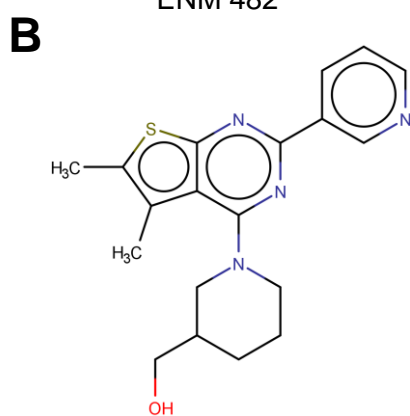
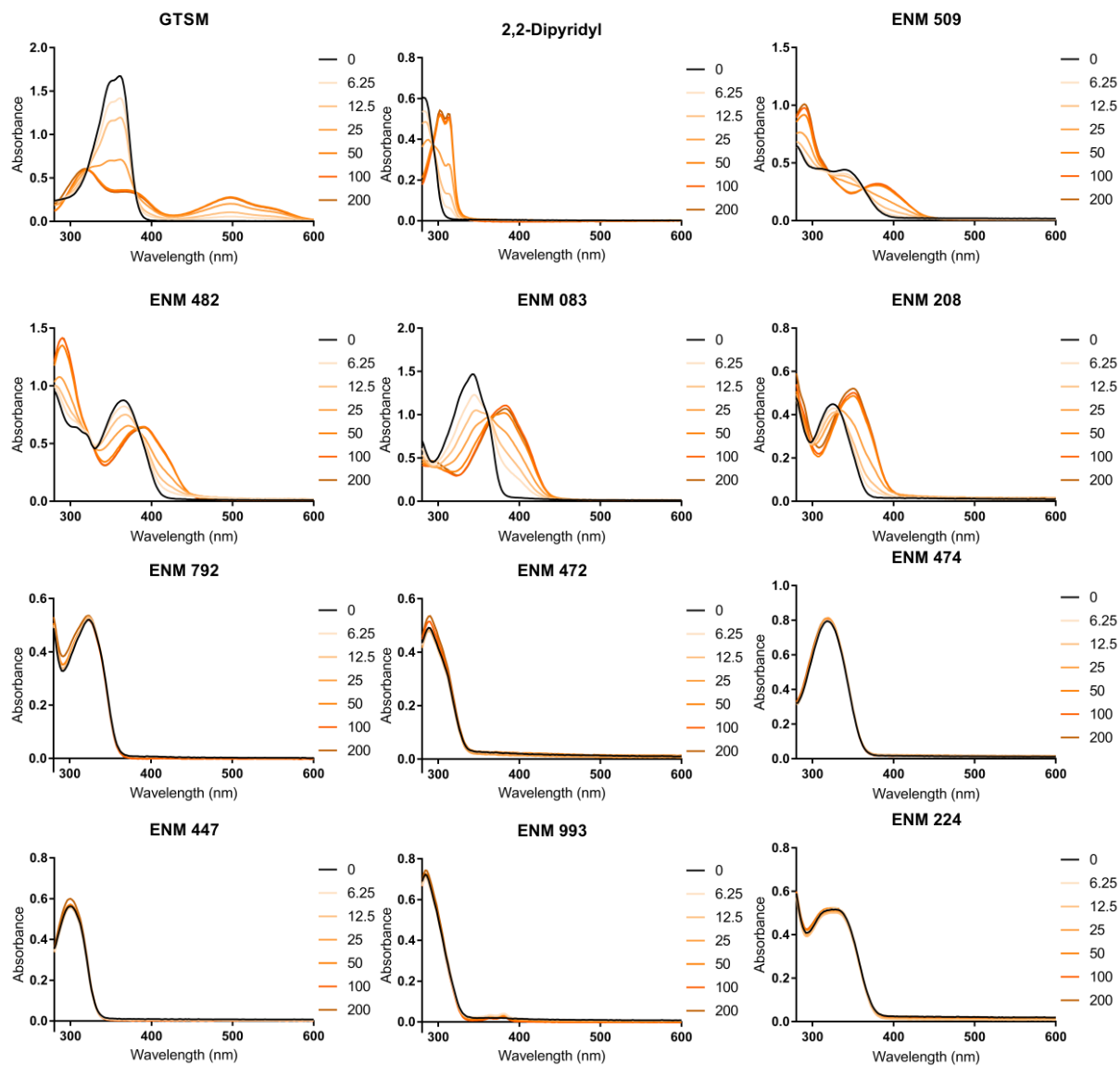


ENM 482

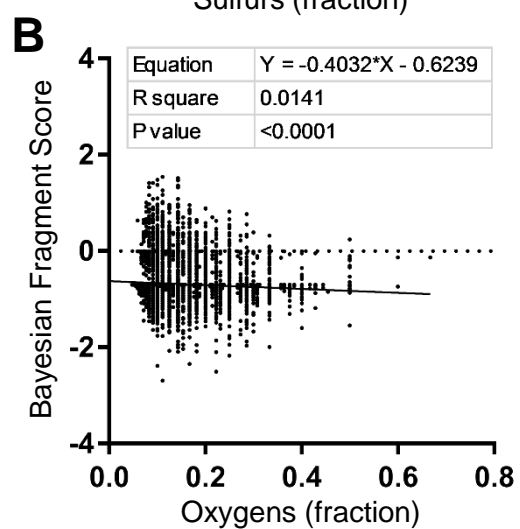
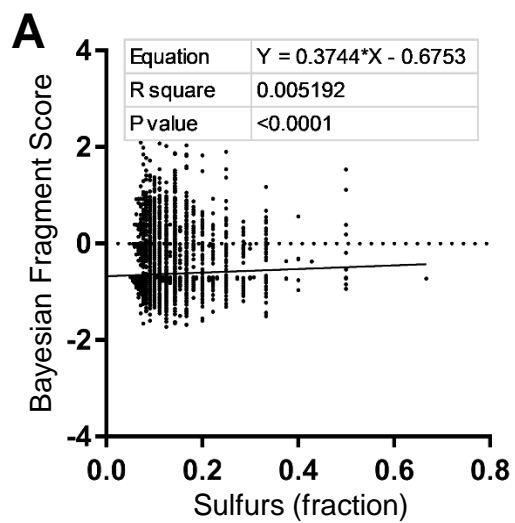


ENM 509

**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 ( $\mu\text{M}$ ) added to  $50\mu\text{M}$  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.

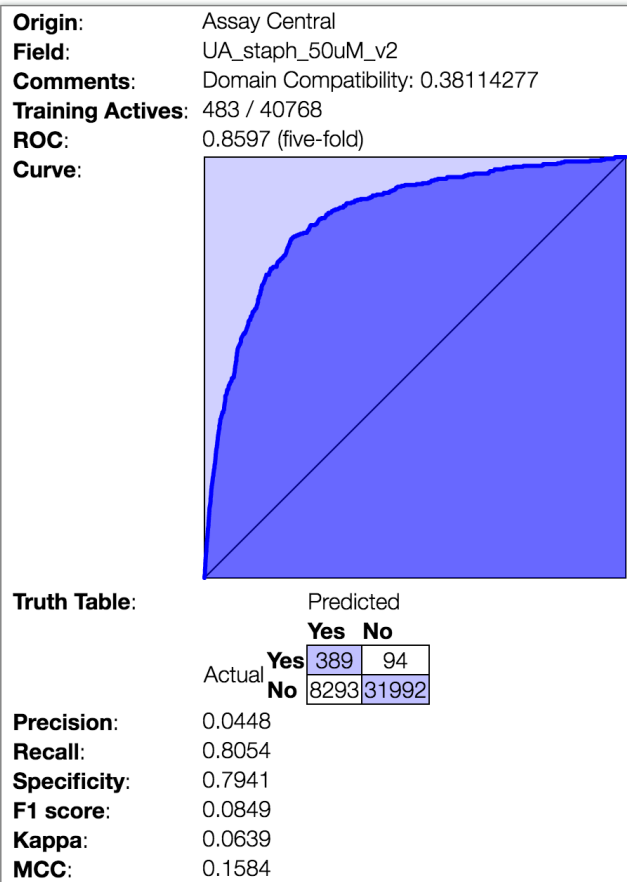
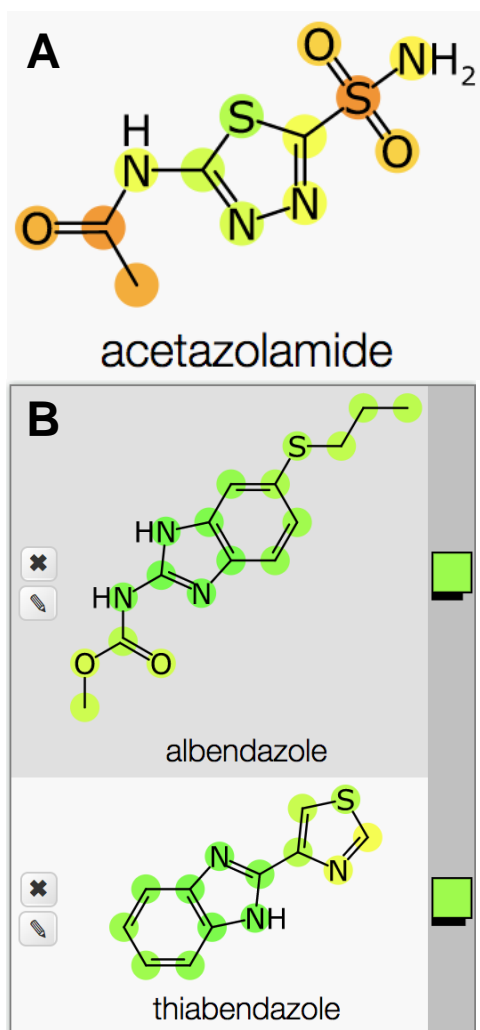


Figure S4. Assay Central 5-fold ROC plot and other statistics.



**Figure S5.** **A**, An example molecule with atomic features of predicted activity colored according to the 50  $\mu$ M 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.