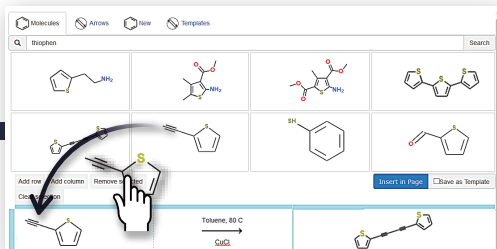




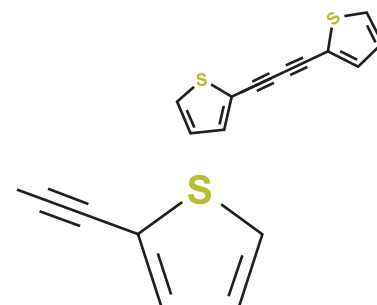
ELN for CHEMISTRY

The chemistry tools for the LabCollector Electronic Notebook are useful for many types of labs. Import structures from LabCollector's Chemical Structures module or design on the fly. Chemical reactions and molecules can be integrated in lab book pages and reporting.

Search



Build



Insert

Amount	10.51 grams		
MW	108.16		214.31

Chemical reactions can be saved and reused

Fully integrated with
LabCollector LIMS:
a collaborative database
for all labs

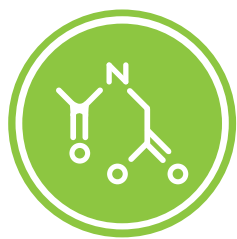
- ▶ Draw or upload molecules directly within LabCollector
- ▶ Supported upload formats: cdx, mol, sdf, cif, pdb
- ▶ Forms autocomplete based on molecule drawn
- ▶ Keep track of exact chemicals and lots used in experiments
- ▶ Create templates for common types of experiments

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Fax: +1 (800) 453 9128

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LabCollector
www.LabCollector.com



CHEMICAL STRUCTURES

LabCollector LIMS Management Module

LabCollector is a web-based **LIMS** allowing laboratories to store, track and share information related to their **R&D** or **production** (storage, stock and order manager, barcode tracking, log activity recorder).

It integrates a specific module to manage **Chemical structures**. It supports **2D/3D structures** (MOL, CIF, PDB and CDX formats) and **spectra**. A powerful **sub-structure search engine** (with molecule designer) can be added to take full advantage of the structures database.

Thousands of molecules can be quickly imported with the integrated SDF or CDX importer.

HOME MODULES & ADD-ONS TOOLS ADMIN HELP ALERTS 6

Search by: Keyword ID

Operator: AND Sort results by: Id ASC strict search + archived records

Name LIKE: From Project: Range: Form is: Structure is: Owned by: From group:

Date created: Filter: Storage filter:

Current Structure Query

Substructure Search:

Substructure Query: Cc1cccs1 Edit/Design query

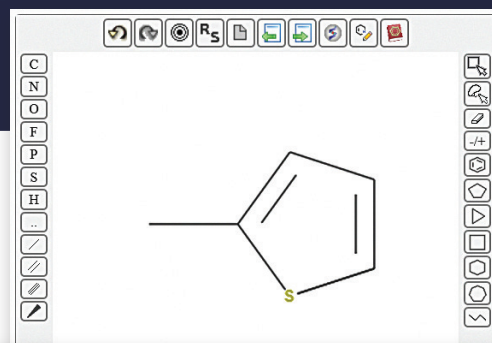
Reset Structure

Current cache from: 2017-01-17 18:55:44 Create New Normalized Cache (Note: This may take several minutes)

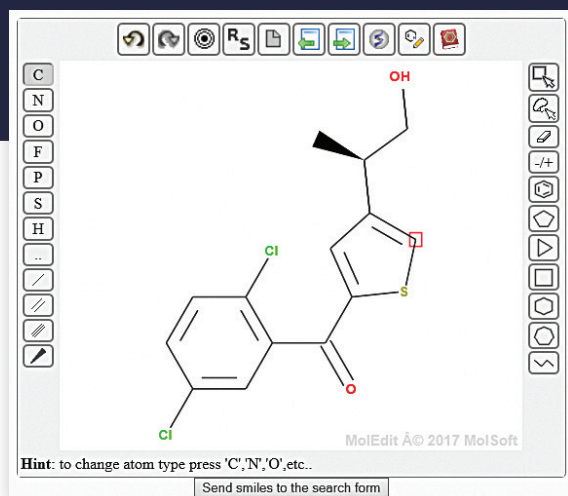
2211 results found | Show/Hide all results on page | Table View

ID	Formula	SMILES	MW	Form	LogP
1	C14H13N3O3		301.31	liquid	45
BB_SC-0001	C8H11O2NS		185.24		
BB_SC-0007	C9H11NO4S		229.25		

Sub structure search



Molecule designer



Design any molecule using the editor.

Current Structure Query

Substructure Search:

Substructure Query: Cc1cccs1 Edit/Design query

Reset Structure

Current cache from: 2017-01-17 18:55:44

Create New Normalized Cache

The molecule designer allows a quick and effective search of all chemical structures stored in LabCollector.

Fully integrated with
LabCollector LIMS:
a collaborative database
for all labs

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