

## Description of Additional Supplementary Files

Filename: Supplementary Data 1

Description: Data used in EVAPA derivation; IC<sub>50</sub> predictions from 4 models on novel anticancer compounds collated from recent literature; Five-fold cross-validation results for five models on GDSC data, split into R, NCC and NCD (only prediction data from the fold with the best EVAPA for each model and split included).

Filename: Supplementary Data 2

Description: Source data for main figures—summary of cross validation of GDSC-derived dataset and prediction error dependence on chemical and biological properties of compounds and cell lines for DeepCDR and DrugCell.