**SUPPLEMENTARY INFORMATION FOR DIFFERENT DRUG EFFECTS ON BC CELL LINES**

## 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 | - |

## 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**