

Publication

A new processing scheme for ultra-high resolution direct infusion mass spectrometry data

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High resolution, high accuracy mass spectrometry is widely used to characterise environmental or biological samples with highly complex composition enabling the identification of chemical composition of often unknown compounds. Despite instrumental advancements, the accurate molecular assignment of compounds acquired in high resolution mass spectra remains time consuming and requires automated algorithms, especially for samples covering a wide mass range and large numbers of compounds. A new processing scheme is introduced implementing filtering methods based on element assignment, instrumental error, and blank subtraction. Optional post-processing incorporates common ion selection across replicate measurements and shoulder ion removal. The scheme allows both positive and negative direct infusion electrospray ionisation (ESI) and atmospheric pressure photoionisation (APPI) acquisition with the same programs. An example application to atmospheric organic aerosol samples using an Orbitrap mass spectrometer is reported for both ionisation techniques resulting in final spectra with 0.8% and 8.4% of the peaks retained from the raw spectra for APPI positive and ESI negative acquisition, respectively.

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