Table 3. Estimated physicochemical and pharmacokinetic parameters by QikProp.[29]

Parameters	**2**	**7**	**22**	**23**	**Range[a] or raccomended value**
QPlogPo/w[b]	3,492	4,653	3,664	4,829	-2 - 6.5
QPlogS[c]	-4,275	-5,808	-4,143	-5,687	-6.5 - 0.5
QPPCaco[d]	1017,626	1017,756	2087,829	2090,597	< 25 poor >500 great
QPlogBB[e]	-0,762	-0,577	-0,517	-0,314	-3 – 1.2
QPPMDCK[f]	504,141	2354,847	1096,232	5127,252	< 25 poor >500 great
Human Oral Absorption Index[g]	3	3	3	3	1:low 2: medium 3: high
Percent Human Oral Absorption[h]	100	100	100	100	< 25% poor >80% great

[a]For 95% of known drugs; [b]predicted octanol/water partition coefficient; [c]predicted aqueous solubility, log S; [d]predicted apparent Caco-2 cell permeability in nm/sec; [e]predicted brain/blood partition coefficient; [f]predicted apparent MDCK cell permeability in nm/sec; [g]predicted qualitative human oral absorption; [h]predicted human oral absorption on 0 to 100% scale.