

Task History

Initiating Search

February 21, 2025, 10:42 AM

Substances:

Filtered By:



Structure Match: As Drawn

Search Tasks

Task	Search Type	View
Returned Substance Results + Filters (2,301)	Substances	View Results
Exported: Retrieved Related Reaction Results + Filters (47)	■ Reactions	View Results
Filtered By:		
Structure Match: As Drawn		
Kept Selected Results		

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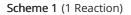


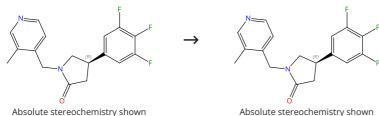
Reactions (44)

View in CAS SciFinder

Steps: 1 Yield: 99%

Steps: 1 Yield: 96%





Absolute stereochemistry shown

Suppliers (22)

Steps: 1 Yield: 99%

Reagents: Deuterium Catalysts: Palladium

Solvents: Dimethylacetamide; -196 °C → rt; 20 h, rt

Experimental Protocols

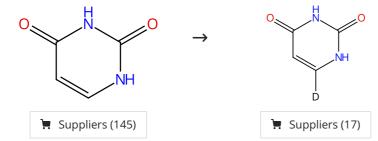
31-614-CAS-39216789

Palladium Nanoparticles for the Deuteration and Tritiation of **Benzylic Positions on Complex Molecules**

By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

Scheme 2 (1 Reaction)



31-116-CAS-4988718

1.1 Reagents: Deuterium, Sodium hydroxide- d

Catalysts: Calcium carbonate, Palladium Solvents: Water-d₂

Steps: 1 Yield: 96%

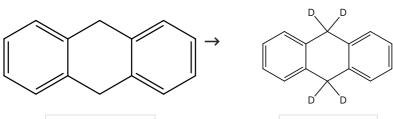
Supplier (1)

Syntheses of [5-2H]-uracil, [5-2H]-cytosine, [6-2H]-uracil and [6-2H]-cytosine

By: Kiritani, Reiko; et al

Journal of Labelled Compounds and Radiopharmaceuticals (1986), 23(2), 207-14.

Scheme 3 (1 Reaction)



> Suppliers (68)

Steps: 1 Yield: 95%

Steps: 1 Yield: 93%

Steps: 1 Yield: 90-92%

Steps: 1 Yield: 92%

31-116-CAS-5203181

I.1 Reagents: Deuterium
Catalysts: Palladium

Catalysts: Palladium Solvents: Acetic acid-d

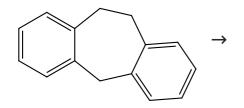
Steps: 1 Yield: 95%

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Scheme 4 (1 Reaction)



☐ Suppliers (40)

D D D

31-116-CAS-11664295

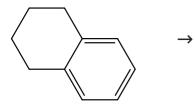
1.1 Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d Steps: 1 Yield: 93%

High-resolution EPR spectroscopic investigations of a homologous set of d 9 -cobalt(0), d 9 -rhodium(0), and d 9 -iridium (0) complexes

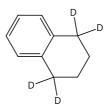
By: Deblon, Stephan; et al

Chemistry - A European Journal (2002), 8(3), 601-611.

Scheme 5 (2 Reactions)



Suppliers (104)



31-116-CAS-11267807

1.1 Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d Steps: 1 Yield: 92%

Hydrogen transfer reactions. 15. The transition state in the dehydrogenation of dihydroarenes by quinones

By: Radtke, Rainer; et al

Chemische Berichte (1990), 123(3), 627-33.

31-116-CAS-3074194

1.1 Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d Steps: 1 Yield: 90%

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Scheme 6 (1 Reaction)

Steps: 1 Yield: 90%

Steps: 1 Yield: 90%

31-116-CAS-9297566

1.1 **Reagents:** Deuterium, Water- d_2

Catalysts: Palladium

Solvents: Water-*d*₂; 16 h, 145 °C

Steps: 1 Yield: 92%

Steps: 1 Yield: 90%

Steps: 1 Yield: 90%

Synthesis of a delta opioid agonist in [${}^{2}H_{6}$], [${}^{2}H_{4}$], [${}^{11}C$], and [${}^{14}C$] labeled forms

By: Elmore, Charles S.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2011), 54(14), 847-854.

Scheme 7 (1 Reaction)

31-116-CAS-4563156

1.1 Reagents: Deuterium chloride, Deuterium

Catalysts: Palladium

Solvents: Methanol-d, Water-d₂; 6 h, 3 bar, 60 °C

1.2 Reagents: Sodium hydroxide

Solvents: Water

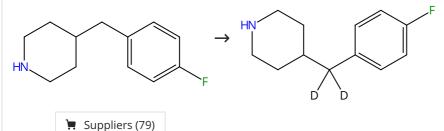
Convenient methods for the synthesis of d_4 , d_2 and d_6 isotop omers of 4-(4-fluorobenzyl)piperidine

By: Proszenyak, Agnes; et al

Journal of Labelled Compounds & Radiopharmaceuticals

(2005), 48(6), 421-427.

Scheme 8 (1 Reaction)



31-116-CAS-11564808

1.1 Reagents: Deuterium chloride, Deuterium

Catalysts: Palladium

Solvents: Methanol-d, Water-d₂; 6 h, 3 bar, 60 °C

1.2 Reagents: Sodium hydroxide

Solvents: Water

Convenient methods for the synthesis of d_4 , d_2 and d_6 isotop omers of 4-(4-fluorobenzyl)piperidine

By: Proszenyak, Agnes; et al

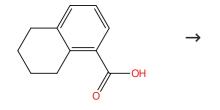
Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(6), 421-427.

Steps: 1 Yield: 88%

Steps: 1 Yield: 87%

Steps: 1 Yield: 85%

Scheme 9 (1 Reaction)



D OH

➤ Suppliers (87)

📜 Supplier (1)

31-116-CAS-7646392

1.1 Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d

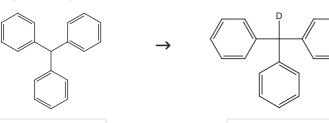
Steps: 1 Yield: 88%

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Scheme 10 (1 Reaction)



Suppliers (85)

₩ Suppliers (2)

31-116-CAS-5486131

1.1 Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d

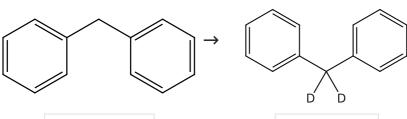
Steps: 1 Yield: 87%

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Scheme 11 (1 Reaction)



Suppliers (87)

➤ Suppliers (4)

31-116-CAS-9493526

1.1 **Reagents:** Deuterium **Catalysts:** Palladium **Solvents:** Acetic acid-*d*

Steps: 1 Yield: 85%

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Steps: 1 Yield: 81%

Steps: 1 Yield: 79%

Page 6

> Suppliers (33)

31-116-CAS-13699197

1.1 Reagents: Calcium carbonate, Deuterium

Catalysts: Palladium Solvents: 1,4-Dioxane 1.2 Reagents: Oxygen Solvents: Acetic acid

Steps: 1 Yield: 83% The preparation of regiospecific tritiated and deuterated dibenzacridines by catalytic exchange and [14-14C]dibenz[a,j] acridine

By: Rosario, Christopher A.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(1), 23-8.

Scheme 13 (1 Reaction)

Suppliers (6)

31-116-CAS-3679279

Reagents: Deuterium Catalysts: Palladium

Solvents: Diethyl ether; 1.5 h, 1 bar, rt

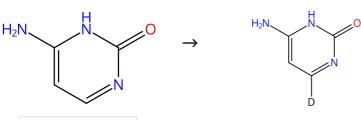
Steps: 1 Yield: 81%

Reactivity of y-chloro-gem-trichloro alkanes with chromous chloride

By: Tisserand, Steve; et al

Tetrahedron Letters (2006), 47(29), 5177-5180.

Scheme 14 (1 Reaction)



Suppliers (129)

31-116-CAS-7264406

Steps: 1 Yield: 79%

Syntheses of [5-2H]-uracil, [5-2H]-cytosine, [6-2H]-uracil and [6-2H]-cytosine

By: Kiritani, Reiko; et al

Journal of Labelled Compounds and Radiopharmaceuticals (1986), 23(2), 207-14.

Reagents: Deuterium, Sodium hydroxide- d Catalysts: Calcium carbonate, Palladium

Solvents: Water-d2

Steps: 1 Yield: 74%

Steps: 1 Yield: 74%

Steps: 1 Yield: 70%

Scheme 15 (1 Reaction)

≒ Suppliers (70)

📜 Supplier (1)

31-116-CAS-975958

1.1 Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d

Steps: 1 Yield: 74%

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Scheme 16 (1 Reaction)

Br → D D D

Br

Suppliers (88)

Supplier (1)

31-116-CAS-17238853

1.1 Reagents: Deuterium Catalysts: Palladium

Solvents: Methanol-d₄; 20 h, rt

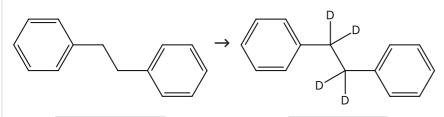
Steps: 1 Yield: 74%

Cobalt-Porphyrin-Catalysed Intramolecular Ring-Closing C-H Amination of Aliphatic Azides: A Nitrene-Radical Approach to Saturated Heterocycles

By: Kuijpers, Petrus F.; et al

Chemistry - A European Journal (2017), 23(33), 7945-7952.

Scheme 17 (1 Reaction)



➤ Suppliers (93)

Supplier (1)

31-116-CAS-3363492

1.1 Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d

Steps: 1 Yield: 70%

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Steps: 1 Yield: 54%

Steps: 1 Yield: 34%

Steps: 1 Yield: 17%

Scheme 18 (1 Reaction)

31-116-CAS-20244030

1.1 **Reagents:** Deuterium **Catalysts:** Palladium

➤ Suppliers (56)

Solvents: Water-*d*₂; 18 h, 2 bar, 150 °C

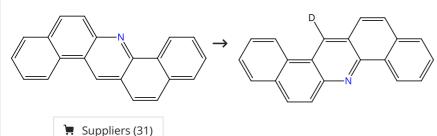
Steps: 1 Yield: 54%

Fine-tuning the efficiency of para-hydrogen-induced hyperpolarization by rational N-heterocyclic carbene design

By: Rayner, Peter J.; et al

Nature Communications (2018), 9(1), 1-11.

Scheme 19 (1 Reaction)



31-116-CAS-2451998

1.1 Reagents: Calcium carbonate, Deuterium

Catalysts: Palladium Solvents: 1,4-Dioxane

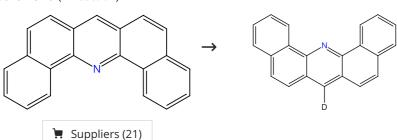
Steps: 1 Yield: 34%

The preparation of regiospecific tritiated and deuterated dibenzacridines by catalytic exchange and [14-¹⁴C]dibenz[a,j] acridine

By: Rosario, Christopher A.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(1), 23-8.

Scheme 20 (1 Reaction)



31-116-CAS-6709832

1.1 **Reagents:** Calcium carbonate, Deuterium

Catalysts: Palladium Solvents: 1,4-Dioxane Reagents: Oxygen Solvents: Acetic acid

Steps: 1 Yield: 17%

The preparation of regiospecific tritiated and deuterated dibenzacridines by catalytic exchange and [14-14C]dibenz[a,j] acridine

By: Rosario, Christopher A.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(1), 23-8.

Scheme 21 (1 Reaction)

Steps: 1

31-614-CAS-36265911

Steps: 1

Supplier (1)

Atomically dispersed palladium catalyzes H/D exchange and isomerization of alkenes via reversible insertion and elimin ation

1.1 Reagents: Deuterium

Suppliers (122)

 $\textbf{Catalysts:} \ \, \textbf{Copper oxide (Cu}_2\textbf{O), Palladium; 450 min, 0.1 M\,Pa,}$

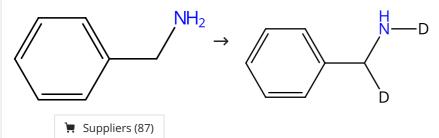
30 °C

By: Liu, Kunlong; et al

Chem Catalysis (2021), 1(7), 1480-1492.

Scheme 22 (1 Reaction)

Steps: 1



31-116-CAS-21488071

Steps: 1

1.1 Reagents: Deuterium

Catalysts: 4-Methylbenzylamine (complexes with palladium),

Palladium (complexes with aryl amines) **Solvents:** Water; 1 h, p H 2, 1 atm, rt

Experimental Protocols

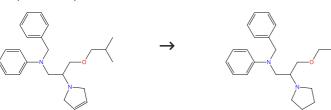
Efficient and Mild Reductive Amination of Carbonyl Compounds Catalyzed by Dual-Function Palladium Nanopar ticles

By: Jv, Xinchun; et al

ACS Sustainable Chemistry & Engineering (2020), 8(3), 1618-1626.

Scheme 23 (1 Reaction)

Steps: 1



31-614-CAS-28234664

Steps: 1

Tritium nuclear magnetic resonance spectroscopy of bepridilpyrrolidine-t

Catalysts: Palladium

Reagents: Deuterium Catalysts: Palladium Solvents: Benzene

By: Kaspersen, Frans M.; et al

Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1986), (4), 585-91.

Scheme 24 (1 Reaction)

Steps: 1

Double bond geometry shown

> Suppliers (58)

Double bond geometry shown

31-614-CAS-36265915

Steps: 1

1.1 Reagents: Deuterium

Catalysts: Copper oxide (Cu₂O), Palladium; 450 min, 0.1 MPa,

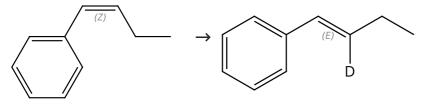
Atomically dispersed palladium catalyzes H/D exchange and isomerization of alkenes via reversible insertion and elimin ation

By: Liu, Kunlong; et al

Chem Catalysis (2021), 1(7), 1480-1492.

Scheme 25 (1 Reaction)

Steps: 1



Double bond geometry shown

Double bond geometry shown

Suppliers (4)

31-614-CAS-36265917

Steps: 1

Reagents: Deuterium

Catalysts: Copper oxide (Cu₂O), Palladium; 450 min, 0.1 MPa,

30 °C

Atomically dispersed palladium catalyzes H/D exchange and isomerization of alkenes via reversible insertion and elimin ation

By: Liu, Kunlong; et al

Chem Catalysis (2021), 1(7), 1480-1492.

Scheme 26 (1 Reaction)

Steps: 1

31-614-CAS-29070914

Steps: 1

Synthesis of tritium-labeled PAM-43

Reagents: Deuterium Catalysts: Palladium

By: Nagaev, Igor Yu.; et al

Mendeleev Communications (2018), 28(1), 64-65.

Scheme 27 (1 Reaction)

Steps: 1

31-614-CAS-26649657

Steps: 1

Catalysts: Trifluoroacetic acid, Palladium diacetate Solvents: 1,1,1,3,3,3-Hexafluoro-2-propanol; 2 h, 40 °C; 40 °C → 23 °C

1.2 Reagents: Cesium carbonate

Catalysts: 2-(Di-tert-butylphosphino)biphenyl

Solvents: 1,1,1,3,3,3-Hexafluoro-2-propanol; 10 min, 23 °C

1.3 Reagents: Deuterium; 18 h, 23 °C

Experimental Protocols

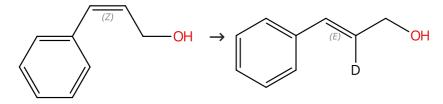
Palladium(II)-Mediated C-H Tritiation of Complex Pharmace uticals

By: Yang, Haifeng; et al

Angewandte Chemie, International Edition (2018), 57(7), 1883-1887.

Scheme 28 (1 Reaction)

Steps: 1



Double bond geometry shown

Double bond geometry shown

□ Suppliers (40)

📜 Supplier (1)

31-614-CAS-36265920

Steps: 1

1.1 Reagents: Deuterium

Catalysts: Copper oxide (Cu₂O), Palladium; 450 min, 0.1 MPa,

30 °C

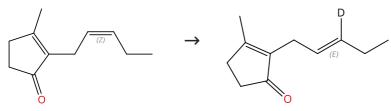
Atomically dispersed palladium catalyzes H/D exchange and isomerization of alkenes via reversible insertion and elimin ation

By: Liu, Kunlong; et al

Chem Catalysis (2021), 1(7), 1480-1492.

Scheme 29 (1 Reaction)

Steps: 1



Double bond geometry shown

Double bond geometry shown

■ Suppliers (68)

31-614-CAS-36265916

Steps: 1

Reagents: Deuterium

Catalysts: Copper oxide (Cu₂O), Palladium; 450 min, 0.1 MPa,

30 °C

Atomically dispersed palladium catalyzes H/D exchange and isomerization of alkenes via reversible insertion and elimin ation

By: Liu, Kunlong; et al

Chem Catalysis (2021), 1(7), 1480-1492.

Scheme 30 (1 Reaction)

Steps: 1

□ Suppliers (73)

📜 Suppliers (11)

31-614-CAS-36089369

Steps: 1

Tripodal Pd metallenes mediated by Nb₂C MXenes for boosting alkynes semihydrogenation

Reagents: Deuterium

Catalysts: Palladium, Niobium carbide (Nb₂C) Solvents: Isopropanol; 0.1 MPa, rt → 298 K

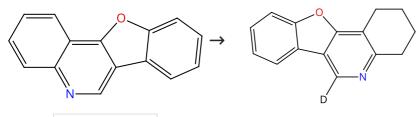
Experimental Protocols

By: Wei, Zhongzhe; et al

Nature Communications (2023), 14(1), 661.

Scheme 31 (1 Reaction)

Steps: 1



📜 Suppliers (2)

31-614-CAS-39390206

Steps: 1

Regioselective Partial Hydrogenation and Deuteration of Tetracyclic (Hetero)aromatic Systems Using a Simple Heterog eneous Catalyst

Reagents: Acetic acid, Deuterium Catalysts: Palladium; 24 h, 80 °C

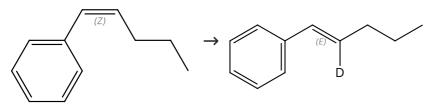
Reagents: Sodium bicarbonate 1.2

By: Kehoe, Roberta A.; et al

Chemistry - A European Journal (2024), 30(17), e202400102.

Scheme 32 (1 Reaction)





Double bond geometry shown

Double bond geometry shown

Suppliers (3)

31-614-CAS-36265914

Steps: 1

Reagents: Deuterium

Catalysts: Copper oxide (Cu₂O), Palladium; 450 min, 0.1 MPa,

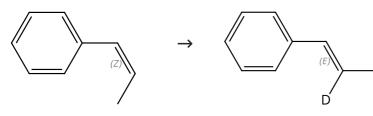
30 °C

Atomically dispersed palladium catalyzes H/D exchange and isomerization of alkenes via reversible insertion and elimin

By: Liu, Kunlong; et al

Chem Catalysis (2021), 1(7), 1480-1492.

Scheme 33 (1 Reaction)



Double bond geometry shown

■ Suppliers (69)

Double bond geometry shown

> Supplier (1)

Steps: 1

31-614-CAS-36265910

1.1 Reagents: Deuterium

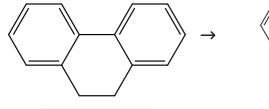
Catalysts: Copper oxide (Cu₂O), Palladium; 450 min, 0.1 MPa,

Atomically dispersed palladium catalyzes H/D exchange and isomerization of alkenes via reversible insertion and elimin ation

By: Liu, Kunlong; et al

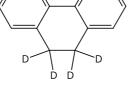
Chem Catalysis (2021), 1(7), 1480-1492.

Scheme 34 (1 Reaction)



Suppliers (52)

Steps: 1



31-116-CAS-7399973

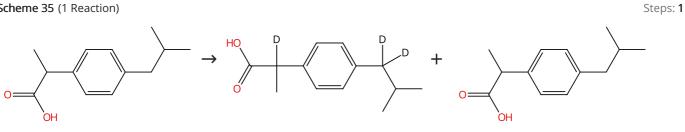
Reagents: Deuterium Catalysts: Palladium Solvents: Acetic acid-d Steps: 1

A selective method for deuterium exchange in hydroar omatic compounds

By: Ofosu-Asante, K.; et al

Journal of Organic Chemistry (1986), 51(26), 5452-4.

Scheme 35 (1 Reaction)



Steps: 1

📜 Suppliers (157)

31-614-CAS-39216784

Reagents: Deuterium Catalysts: Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

Experimental Protocols

Palladium Nanoparticles for the Deuteration and Tritiation of **Benzylic Positions on Complex Molecules**

By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

Steps: 1

Steps: 1

Scheme 36 (1 Reaction)

Steps: 1

Suppliers (101)

31-614-CAS-39216785

Reagents: Deuterium Catalysts: Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

Experimental Protocols

Palladium Nanoparticles for the Deuteration and Tritiation of **Benzylic Positions on Complex Molecules**

By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

Scheme 37 (1 Reaction)

Suppliers (78)

Steps: 1

Palladium Nanoparticles for the Deuteration and Tritiation of Benzylic Positions on Complex Molecules

By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

31-614-CAS-39216773

Reagents: Deuterium 1.1 Catalysts: Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

Experimental Protocols

Scheme 38 (1 Reaction)

> Suppliers (94)

Steps: 1

> Supplier (1)

31-614-CAS-38893217

Reagents: Deuterium Catalysts: Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

Experimental Protocols

Palladium Nanoparticles for the Deuteration and Tritiation of Benzylic Positions on Complex Molecules

By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

Steps: 1

Steps: 1

Scheme 39 (1 Reaction)

HO -

Steps: 1

➤ Suppliers (101)

31-614-CAS-39216778

1.1 Reagents: Deuterium Catalysts: Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

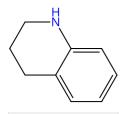
Experimental Protocols

Palladium Nanoparticles for the Deuteration and Tritiation of Benzylic Positions on Complex Molecules

By: Pfeifer, Viktor; et al

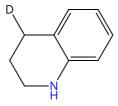
Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

Scheme 40 (1 Reaction)

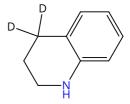


Suppliers (98)





+



➤ Supplier (1)

31-614-CAS-39216772

1.1 Reagents: Deuterium Catalysts: Palladium

Solvents: Tetrahydrofuran; 20 h, 1.1 bar, 50 °C

Experimental Protocols

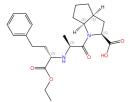
Steps: 1

Palladium Nanoparticles for the Deuteration and Tritiation of Benzylic Positions on Complex Molecules

By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

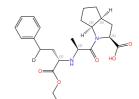
Scheme 41 (1 Reaction)



Absolute stereochemistry shown

Absolute stereochemistry shown

Steps: 1



Absolute stereochemistry shown

Suppliers (102)

31-614-CAS-39216783

1.1 **Reagents:** Deuterium **Catalysts:** Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

Experimental Protocols

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By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

Steps: 1

Scheme 42 (1 Reaction)

N →

➤ Suppliers (80)

31-614-CAS-39216779

1.1 **Reagents:** Deuterium **Catalysts:** Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

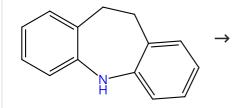
Experimental Protocols

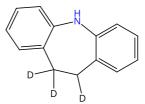
Steps: 1 Palladium Nanoparticles for the Deuteration and Tritiation of Benzylic Positions on Complex Molecules

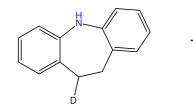
By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

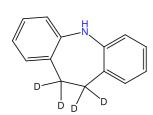
Scheme 43 (1 Reaction)







Suppliers (104)



31-614-CAS-39216768

1.1 Reagents: Deuterium Catalysts: Palladium

Solvents: Dimethylacetamide; 20 h, 1.1 bar, 50 °C

Experimental Protocols

Palladium Nanoparticles for the Deuteration and Tritiation of Benzylic Positions on Complex Molecules

By: Pfeifer, Viktor; et al

Angewandte Chemie, International Edition (2021), 60(51), 26671-26676.

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Steps: 1

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