

PRESS RELEASE
25 January 2018



Enamine expands collaboration with UCSF to explore synthetically feasible chemical space

Enamine REAL database of synthetic compounds accessible via UCSF's online ZINC platform

Kiev, Ukraine, 25 January 2018: Enamine Ltd., a chemical research organization and producer of novel building blocks and screening libraries, has today announced that it has expanded its collaboration on ZINC, a comprehensive online database of purchasable compounds curated by the Irwin and Shoichet laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). Via ZINC, Enamine will provide researchers at UCSF and the global drug-discovery community with access to the company's REAL database, a unique database of more than 300 million novel synthetically feasible chemical structures as an efficient source of potential new compounds for a breadth of drug discovery projects.

The REAL database is the most significant contribution to currently purchasable chemical space, accounting for over 90% of all structures in ZINC. The compounds are conveniently selected in ZINC and then synthesized by Enamine in a single step from its building block stock, ensuring quick delivery and a high success rate.

Michael Bossert, Head of Strategic Alliances at Enamine said: "The number of compounds that Enamine can quickly access with its stock of 150,000 building blocks is astonishing. ZINC is a powerful platform that can efficiently support our endeavors to further expand our chemical space coverage to the global drug discovery community. We are pleased to see the researchers at UCSF benefitting from the diversity and novelty of our structures in the REAL compound arrays."

John Irwin, PhD, Adjunct Professor at the UCSF School of Pharmacy and curator of ZINC agreed: "As we strive to bridge the gap between chemoinformatics and biology, the importance of working within a purchasable chemical space cannot be underestimated. We are pleased to continue our collaboration with Enamine in exploring ways to provide novel chemical compounds, designed and synthesized specifically for each research project, to the global biomedical community."

Most compounds from the REAL database have already been successfully uploaded to ZINC. Over the last year, 92% of the more than 250 compounds ordered from Enamine have been delivered successfully to UCSF.

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Notes to Editors

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About Enamine

Established in Kiev, Ukraine in 1991, Enamine is a chemical company, producer of building blocks and screening libraries. The major asset of the company is the world's largest collection of building blocks. 150,000 in-stock building blocks with 2,000 new ones freshly synthesized each month provide a major competitive advantage in supplying large arrays of building blocks for DNA-encoded library synthesis among other applications. The company's REAL (readily accessible) concept is based on the careful and knowledge-guided enumeration and selection of compounds that can be confidently produced from the stock building blocks using over 60 validated reactions. Visit www.enamine.net for details.

About University California, San Francisco (UCSF)

UC San Francisco (UCSF) is a leading university dedicated to promoting health worldwide through advanced biomedical research, graduate-level education in the life sciences and health professions, and excellence in patient care. It includes top-ranked graduate schools of dentistry, medicine, nursing and pharmacy; a graduate division with nationally renowned programs in basic, biomedical, translational and population sciences; and a preeminent biomedical research enterprise. It also includes UCSF Health, which comprises three top-ranked hospitals, [UCSF Medical Center](#) and UCSF Benioff Children's Hospitals in [San Francisco](#) and [Oakland](#), and other partner and affiliated hospitals and healthcare providers throughout the Bay Area. Visit www.ucsf.edu

About REAL database

The REAL (readily accessible) database is an Enamine's collection of currently 337 million virtual screening compounds. These compounds are a result of careful and knowledge-guided enumeration and selection process ensuring that they can be confidently produced in 2-3 weeks from the stock building blocks just in one synthesis step using over 120 validated reactions. A number of the preselected sets are available to download along with the full database. These include drug-like, lead-like, and fragments, among others.

Visit www.enamine.net/index.php?option=com_content&task=view&id=254 for more details.

About ZINC

ZINC is a database of commercially available compounds for virtual screening. It is freely available to everyone and currently contains over 230 catalogs from 120 vendors, as well as 20 annotated catalogs

such as the ChEMBL medicinal chemistry database. ZINC provides commercially available molecules as 3D biologically-relevant models for docking as well as 2D SMILES for chemoinformatics research. ZINC can be searched using an intuitive user interface and allows subsets by property, vendor, and target to be downloaded in popular, ready-to-use formats.

Visit <http://ZINC15.docking.org> and <http://pubs.acs.org/doi/pdf/10.1021/acs.jcim.5b00559> for details.