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Taipei & ACS Taiwan Chapter



# SciFinder provides an innovative interface that streamlines your research process

The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo. The top right corner contains links for "Preferences", "SciFinder Help", and "Sign Out". Below the logo is a navigation bar with "Explore", "Saved Searches", and "SciPlanner" tabs. The left sidebar contains three main sections: "REFERENCES" (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), "SUBSTANCES" (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and "REACTIONS" (with sub-item: Reaction Structure). The main content area is titled "SUBSTANCES: CHEMICAL STRUCTURE" and features a "Structure Editor" with "Java" and "Non-Java" tabs. The editor shows a chemical structure of a substituted furanone. Below the editor is a "Search" button and an "Advanced Search" link. To the right of the editor are search options: "Search Type" with radio buttons for "Exact Structure", "Substructure" (selected), and "Similarity"; and a checkbox for "Show precision analysis". A "ChemDraw" advertisement is also present. On the far right, there are two sections: "SAVED ANSWER SETS" listing "selective reduction of nitro group" and "Lipitor\_fragment\_patents\_from \_sss" with a "View All | Import" link; and "KEEP ME POSTED" listing recent updates like "carbon nanotubes" with a "View All" link.

SciFinder®

Preferences | SciFinder Help | Sign Out

Explore | Saved Searches | SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw®

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

SAVED ANSWER SETS ?

- selective reduction of nitro group
- Lipitor\_fragment\_patents\_from \_sss
- 143950-76-9
- water\_desalination\_reviewarticle
- MarkShannon1
- macrocycles\_protein
- Autosaved Substance Set

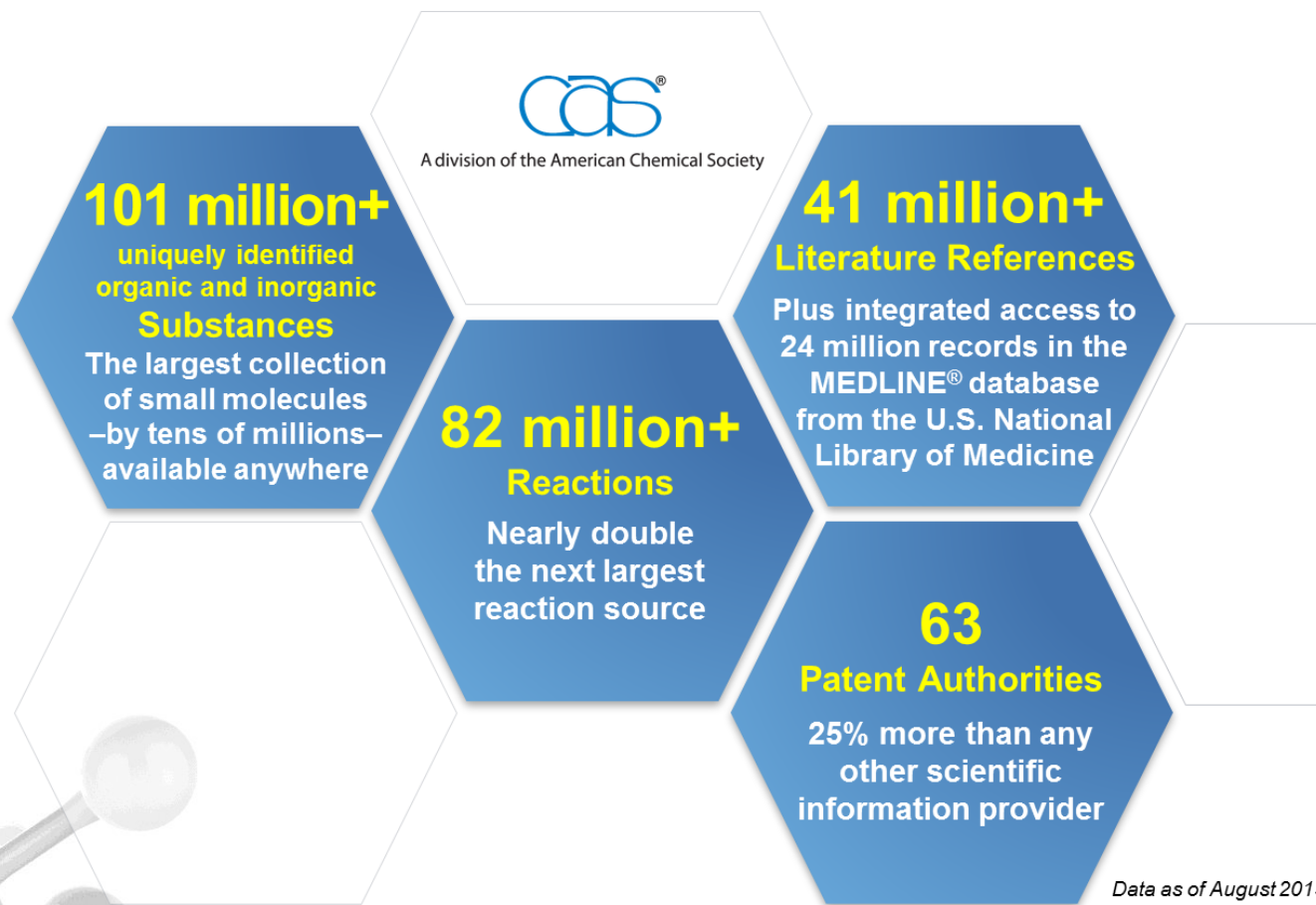
View All | Import

KEEP ME POSTED ?

- carbon nanotubes
- Sep 06, 2014(258)
- Aug 30, 2014(256)
- Aug 23, 2014(268)

View All

# Database growth



# Chemistry: Central Science

CAPlus, produced by CAS, contains more than 41 million chemistry and chemistry related research records categorized in 80 sections, with references in:

## All areas of **biochemistry**

- Agrochemical regulators
- Biochemical genetics
- Fermentation
- Immunochemistry
- Pharmacology

## All areas of **organic chemistry**

- Amino acids
- Biomolecules
- Carbohydrates
- Organometallic compounds
- Steroids

## All areas of **macromolecular chemistry**

- Cellulose, lignin, paper
- Coatings, inks
- Dyes, organic pigments
- Synthetic elastomers
- Textiles, fibers

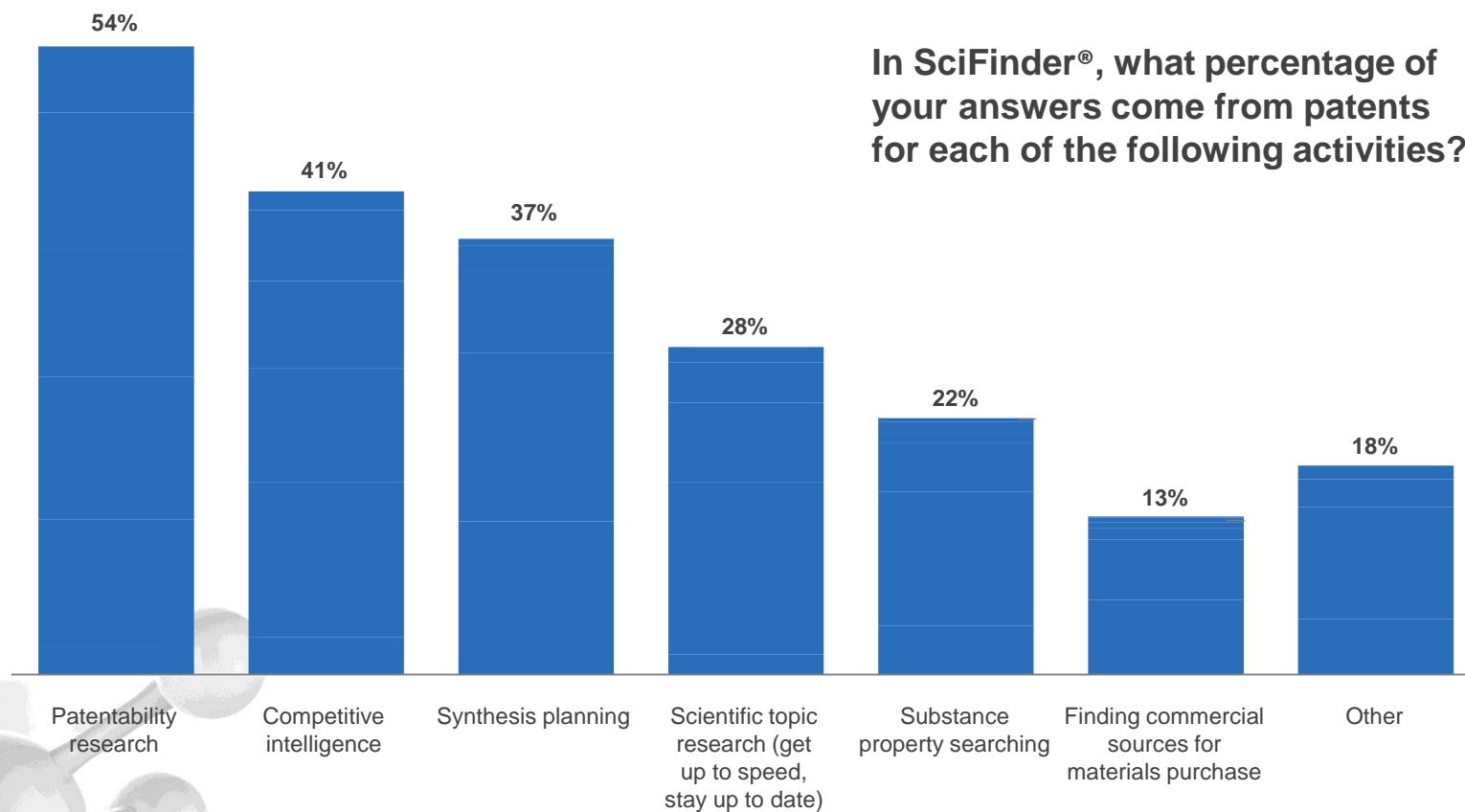
## All areas of **applied chemistry**

- Air pollution
- Ceramics
- Essential oils, cosmetics
- Fossil fuels
- Ferrous metals, alloys

## All areas of **physical, inorganic, analytical chemistry**

- Surface chemistry
- Catalysts
- Phase equilibrium
- Nuclear phenomena
- Electrochemistry

# Patents play a vital role in most research activities



Source: September 2014 SciFinder Patent User Survey

# CAS covers patents from around the world



- Content from 63 patent issuing authorities
- Nine major patent offices available online in CAplus<sup>SM</sup>
  - within two days of publication
  - fully indexed by CAS scientists within 27 days from the date of issue.

# PatentPak™

a robust **patent workflow solution** that allows scientists to **track down and locate the relevant chemistry** in patents using **SciFinder in half the time!**

Viewer Icon →

PDF Icon →

Patent No.	Kind	Language
EP 2851371	A1	English
<b>Patent Family</b>		
FR 3010999	A1	French
WO 2015040209	A1	English

PatentPak™

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ZOOM

DOWNLOAD PDF

Key Substances in Patent

CAS RN 1416788-05-0

Search in SciFinder | View Detail

Analyst Markup Location

page 157

CAS RN 1416788-06-1

1-Piperazinecarboxamide, 4-[5-[(1*S*)-1,2-dihydroxyethyl]-3-fluoro-2-pyridinyl]-4-(5-fluoro-2-benzothiazolyl)-2-methyl-, (2*S*)-, (2*E*)-2-butenedioate (1:1)

Search in SciFinder | View Detail

Analyst Markup Location

page 157

CAS RN 77-76-9

Search in SciFinder | View Detail

Analyst Markup Location

2-Chloro-3-fluoro-5-vinylpyridine (112)


To a solution of 101 (5.00g, 23.8 mmol) and 4,4,6-trimethyl-2-vinyl-1,3,2-dioxaborinane (111, 3.29 g, 21.39 mmol, Sigma-Aldrich) in a mixture of TBAF (30.0 mL) and THF (64.0 mL) under an argon atmosphere was added bis(triphenylphosphine)dichloropalladium(II) catalyst (Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, 1.33 g, 1.90 mmol, Sigma-Aldrich) and K<sub>2</sub>CO<sub>3</sub> (8.20 g, 59.4 mmol). The resulting reaction mixture was heated to 60°C and held for 16 hrs in a sealed bottle. The mixture was cooled to a temperature of about 25°C, diluted with water, and extracted with



# Wouldn't it be nice to click immediately to the patent document?

- Avoid being relegated to hard to use 3<sup>rd</sup> party web sites
- patents are fully searchable and support copy/paste

**PatentPak™**


Preferences | SciFinder Help | Sign Out

Explore ▾
Saved Searches ▾
SciPlanner

Patent "US20080078739" > references (3)

REFERENCES ?

Get Substances    Get Reactions    Get Related Citations

Analyze    Refine    Categorize

Sort by: Accession Number ▾

0 of 3 References Selected

Analyze by:	
Author Name ▾	
Booth Jean Paul	1
Fujita Minoru	1
Hattori Kazuhiro	1
Hibi Mikiharu	1
Kajii Yoshio	1

1. **Capacitively-coupled electrostatic (CCE) processing and methods thereof**

By Booth, Jean-Paul  
From PCT Int. App.


A method for processing a set of characters includes applying a frequency response to a set of characters. The method includes applying a frequency response to a set of characters. The method includes applying a frequency response to a set of characters.

Patent No.	Kind	Language
WO 2010005930	A2	English
<b>Patent Family</b>		
JP 2011527521	T	Japanese
JP 5427888	B2	Japanese
CN 104320899	A	Chinese

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization  
International Bureau

(43) International Publication Date  
14 January 2010 (14.01.2010)



(10) International Publication Number  
**WO 2010/005930 A2**

---

(51) International Patent Classification:  
*H01L 21/66* (2006.01)    *H01L 21/205* (2006.01)  
*H01L 21/3065* (2006.01)

(21) International Application Number:  
PCT/US2009/049757

(22) International Filing Date:  
7 July 2009 (07.07.2009)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:  
61/078,739    7 July 2008 (07.07.2008)    US

(71) Applicant (for all designated States except US): **LAM RESEARCH CORPORATION** [US/US]; 4650 Cushing Parkway, Fremont, CA 94538 (US).

(72) Inventors; and  
**Inventors/Applicants (for US only): BOOTH, Jean-paul** [FR/US]; 4650 Cushing Parkway, Fremont, CA 94538 (US). **KEIL, Douglas, L.** [US/US]; 4650 Cushing Parkway, Fremont, CA 94538 (US).

(74) Agent: **NGUYEN, Joseph, A.**; P.O. Box 700640, San Jose, CA 95170 (US).

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.







(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:  
— without international search report and to be republished upon receipt of that report (Rule 48.2(g))



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- Find patents in English, Chinese, Japanese, Russian, German, French, and Korean

Patent Information				
Patent No.		Kind	Language	Date
EP 2891484	 PatentPak	A1		Jul 8, 2015
US 20150190359	 PatentPak	A1	English	Jul 9, 2015
JP 2015129107	 PatentPak	A	Japanese	Jul 16, 2015
CN 104758249	 PatentPak	A	Chinese	Jul 8, 2015
KR 2015082078	 PatentPak	A	Korean	Jul 15, 2015
WO 2015105458	 PatentPak	A1	English	Jul 16, 2015



Intellectual  
Property  
Office



# Links to key substances in the patent allow scientists to get directly to what matters most in no time at all

**PatentPak™** links to the actual location in the patent where important substances are described in the claims or experimental sections in a unique patent document viewer

1636182-64-3P	Page 127 in PatentPak™
prepn. of triazinane trione derivs. and comps. thereof useful for treatment of diseases	
Biological use, unclassified; Cosmetic use; Food or feed use; Other use, unclassified; Pharmacokinetics; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses	
57-88-5P Cholectrol, preparation	
1626333-91-2P	Page 127 in PatentPak™
1636182-62-1P	Page 127 in PatentPak™
1636182-63-2P	Page 127 in PatentPak™
1636182-65-4P	Page 127 in PatentPak™
1636182-66-5P	Page 128 in PatentPak™
1636182-67-6P	Page 128 in PatentPak™
1636182-68-7P	Page 128 in PatentPak™
1636182-69-8P	Page 128 in PatentPak™
prepn. of triazinane trione derivs. and comps. thereof useful for treatment of diseases	
Biological use, unclassified; Cosmetic use; Food or feed use; Other use, unclassified; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses	

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Key Substances in Patent

CAS RN 1626333-91-2

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Analyst Markup Location

page 127

WO 2014/179562 PCT/US2014/036355

Scheme 1. Exemplary synthesis of certain compounds of Formula (I), wherein R<sup>A</sup> and R<sup>B</sup> are as described herein.

[00269] In one set of experiments, a mixture of compounds 1 and 4 in EtOH was irradiated in the microwave oven at 150 °C for 5 h. The reaction mixture was purified by flash column chromatography to yield a compound of Formula (I). Compound

[00270] Compound 1-1: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.99–4.01 (m, 3H), 3.84–3.88 (m, 3H), 2.30–2.48 (m, 12H), 2.24 (s, 9H), 1.27–1.44 (m, 24H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>29</sub>H<sub>39</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 643.5122, found 643.5203.

[00271] Compound 1-2: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.98–4.00 (m, 3H), 3.83–3.86 (m, 3H), 2.33–2.47 (m, 12H), 2.24 (s, 9H), 1.26–1.46 (m, 36H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>30</sub>H<sub>39</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 727.6056, found 727.6116.

[00272] Compound 1-3: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.99–4.00 (m, 3H), 3.84–3.87 (m, 3H), 2.30–2.47 (m, 12H), 2.24 (s, 9H), 1.26–1.44 (m, 60H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>31</sub>H<sub>41</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 895.7934, found 895.7937.

[00273] Compound 1-4: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.11 (m, 3H), 3.98–3.99 (m, 3H), 3.84–3.87 (m, 3H), 2.33–2.45 (m, 12H), 2.24 (s, 9H), 1.25–1.44 (m, 96H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>30</sub>H<sub>39</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 1148.0751, found 1148.0615.

# A unique patent viewer provides a range of powerful new navigation and exploration tools

**PatentPak™**

Key Substances in Patent

Search in SciFinder | View Detail

Analyst Markup Location  
page 127

**CAS RN 1626333-91-2**

Search in SciFinder | View Detail

Analyst Markup Location  
page 127

**CAS RN 1636182-65-4**

Search in SciFinder | View Detail

Analyst Markup Location  
page 127

**CAS RN 2451-62-9**

Search in SciFinder | View Detail

Analyst Markup Location  
page 127

Visually link the substance from the CAS annotation to the patent text

Navigate through chemistry found in the patent

Search SciFinder from substances identified in the patent text

**Scheme 1.** Exemplary synthesis of certain compounds of Formula (I), wherein R<sup>A</sup> and R<sup>B</sup> are as described herein.

**[00269]** In one set of experiments, a mixture of compounds **1** and **4** in EtOH was irradiated in the microwave oven at 150 °C for 5 h. The reaction mixture was purified by flash column chromatography to yield a compound of Formula (I). Compound

**[00270]** **Compound I-1:** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.99–4.01 (m, 3H), 3.84–3.88 (m, 3H), 2.30–2.48 (m, 12H), 2.24 (s, 9H), 1.27–1.44 (m, 24H), 0.88 (t, *J* = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>33</sub>H<sub>63</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 643.5122, found 643.5203.

**[00271]** **Compound I-2:** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.98–4.00 (m, 3H), 3.83–3.86 (m, 3H), 2.33–2.47 (m, 12H), 2.24 (s, 9H), 1.26–1.46 (m, 36H), 0.88 (t, *J* = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>39</sub>H<sub>79</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 727.6056, found 727.6116.

**[00272]** **Compound I-3:** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.99–4.00 (m, 3H), 3.84–3.87 (m, 3H), 2.30–2.47 (m, 12H), 2.24 (s, 9H), 1.26–1.44 (m, 60H), 0.88 (t, *J* = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>51</sub>H<sub>103</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 895.7934, found 895.7937.

**[00273]** **Compound I-4:** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.11 (m, 3H), 3.98–3.99 (m, 3H), 3.84–3.87 (m, 3H), 2.33–2.45 (m, 12H), 2.24 (s, 9H), 1.25–1.44 (m, 96H), 0.88 (t, *J* = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>69</sub>H<sub>139</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 1148.0751, found 1148.0615.

**Compound I-5:** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.93–3.95 (m, 3H), 3.82–3.84 (m, 3H), 1.34–1.42 (m, 12H), 1.26–1.33 (m, 12H), 1.39–1.41 (m, 12H), 0.89 (t, *J* = 7.0 Hz, 18H). HRMS (ESI) calcd for C<sub>36</sub>H<sub>73</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> found 685.5597.

# Preserve Your Most Valuable Resource – Time



- Instant access to searchable full-text patents from major patent offices around the world
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- Substance location mapping provided through the CAS REGISTRY
- Secure and confidential patent research
- Daily updates
- Interactive viewer with built-in SciFinder search functionality

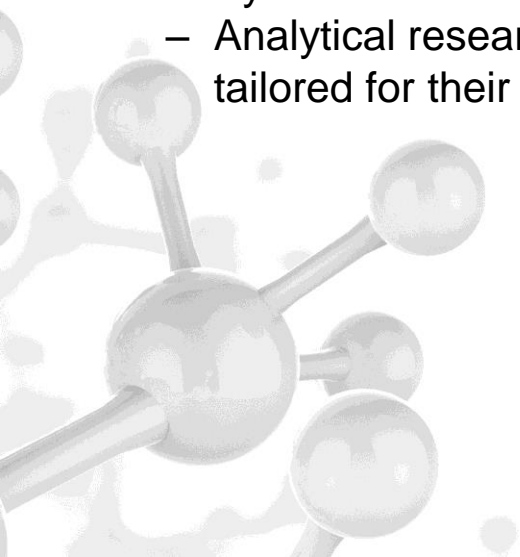
# MethodsNow™ is a complete CAS solution



- Largest single collection of methods information
  - Addresses core chemistry markets
- CAS-quality indexing and new, value-add templating of key methods from important full-text sources
- Covers both synthetic and analytical researcher needs

## So what exactly is MethodsNow?

- A collection of over a million synthetic and analytic methods – with more to come!
  - Focused indexing, step-by-step instruction
  - Details for analytical researchers such as matrix, analyte, instrumentation and comparison capabilities
  
- Interface options right where the user needs them!
  - Synthetic researchers will find relevant content right inside SciFinder
  - Analytical researchers will find relevant content in a newly-designed interface tailored for their search needs



# One product, two interfaces

- Research showed that users interested in synthetic methods were often already in SciFinder, but analytical scientists often weren't (though they might be familiar with it)

*Synthetic chemist looking for great methods?  
They are in SciFinder.*

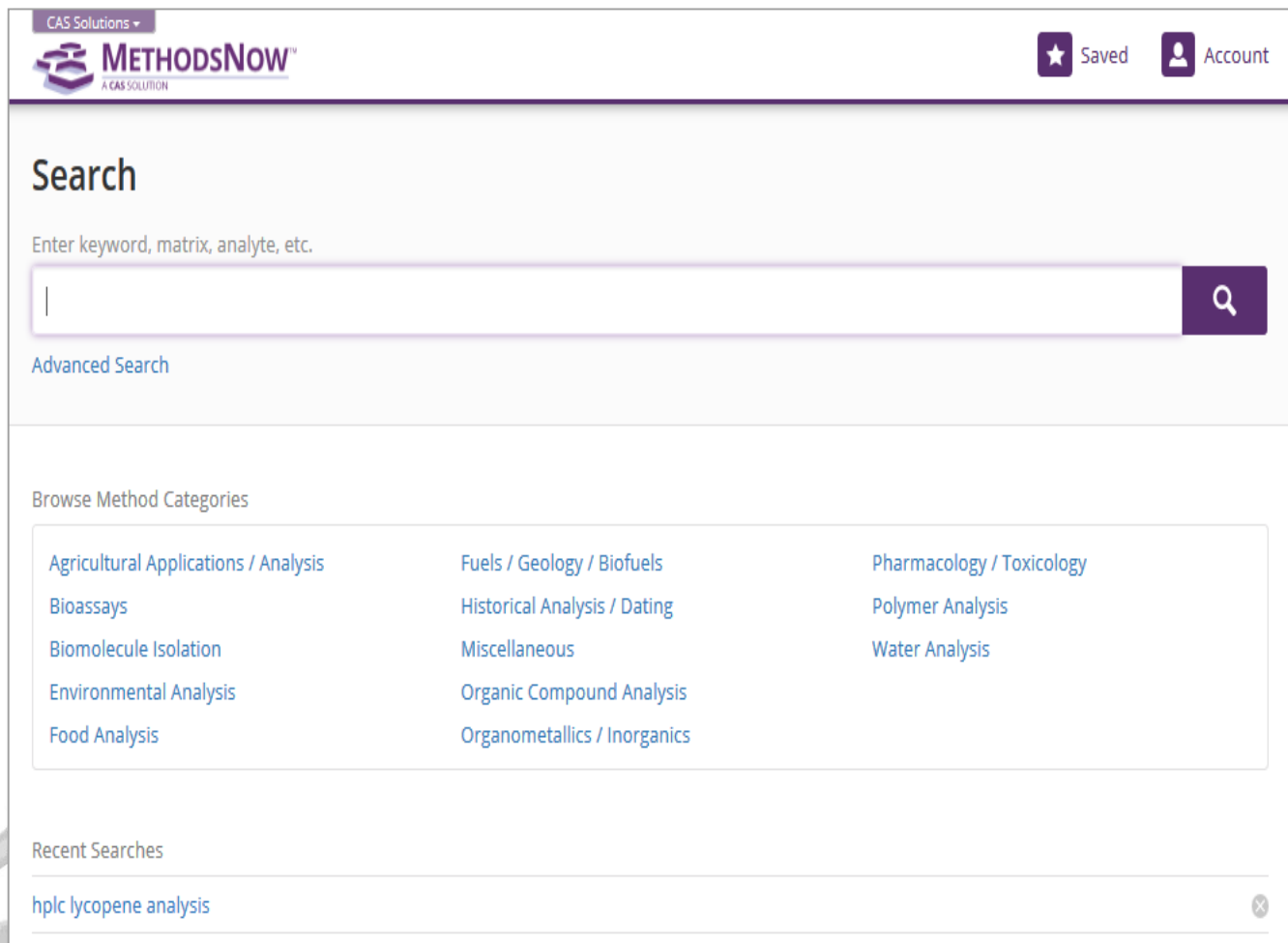
The screenshot shows the SciFinder interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, there's a search bar and a 'SciFinder' logo. The main content area displays a chemical reaction scheme. Below the reaction, there's a 'Procedure' section highlighted with a black oval. The procedure text reads: '1. Stir the mixture of 7-methyl-4-methoxy-carbonylmethyl-2H-chromen-2-one (400 mg, 1.65 mmol), 1-azidoindane (250 mg, 1.83 mmol), copper(II) sulfate pentahydrate (0.17 mmol), (+)-sodium L-ascorbate (300 mg, 1.82 mmol) in 1-BuOH/water (25 mL/25 mL) at room temperature for 4 hours. 2. Add water to the mixture. View more...'.

*Analytical scientist just looking for great methods?  
A new, easy to use interface just for you.*

The screenshot shows the MethodsNow interface. At the top, there's a 'METHODSNow' logo and a 'Saved' button. Below this, there's a search bar with the text 'Enter keyword, matrix, analyte, etc.' and a search icon. Below the search bar, there's an 'Advanced Search' section. The main content area displays a list of method categories: 'Agricultural Applications / Analysis', 'Bioassays', 'Biomolecule Isolation', 'Environmental Analysis', 'Food Analysis', 'Fuels / Geology / Biofuels', 'Historical Analysis / Dating', 'Miscellaneous', 'Organic Compound Analysis', 'Organometallics / Inorganics', 'Pharmacology / Toxicology', 'Polymer Analysis', and 'Water Analysis'. There's also a 'Recent Searches' section at the bottom.



# MethodsNow – Analytical Scientist Interface



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★ Saved    👤 Account

## Search

Enter keyword, matrix, analyte, etc.

Advanced Search

### Browse Method Categories

<a href="#">Agricultural Applications / Analysis</a>	<a href="#">Fuels / Geology / Biofuels</a>	<a href="#">Pharmacology / Toxicology</a>
<a href="#">Bioassays</a>	<a href="#">Historical Analysis / Dating</a>	<a href="#">Polymer Analysis</a>
<a href="#">Biomolecule Isolation</a>	<a href="#">Miscellaneous</a>	<a href="#">Water Analysis</a>
<a href="#">Environmental Analysis</a>	<a href="#">Organic Compound Analysis</a>	
<a href="#">Food Analysis</a>	<a href="#">Organometallics / Inorganics</a>	

### Recent Searches

[hplc lycopene analysis](#) ✕

# Specify one or many advanced search fields

The image displays two overlapping screenshots of the METHODS NOW Advanced Search interface. The top screenshot shows the search criteria selection process, while the bottom screenshot shows the search results page with a dropdown menu open.

**Top Screenshot: Search Criteria Selection**

- Header: CAS Solutions, METHODS NOW A CAS SOLUTION, Saved, Account
- Navigation: Return to Home
- Title: Advanced Search
- Form Fields:
  - Keyword: [Dropdown] [Input]
  - AND [Dropdown] Matrix [Dropdown]
  - AND [Dropdown] Analyte [Dropdown]
- Buttons: Add Search Criteria, Search (Q), Clear

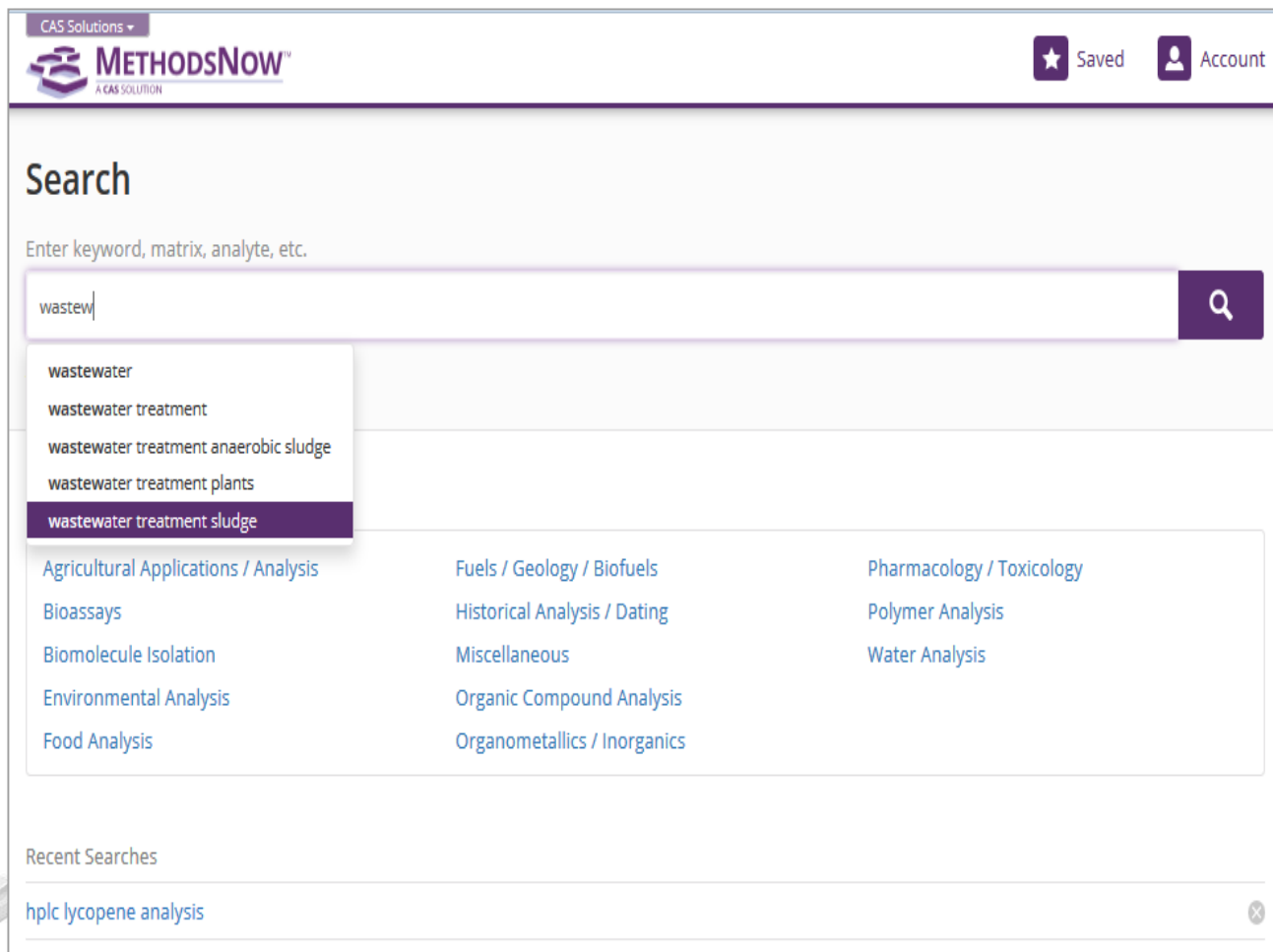
**Bottom Screenshot: Search Results Page**

- Header: CAS Solutions, METHODS NOW A CAS SOLUTION, Saved, Account
- Navigation: Return to Home
- Title: Advanced Search
- Form Fields:
  - Publication Name [Dropdown] [Input]
  - Keyword [Dropdown] [Input]
  - Analyte [Dropdown] [Input]
  - Matrix [Dropdown] [Input]
  - Method Category [Dropdown] [Input]
  - Technique [Dropdown] [Input]
  - CAS Method Number [Input]
  - Publication Name [Dropdown] [Input]
- Buttons: Search (Q), Clear

**Dropdown Menu (Bottom Screenshot):**

- Publication Name (Selected)
- Keyword
- Analyte
- Matrix
- Method Category
- Technique
- CAS Method Number
- Publication Name

# Search for wastewater sludge




CAS Solutions ▾

**METHODSNOW™**  
A CAS SOLUTION

★ Saved    👤 Account

## Search

Enter keyword, matrix, analyte, etc.

wastewater

wastewater treatment

wastewater treatment anaerobic sludge

wastewater treatment plants

wastewater treatment sludge

Agricultural Applications / Analysis

Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

Recent Searches

hplc lycopene analysis



Filters allow you to quickly hone in on the most interesting results

CAS Solutions

**METHODSNow**  
A CAS SOLUTION

wastewater sludge

Results (8923) Sort Relevance

[Return to Home](#)

Analyte  
 Copper (627)  
 Lead (573)  
 Cadmium (495)  
 Nickel (339)  
 Mercury (333)  
[View All](#)

Matrix  
 Drinking waters (3146)  
 River waters (2417)  
 Water (2191)  
 Wastewater (1540)  
 Seawater (1045)  
[View All](#)

Method Category  
 Technique  
 Year

**Analysis of Phosphorus in Wastewater treatment sludge by Dehydration process**  
 CAS MN: 1-143-CAS-4734  
[View Details & Instructions](#) [Add to Compare](#)

Analyte	Phosphorus
Matrix	Municipal wastewater; Wastewater treatment sludge
Other Materials	Reagent: Perchloric acid; Molybdic acid; L-Ascorbic acid; Sulfuric acid Material: Oven
Method Category	Water / Wastewater / Sludge Analysis
Technique	Dehydration process; UV-visible spectroscopy
Equipment Used	UV-VIS spectrometer
Source	Method validation and uncertainty estimation for total phosphorus determination in wastewater sludge samples

# View all on analyte

### Analyte

Alphabetically **By Count**

<input type="checkbox"/> Copper (627)	<input type="checkbox"/> Indeno[1,2,3- <i>cd</i> ]pyrene (119)	<input type="checkbox"/> Polycyclic aromatic hydrocarbons (79)
<input type="checkbox"/> Lead (573)	<input type="checkbox"/> Ciprofloxacin (116)	<input type="checkbox"/> Terbutylazine (79)
<input type="checkbox"/> Cadmium (495)	<input type="checkbox"/> Ethinylestradiol (115)	<input type="checkbox"/> Trimethoprim (79)
<input type="checkbox"/> Nickel (339)	<input type="checkbox"/> Vanadium (115)	<input type="checkbox"/> Dimethyl phthalate (78)
<input type="checkbox"/> Mercury (333)	<input type="checkbox"/> Dibenz[ <i>a,h</i> ]anthracene (112)	<input type="checkbox"/> Selenium (78)
<input type="checkbox"/> Zinc (275)	<input type="checkbox"/> Naproxen (111)	<input type="checkbox"/> Dioctyl phthalate (75)
<input type="checkbox"/> Cobalt (254)	<input type="checkbox"/> Enrofloxacin (110)	<input type="checkbox"/> Diethyl phthalate (74)
<input type="checkbox"/> Chromium (253)	<input type="checkbox"/> Chromium(6+) (107)	<input type="checkbox"/> $\alpha$ -Endosulfan (74)
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<input type="checkbox"/> Arsenic (209)	<input type="checkbox"/> Chlorpyrifos (105)	<input type="checkbox"/> Carbofuran (73)
<input type="checkbox"/> 2,2'-Bis(4-hydroxyphenyl)propane (199)	<input type="checkbox"/> Lead(2+) (104)	<input type="checkbox"/> Sulfadiazine (73)
<input type="checkbox"/> ...	<input type="checkbox"/> ...	<input type="checkbox"/> 2,4,6-Trichlorophenol (72)

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Analyte Carbamazepine

Matrix Wastewater treatment sludge; Wastewater

Other Materials Material: Environmental cartridges; Glass-fiber (0.45mm); Stainless steel vessel (34 mL); LazWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W, continuous).  
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Method Category Active Pharmaceutical Ingredient and Metabolite Analysis; Water / Wastewater / Sludge

Technique Atmospheric pressure chemical ionization mass spectrometry

Equipment Used Milli-Q/Milli-RO system; ASE extractor; Vacuum pump; LDTD-APCI ionization source; Mass Spectrometer

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Title	Analysis of Carbamazepine in Wastewater by Atmospheric pressure chemical ionization mass spectrometry	Analysis of Carbamazepine in Wastewater by Atmospheric pressure chemical ionization mass spectrometry
CAS Method Number	1-101-CAS-27867	1-101-CAS-29149
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis; Water / Wastewater / Sludge Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis; Water / Wastewater / Sludge Analysis
Technique	Atmospheric pressure chemical ionization mass spectrometry	Atmospheric pressure chemical ionization mass spectrometry
Analyte	Carbamazepine	Carbamazepine
Matrix	Wastewater treatment sludge; Wastewater	Wastewater treatment sludge; Wastewater
Other Materials	Environmental cartridges; Glass-fiber (0.45mm); Stainless steel vessel (34 mL); LazWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W)	Environmental cartridges; Glass-fiber (0.45mm); LazWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W, continuous).



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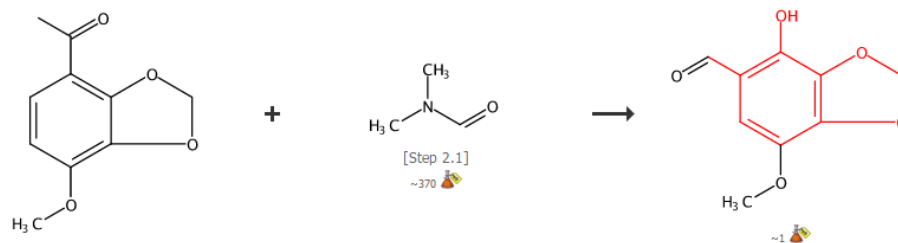
**Procedure**

1. Stir the mixture of 7-ethynyl-4-methoxycarbonylmethyl-2H-chromen-2-one (400 mg, 1.65 mmol), 1-azidoundecane (358 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-sodium L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours.
2. Add water to the mixture.

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Overview

### Steps/Stages

- 1.1 R:Na<sub>2</sub>HPO<sub>4</sub>, R:mCPBA, S:CH<sub>2</sub>Cl<sub>2</sub>, cooled; 1 h, rt
- 1.2 R:KOH, S:MeOH, 2 h, rt
- 1.3 R:HCl, S:H<sub>2</sub>O, acidify
- 2.1 R:POCl<sub>3</sub>, S:DMF, 15 min, 5°C; 5°C → rt; 20 min, rt
- 2.2 rt; rt → 75°C; 2 h, 75°C; 75°C → 0°C
- 2.3 R:H<sub>2</sub>O, 5°C

### Notes

1) Baeyer-Villiger oxidation (stage 1), 2) regioselective, Vilsmeier reaction, Reactants: 2, Reagents: 6, Solvents: 4, Steps: 2, Stages: 6, Most stages in any one step: 3

### References

Total Synthesis of Bulbophylo-B

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By Lin, Jinshun et al

From Journal of Natural Products, 71(11), 1938-1941; 2008

Experimental Procedure



### Step 1

**4-Methoxy-2,3-methylenedioxyphenyl Acetate (8).** To a suspension of **7** (5.0 g, 25.5 mmol) and anhydrous Na<sub>2</sub>HPO<sub>4</sub> (4.7 g, 33.2 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (50 mL) was added *m*-CPBA (85%, 23.4 g, 127.5 mmol), in portions and in an ice-water bath, and the mixture was stirred at room temperature for 1 h. The resulting mixture was refluxed overnight, then cooled and filtered. The filter cake was washed with CH<sub>2</sub>Cl<sub>2</sub> (3 × 30 mL). Evaporation of the solvent *in vacuo* gave a residue, which was directly used in the next reaction. **4-Methoxy-2,3-methylenedioxyphenol (9).** KOH (1.4 g, 25 mmol) in H<sub>2</sub>O (10 mL) was added to the crude **8** (5.5 g, 25.8 mmol) in MeOH (20 mL), and the mixture was stirred for 2 h at room temperature. The mixture was concentrated to 10 mL and acidified with 2 M HCl (5 mL). The aqueous layer was extracted with CHCl<sub>3</sub> (3 × 20 mL), washed with H<sub>2</sub>O (2 × 20 mL) and brine (20 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and concentrated. The residue was purified by column chromatography (CC) (*n*-hexane/EtOAc, 3:1) to give **9** (4.38 g; two steps total yield 78%) as a white solid: **4-Methoxy-2,3-methylenedioxyphenol (9)**, yield 4.38 g, 78% mp 103-105 °C (lit.<sup>12</sup> mp 100-101 °C); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 6.43 (1H, s, H-6), 6.42 (1H, s, H-5), 5.99 (2H, s, OCH<sub>2</sub>O), 4.48 (1H, s, OH), 3.85 (1H, s, OCH<sub>3</sub>).

### Step 2

**2-Hydroxy-3,4-methylenedioxy-5-methoxybenzaldehyde (10).** POCl<sub>3</sub> (5.5 mL, 59.5 mmol) was added dropwise to DMF (10 mL, 129.4 mmol) over 15 min at 5 °C, then stirred at room temperature for 20 min followed by addition of **9** (2.5 g, 14.9 mmol) in portions. The mixture was slowly heated to 75 °C and then stirred at this temperature for 2 h. The resulting mixture was cooled to 5 °C and poured into H<sub>2</sub>O (50 mL). After filtration, the filter cake was purified by CC (*n*-hexane/CHCl<sub>3</sub>, 1:1) to give **10** (2.3 g, 79%) as a white solid: **2-Hydroxy-3,4-methylenedioxy-5-methoxybenzaldehyde (10)**, yield 2.3 g, 79% mp 181-182 °C (lit.<sup>12</sup> mp 179-180 °C); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 10.83 (1H, CHO), 9.73 (1H, s, OH), 6.75 (1H, s, Ar-H), 6.18 (2H, s, OCH<sub>2</sub>O), 3.93 (3H, s, OCH<sub>3</sub>).

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CH<sub>3</sub> (CH<sub>2</sub>)<sub>10</sub>

[Step 2.1] ~59

[Step 4.1] ~145

Overview

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Procedure

1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg, 0

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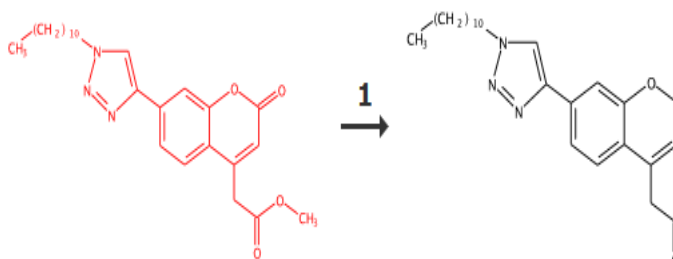
By Jeon, Moon-Kook; Kang, Myoung-Ku; Park, Koon Ha

From Tetrahedron, 68(30), 6038-6053; 2012

Published by Elsevier Ltd.

## Reaction Steps

1 2 3 4



<b>Products</b>	2 <i>H</i> -1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1 <i>H</i> -1,2,3-triazol-4-yl)-2 <i>H</i> -chromen-2-one 1384966-77-1
<b>Reactants</b>	2 <i>H</i> -1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1 <i>H</i> -1,2,3-triazol-4-yl)-2 <i>H</i> -chromen-2-one 1384966-75-9
<b>Reagents</b>	Hydrochloric acid, CAS RN: 7647-01-0 Lithium hydroxide, CAS RN: 1310-65-2
<b>Solvents</b>	Water, CAS RN: 7732-18-5 Tetrahydrofuran, CAS RN: 109-99-9

## MethodsNow

## Procedure

1. Add lithium hydroxide monohydrate (327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1*H*-1,2,3-triazol-4-yl)-2*H*-chromen-2-one (343 mg, 0.780 mmol) in THF/water (25 mL/25 mL) at room temperature.
2. Stir the reaction mixture for 3 hours at room temperature.
3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid.
4. Partition the reaction mixture between ethyl acetate and water.
5. Extract the aqueous layer with ethyl acetate.
6. Dry the combined organic layer over magnesium sulfate.

## Scale

milligram

<sup>1</sup>H NMR

<sup>1</sup>H NMR (300 MHz, acetone-*d*<sub>6</sub>): δ = 7.83 (s, 1H), 8.58 (s, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 6.47 (s, 1H), 4.50 (t, *J* = 7.2 Hz, 2H), 3.99 (s, 2H), 2.00 (quintet, *J* = 7.2 Hz, 2H), 1.32-1.43 (m, 4H), 1.22-1.32 (m, 12H), 0.87 ppm (t, *J* = 6.8 Hz, 3H).

<sup>13</sup>C NMR

<sup>13</sup>C NMR (125 MHz, DMF-*d*<sub>7</sub>, 60 °C): δ = 161.0, 155.1, 154.2, 146.5, 136.0, 127.2, 123.7, 122.1, 120.4, 115.3, 113.5, 51.1, 32.8, 29.9, 27.3, 23.5, 18.7, 14.7 ppm (decarboxylation occurred to give the corresponding 4-methyl derivative).

## IR

IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm<sup>-1</sup>.

## HRMS

HRMS (EI): *m/z* calculated for C<sub>24</sub>H<sub>31</sub>N<sub>3</sub>O<sub>4</sub>: 425.2315 [M<sup>+</sup>]; found: 425.2315.

## Mass Spec

MS (ESI): *m/z*: 426 [M+H<sup>+</sup>].

## MP

235.5±0.8 °C.

## CAS Method Number

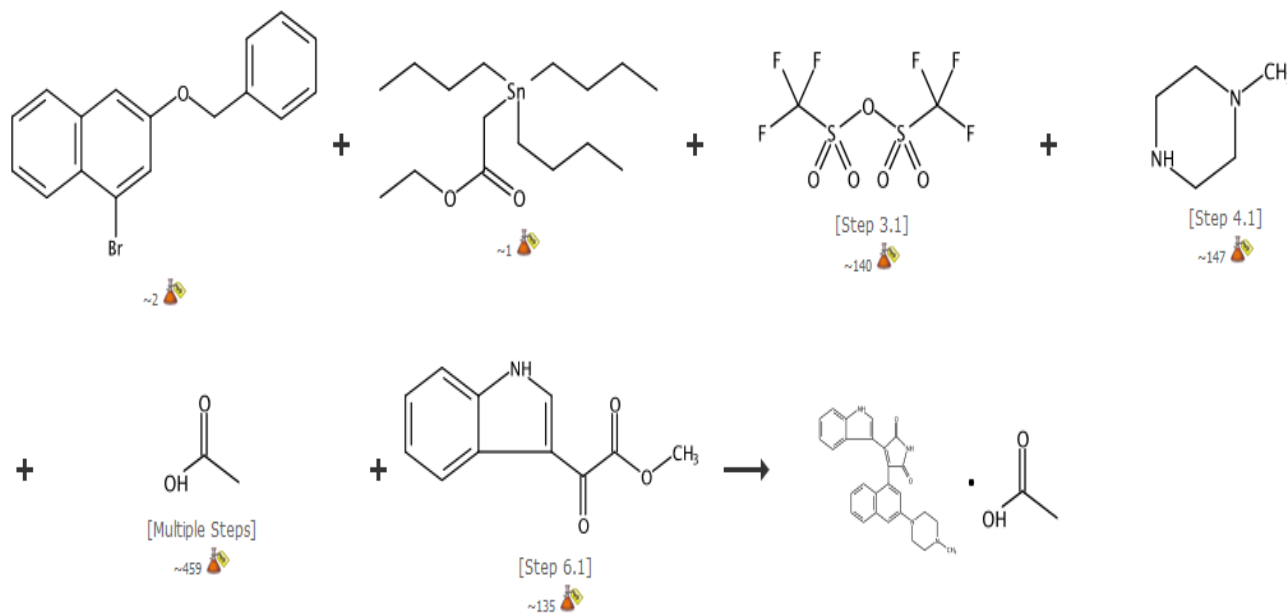
3-352-CAS-78415

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# A reaction with experimental procedure and MethodsNow

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## Procedure

1. Dissolve 3-Benzyloxy-1-bromonaphthalene (5.64 g, 18.01 mmol) in dry DMF (100 ml) under an atmosphere of argon.
2. Add tributyltinyl acetic acid ethyl ester (7.47 g, 10.81 mmol) as well as [bis(tri-*n*-butylphosphino)]palladium(II) dichloride (2.82 g, 2.60 mmol) and zinc(II) bromide (5.27

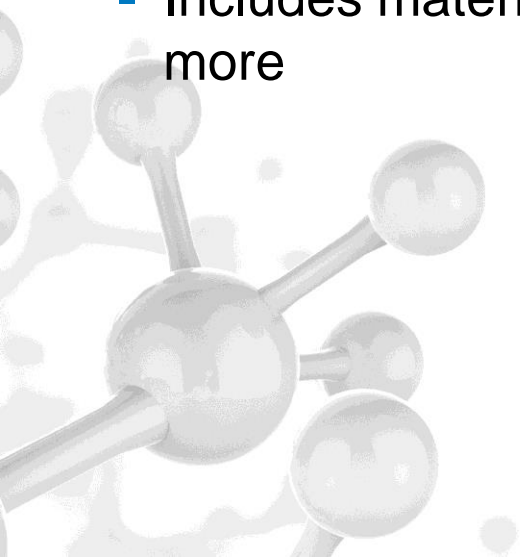
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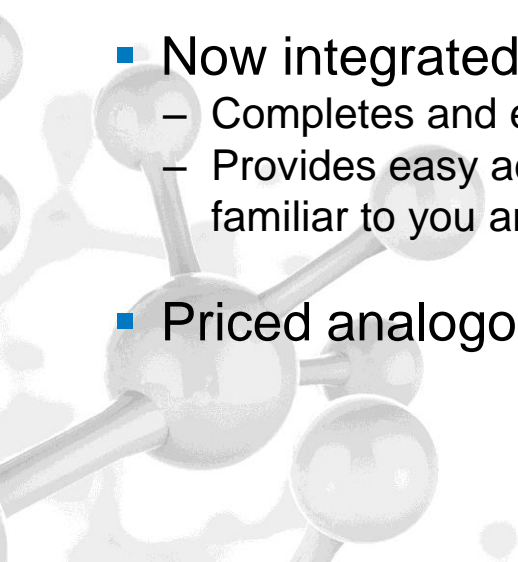
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