Further Reading

STATE OF THE ART: ESI–MS FINGERPRINTING IN COMBINATION WITH PCA

The Approach Analyzing large amounts of smaller molecules in oils can be achieved using an -omics style fingerprint detection approach. This is done by capturing a picture of all components (or as many as possible) in a single fast analysis. This can be performed using different techniques. Here, electrospray ionisation – mass spectrometry (ESI-MS), which is selective to polar species, is used. This soft ionisation technique ideally creates one single molecular ion peak per compound without fragmentation. Combining these both complex and complex datasets  the statistical data analysis, e.g. principal component analysis (PCA) which compresses the data amount based on maximal contained variation, aids in isolating and tracking the impact of components with strongest variation. This information can further be related to critical parameters in optimising approaches.

The Sample Set & Experimental Positive ESI-MS analysis of a set of crude bio-oils derived from lignin rich residue fractions was performed on Agilent 1100 Series LC/MSD. Samples were diluted in DCM and transferred from the autosampler directly to the analyser via PEEK tubing. Ca. 10 scans per analyte peak were averaged and the samples replicated five times. Total analysis time including rinsing per sample < 1 min.

The resulting spectra are seen to be dominated by series of signals with 14 Da spacings (Fig 1). These are indications of –CH₂– chain additions to the base structure of compound classes. In addition, 2 Da spacings indicate the loss of H₂, from a single to yield a double bond.

Novel: 14 Da Spaced Predefined Vectors
To isolate single series and visualise their variance between samples, new 14 Da Spaced vectors were created. 14 Da spaced pulse trains of gaussian peaks were run through the aligned spectra, extracting several 14 Da Spaced signal series. Extracted total abundance values of different series in single samples were then used as new orthogonal basis vectors to describe the system. The series can be ranked by total abundance or largest variance amongst samples. Score plots were created, analogue to those from PCA. The new basis vectors now describe single series and their immediate effect on sample clustering, enabling easier interpretation of the clustering properties.

RESULTS

The method provides fingerprinting and clustering performance similar to that of PCA. Series of signals correlate with compound classes and their singular impact can be directly evaluated.

The method can be used for any regular spaced interval which is believed to have significant impact on the samples based on the two 14 Da candidate vectors now described, analogue to those from PCA. The new basis vectors are created, as described above. The method heavily relies on the ability to distinguish between different classes and, to visualise their variation to assess e.g. catalysis performance.

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