Nontargeted Screening with SCIEX OS Software and ChemSpider

Situation: What To Do When An Unknown Peak Provides No MS/MS Library Matches?

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What: To identify unknown compounds in a complex sample, a typical workflow might start with performing a Suspect Screening to search against a spectral library or database of characterized compounds. When the screen fails to provide a candidate ID, additional processing features and functionality can be employed to determine potential candidate formulae and structures, even beyond the scope of the suspect library.

How: Processing X500R QTOF System data using SCIEX OS Software utilizes using the experimentally determined high-resolution and accurate mass of the detected peak and the FormulaFinder feature to generate candidate empirical formulae for that peak. Candidate formula coupled with MS/MS spectra and the simple interface with the extensive ChemSpider database are used to evaluate candidate structures by matching in silico fragmentation pattern prediction of candidate structures.

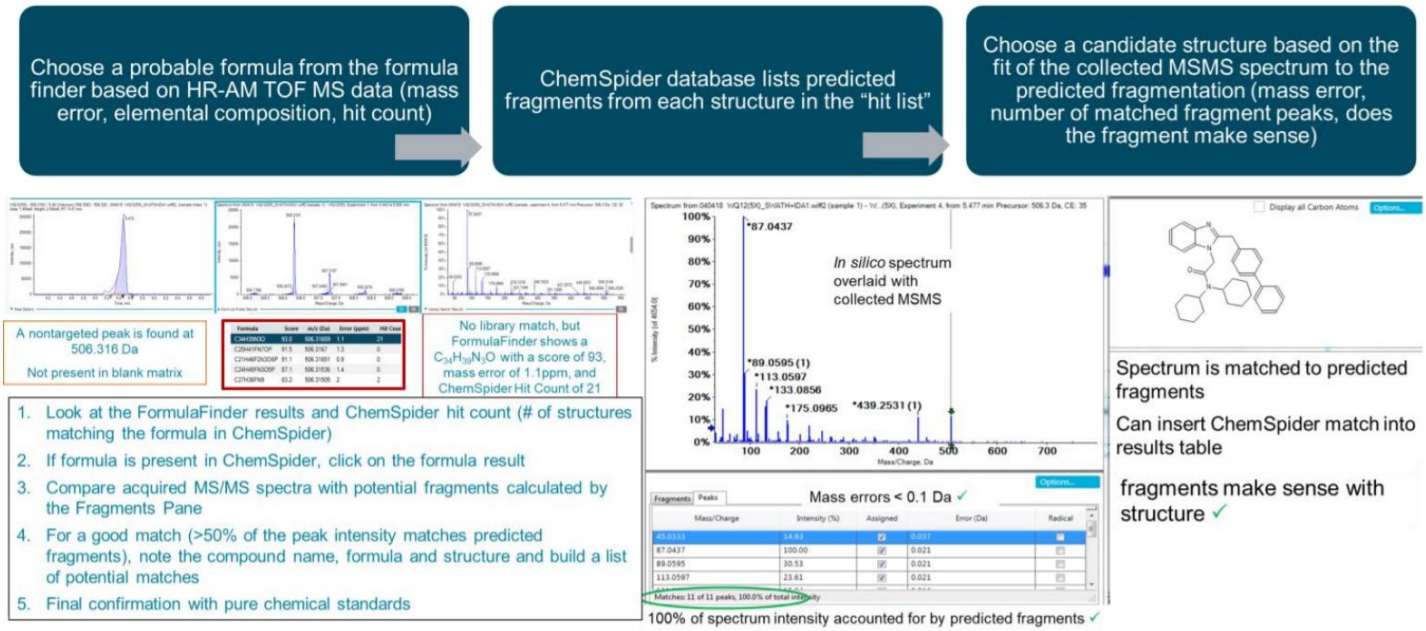

Figure 1. Functionality in Analytics module links ChemSpider Database to FormulaFinder and experimentally derived MS/MS spectral data. An unknown peak which does not have a library match, can still result in a FormulaFinder formula match with low mass error and ChemSpider hit count. ChemSpider can generate candidate structures for each formula with a matching of MS/MS spectra to predicted fragment ions.

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