**Supplement**

# Cancer cell responses to Hsp70 inhibitor JG-98: Comparison with Hsp90 inhibitors and finding synergistic drug combinations.

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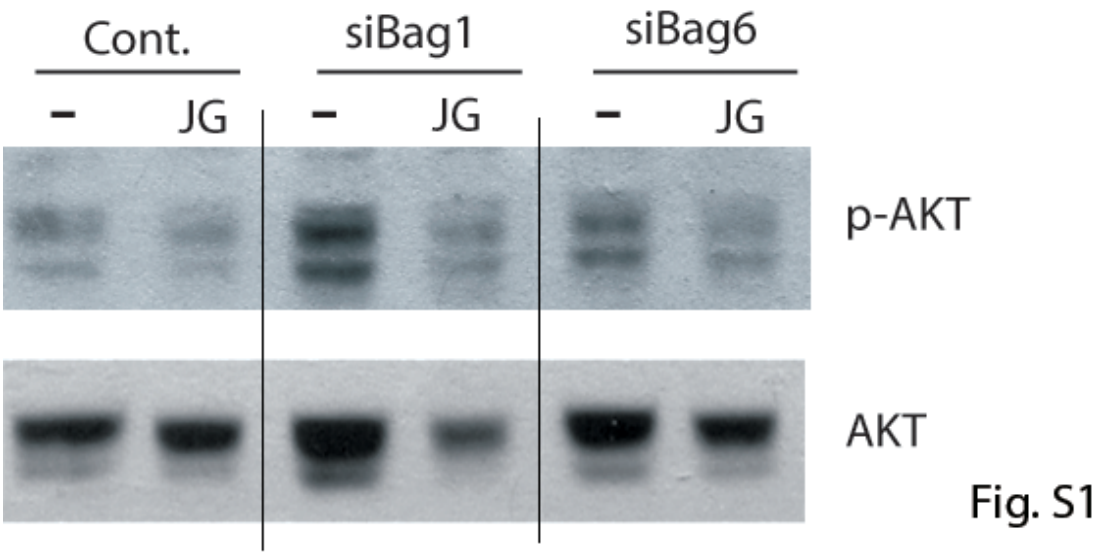


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**Fig. S1. JG-98 downregulates AKT in Bag1- and Bag6-independent manner.** MCF7 cells were transfected with either anti-Bag1 or anti-Bag6 siRNAs (see Materials and Methods) prior to treatment with 2μM of JG-98 for 36h. Levels of Akt and phAkt were determined in cell lysates by immunoblotting with corresponding antibody.

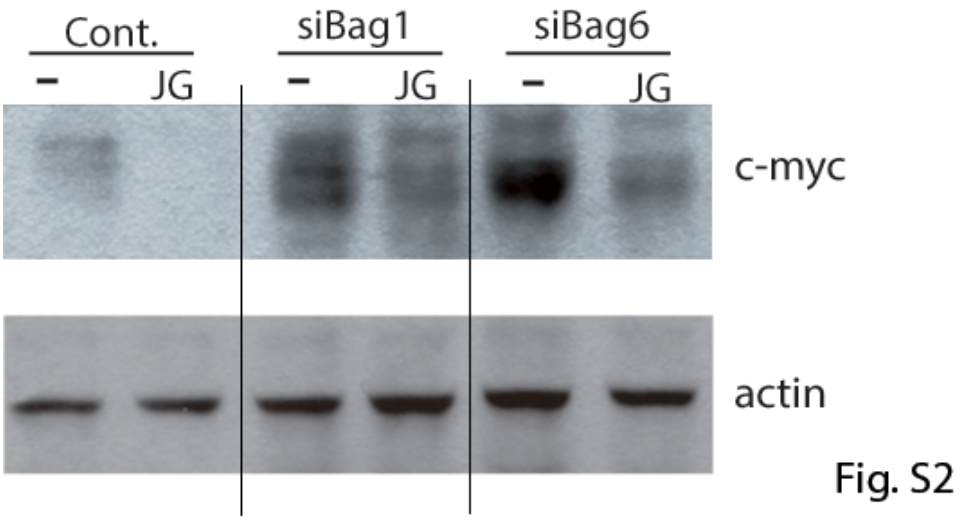



**Fig. S2. JG-98 downregulates c-myc in Bag1- and Bag6-independent manner.** MCF7 cells were transfected with either anti-Bag1 or anti-Bag6 siRNAs as in Fig. S1 and treated with 2μM of JG-98 for 36h. Levels of c-myc were determined in cell lysates by immunoblotting with corresponding antibody.

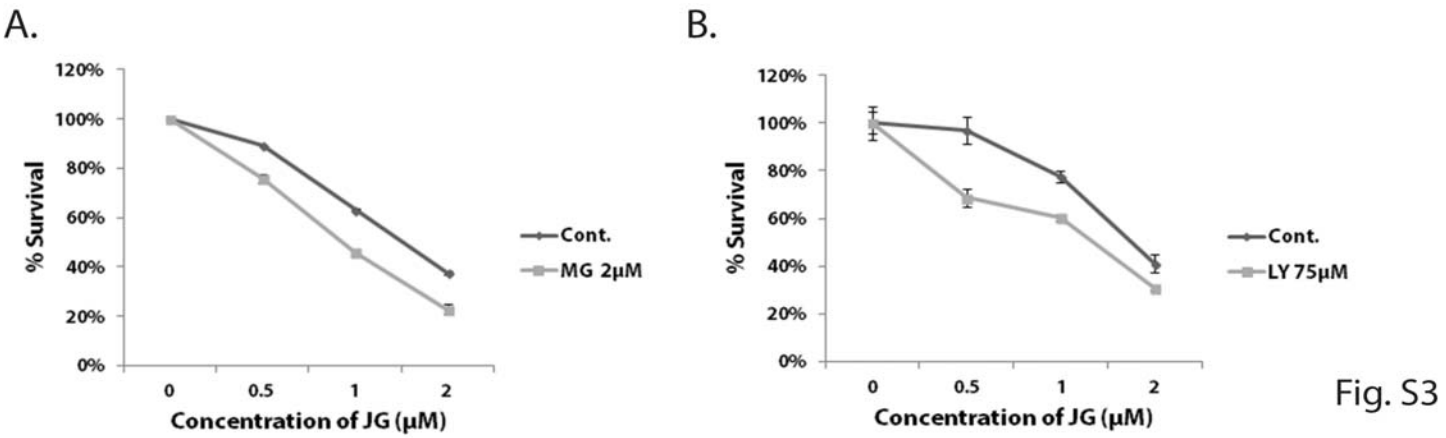
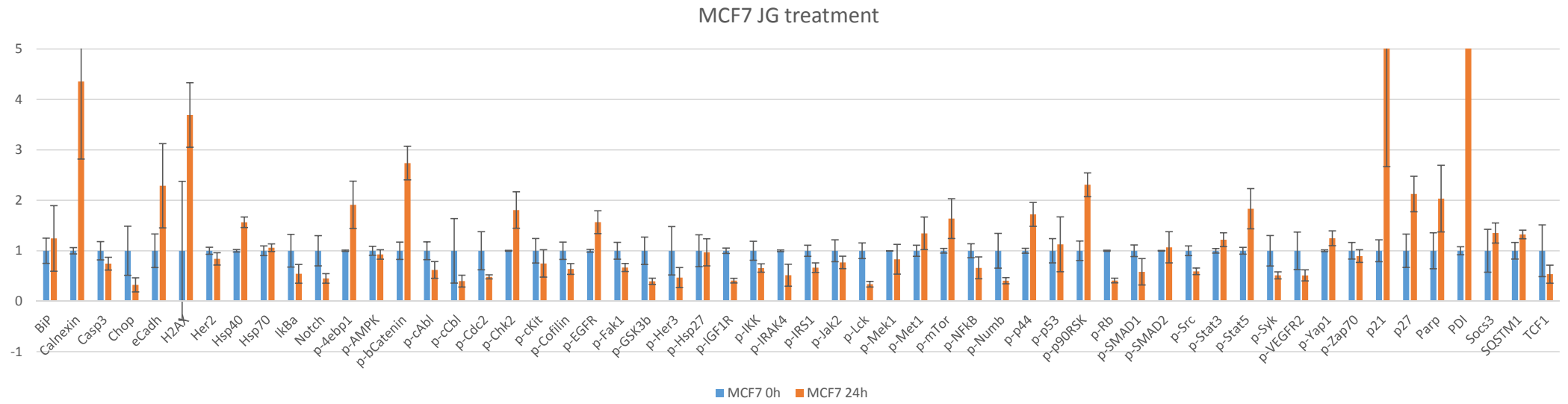



**Fig. S3. Validation of effects of combinations of JG-98 with MG132 and LY294002 in BT474 cells.** Sub-toxic concentrations of drugs were determined and effects of JG-98 either alone or in combination with these drugs were detyermined by MTT assay.


MCF7 JG treatment
5
4
3
2
1
0
-1
BiP
Calnexin
Casp3
Chop
eCadh
H2AX
Her2
Hsp40
Hsp70
IkBa
Notch
p-4ebp1
p-AMPK
p-bCatenin
p-cAbl
p-cCbl
p-Cdc2
p-Chk2
p-cKit
p-Cofilin
p-EGFR
p-Fak1
p-GSK3b
p-Her3
p-Hsp27
p-IGF1R
p-IKK
p-IRAK4
p-IRS1
p-Jak2
p-Lck
p-Mek1
p-Met1
p-mTor
p-NFkB
p-Numb
p-p44
p-p53
p-p90RSK
p-Rb
p-SMAD1
p-SMAD2
p-Src
p-Stat3
p-Stat5
p-Syk
p-VEGFR2
p-Yap1
p-Zap70
p21
p27
Parp
PDI
Socs3
SQSTM1
TCF1
MCF7 0h
MCF7 24h

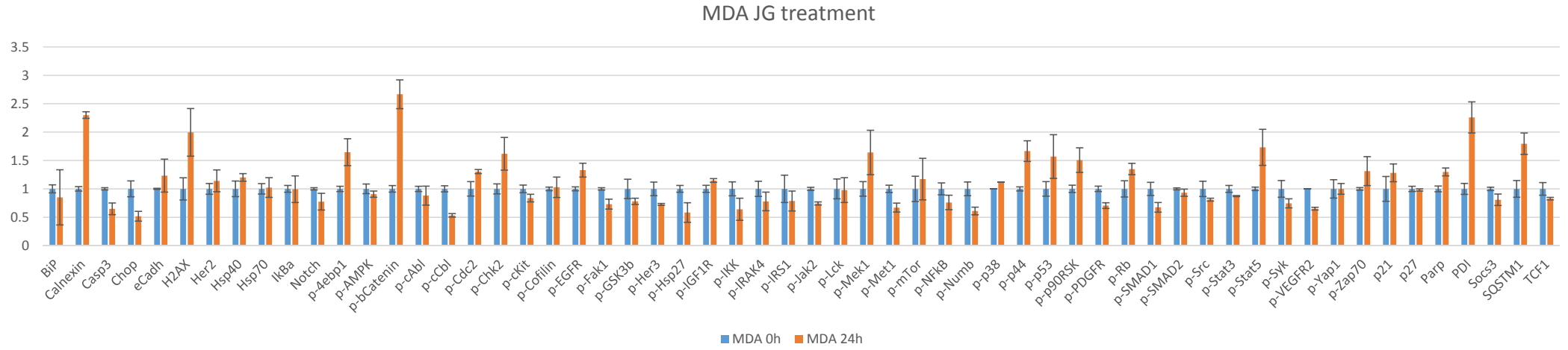

MDA JG treatment
3.5
3
2.5
2
1.5
1
0.5
0
BiP
Calnexin
Casp3
Chop
eCadh
H2AX
Her2
Hsp40
Hsp70
IkBa
Notch
p-4ebp1
p-AMPK
p-bCatenin
p-cAbl
p-cCbl
p-Cdc2
p-Chk2
p-cKit
p-Cofilin
p-EGFR
p-Fak1
p-GSK3b
p-Her3
p-Hsp27
p-IGF1R
p-IKK
p-IRAK4
p-IRS1
p-Jak2
p-Lck
p-Mek1
p-Met1
p-mTor
p-NFkB
p-Numb
p-p38
p-p44
p-p53
p-p90RSK
p-PDGFR
p-Rb
p-SMAD1
p-SMAD2
p-Src
p-Stat3
p-Stat5
p-Syk
p-VEGFR2
p-Yap1
p-Zap70
p21
p27
Parp
PDI
Socs3
SQSTM1
TCF1
MDA 0h
MDA 24h

Fig. S4

**Fig. S4. Effect of JG-98 on multiple signaling proteins.** The experiment was done using the iPAD platform by ActivSignal, Inc., see the text.

**Table S1. Links to the Connectivity Map comparison of effects of JG-98 and tanespimycin.** Links show drugs with connectivity to JG-98 and tanespimycin based on gene expression data in the database.

Table S1 cmap_report

| Cell line | Pert name | Dose(μM) | url_hyperlink |
|---|---|---|---|
| HEPG2 | tanespimycin | 10 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-A61304759_10_n2000.html |
| HT29 | tanespimycin | 10 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-A61304759_10_n2000.html |
| JURKAT | tanespimycin | 10 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-A61304759_10_n2000.html |
| MCF7 | tanespimycin | 10 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-A61304759_10_n2000.html |
| PC3 | tanespimycin | 10 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-A61304759_10_n2000.html |
| HEPG2 | tanespimycin | 3.33333 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-A61304759_3.33333_n2000.html |
| HT29 | tanespimycin | 3.33333 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-A61304759_3.33333_n2000.html |
| JURKAT | tanespimycin | 3.33333 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-A61304759_3.33333_n2000.html |
| MCF7 | tanespimycin | 3.33333 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-A61304759_3.33333_n2000.html |
| PC3 | tanespimycin | 3.33333 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-A61304759_3.33333_n2000.html |
| HEPG2 | tanespimycin | 1.11111 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-A61304759_1.11111_n2000.html |
| HT29 | tanespimycin | 1.11111 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-A61304759_1.11111_n2000.html |
| JURKAT | tanespimycin | 1.11111 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-A61304759_1.11111_n2000.html |
| MCF7 | tanespimycin | 1.11111 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-A61304759_1.11111_n2000.html |
| PC3 | tanespimycin | 1.11111 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-A61304759_1.11111_n2000.html |
| HEPG2 | tanespimycin | 0.37037 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016 |

| | | | |
|---|---|---|---|
| | | | 032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-A61304759_0.37037_n2000.html |
| HT29 | tanespimycin | 0.37037 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-A61304759_0.37037_n2000.html |
| JURKAT | tanespimycin | 0.37037 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-A61304759_0.37037_n2000.html |
| MCF7 | tanespimycin | 0.37037 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-A61304759_0.37037_n2000.html |
| PC3 | tanespimycin | 0.37037 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-A61304759_0.37037_n2000.html |
| HEPG2 | tanespimycin | 0.123457 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-A61304759_0.123457_n2000.html |
| HT29 | tanespimycin | 0.123457 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-A61304759_0.123457_n2000.html |
| JURKAT | tanespimycin | 0.123457 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-A61304759_0.123457_n2000.html |
| MCF7 | tanespimycin | 0.123457 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-A61304759_0.123457_n2000.html |
| PC3 | tanespimycin | 0.123457 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-A61304759_0.123457_n2000.html |
| HEPG2 | tanespimycin | 0.041152 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-A61304759_0.0411523_n2000.html |
| HT29 | tanespimycin | 0.041152 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-A61304759_0.0411523_n2000.html |
| JURKAT | tanespimycin | 0.041152 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-A61304759_0.0411523_n2000.html |
| MCF7 | tanespimycin | 0.041152 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-A61304759_0.0411523_n2000.html |
| PC3 | tanespimycin | 0.041152 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-A61304759_0.0411523_n2000.html |
| HEPG2 | JG-98 | 5 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-U06877554_5_n2000.html |
| HT29 | JG-98 | 5 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-U06877554_5_n2000.html |
| JURKAT | JG-98 | 5 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD |

| | | | |
|---|---|---|---|
| | | | -U06877554_5_n2000.html |
| MCF7 | JG-98 | 5 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-U06877554_5_n2000.html |
| PC3 | JG-98 | 5 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-U06877554_5_n2000.html |
| HEPG2 | JG-98 | 1.66667 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-U06877554_1.66667_n2000.html |
| HT29 | JG-98 | 1.66667 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-U06877554_1.66667_n2000.html |
| JURKAT | JG-98 | 1.66667 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-U06877554_1.66667_n2000.html |
| MCF7 | JG-98 | 1.66667 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-U06877554_1.66667_n2000.html |
| PC3 | JG-98 | 1.66667 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-U06877554_1.66667_n2000.html |
| HEPG2 | JG-98 | 0.555556 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-U06877554_0.555556_n2000.html |
| HT29 | JG-98 | 0.555556 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-U06877554_0.555556_n2000.html |
| JURKAT | JG-98 | 0.555556 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-U06877554_0.555556_n2000.html |
| MCF7 | JG-98 | 0.555556 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-U06877554_0.555556_n2000.html |
| PC3 | JG-98 | 0.555556 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-U06877554_0.555556_n2000.html |
| HEPG2 | JG-98 | 0.185185 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-U06877554_0.185185_n2000.html |
| HT29 | JG-98 | 0.185185 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-U06877554_0.185185_n2000.html |
| JURKAT | JG-98 | 0.185185 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-U06877554_0.185185_n2000.html |
| MCF7 | JG-98 | 0.185185 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-U06877554_0.185185_n2000.html |
| PC3 | JG-98 | 0.185185 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-U06877554_0.185185_n2000.html |

| | | | |
|---|---|---|---|
| HEPG2 | JG-98 | 0.061728 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-U06877554_0.0617284_n2000.html |
| HT29 | JG-98 | 0.061728 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-U06877554_0.0617284_n2000.html |
| JURKAT | JG-98 | 0.061728 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-U06877554_0.0617284_n2000.html |
| MCF7 | JG-98 | 0.061728 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-U06877554_0.0617284_n2000.html |
| PC3 | JG-98 | 0.061728 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-U06877554_0.0617284_n2000.html |
| HEPG2 | JG-98 | 0.020576 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HEPG2_24H_BRD-U06877554_0.0205761_n2000.html |
| HT29 | JG-98 | 0.020576 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_HT29_24H_BRD-U06877554_0.0205761_n2000.html |
| JURKAT | JG-98 | 0.020576 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_JURKAT_24H_BRD-U06877554_0.0205761_n2000.html |
| MCF7 | JG-98 | 0.020576 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_MCF7_24H_BRD-U06877554_0.0205761_n2000.html |
| PC3 | JG-98 | 0.020576 | http://c3.lincscloud.org/~user165/mar23/my_analysis.sig_quest_tool.2016032314335591/query_result/tail.result_WTCS_POL001_PC3_24H_BRD-U06877554_0.0205761_n2000.html |

**Table S2, S3. GSEA report showing pathways that are significantly upregulated (S2) or downregulated (S3) in response of MCF7 cells to JG- 98.** MCF7 cells were treated with 2μM of JG-98 for 36 hours. RNA was isolated and submitted for microarray analysis. Microarray data were analyzed using the Broad Institute software package for gene set enrichment analysis (GSEA) in Boston University Center for Translational Research.

Table S2 downregulated pathways

| NAME | SIZE | FDR q-val | FWER p-val |
|---|---|---|---|
| REACTOME_DNA_REPLICATION | 182 | 0 | 0 |
| REACTOME_CELL_CYCLE | 383 | 0 | 0 |
| REACTOME_CELL_CYCLE_MITOTIC | 301 | 0 | 0 |
| REACTOME_MITOTIC_M_M_G1_PHASES | 162 | 0 | 0 |
| REACTOME_CHROMOSOME_MAINTENANCE | 108 | 0 | 0 |
| REACTOME_S_PHASE | 103 | 0 | 0 |
| SGCGSSAAA_V$E2F1DP2_01 | 164 | 0 | 0 |
| REACTOME_TELOMERE_MAINTENANCE | 65 | 0 | 0 |
| REACTOME_G1_S_TRANSITION | 103 | 0 | 0 |
| REACTOME_DEPOSITION_OF_NEW_CENPA_CONTAINING_NUCLEOSOMES_AT_THE_CENTROMERE | 53 | 0 | 0 |
| REACTOME_SYNTHESIS_OF_DNA | 87 | 0 | 0 |
| REACTOME_MITOTIC_G1_G1_S_PHASES | 127 | 0 | 0 |
| V$E2F1_Q6 | 229 | 0 | 0 |
| V$E2F4DP2_01 | 230 | 0 | 0 |
| V$E2F1DP2_01 | 230 | 0 | 0 |
| V$E2F4DP1_01 | 235 | 0 | 0 |
| REACTOME_PROCESSING_OF_CAPPED_INTRON_CONTAINING_PRE_MRNA | 130 | 0 | 0 |
| V$E2F1DP1_01 | 230 | 0 | 0 |
| REACTOME_DNA_STRAND_ELONGATION | 29 | 0 | 0 |
| V$E2F_02 | 230 | 0 | 0 |
| REACTOME_ACTIVATION_OF_ATR_IN_RESPONSE_TO_REPLICATION_STRESS | 35 | 0 | 0 |
| KEGG_DNA_REPLICATION | 35 | 0 | 0 |
| REACTOME_M_G1_TRANSITION | 75 | 0 | 0 |
| V$E2F1_Q3 | 240 | 0 | 0 |
| V$E2F_Q6 | 227 | 0 | 0 |
| REACTOME_MRNA_SPLICING | 102 | 0 | 0 |
| REACTOME_ACTIVATION_OF_THE_PRE_REPLICATIVE_COMPLEX | 29 | 0 | 0 |
| REACTOME_G2_M_CHECKPOINTS | 41 | 0 | 0 |
| REACTOME_MRNA_PROCESSING | 148 | 0 | 0 |
| V$E2F1DP1RB_01 | 225 | 0 | 0 |
| V$E2F_Q4 | 229 | 0 | 0 |
| REACTOME_MITOTIC_PROMETAPHASE | 83 | 0 | 0 |
| REACTOME_EXTENSION_OF_TELOMERES | 26 | 0 | 0 |
| REACTOME_CELL_CYCLE_CHECKPOINTS | 109 | 0 | 0 |

| | | | |
|---|---|---|---|
| V$E2F_Q3 | 222 | 0 | 0 |
| REACTOME_E2F_MEDIATED_REGULATION_OF_DNA_REPLICATION | 32 | 0 | 0 |
| REACTOME_RNA_POL_I_PROMOTER_OPENING | 47 | 0 | 0 |
| REACTOME_ASSEMBLY_OF_THE_PRE_REPLICATIVE_COMPLEX | 61 | 0 | 0 |
| CHROMOSOME | 120 | 0 | 0 |
| V$E2F_03 | 236 | 0 | 0 |
| V$E2F1_Q6_01 | 232 | 0 | 0 |
| CHROMOSOMAL_PART | 94 | 0 | 0 |
| REACTOME_RNA_POL_I_RNA_POL_III_AND_MITOCHONDRIAL_TRANSCRIPTION | 103 | 0 | 0 |
| KEGG_OXIDATIVE_PHOSPHORYLATION | 111 | 0 | 0 |
| REACTOME_RNA_POL_I_TRANSCRIPTION | 70 | 0 | 0 |
| REACTOME_TRANSCRIPTION | 186 | 0 | 0 |
| REACTOME_TCA_CYCLE_AND_RESPIRATORY_ELECTRON_TRANSPORT | 112 | 0 | 0 |
| V$E2F_Q3_01 | 229 | 0 | 0 |
| REACTOME_RESPIRATORY_ELECTRON_TRANSPORT_ATP_SYNTHESIS_BY_CHEMIOSMOTIC_COUPLING_AND_HEAT_PRODUCTION_BY_UNCOUPLING_PROTEINS_ | 76 | 0 | 0 |
| V$E2F_Q4_01 | 232 | 0 | 0 |
| RNA_SPLICING | 88 | 0 | 0 |
| KRCTCNNNNMANAGC_UNKNOWN | 61 | 0 | 0 |
| REACTOME_CHOLESTEROL_BIOSYNTHESIS | 21 | 0 | 0 |
| KEGG_SPLICEOSOME | 121 | 0 | 0 |
| V$E2F_Q6_01 | 234 | 0 | 0 |
| BIOCARTA_MCM_PATHWAY | 18 | 0 | 0 |
| V$E2F1_Q4_01 | 222 | 0 | 0 |
| REACTOME_ORC1_REMOVAL_FROM_CHROMATIN | 63 | 0 | 0 |
| REACTOME_LAGGING_STRAND_SYNTHESIS | 18 | 0 | 0 |
| MRNA_PROCESSING_GO_0006397 | 70 | 0 | 0 |
| KEGG_PARKINSONS_DISEASE | 107 | 0 | 0 |
| REACTOME_TRANSPORT_OF_MATURE_TRANSCRIPT_TO_CYTOPLASM | 52 | 0 | 0 |
| M_PHASE_OF_MITOTIC_CELL_CYCLE | 84 | 0 | 0 |
| M_PHASE | 113 | 0 | 0 |
| KEGG_CELL_CYCLE | 124 | 0 | 0 |
| REACTOME_REGULATION_OF_MITOTIC_CELL_CYCLE | 74 | 0 | 0 |
| KEGG_SYSTEMIC_LUPUS_ERYTHEMATOSUS | 113 | 0 | 0 |
| REACTOME_G1_S_SPECIFIC_TRANSCRIPTION | 17 | 0 | 0 |
| REACTOME_MEIOTIC_RECOMBINATION | 70 | 0 | 0 |
| ORGANELLE_INNER_MEMBRANE | 71 | 0 | 0 |
| RNA_PROCESSING | 165 | 0 | 0 |
| RIBONUCLEOPROTEIN_COMPLEX | 135 | 0 | 0 |
| REACTOME_AMYLOIDS | 67 | 0 | 0 |
| REACTOME_MEIOSIS | 98 | 0 | 0 |
| CONDENSED_CHROMOSOME | 31 | 0 | 0 |
| REACTOME_RESPIRATORY_ELECTRON_TRANSPORT | 61 | 0 | 0 |
| REACTOME_MRNA_SPLICING_MINOR_PATHWAY | 41 | 0 | 0 |
| CELL_CYCLE_PROCESS | 191 | 0 | 0 |

| | | | |
|---|---|---|---|
| MITOSIS | 81 | 0 | 0 |
| MITOTIC_CELL_CYCLE | 151 | 0 | 0 |
| MITOCHONDRIAL_INNER_MEMBRANE | 63 | 0 | 0 |
| V$E2F_01 | 65 | 0 | 0 |
| CELL_CYCLE_PHASE | 168 | 0 | 0 |
| REACTOME_METABOLISM_OF_NON_CODING_RNA | 44 | 0 | 0 |
| REACTOME_MEIOTIC_SYNAPSIS | 62 | 0 | 0 |
| REACTOME_CLEAVAGE_OF_GROWING_TRANSCRIPT_IN_THE_TERMINATION_REGION_ | 41 | 0 | 0 |
| REPLICATION_FORK | 18 | 0 | 0 |
| REACTOME_DESTABILIZATION_OF_MRNA_BY_AUF1_HNRNP_D0 | 47 | 0 | 0 |
| REACTOME_FORMATION_OF_TUBULIN_FOLDING_INTERMEDIATES_BY_CCT_TRIC | 20 | 0 | 0 |
| KEGG_STEROID_BIOSYNTHESIS | 16 | 0 | 0 |
| KEGG_GLYCOLYSIS_GLUCONEOGENESIS | 60 | 0 | 0 |
| REACTOME_CDT1_ASSOCIATION_WITH_THE_CDC6_ORC_ORIGIN_COMPLEX | 52 | 0 | 0 |
| REACTOME_PACKAGING_OF_TELOMERE_ENDS | 39 | 0 | 0 |
| NUCLEAR_CHROMOSOME | 54 | 0 | 0 |
| CHROMOSOMEPERICENTRIC_REGION | 30 | 9.70E-06 | 0.001 |
| RRNA_METABOLIC_PROCESS | 16 | 9.60E-06 | 0.001 |
| REACTOME_GLYCOLYSIS | 26 | 9.50E-06 | 0.001 |
| KEGG_OOCYTE_MEIOSIS | 111 | 1.91E-05 | 0.002 |
| REACTOME_CYCLIN_A_B1_ASSOCIATED_EVENTS_DURING_G2_M_TRANSITION | 15 | 1.89E-05 | 0.002 |
| REACTOME_APC_C_CDC20_MEDIATED_DEGRADATION_OF_MITOTIC_PROTEINS | 62 | 1.87E-05 | 0.002 |
| REACTOME_MRNA_3_END_PROCESSING | 33 | 1.85E-05 | 0.002 |
| CHROMATIN | 34 | 1.83E-05 | 0.002 |
| REACTOME_GLUCONEOGENESIS | 30 | 4.60E-05 | 0.005 |
| CONDENSED_NUCLEAR_CHROMOSOME | 18 | 8.18E-05 | 0.009 |
| CELL_CYCLE_GO_0007049 | 313 | 8.11E-05 | 0.009 |
| SPINDLE | 39 | 8.03E-05 | 0.009 |
| REACTOME_CYCLIN_E_ASSOCIATED_EVENTS_DURING_G1_S_TRANSITION_ | 60 | 8.85E-05 | 0.01 |
| REACTOME_G0_AND_EARLY_G1 | 23 | 8.77E-05 | 0.01 |
| REACTOME_POST_CHAPERONIN_TUBULIN_FOLDING_PATHWAY | 17 | 9.53E-05 | 0.011 |
| REACTOME_DARPP_32_EVENTS | 24 | 9.44E-05 | 0.011 |
| MITOCHONDRIAL_PART | 136 | 9.36E-05 | 0.011 |
| DNA_REPLICATION | 100 | 1.01E-04 | 0.012 |
| MRNA_METABOLIC_PROCESS | 81 | 1.00E-04 | 0.012 |
| MITOCHONDRIAL_MEMBRANE | 81 | 1.24E-04 | 0.015 |
| REACTOME_APC_C_CDH1_MEDIATED_DEGRADATION_OF_CDC20_AND_OTHER_APC_C_CDH1_TARGETED_PROTEINS_IN_LATE_MITOSIS_EARLY_G1 | 61 | 1.23E-04 | 0.015 |
| DNA_DEPENDENT_DNA_REPLICATION | 55 | 1.70E-04 | 0.021 |
| NUCLEOLAR_PART | 18 | 1.77E-04 | 0.022 |
| REACTOME_GLUCOSE_METABOLISM | 63 | 1.75E-04 | 0.022 |
| MITOTIC_SISTER_CHROMATID_SEGREGATION | 15 | 1.82E-04 | 0.023 |
| REACTOME_DNA_REPAIR | 102 | 2.20E-04 | 0.028 |

| | | | |
|---|---|---|---|
| RRNA_PROCESSING | 15 | 2.34E-04 | 0.03 |
| KEGG_PROGESTERONE_MEDIATED_OOCYTE_MATURATION | 84 | 2.63E-04 | 0.034 |
| SPLICEOSOME | 48 | 2.83E-04 | 0.037 |
| STEROID_BIOSYNTHETIC_PROCESS | 23 | 2.88E-04 | 0.038 |
| MITOCHONDRIAL_MEMBRANE_PART | 49 | 3.01E-04 | 0.04 |
| KEGG_TERPENOID_BACKBONE_BIOSYNTHESIS | 15 | 3.43E-04 | 0.046 |
| RIBONUCLEASE_ACTIVITY | 25 | 3.70E-04 | 0.05 |
| KEGG_BUTANOATE_METABOLISM | 34 | 3.89E-04 | 0.053 |
| REACTOME_HOST_INTERACTIONS_OF_HIV_FACTORS | 116 | 4.58E-04 | 0.062 |
| MITOCHONDRIAL_ENVELOPE | 92 | 5.41E-04 | 0.074 |
| NUCLEAR_CHROMOSOME_PART | 34 | 5.80E-04 | 0.08 |
| REACTOME_HIV_INFECTION | 186 | 5.97E-04 | 0.082 |
| REACTOME_RNA_POL_II_TRANSCRIPTION | 97 | 6.00E-04 | 0.083 |
| MITOCHONDRION | 331 | 6.09E-04 | 0.085 |
| REACTOME_HIV_LIFE_CYCLE | 109 | 6.40E-04 | 0.089 |
| KEGG_BASE_EXCISION_REPAIR | 32 | 6.69E-04 | 0.094 |
| KEGG_MISMATCH_REPAIR | 23 | 6.64E-04 | 0.094 |
| ORGANELLE_ENVELOPE | 163 | 7.55E-04 | 0.108 |
| SMALL_NUCLEAR_RIBONUCLEOPROTEIN_COMPLEX | 22 | 7.84E-04 | 0.112 |
| REACTOME_ABORTIVE_ELONGATION_OF_HIV1_TRANSCRIPT_IN_THE_ABSENCE_OF_TAT | 23 | 8.39E-04 | 0.119 |
| LIPID_BIOSYNTHETIC_PROCESS | 95 | 8.46E-04 | 0.12 |
| ENVELOPE | 163 | 8.60E-04 | 0.123 |
| REACTOME_SCFSKP2_MEDIATED_DEGRADATION_OF_P27_P21 | 51 | 8.92E-04 | 0.129 |
| KEGG_PROTEASOME | 42 | 0.001024 | 0.147 |
| NUCLEOLUS | 122 | 0.001095 | 0.158 |
| REACTOME_TRANSPORT_OF_MATURE_MRNA_DERIVED_FROM_AN_INTRONLESS_TRANSCRIPT | 32 | 0.001133 | 0.164 |
| KEGG_PYRUVATE_METABOLISM | 40 | 0.001138 | 0.165 |
| REACTOME_METABOLISM_OF_CARBOHYDRATES | 230 | 0.001137 | 0.166 |
| CELL_CYCLE_CHECKPOINT_GO_0000075 | 48 | 0.001248 | 0.183 |
| KEGG_PENTOSE_PHOSPHATE_PATHWAY | 27 | 0.001284 | 0.19 |
| REACTOME_CITRIC_ACID_CYCLE_TCA_CYCLE | 18 | 0.001313 | 0.195 |
| KEGG_PYRIMIDINE_METABOLISM | 94 | 0.001311 | 0.196 |
| REACTOME_TRANSCRIPTION_COUPLED_NER_TC_NER | 41 | 0.001302 | 0.196 |
| BIOCARTA_MPR_PATHWAY | 34 | 0.001324 | 0.2 |
| KEGG_VALINE_LEUCINE_AND_ISOLEUCINE_DEGRADATION | 44 | 0.001358 | 0.205 |
| KINETOCHORE | 24 | 0.001368 | 0.208 |
| DNA_METABOLIC_PROCESS | 251 | 0.001383 | 0.211 |
| SISTER_CHROMATID_SEGREGATION | 16 | 0.001392 | 0.213 |
| REACTOME_MITOTIC_G2_G2_M_PHASES | 78 | 0.001402 | 0.216 |
| REACTOME_GLOBAL_GENOMIC_NER_GG_NER | 30 | 0.001393 | 0.216 |
| KEGG_FATTY_ACID_METABOLISM | 40 | 0.001384 | 0.216 |
| CHROMATIN_BINDING | 32 | 0.001376 | 0.216 |
| REACTOME_KINESINS | 24 | 0.00173 | 0.262 |
| REACTOME_GLUCOSE_TRANSPORT | 37 | 0.001737 | 0.265 |
| KEGG_NUCLEOTIDE_EXCISION_REPAIR | 42 | 0.001772 | 0.272 |
| RIBOSOME_BIOGENESIS_AND_ASSEMBLY | 18 | 0.001823 | 0.282 |
| KEGG_HOMOLOGOUS_RECOMBINATION | 28 | 0.002083 | 0.316 |
| KTGGYRSGAA_UNKNOWN | 75 | 0.002104 | 0.321 |

| | | | |
|---|---|---|---|
| ALCOHOL_METABOLIC_PROCESS | 86 | 0.002097 | 0.321 |
| REACTOME_FORMATION_OF_THE_HIV1_EARLY_ELONGATION_COMPLEX | 31 | 0.002157 | 0.329 |
| KEGG_HUNTINGTONS_DISEASE | 165 | 0.002155 | 0.331 |
| REACTOME_NEP_NS2_INTERACTS_WITH_THE_CELLULAR_EXPORT_MACHINERY | 26 | 0.002148 | 0.332 |
| REACTOME_CDK_MEDIATED_PHOSPHORYLATION_AND_REMOVAL_OF_CDC6 | 44 | 0.002218 | 0.343 |
| REACTOME_FATTY_ACYL_COA_BIOSYNTHESIS | 18 | 0.002281 | 0.349 |
| KEGG_PURINE_METABOLISM | 155 | 0.002499 | 0.381 |
| REACTOME_NUCLEOTIDE_EXCISION_REPAIR | 46 | 0.002736 | 0.412 |

Table S3 upregulated pathways

| NAME | FDR q-val | FWER p-val |
|---|---|---|
| REACTOME_UNFOLDED_PROTEIN_RESPONSE | 0 | 0 |
| REACTOME_BMAL1_CLOCK_NPAS2_ACTIVATES_CIRCADIAN_EXPRESSION | 0 | 0 |
| REACTOME_ACTIVATION_OF_CHAPERONE_GENES_BY_XBP1S | 0 | 0 |
| REACTOME_DIABETES_PATHWAYS | 0 | 0 |
| REACTOME_CIRCADIAN_CLOCK | 0.013461 | 0.063 |
| V$ATF6_01 | 0.02439 | 0.131 |
| REACTOME_RORA_ACTIVATES_CIRCADIAN_EXPRESSION | 0.02454 | 0.154 |
| BIOCARTA_P53HYPOXIA_PATHWAY | 0.022521 | 0.161 |
| REACTOME_CIRCADIAN_REPRESSION_OF_EXPRESSION_BY_REV_ERBA | 0.020951 | 0.168 |
| REGULATION_OF_GTPASE_ACTIVITY | 0.024243 | 0.209 |
| TCTATGA,MIR-376A,MIR-376B | 0.07349 | 0.546 |
| BIOCARTA_PML_PATHWAY | 0.06763 | 0.547 |
| REACTOME_CYTOSOLIC_TRNA_AMINOACYLATION | 0.068843 | 0.582 |
| REACTOME_PERK_REGULATED_GENE_EXPRESSION | 0.065437 | 0.586 |
| ER_NUCLEAR_SIGNALING_PATHWAY | 0.068671 | 0.627 |
| KEGG_SNARE_INTERACTIONS_IN_VESICULAR_TRANSPORT | 0.070436 | 0.662 |
| GOLGI_VESICLE_TRANSPORT | 0.068398 | 0.674 |
| REACTOME_ANTIGEN_PRESENTATION_FOLDING_ASSEMBLY_AND_PEPTIDE_LOADING_OF_CLASS_I_MHC | 0.067588 | 0.692 |
| REACTOME_CELL_JUNCTION_ORGANIZATION | 0.072851 | 0.738 |

**Table S4. The list of genes that affect the response to JG-98 identified by the polled shRNA screen in MCF7 and MDA-MB231 cells.**

Table S4

**MCF7**

| Up Genes | Down Genes | | | | |
|---|---|---|---|---|---|
| ACE | ABCB7 | CYP1A2 | HSD17B4 | NR4A3 | RUNX3 |
| ACOT12 | ABCC1 | CYSLTR1 | HSF2 | NRG1 | RUVBL2 |
| ACVR1 | ABCC2 | DNAJA3 | HSP90AB1 | NT5C3 | RXRA |
| ADH1C | ACADVL | DNAJB1 | HSPB1 | NUP214 | SC5DL |
| AK1 | ADCY8 | DRD2 | HSPG2 | OCIAD1 | SF1 |
| APBB2 | ADRA1A | DUSP4 | HTR1F | OPRD1 | SIN3A |
| ARF1 | AGRN | DUSP6 | HTR2B | OXTR | SLC26A2 |
| ARFGAP3 | ALDH4A1 | EEF2 | HTR2C | PAX8 | SMARCA4 |
| ATF2 | AMPD2 | EFTUD2 | HTR3B | PCGF2 | SNRPA1 |
| ATG16L1 | ANP32A | EIF1AX | HTR3C | PDHX | SNRPD2 |
| ATP1A1 | APOBEC3G | EIF2B5 | HTR4 | PGF | SORBS1 |
| ATP5O | AQR | EIF2S2 | HYAL2 | PIK3CG | SP1 |
| ATP6V1E2 | ARFGEF2 | EIF3A | IDH1 | PIK4CA | STRAP |
| ATPGD1 | ATF3 | ELK4 | IGFBP6 | PITX2 | TACR1 |
| C1GALT1 | ATG4A | EMR1 | IL10RB | PLK1 | TBXA2R |
| CACNA1B | ATP6AP1 | EMR3 | IL1R1 | POLR2A | TCF7L1 |
| CACNA1H | ATP6V1G1 | ERCC3 | IL22 | POLR2B | TCOF1 |
| CAMKK1 | ATRX | ESRRA | IRF6 | POLR2D | TEAD2 |
| CAPN10 | BAAT | FBXW7 | IRF8 | POLR2F | TFCP2 |
| CD9 | BAP1 | FOXN1 | JUP | POLR2I | TLE1 |
| CDKL2 | BMP10 | FOXO1 | KCNH7 | POR | TNFSF4 |
| CHEK1 | BNIP3 | FZD3 | KIF11 | PROCR | TNFSF8 |
| CMA1 | BPNT1 | FZD4 | KLRC4 | PSMA1 | TNIP1 |
| COL4A3 | C1ORF103 | FZD7 | KLRK1 | PSMA2 | UBE2L3 |
| FOXK1 | C7 | GAD1 | KPNB1 | PSMA3 | USP9X |
| GGT1 | C9ORF47 | GBX2 | KREMEN1 | PSMB2 | VNN1 |
| IFNA13 | CASK | GCGR | LAT2 | PSMB6 | WARS2 |
| IFNA16 | CBR1 | GGTL3 | LDLR | PSMC2 | WWTR1 |
| INPP5D | CCK | GLP2R | LHX2 | PSMD1 | YY1 |
| KCNJ3 | CCL28 | GNB2L1 | LPHN2 | PSMD2 | |
| LHX8 | CCL3L1 | GPR109B | LRRK2 | PSMD3 | |
| LOC400652 | CD58 | GPR35 | LY75 | PSMD6 | |
| LPO | CDA | GPR37 | MAFK | PTGDR | |
| MAP3K3 | CDC40 | GPR68 | MAML3 | PTGER3 | |
| MYH2 | CDK5 | GPR81 | MAPK8IP3 | RAN | |
| PA2G4 | CDX4 | GRM5 | MBD1 | RBX1 | |
| PIGM | CHD8 | GTF2E2 | MC4R | RECQL | |
| PRKCB1 | CLTC | GTF3C3 | MCM2 | RPA2 | |
| RAC1 | COL5A1 | GZMB | MELK | RPL10 | |

| | | | | |
|---|---|---|---|---|
| RDH14 | COL5A2 | HNRNPC | MOG | RPL11 |
| RENBP | CPO | HNRPK | MYL1 | RPL14 |
| SETD2 | CRY1 | HOXB4 | NACA | RPL30 |
| SMAD2 | CSE1L | HOXB6 | NCL | RPL6 |
| SND1 | CSF2RA | HOXD13 | NEUROG3 | RPS13 |
| TNKS | CXCR3 | HR | NMI | RTF1 |
| XPC | CXCR6 | HRH4 | NR1D1 | RUNX2 |

**MDA-MB231**

| **Up Genes** | **Down Genes** | | | |
|---|---|---|---|---|
| ATP1A1 | ABCC1 | EIF2B5 | PLA2G1B | SEC22B |
| IKZF3 | ABCC2 | EIF3A | PLK1 | SERPINA10 |
| | AKR1C2 | EIF4EBP1 | POLR2A | SHFM1 |
| | ALG11 | EREG | POLR2B | SKP1A |
| | ANAPC4 | FCGR3B | POLR2D | SLAIN1 |
| | AQR | FLT4 | POLR2F | SMC6 |
| | ARD1A | GAPDH | PON3 | SMN1 |
| | ATP1A4 | GBF1 | PPAP2B | SNCB |
| | ATP5G1 | GBX2 | PPP2R2A | SNRNP200 |
| | ATP6AP1 | GNA13 | PRDX2 | SNRPD2 |
| | ATP6V0C | GPX4 | PRKCE | SRP54 |
| | ATP6V0D1 | GSK3A | PRKRA | STAG2 |
| | ATP6V1A | GSTA1 | PRODH | STAR |
| | BAP1 | HES6 | PRPF19 | STAT5A |
| | BCL2L1 | HLA-E | PSMA1 | STRAP |
| | BID | HNRNPC | PSMA2 | THOC4 |
| | BST2 | HNRPK | PSMA3 | TIMELESS |
| | CALM2 | HSD17B1 | PSMA6 | TLN1 |
| | CAPN5 | IFNA17 | PSMA7 | TLR10 |
| | CCL11 | IFNG | PSMB2 | TRAF3 |
| | CCL13 | IGF2R | PSMB4 | TSC2 |
| | CCL2 | IL1RAP | PSMB6 | TUBA1C |
| | CD226 | IL2 | PSMC1 | UBE1 |
| | CDC2L1 | IL4R | PSMC2 | UBE2I |
| | CDC40 | ITGAV | PSMD1 | UBE2L3 |
| | CFLAR | KIF3A | PSMD11 | UBE2V2 |
| | CHD8 | KPNB1 | PSMD12 | USP9X |
| | CHGB | LIAS | PSMD3 | WARS2 |
| | CLEC7A | LOC391656 | PSMD8 | XAB2 |
| | COL8A1 | LPHN3 | PSMF1 | XCL1 |
| | COPS5 | MCM4 | RAB11A | YY1 |
| | COQ7 | MCM6 | RAD21 | ZFP42 |
| | CPSF2 | MTMR1 | RAG1 | |
| | CTNNA1 | MYEF2 | RAN | |
| | CXCR4 | NACA | RARB | |
| | CYP21A2 | NADSYN1 | RBL2 | |

| | | |
|---|---|---|
| DARS | NARS | RBX1 |
| DDHD1 | NRAS | RFX4 |
| DDX41 | NT5C2 | RPA2 |
| DIDO1 | NXT1 | RPL30 |
| DKK4 | PAFAH1B2 | RPL8 |
| DLX3 | PBEF1 | RRM1 |
| DPYSL2 | PENK | RTF1 |
| DSP | PFDN2 | RUVBL2 |
| EFTUD2 | PIK3C3 | SAP18 |
| EIF1AX | PKN1 | SCD5 |

**Table S5. Top 40 connections that are predicted to sensitize cells to JG-98 according to analysis of the Connectivity Map.**

Table S5 Top 40 Connections

| | cmap_id | cmap_name | score_best2 | Target |
|---|---|---|---|---|
| 1 | BRD-K13646352 | midostaurin | 99.822 | TK |
| 2 | BRD-K35960502 | niclosamide | 99.486 | |
| 3 | BRD-K74305673 | IKK-2-inhibitor-V | 99.147 | |
| 4 | BRD-A58564983 | selamectin | 99.404 | |
| 5 | BRD-A08003242 | rhodomyrtoxin-b | 99.134 | |
| 6 | BRD-K01121114 | BRD-K01121114 | 98.875 | |
| 7 | BRD-K92241597 | tosedostat | 98.573 | |
| 8 | BRD-K60623809 | SU-11652 | 99.239 | TK |
| 9 | BRD-K76840893 | RS-17053 | 99.135 | |
| 10 | BRD-K12184916 | NVP-BEZ235 | 98.542 | PI3K |
| 11 | BRD-K38477985 | malonoben | 98.732 | |
| 12 | BRD-K67868012 | PI-103 | 99.207 | PI3K |
| 13 | BRD-K06750613 | GSK-1059615 | 99.598 | PI3K |
| 14 | BRD-K67075780 | TGX-115 | 99.422 | PI3K |
| 15 | BRD-K99582188 | BRD-K99582188 | 97.737 | |
| 16 | BRD-A34462049 | tigecycline | 99.135 | |
| 17 | BRD-K68065987 | MK-2206 | 98.773 | Akt |
| 18 | BRD-A06352508 | SB-218078 | 98.258 | Chk1 |
| 19 | BRD-K33272502 | DG-041 | 97.765 | |
| 20 | BRD-K86574132 | BRD-K86574132 | 99.176 | |
| 21 | BRD-K15616905 | CCCP | 98.324 | |
| 22 | BRD-K55844427 | BRD-K55844427 | 99.228 | |
| 23 | BRD-A50737080 | CGK-733 | 97.079 | |
| 24 | BRD-K88677950 | PD-198306 | 97.378 | |
| 25 | BRD-K50836978 | purvalanol-a | 98.826 | |
| 26 | BRD-K97365803 | PI-828 | 99.261 | PI3K |
| 27 | BRD-K23319301 | BRD-K23319301 | 96.756 | |
| 28 | BRD-A62809825 | thapsigargin | 97.405 | |
| 29 | BRD-K63068307 | ZSTK-474 | 99.11 | PI3K |
| 30 | BRD-K67566344 | KU-0063794 | 99.035 | mTOR |
| 31 | BRD-K28934562 | BRD-K28934562 | 97.185 | |
| 32 | BRD-A59431241 | COL-3 | 95.997 | |
| 33 | BRD-K64642496 | KO-143 | 96.465 | |
| 34 | BRD-K73037408 | KUC111774N | 95.055 | |
| 35 | BRD-K69932463 | AZD-8055 | 96.998 | mTOR |
| 36 | BRD-K40255344 | tyrphostin-A9 | 97.587 | TK |
| 37 | BRD-K59469039 | AG-879 | 98.179 | TK |
| 38 | BRD-A47829399 | artesunate | 97.551 | |
| 39 | BRD-M64432851 | sunitinib | 99.152 | TK |
| 40 | BRD-A11678676 | wortmannin | 97.616 | mTOR |