MOE interface for multidimensional MOPAC scan calculations using the example of prenylating enzymes.

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To date MOPAC [1] reaction coordinate calculations (scan) are rather difficult to prepare. The results, especially of 2D-scans, are arduous to visualize and interpret. Furthermore, fixing a high number of atoms, e.g. backbone atoms of an enzymes active site, is also not yet possible without rather high efforts. MOE already provides a simple interface for setting up MOPAC calculations. However, chemical or enzymatic reactions cannot be handled with this interface.

Here we report a compilation of svl scripts providing a MOE [2] interface for MOPAC 1D and 2D scan calculations. These scripts feature a GUI for simple creation of MOPAC input files and selection of reaction path parameters. Furthermore, it facilitates importing calculation results to molecular databases and simultaneous visualization of the energy hypersurface and corresponding molecular structures. Overall, these scripts provide some straight-forward extensions of the MOE built-in MOPAC functions especially regarding scan calculations. Functionalities of these scripts are demonstrated with the help of MOPAC scan calculations of the reaction path of a monoterpene synthase.

Comprising more than 60,000 compounds terpenoids form the largest family of natural products [3]. Monoterpene synthases catalyze the reaction of geranyl- or linalyl-diphosphate to a broad range of highly diverse monoterpenes. A high number of these enzymes produce a complex, yet specific, spectrum of products, which indicates a, up to some point, similar mechanism of formation of these products. Here the energetic level of the transition state of the respective reaction path decides which product is formed. MOPAC provides an engine for semi-empirical calculations, which are suitable for identification of these reaction paths as well as the corresponding transition states. The scripts mentioned above simplify input preparation and output analysis of MOPAC calculations.

[1] J.J.P Stewart, MOPAC2012, Stewart Computational Chemistry.
[2] Molecular Operating Environment (MOE), 2012.10; Chemical Computing Group Inc., 1010 Sherbooke St. West, Suite #910, Montreal, QC, Canada, H3A 2R7.
[3] Dictionary of Natural Products (DNP), http://dnp.chemnetbase.com, accessed 2014-01-28.