Name Thomas Küttler

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Short Bio

Born in 1992, M.Sc. in 2015, Dr. in 2019 in organic chemistry, joined SGS the same year. As Chemical Scientist I analyse Gasoline, Diesel, and fuels, mainly focused on additives.

Method Name Derivatisation and QTOF-Screening

Method description in brief.

By derivatisation polar groups are introduced to the molecules. This resulting mixture is separated by HPLC and ionized by ESI, utilizing the polar groups. This circumvents the problem caused by a high boiling point. Detection by QTOF-MS provides much information in on run.
The compounds will be separated by their polarity, depending on the attached groups and functional groups.

Applicability of method.

Molecular weights of up to 2000 should be in principle detectable. This method was designed for hydrocarbons. Aromatic compounds can either react very well or hardly, resulting in potential misses. Double bonds may cause an issue.

Quantification can be achieved by comparison to samples of known composition that were derivatised the same way. Responses of similar compounds should be comparable.

Sample preparation required.

Derivation agents need to be added and the sample heated. The resulting mixture is diluted and analysed.

Method strengths.

The high boiling point problem is solved. Different isomers will react to derivatisation differently, allowing for a differentiation.

Estimated time for analysis.

Depending on the complexity of the samples and therefore the complexity of the data processing the analysis should be done in one week, form sample arrival to the finished report.

Method weaknesses.

Some functional groups may interfere one another. Also, the data processing is more complicated than for other methods.

Result interpretation / visualisation / presentation.

The QTOF-MS is used to obtain the mass of the molecule, the formular and the fragments. These come in peaks, which in turn have an integral, that can be used for integration.
As of now, the interpretation is manually done.

Relevant Papers

There are no papers published on this topic yet.