

My Notebook - Table of Contents

New Plan | New Experiment | All Notebooks

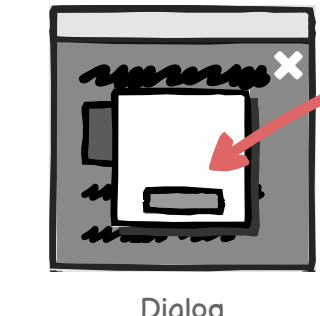
Search experiments [Filter] Search by Structure

Reaction	Date	Title
	7/10/21	Synthesis of 2-amino-2-oxoethyl 5-methyl-1-phenyl-1H-pyrazole-4-carboxylate (SPZ-341)
	6/10/21	Synthesis of cyanomethyl 5-methyl-1-phenyl-1H-pyrazole-4-carboxylate (SPZ-311)
	5/10/21	Synthesis of ethyl 5-methyl-1-phenyl-1H-pyrazole-4-carboxylic acid (SPZ-309)
	4/10/21	Synthesis of ethyl 5-methyl-1-phenyl-1H-pyrazole-4-carboxylate (SPZ-304)

Create new experiment from plan

Add a title for the experiment

Search structure initiates search through Chemical Information Service



Select Experiment Type from list

My Notebook - New Synthesis Plan

Add Title

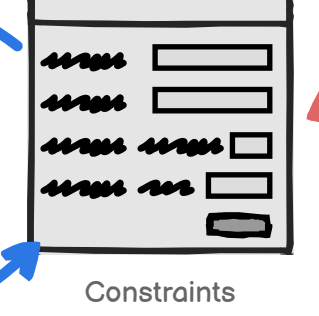
Draw Structure

Search Structure | Choose Service | Add Constraints

Save structure without search

Search by name or code or manually draw structure or reaction

Add constraints to the structure search based on metadata from chemical information



Search Results

Found 41 results out of 184 references with 53 reactions

Structure	IDs	Properties	Links
	66248	C <sub>27</sub> H <sub>32</sub> O <sub>8</sub> 634.453 Identification Spectra Physical Data Drugs Bioactivity Other Data	References Reactions
	66059	C <sub>27</sub> H <sub>32</sub> O <sub>8</sub> 634.453 Identification Spectra Physical Data Drugs Bioactivity Other Data	References Reactions
	42657	C <sub>27</sub> H <sub>32</sub> O <sub>8</sub> 634.47 Identification Spectra Physical Data Drugs Bioactivity Other Data	References Reactions
	58804	C <sub>27</sub> H <sub>32</sub> O <sub>8</sub> 634.453 Identification Spectra Physical Data Drugs Bioactivity Other Data	References Reactions
	22913	C <sub>27</sub> H <sub>32</sub> O <sub>8</sub> 634.28 Identification Spectra	References

Filter structure search by constraints

Click on links to view specific information and data

Import data and metadata from the selected reaction to populate experiment plan

Reactions

Found 20 reactions with 14 references

Steps	Yield	Reference
	77%	Reaction ID: 7849973x
	70%	Reaction ID: 7849973r
	70%	Reaction ID: 7849973r

Article Full Text

Article Abstract

New Synthesis Plan

Reaction

Materials

Safety Information

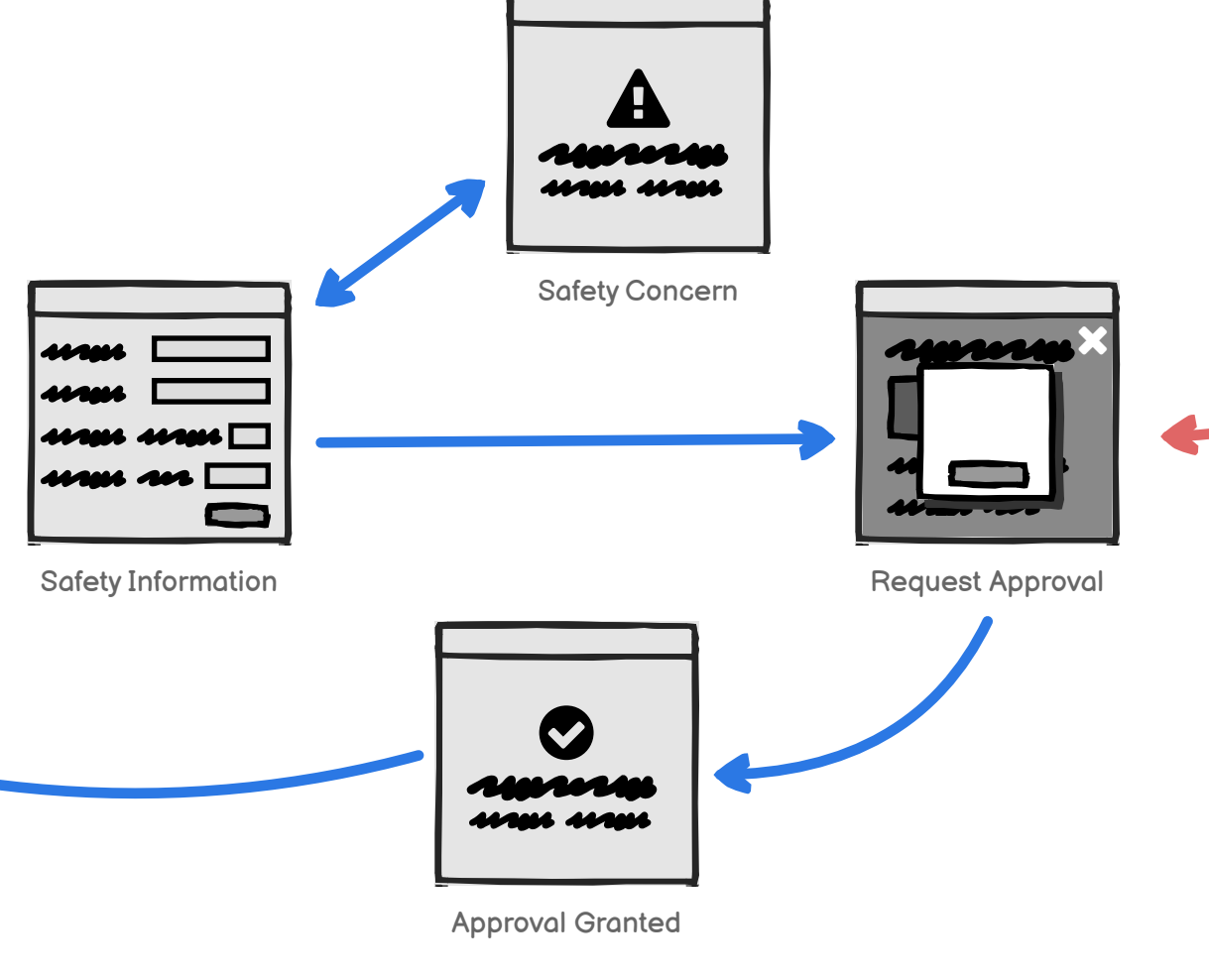
Steps

References

Request Approval | Start Experiment

The different elements of the plan can be modified as required

Some users may need an approval for the plan before they can start the experiment



Some users may need a separate approval for the H&S information

Experiment

Reaction

Author: [Name]

Start: [Date] End: [Date]

Project: [Name] Keywords: [List]

Laboratory/Instrument: [Name]

Status: [Status]

Materials

Safety Information

Steps

Samples

Data

Sketch | TLC | Spectra

Comments

Request Review | Share | Complete Experiment | Publish

User's record of their experiment with added data and interpretations

A mixture of prepopulated and user-generated metadata about the experiment

View materials, and make any changes needed for the experiment (eg quantities)

Safety information from the plan can be viewed

Steps and conditions from the plan can be viewed to help

Add Samples, generate IDs and configure properties

Print barcode label to attach to sample

Add Data Files

View Data in an appropriate viewer, options to annotate and compare data from different sources

Add Comment

Approval Denied

Request Approval

Approval Granted

Some users may need to have their experiment reviewed

Add / Modify Links

Prepopulated and user-defined links

File Selector

Data Viewer

Annotate

Compare Data

Print Barcode / QRCode

Sample ID & properties

Materials

Safety Information

Steps

Data

Links

References

Similar Experiments