

Supplementary Information

Table S1. ZINC codes and docking scores of 48 test compounds (selected from virtual screening).

Compd No.	ZINC Code	Docking Score (kcal/mol)
a1	ZINC00690330	-50.94
a2	ZINC01023194	-49.37
a3	ZINC00859962	-45.39
a4	ZINC00997463	-52.70
a5	ZINC01002704	-49.43
a6	ZINC01793569	-44.06
a7	ZINC00877489	-43.45
a8	ZINC00983690	-43.39
a9	ZINC00994222	-41.04
a10	ZINC02163697	-45.25
a11	ZINC02188322	-41.85
a12	ZINC03098374	-40.39
a13	ZINC00055290	-43.07
a14	ZINC00729256	-42.96
a15	ZINC00704242	-42.89
a16	ZINC00093060	-42.47
a17	ZINC00029018	-42.14
a18	ZINC00665706	-41.74
a19	ZINC01005629	-41.61
a20	ZINC00721097	-41.50
a21	ZINC00207116	-41.06
a22	ZINC00075722	-41.04
a23	ZINC00711632	-41.04
a24	ZINC00311377	-40.96
a25	ZINC02134712	-40.94
a26	ZINC00694083	-40.76
a27	ZINC02051009	-40.52
a28	ZINC04363300	-40.26
a29	ZINC01747386	-40.26
a30	ZINC00695330	-40.08
a31	ZINC08386384	-50.65
a32	ZINC19702623	-48.76
a33	ZINC04046039	-45.50
a34	ZINC00673330	-43.57
a35	ZINC00067613	-42.69
a36	ZINC00203311	-42.67
a37	ZINC08559788	-42.10
a38	ZINC00661157	-41.95
a39	ZINC00915426	-41.93
a40	ZINC00102360	-41.92
a41	ZINC00667327	-40.72
a42	ZINC01028430	-40.42
a43	ZINC19871526	-40.32
a44	ZINC00711462	-40.22

Table S1. *Cont.*

Compd No.	ZINC Code	Docking Score (kcal/mol)
a45	ZINC04578242	-40.03
a46	ZINC00654398	-40.00
a47	ZINC00695335	-40.21
a48	ZINC00789616	-41.06

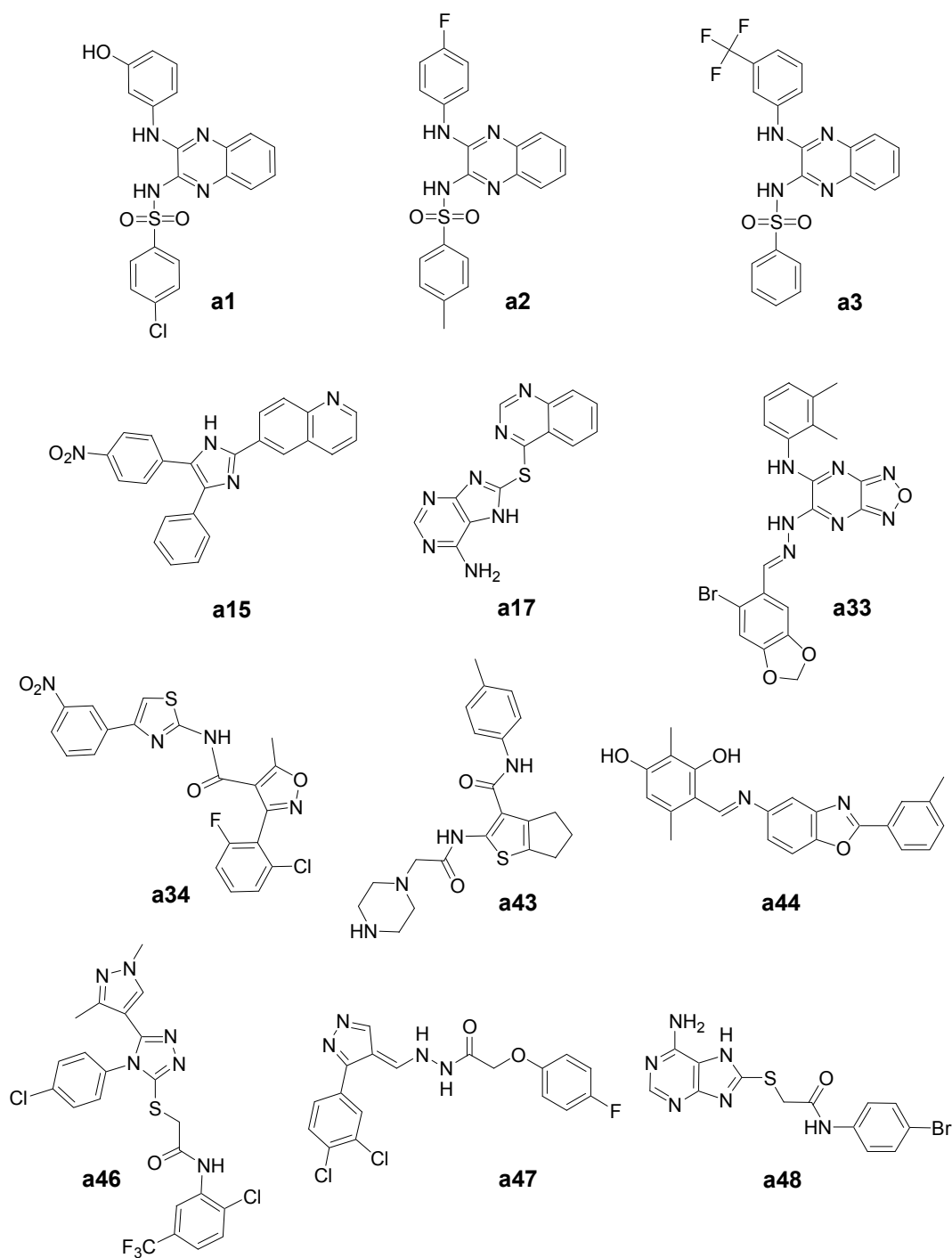


Figure S1. Chemical structures of 12 test compounds that displayed more potent or comparable cytotoxic activity to that of H-89 against HCT-116 human colon cancer cells.