

SUPPLEMENTARY

Prediction of Drug Sensitivity

The cell lines (57) of the CCLE dataset specific to breast cancer were plotted for drug-dose response curves against the drugs present in the CCLE dataset itself. The drugs that did not generate plots for any of the cell lines or generated less than 15 (out of 57) were neglected. This was performed before intersecting the databases to overcome the overlapping cell lines between the CCLE and GDSC datasets.

Table S1. Cell Lines from CCLE Datasets and their Drug Response Records

S.no	Drugs	Rplots generated	Targets	Mechanism of Action	FDA approved
1.	Crizotinib	<15 or 0	c-MET, ALK	c-MET and ALK Inhibitor	TRUE
2.	Dovitinib	28	EGFR, FGFR1, PDGFRbeta, VEGFR-1, KDR	Multi-kinase inhibitor	FALSE
3.	Erlotinib	25	EFGR	EFGR inhibitor	TRUE
4.	Irinotecan	15	Topoisomerase 1	DNA Topoisomerase 1 inhibitor	TRUE
5.	L-685458	25	Gamma Secretase	Gamma-secretase inhibitor	FALSE
6.	Lapatinib	25	EGFR, HER2	EGFR and HER2 inhibitor	TRUE
7.	LBW242	25	IAP	IAP inhibitor	FALSE
8.	Nilotinib	23	Abl/Bcr-Abl	Abl inhibitor	TRUE
9.	Nutlin-3	<15 or 0	MDM2	MDM2 inhibitor	FALSE
10.	Nvp-aew541	<15 or 0	IGF-1R	IGF-1R Inhibitor	FALSE
11.	Nvp-tae 684	<15 or 0	ALK	ALK inhibitor	FALSE
12.	Paclitaxel	<15 or 0	beta-tubulin	Microtubule-Stabilizing Agents	TRUE
13.	Palbociclib	<15 or 0	CDK4/6	CDK4/6 Inhibitor	FALSE
14.	Panobinostat	<15 or 0	HDAC	HDAC inhibitor	TRUE

15.	PD-0325901	<15 or 0	MEK	MEK1 and MEK2 inhibitor	FALSE
16.	PLX4720	<15 or 0	RAF	Raf kinase B inhibitor	FALSE
17.	Sorafenib	<15 or 0	RAF Kinase B, C etc.	Multi-kinase inhibitor	TRUE
18.	Topotecan	<15 or 0	Topoisomerase 1	DNA topoisomerase 1 inhibitor	TRUE
19.	Vandetanib	<15 or 0	Abl, EGFR, Flt3, C-KIT, RET, VEGFR-1, KDR, FLT4	Multi-kinase inhibitor	TRUE

Table S2. Shortlisted Drugs and Cell lines from the CCLE dataset

S.no	Effective Drug(s)	Cell Lines responsive
1.	Dovitinib	(BT-474, HDQ-P1, EFM-19, Hs 578T, HCC70, CAL-85-1, CAMA-1, MDA-MB-453, MDA-MB-468, MDA-MB-415, MDA-MB-436, SK-BR-3, MDA-MB-157, MCF-7, MDA-MB-175-VII, AU565, Hs 739.T, T-47D, HCC1395, BT-20, HMC-1-8, HCC1954, HCC1569, BT-474, BT-549, ZR-75-1)
2.	Erlotinib, L-685458, Lapatinib, LBW242	(HDQ-P1, EFM-19, Hs 578T, HCC70, CAL-85-1, CAMA-1, MDA-MB-453, MDA-MB-468, MDA-MB-415, MDA-MB-436, SK-BR-3, MDA-MB-157, MCF-7, MDA-MB-175-VII, Hs 739.T, T-47D, HCC1395, BT-20, HMC-1-8, HCC1954, HCC1569, BT-474, BT-549, ZR-75-1)
3.	Irinotecan	(HDQ-P1, EFM-19, HCC70, CAL-85-1, CAMA-1, MDA-MB-453, MDA-MB-468, SK-BR-3, MDA-MB-157, MCF-7, AU565, Hs 739.T, BT-20, HMC-1-8, HCC1569, BT-549)
4.	Nilotinib	(HDQ-P1, EFM-19, Hs 578T, HCC70, CAL-85-1, CAMA-1, MDA-MB-453, MDA-MB-468, MDA-MB-415, MDA-MB-436, SK-BR-3, MDA-MB-157, MCF-7, MDA-MB-175-VII, Hs 739.T, T-47D, HCC1395, HMC-1-8, HCC1954, HCC1569, BT-474, BT-549)

Table S3. List of total drugs taken for study

DRUGS	Rplots	Shortlisted via ScRNA-Seq data
5-Fluorouracil	11/11	-
Acetalax	10/11	-
Afatinib	11/11	YES
Afuresertib	10/11	-
AGI-5198	10/11	-
AGI-6780	10/11	-
Alisertib	10/11	-
Alpelisib	10/11	-
AMG-319	10/11	-
AT13148	10/11	-
Axitinib	11/11	-
AZ6102	10/11	-
AZ960	10/11	-
AZD1208	10/11	-
AZD1332	10/11	-
AZD2014	10/11	-
AZD3759	10/11	-
AZD5153	10/11	-

AZD5438	10/11	-
AZD5582	10/11	-
AZD5991	10/11	-
AZD6482	10/11	-
AZD6738	10/11	-
AZD7762	11/11	-
AZD8055	Less than 11	-
AZD8186	Less than 11	-
BDP-00009066	Less than 11	-
BI-2536	Less than 11	-
BIBR-153	Less than 11	-
Bortezomib	11/11	YES
BPD-00008900	Less than 11	-
Buparlisib	Less than 11	-
Camptothecin	11/11	-
Capivasertib///AZD533	Less than 11	-
CDK9_5038	Less than 11	-
CDK9_5576	Less than 11	-
Cediranib	Less than 11	-
Cisplatin	11/11	-

Crizotinib	11/11	-
Cyclophosphamide	Less than 11	-
Cytarabine	Less than 11	-
Dabrafenib	11/11	-
Dactinomycin	11/11	-
Dactolisib	Less than 11	-
Dasatinib	Less than 11	-
Dihydrorotenone	Less than 11	-
Dinaciclib	Less than 11	-
Docetaxel	11/11	-
Doramapimod	Less than 11	-
Eg5_9814	Less than 11	-
Elephantin	Less than 11	-
Entinostat	Less than 11	-
Entospletinib	Less than 11	-
Epirubicin	Less than 11	-
EPZ004777	11/11	-
EPZ5676	11/11	-
ERK_2440	Less than 11	-
ERK_6604	Less than 11	-

Foretinib	Less than 11	-
Fulvestrant	11/11	-
Gallibiscoquinazole	Less than 11	-
GDC0810	Less than 11	-
Gefitinib	Less than 11	-
Gemcitabine	11/11	YES
GSK2578215A	Less than 11	-
GSK2606414	Less than 11	-
GSK343	Less than 11	-
GSK591	Less than 11	-
IAP_5620	Less than 11	-
I-BRD9	Less than 11	-
Ibrutinib	Less than 11	-
IGF1R_3801	Less than 11	-
Ipatasertib	Less than 11	-
IRAK4_4710	Less than 11	-
Irinotecan	11/11	-
IWP-2	Less than 11	-
JAK_8517	Less than 11	-
JAK1_8709	Less than 11	-

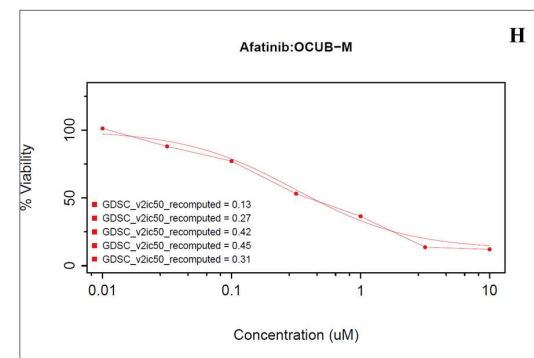
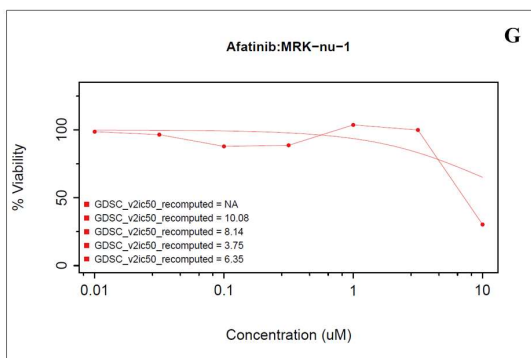
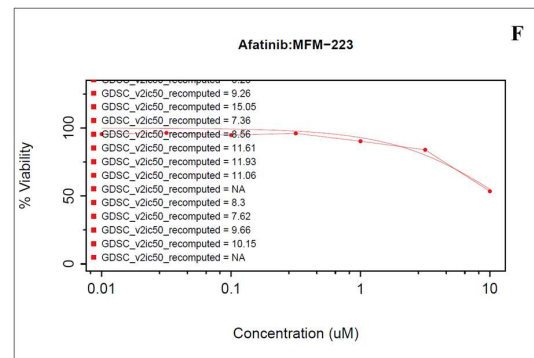
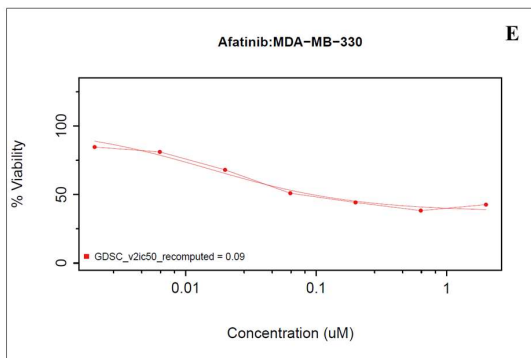
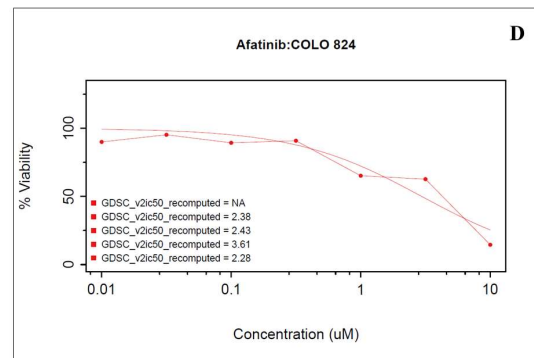
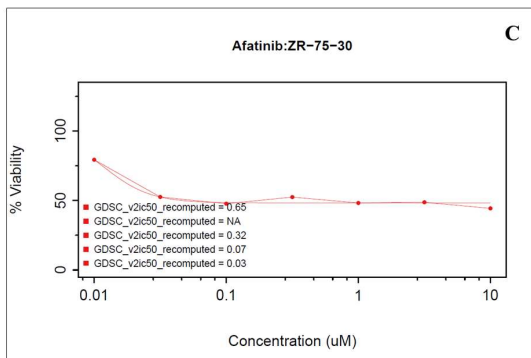
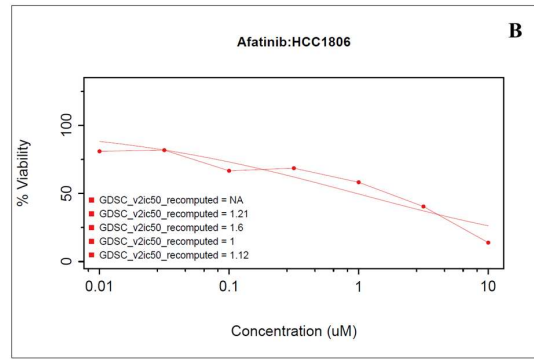
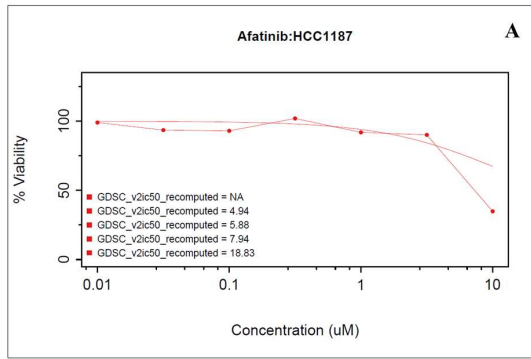
KRAS(G12C) Inhibitor-12	Less than 11	-
KU-55933	Less than 11	-
Lapatinib	11/11	-
LCL161	Less than 11	-
Leflunomide	Less than 11	-
LGK974	11/11	-
Linsitinib	11/11	-
LJI308	Less than 11	-
Luminespib	11/11	-
LY2109761	Less than 11	-
MIM1	Less than 11	-
Mirin	Less than 11	-
Mitoxantrone	Less than 11	-
MK-2206	11/11	-
MK-8776	Less than 11	-
ML323	Less than 11	-
MN-64	Less than 11	-
Navitoclax	11/11	YES
Nelarabine	Less than 11	-

Nilotinib	11/11	-
Niraparib	Less than 11	-
Nutlin-3	Less than 11	-
Nutlin-3a (-)	11/11	-
NVP-ADW742	Less than 11	-
OF-1	Less than 11	-
Olaparib	11/11	-
Osimertinib	Less than 11	-
OTX015	Less than 11	-
Oxaliplatin	11/11	-
P22077	Less than 11	-
Paclitaxel	11/11	-
PAK_533	Less than 11	-
PCI-34051	Less than 11	-
Palbociclib	Less than 11	-
Pevonedistat	Less than 11	-
PF-4708671	Less than 11	-
PFI-3///PFI3	Less than 11	-
Pictilisib	11/11	-
Podophyllotoxin bromide	Less than 11	-

Pyridostatin	Less than 11	-
Ribociclib	Less than 11	
RO-3306	Less than 11	-
Ruxolitinib	Less than 11	-
RVX-208	Less than 11	-
Sabutoclax	Less than 11	-
Sapitinib	11/11	-
Savolitinib	Less than 11	-
SCH772984	11/11	-
Selumetinib	Less than 11	-
Sepantronium bromide	Less than 11	-
Sinularin	Less than 11	-
Sorafenib	11/11	-
TAF1_5496	Less than 11	-
Talazoparib	Less than 11	-
Tamoxifen	11/11	-
Telomerase Inhibitor IX	Less than 11	-
Temozolomide	11/11	-
Teniposide	Less than 11	-
Topotecan	Less than 11	-

Tozasertib	Less than 11	-
TrametinSib	11/11	YES
Ulixertinib	Less than 11	-
ULK1_4989	Less than 11	-
UMI-77	Less than 11	-
Uprosertib	Less than 11	-
VE821	Less than 11	-
Venetoclax	Less than 11	-
Vincristine	Less than 11	-
Vinorelbine	Less than 11	-
Vorinostat	11/11	-
VSP34_8731	Less than 11	-
VX-11e	Less than 11	-
WEHI-539	Less than 11	-
WIKI4	Less than 11	-
WZ4003	Less than 11	-

1.1 Drug-dose response curves



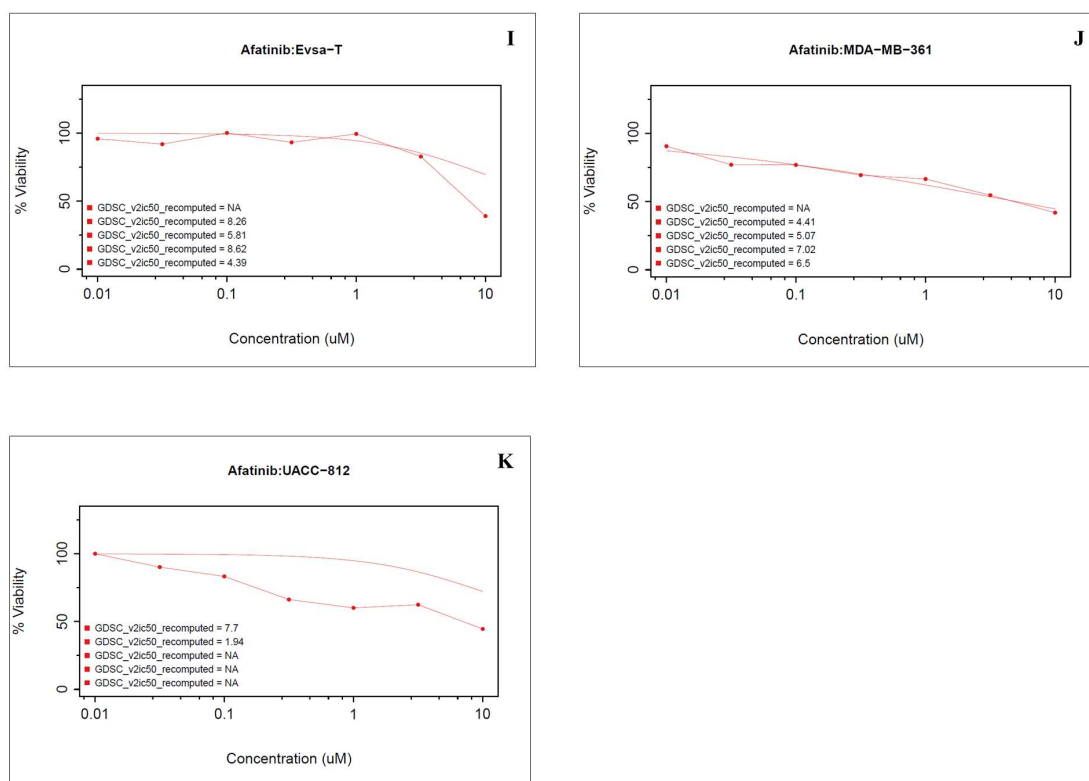
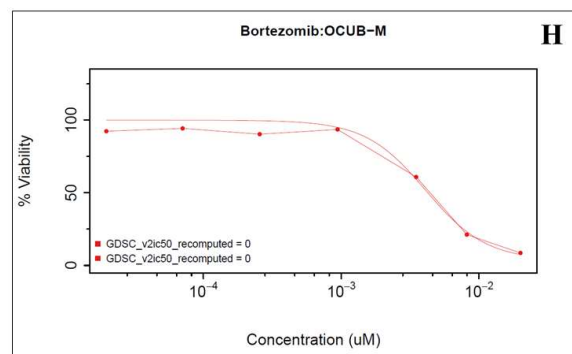
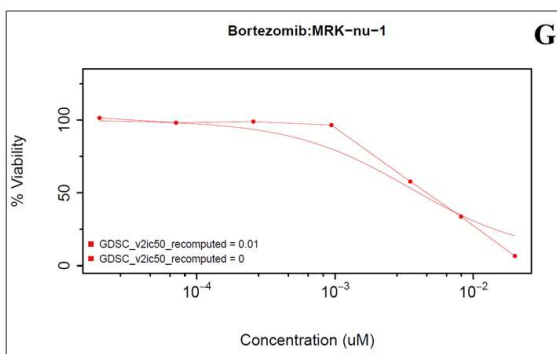
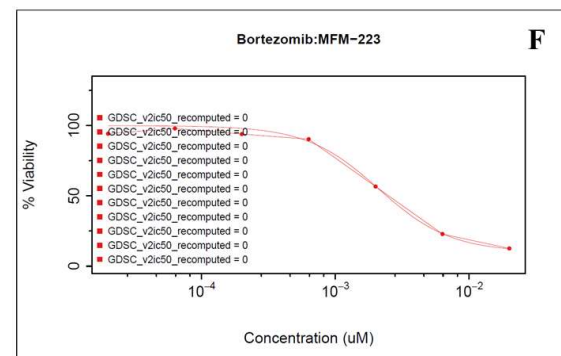
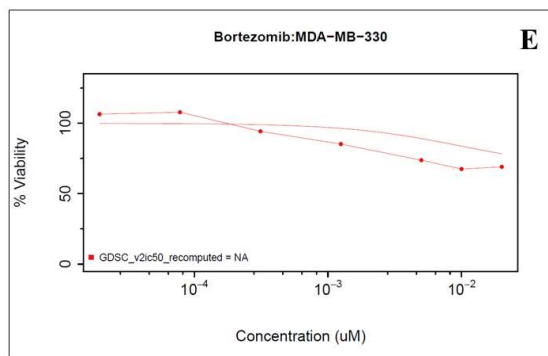
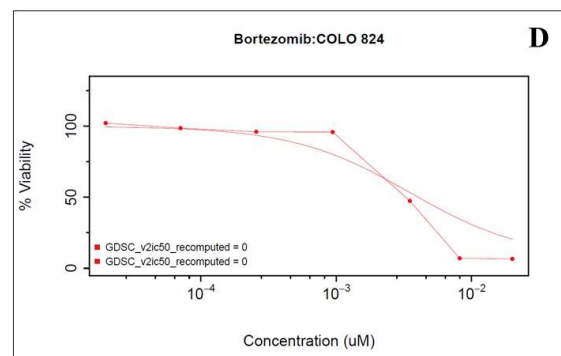
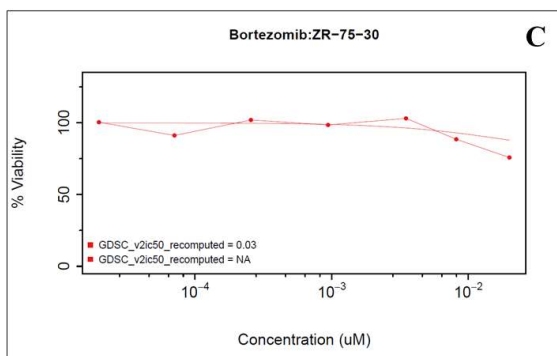
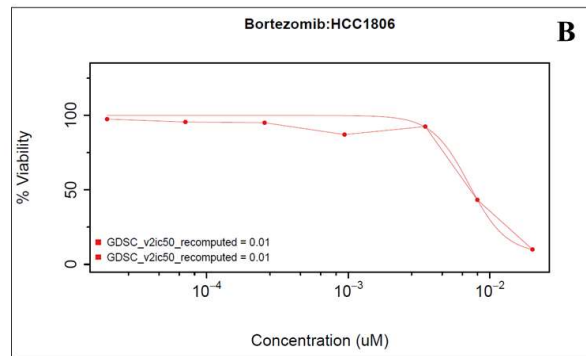
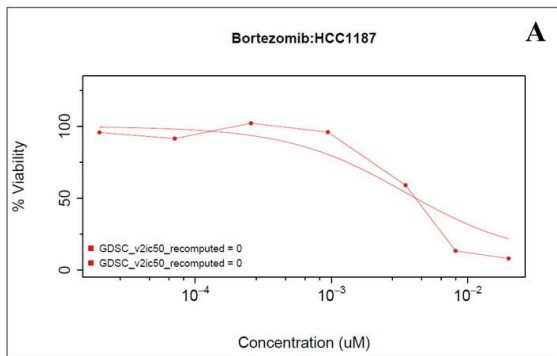


Figure S1. Drug-Dose-Response-Curves of Afatinib drug against 11 breast cancer cell lines (A) HCC1187, The Afatinib drug shows high potency and efficacy at initial concentration and maintains the same response throughout the concentration until 10 micromoles where the decline can be seen. (B)HCC1806, the potency and efficacy at initial concentration is very positive however with increasing concentrations they both decline. (C)ZR-75-30, after the response at initial concentration the drug remains in a steady state with increasing concentrations. (D)COLO824, the drug shows decline in potency and efficacy for this cell line with increasing concentrations. (E)MDA-MB-330, After initial concentrations response, no increase in potency or efficacy is seen. (F)MFM-223, potency of the drug declines rapidly after concentration of 1micromole is administered. (G)MRK-nu-1, a fall in the potency after the initial concentration is interrupted after concentration of 1 micromole. (H)OCUB, Highest potency initially but rapid decline in potency with increasing concentrations. (I)Evsa-T, Graph of this cell line can be seen as fluctuating with sudden increase and decrease in potency as the concentration increases. (J) MDA-MB-361, the cell line shows negative response as with increasing of dosage the potency declines. (K)UACC-812, From initial concentration to final concentration a gradual decrease in potency can be seen.



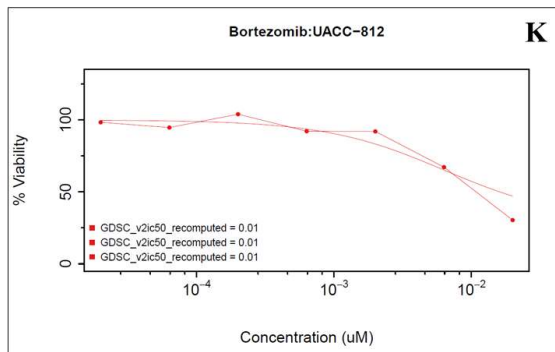
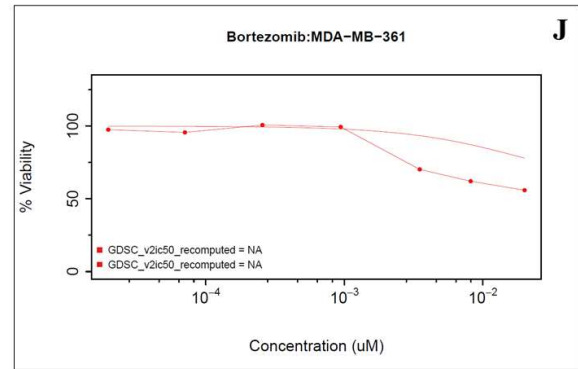
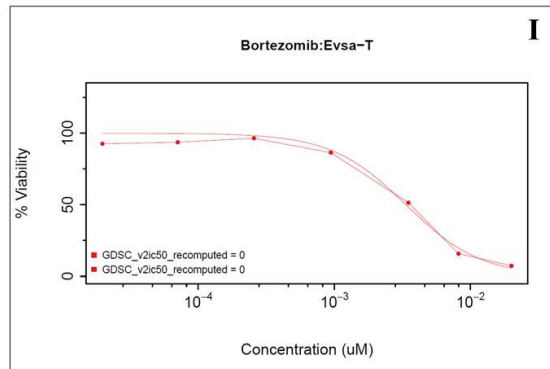
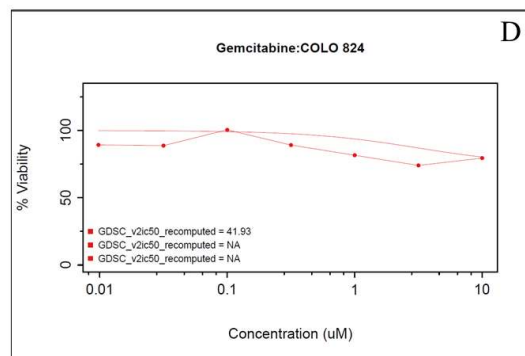
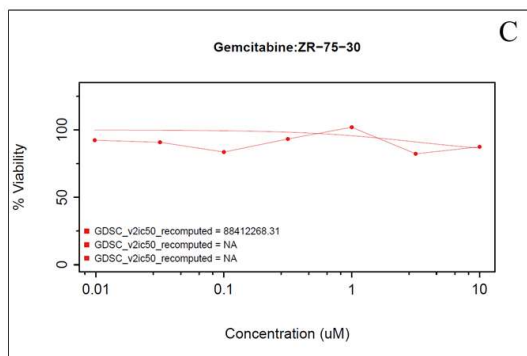
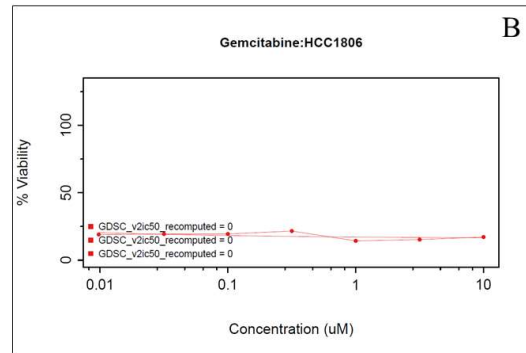
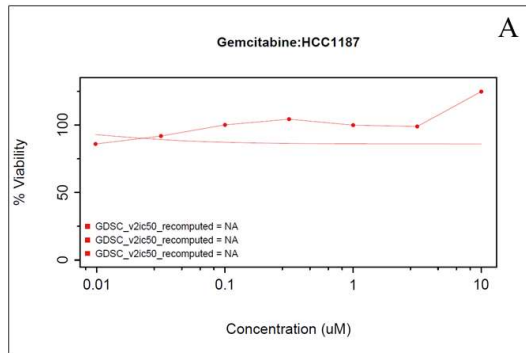


Figure S2. Drug Dose Response Curve of Bortezomib drug against 11 cell lines



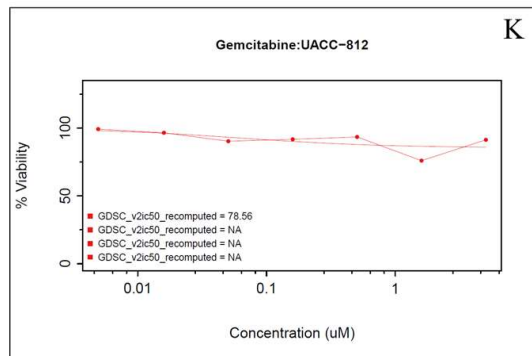
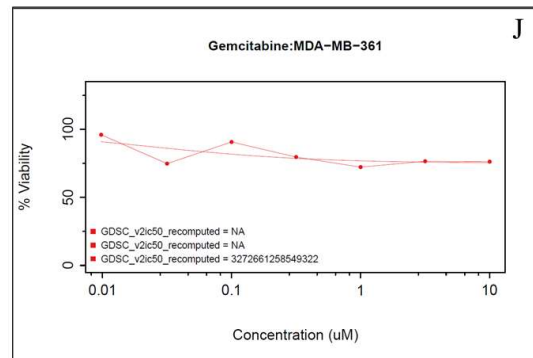
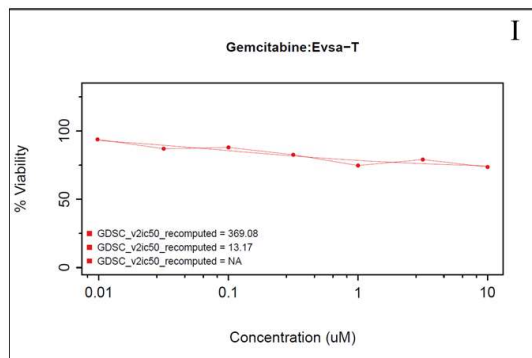
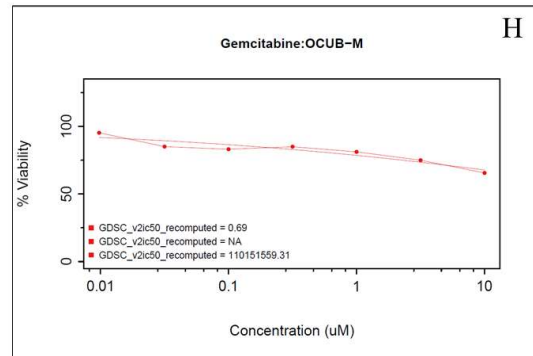
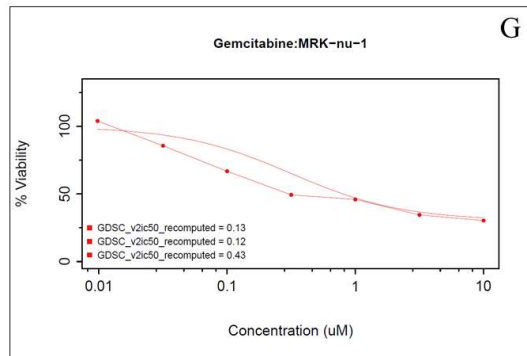
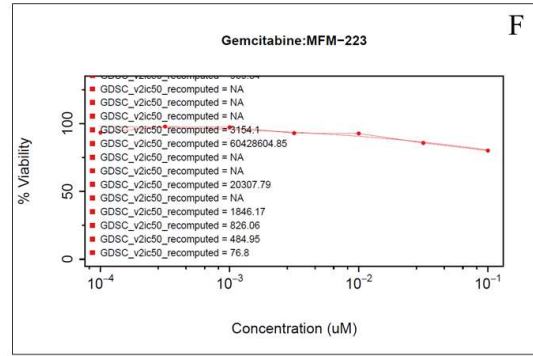
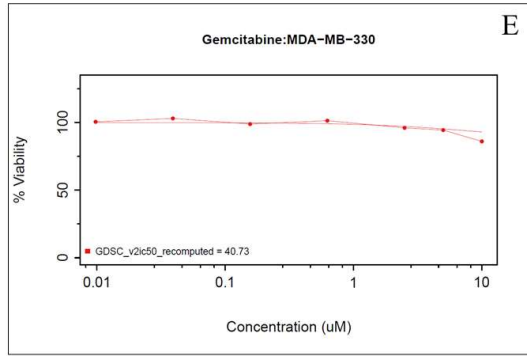
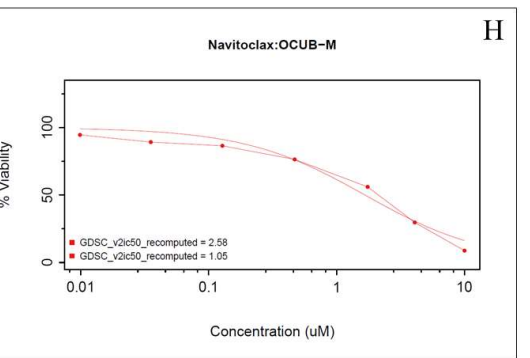
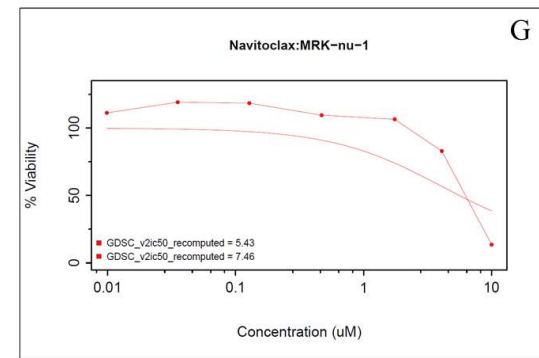
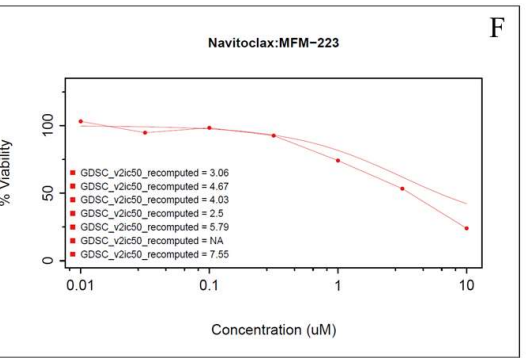
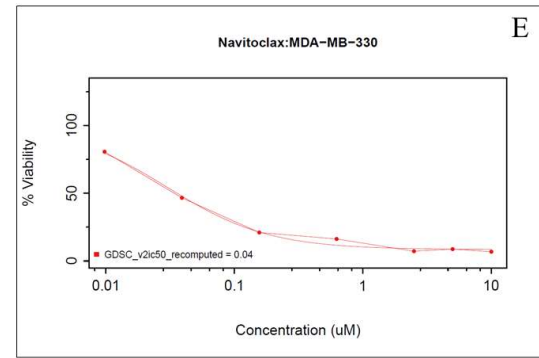
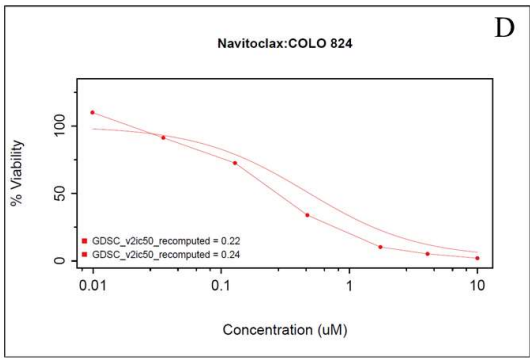
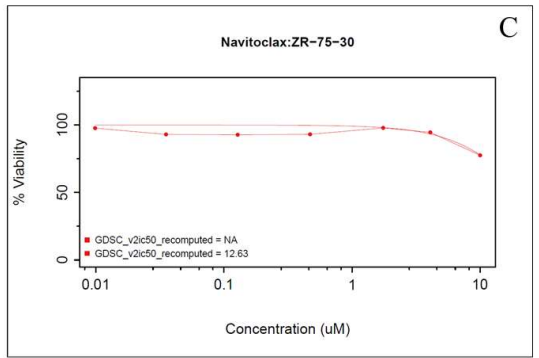
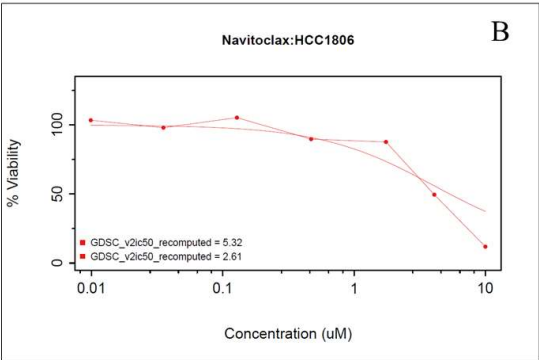
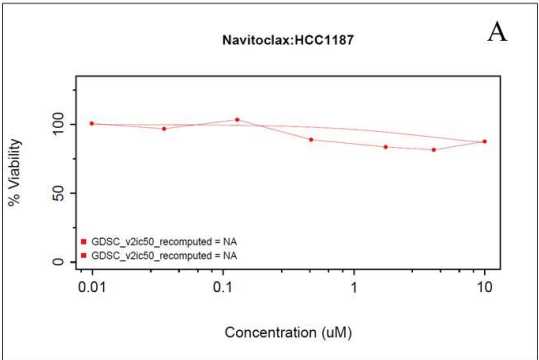


Figure S3. Drug Dose Response Curve of Gemcitabine drug against 11 cell lines



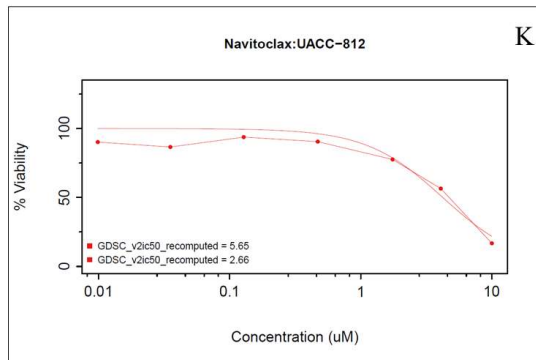
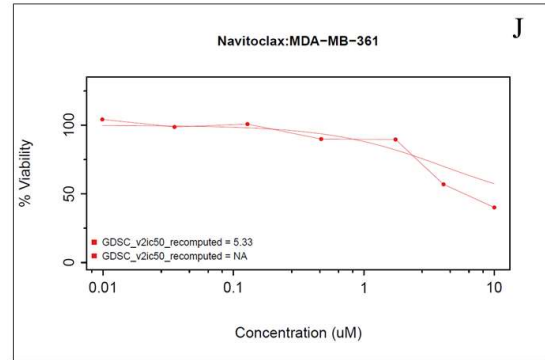
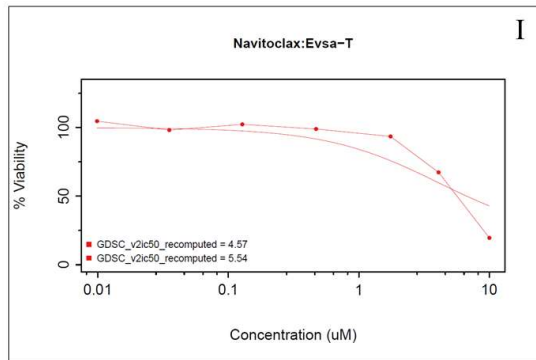
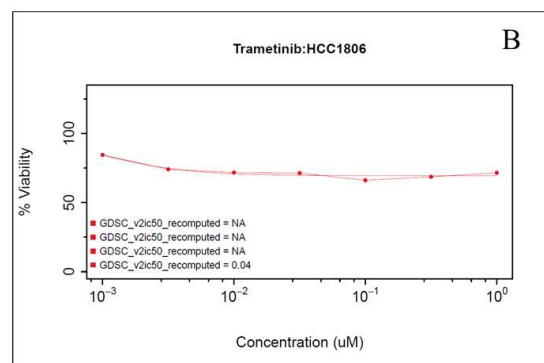
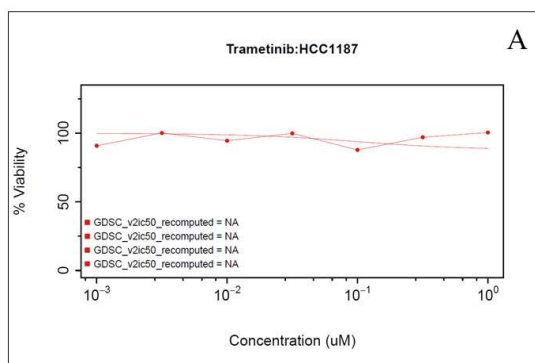
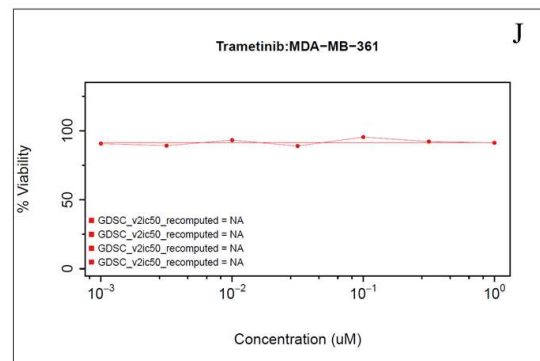
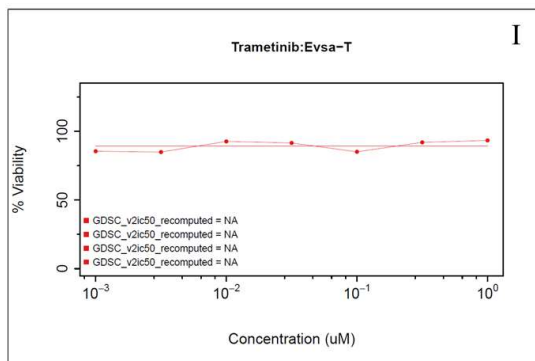
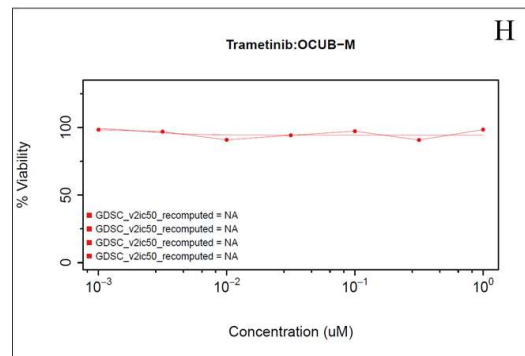
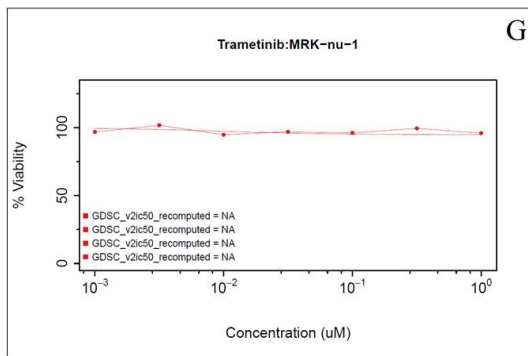
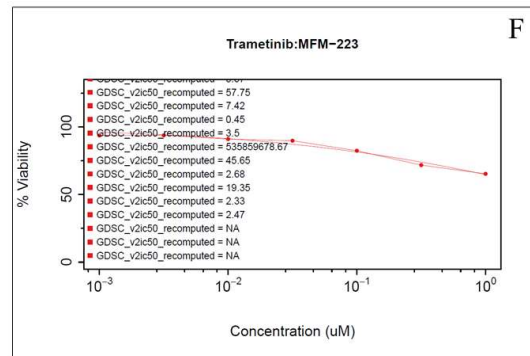
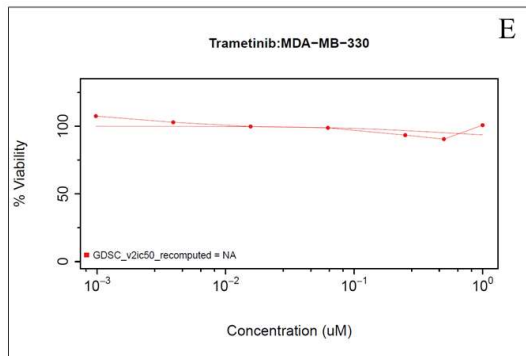
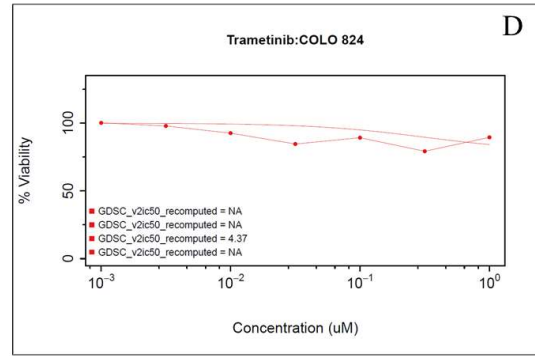
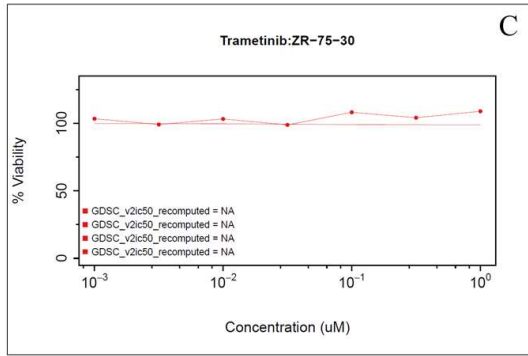


Figure S4. Drug Dose Response Curve of Navitoclax drug against 11 cell lines





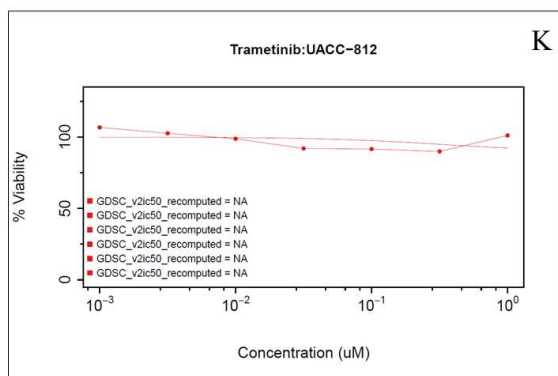


Figure S5. Drug Dose Response Curve of Trametinib drug against 11 cell lines