**Supplementary Legends:**

**Supplementary Figure 1:** Comparison of correlations for *ALK* and *MET***.** Blue, red and grey cells denote significant correlations, significant anti-correlations and non-significant correlations respectively. White cells correspond to combinations that were not tested or are not valid drug-target pairs.

**Supplementary Figure 2:** Comparison of correlations for *HDAC1*, *HDAC2*, *HDAC3*, *HDAC6* and *HDAC8***.** Blue, red and grey cells denote significant correlations, significant anti-correlations and non-significant correlations respectively. White cells correspond to combinations that were not tested or are not valid drug-target pairs.

**Supplementary Figure 3:** Summary of the degree of overlap between the GDSC and CTRP analyses at the transcript level. As GDSC and CTRP provide gene-level expression measurements from different microarray versions (Affymetrix GeneChip HG-U133A in GDSC and HG-U133PLUS2 in CTRP) which potentially detect different isoforms of each gene, we repeated our concordance analysis at the transcript level. The correlation coefficient was calculated for 74 common drugs (targeting drug-target transcript isoforms). The 541 cell lines common in GDSC and CTRP where drug-target transcript isoform expression and AUC values could be obtained were considered.

**Supplementary Table 1:** Spearman correlation values between drug sensitivity and gene expression for 250 drugs studied in the GDSC dataset.

**Supplementary Table 2:** Spearman correlation values between drug sensitivity and gene expression for 481 drugs studied in the CTRP dataset.

**Supplementary Table 3a:** Molecular Targets of the Anticancer Drugs from GDSC, CTRP and DrugBank.Spearman correlation and permutation testing results are provided for both the GDSC and CTRP datasets.

**Supplementary Table 4:** List of drugs where we observe both a correlated and an anti-correlated target in GDSC and CRTP datasets.

**Supplementary Table 5:** Fractions of single cells in each cell line expressing both targets from Figure 3.

**Supplementary Table 6a:** Spearman correlation values between drug sensitivity and target expression for 86 drugs common between GDSC and CTRP.

**Supplementary Table 6b:** Correlation matrix comparing gene expression values.

There are 558 cell lines and 15,934 genes common between both the datasets. Calculated 558x 558 – Correlation matrix comparing gene expression values for 15,934 genes in one cell line from GDSC compared to 15,934 genes in CTRP. Correlation method used was Spearman.

**Supplementary Table 6c:** Spearman correlation values comparing Area under the curve (AUC) values across common cell lines in the GDSC and CTRP datasets for the 86 drugs common between them.

**Supplementary Table 6d:** List of the cell lines where a better gene expression correlation was observed with a different cell line.

**Supplementary Table 7: Transcript isoform aware reanalysis of CTRP-GDSC concordance.** Spearman correlation values between drug sensitivity and drug-target transcript isoforms expression for 74 drugs common between GDSC and CTRP.The 541 cell lines common in GDSC and CTRP where drug-target transcript isoform expression and AUC values could be obtained were considered. As GDSC and CTRP provide gene-level expression measurements from different microarray versions (Affymetrix GeneChip HG-U133A in GDSC and HG-U133PLUS2 in CTRP), which potentially detect different isoforms of each gene, we repeated our analysis at the transcript level.

**Supplementary Table 8:** The top 20 strongest correlations and top 20 strongest anti-correlations between drug sensitivity and gene expression for the GDSC and CTRP datasets.

**Supplementary Table 9:** Drug-target pairs that are significantly correlated in cell lines derived from a cancer subtype but not significantly correlated in the pan-cancer analysis.