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(54) Title: METHOD FOR STRUCTURAL ELUCIDATION OF SMALL MOLECULE COMPONENTS OF A COMPLEX MIXTURE, AND ASSOCIATED APPARATUS AND COMPUTER PROGRAM PRODUCT

(57) Abstract: A method of structurally elucidating small molecule components, comprises determining, per sample, a molecular mass (MM) of a candidate compound (CC) fragment, determining possible molecular formulas (MF) having the fragment MM, and aggregating MS2 spectra for each CC fragment to form a candidate CC MS2 spectrum. Possible MFs and compound structures of an ion in the candidate MS2 spectrum consistent with the possible fragment MFs are determined. Known compounds (KC) similar via MS2 spectrum to the CC, KCs having a compound structure plausibly corresponding to the CC MS2 spectrum, a probability of the MS2 spectrum per fragment having compound substructures, and a combination of known fragment spectra (KFS) forming a compound spectrum statistically similar to the candidate MS2 spectrum of the CC, are determined. The possible MFs and compound structures, KCs, compound substructures, and combination of KFS, are associated with the MS2 spectrum of the CC / fragments thereof.



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