## **Technology**



## Nontargeted Screening with SCIEX OS and ChemSpider

Situation: What to do when an unknown peak provides no MSMS Library matches?

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<u>What:</u> 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 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 formulae coupled with MSMS 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.

Choose a candidate structure based on the Choose a probable formula from the formula fit of the collected MSMS spectrum to the ChemSpider database lists predicted finder based on HR-AM TOF MS data (mass predicted fragmentation (mass error, fragments from each structure in the "hit list" error, elemental composition, hit count) number of matched fragment peaks, does the fragment make sense) 909 In silico spectrum overlaid with 70% collected MSMS 60% 50% 409 C24H20N2O with a score of 93 89.0595 (1) Spectrum is matched to predicted 30% \*133.0856 emSpider Hit Count of 21 fragments 20% \*439.2531(1) 1. Look at the FormulaFinder results and ChemSpider hit count (# of structures Can insert ChemSpider match into matching the formula in ChemSpider) results table 2. If formula is present in ChemSpider, click on the formula result Compare acquired MS/MS spectra with potential fragments calculated by 3. fragments make sense with Mass errors < 0.1 Da the Fragments Pane structure v For a good match (>50% of the peak intensity matches predicted fragments), note the compound name, formula and structure and build a list of potential matches Final confirmation with pure chemical standards 100% of spectrum intensity accounted for by predicted fragments v

Figure 1. Functionality in Analytics module links ChemSpider database to FormulaFinder and experimentally derived MSMS 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 MSMS spectra to predicted fragment ions.

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