RINRUS Toolkit and its Application in Enzymatic Studies

Q. CHENG
University of Memphis, TN, USA

One important aspect in enzymology is the enzyme kinetics, which is the study of catalytic chemical reactions by enzymes. The reaction rate needs to be carefully measured/calibrated under various conditions in wet lab experiments. Using modern computational approaches, the reaction rate can be interpreted by reaction activation energies according to the Arrhenius equation. Multiple computational methods can be used in calculation of activation energies, such as docking, molecular dynamics simulation, quantum mechanics/molecular mechanics, or quantum mechanics-only. Among all these methods, QM-cluster method can often provide more accurate result in energetics, and it is also capable to provide more clear and detailed information in certain chemical reactions such as bond forming/breaking reactions. However, defining the active site is often not systematic, mostly determined with chemical intuition/preference among its practitioners.

As the importance of the residue interaction network (RIN) gets recognized more and more in studying enzyme reactions, RIN has been the foundation of the development of the Residue Interaction Network ResidUe Selector (RINRUS) toolkit. This program takes a PDB file, builds up the residue interaction network according to types of reaction that the user specifies, selects the active site residues, cleans up the edge of the active site, then generates a set of models and input files for QM calculation as well.

This program has been applied in various projects. The QM-cluster calculations constructed by the program have shown promising results which agree well with experimental kinetic data and provide more insights in the field of drug design, novel protein design.