Development and Enhancement of NITER: Expanding Access to Multi-Billion-Scale Compound Libraries and Public Data Sources

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The D ata-Driven Drug Discovery (D4) group at Daiichi Sankyo Co., Ltd., consisting of cheminformaticians and data scientists, aims to improve the success rate of drug discovery through acceleration and optimization of research processes.[1] As part of this initiative, the group has developed NITER (Near-neighbor Investigation Tool for hit-Expansion Research), an integrated compound search platform, based on the fundamental principle that similar compounds exhibit similar properties.

In this presentation, we describe recent expansions of NITER, highlighting the implementation of high-speed search functionality that enables rapid exploration of multi-billion-scale commercial compound catalogs and integration with public data sources. The platform enables researchers to perform comprehensive searches across multiple databases through a unified interface, significantly improving operational efficiency in daily research activities.

In medicinal chemistry research, public data sources such as academic papers, patents, and commercial catalogs serve as rich sources to extract background information, knowledge, and intuition for new ideas. Through case studies, we demonstrate how these enhancements facilitate efficient access to both commercial compounds and various public data sources, providing researchers with valuable insights. By enriching compounds with multifaceted information, researchers can make more informed decisions in compound prioritization and selection. This integrated approach ultimately supports more accurate and efficient drug discovery processes.

[1] Kunimoto R, Bajorath J & Aoki K. From traditional to data-driven medicinal chemistry – a case study. Drug Discov Today 27, 2065-2070, 2022.