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Developing unsupervised computational techniques for the structural elucidation of molecules from complex mixtures.

Knowing the chemical structure of a molecule is fundamental to understanding its properties and predicting its chemical behavior. However, determining the structure of a molecule in a complex mixtures is very challenging, particularly in mixtures such as crude oil and dissolved organic matter. This project hopes to develop a method for determining the chemical structure of molecules in a complex mixture utilizing TIMS-FT-ICR MS and computational tools. This work expands the Software Assisted Molecular Elucidation (SAME)  package by expanding the theoretical tools available. These tools incorporate the ability to assign chemical formulas to generate molecular structures. After optimization, the collisional cross section is calculated for each candidate structure and compared to the experimentally derived values. However, a significant challenge is that the number of potential structures for a given chemical formula increases exponentially as the number of carbon atoms in the formula increases. If unguided, the number of potential structures can quickly, escalate to beyond peta- structures, and becomes computationally impossible to calculate. This project tries to resolve this problem by developing computer software which can undertake this colossal feat of data management. The software will be able to read the raw data obtained from analytical instruments, collect the information which is relevant to the sorting process and store it in a database. This database can then be used to quickly compare the theoretical calculations for the parameters in question and match them with the experimentally derived values.