

	A	B
1	Parameters	Data
2	Drug-Likeness and Physicochemical Properties	
3	molecular_weight	499.534
4	logP	1.0972
5	hydrogen_bond_acceptors	5
6	hydrogen_bond_donors	3
7	Lipinski	4
8	QED	0.5037
9	stereo_centers	6
10	tpsa	131.4
11	AMES	0.3283
12	BBB_Martins	0.8614
13	Bioavailability_Ma	0.5405
14	Metabolism (Cytochrome P450 interactions)	
15	CYP1A2_Veith	0.0003
16	CYP2C19_Veith	0.0427
17	CYP2C9_Substrate_CarbonMangels	0.0303
18	CYP2C9_Veith	0.0089
19	CYP2D6_Substrate_CarbonMangels	0.0971
20	CYP2D6_Veith	0.0179
21	CYP3A4_Substrate_CarbonMangels	0.8528
22	CYP3A4_Veith	0.5945
23	Toxicity and Safety	
24	Carcinogens_Lagunin	0.1027
25	ClinTox	0.3035
26	Skin_Reaction	0.2108
27	hERG	0.5546
28	DILI	0.1703
29	HIA_Hou	0.9736
30	NR-AR-LBD	0.0066
31	NR-AR	0.0215
32	NR-AhR	0.0017
33	NR-Aromatase	0.0305
34	NR-ER-LBD	0.0131
35	NR-ER	0.0266
36	NR-PPAR-gamma	0.0009
37	SR-ARE	0.1515
38	SR-ATAD5	0.0042
39	SR-HSE	0.0062

	A	B
40	SR-MMP	0.0109
41	SR-p53	0.0178
42	Absorption and Distribution	
43	Caco2_Wang	-5.2826
44	Pgp_Broccatelli	0.0719
45	PPBR_AZ	79.6453
46	PAMPA_NCATS	0.812
47	Excretion	
48	Clearance_Hepatocyte_AZ	10.8016
49	Clearance_Microsome_AZ	32.601
50	Half_Life_Obach	-19.9269
51	Solubility and Lipophilicity	
52	Lipophilicity_AstraZeneca	2.4429
53	HydrationFreeEnergy_FreeSolv	-8.6051
54	Solubility_AqSolDB	-4.2309