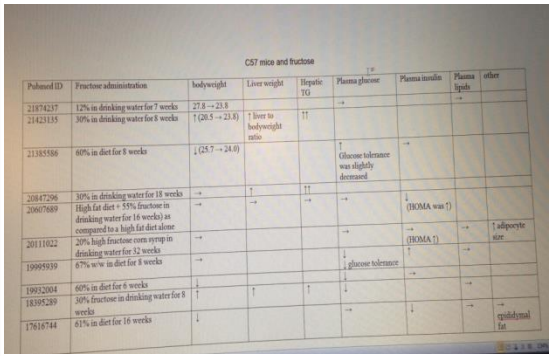
Chuan-Che Liu Ph.D
Senior Account Consultant
tliu2@info.org

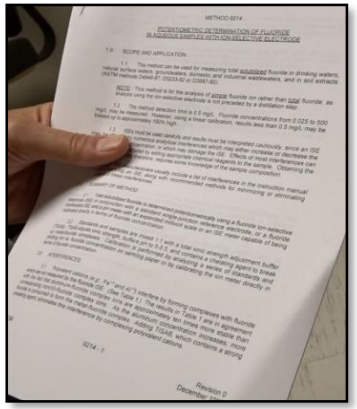
MethodesNow Introduction

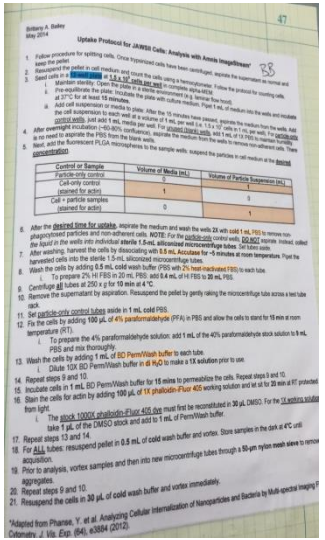
-Immediate access to detailed experimental methods

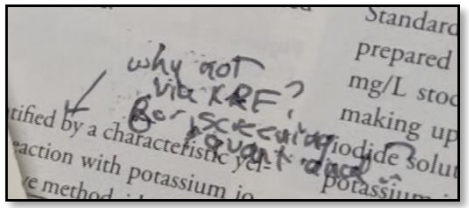
CAS is making it easier for researchers to find methods for their work

Scribbling on papers will become a thing of the past









So what exactly is MethodsNow?

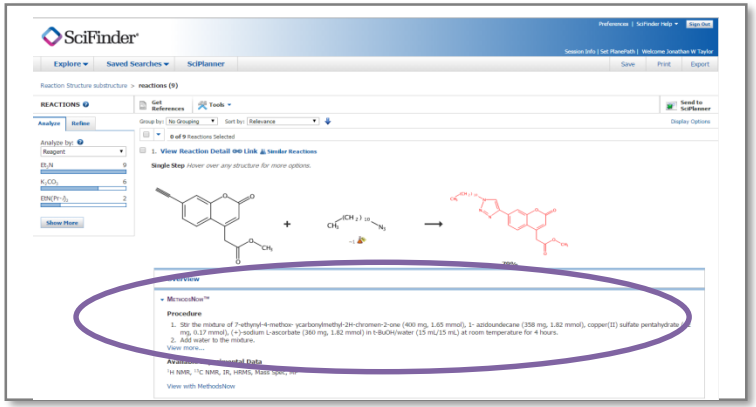
- A collection of over 2 million synthetic and analytic methods – with more to come!
  - Focused indexing, step-by-step instruction
  - Details for analytical researchers such as matrix, analyte, instrumentation and comparison capabilities

- 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

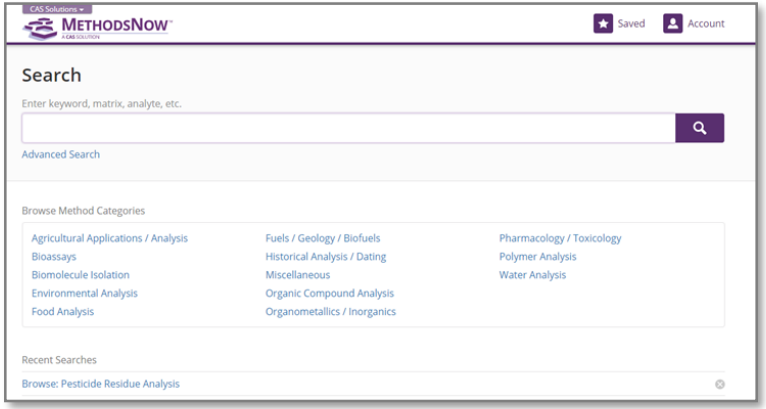
One product, two interfaces

- 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.

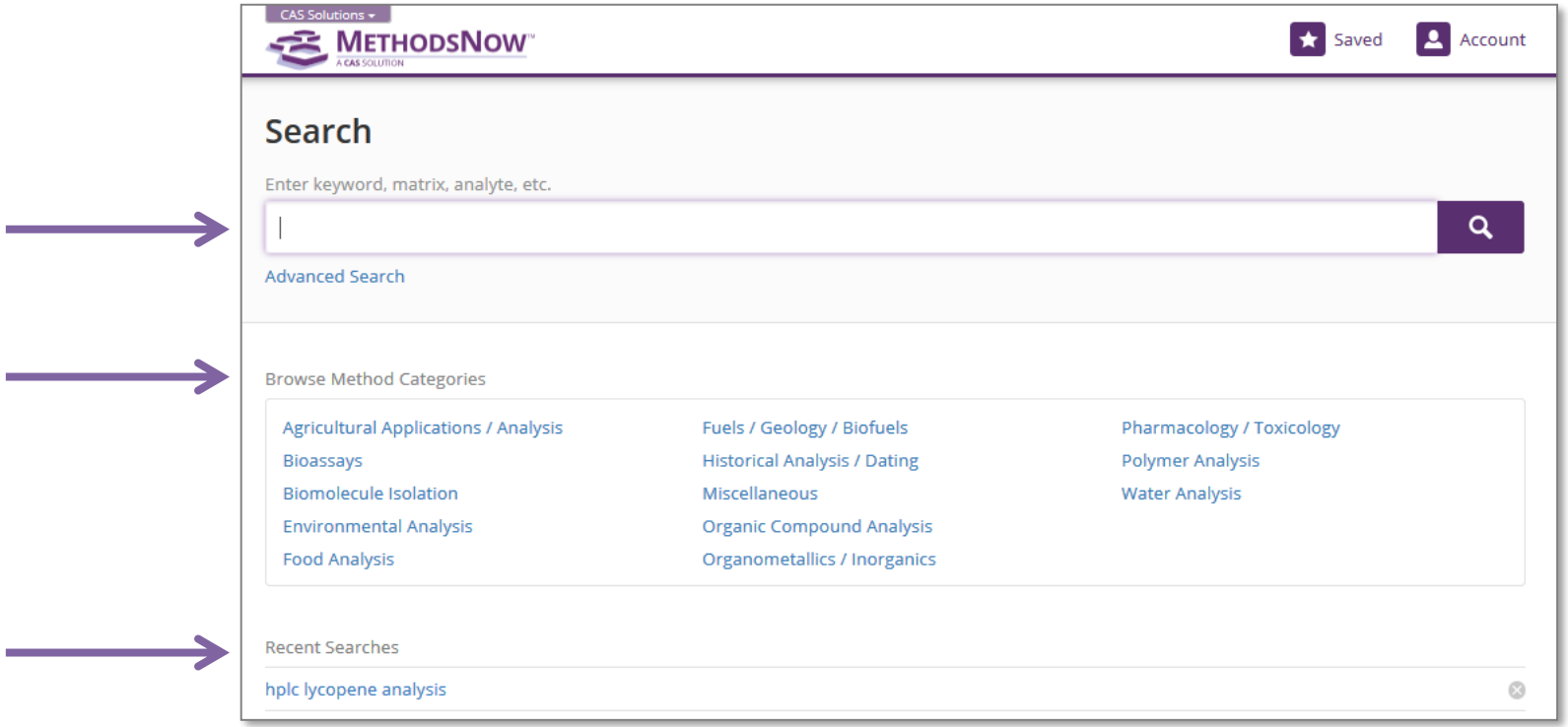


Analytical scientist just looking for great methods? A new, easy to use interface just for you.



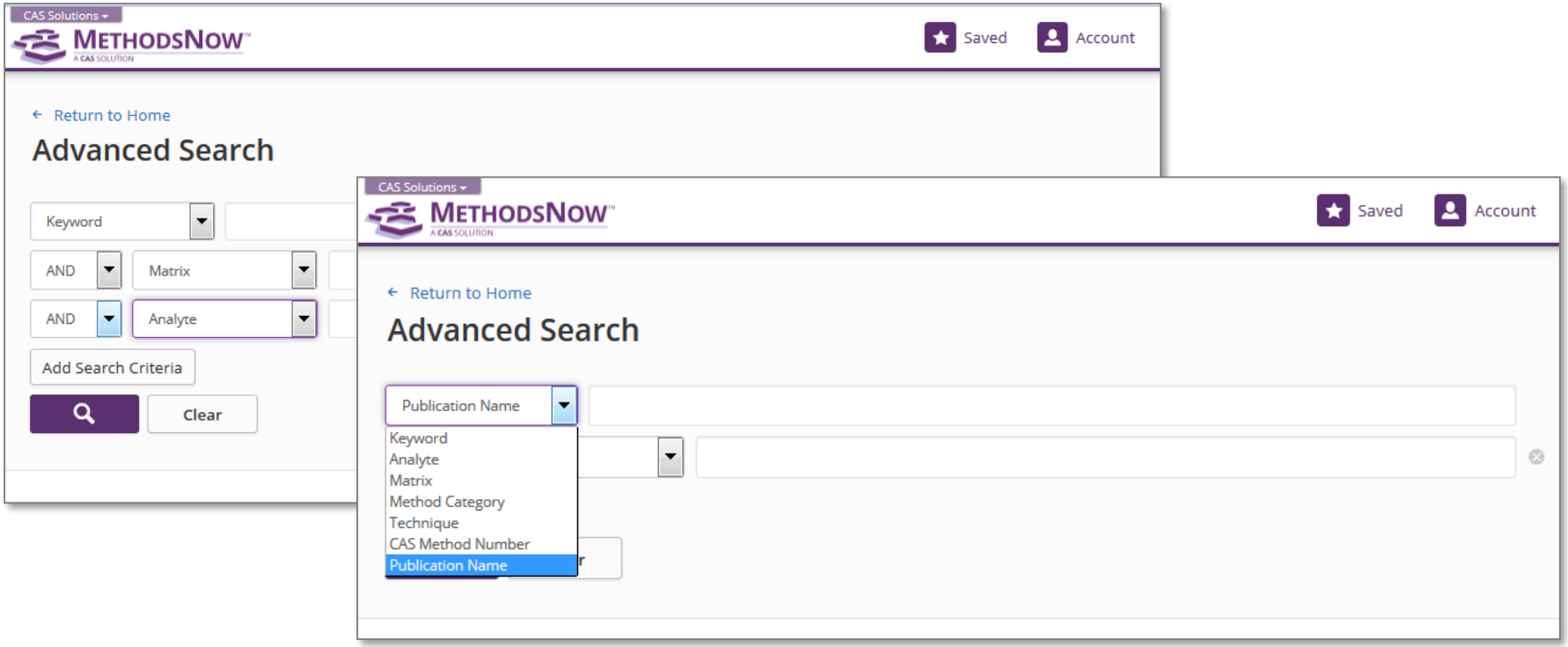
METHODSNOW™
A CAS SOLUTION

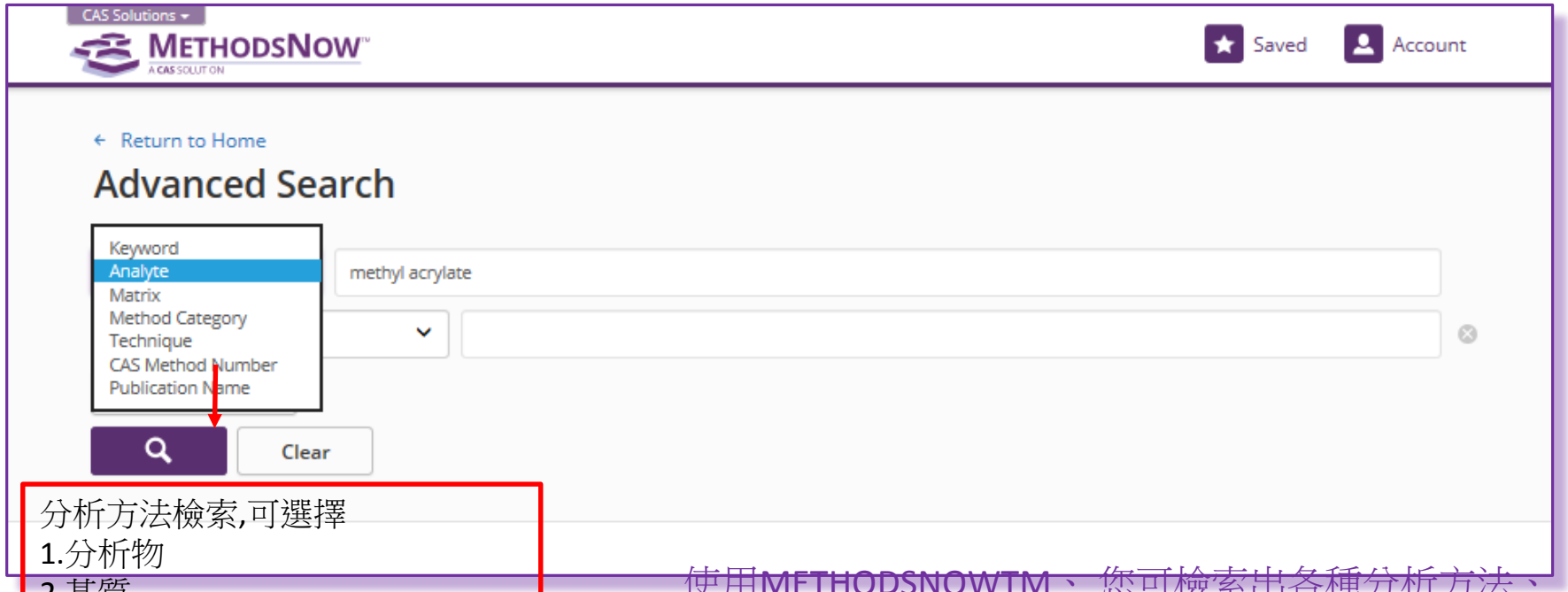
MethodsNow – Analytical Scientist Interface



METHODSNOW™
A CAS SOLUTION

Specify one or many advanced search fields





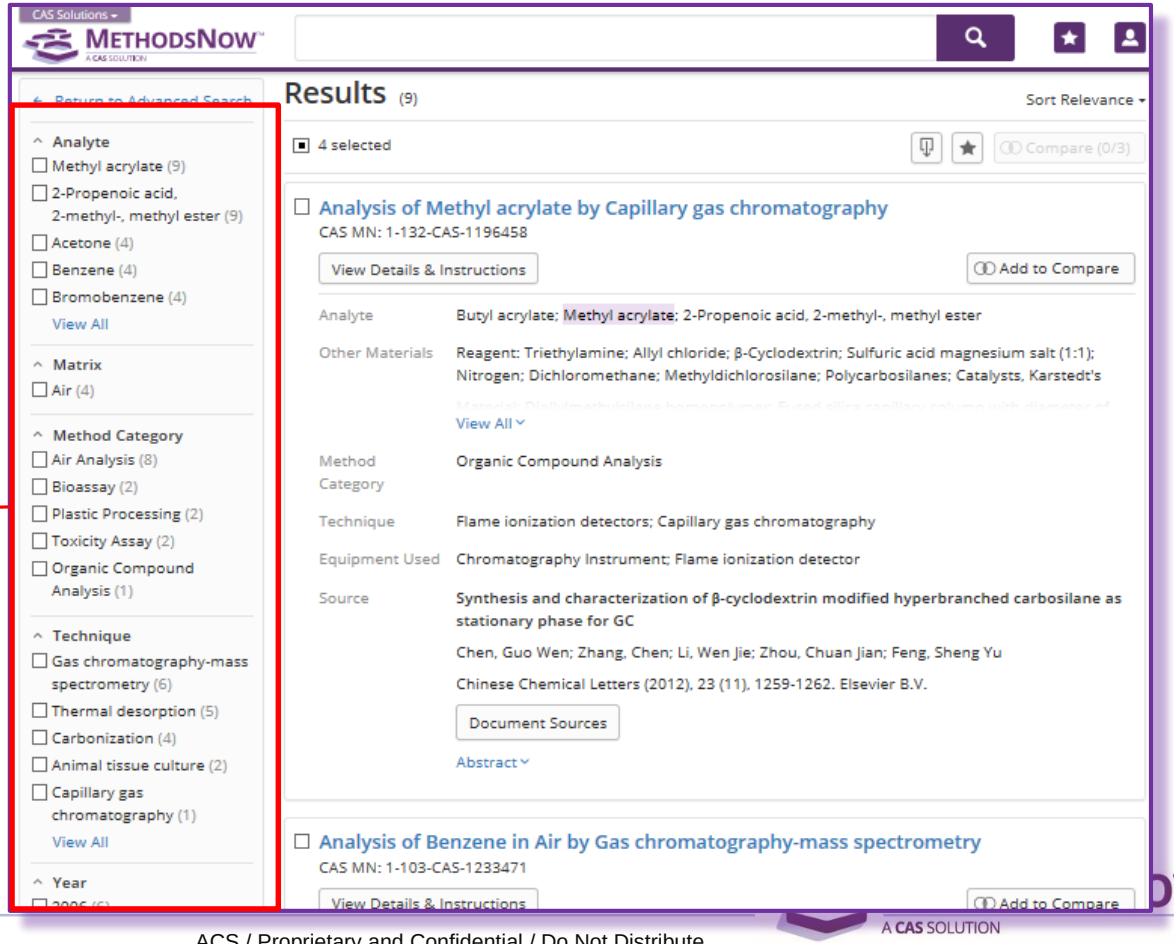
分析方法檢索,可選擇
1.分析物
2.基質
3.方法類別
4.技術
5.CAS方法號
6. 出版物名稱

使用METHODSNOWTM、您可檢索出各種分析方法、並獲取包括實驗步驟、所用材料、所需儀器儀錶、及檢測資料等在內的詳細資訊。如需要，您還可將幾種方法並排對比以便快速地作出選擇。

METHODSNOW™ A CAS SOLUTION

Methal acrylate

篩選結果
1.分析物
2.基質
3.方法類別
4.分析技術
5.文獻年份



Methal acrylate

Equipment Used

TD/GC/MS system, 6890/5973, Agilent

Conditions

Chromatographic

GC Injector temperature- split, 230 °C, split ratio-10:1 ; flow rate- 1 mL/min (35 cm/s) ; Temperature program- -10 °C hold for 3 min, 8 °C min^{-1} to 20 °C, hold for 3 min, 5 °C min^{-1} to 120 °C, hold for 1 min, 20 °C min^{-1} to 250 °C, hold for 1 min ; total run time- 37.15 min

Instrument

MS quad temperature- 150 °C ; MS sorce temperature- 230 °C ; thermal desorption dry purge flow rate- 40 mL/min, Dry purge time- 1 min, Inject time- 1 min

Instructions

Laboratory sample preparation

1. Obtain seven point calibration curves using 2 µL loadings containing 0.3, 0.5, 1, 3, 10, 30 and 100 ng of each compound for scan mode tests.
2. Use duplicate tubes and analyses for this method.

Field sample preparation

1. Randomly select 51 non-smoking homes by phone call, and sample 8 to 10 homes each week.
2. Collect duplicate passive samplers inside and outside of each residence over a 3 to 4 day period.
3. Use a sampling volume of ~2 L.
4. Obtain 4 field blanks each week.
5. Obtain 51 indoor sample measurements and 41 outdoor sample measurements.
6. Analyze using scan mode.
7. Obtain results for each pair in duplicates

檢索呈現
1.摘要
2.分析條件
3.儀器設定
4.樣品配置
5.儀器步驟
6.確效範圍

Methal acrylate

TD/GC/MS Method

1. Use 10 cm length, 6 mm OD and 4 mm ID stainless-steel sampling and thermal desorption tubes with tapered screw threads on both ends.
2. Pack each tube from upstream to downstream with 160 mg of Tenax GR and then 70 mg of Carbosieve SIII separated by glass wool plugs.
3. The 94 target compounds include aromatics, halogenated compounds, terpenes, alkanes and carbonyls.
4. Select the volatile organic compounds (VOCs) based on toxicity and frequency of occurrence.
5. Include fluorobenzene and p-bromo- fluorobenzene as internal standards (IS) for quantification.
6. Analyze laboratory and field samples using an Agilent 6890/5973 GC/MS system running ChemStation (G1701BA, Version B.01, Hewlett-Packard, Palo Alto, CA, USA).
7. Employ a capillary column of 30 m x 0.25 mm id with 0.25 µm film thickness (HP-5MS, Hewlett-Packard, Santa Clarita, CA, USA).
8. Spike each tube (sample or blank) with 2 µL of an internal standard solution containing 2 ng each of fluorobenzene and p-bromo- fluorobenzene.
9. Thermally desorb, cryofocuse and analyze it by gas chromatography mass spectrometry (GC/MS) following methods and quality control procedures.
10. Use identical thermal desorption, gas chromatography (TD/GC) conditions for both scan and SIM methods.

Scan-mode Analysis

1. Run the MS from 1.2-2.5 min after desorption to detect early elution of 1,3-butadiene, an important air toxic, turning the MS off from 2.5 to 4.2 min to avoid the IS solvent peak, and then resuming MS operation from 4.2 to 37.15 min to detect the remaining compounds.

Validation

Limit of Detection	0.026 μgm^{-3}, benzene
	0.033 μgm^{-3}, toluene
	0.019 μgm^{-3}, ethylbenzene
	0.03 μgm^{-3}, p-xylene, m-xylene

檢索呈現
1.摘要
2.分析條件
3.儀器設定
4.樣品配置
5.儀器步驟
6.確效範圍

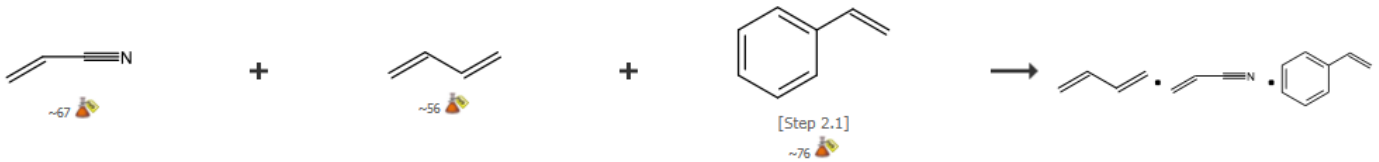
MethodsNow for analytical scientists: Great content sources

Content from years	2000 - present
Number of methods	~220,000 – more than any other single source
Content Coverage	Broad range: Key focus in Pharma, Ag, and chemical as well as others
Source Focus	Full CAplus℠ database. Future investment may include regulatory agencies and instrumentation
Example journal titles	Food Chemistry, Journal of Chromatography A and B, Journal of Agricultural and Food Chemistry, Talanta, Analytica Chimica Acta
Language	English only

MethodsNow – Synthetic Chemist Interface

1. **View Reaction Detail Link**

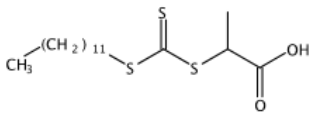
2 Steps *Hover over any structure for more options.*



Overview

Steps/Stages

1.1 R:



R:Et_3N, C:$K_2(S_2O_8)$, 50°C, 2.5-6 bar, pH 10

2.1 C:AIBN, S:PhCl, 12 h, 55°C

Notes

1) inert, azeotropic, monomer conversion = 60%, Reactants: 3, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

References

RAFT-Mediated ab Initio Emulsion Copolymerization of 1,3-Butadiene with Acrylonitrile

Quick View Other Sources

By Hlalele, Lebohang et al

From Macromolecules (Washington, DC, United States), 47(9), 2820-2829; 2014

Experimental Procedure

METHODSNOW™

Procedure

1. Purge the surfactant solution with nitrogen gas for 15 min and subsequently transfer to a pressure stable reactor.
2. Subject the surfactant solution to three nitrogen/vacuum cycles.

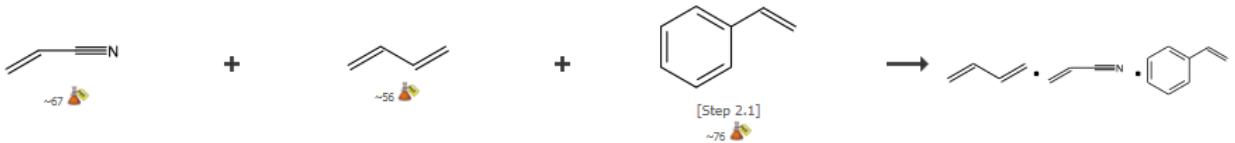
View more...

View with MethodsNow

SciFinder has the largest collection of experimental procedures for reactions

1. **View Reaction Detail** Link

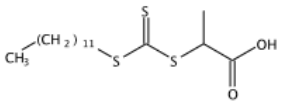
2 Steps *Hover over any structure for more options.*



▾ **Overview**

Steps/Stages

1.1 R:



R:Et_3N, C:$K_2(S_2O_8)$, 50°C, 2.5-6 bar, pH 10

2.1 C:AIBN, S:PhCl, 12 h, 55°C

Notes

1) inert, azeotropic, monomer conversion = 60%, Reactants: 3, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

…e with Acrylonitrile

…4

It is our most popular feature, but you've told us we can do more

▾ **Experimental Procedure**

Macromolecules

Step 1

In a typical copolymerization, the surfactant solution was purged with nitrogen gas for 15 min and subsequently transferred to a pressure stable reactor. Next, the surfactant solution was subjected to three nitrogen/vacuum cycles. A purged solution of DoPAT in acrylonitrile was introduced into the reactor under inert conditions followed by addition of 1,3-butadiene to the reactor via a metal buret, which had been degassed by three nitrogen/vacuum cycles prior to the addition of 1,3-butadiene. The mixture was stirred at 600 rpm and heated to the polymerization temperature (e.g., 50 °C) prior to addition of triethylamine (TEA) base and potassium persulfate (KPS) initiator. The surfactant has been added in such a way that its concentration exceeds the critical micelle concentration. For simplicity, it is assumed that a potential micellar behavior of DoPAT can be ignored. The azeotropic feed composition (38/62) has been confirmed experimentally, indicative of a limited effect of partitioning. It should be stressed that in addition to the temperature the decomposition rate of persulfates is affected by pH and basicity with an increased basicity leading to an increased rate of decomposition. [29-31] The use of base activation of KPS allows for moderate temperatures (45-55 °C) to be employed for the decomposition of the initiator, explaining the aforementioned initiation procedure.

Step 2

NBR Chain Extension in Solution. Trithiocarbonate ω-functional NBR (2.0 g), as obtained via the emulsion RAFT polymerization, was dissolved in chlorobenzene, then styrene (48 mmol) and AIBN (0.015 mmol) were added to the solution. The resulting mixture was degassed by four freeze-pump-thaw cycles and backfilled with nitrogen gas. The flask was subsequently immersed in a preheated oil bath at 55 °C, and the reaction was allowed to proceed for 12 h. The resulting polymer was precipitated in chilled ethanol and dried under vacuum at ambient temperature for 24 h. For the evaluation of the chain extension experiments, an SEC calibration with narrow polystyrene standards was employed.

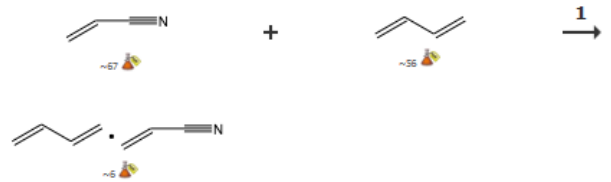
MethodsNow – Step by Step procedure

MethodsNow

RAFT-Mediated ab Initio Emulsion Copolymerization of 1,3-Butadiene with Acrylonitrile

By Hlalele, Lebohang; D'hooge, Dagmar R.; Duerr, Christoph J.; Kaiser, Andreas; Brandau, Sven; Barner-Kowollik, Christopher
From Macromolecules (Washington, DC, United States), 47(9), 2820-2829; 2014
Published by American Chemical Society

Reaction Steps 1 2



Products	Acrylonitrile-butadiene copolymer, CAS RN: 9003-18-3
Reactants	Acrylonitrile, CAS RN: 107-13-1 1,3-Butadiene, CAS RN: 106-99-0
Reagents	2-[[(Dodecylthio)thioxomethyl]thio]propanoic acid, CAS RN: 558484-21-2 Triethylamine, CAS RN: 121-44-8
Catalysts	Potassium persulfate, CAS RN: 7727-21-1
Procedure	1. Purge the surfactant solution with nitrogen gas for 15 min and subsequently transfer to a pressure stable reactor. 2. Subject the surfactant solution to three nitrogen/vacuum cycles. 3. Introduce a purged solution of DoPAT in acrylonitrile into the reactor under inert conditions following with addition of 1,3-butadiene to the reactor via a metal buret, that was degassed by three nitrogen/vacuum cycles prior to the addition of 1,3-butadiene. 4. Stir the mixture at 600 rpm and heat to the polymerization temperature (e.g., 50 °C) prior to addition of triethylamine (TEA) base and potassium persulfate (KPS) initiator. 5. Add surfactant in such a way that its concentration exceeds the critical micelle concentration. 6. Assume that a potential micellar behavior of DoPAT can be ignored.
CAS Method Number	3-614-CAS-2717173

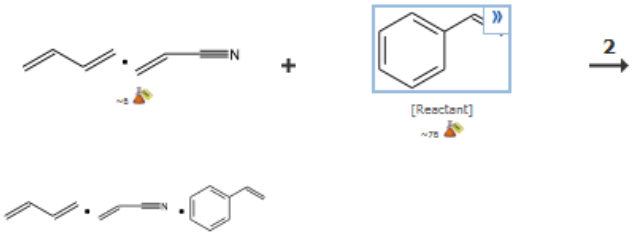
Print/Export Close

MethodsNow

RAFT-Mediated ab Initio Emulsion Copolymerization of 1,3-Butadiene with Acrylonitrile

By Hlalele, Lebohang; D'hooge, Dagmar R.; Duerr, Christoph J.; Kaiser, Andreas; Brandau, Sven; Barner-Kowollik, Christopher
From Macromolecules (Washington, DC, United States), 47(9), 2820-2829; 2014
Published by American Chemical Society

Reaction Steps 1 2



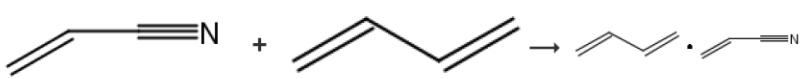
Products	2-Propenenitrile, polymer with 1,3-butadiene and ethenylbenzene, diblock, CAS RN: 749886-85-9
Reactants	Acrylonitrile-butadiene copolymer, CAS RN: 9003-18-3 Styrene, CAS RN: 100-42-5
Catalysts	Azobisisobutyronitrile, CAS RN: 78-67-1
Solvents	Chlorobenzene, CAS RN: 108-90-7
Procedure	1. Dissolve Trithiocarbonate ω-functional NBR (2.0 g) in chlorobenzene. 2. Add styrene (48 mmol) and AIBN (0.015 mmol) to the solution. 3. Degas the resulting mixture with four freeze-pump-thaw cycles and backfill with nitrogen gas. 4. Subsequently immerse the flask in a preheated oil bath at 55 °C. 5. Allow the reaction to proceed for 12 h. 6. Precipitate the the resulting polymer in chilled ethanol. 7. Dry the mixture under vacuum at ambient temperature for 24 h.
CAS Method Number	3-614-CAS-2463870

Print/Export Close

MethodsNow – Export PDF

RAFT-Mediated ab Initio Emulsion Copolymerization of 1,3-Butadiene with Acrylonitrile
By Hlalele, Lebohang; D'hooge, Dagmar R.; Duerr, Christoph J.; Kaiser, Andreas; Brandau, Sven; Barner-Kowollik, Christopher
From Macromolecules (Washington, DC, United States), 47(9), 2820-2829; 2014
Published by American Chemical Society

Step 1

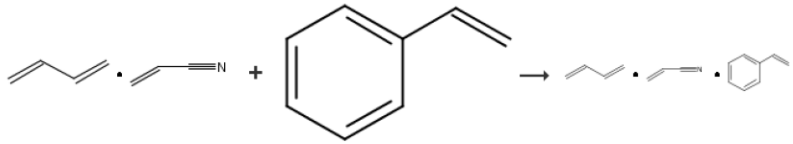


Products	Acrylonitrile-butadiene copolymer, CAS RN: 9003-18-3
Reactants	Acrylonitrile, CAS RN: 107-13-1 1,3-Butadiene, CAS RN: 106-99-0
Reagents	2-[[(Dodecylthio)thioxomethyl]thio]propanoic acid, CAS RN: 558484-21-2 Triethylamine, CAS RN: 121-44-8
Catalysts	Potassium persulfate, CAS RN: 7727-21-1
Procedure	1. Purge the surfactant solution with nitrogen gas for 15 min and subsequently transfe a pressure stable reactor. 2. Subject the surfactant solution to three nitrogen/vacuum cycles. 3. Introduce a purged solution of DoPAT in acrylonitrile into the reactor under inert conditions following with addition of 1,3-butadiene to the reactor via a metal buret, was degassed by three nitrogen/vacuum cycles prior to the addition of 1,3-butadier 4. Stir the mixture at 600 rpm and heat to the polymerization temperature (e.g., 50 °C prior to addition of triethylamine (TEA) base and potassium persulfate (KPS) initiat 5. Add surfactant in such a way that its concentration exceeds the critical micelle concentration. 6. Assume that a potential micellar behavior of DoPAT can be ignored.
CAS Method Number	3-614-CAS-2717173

SciFinder® Page 1

RAFT-Mediated ab Initio Emulsion Copolymerization of 1,3-Butadiene with Acrylonitrile
By Hlalele, Lebohang; D'hooge, Dagmar R.; Duerr, Christoph J.; Kaiser, Andreas; Brandau, Sven; Barner-Kowollik, Christopher
From Macromolecules (Washington, DC, United States), 47(9), 2820-2829; 2014
Published by American Chemical Society

Step 2



[Reactant]

Products	2-Propenenitrile, polymer with 1,3-butadiene and ethenylbenzene, diblock, CAS RN: 749886-85-9
Reactants	Acrylonitrile-butadiene copolymer, CAS RN: 9003-18-3 Styrene, CAS RN: 100-42-5
Catalysts	Azobisisobutyronitrile, CAS RN: 78-67-1
Solvents	Chlorobenzene, CAS RN: 108-90-7
Procedure	1. Dissolve Trithiocarbonate ω-functional NBR (2.0 g) in chlorobenzene. 2. Add styrene (48 mmol) and AIBN (0.015 mmol) to the solution. 3. Degas the resulting mixture with four freeze-pump-thaw cycles and backfill with nitrogen gas. 4. Subsequently immerse the flask in a preheated oil bath at 55 °C. 5. Allow the reaction to proceed for 12 h. 6. Precipitate the the resulting polymer in chilled ethanol. 7. Dry the mixture under vacuum at ambient temperature for 24 h.
CAS Method Number	3-614-CAS-2463870

MethodsNow synthetic chemistry content sources

Content from years	2000 - present
Number of protocols	2.1 million; 3 million later this year
Content Coverage	Small molecule synthesis
Source Focus	180+ journals titles including new coverage from Wiley, RSC and Elsevier in addition to ACS, Springer, Taylor&Francis, WO patents (2010-present)
Example journal titles	Organic Letters, Catalysis Letters, Journal of Coordination Chemistry, Journal of Medicinal Chemistry, Journal of the American Chemical Society, Angewandte Chemie, Tetrahedron, Chemical Science
Language	English only

MethodsNow Benefits

- Readily integrates into your workflow
- Lets you quickly compare analytical methods side by side
- Saves time with easy searching and direct access to method details
- Displays experimental details in easy-to-read table format
- Includes materials, instrumentation, validation data, conditions and more