CERTARA | Chemaxon

Design Hub

A compound design and tracking platform for drug discovery teams and their external collaborators that connects scientific hypotheses, candidate compound selection and computational capabilities.

From scientific rationale to analysis, medicinal chemistry teams share a singular question in the DMTA cycle: Which compound should we make next? Compare new designs, allocate resources, track and prioritize your hypotheses to keep focus in the right place. Your collaboration tool in all this is Design Hub.

Link your hypotheses to design sets

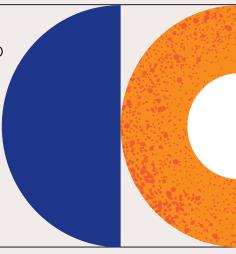Work with your trusted computational models and properties

Share ideas in a single collaboration tool

Customize data access for external partners

- Capture design hypotheses behind compounds ideas (draw and share hypotheses)
- Add or customize property prediction (phys-chem predictors)
- SAR analysis tools to make sense of your assay data
- Virtual library enumeration (scaffold and reaction based)
- Powerful text and chemical structure searching
- Access management controls
- Kanban boards to track project team progress

220 employees

26 years in the field

3 offices in the Americas and Europe

1 M active users serving 9 out of 10 leading pharmaceutical companies

aws

Get in touch