CHIMIA **2005**, *59*, No. 9

Highlights of Analytical Chemistry in Switzerland

High-Speed Identification of Designer Drugs by Multiple Mass Spectrometry

Stephan Kölliker and Michael Oehme*

*Correspondence: Prof. Dr. M. Oehme, Organic Analytical Chemistry, University of Basel, Neuhausstr. 31, CH-4057 Basel

Tel.: +41 61 639 23 01, Fax: +41 61 639 23 00, E-Mail: michael.oehme@unibas.ch

Keywords: Amphetamines · Designer drugs · Multiple mass spectrometry · Structure elucidation

Amphetamines and related drugs are rather frequently used at techno parties. Many different derivatives are on the market. The residues R1, R2 and R3 (also di-substituents) can vary greatly. New modifications show up frequently. The relation between structure and the desired psychedelic effect is largely unknown. The range between any effect and toxic properties can be rather small. Experimenting with dose and intake of different products can be fatal. A quick identification of the active component in pills is therefore important. The questions are: Is the compound already known? If not, what is its structure?

Multiple mass spectrometry (MSn) is a rather new technique introduced in 1995. Our group received the first instrument worldwide and has studied its possibilities for structure elucidation since then. Collision-induced dissociation with defined energies allows the cleavage of specific bonds in an ion trap mass spectrometer. In the case of amphetamines *etc.* the following information is obtained:

Mass spectrum (MS): Mass of compound and hetero atoms present

1st fragmentation (MS2): Loss of -N-R1

2nd fragmentation (MS3): Loss of -R2

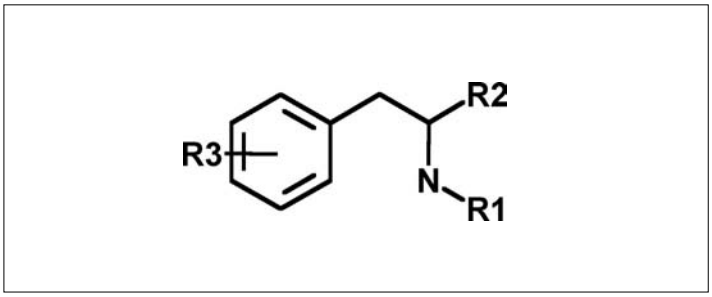
3rd fragmentation (MS4): Number, position and kind of R3 (based on reference spectra unique for ring positions)

This information allows the structure elucidation of a drug in a pill after only dissolution, filtration and a 15 min experiment. By-products can be identified after a pre-separation by high-performance liquid chromatography.

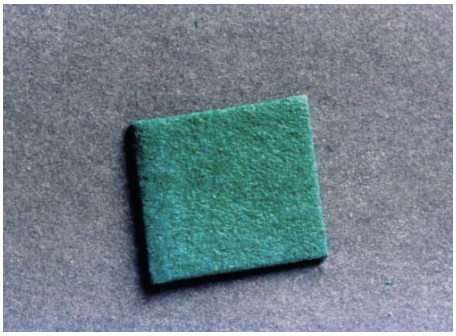
Received: July 6, 2005

Reference

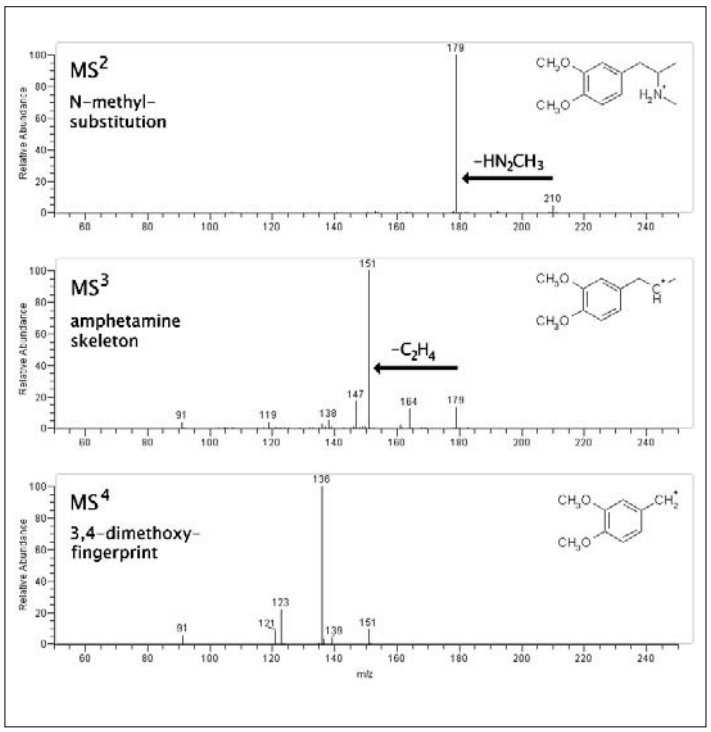
S. Kölliker, M. Oehme, *Anal. Bioanal. Chem.* **2004**, *61*, 215.



Structure of designer drugs with functional groups in various combinations: R1: -NH_2, -$NHCH_3$, -$NHCH_2CH_3$; R2: -H, -CH_3, -CH_2CH_3; R3: -OCH_3, methylenedioxy-, -CH_3, -SCH_3, -Cl, -Br, -I



A designer drug pill



Identification of N-methyl-3,4-dimethoxy-amphetamine as impurity in the pill

Can you show us your analytical highlight?

Please contact: Dr. Veronika R. Meyer, EMPA St.Gallen, Lerchenfeldstrasse 5, 9014 St.Gallen

Phone: 071 274 77 87, Fax: 071 274 77 88, Mail to: veronika.meyer@empa.ch