

Supplemental Table S1

	Bex	A64	A65	A66	A67	A68	A70	A71	A72	A73	A74	A75	A76	A77
MW	348.48	356.47	357.45	355.48	373.21	353.17	350.2	336.18	338.45	350.46	352.18	334.45	334.46	364.2
HBD	1	1	1	1	1	1	1	1	1	1	1	1	1	2
HBA	2	5	6	4	4	5	4	4	4	4	2	2	2	3
cLogP	5.86	4.209	4.556	5.983	6	5.072	5.101	5.177	4.83	5.021	6.57	6.427	6.496	7.287
Violations	1	0	0	1	1	1	1	1	0	1	1	1	1	1
cLogD	3.835	1.86	1.21	3.28	2.91	1.73	1.79	1.84	1.59	1.71	3.15	3.31	3.38	3.79
TPSA	37.3	62.66	75.55	49.77	49.77	77.24	63.08	63.08	63.08	63.08	37.3	37.3	37.3	57.53
LogS	-7.62	-5.443	-5.467	-6.062	-6.315	-5.207	-4.896	-5.254	-5.122	-4.896	-7.603	-7.345	-7.345	-7.397
Water Sol	1	2	2	1	1	2	2	2	2	2	1	1	1	1
Score	3.8	4.4	4.2	3.6	3.7	4	4	4	4.1	4	3.8	3.7	3.7	2.3

Supplemental Table S1. Chemical Properties Used in PCA Analysis (Figure 6). Calculation of HBA, HBD, TPSA, LogS, and cLogP was performed using DataWarrior (Sander, T). Calculation of LogP and water solubility were performed using SwissADME (2). cLogD was calculated using Chemaxon Software (Chemaxon, San Diego, CA). The CNS MPO Score (denoted as Score) was calculated using the algorithm in (3). Violations of Lipinski's Rules (4) were calculated using existing data from the table.

Supplement References.

1. Sander T., Freyss, J., von Korff, M., Rufener, C. 2015. DataWarrior: An Open-Source Program For Chemistry Aware Data Visualization And Analysis. *J. Chem. Info. Model.* 55 (2), 460-473. DOI: 10.1021/ci500588j
2. Daina, A., O. Michielin, O., Zoete, V. 2017. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep.* 7:42717. doi: 10.1038/srep42717.
3. Wager, T.T., Hou, X., Verhoest, P.R., Villalobos, A. 2016. Central Nervous System Multiparameter Optimization Desirability: Application in Drug Discovery. *ACS Chem. Neuro.* 7 (6), 767-775. DOI: 10.1021/acchemneuro.6b00029
4. Lipinski CA. Drug-like properties and the causes of poor solubility and poor permeability. *J. Pharmacology. Toxicol. Methods.* 2000;44:235-249.