

# Searching for Global Minima in Conformational Spaces

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How to locate the global minimum of a biomolecule in conformational space is a challenging problem in computational and theoretical chemistry. We will introduce the most basic concepts relevant to conformational searches, including what a conformational space is, and what the global minimum is. We will also discuss why we need to perform conformational searches, what is needed to perform a conformational search, and how to perform a conformational search. Then we will discuss some of the conformational search methods and energy determination methods and compare their advantages and disadvantages. Taking conformational study of arginine as an example, we discuss successful approaches for medium-sized molecules, for which ab initio computational studies are feasible. Finally, we will focus on simulated annealing simulations and we will suggest how to improve their performance. This discussion will be illustrated by computational results for deoxycytidine and  $\text{H}(\text{NH}_2\text{BH}_2)_n\text{H}$  oligomers.