Supplementary Table S1: The various targets to which the chemical may bind are generally anticipated by the algorithms with likelihood score ranges from 0.376973 to 0.10934.

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Arachidonate 5-lipoxygenase	ALOX5	P09917	CHEMBL 215	Oxidoreductase	0.376973	0 / 42Â Â Â Â Â
3-phosphoinositide dependent protein kinase-1	PDPK1	O15530	CHEMBL 2534	Kinase	0.376973	0 / 1Â Â Â Â Â
Aldose reductase (by homology)	AKR1B1	P15121	CHEMBL 1900	Enzyme	0.149917	3 / 40Â Â Â Â Â
Voltage-gated potassium channel subunit Kv1.3	KCNA3	P22001	CHEMBL 4633	Voltage-gated ion channel	0.149917	0 / 9Â Â Â Â Â
Beta amyloid A4 protein	APP	P05067	CHEMBL 2487	Membrane receptor	0.133684	0 / 15Â Â Â Â Â
Epidermal growth factor receptor erbB1	EGFR	P00533	CHEMBL 203	Kinase	0.117455	5 / 15Â Â Â Â Â
ATP-binding cassette sub-family G member 2	ABCG2	Q9UNQ0	CHEMBL 5393	Primary active transporter	0.10934	1 / 54Â Â Â Â Â
Neuronal acetylcholine receptor protein alpha-7 subunit	CHRNA7	P36544	CHEMBL 2492	Ligand-gated ion channel	0.10934	0 / 11Â Â Â Â Â
Coagulation factor VII/tissue factor	F3	P13726	CHEMBL 4081	Surface antigen	0.10934	0 / 6Â Â Â Â Â
Tubulin beta-1 chain	TUBB1	Q9H4B7	CHEMBL 1915	Structural protein	0.10934	0 / 16Â Â Â Â Â
Monoamine oxidase B	MAOB	P27338	CHEMBL 2039	Oxidoreductase	0.10934	0 / 114Â Â Â Â Â
Protein-tyrosine phosphatase 1B	PTPN1	P18031	CHEMBL 335	Phosphatase	0.10934	6 / 34Â Â Â Â Â
Monoamine oxidase A	MAOA	P21397	CHEMBL 1951	Oxidoreductase	0.10934	0 / 31Â Â Â Â Â
Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL 1978	Cytochrome P450	0.10934	2 / 39Â Â Â Â Â
Nitric oxide synthase, inducible (by homology)	NOS2	P35228	CHEMBL 4481	Enzyme	0.10934	2 / 10Â Â Â Â Â
Ornithine decarboxylase	ODC1	P11926	CHEMBL 1869	Lyase	0.10934	0 / 6Â Â Â Â Â
Telomerase reverse transcriptase	TERT	O14746	CHEMBL 2916	Enzyme	0.10934	0 / 2Â Â Â Â Â
MAP kinase-activated protein kinase 2	MAPKAPK2	P49137	CHEMBL 2208	Kinase	0.10934	0 / 2Â Â Â Â Â
MAP kinase-activated protein kinase 5	MAPKAPK5	Q8IW41	CHEMBL 3094	Kinase	0.10934	0 / 1Â Â Â Â Â
Aldehyde dehydrogenase	ALDH2	P05091	CHEMBL 1935	Oxidoreductase	0.10934	0 / 1Â Â Â Â Â
P-glycoprotein 1	ABCB1	P08183	CHEMBL 4302	Primary active transporter	0.10934	7 / 20Â Â Â Â Â
Acetylcholinesterase	ACHE	P22303	CHEMBL 220	Hydrolase	0.10934	0 / 72Â Â Â Â Â
Cyclooxygenase-1	PTGS1	P23219	CHEMBL 221	Oxidoreductase	0.10934	1 / 13Â Â Â Â Â
Toll-like receptor	TLR9	Q9NR9	CHEMBL	Toll-like and	0.10934	1 / 6Â Â Â Â Â

(TLR7/TLR9)		6	5804	Il-1 receptors		
Thrombin and coagulation factor X	F10	P00742	CHEMBL 244	Protease	0.10934	22 / 0Â Â Â Â Â
Cyclooxygenase-2	PTGS2	P35354	CHEMBL 230	Oxidoreductase	0.10934	1 / 13Â Â Â Â Â
Cysteinyl leukotriene receptor 2	CYSLTR2	Q9NS75	CHEMBL 4330	Family A G protein-coupled receptor	0.10934	0 / 2Â Â Â Â Â
Stem cell growth factor receptor	KIT	P10721	CHEMBL 1936	Kinase	0.10934	0 / 2Â Â Â Â Â
Peroxisome proliferator-activated receptor gamma	PPARG	P37231	CHEMBL 235	Nuclear receptor	0.10934	0 / 18Â Â Â Â Â
Protein kinase C delta	PRKCD	Q05655	CHEMBL 2996	Kinase	0.10934	28 / 1Â Â Â Â Â
Beta-secretase 1	BACE1	P56817	CHEMBL 4822	Protease	0.10934	3 / 22Â Â Â Â Â
Induced myeloid leukemia cell differentiation protein Mcl-1	MCL1	Q07820	CHEMBL 4361	Other cytosolic protein	0	6 / 7Â Â Â Â Â
Alpha-synuclein	SNCA	P37840	CHEMBL 6152	Unclassified protein	0	0 / 3Â Â Â Â Â
ALK tyrosine kinase receptor	ALK	Q9UM73	CHEMBL 4247	Kinase	0	1 / 0Â Â Â Â Â
Nuclear factor NF-kappa-B p65 subunit	RELA	Q04206	CHEMBL 5533	Transcription factor	0	1 / 7Â Â Â Â Â
Urokinase-type plasminogen activator	PLAU	P00749	CHEMBL 3286	Protease	0	6 / 0Â Â Â Â Â
Endoplasmin	HSP90B1	P14625	CHEMBL 1075323	Other membrane protein	0	40 / 0Â Â Â Â Â
Aldo-keto-reductase family 1 member C3	AKR1C3	P42330	CHEMBL 4681	Enzyme	0	0 / 2Â Â Â Â Â
C-X-C chemokine receptor type 4	CXCR4	P61073	CHEMBL 2107	Family A G protein-coupled receptor	0	0 / 1Â Â Â Â Â
Interleukin-8 receptor B	CXCR2	P25025	CHEMBL 2434	Family A G protein-coupled receptor	0	28 / 0Â Â Â Â Â
Butyrylcholinesterase	BCHE	P06276	CHEMBL 1914	Hydrolase	0	0 / 8Â Â Â Â Â
Adenosine A2b receptor	ADORA2B	P29275	CHEMBL 255	Family A G protein-coupled receptor	0	1 / 0Â Â Â Â Â
Rho-associated protein kinase 2	ROCK2	O75116	CHEMBL 2973	Kinase	0	1 / 0Â Â Â Â Â
Arachidonate 12-lipoxygenase	ALOX12	P18054	CHEMBL 3687	Enzyme	0	2 / 0Â Â Â Â Â
Histamine H3 receptor	HRH3	Q9Y5N1	CHEMBL 264	Family A G protein-coupled	0	0 / 1Â Â Â Â Â

				receptor		
Prostanoid EP4 receptor	PTGER4	P35408	CHEMBL1836	Family A G protein-coupled receptor	0	0 / 11Â Â Â Â Â
Prostanoid EP2 receptor	PTGER2	P43116	CHEMBL1881	Family A G protein-coupled receptor	0	0 / 12Â Â Â Â Â
Prostanoid EP3 receptor	PTGER3	P43115	CHEMBL3710	Family A G protein-coupled receptor	0	0 / 11Â Â Â Â Â
Estradiol 17-beta-dehydrogenase 2	HSD17B2	P37059	CHEMBL2789	Enzyme	0	2 / 0Â Â Â Â Â
Estradiol 17-beta-dehydrogenase 1	HSD17B1	P14061	CHEMBL3181	Enzyme	0	2 / 0Â Â Â Â Â
Dihydroorotate dehydrogenase	DHODH	Q02127	CHEMBL1966	Oxidoreductase	0	0 / 1Â Â Â Â Â
Protein kinase C alpha	PRKCA	P17252	CHEMBL299	Kinase	0	29 / 0Â Â Â Â Â
Protein kinase C beta	PRKCB	P05771	CHEMBL3045	Kinase	0	32 / 0Â Â Â Â Â
Protein kinase C epsilon	PRKCE	Q02156	CHEMBL3582	Kinase	0	28 / 0Â Â Â Â Â
C-C chemokine receptor type 4	CCR4	P51679	CHEMBL2414	Family A G protein-coupled receptor	0	7 / 0Â Â Â Â Â
Proteasome assembly chaperone 3	PSMG3	Q9BT73	CHEMBL1075137	Unclassified protein	0	1 / 0Â Â Â Â Â
Prostaglandin E synthase	PTGES	O14684	CHEMBL5658	Enzyme	0	4 / 26Â Â Â Â Â
Cyclin-dependent kinase 5/CDK5 activator 1 CDK5	CDK5R1	Q15078 Q00535	CHEMBL1907600	Kinase	0	0 / 1Â Â Â Â Â
Plasminogen activator inhibitor-1	SERPINE1	P05121	CHEMBL3475	Secreted protein	0	1 / 0Â Â Â Â Â
Interleukin-8 receptor A	CXCR1	P25024	CHEMBL4029	Family A G protein-coupled receptor	0	1 / 0Â Â Â Â Â
Endothelin receptor ET-A (by homology)	EDNRA	P25101	CHEMBL252	Family A G protein-coupled receptor	0	0 / 32Â Â Â Â Â
Inosine-5'-monophosphate dehydrogenase 2	IMPDH2	P12268	CHEMBL2002	Oxidoreductase	0	0 / 22Â Â Â Â Â
Cyclin-dependent kinase 4/cyclin D1	CCND1 CDK4	P24385 P11802	CHEMBL1907601	Kinase	0	2 / 0Â Â Â Â Â
Protein kinase C gamma	PRKCG	P05129	CHEMBL2938	Kinase	0	26 / 0Â Â Â Â Â
Protein kinase C eta	PRKCH	P24723	CHEMBL3616	Kinase	0	27 / 0Â Â Â Â Â
Leukocyte elastase	ELANE	P08246	CHEMBL	Protease	0	0 / 17Â Â Â Â Â

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Retinoic acid receptor gamma	RARG	P13631	CHEMBL 2003	Nuclear receptor	0	0 / 15Â Â Â Â Â
Retinoic acid receptor beta	RARB	P10826	CHEMBL 2008	Nuclear receptor	0	0 / 13Â Â Â Â Â
Retinoic acid receptor alpha	RARA	P10276	CHEMBL 2055	Nuclear receptor	0	0 / 12Â Â Â Â Â
Vascular endothelial growth factor receptor 1	FLT1	P17948	CHEMBL 1868	Kinase	0	0 / 1Â Â Â Â Â
Histone deacetylase 2	HDAC2	Q92769	CHEMBL 1937	Eraser	0	0 / 1Â Â Â Â Â
Platelet-derived growth factor receptor alpha	PDGFRA	P16234	CHEMBL 2007	Kinase	0	0 / 1Â Â Â Â Â
Serine/threonine-protein kinase Aurora-C	AURKC	Q9UQB9	CHEMBL 3935	Kinase	0	0 / 1Â Â Â Â Â
Cathepsin L	CTSL	P07711	CHEMBL 3837	Protease	0	0 / 4Â Â Â Â Â
Squalene monooxygenase (by homology)	SQLE	Q14534	CHEMBL 3592	Enzyme	0	1 / 0Â Â Â Â Â
Apoptosis regulator Bcl-X	BCL2L1	Q07817	CHEMBL 4625	Other ion channel	0	1 / 0Â Â Â Â Â
cAMP-dependent protein kinase alpha-catalytic subunit	PRKACA	P17612	CHEMBL 4101	Kinase	0	10 / 0Â Â Â Â Â
Egl nine homolog 1	EGLN1	Q9GZT9	CHEMBL 5697	Oxidoreductase	0	49 / 0Â Â Â Â Â
Glycogen synthase kinase-3 beta	GSK3B	P49841	CHEMBL 262	Kinase	0	1 / 3Â Â Â Â Â
Receptor protein-tyrosine kinase erbB-2	ERBB2	P04626	CHEMBL 1824	Kinase	0	5 / 2Â Â Â Â Â
C-C chemokine receptor type 5	CCR5	P51681	CHEMBL 274	Family A G protein-coupled receptor	0	1 / 0Â Â Â Â Â
Poly [ADP-ribose] polymerase-1	PARP1	P09874	CHEMBL 3105	Enzyme	0	0 / 15Â Â Â Â Â
Phosphodiesterase 5A	PDE5A	O76074	CHEMBL 1827	Phosphodiesterase	0	2 / 0Â Â Â Â Â
Steryl-sulfatase	STS	P08842	CHEMBL 3559	Enzyme	0	0 / 2Â Â Â Â Â
Isocitrate dehydrogenase [NADP] cytoplasmic	IDH1	O75874	CHEMBL 2007625	Enzyme	0	1 / 0Â Â Â Â Â
Thrombin	F2	P00734	CHEMBL 204	Protease	0	8 / 0Â Â Â Â Â
Fatty acid synthase	FASN	P49327	CHEMBL 4158	Transferase	0	1 / 0Â Â Â Â Â
Dual specificity protein phosphatase 3	DUSP3	P51452	CHEMBL 2635	Phosphatase	0	2 / 0Â Â Â Â Â
Microtubule-associated protein tau	MAPT	P10636	CHEMBL 1293224	Unclassified protein	0	0 / 1Â Â Â Â Â
G-protein coupled receptor 84	GPR84	Q9NQS5	CHEMBL 3714079	Family A G protein-coupled receptor	0	1 / 0Â Â Â Â Â

Tyrosine-protein kinase LCK	LCK	P06239	CHEMBL 258	Kinase	0	0 / 15Â Â Â Â Â
DNA excision repair protein ERCC-5	ERCC5	P28715	CHEMBL 4736	Other nuclear protein	0	2 / 0Â Â Â Â Â
Pyruvate dehydrogenase kinase isoform 1	PDK1	Q15118	CHEMBL 4766	Kinase	0	6 / 0Â Â Â Â Â
Flap endonuclease 1	FEN1	P39748	CHEMBL 5027	Enzyme	0	4 / 0Â Â Â Â Â
Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL 239	Nuclear receptor	0	0 / 9Â Â Â Â Â
Peroxisome proliferator-activated receptor delta	PPARD	Q03181	CHEMBL 3979	Nuclear receptor	0	0 / 4Â Â Â Â Â
ADAMTS5	ADAMTS5	Q9UNA0	CHEMBL 2285	Protease	0	2 / 0Â Â Â Â Â
Alcohol dehydrogenase class III	ADH5	P11766	CHEMBL 4116	Enzyme	0	6 / 0Â Â Â Â Â
Maternal embryonic leucine zipper kinase	MELK	Q14680	CHEMBL 4578	Kinase	0	4 / 0Â Â Â Â Â
Ryanodine receptor 1	RYR1	P21817	CHEMBL 1846	Ligand-gated ion channel	0	1 / 0Â Â Â Â Â