A tree-structured covalent-bond-driven molecular memetic algorithm for optimization of ring-deficient molecules

With enormous success in both science and engineering, the recent advances in evolutionary computation—particularly memetic computing—is gaining increasing attention in the molecular optimization community. In this paper, our interest is to introduce a memetic computational methodology for the discovery of low-energy stable conformations—also known as the stereoisomers—of covalently-bonded molecules, due to the abundance of such molecules in nature and their importance in biology and chemistry. To an optimization algorithm, maintaining the same set of bonds over the course of searching for the stereoisomers is a great challenge. Avoiding the steric effect, i.e. preventing atoms from overlapping or getting too close to each other, is another challenge of molecular optimization. Addressing these challenges, three novel nature-inspired tree-based evolutionary operators are first introduced in this paper. A tree-structured covalent-bond-driven molecular memetic algorithm (TCM-MA)—tailored specifically to deal with molecules that involve covalent bonding but contain no cyclic structures using the three novel evolutionary operators—is then proposed for the efficient search of the stereoisomers of ring-deficient covalently-bonded molecules. Through empirical study using the glutamic acid as a sample molecule of interest, it is witnessed that the proposed TCM-MA discovered as many as up to sixteen times more stereoisomers within as little as up to a five times tighter computational budget compared to two other state-of-the-art algorithms.