Please mark the training sessions that you would like to do.

Name: ____

0	MassMetaSite 3.4	

- Simple example to understand the MassMetaSite seetings
- Batch and auto process
- UNIFI-MassMetaSite connection

• Molecular Discovery Portal.....

- WebMetabase 4.0:
 - Small Molecule:
 - Protocol definition
 - o Experiment and sample list generation
 - o Upload a multiple condition experiment
 - \circ Macros
 - Approval process
 - Analysis tools
 - Single molecule Analysis tools:
 - Metabolic pathway and kinetic analysis
 - 32D docking
 - Metadesign
 - Reporting
 - Multiple molecule analysis tools
 - Search
 - Cluster view
 - Comparator
 - SMRT
 - Fragment analysis
 - MacroMolecule
 - Protocol definition
 - o Experiment and sample list generation
 - o Upload a multiple condition experiment
 - o Macros
 - $\circ \quad \text{Approval process}$
 - o Helm notation
 - o Frequency analysis
 - Site of Cleave predictions

- WebChembase:
 - Chemical degradation experiments
 - Protocol definition
 - Experiment and sample list generation
 - Upload and sample list generation
 - o Macros
 - Approval process
 - o NMR data for structure elucidation
- Compound library:
 - Data collection
 - Data visualization

\circ MetaSite 6.0

- Prediction for:
 - CYP
 - AOX
 - FMO
- Design tools:
 - 32D
 - MetaDesign

◦ MassChemSite 3.0.....□

- Chemistry workflows
 - Late stage functionalization using Mass Spec and NMR data
 - Compound degradation studies
 - Reaction Tracking

Thank you very much for your help in organizing hopefully this unique event.