Table S5. Evaluation parameters of Lipinski's rule of five and its extensions for compounds **5e**, **5f**, and **6a-c,e.**

Compound	mol_MW (<500amu)	donorHB (<5)	accptHB (<10)	QPlogPo/w (<5)	#rotor (0−15)	N of violations (<5)
5e	**548.632**	0.000	9.250	**5.656**	12	2
5f	**548.632**	0.000	9.250	**5.595**	12	2
6a	370.447	0.000	6.000	4.202	7	0
6b	400.473	0.000	6.750	4.283	8	0
6c	384.474	0.000	6.000	4.519	7	0
6e	460.526	0.000	8.250	4.216	10	0

a: QikProp (QP) version 6.5; mol_MW: Molecular weight; donorHB: Number of hydrogen-bond donors (OH, NH, SH); accptHB: Number of hydrogen-bond acceptors (heteroatom O; N; S; F or pairs of transferable electrons); logP: Predicted log *n*-octanol/water partition coefficient; #rotor: Number of non-trivial (not CX3), non-hindered (not alkene, amide, small ring) rotatable bonds. Bold numbers correspond to Lipinski Rule-of Five violations.