

Table S1 Derivatives of ICCB280

Related to Figure 6

#	Similarity	ChemBankID	Primary name	Morphology	NBT assay
1	1	1946343	2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3-(2-methoxyphenyl)quinazolin-4(3H)-one	++	++
2	0.982	1930950	2-[(E)-2-(4-hydroxyphenyl)vinyl]-3-(2-methoxyphenyl)quinazolin-4(3H)-one	-	-
3	0.952	1942907	2-[(E)-2-(2-hydroxyphenyl)vinyl]-3-(2-methoxyphenyl)quinazolin-4(3H)-one	-	-
4	0.931	1935864	2-[(E)-2-(4-hydroxy-3-methoxyphenyl)vinyl]-3-phenylquinazolin-4(3H)-one	-	-
5	0.925	1907892	2-[(E)-2-(4-methoxyphenyl)vinyl]-3-phenylquinazolin-4(3H)-one	-	-
6	0.922	1907894	2-[(E)-2-(3-methoxyphenyl)vinyl]-3-phenylquinazolin-4(3H)-one	-	-
7	0.921	1946347	2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3-phenylquinazolin-4(3H)-one	-	-
8	0.915	1947187	2-[(Z)-2-(4-hydroxy-3-methoxyphenyl)vinyl]-3-(4-hydroxyphenyl)quinazolin-4(3H)-one	+	+
9	0.913	1946179	2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3-(4-methylphenyl)quinazolin-4(3H)-one	-	-
10	0.909	1935740	3-(4-hydroxyphenyl)-2-[(E)-2-(4-methoxyphenyl)vinyl]quinazolin-4(3H)-one	-	-
11	0.902	1942859	3-(4-methoxyphenyl)-2-[(E)-2-(4-methoxyphenyl)vinyl]quinazolin-4(3H)-one	-	-
12	0.9	1946438	2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3-(3-methoxyphenyl)quinazolin-4(3H)-one	+	+
13	0.894	1947133	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-3-(2-methoxyphenyl)quinazolin-4(3H)-one	-	-
14	0.892	1947147	3-(4-hydroxyphenyl)-2-[(Z)-2-(4-hydroxyphenyl)vinyl]quinazolin-4(3H)-one	-	-
15	0.89	1930909	3-(2-methoxyphenyl)-2-[(E)-2-pyridin-3-ylvinyl]quinazolin-4(3H)-one	-	-
16	0.886	1946243	2-[(E)-2-(4-chlorophenyl)vinyl]-3-(2-hydroxyphenyl)quinazolin-4(3H)-one	-	-

17	0.884	1942914	2-[(E)-2-(4-hydroxyphenyl)vinyl]-3-(3-methylphenyl)quinazolin-4(3H)-one	-	-
18	0.879	1947131	3-(4-hydroxyphenyl)-2-[(Z)-2-phenylvinyl]quinazolin-4(3H)-one	-	-
19	0.878	1935741	2-[(E)-2-(3-bromophenyl)vinyl]-3-(2-hydroxyphenyl)quinazolin-4(3H)-one	-	-
20	0.871	1977072	2-[(E)-2-(2-fluorophenyl)vinyl]-6,7-dimethoxy-3-(2-methoxyphenyl)quinazolin-4(3H)-one	-	-
21	0.87	1946261	3-(2-methoxyphenyl)-2-[(Z)-2-(2-nitrophenyl)vinyl]quinazolin-4(3H)-one	-	-
22	0.867	1977078	3-(2-methoxy-4-nitrophenyl)-2-[(E)-2-phenylvinyl]quinazolin-4(3H)-one	-	-
23	0.867	1942635	2-[(E)-2-(1H-indol-3-yl)vinyl]-3-(2-methoxyphenyl)quinazolin-4(3H)-one	-	-
24	0.865	1977185	2-[(E)-2-(2,3-dimethoxyphenyl)vinyl]-3-(4-ethoxyphenyl)quinazolin-4(3H)-one	-	-
25	0.859	1944802	2-[(E)-2-(2-furyl)vinyl]-3-(2-methoxyphenyl)quinazolin-4(3H)-one	+	+
26	0.857	1947051	2-[(E)-2-(2-hydroxy-1-naphthyl)vinyl]-3-(4-hydroxyphenyl)quinazolin-4(3H)-one	-	-
27	0.856	1947092	2-[(Z)-2-(2-hydroxyphenyl)vinyl]-3-(1-naphthyl)quinazolin-4(3H)-one	-	-
28	0.852	1942789	2-[(E)-2-(2-hydroxyphenyl)vinyl]-3-(2-methylphenyl)quinazolin-4(3H)-one	-	+
29	0.849	1919683	2-[(E)-2-(4-methoxyphenyl)vinyl]-3-(4-nitrophenyl)quinazolin-4(3H)-one	-	-
30	0.841	1977126	3-(3,4-dimethoxyphenyl)-2-[(E)-2-(2-hydroxy-3-methoxyphenyl)vinyl]quinazolin-4(3H)-one	-	-
31	0.84	1931136	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-3-(2-naphthyl)quinazolin-4(3H)-one	-	-
32	0.839	1935695	2-[(E)-2-(2-hydroxyphenyl)vinyl]-6-iodo-3-phenylquinazolin-4(3H)-one	-	-
33	0.838	1977205	3-(3,4-dimethoxyphenyl)-2-[(E)-2-(2,3-dimethoxyphenyl)vinyl]quinazolin-4(3H)-one	-	-
34	0.837	1946464	3-(2-hydroxyphenyl)-2-[(E)-2-(3-nitrophenyl)vinyl]quinazolin-4(3H)-one	-	-

35	0.834	1947170	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-3-(3-methylphenyl)quinazolin-4(3H)-one	+	-
36	0.834	1931112	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-3-(1-naphthyl)quinazolin-4(3H)-one	-	-
37	0.832	1951784	3-(2-hydroxyphenyl)-2-[(E)-2-(4-nitrophenyl)vinyl]quinazolin-4(3H)-one	-	-
38	0.831	1977137	methyl 4-[2-[(E)-2-(2,3-dimethoxyphenyl)vinyl]-4-oxoquinazolin-3(4H)-yl]benzoate	-	-
39	0.83	1933589	2-[(Z)-2-(4-chlorophenyl)vinyl]-3-(3-methylphenyl)quinazolin-4(3H)-one	-	-
40	0.828	1931062	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-3-(2-methylphenyl)quinazolin-4(3H)-one	-	-
41	0.826	1930509	4-[4-oxo-2-[(Z)-2-phenylvinyl]quinazolin-3(4H)-yl]benzoic acid	-	-
42	0.826	1977135	3-(4-ethoxyphenyl)-6,7-dimethoxy-2-[(E)-2-(2-methoxyphenyl)vinyl]quinazolin-4(3H)-one	-	-
43	0.826	1946297	3-(2-hydroxyphenyl)-2-[(E)-2-(2-nitrophenyl)vinyl]quinazolin-4(3H)-one	-	-
44	0.825	1935769	2-[(E)-2-(4-chlorophenyl)vinyl]-3-(3-hydroxyphenyl)quinazolin-4(3H)-one	-	-
45	0.822	1907841	5-oxo-N-(pyridin-2-ylmethyl)-2-(trifluoromethyl)-5H-chromeno[2,3-b]pyridine-3-carboxamide	-	-
46	0.821	1931090	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-3-(3-hydroxyphenyl)quinazolin-4(3H)-one	-	-
47	0.819	1946176	2-[(E)-2-(4-chlorophenyl)vinyl]-3-(2-methylphenyl)quinazolin-4(3H)-one	-	-
48	0.819	1946176	2-[(E)-2-(4-bromophenyl)vinyl]-3-(2-methylphenyl)quinazolin-4(3H)-one	-	-
49	0.819	1947169	2-[(Z)-2-[4-(dimethylamino)phenyl]vinyl]-3-(4-hydroxyphenyl)quinazolin-4(3H)-one	-	+
50	0.818	1947148	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-3-(3-methoxyphenyl)quinazolin-4(3H)-one	-	+
51	0.817	1977097	3-(4-ethoxyphenyl)-6,7-dimethoxy-2-[(E)-2-(2,4,5-trimethoxyphenyl)vinyl]quinazolin-4(3H)-one	-	-

52	0.815	1977090	4-[7-chloro-4-oxo-2-[(E)-2-(3,4,5-trimethoxyphenyl)vinyl]quinazolin-3(4H)-yl]benzoic acid	-	-
53	0.809	1973160	2-[(E)-2-(5-bromo-2-hydroxyphenyl)vinyl]-3-(3-hydroxyphenyl)quinazolin-4(3H)-one	-	-
54	0.808	1932943	2-[(E)-2-(1H-indol-3-yl)vinyl]-3-(4-methoxyphenyl)quinazolin-4(3H)-one	-	-
55	0.808	1977099	2-[(Z)-2-(4-fluorophenyl)vinyl]-6,7-dimethoxy-3-(4-methoxyphenyl)quinazolin-4(3H)-one	-	-
56	0.806	1977216	2-[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-6,7-dimethoxy-3-(4-methylphenyl)quinazolin-4(3H)-one	-	-
57	0.806	1942659	2-[(E)-2-(5-methoxy-1,2-dimethyl-1H-indol-3-yl)vinyl]-3-(2-methoxyphenyl)quinazolin-4(3H)-one	-	-
58	0.805	1930929	3-(3-methoxyphenyl)-2-[(E)-2-pyridin-3-ylvinyl]quinazolin-4(3H)-one	-	-
59	0.805	1977220	2-[(E)-2-(2-fluorophenyl)vinyl]-6,7-dimethoxy-3-(4-methoxyphenyl)quinazolin-4(3H)-one	-	+
60	0.803	1944574	2-[(E)-2-(4-hydroxyphenyl)vinyl]-3-(2-nitrophenyl)quinazolin-4(3H)-one	-	-
61	0.801	1972877	4-[2-[(Z)-2-(5-bromo-2-hydroxyphenyl)vinyl]-4-oxoquinazolin-3(4H)-yl]benzoic acid	-	-

Supplemental Experimental Procedures

HPLC-MS analysis was performed with a Waters Alliance-Micromass ZQ instrument, an ESI source, and Waters 2489 UV/visible detector at 254 nm. Analysis was performed using an analytical Waters Symmetry C18 column (3.5 mm, 2.1x100 mm) operating at 0.5 mL/min with a linear gradient of 0–100% of acetonitrile in water (containing 0.1% formic acid, v/v) over 10 min.

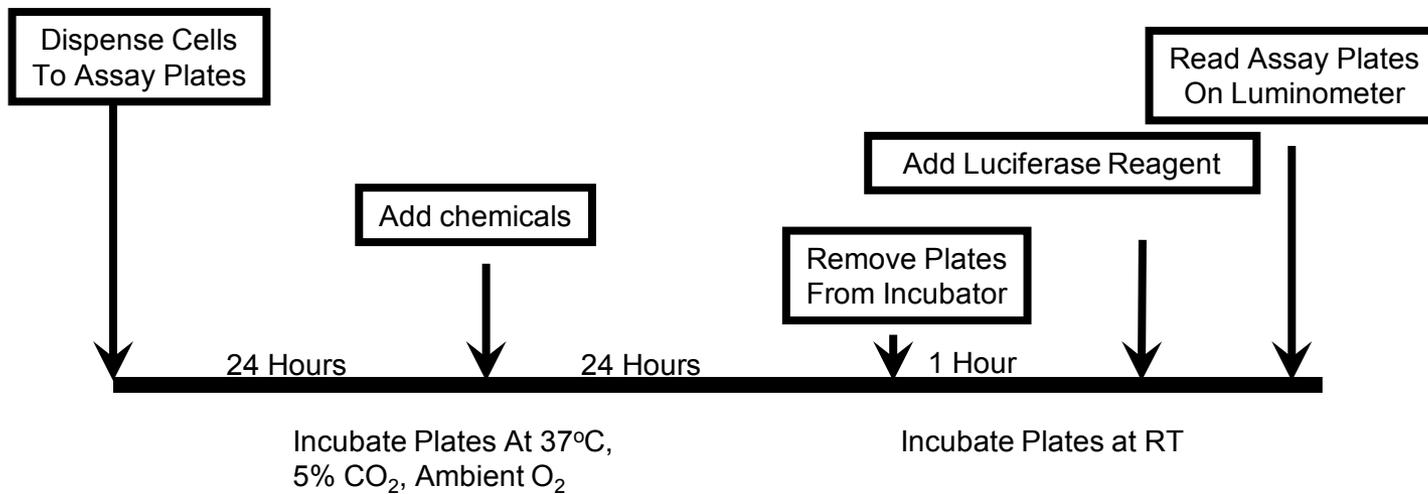


Figure S1 (Related to Figure 2). High-throughput screening assay timeline

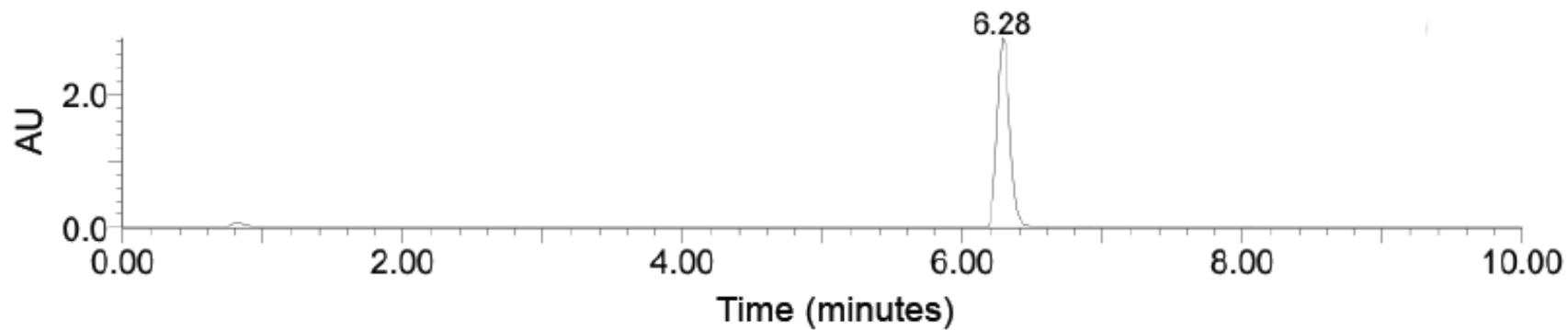


Figure S2 (Related to Figure 3). Assessment of purity of ICCB280. The liquid chromatography injection was monitored at 220 nm using a 0 – 100 %linear acetonitrile to water gradient over 10 minutes and found to elute in high purity at 6.28 minutes.

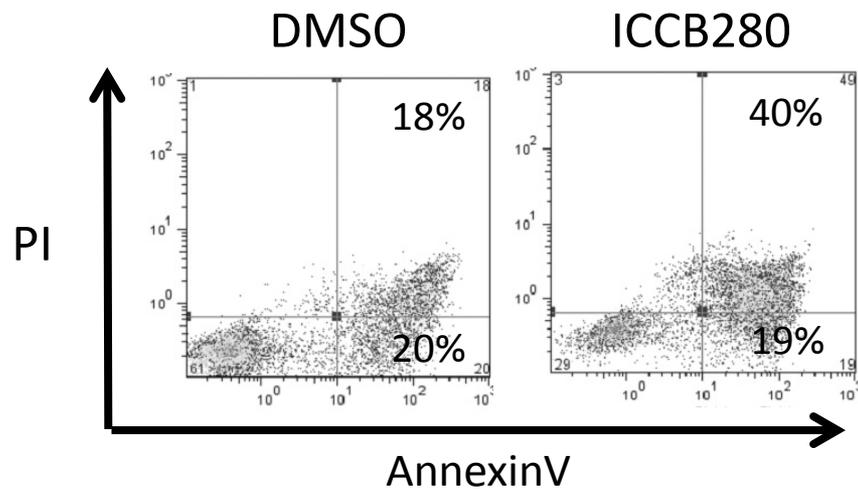


Figure S3 (Related to Figure 3). ICCB280 induces apoptosis in primary AML cells. Mononuclear cells were isolated from the patient# 0505 and treated with either 10 μ M ICCB280 or 0.01% DMSO for 5 days. Cells were stained with Annexin V and PI and subjected to flow cytometric analysis.

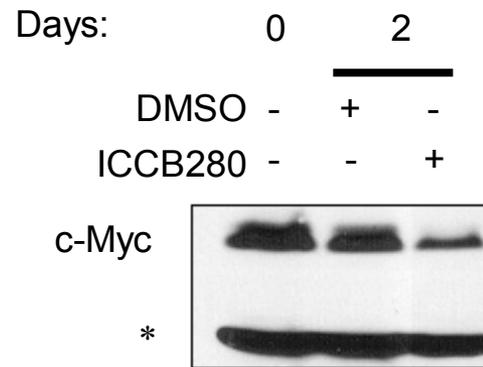


Figure S4 (Related to Figure 4). ICCB280 reduces c-Myc expression. HL-60 cells were treated with 10 μ M ICCB280 or 0.1% DMSO for 2days. Cell extracts were subjected to western blot analysis. Nonspecific bands serve as loading controls (*).