**Figure S1.** Example molecules from the pyridinyl thieno-pyrimidine cluster. A, ENM 482, containing a 2,2-bipyridyl motif. B, ENM 509, containing a 2,3-bipyridyl motif.
Figure S2. Absorbance spectra of selected compounds when mixed with copper. Colored lines indicate amount of copper (µM) added to 50µM of compound, blank subtracted against copper alone. Shifting absorbance spectra under increasing titrations of copper indicates coordination complex formation.
Figure S3. Elemental proportion of ECFP6 fragments correlates with Bayesian model score. A, sulfur positively correlates with fragment score. B, oxygen negatively correlates with fragment score.
Figure S4. Assay Central 5-fold ROC plot and other statistics.
Figure S5. A, An example molecule with atomic features of predicted activity colored according to the 50 µM model. Green indicates a more active feature while red implies an inactive one. This image was taken in the publicly available Assay Central bundle. B, Selected approved drugs predicted as active by the model, colored according to the same scale.