

Table S2 25 molecular descriptors used for principal component analysis (PCA)

No.	Name	Description
1	MW	molecular weight
2	AMW	average molecular weight
3	Sv	sum of atomic van der Waals volumes (scaled on Carbon atom)
4	Mv	mean atomic van der Waals volume (scaled on Carbon atom)
5	Se	sum of atomic Sanderson electronegativities (scaled on Carbon atom)
6	Sp	sum of atomic polarizabilities (scaled on Carbon atom)
7	Me	mean atomic Sanderson electronegativity (scaled on Carbon atom)
8	Mp	mean atomic polarizability (scaled on Carbon atom)
9	a_hyd	number of hydrophobic atoms
10	MLOGP	Moriguchi octanolwater partition coefficient
11	mlogpCX	Moriguchi based lipophilicity descriptor (carbon and halogen atoms)
12	mlogpON	Moriguchi based lipophilicity descriptor (nitrogen and oxygen atoms)
13	mlogpPRX	Moriguchi based lipophilicity descriptor (proximity effect)
14	mlogpUB	Moriguchi based lipophilicity descriptor (unsaturated bonds)
15	mlogpHB	Moriguchi based lipophilicity descriptor (intramolecular H bonds)
16	mlogpPOL	Moriguchi based lipophilicity descriptor (Polar substituents)
17	mlogpAMP	Moriguchi based lipophilicity descriptor (amphotericity)
18	mlogpALK	Moriguchi based lipophilicity descriptor (alkanes and alkenes)
19	mlogpRNG	Moriguchi based lipophilicity descriptor (ring structures)
20	mlogpQN	Moriguchi based lipophilicity descriptor (quarternary nitrogen)
21	mlogpNO2	Moriguchi based lipophilicity descriptor (Nitro groups)
22	mlogpNCS	Moriguchi based lipophilicity descriptor (NCS)
23	mlogpBLM	Moriguchi based lipophilicity descriptor (beta lactam)
24	nHDon	number of hydrogen-bond donors
25	nHAcc	number of hydrogen-bond acceptors