



S5 Fig. The comparison between model-predicted and experimentally-measured in different assays bioactivities of 100 compound-kinase pairs included in our experimental validation. (a,c) Technical variability between two experimental kinase assays. Scatter plots between (a) 82 pK_i values measured in Metz *et al.* study and pIC_{50} values from our experimental assay; (c) 95 pK_d values from Davis *et al.* study and pIC_{50} values from our experimental assay; (b) 73 *in silico*-predicted and measured in Metz *et al.* study pK_i values, excluding compound-kinase pairs blinded in the model training (marked with orange colour in Fig 4a and S2 Table); (d) 95 *in silico*-predicted pK_i values and pK_d readouts from Davis *et al.* study. The values are detailed in S2 Table.