Agenda

[L4-CH] Introduction to Working with Chemical Data

Session 1	
Introduction	Short Intro to KNIME Analytics Platform Chemistry Extensions Chemistry Formats: Readers and Writers
Exploring Chemical Data	De-duplication Calculate Descriptors Interactive Data Exploration and Filtering: Composite Views
Session 2	
Maximum Common Substructure	Maximum Common Substructure Flow Variables
R Group Decomposition	R Group Decomposition Chemical Sketcher Widgets
Session 3	
Clustering	Fingerprints Distance Matrix Hierarchical Clustering
Session 4	
Similarity Search	Similarity Search Functional Group Filtering Configurable Shared Components
Session 5	
Wrap Up Session	**Discussion of last Exercise and Q&A**

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