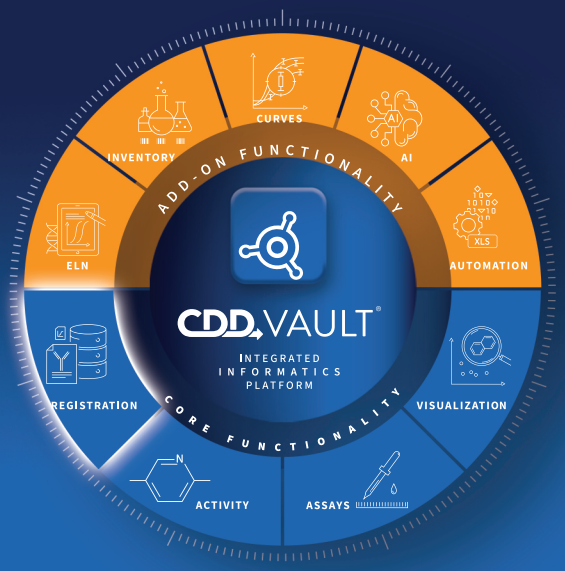
BIOCONJUGATE

REGISTRATION

DATA SHEET



CDD Vault's advanced macromolecule support allows for both biologists and chemists to see relevant information on registered bioconjugate molecules in CDD Vault.

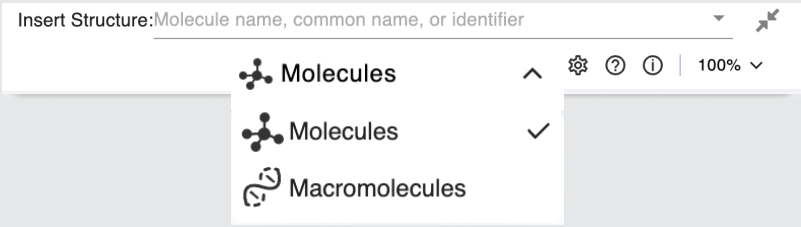
MACROMOLECULE DRAWING MODE

- The CDD Vault drawing tool now includes a macromolecule mode for drawing DNA, RNA, Peptides, as well as unnatural, modified bioconjugates.
- Macromolecules can be viewed as one letter codes, as monomers in a linear snake mode or as monomers in a flexible canvas mode for custom monomer orientations.
- Macromolecule mode includes a built-in library of natural and unnatural amino acid monomers, as well as a nucleotide builder tool for customizing nucleotide phosphates, sugars and bases.
- In addition to drawing molecules in the structure editor, macromolecule mode also supports the import and export of multiple file types, including HELM and IDT.

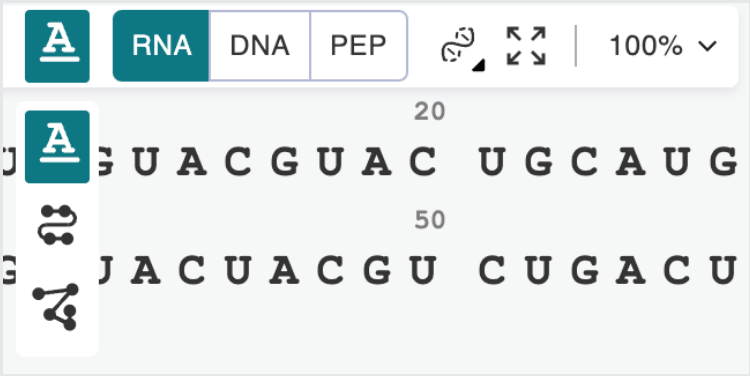
MACROMOLECULE REGISTRATION

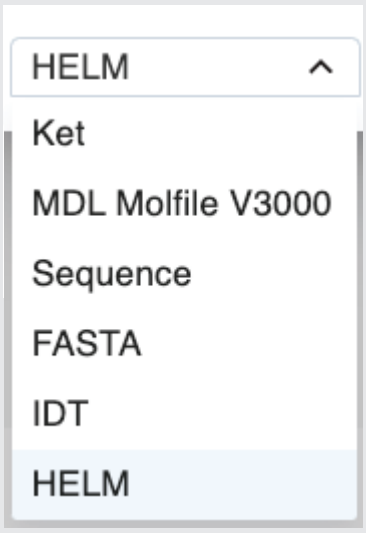
- CDD Vault supports the registration of bioconjugate molecules using molfiles generated by the macromolecule drawing tool to maintain chemical awareness.

Switch between small molecule and macromolecule drawing

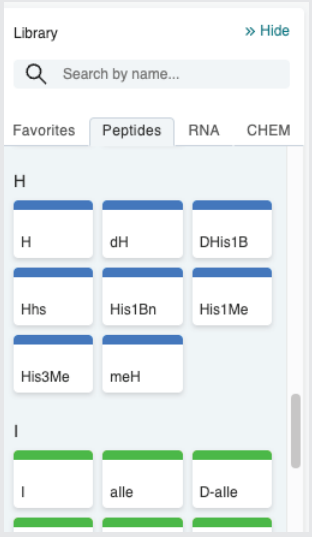


Macromolecule mode drawing options for RNA, DNA and Peptides





Supported file types for import and export into CDD Vault's structure editor



Monomer library included in CDD Vault's macromolecule editor.

CDD VAULT®
Complexity Simplified

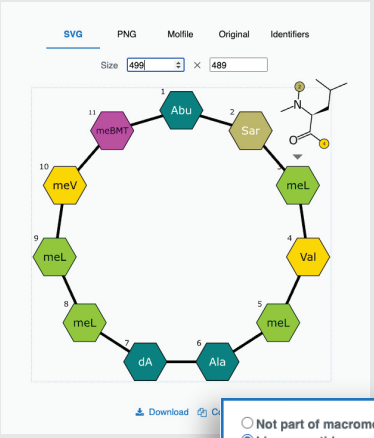
REGISTRATION
DATA SHEET

- Batch linking allows you to track the lifecycle of your registered entities, providing insights into bioconjugate parts.
- Molfiles enable registration and viewing of bioconjugates within CDD Vault while also maintaining the structural information underlying the monomers and connections.
- Molfiles used for registration contain all the information needed for molecule rendering, removing any dependence on custom libraries for proper visualization of bioconjugates.
- Hovering over a monomer in a registered molecule will show the underlying chemical structure of the monomer.

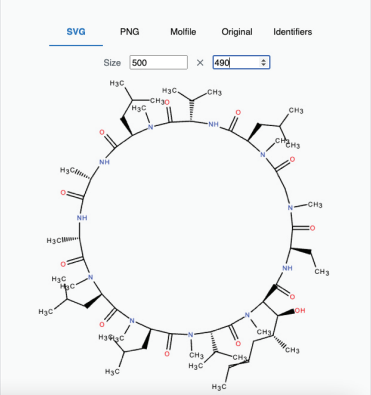
COMPOSE MACROMOLECULE IMPORT MODE

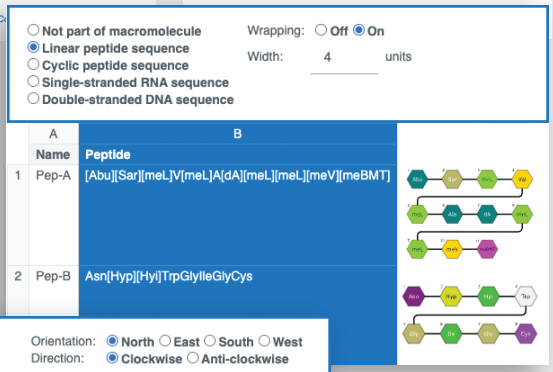
- CDD Vault supports the bulk import of macromolecules within the Import Data tab and the new *Compose Macromolecules* option.
- Uploading a csv or xlsx file enables the bulk creation of linear peptides, cyclic peptides, ssRNAs, and dsDNA molecules.
- To define the monomers during upload, *Compose Macromolecules* supports one or three letter codes for natural monomers, and unnatural monomers contained in brackets as defined at the CDD Vault account level library.
- *Compose Macromolecules* will convert the sequences in a spreadsheet to a molfile that is used to import macromolecule structures and any additional columns can be mapped for molecule data and/or assay data.

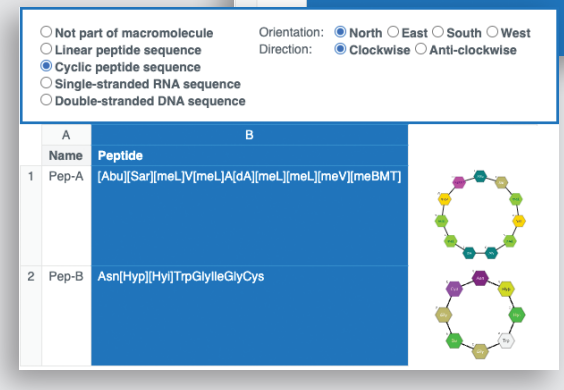
Registered peptide with chemical structure of a monomer being shown

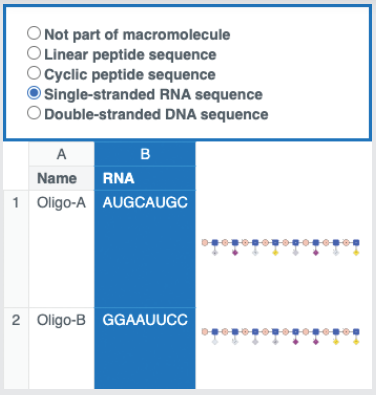


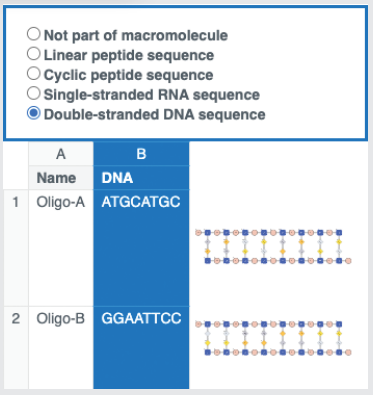
Full atomistic view of registered cyclic peptide











Compose macromolecules mode options

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