AUTOMATED COMPOUND MANAGEMENT **PIPELINE AT THE CZ-OPENSCREEN**

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Introduction

CZ-OPENSCREEN (CZ-OS) is an infrastructure for chemical biology and genetics offering open access to potential users. Our mission is to identify new molecular probes and to develop new tools for the research of chemical compounds – candidates for the development of new potential therapeutics. Compound Management (CM) is an integral part of the High Throughput Screening (HTS) research field and other drug discovery processes where handling of large collections (typically more than hundreds of thousands) of small organic molecules is to be assured.

Methods

The CM department at CZ-OS maintains chemical libraries containing more than 180,000 unique chemical compounds from various commercial and private sources. Typical CM workflow starts with the input/import of the sample data in the proprietary web-based LIMS (ScreenX). Mother samples are kept in 96-wp (Matrix tubes) and stored in an automated storage system (ASM, Hamilton) which is integrated with an automated liquid handling system (Vantage, Hamilton), equipped with 3rd party devices such as: plate labeler, sealer, peeler, centrifuge and decapper. The reformatting employs tip-based pipetting to generate several copies of Echocompatible Daughter plates in 384- and 1536-format. The working set of Daughter plates is stored at 4 °C (TundraStore, HighRes Bio) which is part of the automated HTS platform. The quality of the samples (QC) is monitored by the LC/MS system (Acquity, Waters) compatible with 384-well plates.







Results

At CZ-OS the compound libraries are processed using the robotic systems which allow for an unattended compound dissolving, reformatting, diluting and cherrypicking. Thanks to ScreenX DB the faith of each sample/well is precisely tracked and includes QC checkpoints to assure identity and purity. High emphasis is placed on maintaining the DMSO hydration at minimum level to ensure longterm stability of the compounds and reproducibility of the screening data.

Conclusion

The CM facility at the CZ-OS is equipped with stateof-the-art automation, and together with a dedicated LIMS and database system, ensures optimal conditions for providing a high-level standard of services.

Acknowledgments: This work is supported by The Ministry of Education, Youth, and Sports (LM2023052).

