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Title: **Software Assisted Molecular Elucidation based on TIMS-FT-ICR MS/MS analysis of complex mixtures**.

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## Abstract

The determination of the chemical structure of a molecule within a complex mixture is a challenging analytical problem. In the present work, we describe a workflow based on the analytical characterization of complex mixtures using complementary Trapped Ion Mobility Separation and ultra-high resolution FT-ICR mass separation (TIMS-FT-ICR MS/MS) for the analysis of complex mixtures (e.g., crude oils and dissolved organic matter). In particular, we take advantage of the high mobility resolution and high mass accuracy of TIMS-FT-ICR MS/MS to generate candidate structures using a custom developed theoretical workflow for Software Assisted Molecular Elucidation (SAME) based on the ion-neutral collision cross section (CCS), chemical formula and fragmentation pattern. A significant challenge in candidate assignment is that the number of potential structures for a given chemical formula increases exponentially with the number of atoms in the molecule of interest. If unguided, the number of potential structures can quickly escalate and becomes computationally impossible. In this work, several strategies are discussed to minimize the computational time and to generate a database for targeted molecular structure assignment.