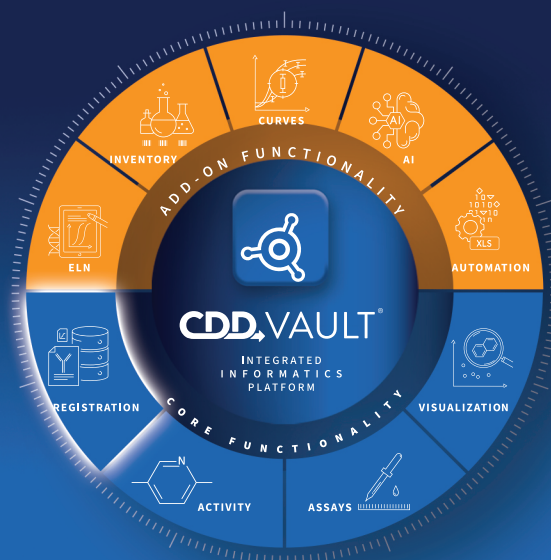




BIOCONJUGATE

# 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

Insert Structure:

- Molecules ^
- Molecules ✓
- Macromolecules

Macromolecule mode drawing options for RNA, DNA and Peptides

RNA DNA PEP

20  
U A C G U A C U G C A U G

50  
J A C U A C G U C U G A C U

HELM ^

Ket

MDL Molfile V3000

Sequence

FASTA

IDT

HELM

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

Monomer library included in CDD Vault's macromolecule editor.

Library >> Hide

Search by name...

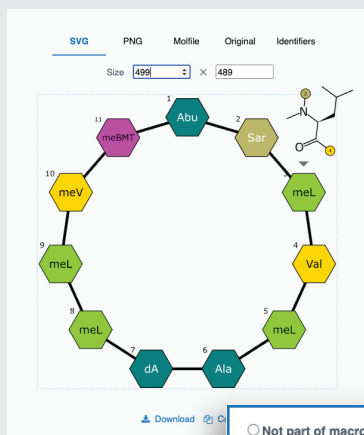
Favorites Peptides RNA CHEM

H		
H	dH	DHis1B
Hhs	His1Bn	His1Me
His3Me	meH	
I		
I	alle	D-alle

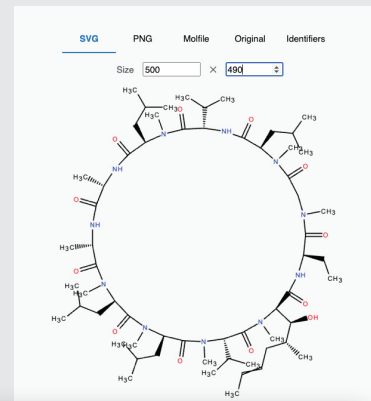


- Batch linking allows you to track the lifecycle of your registered entities, providing insights into bioconjugate parts.
- Molfiles enable registration and viewing of bioconjugates within CDD Vault while also maintaining the structural information underlying the monomers and connections.
- Molfiles 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.

Registered peptide with chemical structure of a monomer being shown



Full atomistic view of registered cyclic peptide



## 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.

Not part of macromolecule  
 Linear peptide sequence  
 Cyclic peptide sequence  
 Single-stranded RNA sequence  
 Double-stranded DNA sequence

Wrapping:  Off  On  
Width: 4 units

	A	B
Name	Peptide	
1 Pep-A	[Abu][Sar][meL][V][meL][A][dA][meL][meL][meV][meBMT]	
2 Pep-B	Asn[Hypp][Hy]TrpGlyIleGlyCys	

Not part of macromolecule  
 Linear peptide sequence  
 Cyclic peptide sequence  
 Single-stranded RNA sequence  
 Double-stranded DNA sequence

Orientation:  North  East  South  West  
Direction:  Clockwise  Anti-clockwise

	A	B
Name	Peptide	
1 Pep-A	[Abu][Sar][meL][V][meL][A][dA][meL][meL][meV][meBMT]	
2 Pep-B	Asn[Hypp][Hy]TrpGlyIleGlyCys	

Not part of macromolecule  
 Linear peptide sequence  
 Cyclic peptide sequence  
 Single-stranded RNA sequence  
 Double-stranded DNA sequence

	A	B
Name	RNA	
1 Oligo-A	AUGCAUGC	
2 Oligo-B	GGAUUUCC	

Not part of macromolecule  
 Linear peptide sequence  
 Cyclic peptide sequence  
 Single-stranded RNA sequence  
 Double-stranded DNA sequence

	A	B
Name	DNA	
1 Oligo-A	ATGCATGC	
2 Oligo-B	GGAATTCC	

Compose macromolecules mode options

Learn more at  
[collaboratedrug.com](http://collaboratedrug.com)  
or contact us at  
[info@collaboratedrug.com](mailto:info@collaboratedrug.com)