

Table S2c Hesperidine docking to nonspecific human blood proteins

PDB ID	Targets	Classification	Energy (kcal/mol)	Dissoc. constant [nM]	Contacting receptor residues
5FFG	Integrin alpha V Beta 6 head	Cell adhesion	-10.89	10.4293486	Phe ²¹ , Val ²³ , Ala ⁹⁶ , Arg ⁹⁹ , Lys ¹⁰¹ , Phe ¹⁵⁹ , Ser ¹⁶⁰ , Asp ¹⁶² , Phe ¹⁶³ , Thr ¹⁶⁴ , Lys ¹⁶⁵ , Tyr ²²⁴ , Ser ²²⁵ , Val ²²⁶ , Ala ²²⁷ , Val ²²⁸ , Asp ²²⁹ , Phe ²⁷⁸ , Ser ²⁷⁹ , Val ²⁸⁰ , Ala ²⁸¹ , Ala ²⁸² , Ala ²⁸³ , Ile ³⁴⁴ , Ala ³⁴⁵ , Pro ³⁴⁶ , Tyr ⁴⁰⁷ , Ser ⁴⁰⁸ , Met ⁴⁰⁹ , Lys ⁴¹⁰
4GWN	Human mature MEPRIN Beta	Hydrolase	-10.58	17.6884277	Cys ¹²⁴ , Trp ¹²⁵ , Ser ¹²⁶ , Thr ¹⁴⁹ , His ¹⁵⁰ , Glu ¹⁵⁵ , His ¹⁵⁶ , His ¹⁶² , Arg ¹⁸⁴ , His ¹⁸⁶ , Asn ¹⁸⁷ , Val ²⁰⁸ , Met ²⁰⁹ , His ²¹⁰ , Tyr ²¹¹ , Ser ²¹² , Ala ²¹⁵ , Phe ²¹⁶ , Gly ²³⁶ , Gln ²³⁷ , Arg ²³⁸
3I7H	Ddb1 (damage specific DNA binding protein 1)	Protein binding	-10.27	29.4979043	Trp ¹¹¹ , Pro ⁴¹² , Tyr ⁴²² , Ser ⁵⁰² , Cys ⁵⁰³ , Asn ⁵⁰⁴ , Cys ⁵⁴⁰ , Leu ⁵⁴¹ , Asp ⁵⁴² , Ile ⁵⁴³ , Thr ⁵⁴⁴ , Pro ⁵⁴⁵ , Leu ⁵⁴⁶ , Arg ⁵⁸⁹ , Ser ⁵⁹⁰ , Ile ⁵⁹¹ , Leu ⁵⁹² , Met ⁵⁹³ , Thr ⁵⁹⁴ , Thr ⁵⁹⁵ , Val ⁶³⁷ , Arg ⁶³⁹ , Thr ⁶⁴⁰ , Arg ⁶⁴² , Cys ⁶⁸⁰ , Pro ⁶⁸¹
4UV8	LSD1(KDM1A)-CoRest	Transcription	-10.1	39.3009297	Gly ³³⁰ , Ala ³³¹ , Val ³³³ , Thr ³³⁵ , Phe ⁵³⁸ , Ala ⁵³⁹ , Asn ⁵⁴⁰ , Trp ⁵⁵² , Asp ⁵⁵³ , Gln ⁵⁵⁴ , Asp ⁵⁵⁵ , Asp ⁵⁵⁶ , Glu ⁵⁵⁹ , His ⁵⁶⁴ , Leu ⁵⁵⁹ , Lys ⁵⁶¹ , Ser ⁷⁶⁰ , Tyr ⁷⁶¹ , Ser ⁷⁶² , Tyr ⁷⁶³ , Val ⁷⁶⁴ , Tyr ⁷⁷³ , Tyr ⁸⁰⁷ , Pro ⁸⁰⁸ , Ala ⁸⁰⁹ , Thr ⁸¹⁰ , His ⁸¹²
2CF9	Recombinant human thrombin	Hydrolase/hydrolase inhibitor	-9.94	51.8341992	Arg ³⁵ , Glu ³⁹ , Leu ⁴⁰ , Leu ⁴¹ , Cys ⁴² , His ⁵⁷ , Cys ⁵⁸ , Trp ⁶⁰ , d, Lys ⁶⁰ , Phe ⁶⁰ , h, Asp ¹⁸⁹ , Ala ¹⁹⁰ , Cys ¹⁹¹ , Glu ¹⁹² , Ser ¹⁹⁵ , Val ²¹³ , Ser ²¹⁴ , Trp ²¹⁵ , Gly ²¹⁵ , Gly ²¹⁹ , Cys ²²⁰ , Gly ²²⁶ , Phe ²²⁷ , Tyr ²²⁸
2FM5	PDE4D2	Hydrolase	-9.88	57.0686953	Tyr ¹⁵⁹ , His ¹⁶⁰ , His ¹⁶⁴ , His ²⁰⁴ , Ser ²⁰⁸ , Asn ²⁰⁹ , Gln ²¹⁰ , Leu ²²⁹ , Gly ²³⁰ , Thr ²⁷¹ , Asp ²⁷² , Met ²⁷³ , Ser ²⁷⁴ , Asp ³¹⁸ , Leu ³¹⁹ , Asn ³²¹ , Pro ³²² , Tyr ³²⁹ , Trp ³³² , Ile ³³⁶ , Phe ³⁴⁰ , Gln ³⁴³ , Ser ³⁵⁵ , Pro ³⁵⁶ , Met ³⁵⁷ , Cys ³⁵⁸ , Gln ³⁶⁹ , Phe ³⁷²
6FFI	MGLUR5 in complex with MMPEP	Membrane protein	-9.77	68.7114375	Leu ⁶³⁵ , Gln ⁶⁴⁷ , Arg ⁶⁴⁸ , Ile ⁶⁵¹ , Gly ⁶⁵² , Met ⁸⁸⁰ , Tyr ⁸⁹⁰ , Leu ⁸⁹¹ , Ile ⁸⁹² , Cys ⁸⁹³ , Asn ⁸⁹⁴ , Thr ⁸⁹⁵ , Thr ⁸⁹⁶ , Gly ⁸⁹⁹ , Val ⁹⁰⁰ , Pro ⁹⁰³ , Leu ⁹⁰⁴ , Tyr ⁹⁵² , Asn ⁹⁵⁶ , Tyr ⁹⁵⁷ , Lys ⁹⁵⁸ , Ile ⁹⁵⁹ , Ile ⁹⁶⁰ , Met ⁹⁶²
4WB7	Camp-dependent protein kinase a (catalytic alpha subunit)	Transferase	-9.46	116.7331172	Lys ² , Asp ³ , Tyr ⁴ , Thr ⁷ , Glu ⁴² , Lys ⁴³ , Glu ⁴⁶ , Glu ⁴⁹ , Ala ⁵⁰ , Phe ³³⁶ , Asn ³⁴¹ , Asn ³⁴⁸ , His ³⁴⁹ , Lys ³⁵⁰ , Phe ³⁵² , Ala ³⁵³
5HEX	Human hexokinase 2	Transferase	-9.36	136.8034375	Asp ⁸⁴ , Leu ⁸⁵ , Gly ⁸⁶ , Asn ⁸⁹ , Phe ⁹⁰ , Arg ⁹¹ , Ile ¹¹¹ , Ser ¹⁵⁵ , Phe ¹⁵⁶ , Asp ²⁰⁹ , Ile ²²⁹ , Gly ²³¹ , Thr ²³² , Gly ²³³ , Ser ²³⁴ , Asn ²³⁵ , Glu ²⁶⁰ , Gly ²⁶² , Glu ²⁹⁴ , Asp ³¹³ , Gly ³¹⁴ , Ser ⁴¹⁵ , Ser ⁴⁴⁵ , Glu ⁴⁴⁶ , Asp ⁴⁴⁷ , Gly ⁴⁴⁸ , Ser ⁴⁴⁹
4FAD	PI3KA	Transferase	-9.35	141.261625	Trp ²⁰¹ , Leu ²⁰⁷ , Pro ²⁰⁸ , Tyr ²¹⁰ , Leu ²¹¹ , Arg ²⁷⁷ , Glu ²⁷⁹ , Gln ²⁹¹ , Trp ²⁹² , Arg ²⁹⁴ , His ²⁹⁵ , Lys ²⁹⁸ , Asn ²⁹⁹ , Asp ⁷⁸⁸ , Arg ⁸⁴⁹ , Glu ⁸⁵² , Glu ⁸⁵⁶ , Leu ⁸⁶⁵ , Pro ⁸⁶⁶ , Tyr ⁸⁶⁷ , Glu ⁸⁸⁰
4U7D	Human RECQ-like helicase	Hydrolase	-9.33	143.9087813	Phe ⁸⁷ , Lys ⁸⁸ , Leu ⁸⁹ , Arg ⁹³ , Thr ¹¹⁵ , Gly ¹¹⁶ , Gly ¹¹⁸ , Lys ¹¹⁹ , Ser ¹²⁰ , Leu ¹²¹ , Tyr ¹²³ , Cys ¹³⁸ , Leu ¹⁴³ , Asp ¹⁴⁶ , Gln ¹⁴⁷ , Val ¹⁵⁰ , Leu ¹⁵⁴ , Asp ²¹⁹ , Glu ²²⁰ , Leu ²⁵³ , Gly ³⁷⁷ , Ile ³⁷⁸ , Asp ³⁷⁹ , Arg ⁴⁰⁷
4NY0	Human focal adhesion kinase	Transferase	-9.23	171.2329219	Arg ³⁶ , Ser ⁸⁸ , Val ⁹⁵ , Arg ¹²⁵ , Ile ¹²⁶ , Arg ¹²⁷ , Leu ¹²⁹ , Phe ¹⁴⁷ , Gln ¹⁵⁰ , Asp ¹⁵⁴ , Glu ¹⁵⁸ , Tyr ²⁵¹ , Arg ²⁵² , Phe ²⁵³ , Lys ²⁵⁵ , Glu ²⁵⁶ , Cys ²⁵⁷ , Asn ³³⁹
4OJ2	Aquaporin	Transport protein	-9.18	186.9406719	His ⁵¹ , Ile ⁶² , Ser ⁶³ , Gly ⁶⁴ , His ⁶⁶ , Cys ⁷⁵ , Gly ⁷⁸ , Cys ⁷⁹ , His ⁸⁰ , Val ⁸¹ , Arg ⁸⁵ , Tyr ⁸⁹ , Ile ¹⁴⁵ , Phe ¹⁴⁶ , Thr ¹⁴⁹ , Asp ¹⁵⁰ , Glu ¹⁵¹ , Arg ¹⁵² , Tyr ²¹⁹ , Asn ²²⁰ , Tyr ²²¹ , Pro ²²⁵ , Ala ²²⁷
1OE9	Myosin V motor	ATPASE/myosin	-9.15	195.9873594	Thr ¹¹² , Arg ¹¹³ , Phe ²⁵¹ , Gln ²⁵² , Ala ²⁵³ , Gly ²⁵⁴ , Glu ²⁵⁶ , Gln ²⁹⁰ , Gly ²⁹¹ , Phe ⁴⁴⁴ , Glu ⁴⁴⁵ , Ile ⁴⁴⁶ , Ser ⁴⁴⁸ , Glu ⁴⁵⁰ , Gln ⁴⁵¹ , Glu ⁵⁶² , Gly ⁵⁶³ , Lys ⁵⁶⁷
4JXJ	Ribosomal RNA small subunit methyltransferase a from rickettsia bellii	Transferase	-9	252.4524063	Asn ²³ , Ile ⁴⁹ , Gly ⁵⁰ , Ile ⁷¹ , Glu ⁷² , Thr ⁷³ , Asp ⁷⁴ , Gln ⁹⁶ , Asp ⁹⁷ , Ala ⁹⁸ , Leu ⁹⁹ , Asn ¹¹⁶ , Leu ¹¹⁷ , Pro ¹¹⁸ , Tyr ¹¹⁹ , His ¹²⁰ , Ile ¹²¹
5CSX	The S156E mutant of human aquaporin 5	Transport protein	-8.87	314.9225625	Ser ⁶⁴ , Gly ⁶⁵ , His ⁶⁷ , Leu ⁷⁶ , Asn ⁸⁰ , Gln ⁸¹ , Ile ⁸² , Arg ⁸⁶ , Tyr ⁹⁰ , Ile ¹⁴⁶ , Phe ¹⁴⁷ , Thr ¹⁵⁰ , Asp ¹⁵¹ , Ser ¹⁵² , Arg ¹⁵³ , Phe ²²² , Asn ²²⁸ , Ile ²³⁸ , Tyr ²⁴³ , Pro ²⁴⁵
5WGS	Human GRK2	Transferase	-8.87	314.9225625	Ile ³² , Leu ³³ , Pro ³⁵ , Asn ¹⁷⁹ , Val ¹⁸⁰ , Asn ¹⁸³ , Ile ¹⁸⁴ , His ¹⁸⁵ , Leu ¹⁸⁶ , Lys ²¹⁰ , Asp ²¹² , Gly ²¹⁷ , Trp ²⁷⁶ , Glu ²⁷⁶ , Arg ⁶¹⁷ , Lys ⁶¹⁸ , Gln ⁶³³ , Cys ⁶³⁴ , Asp ⁶³⁵ , Ser ⁶³⁶ , Asp ⁶³⁷ , Leu ⁶⁴⁰
3R6I	AKR1C3	Oxidoreductase	-8.86	319.2036563	Tyr ²⁴ , Pro ²⁶ , Pro ²⁷ , Leu ⁵⁴ , Tyr ⁵⁵ , Asn ⁵⁶ , Trp ⁸⁶ , His ¹¹⁷ , Ser ¹¹⁸ , Met ¹²⁰ , Leu ¹²² , Asn ¹⁶⁷ , Tyr ²¹⁶ , Arg ²²⁶ , Trp ²²⁷ , Phe ³⁰⁶ , Phe ³¹¹ , Pro ³¹⁸
2QFZ	Human tbc1 domain family member 22a	Hydrolase activator	-8.77	374.7173438	Ser ³⁶ , Phe ³²⁹ , Cys ³⁶⁶ , Lys ³⁶⁹ , Leu ³⁷⁰ , Asp ³⁷² , Gly ³⁷³ , Ile ³⁷⁴ , Gln ³⁷⁵ , Asp ³⁷⁶ , Asn ³⁷⁷ , Gly ³⁸⁴ , Met ³⁸⁷ , Lys ³⁸⁸ , Trp ⁴³⁹ , Tyr ⁴⁴² , Gln ⁴⁴³ , Glu ⁴⁴⁵ , Pro ⁴⁴⁶ , Asp ⁴⁴⁷ , Gly ⁴⁴⁸ , Phe ⁴⁴⁹ , Ser ⁴⁵⁰
4KTV	MAT enzymes: MATA2B	Transferase	-8.74	389.5498125	Glu ²⁷ , Gln ³⁶ , Asp ⁴³ , His ⁸⁹ , Glu ¹⁴⁸ , Val ¹⁵⁵ , His ¹⁵⁸ , Lys ¹⁵⁹ , Ala ¹⁶² , Glu ¹⁶⁶ , Gln ³⁷² , Arg ³⁷³ , Ala ³⁷⁶ , Tyr ³⁷⁷ , Gly ³⁷⁸ , Phe ³⁸⁰ , Gly ³⁸¹ , Arg ³⁸²
4MWS	Human PPCA (trigonal crystal form 1)	Hydrolase	-8.71	411.8625938	Leu ⁶⁷ , Thr ⁶⁸ , Leu ⁷⁴ , Val ⁷⁵ , Gln ⁷⁶ , Asn ²⁴⁵ , Tyr ²⁴⁷ , Asn ²⁴⁸ , Ala ²⁵¹ , Pro ²⁵² , Ala ²⁵⁴ , Cys ³⁰³ , Thr ³⁰⁴ , Asn ³⁰⁵ , Ala ³⁰⁸ , Met ⁴³⁰ , Thr ⁴³³ , Asp ⁴³⁴ , Lys ⁴³⁵ , Pro ⁴³⁶ , Leu ⁴³⁷
4JKJ	The S18Y variant of ubiquitin carboxy-terminal hydrolase 11	Hydrolase	-8.7	419.5806563	Glu ⁷ , Asn ⁹ , Pro ¹⁰ , Glu ¹¹ , Asn ¹⁴ , Leu ¹⁷ , Tyr ¹⁸ , Val ²² , Ala ²³ , Gly ²⁴ , Trp ²⁶ , Arg ²⁷ , Val ²⁹ , Asp ³⁰ , Glu ¹⁰⁹
5FN3	Gamma secretase in class 1 of the apo- state ensemble	Hydrolase	-8.69	430.338875	Leu ²⁶⁰ , Lys ²⁶¹ , Pro ²⁶² , Glu ³¹⁰ , Gln ³¹³ , Lys ³¹⁴ , Ala ³¹⁵ , Pro ³¹⁶ , Val ³¹⁸ , Thr ⁵¹⁷ , Arg ⁵²⁰ , Trp ⁵³³ , Asn ⁵⁷³ , Leu ⁵⁷⁴ , Thr ⁵⁷⁵ , Gly ⁵⁷⁶ , Thr ⁵⁷⁷ , Val ⁵⁷⁸ , Tyr ⁶⁰⁰ , Arg ⁶²² , Ser ⁶²³ , Thr ⁶²⁴
6DK3	Human mitochondrial serine hydrolase 2	Transferase	-8.66	448.88575	Gly ⁹⁹ , Asp ¹¹³ , Glu ¹¹⁶ , Leu ¹¹⁷ , Gln ¹²⁰ , Arg ¹²¹ , Leu ¹²⁴ , Glu ¹²⁵ , Pro ¹³¹ , Gly ¹³⁵ , Val ¹³⁶ , Gln ¹³⁹ , Tyr ²⁹² , Lys ²⁹⁴ , Glu ³¹² , Asn ³¹⁶
5HZJ	Intersectin1 containing wildtype LOV2 domain	Signaling protein	-8.58	512.912875	Gln ¹⁴⁷⁰ , Leu ¹⁵⁸⁸ , Ser ¹⁵⁸⁹ , Glu ¹⁵⁹⁰ , Gln ¹⁵⁹¹ , Leu ¹⁵⁹² , Val ¹⁵⁹³ , Ser ¹⁵⁹⁶ , Val ¹⁵⁹⁷ , Thr ¹⁵⁹⁸ , Asn ¹⁵⁹⁹ , Arg ¹⁶⁰⁴ , Phe ¹⁶²⁹ , Thr ¹⁶⁶¹ , Pro ¹⁶⁶² , Phe ¹⁶⁶⁴ , Asn ¹⁶⁶⁶ , Glu ¹⁶⁶⁷ , His ¹⁶⁸⁷
1W6K	Human OSC	Isomerase	-8.54	552.453875	Asp ²²⁰ , Trp ²²¹ , Ser ²²⁷ , Thr ²²⁸ , Tyr ⁴³⁰ , Gln ⁴³¹ , Lys ⁴³² , Tyr ⁴³⁴ , Arg ⁴³⁵ , Gln ⁴³⁶ , Met ⁴³⁷ , Asn ⁴⁹² , Met ⁴⁹³ , Arg ⁴⁹⁴ , Asn ⁴⁹⁵ , Pro ⁴⁹⁶ , Thr ⁵⁰⁵ , Lys ⁵⁰⁶ , Arg ⁵⁰⁷
4ZWJ	Rhodopsin bound to arrestin	Signaling protein	-8.47	614.4345625	Lys ⁵⁶ , Lys ⁶⁷ , Arg ⁶⁹ , Thr ⁷⁰ , Pro ⁷¹ , Tyr ⁷⁴ , Gly ¹⁴⁹ , Glu ¹⁵⁰ , Asn ¹⁵¹ , His ¹⁵² , Arg ²⁰⁶ , Gln ²⁰⁷⁰ , Glu ²⁰⁷¹ , Asp ²⁰⁷² , Gln ²¹³⁸ , Asp ²¹³⁹ , Val ²¹⁴⁰ , Gly ²¹⁴¹ , Lys ²¹⁴² , Arg ²²⁹²
3HRZ	Human factor B	Immune system	-8.46	624.893125	Arg ¹² , Glu ¹⁶ , Glu ¹⁷ , Gln ¹⁸ , Thr ⁶² , Thr ⁶⁴ , Ser ¹⁰⁴ , Phe ¹⁰⁵ , Met ¹²⁸ , Asp ¹²⁹ , Asn ⁴⁶³ , Lys ⁴⁶⁴ , Lys ⁴⁶⁶ , Ile ⁴⁶⁷ , Phe ⁴⁶⁸ , Asp ⁴⁹¹ , Met ⁵²³
5W45	APOBEC3H	DNA binding protein	-8.42	675.3426875	Leu ¹¹ , Gln ¹² , Asn ¹⁴ , Lys ¹⁶ , Arg ¹⁷ , Arg ¹⁸ , Leu ¹⁹ , Arg ²⁰ , Pro ²² , Tyr ²³ , Tyr ²⁴ , Pro ²⁵ , Arg ²⁶ , Lys ²⁷ , Thr ⁸¹ , Trp ⁸² , Arg ¹¹⁰
3EHT	The extracellular domain of human corticotropin releasing factor receptor	Membrane protein	-8.36	749.84375	His ²⁸⁵ , Asp ²⁵⁴ , Ala ²⁵³ , Arg ²⁵¹ , Tyr ²⁵⁰ , Asn ²⁴⁹ , Gly ²⁴⁸ , Tyr ¹⁷⁸ , Tyr ¹⁷³ , Ile ¹⁷¹ , Glu ²¹¹ , Ile ²⁰ , Met ¹⁹ , Pro ¹⁸ , Asn ¹⁷ , Ile ¹⁶ , Pro ¹⁵ , Gln ¹⁴
2V5Y	The receptor protein tyrosine phosphatase mu ectodomain	Hydrolase	-8.34	775.5878125	Cys ⁴⁰⁰ , Tyr ⁴⁰¹ , Gln ⁴⁰² , Val ⁴⁰³ , Gly ⁴⁰⁴ , Glu ⁴⁰⁷ , Ser ⁴³⁰ , Pro ⁴³¹ , Tyr ⁴³² , Thr ⁴³³ , Asn ⁴³⁴ , Gly ⁴⁸⁵ , Gln ⁴⁸⁸ , Thr ⁴⁸⁹ , Tyr ⁴⁹⁰ , Gly ⁴⁹¹ , Val ⁴⁹² , Ile ⁴⁹³
3VJ9	The human squalene synthase	Transferase	-8.24	918.18875	Glu ¹⁶⁵ , Asp ¹⁶⁹ , Glu ²⁰² , Asn ²⁰³ , Ser ²⁰⁶ , Leu ²⁰⁹ , Lys ²¹³ , Arg ²³⁸ , Tyr ²³⁹ , Glu ²⁶¹ , Thr ²⁶⁴ , Asn ²⁶⁵ , His ²⁶⁸ , His ²⁶⁹ , Asp ²⁷² , Pro ³⁵⁴ , Ser ³⁵⁵ , Lys ³⁵⁸

PDB ID	Targets	Classification	Energy (kcal/mol)	Dissoc. constant [nM]	Contacting receptor residues
5T40	Human EXOG (hexog)	Hydrolase	-8.23	935.3950625	Asp ¹⁰⁸ , Arg ¹⁰⁹ , Lys ¹¹⁰ , Cys ¹¹² , Phe ¹¹⁴ , Ser ¹³⁷ , Arg ¹³⁸ , His ¹⁴⁰ , Pro ¹⁴³ , Ala ¹⁴⁴ , Gly ¹⁴⁵ , Phe ¹⁵⁸ , Phe ¹⁶⁸ , Asn ¹⁷⁶ , Glu ¹⁷⁹ , Arg ¹⁸³ , Arg ³¹⁴
5U2P	Citrate synthase	Transferase	-8.21	952.9238125	Met ⁷² , Arg ⁷³ , Gly ⁷⁴ , Met ⁷⁵ , Gly ⁷⁷ , Leu ⁷⁸ , His ²⁶⁵ , Gly ²⁶⁸ , Asn ²⁶⁹ , Val ²⁷⁰ , His ²⁷³ , Leu ³⁰⁰ , His ³⁰¹ , Gly ³⁴⁸ , Val ³⁴⁹ , Arg ³⁵⁶ , Asn ⁴⁰⁰ , Val ⁴⁰¹ , Asp ⁴⁰² , Arg ⁴²⁸ , Glu ⁴⁴⁷
3MWE	Truncated human ATP-citrate lyase	Transferase	-8.21	962.623	Ser ⁷ , Asp ⁶⁰ , Glu ⁶¹ , Gly ¹⁰⁰ , Asn ¹⁰⁴ , Glu ²³⁷ , Pro ²³⁹ , Pro ²⁴⁰ , Pro ²⁴¹ , Phe ²⁴² , Gly ²⁴³ , Arg ²⁴⁴ , Glu ²⁴⁵ , Ala ²⁴⁶ , Glu ²⁵⁰ , Ala ²⁵¹ , Ala ²⁵⁴
2XMS	Human NDRG2 protein	Signaling protein	-8.18	1002.417063	Asp ¹⁵⁸ , Lys ¹⁶² , His ¹⁷⁰ , Thr ¹⁷³ , Ser ¹⁷⁷ , Gly ¹⁸¹ , Met ¹⁸² , Gly ¹⁸⁵ , His ¹⁸⁶ , Ser ¹⁸⁹ , Gln ¹⁹⁰ , Leu ¹⁹³ , Trp ²²⁰ , Tyr ²²³ , Asn ²²⁴ , Arg ²²⁶ , Pro ²⁵² , His ²⁵³ , Asp ²⁵⁵ , Ala ²⁵⁶
5K10	Isocitrate dehydrogenase (IDH1)	Oxidoreductase	-8.11	1143.465875	Pro ²⁰⁶ , Tyr ²⁰⁸ , Tyr ²³¹ , Lys ²³⁶ , Phe ²³⁹ , Glu ²⁴⁰ , Lys ²⁴³ , Ile ²⁴⁴ , Trp ²⁴⁵ , Glu ²⁴⁷ , Arg ²⁴⁹ , Gln ²⁵⁷ , Ser ²⁶¹ , Glu ²⁶² , Gly ²⁶³ , Gly ²⁶⁴ , Phe ²⁶⁵
2J0S	Exon junction	Hydrolase	-8.09	1172.784875	Pro ¹¹⁴ , Thr ¹¹⁵ , Arg ¹¹⁶ , Gly ¹⁴² , Thr ¹⁶³ , Pro ¹⁶⁴ , Gly ¹⁶⁵ , Arg ¹⁶⁶ , Phe ¹⁹⁷ , Gln ²⁰⁰ , Asn ²⁸⁵ , Thr ²⁸⁶ , Lys ²⁸⁷ , Gly ³⁰⁹ , Asp ³¹⁰ , Arg ³¹⁶ , Thr ³³⁴ , Asp ³³⁵ , Val ³³⁶
3PUF	Human RNase H2 complex	Hydrolase	-8.08	1186.72325	Glu ⁷³ , Arg ¹⁸⁶ , Asp ¹⁸⁷ , Val ¹⁹⁰ , Lys ¹⁹¹ , Trp ¹⁹³ , Gln ¹⁹⁴ , Phe ¹⁹⁵ , Glu ¹⁹⁷ , Lys ¹⁹⁸ , Leu ¹⁹⁹ , Gln ²⁰⁰ , Thr ²⁰⁴ , Tyr ²⁰⁶ , Gly ²⁰⁷ , Ser ²⁰⁸ , Trp ²¹⁹ , Phe ²³³
3DOF	Complex of ARL2 and BART	Signaling protein/hydrolase	-8.06	1233.697375	Lys ⁵ , Gln ¹² , Glu ⁴² , Ser ⁸³ , Thr ⁸⁴ , Asp ⁸⁵ , Arg ¹¹⁴ , Leu ¹¹⁵ , Ala ¹¹⁶ , Gly ¹¹⁷ , Ala ¹¹⁸ , Ile ¹⁷⁶ , Arg ¹⁷⁹ , Ile ¹⁸⁰ , Thr ¹⁸² , Ala ¹⁸³ , Glu ¹⁸⁶ , His ¹⁸⁷
3BYI	Human rho GTPase activating protein 15 (arhgap15)	Signaling protein	-8.04	1278.209	Ile ²⁷⁸ , Arg ²⁸⁹ , Glu ²⁹⁰ , Trp ²⁹⁶ , Phe ²⁹⁷ , Gln ³⁰⁰ , Glu ³⁰³ , Ala ³⁰⁴ , Val ³³² , Glu ³³⁵ , Glu ³³⁶ , Lys ³³⁷ , Leu ³³⁸ , Asn ³³⁹ , Leu ³⁴⁰ , Asp ³⁴¹
1IKN	IKAPBAPALPHA/NF-KAPPA B complex	Transcription factor	-8.04	1289.0415	Lys ²⁸ , Glu ⁴⁹ , Arg ⁵⁰ , Ser ⁵¹ , Thr ⁵² , Glu ²²² , Asp ²²³ , Ile ²²⁴ , Glu ²²⁵ , Val ²²⁶ , Glu ²³⁴ , Ala ²³⁵ , Arg ²³⁶ , Gly ²³⁷ , Ser ²³⁸ , Phe ²³⁹ , Pro ²⁷⁵
3EHI	Human thymidylate synthase M190K	Transferase	-8.01	1337.806	Arg ⁵⁰ , Thr ⁵¹ , Glu ⁸⁷ , Phe ⁹¹ , Asp ¹¹⁶ , Tyr ¹³⁵ , Asn ¹⁸³ , Pro ¹⁸⁴ , His ¹⁹⁶ , Gln ²¹⁴ , Ser ²¹⁶ , Gly ²¹⁷ , Asp ²¹⁸ , Gly ²²² , Phe ²²⁵ , Asn ²²⁶ , His ²⁵⁶ , Tyr ²⁵⁸
6F39	C1R homodimer CUB1-EGF-CUB2	Hydrolase	-7.98	1421.61325	Thr ³⁵ , Gly ³⁶ , Tyr ³⁷ , Arg ³⁸ , Ser ⁶² , Lys ⁶⁶ , Leu ⁶⁸ , Met ⁸⁹ , Ser ⁹⁰ , Gln ⁹¹ , Gly ⁹² , Asn ⁹³ , Lys ⁹⁴ , Met ⁹⁵ , Asp ¹²⁵ , Leu ¹²⁶ , Glu ¹²⁸ , Tyr ¹⁵⁵
5AIU	RNF4-ring domain, UBC13-UB (isopeptide crosslink)	Ligase/signaling protein	-7.97	1440.938875	Tyr ¹⁴³ , Val ¹⁴⁷ , Gly ¹⁵⁰ , Arg ¹⁵¹ , Leu ¹⁵² , Ile ¹⁵³ , Ile ¹⁹² , Tyr ¹⁹³ , Ile ¹⁹⁴ , Gly ¹⁹⁵ , Ser ¹⁹⁶ , Val ¹⁹⁹ , Ser ²⁰⁰ , Cys ²⁰¹ , Pro ²⁰² , His ²²⁵ , Val ²²⁶ , Thr ²⁴⁴
2UW9	PKB-Beta (AKT2)	Transferase	-7.96	1455.60525	Ala ⁸² , Gly ⁸³ , Lys ⁸⁶ , Lys ³⁹⁰ , Gln ³⁹¹ , Arg ³⁹² , Leu ³⁹³ , Gly ³⁹⁴ , Gly ³⁹⁵ , Gly ³⁹⁶ , Pro ³⁹⁷ , Ser ³⁹⁸ , Glu ⁴⁰² , Glu ⁴⁰⁵ , His ⁴⁰⁶ , Arg ⁴⁰⁷
3GR4	Human pyruvate kinase M2	Transferase	-7.96	1460.527125	Arg ²⁵⁵ , Asn ²⁶⁴ , Ile ²⁶⁵ , Lys ²⁶⁶ , Ile ²⁶⁷ , Glu ²⁸⁵ , Ala ²⁸⁶ , Ser ²⁸⁷ , Asp ²⁸⁸ , Gly ³²¹ , Lys ³²² , Pro ³²³ , Lys ³³³ , Ser ⁴³⁴ , Arg ⁴³⁶ , His ⁴³⁹ , Arg ⁴⁴³ , Asn ⁴⁵⁶ , Gln ⁴⁵⁷ , Tyr ⁴⁶⁶ , Ser ⁵¹⁹
3OE9	the chemokine CXCR4 receptor	Signaling protein, hydrolase	-7.91	1581.106375	Asp ¹⁰¹⁰ , Glu ¹⁰¹¹ , Arg ¹⁰¹⁴ , Tyr ¹⁰¹⁸ , Lys ¹⁰¹⁹ , Tyr ¹⁰²⁴ , Thr ¹⁰²⁶ , Gly ¹⁰³⁰ , His ¹⁰³¹ , Leu ¹⁰³² , Asp ¹⁰⁷⁰ , Ala ¹⁰⁷⁴ , Val ¹¹⁰³ , Phe ¹¹⁰⁴ , Gln ¹¹⁰⁵ , Met ¹¹⁰⁶ , Gly ¹¹⁰⁷ , Trp ¹¹³⁸ , Gln ¹¹⁴¹ , Thr ¹¹⁴² , Arg ¹¹⁴⁵
4URW	RAS:SOS complex	Signaling protein	-7.91	1594.505875	Ser ¹⁷ , Ile ²¹ , Tyr ³² , Pro ³⁴ , Thr ³⁵ , Ile ³⁶ , Gly ³⁷ , Tyr ⁴⁰ , Arg ⁴¹ , Asp ⁵⁴ , Ile ⁵⁵ , Leu ⁵⁶ , Asp ⁵⁷ , Thr ⁵⁸ , Ala ⁵⁹ , Gln ⁶¹
5POQ	BRD1 in complex with N10974A	Gene regulation	-7.9	1610.735375	Ile ⁵⁴ , Phe ⁵⁵ , Val ⁵⁹ , Glu ⁶³ , Val ⁶⁴ , Pro ⁶⁵ , Tyr ⁶⁷ , Met ⁷⁵ , Ile ¹⁰² , Asn ¹⁰⁵ , Cys ¹⁰⁶ , Tyr ¹⁰⁹ , Asn ¹¹⁰ , Ala ¹¹¹ , Thr ¹¹⁴ , Phe ¹¹⁶
4ZMV	Human P-cadherin (SS-X-dimer pocket I)	Cell adhesion	-7.82	1846.706875	Ala ¹⁴⁷ , Tyr ¹⁴⁸ , Ser ¹⁴⁹ , Ile ¹⁵⁰ , His ¹⁵¹ , Ser ¹⁵² , Gln ¹⁵³ , Lys ¹⁵⁶ , Asp ¹⁶⁰ , Leu ¹⁶¹ , Met ¹⁶² , Phe ¹⁶³ , Thr ¹⁶⁴ , Ile ¹⁶⁵ , Arg ¹⁶⁷ , Gln ¹⁹² , Gly ¹⁹⁸ , Thr ²⁰²
2CZK	Human myo-inositol mono-phosphatase 2 (impa2)	Hydrolase	-7.74	2113.67775	Arg ⁴⁶ , Gly ⁴⁷ , Gly ⁴⁹ , Arg ⁵⁶ , Leu ⁵⁷ , Arg ⁵⁸ , Val ¹⁵⁹ , Ser ¹⁶⁰ , Gly ¹⁶¹ , Arg ²⁴⁰ , Glu ²⁴¹ , Ala ²⁴² , Gly ²⁴³ , Gly ²⁴⁴ , Ile ²⁴⁵ , Ser ²⁶⁵ , Thr ²⁶⁶ , Arg ²⁶⁷
3OHH	Activated G alpha Q	Signaling protein	-7.72	2197.34375	Ser ²³ , Ile ⁵⁶ , Lys ⁵⁷ , Arg ⁶⁰ , Gly ⁸⁴ , Ser ⁶⁵ , Tyr ⁸⁷ , Phe ⁷⁵ , Leu ⁷⁸ , Val ¹⁸⁴ , Pro ¹⁸⁵ , Thr ¹⁸⁶ , Thr ¹⁸⁷ , Ile ¹⁹⁰ , Tyr ¹⁹² , Pro ¹⁹³ , Phe ¹⁹⁴ , Asp ²⁰⁵
5IOH	Repoman-PP1A (protein phosphatase 1, alpha isoform) holoenzyme	Hydrolase/protein binding	-7.71	2219.709	Arg ⁹⁶ , Asn ¹²⁴ , His ¹²⁵ , Ile ¹³⁰ , Tyr ¹³⁴ , Trp ²⁰⁶ , Asp ²⁰⁸ , Pro ²⁰⁹ , Asp ²¹⁰ , Lys ²¹¹ , Asn ²¹⁹ , Asp ²²⁰ , Arg ²²¹ , Thr ²²⁶ , Gln ²⁴⁹ , Val ²⁵¹ , Glu ²⁵⁶ , Phe ²⁵⁸ , Phe ²⁷⁶
5L6D	The human METTL3-METTL14 complex	Transferase	-7.69	2315.37475	Tyr ⁸⁰ , Leu ⁸¹ , Asp ⁸² , Ser ⁸⁴ , Ile ⁸⁵ , Arg ⁵⁶⁴ , Gln ⁵⁶⁷ , Arg ⁵⁶⁸ , Tyr ⁵⁶⁹ , Pro ⁵⁷⁰ , Asp ⁵⁷¹ , Ile ⁵⁷³ , Ile ⁵⁷⁴ , Ser ⁵⁷⁵ , Lys ⁵⁷⁶
4IA0	The PDE5A1 catalytic domain	Hydrolase	-7.67	2378.7535	Leu ⁵⁵⁴ , Lys ⁵⁵⁵ , Asp ⁵⁵⁸ , Phe ⁵⁵⁹ , Ser ⁵⁶⁰ , Phe ⁵⁶¹ , Ser ⁵⁶² , Glu ⁵⁶⁵ , Leu ⁵⁶⁶ , Thr ⁵⁶⁹ , Lys ⁷⁷⁰ , Pro ⁷⁷¹ , Trp ⁷⁷² , Ile ⁷⁷⁴ , Pro ⁸⁴¹ , Asp ⁸⁴⁴ , Gly ⁸⁴⁵ , Lys ⁸⁴⁸ , Asn ⁸⁴⁹ , Lys ⁸⁵²
4GWG	6-phosphogluconate dehydrogenase apo-form	Oxidoreductase	-7.66	2443.86725	Trp ¹⁷² , Arg ¹⁴² , Ala ¹⁴⁵ , Thr ³⁴⁶ , Gly ³⁴⁹ , Trp ³⁵⁰ , Thr ³⁵¹ , Leu ³⁵² , Asn ³⁵³ , Tyr ³⁵⁴ , Gly ³⁵⁵ , Gly ³⁵⁶ , Lys ³⁷⁶ , Phe ³⁷⁹ , Arg ³⁸⁰ , Pro ³⁸³ , Gln ³⁸⁶
4IRG	The ETS transcription factor ERG	DNA binding protein	-7.65	2464.5785	Gly ²⁹² , Gln ²⁹³ , Gln ²⁹⁵ , Leu ²⁹⁶ , Trp ³³⁴ , Lys ³³⁸ , Lys ³⁴⁰ , Met ³⁴³ , Lys ³⁴⁷ , Leu ³⁴⁸ , Arg ³⁵⁰ , Ala ³⁵¹ , Tyr ³⁵⁴ , Tyr ³⁵⁵ , Lys ³⁵⁸
3R4O	Heat shock protein 90	Chaperone	-7.61	2632.2675	Arg ⁴⁶ , Glu ⁴⁷ , Ser ⁵⁰ , Asn ⁵¹ , Asp ⁵⁴ , Ala ⁵⁵ , Lys ⁵⁸ , Asn ¹⁰⁶ , Leu ¹⁰⁷ , Lys ¹¹² , Gly ¹³² , Gln ¹³³ , Gly ¹³⁵ , Val ¹³⁶ , Gly ¹³⁷ , Phe ¹³⁸ , His ²¹⁰ , Ser ²¹¹ , Gln ²¹² , Phe ²¹³ , Ile ²¹⁴
1ZXN	Human topo IIA ATPase/AMP-PNP	Isomerase	-7.58	2773.6605	Gln ⁵⁹ , Gln ⁶⁰ , Met ⁶¹ , Trp ⁶² , Tyr ⁷² , Arg ²⁴¹ , Lys ³⁰⁶ , Gly ³⁰⁷ , Phe ³⁰⁸ , Gln ³⁰⁹ , Gln ³¹⁰ , Ile ³¹¹ , Ala ³¹⁸ , Ser ³²⁰ , Lys ³²¹ , Gly ³²² , Gly ³²³ , Val ³²⁶
4E+49	Carbonic anhydrase (CA)	Lyase	-7.57	2820.87225	Tyr ⁴⁰ , Asp ⁴¹ , Pro ⁴² , Leu ⁴⁴ , Lys ⁴⁵ , Pro ⁴⁶ , Leu ⁴⁷ , Ser ⁴⁸ , Val ⁴⁹ , Ser ⁵⁰ , Lys ⁸⁰ , Gly ⁸¹ , Gly ⁸² , Glu ¹⁸⁷ , Ser ¹⁸⁸ , Leu ¹⁸⁹ , Asp ¹⁹⁰ , Tyr ¹⁹¹ , Ser ²⁵⁹
1JT3	Human acidic fibroblast growth factor	Hormone/growth factor	-7.56	2888.32175	Asp ²⁸ , Gly ²⁹ , Thr ³⁰ , Val ³¹ , Asp ³² , Asp ⁶⁸ , Thr ⁶⁹ , Leu ⁷² , Val ⁷³ , Tyr ⁷⁴ , Gly ⁷⁵ , Glu ⁸² , Ser ¹¹⁶ , Cys ¹¹⁷ , Lys ¹¹⁸ , Arg ¹¹⁹
5HKJ	Single chain recombinant globular head of the complement system protein C10	Signaling protein	-7.53	3048.61	Asn ²⁰ , Cys ⁶³ , Leu ⁶⁴ , Ser ⁶⁵ , Arg ⁷⁶ , Ser ⁷⁷ , Leu ⁷⁸ , Gly ⁷⁹ , Phe ⁸⁰ , Glu ¹⁰⁹ , Lys ¹¹⁰ , Asp ¹¹¹ , Pro ¹¹² , Gln ¹⁵² , Gln ²⁵⁶ , Gly ²⁵⁷ , Asp ²⁵⁹
4NYH	Pir1 dual specificity phosphatase core	Hydrolase	-7.5	3158.60325	His ³⁰ , Ile ³¹ , Pro ³² , Glu ³³ , Arg ³⁴ , Trp ³⁵ , Lys ³⁶ , Asp ³⁷ , Lys ⁶⁴ , Leu ⁶⁵ , Thr ⁹⁶ , Gln ⁹⁷ , Tyr ⁹⁹ , Thr ¹⁵³ , Arg ¹⁵⁸
3WO2	Human interleukin-18	Immune system	-7.5	3180	Gly ²⁵ , Asn ²⁶ , Arg ²⁷ , Pro ²⁸ , Glu ⁷⁷ , Asn ⁷⁸ , Lys ⁷⁹ , Ile ⁸⁰ , Ile ⁸¹ , Ser ⁸² , Phe ⁸³ , Lys ¹³⁵ , Leu ¹³⁶ , Ile ¹³⁷ , Leu ¹³⁸
2G6P	Truncated (delta 1-89) human methionine aminopeptidase type 1	Hydrolase	-7.49	3234.128	Gln ¹¹³ , Arg ¹¹⁴ , Pro ¹¹⁵ , Asp ¹¹⁶ , Ser ¹²⁷ , Gly ¹⁴³ , Asp ¹⁴⁴ , Glu ¹⁴⁶ , Gly ¹⁴⁷ , Leu ¹⁵⁰ , Tyr ²³³ , Asn ²³⁵ , Gly ²³⁶ , Tyr ²³⁷ , Lys ³⁰⁷ , Leu ³⁰⁸
5HOV	H88A mutated human transthyretin	Transport protein	-7.48	3289.1775	Pro ¹¹ , Glu ⁶¹ , Phe ⁶⁴ , Val ⁶⁵ , Glu ⁶⁶ , Ala ⁹⁷ , Asn ⁹⁸ , Asp ⁹⁹ , Gly ¹⁰¹ , Pro ¹⁰² , Arg ¹⁰³ , Arg ¹⁰⁴ , Tyr ¹⁰⁵ , Asn ¹²⁴
2IYB	Complex between the 3rd LIM domain of TES and the evh1 domain of MENA	Metal-binding	-7.43	3560.72775	Val ¹⁵ , Tyr ¹⁶ , Asp ¹⁷ , Asp ¹⁸ , Ala ¹⁹ , Val ²⁴ , Pro ²⁵ , Ala ²⁶ , Gly ²⁷ , Gly ²⁸ , Val ⁵⁹ , Ile ⁶⁰ , Asn ⁶¹ , Arg ⁸⁴ , Gln ⁸⁵ , Val ⁸⁶ , Tyr ⁸⁷
5Z90	BRD4 bromodomain 1	Transcription	-7.43	3560.72775	Pro ⁴⁵ , Pro ⁴⁶ , Pro ⁴⁸ , Glu ⁴⁹ , Asn ⁵² , Lys ⁵⁵ , Tyr ⁹⁸ , Ile ¹⁰¹ , Lys ¹⁰² , Thr ¹⁰³ , Pro ¹⁰⁴ , Met ¹⁰⁵ , Arg ¹¹³ , Tyr ¹¹⁸ , Asp ¹²⁸ , Thr ¹³¹

PDB ID	Targets	Classification	Energy (kcal/mol)	Dissoc. constant [nM]	Contacting receptor residues
1Z3U	Angiopoietin-2 receptor binding domain	Signaling protein	-7.4	3751.99325	Arg ³²⁸ , Ser ³³² , Val ³³³ , Asp ³³⁴ , Phe ³³⁵ , Gln ³³⁶ , Glu ³⁵² , Gly ⁴⁵⁷ , Met ⁴⁵⁸ , Tyr ⁴⁵⁹ , Tyr ⁴⁶⁰ , Pro ⁴⁶¹ , Gln ⁴⁶⁴ , Lys ⁴⁶⁸ , Asn ⁴⁷⁰
5A2E	Extracellular SRCR domains of human CD6	Immune system	-7.4	3751.99325	Asp ²⁹¹ , Ser ²⁹² , Trp ²⁹⁴ , Arg ²⁹⁴ , Pro ³¹⁵ , Lys ³¹⁶ , Gly ³¹⁷ , Ser ³⁵¹ , Gln ³⁵² , Ser ³⁵³ , Leu ³⁵⁴ , Ala ³⁵⁶ , Arg ³⁵⁷
4A7U	Human I113TSOD1	Oxidoreductase	-7.39	3841.7065	Gly ⁷³ , Pro ⁷⁴ , Lys ⁷⁵ , Asp ⁷⁶ , Gly ⁸⁵ , Asn ⁸⁶ , Val ⁸⁷ , Thr ⁸⁸ , Asp ⁹⁶ , Val ⁹⁷ , Ser ⁹⁸ , Ile ⁹⁹ , Glu ¹⁰⁰ , Leu ¹²⁶ , Lys ¹²⁸
5F6D	UBC9 (K48A/K49A/E54A)	Ligase	-7.36	4020.82775	Asp ¹⁹ , His ²⁰ , Pro ²¹ , Phe ²² , Gly ²³ , Phe ²⁴ , Val ²⁵ , Pro ⁴⁶ , Gly ⁴⁷ , Ala ⁴⁸ , Ala ⁴⁹ , Ala ⁵⁴ , Gly ⁵⁵ , Gly ⁵⁶ , Leu ⁵⁷ , Lys ¹¹⁰ , Leu ¹¹⁴ , Gln ¹¹⁷ , Pro ¹⁵⁷
4IP9	Human serum amyloid A1	Protein binding	-7.34	4172.9355	Ala ¹⁴ , Arg ¹⁵ , Met ¹⁷ , Trp ¹⁸ , Tyr ²¹ , Ile ⁵⁸ , Arg ⁶² , Ile ⁶⁵ , Gln ⁶⁶ , Phe ⁶⁹ , Gly ⁷⁰ , His ⁷¹
2X1X	Structure of VEGF-C in complex with domains 2 and 3 of VEGFR2 in a tetrameric crystal form	Hormone/signaling protein	-7.29	4571.1365	Trp ¹²⁶ , Arg ¹³⁰ , Cys ¹³¹ , Met ¹³² , Pro ¹³³ , Cys ¹⁶⁵ , Cys ¹⁶⁶ , Asn ¹⁶⁷ , Ser ¹⁶⁸ , Leu ¹⁷¹ , Thr ²⁰⁷ , Ser ²⁰⁸ , Cys ²⁰⁹ , Arg ²¹⁰ , Cys ²¹¹ , Met ²¹²
4MXV	Lymphotoxin alpha	Cytokine/immune system	-7.25	4849.3055	Asn ⁴¹ , Ser ⁴² , Leu ⁴³ , Leu ⁴⁴ , Trp ⁴⁵ , Asn ⁶² , Asn ⁶³ , Ser ⁶⁴ , Tyr ⁹⁶ , Gln ¹⁰² , His ¹¹¹ , Ser ¹⁴⁸ , Thr ¹⁴⁹ , His ¹⁵⁰ , Thr ¹⁵¹ , Asp ¹⁵² , Gly ¹⁵³ , Ile ¹⁵⁴
5OKF	Human 14-3-3 sigma with the hspb6 phosphopeptide	Signaling protein	-7.22	5075.406	Trp ⁵⁹ , Arg ⁶⁰ , Ser ⁶³ , Ser ⁶⁴ , Glu ⁶⁶ , Gln ⁶⁷ , Arg ⁸⁵ , Ala ¹³² , Glu ¹³³ , Val ¹³⁴ , Ala ¹³⁵ , Lys ¹⁴⁰ , Tyr ¹⁸¹ , Phe ¹⁸² , Ile ¹⁸³ , Arg ²³⁸
5GNT	BDLP-like folding of Mitofusin 1	Hydrolase	-7.21	5231.9665	Leu ¹⁹⁷ , Ala ¹⁹⁹ , Asp ²⁰⁰ , Val ²⁰¹ , Phe ²⁰² , Leu ²²⁷ , Ser ²²⁸ , Lys ²²⁹ , Pro ²³⁰ , Asn ²³¹ , Ser ³³¹ , Thr ³³⁴ , Thr ³³⁵ , Lys ³³⁶ , Gln ³³⁹
2QX4	Quinone reductase ii	Oxidoreductase	-7.17	5522.3165	Ala ¹⁵² , Glu ¹⁵³ , Tyr ¹⁵⁵ , Thr ¹⁵⁶ , Asp ¹⁶³ , Ser ¹⁶⁴ , Arg ¹⁶⁵ , Leu ¹⁶⁸ , Ala ¹⁸⁵ , Pro ¹⁸⁶ , Gln ¹⁸⁷ , Ile ¹⁸⁸ , Phe ¹⁹⁰ , Met ²⁰³ , Ala ²⁰⁶ , Arg ²¹⁰
2Q7N	LIF receptor (domains 1-5)	CYTOKINE receptor/CYTOKINE	-7.15	5740.907	Thr ¹¹ , Thr ¹² , Asn ¹³ , Asn ¹⁴ , Arg ¹⁶ , Val ¹⁷ , Trp ¹⁸ , Asp ¹⁹ , Pro ⁴⁷ , Leu ⁴⁸ , Glu ⁴⁹ , Thr ⁵⁰ , Asn ⁵² , Lys ⁵³ , Lys ⁵⁴ , Glu ⁸⁹
3ZR0	Human MTH1	Hydrolase	-7.13	5917.996	Arg ³¹ , Leu ¹⁰⁸ , Asp ¹⁰⁹ , Ile ¹¹¹ , Pro ¹¹² , Phe ¹¹³ , Lys ¹¹⁴ , Arg ¹¹⁵ , Met ¹¹⁶ , Trp ¹¹⁷ , Pro ¹¹⁸ , Ser ¹²¹ , Pro ¹²⁵ , Leu ¹²⁸ , Gln ¹²⁹ , Asp ¹⁴³
5U7Z	Human acid ceramidase (ASAH1, aCDase)	Hydrolase	-7.11	6141.874	Lys ⁷⁴ , Val ⁷⁷ , Asn ⁷⁸ , Lys ⁸¹ , Met ⁸⁴ , Gln ⁹⁵ , Asp ⁹⁸ , Ala ¹²⁰ , Ala ¹²¹ , Val ¹²² , Asp ¹²⁴ , Ile ¹²⁵ , Pro ¹²⁶ , Leu ¹²⁷ , Gly ¹²⁸ , Glu ¹²⁹
3H91	Human chromobox homolog 2 (CBX2)	Transcription	-7.08	6428.241	Glu ⁹ , Gln ¹⁰ , Val ¹¹ , Phe ¹² , Arg ²³ , Lys ²⁶ , Glu ²⁸ , Trp ³³ , Ser ⁴² , Trp ⁴³ , Glu ⁴⁴ , Pro ⁴⁵ , Glu ⁴⁷ , Asn ⁴⁸ , Leu ⁵⁰
3UVU	Flap endonuclease 1 (FEN1)	Protein binding/peptide	-7.04	6900.4685	Val ²¹⁵ , Pro ²¹⁶ , Asp ²¹⁷ , Leu ²¹⁸ , Ser ²¹⁹ , Val ²⁵⁷ , Arg ²⁵⁸ , His ²⁶¹ , His ²⁶² , Asn ²⁶³ , Gln ²⁹⁷
1CWF	Human cyclophilin A	Isomerase/immunosuppressant	-7.04	6912.125	Phe ⁷ , Leu ³⁹ , Ser ⁴⁰ , Thr ⁴¹ , Gly ⁴² , Gly ⁴⁵ , Phe ⁴⁶ , Gly ⁴⁷ , Tyr ⁴⁸ , Lys ⁴⁹ , Gly ⁵⁰ , Phe ⁶⁷ , Thr ⁶⁸ , His ⁷⁰ , Lys ⁷⁶ , Asp ¹⁶⁰ , Cys ¹⁶¹ , Gly ¹⁶² , Gln ¹⁶³
4Y5O	CCM2 HHD in complex with MEKK3 NPB1	Transferase	-7.03	7077.3995	Leu ²⁹⁹ , Tyr ³⁰² , Leu ³²² , Tyr ³²⁵ , Arg ³²⁶ , Gly ³²⁸ , Ala ³²⁹ , Ser ³³⁰ , Glu ³⁵³ , Phe ³⁵⁶ , Ile ³⁵⁷ , Pro ³⁵⁸ , Glu ³⁵⁹ , Lys ³⁶⁰ , Asp ³⁶¹
5FUG	A human YL1-H2A.Z-H2B complex	DNA binding protein	-6.96	7964.9745	Leu ⁶⁸ , Asn ⁷¹ , Ala ⁷² , Ser ⁷³ , Lys ⁷⁴ , Asp ⁷⁵ , Leu ⁷⁶ , Lys ⁷⁷ , Val ⁷⁸ , Lys ⁷⁹ , Arg ⁸⁰ , His ⁸⁵ , Leu ⁸⁸ , Ala ⁸⁹ , Gly ⁹²
5D1M	UBCH5B	Ligase	-6.91	8680.963	Leu ¹³ , Ala ¹⁴ , Pro ¹⁷ , Gln ²⁰ , Cys ²¹ , Ser ²² , Ala ²³ , Gly ²⁴ , Gln ³⁴ , Ala ³⁵ , Thr ³⁶ , Met ³⁸ , Val ⁴⁹ , Phe ⁵¹
5VZ3	Growth factor	Signaling protein	-6.78	10738.092	Asp ⁵ , Arg ¹⁶ , Leu ¹⁷ , Gln ⁵¹ , Phe ⁵² , Arg ⁵³ , Ala ⁵⁴ , Gln ⁶⁰ , Lys ¹⁰⁷ , Asp ¹⁰⁸ , Cys ¹⁰⁹ , His ¹¹⁰
6PAX	Human PAX-6 paired domain-DNA complex	Gene regulation	-6.71	12003.441	Pro ⁷³ , Arg ⁷⁴ , Val ⁷⁵ , Ala ⁷⁶ , Pro ⁷⁸ , Val ⁸¹ , Ser ¹¹⁹ , Arg ¹²² , Val ¹²³ , Asn ¹²⁶
1HF0	DNA-binding domain of OCT-1	Transcription	-6.6	14501.163	Glu ¹⁰⁹ , Asn ¹¹¹ , Ile ¹¹² , Val ¹¹⁴ , Ala ¹¹⁵ , Lys ¹¹⁸ , Ser ¹¹⁹ , Glu ¹²² , Ile ¹³⁴ , Gln ¹³⁷ , Leu ¹³⁸ , Asn ¹³⁹
1QE6	Interleukin-8	Immune system	-6.55	15698.361	Leu ²⁵ , Val ²⁷ , Glu ²⁹ , Ser ³⁰ , Ala ³⁵ , Asn ³⁶ , Thr ³⁷ , Ile ³⁹ , Pro ⁵³ , Lys ⁵⁴ , Gln ⁵⁹ , Val ⁶²
1BL1	PTH receptor N-terminus fragment	Hormone receptor	-6.53	16347.319	Phe ⁶ , Leu ⁷ , Glu ¹⁰ , Thr ¹¹ , Arg ¹² , Glu ¹³ , Val ¹⁶ , Ile ²³ , Tyr ²⁴ , Val ²⁶ , Gly ²⁷
5N7E	DBL-homology domain of BCR-ABL	Signaling protein	-6.38	21021.562	Leu ²⁰ , Tyr ³⁷ , Phe ⁴⁹ , Glu ⁵⁰ , Val ⁵¹ , Pro ⁵² , Lys ⁵⁵ , Thr ⁵⁷ , Ala ⁵⁸ , Thr ⁵⁹ , Ile ⁶⁰ , Ser ⁶¹ , Gly ⁶²
4X1L	Protein-induced destabilization of profilin 1 in ALC	Protein binding	-6.35	22001.7	Arg ⁷⁵ , Gly ⁸² , Glu ⁸³ , Ser ⁸⁵ , Gly ¹²² , Leu ¹²³ , Asn ¹²⁵ , Lys ¹²⁶ , Tyr ¹²⁹ , Glu ¹³⁰
2J8B	Human CD59	Lipid binding protein	-6.26	25697.634	Asn ⁵ , Cys ⁶ , Pro ⁷ , Asn ⁹ , Pro ⁹ , Tyr ³⁶ , Asn ³⁷ , Lys ³⁸ , Cys ³⁹ , Arg ⁵³ , Leu ⁵⁴ , Arg ⁵⁵
5M3D	Tuning of CD81LEL (space group p31)	Cell adhesion	-6.26	25871.712	Asp ¹²⁸ , Leu ¹³¹ , Gln ¹³² , Val ¹³⁵ , Val ¹³⁶ , Gly ¹⁵⁸ , Ser ¹⁵⁹ , Ser ¹⁶⁰ , Leu ¹⁶² , Thr ¹⁶³ , Thr ¹⁶⁶ , Thr ¹⁶⁷ , Leu ¹⁷⁰ , His ¹⁹¹
4W9O	The FK1 domain of FKBP51	Isomerase	-6.23	27123.732	Ile ²⁵ , Ser ²⁷ , Thr ⁴⁶ , Pro ⁴⁷ , Met ⁴⁸ , Ile ⁴⁹ , Leu ⁸¹ , Asp ⁹¹ , Ile ⁹² , Ala ⁹⁵ , Thr ⁹⁶
3I69	Apo Glutathione transferase A1-1 GIMF-helix	Transferase	-6.2	28774.302	Met ⁹⁴ , Tyr ⁹⁵ , Gly ⁹⁸ , Asp ¹⁰¹ , Asn ¹³⁰ , Arg ¹³¹ , Tyr ¹³² , Pro ¹³⁴ , Ala ¹³⁵ , Phe ¹³⁶ , Lys ¹³⁸ , Val ¹³⁹
3KLT	A vimentin fragment	Structural protein	-5.9	47182.032	Ala ²¹² , Glu ²¹⁵ , Ser ²¹⁶ , Tyr ²¹⁹ , Arg ²²⁰ , Val ²²³ , Gln ²²⁴