



Quantitative Analysis of different monoterpene isomers using Proton Transfer Reaction LIT and triple quadrupole Mass Spectrometry

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Currently, Proton Transfer Reaction Mass Spectrometry (PTR-MS) allows for quantitative analysis of VOCs in real time at low concentrations, but cannot differentiate isomers or isobaric molecules. Here we present first results of a triple quadrupole (TripleQuad) and a linear quadrupole ion trap (LIT) in combination with proton transfer reaction chemical ionization to provide the advantages of identification capability from MS/MS.

The PTR-LIT instrument couples a PTR source to a linear ion trap using helium as a trapping and collision induced dissociation (CID) gas. Protonated volatile organic compounds are accumulated in the trap up to a few seconds. After the filling time, ions are isolated and manipulated using the technique of dipolar excitation. With the PTR-LIT multi MS (MS^n) is possible with almost unit trapping efficiency. Therefore fragment ions can be isolated and fragmented further with almost no loss in sensitivity.

The Varian MS-320 TripleQuad, using a Townsend discharge as a source of H_3O^+ ions, has two quadrupole mass filters connected by a 180° curved collision cell filled with argon as a CID gas. The first quadrupole is used for preselecting the ions. Afterwards, these ions are fragmented in the collision cell. The resulting fragmentation pattern is recorded using the last quadrupole mass filter.

During laboratory comparison of the two instruments seven monoterpenes were ana-

lyzed. It has been shown that both instruments are able to distinguish between different types of structures, i.e. the double ring structure of α -pinene can be distinguished from the linear structure of ocimene. However, a quantitative analysis of mixtures of monoterpenes in ambient air seems not possible at the moment.