nitroreductase	44	1ETS	-41.23	Thrombin(inhibitor)
45	1TOH	-32.97	Tyrosine hydroxylase	45	1YMJ	-41.23	Adenine nucleotide translocator
46	1XOS	-32.88	PDE 4b	46	1HDT	-41.16	Serine Proteinase alpha-thrombin
47	2FJP	-32.84	Dipeptidyl Peptidase IV (DPP4)	47	1XID	-41.15	D-Xylose Isomerase
48	1XKK	-32.81	Epidermal Growth Factor Receptor(EGFR)	48	1Q0N	-41.14	HPPK
49	2AIG	-32.8	Adamalysin II	49	1EI1	-41.07	DNA Gyrase B Subunit
50	1IJH	-32.73	Cholesterol Oxidase	50	1AEM	-41.06	Peroxidase
51	1R18	-32.67	Methyltransferase	51	2CGR	-41.02	Igg2B Fab Fragment
52	1CBX	-32.67	Carboxypeptidase A	52	1HA3	-41	Elongation Factor Tu
53	1UH5	-32.63	Enoyl ACP reductase	53	1EPP	-41	Elongation Factor Tu

**Compound 7**

Rank	PDB_ID	Energy Scor	TARGET NAME
1	1BBP	-42.44	bilin binding protein (BBP)
2	1GOX	-40.54	Spinach glycolate oxidase
3	1HKV	-38.65	Mycobacterium Diaminopimelate Decarboxylase
4	1YGP	-38.52	Glycogen Phosphorylase, Muscle Form
5	1E1F	-38.09	beta-Glucosidase

**Compound 8**

Rank	PDB_ID	Energy Scor	TARGET NAME
1	1HVR	-29.6	HIV Protease
2	1LBV	-28.04	Inositol 1 phosphatase
3	1Y79	-27.67	Peptidyl dipeptidase
4	1JTV	-27.57	Hydroxysteroid-Dehydrogenase Type 1
5	1D2V	-27.36	Myeloperoxidase

6	2C6C	-37.9	Glutamate carboxypeptidase II	6	1FNO	-27.36	Peptidase
7	1Q5M	-37.75	Alpha hydroxysteroid dehydrogenase	7	2E9W	-27.23	Mast/stem cell growth factor receptor
8	1GOS	-37.6	Amine Oxidase [Flavin-containing] A;	8	1DHF	-26.71	Dihydrofolate Reductase
9	1DKF	-37.54	Retinoid X Receptor	9	1FT2	-26.69	Protein farnesyl transferase
10	1TOH	-37.34	Tyrosine hydroxylase	10	1HA3	-26.4	Elongation Factor Tu
11	1I7B	-37.22	Methionine decarboxylase	11	1OJN	-26.33	Hyaluronate Lyase
12	1PPL	-36.95	Penicillopepsin	12	1XIG	-26.1	D-Xylose Isomerase
13	1TSD	-36.87	Thymidylate Synthetase	13	1JKL	-25.97	Death-Associated Protein Kinase
14	1EJB	-36.73	Lumazine Synthase	14	1H82	-25.97	Polyamine oxidase
15	1NEK	-36.63	Succinate dehydrogenase	15	2FJP	-25.95	Dipeptidyl Peptidase IV (DPP4)
16	1BVY	-36.42	Unspecific Monooxygenase	16	1BGV	-25.9	Glutamate Dehydrogenase
17	1TG7	-36.41	Beta-galactosidase	17	1DXJ	-25.8	Chitinase
18	1DMW	-36.33	Phenylalanine Hydroxylase	18	1DBK	-25.74	Fab' Fragment Of Monoclonal Antibody Db3
19	1HPS	-36.29	HIV Protease	19	1NNC	-25.67	Neuraminidase subtype N9 (TERN)(NA)
20	1HVR	-35.93	Dipeptidyl Peptidase IV (DPP4)	20	1JJC	-25.62	Phenylalanyl-tRNA Synthetase
21	1K4M	-35.91	Nicotinate-nucleotide Adenylyltransferase	21	1B74	-25.58	Glutamate racemase
22	1JS3	-35.86	Aromatic-L-amino-acid Decarboxylase	22	2DDH	-25.51	Acyl CoA oxidase-2
23	1AAQ	-35.84	HIV Protease	23	1KAE	-25.37	Histidinol Dehydrogenase
24	1HS6	-35.78	Leukotriene A4 hydrolase	24	1OPM	-25.28	Peptidylglycine Alpha-Hydroxylating Monooxyg
25	1D6N	-35.76	Hypoxanthine-Guanine Phosphoribosyltransferase	25	1VJT	-25.25	Alpha glucosidase;Glucosidase alpha 1
26	1E55	-35.66	beta-Glucosidase	26	1YMJ	-25.22	Adenine nucleotide translocator
27	1I9C	-35.58	Glutamate Mutase	27	1QHG	-25.21	ATP-Dependent Helicase PcrA
28	1Z57	-35.46	CLK1 protein kinase	28	1BUQ	-25.19	Delta 5-3-ketosteroid isomerase
29	1DWD	-35.36	Serine Proteinase alpha-thrombin	29	1ENT	-25.16	Endothiapepsin
30	1POC	-35.29	Phospholipase A2	30	1K7Y	-25.07	5-methyltetrahydrofolate--homocysteine Methyltransferase
31	1BWK	-35.18	NADPH Dehydrogenase	31	1NM8	-24.94	Carnitine acyltransferase
32	1K6W	-35.13	Cytosine deaminase	32	1DIE	-24.85	D-Xylose Isomerase
33	1JR1	-35.01	Inosine-5'-monophosphate Dehydrogenase 2	33	1IIC	-24.78	Peptide N-myristoyltransferase
34	1IG0	-35	Thiamin Pyrophosphokinase	34	2C0H	-24.77	Beta-mannosidase
35	1FAX	-34.91	Coagulation Factor Xa	35	1YVB	-24.76	falcipain-2
36	1HPV	-34.84	HIV Protease	36	1ED5	-24.73	Nitric Oxide Synthase
37	1NCO	-34.75	Holo-Neocarzinostatin	37	1DID	-24.72	D-Xylose Isomerase
38	1AEG	-34.69	Peroxidase	38	1IMB	-24.72	Inositol-1(or 4)-monophosphatase
39	1Y79	-34.68	Peptidyl dipeptidase	39	1U4O	-24.53	Lactate dehydrogenase
40	1MCS	-34.64	Immunoglobulin lambda Light Chain Dimer (Mcg)	40	1IG3	-24.51	Thiamin Pyrophosphokinase

41	1DBB	-34.53	Fab' Fragment Of The Db3 Anti-Steroid Monoclonal Antibody	41	1DKF	-24.47	Retinoid X Receptor
42	1DIS	-34.53	Dihydrofolate Reductase	42	1Q0N	-24.44	HPPK
43	1X07	-34.52	Undecaprenyl diphosphate synthetase	43	1IN4	-24.35	Holliday Junction DNA Helicase Ruvb
44	1ZFJ	-34.49	Inosine-5'-monophosphate Dehydrogenase;	44	2ANH	-24.3	Alkaline phosphatase
45	1HN4	-34.48	Prophospholipase A2	45	1F2A	-24.26	n/a
46	1K3Y	-34.48	Glutathione Transferase A1-1	46	1J99	-24.09	Alcohol Sulfotransferase
47	1ZKK	-34.44	Histone lysine methyltransferase	47	1DBB	-24.02	Fab' Fragment Of The Db3 Anti-Steroid Monoclonal Antibody
48	1D2V	-34.36	Myeloperoxidase	48	1K3Y	-24.01	Glutathione Transferase A1-1
49	1R0P	-34.32	Hepatocyte Growth Factor Receptor	49	1HVB	-24.01	D-alanyl-D-alanine Carboxypeptidase
50	1PPM	-34.24	Penicillopepsin	50	1CLY	-23.99	n/a
51	2A3L	-34.22	Adenosine phosphate deaminase	51	1IGJ	-23.96	Fab (Igg2A, )
52	1HIH	-34.2	HIV Protease	52	1W50	-23.91	Beta-secretase-1
53	1A94	-34.18	Retroviral protease	53	1DGM	-23.85	Adenosine kinase

#### Compound 9

Rank	PDB_ID	Energy Score	TARGET NAME
1	1U4O	-43.78	Lactate dehydrogenase
2	1FXO	-41.56	Glucose phosphate thymidyltransferase
3	1I9C	-40.83	Glutamate Mutase
4	2FTZ	-40.81	Geranyltranstransferase
5	1TG7	-40.57	Beta-galactosidase
6	1JS3	-40.35	Aromatic-L-amino-acid Decarboxylase
7	1ED5	-38.93	Nitric Oxide Synthase
8	1EG2	-38.87	Modification Methylase Rsri
9	1FNO	-38.68	Peptidase
10	2AUH	-38.59	Insulin Receptor
11	1DGM	-38.19	Adenosine kinase
12	1QHG	-38.03	ATP-Dependent Helicase PcrA
13	2FJP	-37.95	Dipeptidyl Peptidase IV (DPP4)
14	1JJC	-37.49	Phenylalanyl-tRNA Synthetase
15	1HVK	-37.43	HIV Protease
16	1M72	-37.4	Caspase-1
17	1TPL	-37.35	Carbon carbon lyase
18	1Y79	-37.32	Peptidyl dipeptidase

#### Compound 10

Rank	PDB_ID	Energy Score	TARGET NAME
1	1TCO	-47.38	FKBP,tacrolimus binding protein,FK506 binding protein
2	1HVR	-44.99	HIV Protease
3	1OJN	-43.22	Hyaluronate Lyase
4	1DMW	-41.42	Phenylalanine Hydroxylase
5	1HA3	-40.53	Elongation Factor Tu
6	2ER6	-40.13	Endothiapepsin
7	1IFX	-39.94	NH(3)-dependent NAD(+) Synthetase
8	2G63	-39.4	Dipeptidyl Peptidase IV (DPP4)
9	2DDH	-38.92	Acyl CoA oxidase-2
10	1F2A	-38.76	n/a
11	1XIG	-38.74	D-Xylose Isomerase
12	1AL8	-38.69	Oxidase
13	1ICN	-38.61	Intestinal Fatty Acid Binding Protein
14	1HDO	-38.57	Biliverdin Ix Beta Reductase
15	1GRE	-38.49	Glutathione reductase
16	1XEB	-38.39	Acyl CoA acyltransferase
17	1BOB	-38.23	HISTONE ACETYLTRANSFERASE HAT1
18	1HDT	-38.16	Serine Proteinase alpha-thrombin

19	1FT2	-37.3	Protein farnesyl transferase	19	1GPN	-37.97	Acetylcholinesterase
20	1FGK	-37.14	Fibroblast Growth Factor Receptor 1	20	2EU9	-37.96	CLK3 protein kinase
21	1O7D	-37.12	Alpha mannosidase	21	1HVI	-37.94	HIV Protease
22	1DIE	-36.94	D-Xylose Isomerase	22	1FKN	-37.93	Memapsin 2 (Beta-Secretase)
23	1XMC	-36.74	Peroxisomal carnitine O-octanoyltransferase	23	1JNK	-37.82	Jun N terminal kinase
24	1IFX	-36.69	NH(3)-dependent NAD(+) Synthetase	24	2B4Y	-37.64	NAD-dependent deacetylase sirtuin-5
25	2G63	-36.61	Dipeptidyl Peptidase IV (DPP4)	25	1EED	-37.5	Endothiaepsin
26	1HKV	-36.56	Mycobacterium Diaminopimelate Decarboxylase	26	1DMH	-37.46	Catechol 1,2-Dioxygenase
27	1E8W	-36.52	n/a	27	1IYH	-37.44	Hematopoietic Prostaglandin D Synthase
28	1IMB	-36.47	Inositol-1(or 4)-monophosphatase	28	1VRP	-37.38	n/a
29	2ER7	-36.06	Endothiaepsin	29	1EPP	-37.35	Endothiaepsin
30	1FXO	-36.03	Glucose phosphate thymidyltransferase	30	1FNO	-37.03	Peptidase
31	1OEC	-35.84	Fibroblast Growth Factor Receptor 2	31	2G5T	-37	Dipeptidyl peptidase IV
32	2G5P	-35.73	Dipeptidyl Peptidase IV (DPP4)	32	1HPX	-36.93	HIV Protease
33	1Q3E	-35.7	Potassium/Sodium Hyperpolarization-Activated	33	1IMB	-36.9	Inositol-1(or 4)-monophosphatase
34	1PS9	-35.68	2,4-Dienoyl-Coa Reductase	34	1TMN	-36.83	Thermolysin
35	1LNA	-35.67	Thermolysin	35	1ED5	-36.76	Nitric Oxide Synthase
36	1VKG	-35.57	Histone deacetylase-8	36	1IIC	-36.75	Peptide N-myristoyltransferase
37	1GPN	-35.53	Acetylcholinesterase	37	1AE8	-36.67	Serine Proteinase alpha-thrombin
38	1QPJ	-35.25	T-cell specific kinase family	38	1CSN	-36.64	Casein kinase I
39	1HVL	-35.17	HIV Protease	39	1PS9	-36.6	2,4-Dienoyl-Coa Reductase
40	2G5T	-35.06	Dipeptidyl peptidase IV	40	7UPJ	-36.58	HIV Protease
41	1DIF	-34.97	HIV Protease	41	1DBB	-36.5	Fab' Fragment Of The Db3 Anti-Steroid Monoclonal Antibody
42	2ER6	-34.95	Endothiaepsin	42	1AEC	-36.45	Actinidin
43	1K3Y	-34.93	Glutathione Transferase A1-1	43	2ER7	-36.44	Endothiaepsin
44	1DIA	-34.88	Methylenetetrahydrofolate Reductase	44	1IGJ	-36.22	Fab (Igg2A, )
45	1DGD	-34.87	Dialkylglycine decarboxylase	45	1GP6	-36.21	n/a
46	1MUO	-34.69	Aurora-2 protein kinase	46	1DV1	-35.98	Biotin Carboxylase
47	2DDH	-34.62	Acyl CoA oxidase-2	47	1DGM	-35.92	Adenosine kinase
48	1PMT	-34.52	Glutathione transferase	48	1J4R	-35.86	Fk506-binding Protein 1a
49	1PS9	-34.36	2,4-Dienoyl-Coa Reductase	49	9HVP	-35.85	HIV Protease
50	1YVB	-34.34	falcipain-2	50	1PPK	-35.85	Penicillopepsin
51	1W08	-34.31	Lysozyme	51	1JKL	-35.81	Death-Associated Protein Kinase
52	1E7W	-34.23	Flavo-hemoglobin	52	1HVJ	-35.79	HIV Protease
53	1K7Y	-34.22	5-methyltetrahydrofolate--homocysteine M	53	1PTG	-35.76	1-phosphatidylinositol-4,5-bisphosphate Pbl



Compound 11				Compound 12			
Rank	PDB_ID	Energy Scor	TARGET NAME	Rank	PDB_ID	Energy Scor	TARGET NAME
1	1FNO	-46.39	Peptidase	1	1DID	-41.35	D-Xylose Isomerase
2	1ZSX	-41.17	Voltage gated potassium channel	2	1Y79	-39.86	Peptidyl dipeptidase
3	2FTZ	-40.69	Geranyltranstransferase	3	1XIE	-39.71	D-Xylose Isomerase
4	2AHE	-40.16	Chloride channel	4	1OJN	-37.77	Hyaluronate Lyase
5	1Y79	-39.92	Peptidyl dipeptidase	5	1D2T	-37.76	Acid phosphatase
6	1JKL	-39.89	Death-Associated Protein Kinase	6	1LGR	-36.95	Glutamine Synthetase
7	1OEC	-39.85	Fibroblast Growth Factor Receptor 2	7	2FJP	-36.87	Dipeptidyl Peptidase IV (DPP4)
8	1NNB	-39.2	Neuramidase	8	1PIG	-36.37	alpha-Amylase
9	1O6L	-38.97	Activated Akt/Protein Kinase B	9	1Q0N	-36.09	HPPK
10	1DXJ	-38.96	Chitinase	10	2G5T	-35.81	Dipeptidyl peptidase IV
11	1JQH	-38.76	Insulin-like Growth Factor I Receptor	11	1GL3	-35	Aspartate-semialdehyde Dehydrogenase
12	2G63	-38.55	Dipeptidyl Peptidase IV (DPP4)	12	1H82	-34.84	Polyamine oxidase
13	1WOH	-38.33	Agmatinase	13	1IIC	-34.76	Peptide N-myristoyltransferase
14	1H8P	-38.32	Seminal Plasma Protein Pdc-109	14	1FT2	-34.64	Protein farnesyl transferase
15	1XIE	-38.11	D-Xylose Isomerase	15	1K3Y	-34.49	Glutathione Transferase A1-1
16	2EU9	-38.02	CLK3 protein kinase	16	1P42	-34.45	N-acetylglucosamine deacetylase
17	2C6C	-37.26	Glutamate carboxypeptidase II	17	2G63	-34.33	Dipeptidyl Peptidase IV (DPP4)
18	1CRK	-37.16	Basic-type creatine kinase	18	1BMT	-34.28	5-methyltetrahydrofolate--homocysteine Methyltransferase
19	1YVB	-36.88	falcipain-2	19	2G5P	-34.21	Dipeptidyl Peptidase IV (DPP4)
20	1FGK	-36.66	Fibroblast Growth Factor Receptor 1	20	1FNO	-34.12	Peptidase
21	1HM6	-36.55	Annexin A10	21	1JJC	-33.81	Phenylalanyl-tRNA Synthetase
22	1TC1	-36.49	Hypoxanthine phosphoribosyltransferase	22	1ES7	-33.64	BONE MORPHOGENETIC PROTEIN-2(bmp2)
23	1K3Y	-36.21	Glutathione Transferase A1-1	23	1FXO	-33.57	Glucose phosphate thymidyltransferase
24	1HVJ	-36.13	HIV Protease	24	1KAE	-33.47	Histidinol Dehydrogenase
25	1VKG	-36.01	Histone deacetylase-8	25	1DXJ	-33.37	Chitinase
26	1YVJ	-35.91	Jak3 tyrosine kinase	26	2AUH	-33.36	Insulin Receptor
27	2ANH	-35.84	Alkaline phosphatase	27	2BH9	-33.36	Glucose-6-phosphate dehydrogenase
28	1R82	-35.77	Glycosyltransferase	28	1X50	-33.12	Galectin-4
29	1U4O	-35.69	Lactate dehydrogenase	29	1NSD	-33.06	Neuramidase
30	1OXO	-35.62	Aspartate Aminotransferase, Cytoplasmic	30	1TYP	-32.84	Trypanothione Reductase
31	1PJK	-35.15	Casein Kinase II, Alpha Chain	31	1TC1	-32.73	Hypoxanthine phosphoribosyltransferase
32	1IA9	-35.08	Transient Receptor Potential-Related Protein;	32	1F2A	-32.58	n/a
33	1DI8	-35.07	Cyclin-Dependent Kinase 2 (Cdk2)	33	1MCB	-32.56	Immunoglobulin lambda Light Chain Dimer

34	1NN6	-34.97	Chymase	34	1APT	-32.06	Penicillopepsin
35	1ES7	-34.87	BONE MORPHOGENETIC PROTEIN-2(bmp2)	35	2CBI	-32.01	Hyaluronidase
36	1R12	-34.74	NAD+ nucleosidase *download file*	36	1NDF	-31.96	Carnitine Acetyltransferase
37	1INF	-34.74	Influenza Virus B/Lee/40 Neuraminidase - Influenzavirus B Influenza B virus	37	1G1T	-31.8	E-selectin
38	1CKN	-34.68	RNA Triphosphatase	38	1ITU	-31.8	Dipeptidase
39	1K3Y	-34.66	Glutathione Transferase A1-1	39	1TPL	-31.77	Carbon carbon lyase
40	1HVR	-34.58	HIV Protease	40	1YVB	-31.77	falcipain-2
41	1W08	-34.53	Lysozyme	41	1JWH	-31.71	Casein Kinase II, Alpha Chain
42	2G5T	-34.52	Dipeptidyl peptidase IV	42	1L1E	-31.68	Mycolic Acid Synthase
43	1EKV	-34.47	Branched Chain Amino Acid-dependent Aminotransferase	43	1QD6	-31.56	Phospholipase A1
44	1TG7	-34.43	Beta-galactosidase	44	1HKV	-31.43	Mycobacterium Diaminopimelate Decarboxylase
45	1PTG	-34.24	1-phosphatidylinositol-4,5-bisphosphate Phosphodiesterase beta 1	45	1CRK	-31.36	Basic-type creatine kinase
46	1Y TZ	-34.05	Troponin T	46	1DGM	-31.29	Adenosine kinase
47	1KAE	-34.03	Histidinol Dehydrogenase	47	2CPP	-31.25	Cytochrome P450 Reductase
48	1BHS	-33.93	17-beta Hydroxysteroid-Dehydrogenase Type 1;	48	2AGT	-31.19	Aldehyde Reductase
49	1LCP	-33.88	Adipocyte-derived Leucine Aminopeptidase	49	9ICD	-31.17	Isocitrate dehydrogenase
50	1PBN	-33.73	Purine Nucleoside Phosphorylase	50	1IVD	-31.16	Influenza A Subtype N2 Neuraminidase
51	1Z93	-33.32	Carbonic anhydrase-III	51	1EED	-30.75	Endothiaepsin
52	1Y0S	-33.26	Peroxisome Proliferator Activated Receptor delta(PPAR delta)	52	1D2V	-30.7	Myeloperoxidase
53	1JS6	-33.18	Dopa decarboxylase	53	1E3V	-30.61	Steroid Delta-Isomerase

#### Compound 13

Rank	PDB_ID	Energy Score	TARGET NAME
1	1A94	-58.76	Retroviral protease
2	1TPL	-44.45	Carbon carbon lyase
3	1YTV	-41.95	Vasopressin V1a receptor
4	1YVB	-41.86	falcipain-2
5	1HVR	-40.95	HIV Protease
6	2CWC	-40.46	ADP ribosylglycohydrolase
7	1VKG	-38.85	Histone deacetylase-8
8	1PPL	-38.74	Penicillopepsin
9	1K3Y	-38.08	Glutathione Transferase A1-1
10	1FT2	-38.02	Protein farnesyl transferase

#### Compound 14

Rank	PDB_ID	Energy Score	TARGET NAME
1	1XIE	-45.27	D-Xylose Isomerase
2	1O6L	-41.37	Activated Akt/Protein Kinase B
3	2G5T	-39.31	Dipeptidyl peptidase IV
4	2G63	-38.39	Dipeptidyl Peptidase IV (DPP4)
5	2C0H	-38.1	Beta-mannosidase
6	1QD6	-37.93	Phospholipase A1
7	1FT2	-37.84	Protein farnesyl transferase
8	1JJC	-37.63	Phenylalanyl-tRNA Synthetase
9	1VKG	-37.24	Histone deacetylase-8
10	1YVB	-37.14	falcipain-2

11	2FJP	-38.01	Dipeptidyl Peptidase IV (DPP4)	11	1PPI	-36.16	alpha-Amylase
12	1XKK	-37.29	Epidermal Growth Factor Receptor(EGFR)	12	2G5P	-34.52	Dipeptidyl Peptidase IV (DPP4)
13	1DXJ	-37.23	Chitinase	13	1K7Y	-34.39	5-methyltetrahydrofolate--homocysteine
14	2G5T	-36.99	Dipeptidyl peptidase IV	14	1CGH	-33.88	Cathepsin G
15	1R82	-36.95	Glycosyltransferase	15	1ED5	-33.8	Nitric Oxide Synthase
16	1HOS	-36.95	HIV Protease	16	1HVR	-33.77	HIV Protease
17	1B8P	-36.94	malate dehydrogenase	17	1ME8	-33.74	Inosine Monophosphate Dehydrogenase
18	1FNO	-36.82	Peptidase	18	1IGJ	-33.25	Fab (Igg2A, )
19	1JJC	-36.54	Phenylalanyl-tRNA Synthetase	19	1YMJ	-33.22	Adenine nucleotide translocator
20	1R31	-36.5	HMG CoA reductase	20	1K3Y	-33.06	Glutathione Transferase A1-1
21	1VRP	-36.4	n/a	21	1UEA	-32.84	Metalloprotease 3
22	1ES7	-36.31	BONE MORPHOGENETIC PROTEIN-2(bmp2)	22	2FOJ	-32.8	Ubiquitin thiolesterase-7
23	1AM5	-36.04	Pepsin	23	1QM4	-32.68	Methionine adenosyltransferase
24	1FXO	-35.98	Glucose phosphate thymidyltransferase	24	1OXO	-32.67	Aspartate Aminotransferase, Cytoplasmic
25	2BH9	-35.95	Glucose-6-phosphate dehydrogenase	25	1WNY	-32.65	Isoleucyl tRNA synthetase
26	1O6L	-35.77	Activated Akt/Protein Kinase B	26	1TNH	-32.58	Trypsin
27	1DWD	-35.66	Serine Proteinase alpha-thrombin	27	1ISS	-32.55	Metabotropic Glutamate Receptor 1;
28	1F2Q	-35.58	Immunoglobulin E	28	1TDB	-32.5	Thymidylate Synthetase
29	1CSN	-35.54	Casein kinase I	29	1CI0	-32.44	Pnp Oxidase
30	1DWB	-35.53	Serine Proteinase alpha-thrombin	30	1B5L	-32.37	Tau protein
31	1JNW	-35.51	Pyridoxal Phosphate Biosynthetic Protein Pdxj;	31	1FNO	-32.31	Peptidase
32	1F2A	-35.45	n/a	32	1CYN	-32.28	Cyclophilin Receptor
33	1INF	-35.38	Influenza Virus B/Lee/40 Neuraminidase - Influenzavirus B Influenza B virus	33	1OS0	-32.26	Thermolysin
34	1GPM	-35.31	GMP synthetase	34	1B09	-32.2	C-reactive protein
35	1HDT	-35.3	Serine Proteinase alpha-thrombin	35	1G0Y	-32.17	Type I IL-1 receptor
36	1HP7	-35.15	Alpha 1 antitrypsin	36	1R53	-32.11	Chorismate synthase
37	2G5P	-35	Dipeptidyl Peptidase IV (DPP4)	37	1LBV	-32.11	Inositol 1 phosphatase
38	1TG7	-34.81	Beta-galactosidase	38	2ANY	-32.08	Kallikrein
39	1IVD	-34.79	Influenza A Subtype N2 Neuraminidase	39	1GPM	-32.07	GMP synthetase
40	1GL3	-34.69	Aspartate-semialdehyde Dehydrogenase	40	2FJP	-31.98	Dipeptidyl Peptidase IV (DPP4)
41	1UDH	-34.64	Glycosylase	41	2B3K	-31.89	Methionine aminopeptidase
42	1PTY	-34.51	Protein Tyrosine Phosphatase 1b	42	1XBA	-31.88	Syk tyrosine kinase
43	1DV1	-34.47	Biotin Carboxylase;	43	2ANH	-31.84	Alkaline phosphatase
44	2G63	-34.42	Dipeptidyl Peptidase IV (DPP4)	44	1OEC	-31.81	Fibroblast Growth Factor Receptor 2

45	1ELA	-34.32	Elastase 1	45	1JWH	-31.69	Casein Kinase II, Alpha Chain
46	8CAT	-34.22	Catalase	46	1HKV	-31.68	Mycobacterium Diaminopimelate Decarboxylase
47	1QPJ	-34.14	T-cell specific kinase family	47	1HKV	-31.63	Mycobacterium Diaminopimelate Decarboxylase
48	1D2V	-34.04	Myeloperoxidase	48	1J02	-31.6	Oxygenase
49	1TNG	-33.98	Trypsin	49	1BGV	-31.56	Glutamate Dehydrogenase
50	1JAP	-33.93	Metalloprotease 8	50	1LCL	-31.52	Lysophospholipase
51	1G0Y	-33.88	Type I IL-1 receptor	51	1NSD	-31.48	Neuramidase
52	1EPP	-33.82	Endothiapepsin	52	1E4X	-31.47	Anti-Tgf alpha Antibody Fab-Fragment
53	1HPX	-33.72	HIV Protease	53	1INF	-31.46	Influenza Virus B/Lee/40 Neuraminidase - Influenzavirus B Influenza B virus

#### Compound 15

Rank	PDB_ID	Energy Score	TARGET NAME
1	1OOQ	-37.82	Dihydropteridine Reductase
2	6TMN	-35.92	Thermolysin
3	1K3Y	-35.39	Glutathione Transferase A1-1
4	1PS9	-35.31	2,4-Dienoyl-Coa Reductase
5	1HVI	-35	HIV Protease
6	1FT2	-34.98	Protein farnesyl transferase
7	2ANY	-34.92	Kallikrein
8	1I9C	-34.73	Glutamate Mutase
9	1BGV	-34.46	Glutamate Dehydrogenase
10	1R12	-34.42	NAD
11	1OJN	-34.4	Hyaluronate Lyase
12	1IGJ	-34.2	Fab (Igg2A, )
13	1KAE	-34.14	Histidinol Dehydrogenase
14	1JNK	-34.13	Jun N terminal kinase
15	1PS9	-33.99	2,4-Dienoyl-Coa Reductase
16	1Y79	-33.9	Peptidyl dipeptidase
17	1WDA	-33.89	Protein arginine deiminase IV
18	1JJC	-33.76	Phenylalanyl-tRNA Synthetase
19	2CWC	-33.66	ADP ribosylglycohydrolase
20	1JKL	-33.56	Death-Associated Protein Kinase
21	2G63	-33.55	Dipeptidyl Peptidase IV (DPP4)
22	2ETR	-33.46	Rho-associated protein kinase 1; ROCK I
23	1YVB	-33.34	falcipain-2
24	1DIH	-32.97	Microbial Dihydrofolate Reductase

#### Compound 16

Rank	PDB_ID	Energy Score	TARGET NAME
1	1I9C	-41.17	Glutamate Mutase
2	1K3Y	-39.58	Glutathione Transferase A1-1
3	1OOQ	-39.24	Dihydropteridine Reductase
4	1YVB	-38.15	falcipain-2
5	1PS9	-37.83	2,4-Dienoyl-Coa Reductase
6	1ED5	-37.58	Nitric Oxide Synthase
7	1OJN	-36.93	Hyaluronate Lyase
8	1FNO	-36.73	Peptidase
9	1VRP	-36.54	n/a
10	1HDT	-36.48	Serine Proteinase alpha-thrombin
11	1CRK	-36.36	Basic-type creatine kinase
12	1JWH	-36.16	Casein Kinase II, Alpha Chain
13	1W50	-36.09	Beta-secretase-1
14	1BGV	-36.04	Glutamate Dehydrogenase
15	1GL3	-35.77	Aspartate-semialdehyde Dehydrogenase
16	1K3Y	-35.31	Glutathione Transferase A1-1
17	1XIE	-35.08	D-Xylose Isomerase
18	1Y79	-34.99	Peptidyl dipeptidase
19	1PPL	-34.91	Penicillopepsin
20	1TYP	-34.7	Trypanothione Reductase
21	1YTV	-34.65	Vasopressin V1a receptor
22	1JTV	-34.59	Hydroxysteroid-Dehydrogenase Type 1
23	1F2A	-34.43	n/a
24	1JKL	-34.32	Death-Associated Protein Kinase

25	1O7D	-32.92	Alpha mannosidase	25	1C10	-34.32	Pnp Oxidase
26	1LNA	-32.89	Thermolysin	26	2ANY	-34.3	Kallikrein
27	1CRK	-32.83	Basic-type creatine kinase	27	2G63	-34.17	Dipeptidyl Peptidase IV (DPP4)
28	1NM8	-32.66	Carnitine acyltransferase	28	1K7Y	-33.92	5-methyltetrahydrofolate--homocysteine Methyltransferase;
29	2G5T	-32.31	Dipeptidyl peptidase IV	29	1AM5	-33.89	Pepsin
30	1HKV	-32.26	Mycobacterium Diaminopimelate Decarboxylase	30	1CTR	-33.75	Calmodulin
31	1W50	-32.25	Beta-secretase-1	31	1NN6	-33.58	Chymase
32	2ANH	-32.23	Alkaline phosphatase	32	1IIC	-33.41	Peptide N-myristoyltransferase
33	1DXJ	-32.09	Chitinase	33	1O6L	-33.4	Activated Akt/Protein Kinase B
34	1ED5	-31.85	Nitric Oxide Synthase	34	1BMT	-33.39	5-methyltetrahydrofolate--homocysteine Methyltransferase
35	1CTR	-31.78	Calmodulin	35	2AUH	-33.37	Insulin Receptor
36	1PPL	-31.7	Penicillopepsin	36	1C4K	-33.25	Ornithine Decarboxylase
37	1F57	-31.63	Cysteine carboxypeptidase	37	1JJC	-33.22	Phenylalanyl-tRNA Synthetase
38	1JWH	-31.55	Casein Kinase II, Alpha Chain	38	1KAE	-33.12	Histidinol Dehydrogenase
39	1JWH	-31.36	Casein Kinase II, Alpha Chain	39	1XEY	-33.11	Glutamate decarboxylase
40	1TMN	-31.33	Thermolysin	40	1XKK	-33.02	Epidermal Growth Factor Receptor(EGFR)
41	1PPM	-31.2	Penicillopepsin	41	2BH9	-32.96	Glucose-6-phosphate dehydrogenase
42	1AEC	-31.19	Actinidin	42	1AEC	-32.95	Actinidin
43	1HDT	-31.05	Serine Proteinase alpha-thrombin	43	1INF	-32.91	Influenza Virus B/Lee/40 Neuraminidase - Influenzavirus B Influenza B virus
44	1ENT	-31.02	Endothiapepsin	44	1ICR	-32.85	Nitroreductase
45	1HDT	-31.02	Serine Proteinase alpha-thrombin	45	1ADF	-32.75	Alcohol Dehydrogenase
46	1H82	-30.99	Polyamine oxidase	46	1EVZ	-32.53	Glycerol-3-phosphate dehydrogenase
47	1FNO	-30.97	Peptidase	47	1TC1	-32.47	Hypoxanthine phosphoribosyltransferase
48	2G5P	-30.74	Dipeptidyl Peptidase IV (DPP4)	48	1D2V	-32.41	Myeloperoxidase
49	2BH9	-30.7	Glucose-6-phosphate dehydrogenase	49	2B7A	-32.32	Jak2 tyrosine kinase
50	1INF	-30.65	Influenza Virus B/Lee/40 Neuraminidase - Influenzavirus B Influenza B virus	50	1VJT	-32.31	Alpha glucosidase
51	1ZVU	-30.64	Topoisomerase IV	51	1E7W	-32.2	Flavoheмоglobin
52	1K7Y	-30.61	5-methyltetrahydrofolate--homocysteine Methyltransferase;	52	1CKN	-32.08	RNA Triphosphatase
53	2FJP	-30.58	Dipeptidyl Peptidase IV (DPP4)	53	2EU9	-32.06	CLK3 protein kinase

Compound 17

Rank PDB\_ID Energy Scor TARGET NAME

Compound 18

Rank PDB\_ID Energy Scor TARGET NAME

1	1TYP	-42.44	Trypanothione Reductase	1	1GOX	-33.4	Spinach glycolate oxidase
2	2AUH	-39.42	Insulin Receptor	2	1YTV	-32.54	Vasopressin V1a receptor
3	1Y79	-38.92	Peptidyl dipeptidase	3	1DIE	-32.53	D-Xylose Isomerase
4	1D2V	-38.75	Myeloperoxidase	4	1Q5M	-32.37	Alpha hydroxysteroid dehydrogenase
5	1DTL	-38.36	Cardiac Troponin C (ctnc);	5	1HKV	-32.07	Mycobacterium Diaminopimelate Decarboxylase
6	1JR1	-38.22	Inosine-5'-monophosphate Dehydrogenase 2;	6	1J96	-31.31	Aldo-Keto Reductase Family 1 Member C3
7	2EU9	-37.7	CLK3 protein kinase	7	1JR1	-30.27	Inosine-5'-monophosphate Dehydrogenase 2
8	1FNO	-37.33	Peptidase	8	1K6W	-30.08	Cytosine deaminase
9	2FW3	-36.54	Carnitine O-palmitoyltransferase II, mitochondrial	9	2FTZ	-29.88	Geranyltranstransferase
10	1XID	-36.29	D-Xylose Isomerase	10	1XIE	-29.81	D-Xylose Isomerase
11	1IVD	-36.26	Influenza A Subtype N2 Neuraminidase	11	1PVG	-29.71	DNA Topoisomerase II
12	2C6C	-36.02	Glutamate carboxypeptidase II	12	1ZFJ	-29.66	Inosine-5'-monophosphate Dehydrogenase
13	1VRP	-35.7	n/a	13	2C6Q	-29.47	GMP reductase
14	1DIF	-34.74	HIV Protease	14	1DID	-29.1	D-Xylose Isomerase
15	1FT2	-34.53	Protein farnesyl transferase	15	1POC	-28.6	Phospholipase A2
16	1CTR	-34.37	Calmodulin	16	1NEK	-28.58	Succinate dehydrogenase
17	1DXJ	-34.26	Chitinase	17	1HTG	-28.57	HIV Protease
18	1O6L	-34.19	Activated Akt/Protein Kinase B	18	1OYA	-28.51	NADPH Dehydrogenase
19	1AH2	-34.06	Serine protease	19	1P42	-28.48	N-acetylglucosamine deacetylase
20	1PJK	-34.05	Casein Kinase II, Alpha Chain	20	1IG3	-28.47	Thiamin Pyrophosphokinase
21	1HA3	-34.02	Elongation Factor Tu	21	2C6C	-28.45	Glutamate carboxypeptidase II
22	1MCR	-33.84	Immunoglobulin lambda Light Chain Dimer (Mcg)	22	1BBP	-28.43	bilin binding protein (BBP)
23	1LGR	-33.79	Glutamine Synthetase	23	1HS6	-28.41	Leukotriene A4 hydrolase
24	1TCO	-33.74	FKBP,tacrolimus binding protein,FK506 binding	24	1DMW	-28.34	Phenylalanine Hydroxylase
25	1E3V	-33.69	Steroid Delta-Isomerase	25	1HKV	-28.27	Mycobacterium Diaminopimelate Decarboxylase
26	1JTV	-33.09	Hydroxysteroid-Dehydrogenase Type 1	26	1U0F	-28.27	Glucose-6-phosphate Isomerase
27	1HKV	-33.07	Mycobacterium Diaminopimelate Decarboxylase	27	1ICR	-28.27	Nitroreductase
28	1HVR	-32.92	HIV Protease	28	1E6U	-28.22	GDP fucose synthetase
29	1ENT	-32.76	Endothiapepsin	29	1D2V	-28.21	Myeloperoxidase
30	1OXO	-32.75	Aspartate Aminotransferase, Cytoplasmic	30	1TUI	-28.15	Elongation Factor 1-alpha
31	1C9C	-32.72	Aspartate Aminotransferase, Cytoplasmic	31	1Y79	-27.99	Peptidyl dipeptidase
32	1IMB	-32.71	Inositol-1(or 4)-monophosphatase	32	1AJX	-27.98	HIV Protease
33	1DMW	-32.7	Phenylalanine Hydroxylase	33	2DBL	-27.96	UNDEFINED
34	1PPL	-32.54	Penicillopepsin	34	1EFR	-27.89	Bovine Mitochondrial F1-ATPase
35	1LCP	-32.51	Adipocyte-derived Leucine Aminopeptidase	35	1H7X	-27.86	Dihydropyrimidine dehydrogenase
36	1QPJ	-32.49	T-cell specific kinase family	36	2FW3	-27.81	Carnitine O-palmitoyltransferase II, mitochondrial

37	2G63	-32.38	Dipeptidyl Peptidase IV (DPP4)	37	1JCN	-27.81	IMP-1 dehydrogenase
38	2G5T	-32.35	Dipeptidyl peptidase IV	38	1ILH	-27.72	Pregnane X receptor
39	1CRK	-32.26	Basic-type creatine kinase	39	1IDA	-27.69	HIV-2 Protease
40	1W08	-32.2	Lysozyme	40	1PG5	-27.56	Aspartate Carbamoyltransferase
41	1PG5	-32.18	Aspartate Carbamoyltransferase	41	1CY1	-27.54	DNA Topoisomerase
42	1DGM	-32.15	Adenosine kinase	42	1CEV	-27.51	Arginase
43	1DGD	-32.15	Dialkylglycine decarboxylase	43	1DBK	-27.49	Fab' Fragment Of Monoclonal Antibody Db3
44	1MMQ	-31.99	Matrilysin	44	1CVI	-27.4	Prostatic acid phosphatase
45	1BMT	-31.87	5-methyltetrahydrofolate--homocysteine Methyltransferase	45	1XEB	-27.39	Acyl CoA acyltransferase
46	1HVI	-31.85	HIV Protease	46	1HTF	-27.35	HIV Protease
47	1JWH	-31.85	Casein Kinase II, Alpha Chain	47	1OHY	-27.32	4-AMINO BUTYRATE AMINOTRANSFERASE
48	1JJC	-31.82	Phenylalanyl-tRNA Synthetase	48	1NSC	-27.28	Neuramidase
49	1DIA	-31.78	Methylenetetrahydrofolate Reductase	49	1GL3	-27.23	Aspartate-semialdehyde Dehydrogenase
50	1JS3	-31.78	Aromatic-L-amino-acid Decarboxylase	50	1HDO	-27.16	Biliverdin Ix Beta Reductase
51	1DMH	-31.77	Catechol 1,2-Dioxygenase	51	1ZKK	-27.09	Histone lysine methyltransferase
52	1R12	-31.77	NAD+ nucleosidase *download file*	52	1DBM	-27.08	Fab' Fragment Of Monoclonal Antibody Db3
53	1TX4	-31.67	Transforming protein RhoA	53	1FEN	-27.03	Retinol Binding Protein

**Compound 19**

Rank	PDB_ID	Energy Score	TARGET NAME
1	1FT2	-38.82	Protein farnesyl transferase
2	1K7Y	-38.37	5-methyltetrahydrofolate--homocysteine Methyltransferase;
3	1DID	-37.56	D-Xylose Isomerase
4	1IVE	-35.81	Neuraminidase
5	1DXJ	-35.07	Chitinase
6	1OJN	-34.82	Hyaluronate Lyase
7	2BH9	-34.78	Glucose-6-phosphate dehydrogenase
8	1PPL	-34.65	Penicillopepsin
9	1IFX	-34.4	NH(3)-dependent NAD(+) Synthetase
10	1TC1	-34.16	Hypoxanthine phosphoribosyltransferase
11	1CRK	-34.12	Basic-type creatine kinase
12	1YVB	-34.07	falcipain-2
13	1JWH	-33.74	Casein Kinase II, Alpha Chain
14	1AEC	-33.67	Actinidin
15	1GRE	-33.55	Glutathione reductase

16	1I6V	-33.28	DNA-directed RNA Polymerase II 19 KDa
17	1CY1	-33.24	DNA Topoisomerase
18	2G5T	-33.19	Dipeptidyl peptidase IV
19	1PPH	-32.93	Trypsin
20	2EU9	-32.91	CLK3 protein kinase
21	1DIE	-32.76	D-Xylose Isomerase
22	1APU	-32.74	Penicillopepsin
23	1JJC	-32.71	Phenylalanyl-tRNA Synthetase
24	1CKN	-32.55	RNA Triphosphatase
25	1AM5	-32.35	Pepsin
26	1JTV	-32.33	Hydroxysteroid-Dehydrogenase Type 1
27	1DIF	-32.27	HIV Protease
28	1YTV	-32.1	Vasopressin V1a receptor
29	1IG3	-32.07	Thiamin Pyrophosphokinase
30	1BMT	-32.03	5-methyltetrahydrofolate--homocysteine Methyltransferase
31	1PJK	-31.9	Casein Kinase II, Alpha Chain
32	1NSD	-31.73	Neuramidase
33	1J99	-31.61	Alcohol Sulfotransferase
34	1HVI	-31.51	HIV Protease
35	2AEE	-31.5	Orotate phosphoribosyltransferase
36	1WEI	-31.37	A-G adenine DNA glycosylase
37	1H82	-31.29	Polyamine oxidase
38	2C6C	-31.19	Glutamate carboxypeptidase II
39	1WOH	-31.11	Agmatinase
40	1M4H	-30.88	Memapsin 2
41	1R31	-30.74	HMG CoA reductase
42	1JKL	-30.63	Death-Associated Protein Kinase
43	2CBI	-30.61	Hyaluronidase
44	1W08	-30.6	Lysozyme
45	1AL8	-30.59	Oxidase
46	1JBQ	-30.53	Cystathionine beta-synthase
47	1TYP	-30.51	Trypanothione Reductase
48	1PS9	-30.45	2,4-Dienoyl-Coa Reductase
49	1E7W	-30.44	Flavo-hemoglobin
50	1PFX	-30.37	Coagulation Factor IX



51	1TG7	-30.26	Beta-galactosidase
52	1CYN	-30.22	Cyclophilin Receptor
53	1FGK	-30.2	Fibroblast Growth Factor Receptor 1