Solutions for Chemistry, Pharma DMPK, BioPharma, OMICS and computational chemistry

Mass Analytica

EUROPEAN
TRAINING AND USER MEETING

Molecular Discovery Headquarters in Montelino, Italy

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Training: 18th-20th of September 2023
User Meeting: 20th-22nd of September 2023

FROM 18TH TO 22ND SEPTEMBER

EUROPEAN TRAINING AND USER MEETING 2023

Molecular Discovery Headquarters in Montelino (Italy)

We are glad to announce that Mass Analytica (Lead Molecular Design, Molecular Discovery and Molecular Horizon) are organizing a Training (18th-20th of September 2023) and the User meeting (20th-22nd of September 2023) at the Molecular Discovery Headquarters in Montelino (Italy).

The training will be divided into different sessions depending on the interest and expertise. The idea is to have dedicated groups for each software and if possible, also divided by expertise and/or interest in using the applications.

The applications cover all branches of Mass Spec. Data analysis: Lipostar, Mars, Lipostar MSI, Pyxis, MassMetaSite, MassChemSite and Oniro (WebMetabase, WebChembase, WebQuant and Compound Library)

At the meeting we will show all the new features that we have been working on:

- **MassMetaSite:** New settings and all the new Macromolecule module.
- **WebMetabase:** New chromatographic and modeling tools, and Macromolecule module. AI for peak selection
- **WebQuant:** new module for quantification based on automatic calibration lines, automation and the easy ADME workflows. Automation of Quan-Qual workflow.
- **Compound Library:** the new link across experiments, connection to prediction tools and self-made model building.
- **LipostarMSI:** focusing on export for LMD, MALDI-IHC-guided analysis, and upgrades in identification.
- **Pyxis:** ion mobility MSI data analysis and isobars scout algorithm.
- **Lipostar:** significant upgrades for quantification, ion mobility, identification.
- **MARS:** New software for LC-MS based metabolomics and beyond

As you know in this user meeting, we would like to have a major part of the time users bringing up their cases so we can have an open discussion on what needs to be improved and what is the direction.

We have a limited number of seats, so please, if you are interested in coming to the training or the user meeting or both, complete the form. If you need further information do not hesitate to contact me.

Training topics

Please, mark the topics you are interested on:

MassMetaSite:

- ☐ Settings for small molecules
- ☐ Settings for macro molecules
- ☐ Batch process
- ☐ Autoprocess

Oniro/WebMetabase:

- ☐ Template definition (small and macro molecule)
- ☐ Protocol definition (small and macro molecule)
- ☐ Running MassMetaSite within WebMetabase (small and macro)
- ☐ Processing Small Molecule experiment
- ☐ Single molecule analysis tools: Report, Docking, MetaDesign, Metabolic Pathway
- ☐ Tools:
    - Search
    - Multiple experiment analysis tools:
        - Comparator
        - Cluster view
        - Structure metabolism relationship table
        - Fragment analysis
    - Monomer database (macro molecule)

Oniro/WebQuant:

- ☐ Template definition for an ADME experiment set up
- ☐ Template definition for Quantitative analysis
- ☐ Process an experiment

MassChemSite:

- Derivatization workflow:
  - Forced degradation studies
  - Late-stage functionalization
  - Degradation of pesticides in soil samples
- Compound monitoring:
  - Find pesticides in vegetables samples
  - Find 384 pesticides on a single standard sample
- Reaction tracking:
  - Using the Mass spec to follow chemical reaction crudes

Compound Library:

- Predict chemical properties
- Model building for CCS, clearance, fragmentation
- Combining different experiment on a single report

Lipostar

- The DB Manager
- Dealing with IMS data
- Quantification
- Identification

MARS

- Generation of databases for metabolomics and exposomics
- Identification
- The MS/MS validator
- Pathway analysis

Lipostar MSI

- Export for laser-capture microdissection
- MALDI-IHC-guided targeted and untargeted data analysis
- MRM and quantification
- Identification and drug MetID

Pyxis

- Targeted and untargeted workflow for spectral and image analysis in 3D: m/z, CCS, intensity
- Isobars scout
- Identification

European Training and User Meeting in Montelino (Italy) 18th-22nd September 2023

Molecular Discovery, Lead Molecular Design and Molecular Horizon

Training (18th-20th of September 2023) /
User meeting (20th-22nd of September 2023)

Registration form

Company: _____

Name: _____Job title: _____

_____

Telephone: _____ E-mail: _____

☐ Training (18-20th September)

☐ One day training

- ☐ 18th September
- ☐ 19th September
- ☐ 20th September

☐ User Meeting (20-22nd September)

** Training: 500€*

**One day training: 250€*

Other information:

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Training location: Montelino, Italy.