New Drug

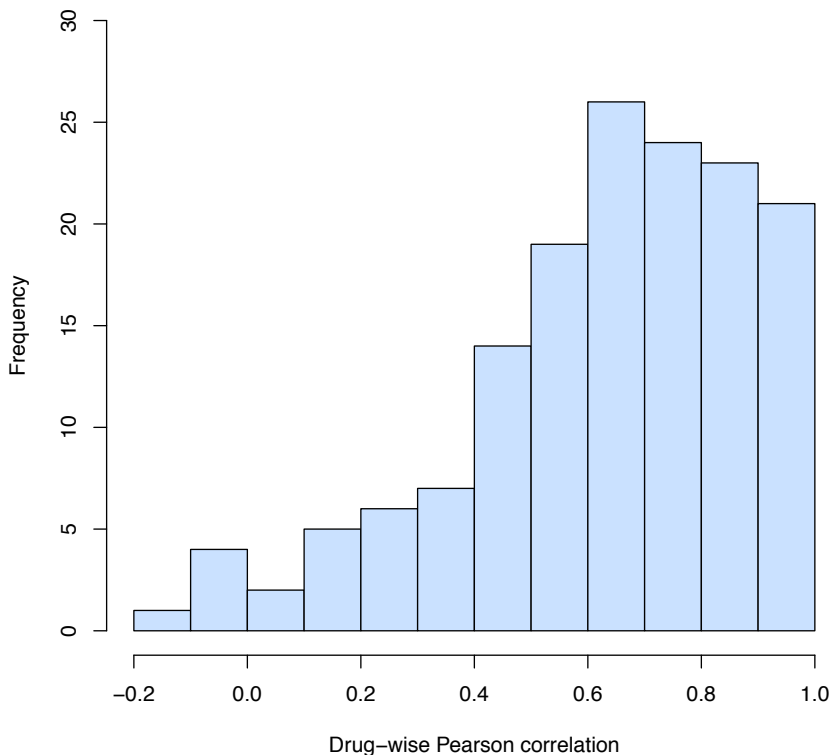**S3 Fig. Distribution of 152 drug-wise Pearson correlation values between compound-kinase binding affinities (pK_i) measured in the Metz *et al*. study and their model predictions under the *New Drug* scenario.** The predictions were made using KronRLS algorithm with the best pair of drug and protein 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.