

**Table S1.** Top-7 (those with better Fit Score) human proteins found for compounds I-VIII

Rank	PDB ID	Target Name	Number of Features	Fit Score	Normalized Fit Score	z'-score
<b>I</b>						
1	1F86	Transthyretin	3	2.984	0.9947	0.77242
2	3DEJ	Caspase-3	3	2.977	0.9922	0.91843
3	1PQ9	Oxysterols receptor LXR-beta	3	2.97	0.9901	0.83174
4	2VWU	Ephrin type-B receptor 4	3	2.968	0.9892	0.88698
5	1VEC	Probable ATP-dependent RNA helicase DDX6	3	2.957	0.9857	0.92884
6	1UDU	cGMP-specific 3,5-cyclic phosphodiesterase	3	2.953	0.9842	0.84906
7	1PMV	Mitogen-activated protein kinase 10	3	2.951	0.9837	0.53892
<b>II</b>						
1	2AGT	Aldose reductase	3	2.992	0.9974	0.84748
2	1BM6	Stromelysin-1	3	2.978	0.9927	0.58522
3	1LBK	Glutathione S-transferase P	3	2.974	0.9913	0.6646
4	1PQ9	Oxysterols receptor LXR-beta	3	2.968	0.9894	0.68102
5	1UNH	Cyclin-dependent kinase 5 activator 1	3	2.964	0.988	0.76718
6	1PMV	Mitogen-activated protein kinase 10	3	2.961	0.9868	0.35032
7	1PME	Mitogen-activated protein kinase 1	3	2.959	0.9863	0.57058
<b>III</b>						
1	1LBK	Glutathione S-transferase P	3	2.987	0.9956	0.76515
2	1DVZ	Transthyretin	3	2.986	0.9954	0.74064
3	3DEJ	Caspase-3	3	2.982	0.9939	0.82835
4	2C3I	Proto-oncogene serine/threonine-protein kinase Pim-1	3	2.979	0.993	0.76856
5	1UDU	cGMP-specific 3,5-cyclic phosphodiesterase	3	2.979	0.9929	0.81934
6	1VEC	Probable ATP-dependent RNA helicase DDX6	3	2.978	0.9925	0.88084
7	1PMV	Mitogen-activated protein kinase 10	3	2.974	0.9912	0.47884
<b>IV</b>						
1	1VEC	Probable ATP-dependent RNA helicase DDX6	3	2.971	0.9904	0.92058
2	2UYI	Kinesin-like protein KIF11	3	2.971	0.9903	0.86973
3	1PMV	Mitogen-activated protein kinase 10	3	2.97	0.9898	0.54878
4	1PQ9	Oxysterols receptor LXR-beta	3	2.968	0.9894	0.78082
5	1DVZ	Transthyretin	3	2.961	0.987	0.72532

<b>6</b>	<b>1UDU</b>	cGMP-specific 3,5-cyclic phosphodiesterase	3	2.927	0.9755	0.7342
<b>7</b>	<b>1UKI</b>	Mitogen-activated protein kinase 8	3	2.919	0.9728	0.52367
<b>V</b>						
<b>1</b>	<b>1PMV</b>	Mitogen-activated protein kinase 10	3	2.979	0.9931	0.45302
<b>2</b>	<b>1DVZ</b>	Transthyretin	3	2.978	0.9927	0.67553
<b>3</b>	<b>1PQ9</b>	Oxysterols receptor LXR-beta	3	2.971	0.9903	0.70581
<b>4</b>	<b>1W8M</b>	Peptidyl-prolyl cis-trans isomerase A	3	2.966	0.9888	0.67479
<b>5</b>	<b>1BM6</b>	Stromelysin-1	3	2.964	0.9881	0.56266
<b>6</b>	<b>1UKI</b>	Mitogen-activated protein kinase 8	3	2.952	0.9841	0.5335
<b>7</b>	<b>1VEC</b>	Probable ATP-dependent RNA helicase DDX6	3	2.938	0.9794	0.73317
<b>VI</b>						
<b>1</b>	<b>1F86</b>	Transthyretin	3	2.987	0.9955	0.59933
<b>2</b>	<b>1W7H</b>	Mitogen-activated protein kinase 14	3	2.982	0.994	0.8043
<b>3</b>	<b>1PMV</b>	Mitogen-activated protein kinase 10	3	2.972	0.9907	0.44316
<b>4</b>	<b>1PQ9</b>	Oxysterols receptor LXR-beta	3	2.971	0.9905	0.71801
<b>5</b>	<b>1VEC</b>	Probable ATP-dependent RNA helicase DDX6	3	2.966	0.9888	0.82767
<b>6</b>	<b>1SMD</b>	Alpha-amylase 1	3	2.955	0.9851	0.84318
<b>7</b>	<b>1UKI</b>	Mitogen-activated protein kinase 8	3	2.943	0.9811	0.51972
<b>VII</b>						
<b>1</b>	<b>1BM6</b>	Stromelysin-1	3	2.989	0.9962	0.81483
<b>2</b>	<b>1PQ9</b>	Oxysterols receptor LXR-beta	3	2.969	0.9897	0.84838
<b>3</b>	<b>1PMV</b>	Mitogen-activated protein kinase 10	3	2.946	0.9819	0.54626
<b>4</b>	<b>2NMX</b>	Carbonic anhydrase 1	3	2.942	0.9806	0.83863
<b>5</b>	<b>1SMD</b>	Alpha-amylase 1	3	2.932	0.9773	0.90627
<b>6</b>	<b>1UKI</b>	Mitogen-activated protein kinase 8	3	2.924	0.9746	0.61508
<b>7</b>	<b>1W8M</b>	Peptidyl-prolyl cis-trans isomerase A	3	2.923	0.9743	0.70825
<b>VIII</b>						
<b>1</b>	<b>2F6T</b>	Tyrosine-protein phosphatase non-receptor type 1	3	2.994	0.998	0.79482
<b>2</b>	<b>1VEC</b>	Probable ATP-dependent RNA helicase DDX6	3	2.98	0.9932	0.82852
<b>3</b>	<b>1PMV</b>	Mitogen-activated protein kinase 10	3	2.976	0.9921	0.40405
<b>4</b>	<b>1PQ9</b>	Oxysterols receptor LXR-beta	3	2.972	0.9907	0.687
<b>5</b>	<b>2JBP</b>	MAP kinase-activated protein kinase 2	3	2.961	0.9871	0.52817

<b>6</b>	<b>1UKI</b>	Mitogen-activated protein kinase 8	3	2.949	0.983	0.50611
<b>7</b>	<b>2Q08</b>	Carbonic anhydrase 2	3	2.948	0.9827	0.69319