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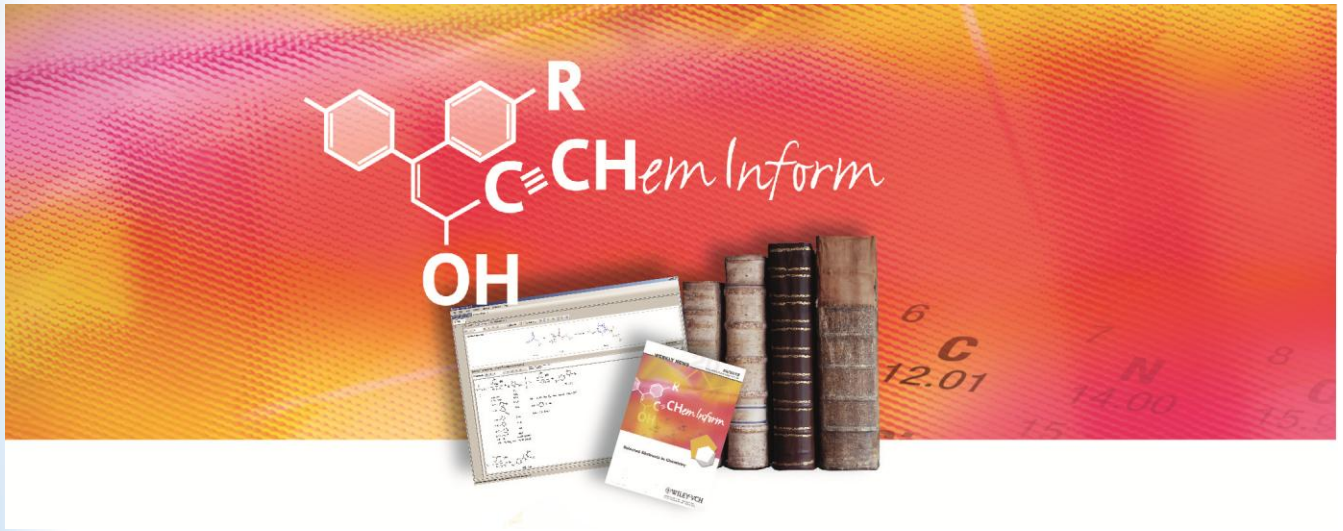

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WILEY

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Facts:

Scope of chemistry covered:	synthetic, organic, inorganic, organometallic chemistry
Chemical reactions:	over 1,7 million (70,000 reactions added per year)
Number of substances:	over 1,5 million
Updating:	weekly
Journals covered:	about 100 (the most important ones)
Dates covered:	1991 - present

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The abstracts in the ChemInform provide you with the latest developments in preparative chemistry, including:

- novel catalysts and reagents
- protecting groups
- functional group transformations
- approaches to heterocyclic scaffolds
- new strategies in natural product synthesis

ChemInform®

Search in the pool of ChemInform reactions for:

- structures and substructures
- reaction types
- experimental conditions (e.g. reagent, solvent, yield, e.e.)
- bibliographic data (e.g. author, journal, year, title)
- combinations thereof

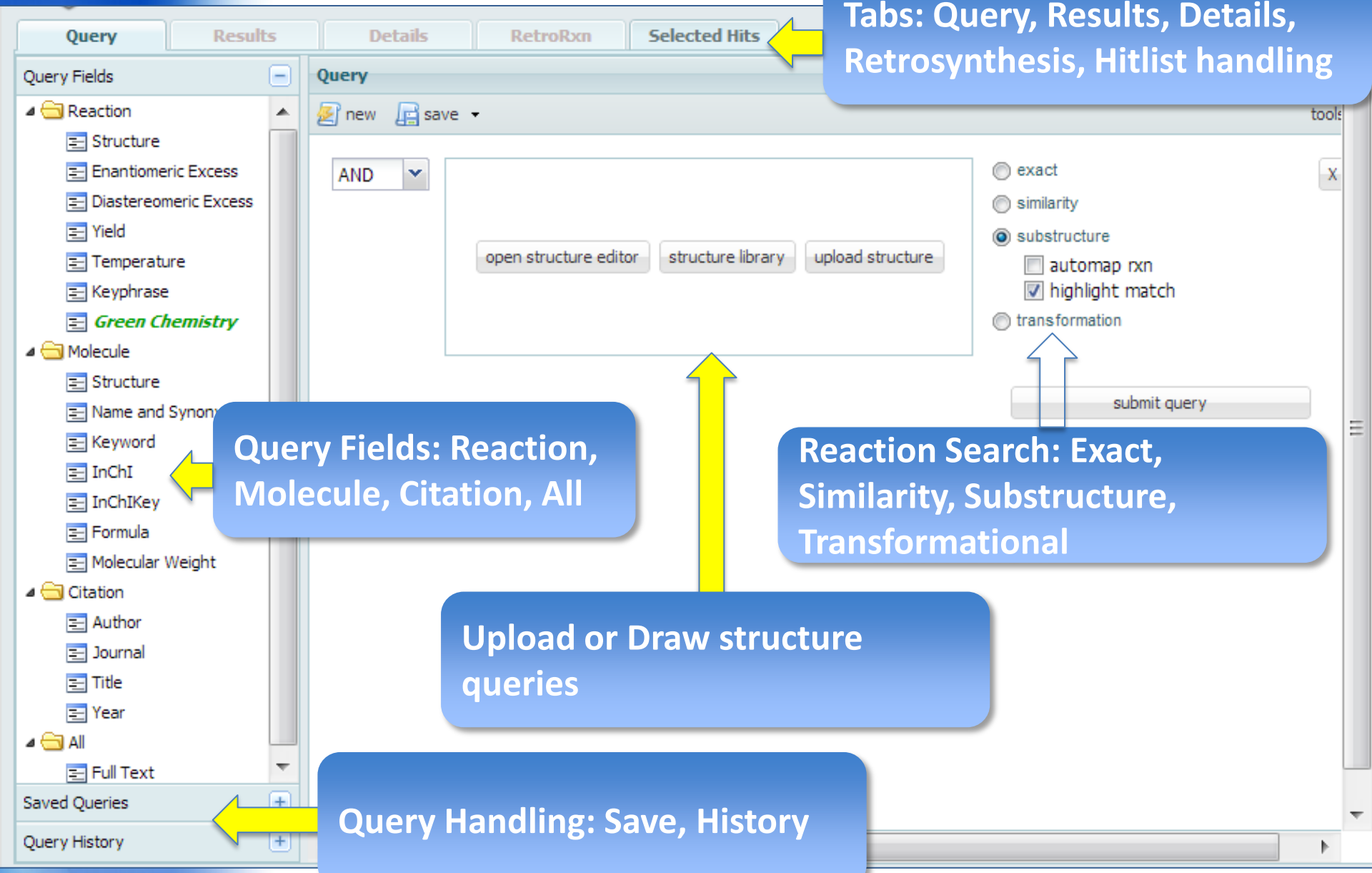
Chemical Reactions

One of the main tasks of researchers in chemical and pharmaceutical Industry is to synthesize new chemical compounds applied in the areas agriculture, pharma, intermediates, dyes and more.

Most efficient tool to make this work succesful is reaction databases with carefully selected and curated experimental data.
Besides the reaction centers conditions and yield is the Information the researcher is interested in

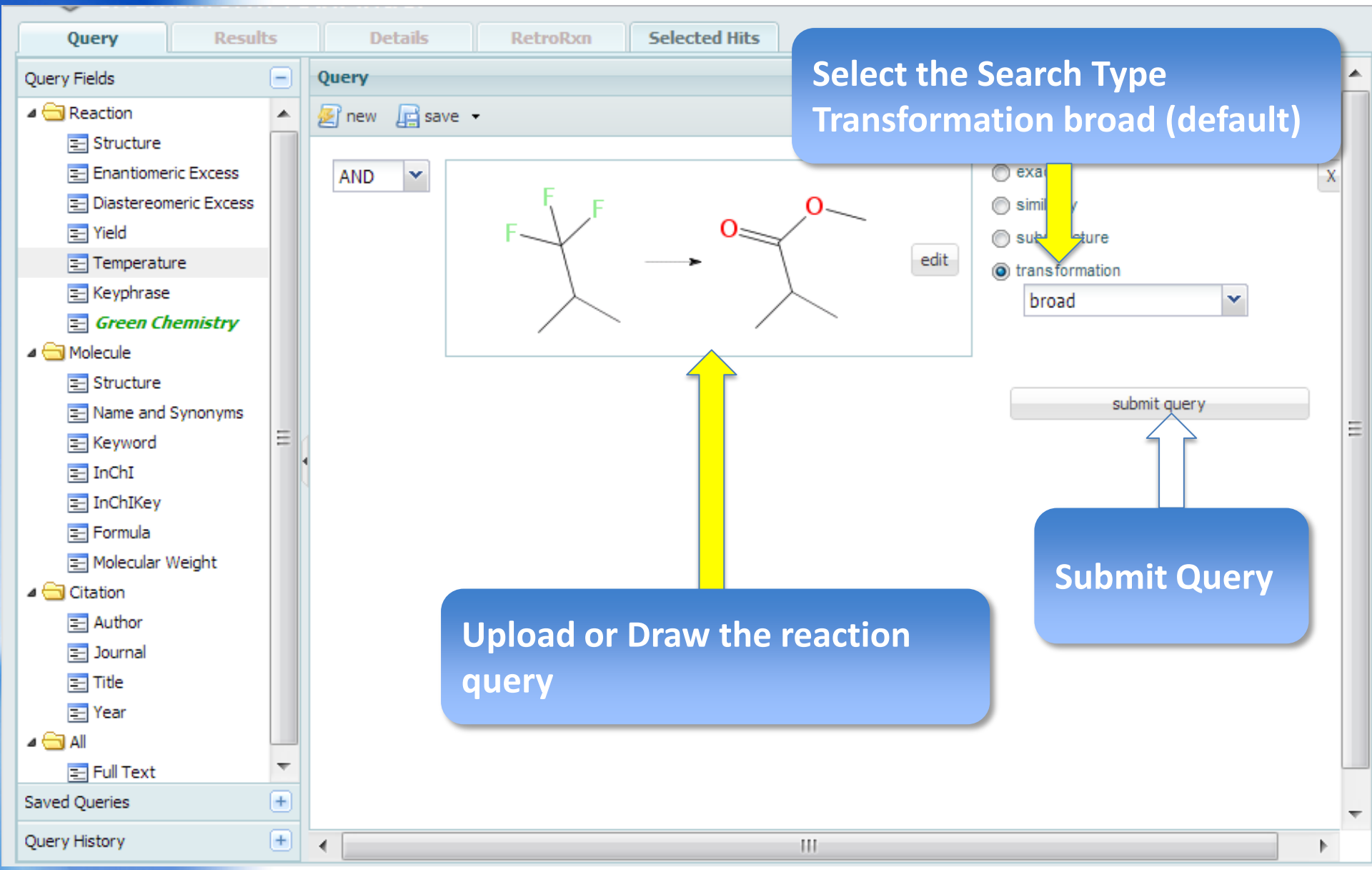
Table-of-contents

Section 1: RxnFinder User Interface



Section 2: Transformational Search, Schemes, Reaction Details

Use case: One of the most powerful reaction searches is the reaction center search or **transformational search**. Reactions with similar reaction centers can be identified using this technique. An example is the functional group transformation, e.g., from a trifluoromethyl to a carboxyl group.


Query
Results
Details
RetroRxn
Selected Hits
Query Fields
Reaction
Structure
Enantiomeric Excess
Diastereomeric Excess
Yield
Temperature
Keyphrase
Green Chemistry
Molecule
Structure
Name and Synonyms
Keyword
InChI
InChIKey
Formula
Molecular Weight
Citation
Author
Journal
Title
Year
All
Full Text
Saved Queries
Query History
Query
new
save
AND
edit
transformation
broad
submit query
Select the Search Type
Transformation broad (default)
Upload or Draw the reaction query
Submit Query

13 Hits match the Query

Query | Results | Details | RetroRxn | Selected Hits

Cluster Analysis

Author

Catalyst

Catalyst	n
none	13

Reagent

Solvent

Temperature (min.)

Temperature (max.)

Year

Yield

Classification: broad

Classification: medium

Classification: narrow

Resultset

reset filter | add filter to query | 13 Hits

Yield	Condition	Reference
90	fuming H_2SO_4	WANG, K.; LI, H.; WEN, J.; J Fluorine Chem [JFLCAR] 2001, 109 (2), 205-208. [open scheme] [open article] [save pdf] [show details]
90	0·5M aq. NaOH dioxane	KING, J. F.; GILL, M. S.; J Org Chem [JOCEAH] 1996, 61 (21), 7250-7255. [open scheme] [open article] [save pdf] [show details]

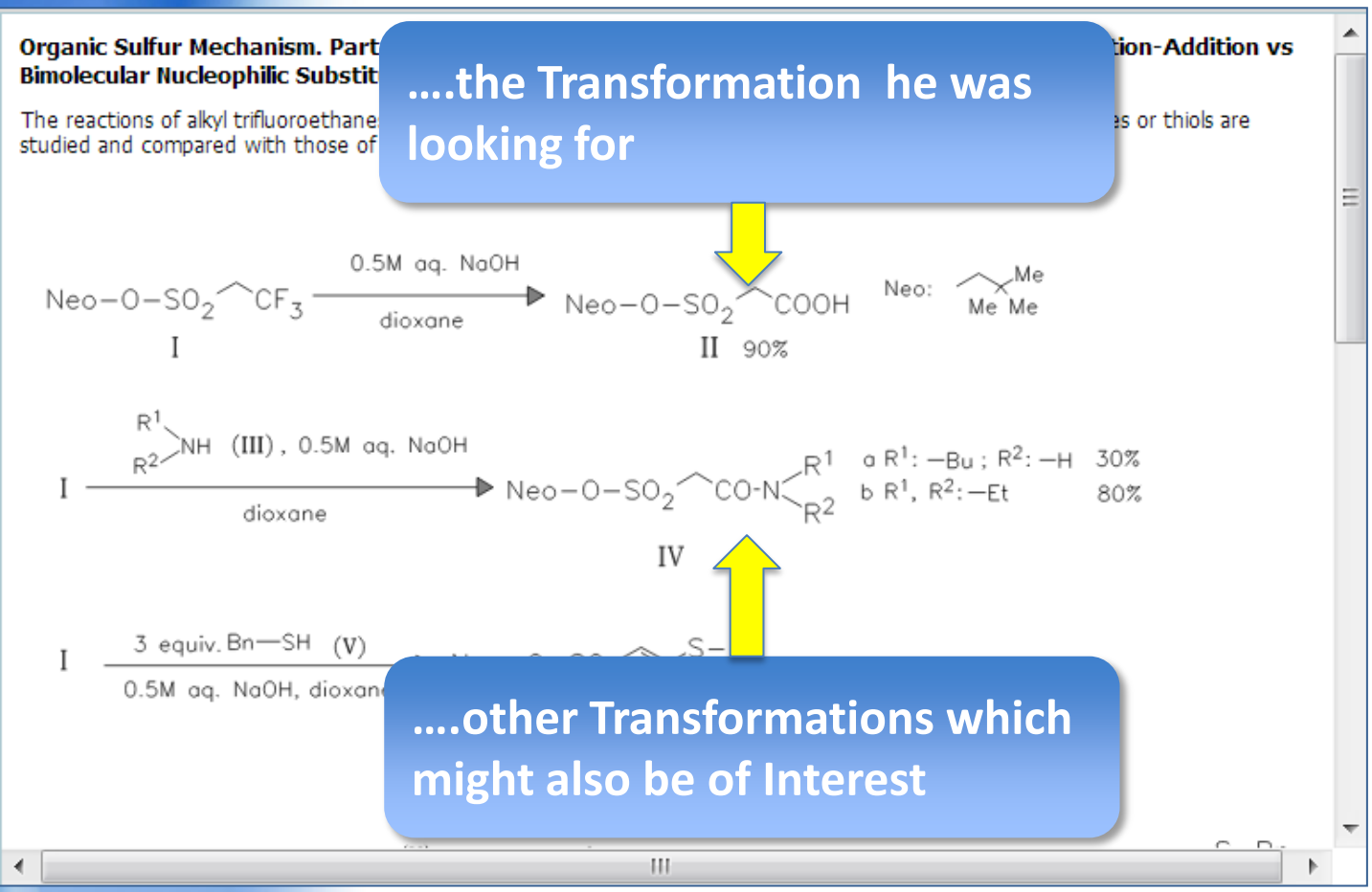
Open the Reaction Scheme

Page 1 of 1 | Displaying Reactions 1 - 13 of 13

Clipboard

Reference

no reactions on clipboard



The **scheme** is a comprehensive summary of the most important reactions in an article.

At a glance the chemist gets the crucial details of reactions.....

Query | Results | Details | RetroRxn | Selected Hits

Cluster Analysis

Author

Catalyst

Catalyst	n
none	13

Reagent

Solvent

Temperature (min.)

Temperature (max.)

Year

Yield

Classification: broad

Classification: medium

Classification: narrow

Resultset

reset filter | add filter to query | 13 Hits

Yield	Condition	Reference
90	fuming H_2SO_4	WANG, K.; LI, H.; WEN, J.; J Fluorine Chem [JFLCAR] 2001, 109 (2), 205-208. [open scheme] [open article] [save pdf] [show details]
90	0·5M aq. NaOH dioxane	KING, J. F.; GILL, M. S.; J Org Chem [JOCEAH] 1996, 61 (21), 7250-7255. [open scheme] [open article] [save pdf] [show details]

Page 1 of 1 | Displaying Reactions 1 - 13 of 13

Clipboard

Reference

no reactions on clipboard

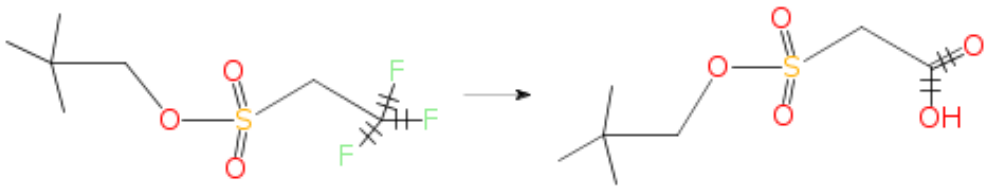
To display the Reaction Details the link Show Details is clicked

Query | Results | Details | RetroRxn | Selected Hits

Source Information

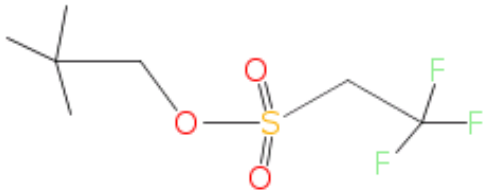
KING, J. F.; GILL, M. S.; J Org Chem 61 (1996) 21, 7250-

Reaction RXCI90428854



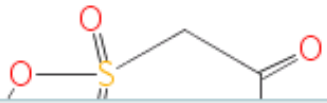
max. overall yield: 90%; Keyphrases: alkylation, O-alkylation

Reactant



$C_7H_{13}F_3O_3S$ (mw: 234.23652)
Keywords: halide, halide (F), sulfonate ester, sulfur
InChI: InChI=1S/C7H13F3O3S/c1-6(2,3)4-13-14(11,12)5-7(8,9)10/h4-5H2,1-3H3
InChIKey: WQWGDQFECKBTJN-UHFFFAOYSA-N

Product



Reaction 3 of 13

This reaction details page displays:

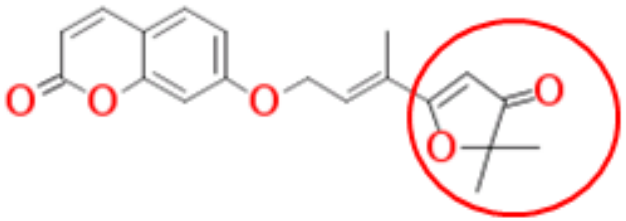
- Products
  Reactants
- Catalysts
- Solvents

and

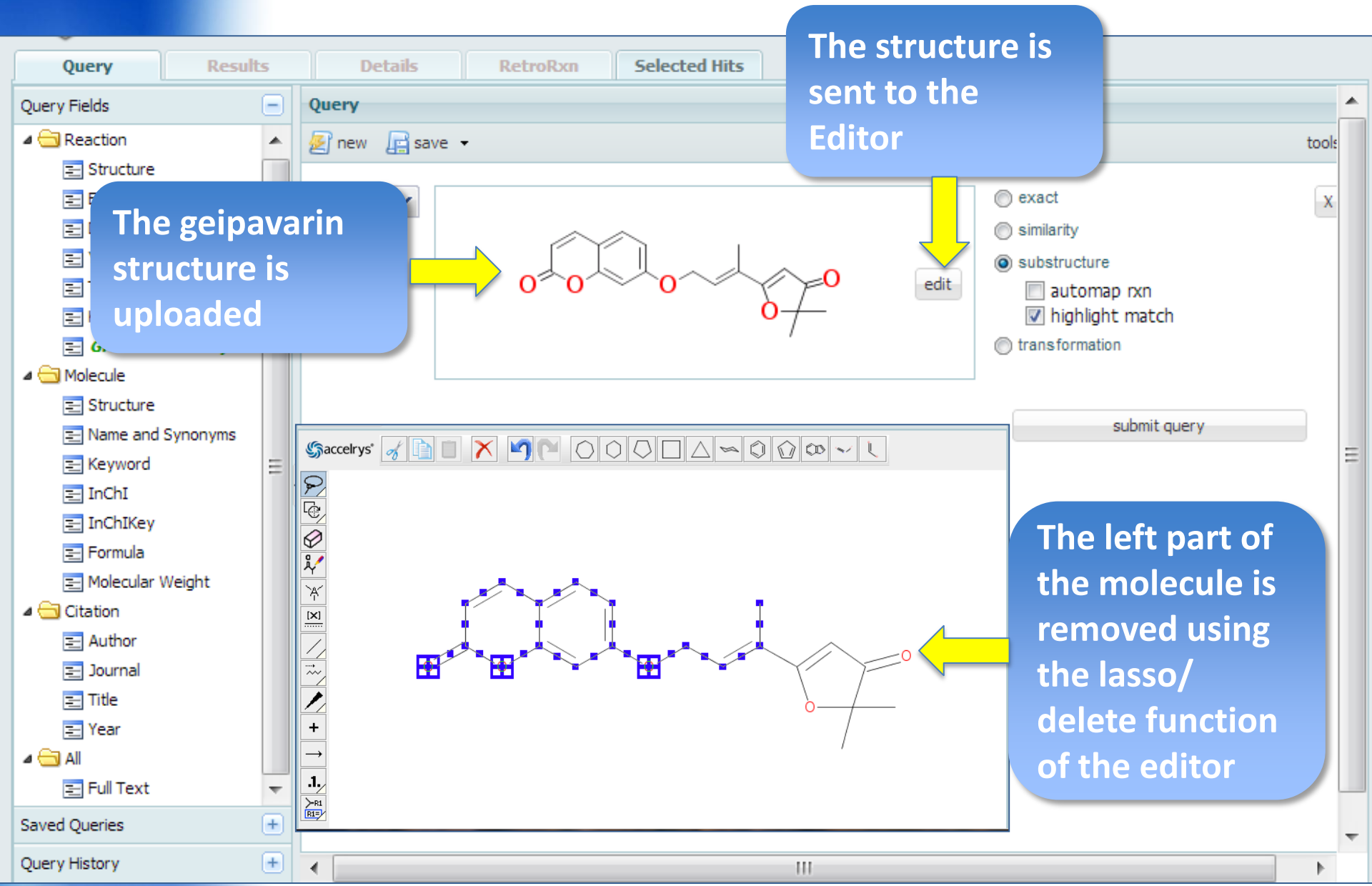
- Keywords
- Structure
  Properties
- Yield
- Temperature

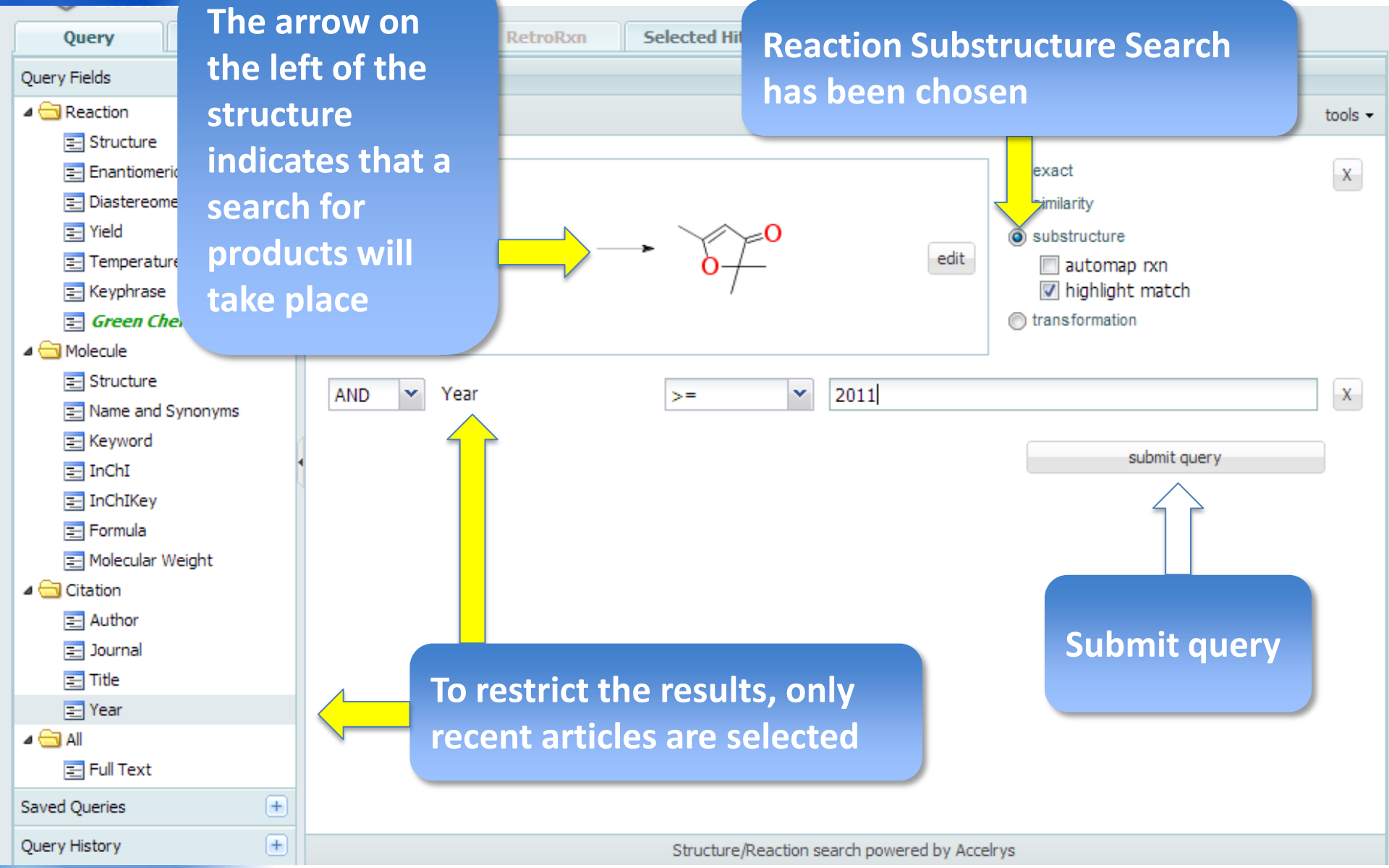
Section 3: Substructure Search, Filters, Cluster Analysis

Use case: Geipavarin is a natural compound known as a potential anti-cancer drug



A pharma researcher identifies the 5-membered ring as being a potential pharmacophore (important part of the molecule) and wants to find products including this ring.


Query
Results
Details
RetroRxn
Selected Hits
Query Fields
Reaction
Structure
Molecule
Structure
Name and Synonyms
Keyword
InChI
InChIKey
Formula
Molecular Weight
Citation
Author
Journal
Title
Year
All
Full Text
Saved Queries
Query History
Query
new
save
tools
edit
exact
similarity
substructure
automap rxn
highlight match
transformation
submit query
accelrys
The structure is sent to the Editor
The geipavarin structure is uploaded
The left part of the molecule is removed using the lasso/ delete function of the editor



The arrow on the left of the structure indicates that a search for products will take place

Reaction Substructure Search has been chosen

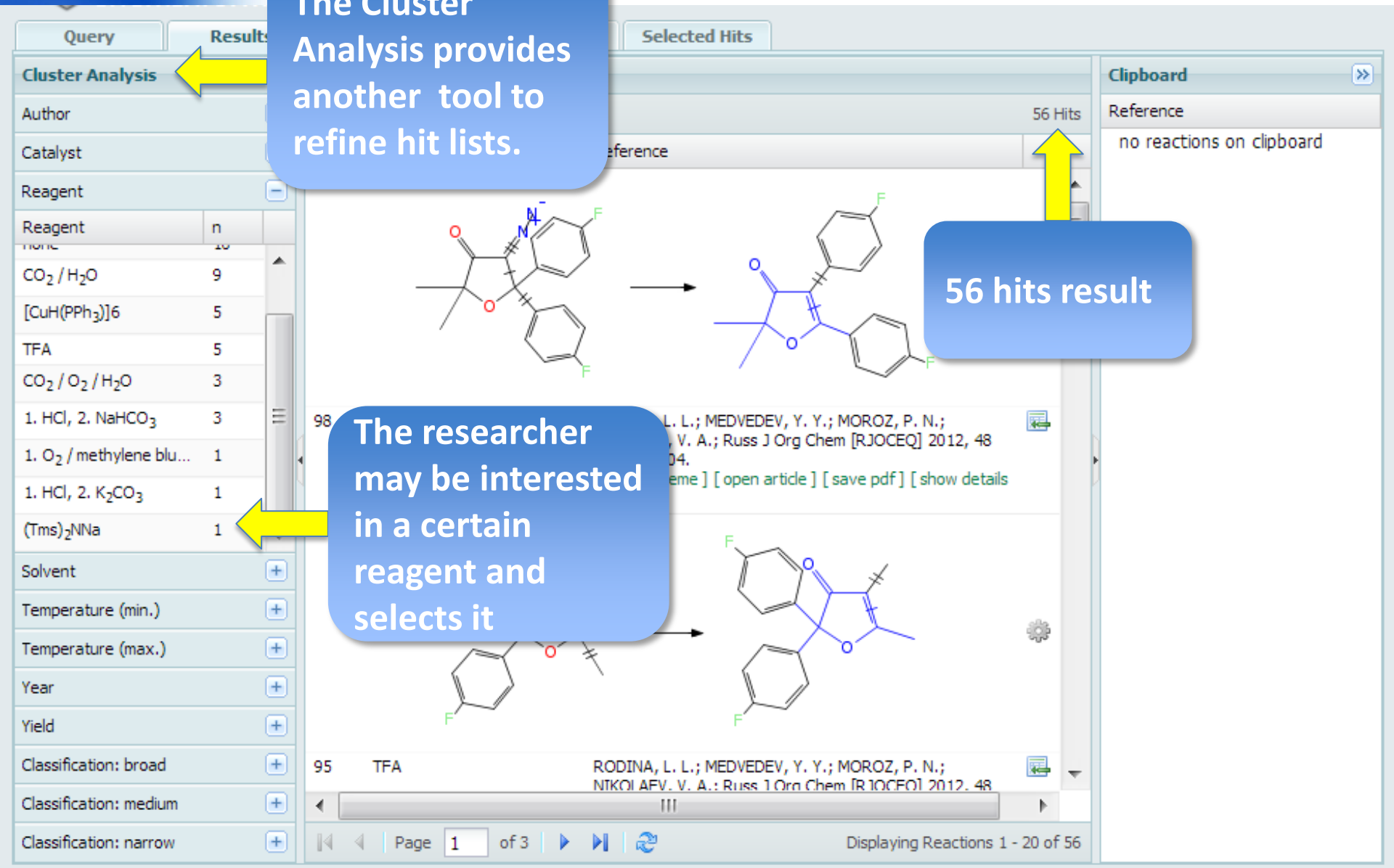
To restrict the results, only recent articles are selected

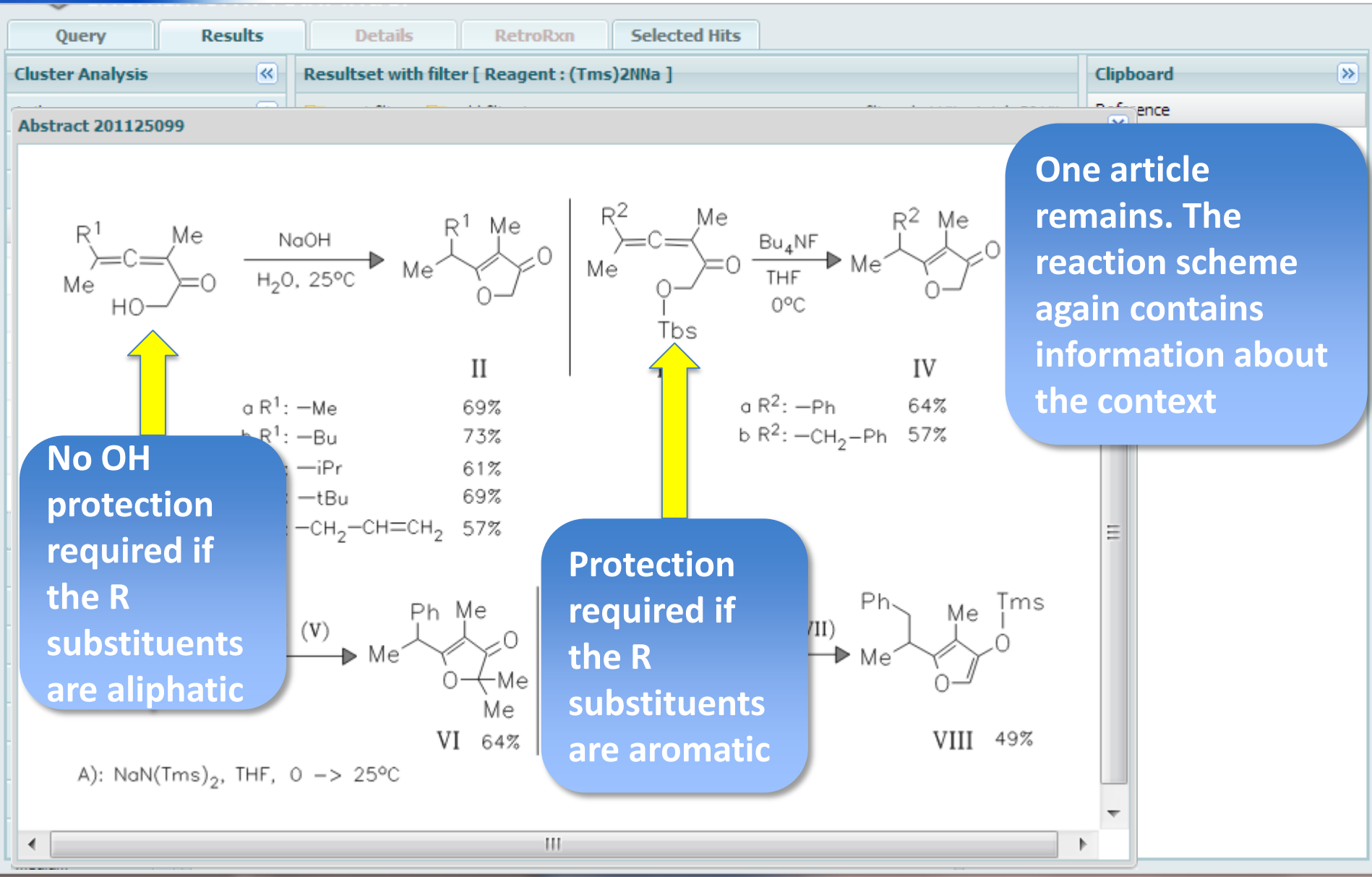
Submit query

The Cluster Analysis provides another tool to refine hit lists.

56 hits result

The researcher may be interested in a certain reagent and selects it

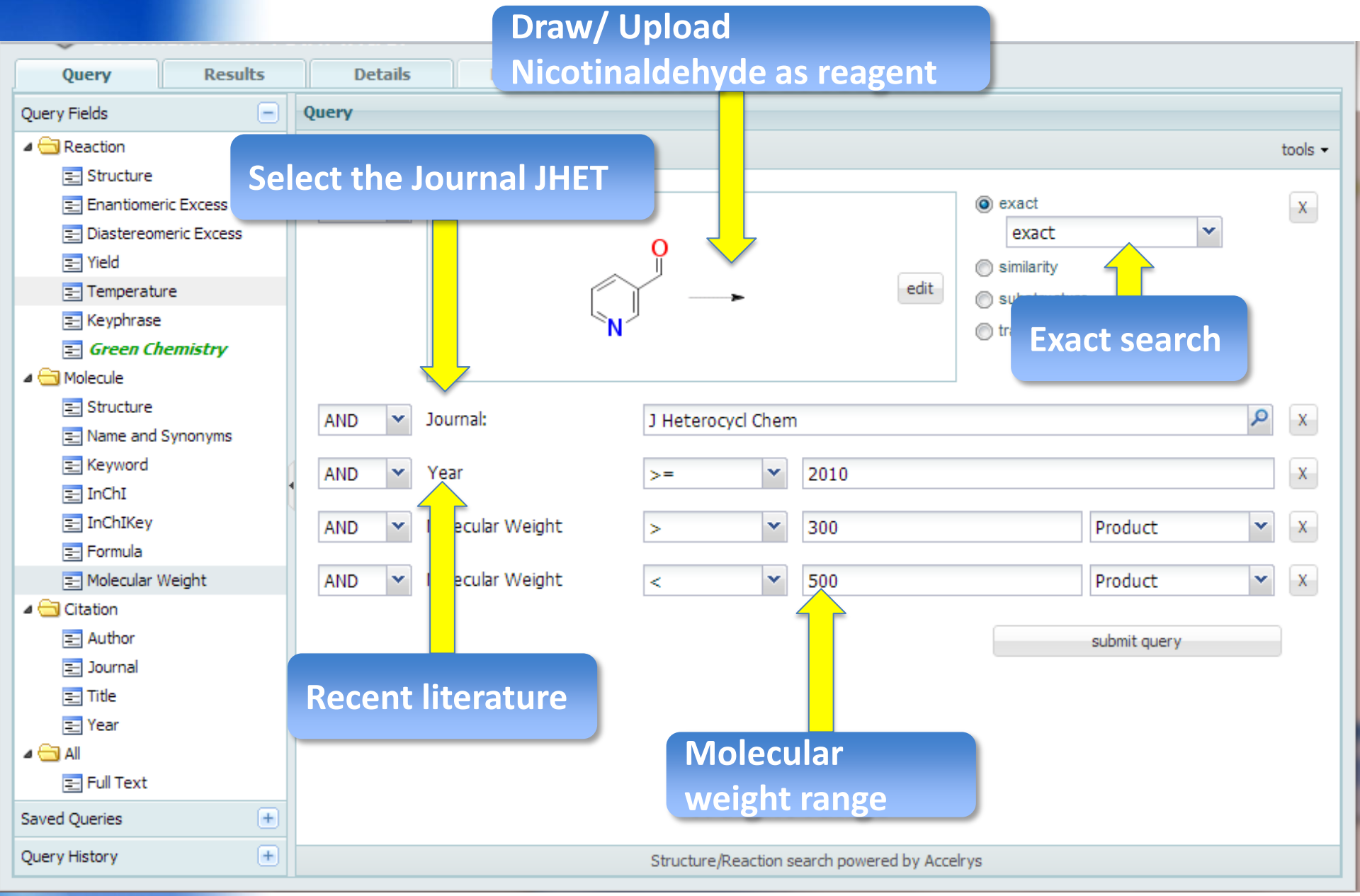



Query
Results
Details
RetroRxn
Selected Hits
Cluster Analysis
Resultset with filter [Reagent : (Tms)2NNa]
Clipboard
Abstract 201125099
NaOH
H2O, 25°C
II
a R1: –Me 69%
b R1: –Bu 73%
–iPr 61%
–tBu 69%
–CH2–CH=CH2 57%
Bu4NF
THF
0°C
Tbs
IV
a R2: –Ph 64%
b R2: –CH2–Ph 57%
(V)
VI 64%
VII)
VIII 49%
A): NaN(Tms)2, THF, 0 –> 25°C
No OH protection required if the R substituents are aliphatic
Protection required if the R substituents are aromatic
One article remains. The reaction scheme again contains information about the context

Section 4: From RxnFinder to Wiley‘s Smart Article

Use Case : A research chemist who works on heterocycles wants to start from nicotinaldehyde as the reagent. The products shall have molecular weights in the range 300 to 500 Dalton (see Lipinsky‘s „Rule of 5“ defining drug likeness with 5 criteria)

What has recently been published in the **Journal of Heterocyclic Chemistry** on this research field?


Draw/ Upload
Nicotinaldehyde as reagent
Select the Journal JHET
Exact search
Recent literature
Molecular
weight range
Query
Results
Details
Query Fields
Reaction
Structure
Enantiomeric Excess
Diastereomeric Excess
Yield
Temperature
Keyphrase
Green Chemistry
Molecule
Structure
Name and Synonyms
Keyword
InChI
InChIKey
Formula
Molecular Weight
Citation
Author
Journal
Title
Year
All
Full Text
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Query History
tools
edit
exact
exact
similarity
AND
Journal:
J Heterocycl Chem
AND
Year
>=
2010
AND
ecular Weight
>
300
Product
AND
ecular Weight
<
500
Product
submit query
Structure/Reaction search powered by Accelrys

Query | Results | Details | RetroRxn | Selected Hits

Cluster Analysis

- Author
- Catalyst
- Reagent

Reagent	n
none	10
molecular sieves	8
DBU	2

- Solvent
- Temperature (min.)
- Temperature (max.)
- Year
- Yield
- Classification: broad
- Classification: medium
- Classification: narrow

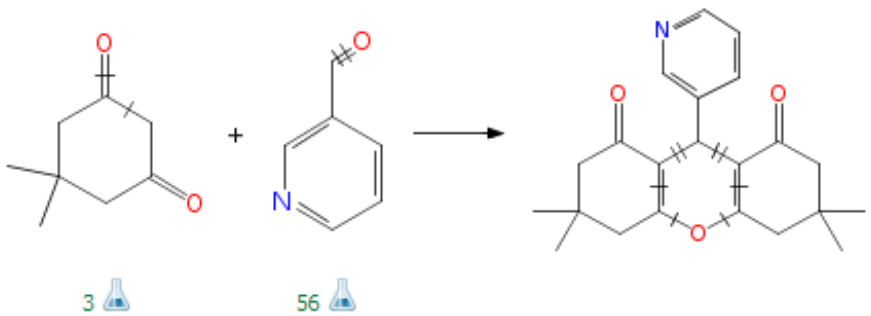
Resultset

reset filter | add filter

20 Hits result

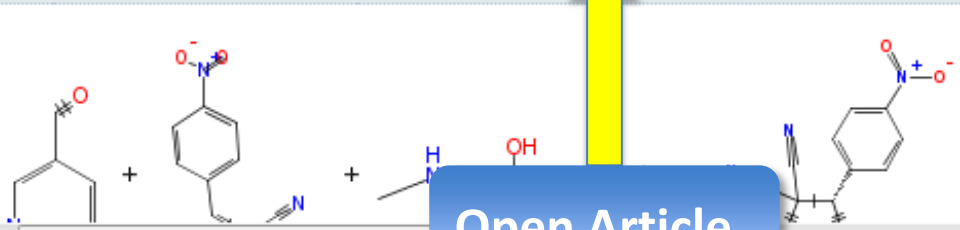
20 Hits

Yield	Condition	
75	mol. sieves toluene	GHANDI, M.; TAHERI, A.; ABBASI, A.; J Heterocycl Chem [JHTCAD] 2010, 47 (3), 611-615. [open scheme] [open article] [save pdf] [show details]



3 56

71	silica-$(CH_2)_3$-S-SO_3H (cat.) EtOH	NIKNAM, K.; PANAHI, F.; SABERI, D.; MOHAGHEGHNEJAD, M.; J Heterocycl Chem [JHTCAD] 2010, 47 (2), 292-300. [open scheme] [open article] [save pdf] [show details]



Open Article

Page 1 of 1 | Displaying Reactions 1 - 20 of 20

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Article

Silica-bonded *S*-sulfonic acid as recyclable catalyst for the synthesis of 1,8-dioxo-decahydroacridines and 1,8-dioxo-octahydroxanthenes

Khodabakhsh Niknam*, Farhad Panahi, Dariush Saberi, Molki Mohagheghnejad

Article first published online: 23 FEB 2010
DOI: 10.1002/jhet.303

Issue

Journal of Heterocyclic Chemistry
Volume 47, Issue 2, pages 292–300, March 2010

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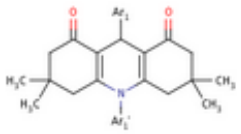
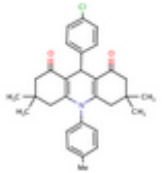


Compound 5

Molecular Weight:
Molecular Formula: Not Available
InChIKey: Not Available

View compound in article | Full details | Search this compound

Exact structure search in Wiley Online Library

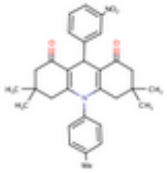


Compound 5a

Molecular Weight: 474.034
Molecular Formula: C30H32ClNO2
InChIKey: DCOWGQSTQYZTOB-UHFFFAOYSA-N

View compound in article

Views all instances of the compound in the article

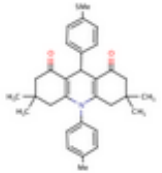


Compound 5b

Molecular Weight: 484.5861
Molecular Formula: C30H32N2O4
InChIKey: KKEFCOAMTHBVAX-UHFFFAOYSA-N

View compound in article | Full details

Links to the compound record with properties, molfile export, external links to Google, PubChem, ChemSpider



Compound 5c

Molecular Weight: 485.68
Molecular Formula: C31H35NO2S
InChIKey: MYOSQCRLRGHSNO-UHFFFAOYSA-N

View compound in article | Full details | Search this compound

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- ‘Failed reactions’ are also included (Yield = 0).

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