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Abstract:

One of the key challenges in drug discovery is ensuring that project leaders and decision makers have access to the latest and most relevant data for their projects. While database architects can skillfully develop systems to search large volumes of complex data at high speed, end users typically don't have the necessary technical knowledge to set up queries and easily extract relevant results. In this paper, we will describe the development of a graphical tool for user-friendly creation, sharing and execution of structured database queries. This is seamlessly linked with a comprehensive software environment, in which the resulting data can be used to guide effective decisions in the selection and design of high quality compounds for drug discovery and other chemistry fields.

Physiochemical and biological results for the chemical concept, salt and batch are pre-aggregated from the data management system (BioRails™) on a scheduled basis, using a separate data mart. Complex queries can then be easily constructed to access the data mart, simply by dragging-and-dropping query terms and editing the criteria in-place. The results of running a query are preprocessed to assign units and errors and remove redundant columns, before being returned directly as a data set in StarDrop.

StarDrop's intuitive data visualisation tools help to identify key structure-activity relationships and new optimisation strategies. Coupled with multi-parameter optimisation, in silico modelling, de novo and structure-based design capabilities, the resulting information can guide design of novel compounds that improve the overall balance of target activity, physicochemical and

User-friendly Database Querying for Decision-Making in Drug Discovery

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ADME properties required for a successful candidate drug. When new experimental results are available, StarDrop can use the original query to instantly update the data set and new compounds and data are highlighted for the user's attention. The connectivity between design and decision making tools and the data management system ensures that project teams have access to the latest information without needing to compile the data manually from many sources. This leads to better decisions and shorter project timelines.

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