Compound logistics course

Date: March 17 - 18, 2022
Location: Institute of Molecular Genetics of the ASCR, v. v. i.
Prague, Czech Republic

Time | Topic
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11:00 | **Lab tour over CZ-OPENSEEN** (National infrastructure for chemical biology) laboratories, introduction of the High-Throughput-Screening (HTS) laboratory automation, description of the typical HTS Project stages from assay development to hit validation
12:00 | **Lab tour over CZ-OPENSEEN Compound Management facility**, introduction of the standalone instruments and tools, introduction of the Automated storage system (Hamilton ASM) and Automated Liquid handling workstation (Hamilton Vantage), introduction of the Quality Control (QC) instrumentation (Waters I-Class UPLC-MS)
13:00 | Lunch
14:00 | **Introduction of ScreenX DB** (web-based in-house developed LIMS database) and functionalities essential for CM, Introduction of PROBES and DRUGS portal – a tool for high quality chemical probes and approved drugs selection
16:00 | **Compound Management workflow** (theory vs. our approach)
   - Types of compound libraries (diversity, bioactive, academic, focused libraries, sub-libraries, fragment, etc) and their specifics
   - Compound acquiring (purchase x donation), approved commercial vendors, electronic data needed for effective compound registration
   - Compound registration/dissolving, preparing of Mother plates, Storage tube options, barcoding
   - Sample storage, storing dry samples x DMSO solutions, optimal storage conditions, environment control, sensitive samples with special storage needs
   - Library reformattting, preparing of Daughter plates (assay-ready plates), Z-reformat, types of suitable labware
   - Cherrypicking, hit selection, preparing dilution series for dose response experiments
19:30 | Dinner

Day 2 (Friday, March 18th, 2022)

Time | Topic
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9:30 | Hands-on training - Automated storage system (Hamilton ASM), setting up processes to introduce and retrieve samples, sample list formats, Cherrypicking, etc.
11:00 | Hands-on training - Automated Liquid handling workstation (Hamilton Vantage), system structure, 3rd party devices, programming new assay, pipetting tools and parameters, troubleshooting and error recovery
13:00 | Lunch
14:00 | Hands-on training – QC by UPLC-MS, sample list creation from ScreenX, sample preparation for LC-MS, LC parameters optimization, automated result validation and reporting, single sample reporting, upload to the DB, the difficulties related to the LC-MS of large screening libraries
16:00 | End of the course

Final program can be customized depending on the specific interests of the individual attendees, covering and discussing the suggested topics more in depth.

For our instrumental equipment please refer to: [https://openscreen.cz/en/node/181](https://openscreen.cz/en/node/181)