

## Supplementary file

smiles	LogS	LogD	LogP	Pgp-inh	Pgp-sub	HIA	F(20%)	F(30%)	Caco-2
<chem>COc1ccc2c(c1)OC[C@H](c1ccc(O)cc1OC)C2</chem>	-4.083	3.482	3.574	0.016	0.552	0.004	0.518	0.137	-4.816
<chem>COc1cc(OC)c2c(c1)O[C@H](c1ccc3c(c1)OCO3)[C@H](O)C2</chem>	-5.149	3.251	3.178	0.925	0.002	0.003	0.002	0.002	-4.944
<chem>COc1cc2c(cc1O)C(Cc1ccc(OC)c(OC)c1)N(C)CC2</chem>	-2.283	3.038	2.316	0.538	0.69	0.004	0.234	0.805	-4.615
<chem>NC(=O)c1cc(Cl)c(OCc2ccccc2)c(Cl)c1</chem>	-4.91	3.034	3.594	0.839	0.002	0.003	0.002	0.516	-4.681
<chem>COc1cc2c(cc1OC)-c1c(OC)c(OC)cc3c1[C@H](C2)N(C)CC3</chem>	-3.1	3.035	2.733	0.886	0.985	0.003	0.341	0.705	-4.905

MDCK	BBB	PPB	VDss	Fu	CYP1A2-inh	CYP1A2-sub	CYP2C19-inh	CYP2C19-sub	CYP2C9-inh	CYP2C9-sub	CYP2D6-inh	CYP2D6-sub	CYP3A4-inh	CYP3A4-sub
2.48E-05	0.088	96.26%	1.015	4.36%	0.96	0.965	0.939	0.863	0.705	0.942	0.831	0.953	0.802	0.716
4.62E-05	0.892	94.97%	0.861	3.75%	0.817	0.908	0.869	0.824	0.715	0.901	0.941	0.913	0.961	0.784
1.90E-05	0.987	74.15%	1.783	14.54%	0.147	0.966	0.137	0.95	0.014	0.662	0.473	0.948	0.053	0.927
1.63E-05	0.706	99.98%	0.627	1.33%	0.961	0.731	0.863	0.074	0.795	0.401	0.074	0.21	0.065	0.186
3.08E-05	0.971	63.28%	1.752	25.54%	0.165	0.982	0.086	0.957	0.013	0.81	0.064	0.941	0.081	0.93

T12	hERG	H-HT	DILI	Ames	ROA	FDAMDD	SkinSen	Carcinogenicity	EC	EI	Respiratory	BCF	IGC50
0.563	0.153	0.272	0.472	0.322	0.083	0.929	0.672	0.845	0.004	0.55	0.726	2.274	4.816
0.225	0.159	0.213	0.79	0.237	0.029	0.325	0.269	0.892	0.003	0.032	0.661	2.018	4.167

0.849	0.766	0.19	0.419	0.152	0.438	0.906	0.587	0.059	0.003	0.01	0.927	1.845	4.53
0.214	0.448	0.109	0.939	0.059	0.053	0.423	0.087	0.565	0.003	0.027	0.016	1.18	4.181
0.471	0.388	0.16	0.739	0.227	0.857	0.948	0.164	0.037	0.003	0.01	0.944	2.593	4.242

LC50	LC50DM	NR-AR	NR-AR-LBD	NR-AhR	NR-Aromatase	NR-ER	NR-ER-LBD	NR-PPAR-gamma	SR-ARE	SR-ATAD5	SR-HSE	SR-MMP	SR-p53	MW
5.858	6.482	0.484	0.099	0.876	0.46	0.854	0.89	0.003	0.772	0.798	0.06	0.829	0.672	286.12
5.746	6.464	0.028	0.137	0.856	0.266	0.161	0.006	0.011	0.148	0.43	0.037	0.298	0.555	330.11
4.917	6.583	0.282	0.009	0.434	0.043	0.084	0.011	0.004	0.363	0.031	0.011	0.256	0.159	343.18
4.545	4.498	0.169	0.009	0.834	0.072	0.169	0.008	0.004	0.435	0.021	0.013	0.349	0.168	295.02
6.584	7.087	0.39	0.043	0.868	0.657	0.058	0.04	0.005	0.577	0.133	0.014	0.472	0.822	355.18

Vol	Dense	nHA	nHD	TPSA	nRot	nRing	MaxRing	nHet	fChar	nRig	Flex	nStereo	NonBiodegradable
296.261	0.966	4	1	47.92	3	3	10	4	0	17	0.176	1	0
322.581	1.023	6	1	66.38	3	4	10	6	0	21	0.143	2	0

359.146	0.956	5	1	51.16	5	3	10	5	0	17	0.294	1	0
274.131	1.076	3	2	52.32	4	2	6	5	0	13	0.308	0	1
367.885	0.965	5	0	40.16	4	4	16	5	0	20	0.2	1	0

SureChEMBL	LD50_oral	Skin_Sensitization	Acute_Aquatic_Toxicity	Toxicophores	Genotoxic_Carcinogenicity_Mutagenicity	QED	Synth	Fsp3
0	0	1	0	1	0	0.941	2.669	0.294
0	0	2	2	1	0	0.933	3.149	0.333
0	0	5	0	1	0	0.904	2.685	0.4
0	0	1	1	0	0	0.935	1.749	0.071
0	0	1	0	0	3	0.84	2.929	0.429

Chelating	PAINS	Lipinski	Pfizer	GSK	GoldenTriangle
0	0	Accepted	Rejected	Accepted	Accepted
0	0	Accepted	Rejected	Accepted	Accepted
1	0	Accepted	Accepted	Accepted	Accepted
0	0	Accepted	Rejected	Accepted	Accepted
0	0	Accepted	Accepted	Accepted	Accepted