Figure S1: Schematic representation of the parameters Gr (Grid Radius), Nt (Near Threshold) and Ft (Far Threshold).

**Examples**

Near Threshold: 3Å, Far Threshold: 6Å

Near Threshold: 5Å, Far Threshold: 15 Å

Figure S1: This figure shows a schematic representation of how the results can be modulated by the choice of different values for the parameters Gr (Grid Radius), Nt (Near Threshold) and Ft (Far Threshold).
Figure S2: In this figure, three potential ligand-binding sites are shown. These sites were predicted in the protein 3U90 by the Metapocket Software. In the red square is tagged the site that corresponds to the similar 3D pattern detected by Geomfinder.
Figure S3: Structure of Monoamine Oxidase B Co-cristalized compounds.

In this figure, 32 different compounds which have been co-crystallized with the Monoamine Oxidase B enzyme. The three letter code, which is shown in the blue squares below of each structure, correspond to the ID of the ligands stored in the Protein Data Bank database.