

ELN

Search entries

The screenshot displays the ELN interface with a search bar and filter options. A callout box explains search syntax: "Search for term(s)" with bullet points: "Wildcard: *", "Use leading zeros for IDs", and "Use double quotes for exact search". Another callout points to the search button: "Search for substructure". A third callout points to the filter dropdown: "Filter entries by" with options "Author" and "Status".

On the left sidebar, a callout box states: "ELN entries associated with a project" pointing to the "Projects" section, and another callout states: "ELN entries" with a bullet point "Click to open" pointing to the "Public Data" section.

The main table lists entries with columns: ID, Title, Author, Modified, Created, and Status. The entries are:

ID	Title	Author	Modified	Created	Status
1186	Diels-Alder reaction of 1,3-butadiene ...	Heather Mattson Ar...	2018-11-27	2018-03-26	Open
3101	Analysis of 5-[2-chloro-5-(trifluoromet...	Heather Mattson Ar...	2018-11-02	2018-10-17	Open
2935	Coomassie Blue Analysis w				
1187	Principles of Early Drug Dis				
1367	Squamous cell tumors				
2202	Quinone methide synthesis				

An inset window shows a search for "mice" with the filter "with structure". It displays the entry for ID 1367, "Squamous cell tumors" by Heather Mattson Ar... The entry body contains text with "mice" in bold. A callout box states: "Search terms appear in bold in context". Another callout box states: "Attached MS Office documents, PDF and text files are searched".

At the bottom of the inset, two chemical structures are shown: a 2,4-dichlorophenyl ring and a piperazine ring.

ELN

Create new entry

Explore Data **ELN** Imp

+ Create a new ...

Protocol

Molecule

Project

ELN Entry

Select Create a new > ELN Entry

Select Project

Project ABC

Select project

Begin Editing

Duplicate an existing ELN entry

Finalize entry once complete

Print entry to PDF

Download attached files as .zip file

Synthesis of 2,2,2-trifluoroethyl (1S)-cyclohex-3-ene-1-carboxylate

Title

ID: 2367

Project: Project ABC

PI

Project code

Location: NA

Date

File

Upload File

Add metadata fields in Settings>Vault>ELN Fields

Normal Text

B / U

Save status: auto-saves 8 times per second

Save

Duplicate of: Entry: 1186 - Diels-Alder reaction of 1,3-butadiene and 2,2,2-trifluoroethyl prop-2-enoate to form 2,2,2-trifluoroethyl (1S)-cyclohex-3-ene-1-carboxylate (hereafter referred to as 'product'). The product will be isolated by vacuum filtration and weighed. The product will be analyzed using melting point.

Elements

- Insert a link
 - URL
 - CDD object
- Attach file
 - Click icon
 - Drag and drop
- Insert table
 - Click icon
 - Copy/paste from Excel
- Insert structure
- Insert assay annotation

C=CC=C + C=CC(=O)OCC(F)(F)F >> C1=CCCCC1C(=O)OCC(F)(F)F

ELN Elements

Links

Search for CDD object or paste URL

Insert CDD Objects:

- Molecules
- Protocols
- Protocol runs
- ELN entries

Display Options

- Text
- Caspase 12 Assay - 2018-08-10

Select display

- Custom text
 - URL entered if blank
- Default text
- Structure (molecules only)

Display in ELN Entry

Click link to go to object

Mouse over link to edit or attach Run Export (runs only)

Attached Run Export

Active hyperlinks

<https://www.ncbi.nlm.nih.gov/pubmed/28203483>

File Attachments

Image files and first page of PDF files rendered

PDB files rendered in an interactive viewer

- Drag to rotate
- Shift + drag to zoom

Additional file types appear as links

Import data from CSV or SDF files

View imported data

Assay results

- [Inhibition Data.csv](#)
- [Inhibition Data.csv](#)
- [Inhibition Data.csv](#)

[betaLactams.sdf](#)

[Explore imported data](#)

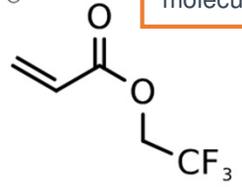
Molecules and Reactions



Registration number link added to drawn structures already registered

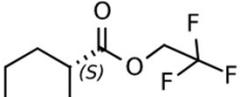
HADV-0035551

Register molecule

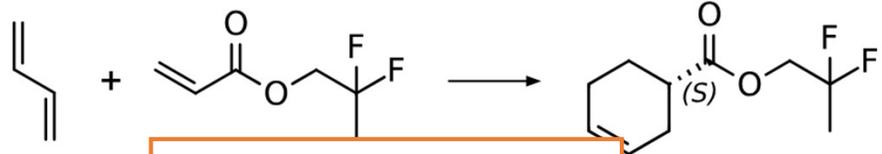


Only displayed molecules are substructure searchable

Link to registered molecule record



HADV-0000170 (003)



Attach CDX or CDXML files from ChemDraw to add reaction and stoichiometry table

Reactants				
Formula	C4H6	C6H8F2O2	Formula	C10H14F2O2
MW	54.09	150.12	MW	204.22
Limiting?	Yes	No	Equivalents	

Tables

ID	Inhibition	SEM
HADV-0000170	-10.336685	4.597
	3609	6.568486

Edit Table

- Insert link
- Insert file
- Insert structure
- Insert/delete row or column
- Delete table

Assay Annotation

In ELN Entry

Assay Annotation

This is an assay to identify potential treatments for an unknown disease, by investigating the biological process of target from **Mus musculus**.

This is a **ADMET/functional/plasma stability assay** in , using , with physical detection method, using an unknown detection instrument

Auto-generated text from annotations

Target

Bioassay Type

- ADMET
- functional

Mode Of Action

- inhibition

Summary of annotations

Method

Bioassay

- plasma stability assay

Assay Cell Line

- 184B5 cell



Dialog

TARGET
METHOD

bioassay type
 ADMET functional

Mode Of Action (click to see proposals)

Proposals

inhibition

activation

Proposals are above dotted line

Start typing to select desired value
 Note: Add custom annotations by typing desired value