Global Reaction Root Mapping in Free Energy of Alanine Tripeptide in Water

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In chemical reactions, the maximum likelihood paths connect equilibrium structures (EQ) of reactant, transition structures (TS) and EQs of products. Such paths are called minimum free-energy path (MFEP), and the characterization of free energy landscapes to find MFEPs is one of the fundamental tasks of molecular dynamics simulations. In our study, we proposed a global reaction root mapping method in the free energy (GRRM-FE). In this method, we use umbrella integration [1] to optimize structures of EQ and TS points, and the anharmonic downward distortion following (ADDF) method [2] to search TS points. This method makes it possible to find EQs, TSs and MFEPs automatically. We chose alanine tripeptide (Fig. 1) in water as a small model of a protein. The conformation of alanine tripeptide can be identified by 4 dihedral angles, so we performed GRRM-FE calculations in 4 dimensions. Fig. 2 shows the results: green squares are EQ points and the gray circles are TS points. We analyzed the structure of reaction paths, and the result shows that almost all important structures were found.

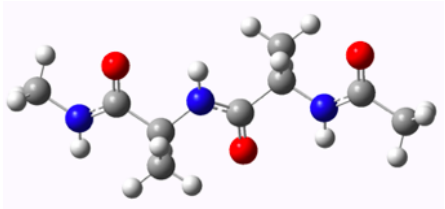

Fig.1 The structure of an alanine tripeptide.

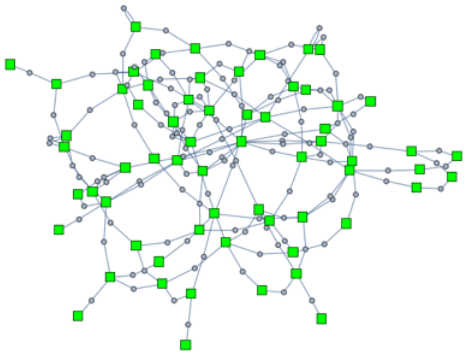

Fig. 2 The figure of graph theory in reaction paths of alanine tripeptide in water.

[1] Matthias U. Bohner, and Johannes Kästner. Journal of Chemical Physics 137.3 (2012): 034105.

[2] Satoshi Maeda, Koichi Ohno, and Keiji Morokuma. Physical Chemistry Chemical Physics 15.11 (2013): 3683-3701.