

Introducing

Design Hub

by  ChemAxon

In ChemAxon's earlier application, Marvin Live, there wasn't a good solution to capturing the scientific rationale connected to design compounds. To address this issue, we spent most of 2019 developing new systems that all culminated in a quite new application we decided to give a separate name. Meet Design Hub.

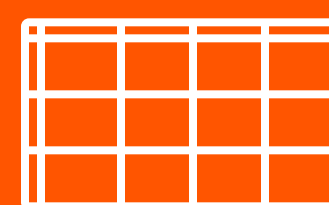


Scientific rationale

Capture your analysis results and observations with chemical structures, charts, arrows, annotations, attached files, all organized on several pages (or slides). The discussions originating from this can lead to new hypothesis to be proven or disproven with new compounds and new assays.

Guided design

Use the full informatics landscape to guide your chemical series to compounds with advantageous phys-chem properties, good binding affinity, no patentability concerns, understood toxicology profile and high synthetic feasibility. Simple compounds, scaffold based enumeration and reactions are all supported.

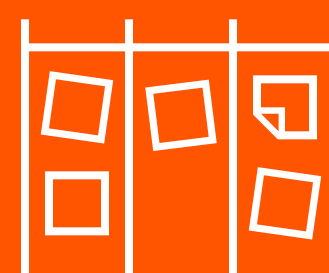


Virtual registration

When your hypothesis and compounds are ready for review, just click the share button. Design Hub can run quality checks, compare compounds with public or patented ones, take care of virtual ID generation and update you when the compound is eventually synthesized.

Kanban

Compound progression, chemical series status or a hypothesis level view of the project are all easy with kanban boards that let everyone keep an eye on the next team meeting's agenda, recent successes, stuck compounds or overloaded colleagues in need of help.



Universal search

All this data can be used as a foundational piece of a continuously learning medicinal chemistry department. Disproven hypotheses, failed syntheses are all great teachers worth having. Just define your text or chemical structure query to get all relevant answers from the knowledge base.

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