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## SINTEF Ocean AS


Senior Research Scientist Lisbet Sørensen has a PhD in analytical chemistry, and > 10 years of research experience in developing and applying a combination of high-resolution separation and mass spectrometry with high throughput data algorithms to characterize complex chemical mixtures and correlate to their properties.

# Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICRMS)

## Method description in brief.

The sample is typically introduced directly in the mass spectrometer (without prior instrumental separation) from a solvent extract or, where appropriate, from a solid sample deposit. Several ion sources can be applied. Atmospheric pressure photoionization (APPI) in combination with electrospray (ESI) are the most applied for petroleum analysis. Atmospheric pressure chemical ionization (APCI), laser desorption and field desorption have also been investigated. After ionization, the mass-to-charge ratio of produced ions is measured in the ICR ion trap as a function of their frequency of cyclotron rotation in the high magnetic field.

## Applicability of method.

Depending on the selected ionization technique, FT-ICRMS is in theory applicable to all or most organic compound classes, and a wide range of compound masses/carbon number. The different ionization techniques may, however, favour detection of certain functional groups. The mass resolution (>100,000) allows accurate mass determination and elemental composition identification.

## Sample preparation required.

Sample preparation may be as easy as dissolution in appropriate solvent. Measures (like fractionation) to simplify matrix may be applied and has been and is currently investigated.

## Method strengths.

The key strength of this method is the resolution power and ability to identify a wide range of compounds and classify them by elemental composition. As such, it lends itself to characterization of very complex samples – and to compare variation in composition of such samples. It also does not rely on compounds being both amenable to and stabile throughout an online chemical separation, overcoming challenges observed in e.g., gas chromatography-based techniques, allowing detection of larger and more polar chemicals.

## Estimated time for analysis.

Depends on selected sample pre-treatment strategies. In an ideal situation and without time-consuming pre-treatment, sample analysis and data treatment can be accomplished in 1-2 days.

## Method weaknesses.

The main weaknesses of the analytical method(s) lie in matrix dependency and ion suppression, challenging the extent of potential for cross-sample comparisons. Quantification of identified compounds is questionable due to the large number and differences in properties of compounds potentially identified. No direct information on chemical structure.

## Result interpretation / visualisation / presentation.

Raw data (detected masses) is transformed into chemical elemental composition based on accurate mass predictions. Depending on the question at hand, various multi-dimensional visual data representations are commonly applied. Classification by carbon number, double-bond equivalents, H/C-, O/C-ratios may be used for binning masses in two dimensions and the summed intensity/abundance applied in the second dimension.