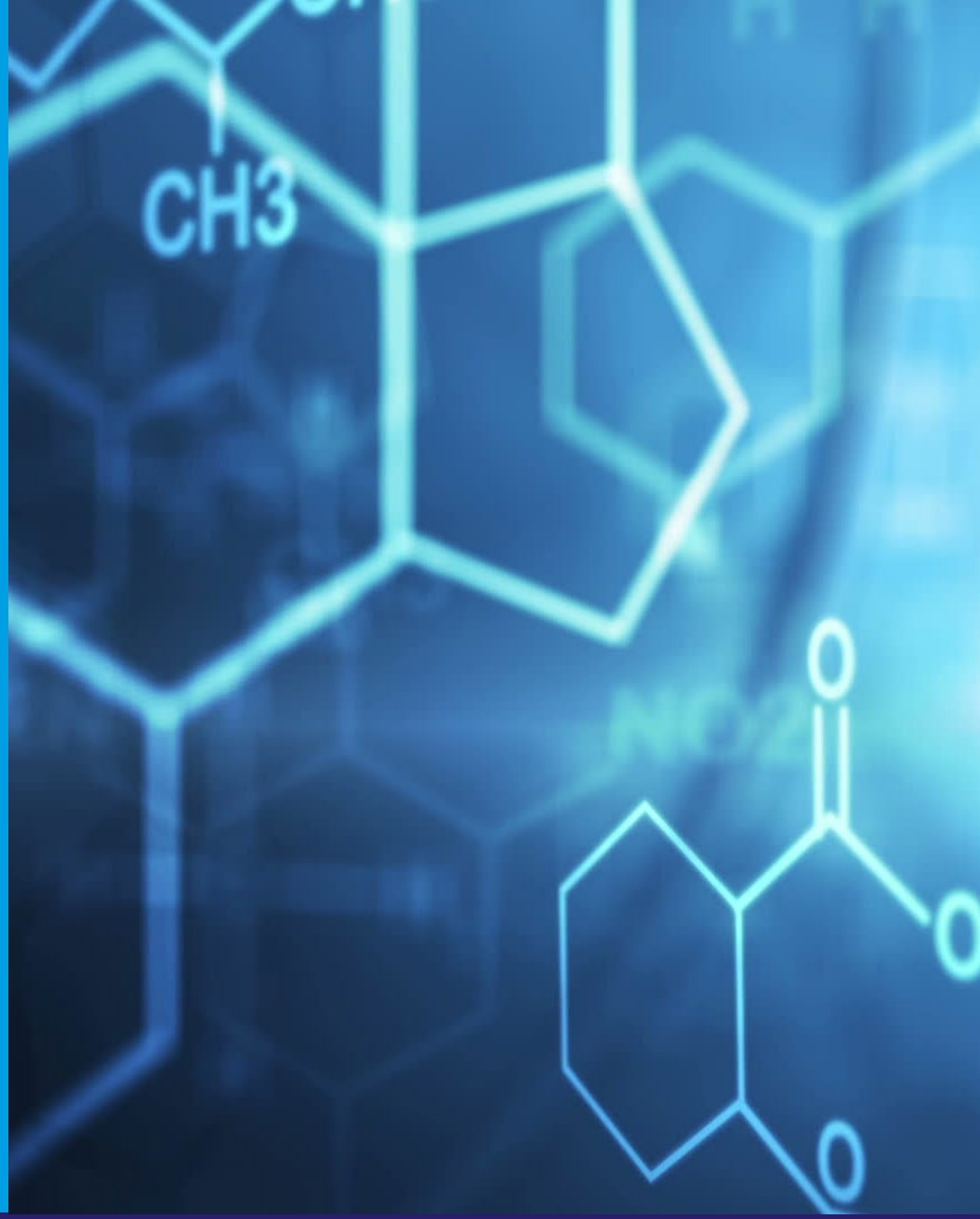
# IDBS & ChemAxon: Our Strategic Partnership

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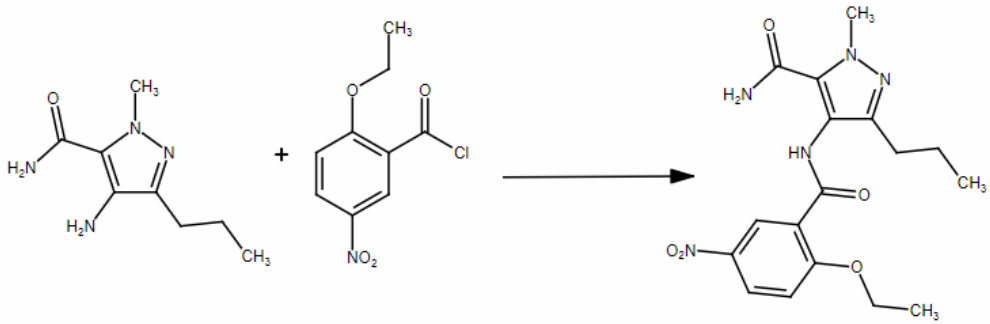
E-WorkBook CHEMISTRY | Save | Stoichiometry | Show title | Done

Overview

Total reaction mass
46.398 g

Total reaction volume
141.354 mL



Edit reaction
Find component
Print worksheet
Clear reaction

Components | Conditions | Health & Safety | Procedure | Registration | Analytical

Columns

| Reactants | Add new | Limit | Equiv. | Mass | Volume | MW (g/mol) | Purity (%) | Quantifier | n | Supplier ID | Batch ID | CAS Number | Synonym |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| (R1) 4-amino-2-methyl-5-propylpyrazo... | | ✓ | 1 | 10 g | | 182.227 | 100 | | 54.877 mmol | Internal | | | |
| (R2) 2-ethoxy-5-nitrobenzoyl chloride | | | 1.2 | 15.121 g | 12.601 mL | 229.62 | 100 | 1.2 g/mL | 65.852 mmol | | | | |

| Agents | Add new | Limit | Equiv. | Mass | Volume | Purity (%) | Quantifier | n | MW (g/mol) | IUPAC name |
|---|---|---|---|---|---|---|---|---|---|---|
| (A1) DIPEA | | | 3 | 21.277 g | 28.753 mL | 100 | 0.74 g/mL | 164.63 mmol | 129.243 | N,N-diisopropylethylamine |

| Solvents | Add new | Volume | Molarity | Solvent Vols | Comment |
|---|---|---|---|---|---|
| (S1) DCE | | 100 mL | 0.549 M | 10 | |

| Catalysts | Add new |
|---|---|

| Products | Add new | Formula | Mass [expected] | Mass [actual] | Purity (%) | n [expected] | n [actual] | Yield |
|---|---|---|---|---|---|---|---|---|
| (P1) 4-(2-ethoxy-5-nitrobenzamido)-2-... | | $C_{17}H_{21}N_5O_5$ | 20.6 g | 19.8 g | 97 | 54.877 mmol | 51.163 mmol | |

Stoichiometry with integrations to reagent sources, analytical services and registration

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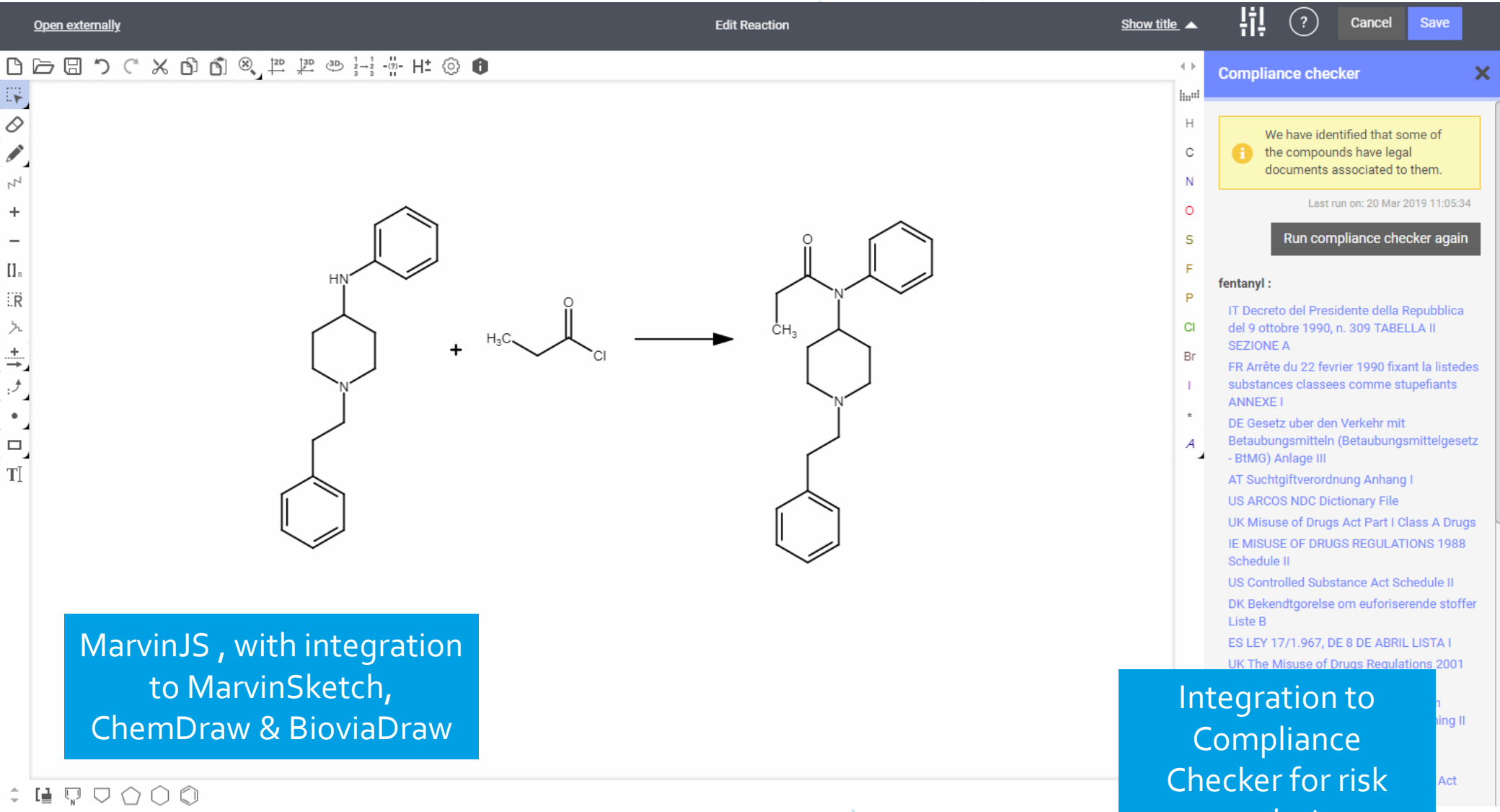


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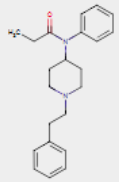
Registration Upload Staging Search

Quick search: type here any ID...

admin

Tree Browser

- CXN319
  - CXN319A
    - CXN319-001
    - CXN319-002

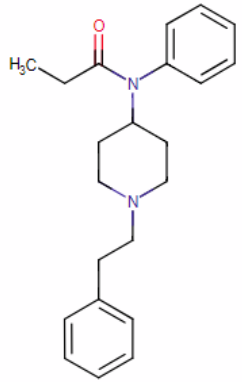


# CXN319-002

Using source **REGISTRAR** • Created on **2019-03-20 11:14:00**

Edit ··· More actions

| LnbRef | Created by | Molecular Formula | Mol Weight | Submitter |
|---|---|---|---|---|
| CXN319-002 | Ian | C22H28N2O | 336.479 | Ian |



**Additional Data**

| Project | Comment |
|---|---|
| | -- |

**Characterization**

NMR
structure consistent with spect
rum

**Uncategorized Data**

| % Yield | Experiment ID | Mass |
|---|---|---|
| 96.07 | Ian-0069 | 6.41 |

Project ID
aaa31f40350011e99fe400000
a0e0159

Oauth Single Sign-on

Direct access to the ChemAxon Registration record

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E-WorkBook ELN

Navigator | 1 My tasks | My workflows | Activity | Search

Search for Reactions | Search | Hide detail (3) | Options

Match ALL search terms

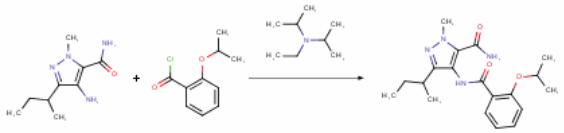
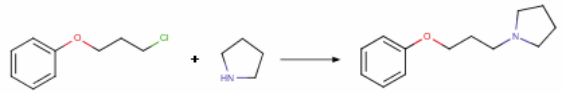
New...

Reaction chemistry
**Structure**
Defined
Substructure (Ignore stereo)

Experiment
**Created by**
is
Ian

Reaction chemistry
**Yield of Product**
greater than
70 %

Download ...

| Reaction | Title | Created By | Created At | Product Yield |
|---|---|---|---|---|
|  | Ian-0046 | Ian | 18 Jul 2018 14:59 19s | 88.151% (P1) |
|  | EXP-Ian1189 | Ian | 28 Mar 2018 11:17 8s | 98.078% (P1) |
| | EXP-Ian1393 | Ian | 26 Feb 2018 | 88.800% (P1) |

Search combining experimental and chemical information (JCHEM backend)

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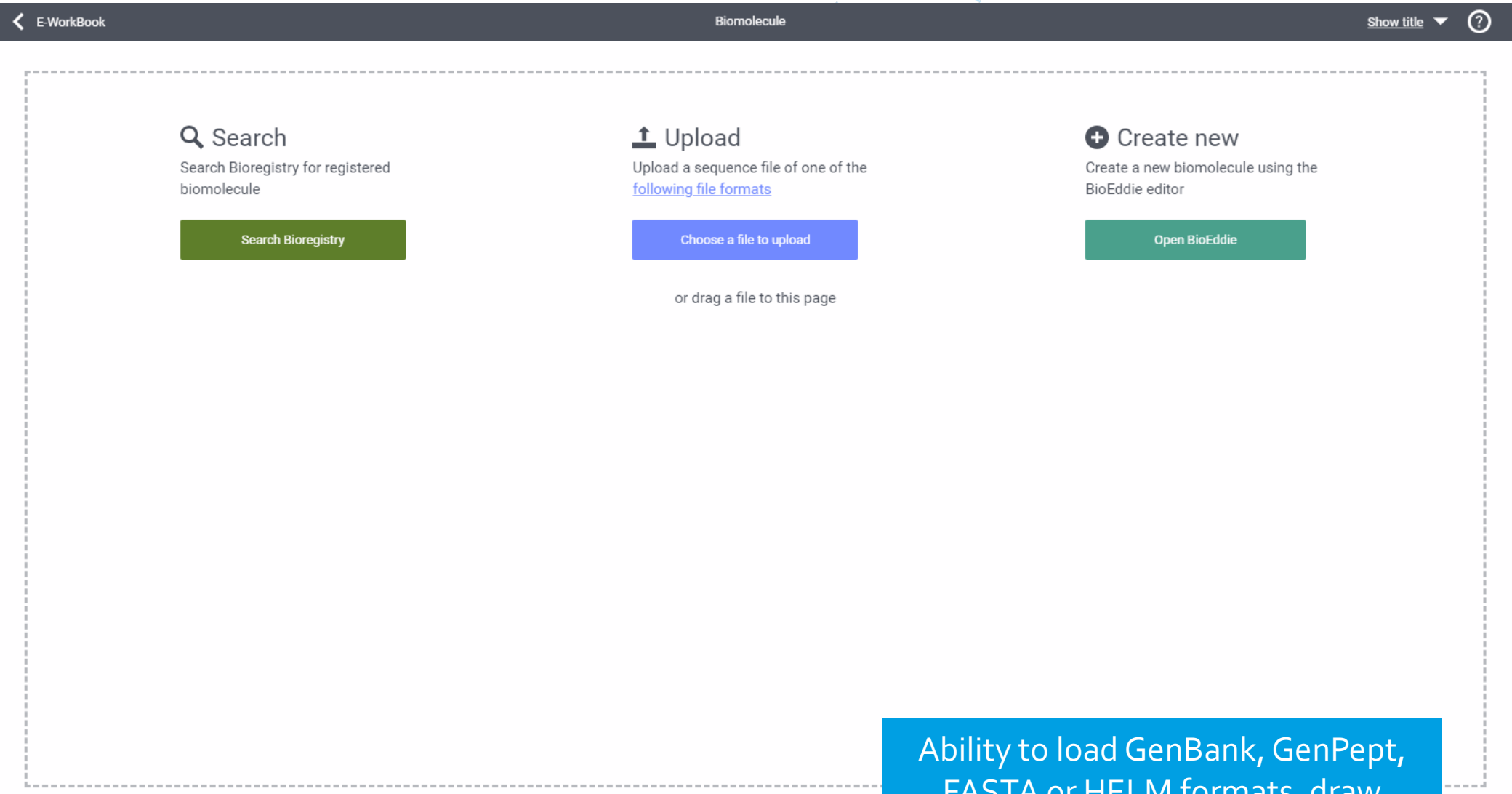


Ability to load GenBank, GenPept, FASTA or HELM formats, draw HELM and query bio-registration

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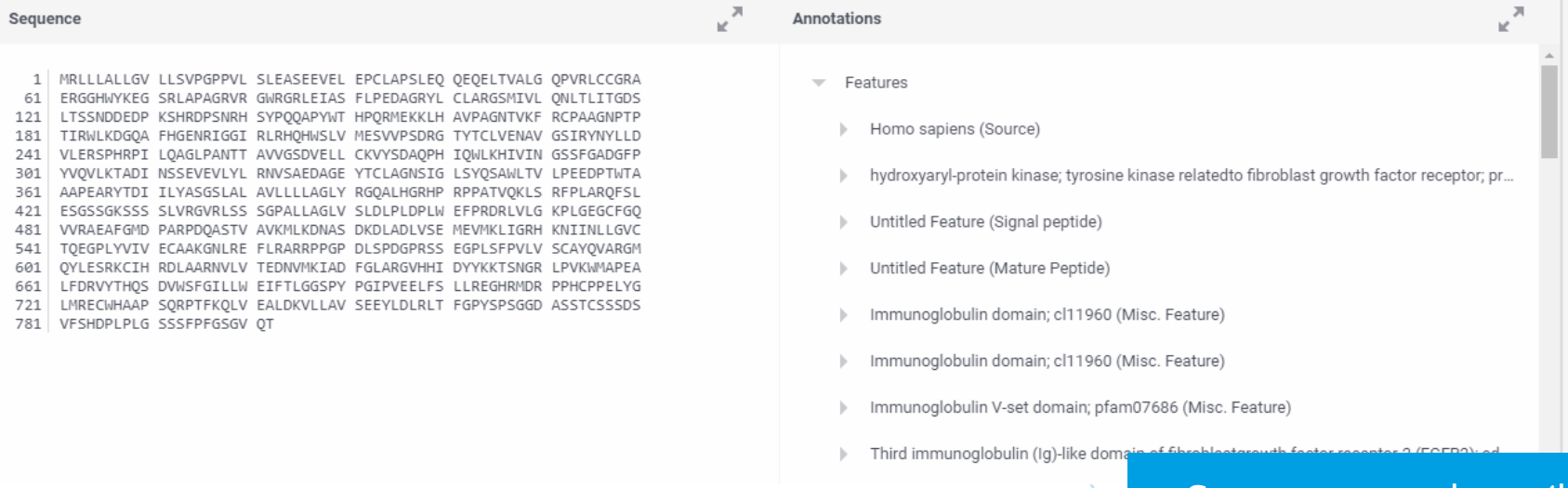





# Sequence renderer (linear/cyclic)

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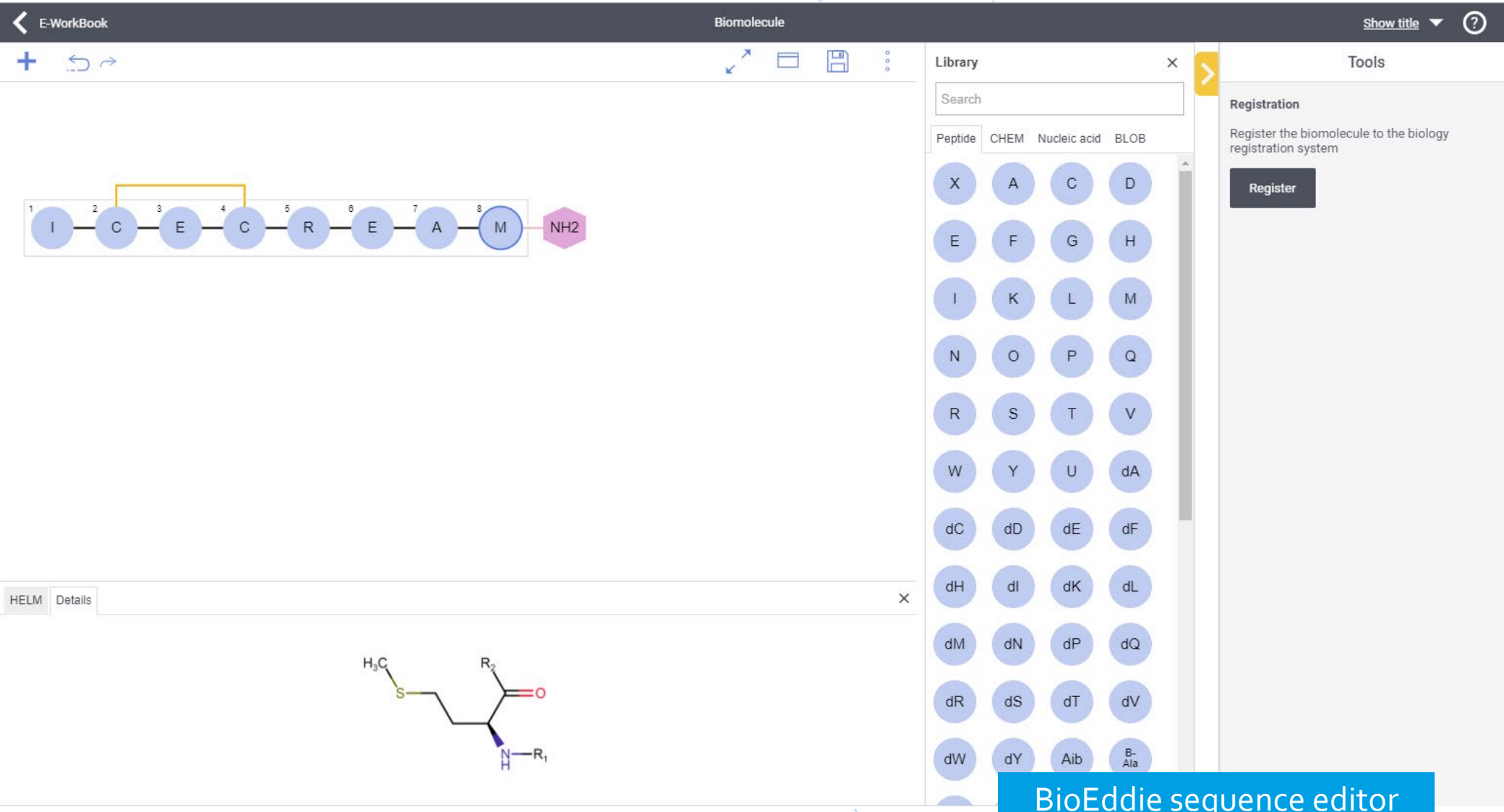


BioEddie sequence editor (BMT backend)

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E-WorkBook BIOREGISTRY

Help

# Search results

Search for a biomolecule | by properties

Refine results

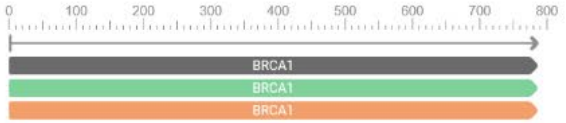
Clear all

Type

- Clear
- Protein
- Vector
- Antibody
- Enzyme

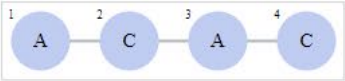
## BA_Ab1

| | |
|---|---|
| Sequence ID | CXN32 |
| Type | Antibody |
| Species | Arabidopsis thaliana |
| Accession Number | BA123 |



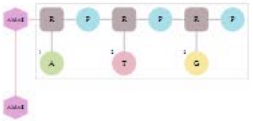

## d

| | |
|---|---|
| Sequence ID | CXN24 |
| Type | Antibody |
| Species | |
| Accession Number | |




## Delic

| | |
|---|---|
| Sequence ID | CXN18 |
| Type | Enzyme |
| Species | Escherichia coli |
| Accession Number | BHB12 |



## Drosophila melanogaster MIP31231 full insert cDNA

| | |
|---|---|
| Sequence ID | CXN15 |
| Type | Antibody |
| Species | |
| Accession Number | BT128753 |

IP Ian Peirson

Bio-Registration search by sequence/type (BMT backend)

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# Thank you!

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