MetaSite MassMetaSite
WebMetabase
MassChemsite

2020 EUROPEAN TRAINING

MD MOLECULAR DISCOVERY

lead molecular design

11th, 12th and 13th May

MONTELINO
ITALY (EU)

MetaSite / MassMetaSite / WebMetabase / MassChemsite

2020 Training

Day 1. 11th May 2020.

Afternoon session

5:00PM

Opening Pre-Training Presentation on MD platform system: "Introduction to MD platform: All tools the Molecular Discovery at your fingertip"

Day 2. 12th May 2020.

Morning session

9:00AM Presentation, demo and tutorial for the new features in MassMetaSite 4.0:

- Presentation: "**MassMetaSite 4.0: Simplification**"
- Demo:
    - New Graphical Interface:
        1. Single experiment
        2. Batch processing
        3. Autoprocess
    - Isotope labeling and GSH workflow

10:30AM – 1:30PM Tutorial:

1. Single experiment:
    - 1.1 Just run an experiment.
    - 1.2 Study of the impact of the different settings in the output
2. Batch processing:
    - 2.1 Import settings from previous versions
    - 2.2 Starting from a Sample list
    - 2.3 Starting from a WebMetabase connection
3. Autoprocess:
    - 3.1 Import settings from previous versions
    - 3.2 Setting up a calculation

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Day 2. 12th May 2020.

Afternoon session

2:30PM

Presentation, demo and tutorial for the new features in WebMetabase 4.1:

- Presentation: "**WebMetabase 4.1: Making the workflows simple, less effort more throughput**"
- Demo:
    - Protocol Template system
    - Running MassMetaSite from WebMetabase
    - External connection to:
        1. Assay catalogs
        2. Molecular Structures database
        3. WMB-MMS-UNIFI

4:00PM – 7:00PM Tutorial:

- **Block 1:** Templates, protocol, experiments
- **Block 2:** Workflows:
    - WMB – sample list – MMS
    - MMS within WMB
    - WMB-MMS-UNIFI
- **Block 3:** Experiment analysis:
    - Small Molecule:
        1. Single condition:
            1.1 GSH trapping: with and without isotope labeling
        2. Multiple conditions:
            2.1 Kinetic Analysis
            2.2 Species comparison
            2.3 Cytochrome Reaction Phenotyping
    - Macro Molecule
        1. Single condition:
            1.1 Monomer management.
        2. Multiple condition:
            2.1 Kinetic analysis
            2.2 Matrix comparison

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Day 3. 13th May 2020.

Morning session

9:00AM – 1:00PM Tutorial:

- **Block 4:** Analysis tools
    - Small Molecule:
        1. Single experiment:
            - 1.1 Reporting
            - 1.2 Docking
            - 1.3 MetaDesign
            - 1.4 Metabolic Pathway
        2. Multiple experiments:
            - 2.1 Search: Multi-condition search
            - 2.2 Cluster View
            - 2.3 Comparator
            - 2.4 Protocol comparison
            - 2.5 Structure Metabolism Relationship table
            - 2.6 Fragment Analysis
    - Macro Molecule:
        1. Single Experiment:
            - 1.1 Reporting
        2. Multiple experiments:
            - 2.1 Frequency Analysis

- **Block 5:** System maintenance
    - Installation
    - Settings managements
    - User managements

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Day 3. 13th May 2020.

Afternoon session

2:00PM Presentation, demo and Tutorial for the new features in Compound Library 1.0

- Presentation: **What is the compound library, why it might be relevant for my work?**
- Demo:
    - Comparing experiments for the same compound
        1. Comparator
        2. Reporting
    - Prediction capabilities
        1. Phys Chem properties
        2. Metabolism
        3. ADME

3:00PM – 5:00PM Tutorial

- Comparing experiments for the same compound
    1. Comparator
    2. Reporting
- Prediction capabilities
    1. Phys Chem properties
    2. Metabolism
    3. ADME

5:00PM – 6:00PM Presentation, demo and Tutorial for the new features in WebQuant

- Presentation: **What is WebQuant?**
- Demo:
    - Clearance calculation
- Tutorial:
    - Clearance calculation