



Supplementary Fig. 2: ~ 500 non-redundant proteins that have the best 3D matches with the Class A β -lactamase motif. We demonstrate that electrostatic conformity leads to a considerable reduction in false positives. The dashed line denotes the highest scoring β -lactamase (PDB id: 2QZ6). When 3D conformity is the sole criteria, there are 80% of the proteins that are below this score, and qualify as possible β -lactamases. This number reduces to 20% when electrostatic conformity is combined with 3D congruence. This analysis was performed on a set of ~ 500 proteins that were the best candidates using a quick 3D match on all the $\sim 50,000$ proteins in the PDB database. It is to be noted that the 4 fold enrichment achieved on this set is an underestimation of the power of our method since the chosen set of proteins was a filtered category through 3D congruence.