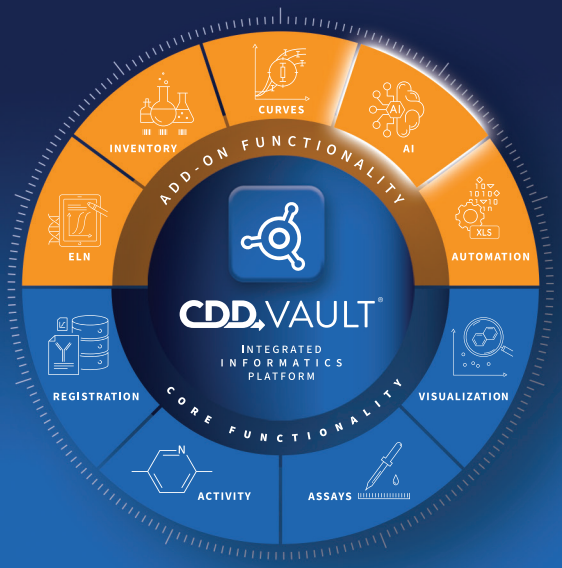
AI

DATASHEET

Improve your drug discovery pipeline using CDD Vault's built-in AI capabilities

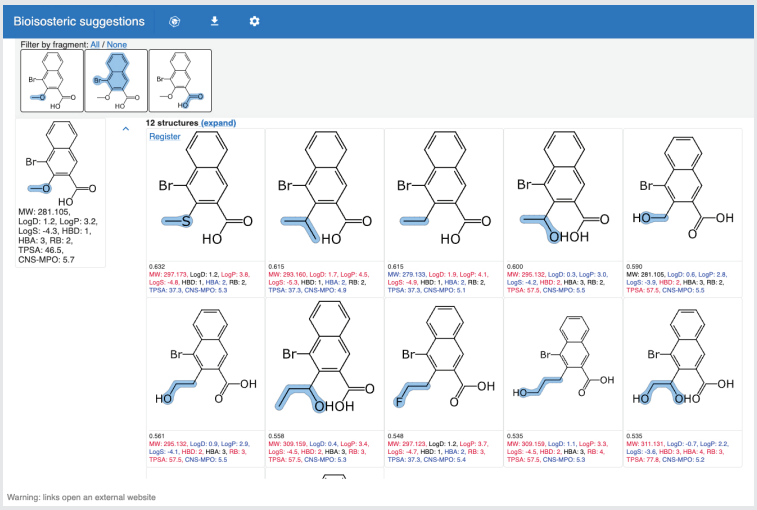


AI READY STRUCTURED DATA

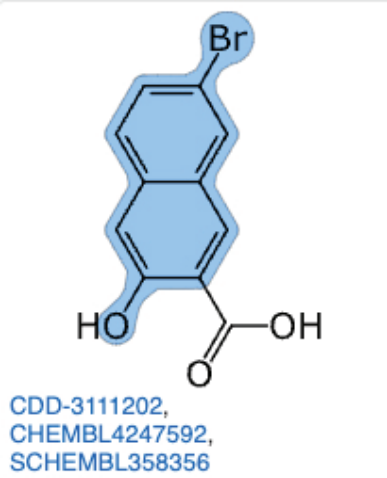
- Use CDD Vault's registration system to create standardized datasets.

BIOISOSTERIC SUGGESTIONS

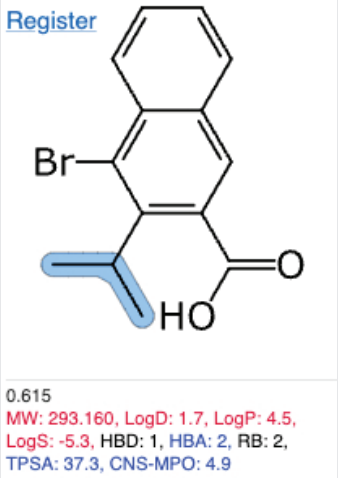
- Improve molecule design and streamline the development of new therapies using CDD Vault's advanced bioisosteric suggestion algorithms to suggest drug-like molecules based on stability.
- Vault's bioisosteric suggestion algorithm will suggest new fragments for your selected molecule, with a bias towards synthesizable results.
- CDD Vault makes it easy to focus on novelty by cross-referencing bioisostere suggestions versus molecules already published in ChEMBL, SureChEMBL, Enamine or CDD Public databases.
- Customize your bioisostere suggestion results with predicted properties and similarity to your original molecules.
- Easily register suggested bioisosteres directly into your Vault for further development of molecules of interest.



Bioiosostere suggestion results



Results include references to external databases for published molecules



Customize results with predicted properties and easily register bioisosteres

CDD VAULT®
Complexity Simplified

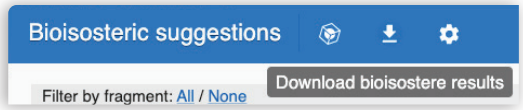
AI
DATA SHEET

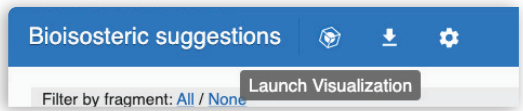
ENHANCED SEARCHING

- Use Vault's advanced AI search to rapidly search compounds similar to yours in ChEMBL, SureChEMBL, Enamine and CDD Public databases safely from the CDD Vault servers.
- CDD Vault's AI search results group similar structures by scaffold and allow for a variety of properties to be viewed for further analysis.

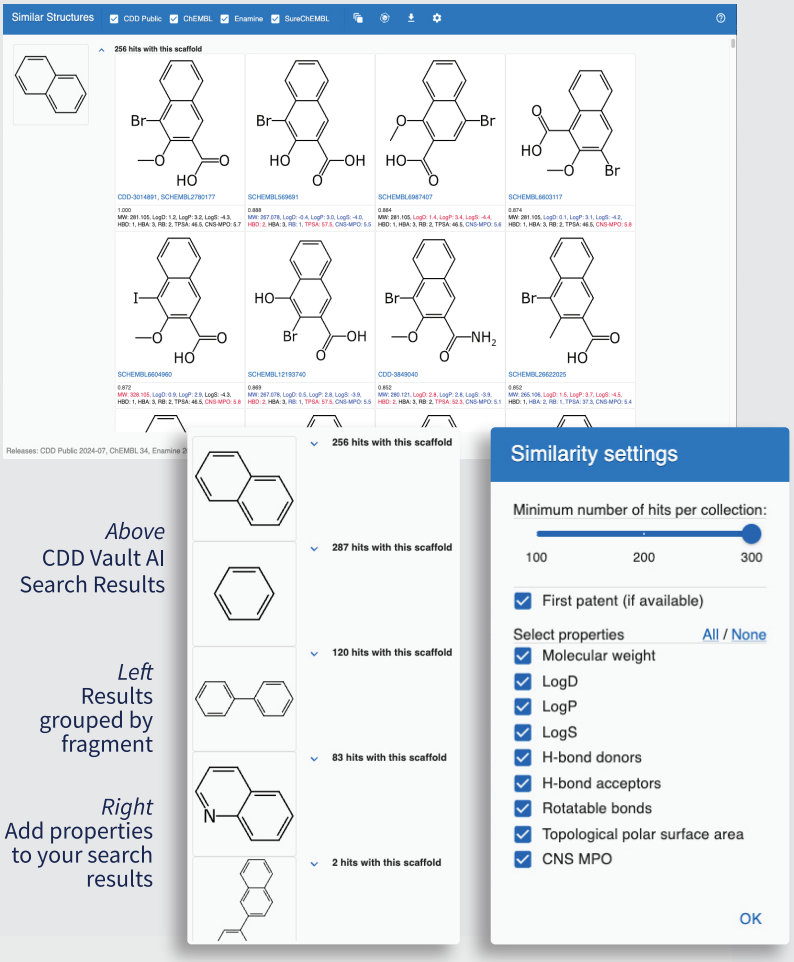
DATA ACCESSIBILITY

- Search results and bioisostere suggestions can be analyzed offline by downloading the dataset, or pushed directly into CDD Vault's built in Visualization tool.
- Both advanced AI searching and bioisostere molecule suggestions can be accessed directly from a registered molecule or from the CDD Vault molecule editor on any drawn molecule.
- Embed our deep learning technology into your analytical workflows.
- Build your own predictive models and optimize the properties of your leads to generate new ideas.





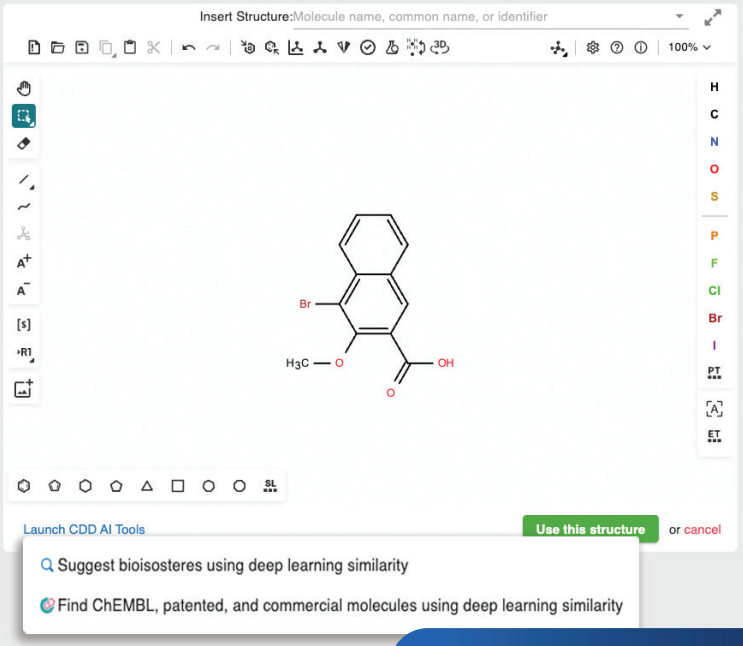
Download results or push them into Visualization



Above CDD Vault AI Search Results

Left Results grouped by fragment

Right Add properties to your search results



Use AI Tools directly in CDD Vault molecule editor on any virtual molecule

Learn more at
collaborativedrug.com

or contact us at
info@collaborativedrug.com