

Supplementary Table 2 List of compounds and their IC50 data on glioblastoma cell lines (S1) from ChEMBL.

pert_iname	Standard Value IC50	Activity
A-443644	248.2	Effective
AZD-8055	1750.77	Effective
BI-2536	188.24	Effective
BMS-754807	1527.21	Effective
bortezomib	0.925	Effective
BX-795	3714.94	Effective
camptothecin	12.76	Effective
CGP-60474	130.2	Effective
cytarabine	2181.22	Effective
dasatinib	354.1	Effective
doxorubicin	323.02	Effective
elesclomol	22.52	Effective
entinostat	3035.13	Effective
epothilone	3.915	Effective
etoposide	8732.725	Effective
FH-535	9111.22	Effective
floxuridine	5570	Effective
foretinib	960	Effective
GDC-0941	4885.57	Effective
gemcitabine	37.24	Effective
GW-843682X	97.86	Effective
MG-132	3242.62	Effective
midostaurin	659.03	Effective
narciclasine	48	Effective
NVP-AUY922	30.275	Effective
NVP-BEZ235	69.31	Effective
NVP-TAE684	2654.14	Effective
palbociclib	9865.075	Effective
PD-0325901	1843.45	Effective
podophyllotoxin	5690	Effective
ponatinib	1862.66	Effective
saracatinib	3650	Effective
sirolimus	581.52	Effective
tanespimycin	117.81	Effective
thapsigargin	14.81	Effective
torin-1	63.41	Effective
trifluoperazine	9900	Effective
TW-37	443.26	Effective

vinblastine	15.045	Effective
vorinostat	4428.19	Effective
ZM-447439	9769.315	Ineffective
afatinib	25724.69	Ineffective
AKT-inhibitor-1-2	28588.94	Ineffective
axitinib	31134.88	Ineffective
AZ-628	17761.21	Ineffective
AZD-6482	10791.28	Ineffective
betulinic-acid	22000	Ineffective
bicalutamide	71901.92	Ineffective
bosutinib	30754.45	Ineffective
CHIR-99021	79955.32	Ineffective
crizotinib	84165.32	Ineffective
curcumin	17500	Ineffective
cyclopamine	425814.6	Ineffective
doramapimod	554480	Ineffective
epigallocatechin	166000	Ineffective
erlotinib	109168.2	Ineffective
gefitinib	16327.03	Ineffective
genistein	89410	Ineffective
GSK-650394	33002.79	Ineffective
harmine	24000	Ineffective
HSP90-inhibitor	19571.69	Ineffective
HY-11007	77778.34	Ineffective
IKK3-inhibitor-IX	414343.8	Ineffective
imatinib	97521.71	Ineffective
KU-55933	101264.4	Ineffective
lapatinib	104774.9	Ineffective
lenalidomide	307372.6	Ineffective
metformin	32700267	Ineffective
methotrexate	15399.78	Ineffective
MK-2206	12809.5	Ineffective
motesanib	64428.02	Ineffective
mycophenolic-acid	10690	Ineffective
navitoclax	53437.78	Ineffective
nilotinib	100117.2	Ineffective
NU-7441	21412.72	Ineffective
olaparib	66171.24	Ineffective
PAC-1	61639.26	Ineffective
parthenolide	48984.54	Ineffective
pazopanib	35958.63	Ineffective
PD-173074	46078.77	Ineffective

PD-184352	11664.17	Ineffective
PF-562271	10460.83	Ineffective
PHA-665752	170164.1	Ineffective
piperlongumine	11130	Ineffective
PLX-4720	131089.6	Ineffective
pyrimethamine	655756.2	Ineffective
QS-11	32602.47	Ineffective
RO-3306	130460.9	Ineffective
roscovitine	167901.1	Ineffective
rucaparib	35722.04	Ineffective
SB-216763	285569.2	Ineffective
selumetinib	45596.15	Ineffective
sorafenib	159882.3	Ineffective
SYK-inhibitor	14185.47	Ineffective
temozolomide	724500	Ineffective
tipifarnib-P2	10127.17	Ineffective
tozasertib	10076	Ineffective
tretinoin	294287.8	Ineffective
veliparib	306388.3	Ineffective
VX-702	128809.7	Ineffective
WH-4023	13159.99	Ineffective

Effective designated as IC50 < 10 µM and ineffective is designated as IC50 >= 10 µM