

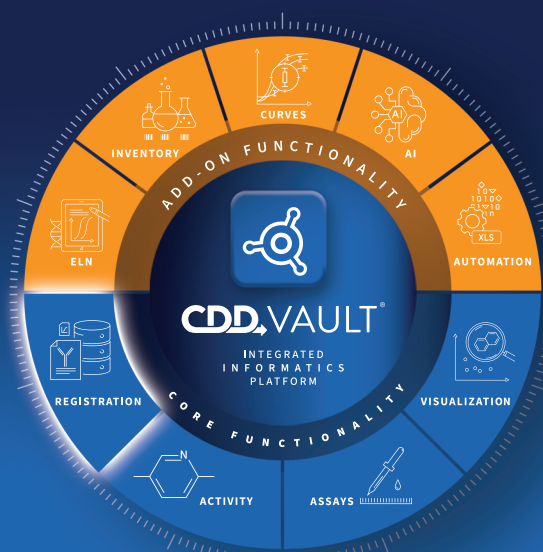


siRNA

REGISTRATION

DATA SHEET

CDD Vault simplifies registration of small interfering RNA (siRNA) molecules through the compose macromolecule editor, allowing seamless entity rendering, and data capture of complex nucleotide modalities.

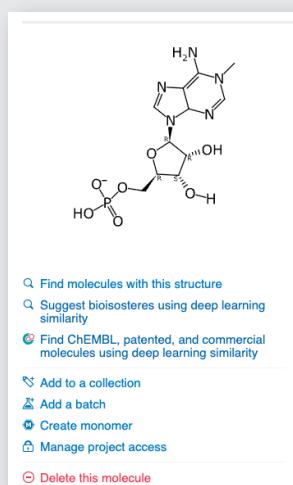


CUSTOM NUCLEOTIDE MONOMERS

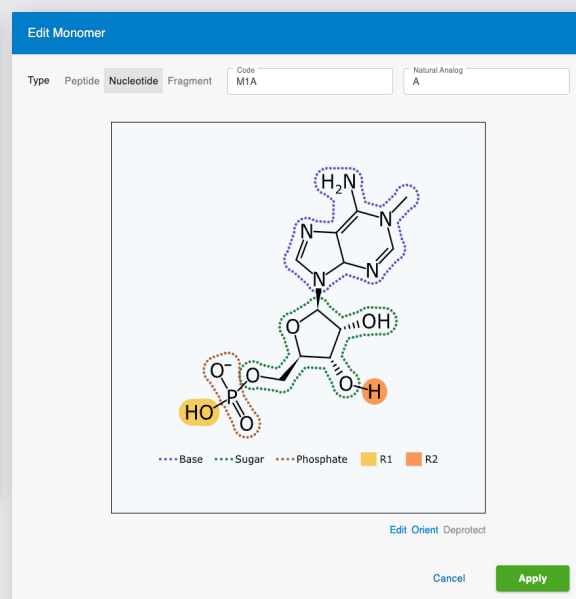
- CDD Vault's monomer library allows users to register small molecule monomers in CDD Vault and add them to the monomer library.
- CDD Vault's built-in molecule sketcher allows users to mark their R1 and R2 leaving groups as well as the sub-components (Sugar, Phosphate and Base) of the monomers for proper rendering in siRNA complexes.
- Customer monomer annotation is stored alongside the registered small molecule to allow Vault to easily remove leaving groups during siRNA construction.
- In addition to single monomer creation, small molecules can be uploaded as monomers in bulk using the import data tab of CDD Vault for mass imports.

siRNA UPLOAD AND RENDERING

- CDD Vault's macromolecule upload has capabilities for "Chemically Aware" siRNAs for biologists and chemists.
- CDD Vault will automatically render siRNA images based on sequences provided and available metadata.



Create monomer option in CDD Vault



Monomer code creation and annotation

	A → Structure	B	C → Natural	D → Code	
	SDF Molfile	Molecule Name	Natural	Code	2D-MOE-A*
1		RJT-0010033	A	Z'-MOE-A*	
2		RJT-0010032	C	dM-C*	
3		RJT-0010031	A	dA*	
4		RJT-0010030	T	dT*	
5		RJT-0010029	G	dG*	

Bulk monomer import



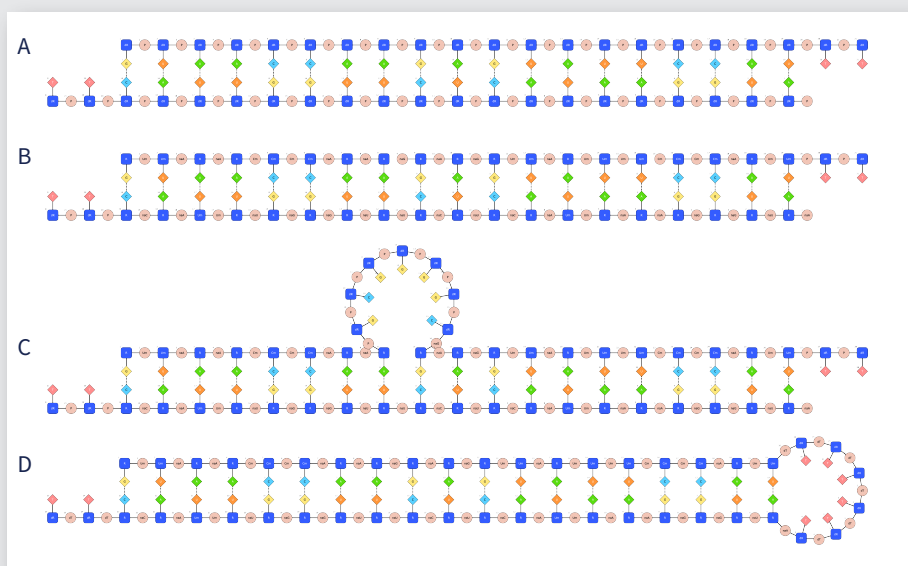
- siRNA sense and antisense strands can be uploaded as linear nucleotide sequences that include natural or custom nucleotide codes, and with a default DNA or RNA sugar backbone.
- Metadata can be appended to the strand sequences to map the location of strand hybridization, mark any chain breaks, and denote end-to-end chain connections.
- Vault will register both sense and antisense strands with the phosphate, sugar and bases color coded for easy identification.
- All siRNA entities are stored as a Self-Contained Sequence Representation (SCSR) molfile, ensuring the storage of molecular structures and monomer annotations in an interoperable format.

CONNECTED CDD VAULT ECOSYSTEM

- siRNA composer easily pulls monomers from the built-in CDD Vault monomer library for seamless reference based on monomer code.
- Capture precise atomistic data for better AI/ML application and facile integration with customer data ecosystem via UI or API.
- Registration IDs can be used to quickly associate assay data to your siRNA entities and viewed within a search report table.
- Referencing siRNAs in the ELN will automatically create a breadcrumb link to the ELN entry from the molecule page.
- All siRNA entities are stored as SCSR based molfiles that provide a machine readable format for all metadata, sequence and structure information.

A	B	C
Name	Sense	Antisense
1 siRNA Natural	GUAACCAAGAGUAUCCAUTT{1-19:1}	AUGGAUACUCUUGGUUACTT{19:1}
2 siRNA Custom	[naG][Um][naA][naA][Cm][naA][naG][naA][naG][Um][naA][Um][Um][Cm][naA][Um]TT{1-19:1}	[naA][naU][naG][naA][naA][Um][naA][naC][naU][naC][naU][naG][naC][naU][naA][naC]TT{19:1}
3 siRNA with Bubbles	[naG][Um][naA][naA][Cm][naA][naA][GCGGGGC][naA][naG][Um][Um][Um][Cm][naA][Um]TT{1-6:1}{16-26:2}	[naA][naU][naG][naA][naA][Um][naA][naC][naU][naC][naU][naG][naC][naU][naA][naC]TT{19:1}{11:2}
4 siRNA with Breaks	[naG][Um][naA][naA][Cm][naA][naA][naG][naA][naG][Um][naA][Um][Um][Cm][naA][Um]TT{1-19:1}	[naA][naU][naG][naA][naA][Um][naA][naC][naU][naC][naU][naU][naG][naC][naU][naA][naC]TT{19:1}
5 siRNA Connected	[naG][Um][naA][naA][Cm][naA][naA][naG][naA][naG][Um][naA][Um][Um][Cm][naA][Um]dT{1-19:1}{8:1}	{A:1}{dT}{dT}{dT}{dT}{dT}[naA][naU][naG][naG][naA][naA][Um][naA][naC][naU][naC][naU][naA][naC]dT{23:1}

Sense and antisense strands mapped and siRNA rendered



Different siRNA rendering options:

A: siRNA with 2 base overhangs

B: siRNA with sense strand breaks

C: siRNA with sense strand bubble

D: siRNA with terminal hairpin

1 Selected: Launch Visualization Export Add to collection Build model Flag outliers Customize your report Save this search									
Select...	Properties	Molecule Fields	Batch Fields	PK Intravenous Dosing: Exponential Decay Equation	Inventory Summary	Area under the curve	Tau	Plot Time - Measured Concentration	
all	log P	log D	ELN Entry	Type	Sample Count: 1	58.3	1.20		
none					Amount Remaining: 57.0 g			Flag outliers & Override	
	-75.3	-111.1	Ex-000001 - siRNA Synthesis	siRNA					
BioV-0000058 KayTee Therapeutics									

siRNA in a Vault search results table with molecule properties, ELN link, inventory summary and assay information

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