Supporting Information

Synthesis, activity and pharmacophore development for isatin-b-thiosemicarbazones with MDR1-selective activity

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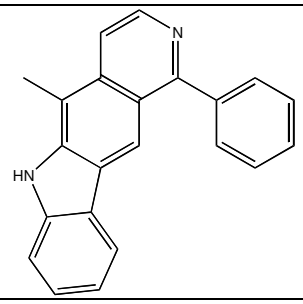
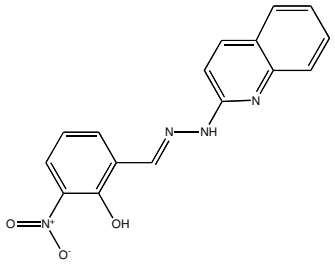
Supporting information Figure S1. Structures and names of non-thiosemicarbazone compounds that satisfied at least 3 of 7 sites, including AH_1R_1, pharmacophore site matches for each compound.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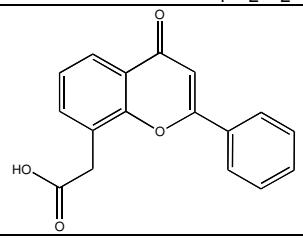	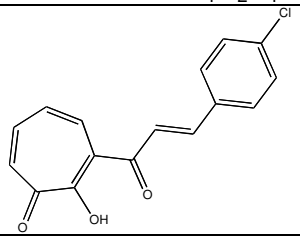
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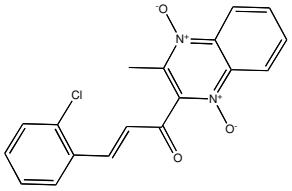	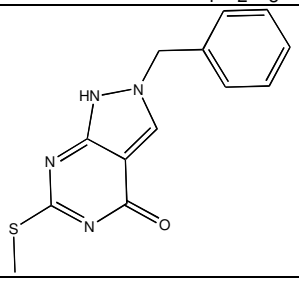
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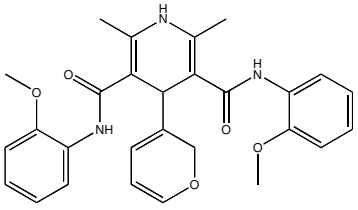	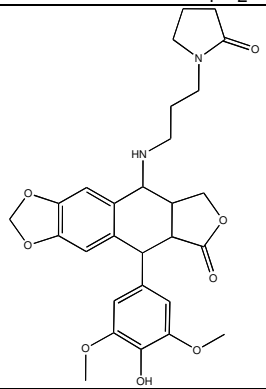
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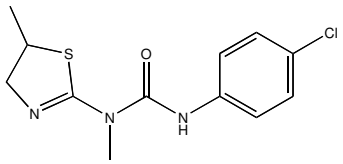	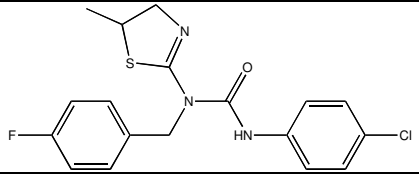
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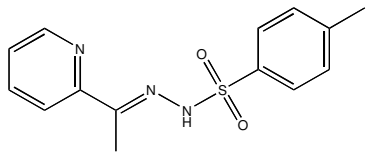	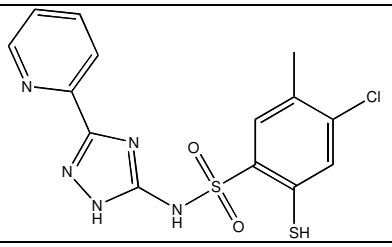
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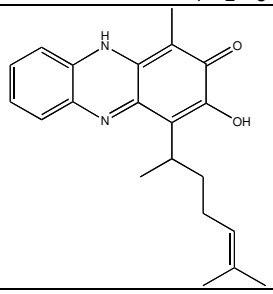	
NSC697120: $AH_1H_2R_2$	

Supporting information Table S1. List of kinases examined, and summary of data from kinase inhibition assay against NSC73306. Compounds were tested for 10 doses starting at 20 μM with 3-fold serial dilutions. The kinase reactions were run at 1 μM ATP and 1% DMSO final concentration. For IC_{50} values >50, partial inhibition was observed at the highest dose-point, however this was not adequate to generate an IC_{50} value.

Kinase	IC_{50} (uM) Staurosporine	IC_{50} (uM) NSC73306
ABL1	0.136	>50.00
AKT1	0.006	-
Aurora A	0.022	-
BTK	0.036	-
CAMK2β	<0.0001	-
CDK1/cyclin B	0.0016	-
CDK2/cyclin A	0.00036	>50.00
CHK1	<0.0001	>50.00
CHK2	0.0067	-
c-MET	0.103	-
c-SRC	0.0013	-
DAPK1	0.0005	-
EGFR	0.132	-
EPHA3	0.048	-
EPHB4	0.233	-
ERBB4	0.282	-
ERK1	7.791	-
ERK2	4.491	-
FGFR1	0.009	-
FGFR2	0.034	-
FGFR3	0.018	-
FLT1	0.019	-
FLT3	0.0010	>50.00
FLT4	0.0019	-
GSK3β	0.0052	-
HIPK1	2.639	-
IR	0.0085	-
IRAK4	0.034	-
JAK2	0.0047	-
JAK3	0.00015	-
KDR	0.0035	-
LCK	0.004	-
LYN	0.00049	-
MINK	0.00049	-
MST2	0.00041	-
P38α	No inhibition	-
PAK2	0.0010	-
PDGFRα	<0.0001	-
PHKγ2	<0.0001	-
PIM1	0.0027	>50.00
PKA	0.00031	-
PKCα	0.00070	>50.00
PLK2	0.197	>50.00
RET	0.00046	-
ROCK1	0.0011	>50.00

RSK1	<0.0001	34.90
SYK	<0.0001	-
TAK1-TAB1	0.035	-
TIE2/TEK	0.052	-
TRKA	0.0017	-