Efficient Cysteine Conformers Search by a Bayesian Optimization Method

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Cysteine is a fundamental amino acid and has applications in different fields. In recent years, the conformers of isolated cysteine molecules have been widely studied with theoretical simulations and experimental methods [1,2,3,4], however, accurate cysteine conformers prediction with ab initio methods remains time-consuming and low efficiency. In order to do such search, several thousands starting structures needed be relaxed [2]. Here, we adopt a machine learning method based on Bayesian optimization combining with Density Functional Theory (DFT) [5] to search conformers of cysteine efficiently. In our new process, we only need 400 single-point energy calculations to find the global and local minimum structures. The tens of local minimum structures are further relaxed by DFT and corrected by vibration energy. Comparing to the previous studies, the energy order of six low-energy conformers predicted agrees with experimental results [1] and some new conformers have been predicted. This method can be easily extended to the conformer search of other molecules and nanostructures.

References

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