Supplementary Information

Plant-derived natural polyphenols as potential antiviral drugs against SARS-CoV-2 *via* RNA-dependent RNA polymerase (RdRp) inhibition: An *in-silico* analysis

Satyam Singh[1], Md Fulbabu Sk[1], Avinash Sonawane[1], Parimal Kar[1], Sushabhan Sadhukhan[2*]

[1]Discipline of Biosciences and Biomedical Engineering, Indian Institute of Technology Indore, Madhya Pradesh 453 552, India

[2]Discipline of Chemistry, Indian Institute of Technology Palakkad, Kerala 678 557, India

*Corresponding author. *E-mail address*: sushabhan@iitpkd.ac.in (S. Sadhukhan).

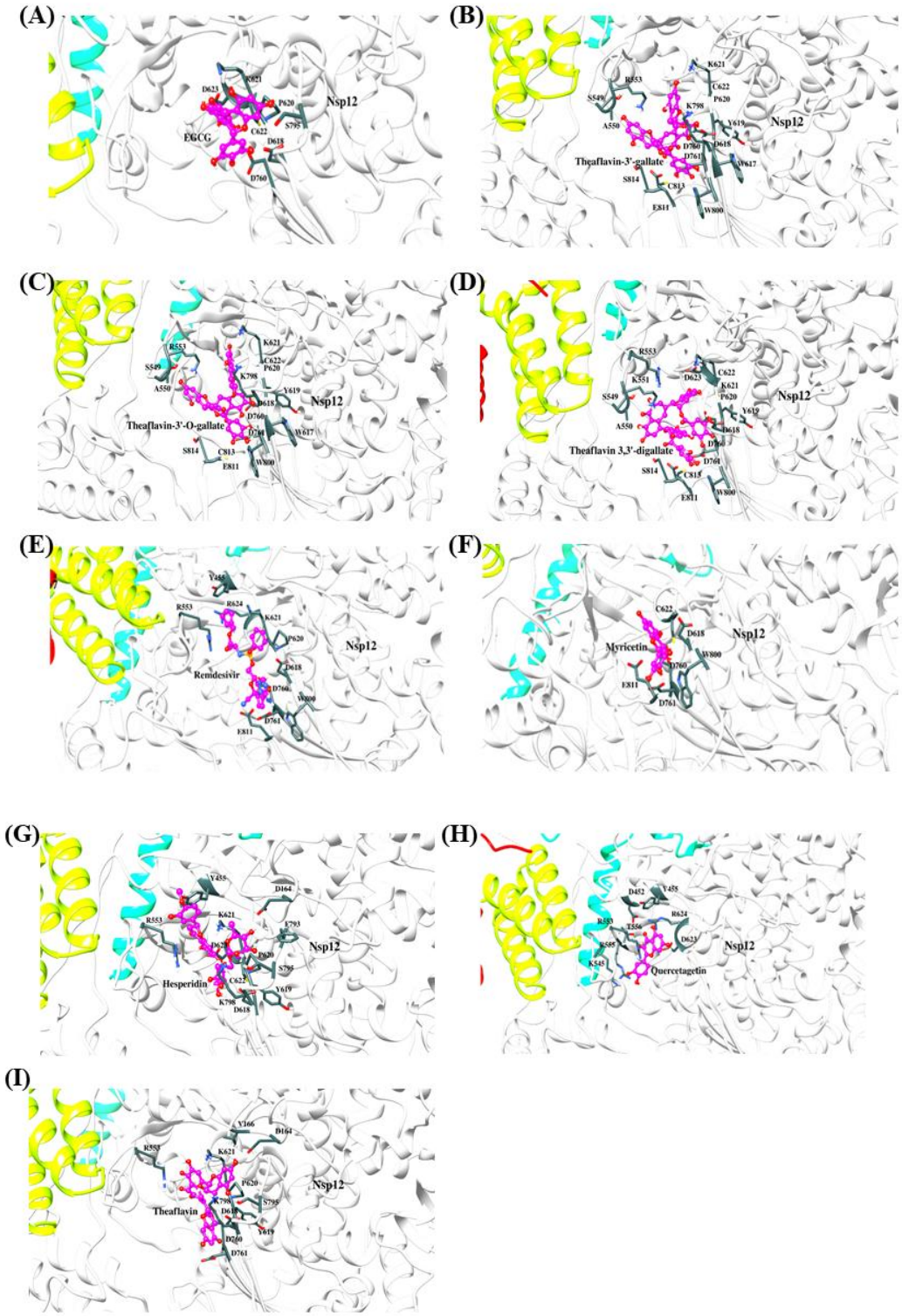


Figure S1. Best docked conformation of SARS-CoV-2 RdRp complexed with (A) EGCG, (B) TF2a, (C) TF2b, (D) TF3, (E) remdesivir, (F) myricetin, (G) hesperidin, (H) quercetagetin, (I) TF1.

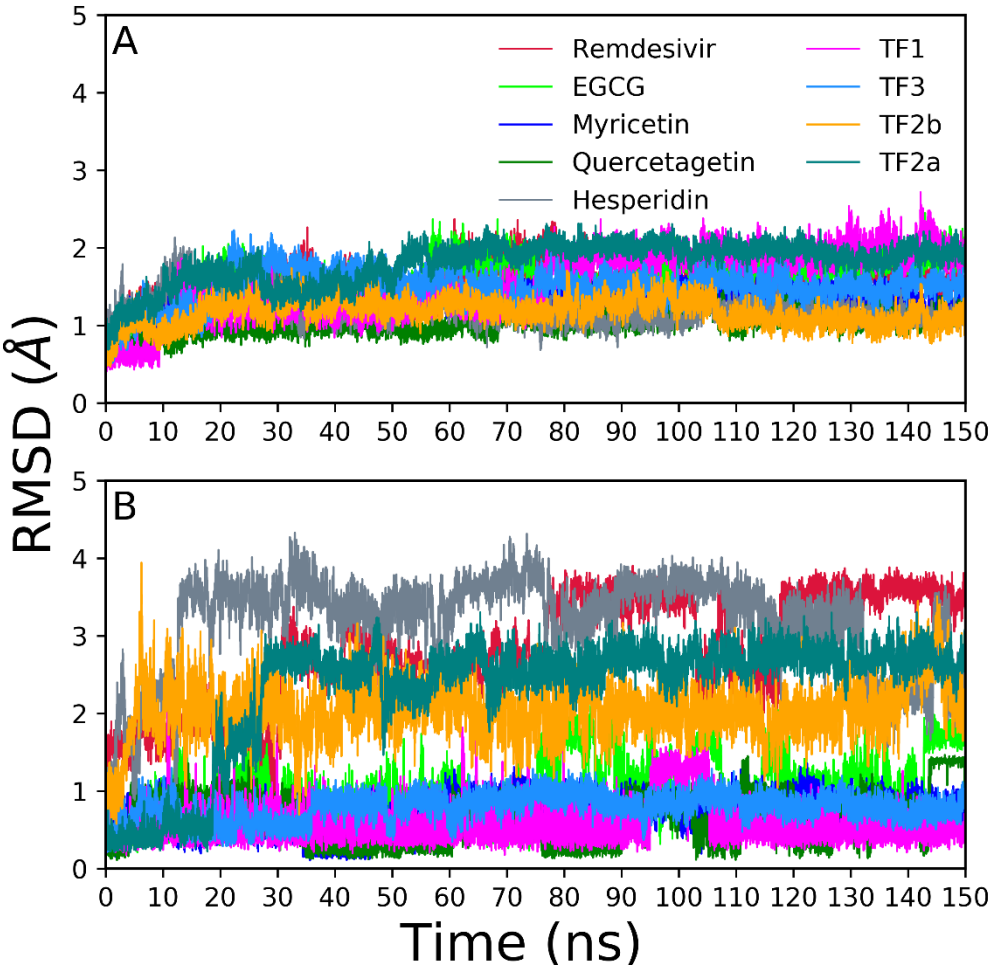


Figure S2. Time evolution of root-mean-square deviations (RMSDs) relative to their initial conformation of the RdRp complexes (**A**) for residue backbone atoms of binding pocket (5 Å around the ligand), and (**B**) for the ligands.

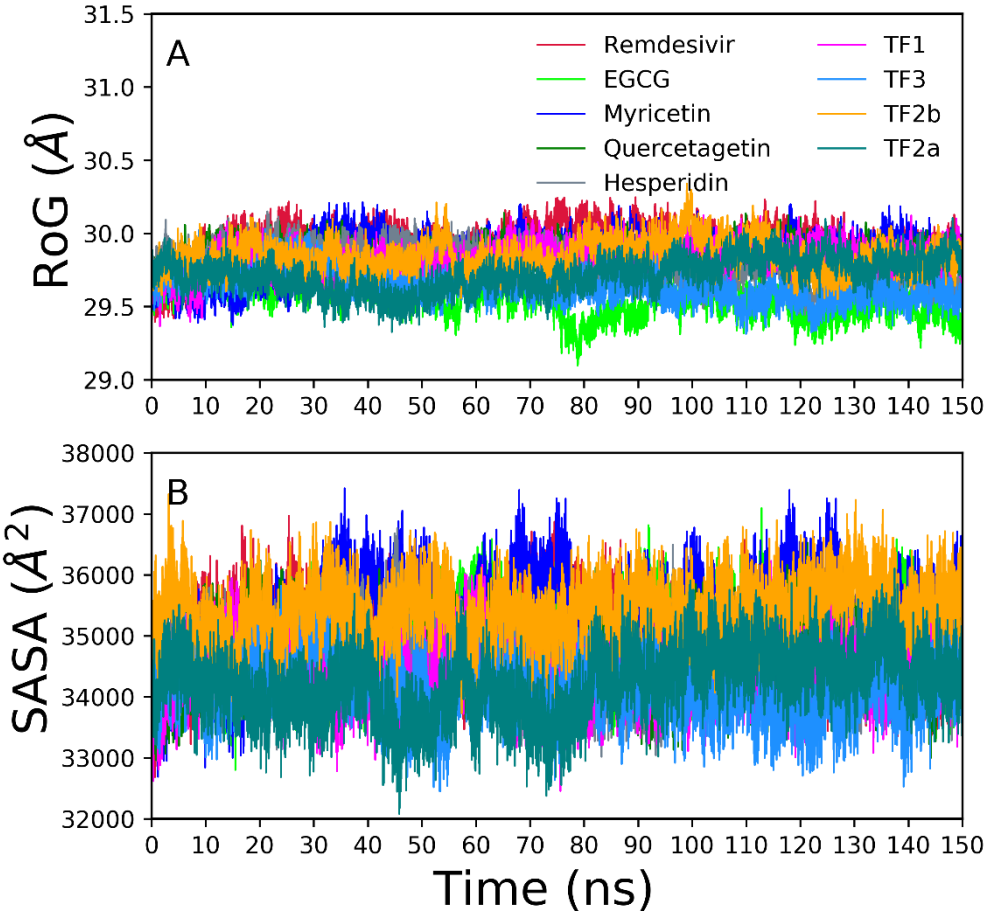
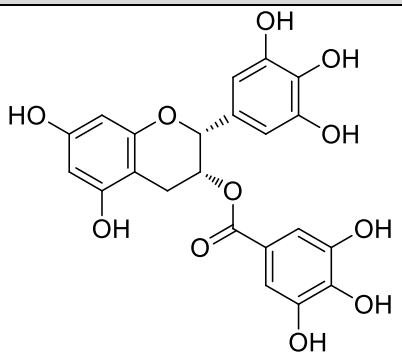
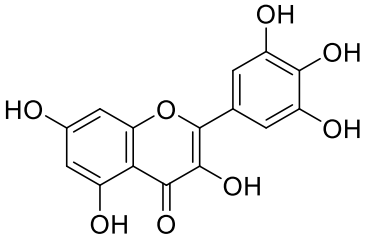
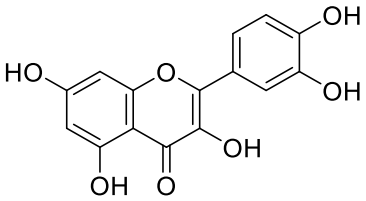
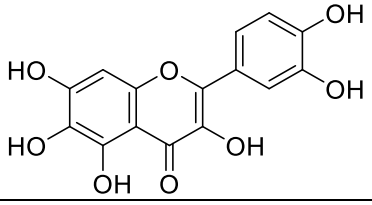
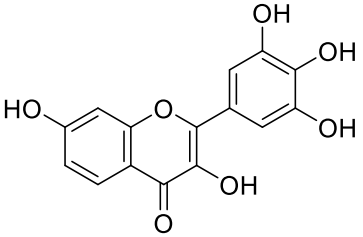
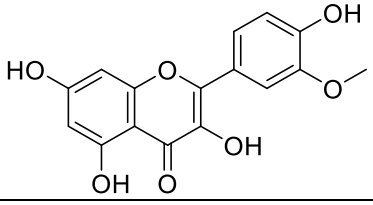
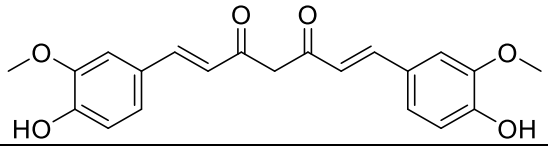
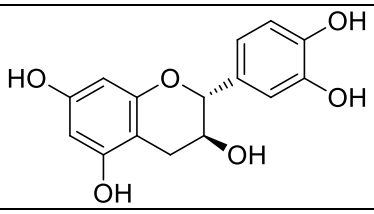
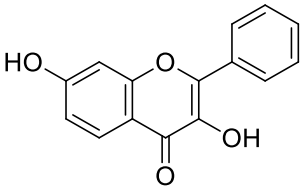
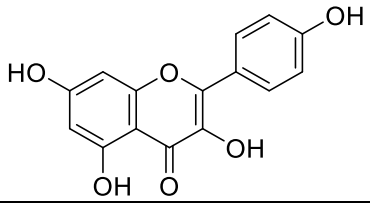
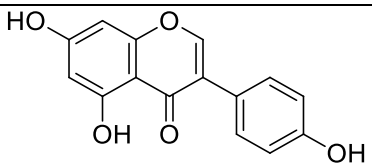
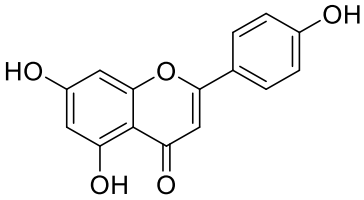
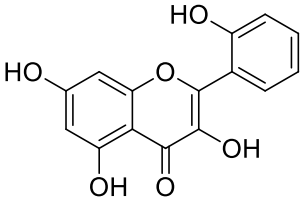
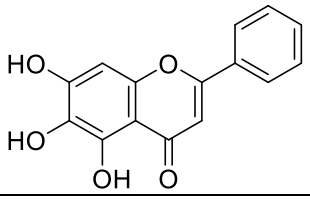
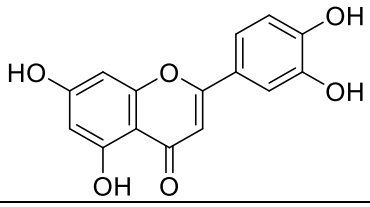
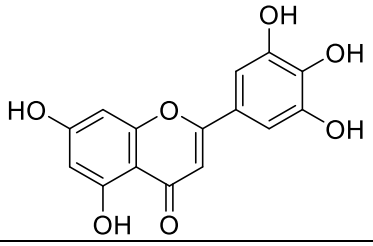
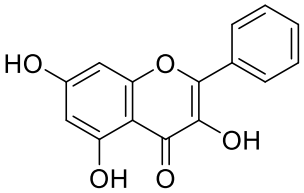
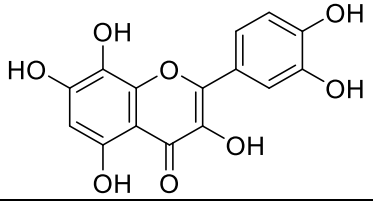
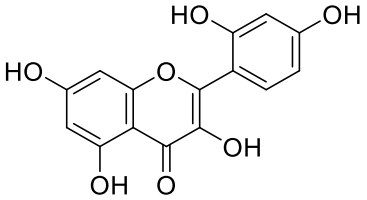
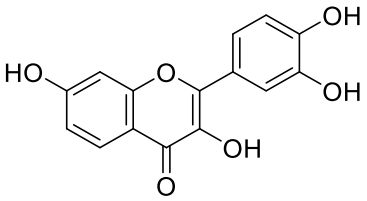
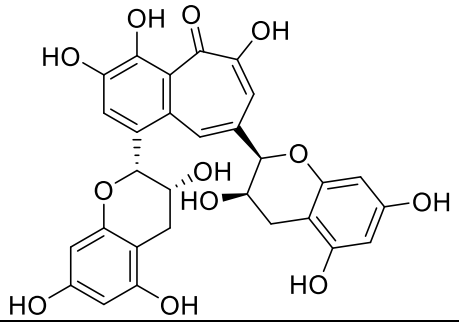
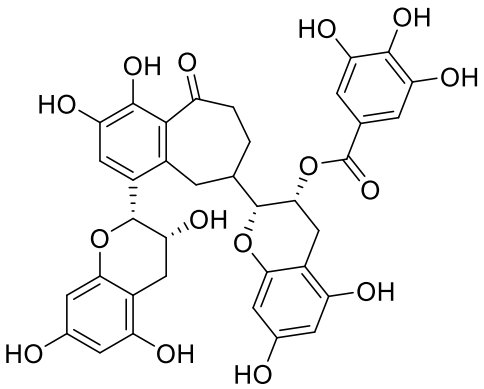


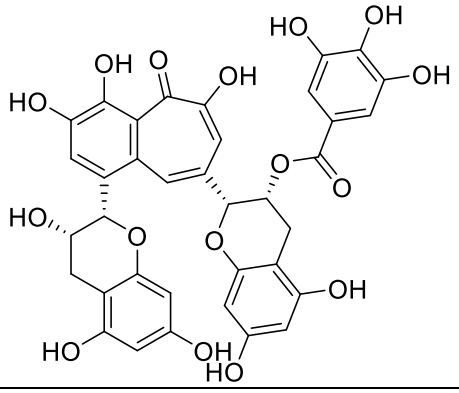
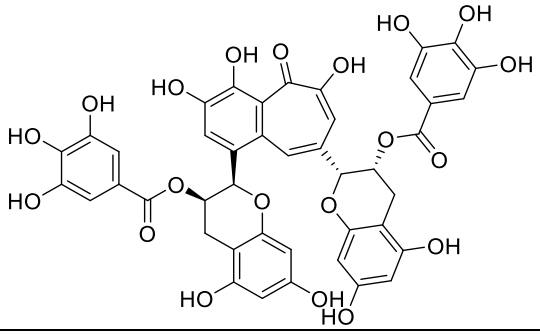
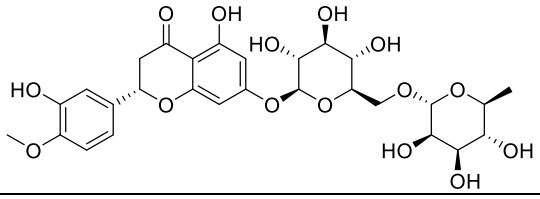
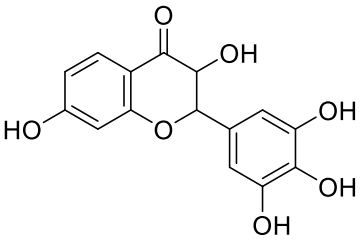
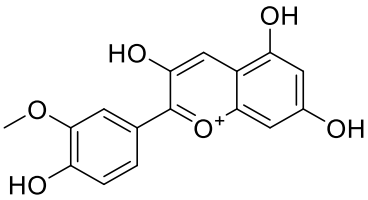
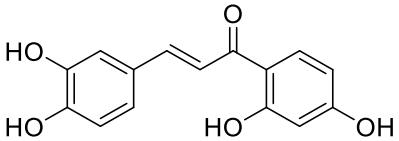
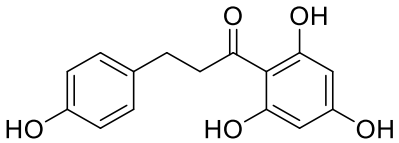
Figure S3. The time evolution of (**A**) the radius of gyration (RoG) and (**B**) solvent accessible surface area (SASA) of the RdRp complexes during MD simulations.

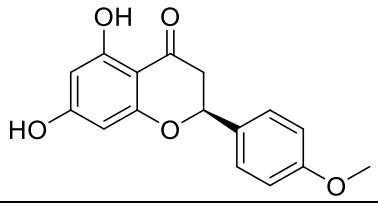
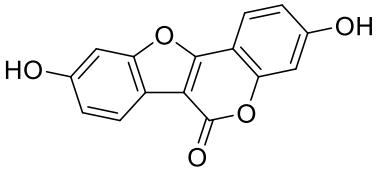
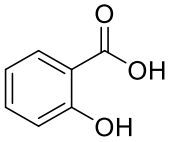
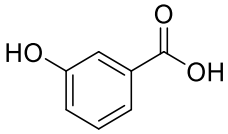
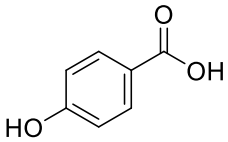
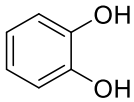
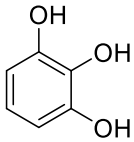
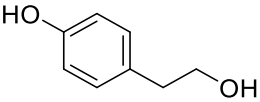
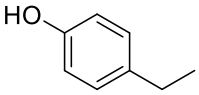
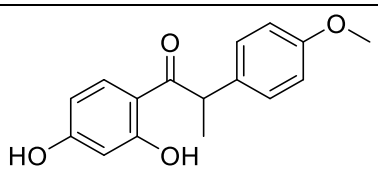
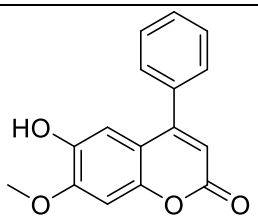
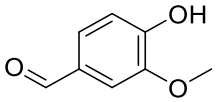
Table S1. Chemical structure and natural source for the hundred polyphenols selected for the current study.

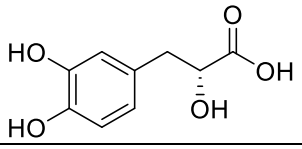
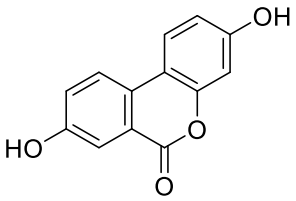
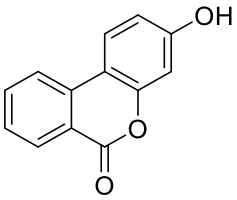
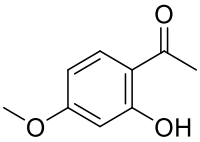
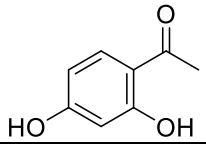
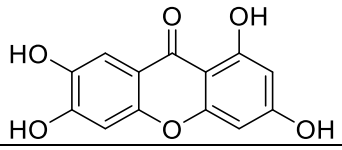
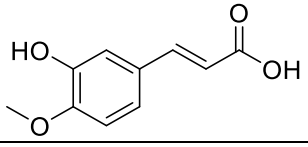
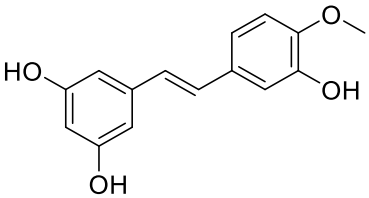
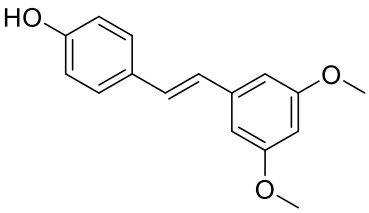
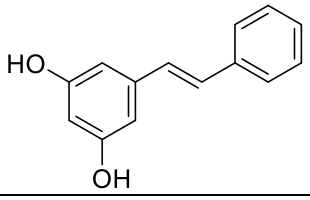
S. No.	Compound (PubChem CID No.)	Structure	Common Sources
1	EGCG (65064)		*Camellia sinensis*
2	Myricetin (5281672)		*Myristica fragrans*
3	Quercetin (5280343)		*Azadirachta indica*
4	Quercetagetin (5281680)		*Eupatorium gracile*
5	Robinetin (5280647)		*Vaccinium corymbosum*
6	Isorhamnetin (5281654)		*Solanum lycopersicum*

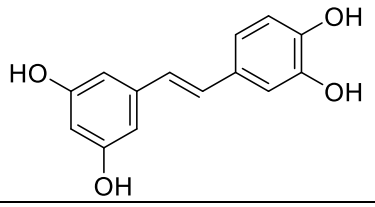
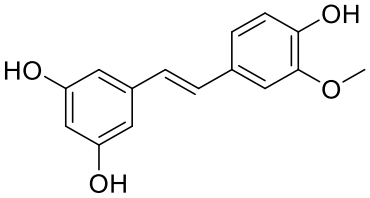
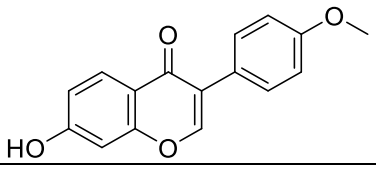
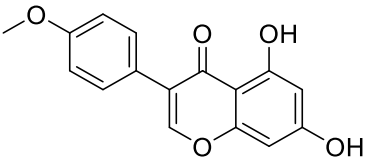
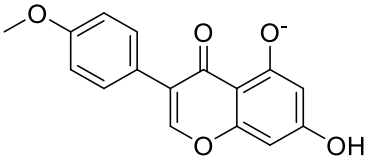
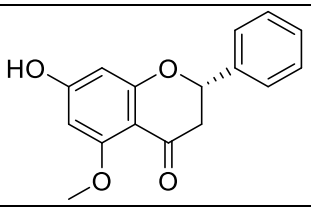
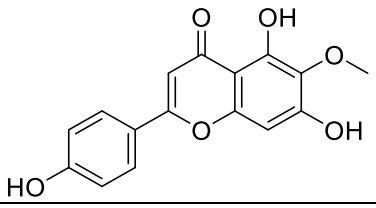
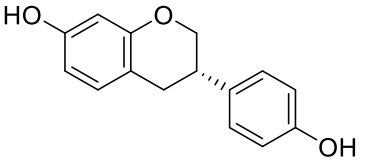
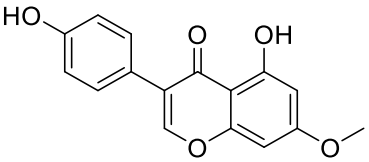
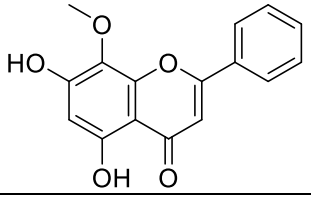
7	Curcumin (969516)		*Curcuma longa*
8	Catechin (73160)		*Vitis vinifera*
9	5-Deoxygalangin (5393152)		*Spatholobus subrectus*
10	Kaempferol (5280863)		*Brassica oleracea var. italica*
11	Genistein (5280961)		*Coffea arabica*
12	Apigenin (5280443)		*Camellia sinensis*
13	Datiscetin (5281610)		*Datisca cannabina*
14	Baicalein (5281605)		*Scutellaria baicalensis*
15	Luteolin (5280445)		*Bacopa moneirra*

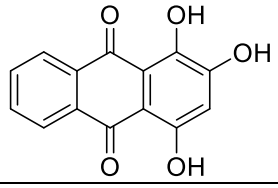
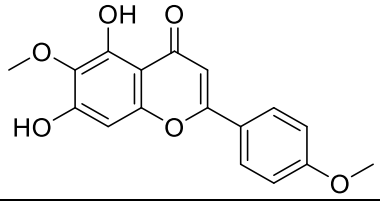
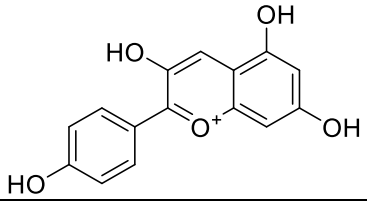
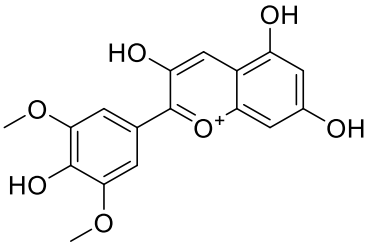
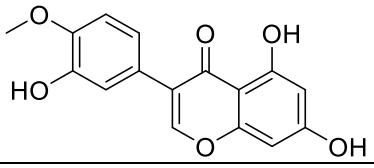
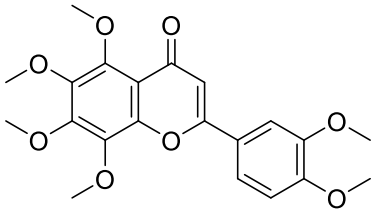
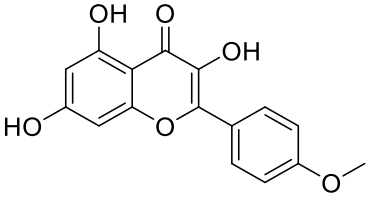
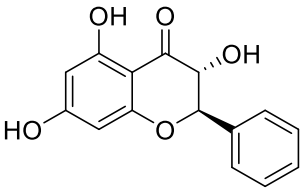
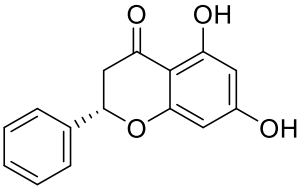
16	Tricetin (5281701)		*Eucalyptus globus*
17	Galangin (5281616)		*Alpinia officinarum*
18	Gossypetin (5280647)		*Hibiscus sabdariffa*
19	Morin (5281670)		*Artocarpus heterophyllus*
20	Fisetin (5281614)		*Rhus cotinus*
21	Theaflavin (135403798)		*Camellia sinensis*
22	Theaflavin-3’-O-gallate (71307578)		*Camellia sinensis*

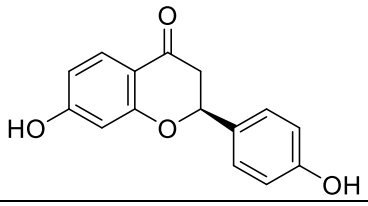
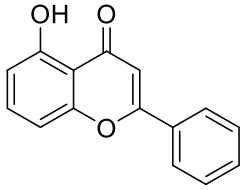
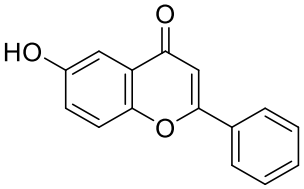
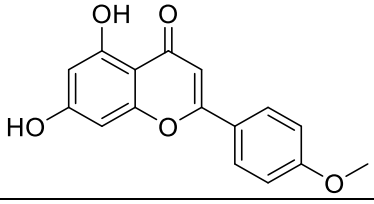
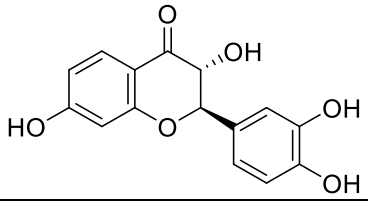
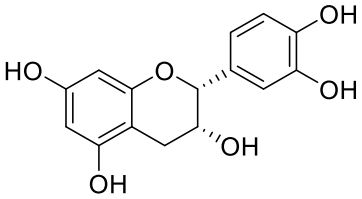
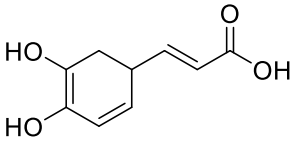
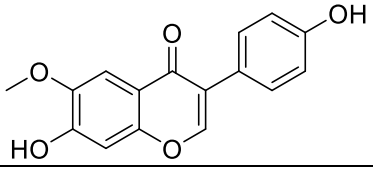
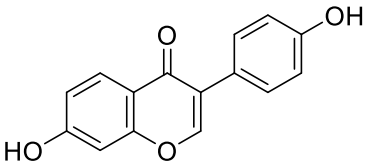
23	Theaflavin 3'-gallate (136825043)		*Camellia sinensis*
24	Theaflavin 3, 3'-digallate (135403795)		*Camellia sinensis*
25	Hesperidin (10621)		*Citrus medica*
26	Dihydrorobinetin (203990		*Vaccinium corymbosum*
27	Peonidin (441773)		*Paeonia lactiflora*
28	Butein (5281222)		*Butea monosperma*
29	Phloretin (4788)		*Malus domestica*

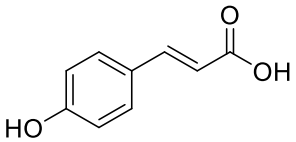
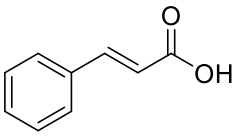
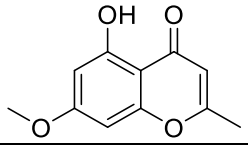
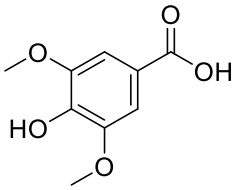
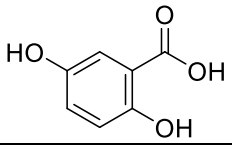
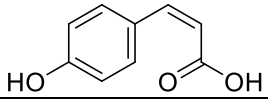
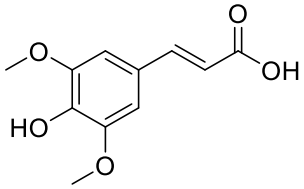
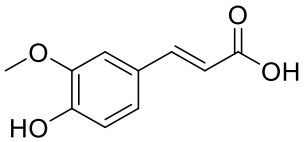
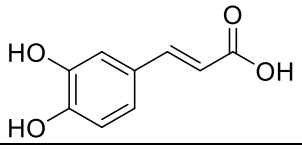
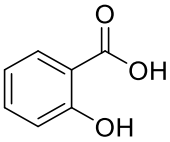
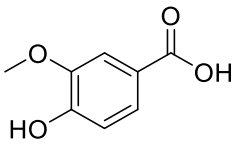
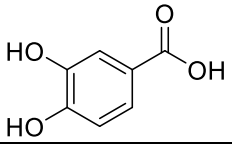
30	Isosakuranetin (160481)		*Salvia elegans*
31	Coumestrol (5281707)		*Medicago sativa*
32	2-hydroxybenzoic acid (450660)		*Catharanthus roseus*
33	3-hydroxybenzoic acid (7420)		*Catharanthus roseus*
34	4-hydroxybenzoic acid (135)		*Catharanthus roseus*
35	Catechol (289)		*Senegalia catechu*
36	Pyrogallol (1057)		*Myriophyllum spicatum*
37	Tyrosol (10393)		*Olea europaea*
38	4-ethylphenol (31242)		*Larrea divaricata*
39	Angolensin (3584988)		*Trifolium pratense*
40	Dalbergin (442768)		*Mesua thwaitesii*
41	Vanillin (1183)		*Vanillia planifolia*

42	Danshensu (11600642)		*Salvia clandestina*
43	Urolithin A (5488186)		*Punica grantum*
44	Urolithin B (5380406)		*Punica grantum*
45	Paeonol (11092)		*Paeonia suffruticosa*
46	Resacetophenone (6990)		*Cistus monospeliensis*
47	Norathyriol (5281656)		*Gracinia mangostana*
48	Isoferulic acid (736186)		*Capsicum annuum*
49	Rhapontigenin (5320954)		*Vitis coignetiae*
50	Pterostilbene (5281727)		*Pterocarpus marsupium*
51	Pinosylvin (5280457)		*Gnetum cliestostachyum*

52	Piceatannol (667639)		*Laburnum anagyroides*
53	Isorhapontigenin (5318650)		*Vitis coignetiae*
54	Formononetin (5280378)		*Trifolium pratense*
55	Biochanin A (528073)		*Medicago sativa*
56	Biochanin (1-) A (25203224)		*Medicago sativa*
57	Alpinetin (154279)		*Alpinia katsumadai*
58	Hispidulin (5281628)		*Grindelia argentina*
59	R-(+) Equol (6950272)		*Pueraria mirifica*
60	Prunetin (5281804)		*Prunus emarginata*
61	Wogonin (5281703)		*Scutellaria baicalensis*

62	Purpurin (6683)		*Tephrosia purpurea*
63	Pectolinarigenin (5320438)		*Clerodendrum phlomidis*
64	Pelargonidin (440832)		*Rubus fruticosus*
65	Malvidin (159287)		*Vitis vinifera*
66	Pratensein (5281803)		*Trifolium pratense*
67	Nobiletin (72344)		*Citrus reticulata*
68	Kaempferide (5281666)		*Acalypha indica*
69	Pinobanksin (73202)		*Populus nigra*
70	Pinocembrin (68071)		*Populus nigra*

71	Pinostrobin (73201)		*Populus nigra*
72	Liquiritigenin (114829)		*Glyccheriza glabra*
73	5-hydroxyflavone (68112)		*Barleria prionitis*
74	6-hydroxyflavone (72279)		*Barleria prionitis*
75	Acacetin (5280442)		*Ammi visnaga*
76	Fustin (5317435)		*Cotinus coggygria*
77	(-) Epicatechin (72276)		*Camellia sinensis*
78	Dihydro-caffeic acid (15847196)		*Coffea arabica*
79	Glycitein (5317750)		*Trifolium pratense*
80	Daidzein (5281708)		*Pueraria mirifica*

81	4-hydroxycinnamic acid (637542)		*Artemisia vulgaris*
82	Cinnamic acid (444539)		*Artemisia vulgaris*
83	Eugenin (10189)		*Rosa damascena*
84	Syringic acid (10742)		*Larrea divaricata*
85	Gentisic acid (3469)		*Alchornea cordifolia*
86	P-coumeric acid (1549106)		*Larrea divaricata*
87	Sinapic acid (637775)		*Arabidopsis thaliana*
88	Ferulic acid (445858)		*Capsicum annuum*
89	Caffeic acid (689043)		*Beta vulgaris*
90	Salicyclic acid (338)		*Catharanthus roseus*
91	Vanillic acid (8468)		*Catharanthus roseus*
92	Protocatechuic acid (72)		*Prunus amygdalus*

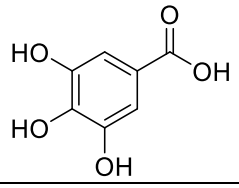
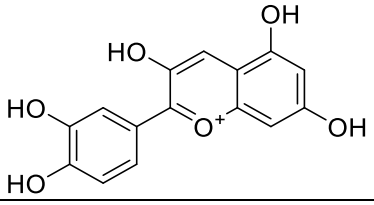
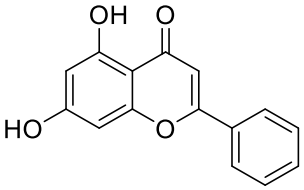
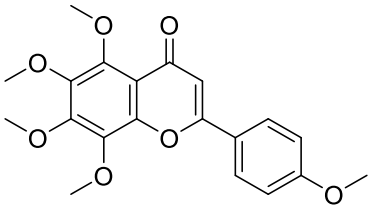
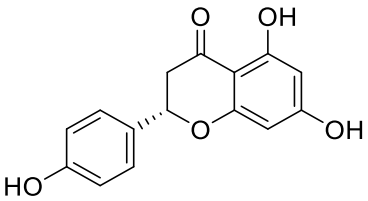
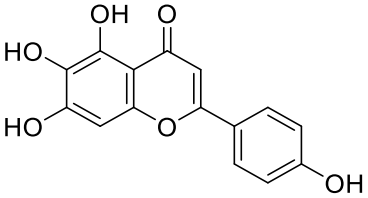
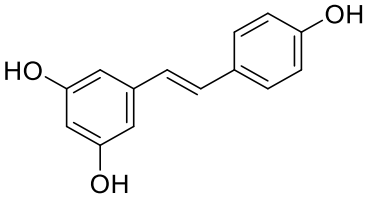
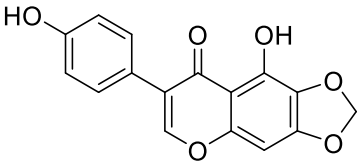
93	Gallic acid (370)		*Terminalia chebula*
94	Cyanidin (128861)		*Prunus avium*
95	Chrysin (5281607)		*Oroxylum indicum*
96	Tangeritin (68077)		*Citrus sinensis*
97	Naringenin (932)		*Citrus sinensis*
98	Scutellarein (5281697)		*Scutellaria baicalensis*
99	Resveratrol (445154)		*Vitis vinifera*
100	Irilone (5281779)		*Trifolium pratense*

Table S2. Energetic components of the binding free energy of RdRp and natural polyphenols along with remdesivir complexes in kcal/mol. Data are represented as average ± SEM.

Components	Myricetin	Quercetagetin	Hesperidin	TF1	Remdesivir
ΔE_{vdW}	-29.13 ± 0.29	-18.81 ± 0.33	-33.54 ± 0.14	-28.28 ± 0.27	-31.85 ± 0.15
ΔE_{elec}	-21.37 ± 0.84	-43.11 ± 1.10	-32.60 ± 0.65	-29.41 ± 0.46	-98.40 ± 0.70
ΔG_{pol}	37.45 ± 0.45	51.27 ± 0.75	54.20 ± 0.70	47.49 ± 0.50	109.97 ± 0.57
ΔG_{np}	-3.16 ± 0.00	-2.83 ± 0.00	-4.31± 0.00	-3.19 ± 0.00	-4.29 ± 0.01
ΔG_{solv} [a]	34.29 ± 0.45	48.44 ± 0.75	49.89 ±0.70	44.30 ± 0.50	105.68 ± 0.57
$\Delta G_{pol + elec}$ [b]	16.08 ± 0.95	8.16 ± 1.33	21.60 ± 0.95	18.08 ± 0.67	11.57 ± 0.90
ΔE_{MM} [c]	-50.50 ± 0.88	-61.92 ± 1.14	-66.14 ± 0.66	-57.69 ± 0.53	-130.25± 0.71
ΔG_{bind} [sim]	-16.21 ± 0.98	-13.48 ± 1.36	-16.25 ± 0.96	-13.39 ± 0.72	-24.57 ± 0.91

[a]$\Delta G_{solv} = \Delta G_{np} + \Delta G_{pol}$, [b]$\Delta G_{pol + elec} = \Delta E_{elec} + \Delta G_{pol,}$ [c]$\Delta E_{MM} = \Delta E_{vdW} + \Delta E_{elec}$.

Table S3. Predicted absorption properties of remdesivir, EGCG, TF2a, TF2b and TF3

Properties	Remdesivir	EGCG	TF2a	TF2b	TF3
Water solubility log mol/L	-3.07	-2.894	-2.892	-2.892	-2.892
Caco2 permeability Log 10^{-6} cm/s	0.635	-1.521	0.027	-1.293	-1.643
Human intestinal absorption (%)	71.109	47.395	50.555	37.409	36.043
Skin permeability log Kp	-2.735	-2.735	-2.735	-2.735	-2.735
P-glycoprotein substrate	Yes	Yes	Yes	Yes	Yes
P-glycoprotein I inhibitor	Yes	No	Yes	Yes	No
P-glycoprotein II inhibitor	No	Yes	Yes	Yes	Yes

Table S4. Predicted distribution properties of remdesivir, EGCG, TF2a, TF2b and TF3

Properties	Remdesivir	EGCG	TF2a	TF2b	TF3
VDss (log L/kg)	0.307	0.806	0.742	-0.021	-0.088
Fraction unbound (human) (Fu)	0.005	0.215	0.22	0.319	0.371
BBB permeability (log BB)	-2.056	-2.184	-2.092	-2.665	-3.442
CNS permeability (log PS)	-4.675	-3.96	-4.159	-4.406	-5.115

Table S5. Predicted metabolic fates of remdesivir, EGCG, TF2a, TF2b and TF3

Properties	Remdesivir	EGCG	TF2a	TF2b	TF3
CYP2D6 substrate	No	No	No	No	No
CYP3A4 substrate	Yes	No	Yes	No	Yes
CYP1A2 inhibitor	No	No	No	No	No
CYP2C19 inhibitor	No	No	No	No	No
CYP2C9 inhibitor	No	No	No	No	No
CYP2D6 inhibitor	No	No	No	No	No
CYP3A4 inhibitor	No	Yes	No	No	No

Table S6. Predicted excretion routes of remdesivir, EGCG, TF2a, TF2b and TF3

Properties	Remdesivir	EGCG	TF2a	TF2b	TF3
Total clearance log ml/min/kg	0.198	0.292	-1.535	-0.019	-0.039
Renal OCT2 substrate	No	No	No	Yes	Yes

Table S7: SwissTargetPrediction report obtained using EGCG as the query molecule

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Microtubule-associated protein tau	MAPT	P10636	CHEMBL1293224	Unclassified protein	1.0	2 / 1
DNA (cytosine-5)-methyltransferase 1	DNMT1	P26358	CHEMBL1993	Writer	1.0	1 / 1
Dual-specificity tyrosine-phosphorylation regulated kinase 1A	DYRK1A	Q13627	CHEMBL2292	Kinase	1.0	10 / 1
Beta amyloid A4 protein	APP	P05067	CHEMBL2487	Membrane receptor	1.0	3 / 2
MAP kinase p38 alpha	MAPK14	Q16539	CHEMBL260	Kinase	1.0	2 / 2
Telomerase reverse transcriptase	TERT	O14746	CHEMBL2916	Enzyme	1.0	5 / 2
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	1.0	8 / 6
6-phosphogluconate dehydrogenase	PGD	P52209	CHEMBL3404	Enzyme	1.0	4 / 4
Hepatocyte growth factor receptor	MET	P08581	CHEMBL3717	Kinase	1.0	6 / 6
Matrix metalloproteinase 14	MMP14	P50281	CHEMBL3869	Protease	1.0	5 / 4
P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	1.0	3 / 99
Beta-secretase 1	BACE1	P56817	CHEMBL4822	Protease	1.0	14 / 14
Apoptosis regulator Bcl-2	BCL2	P10415	CHEMBL4860	Other ion channel	1.0	5 / 7
Signal transducer and activator of transcription 1-alpha/ beta	STAT1	P42224	CHEMBL6101	Transcription factor	1.0	1 / 1
Squalene monooxygenase (by homology)	SQLE	Q14534	CHEMBL3592	Enzyme	1.0	1 / 9
HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0.779416251511	1 / 1
CMP-N-acetylneuraminate-beta-1,4-galactoside alpha-2,3-sialyltransferase	ST3GAL3	Q11203	CHEMBL3596076	Transferase	0.544613584146	1 / 1
Alpha-(1,3)-fucosyltransferase 7	FUT7	Q11130	CHEMBL3596077	Transferase	0.544613584146	1 / 1
Fucosyltransferase 4	FUT4	P22083	CHEMBL4996	Enzyme	0.544613584146	1 / 1
GABA-A receptor; alpha-1/ beta-2/ gamma-2	GABRA1 GABRB2 GABRG2	P14867 P47870 P18507	CHEMBL2095172	Ligand-gated ion channel	0.109013467516	0 / 1
Carbonic anhydrase III	CA3	P07451	CHEMBL2885	Lyase	0.100634432184	0 / 2
Matrix	MMP12	P39900	CHEMBL4393	Protease	0.100634432184	2 / 6

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
metalloproteinase 12						
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.100634432184	6 / 2
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.100634432184	7 / 2
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.100634432184	5 / 8
Hypoxia-inducible factor 1 alpha	HIF1A	Q16665	CHEMBL4261	Transcription factor	0.100634432184	0 / 6
Carbonic anhydrase VII	CA7	P43166	CHEMBL2326	Lyase	0.100634432184	5 / 8
Carbonic anhydrase VI	CA6	P23280	CHEMBL3025	Lyase	0.100634432184	2 / 2
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.100634432184	6 / 1
Carbonic anhydrase VB	CA5B	Q9Y2D0	CHEMBL3969	Lyase	0.100634432184	2 / 2
Carbonic anhydrase VA	CA5A	P35218	CHEMBL4789	Lyase	0.100634432184	2 / 2
Cyclooxygenase-1	PTGS1	P23219	CHEMBL221	Oxidoreductase	0.100634432184	1 / 14
Matrix metalloproteinase 9	MMP9	P14780	CHEMBL321	Protease	0.100634432184	7 / 6
ATP-binding cassette sub-family G member 2	ABCG2	Q9UNQ0	CHEMBL5393	Primary active transporter	0.100634432184	0 / 11
Carbonic anhydrase IV	CA4	P22748	CHEMBL3729	Lyase	0.100634432184	2 / 8
Kallikrein 1	KLK1	P06870	CHEMBL2319	Protease	0.100634432184	0 / 1
Kallikrein 2	KLK2	P20151	CHEMBL2442	Protease	0.100634432184	0 / 1
Matrix metalloproteinase 13	MMP13	P45452	CHEMBL280	Protease	0.100634432184	1 / 3
Multidrug resistance-associated protein 1	ABCC1	P33527	CHEMBL3004	Primary active transporter	0.100634432184	2 / 6
Carbonic anhydrase XIII	CA13	Q8N1Q1	CHEMBL3912	Lyase	0.100634432184	2 / 1
Taste receptor type 2 member 31	TAS2R31	P59538	CHEMBL2034804	Taste family G protein-coupled receptor	0.100634432184	0 / 3
Placenta growth factor	PGF	P49763	CHEMBL1697671	Unclassified protein	0.100634432184	0 / 3
Vascular endothelial growth factor A	VEGFA	P15692	CHEMBL1783	Secreted protein	0.100634432184	0 / 3
Dynamin-1	DNM1	Q05193	CHEMBL4958	Enzyme	0.100634432184	4 / 0
Stem cell growth factor receptor	KIT	P10721	CHEMBL1936	Kinase	0.0	0 / 3
Vascular endothelial growth factor receptor 2	KDR	P35968	CHEMBL279	Kinase	0.0	0 / 6
Fibroblast growth factor receptor 1	FGFR1	P11362	CHEMBL3650	Kinase	0.0	0 / 3
Testis-specific androgen-binding protein	SHBG	P04278	CHEMBL3305	Secreted protein	0.0	0 / 2

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Carbonyl reductase [NADPH] 1	CBR1	P16152	CHEMBL5586	Enzyme	0.0	0 / 1
Neuronal acetylcholine receptor protein alpha-7 subunit	CHRNA7	P36544	CHEMBL2492	Ligand-gated ion channel	0.0	3 / 0
Dopamine D2 receptor (by homology)	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0.0	0 / 35
Adenosine A3 receptor	ADORA3	P0DMS8	CHEMBL256	Family A G protein-coupled receptor	0.0	0 / 3
Heat shock protein HSP 90-alpha	HSP90AA1	P07900	CHEMBL3880	Other cytosolic protein	0.0	2 / 0
Retinoid X receptor alpha	RXRA	P19793	CHEMBL2061	Nuclear receptor	0.0	0 / 14
Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL1978	Cytochrome P450	0.0	1 / 40
Plasminogen activator inhibitor-1	SERPINE1	P05121	CHEMBL3475	Secreted protein	0.0	8 / 16
Alpha-synuclein	SNCA	P37840	CHEMBL6152	Unclassified protein	0.0	20 / 0
Estrogen receptor alpha	ESR1	P03372	CHEMBL206	Nuclear receptor	0.0	8 / 84
DNA polymerase beta (by homology)	POLB	P06746	CHEMBL2392	Enzyme	0.0	0 / 3
Estradiol 17-beta-dehydrogenase 2	HSD17B2	P37059	CHEMBL2789	Enzyme	0.0	34 / 0
Phospholipase A2 group IIA	PLA2G2A	P14555	CHEMBL3474	Enzyme	0.0	0 / 5
Phospholipase A2 group V	PLA2G5	P39877	CHEMBL4323	Enzyme	0.0	0 / 1
Group X secretory phospholipase A2	PLA2G10	O15496	CHEMBL4342	Enzyme	0.0	0 / 1
14-3-3 protein gamma	YWHAG	P61981	CHEMBL1293296	Unclassified protein	0.0	1 / 0
Serine/threonine-protein kinase RAF	RAF1	P04049	CHEMBL1906	Kinase	0.0	31 / 0
Serine/threonine-protein kinase B-raf	BRAF	P15056	CHEMBL5145	Kinase	0.0	33 / 0
Eukaryotic initiation factor 4A-I	EIF4A1	P60842	CHEMBL2052028	Hydrolase	0.0	0 / 29
Thyroid hormone receptor alpha	THRA	P10827	CHEMBL1860	Nuclear receptor	0.0	4 / 0
Thyroid hormone receptor beta-1	THRB	P10828	CHEMBL1947	Nuclear receptor	0.0	4 / 0
Pyruvate dehydrogenase kinase isoform 1	PDK1	Q15118	CHEMBL4766	Kinase	0.0	37 / 0
Alkaline phosphatase, tissue-nonspecific isozyme	ALPL	P05186	CHEMBL5979	Enzyme	0.0	1 / 0
NADH-ubiquinone	MT-ND4	P03905	CHEMBL4499	Oxidoreductase	0.0	0 / 4

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
oxidoreductase chain 4						
Elastase 1	CELA1	Q9UNI1	CHEMBL3000	Protease	0.0	1 / 0
Prolyl endopeptidase	PREP	P48147	CHEMBL3202	Protease	0.0	1 / 0
Tyrosyl-DNA phosphodiesterase 1	TDP1	Q9NUW8	CHEMBL1075138	Enzyme	0.0	0 / 2
Estradiol 17-beta-dehydrogenase 1	HSD17B1	P14061	CHEMBL3181	Enzyme	0.0	34 / 1
Poly [ADP-ribose] polymerase-1	PARP1	P09874	CHEMBL3105	Enzyme	0.0	1 / 0
Carbonic anhydrase XIV	CA14	Q9ULX7	CHEMBL3510	Lyase	0.0	4 / 0
Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	0.0	0 / 92
5-lipoxygenase activating protein	ALOX5AP	P20292	CHEMBL4550	Other cytosolic protein	0.0	6 / 0
Peroxisome proliferator-activated receptor gamma	PPARG	P37231	CHEMBL235	Nuclear receptor	0.0	0 / 75
Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	0.0	0 / 73
Diacylglycerol O-acyltransferase 1	DGAT1	O75907	CHEMBL6009	Enzyme	0.0	4 / 0
C-C chemokine receptor type 5	CCR5	P51681	CHEMBL274	Family A G protein-coupled receptor	0.0	6 / 0
Cytochrome P450 1B1	CYP1B1	Q16678	CHEMBL4878	Cytochrome P450	0.0	1 / 6
Cyclin-dependent kinase 5/CDK5 activator 1	CDK5R1 CDK5	Q15078 Q00535	CHEMBL1907600	Kinase	0.0	7 / 0
Zinc finger protein GLI2	GLI2	P10070	CHEMBL5119	Transcription factor	0.0	1 / 0
Zinc finger protein GLI1	GLI1	P08151	CHEMBL5461	Transcription factor	0.0	1 / 0
Serine/threonine-protein kinase Chk1	CHEK1	O14757	CHEMBL4630	Kinase	0.0	15 / 0
Serine/threonine-protein kinase WEE1	WEE1	P30291	CHEMBL5491	Kinase	0.0	7 / 0
Phospholipase A2 group 1B	PLA2G1B	P04054	CHEMBL4426	Enzyme	0.0	0 / 1
Voltage-gated potassium channel subunit Kv1.3	KCNA3	P22001	CHEMBL4633	Voltage-gated ion channel	0.0	0 / 1
Tyrosine-protein kinase ABL	ABL1	P00519	CHEMBL1862	Kinase	0.0	1 / 0
Platelet-derived growth factor receptor beta	PDGFRB	P09619	CHEMBL1913	Kinase	0.0	1 / 0
Tyrosine-protein kinase receptor FLT3	FLT3	P36888	CHEMBL1974	Kinase	0.0	2 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Beta-galactoside alpha-2,6-sialyltransferase 1	ST6GAL1	P15907	CHEMBL3596075	Transferase	0.0	0 / 2
Serine/threonine-protein kinase Chk2	CHEK2	O96017	CHEMBL2527	Kinase	0.0	1 / 0
Sphingosine kinase 2	SPHK2	Q9NRA0	CHEMBL3023	Enzyme	0.0	2 / 0
Sphingosine kinase 1	SPHK1	Q9NYA1	CHEMBL4394	Enzyme	0.0	2 / 0
Insulin receptor	INSR	P06213	CHEMBL1981	Kinase	0.0	3 / 0

Table S8: SwissTargetPrediction report obtained using TF3 as the query molecule

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Apoptosis regulator Bcl-2	BCL2	P10415	CHEMBL4860	Other ion channel	0.53418213932	4 / 7
Squalene monooxygenase (by homology)	SQLE	Q14534	CHEMBL3592	Enzyme	0.179721075113	6 / 4
Microtubule-associated protein tau	MAPT	P10636	CHEMBL1293224	Unclassified protein	0.0927518343406	0 / 1
DNA (cytosine-5)-methyltransferase 1	DNMT1	P26358	CHEMBL1993	Writer	0.0927518343406	0 / 1
Dual-specificity tyrosine-phosphorylation regulated kinase 1A	DYRK1A	Q13627	CHEMBL2292	Kinase	0.0927518343406	0 / 1
HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0.0927518343406	0 / 1
Beta amyloid A4 protein	APP	P05067	CHEMBL2487	Membrane receptor	0.0927518343406	0 / 2
MAP kinase p38 alpha	MAPK14	Q16539	CHEMBL260	Kinase	0.0927518343406	0 / 2
Telomerase reverse transcriptase	TERT	O14746	CHEMBL2916	Enzyme	0.0927518343406	0 / 1
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	0.0927518343406	0 / 4
6-phosphogluconate dehydrogenase	PGD	P52209	CHEMBL3404	Enzyme	0.0927518343406	0 / 4
CMP-N-acetylneuraminate-beta-1,4-galactoside alpha-2,3-sialyltransferase	ST3GAL3	Q11203	CHEMBL3596076	Transferase	0.0927518343406	0 / 1
Alpha-(1,3)-fucosyltransferase 7	FUT7	Q11130	CHEMBL3596077	Transferase	0.0927518343406	0 / 1
Hepatocyte growth factor receptor	MET	P08581	CHEMBL3717	Kinase	0.0927518343406	0 / 5
Matrix metalloproteinase 14	MMP14	P50281	CHEMBL3869	Protease	0.0927518343406	0 / 4
Fucosyltransferase 4	FUT4	P22083	CHEMBL4996	Enzyme	0.0927518343406	0 / 1
Signal transducer and activator of transcription 1-alpha/ beta	STAT1	P42224	CHEMBL6101	Transcription factor	0.0927518343406	0 / 1
P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	0.0833265263612	2 / 68
Beta-secretase 1	BACE1	P56817	CHEMBL4822	Protease	0.0738845559978	8 / 12
GABA-A receptor; alpha-1/ beta-2/ gamma-2	GABRA1 GABRB2 GABRG2	P14867 P47870 P18507	CHEMBL2095172	Ligand-gated ion channel	0.0642387798076	0 / 1
Carbonic anhydrase	CA3	P07451	CHEMBL2885	Lyase	0.0642387798076	0 / 2

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
III						
Carbonic anhydrase VI	CA6	P23280	CHEMBL3025	Lyase	0.0642387798076	0 / 2
Carbonic anhydrase VB	CA5B	Q9Y2D0	CHEMBL3969	Lyase	0.0642387798076	0 / 2
Carbonic anhydrase VA	CA5A	P35218	CHEMBL4789	Lyase	0.0642387798076	0 / 2
Matrix metalloproteinase 13	MMP13	P45452	CHEMBL280	Protease	0.0642387798076	0 / 1
Matrix metalloproteinase 12	MMP12	P39900	CHEMBL4393	Protease	0.0642387798076	0 / 4
Cyclooxygenase-1	PTGS1	P23219	CHEMBL221	Oxidoreductase	0.0642387798076	0 / 6
Hypoxia-inducible factor 1 alpha	HIF1A	Q16665	CHEMBL4261	Transcription factor	0.0642387798076	0 / 4
Carbonic anhydrase XIII	CA13	Q8N1Q1	CHEMBL3912	Lyase	0.0642387798076	0 / 1
Multidrug resistance-associated protein 1	ABCC1	P33527	CHEMBL3004	Primary active transporter	0.0	0 / 6
ATP-binding cassette sub-family G member 2	ABCG2	Q9UNQ0	CHEMBL5393	Primary active transporter	0.0	0 / 11
Matrix metalloproteinase 9	MMP9	P14780	CHEMBL321	Protease	0.0	0 / 3
Cytochrome P450 1B1	CYP1B1	Q16678	CHEMBL4878	Cytochrome P450	0.0	0 / 6
Apoptosis regulator Bcl-X	BCL2L1	Q07817	CHEMBL4625	Other ion channel	0.0	5 / 0
Carbonic anhydrase VII	CA7	P43166	CHEMBL2326	Lyase	0.0	1 / 8
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.0	2 / 8
Carbonic anhydrase IV	CA4	P22748	CHEMBL3729	Lyase	0.0	1 / 8
Dopamine D2 receptor (by homology)	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0.0	0 / 25
Induced myeloid leukemia cell differentiation protein Mcl-1	MCL1	Q07820	CHEMBL4361	Other cytosolic protein	0.0	3 / 0
Bcl-2-related protein A1	BCL2A1	Q16548	CHEMBL6044	Unclassified protein	0.0	2 / 0
Taste receptor type 2 member 31	TAS2R31	P59538	CHEMBL2034804	Taste family G protein-coupled receptor	0.0	0 / 3
AMY1C	AMY1A	P04745	CHEMBL2478	Enzyme	0.0	1 / 0
Placenta growth factor	PGF	P49763	CHEMBL1697671	Unclassified protein	0.0	0 / 3
Vascular endothelial growth factor A	VEGFA	P15692	CHEMBL1783	Secreted protein	0.0	0 / 3

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Ribosomal protein S6 kinase alpha 3	RPS6KA3	P51812	CHEMBL2345	Kinase	0.0	9 / 0
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.0	1 / 2
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.0	1 / 2
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.0	1 / 1
Thrombin	F2	P00734	CHEMBL204	Protease	0.0	4 / 0
Calcitonin-gene-related peptide receptor, CALCRL/ RAMP1	CALCRL RAMP1	Q16602 O60894	CHEMBL2107838	Other membrane protein	0.0	1 / 0
Nitric oxide synthase, inducible (by homology)	NOS2	P35228	CHEMBL4481	Enzyme	0.0	2 / 0
Stem cell growth factor receptor	KIT	P10721	CHEMBL1936	Kinase	0.0	0 / 3
Vascular endothelial growth factor receptor 2	KDR	P35968	CHEMBL279	Kinase	0.0	0 / 4
Fibroblast growth factor receptor 1	FGFR1	P11362	CHEMBL3650	Kinase	0.0	0 / 3
Integrin alpha-3	ITGA3	P26006	CHEMBL3525	Membrane receptor	0.0	3 / 0
Eukaryotic initiation factor 4A-I	EIF4A1	P60842	CHEMBL2052028	Hydrolase	0.0	0 / 25
Retinoid X receptor alpha	RXRA	P19793	CHEMBL2061	Nuclear receptor	0.0	0 / 12
Estradiol 17-beta-dehydrogenase 1	HSD17B1	P14061	CHEMBL3181	Enzyme	0.0	0 / 1
Testis-specific androgen-binding protein	SHBG	P04278	CHEMBL3305	Secreted protein	0.0	0 / 1
Carbonyl reductase [NADPH] 1	CBR1	P16152	CHEMBL5586	Enzyme	0.0	0 / 1
Estrogen receptor beta	ESR2	Q92731	CHEMBL242	Nuclear receptor	0.0	0 / 74
Receptor-type tyrosine-protein phosphatase alpha	PTPRA	P18433	CHEMBL3918	Phosphatase	0.0	1 / 0
Heat shock protein 75 kDa, mitochondrial	TRAP1	Q12931	CHEMBL1075132	Other cytosolic protein	0.0	2 / 0
Heat shock protein HSP 90-alpha	HSP90AA1	P07900	CHEMBL3880	Other cytosolic protein	0.0	2 / 0
Heat shock protein HSP 90-beta	HSP90AB1	P08238	CHEMBL4303	Other cytosolic protein	0.0	2 / 0
Monoamine oxidase B	MAOB	P27338	CHEMBL2039	Oxidoreductase	0.0	0 / 56
Adenosine A1 receptor (by homology)	ADORA1	P30542	CHEMBL226	Family A G protein-coupled receptor	0.0	0 / 4

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Adenosine A3 receptor	ADORA3	P0DMS8	CHEMBL256	Family A G protein-coupled receptor	0.0	0 / 2
Metastin receptor	KISS1R	Q969F8	CHEMBL5413	Family A G protein-coupled receptor	0.0	2 / 0
cAMP-dependent protein kinase alpha-catalytic subunit	PRKACA	P17612	CHEMBL4101	Kinase	0.0	2 / 0
Acetylcholinesterase	ACHE	P22303	CHEMBL220	Hydrolase	0.0	0 / 3
Tyrosine-protein kinase SYK	SYK	P43405	CHEMBL2599	Kinase	0.0	1 / 0
DNA polymerase beta (by homology)	POLB	P06746	CHEMBL2392	Enzyme	0.0	0 / 2
Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	0.0	0 / 63
Beta-galactoside alpha-2,6-sialyltransferase 1	ST6GAL1	P15907	CHEMBL3596075	Transferase	0.0	0 / 2
Phospholipase A2 group IIA	PLA2G2A	P14555	CHEMBL3474	Enzyme	0.0	0 / 5
Phospholipase A2 group V	PLA2G5	P39877	CHEMBL4323	Enzyme	0.0	0 / 1
Group X secretory phospholipase A2	PLA2G10	O15496	CHEMBL4342	Enzyme	0.0	0 / 1
NADH-ubiquinone oxidoreductase chain 4	MT-ND4	P03905	CHEMBL4499	Oxidoreductase	0.0	0 / 4
Lysine-specific histone demethylase 1	KDM1A	O60341	CHEMBL6136	Eraser	0.0	1 / 0
Bile salt export pump	ABCB11	O95342	CHEMBL6020	Primary active transporter	0.0	1 / 0
Tyrosyl-DNA phosphodiesterase 1	TDP1	Q9NUW8	CHEMBL1075138	Enzyme	0.0	0 / 2
Phospholipase A2 group 1B	PLA2G1B	P04054	CHEMBL4426	Enzyme	0.0	0 / 1
FK506-binding protein 1A	FKBP1A	P62942	CHEMBL1902	Isomerase	0.0	1 / 0
Peptidyl-prolyl cis-trans isomerase FKBP5	FKBP5	Q13451	CHEMBL2052031	Enzyme	0.0	1 / 0
Carbonic anhydrase XIV	CA14	Q9ULX7	CHEMBL3510	Lyase	0.0	1 / 0
Lysine-specific demethylase 2A	KDM2A	Q9Y2K7	CHEMBL1938210	Eraser	0.0	1 / 0
Lysine-specific demethylase 6B	KDM6B	O15054	CHEMBL1938211	Eraser	0.0	1 / 0
Phosphodiesterase 5A	PDE5A	O76074	CHEMBL1827	Phosphodiesterase	0.0	1 / 0
Pyruvate dehydrogenase kinase isoform 1	PDK1	Q15118	CHEMBL4766	Kinase	0.0	1 / 0
Pregnane X receptor	NR1I2	O75469	CHEMBL3401	Nuclear receptor	0.0	1 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Caspase-1	CASP1	P29466	CHEMBL4801	Protease	0.0	1 / 0
Cannabinoid receptor 1 (by homology)	CNR1	P21554	CHEMBL218	Family A G protein-coupled receptor	0.0	0 / 45
Cannabinoid receptor 2	CNR2	P34972	CHEMBL253	Family A G protein-coupled receptor	0.0	0 / 47
Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL1978	Cytochrome P450	0.0	2 / 36
Coagulation factor VII	F7	P08709	CHEMBL3991	Protease	0.0	2 / 0
Sulfonylurea receptor 2	ABCC9	O60706	CHEMBL1971	Primary active transporter	0.0	0 / 1
Leukotriene B4 receptor 1	LTB4R	Q15722	CHEMBL3911	Family A G protein-coupled receptor	0.0	0 / 11
Peroxisome proliferator-activated receptor gamma	PPARG	P37231	CHEMBL235	Nuclear receptor	0.0	0 / 34
Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	0.0	0 / 36

Table S9: SwissTargetPrediction report obtained using TF2a as the query molecule

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Beta amyloid A4 protein	APP	P05067	CHEMBL2487	Membrane receptor	0.0498457217793	3 / 2
Microtubule-associated protein tau	MAPT	P10636	CHEMBL1293224	Unclassified protein	0.0498457217793	0 / 1
Dual-specificity tyrosine-phosphorylation regulated kinase 1A	DYRK1A	Q13627	CHEMBL2292	Kinase	0.0498457217793	0 / 1
Telomerase reverse transcriptase	TERT	O14746	CHEMBL2916	Enzyme	0.0498457217793	0 / 2
6-phosphogluconate dehydrogenase	PGD	P52209	CHEMBL3404	Enzyme	0.0498457217793	0 / 4
CMP- N-acetylneuraminate-beta-1,4-galactoside alpha-2,3-sialyltransferase	ST3GAL3	Q11203	CHEMBL3596076	Transferase	0.0498457217793	0 / 1
Alpha-(1,3)-fucosyltransferase 7	FUT7	Q11130	CHEMBL3596077	Transferase	0.0498457217793	0 / 1
Fucosyltransferase 4	FUT4	P22083	CHEMBL4996	Enzyme	0.0498457217793	0 / 1
Signal transducer and activator of transcription 1-alpha/ beta	STAT1	P42224	CHEMBL6101	Transcription factor	0.0498457217793	0 / 1
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	0.0498457217793	27 / 12
Apoptosis regulator Bcl-2	BCL2	P10415	CHEMBL4860	Other ion channel	0.0498457217793	34 / 7
HERG	KCNH2	Q12809	CHEMBL240	Voltage- gated ion channel	0.0498457217793	58 / 2
Beta- secretase 1	BACE1	P56817	CHEMBL4822	Protease	0.0498457217793	86 / 12
Squalene monooxygenase (by homology)	SQLE	Q14534	CHEMBL3592	Enzyme	0.0498457217793	1 / 5
P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	0.0498457217793	6 / 58
Hepatocyte growth factor receptor	MET	P08581	CHEMBL3717	Kinase	0.0498457217793	7 / 5
Matrix metalloproteinase 14	MMP14	P50281	CHEMBL3869	Protease	0.0498457217793	7 / 4
DNA (cytosine-5)-methyltransferase 1	DNMT1	P26358	CHEMBL1993	Writer	0.0	1 / 1
Thrombin	F2	P00734	CHEMBL204	Protease	0.0	161 / 0
MAP kinase p38 alpha	MAPK14	Q16539	CHEMBL260	Kinase	0.0	3 / 2
Plasminogen (by homology)	PLG	P00747	CHEMBL1801	Protease	0.0	55 / 0
Trypsin I (by homology)	PRSS1	P07477	CHEMBL209	Protease	0.0	75 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Trypsin III (by homology)	PRSS3	P35030	CHEMBL4551	Protease	0.0	16 / 0
Tissue-type plasminogen activator	PLAT	P00750	CHEMBL1873	Protease	0.0	15 / 0
Thymidylate synthase (by homology)	TYMS	P04818	CHEMBL1952	Transferase	0.0	2 / 0
GABA-A receptor; alpha-1/beta-2/ gamma-2	GABRA1 GABRB2 GABRG2	P14867 P47870 P18507	CHEMBL2095172	Ligand-gated ion channel	0.0	0 / 1
Proteinase-activated receptor 1	F2R	P25116	CHEMBL3974	Family A G protein-coupled receptor	0.0	9 / 0
Cyclin-dependent kinase 2/cyclin E	CCNE2 CDK2 CCNE1	O96020 P24941 P24864	CHEMBL2094126	Other cytosolic protein	0.0	2 / 0
Protein-tyrosine phosphatase 1B	PTPN1	P18031	CHEMBL335	Phosphatase	0.0	8 / 21
Insulin-degrading enzyme	IDE	P14735	CHEMBL1293287	Enzyme	0.0	3 / 0
Beta-3 adrenergic receptor	ADRB3	P13945	CHEMBL246	Family A G protein-coupled receptor	0.0	71 / 0
Renin	REN	P00797	CHEMBL286	Protease	0.0	92 / 0
Tryptase beta-1	TPSAB1	Q15661	CHEMBL2617	Protease	0.0	3 / 0
Urokinase-type plasminogen activator	PLAU	P00749	CHEMBL3286	Protease	0.0	45 / 0
Transmembrane protease serine 11D	TMPRSS11D	O60235	CHEMBL1795138	Protease	0.0	1 / 0
Angiotensin-converting enzyme	ACE	P12821	CHEMBL1808	Protease	0.0	5 / 0
Anandamide amidohydrolase	FAAH	O00519	CHEMBL2243	Enzyme	0.0	5 / 0
Adenosine A2a receptor (by homology)	ADORA2A	P29274	CHEMBL251	Family A G protein-coupled receptor	0.0	17 / 0
Monoglyceride lipase	MGLL	Q99685	CHEMBL4191	Enzyme	0.0	4 / 0
Monoacylglycerol lipase ABHD6 (by homology)	ABHD6	Q9BV23	CHEMBL2189127	Enzyme	0.0	4 / 0
Beta-1 adrenergic receptor	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor	0.0	82 / 0
Serotonin 1a (5-HT1a) receptor	HTR1A	P08908	CHEMBL214	Family A G protein-coupled receptor	0.0	21 / 0
Interleukin-1 receptor-associated kinase 4	IRAK4	Q9NWZ3	CHEMBL3778	Kinase	0.0	30 / 0
Furin	FURIN	P09958	CHEMBL2611	Protease	0.0	2 / 0
Kallikrein 2	KLK2	P20151	CHEMBL2442	Protease	0.0	0 / 1

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Macrophage colony stimulating factor receptor (by homology)	CSF1R	P07333	CHEMBL1844	Kinase	0.0	13 / 0
Serine/threonine-protein kinase mTOR	MTOR	P42345	CHEMBL2842	Kinase	0.0	92 / 0
PI3-kinase p110-alpha subunit	PIK3CA	P42336	CHEMBL4005	Enzyme	0.0	65 / 0
Somatostatin receptor 4	SSTR4	P31391	CHEMBL1853	Family A G protein-coupled receptor	0.0	3 / 0
Adrenergic receptor beta	ADRB2	P07550	CHEMBL210	Family A G protein-coupled receptor	0.0	81 / 0
Muscarinic acetylcholine receptor M2	CHRM2	P08172	CHEMBL211	Family A G protein-coupled receptor	0.0	12 / 0
Muscarinic acetylcholine receptor M3	CHRM3	P20309	CHEMBL245	Family A G protein-coupled receptor	0.0	11 / 0
Cathepsin D	CTSD	P07339	CHEMBL2581	Protease	0.0	9 / 0
Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL1978	Cytochrome P450	0.0	0 / 35
Xaa-Pro aminopeptidase 1	XPNPEP1	Q9NQW7	CHEMBL3782	Protease	0.0	1 / 0
Leucine aminopeptidase	LAP3	P28838	CHEMBL3965	Protease	0.0	2 / 0
Ribosomal protein S6 kinase 1	RPS6KB1	P23443	CHEMBL4501	Kinase	0.0	7 / 0
Xaa-Pro aminopeptidase 2	XPNPEP2	O43895	CHEMBL4610	Protease	0.0	1 / 0
Serine/threonine-protein kinase Chk1	CHEK1	O14757	CHEMBL4630	Kinase	0.0	21 / 0
Serine protease hepsin	HPN	P05981	CHEMBL2079849	Protease	0.0	7 / 0
Matriptase	ST14	Q9Y5Y6	CHEMBL3018	Protease	0.0	10 / 0
Hepatocyte growth factor activator	HGFAC	Q04756	CHEMBL3351190	Unclassified protein	0.0	8 / 0
Proteasome Macropain subunit	PSMB2	P49721	CHEMBL3492	Protease	0.0	3 / 0
Mitogen-activated protein kinase kinase kinase 14	MAP3K14	Q99558	CHEMBL5888	Kinase	0.0	86 / 0
Bradykinin B1 receptor	BDKRB1	P46663	CHEMBL4308	Family A G protein-coupled receptor	0.0	20 / 0
Coagulation factor IX	F9	P00740	CHEMBL2016	Protease	0.0	9 / 0
Estradiol 17-beta-dehydrogenase 2	HSD17B2	P37059	CHEMBL2789	Enzyme	0.0	15 / 0
Endothelin-converting enzyme 1	ECE1	P42892	CHEMBL4791	Protease	0.0	2 / 0
Coagulation factor XI	F11	P03951	CHEMBL2820	Protease	0.0	8 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Dipeptidyl peptidase IV	DPP4	P27487	CHEMBL284	Protease	0.0	6 / 0
Dipeptidyl peptidase II	DPP7	Q9UHL4	CHEMBL3976	Protease	0.0	5 / 0
Dipeptidyl peptidase VIII	DPP8	Q6V1X1	CHEMBL4657	Protease	0.0	5 / 0
PDZ-binding kinase	PBK	Q96KB5	CHEMBL4896	Kinase	0.0	4 / 0
Receptor-type tyrosine-protein phosphatase F (LAR)	PTPRF	P10586	CHEMBL3521	Membrane receptor	0.0	0 / 2
Indoleamine 2,3-dioxygenase	IDO1	P14902	CHEMBL4685	Enzyme	0.0	0 / 3
Dihydrofolate reductase (by homology)	DHFR	P00374	CHEMBL202	Oxidoreductase	0.0	9 / 0
Coagulation factor VII	F7	P08709	CHEMBL3991	Protease	0.0	11 / 0
Retinoid X receptor alpha	RXRA	P19793	CHEMBL2061	Nuclear receptor	0.0	0 / 10
Caspase-3	CASP3	P42574	CHEMBL2334	Protease	0.0	1 / 0
Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1	Q02750	CHEMBL3587	Kinase	0.0	2 / 0
Serotonin 1b (5-HT1b) receptor	HTR1B	P28222	CHEMBL1898	Family A G protein-coupled receptor	0.0	12 / 0
Neprilysin	MME	P08473	CHEMBL1944	Protease	0.0	1 / 0
Serotonin 1d (5-HT1d) receptor	HTR1D	P28221	CHEMBL1983	Family A G protein-coupled receptor	0.0	23 / 0
Alpha-1a adrenergic receptor	ADRA1A	P35348	CHEMBL229	Family A G protein-coupled receptor	0.0	15 / 0
Vanilloid receptor (by homology)	TRPV1	Q8NER1	CHEMBL4794	Voltage-gated ion channel	0.0	16 / 0
Tyrosine-protein kinase JAK2	JAK2	O60674	CHEMBL2971	Kinase	0.0	14 / 0
Cyclin-dependent kinase 2	CDK2	P24941	CHEMBL301	Kinase	0.0	11 / 0
Phosphatidylinositol 3-kinase catalytic subunit type 3	PIK3C3	Q8NEB9	CHEMBL1075165	Enzyme	0.0	4 / 0
PI3-kinase p110-delta subunit	PIK3CD	O00329	CHEMBL3130	Enzyme	0.0	18 / 0
DNA-dependent protein kinase	PRKDC	P78527	CHEMBL3142	Kinase	0.0	17 / 0
PI3-kinase p110-beta subunit	PIK3CB	P42338	CHEMBL3145	Enzyme	0.0	29 / 0
PI3-kinase p110-gamma subunit	PIK3CG	P48736	CHEMBL3267	Enzyme	0.0	20 / 0
Thrombin and coagulation factor X	F10	P00742	CHEMBL244	Protease	0.0	108 / 3

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Bromodomain-containing protein 4	BRD4	O60885	CHEMBL1163125	Reader	0.0	15 / 0
P2X purinoceptor 3	P2RX3	P56373	CHEMBL2998	Ligand-gated ion channel	0.0	23 / 0
Serotonin 7 (5-HT7) receptor	HTR7	P34969	CHEMBL3155	Family A G protein-coupled receptor	0.0	2 / 0
Bone morphogenetic protein 1	BMP1	P13497	CHEMBL3898	Protease	0.0	9 / 0
Neuropeptide Y receptor type 1	NPY1R	P25929	CHEMBL4777	Family A G protein-coupled receptor	0.0	11 / 0
WD repeat-containing protein 5	WDR5	P61964	CHEMBL1075317	Unclassified protein	0.0	1 / 0
Cyclin-dependent kinase 1	CDK1	P06493	CHEMBL308	Kinase	0.0	8 / 0

Table S10: SwissTargetPrediction report obtained using TF2b as the query molecule

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Apoptosis regulator Bcl-2	BCL2	P10415	CHEMBL4860	Other ion channel	0.950473054407	5 / 7
Microtubule-associated protein tau	MAPT	P10636	CHEMBL1293224	Unclassified protein	0.0841390721621	0 / 1
DNA (cytosine-5)-methyltransferase 1	DNMT1	P26358	CHEMBL1993	Writer	0.0841390721621	0 / 1
Dual-specificity tyrosine-phosphorylation regulated kinase 1A	DYRK1A	Q13627	CHEMBL2292	Kinase	0.0841390721621	0 / 1
HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0.0841390721621	0 / 1
Beta amyloid A4 protein	APP	P05067	CHEMBL2487	Membrane receptor	0.0841390721621	0 / 2
MAP kinase p38 alpha	MAPK14	Q16539	CHEMBL260	Kinase	0.0841390721621	0 / 2
Telomerase reverse transcriptase	TERT	O14746	CHEMBL2916	Enzyme	0.0841390721621	0 / 1
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	0.0841390721621	0 / 4
6-phosphogluconate dehydrogenase	PGD	P52209	CHEMBL3404	Enzyme	0.0841390721621	0 / 4
CMP-N-acetylneuraminate-beta-1,4-galactoside alpha-2,3-sialyltransferase	ST3GAL3	Q11203	CHEMBL3596076	Transferase	0.0841390721621	0 / 1
Alpha-(1,3)-fucosyltransferase 7	FUT7	Q11130	CHEMBL3596077	Transferase	0.0841390721621	0 / 1
Hepatocyte growth factor receptor	MET	P08581	CHEMBL3717	Kinase	0.0841390721621	0 / 5
Matrix metalloproteinase 14	MMP14	P50281	CHEMBL3869	Protease	0.0841390721621	0 / 4
Fucosyltransferase 4	FUT4	P22083	CHEMBL4996	Enzyme	0.0841390721621	0 / 1
Signal transducer and activator of transcription 1-alpha/ beta	STAT1	P42224	CHEMBL6101	Transcription factor	0.0841390721621	0 / 1
P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	0.0841390721621	3 / 68
Squalene monooxygenase (by homology)	SQLE	Q14534	CHEMBL3592	Enzyme	0.0841390721621	7 / 4
Beta-secretase 1	BACE1	P56817	CHEMBL4822	Protease	0.0742995456363	8 / 12
GABA-A receptor; alpha-1/ beta-2/	GABRA1 GABRB2	P14867 P47870	CHEMBL2095172	Ligand-gated ion channel	0.0345221577323	0 / 1

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
gamma-2	GABRG2	P18507				
Carbonic anhydrase III	CA3	P07451	CHEMBL2885	Lyase	0.0345221577323	0 / 2
Carbonic anhydrase VI	CA6	P23280	CHEMBL3025	Lyase	0.0345221577323	0 / 2
Carbonic anhydrase VB	CA5B	Q9Y2D0	CHEMBL3969	Lyase	0.0345221577323	0 / 2
Carbonic anhydrase VA	CA5A	P35218	CHEMBL4789	Lyase	0.0345221577323	0 / 2
Matrix metalloproteinase 13	MMP13	P45452	CHEMBL280	Protease	0.0345221577323	0 / 1
Matrix metalloproteinase 12	MMP12	P39900	CHEMBL4393	Protease	0.0345221577323	0 / 4
Cyclooxygenase-1	PTGS1	P23219	CHEMBL221	Oxidoreductase	0.0345221577323	0 / 6
Carbonic anhydrase VII	CA7	P43166	CHEMBL2326	Lyase	0.0345221577323	4 / 8
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.0345221577323	11 / 8
Carbonic anhydrase IV	CA4	P22748	CHEMBL3729	Lyase	0.0345221577323	2 / 8
Hypoxia-inducible factor 1 alpha	HIF1A	Q16665	CHEMBL4261	Transcription factor	0.0345221577323	0 / 4
Apoptosis regulator Bcl-X	BCL2L1	Q07817	CHEMBL4625	Other ion channel	0.0345221577323	6 / 0
Carbonic anhydrase XIII	CA13	Q8N1Q1	CHEMBL3912	Lyase	0.0345221577323	0 / 1
ATP-binding cassette sub-family G member 2	ABCG2	Q9UNQ0	CHEMBL5393	Primary active transporter	0.0	0 / 11
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.0	10 / 2
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.0	9 / 2
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.0	10 / 1
Matrix metalloproteinase 9	MMP9	P14780	CHEMBL321	Protease	0.0	0 / 3
cAMP-dependent protein kinase alpha-catalytic subunit	PRKACA	P17612	CHEMBL4101	Kinase	0.0	15 / 0
Cytochrome P450 1B1	CYP1B1	Q16678	CHEMBL4878	Cytochrome P450	0.0	0 / 6
Ribosomal protein S6 kinase alpha 3	RPS6KA3	P51812	CHEMBL2345	Kinase	0.0	13 / 0
Coagulation factor VII	F7	P08709	CHEMBL3991	Protease	0.0	2 / 0
Transitional endoplasmic reticulum ATPase	VCP	P55072	CHEMBL1075145	Primary active transporter	0.0	2 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Troponin, cardiac muscle	TNNC1 TNNT2 TNNI3	P63316 P45379 P19429	CHEMBL2095202	Unclassified protein	0.0	1 / 0
Dopamine D2 receptor (by homology)	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor	0.0	0 / 25
Taste receptor type 2 member 31	TAS2R31	P59538	CHEMBL2034804	Taste family G protein-coupled receptor	0.0	0 / 3
Tyrosine-protein kinase LCK	LCK	P06239	CHEMBL258	Kinase	0.0	1 / 0
DNA-3-methyladenine glycosylase	MPG	P29372	CHEMBL3396943	Enzyme	0.0	1 / 0
Induced myeloid leukemia cell differentiation protein Mcl-1	MCL1	Q07820	CHEMBL4361	Other cytosolic protein	0.0	4 / 0
Placenta growth factor	PGF	P49763	CHEMBL1697671	Unclassified protein	0.0	0 / 3
Vascular endothelial growth factor A	VEGFA	P15692	CHEMBL1783	Secreted protein	0.0	0 / 3
Carbonic anhydrase XIV	CA14	Q9ULX7	CHEMBL3510	Lyase	0.0	5 / 0
Heat shock protein 75 kDa, mitochondrial	TRAP1	Q12931	CHEMBL1075132	Other cytosolic protein	0.0	2 / 0
Heat shock protein HSP 90-alpha	HSP90AA1	P07900	CHEMBL3880	Other cytosolic protein	0.0	3 / 0
Heat shock protein HSP 90-beta	HSP90AB1	P08238	CHEMBL4303	Other cytosolic protein	0.0	2 / 0
Integrin alpha-3	ITGA3	P26006	CHEMBL3525	Membrane receptor	0.0	3 / 0
Receptor-type tyrosine-protein phosphatase alpha	PTPRA	P18433	CHEMBL3918	Phosphatase	0.0	1 / 0
Metastin receptor	KISS1R	Q969F8	CHEMBL5413	Family A G protein-coupled receptor	0.0	9 / 0
Thrombin	F2	P00734	CHEMBL204	Protease	0.0	12 / 0
Lysine-specific demethylase 2A	KDM2A	Q9Y2K7	CHEMBL1938210	Eraser	0.0	1 / 0
Lysine-specific demethylase 6B	KDM6B	O15054	CHEMBL1938211	Eraser	0.0	1 / 0
Stem cell growth factor receptor	KIT	P10721	CHEMBL1936	Kinase	0.0	0 / 3
Vascular endothelial growth factor receptor 2	KDR	P35968	CHEMBL279	Kinase	0.0	0 / 4
Fibroblast growth factor receptor 1	FGFR1	P11362	CHEMBL3650	Kinase	0.0	0 / 3
Eukaryotic initiation factor 4A-I	EIF4A1	P60842	CHEMBL2052028	Hydrolase	0.0	0 / 25

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Thymidylate synthase (by homology)	TYMS	P04818	CHEMBL1952	Transferase	0.0	1 / 0
Nitric oxide synthase, inducible (by homology)	NOS2	P35228	CHEMBL4481	Enzyme	0.0	1 / 0
Retinoid X receptor alpha	RXRA	P19793	CHEMBL2061	Nuclear receptor	0.0	0 / 12
Estradiol 17-beta-dehydrogenase 1	HSD17B1	P14061	CHEMBL3181	Enzyme	0.0	0 / 1
Testis-specific androgen-binding protein	SHBG	P04278	CHEMBL3305	Secreted protein	0.0	0 / 1
Carbonyl reductase [NADPH] 1	CBR1	P16152	CHEMBL5586	Enzyme	0.0	0 / 1
Phosphodiesterase 5A	PDE5A	O76074	CHEMBL1827	Phosphodiesterase	0.0	1 / 0
Glucagon receptor	GCGR	P47871	CHEMBL1985	Family B G protein-coupled receptor	0.0	1 / 0
Estrogen receptor beta	ESR2	Q92731	CHEMBL242	Nuclear receptor	0.0	0 / 74
Dynamin-2	DNM2	P50570	CHEMBL5812	Enzyme	0.0	1 / 0
Xanthine dehydrogenase	XDH	P47989	CHEMBL1929	Oxidoreductase	0.0	1 / 0
Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL1978	Cytochrome P450	0.0	2 / 36
Protein kinase C (PKC)	PRKCZ	Q05513	CHEMBL3438	Kinase	0.0	4 / 0
Monoamine oxidase B	MAOB	P27338	CHEMBL2039	Oxidoreductase	0.0	0 / 56
Adenosine A1 receptor (by homology)	ADORA1	P30542	CHEMBL226	Family A G protein-coupled receptor	0.0	0 / 4
Adenosine A3 receptor	ADORA3	P0DMS8	CHEMBL256	Family A G protein-coupled receptor	0.0	0 / 2
Multidrug resistance-associated protein 1	ABCC1	P33527	CHEMBL3004	Primary active transporter	0.0	1 / 6
Bcl-2-related protein A1	BCL2A1	Q16548	CHEMBL6044	Unclassified protein	0.0	2 / 0
Maternal embryonic leucine zipper kinase	MELK	Q14680	CHEMBL4578	Kinase	0.0	14 / 0
DNA polymerase beta (by homology)	POLB	P06746	CHEMBL2392	Enzyme	0.0	0 / 2
Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	0.0	0 / 63
Beta-galactoside alpha-2,6-sialyltransferase 1	ST6GAL1	P15907	CHEMBL3596075	Transferase	0.0	0 / 2
Kallikrein 1	KLK1	P06870	CHEMBL2319	Protease	0.0	1 / 1

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Kallikrein 2	KLK2	P20151	CHEMBL2442	Protease	0.0	1 / 1
Integrin alpha-4/ beta-1	ITGB1 ITGA4	P05556 P13612	CHEMBL1907599	Membrane receptor	0.0	1 / 0
Pyruvate dehydrogenase kinase isoform 1	PDK1	Q15118	CHEMBL4766	Kinase	0.0	5 / 0
Phospholipase A2 group IIA	PLA2G2A	P14555	CHEMBL3474	Enzyme	0.0	0 / 5
Phospholipase A2 group V	PLA2G5	P39877	CHEMBL4323	Enzyme	0.0	0 / 1
Group X secretory phospholipase A2	PLA2G10	O15496	CHEMBL4342	Enzyme	0.0	0 / 1
NADH-ubiquinone oxidoreductase chain 4	MT-ND4	P03905	CHEMBL4499	Oxidoreductase	0.0	0 / 4
AMY1C	AMY1A	P04745	CHEMBL2478	Enzyme	0.0	1 / 0
Lysine-specific histone demethylase 1	KDM1A	O60341	CHEMBL6136	Eraser	0.0	1 / 0
Phospholipase A2 group 1B	PLA2G1B	P04054	CHEMBL4426	Enzyme	0.0	0 / 1
FK506-binding protein 1A	FKBP1A	P62942	CHEMBL1902	Isomerase	0.0	1 / 0
Peptidyl-prolyl cis-trans isomerase FKBP5	FKBP5	Q13451	CHEMBL2052031	Enzyme	0.0	1 / 0

Table S11: SwissTargetPrediction report obtained using remdesivir as the query molecule

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Adenosine A3 receptor	ADORA3	P0DMS8	CHEMBL256	Family A G protein-coupled receptor	0.0822215166115	855 / 0
Purinergic receptor P2Y12	P2RY12	Q9H244	CHEMBL2001	Family A G protein-coupled receptor	0.0822215166115	55 / 0
Transmembrane domain-containing protein TMIGD3	TMIGD3	P0DMS9	CHEMBL3712907	Unclassified protein	0.0822215166115	34 / 0
Adenosine A1 receptor	ADORA1	P30542	CHEMBL226	Family A G protein-coupled receptor	0.0822215166115	1181 / 0
Acyl-CoA desaturase	SCD	O00767	CHEMBL5555	Enzyme	0.0822215166115	55 / 0
Phosphodiesterase 10A	PDE10A	Q9Y233	CHEMBL4409	Phosphodiesterase	0.0822215166115	583 / 0
Cyclin-dependent kinase 5/CDK5 activator 1	CDK5R1 CDK5	Q15078 Q00535	CHEMBL1907600	Kinase	0.0822215166115	102 / 0
Cyclin-dependent kinase 2/cyclin A	CDK2 CCNA1 CCNA2	P24941 P78396 P20248	CHEMBL2094128	Other cytosolic protein	0.0822215166115	108 / 0
CDK9/ cyclin T1	CDK9 CCNT1	P50750 O60563	CHEMBL2111389	Other cytosolic protein	0.0822215166115	40 / 0
Dual-specificity tyrosine-phosphorylation regulated kinase 1A	DYRK1A	Q13627	CHEMBL2292	Kinase	0.0822215166115	69 / 0
Casein kinase I alpha	CSNK1A1	P48729	CHEMBL2793	Kinase	0.0822215166115	12 / 0
Dual specificty protein kinase CLK1 (by homology)	CLK1	P49759	CHEMBL4224	Kinase	0.0822215166115	19 / 0
Insulin-like growth factor I receptor	IGF1R	P08069	CHEMBL1957	Kinase	0.0822215166115	246 / 0
Interleukin-8 receptor B	CXCR2	P25025	CHEMBL2434	Family A G protein-coupled receptor	0.0822215166115	178 / 0
Adenosine A2a receptor	ADORA2A	P29274	CHEMBL251	Family A G protein-coupled receptor	0.0822215166115	896 / 0
Vascular endothelial growth factor receptor 2	KDR	P35968	CHEMBL279	Kinase	0.0822215166115	490 / 0
Cyclin-dependent kinase 2	CDK2	P24941	CHEMBL301	Kinase	0.0822215166115	226 / 0
Cyclin-dependent kinase 9	CDK9	P50750	CHEMBL3116	Kinase	0.0822215166115	64 / 0
ADAM17	ADAM17	P78536	CHEMBL3706	Protease	0.0822215166115	220 / 0
Geranylgeranyl transferase type I	PGGT1B FNTA	P53609 P49354	CHEMBL2095164	Enzyme	0.0822215166115	7 / 0
Cyclin-dependent kinase 2/cyclin E	CCNE2 CDK2 CCNE1	O96020 P24941 P24864	CHEMBL2094126	Other cytosolic protein	0.0822215166115	96 / 0
Cathepsin K	CTSK	P43235	CHEMBL268	Protease	0.0822215166115	119 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
PI3-kinase p110-gamma subunit	PIK3CG	P48736	CHEMBL3267	Enzyme	0.0822215166115	307 / 0
Interleukin-1 receptor-associated kinase 4	IRAK4	Q9NWZ3	CHEMBL3778	Kinase	0.0822215166115	98 / 0
Nerve growth factor receptor Trk-A	NTRK1	P04629	CHEMBL2815	Kinase	0.0822215166115	230 / 0
Serine/threonine-protein kinase B-raf	BRAF	P15056	CHEMBL5145	Kinase	0.0822215166115	156 / 0
Cholecystokinin B receptor	CCKBR	P32239	CHEMBL298	Family A G protein-coupled receptor	0.0822215166115	88 / 0
GABA receptor alpha-5 subunit	GABRA5	P31644	CHEMBL5112	Ligand-gated ion channel	0.0822215166115	136 / 0
Matrix metalloproteinase 13	MMP13	P45452	CHEMBL280	Protease	0.0822215166115	308 / 0
Matrix metalloproteinase 3	MMP3	P08254	CHEMBL283	Protease	0.0822215166115	167 / 0
Matrix metalloproteinase 9	MMP9	P14780	CHEMBL321	Protease	0.0822215166115	226 / 0
Matrix metalloproteinase 1	MMP1	P03956	CHEMBL332	Protease	0.0822215166115	332 / 0
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	0.0822215166115	257 / 0
Hepatocyte growth factor receptor	MET	P08581	CHEMBL3717	Kinase	0.0822215166115	256 / 0
Matrix metalloproteinase 8	MMP8	P22894	CHEMBL4588	Protease	0.0822215166115	103 / 0
Epidermal growth factor receptor erbB1	EGFR	P00533	CHEMBL203	Kinase	0.0822215166115	545 / 0
Neurokinin 2 receptor	TACR2	P21452	CHEMBL2327	Family A G protein-coupled receptor	0.0822215166115	91 / 0
Sodium/glucose cotransporter 2	SLC5A2	P31639	CHEMBL3884	Electrochemical transporter	0.0822215166115	519 / 0
MAP kinase ERK2	MAPK1	P28482	CHEMBL4040	Kinase	0.0822215166115	370 / 0
ADAM10	ADAM10	O14672	CHEMBL5028	Protease	0.0822215166115	16 / 0
PI3-kinase p110-beta subunit	PIK3CB	P42338	CHEMBL3145	Enzyme	0.0822215166115	257 / 0
PI3-kinase p110-alpha subunit	PIK3CA	P42336	CHEMBL4005	Enzyme	0.0822215166115	1130 / 0
ALK tyrosine kinase receptor	ALK	Q9UM73	CHEMBL4247	Kinase	0.0822215166115	76 / 0
Endothelin receptor ET-B	EDNRB	P24530	CHEMBL1785	Family A G protein-coupled receptor	0.0822215166115	96 / 0
Endothelin receptor ET-A	EDNRA	P25101	CHEMBL252	Family A G protein-coupled receptor	0.0822215166115	160 / 0
Adenosine A2b receptor	ADORA2B	P29275	CHEMBL255	Family A G protein-coupled receptor	0.0822215166115	84 / 0
Protein kinase C alpha	PRKCA	P17252	CHEMBL299	Kinase	0.0822215166115	179 / 0
RAS guanyl	RASGRP3	Q8IV61	CHEMBL3638	Other cytosolic	0.0822215166115	50 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
releasing protein 3				protein		
Tyrosine-protein kinase SYK	SYK	P43405	CHEMBL2599	Kinase	0.0822215166115	600 / 0
Proteasome Macropain subunit	PSMB2	P49721	CHEMBL3492	Protease	0.0822215166115	4 / 0
Tyrosine-protein kinase TYK2	TYK2	P29597	CHEMBL3553	Kinase	0.0822215166115	90 / 0
Matrix metalloproteinase 14	MMP14	P50281	CHEMBL3869	Protease	0.0822215166115	99 / 0
Matrix metalloproteinase 7	MMP7	P09237	CHEMBL4073	Protease	0.0822215166115	49 / 0
26S proteosome	PSMB1	P20618	CHEMBL4208	Protease	0.0822215166115	2 / 0
Proteasome Macropain subunit MB1	PSMB5	P28074	CHEMBL4662	Protease	0.0822215166115	16 / 0
Phosphodiesterase 5A	PDE5A	O76074	CHEMBL1827	Phosphodiesterase	0.0822215166115	221 / 0
Serine/threonine-protein kinase mTOR	MTOR	P42345	CHEMBL2842	Kinase	0.0822215166115	966 / 0
Hexokinase type IV	GCK	P35557	CHEMBL3820	Enzyme	0.0822215166115	139 / 0
Caspase-1 (by homology)	CASP1	P29466	CHEMBL4801	Protease	0.0822215166115	135 / 0
Matrix metalloproteinase 10	MMP10	P09238	CHEMBL4270	Protease	0.0822215166115	3 / 0
Tyrosine kinase non-receptor protein 2	TNK2	Q07912	CHEMBL4599	Kinase	0.0822215166115	92 / 0
Equilibrative nucleoside transporter 1	SLC29A1	Q99808	CHEMBL1997	Electrochemical transporter	0.0822215166115	75 / 0
Mammalian target of Rapamycin (mTORC1)	FKBP1A MTOR	P62942 P42345	CHEMBL2221341	Kinase	0.0822215166115	38 / 0
3-phosphoinositide dependent protein kinase-1	PDPK1	O15530	CHEMBL2534	Kinase	0.0822215166115	99 / 0
Cathepsin D	CTSD	P07339	CHEMBL2581	Protease	0.0822215166115	228 / 0
Cathepsin S	CTSS	P25774	CHEMBL2954	Protease	0.0822215166115	97 / 0
Thymidine phosphorylase	TYMP	P19971	CHEMBL3106	Enzyme	0.0822215166115	3 / 0
Caspase-8	CASP8	Q14790	CHEMBL3776	Protease	0.0822215166115	104 / 0
Beta-secretase 1	BACE1	P56817	CHEMBL4822	Protease	0.0822215166115	802 / 0
Mitogen-activated protein kinase kinase kinase 14	MAP3K14	Q99558	CHEMBL5888	Kinase	0.0822215166115	340 / 0
Serotonin 2b (5-HT2b) receptor	HTR2B	P41595	CHEMBL1833	Family A G protein-coupled receptor	0.0822215166115	30 / 0
Serine/threonine-protein kinase	AURKB	Q96GD4	CHEMBL2185	Kinase	0.0822215166115	184 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Aurora-B						
Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1	Q02750	CHEMBL3587	Kinase	0.0822215166115	197 / 0
Serine/threonine-protein kinase Aurora-A	AURKA	O14965	CHEMBL4722	Kinase	0.0822215166115	280 / 0
Glyceraldehyde-3-phosphate dehydrogenase liver	GAPDH	P04406	CHEMBL2284	Oxidoreductase	0.0822215166115	10 / 0
Tyrosine-protein kinase ITK/TSK	ITK	Q08881	CHEMBL2959	Kinase	0.0822215166115	78 / 0
Cyclin-dependent kinase 1	CDK1	P06493	CHEMBL308	Kinase	0.0822215166115	223 / 0
Interleukin-8 receptor A	CXCR1	P25024	CHEMBL4029	Family A G protein-coupled receptor	0.0822215166115	51 / 0
DNA polymerase alpha subunit	POLA1	P09884	CHEMBL1828	Transferase	0.0822215166115	3 / 0
Cyclin-dependent kinase 2/cyclin E1	CCNE1 CDK2	P24864 P24941	CHEMBL1907605	Kinase	0.0822215166115	85 / 0
Arachidonate 5-lipoxygenase	ALOX5	P09917	CHEMBL215	Oxidoreductase	0.0822215166115	94 / 0
Tyrosine-protein kinase SRC	SRC	P12931	CHEMBL267	Kinase	0.0822215166115	246 / 0
Phosphodiesterase 4D	PDE4D	Q08499	CHEMBL288	Phosphodiesterase	0.0822215166115	53 / 0
Cyclin-dependent kinase 5/CDK5 activator 1	CDK5	Q00535	CHEMBL4036	Kinase	0.0822215166115	47 / 0
Sodium channel protein type IX alpha subunit	SCN9A	Q15858	CHEMBL4296	Voltage-gated ion channel	0.0822215166115	245 / 0
Tyrosine-protein kinase JAK3	JAK3	P52333	CHEMBL2148	Kinase	0.0822215166115	195 / 0
Tyrosine-protein kinase JAK1	JAK1	P23458	CHEMBL2835	Kinase	0.0822215166115	171 / 0
Tyrosine-protein kinase JAK2	JAK2	O60674	CHEMBL2971	Kinase	0.0822215166115	314 / 0
Matrix metalloproteinase 12	MMP12	P39900	CHEMBL4393	Protease	0.0822215166115	31 / 0
Sodium/glucose cotransporter 1	SLC5A1	P13866	CHEMBL4979	Electrochemical transporter	0.0822215166115	145 / 0
Tyrosine-protein kinase FYN	FYN	P06241	CHEMBL1841	Kinase	0.0822215166115	16 / 0
Complement factor D	CFD	P00746	CHEMBL2176771	Protease	0.0822215166115	125 / 0
HERG	KCNH2	Q12809	CHEMBL240	Voltage-gated ion channel	0.0822215166115	277 / 0
MAP kinase p38 alpha (by	MAPK14	Q16539	CHEMBL260	Kinase	0.0822215166115	384 / 0

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
homology)						
Cyclin-dependent kinase 4	CDK4	P11802	CHEMBL331	Kinase	0.0822215166115	154 / 0
Acetyl-coenzyme A transporter 1	SLC33A1	O00400	CHEMBL3638338	Electrochemical transporter	0.0822215166115	65 / 0
Transient receptor potential cation channel subfamily A member 1	TRPA1	O75762	CHEMBL6007	Voltage-gated ion channel	0.0822215166115	9 / 0
Gamma-secretase	PSEN2 PSENEN NCSTN APH1A PSEN1 APH1B	P49810 Q9NZ42 Q92542 Q96BI3 P49768 Q8WW43	CHEMBL2094135	Protease	0.0822215166115	94 / 0
Cyclin-dependent kinase 7/ cyclin H	CDK7 CCNH	P50613 P51946	CHEMBL2111288	Other cytosolic protein	0.0822215166115	46 / 0
PI3-kinase p110-delta subunit	PIK3CD	O00329	CHEMBL3130	Enzyme	0.0822215166115	250 / 0