



## High Mass Accuracy Filtering For Improved Spectral Matching Of High-Resolution Gas Chromatography-Mass Spectrometry Data Against Unit-Resolution Reference Databases

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### The Invention

The invention provides methods, systems and algorithms for identifying high-resolution mass spectra. In some embodiments, an analyte is ionized and analyzed using high-resolution mass spectrometry (MS) at high mass accuracy (such as  $\leq 75$  ppm or  $\leq 30$  ppm) and the obtained mass spectra are matched with one or more prospective candidate molecules or chemical formulas. The invention provide, for example, methods and systems wherein the possible fragments that can be generated from the candidate molecules or chemical formulas are determined as well as the masses of each of these fragments. The invention provide, for example, methods and systems wherein the high-resolution mass spectra are then compared with the calculated fragment masses for each of the candidate molecules or chemical formula, and the portion of the high-resolution mass spectra that corresponds or can be explained by the calculated fragment masses is determined.

### Additional Information

#### For More Information About the Inventors

- [Joshua Coon](#)

#### Tech Fields

- [Analytical Instrumentation, Methods & Materials : Mass spectrometry.](#)

For current licensing status, please contact Jennifer Gottwald at [jennifer@warf.org](mailto:jennifer@warf.org) or 608-960-9854