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Waters METLIN MS/MS Library for Progenesis QI Software

Confidently identify metabolites in complex samples with the original and most comprehensive MS/MS database

STREAMLINE YOUR LIBRARY SEARCH CAPABILITIES

Compound identification is a critical component to any untargeted metabolomics experiment aimed at understanding the global metabolic changes that can occur in a biological system. The confidence level in identification is directly dependent on the quality of the database used.

The Waters® METLIN™ MS/MS Library is now available as a plugin for Progenesis® QI opening up fast, batch searching of metabolomics data against the original and most comprehensive MS/MS metabolite database. The Waters METLIN MS/MS library consists of metabolite MS/MS data specifically generated for Waters QTof instruments in both positive and negative ion data.

METLIN is the largest MS/MS collection of data and is suitable for a wide range of metabolomic studies including health sciences, food research and environmental analysis. It includes molecules ranging from lipids, steroids, plant & bacteria metabolites, small peptides, carbohydrates, exogenous drugs/metabolites, central carbon metabolites and toxicants. Data from over 14,000 metabolites have been collected and another 200,000 molecules have *in silico* MS/MS data.

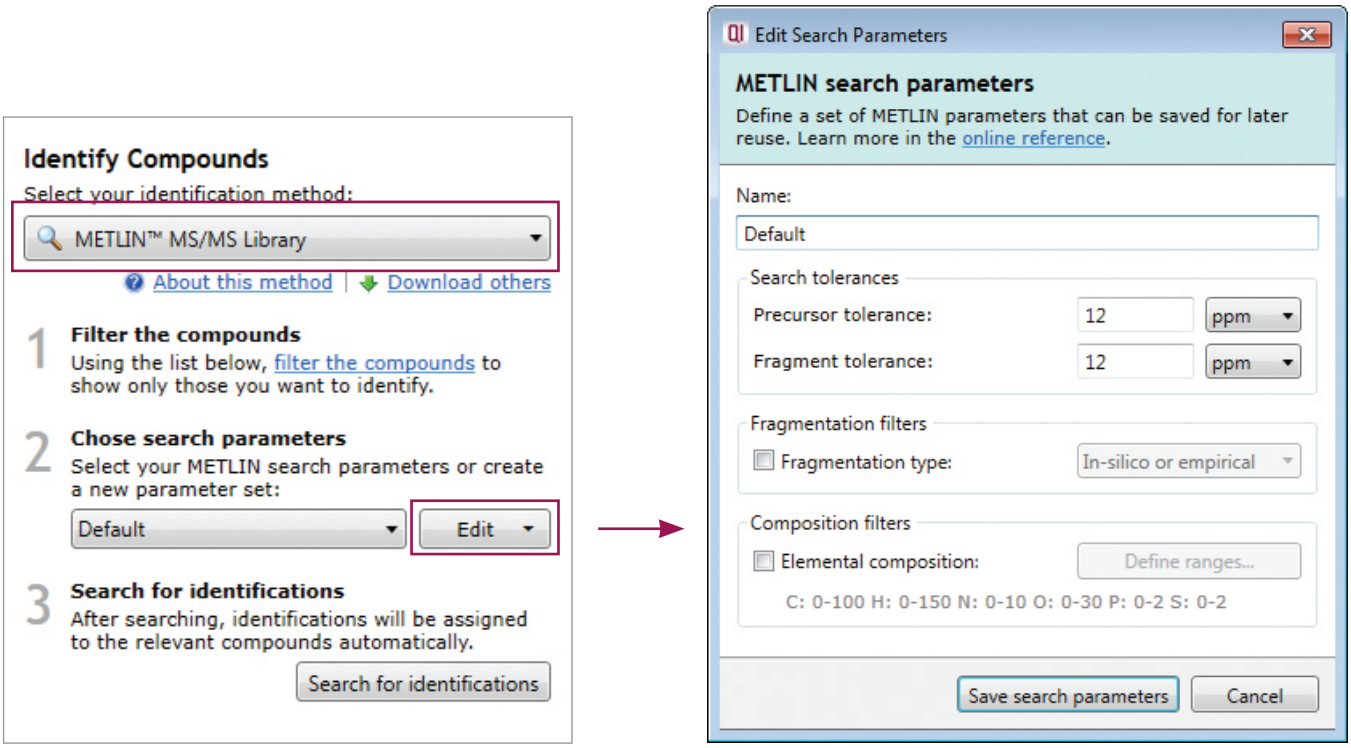

Figure 1. To identify compounds in Progenesis QI, simply select METLIN Library and enter the desired parameters for the search, including precursor and fragment ion tolerances and optional filters for fragmentation type and elemental composition.

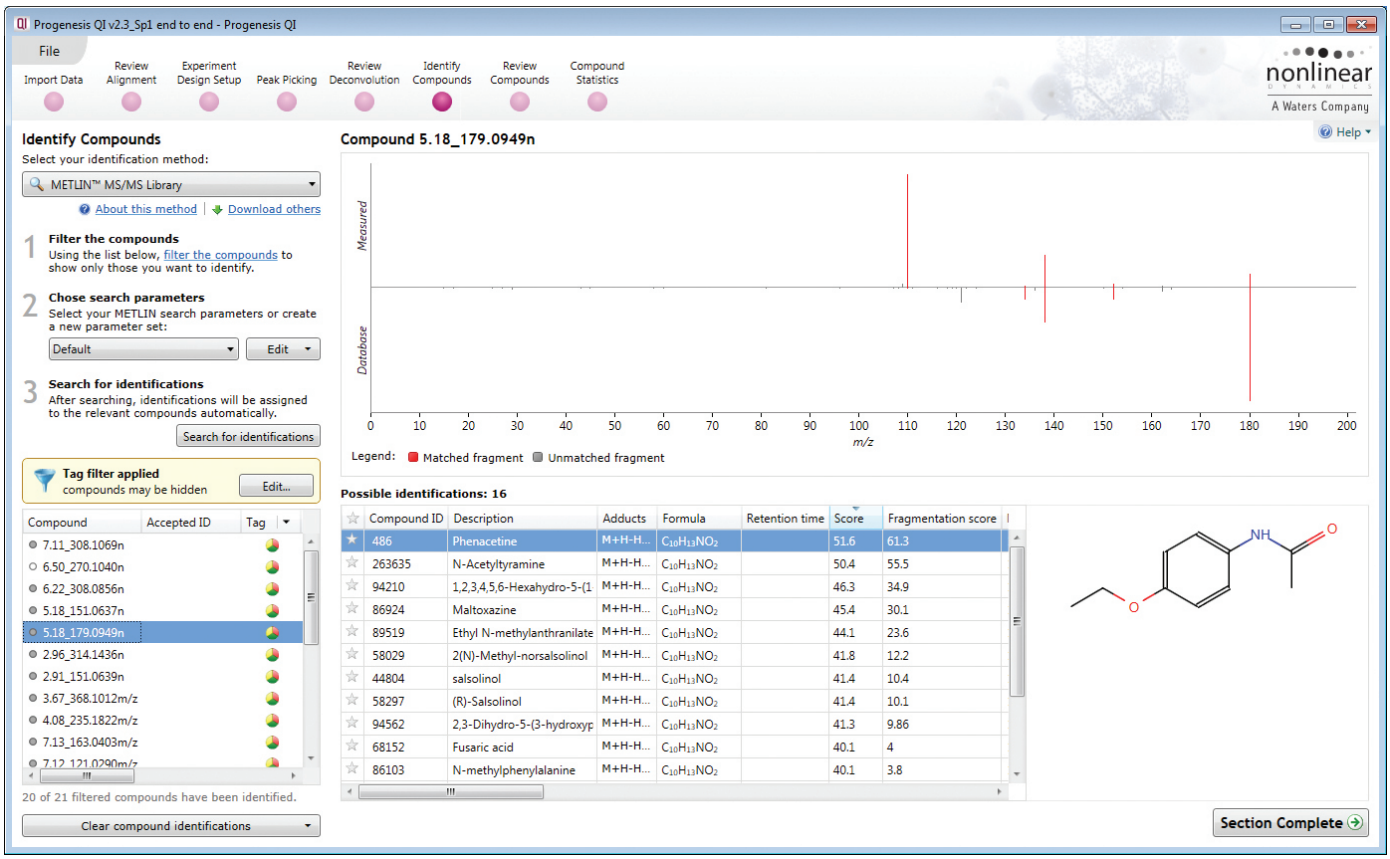

Figure 2. Compound identities returned in Progenesis QI from a human urine sample that was spiked with an analgesic mix. Identified component is phenacetine with a search score of 51.6 with experimentally measured spectra uppermost and database spectra lowermost on the mirror plot.

With the Waters METLIN MS/MS library, metabolomics researchers now have the ability to easily search a comprehensive MS/MS compound library directly from within Progenesis QI, easily identifying more components in their samples with greater confidence. This local copy of the Waters METLIN library is fast to search and is an excellent addition to the wide range of compound databases already available for Progenesis QI.

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