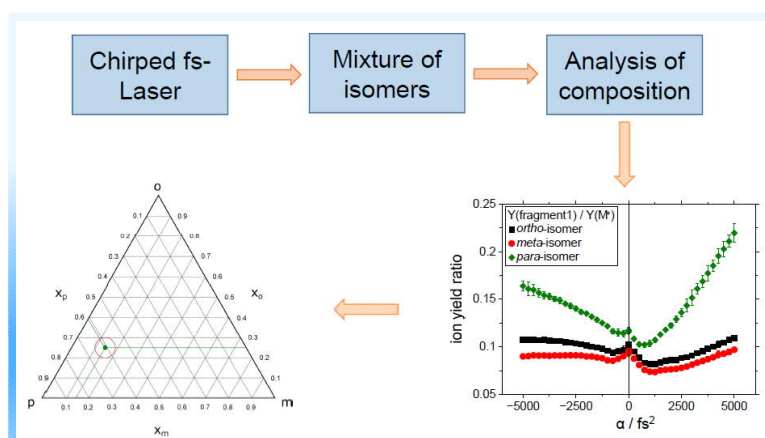


Mass spectrometric data analysis allowing quantitative determination of structural isomers within Mixtures of Compounds

Mass spectrometry, fs-LIMS, data analysis, data acquisition, quantitative analysis of mixtures of structural isomers

DESCRIPTION OF TECHNOLOGY

Quantitative mass spectrometry is one of the most powerful tools for chemical analysis in many areas, e.g. science, environmental analysis, in-line process analysis, forensic investigations etc. Often it is important to discern between structural isomers of a certain compound within a mixture of compounds. Usually then it is necessary to perform a separation of the substances / isomers forming the mixture, e. g. via chromatography, before analysing the separated substances / isomers via mass spectrometry.



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The new analytical method presented herein allows the qualitative and quantitative analysis of structurally isomeric compounds of a mixture by mass spectrometry without the need of separating the constituents of the mixture beforehand.

This is achieved by an advanced way of data acquisition and data analysis where the intricate differences within the mass spectra of structural isomers are analysed in time. This multidimensional approach makes use of ultra-short laser pulses, which are being modulated in their spectral phase $\varphi(\omega)$, thus leading to a multitude of information being contained in the signals of every acquired mass spectrum. These „hidden informations“ are then subsequently evaluated by means of data mining within the mass spectra.

AT A GLANCE ...

Application Fields

- Mass spectrometry
- Environmental analysis
- Process analysis in chemical industry

Business

- Manufacturers of mass spectrometers
- Manufacturers of equipment for mass spectrometry

USP

- Reduction of need for sample preparation/ chemical separation
- Direct quantitative distinction of structural isomers

Development Status

- Laboratory setup available for exemplarily testing

Patent Status

Priority application filed on 05.03.2020 at the European Patent Office.

APPLICATION FIELDS

The current technology offer enhances the analytical possibilities provided by mass spectroscopy and at the same time reduces the need for sample preparation to a great extent. It may therefore be applied in nearly all fields of chemical analytics where mass spectrometry is applied.

ADVANTAGES OVER THE PRIOR ART

The technology simplifies, resp. even eliminates sample preparation / chemical separation for mass spectroscopic analysis and by doing so saves time and cost of chemical analysis.

STATE OF THE PRODUCT DEVELOPMENT

A laboratory set-up for performing sample analyses is existing at the Philipps-Universität Marburg.

MARKET POTENTIAL

Taken TOF LC MS as an exemplary sub-segment of the whole mass spectrometer market (estimated revenue by Frost&Sullivan to be about 4 billion US-\$ in 2020), the global market for the technology presented herein may be guessed to be about 740 million US-\$ in 2020.

COOPERATION OPPORTUNITIES

On behalf of its shareholder Philipps-Universität Marburg TransMIT GmbH is looking for licensees or cooperation partners for further development in the US, Far East or Europe.

A TECHNOLOGY OF



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SYSTEM PARTNER FOR INNOVATION

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