

Table S1 Results of six retrieved compounds for pharmacokinetics parameters obtained from Lipinski's rule of five filter parameters and ADMET descriptors.

Compd	Lipinski's rule of five			ADMET parameters		
	mw	Num_HBA	Num_HBD	AlogP98 (≥ 3) ^a	LogS (≥ -6) ^a	PSA (≤ 112) ^a
FX-01	432.877	4	1	5.737	-5.596	90.465
FX-02	437.922	5	3	3.774	-5.04	91.607
FX-03	472.367	5	3	4.439	-5.908	90.532
FX-04	408.495	4	1	5.839	-5.539	80.384
FX-05	401.458	5	3	3.757	-5.986	84.207
FX-06	408.452	5	2	4.188	-5.276	93.651

^a AlogP98 ≥ 3 , LogS ≥ -6 and PSA ≤ 112 were used as control.