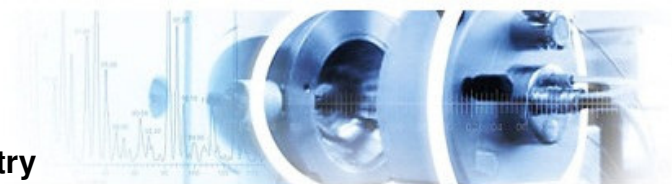




IOCB AS CR, v.v.i.

Research – Service Team Mass Spectrometry



Third Short Mass Spectrometry Courses

MINIŠKOLA HMOTNOSTNÍ SPEKTROMETRIE

November 14 – 15, 2011

Why “Miniškola”?

Information for our colleagues – the MS service users

- services provided by the MS group
- organization of the service work
- news and future plans
- basic interpretation of data

Demonstration of MS instruments

User training for open-access instruments

Discussion, user feedback

Agenda

Monday, November 14

Mass Spectrometry Basics (IOCB Lecture Hall)

- 9.00 - 9.30 Opening (J. Cvačka)
9.30 - 9.45 Introduction to mass spectrometry (J. Cvačka)
9.45 - 10.30 MS instrumentation (V. Vrkoslav)

break, refreshment

Services of the MS Group (IOCB Lecture Hall)

- 11:00 - 11.30 Small molecules (A. Březinová)
11.30 - 11.50 Biomolecules (Z. Demianová)

Demonstration of instruments (lab. 107, 33, 53)

- 14.00 - 17.30 Orbitrap – High resolution and proteomics (Z. Demianová)
MALDI – Large and small molecules (V. Vrkoslav)
ESI MSⁿ – Tandem MS for structure elucidation (J. Cvačka)

Agenda

Tuesday, November 15

Interpretation of MS data (IOCB Lecture Hall)

- 9.00 - 10.20 Spectra interpretation – small molecules (J. Cvačka)
10.20 - 11.00 MS-based proteomics (Z. Demianová)

break, refreshment

News (IOCB Lecture Hall)

- 11.30 - 12.00 TripleTOF 5600 System (T. Korba, AB SCIEX)
12.00 - 12.30 MALDI-TOF/TOF ultrafleXtreme (M. Boháč, Bruker)
12.30 - 13.00 New request management system of MS lab (M. Strohaln)

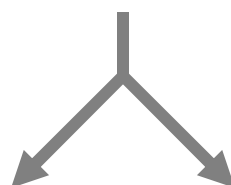
Training for open access instruments (lab.107, 53)

- 14.00 - 15.00 Training for open-access GC/MS (V. Vrkoslav)
Training for open-access LC/MS (A. Březinová)

Research-Service Team Mass Spectrometry



& students (4 PhD, 4 MSc)



Research

- Identification of organic compounds by common MS methods
- New procedures for analysis of organic compounds based on MS and chromatography

Services

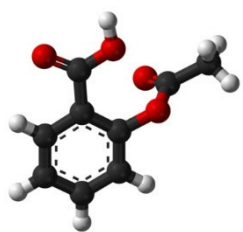
- Services towards characterization and structure elucidation of organic compounds



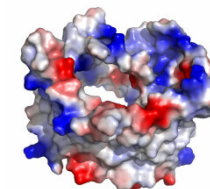
<http://www.uochb.cz/web/structure/200.html>

Services

**Analysis
of Small
Molecules**



**Analysis
of Bio-
molecules**



**Open Access
Instruments**

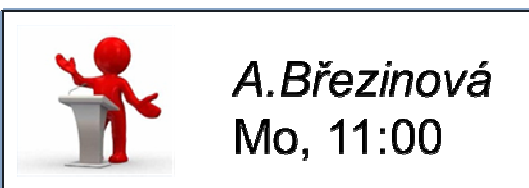
Services: Small molecules

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)



Anna Březinová (tel. 302)

Services: Biomolecules

Routine services:

➤ Determination of molecular weight of biomolecules
MALDI or ESI-MS analysis

➤ Identification of proteins
peptide mass fingerprinting (MALDI-TOF)
identification using ESI-MS/MS

On demand services:

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



Z. Demianová
Mon, 11:30



Zuzana Demianová (tel. 237)

Services: Open access instruments

The open access instruments:

- **2 GC/MS** (LR EI, nonpolar and polar column)
- **LC/MS** (LR ESI, APCI, MSⁿ)



Room 107 (SV)
7/24



Room 53 (LS)
working hours

Authorized users:

IOCB employees and students trained by the MS staff

Notes and rules:

- *the instruments can be reserved (use calendars by the instruments)*
- *each measurement must be registered in a logbook*
- *the users are responsible for damages caused by misuse of the instruments*
- *priority of the MS staff for routine services, maintenance etc.*

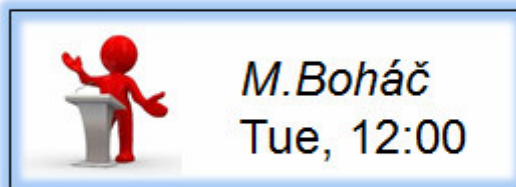


Vladimír Vrkoslav (tel. 237)

Mass spectrometers



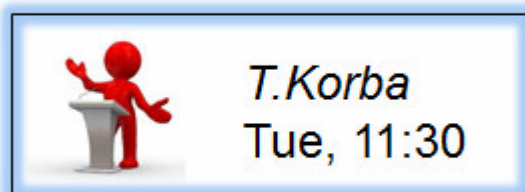
Q-TOF micro (Waters)
Small molecules
(LR); ESI, APCI



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



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



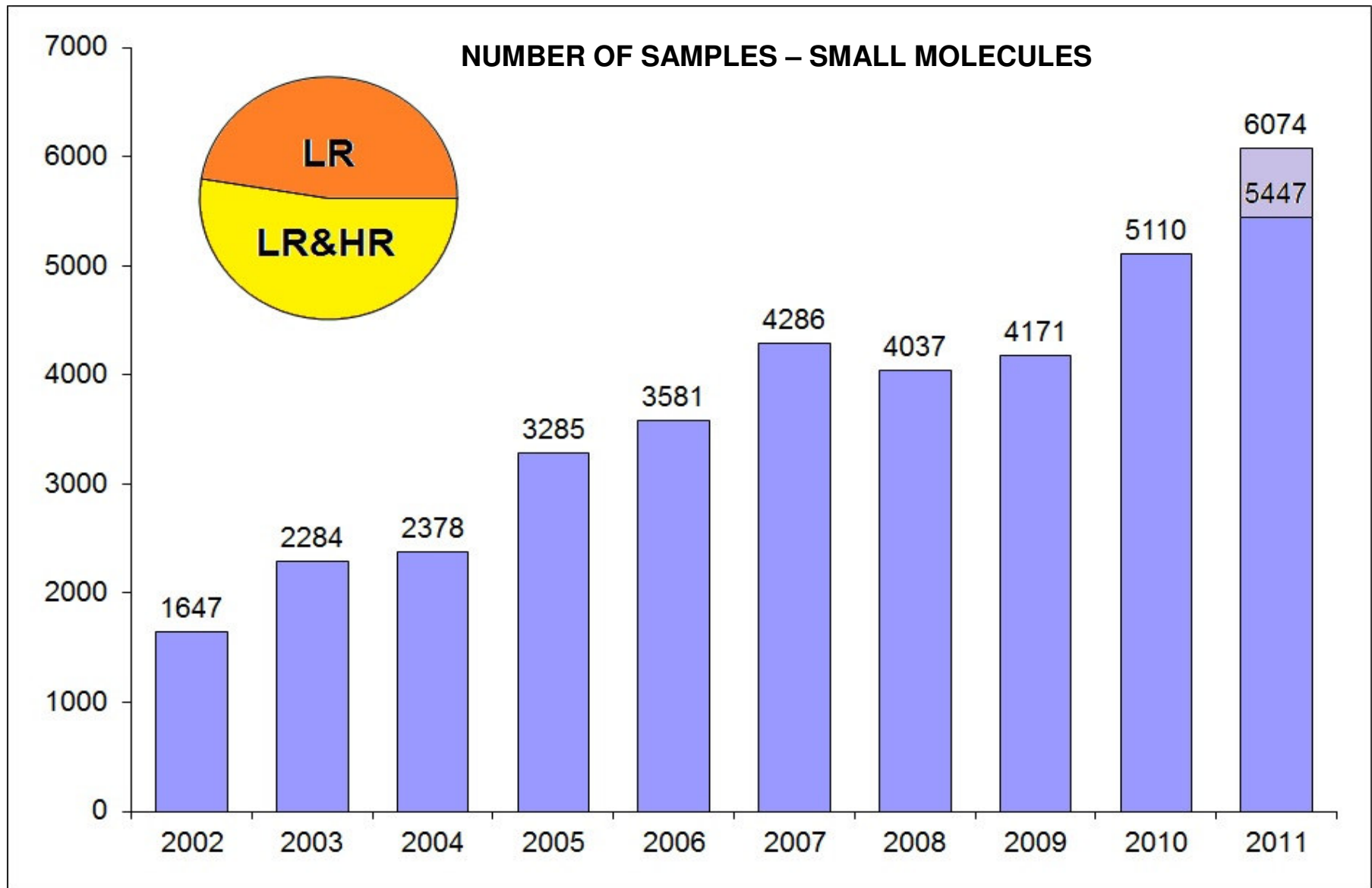
TripleTOF (ABSciex)
Biomolecules
(HR); nanoESI



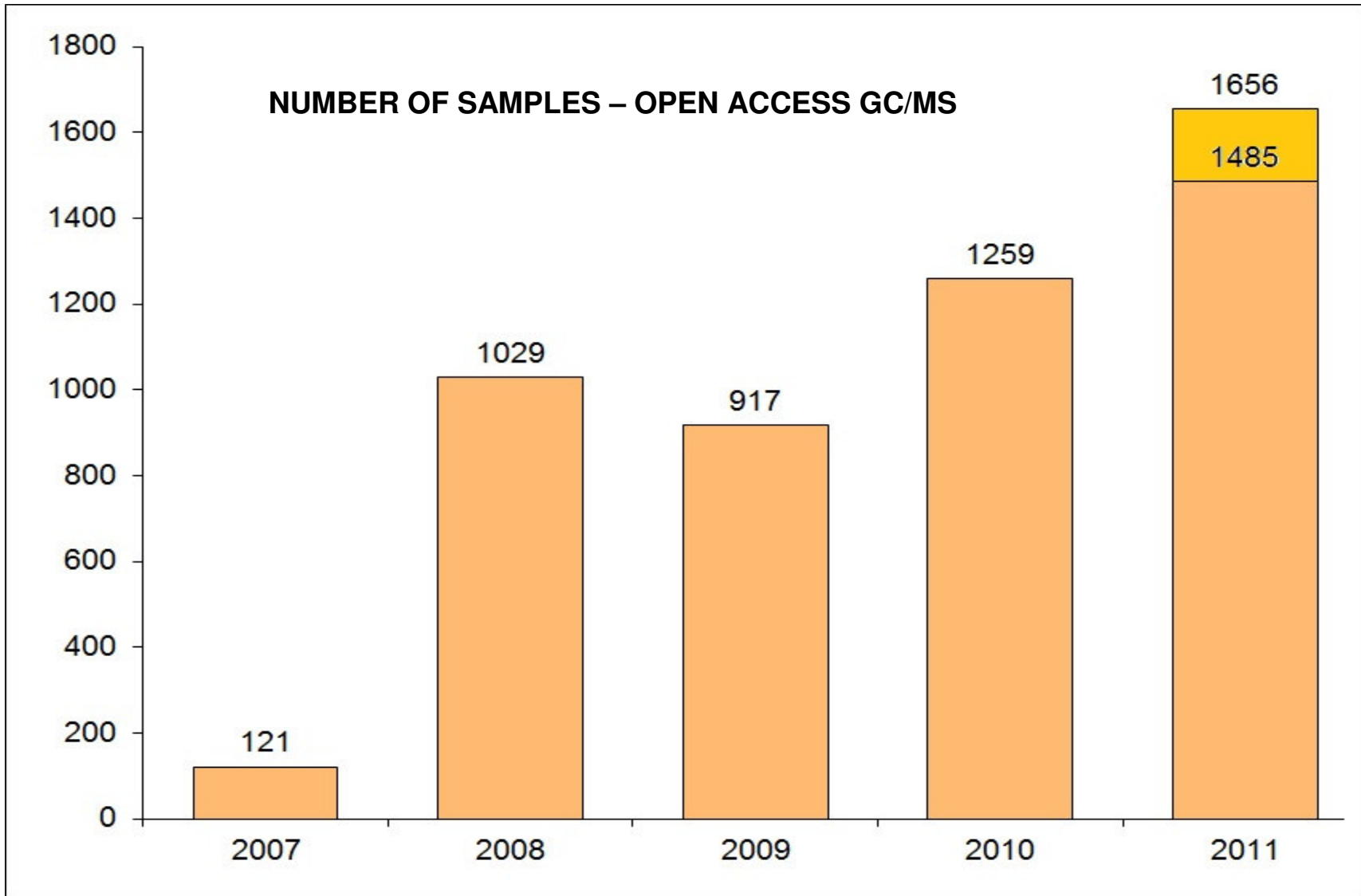
GCT Premier (Waters)
Small molecules
(HR); EI, CI



MS services seen by statistics



MS services seen by statistics



Sample measurement workflow - Current

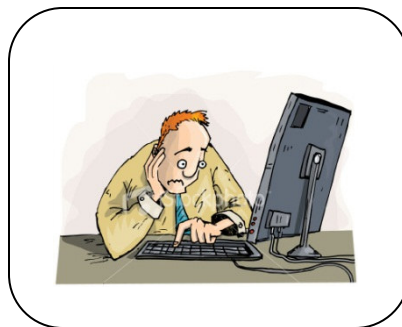
Sample & completed form



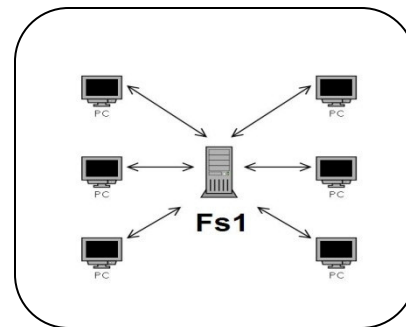
Sample registration in a logbook



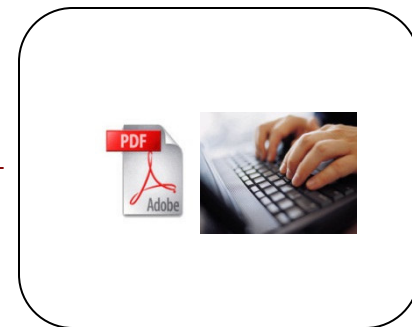
Sample analysis



Data viewing (**pdf**)



Data upload to local network



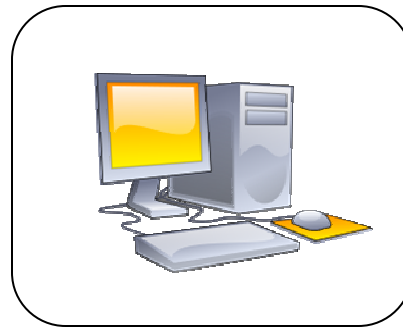
Data analysis & conversion to **pdf**

Sample measurement workflow – Near future

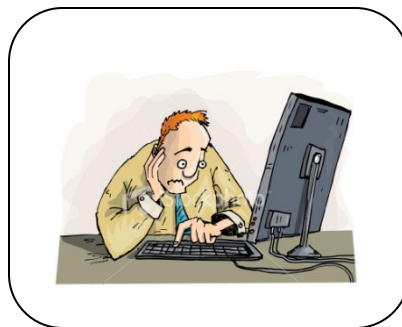
Sample & completed form



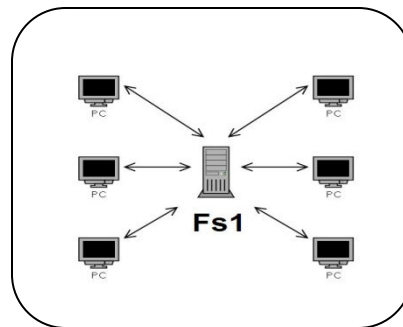
Sample registration from any computer



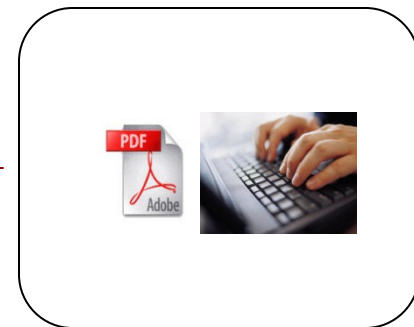
Sample analysis



Data viewing (**pdf**)



Data upload to local network



Data analysis & conversion to ***.pdf**

Sample measurement workflow – Near future

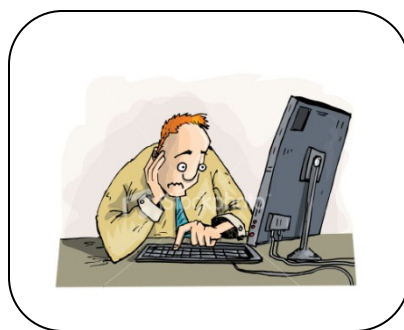
Sample & completed form



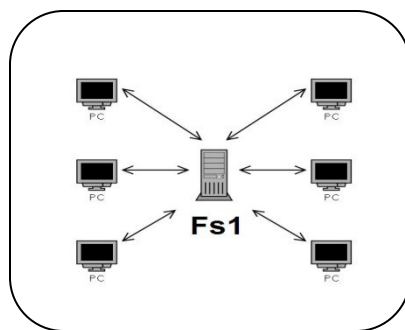
Sample registration from any computer



Sample analysis



Data viewing (**pdf**)



Data upload to local network



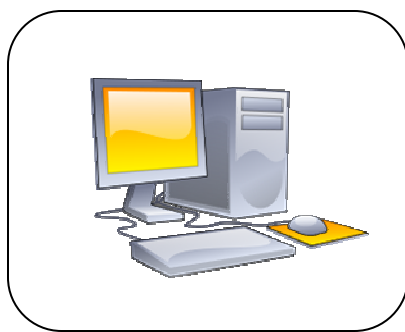
Data analysis & Conversion to ***.msd** (mzXML)

Sample measurement workflow – Near future

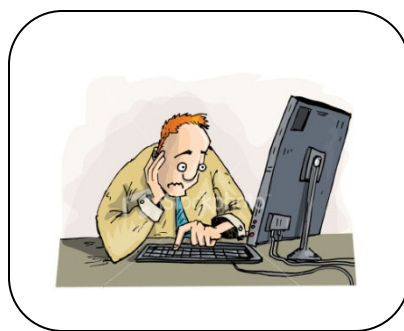
Sample & completed form



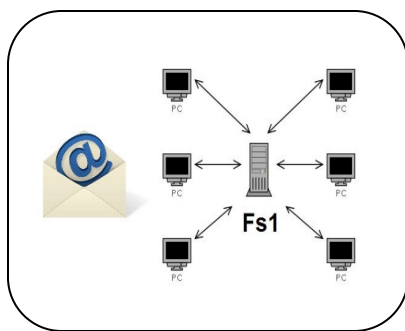
Sample registration from any computer



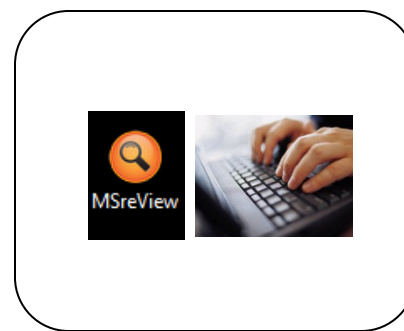
Sample analysis



Data viewing (**pdf**)



Data upload to network, e-mail notification

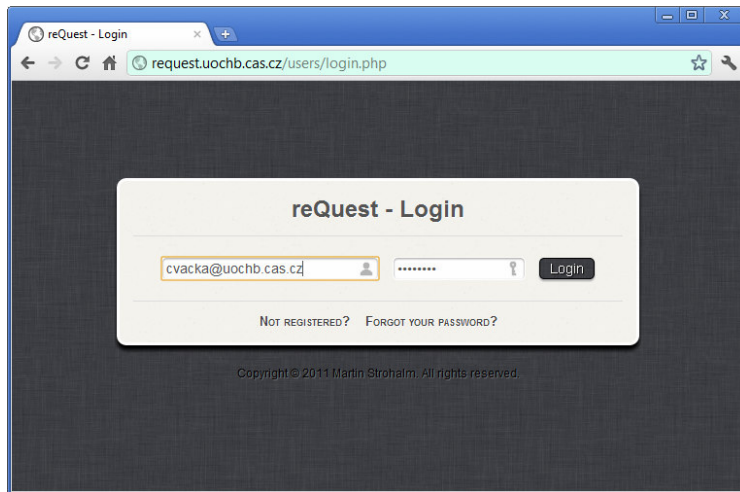


Data analysis & Conversion to ***.msd** (mzXML)

MSreQuest - MSreView

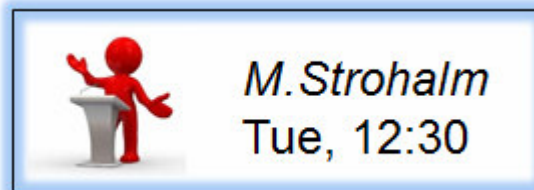
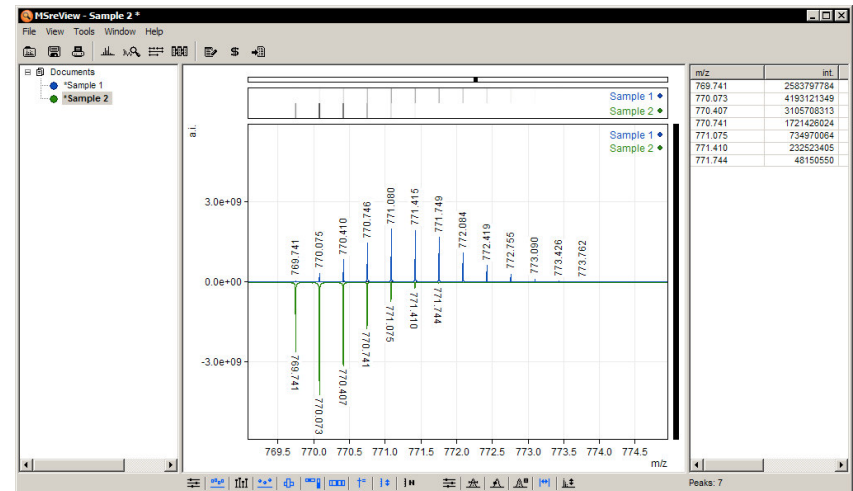
MSreQuest

Web-based sample submission

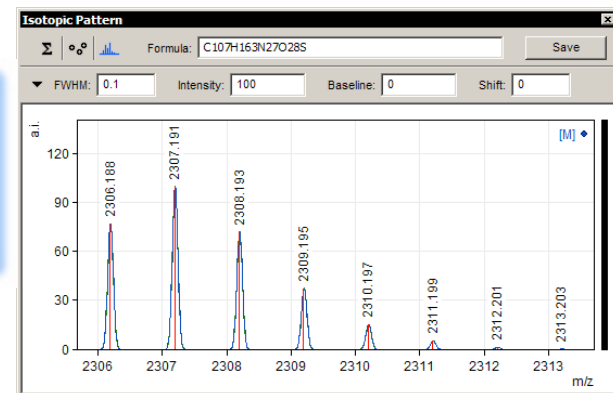


MSreView

Software for working with mass spectra



<http://request.uochb.cas.cz>



Moving labs

1/2012

106/107 SV → 64/64a SZ

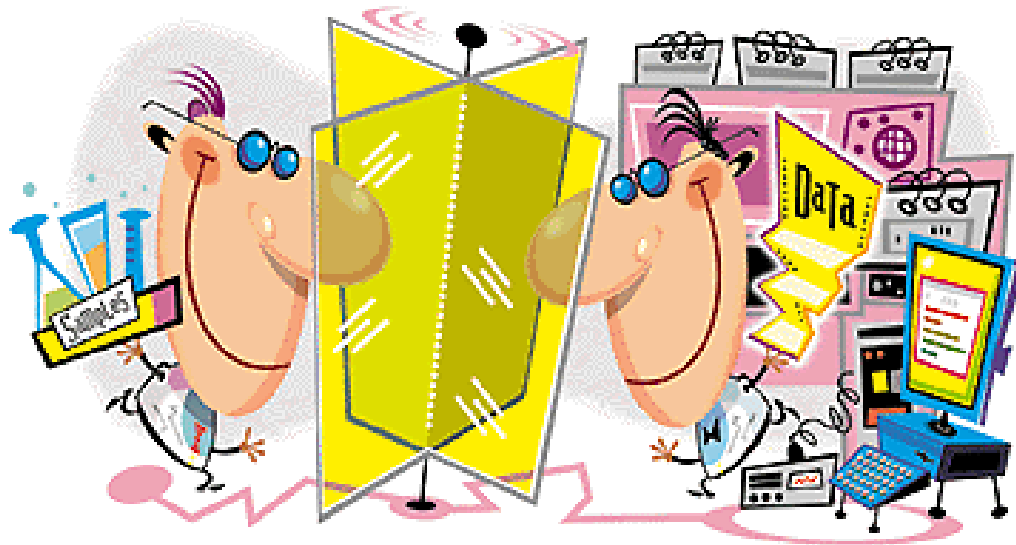
Interruption of Orbitrap and GC/MS operation
(HR small molecules, open access GC/MS)

2013



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. .



Acknowledgements

Organizers:

Anička Březinová, Zuzka Demianová, Kveta Kertisová, Katka Nováková,
Eva Mikolášová, Vláďa Vrkoslav

Invited speakers:

Michal Boháč, Tomáš Korba, Martin Strohalm

Financial support:

IOCB AS CR, v.v.i.