Macromolecular Conformation Analysis by the LIL-ADMA Method: How to Deal With Many Atoms Moving in All Directions?

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In searching for a target conformation, such as a local energy minimum of a macromolecule, a compromise involving lower accuracy in an early, crude stage of the search, testing many conformations by some quick, but less accurate method, followed by only a few, more accurate, and more expensive computations near the crudely-located target conformation is advantageous. One such approach is a combination of the Adjustable Density Matrix Assembler (ADMA, an *ab initio* quality linear scaling method, [1-4]), and the rather quick Löwdin-Inverse-Löwdin (LIL) density matrix extrapolation method [3,5], both involving the same type of density matrices on a common AO basis, ensuring perfect compatibility.
Starting with some initial, *ab initio* quality density matrix, a quick and detailed search of the conformational space can be performed by the LIL density matrix extrapolation method, leading to a new candidate conformation to be recalculated by the more accurate, *ab initio* quality method. These steps can be repeated in an iterative fashion, combining the advantages of speed and accuracy.

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