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Number of substances:	over 1,5 million
Updating:	weekly
Journals covered:	about 100 (the most important ones)
Dates covered:	1991 - present



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



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 successful 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

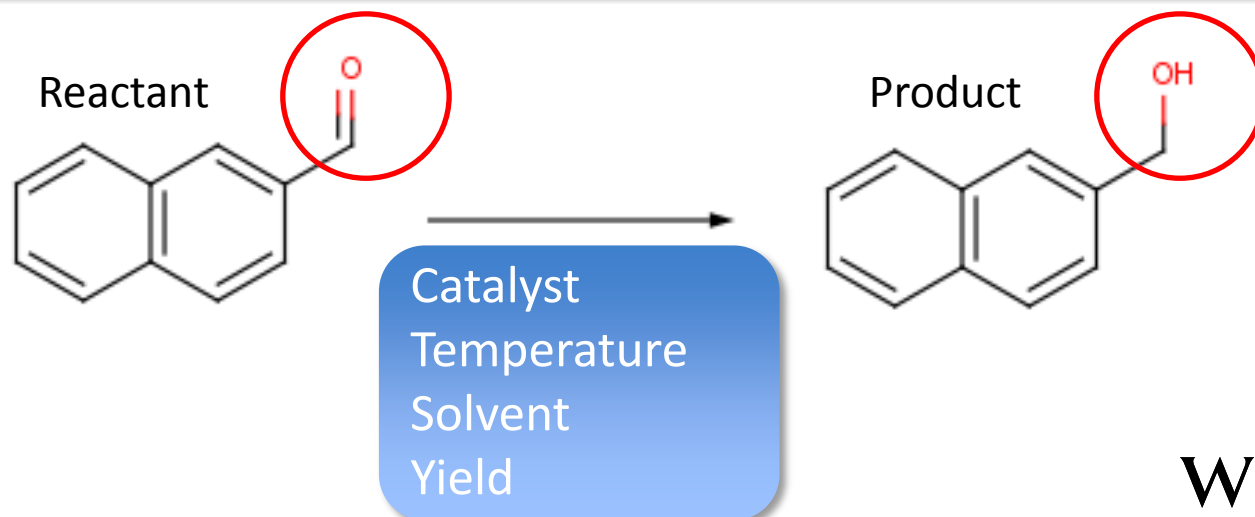


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Section 1: RxnFinder User Interface

The screenshot displays the RxnFinder web application interface. At the top, there are five tabs: Query, Results, Details, RetroRxn, and Selected Hits. A callout box points to these tabs, stating: "Tabs: Query, Results, Details, Retrosynthesis, Hitlist handling".

On the left side, there is a "Query Fields" panel with a tree view. It includes categories for Reaction (Structure, Enantiomeric Excess, Diastereomeric Excess, Yield, Temperature, Keyphrase, Green Chemistry), Molecule (Structure, Name and Synonym, Keyword, InChI, InChIKey, Formula, Molecular Weight), Citation (Author, Journal, Title, Year), and All (Full Text). A callout box points to this panel: "Query Fields: Reaction, Molecule, Citation, All".

The main "Query" area contains a search box with a dropdown menu set to "AND". Below the search box are three buttons: "open structure editor", "structure library", and "upload structure". A callout box points to these buttons: "Upload or Draw structure queries".

To the right of the search box, there are radio buttons for search types: "exact", "similarity", "substructure", and "transformation". Under "substructure", there are checkboxes for "automap rxn" and "highlight match". A "submit query" button is located at the bottom right. A callout box points to these options: "Reaction Search: Exact, Similarity, Substructure, Transformational".

At the bottom left, there are sections for "Saved Queries" and "Query History", each with a plus sign icon. A callout box points to these sections: "Query Handling: Save, History".

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.

The screenshot shows a web-based chemical query interface. On the left is a sidebar with 'Query Fields' categorized into 'Reaction' (Structure, Enantiomeric Excess, Diastereomeric Excess, Yield, Temperature, Keyphrase, Green Chemistry) and 'Molecule' (Structure, Name and Synonyms, Keyword, InChI, InChIKey, Formula, Molecular Weight). Below are 'Citation' (Author, Journal, Title, Year) and 'All' (Full Text) sections, along with 'Saved Queries' and 'Query History' buttons.

The main 'Query' area has tabs for 'Query', 'Results', 'Details', 'RetroRxn', and 'Selected Hits'. It contains a 'new' and 'save' button, a dropdown menu set to 'AND', and a central workspace for drawing or uploading a reaction. A reaction is shown: a tert-butyl fluoride derivative (left) reacting to form a tert-butyl ester (right). A yellow arrow points from a blue callout box below to this reaction.

On the right, there are radio buttons for search types: 'exact', 'similarity', 'substructure', and 'transformation' (which is selected). Below these is a dropdown menu set to 'broad'. A yellow arrow points from a blue callout box above to this dropdown. Below the search type options is a 'submit query' button. A white arrow points from a blue callout box below to this button.

Annotations include three blue callout boxes with white text: 'Select the Search Type Transformation broad (default)' (top right), 'Submit Query' (bottom right), and 'Upload or Draw the reaction query' (bottom center). A yellow arrow points from the 'Submit Query' box to the 'submit query' button. Another yellow arrow points from the 'Upload or Draw the reaction query' box to the reaction drawing area. A third yellow arrow points from the 'Submit Query' box to the 'transformation' radio button.

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 ₂ SO 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]

Clipboard >> Reference no reactions on clipboard

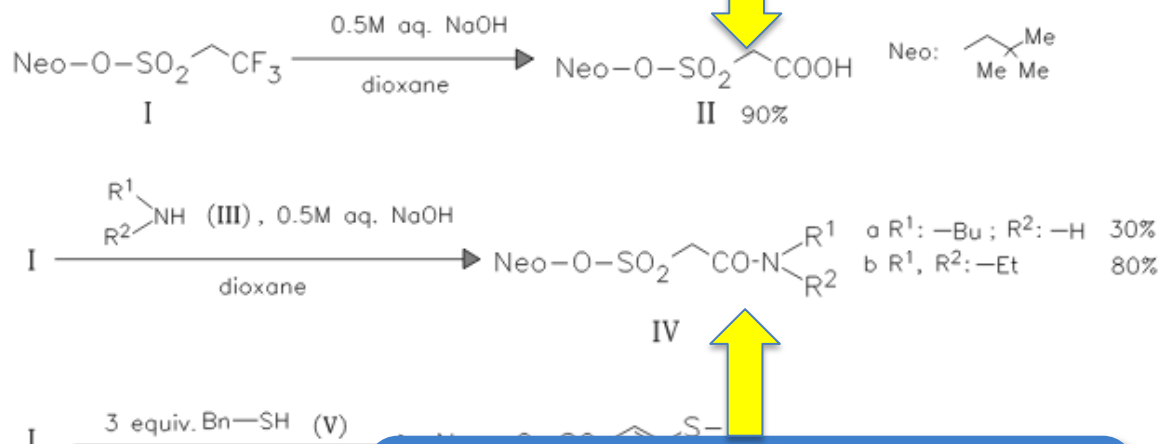
Page 1 of 1 Displaying Reactions 1 - 13 of 13

Open the Reaction Scheme

Organic Sulfur Mechanism. Part
Bimolecular Nucleophilic Substitution

The reactions of alkyl trifluoroethane
studied and compared with those of

...the Transformation he was
looking for



...other Transformations which
might also be of Interest

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 ₂ SO ₄	WANG, K.; LI, H.; WEN, J.; J Fluorine Chem [JFLCAR] 2001, 109 (2), 205-208. [open scheme] [open article] [save pdf] [show details]
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no reactions on clipboard

Displaying Reactions 1 - 13 of 13

Page 1 of 1

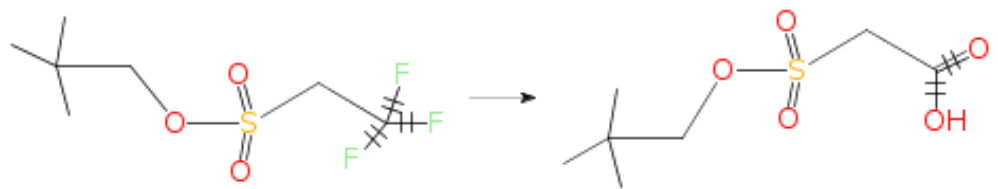
To display the Reaction Details the link Show Details is clicked

The screenshot shows a chemical database interface with a sidebar on the left containing filters for Author, Catalyst, Reagent, Solvent, Temperature, Year, Yield, and Classification. The main area displays a table of search results with columns for Yield, Condition, and Reference. Two reaction entries are visible, each with a chemical structure and a 'show details' link. A blue callout box with a white arrow points to the 'show details' link of the second reaction. The bottom of the interface shows pagination information: 'Page 1 of 1' and 'Displaying Reactions 1 - 13 of 13'.

Query Results Details **RetroRxn** Selected Hits

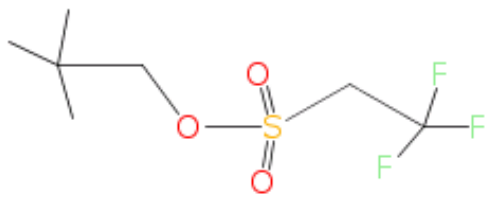
Source Information
 KING, J. F.; GILL, M. S.; J Org Chem 61 (1996) 21, 7250-

Reaction RXCI90428854



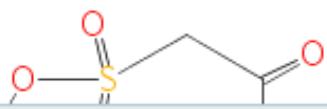
max. overall yield: 90%; Keyphrases: alkylation, O-alkylation

Reactant



C₇H₁₃F₃O₃S (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



CS: 100% Yield: 90%

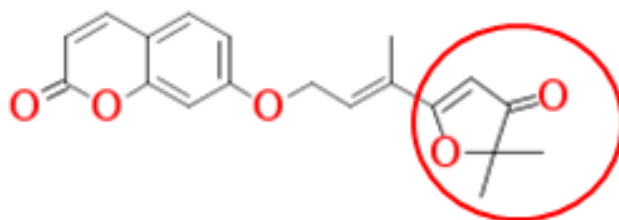
Reaction 3 of 13

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.

The screenshot displays a chemical software interface with several panels. On the left, a sidebar lists 'Query Fields' and 'Molecule' categories with various search criteria. The main window is titled 'Query' and contains a chemical structure of a complex molecule. A blue callout box with a yellow arrow pointing to the structure says 'The geipavarin structure is uploaded'. To the right of the structure is an 'edit' button, with another blue callout box and a yellow arrow pointing to it saying 'The structure is sent to the Editor'. Below the main window is a smaller 'accelrys' editor window. A blue callout box with a yellow arrow pointing to the left side of the molecule in this editor says 'The left part of the molecule is removed using the lasso/delete function of the editor'. The editor window shows the same molecule with blue selection boxes around the left portion, indicating it is being prepared for deletion. The interface also includes a 'submit query' button and various search options like 'exact', 'similarity', 'substructure', 'automap rxn', 'highlight match', and 'transformation'.

Query Fields

- Reaction
 - Structure
- Molecule
 - Structure
 - Name and Synonyms
 - Keyword
 - InChI
 - InChIKey
 - Formula
 - Molecular Weight
- Citation
 - Author
 - Journal
 - Title
 - Year
- All
 - Full Text

Query

new save

edit

submit query

exact

similarity

substructure

automap rxn

highlight match

transformation

accelrys

The geipavarin structure is uploaded

The structure is sent to the Editor

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 screenshot shows a chemical search interface. On the left, a 'Query Fields' sidebar lists categories: Reaction (Structure, Enantiomeric, Diastereome, Yield, Temperature, Keyphrase, Green Chem) and Molecule (Structure, Name and Synonyms, Keyword, InChI, InChIKey, Formula, Molecular Weight). Below these are Citation (Author, Journal, Title, Year) and All (Full Text) fields. A yellow arrow points from the 'Reaction' folder to a central chemical structure of a cyclic enone. Another yellow arrow points from the 'Reaction' folder to the 'substructure' option in the search criteria panel. The search criteria panel includes options for 'exact', 'similarity', 'substructure' (selected), 'automap rxn', 'highlight match' (checked), and 'transformation'. Below this is a search filter: 'AND Year >= 2011'. A 'submit query' button is located below the filter. A yellow arrow points from the 'submit query' button to a blue callout box. At the bottom, the text 'Structure/Reaction search powered by Accelrys' is visible.

The Cluster Analysis provides another tool to refine hit lists.

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

56 hits result

The screenshot displays a search results page with a 'Query' tab and a 'Results' tab. The 'Cluster Analysis' section is highlighted with a yellow arrow. The 'Reagent' filter is set to '(Tms)₂NNa', which is also highlighted with a yellow arrow. The 'Clipboard' section shows 'no reactions on clipboard'. The main content area displays two chemical reactions, each with a reference entry below it. The first reaction is labeled '98' and the second is labeled '95'. The page footer indicates 'Page 1 of 3' and 'Displaying Reactions 1 - 20 of 56'.

Reagent	n
none	10
CO ₂ / H ₂ O	9
[CuH(PPh ₃)] ₆	5
TFA	5
CO ₂ / O ₂ / H ₂ O	3
1. HCl, 2. NaHCO ₃	3
1. O ₂ / methylene blu...	1
1. HCl, 2. K ₂ CO ₃	1
(Tms) ₂ NNa	1

Reference

98

95

TFA

RODINA, L. L.; MEDVEDEV, Y. Y.; MOROZ, P. N.; NIKOLAEV, V. A.; Russ J Org Chem [RJOCEQ] 2012, 48

RODINA, L. L.; MEDVEDEV, Y. Y.; MOROZ, P. N.; NIKOLAEV, V. A.; Russ J Org Chem [RJOCEQ] 2012, 48

Page 1 of 3

Displaying Reactions 1 - 20 of 56

Query Results Details RetroRxn Selected Hits

Cluster Analysis Resultset with filter [Reagent : (Tms)2NNa] Clipboard

Abstract 201125099

R^1

 Me

 Me

 HO-CH_2

 $\xrightarrow[\text{H}_2\text{O}, 25^\circ\text{C}]{\text{NaOH}}$

 Me

 R^1

 Me

 O

II

R^2

 Me

 Me

 O-Tbs

 $\xrightarrow[\text{THF}, 0^\circ\text{C}]{\text{Bu}_4\text{NF}}$

 Me

 R^2

 Me

 O

IV

a R ¹ : -Me	69%
b R ¹ : -Bu	73%
-iPr	61%
-tBu	69%
-CH ₂ -CH=CH ₂	57%

Ph

 Me

 Me

 O

 Me

VI 64%

Ph

 Me

 Me

 O-Tms

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

The screenshot shows a chemical search interface with a sidebar on the left and a main search area. The sidebar contains a tree view of search 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), and All (Full Text). The main search area has a 'Query' tab and a 'Query' field containing a chemical structure of nicotinaldehyde. Below the query field are search criteria: Journal (J Heterocycl Chem), Year (>= 2010), Molecular Weight (> 300), and Molecular Weight (< 500). The search criteria are applied to the 'Product' field. A 'submit query' button is at the bottom right. The footer text reads 'Structure/Reaction search powered by Accelrys'.

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

Query

Journal: J Heterocycl Chem

Year: >= 2010

Molecular Weight: > 300

Molecular 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 +

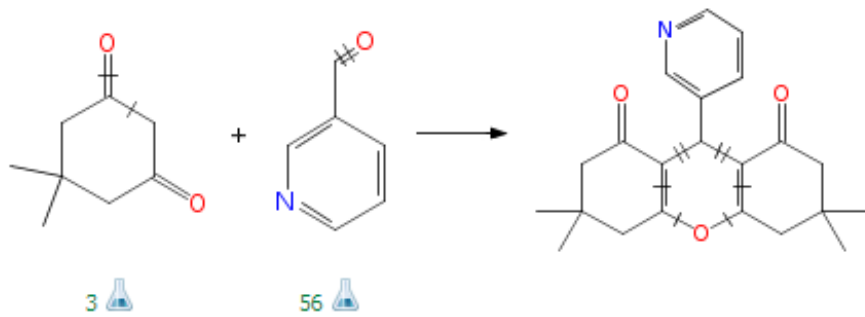
Resultset

20 Hits result

20 Hits

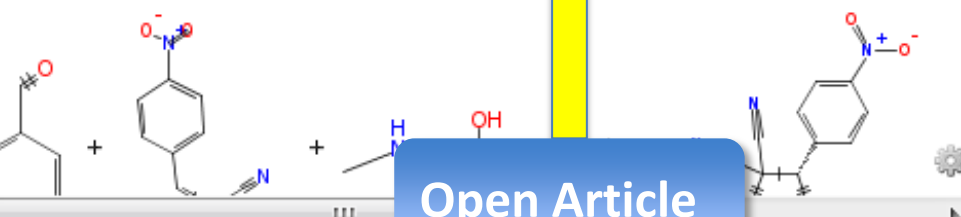
Yield Condition

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-(CH₂)₃-S-SO₃H (cat.) EtOH NIKNAM, K.; PANAH, 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

Clipboard

Reference

no reactions on clipboard

LOGIN






 Enter e-mail address

 Enter password

 REMEMBER ME

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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

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Issue



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

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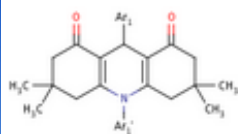
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All compounds identified by the author as primary are displayed on the Abstract page

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Compound 5

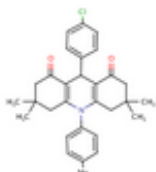
Molecular Weight:

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

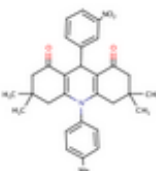
Molecular Weight: 474.034

Molecular Formula: C₃₀H₃₂ClNO₂

InChIKey: DCOWGQSTQYZTOB-UHFFFAOYSA-N

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Views all instances of
the compound in the
article



Compound 5b

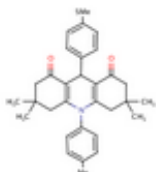
Molecular Weight: 484.5861

Molecular Formula: C₃₀H₃₂N₂O₄

InChIKey: KKEFCOAMTHBVAX-UHFFFAOYSA-N

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



Compound 5c

Molecular Weight: 485.68

Molecular Formula: C₃₁H₃₅N₂O₂S

InChIKey: MYOSQCRLRGHSNO-UHFFFAOYSA-N

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