

## Supplementary Information

### **An *in-silico* study on selected organosulfur compounds as potential drugs for SARS-CoV-2 infection *via* binding multiple drug targets**

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**Table S1.** SwissTargetPrediction report obtained using Lurasidone as the query molecule

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Serotonin 2a (5-HT <sub>2a</sub> ) receptor	HTR2A	P28223	CHEMBL224	Family A G protein-coupled receptor	0.608268278407	1243 / 163
Dopamine D2 receptor (by homology)	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0.599434549737	2915 / 337
Serotonin 1a (5-HT <sub>1a</sub> ) receptor	HTR1A	P08908	CHEMBL214	Family A G protein-coupled receptor	0.110612204199	1192 / 151
Serotonin 1b (5-HT <sub>1b</sub> ) receptor	HTR1B	P28222	CHEMBL1898	Family A G protein-coupled receptor	0.110612204199	392 / 3
Sigma opioid receptor	SIGMAR1	Q99720	CHEMBL287	Membrane receptor	0.110612204199	810 / 1
Serotonin 7 (5-HT <sub>7</sub> ) receptor	HTR7	P34969	CHEMBL3155	Family A G protein-coupled receptor	0.110612204199	639 / 49
C-C chemokine receptor type 3	CCR3	P51677	CHEMBL3473	Family A G protein-coupled receptor	0.110612204199	451 / 0
Delta opioid receptor	OPRD1	P41143	CHEMBL236	Family A G protein-coupled receptor	0.110612204199	1012 / 0
Melanocortin receptor 4	MC4R	P32245	CHEMBL259	Family A G protein-coupled receptor	0.110612204199	704 / 0
Melanocortin receptor 1	MC1R	Q01726	CHEMBL3795	Family A G protein-coupled receptor	0.110612204199	102 / 0
Melanocortin receptor 3	MC3R	P41968	CHEMBL4644	Family A G protein-coupled receptor	0.110612204199	146 / 0
Neurokinin 2 receptor	TACR2	P21452	CHEMBL2327	Family A G protein-coupled receptor	0.110612204199	175 / 0
Neurokinin 3 receptor	TACR3	P29371	CHEMBL4429	Family A G protein-coupled receptor	0.110612204199	126 / 0
P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	0.110612204199	125 / 0
Cathepsin L	CTSL	P07711	CHEMBL3837	Protease	0.110612204199	34 / 0
Serotonin 6 (5-HT <sub>6</sub> ) receptor	HTR6	P50406	CHEMBL3371	Family A G protein-coupled receptor	0.110612204199	220 / 30
ATP-sensitive inward rectifier potassium channel 1	KCNJ1	P48048	CHEMBL1293292	Voltage-gated ion channel	0.110612204199	20 / 0
Histamine H3 receptor	HRH3	Q9Y5N1	CHEMBL264	Family A G protein-coupled receptor	0.110612204199	544 / 0
Protein farnesyltransferase	FNTA FNTB	P49354 P49356	CHEMBL2094108	Enzyme	0.110612204199	126 / 0
Neurokinin 1 receptor	TACR1	P25103	CHEMBL249	Family A G protein-coupled receptor	0.110612204199	277 / 0
Beta-secretase 1	BACE1	P56817	CHEMBL4822	Protease	0.110612204199	111 / 0
Acetyl-CoA carboxylase 1	ACACA	Q13085	CHEMBL3351	Enzyme	0.110612204199	44 / 0
Phosphodiesterase 9A	PDE9A	O76083	CHEMBL3535	Phosphodiesterase	0.110612204199	14 / 0
Phosphodiesterase 1C	PDE1C	Q14123	CHEMBL4619	Phosphodiesterase	0.110612204199	12 / 0
Acetyl-CoA carboxylase 2	ACACB	O00763	CHEMBL4829	Ligase	0.110612204199	79 / 0
Dipeptidyl peptidase II	DPP7	Q9UHL4	CHEMBL3976	Protease	0.110612204199	149 / 0
Dipeptidyl peptidase VIII	DPP8	Q6V1X1	CHEMBL4657	Protease	0.110612204199	165 / 0
Alpha-1a adrenergic receptor	ADRA1A	P35348	CHEMBL229	Family A G protein-coupled receptor	0.110612204199	633 / 73

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Synaptic vesicular amine transporter (by homology)	SLC18A2	Q05940	CHEMBL1893	Electrochemical transporter	0.110612204199	20 / 0
Equilibrative nucleoside transporter 1	SLC29A1	Q99808	CHEMBL1997	Electrochemical transporter	0.110612204199	3 / 0
Alpha-2a adrenergic receptor	ADRA2A	P08913	CHEMBL1867	Family A G protein-coupled receptor	0.110612204199	81 / 0
Adrenergic receptor alpha-2	ADRA2C	P18825	CHEMBL1916	Family A G protein-coupled receptor	0.110612204199	70 / 0
Alpha-2b adrenergic receptor	ADRA2B	P18089	CHEMBL1942	Family A G protein-coupled receptor	0.110612204199	66 / 0
Max-like protein X	MLX	Q9UH92	CHEMBL2062357	Unclassified protein	0.110612204199	7 / 0
C-C chemokine receptor type 4	CCR4	P51679	CHEMBL2414	Family A G protein-coupled receptor	0.110612204199	31 / 0
Arachidonate 5-lipoxygenase	ALOX5	P09917	CHEMBL215	Oxidoreductase	0.110612204199	6 / 0
Poly [ADP-ribose] polymerase-1	PARP1	P09874	CHEMBL3105	Enzyme	0.110612204199	431 / 0
Serotonin 4 (5-HT4) receptor	HTR4	Q13639	CHEMBL1875	Family A G protein-coupled receptor	0.110612204199	53 / 0
Voltage-gated N-type calcium channel alpha-1B subunit	CACNA1B	Q00975	CHEMBL4478	Voltage-gated ion channel	0.110612204199	28 / 0
Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 4	HCN4	Q9Y3Q4	CHEMBL1250417	Voltage-gated ion channel	0.110612204199	18 / 0
Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 1	HCN1	O60741	CHEMBL1795171	Voltage-gated ion channel	0.110612204199	21 / 0
Inhibitor of nuclear factor kappa B kinase beta subunit	IKBKB	O14920	CHEMBL1991	Kinase	0.110612204199	32 / 0
Thrombin	F2	P00734	CHEMBL204	Protease	0.110612204199	397 / 0
Melanocortin receptor 5	MC5R	P33032	CHEMBL4608	Family A G protein-coupled receptor	0.110612204199	108 / 0
Ghrelin receptor	GHSR	Q92847	CHEMBL4616	Family A G protein-coupled receptor	0.110612204199	185 / 0
HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0.110612204199	712 / 28
C-C motif chemokine 5	CCL5	P13501	CHEMBL1275217	Family A G protein-coupled receptor	0.110612204199	22 / 0
Serotonin 3a (5-HT3a) receptor	HTR3A	P46098	CHEMBL1899	Ligand-gated ion channel	0.110612204199	70 / 0
LDL-associated phospholipase A2	PLA2G7	Q13093	CHEMBL3514	Enzyme	0.110612204199	12 / 0
Butyrylcholinesterase	BCHE	P06276	CHEMBL1914	Hydrolase	0.110612204199	93 / 0
Glucocorticoid receptor	NR3C1	P04150	CHEMBL2034	Nuclear receptor	0.110612204199	32 / 0
Vasopressin V2 receptor	AVPR2	P30518	CHEMBL1790	Family A G protein-	0.110612204199	75 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
				coupled receptor		
Oxytocin receptor	OXTR	P30559	CHEMBL2049	Family A G protein-coupled receptor	0.110612204199	52 / 0
Telomerase reverse transcriptase	TERT	O14746	CHEMBL2916	Enzyme	0.110612204199	25 / 0
Arachidonate 15-lipoxygenase	ALOX15	P16050	CHEMBL2903	Enzyme	0.110612204199	4 / 0
Kir3.1/Kir3.4	KCNJ5 KCNJ3	P48544 P48549	CHEMBL3038488	Voltage-gated ion channel	0.110612204199	20 / 0
C-X-C chemokine receptor type 3	CXCR3	P49682	CHEMBL4441	Family A G protein-coupled receptor	0.110612204199	73 / 0
Neuropeptide Y receptor type 2	NPY2R	P49146	CHEMBL4018	Family A G protein-coupled receptor	0.110612204199	26 / 0
Isocitrate dehydrogenase [NADP] cytoplasmic	IDH1	O75874	CHEMBL2007625	Enzyme	0.110612204199	12 / 0
Complement factor D	CFD	P00746	CHEMBL2176771	Protease	0.110612204199	63 / 0
Norepinephrine transporter	SLC6A2	P23975	CHEMBL222	Electrochemical transporter	0.110612204199	145 / 0
Lysosomal Pro-X carboxypeptidase	PRCP	P42785	CHEMBL2335	Protease	0.110612204199	147 / 0
Geranylgeranyl transferase type I beta subunit	PGGT1B	P53609	CHEMBL4135	Enzyme	0.110612204199	8 / 0
Tyrosine-protein kinase SYK	SYK	P43405	CHEMBL2599	Kinase	0.110612204199	137 / 0
Adenosylhomocysteinase	AHCY	P23526	CHEMBL2664	Enzyme	0.110612204199	31 / 0
Hematopoietic cell protein-tyrosine phosphatase 70Z-PEP	PTPN22	Q9Y2R2	CHEMBL2889	Phosphatase	0.110612204199	4 / 0
Cyclin-dependent kinase 2	CDK2	P24941	CHEMBL301	Kinase	0.110612204199	33 / 0
Serine/threonine-protein kinase PAK 4	PAK4	O96013	CHEMBL4482	Kinase	0.110612204199	37 / 0
Sphingosine 1-phosphate receptor Edg-3	S1PR3	Q99500	CHEMBL3892	Family A G protein-coupled receptor	0.110612204199	7 / 0
Hepatocyte growth factor receptor	MET	P08581	CHEMBL3717	Kinase	0.110612204199	126 / 0
c-Jun N-terminal kinase 1	MAPK8	P45983	CHEMBL2276	Kinase	0.110612204199	29 / 0
3-phosphoinositide dependent protein kinase-1	PDPK1	O15530	CHEMBL2534	Kinase	0.110612204199	46 / 0
Phospholipase D1	PLD1	Q13393	CHEMBL2536	Hydrolase	0.110612204199	71 / 0
c-Jun N-terminal kinase 3	MAPK10	P53779	CHEMBL2637	Kinase	0.110612204199	28 / 0
Phospholipase D2	PLD2	O14939	CHEMBL2734	Hydrolase	0.110612204199	60 / 0
Bcl2-antagonist of cell death (BAD)	BAD	Q92934	CHEMBL3817	Other cytosolic protein	0.110612204199	5 / 0
Apoptosis regulator Bcl-2	BCL2	P10415	CHEMBL4860	Other ion channel	0.110612204199	28 / 0
Heat shock protein HSP 90-alpha	HSP90AA1	P07900	CHEMBL3880	Other cytosolic protein	0.110612204199	56 / 0
Voltage-gated T-type calcium channel	CACNA1H	O95180	CHEMBL1859	Voltage-gated ion channel	0.110612204199	26 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
alpha-1H subunit						
Cannabinoid receptor 1	CNR1	P21554	CHEMBL218	Family A G protein-coupled receptor	0.110612204199	95 / 0
Adenosine A3 receptor	ADORA3	P0DMS8	CHEMBL256	Family A G protein-coupled receptor	0.110612204199	13 / 0
Poly [ADP-ribose] polymerase 2	PARP2	Q9UGN5	CHEMBL5366	Enzyme	0.110612204199	32 / 0
Voltage-gated T-type calcium channel alpha-11 subunit	CACNA11	Q9P0X4	CHEMBL5558	Voltage-gated ion channel	0.110612204199	17 / 0
Histamine H2 receptor	HRH2	P25021	CHEMBL1941	Family A G protein-coupled receptor	0.110612204199	22 / 0
Epidermal growth factor receptor erbB1	EGFR	P00533	CHEMBL203	Kinase	0.110612204199	298 / 0
Adrenergic receptor beta	ADRB2	P07550	CHEMBL210	Family A G protein-coupled receptor	0.110612204199	12 / 0
Beta-1 adrenergic receptor	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor	0.110612204199	21 / 0
Glycogen synthase kinase-3 beta	GSK3B	P49841	CHEMBL262	Kinase	0.110612204199	44 / 0
Thymidine kinase, cytosolic	TK1	P04183	CHEMBL2883	Transferase	0.110612204199	2 / 0
Sphingosine-1-phosphate lyase 1	SGPL1	O95470	CHEMBL3286061	Enzyme	0.110612204199	13 / 0
MAP kinase ERK2	MAPK1	P28482	CHEMBL4040	Kinase	0.110612204199	131 / 0
ATP-binding cassette sub-family G member 2	ABCG2	Q9UNQ0	CHEMBL5393	Primary active transporter	0.110612204199	22 / 0
Serine/threonine-protein kinase MARK1	MARK1	Q9P0L2	CHEMBL5940	Kinase	0.110612204199	4 / 0
Tissue-type plasminogen activator	PLAT	P00750	CHEMBL1873	Protease	0.110612204199	20 / 0
C-X-C chemokine receptor type 7	ACKR3	P25106	CHEMBL2010631	Family A G protein-coupled receptor	0.110612204199	25 / 0
Trypsin I	PRSS1	P07477	CHEMBL209	Protease	0.110612204199	76 / 0
Gamma-secretase	PSEN2 PSENEN NCSTN APH1A PSEN1 APH1B	P49810 Q9NZ42 Q92542 Q96BI3 P49768 Q8WW43	CHEMBL2094135	Protease	0.110612204199	96 / 0
Vascular endothelial growth factor receptor 2	KDR	P35968	CHEMBL279	Kinase	0.110612204199	196 / 0
Protein kinase C beta	PRKCB	P05771	CHEMBL3045	Kinase	0.110612204199	150 / 0
Neuropeptide Y receptor type 5	NPY5R	Q15761	CHEMBL4561	Family A G protein-coupled receptor	0.110612204199	21 / 0

**Table S2.** SwissTargetPrediction report obtained using Lurasidone\_Exo as the query molecule

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Dopamine D2 receptor (by homology)	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0.693886270949	677 / 291
Serotonin 2a (5-HT2a) receptor	HTR2A	P28223	CHEMBL224	Family A G protein-coupled receptor	0.449078210826	440 / 145
Sigma opioid receptor	SIGMAR1	Q99720	CHEMBL287	Membrane receptor	0.103186936728	296 / 1
Serotonin 1b (5-HT1b) receptor	HTR1B	P28222	CHEMBL1898	Family A G protein-coupled receptor	0.103186936728	83 / 1
Scavenger receptor class B member 1 (by homology)	SCARB1	Q8WTV0	CHEMBL1914272	Unclassified protein	0.103186936728	13 / 0
Serotonin 1a (5-HT1a) receptor	HTR1A	P08908	CHEMBL214	Family A G protein-coupled receptor	0.103186936728	256 / 102
Neurokinin 3 receptor	TACR3	P29371	CHEMBL4429	Family A G protein-coupled receptor	0.103186936728	18 / 0
Cyclin-dependent kinase 9	CDK9	P50750	CHEMBL3116	Kinase	0.103186936728	85 / 0
Apoptosis regulator Bcl-2	BCL2	P10415	CHEMBL4860	Other ion channel	0.103186936728	225 / 0
Neurokinin 2 receptor	TACR2	P21452	CHEMBL2327	Family A G protein-coupled receptor	0.103186936728	215 / 0
Delta opioid receptor	OPRD1	P41143	CHEMBL236	Family A G protein-coupled receptor	0.103186936728	484 / 0
C-C chemokine receptor type 3	CCR3	P51677	CHEMBL3473	Family A G protein-coupled receptor	0.103186936728	190 / 0
HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0.103186936728	475 / 30
Dopamine transporter (by homology)	SLC6A3	Q01959	CHEMBL238	Electrochemical transporter	0.103186936728	319 / 0
Orexin receptor 2	HCRTR2	O43614	CHEMBL4792	Family A G protein-coupled receptor	0.103186936728	9 / 0
Orexin receptor 1	HCRTR1	O43613	CHEMBL5113	Family A G protein-coupled receptor	0.103186936728	9 / 0
Beta-secretase 1	BACE1	P56817	CHEMBL4822	Protease	0.103186936728	744 / 0
Cathepsin D	CTSD	P07339	CHEMBL2581	Protease	0.103186936728	266 / 0
Adrenergic receptor beta	ADRB2	P07550	CHEMBL210	Family A G protein-coupled receptor	0.103186936728	302 / 0
Histamine H2 receptor	HRH2	P25021	CHEMBL1941	Family A G protein-coupled receptor	0.103186936728	14 / 0
3-phosphoinositide dependent protein kinase-1	PDPK1	O15530	CHEMBL2534	Kinase	0.103186936728	68 / 0
Serine/ threonine-protein kinase AKT	AKT1	P31749	CHEMBL4282	Kinase	0.103186936728	140 / 0
Acetyl-CoA carboxylase 1	ACACA	Q13085	CHEMBL3351	Enzyme	0.103186936728	2 / 0
Acetyl-CoA carboxylase 2	ACACB	O00763	CHEMBL4829	Ligase	0.103186936728	65 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
p53-binding protein Mdm-2	MDM2	Q00987	CHEMBL5023	Other nuclear protein	0.103186936728	165 / 0
Tyrosine-protein kinase FYN	FYN	P06241	CHEMBL1841	Kinase	0.103186936728	19 / 0
Platelet-derived growth factor receptor beta	PDGFRB	P09619	CHEMBL1913	Kinase	0.103186936728	25 / 0
Tyrosine-protein kinase YES	YES1	P07947	CHEMBL2073	Kinase	0.103186936728	14 / 0
Tyrosine-protein kinase LCK	LCK	P06239	CHEMBL258	Kinase	0.103186936728	75 / 0
Tyrosine-protein kinase SRC	SRC	P12931	CHEMBL267	Kinase	0.103186936728	169 / 0
Vascular endothelial growth factor receptor 2	KDR	P35968	CHEMBL279	Kinase	0.103186936728	277 / 0
Melanin-concentrating hormone receptor 1	MCHR1	Q99705	CHEMBL344	Family A G protein-coupled receptor	0.103186936728	287 / 0
Fibroblast growth factor receptor 1	FGFR1	P11362	CHEMBL3650	Kinase	0.103186936728	97 / 0
Inhibitor of apoptosis protein 3	XIAP	P98170	CHEMBL4198	Other cytosolic protein	0.103186936728	124 / 0
HLA-DR antigens-associated invariant chain	CD74	P04233	CHEMBL4692	Surface antigen	0.103186936728	5 / 0
Alpha-1a adrenergic receptor	ADRA1A	P35348	CHEMBL229	Family A G protein-coupled receptor	0.103186936728	193 / 58
Norepinephrine transporter	SLC6A2	P23975	CHEMBL222	Electrochemical transporter	0.103186936728	110 / 0
Histamine H3 receptor	HRH3	Q9Y5N1	CHEMBL264	Family A G protein-coupled receptor	0.103186936728	257 / 0
6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase 3	PFKFB3	Q16875	CHEMBL2331053	Enzyme	0.103186936728	84 / 0
Neuropeptide Y receptor type 1	NPY1R	P25929	CHEMBL4777	Family A G protein-coupled receptor	0.103186936728	74 / 0
Voltage-gated T-type calcium channel alpha-1H subunit	CACNA1H	O95180	CHEMBL1859	Voltage-gated ion channel	0.103186936728	8 / 0
Alpha-2a adrenergic receptor	ADRA2A	P08913	CHEMBL1867	Family A G protein-coupled receptor	0.103186936728	69 / 0
Adrenergic receptor alpha-2	ADRA2C	P18825	CHEMBL1916	Family A G protein-coupled receptor	0.103186936728	70 / 0
Alpha-2b adrenergic receptor	ADRA2B	P18089	CHEMBL1942	Family A G protein-coupled receptor	0.103186936728	60 / 0
Melanocortin receptor 4	MC4R	P32245	CHEMBL259	Family A G protein-coupled receptor	0.103186936728	128 / 0
PI3-kinase p110-delta subunit	PIK3CD	O00329	CHEMBL3130	Enzyme	0.103186936728	126 / 0
Glycine transporter 1	SLC6A9	P48067	CHEMBL2337	Electrochemical transporter	0.103186936728	65 / 0
Methionine	METAP1	P53582	CHEMBL2474	Protease	0.103186936728	11 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
aminopeptidase 1						
DNA-dependent protein kinase	PRKDC	P78527	CHEMBL3142	Kinase	0.103186936728	92 / 0
Serine/threonine-protein kinase AKT2	AKT2	P31751	CHEMBL2431	Kinase	0.103186936728	60 / 0
Heat shock protein HSP 90-beta	HSP90AB1	P08238	CHEMBL4303	Other cytosolic protein	0.103186936728	42 / 0
Serine/threonine-protein kinase AKT	AKT3	Q9Y243	CHEMBL4816	Kinase	0.103186936728	39 / 0
Insulin-like growth factor I receptor	IGF1R	P08069	CHEMBL1957	Kinase	0.103186936728	214 / 0
Phosphodiesterase 8B	PDE8B	O95263	CHEMBL4408	Phosphodiesterase	0.103186936728	23 / 0
Vesicular acetylcholine transporter	SLC18A3	Q16572	CHEMBL4767	Electrochemical transporter	0.103186936728	148 / 0
Tyrosine-protein kinase JAK3	JAK3	P52333	CHEMBL2148	Kinase	0.103186936728	119 / 0
Tyrosine-protein kinase JAK2	JAK2	O60674	CHEMBL2971	Kinase	0.103186936728	185 / 0
Protein kinase C beta	PRKCB	P05771	CHEMBL3045	Kinase	0.103186936728	113 / 0
P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	0.103186936728	138 / 0
Synaptic vesicular amine transporter (by homology)	SLC18A2	Q05940	CHEMBL1893	Electrochemical transporter	0.103186936728	61 / 0
Phosphodiesterase 9A	PDE9A	O76083	CHEMBL3535	Phosphodiesterase	0.103186936728	17 / 0
Phosphodiesterase 1C	PDE1C	Q14123	CHEMBL4619	Phosphodiesterase	0.103186936728	11 / 0
Cannabinoid receptor 2 (by homology)	CNR2	P34972	CHEMBL253	Family A G protein-coupled receptor	0.103186936728	205 / 0
Cystic fibrosis transmembrane conductance regulator	CFTR	P13569	CHEMBL4051	Other ion channel	0.103186936728	4 / 0
Vasopressin V2 receptor	AVPR2	P30518	CHEMBL1790	Family A G protein-coupled receptor	0.103186936728	37 / 0
Oxytocin receptor	OXTR	P30559	CHEMBL2049	Family A G protein-coupled receptor	0.103186936728	37 / 0
Beta-1 adrenergic receptor	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor	0.103186936728	268 / 0
Serotonin 7 (5-HT7) receptor	HTR7	P34969	CHEMBL3155	Family A G protein-coupled receptor	0.103186936728	76 / 33
Vasopressin V1a receptor (by homology)	AVPR1A	P37288	CHEMBL1889	Family A G protein-coupled receptor	0.103186936728	37 / 0
Glycine transporter 2	SLC6A5	Q9Y345	CHEMBL3060	Electrochemical transporter	0.103186936728	6 / 0
Beta amyloid A4 protein	APP	P05067	CHEMBL2487	Membrane receptor	0.103186936728	27 / 0
Sphingosine kinase 2	SPHK2	Q9NRA0	CHEMBL3023	Enzyme	0.103186936728	41 / 0



Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Sphingosine kinase 1	SPHK1	Q9NYA1	CHEMBL4394	Enzyme	0.103186936728	77 / 0
ATP-sensitive inward rectifier potassium channel 1	KCNJ1	P48048	CHEMBL1293292	Voltage-gated ion channel	0.103186936728	50 / 0
Epidermal growth factor receptor erbB1	EGFR	P00533	CHEMBL203	Kinase	0.103186936728	279 / 0
Gamma-secretase	PSEN2 PSENEN NCSTN APH1A PSEN1 APH1B	P49810 Q9NZ42 Q92542 Q96BI3 P49768 Q8WW43	CHEMBL2094135	Protease	0.103186936728	72 / 0
Neuropeptide Y receptor type 5	NPY5R	Q15761	CHEMBL4561	Family A G protein-coupled receptor	0.103186936728	15 / 0
Serotonin 1d (5-HT1d) receptor	HTR1D	P28221	CHEMBL1983	Family A G protein-coupled receptor	0.103186936728	90 / 0
Voltage-gated T-type calcium channel alpha-1I subunit	CACNA1I	Q9P0X4	CHEMBL5558	Voltage-gated ion channel	0.103186936728	4 / 0
Bromodomain-containing protein 4	BRD4	O60885	CHEMBL1163125	Reader	0.103186936728	17 / 0
Cyclin-dependent kinase 4/cyclin D1	CCND1 CDK4	P24385 P11802	CHEMBL1907601	Kinase	0.103186936728	59 / 0
Thrombin	F2	P00734	CHEMBL204	Protease	0.103186936728	148 / 0
Cyclin-dependent kinase 2/cyclin E	CCNE2 CDK2 CCNE1	O96020 P24941 P24864	CHEMBL2094126	Other cytosolic protein	0.103186936728	70 / 0
ATPase family AAA domain-containing protein 2	ATAD2	Q6PL18	CHEMBL2150837	Reader	0.103186936728	6 / 0
Serine/threonine-protein kinase mTOR	MTOR	P42345	CHEMBL2842	Kinase	0.103186936728	604 / 0
Heat shock protein HSP 90-alpha	HSP90AA1	P07900	CHEMBL3880	Other cytosolic protein	0.103186936728	100 / 0
PI3-kinase p110-alpha subunit	PIK3CA	P42336	CHEMBL4005	Enzyme	0.103186936728	485 / 0
Butyrylcholinesterase	BCHE	P06276	CHEMBL1914	Hydrolase	0.103186936728	20 / 0
Protein farnesyltransferase	FNTA FNTB	P49354 P49356	CHEMBL2094108	Enzyme	0.103186936728	49 / 0
Tyrosine-protein kinase SYK	SYK	P43405	CHEMBL2599	Kinase	0.103186936728	417 / 0
Poly [ADP-ribose] polymerase-1	PARP1	P09874	CHEMBL3105	Enzyme	0.103186936728	58 / 0
Tyrosine-protein kinase receptor FLT3	FLT3	P36888	CHEMBL1974	Kinase	0.103186936728	98 / 0
Cyclin-dependent kinase 2/cyclin A	CDK2 CCNA1 CCNA2	P24941 P78396 P20248	CHEMBL2094128	Other cytosolic protein	0.103186936728	38 / 0
Gonadotropin-releasing hormone receptor	GNRHR	P30968	CHEMBL1855	Family A G protein-coupled receptor	0.103186936728	79 / 0
Vitamin D receptor	VDR	P11473	CHEMBL1977	Nuclear receptor	0.103186936728	66 / 0
Beta-3 adrenergic	ADRB3	P13945	CHEMBL246	Family A G protein-	0.103186936728	235 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
receptor				coupled receptor		
Programmed cell death 1 ligand 1	CD274	Q9NZQ7	CHEMBL3580522	Unclassified protein	0.103186936728	3 / 0
Urotensin II receptor	UTS2R	Q9UKP6	CHEMBL3764	Family A G protein-coupled receptor	0.103186936728	35 / 0
Dual specificity protein kinase TTK	TTK	P33981	CHEMBL3983	Kinase	0.103186936728	26 / 0
Potassium channel subfamily K member 3	KCNK3	O14649	CHEMBL2321613	Voltage-gated ion channel	0.103186936728	2 / 0