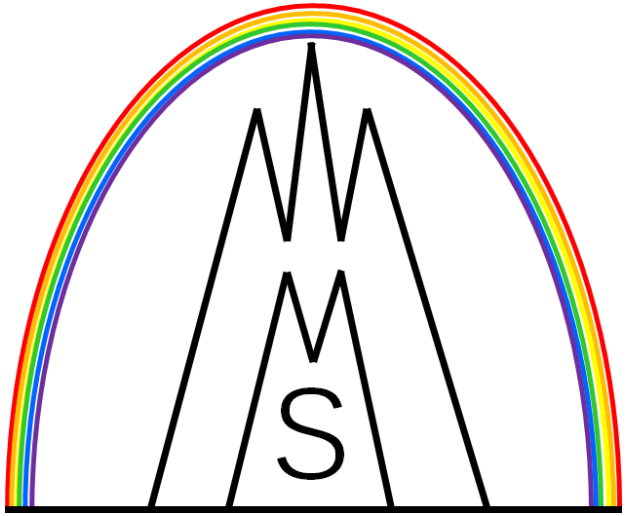
ÚOCHB AV ČR
IOCB PRAGUE

Research - Service Group Mass Spectrometry:



5th Short Mass Spectrometry Courses

IOCB Prague, March 31 – April 1, 2016

Why MS courses?

Information for our colleagues – the MS service users

- services provided by the MS group
- organization of the service work
- basics of data interpretation

Demonstration of MS instruments

User training for open-access GC/MS

Discussion, user feedback

Agenda

Thursday, March 31

Opening & Mass spectrometry basics (IOCB Club)

9:00 - 9:30	MS group: research and services (J. Cvačka)
9:30 - 9:50	What is mass spectrometry? (M. Hubálek)
9:50 – 10:20	Ionization and ion sources (V. Vrkoslav)
	break & refreshment
10:50 – 11:20	Ion analyzers (V. Vrkoslav)

Services of the MS group (IOCB Club)

11:20 - 11:50	Small molecules (M. Svoboda)
11:50 - 12:20	Biomolecules (M. Hubálek)

Guided tour & demonstration of the instruments (lab. A.1.80 and A.1.83)

13:30 - 16:30	Orbitrap – High resolution and tandem MS (A.1.83; J. Cvačka)
	MALDI – Large and small molecules (A.1.80; V. Vrkoslav)

Agenda

Friday, April 1

Acquiring & interpreting MS data (IOCB Club)

9:00 – 10:20	Understanding mass spectra of small molecules (J. Cvačka)
	break & refreshment
10:50 – 12:10	Experimental strategies in proteomics (J. Březinová/M. Hubálek)

Guided tour & demonstration of the instruments; Open-access GC/MS training (lab. A.1.83 & A.1.88A)

14:00 - 16:30	Proteomics data interpretation (A.1.83; M. Hubálek)
	Training for open-access GC/MS (A.1.88A; V. Vrkoslav)

Mass Spectrometry Group

PhD (4) and MSc (2) students

RESEARCH **SERVICES**

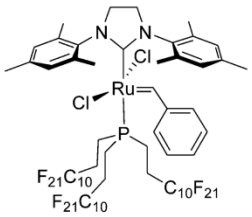
Phone contacts:
303: group leader
508: small molecule services
117: biomolecule services
347: open-access instruments

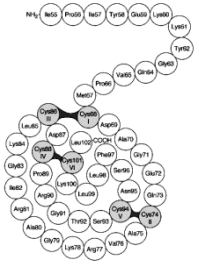
Our location: A, 1st floor, SE wing

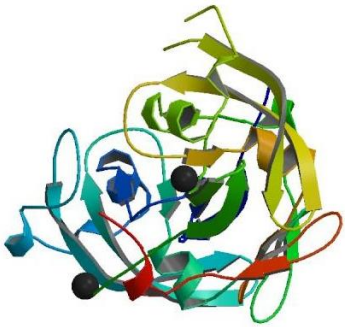
http://www.uochb.cz/web/structure/200.html

Research - collaborative

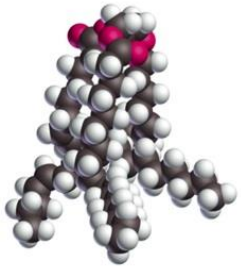
- Structure elucidation of natural products (small molecules)
- Structure elucidation of synthetic compounds
- Structure elucidation of peptides
- Identification and quantification of proteins







Research – group projects



<u>New</u> analytical methods for lipids and related molecules

- Chromatography for separation of complex mixtures
- Mass spectrometry for structure elucidation
- MALDI imaging applications

Technical development of MS instrumentation

- Development and applications of DAPPI & DESI
- Miniaturization of APCI and APPI sources
- Combining electrochemistry and ESI-MS

I. Lipids of vernix caseosa

Vernix caseosa
Waxy or cheese-like white substance found coating the skin of newborn human babies

Composition:

shed epithelium cells and lipid secretions of sebaceous glands
water, proteins & peptides, lipids

Function:

protection from amniotic fluid maceration; minimizes friction in delivery

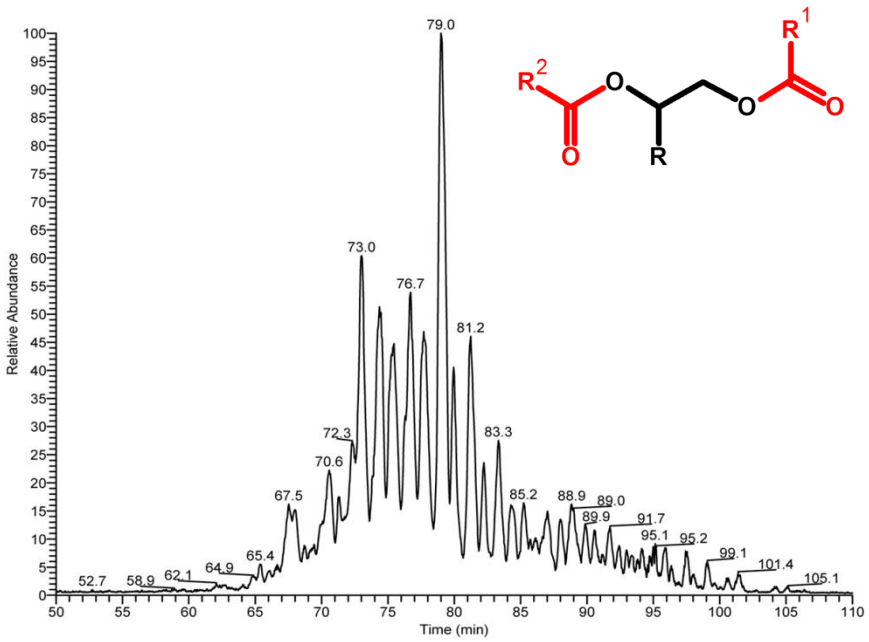
Properties:

wound healing, antimicrobial, antioxidation, moisturizing

Artificial vernix attractive for medicine: *serious skin burn healing, venous ulcers healing, treatment for premature babies etc.*

I. Lipids of vernix caseosa

1,2-Diol Diesters



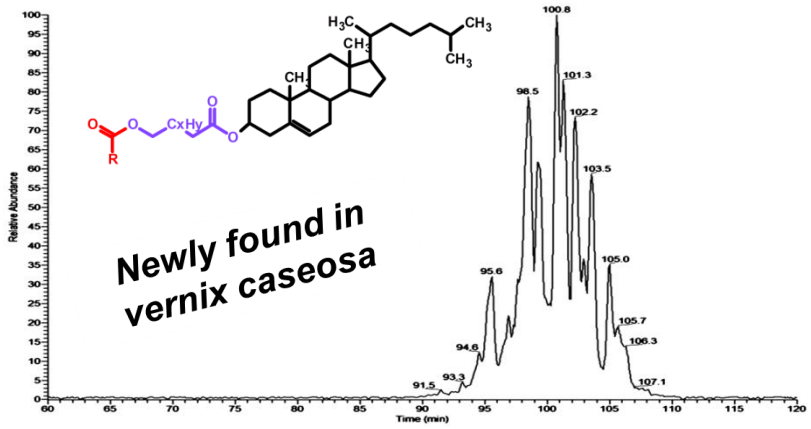
> 2200 molecular species detected

48 - 65 carbons

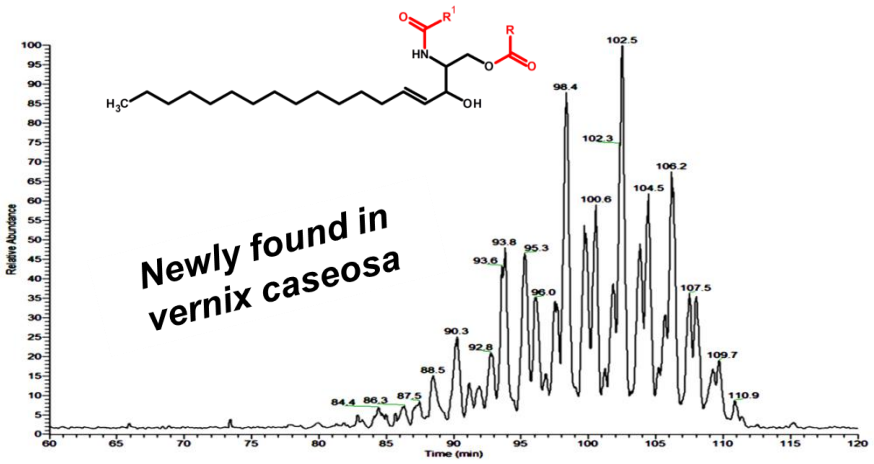
0 - 3 double bonds (mostly n-7)

72 diols, 62 fatty acyls

Cholesteryl OHFA Diesters

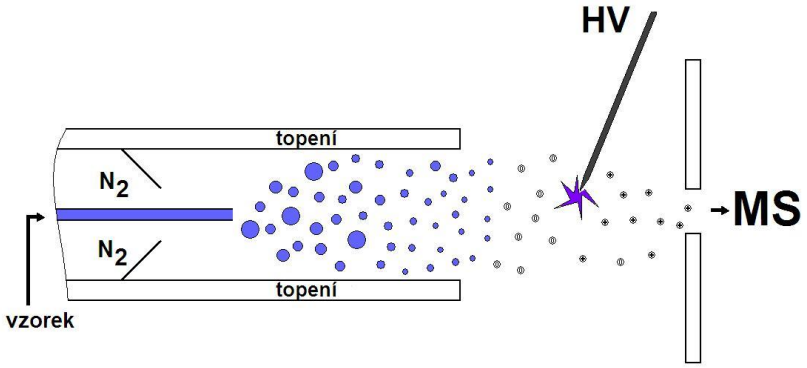


O-Acyl Ceramides



II. Localization of double bonds

Ion source for APCI



GAS-PHASE CHEMICAL REACTIONS OF ACETONITRILE IN THE APCI SOURCE

1/ formation of a reactive specie

$H_2C{=}C{=}N^{+\bullet}{-}CH_3$

2/ reaction of the reactive specie with double bond(s); formation of $[M+55]^{+\bullet}$

$[M + C_3H_5N]^{+\bullet}$

Localization of double bonds in the aliphatic chains:

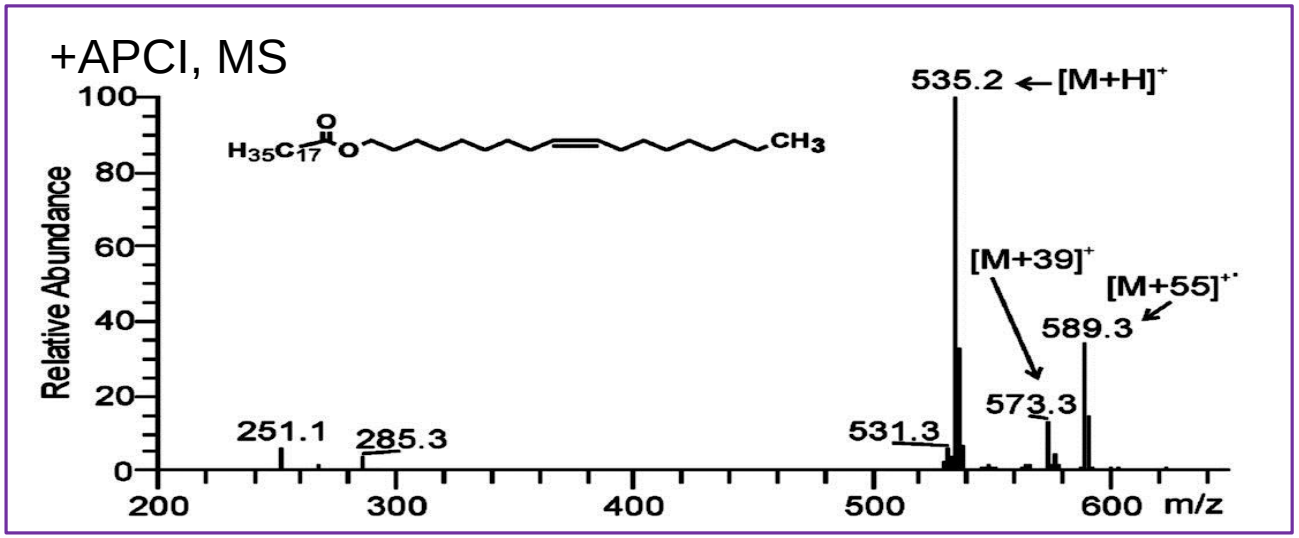
MS/MS (CID) of the $[M + 55]^{+\bullet}$; fragmentation of the C=C bond

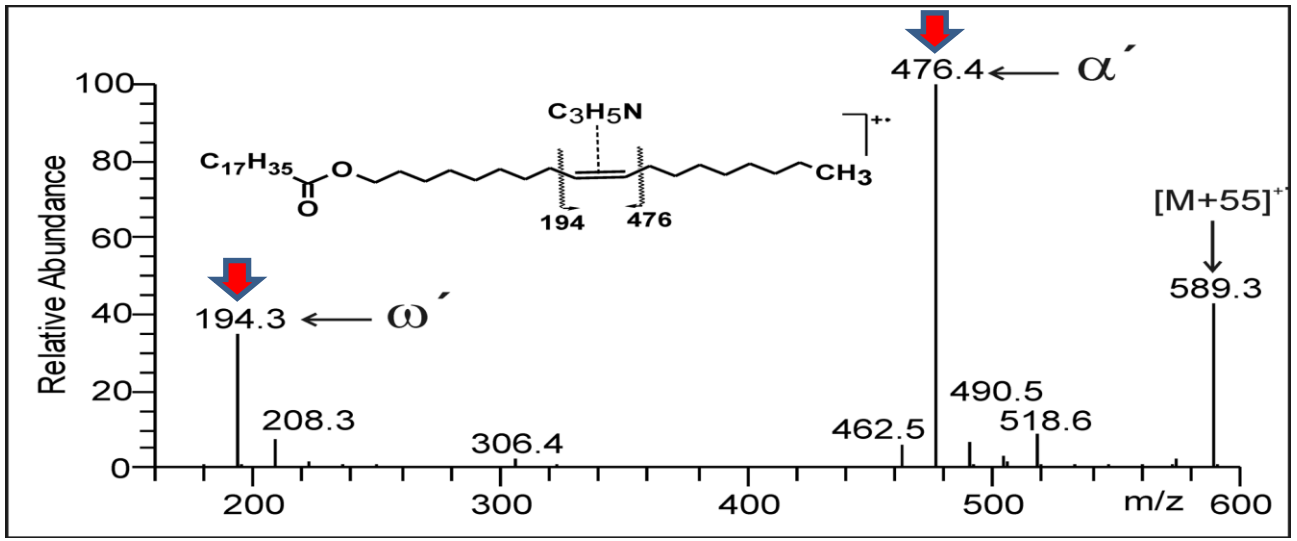
II. Localization of double bonds

Full-scan APCI MS spectrum

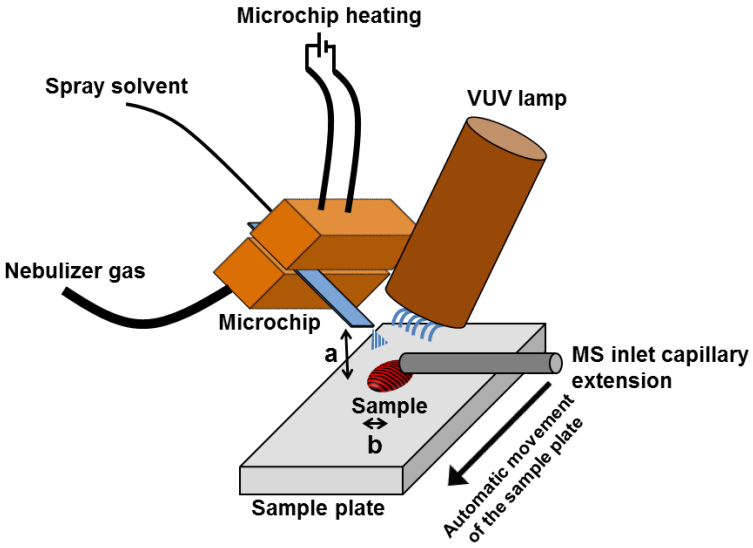
CID

MS/MS spectrum



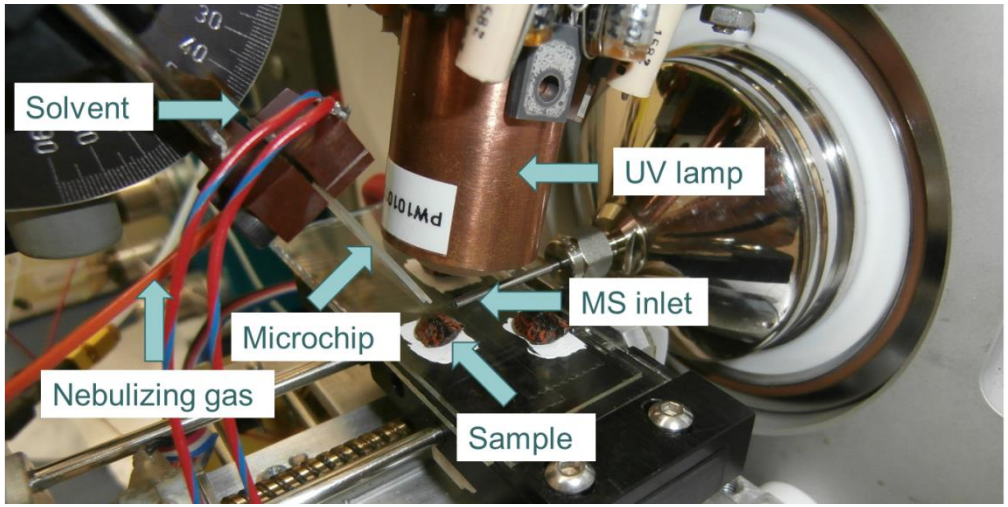


III. DAPPI-MS



UNIVERSITY OF HELSINKI

IOCB DEVELOPMENT WORKSHOPS

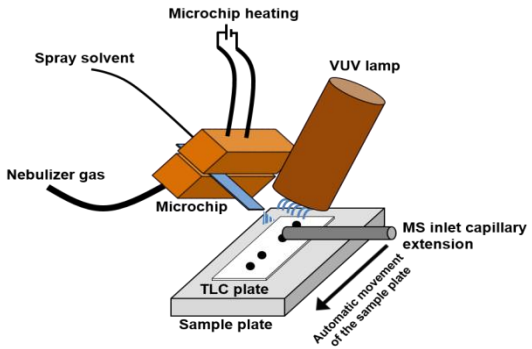


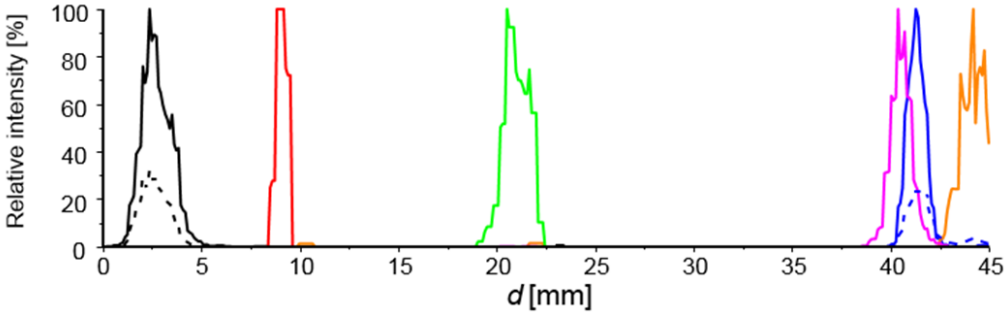
Desorption atmospheric pressure photoionization (DAPPI) is an ambient ionization technique for MS that uses hot solvent vapor for desorption in conjunction with photoionization.

Applications and instrumental development for non-planar objects

III. DAPPI-MS

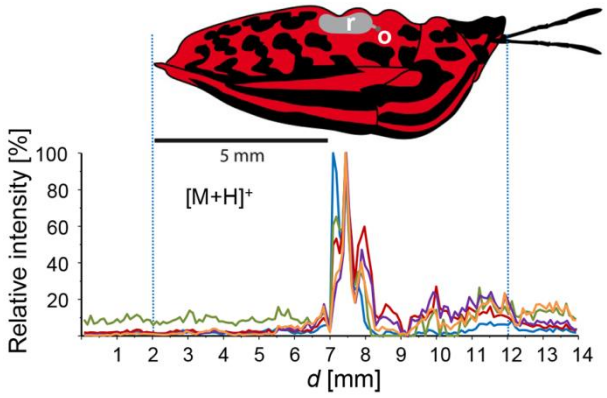
1/ TLC/DAPPI of lipids



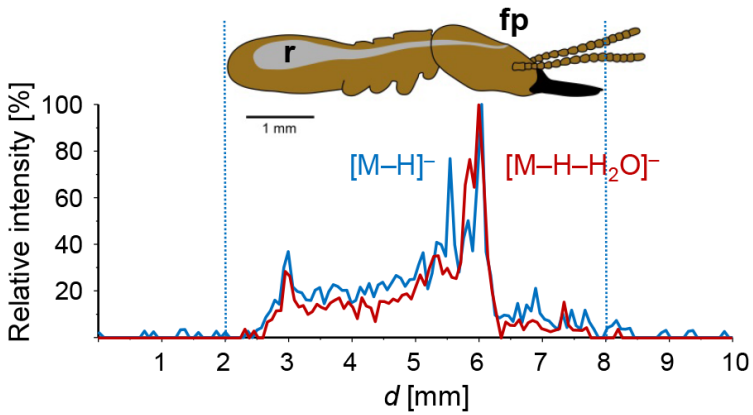


Cholesterol, TG, 1,2-DDE, WE, CholE, squalene.

2/ Spatial distribution of insect defense compounds



Unsaturated aldehydes in stink bug

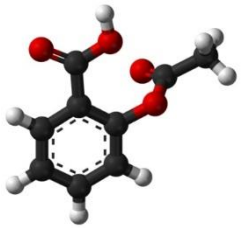


1-Nitropentadecene in termite

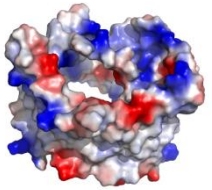
Services

Analysis of Small Molecules

Analysis of Bio-molecules



Open Access Instruments



Services: Small molecules

Routine services:

- Low resolution MS spectra of small molecules
  EI/CI, ESI, APCI, MALDI; (+/-)

- High resolution MS spectra of small molecules
  EI/CI, ESI, APCI, MALDI; (+/-)

On demand services:

- HPLC/MS, GC/MS
- Fragmentation spectra (MS/MS)
- Ion mobility experiments

M. Svoboda
Thu 11:20

Services: Biomolecules

Routine services:

- Determination of molecular weight of biomolecules

  MALDI or ESI-MS analysis

- Identification of proteins

identification using ESI-MS/MS

M.Hubálek
Thu 11:50

On demand services:

- *Protein quantification (label free, SILAC, iTRAQ)*
- *Post-translation modifications*

Services: Open access instrument

The open access instrument:

- **GC/MS** (LR EI, nonpolar column)

  - now accessible in working hours; keys for users will be available after April 10 (7/24)

Room A.1.88a

Authorized users:

IOCB employees and students *trained by the MS staff*

Google Calendar

on-line reservations

Notes and rules:

- the instruments can be reserved

- each measurement must be registered in a logbook

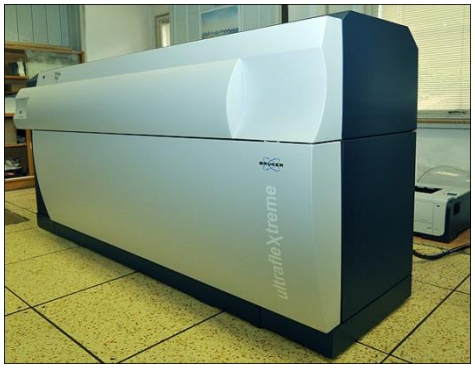
- the users are responsible for damages cased by misuse of the instruments

- priority of the MS staff for routine services, maintenance etc.

Vladimír Vrkoslav (tel. 347)

Mass spectrometers

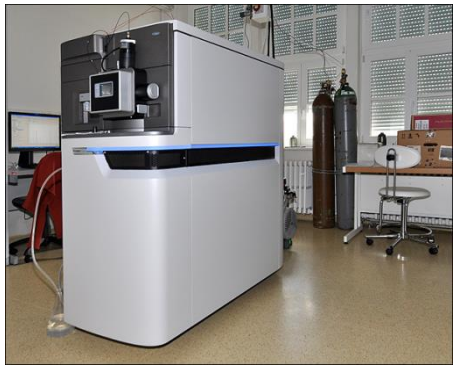
Q-TOF micro (Waters)
Small molecules
(LR); ESI, APCI



UltraflexTreme (Bruker)
Small molecules, biomolecules
(LR, HR); MALDI

LTQ Orbitrap XL (Thermo)
Small molecules, biomolecules
(HR); ESI, APCI, nanoESI

TripleTOF (AB Sciex)
Biomolecules
(HR); nanoESI

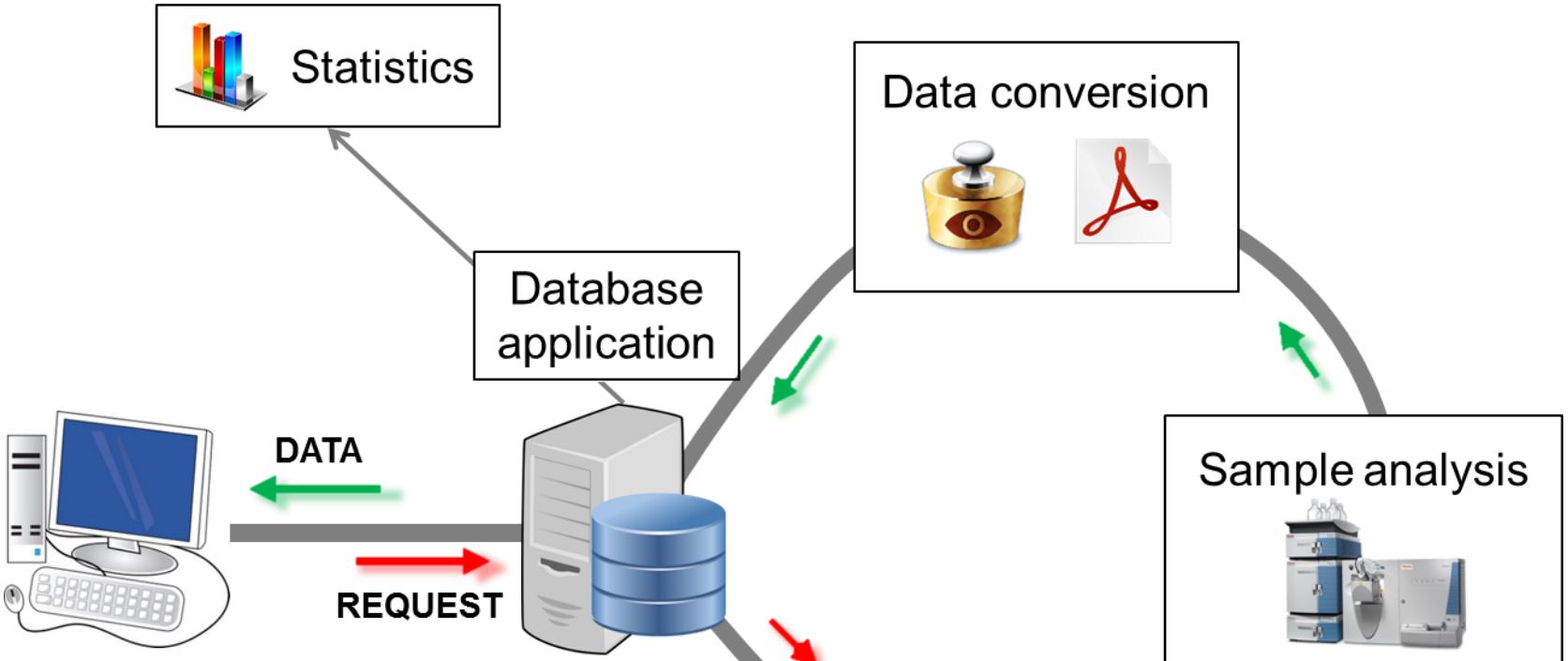


Synapt G2 (Waters)
Ion mobility, small & biomolecules
(HR); nanoESI, ESI, APCI

GCT Premier (Waters)
Small molecules
(HR); EI, CI

Sample submission

http://request.uochb.cas.cz



M. Svoboda Thu 11:20

M.Hubálek Thu 11:50

Measured data

Small molecules:

Two optional data formats:

pdf

msd *

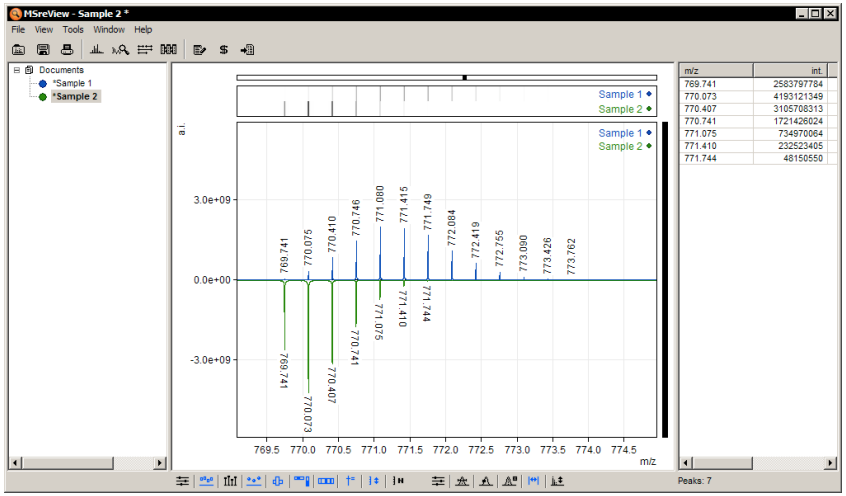
Biomolecules:

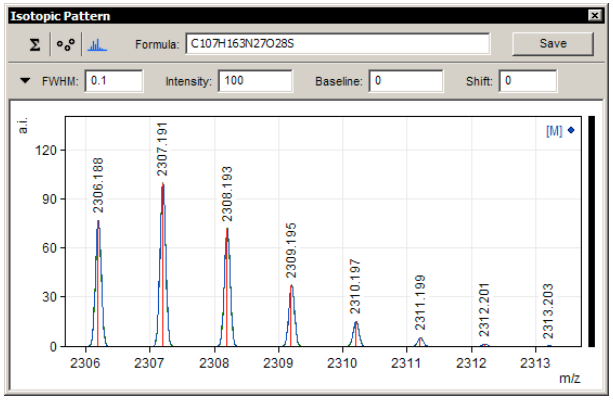
Various data formats (mostly txt, docx)

* *http://www.mmass.org/*

MSreView

Software for working with mass spectra





MS services: Usage statistics 2015

183 users from 29 groups
6624 requests
2.5 working days (average for data delivery)

Small molecules

51 users from 16 groups
246 requests
10 working days (average for data delivery)

Proteomics

1442 GC/MS runs

Open Access

MS services: Usage statistics

ReQuest users:

Year	Number of groups	Number of users
2013	29	172
2014	33	202
2015	35	218

MS Service is here for you…

We value your thoughts and opinions! Please feel free to contact us with your comments, questions or special service needs.