



## RESEARCH AREAS

## NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY

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### FRAUNHOFER IME APPLIED ECOLOGY DIVISION

The overall aim of the Applied Ecology Division is to investigate and assess the risks presented by synthetic chemicals and natural substances towards ecosystems, and towards humans via contaminated food, feed and consumer products.

#### Our current topics and business areas are:

- Chemical and Product Safety
- Fate and Effect of Agrochemicals
- Uptake and Metabolism of Agrochemicals
- Food and Feed Safety
- Environmental Monitoring
- Soil and Water Protection



# YOUR PARTNER FOR THE STRUCTURAL ANALYSIS OF ORGANIC SUBSTANCES, ALSO FROM COMPLEX MATRICES

## BACKGROUND

All organic compounds undergo transformation and degradation processes that generate new substances with completely different properties. This also applies to anthropogenic organic chemicals.

Before plant protection products can be registered, it is therefore necessary to understand how they are metabolized in plants and animals, and how they are degraded in different environmental matrices, to ensure that no persistent or toxic degradation products are formed.

Complex studies are required to produce the necessary data, involving comprehensive and highly-specific chemical analysis procedures.

The Fraunhofer IME has many years of experience in this area, and carries out comprehensive tests to determine the fate of substances metabolized by plants and animals and degraded in the environment. To keep pace with the state-of-the-art testing methods required by the regulatory authorities, the Fraunhofer IME invests in novel analytical methods and continuously expands its spectrum of research, development and services.



## INCREASING DEMANDS FOR ENVIRONMENTAL ANALYSIS

Regulatory approval procedures for the environmental analysis of organic compounds are challenging because highly-sensitive analytical methods are needed to detect and identify the minute quantities of transformation products generated by metabolism and environmental degradation.

## NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY AT THE FRAUNHOFER IME

Nuclear magnetic resonance (NMR) spectroscopy is the most efficient analytical method for determining the structure of organic substances. The Fraunhofer IME offers a 700 MHz NMR spectrometer equipped with a 1.7 mm cryoprobe, which is ideal for the high-resolution analysis of small substance quantities (up 10 µg). The NMR suite is supported by a high-resolution Orbitrap™ Hybrid FT mass spectrometer that can determine the chemical formulae of unknown substances to complement the structural data. A LC-SPE unit is used to isolate and concentrate samples, e.g. from environmental simulation experiments.

*Figure: Our LC-SPE system*



Our NMR suite brings together Fraunhofer IME's expertise in testing the environmental behavior of plant protection products, biocides, pharmaceuticals and industrial chemical products with the additional capability of identifying unknown organic substances.

All the analytical methods we offer are compatible with radio-labelling (<sup>14</sup>C) allowing the clear identification of unknown transformation products. This is the standard approach to determine the environmental fate of organic substances and to identify metabolic products in plants and animals. This means that all investigations, such as studies required for pesticide registration, can be carried out in one test facility without loss of time or information. We also offer structural determination by NMR spectroscopy as a direct and independent service.

All substance identification studies are carried out according to good laboratory practice (GLP). Compliance with GLP is monitored by our in-house quality assurance unit and regular external audits.

*Figure: Our NMR cryoprobe*