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Innovative Chemical Database Design for Drug Discovery

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A distributed and extensible structure and activity related information database is described. Research groups working on similar projects within a single company often can't benefit from each others' work because their data is stored in disconnected repositories. Thus the necessity of a integrated chemical database in the field of drug discovery to significantly improve the lead identification, lead optimization and prioritization process is explained. The technology supporting data acquisition, data access, and data sharing from an in house database in an easy to use user interface for a researcher is elaborated. This allows researcher to focus on research and not the tools for research

Depending on the type of data like chemical, physical, biological, pharmacological data, etc, a database can be classification as target based, disease based, pharmacokinetic, reaction, medicinal chemistry, natural products, mechanism based toxicity database, etc, for the convenience of a researcher. The advantages of chemical databases are elucidated which primarily accelerates research and expands knowledge by rapidly enabling researchers to search, view, and analyze chemical and biological data from a available repository of all published/patented information to drug discovery scientists. Molecules can also be queried/ retrieved based on any one or more fields of interest like scaffolds, specific protein targets, molecular weight, assay type, activity ranges etc. using various query methods thus reducing enormous amount of time.

Thus structure and activity related chemical databases play a major role in enhancing the ability to generate a better set of molecules from chemical libraries for virtual screening, which will improve the probability of success and the productivity of the drug discovery process.