Supplementary Table S1. Drug-likeness properties of metabolite

Molecule	Canonical SMILES	Formula	MW
Hydroperoxide, 1-methylbutyl	CC(OO)CCC	C5H12O2	104.15
Trimethylsilyl ethaneperoxoate	CC(=O)OO[Si](C)(C)C	C5H12O3Si	148.23
4-Hydroxy-2-butanone	CC(=O)CCO	C4H8O2	88.11
2-(isobutoxymethyl)oxirane	CC(COCC1CO1)C	C7H14O2	130.18
2,4-Di-tert-butylphenol	CC(COCC1CO1)C	C7H14O2	130.18
Nyasol	C=C[C@@H](c1ccc(cc1)O)/C=C\c1ccc(cc1)O	C17H16O2	252.31
trans-4,4'-Dimethoxy-beta-methylchalcone	COc1ccc(cc1)/C(=C/C(=O)c1ccc(cc1)OC)/C	C18H18O3	282.33
Pent-3-ene-2-one, 3-phenyl-, oxime	C/C=C(\c1ccccc1)/C(=N/O)/C	C11H13NO	175.23

#Heavy atoms	#Aromatic heavy atoms	Fraction Csp3	#Rotatable bonds	#H-bond acceptors	#H-bond donors
7	0	1	3	2	1
9	0	0.8	3	3	0
6	0	0.75	2	2	1
9	0	1	4	2	0
9	0	1	4	2	0
19	12	0.06	4	2	2
21	12	0.17	5	3	0
13	6	0.18	2	2	1

MR	TPSA	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P	Consensus Log P
28.81	29.46	1.82	1.27	1.66	1.04	0.35	1.23
36.39	35.53	2.29	1.59	1.32	0.83	-1	1
22.7	37.3	0.71	-0.8	-0.04	-0.33	0.13	-0.06
35.82	21.76	2.27	1.32	1.06	0.57	1.84	1.41
35.82	21.76	2.27	1.32	1.06	0.57	1.84	1.41
79.01	40.46	2.42	4.38	3.97	3.54	4	3.66
84.04	35.53	3.26	4.26	3.99	2.9	4.25	3.73
55.37	32.59	2.28	2.66	2.94	2.49	2.57	2.59

ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)
-1.09	8.51	0.0817	Very soluble	-1.49	3.39
-1.56	4.06	0.0274	Very soluble	-1.95	1.67
0.25	157	1.78	Highly soluble	0.5	276
-1.21	7.94	0.061	Very soluble	-1.38	5.45
-1.21	7.94	0.061	Very soluble	-1.38	5.45
-4.37	0.0108	0.0000429	Moderately soluble	-4.95	0.00286
-4.37	0.0121	0.0000429	Moderately soluble	-4.72	0.00541
-2.81	0.27	0.00154	Soluble	-3	0.177

Ali Solubility (mol/l)	Ali Class	Silicos-IT LogSw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)
0.0325	Very soluble	-0.61	25.8	0.248
0.0113	Very soluble	-0.94	16.9	0.114
3.13	Highly soluble	-0.35	39.4	0.448
0.0419	Very soluble	-1.28	6.88	0.0528

0.0419	Very soluble	-1.28	6.88	0.0528
0.0000113	Moderately soluble	-4.35	0.0112	0.0000443
0.0000191	Moderately soluble	-5.59	0.000722	0.00000256
0.00101	Soluble	-2.78	0.293	0.00167

Silicos-IT class	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor
Soluble	High	Yes	No	No	No
Soluble	High	Yes	No	No	No
Soluble	High	No	No	No	No
Soluble	High	Yes	No	No	No
Soluble	High	Yes	No	No	No
Moderately soluble	High	Yes	No	Yes	No
Moderately soluble	High	Yes	No	Yes	Yes
Soluble	High	Yes	No	No	No

CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp (cm/s)	Lipinski #violations	Ghose #violations	Veber #violations
No	No	No	-6.03	0	3	0
No	No	No	-6.08	0	2	0
No	No	No	-7.41	0	3	0
No	No	No	-6.16	0	2	0
No	No	No	-6.16	0	2	0
Yes	Yes	Yes	-4.73	0	0	0
Yes	Yes	Yes	-5	0	0	0

No	No	No	-5.48	0	0	0

Egan #violations	Muegge #violations	Bioavailability Score	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility
0	1	0.55	0	1	1	2.61
0	1	0.55	0	2	1	3.3
0	2	0.55	0	0	1	1
0	1	0.55	0	1	1	2.78
0	1	0.55	0	1	1	2.78
0	0	0.55	0	1	1	3.05
0	0	0.55	0	1	1	2.61
0	1	0.55	0	3	1	2.47