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Database “independent” dereplication

As part of our on-going effort to develop methods for compound identification[1,2], here we present a new approach (under development)[3] for a network based dereplication that starts with MSMS and ends with an NMR-network match for high confidence level. Briefly, the high resolution MSMS data of a given sample, a candidate list of structural formula is submitted to chemical shift simulation (using the nmrshiftdb prediction mechanism).[4] HSQC and HMBC-like data are then simulated accordingly ($^{n}J_{CH}$) ssing the predicted annotated chemical shift; this data is organized into networks and storage. Once the *J*-based heteronuclear 2D NMR experiments (HSQC, HMBC and HSQC-TOCSY) of that same sample are collected, all correlated peaks are filtered and organized as “individual” networks. The similarity among the predicted spectra of the candidate list and the measured spectra of that same sample is taken as an indication of the most likely candidates for its constituents, together with the spectral match to clusters built by the network analysis. We highlight the application of an algorithm combining MS and NMR spectroscopy and a robust $^{n}J_{CH}$ network analysis for a reliable identification routine.

References:

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