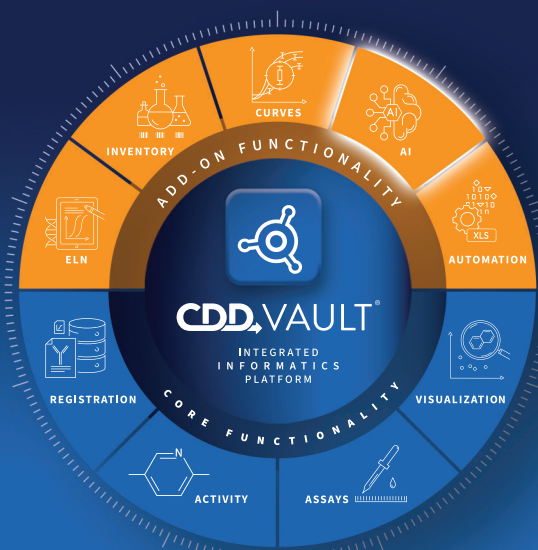




AI DATASHEET

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.

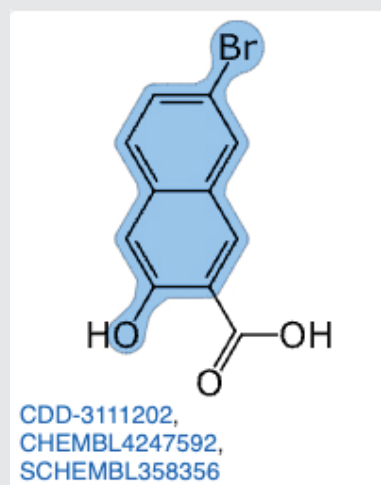
BIOISOSTERIC SUGGESTIONS

- 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.

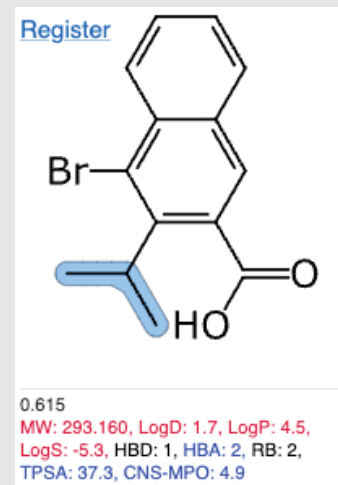
The screenshot shows the 'Bioisosteric suggestions' interface. It features a filter bar at the top, a grid of 12 suggested molecules, and a 'Register' button. Each molecule is represented by its chemical structure and a list of properties: MW, LogD, LogP, LogS, HBD, HBA, RB, TPSA, and CNS-MPO.

Structure	MW	LogD	LogP	LogS	HBD	HBA	RB	TPSA	CNS-MPO
0.632	291.105	1.2	3.2	-4.3	1	3	2	46.5	5.7
0.632	291.170	1.2	LogP: 3.8	-4.8	1	3	2	37.3	5.3
0.615	293.160	1.7	LogP: 4.5	-5.3	1	2	2	37.3	4.9
0.615	279.155	1.8	LogP: 4.1	-4.9	1	3	2	37.3	5.1
0.600	293.160	LogD: 0.3	LogP: 3.0	-4.2	1	3	2	37.3	5.5
0.690	291.105	LogD: 0.6	LogP: 3.4	-3.9	1	3	2	37.3	5.3
0.681	295.150	LogD: 0.9	LogP: 2.9	-4.1	1	3	2	37.3	5.5
0.656	309.159	LogD: 0.4	LogP: 3.4	-6.1	1	3	2	37.3	5.3
0.648	297.120	LogD: 1.2	LogP: 3.7	-4.7	1	3	2	37.3	5.4
0.630	309.159	LogD: 1.1	LogP: 3.3	-4.3	1	3	2	37.3	5.3
0.636	311.131	LogD: 0.7	LogP: 2.2	-5.6	1	3	2	37.3	5.2

Bioisostere suggestion results



Results include references to external databases for published molecules



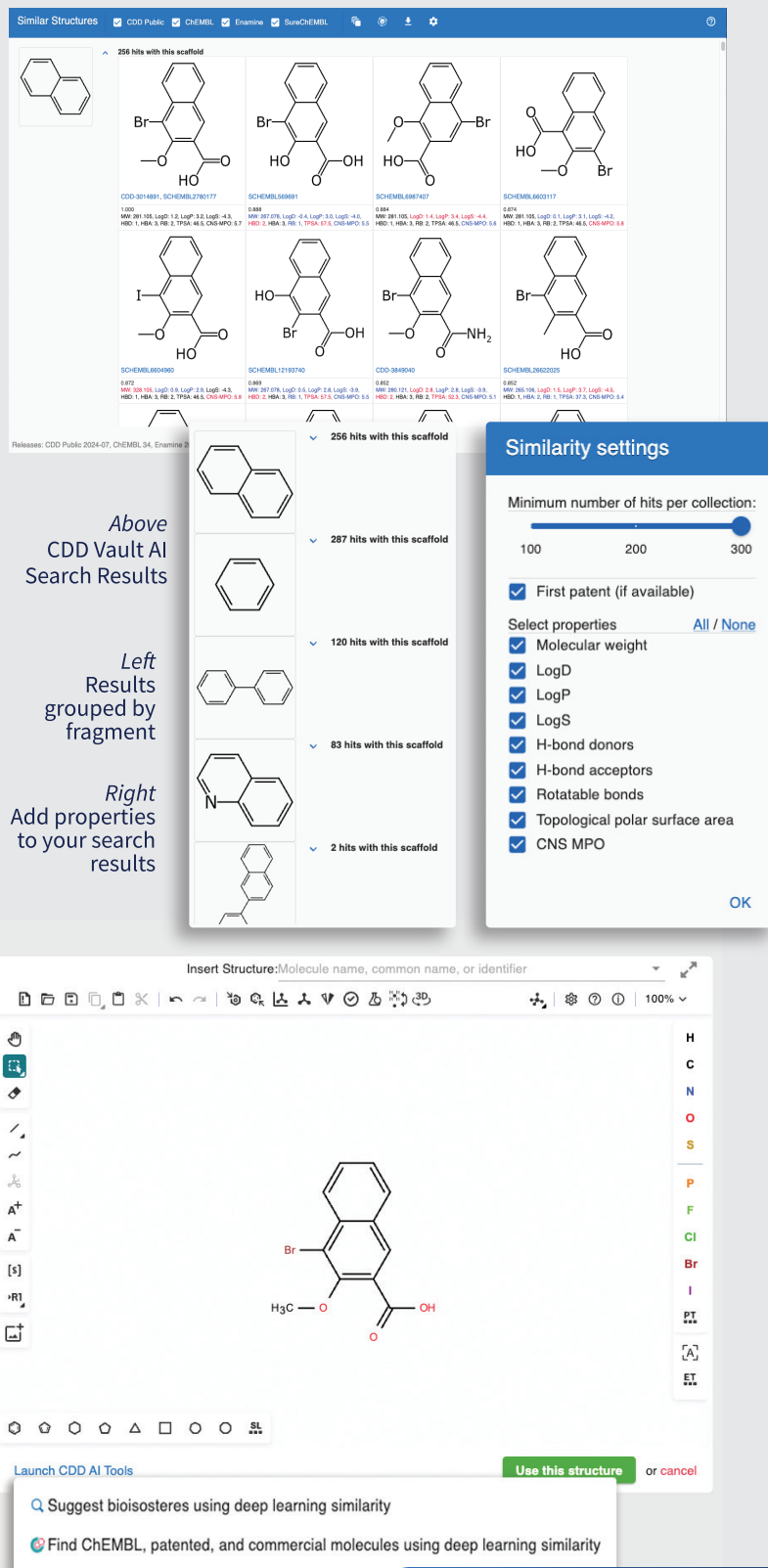
Customize results with predicted properties and easily register bioisosteres

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.






The screenshot displays the CDD Vault AI search interface. At the top, it shows 'Similar Structures' with a grid of chemical structures and their associated identifiers (e.g., CDD-3014891, SCHEMBL278177). Below this, a 'Similarity settings' panel is visible, allowing users to adjust the 'Minimum number of hits per collection' (ranging from 100 to 300) and select properties for analysis, such as Molecular weight, LogD, LogP, LogS, H-bond donors, H-bond acceptors, Rotatable bonds, Topological polar surface area, and CNS MPO.



On the left side, a vertical list of scaffolds is shown with the number of hits for each: 256 hits with this scaffold, 287 hits with this scaffold, 120 hits with this scaffold, 83 hits with this scaffold, and 2 hits with this scaffold. Annotations indicate that these results are 'Above CDD Vault AI Search Results' and 'Left Results grouped by fragment'. A note on the right says 'Right Add properties to your search results'.


At the bottom, the 'Molecule editor' is shown with a chemical structure of a substituted benzene ring. The editor includes a toolbar with various drawing tools and a legend on the right side listing elements: H, C, N, O, S, P, F, Cl, Br, I, PT, and ET. A 'Use this structure' button is present at the bottom right of the editor.

Two pop-up boxes are visible at the bottom of the editor: 'Suggest bioisosteres using deep learning similarity' and 'Find ChEMBL, patented, and commercial molecules using deep learning similarity'.

Bioisosteric suggestions  

Filter by fragment: All / None  Download bioisostere results

Bioisosteric suggestions  

Filter by fragment: All / None  Launch Visualization

Download results or push them into Visualization

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

Learn more at collaboratedrug.com
or contact us at info@collaboratedrug.com