AN INTRODUCTION TO SMARTS PATTERNS & THEIR APPLICATIONS

WORKSHOP CONTENTS

In this 2-hour workshop, participants will learn the basics of designing SMARTS patterns. After a 30-minute introduction to understanding and generating SMARTS expressions and their application in drug discovery for filtering assay-interfering small molecules, participants will be introduced to the standalone tool SMARTSeditor (https://www.zbh.uni-hamburg.de/forschung/amd/software/smartseditor.html). They will derive SMARTS patterns to filter assay interference compounds. This graphical user interface (GUI) tool enables the participants to design patterns in a highly intuitive chemistry-aware manner.

After a short break, the online web service SMARTSplus (https://smarts.plus) will be presented. There, participants will visualize the generated SMARTS patterns in a chemically highly intuitive manner (SMARTSview). Next, SMARTSsearch will be used to find similar SMARTS patterns in SMARTS collections to detect frequent hitters. SMARTScompare will then be applied to detect the distinct similarities between the designed pattern and available patterns, which is especially helpful to optimize individual SMARTS collections.

LEARNING GOALS

- understanding SMARTS expressions and their applications
- using sets of wanted and unwanted molecules to design discriminative SMARTS patterns with SMARTSminer
- modifying and optimizing SMARTS patterns with SMARTSeditor
- comparing SMARTS strings and visualizing their differences on SMARTSplus

PREPARATION INSTRUCTIONS

- participants are asked to install the standalone GUI tool SMARTSeditor by registering at https://uhh.de/naomi, downloading the package for their operating system, and follow the installation instructions at https://umfragen.uni-hamburg.de/index.php/853563?lang=en
- participants will need internet access and a web browser to follow the instructions in the second part of the workshop
- contact software.zbh@uni-hamburg.de if you need any further support