

[L4-CA] Machine Learning for Chemical Applications

Session 1	
Introduction	Short Intro to KNIME Analytics Platform Chemistry Extensions Chemistry Formats: Readers and Writers
Access and Transformation of Chemical Data	Read in Data from Files and Databases Interactive Data Exploration and Clustering: Composite Views
Session 2	
Machine Learning	Parameter Optimization Loop Model Learner and Predictor Model Evaluation
Session 3	
Multi-objective Optimization	Reading in Models Pareto Ranking Interactive View to Explore Results
Session 4	
Matched Molecular Pair Analysis	Preprocessing of Molecules Fragmentation and Molecular Pairs Finding Exploring the Results
Session 5	
Wrap Up Session	Discussion of last Exercise and Q&A