

Genetic Algorithms in Conformational Searching

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I. ABSTRACT

Conformational searching algorithms are used to find a host of low energy configurations for a given molecule. The large space of possible configurations for molecules grows quickly with the number of atoms, particularly those with many rotatable bonds. Thus, the search for all low energy configurations quickly becomes intractable. Similar problems in global optimization have been approached with genetic algorithms in related fields, but relatively little effort has gone into applying such approaches to problems in computational chemistry, outside of cheminformatics. In this presentation we review a recent application of genetic algorithms as a means of finding many low energy conformers of a set of dipeptide molecules. The algorithm is able to successfully find more low energy conformers than other approaches and shows promise as a means of finding several energy minima in a high dimensional space with reduced computational cost.