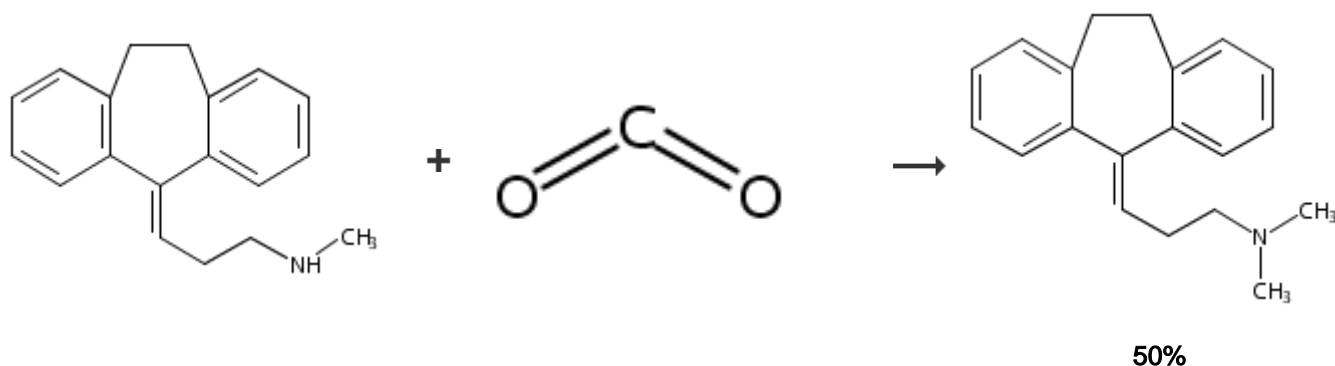


1. Single Step



Overview

Steps/Stages

- 1.1 R:Poly(methyl siloxane), C:K₃PO₄, C:18-Crown-6, S:MeCN, 72 h, 80°C, 1 atm

Notes

glovebox used, sealed tube used, Reactants: 2, Reagents: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

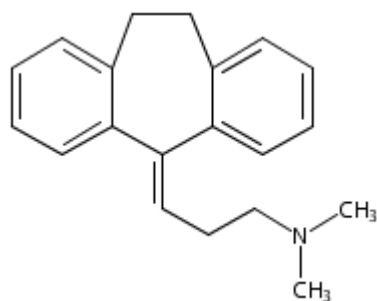
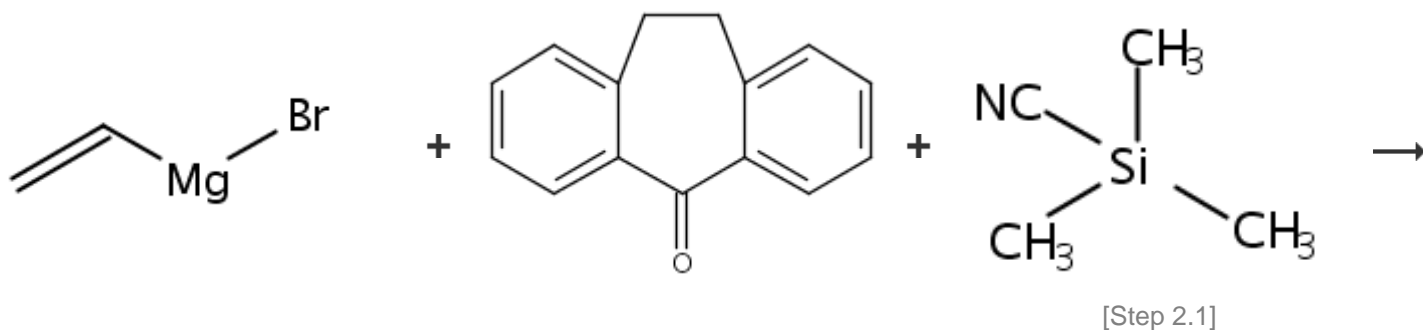
[Scalable direct N-methylation of drug-like amines using ¹²CO₂/¹³CO₂ by simple inorganic base catalysis](#)

By Lu, Chunlei et al

From Science Bulletin, 64(11), 723-729; 2019

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2. 4 Steps



Overview

Steps/Stages

Notes

- 1.1 S:THF, 0°C; 0.5 h, 0°C; 0°C → rt; 2-5 h, rt
 1.2 R:NH₄Cl, S:H₂O, rt
 2.1 C:I₂, C:Li₂CO₃, S:CH₂Cl₂, 5 h, 35°C
 2.2 R:Na₂S₂O₃, S:H₂O
 3.1
 4.1

1) Grignard reaction, Et₂O solvent may also be used (stage 1), 2) sealed tube used, 3) literature preparation, no experimental detail, 4) no experimental detail, Reactants: 3, Reagents: 2, Catalysts: 2, Solvents: 3, Steps: 4, Stages: 6, Most stages in any one step: 2

References

[I₂/Li₂CO₃-promoted cyanation of diarylalcohols through a dual activation process](#)

By Hu, Liangzhen et al

From Tetrahedron, 75(2), 308-314; 2019

Reaction Protocol

Procedure

1. Load a two-necked flask under argon atmosphere with a solution of ketone (5 mmol) in anhydrous THF (5 mL).
2. Add Grignard reagent (1.0 M in THF, 5.5 mL, 5.5 mmol, 1.1 equivalents) dropwise via syringe in ice-bath under vigorous stirring.

[View more...](#)

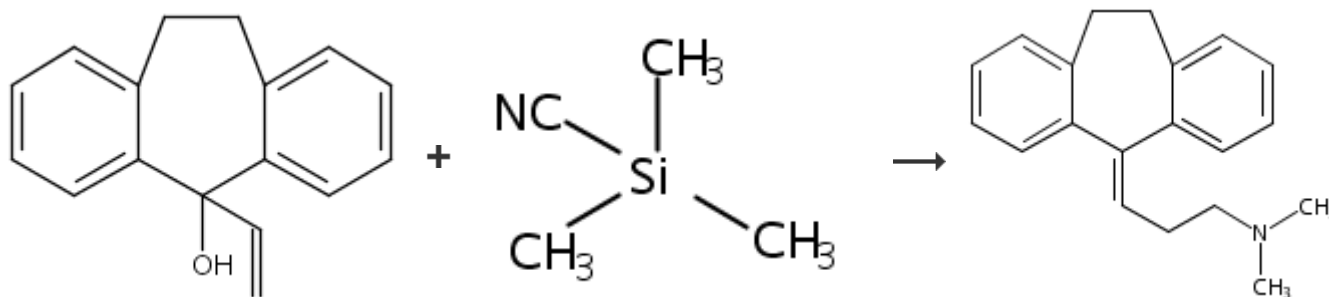
Available Experimental Data

¹H NMR, ¹³C NMR, MP, State

[View with MethodsNow](#)

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3. 3 Steps



[Overview](#)

Steps/Stages

Notes

1.1 C:I₂, C:Li₂CO₃, S:CH₂Cl₂, 5 h, 35 °C

1.2 R:Na₂S₂O₃, S:H₂O

2.1

3.1

1) sealed tube used, 2) literature preparation, no experimental detail, 3) no experimental detail, Reactants: 2, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 3, Stages: 4, Most stages in any one step: 2

References

[I₂/Li₂CO₃-promoted cyanation of diarylalcohols through a dual activation process](#)

By Hu, Liangzhen et al

From Tetrahedron, 75(2), 308-314; 2019

Reaction Protocol

Procedure

1. Charge a round-bottomed flask with allylic alcohol (0.3 mmol) in DCM (5 mL), Li₂CO₃ (0.06 mmol), TMSCN (1.35 mmol) and I₂ (0.54 mmol) in sequence successively.
2. Stir the resulting mixture under closed conditions at 35 °C (water bath temperature) for 5 hours.

[View more...](#)

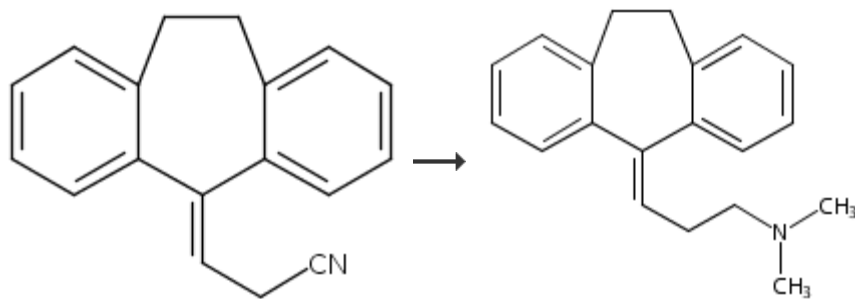
Available Experimental Data

¹H NMR, ¹³C NMR, MP, State

[View with MethodsNow](#)

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4. 2 Steps



Overview

Steps/Stages

1.1

2.1

Notes

1) literature preparation, no experimental detail, 2) no experimental detail, Reactants: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

References

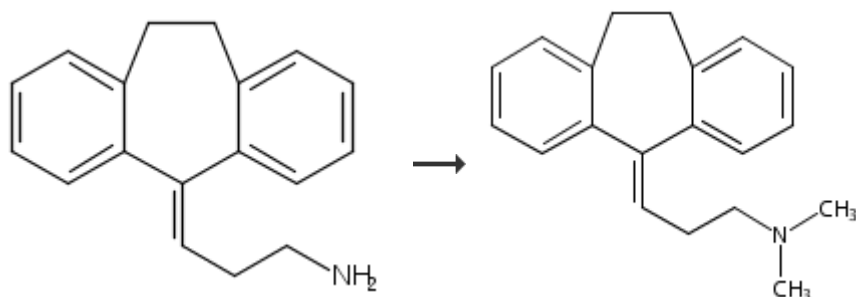
[I₂/Li₂CO₃-promoted cyanation of diarylalcohols through a dual activation process](#)

By Hu, Liangzhen et al

From Tetrahedron, 75(2), 308-314; 2019

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5. Single Step



[Overview](#)

Steps/Stages

1.1

Notes

no experimental detail, Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

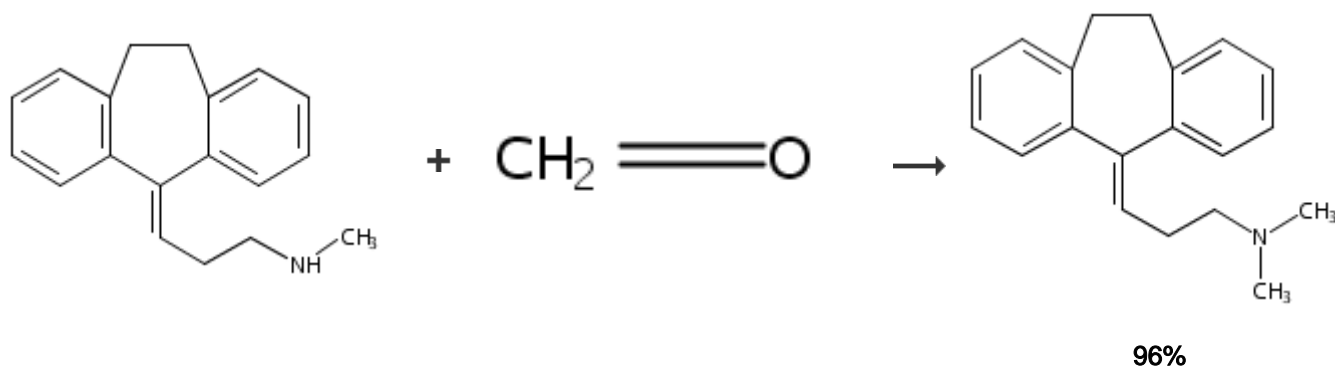
[I₂/Li₂CO₃-promoted cyanation of diarylalcohols through a dual activation process](#)

By Hu, Liangzhen et al

From Tetrahedron, 75(2), 308-314; 2019

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6. Single Step



[Overview](#)

Steps/Stages

Notes

1.1 R:Disodium carbonate, C:Fe, S:DMSO, S:H₂O, 24 h, 130°C

chemoselective, pressure tube used, catalyst prepared and used, reusable catalyst, paraformaldehyde used, solid-supported catalyst, Reactants: 2, Reagents: 1, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

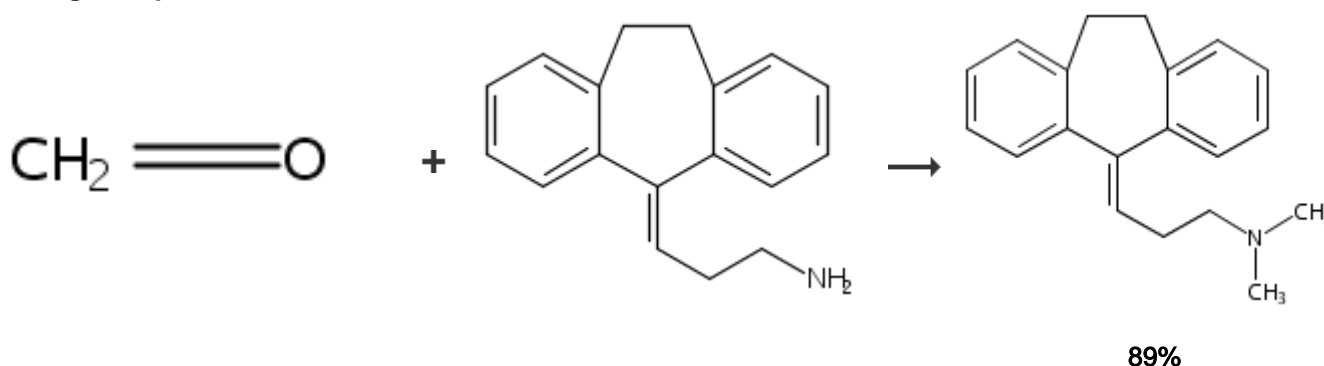
[Convenient iron-catalyzed reductive aminations without hydrogen for selective synthesis of N-methylamines](#)

By Natte, Kishore et al

From Nature Communications, 8(1), 1-9; 2017

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7. Single Step



Overview

Steps/Stages

1.1 R:HCO₂H, R:Et₃N, C:Co₃O₄ on nitrogen doped graphene (carbon), S:H₂O, S:*t*-BuOH, 14 h, 100°C

Notes

catalyst prepared and used, recyclable catalyst, reusable catalyst, sealed pressure tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

[Expedient Synthesis of N-Methyl- and N-Alkylamines by Reductive Amination using Reusable Cobalt Oxide Nanoparticles](#)

By Senthamarai, Thirusangumurugan et al

From ChemCatChem, 10(6), 1235-1240; 2018

Reaction Protocol

Procedure

1. Charge an oven-dried 15 mL ACE pressure tube with stir bar and Co₃O₄/NGr@C (80 mg), amine (1 mmol), formaldehyde (200 μL aqueous formaldehyde (37 wt. % in H₂O)), HCOOH:Et₃N (5:2 ratio) (2 mmol) and *t*butanol (3 mL).
2. Flush the pressure tube with argon, close with screw cap and allow the reaction to progress at 100 °C for 24 hours.

[View more...](#)

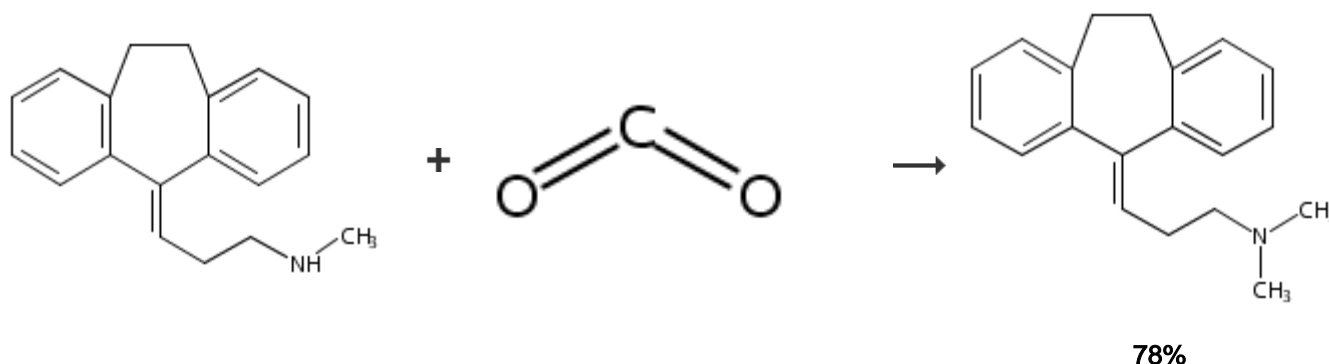
Available Experimental Data

¹H NMR, ¹³C NMR, HRMS, State

[View with
MethodsNow](#)

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8. Single Step



Overview

Steps/Stages

1.1 R:18-Crown-6, C:K₃PO₄, S:MeCN, 72 h, 80°C, 1 bar

Notes

methyl hydrogen polysiloxane used, glovebox used, green chemistry, Reactants: 2, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

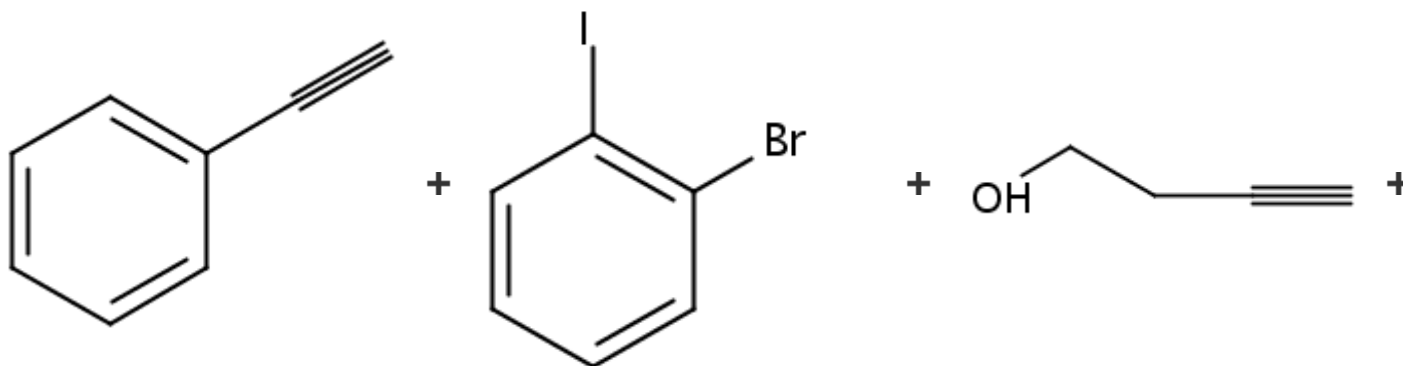
[Process for methylation of amine](#)

By Lin, Bailin et al

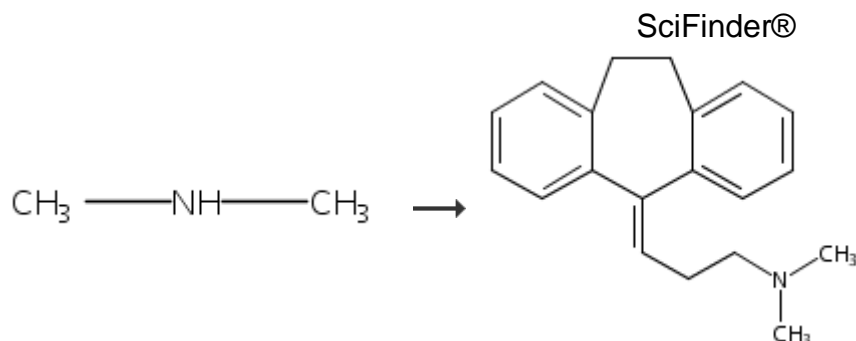
From Faming Zhuanli Shenqing, 107337606, 10 Nov 2017

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9. 5 Steps



[Step 3.1]



[Step 4.3]

Overview**Steps/Stages**

- 1.1 R:Et₃N, C:Cul, C: PdCl₂(PPh₃)₂, S:MeCN, 0°C; 22 h, rt
- 1.2 R:NaHCO₃, S:H₂O
- 2.1 R:H₂, C: Pd, S:AcOEt, 6 h, rt
- 3.1 R:Cs₂CO₃, C:657408-07-6, C: PdCl₂(CH₃CN)₂, S:MeCN, 6.5 h, 60°C
- 4.1 R:Et₃N, R:MeSO₂Cl, S:CH₂Cl₂, 2.5 h, 0°C
- 4.2 R:NaHCO₃, S:H₂O
- 4.3 S:H₂O, S:EtOH, 2 h, 50°C
- 5.1 C:Triflic acid, S:CH₂Cl₂, 10 min, 0°C
- 5.2 R:NaHCO₃, S:H₂O

Notes

1) Sonogashira coupling, 5) Friedel-Crafts alkylation, regioselective, Reactants: 4, Reagents: 5, Catalysts: 6, Solvents: 5, Steps: 5, Stages: 9, Most stages in any one step: 3

References

[Construction of dibenzo-fused seven- to nine-membered carbocycles via Bronsted acid-promoted intramolecular Friedel-Crafts-type alkylation](#)

By Otani, Takashi et al

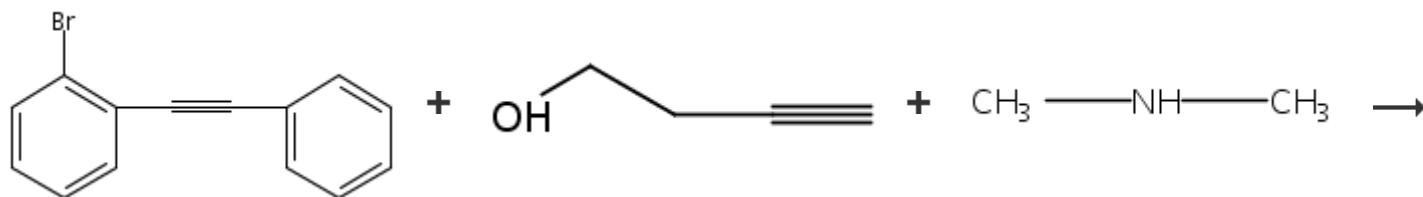
From Chemical Communications (Cambridge, United Kingdom), 51(37), 7895-7898; 2015

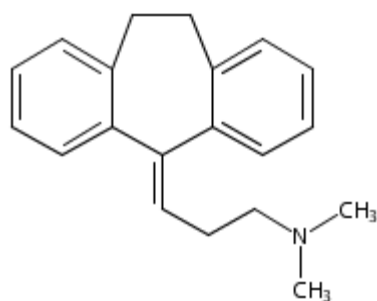
Reaction Protocol**Procedure**

1. Add PdCl₂(PPh₃)₂ (70.2 mg, 100 μmol, 1 mol%) and Cul (38.5 mg, 202 μmol, 2 mol%) to a mixture of 1-bromo-2-iodobenzene (1.25 mL, 10.0 mmol), triethylamine (40 mL) and CH₃CN (40 mL).
2. Cool the mixture to 0 °C.

[View more...](#)**Available Experimental Data**¹H NMR, ¹³C NMR, HRMS, State[View with MethodsNow](#)

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10. 4 Steps



Overview

Steps/Stages

- 1.1 R:H₂, C: Pd, S: AcOEt, 6 h, rt
- 2.1 R: Cs₂CO₃, C: 657408-07-6, C: PdCl₂(CH₃CN)₂, S: MeCN, 6.5 h, 60°C
- 3.1 R: Et₃N, R: MeSO₂Cl, S: CH₂Cl₂, 2.5 h, 0°C
- 3.2 R: NaHCO₃, S: H₂O
- 3.3 S: H₂O, S: EtOH, 2 h, 50°C
- 4.1 C: Triflic acid, S: CH₂Cl₂, 10 min, 0°C
- 4.2 R: NaHCO₃, S: H₂O

Reaction Protocol

Procedure

1. Stir a suspension of 1-bromo-2-(phenylethynyl)benzene (974 mg) and 10% Pd/C (200 mg, 188 μmol) in ethyl acetate (15 mL) under a balloon of hydrogen for 6 hours at room temperature.
2. Dilute the reaction mixture with ethyl acetate.

[View more...](#)

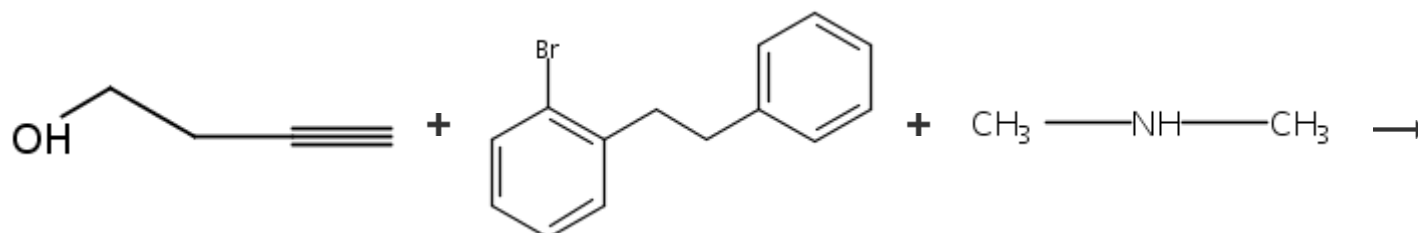
Available Experimental Data

¹H NMR, ¹³C NMR, HRMS, State

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11. 3 Steps



[Step 2.3]

Notes

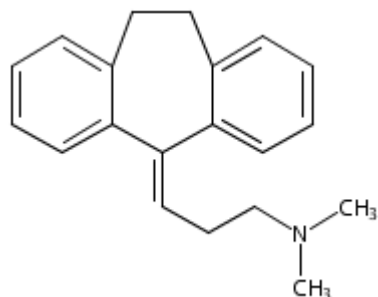
4) Friedel-Crafts alkenylation, regioselective, Reactants: 3, Reagents: 5, Catalysts: 4, Solvents: 5, Steps: 4, Stages: 7, Most stages in any one step: 3

References

[Construction of dibenzo-fused seven- to nine-membered carbocycles via Bronsted acid-promoted intramolecular Friedel-Crafts-type alkenylation](#)

By Otani, Takashi et al

From Chemical Communications (Cambridge, United Kingdom), 51(37), 7895-7898; 2015



Overview

Steps/Stages

- 1.1 R:Cs₂CO₃, C:657408-07-6, C:PdCl₂(CH₃CN)₂, S:MeCN, 6.5 h, 60 °C
- 2.1 R:Et₃N, R:MeSO₂Cl, S:CH₂Cl₂, 2.5 h, 0 °C
- 2.2 R:NaHCO₃, S:H₂O
- 2.3 S:H₂O, S:EtOH, 2 h, 50 °C
- 3.1 C:Triflic acid, S:CH₂Cl₂, 10 min, 0 °C
- 3.2 R:NaHCO₃, S:H₂O

Notes

3) Friedel-Crafts alkenylation, regioselective, Reactants: 3, Reagents: 4, Catalysts: 3, Solvents: 4, Steps: 3, Stages: 6, Most stages in any one step: 3

References

Construction of dibenzo-fused seven- to nine-membered carbocycles via Bronsted acid-promoted intramolecular Friedel-Crafts-type alkenylation

By Otani, Takashi et al

From Chemical Communications (Cambridge, United Kingdom), 51(37), 7895-7898; 2015

Reaction Protocol

Procedure

1. Add 3-butyn-1-ol (230 μL, 3.00 mmol) to a mixture of 1-bromo-2-phenethylbenzene (261 mg), SPhos (27.6 mg, 67.2 μmol, 7 mol%), PdCl₂(CH₃CN)₂ (5.2 mg, 20 μmol, 2 mol%), Cs₂CO₃ (793 mg, 2.43 mmol) and dry CH₃CN (10 mL).
2. Stir the mixture at 60 °C for 6.5 hours.

[View more...](#)

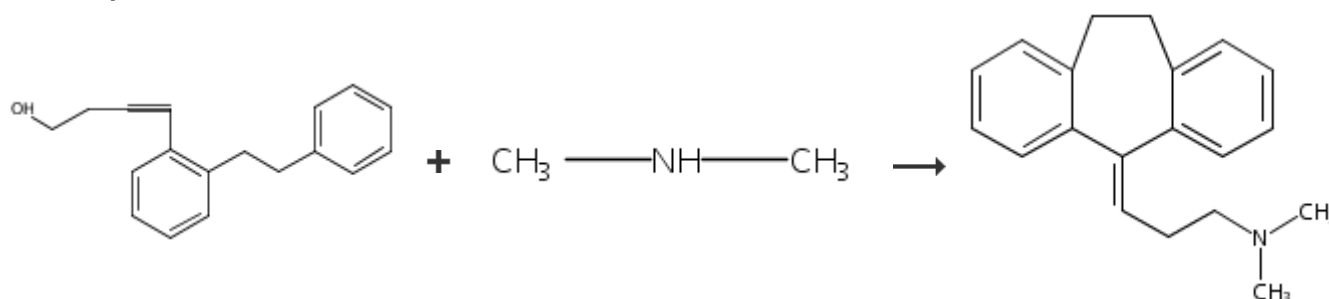
Available Experimental Data

¹H NMR, ¹³C NMR, HRMS, State

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12. 2 Steps



[Overview](#)**Steps/Stages**

- 1.1 R:Et₃N, R:MeSO₂Cl, S:CH₂Cl₂, 2.5 h, 0°C
 1.2 R:NaHCO₃, S:H₂O
 1.3 S:H₂O, S:EtOH, 2 h, 50°C
 2.1 C:Triflic acid, S:CH₂Cl₂, 10 min, 0°C
 2.2 R:NaHCO₃, S:H₂O

Notes

2) Friedel-Crafts alkenylation, regioselective, Reactants: 2, Reagents: 3, Catalysts: 1, Solvents: 3, Steps: 2, Stages: 5, Most stages in any one step: 3

References

[Construction of dibenzo-fused seven- to nine-membered carbocycles via Bronsted acid-promoted intramolecular Friedel-Crafts-type alkenylation](#)

By Otani, Takashi et al

From Chemical Communications (Cambridge, United Kingdom), 51(37), 7895-7898; 2015

[Reaction Protocol](#)**Procedure**

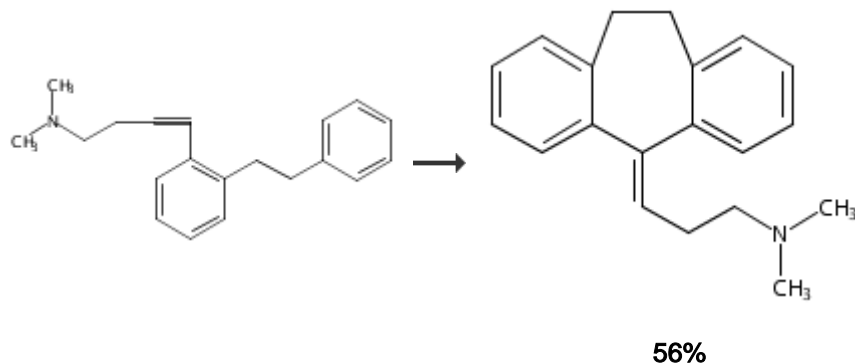
1. Add methanesulfonyl chloride (40.0 μL, 300 μmol) to a mixture of 4-(2-phenethyl-phenyl)but-3-yn-1-ol (53.6 mg), triethylamine (60 μL, 400 μmol) and CH₂Cl₂ (2.0 mL) at 0 °C.
2. Stir the mixture at 0 °C for 2.5 hours.

[View more...](#)**Available Experimental Data**

¹H NMR, ¹³C NMR, HRMS, State

[View with MethodsNow](#)

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13. Single Step[Overview](#)**Steps/Stages****Notes**

1.1 C:Triflic acid, S:CH₂Cl₂, 10 min, 0°C

1.2 R:NaHCO₃, S:H₂O

Friedel-Crafts alkenylation, regioselective,
Reactants: 1, Reagents: 1, Catalysts: 1,
Solvents: 2, Steps: 1, Stages: 2, Most stages
in any one step: 2

References

[Construction of dibenzo-fused seven- to nine-membered carbocycles via Bronsted acid-promoted intramolecular Friedel-Crafts-type alkenylation](#)

By Otani, Takashi et al

From Chemical Communications (Cambridge, United Kingdom), 51(37), 7895-7898; 2015

Reaction Protocol

Procedure

1. Add TfOH (21.9 μ L, 250 μ mol) to a mixture of N,N-dimethyl-4-(2-phenethylphenyl)but-3-yn-1-amine (13.8 mg) in CH₂Cl₂ (0.5 mL) at 0 °C.
2. Stir the mixture at 0 °C for 10 minutes.

[View more...](#)

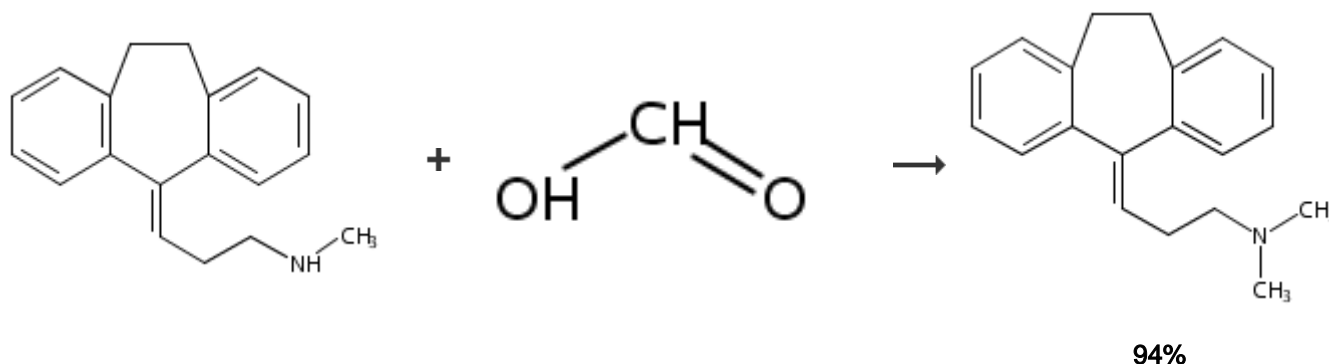
Available Experimental Data

¹H NMR, State

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14. Single Step



Overview

Steps/Stages

1.1 C:11057-89-9, C:Ph₂P(CH₂)₃PPh₂, S:THF, 10 min, rt

1.2 R:PhSiH₃, 18 h, 60°C

1.3 R:NaOH, S:H₂O, S:AcOEt, rt; 3 h, rt

Notes

Schlenk tube used, conversion 97%,
Reactants: 2, Reagents: 2, Catalysts: 2,
Solvents: 3, Steps: 1, Stages: 3, Most stages
in any one step: 3

References

[General catalytic methylation of amines with formic acid under mild reaction conditions](#)

By Sorribes, Ivan et al

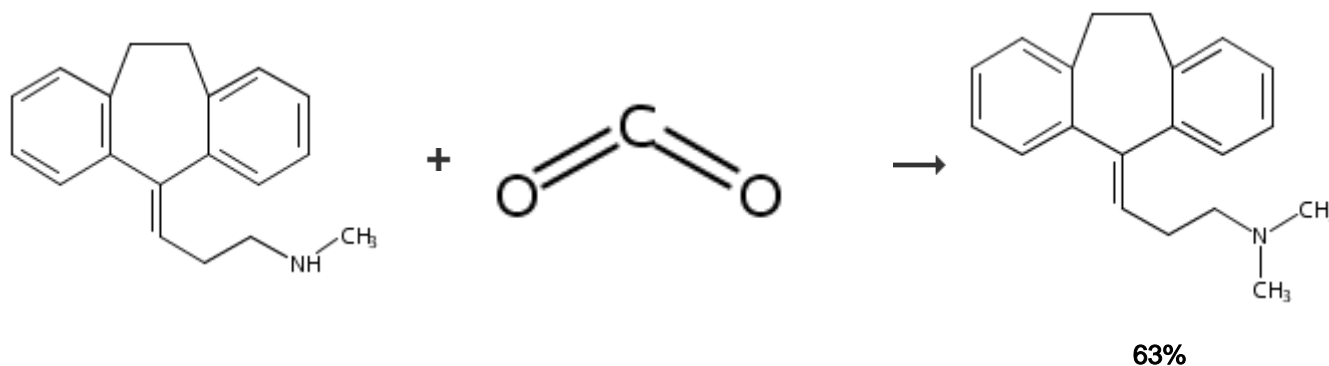
From Chemistry - A European Journal, 20(26), 7878-7883; 2014

[Reaction Protocol](#)

- Procedure**
1. Dissolve dppp (2.1 mg, 0.005 mmol) in dry nBu₂O (1 mL) in a Schlenk tube under argon atmosphere.
 2. Add Karstedt's catalyst (57 μL, 0.005 mmol), leading to the formation of a slightly yellow solution.

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15. Single Step[Overview](#)**Steps/Stages**

- 1.1 R:NaH, C:141556-42-5, S:DMF, 30 min, rt
- 1.2 R:Ph₂SiH₂, S:DMF, 24-48 h, 50°C, 1 atm
- 1.3 R:(NH₄)F, S:H₂O, overnight, rt

Notes

chemoselective, Reactants: 2, Reagents: 3, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 3, Most stages in any one step: 3

References

[Metal-Free Catalyst for the Chemoselective Methylation of Amines Using Carbon Dioxide as a Carbon Source](#)

By Das, Shoubhik et al

From *Angewandte Chemie, International Edition*, 53(47), 12876-12879; 2014

[Reaction Protocol](#)

- Procedure**
1. In the glovebox, place imidazolium salt (0.05 mmol) and NaH (0.05 mmol) in a 10 mL Schlenk tube.
 2. Using Schlenk techniques, add 2 mL of dry DMF to the Schlenk tube.

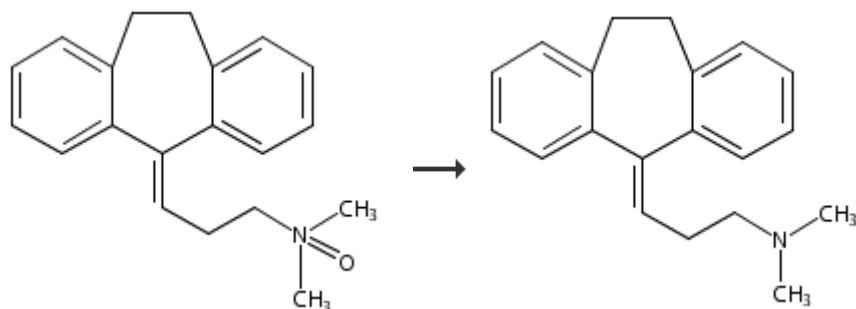
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Available Experimental Data ¹H NMR, ¹³C NMR, HRMS, State

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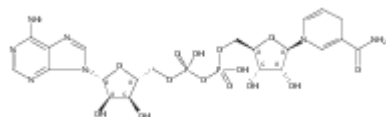
16. Single Step



Overview

Steps/Stages

1.1 R:



R:O₂, S:H₂O, 3 min, 37°C; 15 min, 37°C

Notes

biotransformation, enzymic, mitochondrial amidoxime reducing component, cytochrome b5, cytochrome b5 reductase enzyme used, buffered solution used, Reactants: 1, Reagents: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

[The Mitochondrial Amidoxime Reducing Component \(mARC\): Involvement in Metabolic Reduction of N-Oxides, Oximes and N-Hydroxyamidinohydrazones](#)

By Jakobs, Heyka H. et al

From ChemMedChem, 9(10), 2381-2387; 2014

Reaction Protocol

Procedure

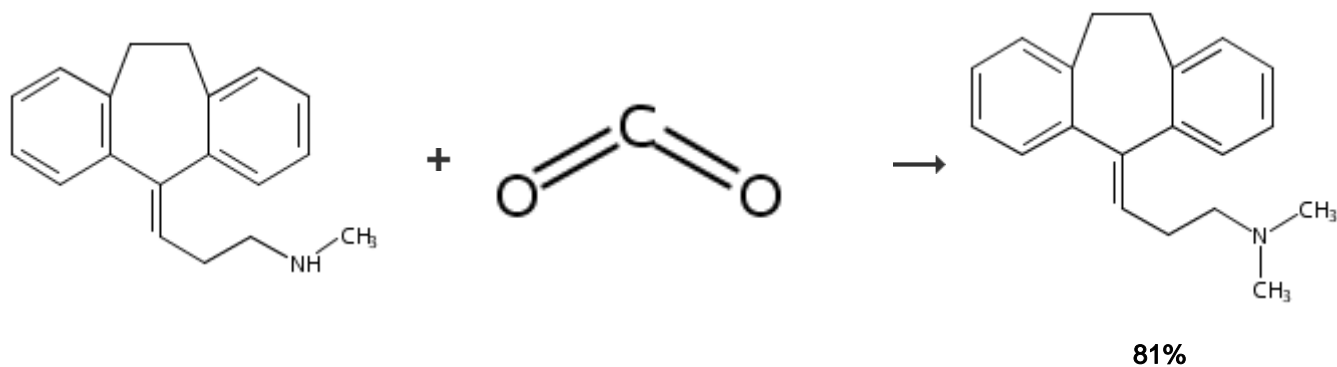
1. Unless otherwise stated, a standard incubation mixture consisted of 3 mM substrate (2 mM in case of nicotinamide-N-oxide) and 1 mM NADH in a total volume of 150 μ L in 20 mM 2-(N-morpholino)ethansulfonic acid (MES) buffer, pH 6.0 for recombinant proteins or potassium phosphate buffer, consisting of 50 mM K₂HPO₄ and 50 mM KH₂PO₄, pH 6.0 for subcellular fractions.
2. Add 3% dimethyl sulfoxide (DMSO) to enhance solubility of the substrate.

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17. Single Step



Overview

Steps/Stages

- 1.1 R:H₂, C:14284-93-6, C:22031-12-5, C:LiCl, S:THF, 24 h, rt → 140°C, 60 atm

Notes

high pressure, autoclave used, Reactants: 2, Reagents: 1, Catalysts: 3, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

[Selective Methylation of Amines with Carbon Dioxide and H₂](#)

By Li, Yuehui et al

From *Angewandte Chemie, International Edition*, 52(46), 12156-12160; 2013

Reaction Protocol

Procedure

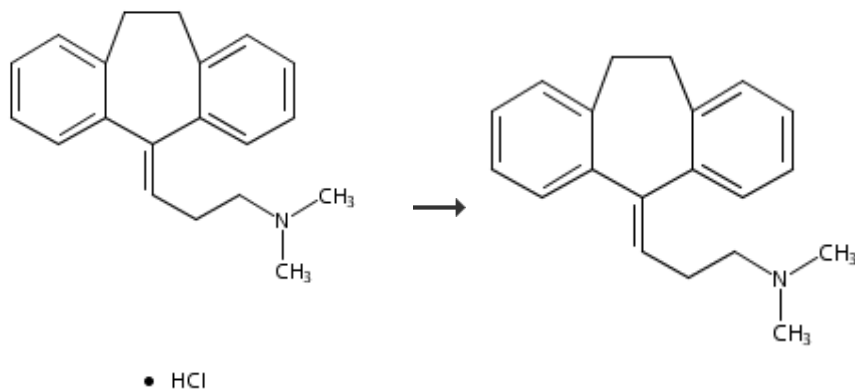
1. Charge [Ru(acac)₃] (2.0 mg), triphos (6.2 mg) and MSA (0.51 μL, 7.5 μmol) to the 4 mL glass vial containing a stir bar inside the autoclave.
2. Add dry THF (2.0 mL) and the amine substrate (0.5 mmol) to the vial.

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18. Single Step



Overview

Steps/Stages1.1 R:NaOH, S:H₂O, basify**Notes**

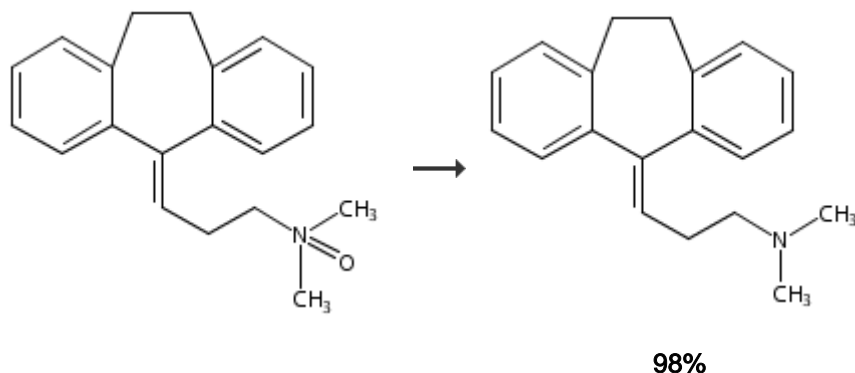
Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References[Novel method for the synthesis of stable Amitriptyline N-Oxide](#)

By Ramesh, Andagar Ramakrishna and Roy, Anjan Kumar

From Indian Pat. Appl., 2009CH02050, 04 Mar 2011

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19. Single Step[Overview](#)**Steps/Stages**1.1 C:Ni, S:H₂O, 10 min, 60°C1.2 R:NaBH₄, 15-20 min, 60°C; 2 h, 60°C**Notes**

chemoselective, green chemistry-solvent, incremental addition (stage 2), Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References[A chemoselective deoxygenation of N-oxides by sodium borohydride-Raney nickel in water](#)

By Gowda, Narendra B. et al

From Tetrahedron Letters, 51(43), 5690-5693; 2010

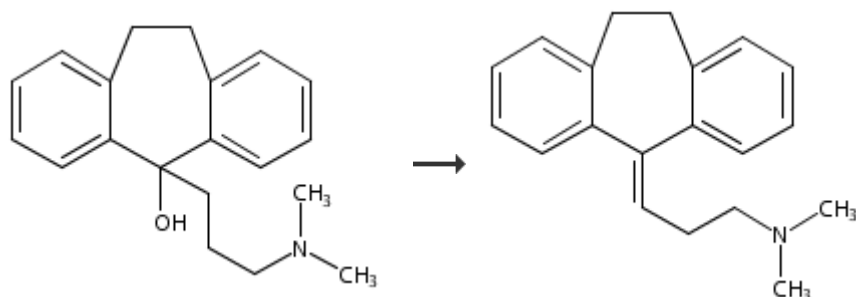
[Reaction Protocol](#)**Procedure**

1. Dissolve (1 mmol) of amitriptyline N-oxide in 2.5 mL of water at 60 °C.
2. Add Raney nickel (0.10 g, W6 grade) to the solution.

[View more...](#)**Available Experimental Data**¹H NMR, ¹³C NMR, Mass Spec[View with MethodsNow](#)

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20. Single Step



Overview

Steps/Stages

1.1

Notes

Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

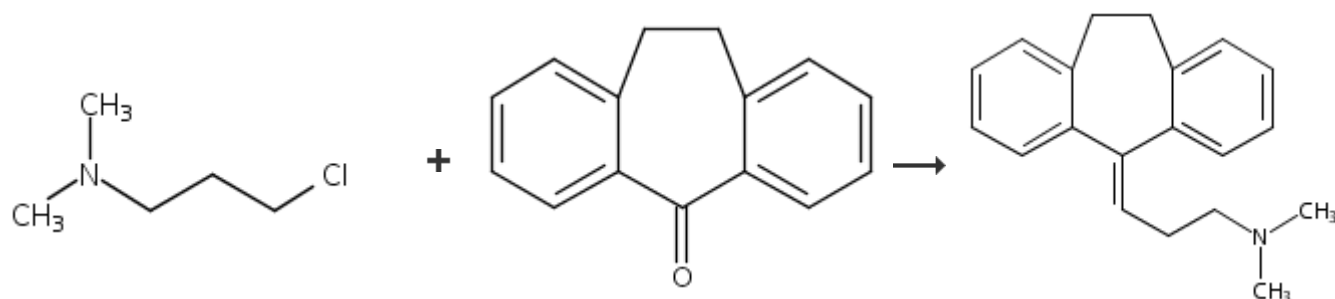
[Preparation of amitriptyline hydrochloride](#)

By Darabantu, Mircea et al

From Rom., 91179, 30 Apr 1987

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21. 2 Steps



Overview

Steps/Stages

1.1

2.1

Notes

Reactants: 2, Steps: 2, Stages: 2, Most stages in any one step: 1

References

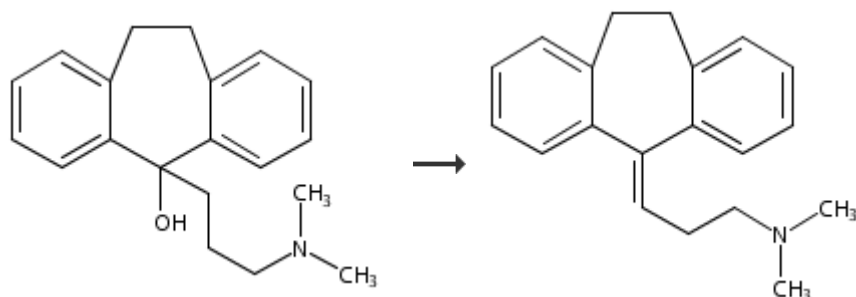
[Tricyclic antidepressants](#)

By Mayer, Jiri et al

From Czech., 232331, 16 Jan 1985

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22. Single Step



[Overview](#)

Steps/Stages

1.1

Notes

Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

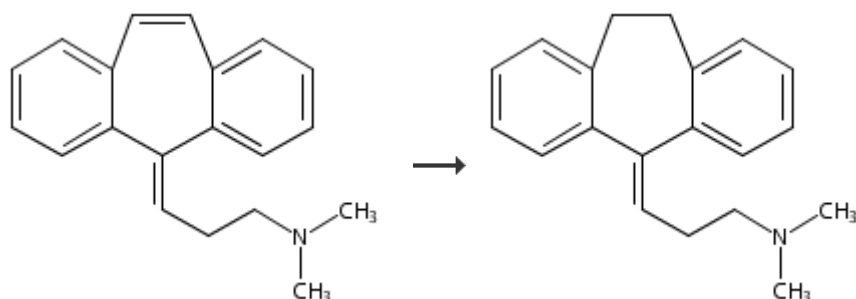
[Tricyclic antidepressants](#)

By Mayer, Jiri et al

From Czech., 232331, 16 Jan 1985

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23. Single Step



[Overview](#)

Steps/Stages

1.1

Notes

Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

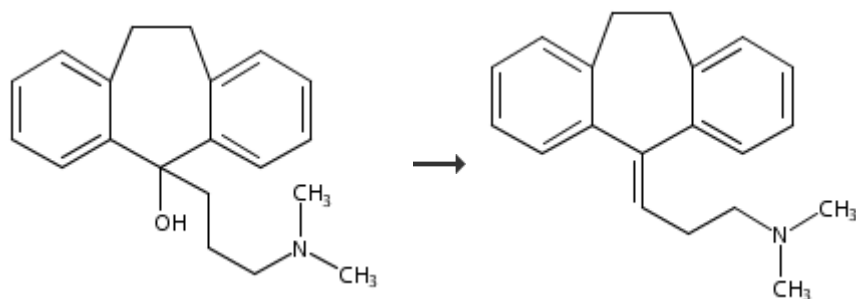
[Tritium labeling of antidepressants with regard to their chemical structure](#)

By Buchman, Ouri et al

From Journal of Labelled Compounds and Radiopharmaceuticals, 20(7), 887-900; 1983

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24. Single Step



Overview

Steps/Stages

1.1 R:HCl, S:Me₂CHOH

Notes

Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

[Amitriptyline hydrochloride](#)

By Pop, Emil et al

From Rom., 76312, 30 Apr 1981

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