S3 Fig. Distribution of 152 drug-wise Pearson correlation values between compound-kinase binding affinities (pKᵢ) measured in the Metz et al. study and their model predictions under the New Drug scenario. The predictions were made using KronRLS algorithm with the best pair of drug and protein kernels (KD-sp and KP-GS) under the leave-drug-out cross-validation. 125 out of 152 correlations are statistically significant (p < 0.0001), and 58 correlation values are greater than 0.75.