

[L4-CH] Introduction to Working with Chemical Data

| Session 1 | |
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| 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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