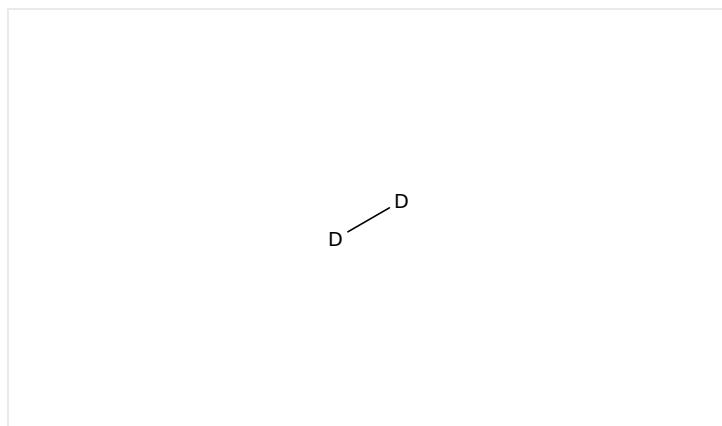


Initiating Search

February 23, 2025, 9:23 PM



 Substances:

Filtered By:



Structure Match: As Drawn

Search Tasks

Task	Search Type	View
Returned Substance Results + Filters (2,302)	 Substances	View Results
Exported: Retrieved Related Reaction Results + Filters (185)	 Reactions	View Results
Filtered By: Substance Role: Catalyst:	<p>1,1'-Bis[(11a<i>R</i>)-10,11,12,13-tetrahydro-4<i>H</i>-diindeno[7,1-<i>cd</i>:1',7'-<i>ef</i>]phosphocin-5(6<i>H</i>)-yl]ferrocene, 1,1'-Bis[(11a<i>S</i>)-10,11,12,13-tetrahydro-4<i>H</i>-diindeno[7,1-<i>cd</i>:1',7'-<i>ef</i>]phosphocin-5(6<i>H</i>)-yl]ferrocene, 1,1'-Bis[(11b<i>R</i>)-3,5-dihydro-4<i>H</i>-dinaphtho[2,1-<i>c</i>:1',2'-<i>e</i>]phosphopin-4-yl]ferrocene, 1,1'-Bis[(11b<i>S</i>)-3,5-dihydro-4<i>H</i>-dinaphtho[2,1-<i>c</i>:1',2'-<i>e</i>]phosphopin-4-yl]ferrocene, 1,1'-Bis[(1,1-dimethylethyl)-2-pyridinylphosphino]ferrocene, 1,1-Bis(diphenylphosphino)ferrocene, (1<i>R</i>)-1-[(1<i>R</i>)-1-[Bis(3,5-dimethylphenyl)phosphino]ethyl]-2-[bis(3,5-dimethylphenyl)phosphino]phenyl]ferrocene, (1<i>R</i>)-1-[(1<i>R</i>)-1-(Dicyclohexylphosphino)ethyl]-2-[2-(diphenylphosphino)phenyl]ferrocene, (1<i>R</i>,1'<i>R</i>)-1,1'-Bis(dicyclohexylphosphino)-2,2'-bis[(<i>R</i>)-(dimethylamino)phenylmethyl]ferrocene, (1<i>S</i>)-1,1'-Bis[bis(4-methoxy-3,5-dimethylphenyl)phosphino]-2-[(1<i>S</i>)-1-[[[3,5-bis(trifluoromethyl)phenyl]amino]thioxomethyl]amino]ethyl]ferrocene, (1<i>S</i>)-1-[Bis(1,1-dimethylethyl)phosphino]-2-[(1<i>R</i>)-1-(diphenylphosphino)ethyl]ferrocene, (1<i>S</i>,1"<i>S</i>)-2,2"-Bis[(1<i>S</i>)-1-(diphenylphosphino)ethyl]-1,1"-biferrocene, (2<i>R</i>)-1-[(1<i>R</i>)-1-[[[3,5-Bis(trifluoromethyl)phenyl]amino]thioxomethyl]amino]ethyl]-1',2-bis(diphenylphosphino)ferrocene, (2<i>R</i>)-1-[(1<i>R</i>)-1-[Bis(1,1-dimethylethyl)phosphino]ethyl]-2-[bis[4-(trifluoromethyl)phenyl]phosphino]ferrocene, (2<i>R</i>)-1-[(1<i>R</i>)-1-[Bis(1,1-dimethylethyl)phosphino]ethyl]-2-(di-2-furanylphosphino)ferrocene, (2<i>R</i>)-1-[(1<i>R</i>)-1-[Bis(1,1-dimethylethyl)phosphino]ethyl]-2-(diphenylphosphino)ferrocene, (2<i>R</i>)-1-[(1<i>S</i>)-1-[Bis(1,1-</p>	

dimethylethyl)phosphino]ethyl]-2-(diphenylphosphino)ferrocene, (2*S*)-1-[(1*S*)-1-[[[3,5-Bis(trifluoromethyl)phenyl]amino]thioxomethyl]amino]ethyl]-1',2-bis(diphenylphosphino)ferrocene, (2*S*)-1-[(1*S*)-1-[[[3,5-Bis(trifluoromethyl)phenyl]amino]thioxomethyl]methylamino]ethyl]-1',2-bis(diphenylphosphino)ferrocene, (2*S*)-1-[(1*S*)-1-[Bis(1,1-dimethylethyl)phosphino]ethyl]-2-(diphenylphosphino)ferrocene, (η^5 -2,4-Cyclopentadien-1-yl)[(1,2,3,3a,9b- η)-(3a*S*)-3a*H*-cyclopenta[*c*]quinolin-3a-yl]iron, Borate(1-), tetrafluoro-, iron(2+) (2:1), Dichloro[*N,N'*-[(2,6-pyridinediyl- κ *M*)diethylidyne]bis[2,6-diethylbenzenamine- κ *M*]]iron, Ferrocene, 1,1'-bis(diphenylphosphino)-2-[(1*R*)-1-[methyl[2-(1-piperidinyl)ethyl]amino]ethyl]-, (2*R*)-, Ferrocene, 1-[(1*R*)-1-[[[3,5-bis(trifluoromethyl)phenyl]amino]thioxomethyl]methylamino]ethyl]-1',2-bis(diphenylphosphino)-, (2*S*)-, Ferrocene, 1-[(1*R*)-1-[bis(3,5-dimethylphenyl)phosphino]ethyl]-2-[bis(4-methoxy-3,5-dimethylphenyl)phosphino]-, (2*R*)-, Ferrocene, 1-[(1*S*)-1-[[[3,5-bis(trifluoromethyl)phenyl]amino]thioxomethyl]amino]ethyl]-1',2-bis(di-2-naphthalenylphosphino)-, (2*S*)-, Iridium(1+), [(2*R*)-1-[(1*R*)-1-[bis(4-methoxy-3,5-dimethylphenyl)phosphino- κ *P*]ethyl]-2-(dicyclohexylphosphino- κ *P*)ferrocene][(1,2,5,6- η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (1:1), Iron(1+), (*N,N*-dimethylboranamine- κ *H*¹, κ *H*¹)hydro[*N,N'*-(2,6-pyridinediyl- κ *M*)bis[*N*-methyl-*P,P*-bis(1-methylethyl)phosphinous amide- κ *P*]-, (OC-6-13)-, tetraphenylborate(1-) (1:1), Iron(1+), tricarbonyl[(4a,5,6,7,7a- η)-2,3,4,4a-tetrahydro-1,4-dimethyl-6-[(1-methylethyl)amino]-5,7-diphenyl-1*H*-cyclopenta[*b*]pyrazin-4a-yl]-, tetrafluoroborate(1-) (1:1), Iron, [6-[[bis(1,1-dimethylethyl)phosphino- κ *P*]methyl]-2,2'-bipyridine- κ *N*¹, κ *N*¹]dichloro-, (SP-5-13)-, Iron alloy, nonbase, Fe,Pd,Pt, Iron, compd. with nickel (3:1), Iron, [[*N,N'*-(1,3-dimethyl-1,3-propanediylidene)bis[2,6-bis(1-methylethyl)benzenaminato- κ *M*]](1-)] [(trimethylsilyl)methyl]-, Iron, tricarbonyl(13*H*-cyclopenta[1,2:3,4]dicycloocten-13-one)-, Methanesulfonic acid, 1,1,1-trifluoro-, iron(2+) salt (2:1), [[*N,N'*-(1,3-Dimethyl-1,3-propanediylidene)bis[2,6-dimethylbenzenaminato- κ *M*]](1-)] [(trimethylsilyl)methyl]iron, (OC-6-12)-Dibromocarbonyl[2-(dicyclohexylphosphino- κ *P*)-*N*-[2-(dicyclohexylphosphino- κ *P*)ethyl]ethanamine- κ *M*]iron, (S)-1-[(*R*_p)-[2-(Dicyclohexylphosphino)ferrocenyl]ethyl]diphenylphosphine, (SP-5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl- κ *M*)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-2-ylidene- κ *C*]]iron, (SP-5-13)-Bis(dinitrogen)[*N,N'*-[(2,6-pyridinediyl- κ *M*)diethylidyne]bis[2,6-bis(1-methylethyl)benzenamine- κ *M*]]iron, (SP-5-14)-Dichloro[*N*-[1-[8-[(4*S*)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl- κ *N*³]-2-quinoliny- κ *M*]ethylidene]-2,6-bis(1-methylethyl)benzenamine- κ *M*]iron, (TB-5-11)-Tricarbonylbis(trimethylphosphine)iron, Tricarbonyl[(3a,4,6,6a- η)-2,3-dihydro-2-[(4-methylphenyl)sulfonyl]-4,6-bis[tris(1-methylethyl)silyl]cyclopenta[*c*]pyrrol-5(1*H*)-one]iron

Document

Type:

Language:

Journal


English

Reactions (17)

[View in CAS SciFinder](#)

Scheme 1 (1 Reaction)

Steps: 1 Yield: 100%


 Suppliers (137)

31-614-CAS-30411019

Steps: 1 Yield: 100%

Iron-catalysed tritiation of pharmaceuticals

1.1 Reagents: Deuterium

Catalysts: (*SP*-5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl-κ*N*)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*]]iron

Solvents: Tetrahydrofuran; 4 atm, -196 °C; 24 h, 45 °C

1.2 Reagents: Oxygen

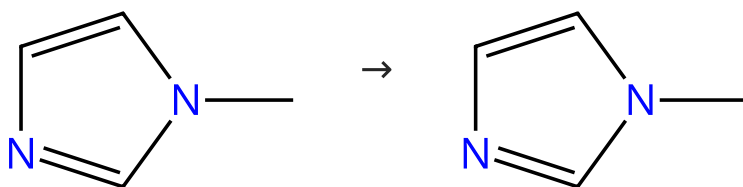
Experimental Protocols

By: Pony Yu, Renyuan; et al

Nature (London, United Kingdom) (2016), 529(7585), 195-199.

Scheme 2 (1 Reaction)

Steps: 1 Yield: 98%


 Suppliers (122)

31-614-CAS-26895108

Steps: 1 Yield: 98%

Iron-catalysed tritiation of pharmaceuticals

1.1 Reagents: Deuterium

Catalysts: (*SP*-5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl-κ*N*)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*]]iron

Solvents: Tetrahydrofuran; -196 °C; 24 h, 45 °C

1.2 Reagents: Oxygen

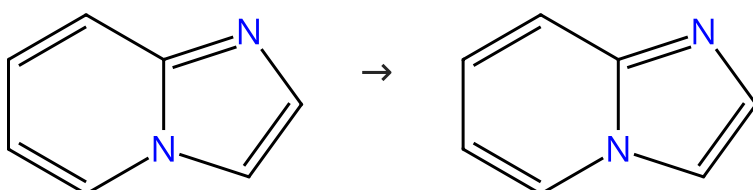
Experimental Protocols

By: Pony Yu, Renyuan; et al

Nature (London, United Kingdom) (2016), 529(7585), 195-199.

Scheme 3 (1 Reaction)

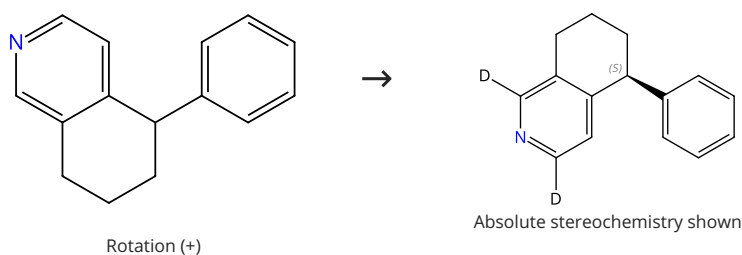
Steps: 1 Yield: 93%


 Suppliers (91)

31-614-CAS-30391572	Steps: 1 Yield: 93%	Iron-catalysed tritiation of pharmaceuticals
1.1 Reagents: Deuterium Catalysts: (<i>SP</i> -5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl- κ <i>M</i>)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2 <i>H</i> -imidazol-2-ylidene- κ <i>C</i>]]iron Solvents: Tetrahydrofuran; 4 atm, -196 °C; 24 h, 45 °C	By: Pony Yu, Renyuan; et al Nature (London, United Kingdom) (2016), 529(7585), 195-199.	
1.2 Reagents: Oxygen		
Experimental Protocols		

Scheme 4 (1 Reaction)

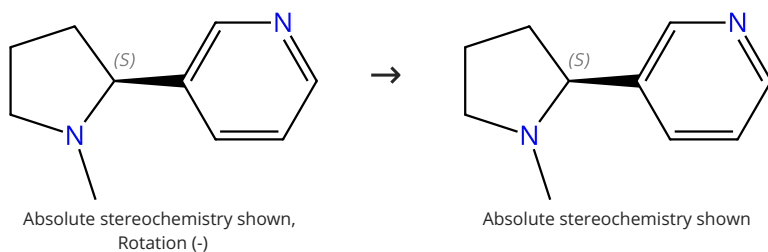
Steps: 1 Yield: 92%



31-116-CAS-18697970	Steps: 1 Yield: 92%	Ruthenium-Catalyzed Chemo- and Enantioselective Hydrogenation of Isoquinoline Carbocycles
1.1 Catalysts: Ruthenium, [(1,2,5,6- η)-1,5-cyclooctadiene]bis[(1,2,3- η)-2-methyl-2-propenyl]-, (1 <i>S</i> ,1'' <i>S</i>)-2,2''-Bis[(1 <i>S</i>)-1-(diphenylphosphino)ethyl]-1,1''-biferrocene Solvents: Tetrahydrofuran; 8 h, rt	By: Jin, Yushu; et al Journal of Organic Chemistry (2018), 83(7), 3829-3839.	
1.2 Reagents: Potassium carbonate, Deuterium Solvents: Isopropanol; 48 h, 80 °C		
Experimental Protocols		

Scheme 5 (1 Reaction)

Steps: 1 Yield: 91%

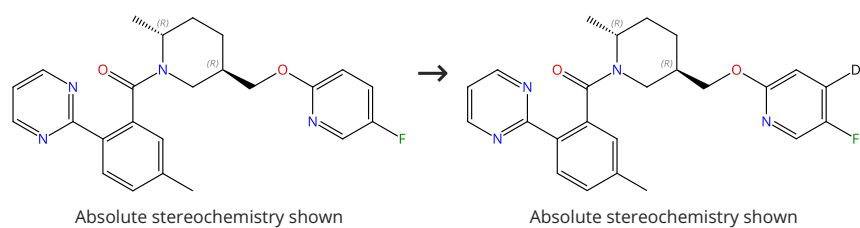


Suppliers (95)

31-614-CAS-26015007	Steps: 1 Yield: 91%	Iron-catalysed tritiation of pharmaceuticals
1.1 Reagents: Deuterium Catalysts: (<i>SP</i> -5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl- κ <i>M</i>)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2 <i>H</i> -imidazol-2-ylidene- κ <i>C</i>]]iron Solvents: Tetrahydrofuran; 4 atm, -196 °C; 24 h, 45 °C	By: Pony Yu, Renyuan; et al Nature (London, United Kingdom) (2016), 529(7585), 195-199.	
1.2 Reagents: Oxygen		
Experimental Protocols		

Scheme 6 (1 Reaction)

Steps: 1 Yield: 85%



Suppliers (52)

31-614-CAS-28636814

Steps: 1 Yield: 85%

Iron-catalysed tritiation of pharmaceuticals

1.1 Reagents: Deuterium

Catalysts: (*SP*-5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl- κ *N*)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-2-ylidene- κ *C*]]iron

Solvents: *N*-Methyl-2-pyrrolidone; -196 °C; 24 h, 45 °C; 1 atm, 23 °C

1.2 Reagents: Oxygen

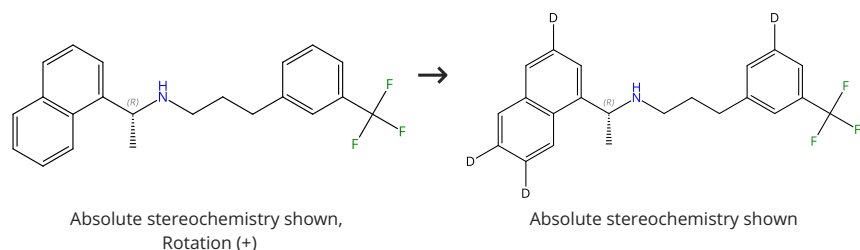
Experimental Protocols

By: Pony Yu, Renyuan; et al

Nature (London, United Kingdom) (2016), 529(7585), 195-199.

Scheme 7 (1 Reaction)

Steps: 1 Yield: 85%



Suppliers (69)

31-116-CAS-8590858

Steps: 1 Yield: 85%

Iron-catalysed tritiation of pharmaceuticals

1.1 Reagents: Deuterium

Catalysts: (*SP*-5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl- κ *N*)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-2-ylidene- κ *C*]]iron

Solvents: *N*-Methyl-2-pyrrolidone; -196 °C; 24 h, 45 °C; 1 atm, 23 °C

1.2 Reagents: Oxygen

Experimental Protocols

By: Pony Yu, Renyuan; et al

Nature (London, United Kingdom) (2016), 529(7585), 195-199.

Scheme 8 (1 Reaction)

Steps: 1 Yield: 82%

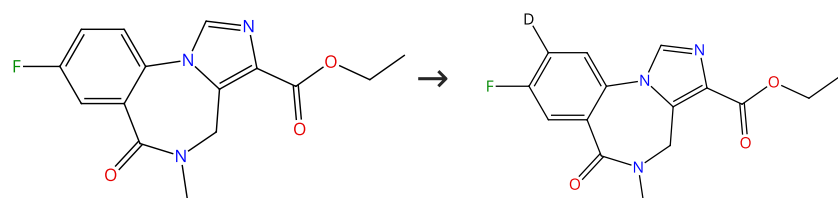


Suppliers (123)

31-614-CAS-29336627 Steps: 1 Yield: 82%	Iron-catalysed tritiation of pharmaceuticals
1.1 Reagents: Deuterium Catalysts: (<i>SP</i> -5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl-κ <i>M</i>)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2 <i>H</i> -imidazol-2-ylidene-κ <i>C</i>]]iron Solvents: Tetrahydrofuran; 4 atm, -196 °C; 24 h, 45 °C 1.2 Reagents: Oxygen	By: Pony Yu, Renyuan; et al Nature (London, United Kingdom) (2016), 529(7585), 195-199.
Experimental Protocols	

Scheme 9 (1 Reaction)

Steps: 1 Yield: 81%

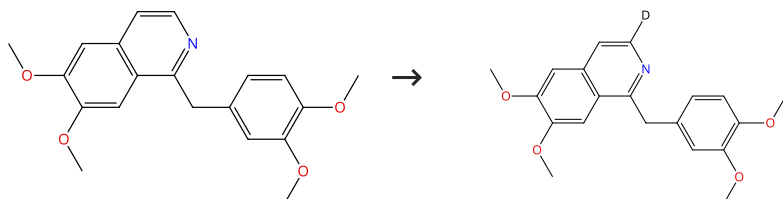


Suppliers (117)

31-116-CAS-5086782 Steps: 1 Yield: 81%	Iron-catalysed tritiation of pharmaceuticals
1.1 Reagents: Deuterium Catalysts: (<i>SP</i> -5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl-κ <i>M</i>)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2 <i>H</i> -imidazol-2-ylidene-κ <i>C</i>]]iron Solvents: <i>N</i> -Methyl-2-pyrrolidone; -196 °C; 24 h, 45 °C; 1 atm, 23 °C 1.2 Reagents: Oxygen	By: Pony Yu, Renyuan; et al Nature (London, United Kingdom) (2016), 529(7585), 195-199.
Experimental Protocols	

Scheme 10 (1 Reaction)

Steps: 1 Yield: 80%

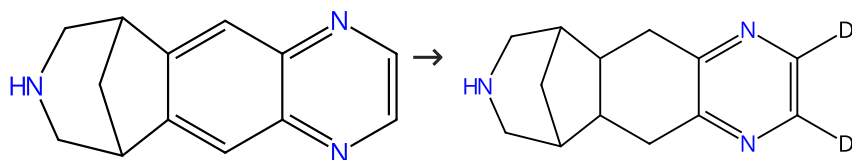


Suppliers (33)

31-116-CAS-13505597 Steps: 1 Yield: 80%	Iron-catalysed tritiation of pharmaceuticals
1.1 Reagents: Deuterium Catalysts: (<i>SP</i> -5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl-κ <i>M</i>)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2 <i>H</i> -imidazol-2-ylidene-κ <i>C</i>]]iron Solvents: <i>N</i> -Methyl-2-pyrrolidone; -196 °C; 24 h, 45 °C; 1 atm, 23 °C 1.2 Reagents: Oxygen	By: Pony Yu, Renyuan; et al Nature (London, United Kingdom) (2016), 529(7585), 195-199.
Experimental Protocols	

Scheme 11 (1 Reaction)

Steps: 1 Yield: 76%



Suppliers (69)

31-116-CAS-9255038

Steps: 1 Yield: 76%

Iron-catalysed tritiation of pharmaceuticals

1.1 Reagents: Deuterium

Catalysts: (*SP*-5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl-κ*N*)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*]]iron

Solvents: *N*-Methyl-2-pyrrolidone; -196 °C; 24 h, 45 °C; 1 atm, 23 °C

1.2 Reagents: Oxygen

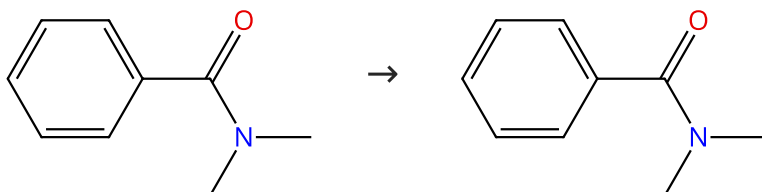
Experimental Protocols

By: Pony Yu, Renyuan; et al

Nature (London, United Kingdom) (2016), 529(7585), 195-199.

Scheme 12 (1 Reaction)

Steps: 1 Yield: 74%



Suppliers (75)

31-614-CAS-27865031

Steps: 1 Yield: 74%

Iron-catalysed tritiation of pharmaceuticals

1.1 Reagents: Deuterium

Catalysts: (*SP*-5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl-κ*N*)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*]]iron

Solvents: Tetrahydrofuran; 4 atm, -196 °C; 24 h, 45 °C

1.2 Reagents: Oxygen

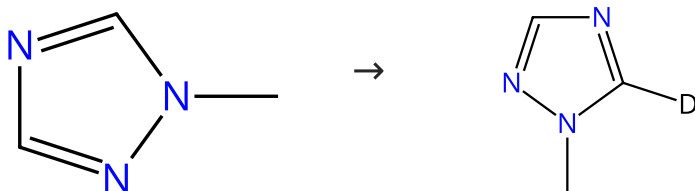
Experimental Protocols

By: Pony Yu, Renyuan; et al

Nature (London, United Kingdom) (2016), 529(7585), 195-199.

Scheme 13 (1 Reaction)

Steps: 1



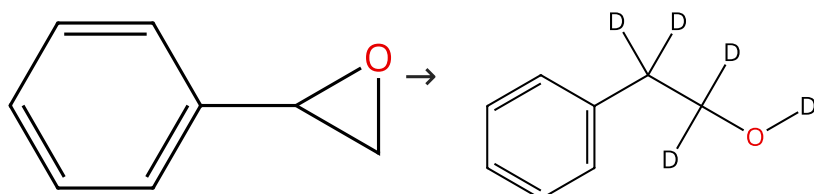
Suppliers (77)

Supplier (1)

31-116-CAS-14882506	Steps: 1	Iron-catalysed tritiation of pharmaceuticals
1.1 Reagents: Deuterium Catalysts: (<i>SP</i> -5-12)-Bis(dinitrogen)[1,1'-(2,6-pyridinediyl- κ M)bis[3-[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2 <i>H</i> -imidazol-2-ylidene- κ C]]iron Solvents: Tetrahydrofuran; 4 atm, -196 °C; 24 h, 45 °C		By: Pony Yu, Renyuan; et al Nature (London, United Kingdom) (2016), 529(7585), 195-199.
1.2 Reagents: Oxygen		
Experimental Protocols		

Scheme 14 (1 Reaction)

Steps: 1

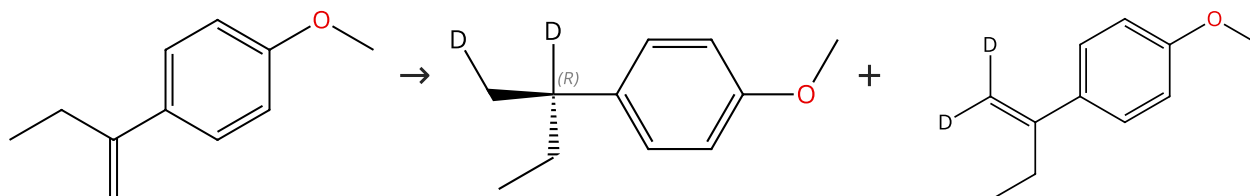


Suppliers (70)

31-614-CAS-25104369	Steps: 1	Regiodivergent Reductive Opening of Epoxides by Catalytic Hydrogenation Promoted by a (Cyclopentadienone)iron Complex
1.1 Catalysts: Trimethylamine oxide, Iron, tricarbonyl(13 <i>H</i> -cyclopenta[1,2:3,4]dicycloocten-13-one)- Solvents: Toluene; 20 min, rt		By: Tadiello, Laura; et al ACS Catalysis (2022), 12(1), 235-246.
1.2 Reagents: Deuterium Solvents: Toluene; 22 h, 20 bar, 150 °C		
Experimental Protocols		

Scheme 15 (1 Reaction)

Steps: 1 Yield: 73%

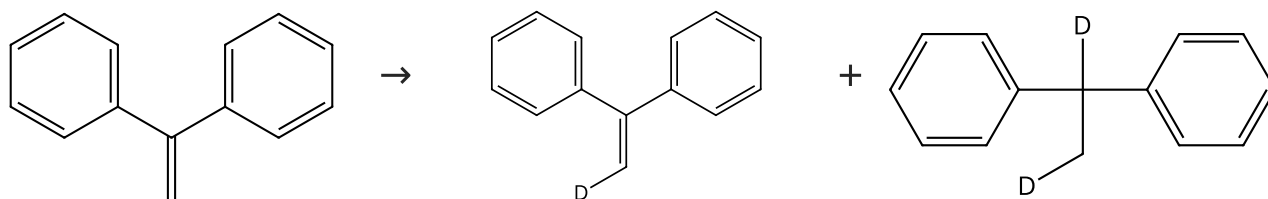


Suppliers (6)

31-116-CAS-23910434	Steps: 1 Yield: 73%	Iron-Catalyzed Highly Enantioselective Hydrogenation of Alkenes
1.1 Catalysts: Acetonitrile, Sodium triethylborohydride, Octadecylsilane, (<i>SP</i> -5-14)-Dichloro[<i>N</i> -[1-[8-[(4 <i>S</i>)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl- κ N ³]-2-quinoliny- κ M]ethylidene]-2,6-bis(1-methylethyl)benzenamine- κ M]iron Solvents: Toluene, Tetrahydrofuran; rt; 5 min, rt		By: Lu, Peng; et al Journal of the American Chemical Society (2021), 143(32), 12433-12438.
1.2 Reagents: Deuterium; 4 h, rt		
1.3 -		
Experimental Protocols		

Scheme 16 (1 Reaction)

Steps: 1



Suppliers (77)

Suppliers (2)

Supplier (1)

31-116-CAS-22876134

Steps: 1

Zero valent iron complexes as base partners in frustrated Lewis pair chemistry

By: Tinnermann, Hendrik; et al

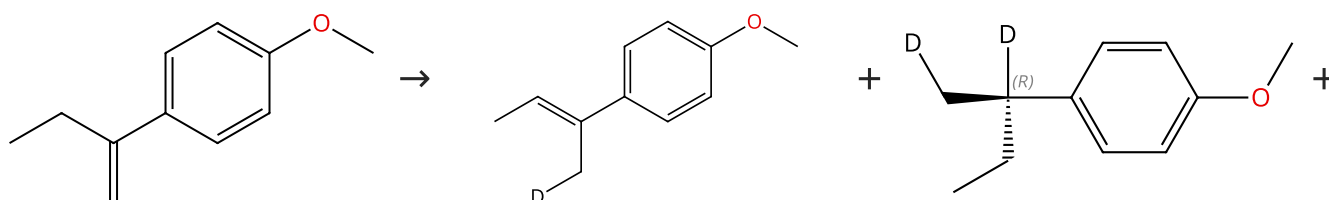
Dalton Transactions (2020), 49(43), 15184-15189.

1.1 **Reagents:** Deuterium
Catalysts: Tris(pentafluorophenyl)borane, (*TB*-5-11)-Tricarbonylbis(trimethylphosphine)iron
Solvents: Benzene; 3 d, 60 °C

Experimental Protocols

Scheme 17 (1 Reaction)

Steps: 1 Yield: 42%



Suppliers (6)

Absolute stereochemistry shown

31-116-CAS-23906715

Steps: 1 Yield: 42%

Iron-Catalyzed Highly Enantioselective Hydrogenation of Alkenes

By: Lu, Peng; et al

Journal of the American Chemical Society (2021), 143(32), 12433-12438.

1.1 **Catalysts:** Sodium triethylborohydride, (*SP*-5-14)-Dichloro[*N*-[1-[8-[(4*S*)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κ^N]-2-quinolinyl-κ^N]ethylidene]-2,6-bis(1-methylethyl)benzenamine-κ^N]iron

Solvents: Toluene, Tetrahydrofuran; rt; 5 min, rt1.2 **Reagents:** Deuterium; 4 h, rt

1.3 -

Experimental Protocols