

innovations

from the University of Vermont

TITLE: ERS STANDARD CALCULATION FOR EM-MS

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DESCRIPTION: A major challenge posed in the assessment of risk at remediation sites and when detecting explosives is the ability to detect, quantify and determine the structure of compounds and their metabolites. Precise structural identification of chemicals is crucial, because chemical structure dictates biological, toxicological, and explosive activity. Moreover, accurate quantification is important to assess hazard and estimate risk. The coupling of electron monochromators to mass spectrometers (EM-MS) provides a potentially powerful tool for such molecular identification. EM-MS expands the sensitivity of traditional MS through the inclusion of a new dimension in the space of molecular characteristics – the electron resonance energy (ER) spectrum. However, before this technique can fulfill its full potential a library of ER spectra standards must be obtained in order to associate a spectrum with the molecule or class of molecules from which it arose, a likely cost-prohibitive venture. This invention provides a method to obtain these standards and enabling EM-MS by supplementing direct measurement with chemical inference and quantum scattering.

ADVANTAGES: Creation of a library of ER spectra for all molecules of potential interest is cost-prohibitive due to the large number of standards needed. The direct calculation method provided here offers a reduced cost method to obtain these spectra as needed and to quickly enable this important and powerful tool.

PATENT STATUS: Patent pending

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