

Supporting information for

**A multi-disciplinary team-based classroom exercise for small molecule
drug discovery**

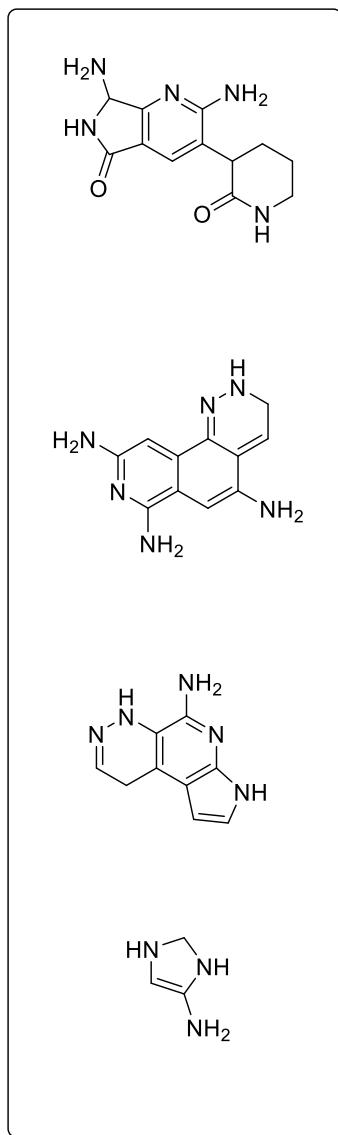
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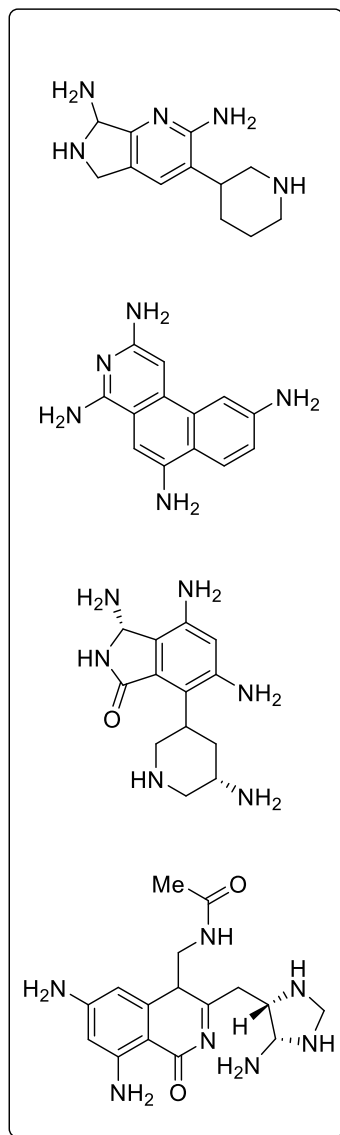
Example of student-designed compound progression

Round 1



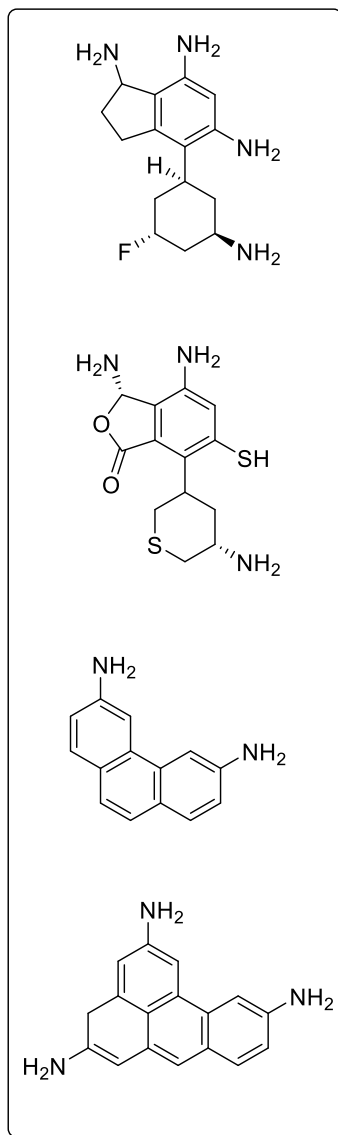
Dose-response (IC_{50} values)

Round 2



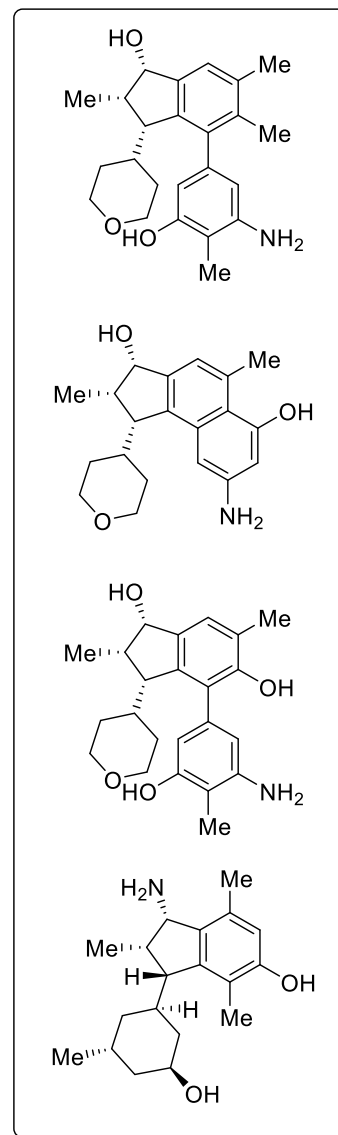
Dose-response (IC_{50} values)

Round 3



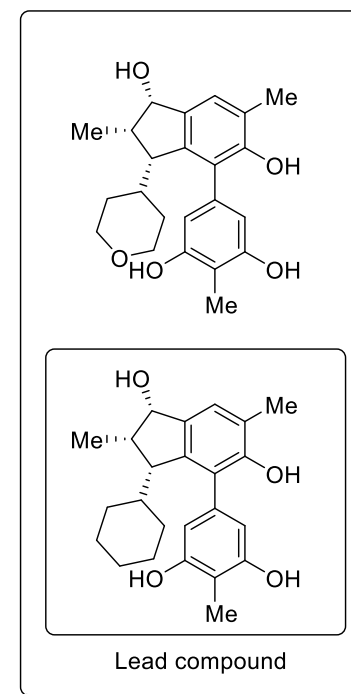
Dose-response (IC_{50} values)

Round 4



Dose-response (IC_{50} values)

Round 5



Genotoxicity assay (Comet assay) (x2)

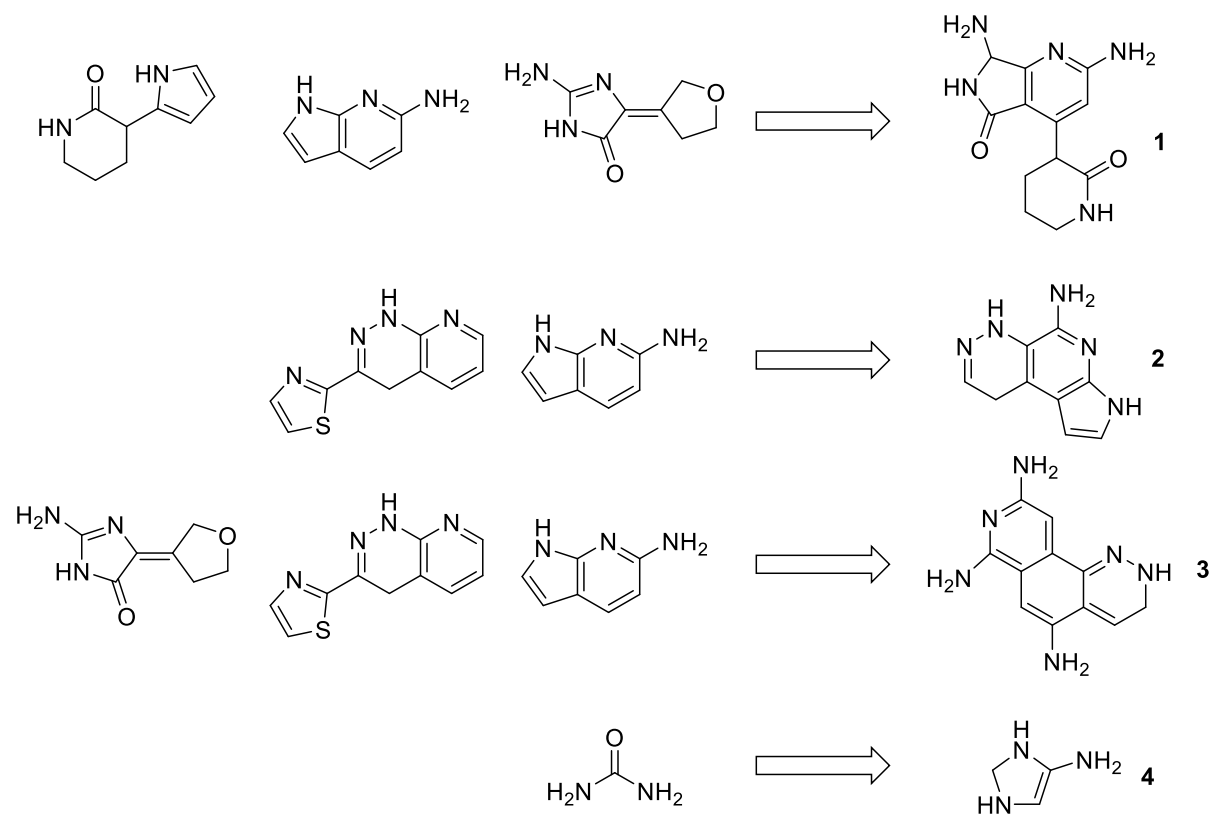
Plasma protein binding assay (x2)

MTT assay (x2)

CaCo2 assay (x1)

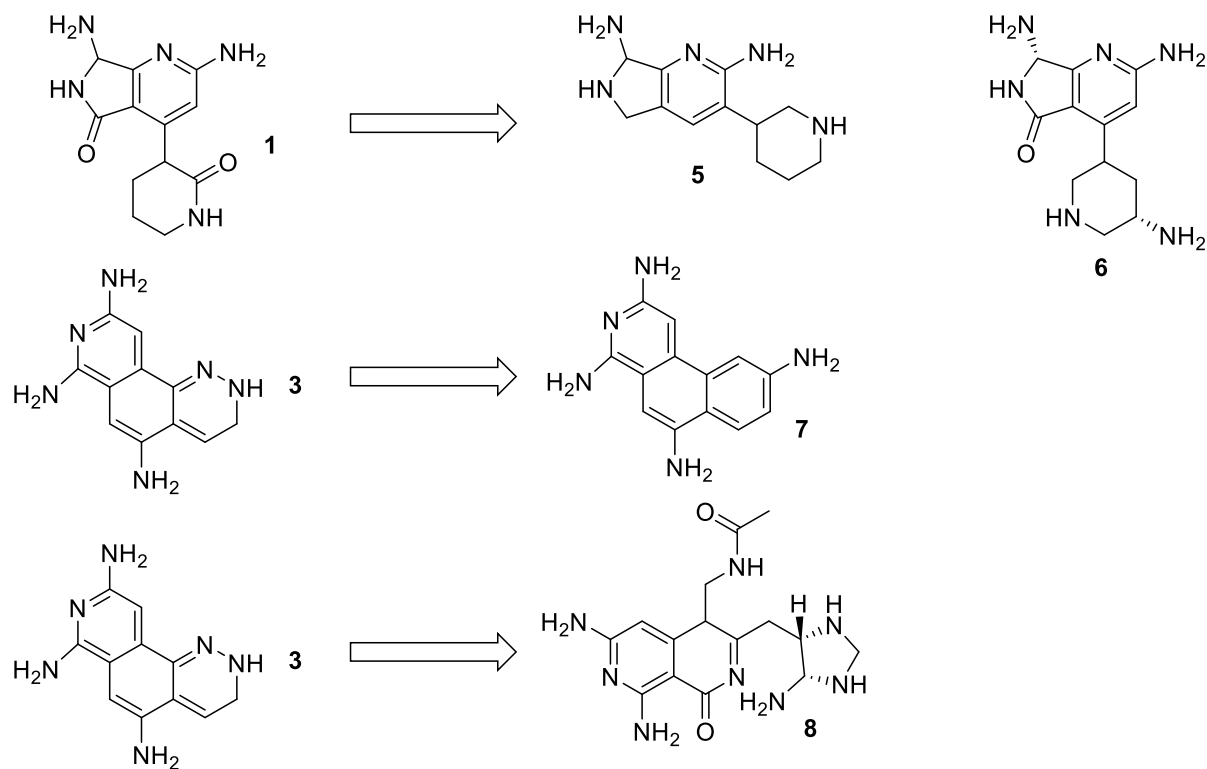
Dose-response (IC_{50} values) (x1)

Round 1



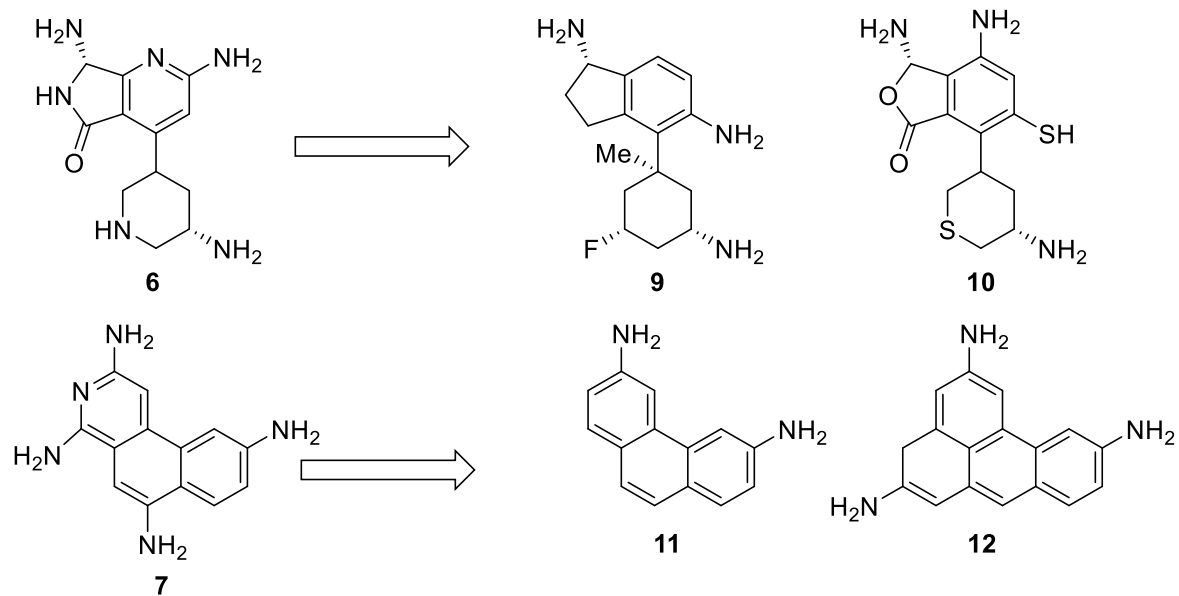
	1	2	3	4
cLogP	-2.16	-1.20	-1.29	0.43
logD _{7.4}	-1.55	-2.10	-3.41	-0.93
logS	-2.39	-3.31	-0.77	-0.89
tPSA (Å ²)	123.13	78.56	115.34	50.08
IC ₅₀ (μM)	99 ± 1	165 ± 1	257 ± 1	1020 ± 24

Round 2



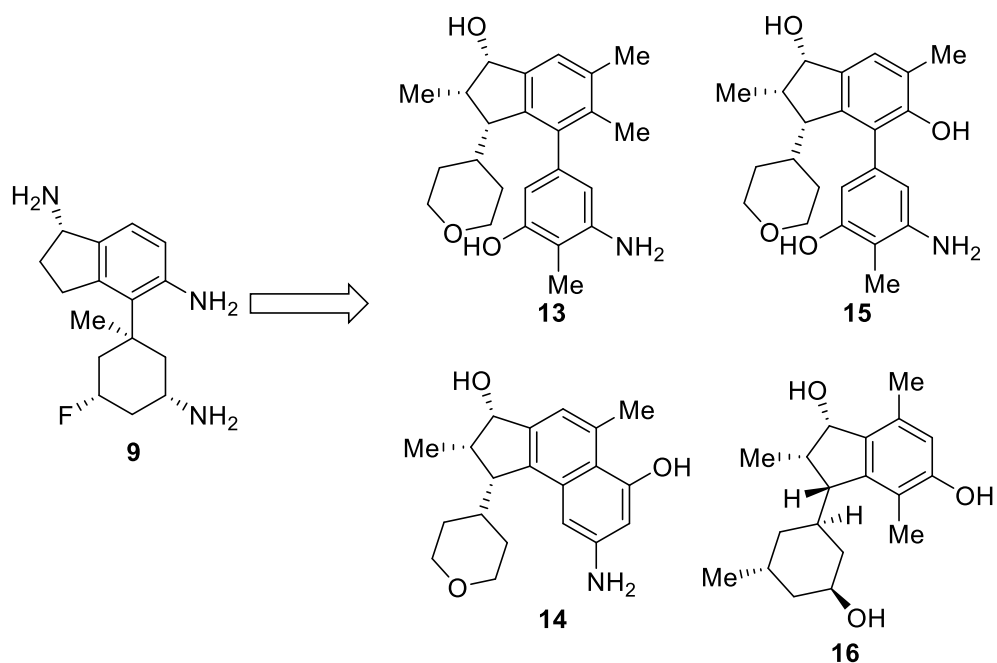
	5	6	7	8
cLogP	-1.65	<-2	1.21	<-2
logD _{7.4}	-4.09	-6.67	1.15	-2.43
logS	0.63	0.56	-1.56	0.46
tPSA (Å ²)	88.99	145.21	116.97	160.65
IC ₅₀ (μM)	126 ± 1	87 ± 1	47 ± 1	389 ± 1

Round 3



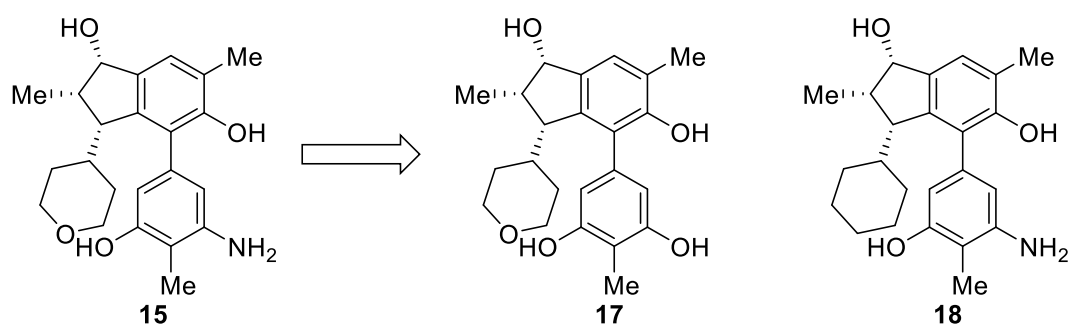
	9	10	11	12
cLogP	0.03	0.35	2.40	2.87
logD _{7.4}	-4.00	-2.35	2.39	0
logS	0.56	-0.94	-4.14	-4.58
tPSA (Å ²)	104.08	168.46	52.04	78.06
IC ₅₀ (μM)	11 ± 1	139 ± 1	18 ± 1	4.3 ± 0.1

Round 4



	13	14	15	16
cLogP	4.80	3.61	3.83	3.32
logD _{7.4}	-4.35	3.61	3.83	1.24
logS	-4.35	-3.61	-3.57	-0.84
tPSA (Å ²)	75.71	75.71	95.94	66.48
IC ₅₀ (μM)	--	--	0.82 ± 0.01	0.64 ± 0.02

Round 5



	17	18
cLogP	3.92	4.96
logD _{7.4}	3.92	4.96
logS	-3.38	-4.47
tPSA (Å ²)	90.15	80.92
IC ₅₀ (μM)	0.940 ± 0.001	0.150 ± 0.001