**Wednesday, May 28th**

**9.00 – 10.30**

**Basics of Python and Jupyter Notebooks**

Introduction to scientific modules in Python and Jupyter Notebooks.

**10.30 – 11.00**

**Coffee break**

**11.00 – 12.30**

**Digital chemical reactions**

Introduction to SMARTS strings, using RDKit to set up digital reactions and automating reactions with multiple substrates.

**12.30 – 14.00**

**Descriptors and featurization**

How to featurize molecules with chemical properties, electronic and steric parameters, etc. Using AQME to generate QM descriptors in an automated manner.

**14.00 – 16.00**

**Lunch break**

**16.00 – 17.30**

**Chemical space exploration, dimensionality reduction and clustering**

Introduction to the concept of chemical space, using dimensionality reduction to simplify visualization, and using molecular clustering to select and organize molecules using their properties.

**Thursday, May 29th**

**9.00 – 10.30**

**ML to predict chemical outcomes**

Supervised ML methods and examples to predict chemical outcomes such as reactions results and molecular properties. Data curation and evaluation of ML models.

**10.30 – 11.00**

**Coffee break**

**11.00 – 12.30**

**Automation of ML protocols with ROBERT and easyROB**

Automated ML workflows for prediction: from CSV or ChemDraw to ML predictors. Beta testing of the easyROB executable.

**12.30 – 14.00**

**Custom problems**

If there is enough time, we can go over problems from the participants’ research.