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Supplementary material:

Table 1: Principal Descriptors calculated by Lipinski's Rule of Five

Lead molecules[a]	MW[b]	Number of HBA[c]	Number of HBD[d]	Mol LogP[e]	Mol LogS[f]
Synthetic compounds					
ASN03576800	285.03	7	2	-0.09	-2.68
ASN07462345	411.16	5	1	3.90	-5.83
ASN06396768	336.01	5	1	3.22	-4.66
ASN05439185	478.10	6	2	3.85	-6.54
ASN01516681	393.15	4	2	3.98	-5.63
Natural compounds					
693	194.41	9	4	-1.87	-0.91
234	313.35	5	3	2.71	-4.13
86	180.19	0	4	-0.20	-0.04
3	212.24	2	2	3.03	-2.90
358	290.27	7	5	0.29	-2.52

a. Ligand molecule IDs of Asinex database
b. Molecular weight of the molecule (160 to 500)
c. Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution (not more than 10).
d. Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution (not more than 5).
e. Log P for octanol / water (-2.0 – 6.5).
f. Predicted aqueous solubility, log S. S in mol dm–3 is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid (-6.5 – 0.5).

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