

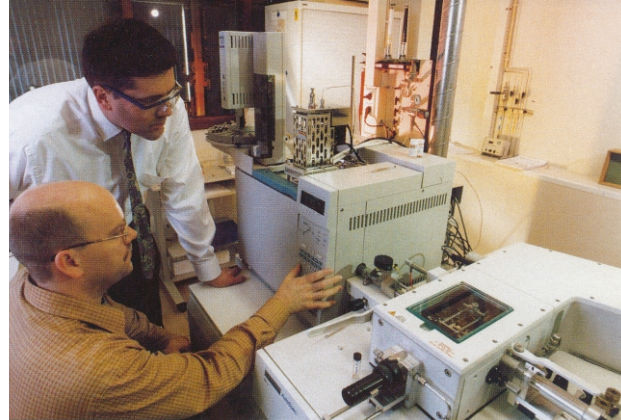
## Identification of unknown substances using mass spectrometry

### Application note Resolve 03-06

The identification of unknown substances is a common analytical problem. Examples are the establishment of the structure of main and side products of new synthesis routes, the identification of the structure of purified products, the identification of unknown peaks in chromatograms, the analysis of competitor's products and material characterization studies.

One of the techniques that have been successfully used in structure identification is mass spectrometry (MS). This technique, often used in combination with other techniques, can analyze pure substances as well as components in mixtures in concentrations ranging from percentages to ppb's. Polar, non-polar, ionogenic, volatile and nonvolatile components with molecular masses ranging from 2 to 100,000 can be identified

There are plenty of examples of successful MS applications at DSM Research. Coupling of MS with chromatographic techniques, for example, helps to identify unknown peaks in chromatograms,



especially when we use the extensive spectrum libraries we have compiled over many years. Furthermore, the use of flow injection analysis followed by MS helps verify molar masses of synthetic products and impurities. Probe-MS and tandem MS give additional structure information where bench-top GC-MS does not suffice. Thermally unstable components (biomolecules, pharmaceutical products and complicated hydrocarbon mixtures) can be identified using 'soft ionization' techniques such as chemical ionization and field desorption. Finally, selective MS-techniques, for example GC-GC-chemical ionization tandem mass spectrometry and LC-MS, can be used to quantify trace components at sub ppm or ppb level in difficult matrices.

To involve our experts in your research programs or to obtain additional information on mass spectrometry please contact us.

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