SYSTEMS AND METHODS FOR MAPPING BINDING SITE VOLUMES IN MACROMOLECULES

ABSTRACT

Systems, methods, and apparatus for evaluating a binding site of a macromolecule are disclosed in which the binding site is identified and a binding site volume map of the binding site is constructed. The binding site volume map has a surface with a plurality of regions. Each respective region in the plurality of regions of the surface is classified based upon a first characteristic that is complementary to a second characteristic of a portion of the macromolecule that is nearest to the respective region, thereby creating an interaction map. Systems, methods, and apparatus for comparing macromolecules are also disclosed in which a binding site volume map is constructed for each of the macromolecules. Then, a composite binding site volume map that comprises a volumetric combination of each of the binding site volume maps is constructed. An interaction map can be constructed from the composite binding site volume map.

Figure 1