CAS SciFinder

Task History

Initiating Search

February 21, 2025, 8:21 PM

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 (880)	Reactions	View Results

Filtered By:

Substance Role: **Reagent**

Catalyst: **[(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium, [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)iridium(1+), [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+), [(1,2,5,6-η)-1,5-Cyclooctadiene][(1*S*)-7'-(diphenylphosphino-κ*P*)-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-indene]-7-carboxylato-κ*O*]iridium, [(1,2,5,6-η)-1,5-Cyclooctadiene](2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium, [μ-[1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-4-yl-2-ylidene-κ*C*^{2}:κ*C*^{4}]][(1,2,5,6-η)-1,5-cyclooctadiene][tris(2,3,4,5,6-pentafluorophenyl)boron]iridium, [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium, Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium, Chloro(1,5-cyclooctadiene)(1,3-**

dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium, Chloro[(2,2-dimethyl-1,2-ethanediyl)[3-(1,1-dimethylethyl)-1*H*-imidazol-1-yl-2(3*H*)-ylidene]][(2,2-dimethyl-1,2-ethanediyl)[3-(1,1-dimethylethyl-κC^2,κH^2)-1*H*-imidazol-1-yl-2(3*H*)-ylidene]]iridium, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Dihydrobis(2-propanone)bis(triphenylphosphine)iridium(1+), Iridium, Iridium(1+), [1,1'-[1,1'-biphenyl]-2,2'-diylbis[1,1-diphenylphosphine-κ*P*]][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(11a*S*)-4,8-bis(1,1-dimethylethyl)-6-[[(1*R*,2*R*)-2-[(2,6-dimethylphenyl)thio-κ*S*]cyclohexyl]oxy]-1,2,10,11-tetramethyldibenzo[*d*,*f*][1,3,2]dioxaphosphepin-κP^6][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,1'-(1,2-ethanediyl)bis[1,1-diphenylphosphine-κ*P*]]-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](pyridine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(pyridine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(tributylphosphine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(tricyclohexylphosphine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1-[(4*S*,5*R*)-4,5-dihydro-5-methyl-2-phenyl-4-oxazolyl-κN^3]-2-phenyl-1-(phenylmethyl)ethyl diphenylphosphinite-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-),

Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1-[(4*S*,5*S*)-4,5-dihydro-5-methyl-2-phenyl-4-oxazolyl-κ*N*^{3}]-2-phenyl-1-(phenylmethyl)ethyl dicyclohexylphosphinite-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(3a*S*,8a*R*)-2-[(1 *S*)-2'-(diphenylphosphino-κ*P*)[1,1'-biphenyl]-2-yl]-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*R*)-2-[2-(diphenylphosphino-κ*P*)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-2-(1,1-dimethylethyl)-4-[2-(diphenylphosphino-κ*P*)ethyl]-4,5-dihydrooxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-2-[(1 *S*)-2'-(diphenylphosphino-κ*P*)[1,1'-biphenyl]-2-yl]-4,5-dihydro-4-(1-methylethyl)oxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-2-[(1 *S*)-2'-(diphenylphosphino-κ*P*)[1,1'-biphenyl]-2-yl]-4,5-dihydro-4-phenyloxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-4-[2-(diphenylphosphino-κ*P*)ethyl]-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yloxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(7*S*)-6,7-dihydro-4-methyl-2-(2,4,6-trimethylphenyl)-5*H*-cyclopenta[*b*]pyridin-7-yl *P*,*P*-dicyclohexylphosphinite-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(8*R*)-8-[(diphenylphosphino-κ*P*)methyl]-5,6,7,8-tetrahydro-2-phenylimidazo[1,2-*a*]pyridine-κ*N*^{1}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(pyridine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(pyridine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][[*P*(*S*)]-*N*-[(1 *R*)-1-[(4*S*)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κ*N*^{3}]-2-methylpropyl]-*P*-(1,1-dimethylethyl)-*P*-

methylphosphinous amide-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris(triphenylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-, Iridium(1+), [1,4-butanediylbis[diphenylphosphine-κ*P*]][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-), Iridium(1+), [(1*R*,3*S*,4*S*)-2-[bis(2-methylphenyl)phosphino-κ*P*]-3-(4-phenyl-2-thiazolyl-κ*N*^{3})-2-azabicyclo[2.2.1]heptane][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1*S*,3*R*,4*R*)-2-[bis(2-methylphenyl)phosphino-κ*P*]-3-(4,5-dihydro-4,4-diphenyl-2-oxazolyl-κ*N*^{3})-2-azabicyclo[2.2.1]heptane][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [2-[(1*S*)-7'-[bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-4,5-dihydrooxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), 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), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ*N*^{1},κ*N*$^{1'}$]bis[2-(2-pyridinyl-κ*N*)phenyl-κ*C*]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ*N*^{1},κ*N*$^{1'}$]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κ*N*]phenyl-κ*C*]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(4*S*)-2-[(1*S*)-7'-[bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-4,5-

dihydro-4-methyloxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(4*S*)-2-[(1*S*)-7'-[bis(3,5-dimethylphenyl)phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-4,5-dihydro-4-(1-naphthalenylmethyl)oxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(4*S*)-2-[2-[bis(4-fluorophenyl)phosphino-κ*P*]phenyl]-4-(1,1-dimethylethyl)-4,5-dihydrooxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, stereoisomer, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-), Iridium(1+), [(4*S*)-2-[[bis(1,1-dimethylethyl)phosphino-κ*P*]methyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), bis[1,1'-(1*S*)-[1,1'-binaphthalene]-2,2'-diylbis[1,1-diphenylphosphine-κ*P*]]tri-μ-chlorodihydrodi-, chloride (1:1), stereoisomer, Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1), Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), dihydrobis(2-propanone)bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(2+), aqua([4,4'-bipyrimidine]-2,2',6,6'(1*H*,1'*H*,3*H*,3'*H*)-tetrone-κ*N*^{3},κ*N*^{3}')[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, sulfate (1:1), Iridium, chloro[(2,2-dimethyl-1,2-ethanediyl)[3-(1,1-dimethylethyl)-1*H*-imidazol-1-yl-2(3*H*)-ylidene]][1-(1,1-dimethylethyl-κ*C*^{2},κ*H*^{2})-3-(1,1-dimethylethyl)-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*]hydro-, Iridium, compd. with ruthenium (1:2), Iridium, compd. with ruthenium (2:1), Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Iridium trichloride, (*OC*-6-53)-[*N*-[(1'*R*)-7'-[Bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-1,3-dithiane-2-methanamine-κ*N*^{2},κ*S*^{1}]chlorodihydroiridium, (*OC*-6-53)-[*N*-[(1*R*)-7'-[Bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-6-methyl-2-pyridinemethanamine-κ*N*^{1},κ*N*^{2}]chlorodihydroiridium, (*SP*-5-43)-[2,6-Bis[[bis(1,1-dimethylethyl)phosphino-κ*P*]oxy]phenyl-κ*C*]chlorohydroiridium, (*SP*-5-43)-[2,6-Bis[[bis(1-methylethyl)phosphino-κ*P*]oxy]phenyl-κ*C*]chlorohydroiridium,

	Stereoisomer of chloro[(1,2-η)-cyclooctene]bis(1,3-dicyclohexyl-1,3-dihydro-2*H*-imidazol-2-ylidene)iridium, Tantalum, [dihydro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium]tris(2,2-dimethylpropyl)-, (*Ir*-*Ta*)
Document Type:	Journal
Language:	English

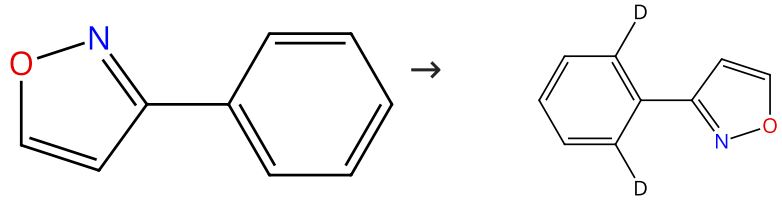
CAS SciFinder

Reactions (488)

View in CAS SciFinder

Scheme 1 (1 Reaction)

Steps: **1** Yield: **100%**



Suppliers (50)

31-116-CAS-3002656

Steps: **1** Yield: **100%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

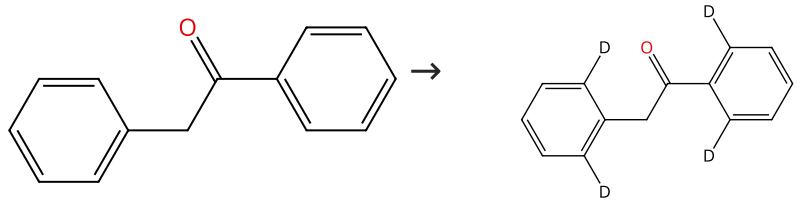
Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 2 (1 Reaction)

Steps: **1** Yield: **100%**



Suppliers (103)

31-116-CAS-22583930

Steps: **1** Yield: **100%**

1.1 **Reagents:** Deuterium, Tritium
Catalysts: [μ-[1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-4-yl-2-ylidene-κC^2:κC^4]][(1,2,5,6-η)-1,5-cyclooctadiene][tris(2,3,4,5,6-pentafluorophenyl)boron]iridium
Solvents: Cyclohexane; 3 h, 1 atm, rt

Experimental Protocols

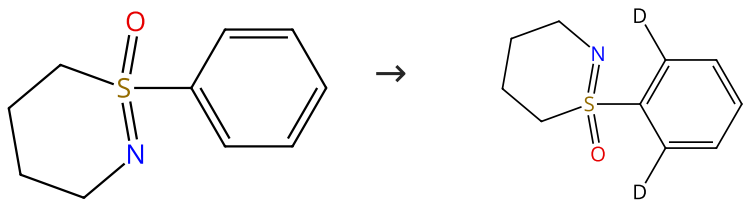
Iridium(I) Complexes with Anionic N-Heterocyclic Carbene Ligands as Catalysts for H/D Exchange in Nonpolar Media

By: Koneczny, Marvin; et al

Advanced Synthesis & Catalysis (2020), 362(18), 3857-3863.

Scheme 3 (1 Reaction)

Steps: **1** Yield: **100%**



31-614-CAS-42989284 Steps: **1** Yield: **100%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

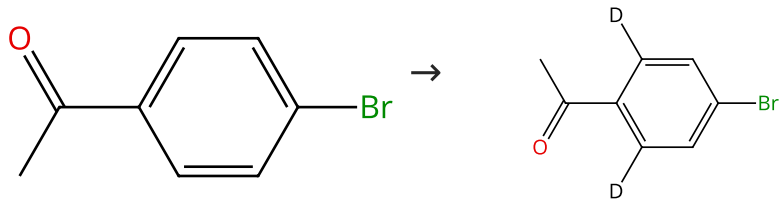
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 4 (2 Reactions) Steps: **1** Yield: **100%**



Suppliers (92)

31-116-CAS-1507860 Steps: **1** Yield: **100%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 66 - 68 h, rt

The mediation of aryl ketone deuteration by $[Ir(PPh_3)_3(cod)]^+.BF^-_4$

By: Herbert, John M.

Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(5), 317-322.

31-116-CAS-342649 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

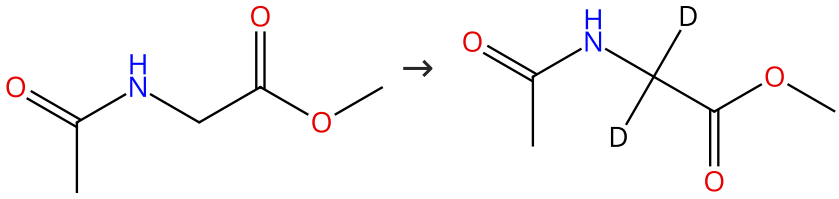
Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 5 (1 Reaction) Steps: **1** Yield: **99%**



Suppliers (61)

31-116-CAS-18953291 Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

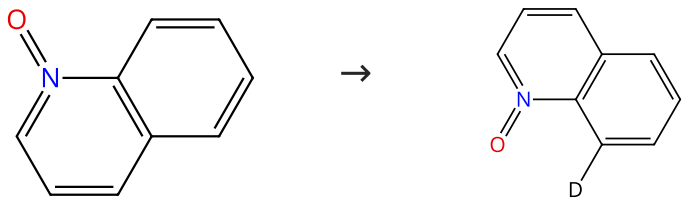
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 6 (1 Reaction)

Steps: **1** Yield: **99%**



Suppliers (57)

Supplier (1)

31-614-CAS-36762216

Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

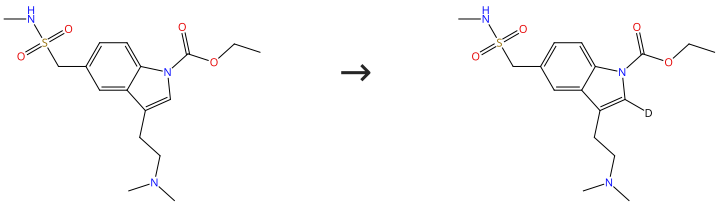
Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 7 (1 Reaction)

Steps: **1** Yield: **99%**



31-116-CAS-18343792

Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 36 h, 25 °C

Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 8 (1 Reaction)

Steps: **1** Yield: **99%**

Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-18953305

Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

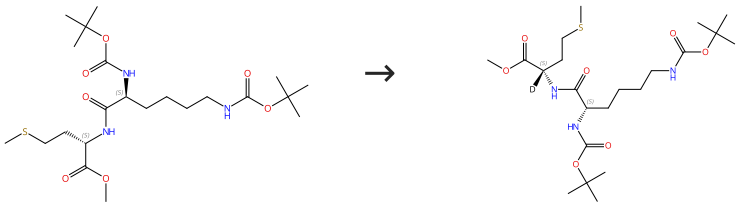
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 9 (1 Reaction)

Steps: **1** Yield: **99%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-18953306

Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 10 (1 Reaction)

Steps: **1** Yield: **99%**

Suppliers (84)

31-614-CAS-29440452

Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Chlorobenzene; 2.5 h, 803 mbar, 120 °C

Experimental Protocols

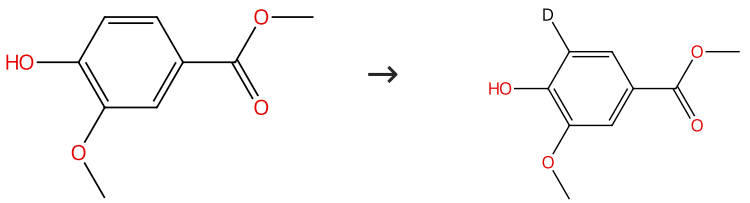
Tritium hydrogen-isotope exchange with electron-poor tertiary benzenesulfonamide moiety; application in late-stage labeling of T0901317

By: Yongsong, Tian; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2022), 65(2), 36-44.

Scheme 11 (1 Reaction)

Steps: **1** Yield: **99%**



Suppliers (104)

31-614-CAS-24835972

Steps: **1** Yield: **99%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

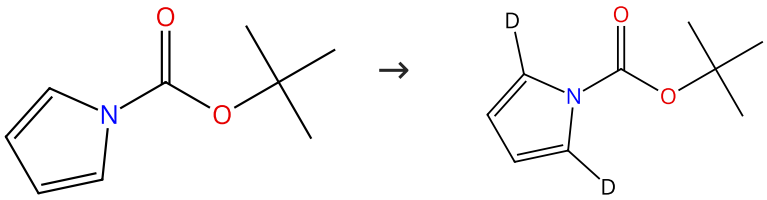
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 12 (1 Reaction)

Steps: **1** Yield: **99%**



Suppliers (74)

31-116-CAS-22583924

Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: [μ-[1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-4-yl-2-ylidene-κC^2:κC^4]][(1,2,5,6-η)-1,5-cyclooctadiene][tris(2,3,4,5,6-pentafluorophenyl)boron]iridium
Solvents: Cyclohexane; 3 h, 1 atm, rt

Experimental Protocols

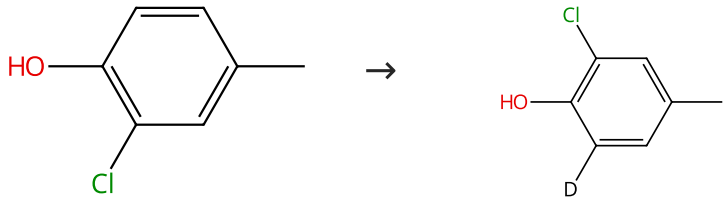
Iridium(I) Complexes with Anionic N-Heterocyclic Carbene Ligands as Catalysts for H/D Exchange in Nonpolar Media

By: Koneczny, Marvin; et al

Advanced Synthesis & Catalysis (2020), 362(18), 3857-3863.

Scheme 13 (1 Reaction)

Steps: **1** Yield: **99%**



Suppliers (75)

31-614-CAS-24835963

Steps: **1** Yield: **99%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

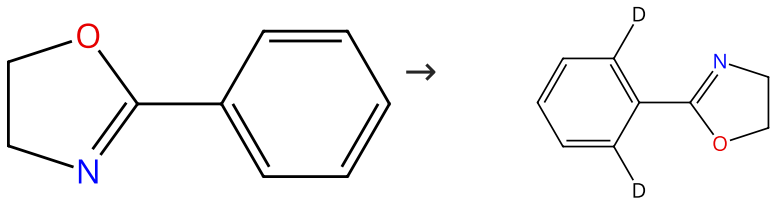
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 14 (4 Reactions)

Steps: **1** Yield: **96-99%**



Suppliers (68)

31-116-CAS-3331913

Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

31-614-CAS-35597980 Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

31-614-CAS-23969793 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

31-116-CAS-17237224 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

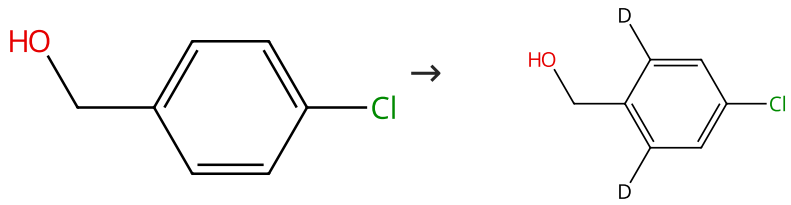
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 15 (1 Reaction) Steps: **1** Yield: **99%**



Suppliers (93)

31-614-CAS-24836030 Steps: **1** Yield: **99%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

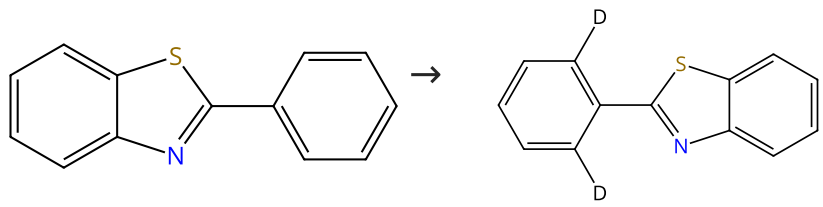
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 16 (2 Reactions) Steps: **1** Yield: **99%**



Suppliers (77)

31-116-CAS-4803935 Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

31-614-CAS-23969783 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

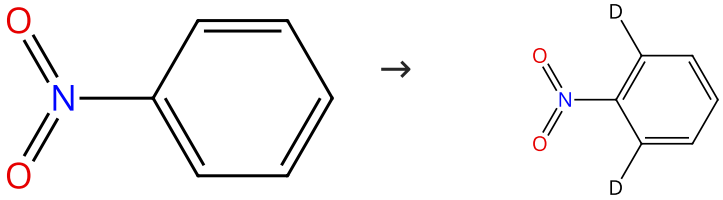
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 17 (6 Reactions) Steps: **1** Yield: **97-99%**



Suppliers (107)

31-116-CAS-16442679 Steps: **1** Yield: **99%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Hydrogen isotope exchange with highly active iridium(I) NH C/phosphine complexes: a compar ative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

31-116-CAS-1837133 Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-13113114 Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-15242112 Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-614-CAS-23969802 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

31-116-CAS-17237226 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

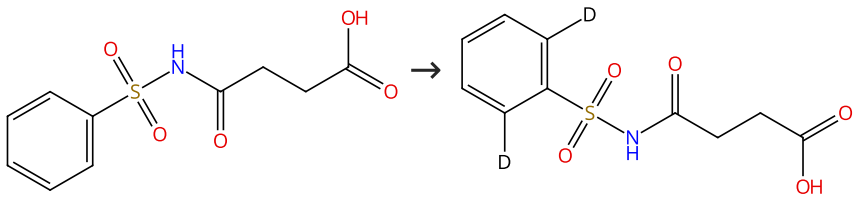
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 18 (1 Reaction) Steps: **1** Yield: **98%**



Suppliers (41)

31-116-CAS-17006218 Steps: **1** Yield: **98%**

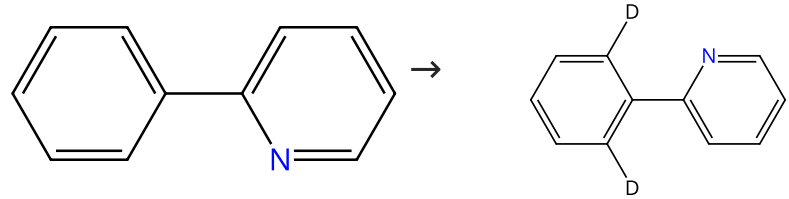
1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 19 (14 Reactions) Steps: **1** Yield: **38-98%**



Suppliers (94)

Supplier (1)

31-116-CAS-8565624 Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-3267916 Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: *tert*-Butyl methyl ether; rt → - 78 °C; 2 h, 25 °C

Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-4581817 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-2461233 Steps: **1** Yield: **38%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-614-CAS-23969786 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

31-116-CAS-17237220 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

31-116-CAS-9943079 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; 1 atm, -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

31-116-CAS-10629851 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Silver hexafluoroantimonate, (*SP*-5-43)-[2,6-Bis[[bis(1,1-dimethylethyl)phosphino-κ*P*]oxy]phenyl-κ*C*]chlorohydroiridium
Solvents: Dichloromethane; 4 h, rt

Application of iridium pincer complexes in hydrogen isotope exchange reactions

By: Traeff, Annika; et al

Journal of Organometallic Chemistry (2007), 692(25), 5529-5531.

31-116-CAS-7431955 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-3515880 Steps: **1**

1.1 **Catalysts:** Triphenylphosphine (polystyrene-bound), Iridium (1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 2 h, rt

1.2 **Reagents:** Deuterium
Solvents: Dichloromethane; 4 h, rt; 18 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-9570109 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-5302798 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-11260873 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

31-116-CAS-12372059 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

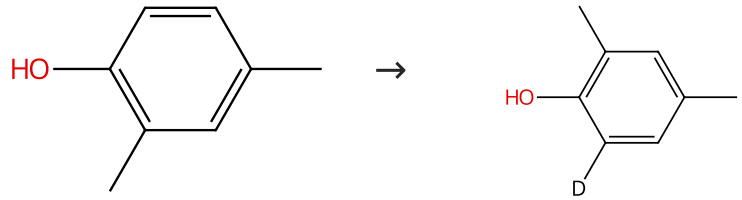
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 20 (1 Reaction)

Steps: **1** Yield: **98%**



Suppliers (81)

31-614-CAS-24835999

Steps: **1** Yield: **98%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

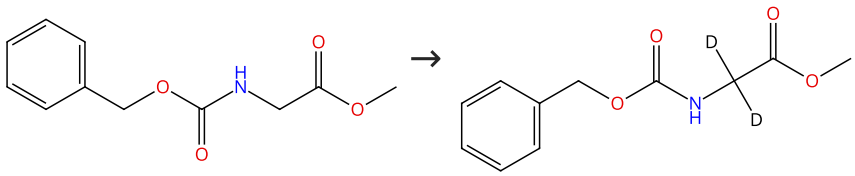
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 21 (1 Reaction)

Steps: **1** Yield: **98%**



Suppliers (70)

31-116-CAS-18953292

Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

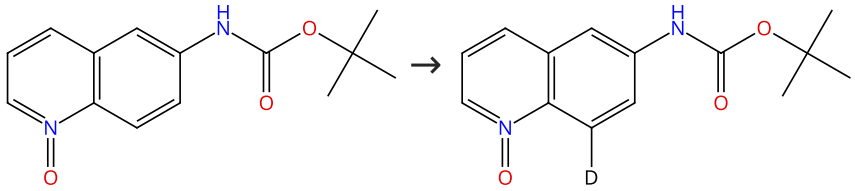
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 22 (1 Reaction)

Steps: **1** Yield: **98%**



31-614-CAS-36762229

Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

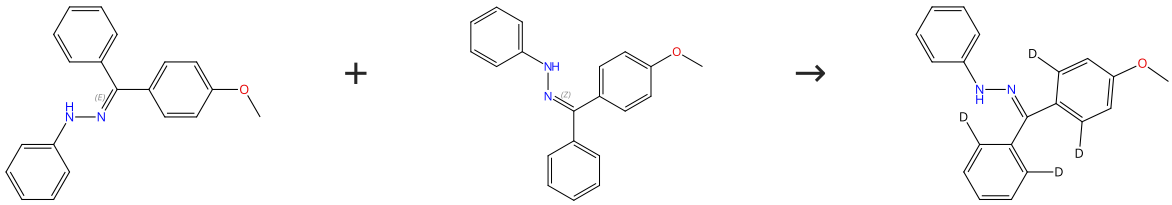
Selective Deuteration of Heterocycle N-Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 23 (1 Reaction)

Steps: **1** Yield: **98%**



Double bond geometry shown

Double bond geometry shown

Suppliers (2)

Supplier (1)

31-614-CAS-25896424

Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C; 16 h, 25 °C

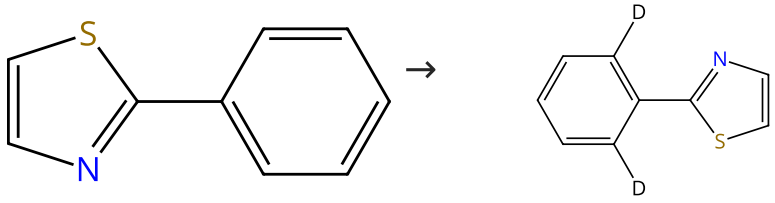
Transition-Metal-Free Coupling of 1,3-Dipoles and Boronic Acids as a Sustainable Approach to C-C Bond Formation

By: Livingstone, Keith; et al

Chemistry - A European Journal (2020), 26(46), 10591-10597.

Scheme 24 (1 Reaction)

Steps: **1** Yield: **98%**



Suppliers (79)

31-116-CAS-1153042

Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

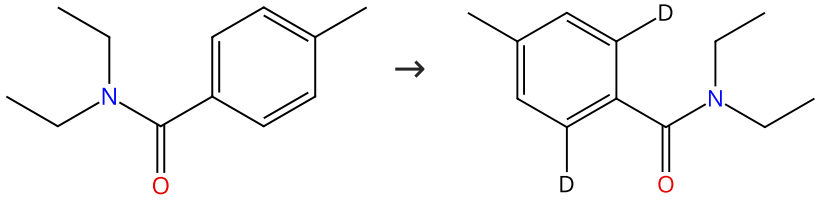
Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 25 (6 Reactions)

Steps: **1** Yield: **81-98%**



Suppliers (50)

31-116-CAS-2169469

Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-4292161 Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-6441962 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-9338727 Steps: **1** Yield: **85%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: 2-Methyltetrahydrofuran; rt → -78 °C; 16 h, 25 °C

Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-16442677 Steps: **1** Yield: **81%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

31-116-CAS-1465271 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; 1 atm, -78 °C → 25 °C; 16 h, 25 °C

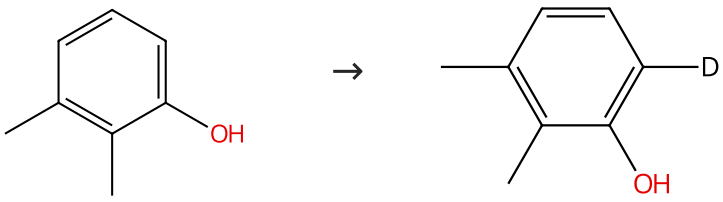
Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 26 (1 Reaction) Steps: **1** Yield: **98%**



Suppliers (69)

31-614-CAS-24835980 Steps: **1** Yield: **98%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Ethyl acetate; 10 h, 1 atm, 35 °C

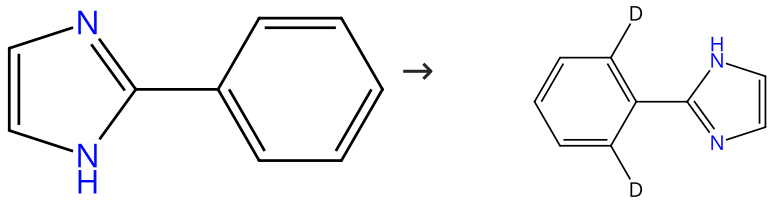
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 27 (7 Reactions) Steps: **1** Yield: **34-98%**



Suppliers (94)

31-116-CAS-3709201 Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

31-116-CAS-6798169 Steps: **1** Yield: **34%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-17237212 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κN^3]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: *tert*-Butyl methyl ether; 2 h, 1 atm, rt

Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

31-116-CAS-3229112 Steps: **1**

1.1 **Catalysts:** Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C
1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

31-116-CAS-7483184 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; 1 atm, -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

31-116-CAS-13119513 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

31-116-CAS-13983956 Steps: 1

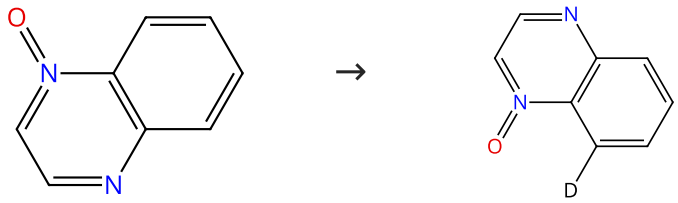
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), dihydrobis(2-propanone)bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane

Investigation of iridium hydride complex [$IrH_2(Me_2CO)_2(PPh_3)_2$]BF_4 as a catalyst of hydrogen isotope exchange of substrates in solution

By: Heys, Richard

Journal of the Chemical Society, Chemical Communications (1992), (9), 680-1.

Scheme 28 (1 Reaction) Steps: **1** Yield: **98%**



Suppliers (46)

31-614-CAS-36762230 Steps: **1** Yield: **98%**

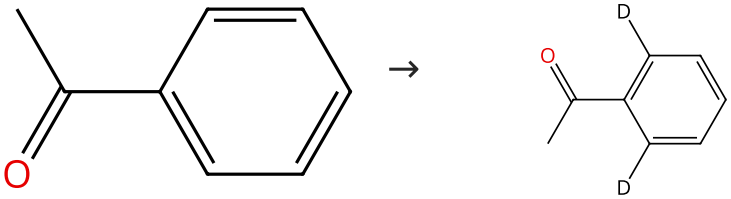
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

Selective Deuteration of Heterocycle N-Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 29 (13 Reactions) Steps: **1** Yield: **33-98%**



Suppliers (109) Supplier (1)

31-116-CAS-11024240 Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

Experimental Protocols

31-116-CAS-8894818 Steps: **1** Yield: **98%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-16441556 Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

31-116-CAS-1491623 Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Diethyl ether; rt → - 78 °C; 1 h, 25 °C

Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-4599727 Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-614-CAS-35597982 Steps: **1** Yield: **43%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

31-116-CAS-22583916 Steps: **1** Yield: **33%**

1.1 **Reagents:** Deuterium
Catalysts: [μ-[1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-4-yl-2-ylidene-κC^2:κC^4]][(1,2,5,6-η)-1,5-cyclooctadiene][tris(2,3,4,5,6-pentafluorophenyl)boron]iridium
Solvents: Cyclohexane; 3 h, 1 atm, rt

Experimental Protocols

Iridium(I) Complexes with Anionic N-Heterocyclic Carbene Ligands as Catalysts for H/D Exchange in Nonpolar Media

By: Koneczny, Marvin; et al

Advanced Synthesis & Catalysis (2020), 362(18), 3857-3863.

31-614-CAS-23969785 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

31-116-CAS-3945956 Steps: **1**

1.1 **Catalysts:** Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C

1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

31-116-CAS-9758932 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Anion effects to deliver enhanced iridium catalysts for hydrogen isotope exchange processes

By: Kennedy, Alan R.; et al

Organic & Biomolecular Chemistry (2014), 12(40), 7927-7931.

31-116-CAS-14296314 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Anion effects to deliver enhanced iridium catalysts for hydrogen isotope exchange processes

By: Kennedy, Alan R.; et al

Organic & Biomolecular Chemistry (2014), 12(40), 7927-7931.

31-116-CAS-9664837 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

31-116-CAS-8434780 Steps: **1**

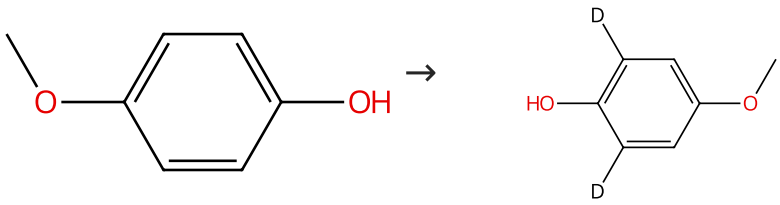
1.1 **Reagents:** Sodium carbonate, Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 30 (1 Reaction) Steps: **1** Yield: **97%**



Suppliers (127)

31-614-CAS-24835946 Steps: **1** Yield: **97%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

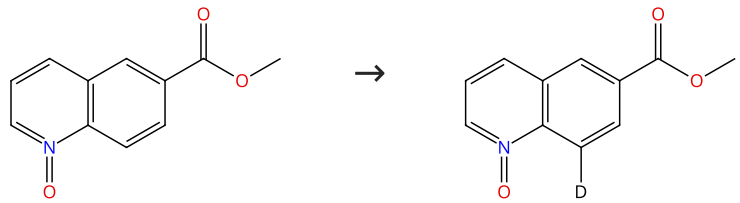
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 31 (1 Reaction)

Steps: **1** Yield: **97%**



Suppliers (6)

31-614-CAS-36762228

Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

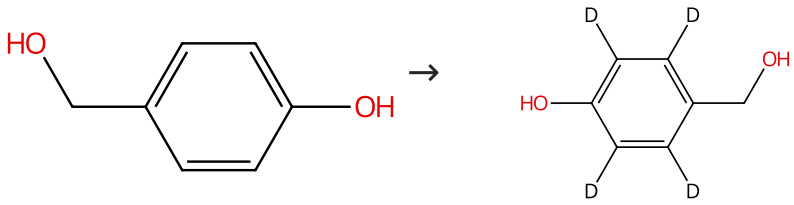
Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 32 (1 Reaction)

Steps: **1** Yield: **97%**



Suppliers (122)

31-614-CAS-24835983

Steps: **1** Yield: **97%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

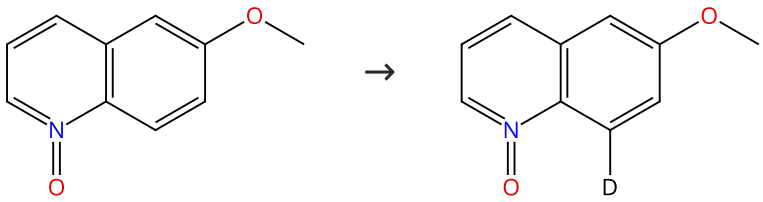
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 33 (1 Reaction)

Steps: **1** Yield: **97%**



Suppliers (59)

31-614-CAS-36762222

Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

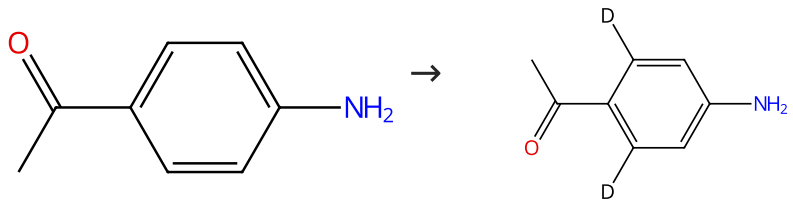
Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 34 (2 Reactions)

Steps: **1** Yield: **96-97%**



Suppliers (114)

31-116-CAS-21775900

Steps: **1** Yield: **97%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; 12 h, 50 °C

Experimental Protocols

Mesoionic Carbene-Iridium Complex Catalyzed Ortho-Selective Hydrogen Isotope Exchange of Anilines with High Functional Group Tolerance

By: Liu, Wei; et al

Organic Letters (2020), 22(6), 2210-2214.

31-116-CAS-21775901

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](triphenyl phosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 12 h, 50 °C

Experimental Protocols

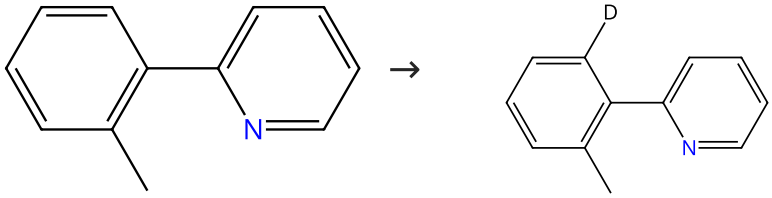
Mesoionic Carbene-Iridium Complex Catalyzed Ortho-Selective Hydrogen Isotope Exchange of Anilines with High Functional Group Tolerance

By: Liu, Wei; et al

Organic Letters (2020), 22(6), 2210-2214.

Scheme 35 (1 Reaction)

Steps: **1** Yield: **96%**



Suppliers (67)

31-614-CAS-35597975

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 300 mbar, rt

Experimental Protocols

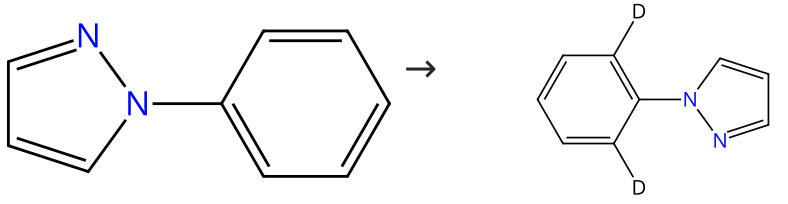
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 36 (7 Reactions)

Steps: **1** Yield: **93-96%**



Suppliers (90)

31-116-CAS-6712149 Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-8849072 Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-10981012 Steps: **1** Yield: **93%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-614-CAS-23969803 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

31-116-CAS-17237225 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

31-116-CAS-7537426 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Diethyl ether; rt → - 78 °C; 1 h, 25 °C

Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-2973744 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; 1 atm, -78 °C → 25 °C; 16 h, 25 °C

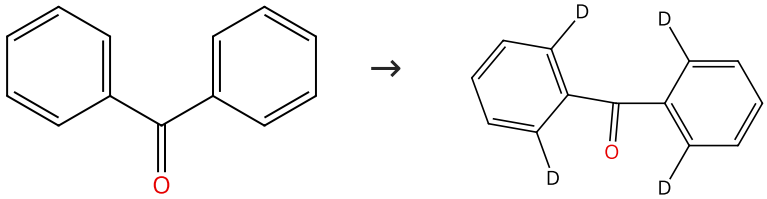
Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 37 (8 Reactions) Steps: **1** Yield: **95-96%**



Suppliers (142) Supplier (1)

31-116-CAS-7041357 Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-4907624 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-9172820 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-14868724 Steps: **1**

1.1 **Catalysts:** Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C

1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

31-116-CAS-5355335 Steps: **1**

1.1 **Catalysts:** Triphenylphosphine (polystyrene-bound), Iridium (1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 2 h, rt

1.2 **Reagents:** Deuterium
Solvents: Dichloromethane; 4 h, rt; 18 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-14169477 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-12034294 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-9899249 Steps: **1**

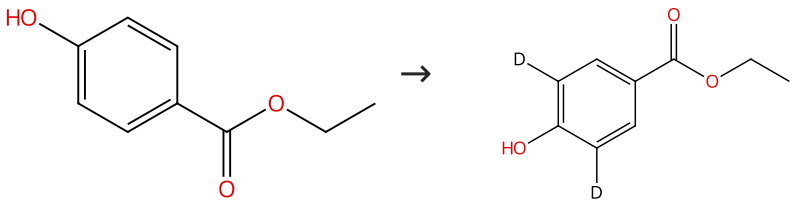
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

Scheme 38 (1 Reaction) Steps: **1** Yield: **96%**



Suppliers (141)

31-614-CAS-24835957 Steps: **1** Yield: **96%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

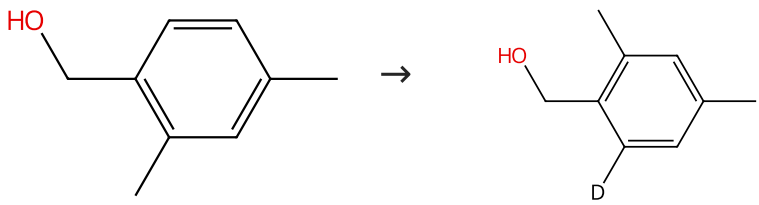
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 39 (1 Reaction) Steps: **1** Yield: **96%**



Suppliers (79)

31-614-CAS-24836015 Steps: **1** Yield: **96%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

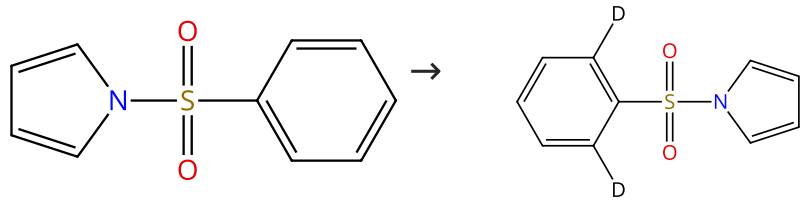
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 40 (1 Reaction) Steps: **1** Yield: **96%**



Suppliers (84)

31-116-CAS-17006208 Steps: **1** Yield: **96%**

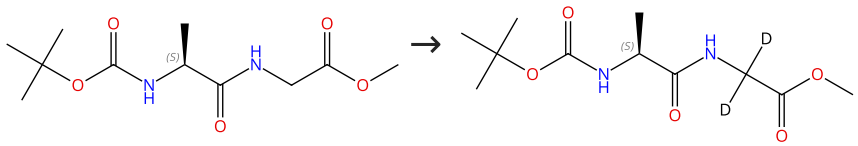
1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 41 (1 Reaction) Steps: **1** Yield: **96%**



Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (14)

31-116-CAS-18953301 Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenyl phosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

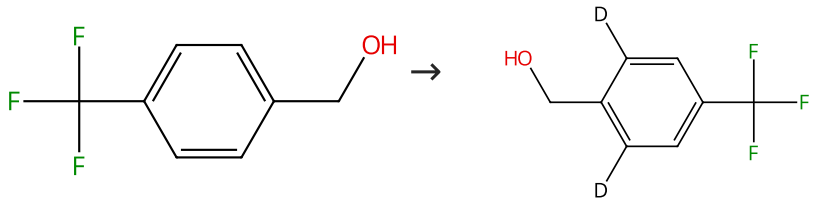
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 42 (1 Reaction) Steps: **1** Yield: **96%**



Suppliers (85)

31-614-CAS-24836022 Steps: **1** Yield: **96%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

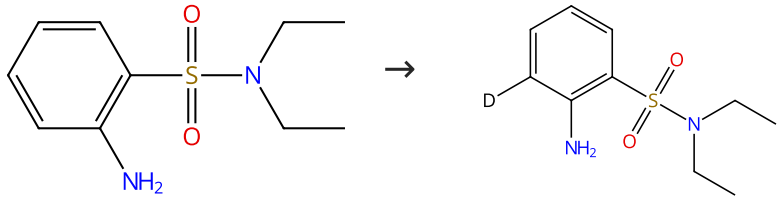
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 43 (1 Reaction) Steps: **1** Yield: **96%**



Suppliers (54)

31-116-CAS-17006202 Steps: **1** Yield: **96%**

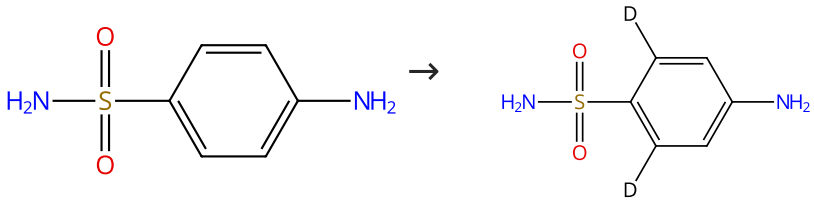
1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 44 (2 Reactions) Steps: **1** Yield: **96%**



Suppliers (159)

31-116-CAS-21775903 Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 12 h, 50 °C

Experimental Protocols

Mesoionic Carbene-Iridium Complex Catalyzed Ortho-Selective Hydrogen Isotope Exchange of Anilines with High Functional Group Tolerance

By: Liu, Wei; et al

Organic Letters (2020), 22(6), 2210-2214.

31-116-CAS-740933 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

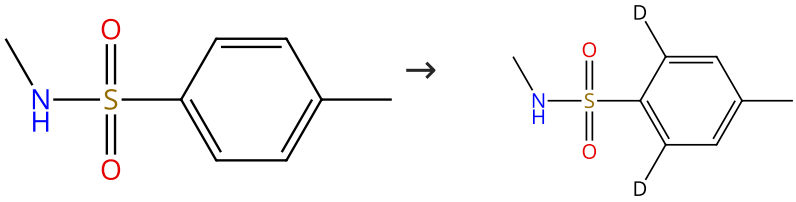
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 45 (1 Reaction)

Steps: **1** Yield: **96%**



Suppliers (81)

31-116-CAS-17006183

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

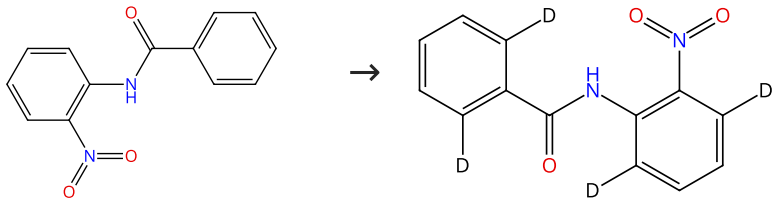
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 46 (3 Reactions)

Steps: **1** Yield: **92-96%**



Suppliers (43)

31-116-CAS-2194871

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-4215246

Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-6381842

Steps: **1** Yield: **92%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

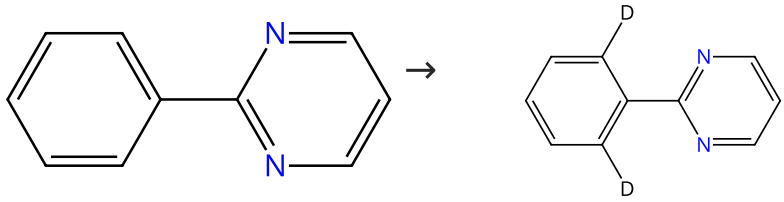
Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

Scheme 47 (1 Reaction)

Steps: **1** Yield: **96%**



Suppliers (64)

31-116-CAS-10170512

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

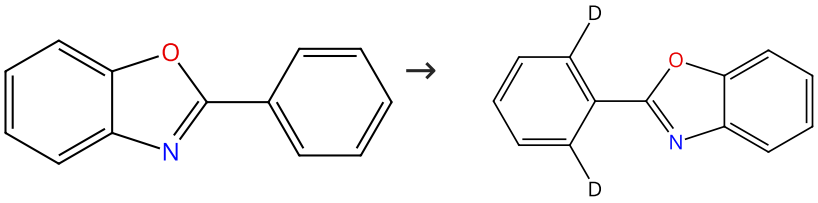
Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 48 (1 Reaction)

Steps: **1** Yield: **96%**



Suppliers (75)

31-116-CAS-557991

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

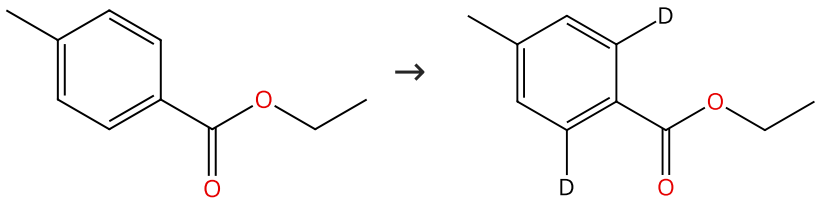
Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 49 (1 Reaction)

Steps: **1** Yield: **96%**



Suppliers (69)

Suppliers (2)

31-116-CAS-16442673

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

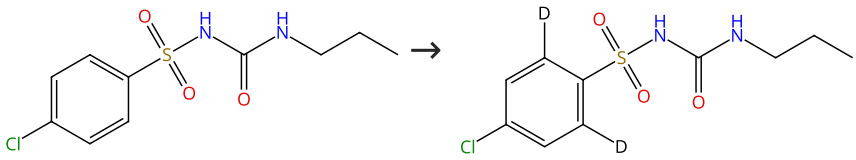
Hydrogen isotope exchange with highly active iridium(I) NH C/phosphine complexes: a compar ative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

Scheme 50 (1 Reaction)

Steps: **1** Yield: **96%**



Suppliers (85)

31-116-CAS-17006214

Steps: **1** Yield: **96%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

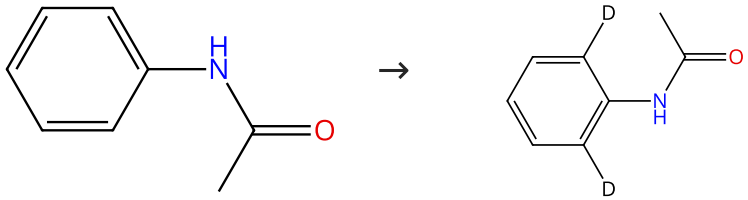
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 51 (9 Reactions)

Steps: **1** Yield: **70-95%**



Suppliers (108)

31-116-CAS-6111797

Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-3979468

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-15519155

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-11462526 Steps: **1** Yield: **70%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: 2-Methyltetrahydrofuran; rt → -78 °C; 16 h, 25 °C

Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-17237218 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

31-116-CAS-5692037 Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](pyridine)-, hexafluorophosphate(1-)
Solvents: Dichloromethane; rt → -78 °C

1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

31-116-CAS-3258509 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; 1 atm, -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

31-116-CAS-430228 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 4 h, rt

Application of iridium pincer complexes in hydrogen isotope exchange reactions

By: Traeff, Annika; et al

Journal of Organometallic Chemistry (2007), 692(25), 5529-5531.

31-116-CAS-1712423 Steps: **1**

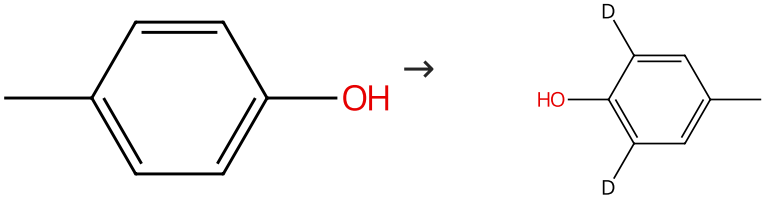
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 52 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (100) Suppliers (4)

31-614-CAS-24835950 Steps: **1** Yield: **95%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

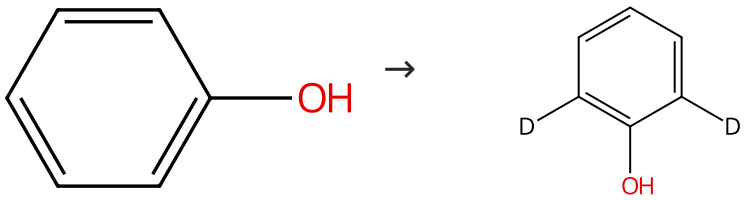
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 53 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (220)

31-614-CAS-24835956 Steps: **1** Yield: **95%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 54 (1 Reaction) Steps: **1** Yield: **95%**

Suppliers (7)

31-614-CAS-36762223 Steps: **1** Yield: **95%**

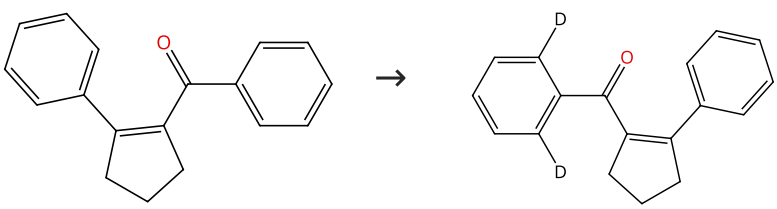
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 55 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (3)

31-614-CAS-36064974 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*R*)-2-[2-(diphenylphosphino-κ*P*)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN^3]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 3 h, 1 bar, 30 °C

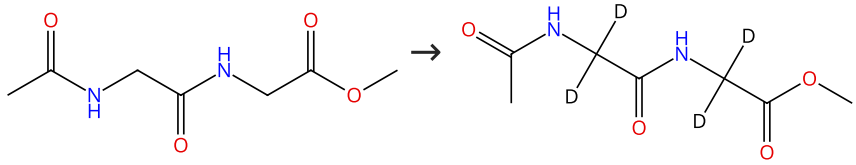
Experimental Protocols

Asymmetric Hydrogenation of Tetrasubstituted α,β-Unsaturated Ketones: Access to Chiral 2-Substituted Cyclopentyl Aryl Ketones

By: Ding, Zhengdong; et al

Precision Chemistry (2023), 1(3), 146-152.

Scheme 56 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (10)

31-116-CAS-18953299 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

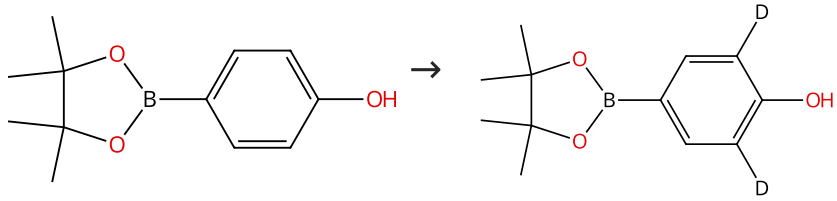
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 57 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (98)

31-614-CAS-24835965 Steps: **1** Yield: **95%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

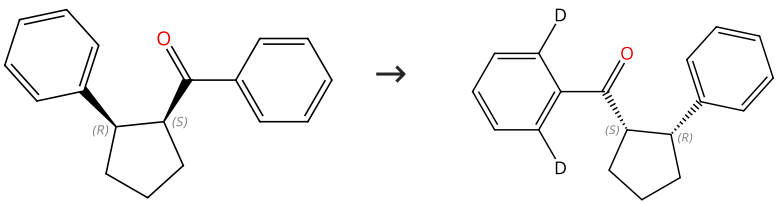
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 58 (1 Reaction) Steps: **1** Yield: **95%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-614-CAS-36064968 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*R*)-2-[2-(diphenylphosphino-κ*P*)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN^3]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 3 h, 1 bar, 30 °C

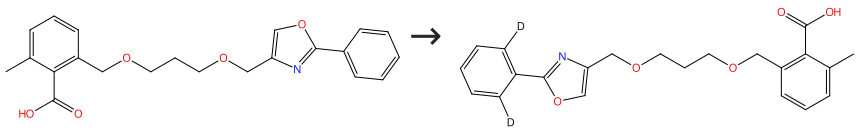
Experimental Protocols

Asymmetric Hydrogenation of Tetrasubstituted α,β-Unsaturated Ketones: Access to Chiral 2-Substituted Cyclopentyl Aryl Ketones

By: Ding, Zhengdong; et al

Precision Chemistry (2023), 1(3), 146-152.

Scheme 59 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (16)

31-116-CAS-5224125 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

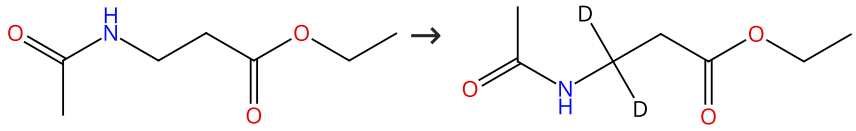
Experimental Protocols

Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceutically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 60 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (8)

31-116-CAS-18953296 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

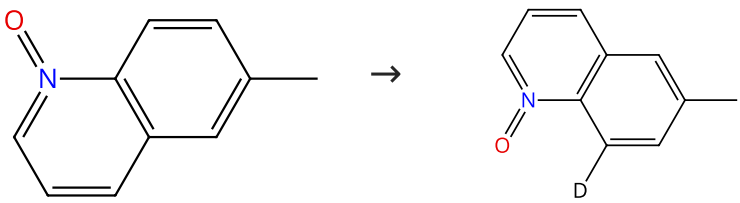
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 61 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (12)

31-614-CAS-36762209 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 62 (1 Reaction) Steps: **1** Yield: **95%**

Suppliers (67)

31-614-CAS-24836036 Steps: **1** Yield: **95%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

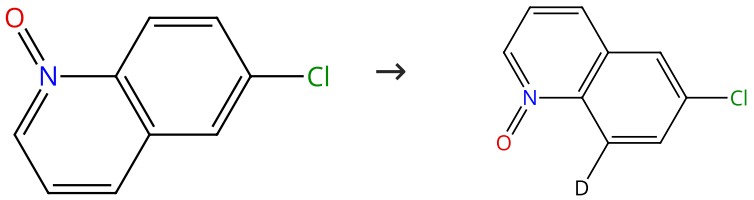
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 63 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (8)

31-614-CAS-36762207 Steps: **1** Yield: **95%**

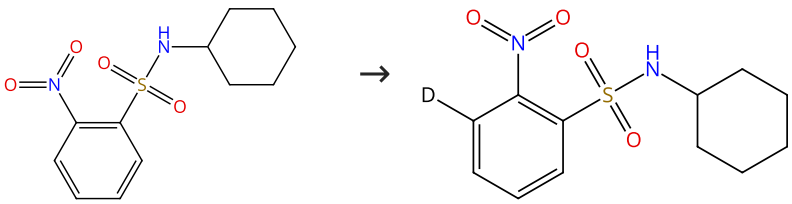
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 64 (1 Reaction) Steps: **1** Yield: **95%**



Suppliers (37)

31-116-CAS-17006189 Steps: **1** Yield: **95%**

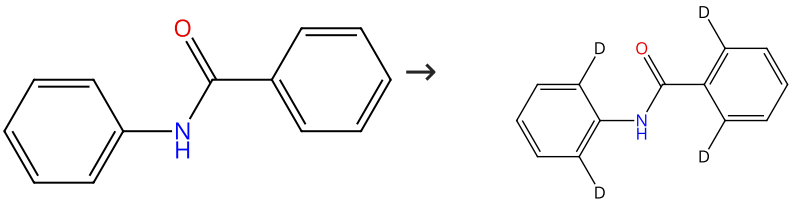
1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 65 (6 Reactions) Steps: **1** Yield: **91-95%**



Suppliers (89)

31-116-CAS-8514557 Steps: **1** Yield: **95%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-13875018 Steps: **1** Yield: **93%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: 2-Methyltetrahydrofuran; rt → -78 °C; 1 h, 25 °C

Experimental Protocols

Practically convenient and industr ially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-14495287 Steps: **1** Yield: **91%**

1.1 **Catalysts:** Triphenylphosphine (polystyrene-bound), Iridium (1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 2 h, rt

1.2 **Reagents:** Deuterium
Solvents: Dichloromethane; 4 h, rt; 18 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-13828080 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-409693 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-11698681 Steps: **1**

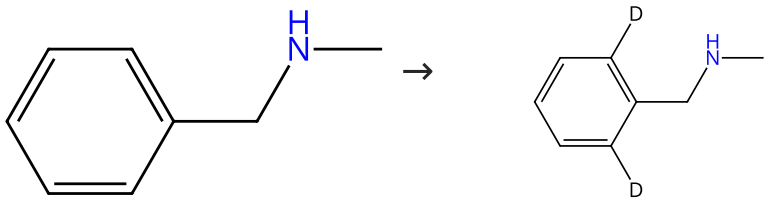
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis (triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

Scheme 66 (2 Reactions) Steps: **1** Yield: **94%**



Suppliers (92)

31-116-CAS-135911 Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-1664527 Steps: **1**

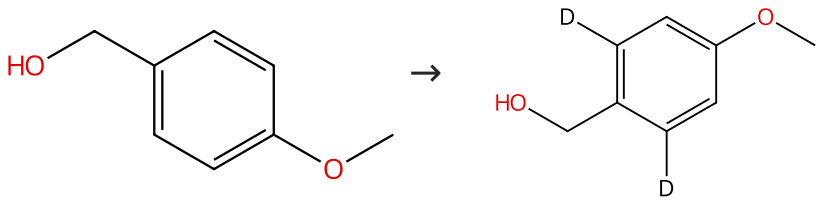
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 67 (1 Reaction) Steps: **1** Yield: **94%**



Suppliers (108)

31-614-CAS-24836026 Steps: **1** Yield: **94%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

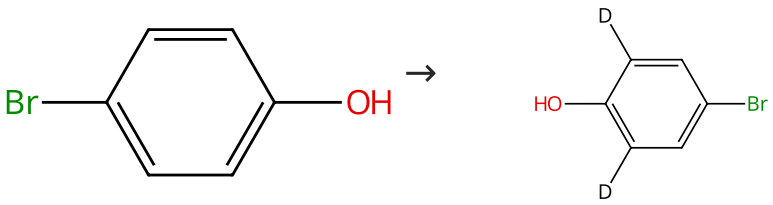
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 68 (1 Reaction)

Steps: **1** Yield: **94%**



Suppliers (88)

Suppliers (6)

31-614-CAS-24835951

Steps: **1** Yield: **94%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

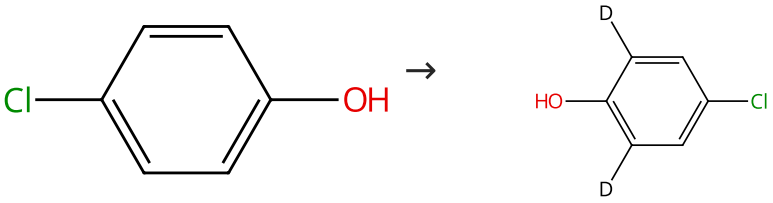
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 69 (1 Reaction)

Steps: **1** Yield: **94%**



Suppliers (98)

31-614-CAS-24835955

Steps: **1** Yield: **94%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

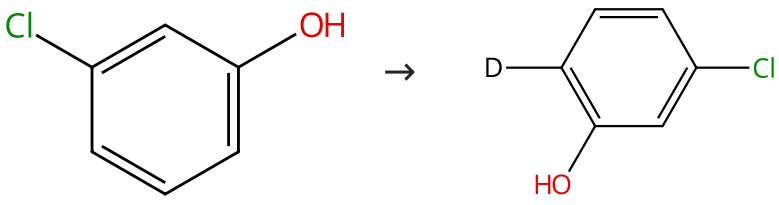
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 70 (1 Reaction)

Steps: **1** Yield: **94%**



Suppliers (89)

31-614-CAS-24835991

Steps: **1** Yield: **94%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Dichloromethane; 10 h, 1 atm, 35 °C

Experimental Protocols

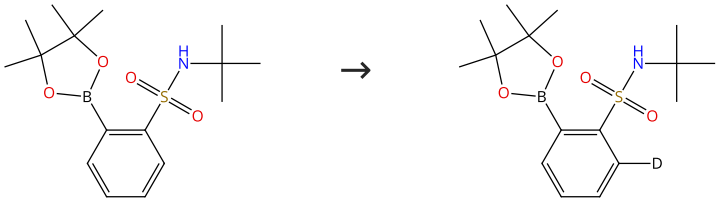
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 71 (1 Reaction)

Steps: **1** Yield: **94%**



Suppliers (21)

31-116-CAS-17006200

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

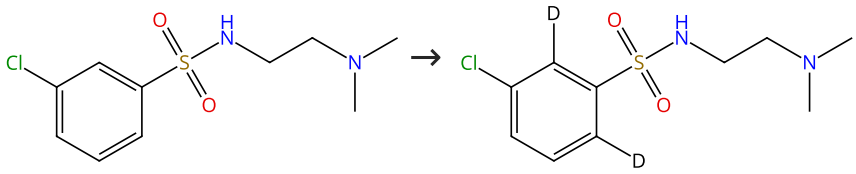
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 72 (1 Reaction)

Steps: **1** Yield: **94%**



Supplier (1)

31-116-CAS-17006197

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

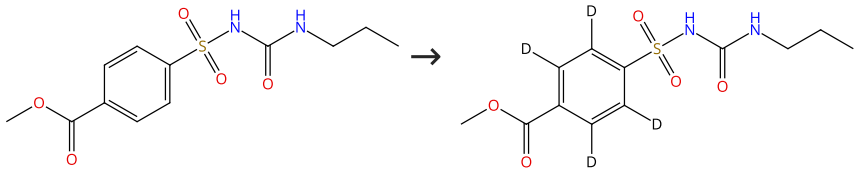
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 73 (1 Reaction)

Steps: **1** Yield: **94%**



31-116-CAS-17006216

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

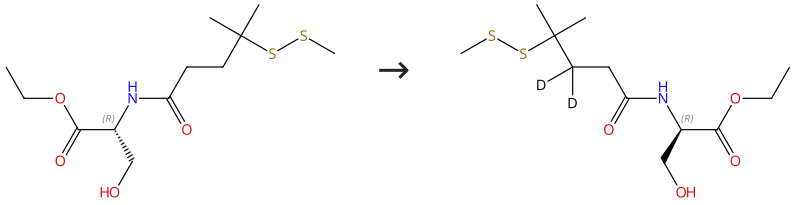
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 74 (1 Reaction)

Steps: **1** Yield: **94%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-18953284

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 80 °C

Experimental Protocols

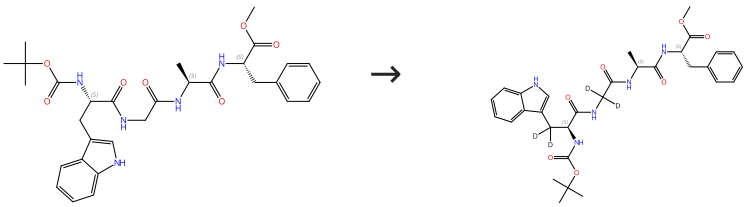
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 75 (1 Reaction)

Steps: **1** Yield: **94%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-18953307

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

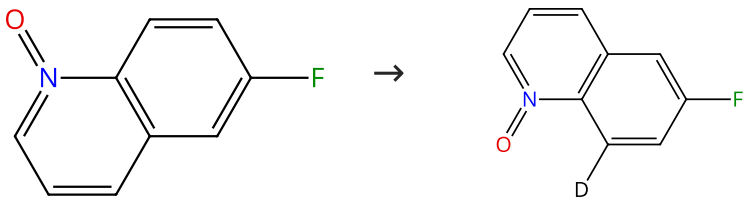
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 76 (1 Reaction)

Steps: **1** Yield: **94%**



Suppliers (9)

31-614-CAS-36762206

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

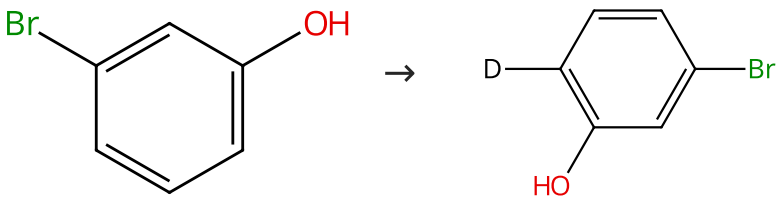
Selective Deuteration of Heterocycle N-Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 77 (1 Reaction)

Steps: **1** Yield: **94%**



Suppliers (82)

31-614-CAS-24835995

Steps: **1** Yield: **94%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Dichloromethane; 10 h, 1 atm, 35 °C

Experimental Protocols

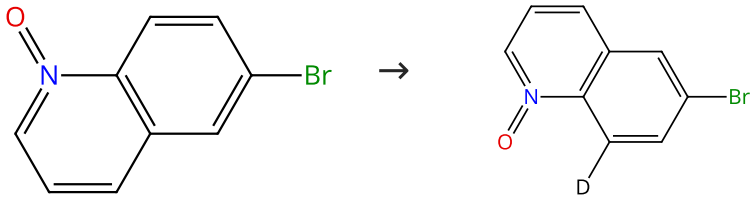
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 78 (1 Reaction)

Steps: **1** Yield: **94%**



Suppliers (35)

31-614-CAS-36762224

Steps: **1** Yield: **94%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

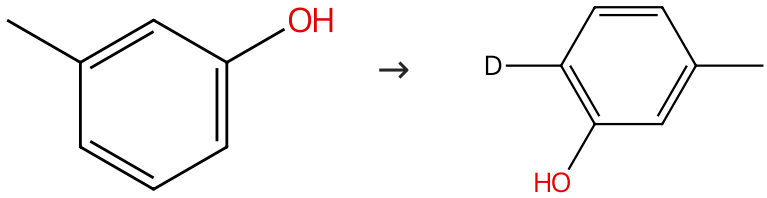
Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 79 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (94)

31-614-CAS-24835964

Steps: **1** Yield: **93%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Ethyl acetate; 10 h, 1 atm, 35 °C

Experimental Protocols

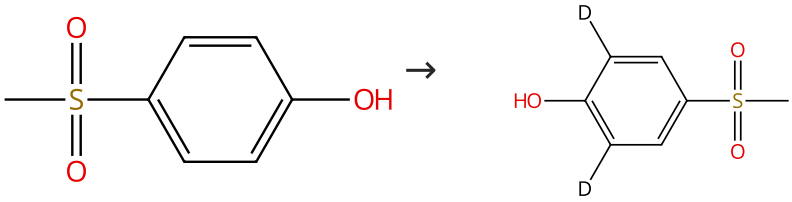
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 80 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (82)

31-614-CAS-24835970

Steps: **1** Yield: **93%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

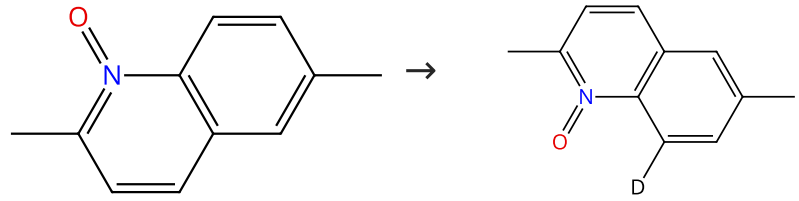
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 81 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (3)

31-614-CAS-36762204

Steps: **1** Yield: **93%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

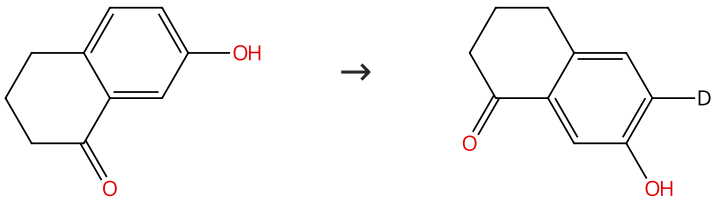
Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 82 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (80)

31-614-CAS-24835996

Steps: **1** Yield: **93%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

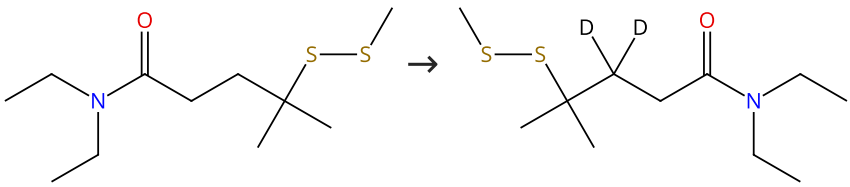
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 83 (1 Reaction)

Steps: **1** Yield: **93%**



31-116-CAS-18953281

Steps: **1** Yield: **93%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 80 °C

Experimental Protocols

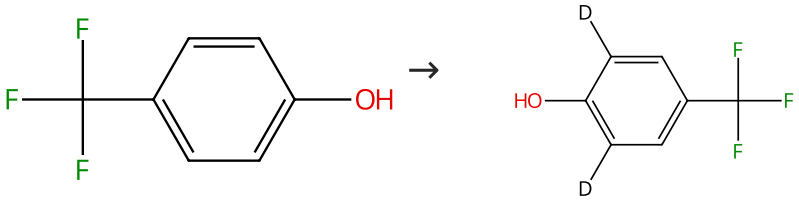
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 84 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (105)

31-614-CAS-24835952

Steps: **1** Yield: **93%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 85 (1 Reaction)

Steps: **1** Yield: **93%**

Suppliers (2)

31-614-CAS-36762202

Steps: **1** Yield: **93%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

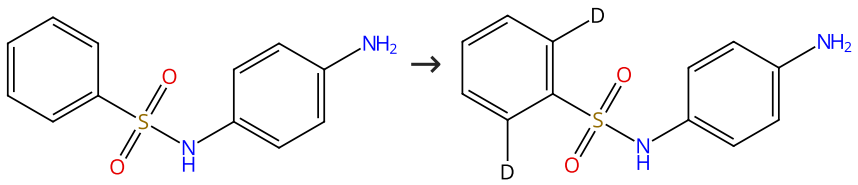
Selective Deuteration of Heterocycle N-Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 86 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (20)

31-116-CAS-17006187

Steps: **1** Yield: **93%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

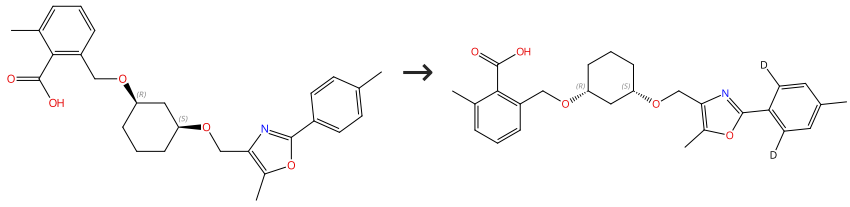
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 87 (1 Reaction)

Steps: **1** Yield: **93%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-15414068

Steps: **1** Yield: **93%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Tetrahydrofuran; 1 h, 50 °C

Experimental Protocols

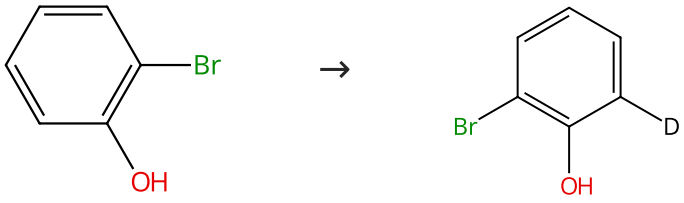
Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 88 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (86)

31-614-CAS-24835974

Steps: **1** Yield: **93%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Dichloromethane; 10 h, 1 atm, 35 °C

Experimental Protocols

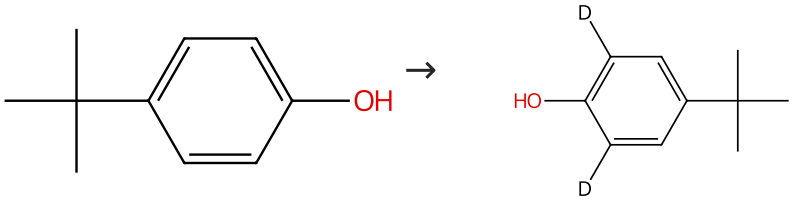
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 89 (1 Reaction)

Steps: **1** Yield: **93%**



Suppliers (90)

31-614-CAS-24835968

Steps: **1** Yield: **93%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

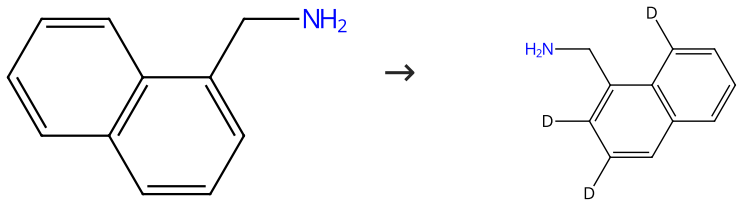
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 90 (1 Reaction)

Steps: **1** Yield: **92%**



Suppliers (96)

31-116-CAS-22583929

Steps: **1** Yield: **92%**

1.1 **Reagents:** Deuterium, Tritium
Catalysts: [μ-[1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-4-yl-2-ylidene-κC^2:κC^4]][(1,2,5,6-η)-1,5-cyclooctadiene][tris(2,3,4,5,6-pentafluorophenyl)boron]iridium
Solvents: Cyclohexane; 3 h, 1 atm, rt

Experimental Protocols

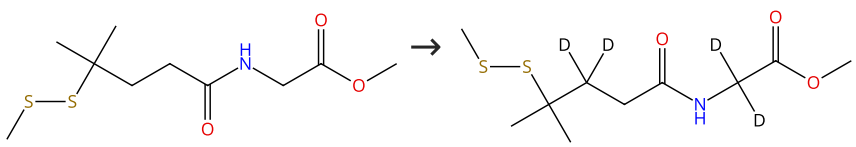
Iridium(I) Complexes with Anionic N-Heterocyclic Carbene Ligands as Catalysts for H/D Exchange in Nonpolar Media

By: Koneczny, Marvin; et al

Advanced Synthesis & Catalysis (2020), 362(18), 3857-3863.

Scheme 91 (1 Reaction)

Steps: **1** Yield: **92%**



31-116-CAS-18953285

Steps: **1** Yield: **92%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 80 °C

Experimental Protocols

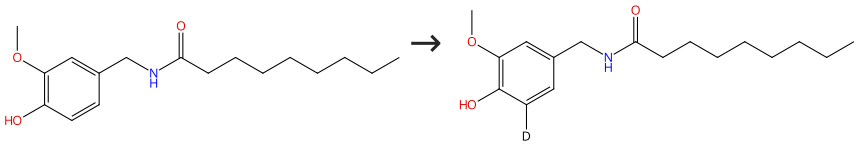
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 92 (1 Reaction)

Steps: **1** Yield: **92%**



Suppliers (116)

31-614-CAS-24835992

Steps: **1** Yield: **92%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 24 h, 1 atm, 70 °C

Experimental Protocols

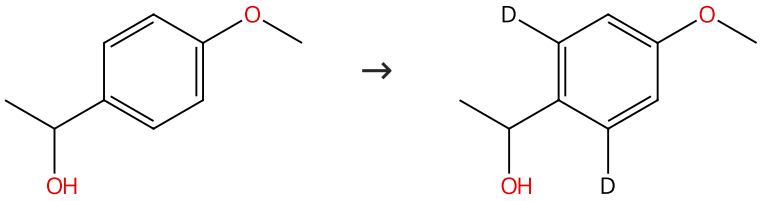
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 93 (1 Reaction)

Steps: **1** Yield: **92%**



Suppliers (75)

31-614-CAS-24836020

Steps: **1** Yield: **92%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

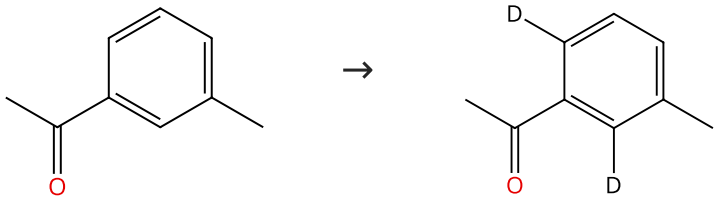
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 94 (6 Reactions)

Steps: **1** Yield: **92%**



Suppliers (86)

31-116-CAS-12744537

Steps: **1** Yield: **92%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 66 - 68 h, rt

The mediation of aryl ketone deuteration by $[Ir(PPh_3)_3(cod)]^+.BF^-_4$

By: Herbert, John M.

Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(5), 317-322.

31-116-CAS-1371104 Steps: **1**

1.1 **Catalysts:** Triphenylphosphine (polystyrene-bound), Iridium (1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 2 h, rt

1.2 **Reagents:** Deuterium
Solvents: Dichloromethane; 4 h, rt; 18 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-3181938 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-1049959 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-14437543 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-777206 Steps: **1**

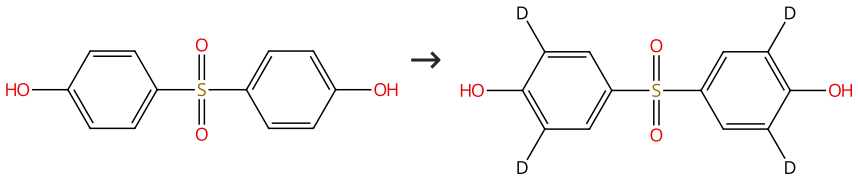
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 95 (1 Reaction) Steps: **1** Yield: **92%**



Suppliers (104) Supplier (1)

31-614-CAS-24835989 Steps: **1** Yield: **92%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 24 h, 1 atm, 70 °C

Experimental Protocols

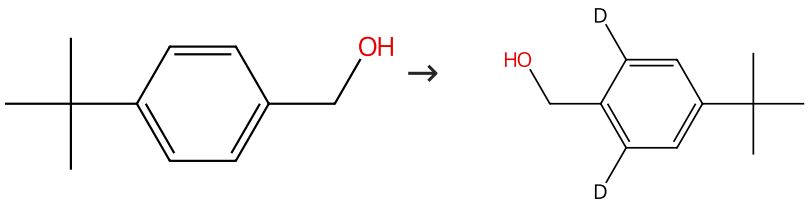
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 96 (1 Reaction)

Steps: **1** Yield: **92%**



Suppliers (78)

31-614-CAS-24836012

Steps: **1** Yield: **92%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

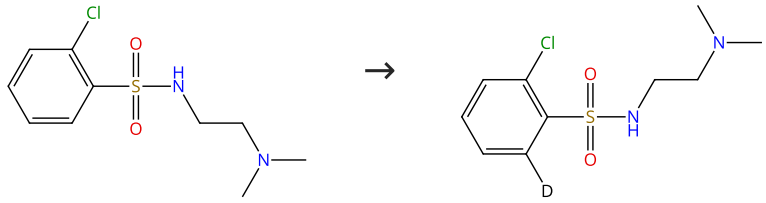
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 97 (1 Reaction)

Steps: **1** Yield: **91%**



Suppliers (5)

31-116-CAS-17006196

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 98 (1 Reaction)

Steps: **1** Yield: **91%**

Suppliers (17)

31-614-CAS-36762221

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

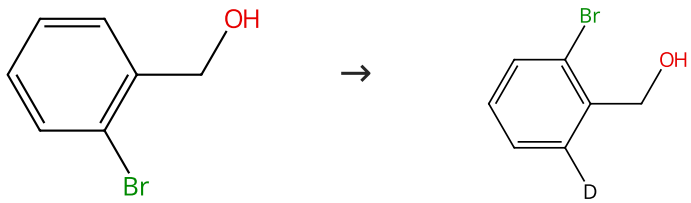
Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 99 (1 Reaction)

Steps: **1** Yield: **91%**



Suppliers (96)

31-614-CAS-24836019

Steps: **1** Yield: **91%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Dichloromethane; 10 h, 1 atm, 35 °C

Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 100 (1 Reaction)

Steps: **1** Yield: **91%**

Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (80)

31-116-CAS-17006220

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

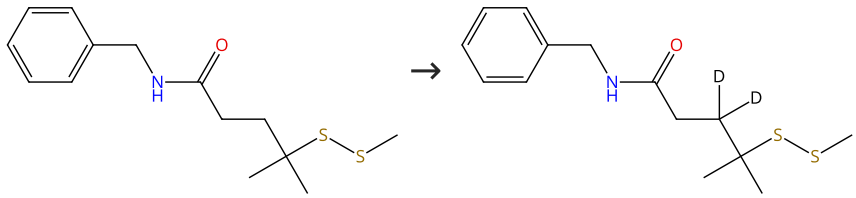
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 101 (1 Reaction)

Steps: **1** Yield: **91%**



31-116-CAS-18953282

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 80 °C

Experimental Protocols

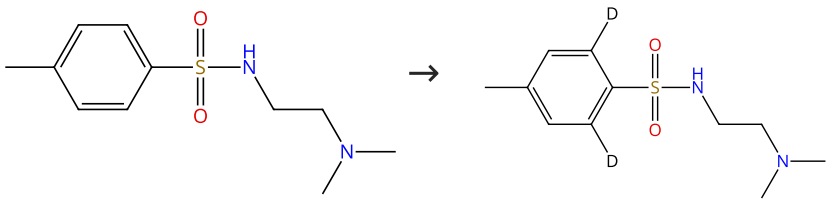
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 102 (1 Reaction)

Steps: **1** Yield: **91%**



Suppliers (11)

31-116-CAS-17006195

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

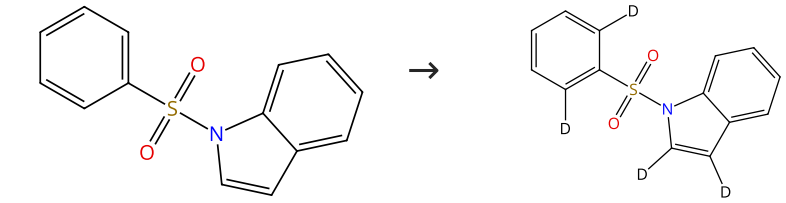
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 103 (1 Reaction)

Steps: **1** Yield: **91%**



Suppliers (79)

31-116-CAS-17006211

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

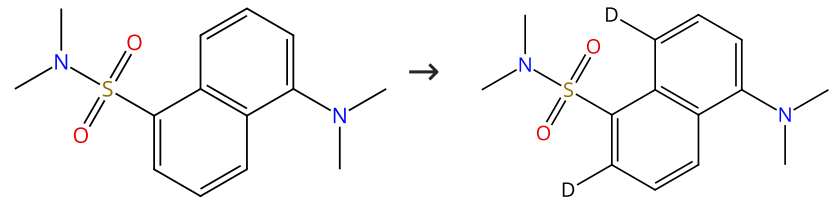
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 104 (1 Reaction)

Steps: **1** Yield: **91%**



Suppliers (15)

31-116-CAS-17006203

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

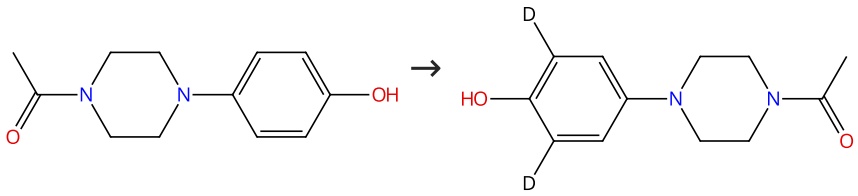
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 105 (1 Reaction)

Steps: **1** Yield: **91%**



Suppliers (92)

31-614-CAS-24835958

Steps: **1** Yield: **91%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

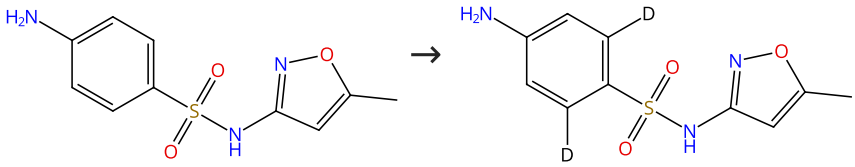
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 106 (1 Reaction)

Steps: **1** Yield: **91%**



Suppliers (129)

31-116-CAS-17006219

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

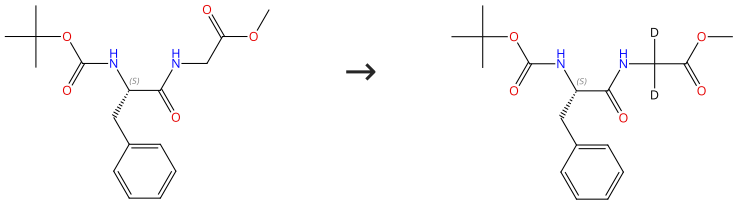
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 107 (1 Reaction)

Steps: **1** Yield: **91%**



Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (53)

31-116-CAS-18953303

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

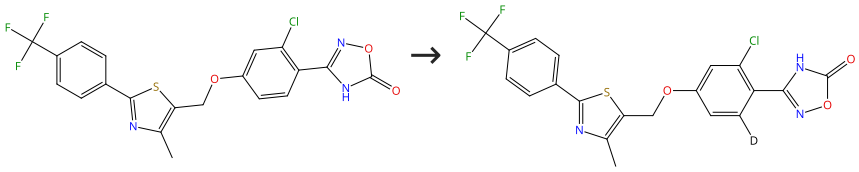
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 108 (1 Reaction)

Steps: **1** Yield: **91%**



Supplier (1)

31-116-CAS-6559694

Steps: **1** Yield: **91%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Tetrahydrofuran; 1 h, 50 °C

Experimental Protocols

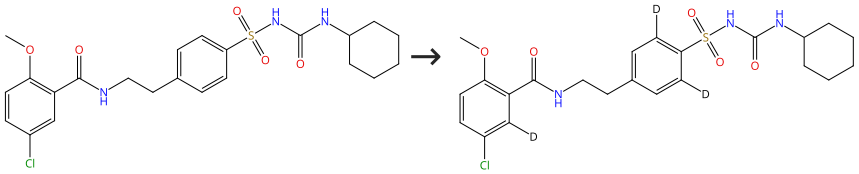
Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 109 (1 Reaction)

Steps: **1** Yield: **90%**



Suppliers (122)

31-116-CAS-17006223

Steps: **1** Yield: **90%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

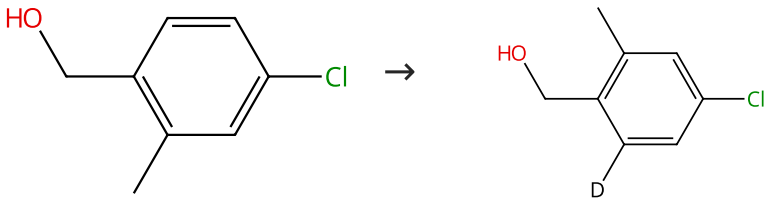
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 110 (1 Reaction)

Steps: **1** Yield: **90%**



Suppliers (73)

31-614-CAS-24836016

Steps: **1** Yield: **90%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

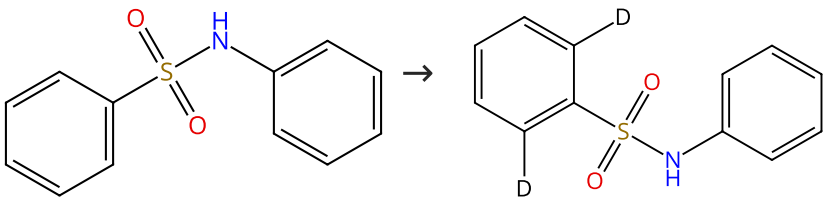
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 111 (1 Reaction)

Steps: **1** Yield: **90%**



Suppliers (72)

31-116-CAS-17006184

Steps: **1** Yield: **90%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

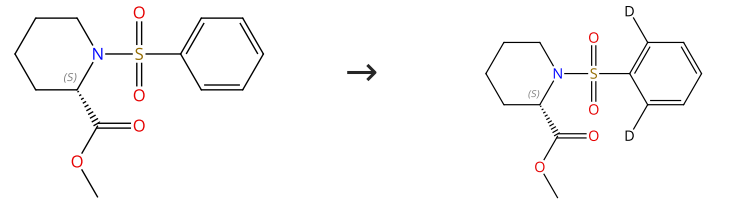
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 112 (1 Reaction)

Steps: **1** Yield: **90%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-17006205

Steps: **1** Yield: **90%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

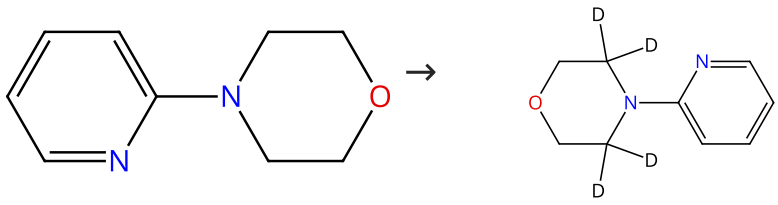
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 113 (1 Reaction)

Steps: **1** Yield: **90%**



Suppliers (57)

31-116-CAS-19412266

Steps: **1** Yield: **90%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

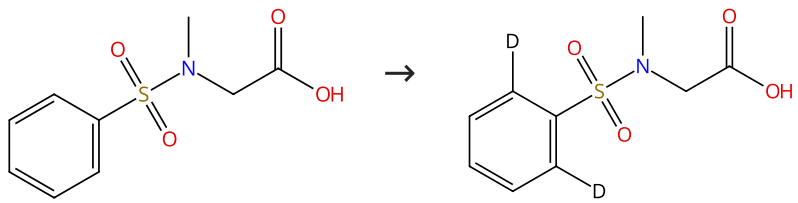
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 114 (1 Reaction)

Steps: **1** Yield: **90%**



Suppliers (58)

31-116-CAS-17006204

Steps: **1** Yield: **90%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

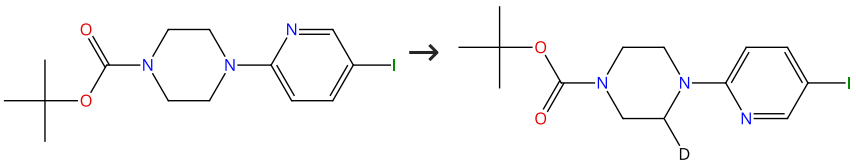
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 115 (1 Reaction)

Steps: **1** Yield: **90%**



Suppliers (49)

31-116-CAS-1056040

Steps: **1** Yield: **90%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 16 h, 0.46 - 1 atm, rt

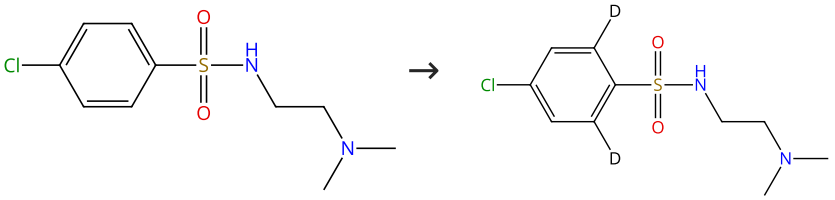
Hydrogen isotope exchange at alkyl positions using Crabtree's catalyst and its application to the tritiation of methapyrilene

By: Bushby, Nick; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 519-520.

Scheme 116 (1 Reaction)

Steps: **1** Yield: **90%**



Suppliers (7)

31-116-CAS-17006198

Steps: **1** Yield: **90%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

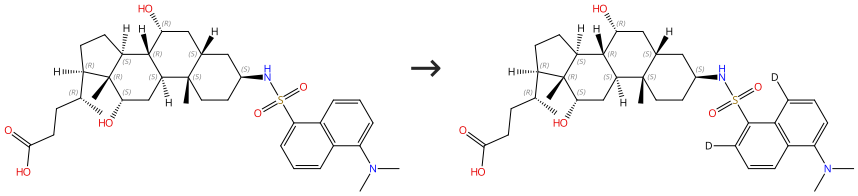
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 117 (1 Reaction)

Steps: **1** Yield: **89%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-17006225

Steps: **1** Yield: **89%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

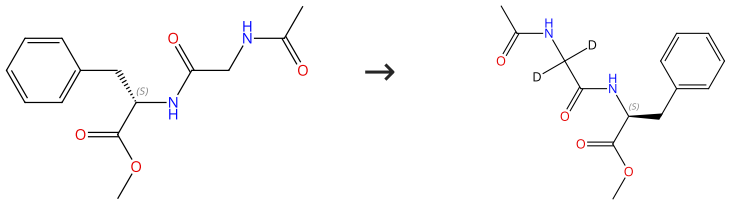
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 118 (1 Reaction)

Steps: **1** Yield: **89%**



Absolute stereochemistry shown

Absolute stereochemistry shown

Suppliers (3)

31-116-CAS-18953297

Steps: **1** Yield: **89%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

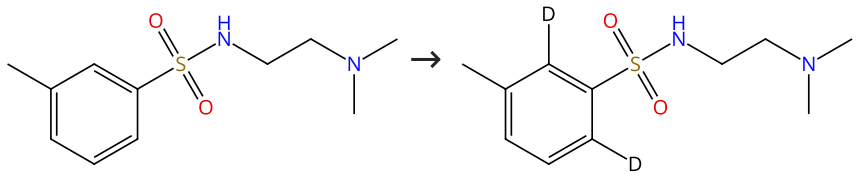
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 119 (1 Reaction)

Steps: **1** Yield: **89%**



Supplier (1)

31-116-CAS-17006194

Steps: **1** Yield: **89%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

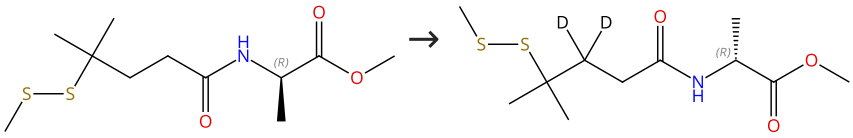
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 120 (1 Reaction)

Steps: **1** Yield: **89%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-18953283

Steps: **1** Yield: **89%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 80 °C

Experimental Protocols

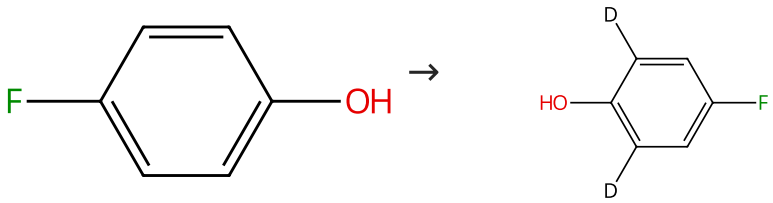
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 121 (1 Reaction)

Steps: **1** Yield: **89%**



Suppliers (97)

Supplier (1)

31-614-CAS-24835966

Steps: **1** Yield: **89%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

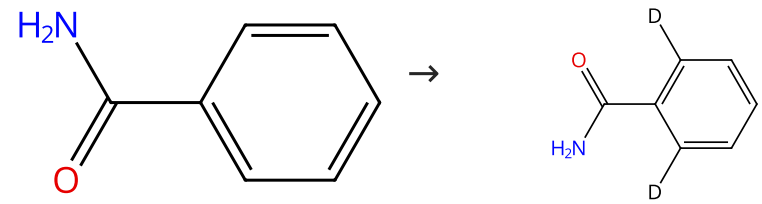
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 122 (5 Reactions)

Steps: **1** Yield: **32-89%**



Suppliers (115)

31-116-CAS-12086536

Steps: **1** Yield: **89%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: 2-Methyltetrahydrofuran; rt → -78 °C; 16 h, 25 °C

Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-13438671 Steps: **1** Yield: **79%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-15291 Steps: **1** Yield: **75%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-11294784 Steps: **1** Yield: **32%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 16 h, rt

Experimental Protocols

Highly active iridium(I) complexes for catalytic hydrogen isotope exchange

By: Brown, Jack A.; et al

Chemical Communications (Cambridge, United Kingdom) (2008), (9), 1115-1117.

31-116-CAS-10321712 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; 1 atm, -78 °C → 25 °C; 16 h, 25 °C

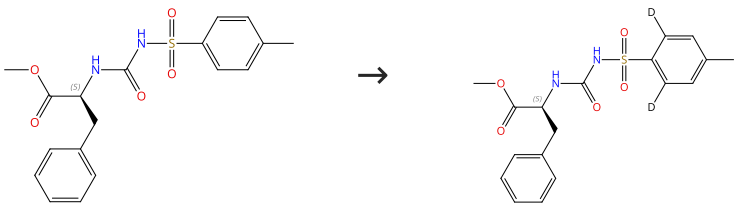
Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 123 (1 Reaction) Steps: **1** Yield: **89%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-17006217 Steps: **1** Yield: **89%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

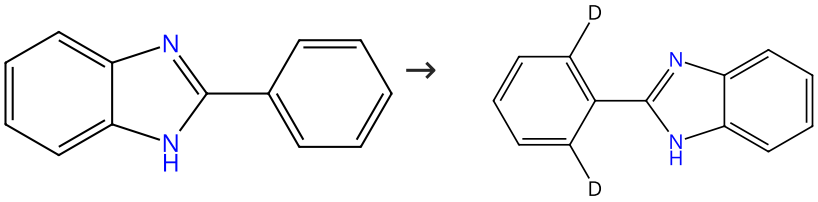
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 124 (1 Reaction)

Steps: **1** Yield: **89%**



Suppliers (78)

31-116-CAS-7552820

Steps: **1** Yield: **89%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

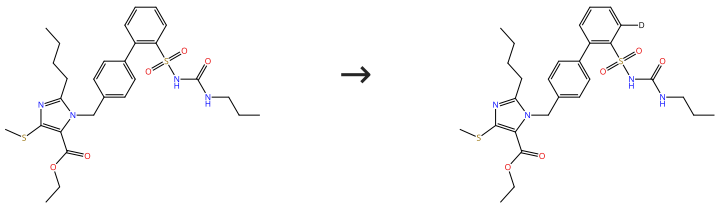
Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceu tically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Scheme 125 (1 Reaction)

Steps: **1** Yield: **88%**



Suppliers (3)

31-116-CAS-17006226

Steps: **1** Yield: **88%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

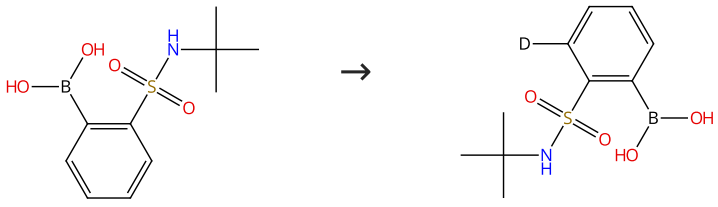
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 126 (1 Reaction)

Steps: **1** Yield: **88%**



Suppliers (66)

31-116-CAS-17006199

Steps: **1** Yield: **88%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

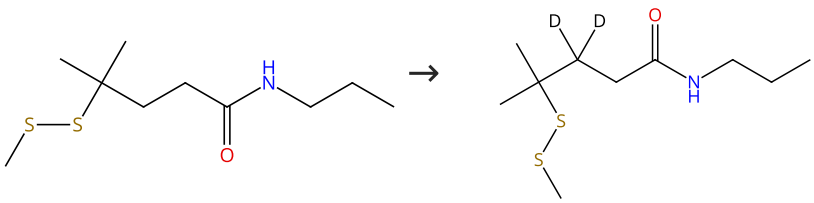
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 127 (1 Reaction)

Steps: **1** Yield: **88%**



31-116-CAS-18953280

Steps: **1** Yield: **88%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 80 °C

Experimental Protocols

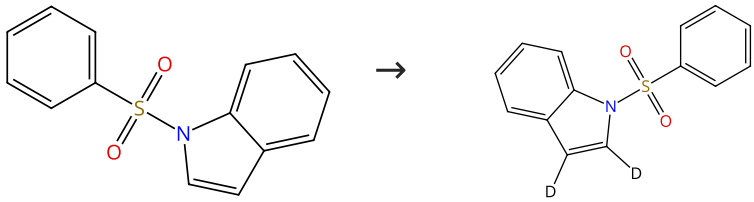
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 128 (1 Reaction)

Steps: **1** Yield: **88%**



Suppliers (79)

31-116-CAS-17006210

Steps: **1** Yield: **88%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

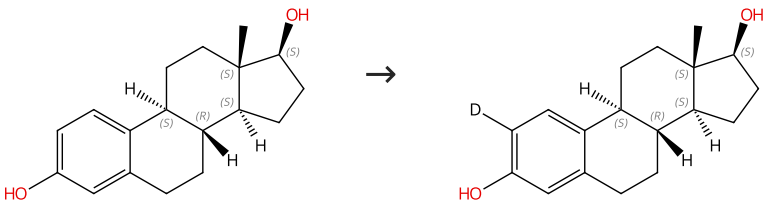
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 129 (1 Reaction)

Steps: **1** Yield: **88%**



Absolute stereochemistry shown

Suppliers (142)

Absolute stereochemistry shown

Supplier (1)

31-614-CAS-24836006

Steps: **1** Yield: **88%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 24 h, 1 atm, 70 °C

Experimental Protocols

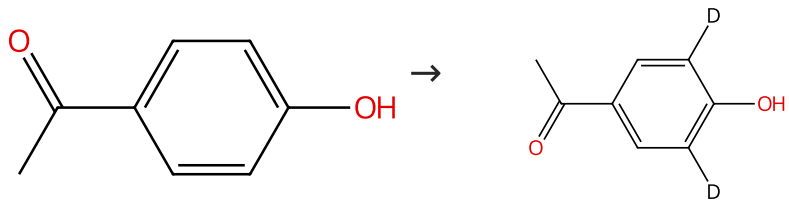
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 130 (1 Reaction)

Steps: **1** Yield: **88%**



Suppliers (135)

31-614-CAS-24835953

Steps: **1** Yield: **88%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

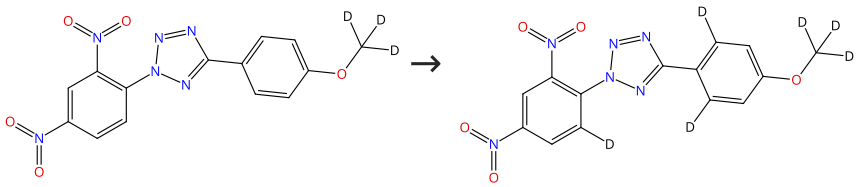
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 131 (1 Reaction)

Steps: **1** Yield: **87%**



31-614-CAS-35202557

Steps: **1** Yield: **87%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → rt; 24 h, rt

Experimental Protocols

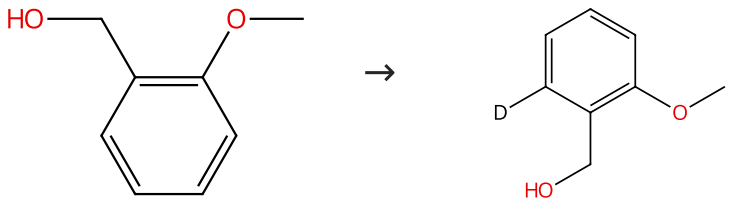
Functionalized Tetrazoles as Latent Active Esters in the Synthesis of Amide Bonds

By: Elwood, Jessica M. L.; et al

Organic Letters (2022), 24(51), 9491-9496.

Scheme 132 (1 Reaction)

Steps: **1** Yield: **87%**



Suppliers (95)

31-614-CAS-24836013

Steps: **1** Yield: **87%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Dichloromethane; 10 h, 1 atm, 35 °C

Experimental Protocols

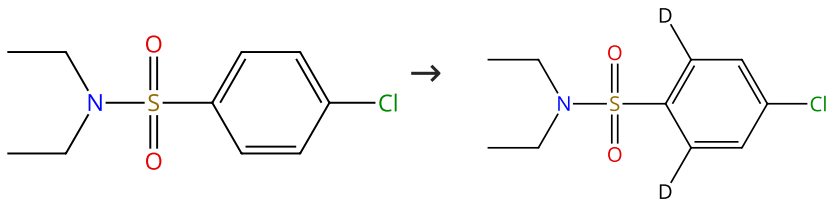
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 133 (1 Reaction)

Steps: **1** Yield: **87%**



Suppliers (24)

31-116-CAS-17006201

Steps: **1** Yield: **87%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

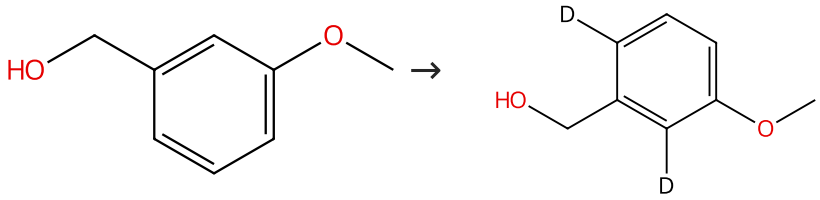
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 134 (1 Reaction)

Steps: **1** Yield: **87%**



Suppliers (85)

31-614-CAS-24836046

Steps: **1** Yield: **87%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Dichloromethane; 10 h, 1 atm, 35 °C

Experimental Protocols

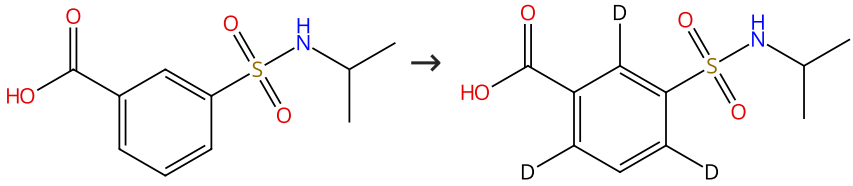
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 135 (1 Reaction)

Steps: **1** Yield: **87%**



Suppliers (42)

31-116-CAS-17006190

Steps: **1** Yield: **87%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

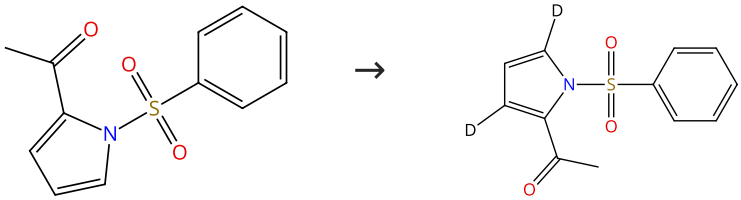
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 136 (1 Reaction)

Steps: **1** Yield: **87%**



Suppliers (18)

31-116-CAS-17006212

Steps: **1** Yield: **87%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

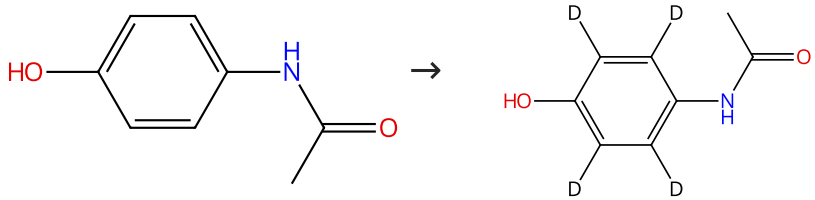
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 137 (1 Reaction)

Steps: **1** Yield: **86%**



Suppliers (147)

Suppliers (60)

31-614-CAS-24835982

Steps: **1** Yield: **86%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

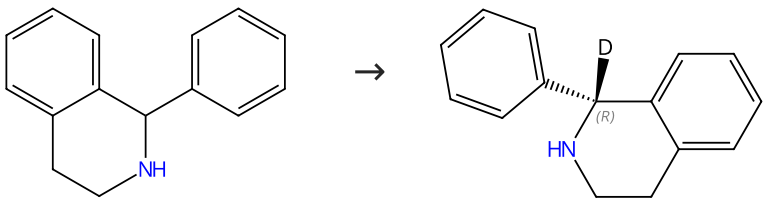
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 138 (1 Reaction)

Steps: **1** Yield: **86%**



Absolute stereochemistry shown, Rotation (-)

Suppliers (93)

31-116-CAS-14492719 Steps: **1** Yield: **86%**

1.1 **Catalysts:** Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene] diiridium, 1,1'-[(5*R*)-2,2',3,3'-Tetrahydro[5,5'-bi-1,4-benzodioxin]-6,6'-diyl]bis[1,1-diphenylphosphine]
Solvents: 1,2-Dichloroethane; 10 min, rt

1.2 **Reagents:** *N*-Bromosuccinimide, Sodium carbonate
Solvents: 1,2-Dichloroethane; 10 min, rt

1.3 **Reagents:** Deuterium; 36 h, 500 psi, 30 °C

1.4 **Reagents:** Sodium bicarbonate
Solvents: Water; 10 - 15 min

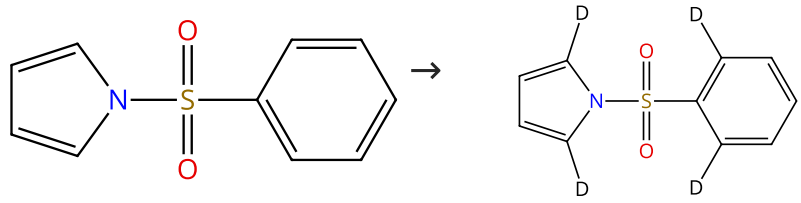
Experimental Protocols

Concise Redox Deracemization of Secondary and Tertiary Amines with a Tetrahydroisoquinoline Core via a Nonenzymatic Process

By: Ji, Yue; et al

Journal of the American Chemical Society (2015), 137(33), 10496-10499.

Scheme 139 (1 Reaction) Steps: **1** Yield: **85%**



Suppliers (84)

31-116-CAS-17006209 Steps: **1** Yield: **85%**

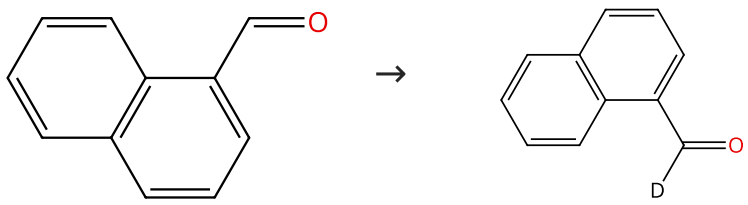
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 140 (1 Reaction) Steps: **1** Yield: **85%**



Suppliers (92) Supplier (1)

31-116-CAS-17347304 Steps: **1** Yield: **85%**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

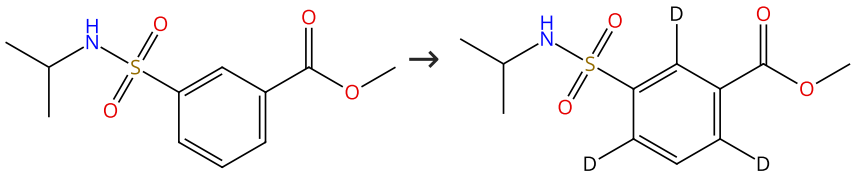
Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 141 (1 Reaction)

Steps: **1** Yield: **85%**



Suppliers (11)

31-116-CAS-17006192

Steps: **1** Yield: **85%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

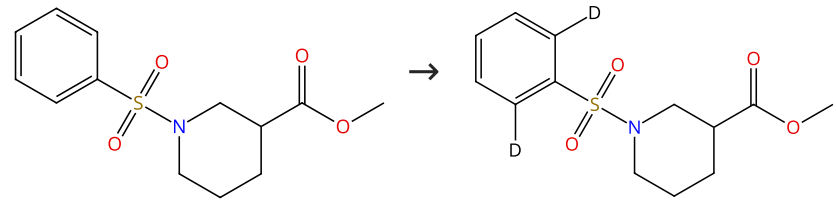
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 142 (1 Reaction)

Steps: **1** Yield: **84%**



Suppliers (22)

31-116-CAS-17006206

Steps: **1** Yield: **84%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

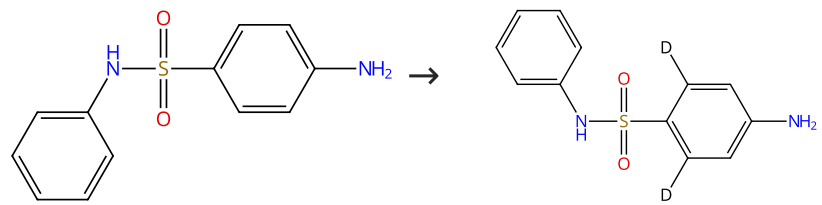
Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 143 (1 Reaction)

Steps: **1** Yield: **84%**



Suppliers (65)

31-116-CAS-17006185

Steps: **1** Yield: **84%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 144 (1 Reaction)

Steps: **1** Yield: **84%**

Suppliers (58)

31-614-CAS-24835988

Steps: **1** Yield: **84%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 24 h, 1 atm, 70 °C

Experimental Protocols

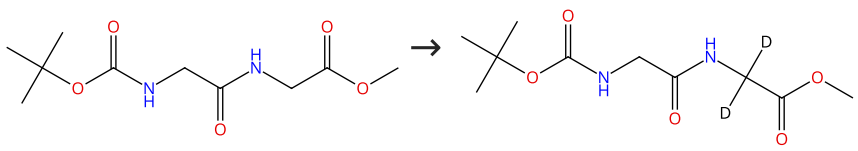
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 145 (1 Reaction)

Steps: **1** Yield: **84%**



Suppliers (6)

31-116-CAS-18953300

Steps: **1** Yield: **84%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

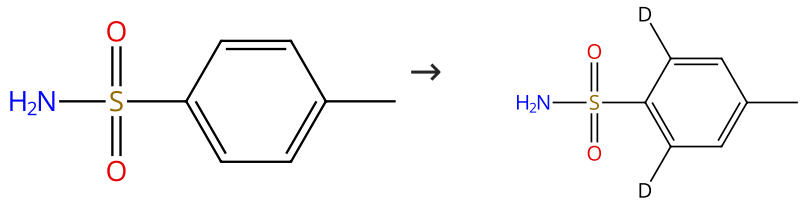
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 146 (2 Reactions)

Steps: **1** Yield: **84%**



Suppliers (99)

31-116-CAS-5568762

Steps: **1** Yield: **84%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

31-116-CAS-17237245 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

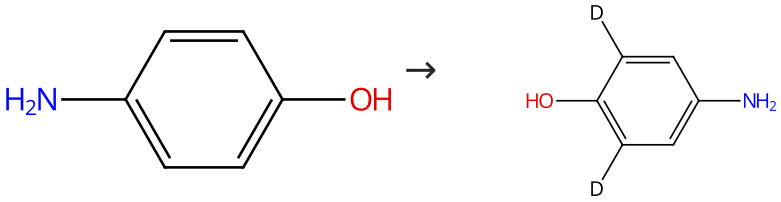
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 147 (1 Reaction) Steps: **1** Yield: **83%**



Suppliers (106) Suppliers (2)

31-614-CAS-24835993 Steps: **1** Yield: **83%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

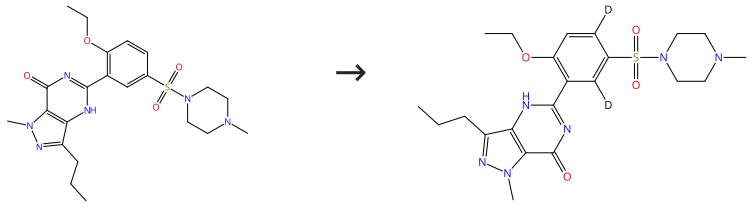
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 148 (1 Reaction) Steps: **1** Yield: **83%**



Suppliers (63)

31-116-CAS-17006221 Steps: **1** Yield: **83%**

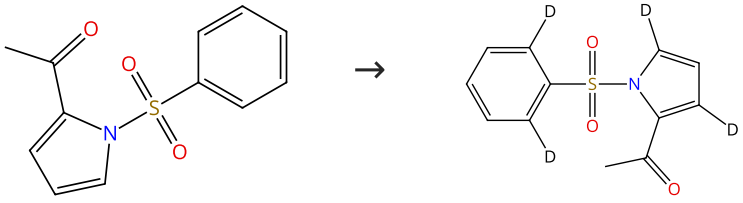
1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 149 (1 Reaction) Steps: **1** Yield: **83%**



Suppliers (18)

31-116-CAS-17006213 Steps: **1** Yield: **83%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 150 (1 Reaction) Steps: **1** Yield: **83%**

Suppliers (85)

31-614-CAS-24835959 Steps: **1** Yield: **83%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Ethyl acetate; 10 h, 1 atm, 35 °C

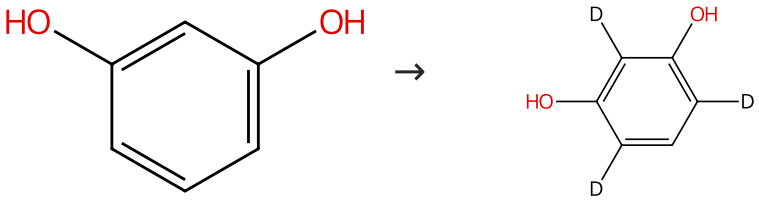
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 151 (1 Reaction) Steps: **1** Yield: **82%**



Suppliers (121) Supplier (1)

31-614-CAS-24835973 Steps: **1** Yield: **82%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

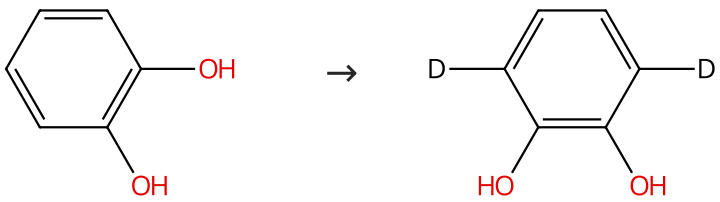
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 152 (1 Reaction) Steps: **1** Yield: **82%**



Suppliers (114)

31-614-CAS-24836008 Steps: **1** Yield: **82%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

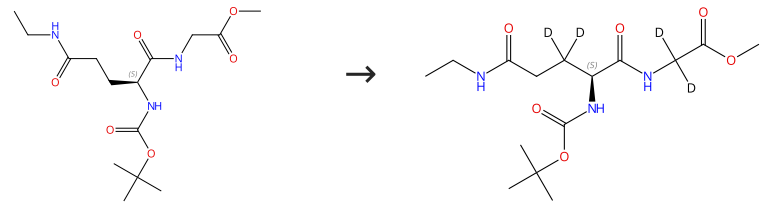
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 153 (1 Reaction) Steps: **1** Yield: **82%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-18953304 Steps: **1** Yield: **82%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

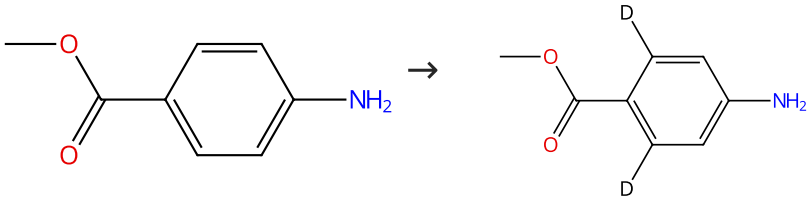
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 154 (1 Reaction) Steps: **1** Yield: **82%**



Suppliers (95)

31-116-CAS-21775899 Steps: **1** Yield: **82%**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; 12 h, 50 °C

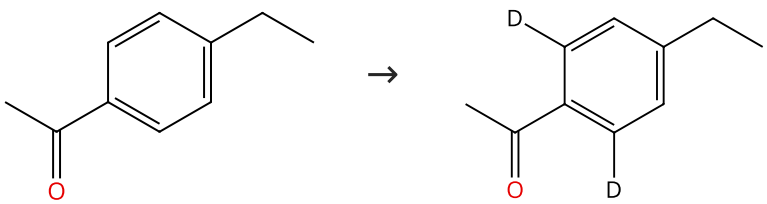
Experimental Protocols

Mesoionic Carbene-Iridium Complex Catalyzed Ortho-Selective Hydrogen Isotope Exchange of Anilines with High Functional Group Tolerance

By: Liu, Wei; et al

Organic Letters (2020), 22(6), 2210-2214.

Scheme 155 (1 Reaction) Steps: **1** Yield: **82%**



Suppliers (80)

31-116-CAS-22426899 Steps: **1** Yield: **82%**

1.1 **Reagents:** Deuterium
Catalysts: Water-d_2, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 32 h, 1 atm, rt

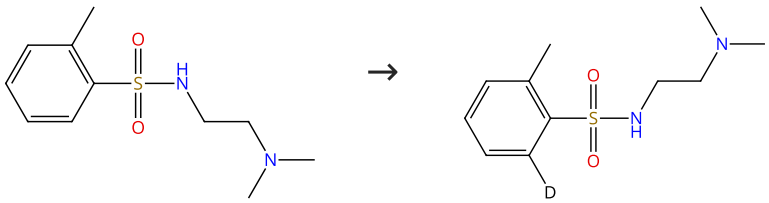
Experimental Protocols

Mechanistic Interrogation of Alkyne Hydroarylations Catalyzed by Highly Reduced, Single-Component Cobalt Complexes

By: Suslick, Benjamin A.; et al

Journal of the American Chemical Society (2020), 142(25), 11203-11218.

Scheme 156 (1 Reaction) Steps: **1** Yield: **81%**



Suppliers (3)

31-116-CAS-17006193 Steps: **1** Yield: **81%**

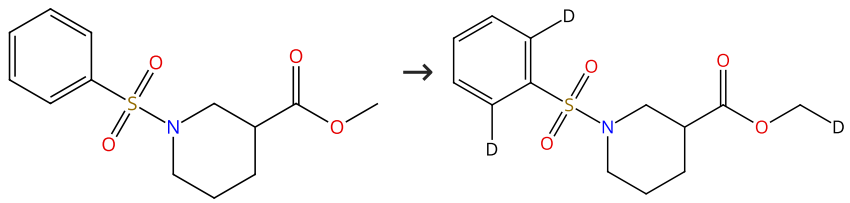
1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Chlorobenzene; 1 h, 1 atm, 120 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 157 (1 Reaction) Steps: **1** Yield: **80%**



Suppliers (22)

31-116-CAS-17006207 Steps: **1** Yield: **80%**

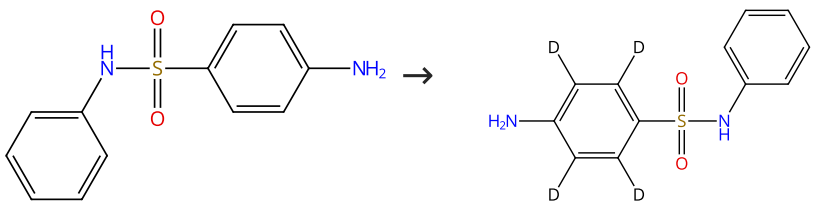
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 158 (1 Reaction) Steps: **1** Yield: **80%**



Suppliers (65)

31-116-CAS-17006186 Steps: **1** Yield: **80%**

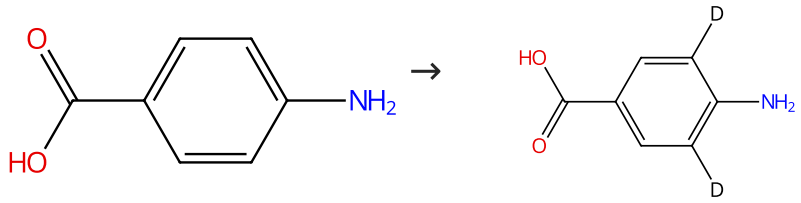
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 159 (2 Reactions) Steps: **1** Yield: **80%**



Suppliers (137)

31-116-CAS-2872308 Steps: **1** Yield: **80%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-2460885 Steps: **1**

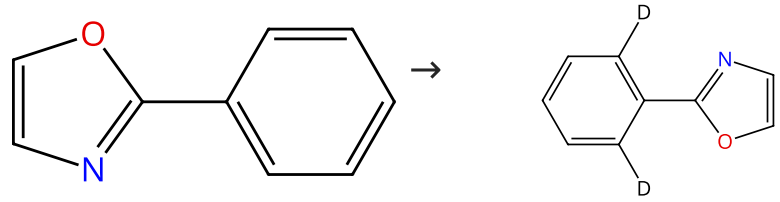
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 160 (2 Reactions) Steps: **1** Yield: **80%**



Suppliers (57)

31-116-CAS-12462760 Steps: **1** Yield: **80%**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Expanded applicability of iridium(I) NHC/phosphine catalysts in hydrogen isotope exchange processes with pharmaceutically-relevant heterocycles

By: Atzrodt, Jens; et al

Tetrahedron (2015), 71(13), 1924-1929.

Experimental Protocols

31-614-CAS-35597974 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

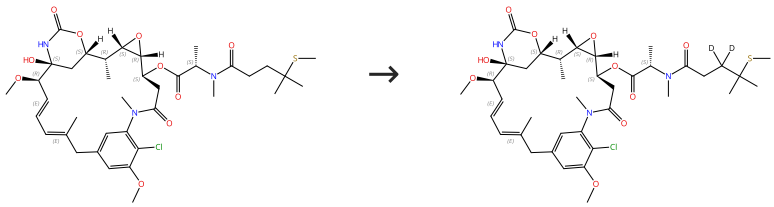
Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 161 (1 Reaction) Steps: **1** Yield: **80%**



Absolute stereochemistry shown
Double bond geometry shown

Absolute stereochemistry shown
Double bond geometry shown

31-116-CAS-18953287 Steps: **1** Yield: **80%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 50 °C

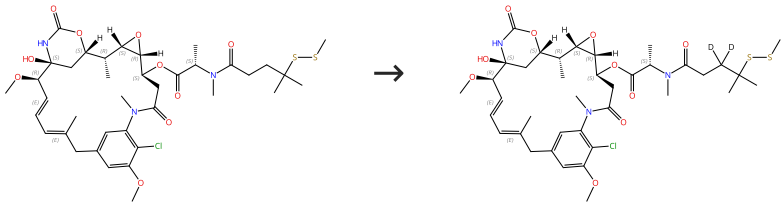
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 162 (1 Reaction) Steps: **1** Yield: **80%**



Absolute stereochemistry shown
Double bond geometry shown

Absolute stereochemistry shown
Double bond geometry shown

31-116-CAS-18953288 Steps: **1** Yield: **80%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 50 °C

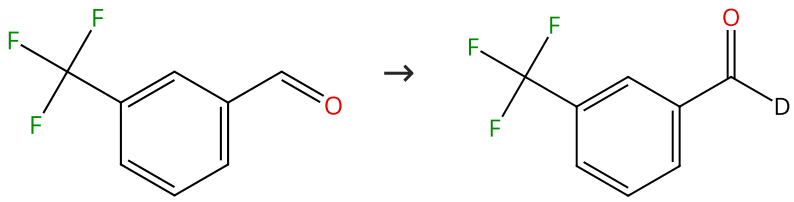
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 163 (1 Reaction) Steps: **1** Yield: **80%**



Suppliers (109)

31-116-CAS-17347301 Steps: **1** Yield: **80%**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

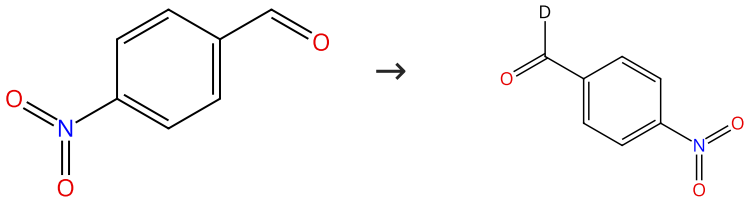
Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 164 (1 Reaction) Steps: **1** Yield: **80%**



Suppliers (96) Supplier (1)

31-116-CAS-17347298 Steps: **1** Yield: **80%**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

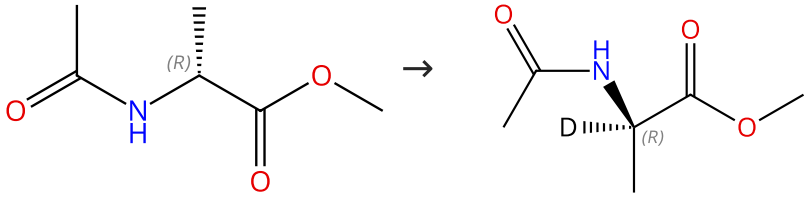
Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 165 (1 Reaction) Steps: **1** Yield: **78%**



Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (64)

31-116-CAS-18953295 Steps: **1** Yield: **78%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

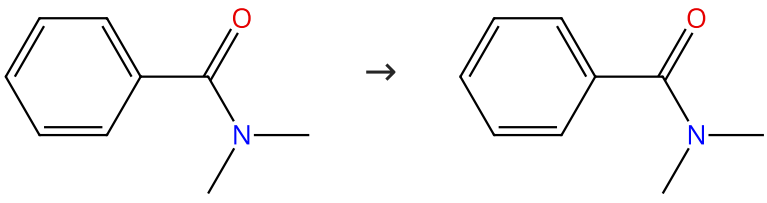
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 166 (2 Reactions) Steps: **1**



Suppliers (75)

31-614-CAS-26654608 Steps: **1**

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (polystyrene-supported)
Solvents: Dichloromethane; 1 h, rt

31-614-CAS-28254612 Steps: **1**

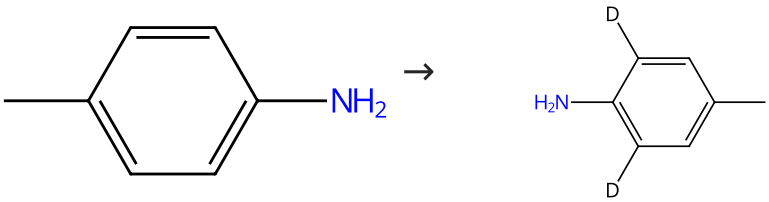
Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

Scheme 167 (2 Reactions) Steps: **1** Yield: **77%**



Suppliers (78)

31-116-CAS-737228 Steps: **1** Yield: **77%**

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

31-116-CAS-13728664 Steps: **1**

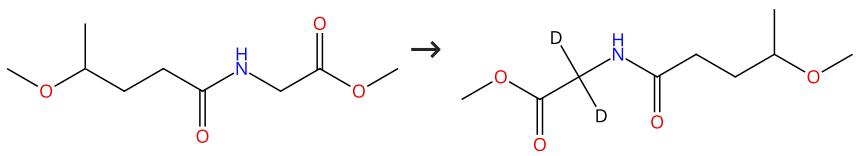
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Scheme 168 (1 Reaction) Steps: **1** Yield: **76%**



Suppliers (2)

31-116-CAS-18953289 Steps: **1** Yield: **76%**

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

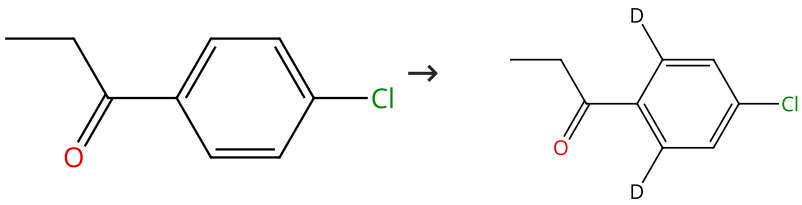
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Scheme 169 (1 Reaction)

Steps: **1** Yield: **76%**



Suppliers (86)

31-116-CAS-8489440

Steps: **1** Yield: **76%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 66 - 68 h, rt

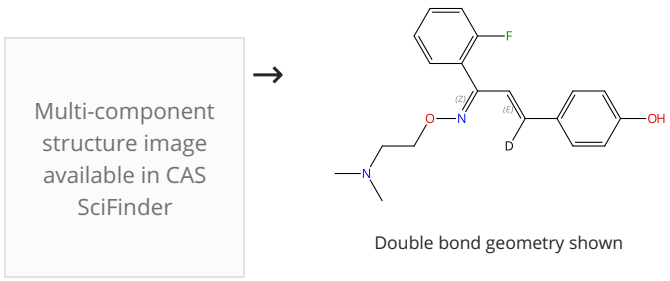
The mediation of aryl ketone deuteration by $[Ir(PPh_3)_3(cod)]^+.BF^-_4$

By: Herbert, John M.

Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(5), 317-322.

Scheme 170 (1 Reaction)

Steps: **1** Yield: **75%**



Double bond geometry shown

Suppliers (40)

31-116-CAS-6951659

Steps: **1** Yield: **75%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 70 h, rt

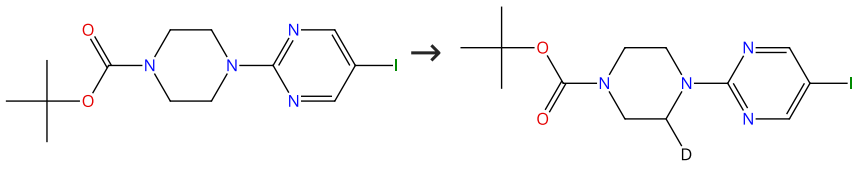
Iridium-mediated β-deuteration of enones

By: Gibson, Jennifer S.; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(6), 531-537.

Scheme 171 (1 Reaction)

Steps: **1** Yield: **74%**



Suppliers (48)

31-116-CAS-3434199

Steps: **1** Yield: **74%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 16 h, 0.46 - 1 atm, rt

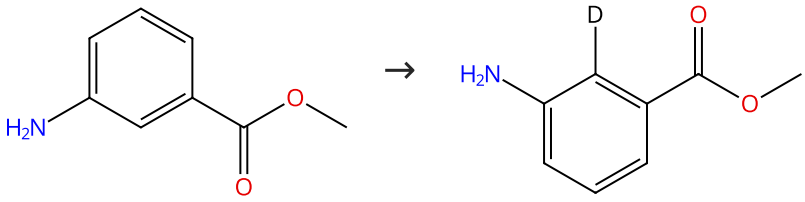
Hydrogen isotope exchange at alkyl positions using Crabtree's catalyst and its application to the tritiation of methapyrilene

By: Bushby, Nick; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 519-520.

Scheme 172 (1 Reaction)

Steps: **1** Yield: **74%**



Suppliers (101)

31-116-CAS-21775904

Steps: **1** Yield: **74%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](triphenyl phosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 12 h, 50 °C

Experimental Protocols

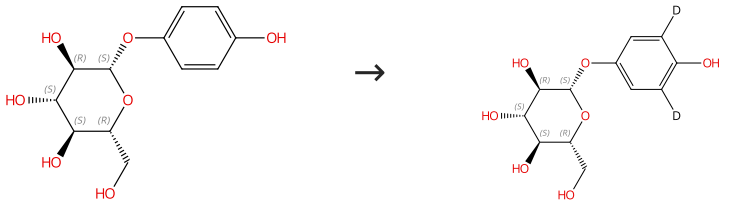
Mesoionic Carbene-Iridium Complex Catalyzed Ortho-Selective Hydrogen Isotope Exchange of Anilines with High Functional Group Tolerance

By: Liu, Wei; et al

Organic Letters (2020), 22(6), 2210-2214.

Scheme 173 (1 Reaction)

Steps: **1** Yield: **74%**



Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (108)

31-614-CAS-24836001

Steps: **1** Yield: **74%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 24 h, 1 atm, 70 °C

Experimental Protocols

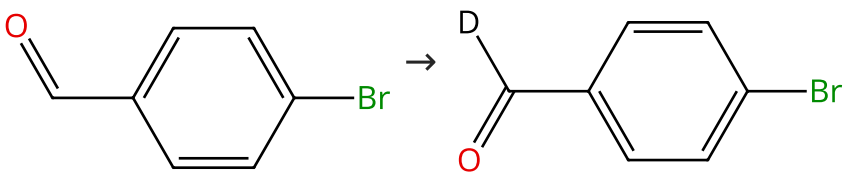
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 174 (1 Reaction)

Steps: **1** Yield: **73%**



Suppliers (98)

31-116-CAS-17347297

Steps: **1** Yield: **73%**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

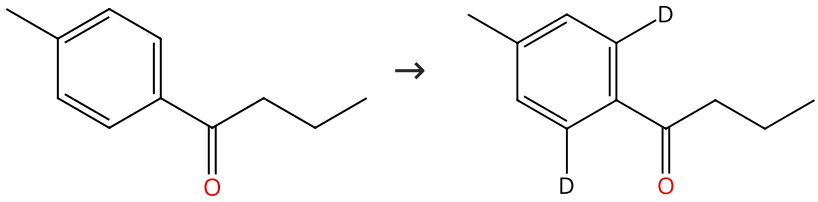
Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 175 (1 Reaction)

Steps: **1** Yield: **73%**



Suppliers (62)

31-116-CAS-6366622

Steps: **1** Yield: **73%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 66 - 68 h, rt

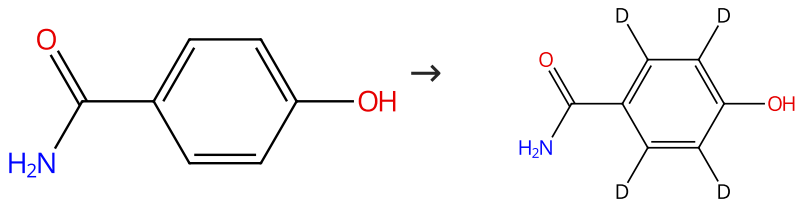
The mediation of aryl ketone deuteration by [Ir(PPh$_3$)$_3$(cod)]$^+$.BF$^-_4$

By: Herbert, John M.

Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(5), 317-322.

Scheme 176 (1 Reaction)

Steps: **1** Yield: **73%**



Suppliers (81)

31-614-CAS-24835981

Steps: **1** Yield: **73%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 12 h, 1 atm, 50 °C

Experimental Protocols

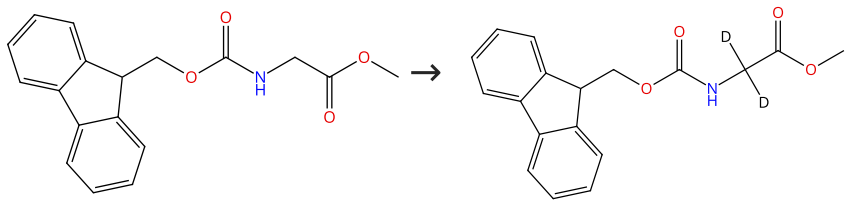
Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 177 (1 Reaction)

Steps: **1** Yield: **72%**



Suppliers (28)

31-116-CAS-18953293

Steps: **1** Yield: **72%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenyl phosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

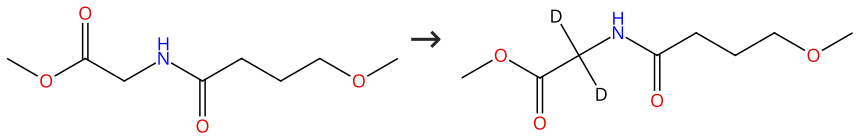
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 178 (1 Reaction)

Steps: **1** Yield: **72%**



Suppliers (3)

31-116-CAS-18953290

Steps: **1** Yield: **72%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

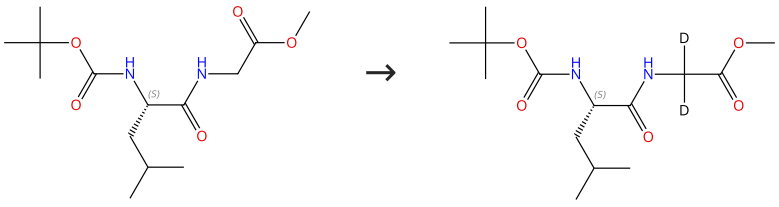
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 179 (1 Reaction)

Steps: **1** Yield: **72%**



Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (11)

31-116-CAS-18953302

Steps: **1** Yield: **72%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

Experimental Protocols

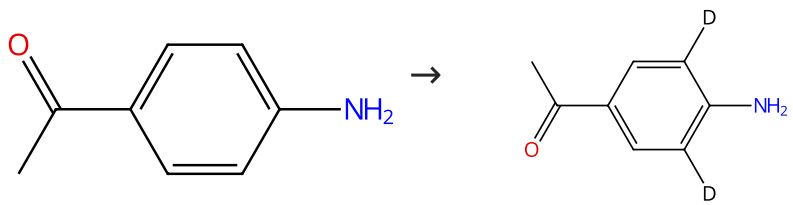
Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 180 (2 Reactions)

Steps: **1** Yield: **72%**



Suppliers (114)

31-116-CAS-13463455

Steps: **1** Yield: **72%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-6721898 Steps: **1**

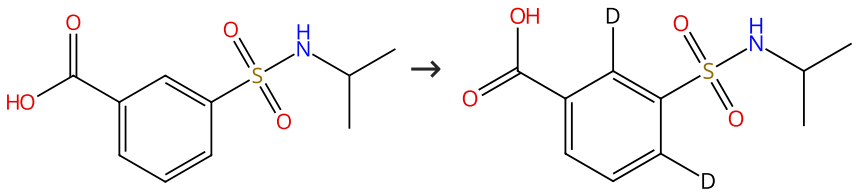
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 181 (1 Reaction) Steps: **1** Yield: **71%**



Suppliers (42)

31-116-CAS-17006191 Steps: **1** Yield: **71%**

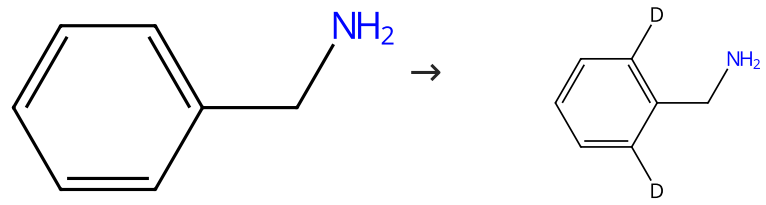
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κN^3]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 182 (1 Reaction) Steps: **1** Yield: **70%**



Suppliers (87)

31-116-CAS-13527360 Steps: **1** Yield: **70%**

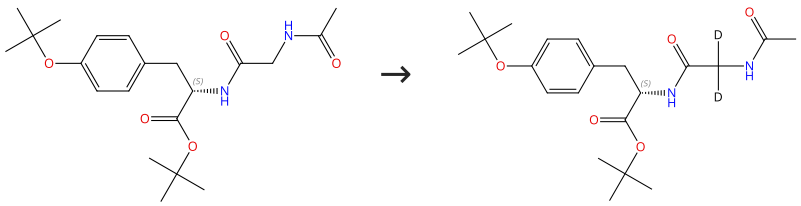
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 183 (1 Reaction) Steps: **1** Yield: **70%**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-18953298 Steps: **1** Yield: **70%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

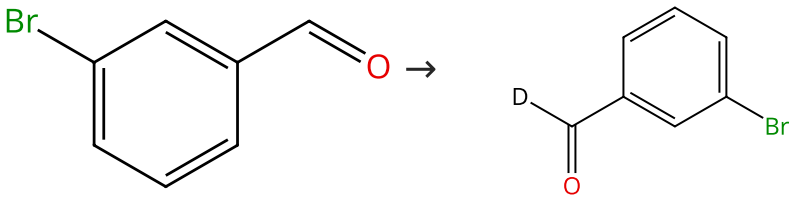
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 184 (1 Reaction) Steps: **1** Yield: **70%**



Suppliers (102)

31-116-CAS-17347299 Steps: **1** Yield: **70%**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

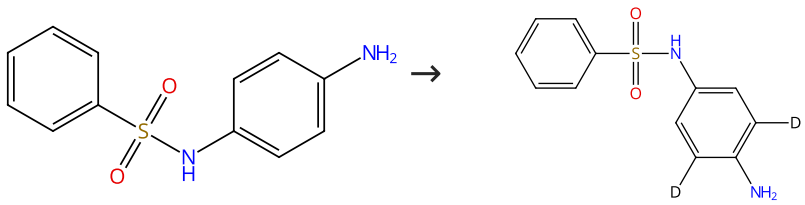
Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 185 (1 Reaction) Steps: **1** Yield: **70%**



Suppliers (20)

31-116-CAS-17006188 Steps: **1** Yield: **70%**

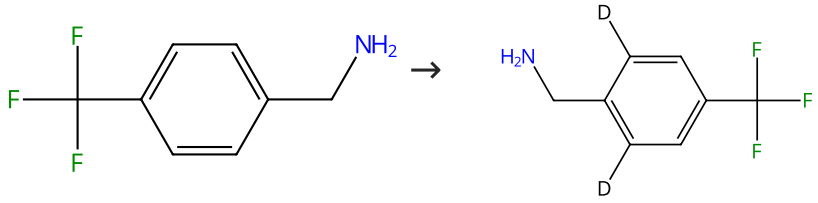
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chlorobenzene; 2 h, 1 atm, 100 °C

Hydrogen-Isotope Exchange (HIE) Reactions of Secondary and Tertiary Sulfonamides and Sulfonylureas with Iridium(I) Catalysts

By: Burhop, Annina; et al

European Journal of Organic Chemistry (2017), 2017(11), 1418-1424.

Scheme 186 (2 Reactions) Steps: **1** Yield: **69%**



Suppliers (91)

31-116-CAS-4669322 Steps: **1** Yield: **69%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-8631893 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 187 (2 Reactions) Steps: **1** Yield: **68%**

Suppliers (68)

31-116-CAS-10611266 Steps: **1** Yield: **68%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 66 - 68 h, rt

The mediation of aryl ketone deuteration by $[Ir(PPh_3)_3(cod)]^+.BF^-_4$

By: Herbert, John M.

Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(5), 317-322.

31-116-CAS-14783185 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 188 (1 Reaction) Steps: **1** Yield: **66%**

Suppliers (57) Suppliers (5)

31-614-CAS-36762225 Steps: **1** Yield: **66%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

1.2 **Reagents:** Phosphorus trichloride
Solvents: Chloroform; 24 h, 40 °C

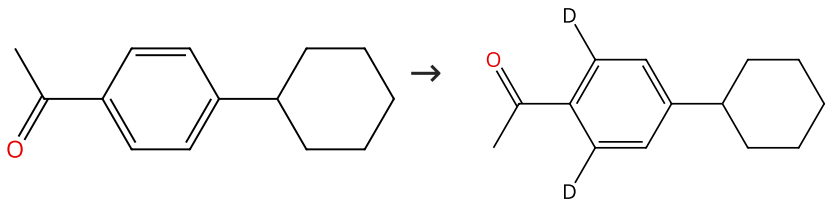
Selective Deuteration of Heterocycle N-Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 189 (1 Reaction)

Steps: **1** Yield: **66%**



Suppliers (78)

31-116-CAS-3624841

Steps: **1** Yield: **66%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 66 - 68 h, rt

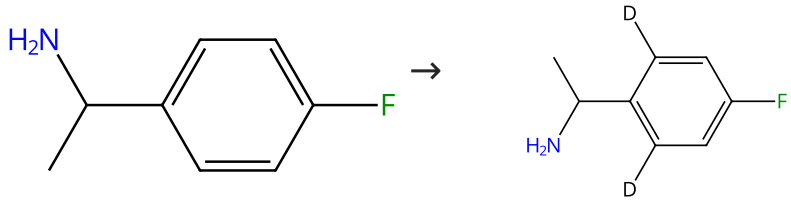
The mediation of aryl ketone deuteration by [Ir(PPh$_3$)$_3$(cod)]$^+$.BF$^-_4$

By: Herbert, John M.

Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(5), 317-322.

Scheme 190 (2 Reactions)

Steps: **1** Yield: **66%**



Suppliers (67)

31-116-CAS-2544329

Steps: **1** Yield: **66%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-6876659

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 191 (1 Reaction)

Steps: **1** Yield: **66%**

Suppliers (77)

Supplier (1)

31-116-CAS-11961779 Steps: **1** Yield: **66%**

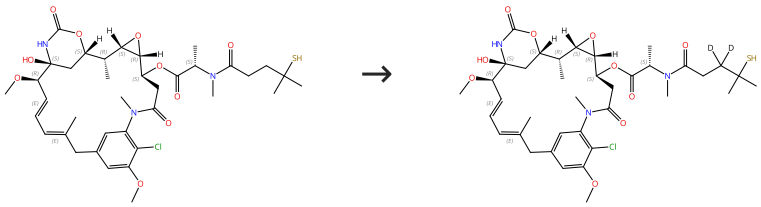
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 16 h, 0.46 - 1 atm, rt

Hydrogen isotope exchange at alkyl positions using Crabtree's catalyst and its application to the tritiation of methapyrilene

By: Bushby, Nick; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 519-520.

Scheme 192 (1 Reaction) Steps: **1** Yield: **65%**



Absolute stereochemistry shown
Double bond geometry shown

Absolute stereochemistry shown
Double bond geometry shown

31-116-CAS-18953286 Steps: **1** Yield: **65%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 3 h, 1 atm, 50 °C

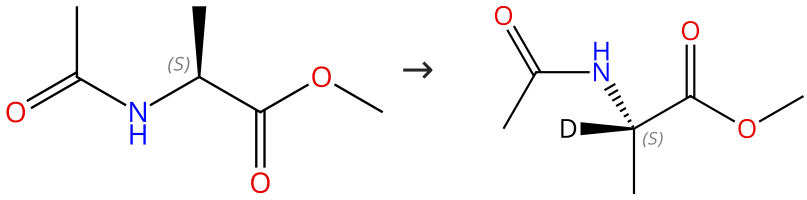
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 193 (1 Reaction) Steps: **1** Yield: **65%**



Absolute stereochemistry shown,
Rotation (+)

Absolute stereochemistry shown

Suppliers (65)

31-116-CAS-18953294 Steps: **1** Yield: **65%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+)
Solvents: Isopropyl acetate; 8 h, 1 atm, 80 °C

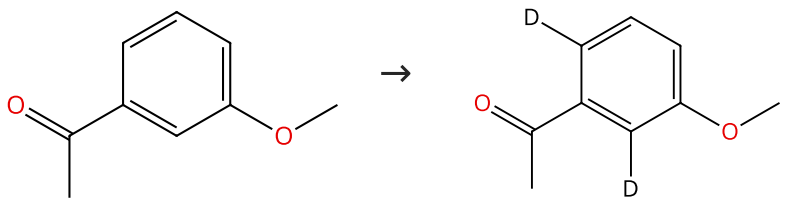
Experimental Protocols

Highly selective directed iridium-catalyzed hydrogen isotope exchange reactions of aliphatic amides

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2018), 57(27), 8159-8163.

Scheme 194 (2 Reactions) Steps: **1** Yield: **64%**



Suppliers (96)

31-116-CAS-14888993 Steps: **1** Yield: **64%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 66 - 68 h, rt

The mediation of aryl ketone deuteration by $[Ir(PPh_3)_3(cod)]^+.BF^-_4$

By: Herbert, John M.

Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(5), 317-322.

31-116-CAS-14172611 Steps: **1**

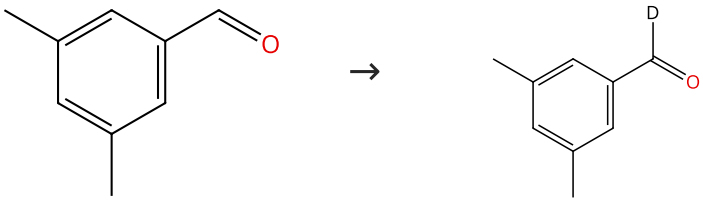
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 195 (1 Reaction) Steps: **1** Yield: **63%**



Suppliers (98) Supplier (1)

31-116-CAS-17347302 Steps: **1** Yield: **63%**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 196 (1 Reaction) Steps: **1** Yield: **56%**

Suppliers (47)

31-116-CAS-9839984 Steps: **1** Yield: **56%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 16 h, 0.46 - 1 atm, rt

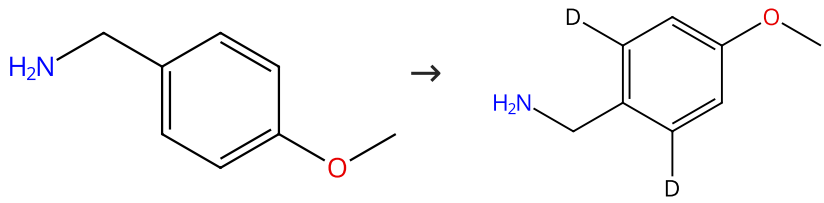
Hydrogen isotope exchange at alkyl positions using Crabtree's catalyst and its application to the tritiation of methapyrilene

By: Bushby, Nick; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 519-520.

Scheme 197 (2 Reactions)

Steps: **1** Yield: **55%**



Suppliers (93)

31-116-CAS-366083

Steps: **1** Yield: **55%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-8677826

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

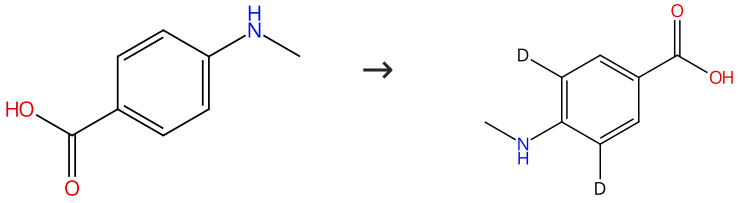
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 198 (1 Reaction)

Steps: **1** Yield: **53%**



Suppliers (83)

31-116-CAS-5001667

Steps: **1** Yield: **53%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

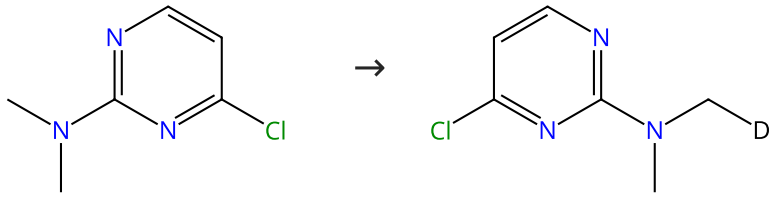
Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 199 (1 Reaction)

Steps: **1** Yield: **52%**



Suppliers (57)

31-116-CAS-5567925 Steps: **1** Yield: **52%**

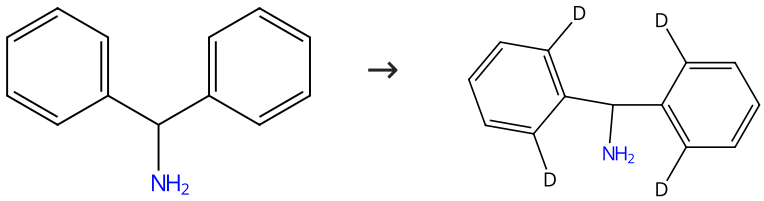
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 16 h, 0.46 - 1 atm, rt

Hydrogen isotope exchange at alkyl positions using Crabtree's catalyst and its application to the tritiation of methapyrilene

By: Bushby, Nick; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 519-520.

Scheme 200 (2 Reactions) Steps: **1** Yield: **50%**



Suppliers (93)

31-116-CAS-8934687 Steps: **1** Yield: **50%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-11142245 Steps: **1**

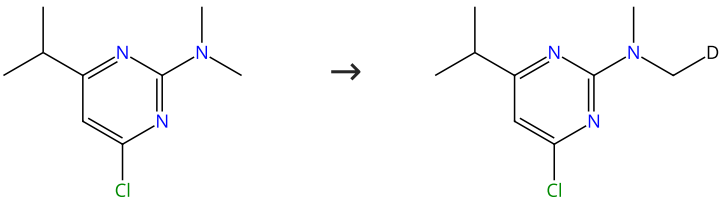
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 201 (1 Reaction) Steps: **1** Yield: **47%**



Suppliers (22)

31-116-CAS-7710947 Steps: **1** Yield: **47%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 16 h, 0.46 - 1 atm, rt

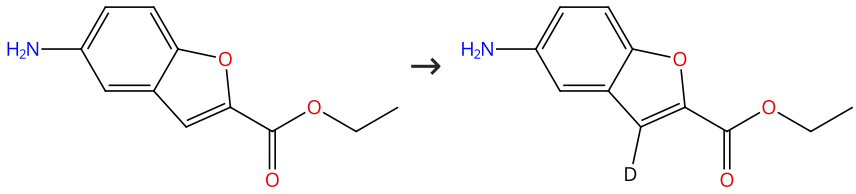
Hydrogen isotope exchange at alkyl positions using Crabtree's catalyst and its application to the tritiation of methapyrilene

By: Bushby, Nick; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 519-520.

Scheme 202 (1 Reaction)

Steps: **1** Yield: **45%**



Suppliers (78)

31-116-CAS-21775905

Steps: **1** Yield: **45%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](triphenyl phosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 12 h, 50 °C

Experimental Protocols

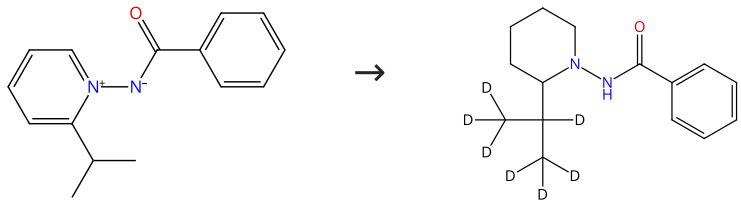
Mesoionic Carbene-Iridium Complex Catalyzed Ortho-Selective Hydrogen Isotope Exchange of Anilines with High Functional Group Tolerance

By: Liu, Wei; et al

Organic Letters (2020), 22(6), 2210-2214.

Scheme 203 (1 Reaction)

Steps: **1** Yield: **42%**



Supplier (1)

31-614-CAS-26580688

Steps: **1** Yield: **42%**

1.1 **Catalysts:** Iodine, Iridium(1+), [(4*S*)-2-[2-[bis(4-fluorophenyl) phosphino-κ*P*]phenyl]-4-(1,1-dimethylethyl)-4,5-dihydroo xazole-κN^3][(1,2,5,6-η)-1,5-cyclooctadiene]-, stereoisomer, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-)
Solvents: Toluene; 8 h, rt

1.2 **Reagents:** Deuterium; 6 h, 400 psi, rt

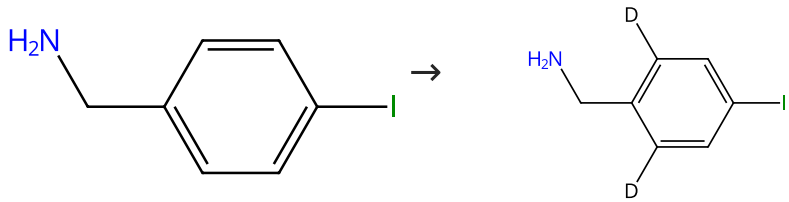
Iridium catalyzed enantioselective hydrogenation of N-iminopyridinium ylides: mechanistic insights

By: Legault, Claude Y.; et al

Heterocycles (2008), 76(2), 1271-1283.

Scheme 204 (1 Reaction)

Steps: **1** Yield: **42%**



Suppliers (93)

31-116-CAS-11675504

Steps: **1** Yield: **42%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafl uoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

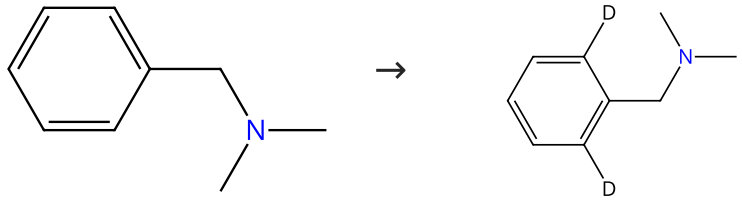
Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 205 (2 Reactions)

Steps: **1** Yield: **35%**



Suppliers (67)

31-116-CAS-9537415

Steps: **1** Yield: **35%**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-5885793

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylformamide; 4 h, rt

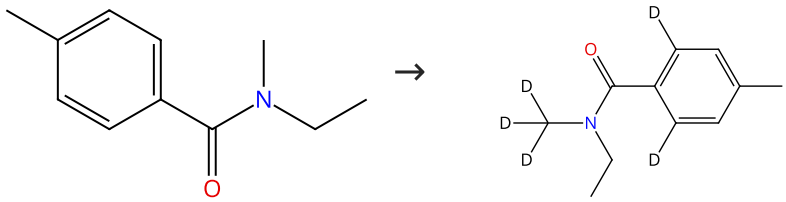
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 206 (1 Reaction)

Steps: **1** Yield: **31%**



Suppliers (4)

31-116-CAS-7355765

Steps: **1** Yield: **31%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: *tert*-Butyl methyl ether; rt → - 78 °C; 2 h, 25 °C

Experimental Protocols

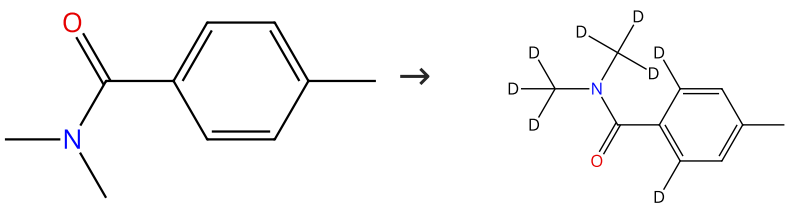
Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

Scheme 207 (1 Reaction)

Steps: **1** Yield: **22%**



Suppliers (23)

31-116-CAS-14216473 Steps: **1** Yield: **22%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: 2-Methyltetrahydrofuran; rt → -78 °C; 1 h, 25 °C

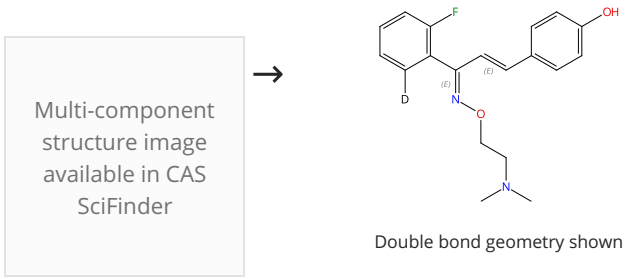
Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

Scheme 208 (1 Reaction) Steps: **1** Yield: **15%**



Double bond geometry shown

Suppliers (2)

31-116-CAS-11217012 Steps: **1** Yield: **15%**

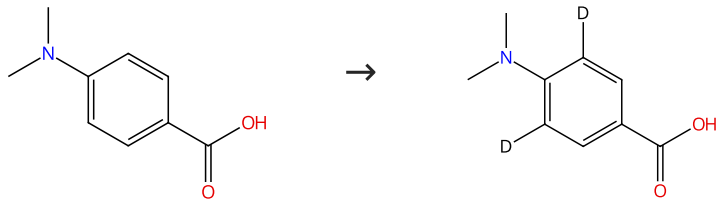
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 70 h, rt

Iridium-mediated β-deuteration of enones

By: Gibson, Jennifer S.; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(6), 531-537.

Scheme 209 (1 Reaction) Steps: **1** Yield: **11%**



Suppliers (90)

31-116-CAS-7109174 Steps: **1** Yield: **11%**

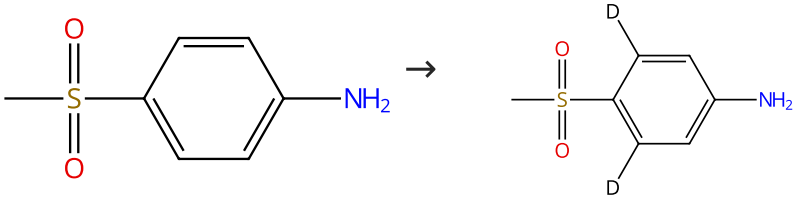
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 210 (1 Reaction) Steps: **1** Yield: **7%**



Suppliers (83)

31-116-CAS-21775902 Steps: **1** Yield: **7%**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](triphenyl phosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 12 h, 50 °C

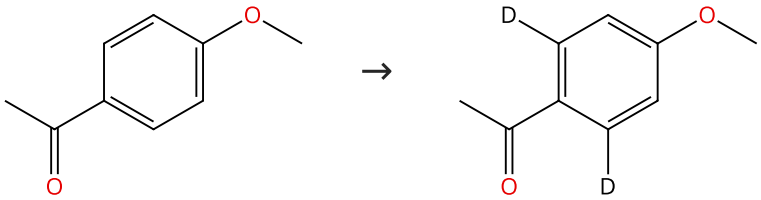
Experimental Protocols

Mesoionic Carbene-Iridium Complex Catalyzed Ortho-Selective Hydrogen Isotope Exchange of Anilines with High Functional Group Tolerance

By: Liu, Wei; et al

Organic Letters (2020), 22(6), 2210-2214.

Scheme 211 (1 Reaction) Steps: **1**



Suppliers (103)

31-116-CAS-9007388 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 212 (2 Reactions) Steps: **1**

Suppliers (83)

31-614-CAS-27218708 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (polystyrene-supported)
Solvents: Dichloromethane; 1 h, rt

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

31-614-CAS-28029446 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

Scheme 213 (1 Reaction)

Steps: **1**

Suppliers (83)

31-116-CAS-15661324

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 40 °C; 1 h, 40 °C

Experimental Protocols

Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 214 (1 Reaction)

Steps: **1**

Suppliers (83)

mixture with monodeuterated analog

31-116-CAS-15602382

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 215 (1 Reaction)

Steps: **1**

Suppliers (83)

31-116-CAS-16442685

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

Scheme 216 (5 Reactions)

Steps: **1**

Suppliers (83)

31-116-CAS-16442681

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

31-116-CAS-2906518

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-777121

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-12309474

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-14773691

Steps: **1**

1.1 **Catalysts:** Triphenylphosphine (polystyrene-bound), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 2 h, rt

1.2 **Reagents:** Deuterium
Solvents: Dichloromethane; 4 h, rt; 18 h, rt

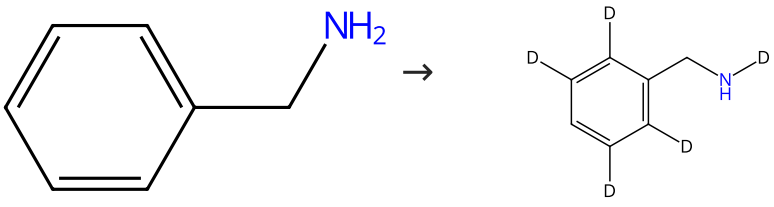
A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

Scheme 217 (1 Reaction)

Steps: **1**



Suppliers (87)

31-116-CAS-20812383 Steps: **1**

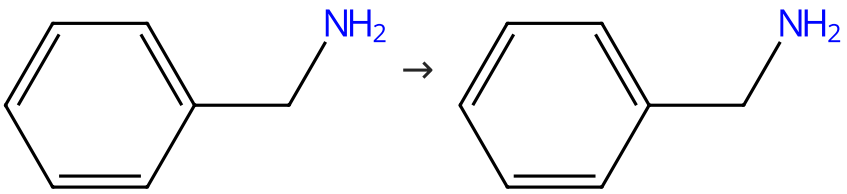
1.1 **Reagents:** Deuterium
Catalysts: Tantalum, [dihydro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium]tris(2,2-dimethylpropyl)-, (*Ir-Ta*) (silica-supported, hydrogenation of)
Solvents: Pentane; 24 h, 800 mbar, 25 °C

Metal-Metal Synergy in Well-Defined Surface Tantalum-Iridium Heterobimetallic Catalysts for H/D Exchange Reactions

By: Lassalle, Sebastien; et al

Journal of the American Chemical Society (2019), 141(49), 19321-19335.

Scheme 218 (1 Reaction) Steps: **1**



Suppliers (87)

31-614-CAS-30162230 Steps: **1**

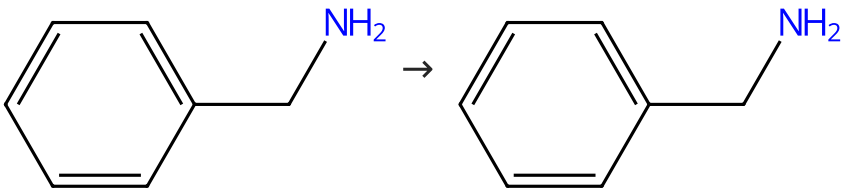
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 219 (1 Reaction) Steps: **1**



Suppliers (87)

31-614-CAS-26526781 Steps: **1**

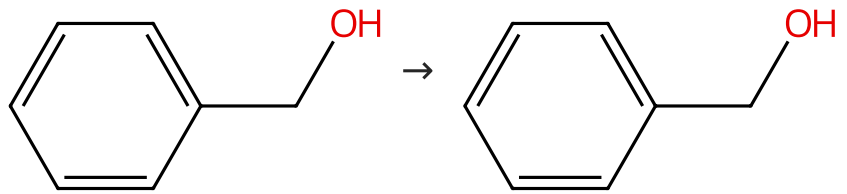
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 220 (1 Reaction) Steps: **1**



Suppliers (161)

31-614-CAS-28126674 Steps: **1**

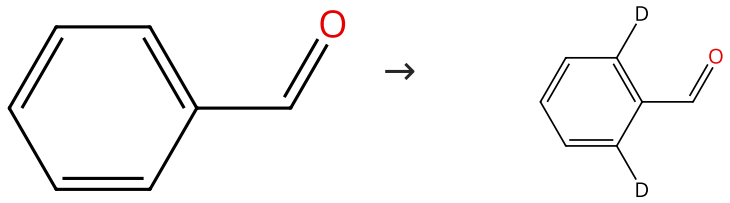
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 221 (1 Reaction) Steps: **1**



Suppliers (80)

31-116-CAS-17237217 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}] ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl] borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

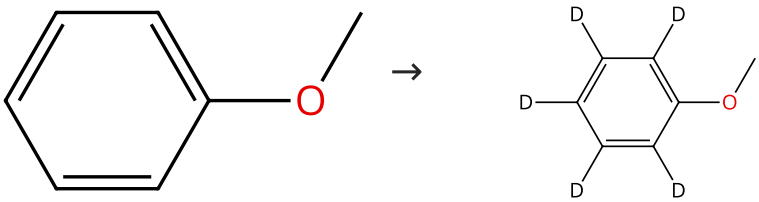
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 222 (1 Reaction) Steps: **1**



Suppliers (89) Suppliers (23)

31-116-CAS-20812384 Steps: **1**

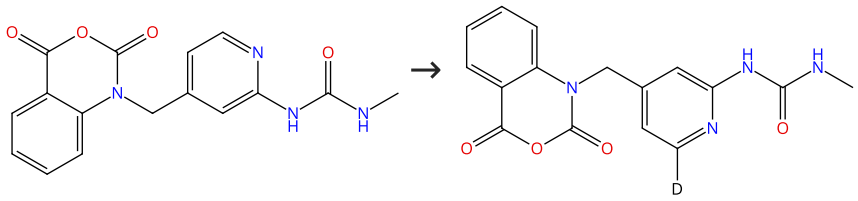
1.1 **Reagents:** Deuterium
Catalysts: Tantalum, [dihydro[(1,2,3,4,5-η)-1,2,3,4,5-pentam ethyl-2,4-cyclopentadien-1-yl]iridium]tris(2,2-dimethylpropyl)-, (*Ir-Ta*) (silica-supported, hydrogenation of)
Solvents: Pentane; 24 h, 800 mbar, 25 °C

Metal-Metal Synergy in Well-Defined Surface Tantalum-Iridium Heterobimetallic Catalysts for H/D Exchange Reactions

By: Lassalle, Sebastien; et al

Journal of the American Chemical Society (2019), 141(49), 19321-19335.

Scheme 223 (1 Reaction) Steps: **1**



31-116-CAS-6694406 Steps: **1**

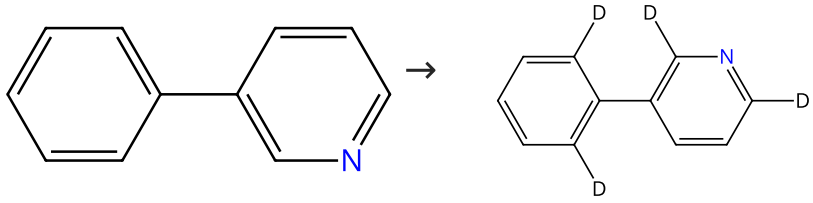
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1457 - 1639 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 224 (1 Reaction) Steps: **1**



Suppliers (84)

31-116-CAS-22794804 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

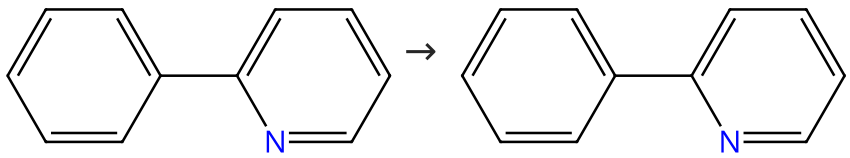
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 225 (1 Reaction) Steps: **1**



Suppliers (94)

deuterated

31-614-CAS-29493769 Steps: **1**

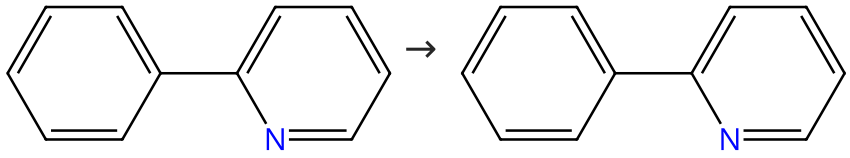
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(tributylphosphine)-, hexafluorophosphate(1-)
Solvents: Dichloromethane; overnight, 500 mbar, rt

Investigation of isotopic exchange reactions using N-heterocyclic iridium (I) complexes

By: Powell, Mark E.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 523-525.

Scheme 226 (2 Reactions) Steps: **1**



Suppliers (94)

31-614-CAS-27321457 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis (dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (polystyrene-supported)
Solvents: Dichloromethane; 1 h, rt

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

31-614-CAS-28132263 Steps: **1**

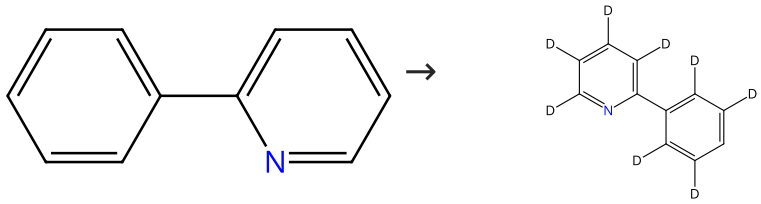
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

Scheme 227 (1 Reaction) Steps: **1**



Suppliers (94)

31-116-CAS-22794803 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

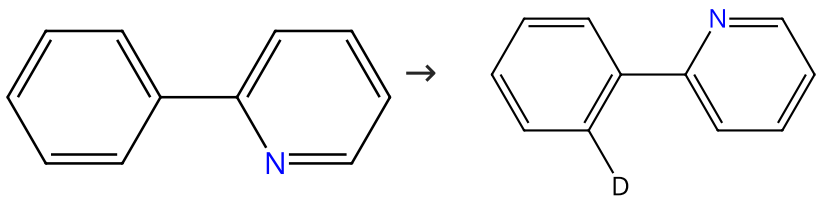
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 228 (1 Reaction) Steps: **1**



Suppliers (94)

Suppliers (6)

31-116-CAS-4459601 Steps: **1**

1.1 **Catalysts:** Triphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

1.2 **Reagents:** Deuterium

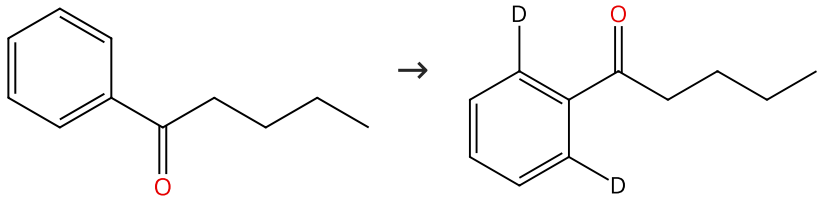
Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 229 (1 Reaction)

Steps: **1**



Suppliers (90)

31-116-CAS-14909808

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

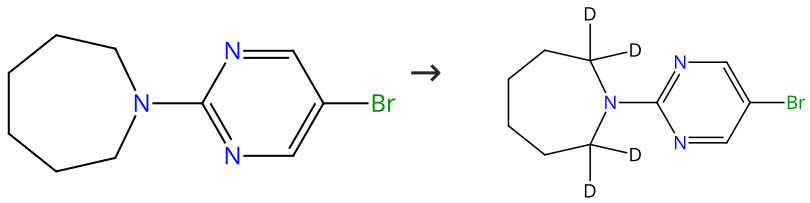
Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 230 (1 Reaction)

Steps: **1**



Suppliers (40)

31-116-CAS-19414261

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

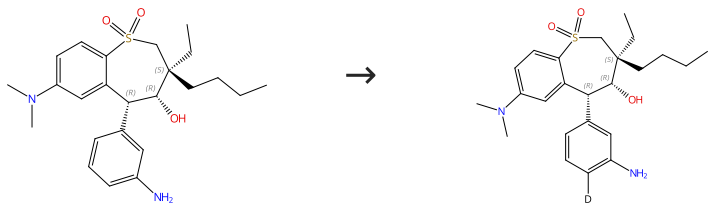
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 231 (1 Reaction)

Steps: **1**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-22794830

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

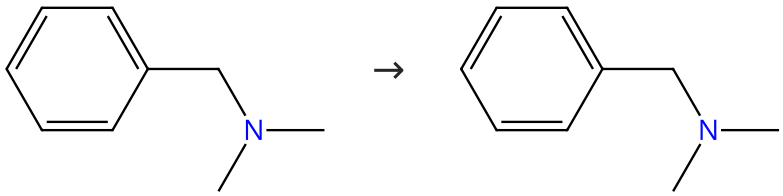
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 232 (1 Reaction)

Steps: **1**



Suppliers (67)

31-614-CAS-27315935

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

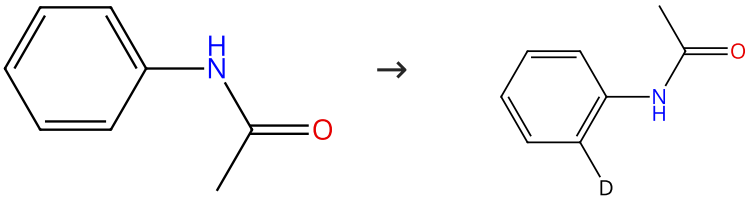
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 233 (1 Reaction)

Steps: **1**



Suppliers (108)

with and without addnl. ortho deuterium

31-116-CAS-12979802

Steps: **1**

1.1 **Catalysts:** Methyldiphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

1.2 **Reagents:** Deuterium

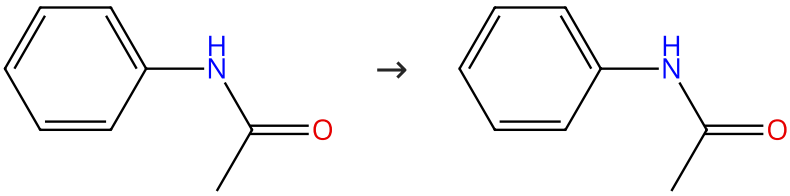
Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 234 (1 Reaction)

Steps: **1**



Suppliers (108)

31-614-CAS-26309012

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

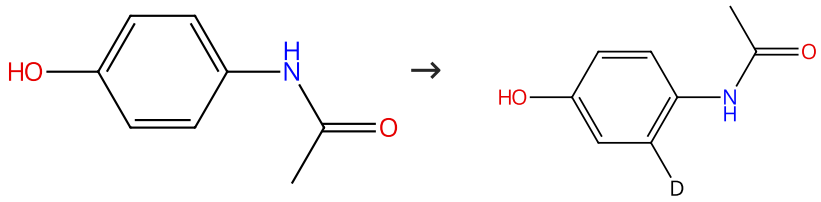
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 235 (1 Reaction)

Steps: **1**



Suppliers (147)

31-116-CAS-6832748

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 6 h, 0.9 atm, rt

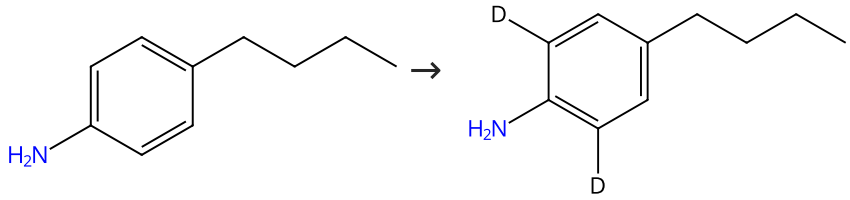
Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

Scheme 236 (2 Reactions)

Steps: **1**



Suppliers (78)

Supplier (1)

31-116-CAS-22794815

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

31-116-CAS-21649660

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

Experimental Protocols

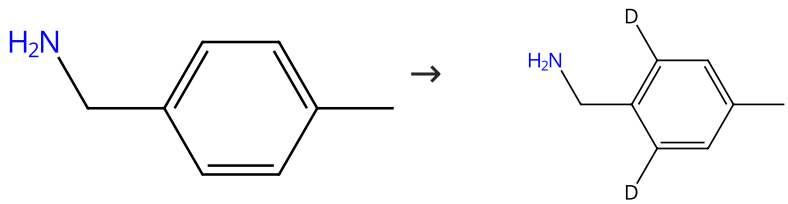
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 237 (1 Reaction)

Steps: **1**



Suppliers (86)

31-116-CAS-6833133 Steps: **1**

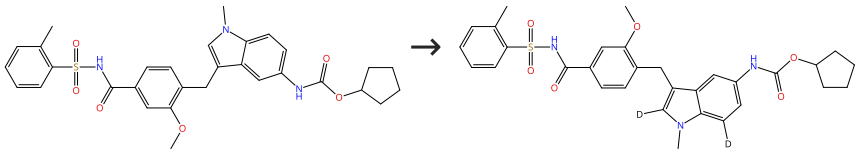
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 238 (1 Reaction) Steps: **1**



Suppliers (84)

31-116-CAS-22794822 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

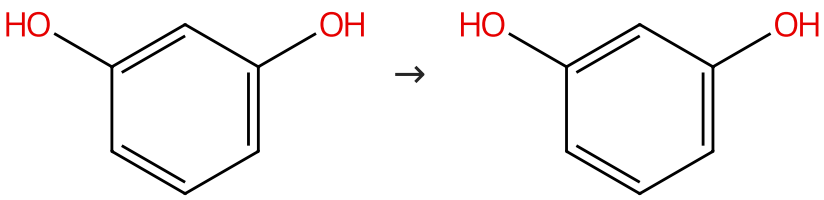
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 239 (1 Reaction) Steps: **1**



Suppliers (121)

31-614-CAS-27099263 Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

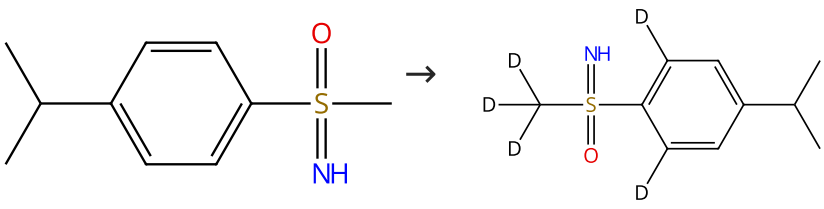
Experimental Protocols

Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 240 (1 Reaction) Steps: **1**



Suppliers (31)

31-614-CAS-42989262 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Diethyl ether; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

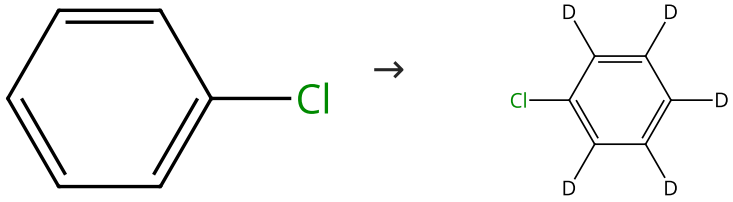
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 241 (1 Reaction) Steps: **1**



Suppliers (140) Suppliers (64)

31-116-CAS-20812385 Steps: **1**

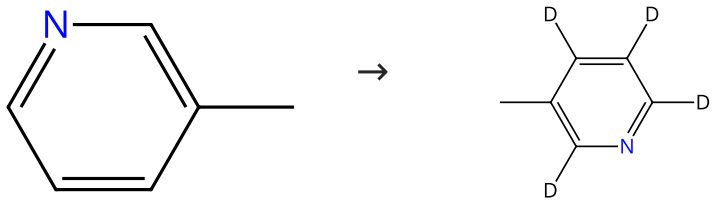
1.1 **Reagents:** Deuterium
Catalysts: Tantalum, [dihydro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium]tris(2,2-dimethylpropyl)-, (*Ir-Ta*) (silica-supported, hydrogenation of)
Solvents: Pentane; 24 h, 800 mbar, 25 °C

Metal-Metal Synergy in Well-Defined Surface Tantalum-Iridium Heterobimetallic Catalysts for H/D Exchange Reactions

By: Lassalle, Sebastien; et al

Journal of the American Chemical Society (2019), 141(49), 19321-19335.

Scheme 242 (1 Reaction) Steps: **1**



Suppliers (76) Suppliers (4)

31-116-CAS-22794806 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

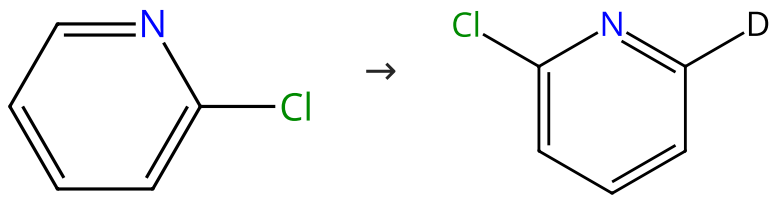
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 243 (1 Reaction) Steps: **1**



Suppliers (70) Suppliers (3)

31-116-CAS-8878827 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooc tadiene](pyridine)(tricyclohexylphosphine)-, hexafluoro phosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 244 (1 Reaction) Steps: **1**

Suppliers (221) Suppliers (161)

31-116-CAS-22794807 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxyd iiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

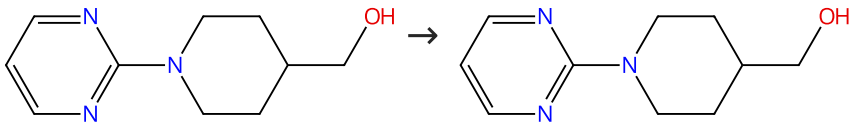
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmace uticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 245 (1 Reaction) Steps: **1**



Suppliers (51)

31-614-CAS-27811784 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

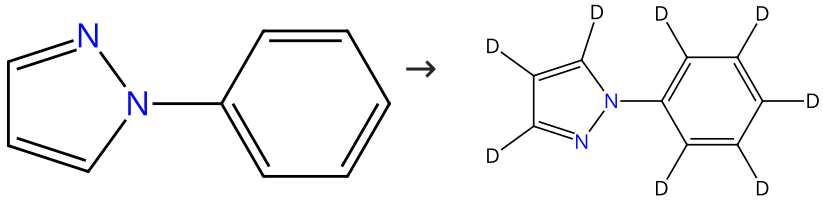
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 246 (1 Reaction) Steps: **1**



Suppliers (90) Suppliers (4)

31-116-CAS-22794812 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

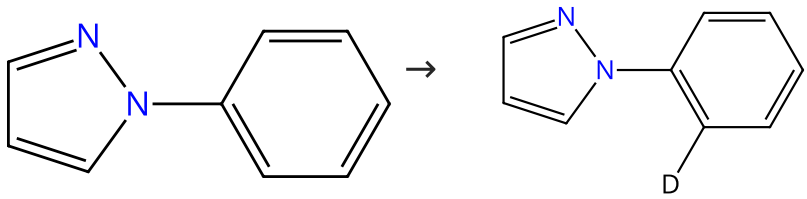
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 247 (1 Reaction) Steps: **1**



Suppliers (90)

31-116-CAS-6599115 Steps: **1**

1.1 **Catalysts:** Methyldiphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

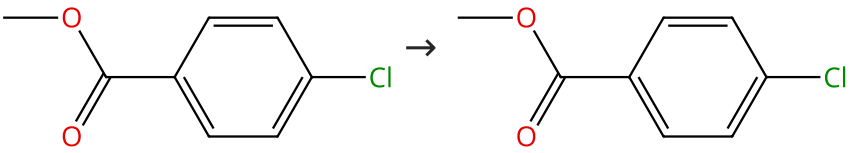
1.2 **Reagents:** Deuterium

Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 248 (1 Reaction) Steps: **1**



Suppliers (93)

mixture with deuterated analog

31-614-CAS-26009305 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

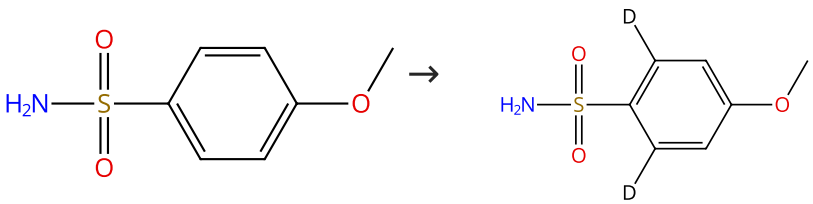
Experimental Protocols

Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 249 (1 Reaction) Steps: **1**



Suppliers (66)

31-116-CAS-14191354 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

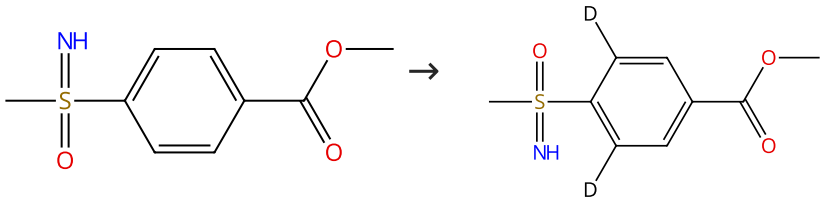
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 250 (1 Reaction) Steps: **1**



Suppliers (38)

31-614-CAS-42989291 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

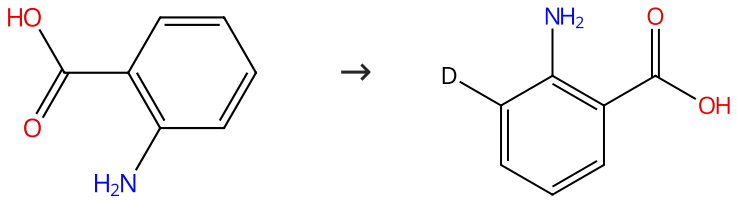
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 251 (1 Reaction) Steps: **1**



Suppliers (48)

31-116-CAS-9207438 Steps: **1**

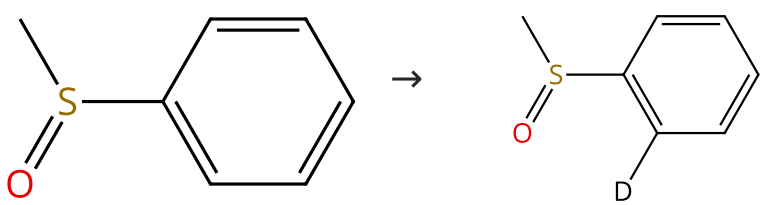
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 252 (1 Reaction) Steps: **1**



Suppliers (82)

31-116-CAS-10577091 Steps: **1**

1.1 **Catalysts:** Methyldiphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

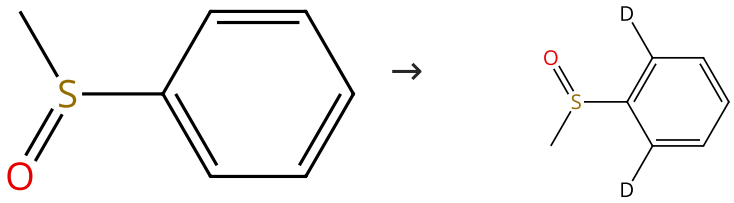
1.2 **Reagents:** Deuterium

Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 253 (1 Reaction) Steps: **1**



Suppliers (82)

31-116-CAS-8159306 Steps: **1**

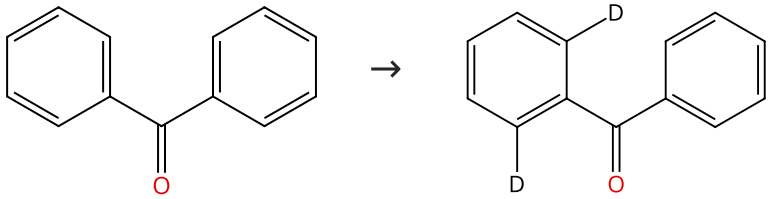
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 254 (1 Reaction) Steps: **1**



Suppliers (142)

31-116-CAS-54507 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

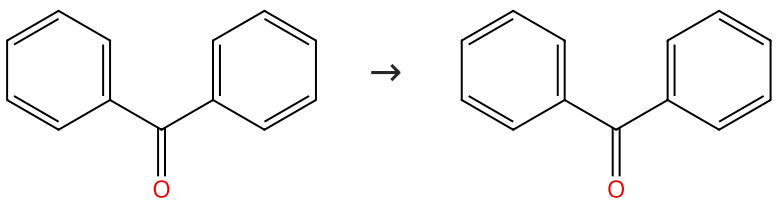
Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 255 (2 Reactions) Steps: **1**



Suppliers (142)

31-614-CAS-26429046 Steps: **1**

Tritium-labeling via an iridium-based solid-phase catalyst

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

31-614-CAS-25607125 Steps: **1**

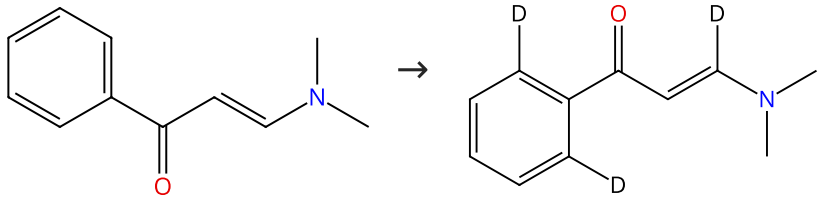
Tritium-labeling via an iridium-based solid-phase catalyst

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (polystyrene-supported)
Solvents: Dichloromethane; 1 h, rt

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

Scheme 256 (1 Reaction) Steps: **1**



Suppliers (68)

31-116-CAS-12158023 Steps: **1**

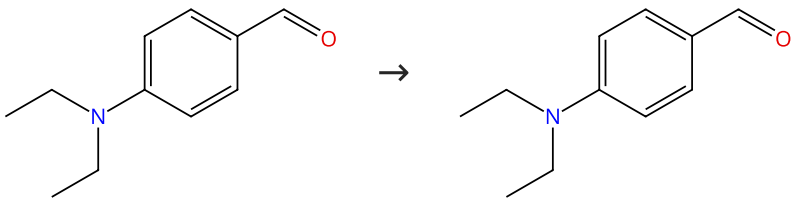
Iridium-mediated β-deuteration of enones

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 70 h, rt

By: Gibson, Jennifer S.; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(6), 531-537.

Scheme 257 (1 Reaction) Steps: **1**



Suppliers (96)

deuterated

31-614-CAS-25223970 Steps: **1**

Investigation of isotopic exchange reactions using N-hetero cyclic iridium (I) complexes

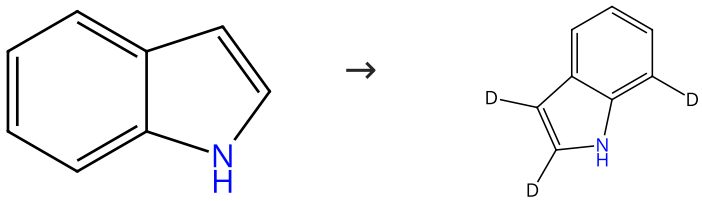
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; overnight, 500 mbar, rt

By: Powell, Mark E.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 523-525.

Scheme 258 (1 Reaction)

Steps: **1**



Suppliers (117)

31-116-CAS-22794808

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

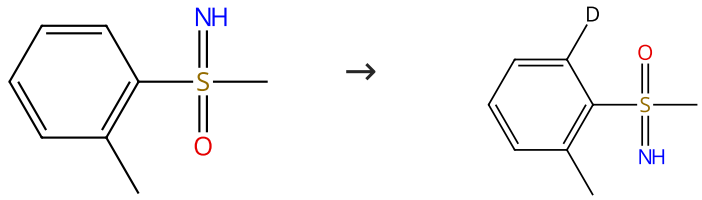
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 259 (1 Reaction)

Steps: **1**



Suppliers (26)

31-614-CAS-42989265

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

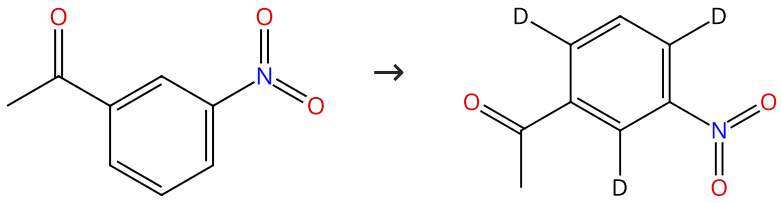
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 260 (1 Reaction)

Steps: **1**



Suppliers (92)

Supplier (1)

31-116-CAS-9912057

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

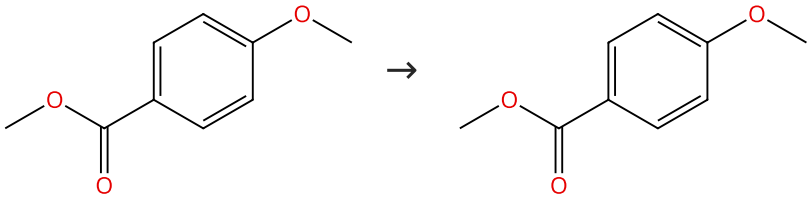
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 261 (1 Reaction)

Steps: **1**



Suppliers (91)

mixture with deuterated analog

31-614-CAS-29312279

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

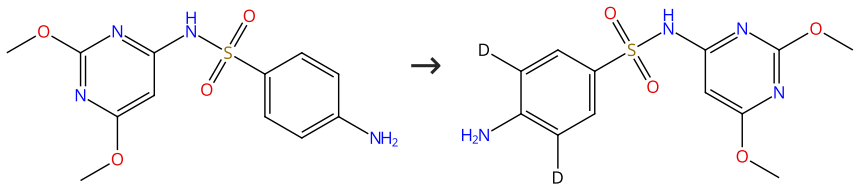
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 262 (1 Reaction)

Steps: **1**



Suppliers (95)

31-116-CAS-21649684

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

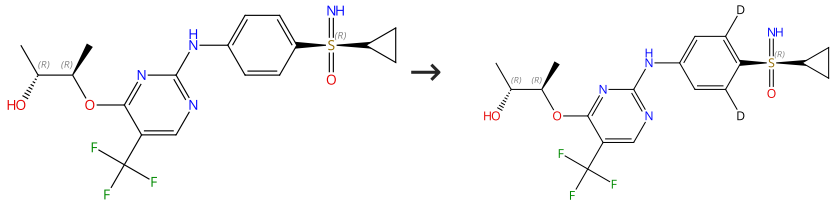
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 263 (1 Reaction)

Steps: **1**



Absolute stereochemistry shown

Relative stereochemistry shown

Suppliers (39)

31-614-CAS-42989303

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Ethyl acetate; -78 °C → 50 °C; 16 h, 50 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

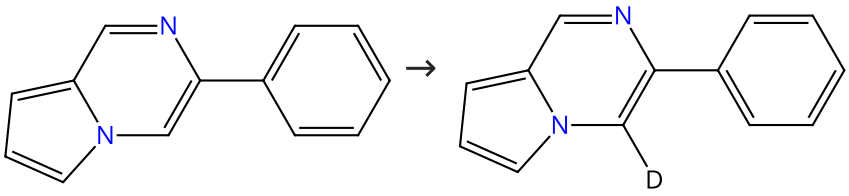
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 264 (1 Reaction)

Steps: **1**



31-116-CAS-17911540

Steps: **1**

1.1 **Catalysts:** Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene] diiridium, 1,1'-[(1*R*)-4,4',6,6'-Tetramethoxy[1,1'-biphenyl]-2,2'-diyl]bis[1,1-bis[3,5-bis(trifluoromethyl)phenyl]phosphine
Solvents: Tetrahydrofuran; 5 min, rt

1.2 **Reagents:** Deuterium
Solvents: Tetrahydrofuran; 3 h, 1.96 M Pa, 60 °C

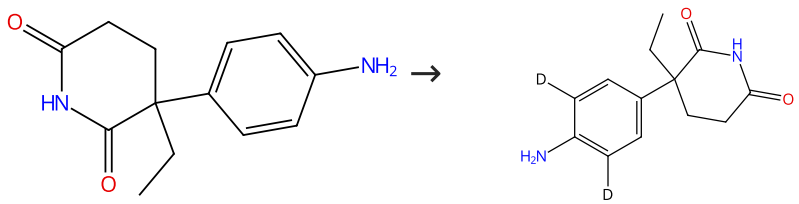
Enantioselective Hydrogenation of Pyrrolo[1,2-a]pyrazines, Heteroaromatics Containing Two Nitrogen Atoms

By: Hu, Shu-Bo; et al

Advanced Synthesis & Catalysis (2017), 359(16), 2762-2767.

Scheme 265 (2 Reactions)

Steps: **1**



Suppliers (73)

31-116-CAS-22794831

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

31-116-CAS-21649683

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

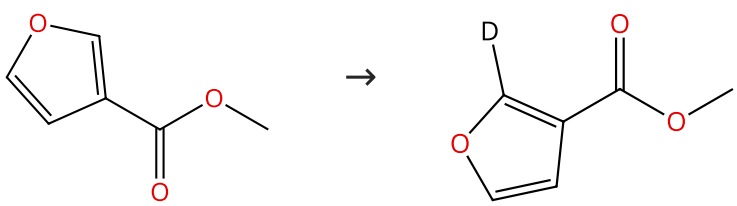
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 266 (1 Reaction)

Steps: **1**



Suppliers (68)

31-116-CAS-593271 Steps: 1

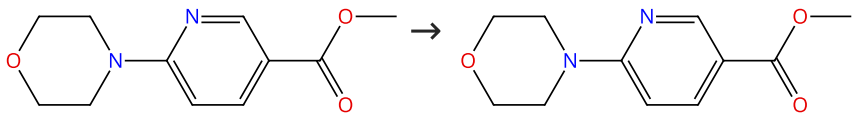
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), dihydrobis(2-propanone)bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane

Investigation of iridium hydride complex $[IrH_2(Me_2CO)_2(PPh_3)_2]BF_4$ as a catalyst of hydrogen isotope exchange of substrates in solution

By: Heys, Richard

Journal of the Chemical Society, Chemical Communications (1992), (9), 680-1.

Scheme 267 (1 Reaction) Steps: **1**



Suppliers (57)

31-614-CAS-30254870 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

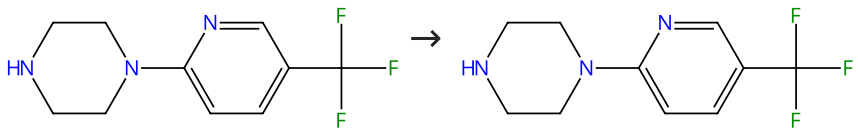
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 268 (1 Reaction) Steps: **1**



Suppliers (80)

31-614-CAS-30197731 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

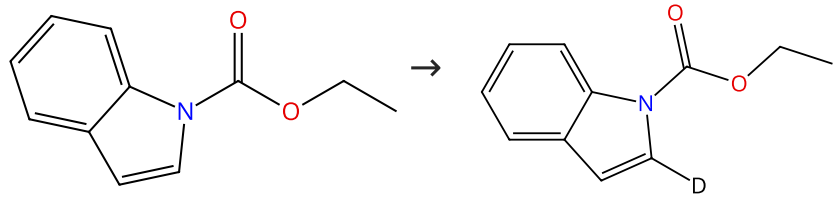
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 269 (1 Reaction) Steps: **1**



Suppliers (12)

31-116-CAS-18343776 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

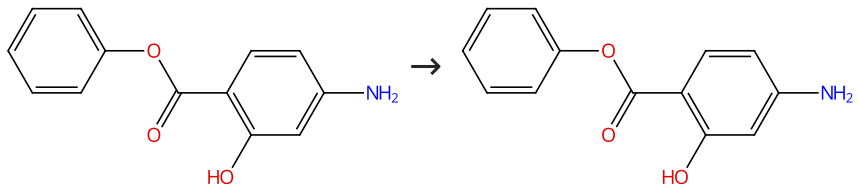
Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 270 (1 Reaction) Steps: **1**



Suppliers (48)

31-614-CAS-25649581 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

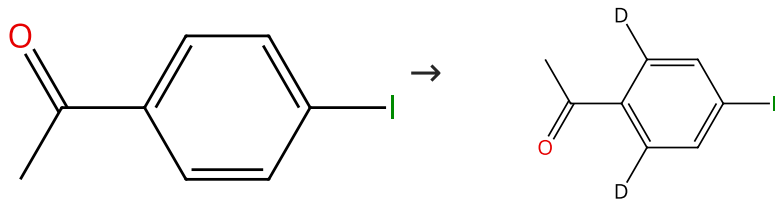
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 271 (1 Reaction) Steps: **1**



Suppliers (93)

31-116-CAS-11293701 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

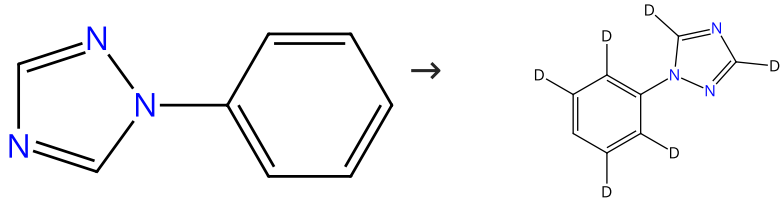
Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 272 (1 Reaction) Steps: **1**



Suppliers (60)

31-116-CAS-22794813 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

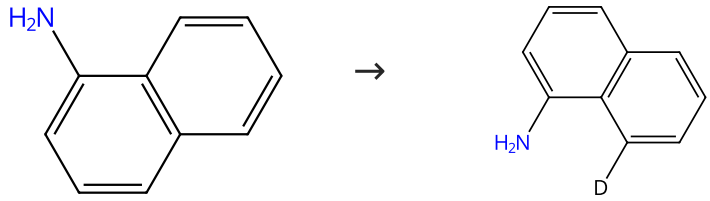
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 273 (1 Reaction) Steps: **1**



Suppliers (73)

31-116-CAS-17237214 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

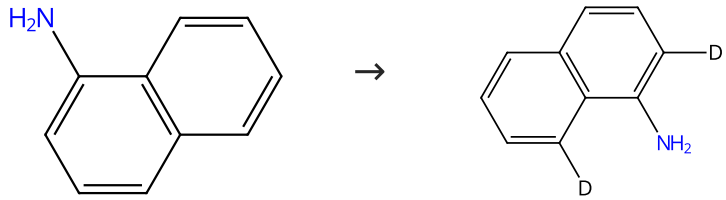
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 274 (1 Reaction) Steps: **1**



Suppliers (73)

31-116-CAS-21649665 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

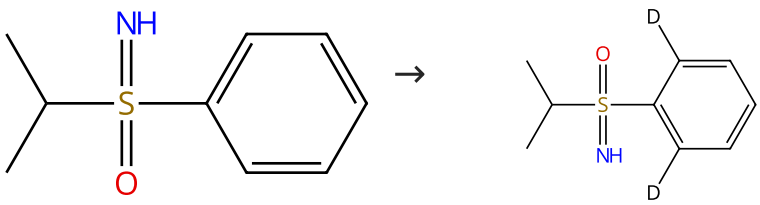
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 275 (1 Reaction) Steps: **1**



Suppliers (6)

31-614-CAS-42989274 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

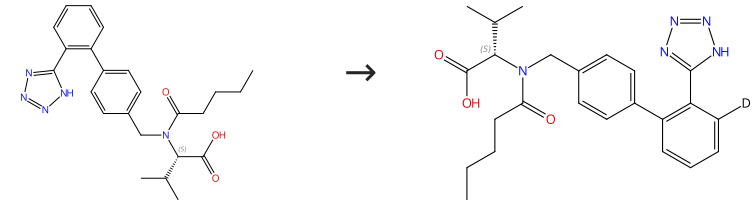
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 276 (1 Reaction) Steps: **1**



Absolute stereochemistry shown

Absolute stereochemistry shown

Suppliers (124)

31-116-CAS-15607199 Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 6 h, 1 atm, 50 °C

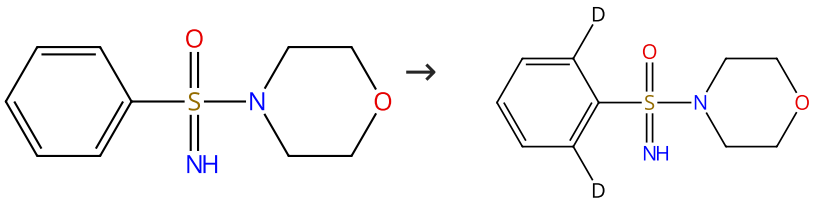
Experimental Protocols

Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 277 (1 Reaction) Steps: **1**



Suppliers (6)

31-614-CAS-42989286 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

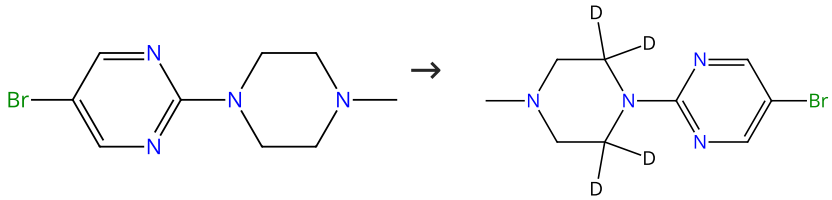
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 278 (1 Reaction)

Steps: **1**



Suppliers (58)

31-116-CAS-19412276

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

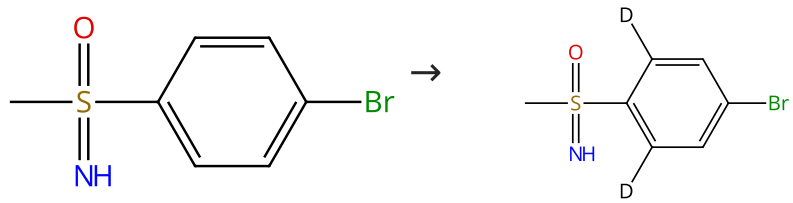
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 279 (1 Reaction)

Steps: **1**



Suppliers (50)

31-614-CAS-42989266

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

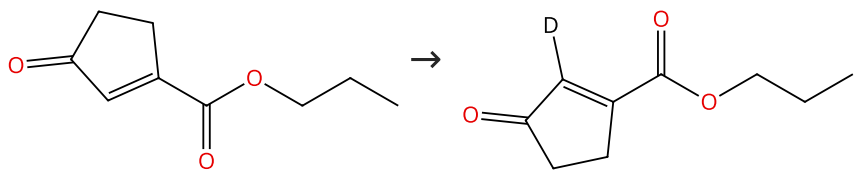
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 280 (1 Reaction)

Steps: **1**



Suppliers (2)

31-116-CAS-16073166 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 10 min, 25 °C

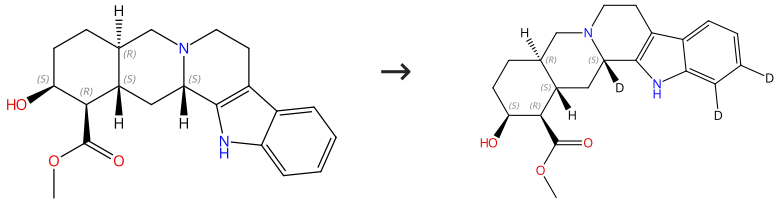
Experimental Protocols

The labeling of unsaturated γ-hydroxybutyric acid by heavy isotopes of hydrogen: iridium complex-mediated H/D exchange by C-H bond activation vs reduction by boro-deuterides/tritides

By: Marek, Ales; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(12), 476-483.

Scheme 281 (1 Reaction) Steps: **1**



Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown

Suppliers (46)

31-116-CAS-22794824 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

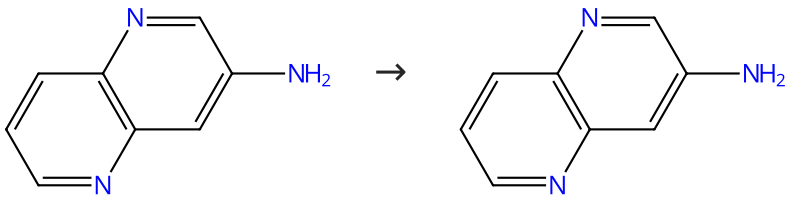
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 282 (1 Reaction) Steps: **1**



Suppliers (69)

31-614-CAS-27488765 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

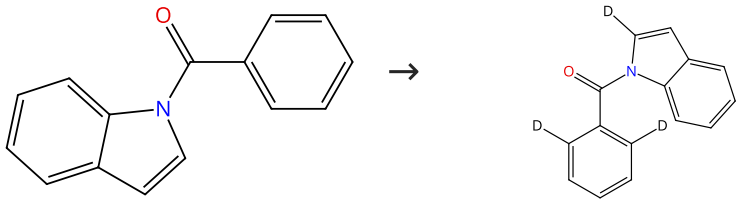
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 283 (1 Reaction) Steps: **1**



Suppliers (20)

31-116-CAS-18343778 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 24 h, 1 atm, 25 °C

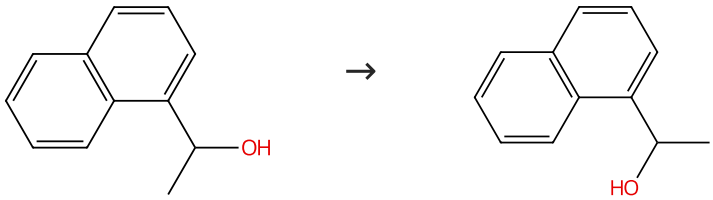
Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 284 (1 Reaction) Steps: **1**



Suppliers (85)

31-614-CAS-29617115 Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

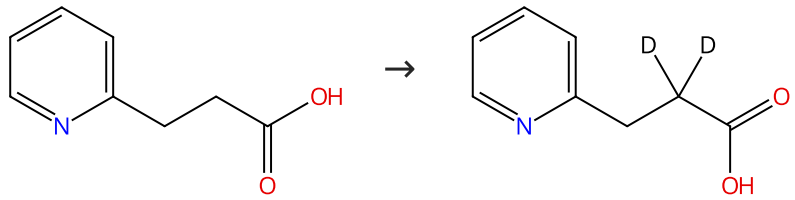
Experimental Protocols

Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 285 (1 Reaction) Steps: **1**



Suppliers (76)

31-116-CAS-19412283 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

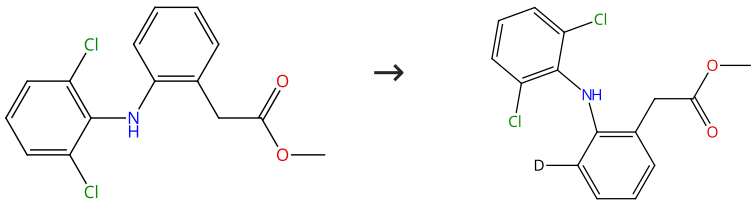
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 286 (1 Reaction) Steps: **1**



Suppliers (75)

31-116-CAS-22794833 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

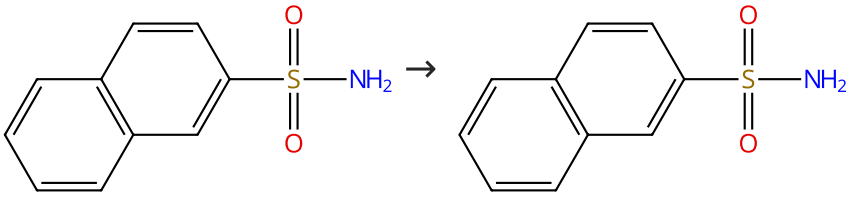
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 287 (1 Reaction) Steps: **1**



Suppliers (57)

31-614-CAS-28058180 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

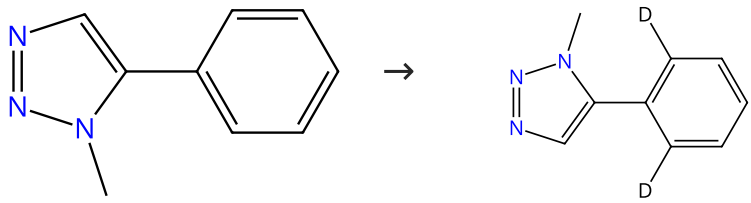
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 288 (1 Reaction) Steps: **1**



Suppliers (7)

31-116-CAS-15600073 Steps: **1**

1.1 **Reagents:** Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

Experimental Protocols

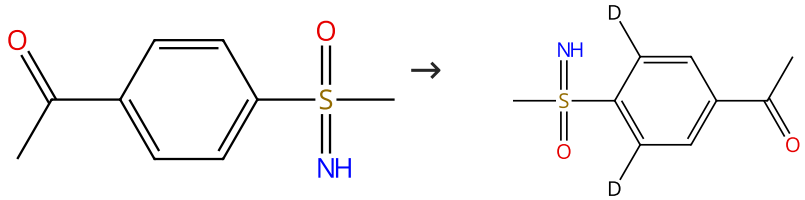
Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 289 (1 Reaction)

Steps: **1**



Suppliers (25)

31-614-CAS-42989298

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

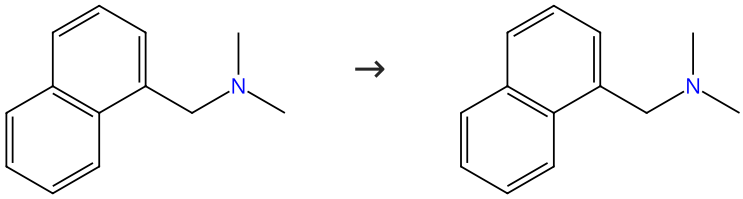
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 290 (1 Reaction)

Steps: **1**



Suppliers (44)

31-614-CAS-26077175

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

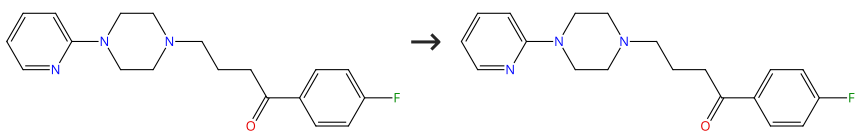
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 291 (1 Reaction)

Steps: **1**



Suppliers (90)

31-614-CAS-26493494 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

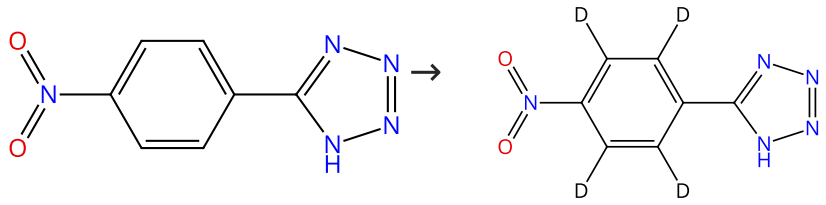
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 292 (1 Reaction) Steps: **1**



Suppliers (63)

31-116-CAS-17238346 Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

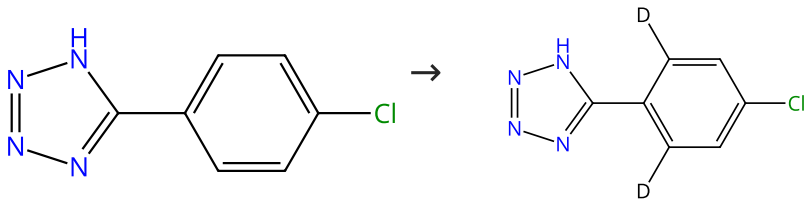
Experimental Protocols

Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 293 (1 Reaction) Steps: **1**



Suppliers (64)

31-116-CAS-15553847 Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

Experimental Protocols

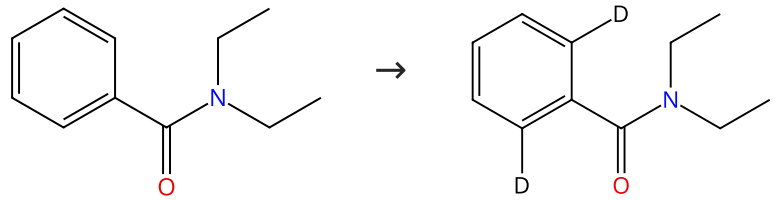
Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 294 (2 Reactions)

Steps: **1**



Suppliers (68)

31-116-CAS-17237228

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

31-116-CAS-11810092

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C

1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

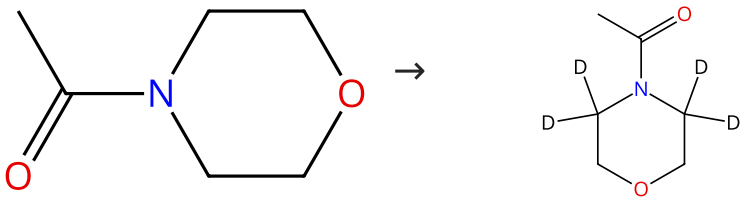
Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

Scheme 295 (1 Reaction)

Steps: **1**



Suppliers (81)

Supplier (1)

31-116-CAS-19412271

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: *tert*-Butyl methyl ether; 3 h, 50 °C

Experimental Protocols

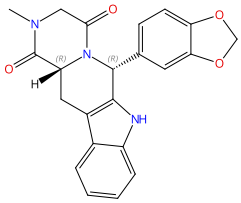
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

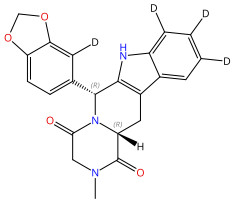
ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 296 (1 Reaction)

Steps: **1**



Absolute stereochemistry shown, Rotation (+)



Absolute stereochemistry shown

Suppliers (97)

31-116-CAS-22794825 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

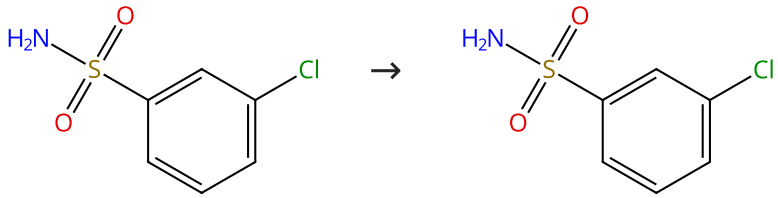
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 297 (1 Reaction)

Steps: **1**



Suppliers (62)

31-614-CAS-29579295 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

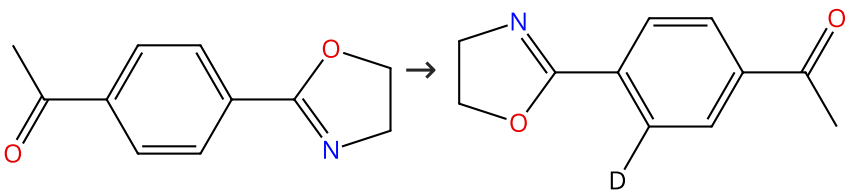
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 298 (1 Reaction)

Steps: **1**



Suppliers (5)

31-614-CAS-23969799 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

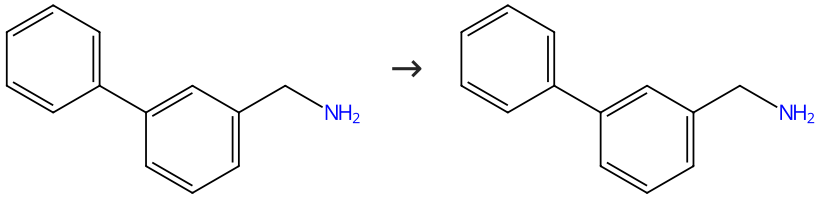
Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 299 (1 Reaction)

Steps: **1**



Suppliers (75)

31-614-CAS-28322820

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

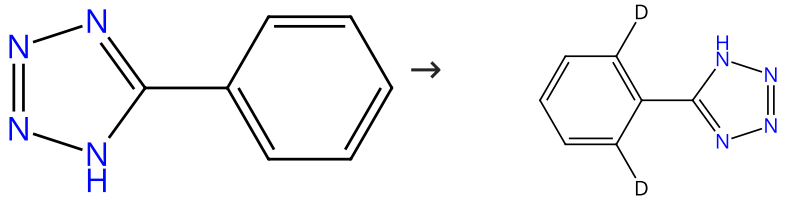
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 300 (1 Reaction)

Steps: **1**



Suppliers (105)

31-116-CAS-15591230

Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

Experimental Protocols

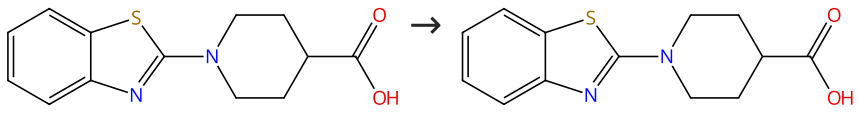
Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 301 (1 Reaction)

Steps: **1**



Suppliers (25)

31-614-CAS-25259669

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: 2-Methyltetrahydrofuran; 1 h, 25 °C

Experimental Protocols

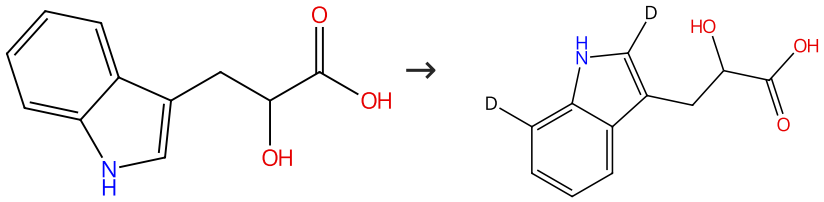
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 302 (1 Reaction)

Steps: **1**



Suppliers (90)

31-116-CAS-22794823

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

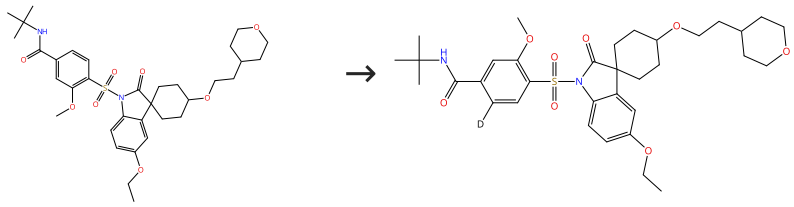
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 303 (1 Reaction)

Steps: **1**



31-116-CAS-2891708

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 42 h, rt

Experimental Protocols

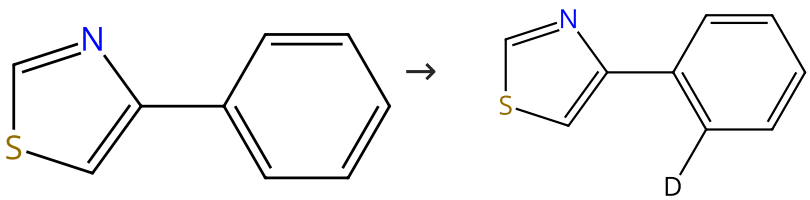
Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

Scheme 304 (1 Reaction)

Steps: **1**



Suppliers (62)

with and without addnl. ortho deuterium

31-116-CAS-10838848

Steps: **1**

1.1 **Catalysts:** Triphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

1.2 **Reagents:** Deuterium

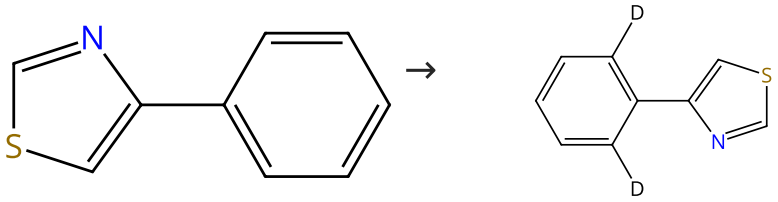
Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 305 (1 Reaction)

Steps: **1**



Suppliers (62)

Supplier (1)

31-116-CAS-3176986

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

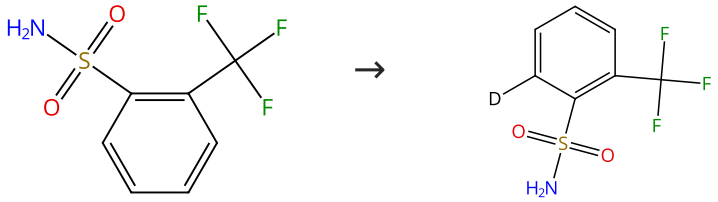
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 306 (1 Reaction)

Steps: **1**



Suppliers (71)

31-116-CAS-119095

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 40 °C; 2 h, 40 °C

Experimental Protocols

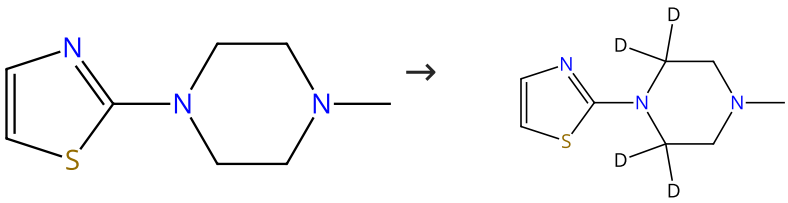
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 307 (1 Reaction)

Steps: **1**



Suppliers (46)

31-116-CAS-19412277

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

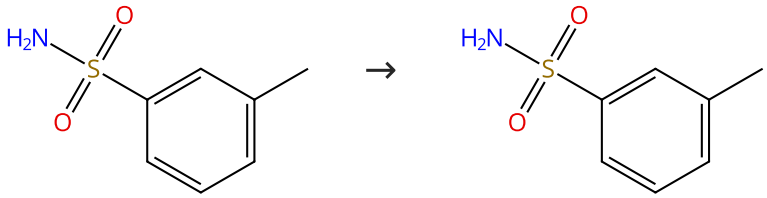
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 308 (1 Reaction)

Steps: **1**



Suppliers (63)

31-614-CAS-28765236

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

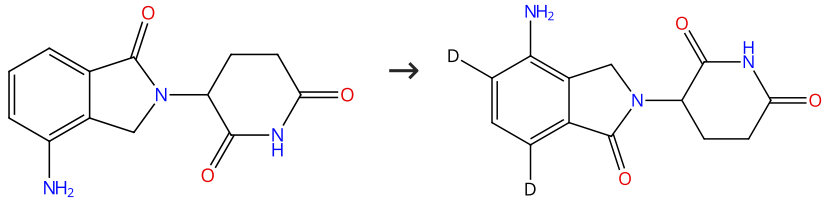
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 309 (1 Reaction)

Steps: **1**



Suppliers (126)

31-116-CAS-22794832

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

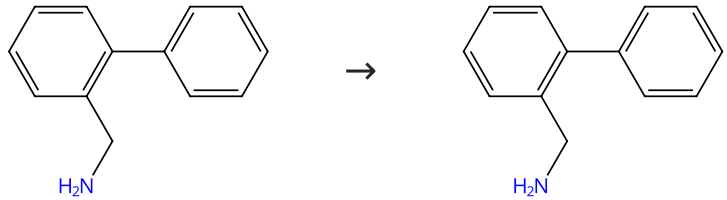
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 310 (1 Reaction)

Steps: **1**



Suppliers (69)

31-614-CAS-26722304

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

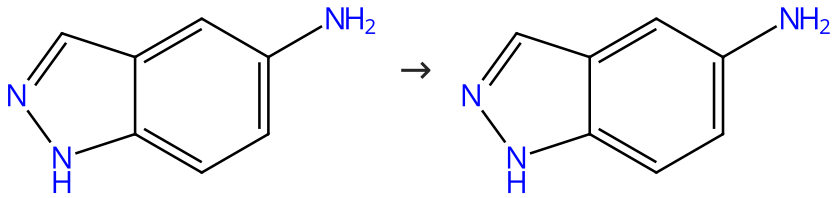
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 311 (1 Reaction)

Steps: **1**



Suppliers (96)

31-614-CAS-26697126

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 312 (1 Reaction)

Steps: **1**

Suppliers (55)

31-116-CAS-21649679

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

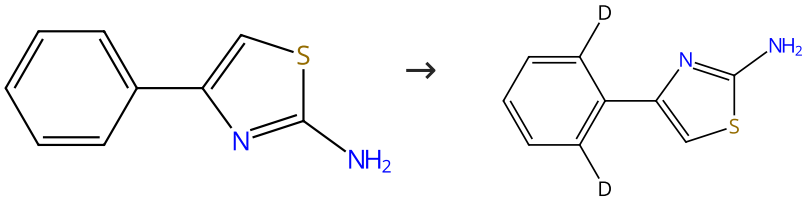
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 313 (1 Reaction)

Steps: **1**



Suppliers (106)

31-116-CAS-8109012

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

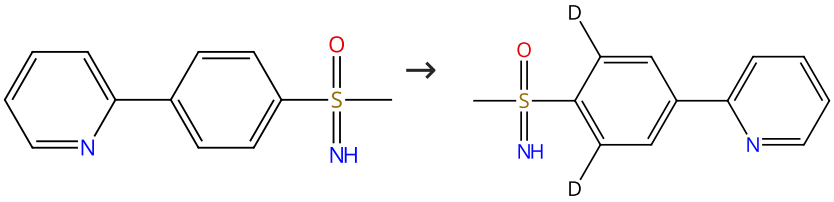
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 314 (1 Reaction)

Steps: **1**



31-614-CAS-42989296

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

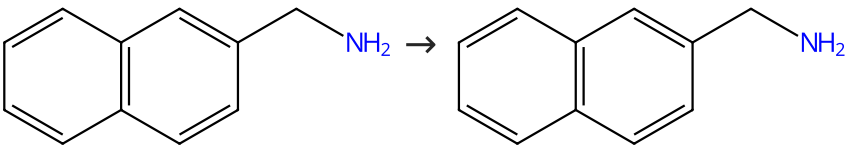
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 315 (1 Reaction)

Steps: **1**



Suppliers (68)

31-614-CAS-26825505

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

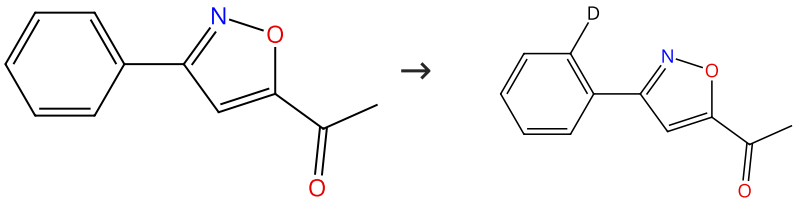
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 316 (1 Reaction)

Steps: **1**



Suppliers (53)

with and without addnl. ortho deuterium

31-116-CAS-8720939

Steps: **1**

1.1 **Catalysts:** Triphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

1.2 **Reagents:** Deuterium

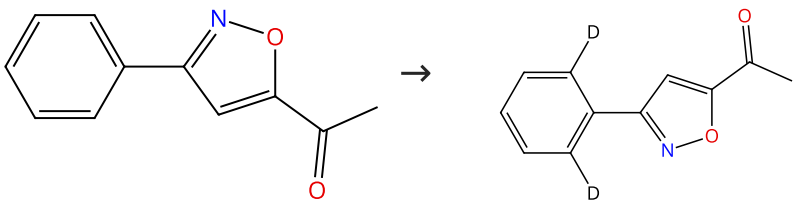
Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 317 (1 Reaction)

Steps: **1**



Suppliers (53)

31-116-CAS-10232859

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

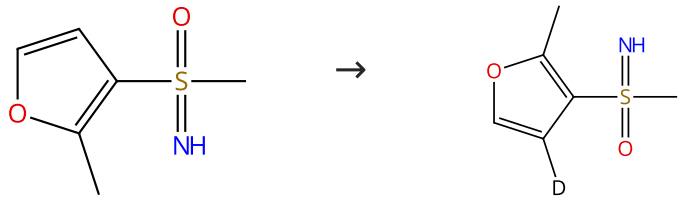
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 318 (1 Reaction)

Steps: **1**



Suppliers (22)

31-614-CAS-42989280

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

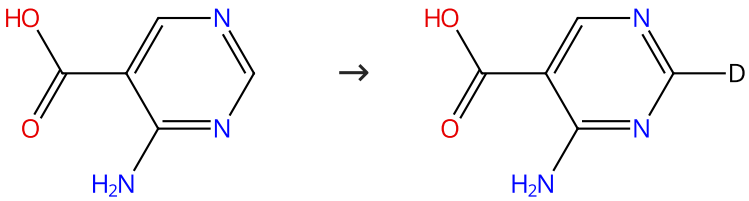
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 319 (1 Reaction)

Steps: **1**



Suppliers (75)

31-116-CAS-10665266

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

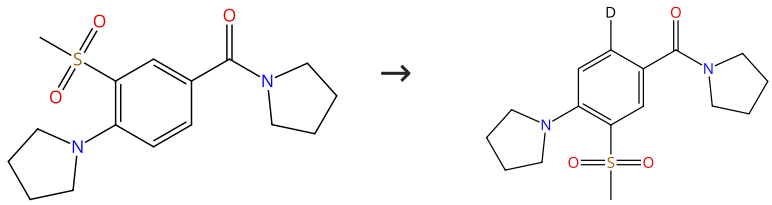
The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 320 (1 Reaction)

Steps: **1**



31-116-CAS-17237227

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

Experimental Protocols

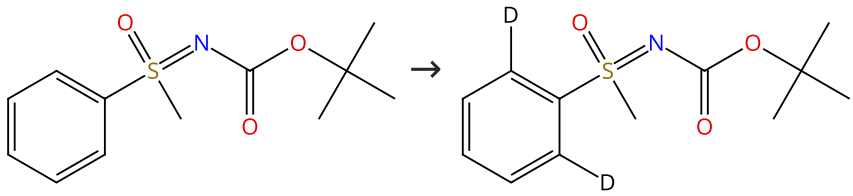
Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 321 (1 Reaction)

Steps: **1**



Suppliers (2)

31-614-CAS-42989295

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 30 °C; 1 h, 30 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

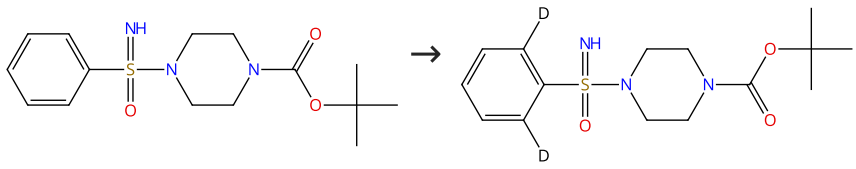
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 322 (1 Reaction)

Steps: **1**



31-614-CAS-42989287

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

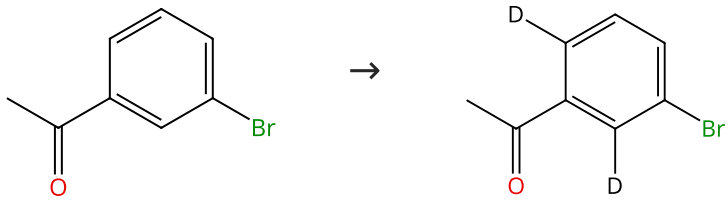
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 323 (1 Reaction)

Steps: **1**



Suppliers (96)

31-116-CAS-3503790

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis (triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

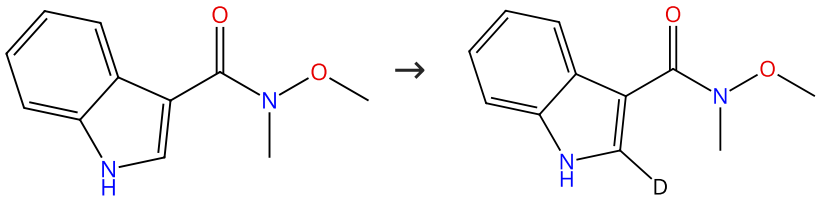
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 324 (1 Reaction)

Steps: **1**



Suppliers (28)

31-116-CAS-18343779

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene] (triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

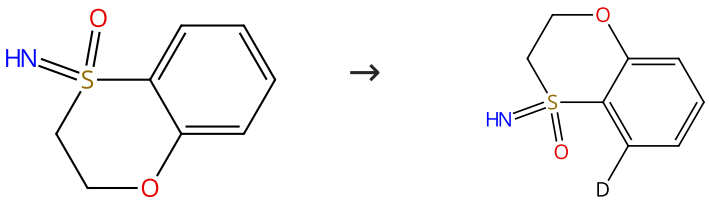
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 325 (1 Reaction)

Steps: **1**



Suppliers (15)

31-614-CAS-42989282

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene] (triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl] borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

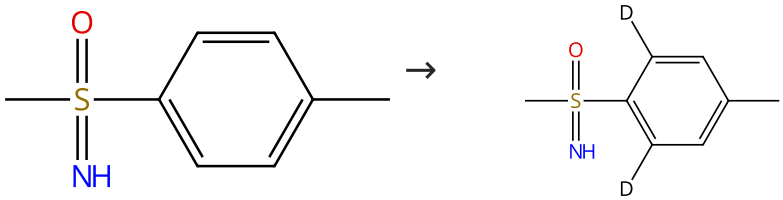
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 326 (1 Reaction)

Steps: **1**



Suppliers (51)

31-614-CAS-42989267

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

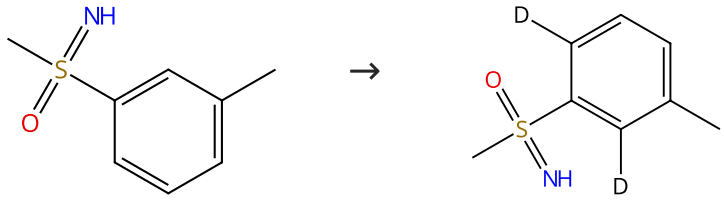
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 327 (1 Reaction)

Steps: **1**



Suppliers (44)

31-614-CAS-42989263

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

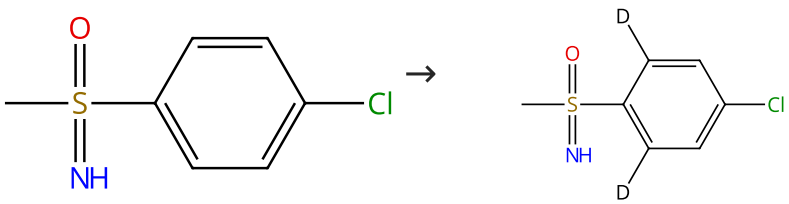
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 328 (1 Reaction)

Steps: **1**



Suppliers (51)

31-614-CAS-42989268 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 329 (1 Reaction) Steps: **1**

Suppliers (31)

31-614-CAS-42989276 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

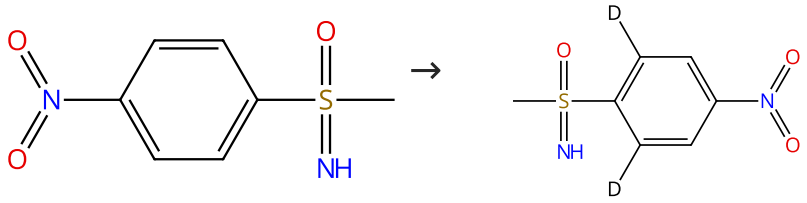
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 330 (1 Reaction) Steps: **1**



Suppliers (40)

31-614-CAS-42989299 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Ethanol; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

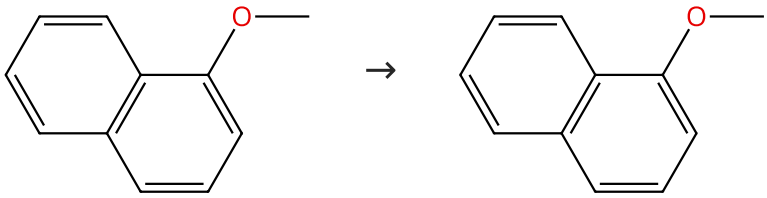
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 331 (1 Reaction)

Steps: **1**



Suppliers (87)

31-614-CAS-27909232

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

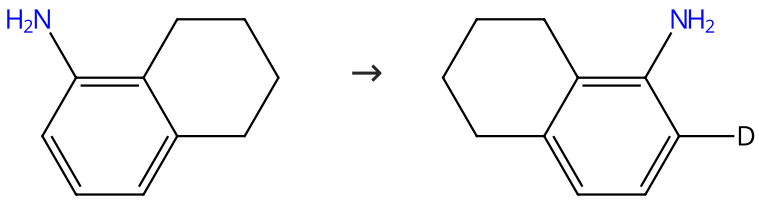
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 332 (1 Reaction)

Steps: **1**



Suppliers (62)

31-116-CAS-21649667

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

Experimental Protocols

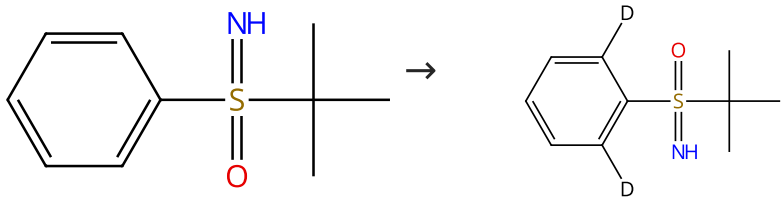
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 333 (1 Reaction)

Steps: **1**



Suppliers (2)

31-614-CAS-42989278 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

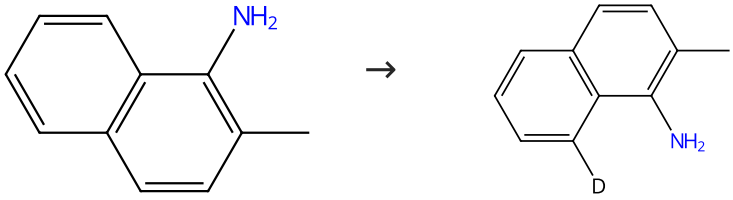
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 334 (1 Reaction) Steps: **1**



Suppliers (79)

31-116-CAS-21649666 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

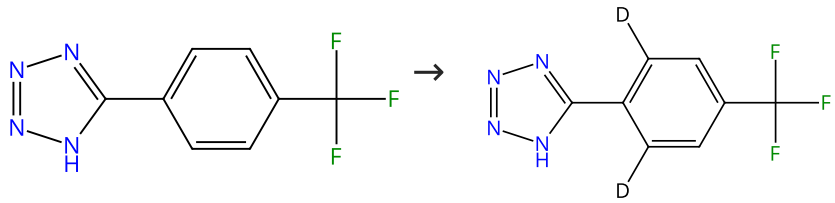
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 335 (1 Reaction) Steps: **1**



Suppliers (55)

31-116-CAS-15567817 Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

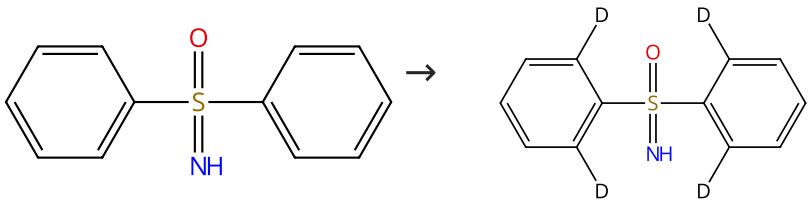
Experimental Protocols

Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 336 (1 Reaction) Steps: **1**



Suppliers (46)

31-614-CAS-42989277 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

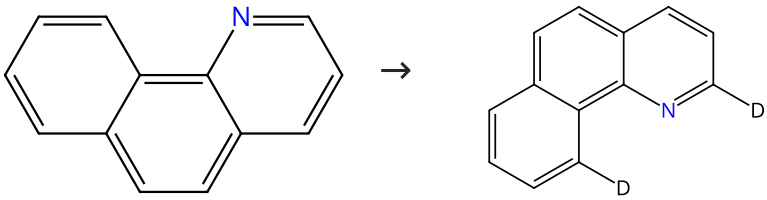
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 337 (1 Reaction) Steps: **1**



Suppliers (81)

31-116-CAS-2737976 Steps: **1**

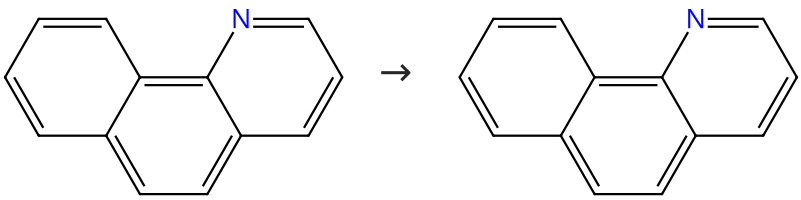
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), dihydrobis(2-propanone)bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane

Investigation of iridium hydride complex $[IrH_2(Me_2CO)_2(PPh_3)_2]BF_4$ as a catalyst of hydrogen isotope exchange of substrates in solution

By: Heys, Richard

Journal of the Chemical Society, Chemical Communications (1992), (9), 680-1.

Scheme 338 (1 Reaction) Steps: **1**



Suppliers (81)

31-614-CAS-30678547 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (polystyrene-supported)
Solvents: Dichloromethane; 1 h, rt

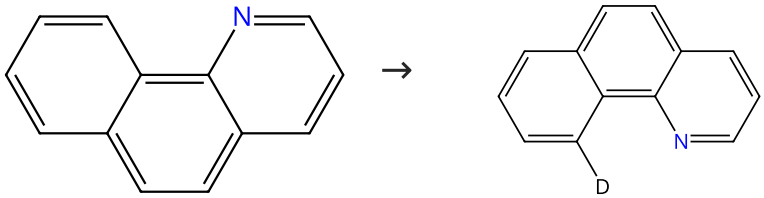
Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

Scheme 339 (3 Reactions)

Steps: **1**



Suppliers (81)

31-116-CAS-3239214

Steps: **1**

1.1 **Catalysts:** Triphenylphosphine (polystyrene-bound), Iridium (1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 2 h, rt

1.2 **Reagents:** Deuterium
Solvents: Dichloromethane; 4 h, rt; 18 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-7773118

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-15521176

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

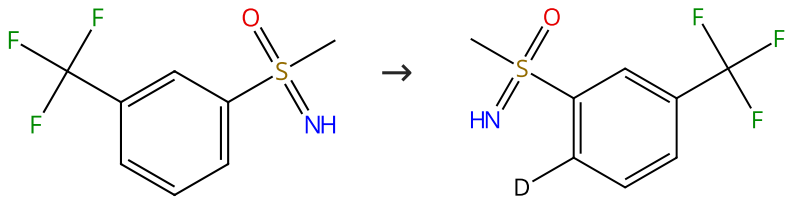
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 340 (1 Reaction)

Steps: **1**



Suppliers (23)

31-614-CAS-42989270

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

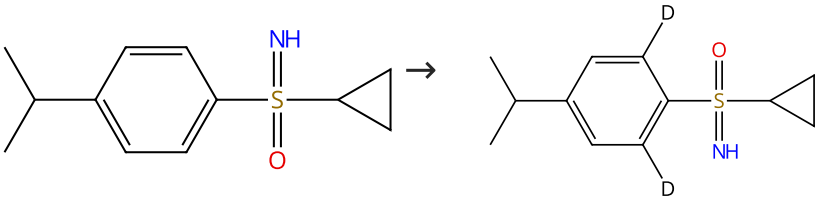
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 341 (1 Reaction)

Steps: **1**



Suppliers (3)

31-614-CAS-42989275

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

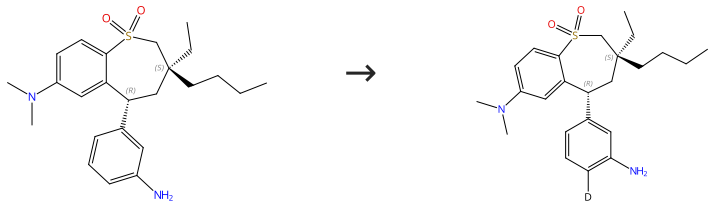
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 342 (1 Reaction)

Steps: **1**



Absolute stereochemistry shown

Absolute stereochemistry shown

31-116-CAS-21649688

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

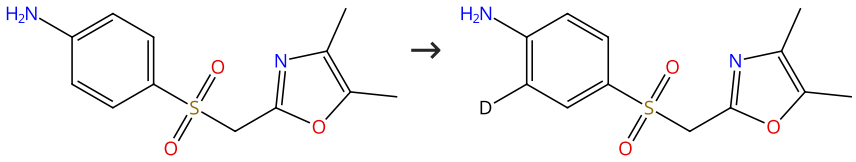
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 343 (1 Reaction)

Steps: **1**



31-116-CAS-21649685

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

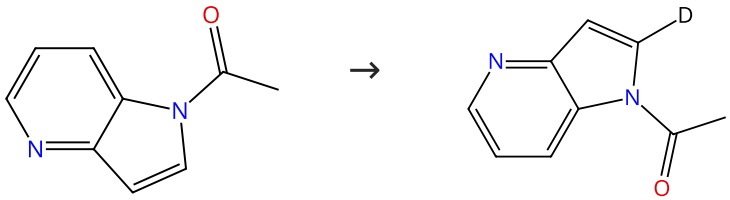
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 344 (1 Reaction)

Steps: **1**



Suppliers (16)

31-116-CAS-18343782

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

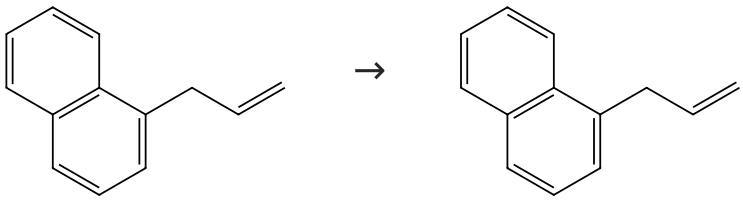
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 345 (1 Reaction)

Steps: **1**



Suppliers (74)

31-614-CAS-30416977

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

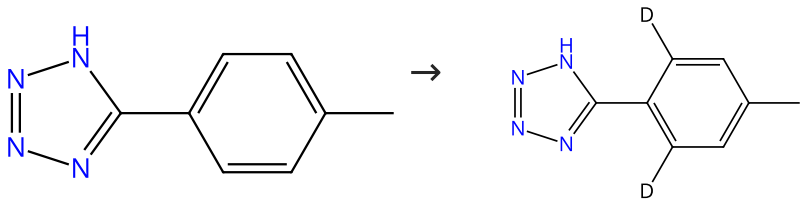
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 346 (1 Reaction)

Steps: **1**



Suppliers (86)

31-116-CAS-15612813

Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

Experimental Protocols

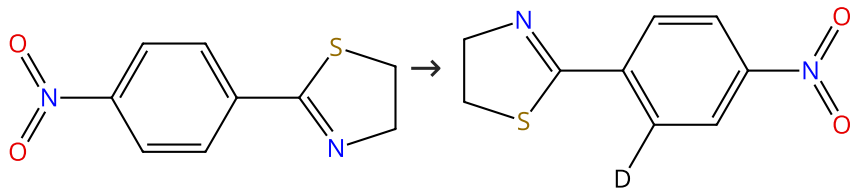
Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 347 (1 Reaction)

Steps: **1**



Suppliers (7)

31-614-CAS-23969801

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

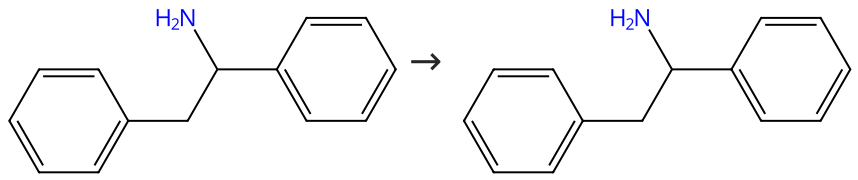
Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 348 (1 Reaction)

Steps: **1**



Suppliers (62)

31-614-CAS-27879631

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylformamide; 4 h, rt

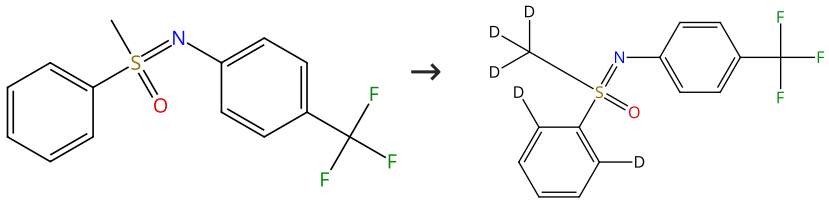
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 349 (1 Reaction)

Steps: **1**



Supplier (1)

31-614-CAS-42989292 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 4 h, 25 °C

1.2 **Reagents:** Acetonitrile

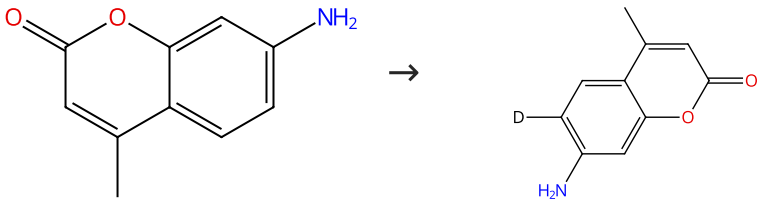
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 350 (1 Reaction) Steps: **1**



Suppliers (113)

31-116-CAS-21649669 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

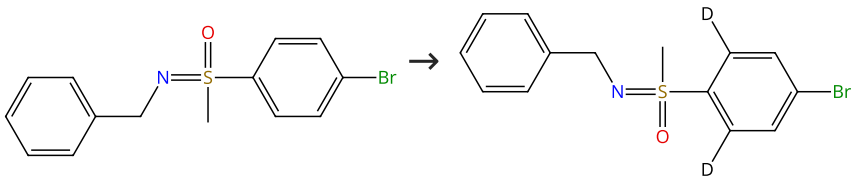
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 351 (1 Reaction) Steps: **1**



31-614-CAS-42989293 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 30 °C; 1 h, 30 °C

1.2 **Reagents:** Acetonitrile

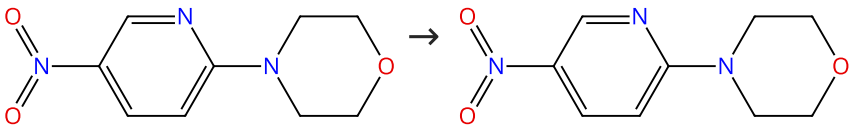
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 352 (1 Reaction) Steps: **1**



Suppliers (69)

31-614-CAS-27040526 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

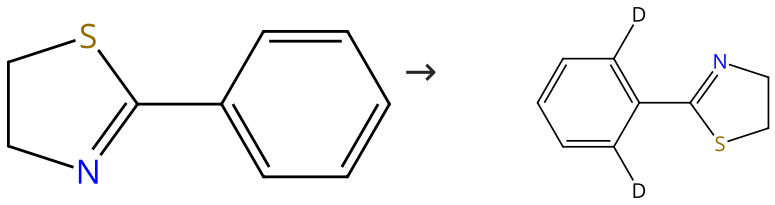
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 353 (1 Reaction) Steps: **1**



Suppliers (8)

31-614-CAS-23969781 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

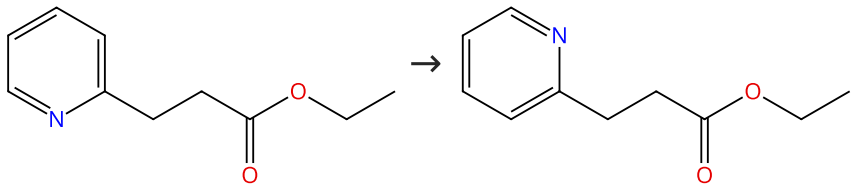
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 354 (1 Reaction) Steps: **1**



Suppliers (58)

31-614-CAS-29122613 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 355 (1 Reaction)

Steps: **1**

Suppliers (101)

Suppliers (31)

31-116-CAS-22794810

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

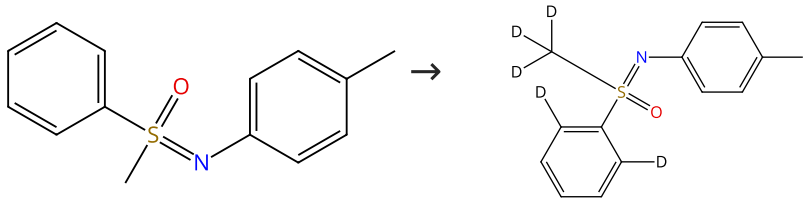
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 356 (1 Reaction)

Steps: **1**



Supplier (1)

31-614-CAS-42989288

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 4 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

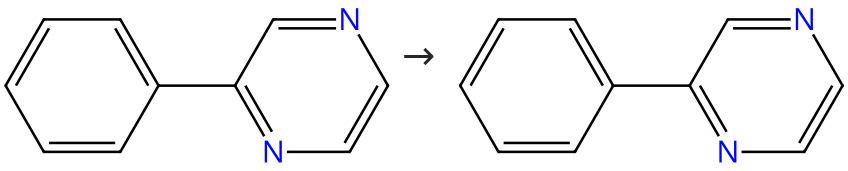
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 357 (1 Reaction)

Steps: **1**



Suppliers (34)

31-614-CAS-26404542

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

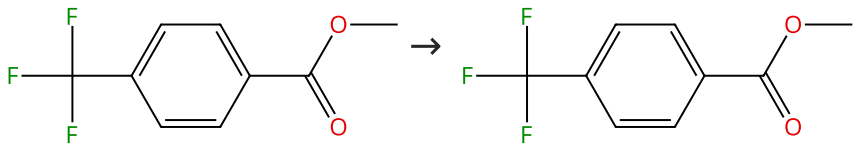
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 358 (1 Reaction)

Steps: **1**



Suppliers (78)

mixture with deuterated analog

31-614-CAS-25027778

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 40 °C; 1 h, 40 °C

Experimental Protocols

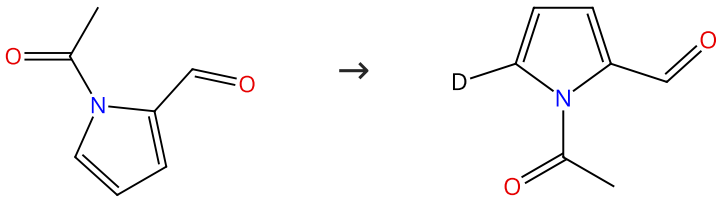
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 359 (1 Reaction)

Steps: **1**



Suppliers (7)

31-116-CAS-18343789

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

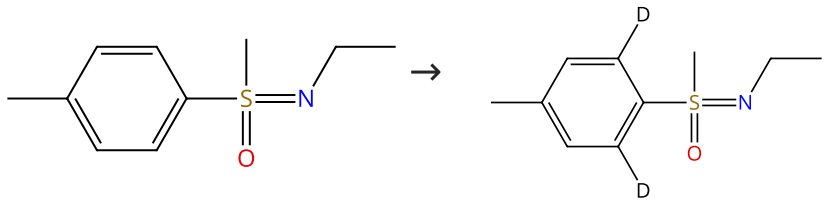
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 360 (1 Reaction)

Steps: **1**



31-614-CAS-42989283

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

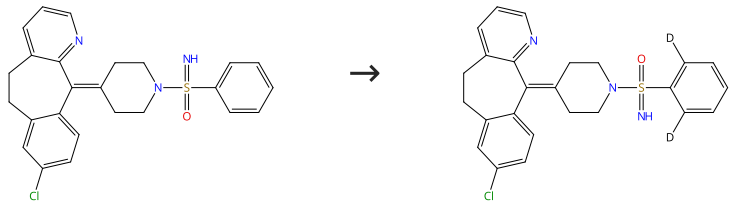
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 361 (1 Reaction)

Steps: **1**



31-614-CAS-42989294

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

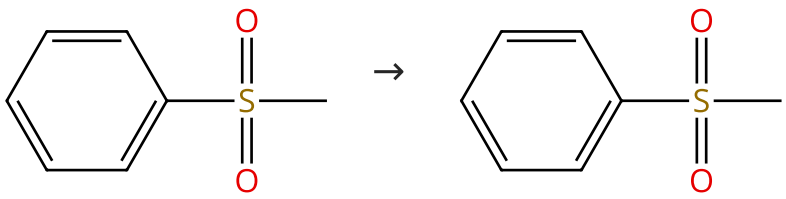
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 362 (2 Reactions)

Steps: **1**



Suppliers (84)

31-614-CAS-26188081

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

31-614-CAS-30314017

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

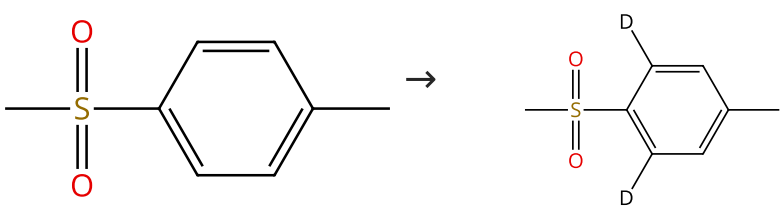
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 363 (1 Reaction)

Steps: **1**



Suppliers (76)

31-116-CAS-17237239 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

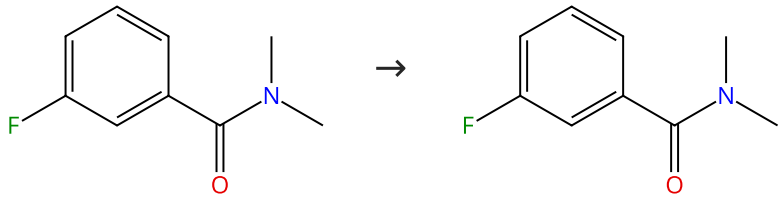
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 364 (1 Reaction) Steps: **1**



Suppliers (9)

31-614-CAS-29475384 Steps: **1**

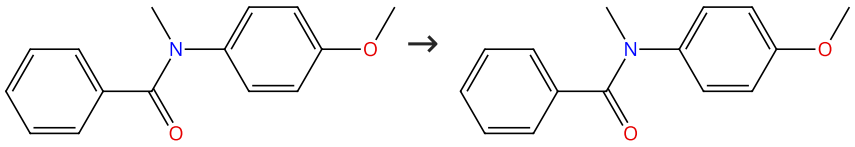
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane-d_2

Meta-substituent effects on organoiridium-catalyzed ortho-hydrogen isotope exchange

By: Heys, J. Richard; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(6), 189-200.

Scheme 365 (2 Reactions) Steps: **1**



Suppliers (9)

31-116-CAS-9468428 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,1'-(1,2-ethanediyl)bis[1,1-diphenylphosphine-κ*P*]]-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 2 - 3 h, rt

The development and use of iridium(I) phosphine systems for ortho-directed hydrogen-isotope exchange

By: Salter, Rhys

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 645-657.

31-116-CAS-7327090 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 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)
Solvents: Dichloromethane; 2 - 3 h, rt

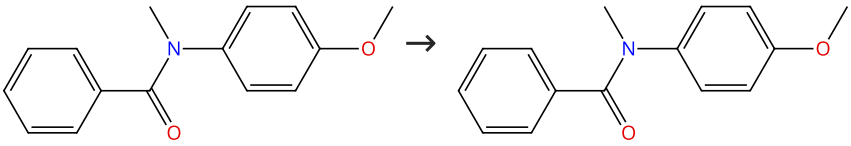
The development and use of iridium(I) phosphine systems for ortho-directed hydrogen-isotope exchange

By: Salter, Rhys

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 645-657.

Scheme 366 (1 Reaction)

Steps: **1**



Suppliers (9)

deuterated

31-614-CAS-25847334

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(triphenyl phosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; overnight, 500 mbar, rt

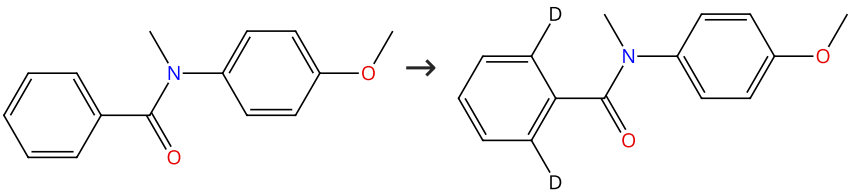
Investigation of isotopic exchange reactions using N-heterocyclic iridium (I) complexes

By: Powell, Mark E.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 523-525.

Scheme 367 (1 Reaction)

Steps: **1**



Suppliers (9)

31-116-CAS-7494068

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Butyl-3-methylimidazolium trifluoromethanesulfonate; 6 h, rt

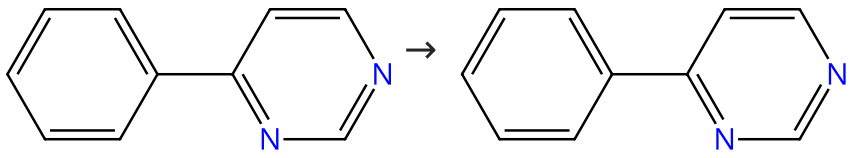
Application of 1-butyl-3-methylimidazolium hexafluorophosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

Scheme 368 (1 Reaction)

Steps: **1**



Suppliers (61)

31-614-CAS-25582927

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

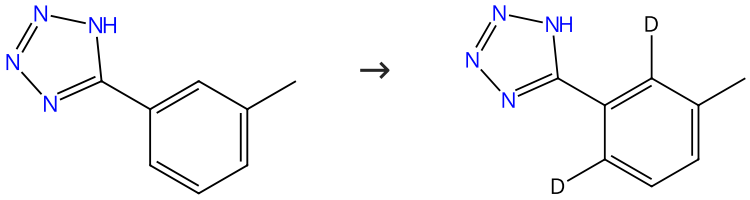
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 369 (1 Reaction)

Steps: **1**



Suppliers (63)

31-116-CAS-15673933

Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

Experimental Protocols

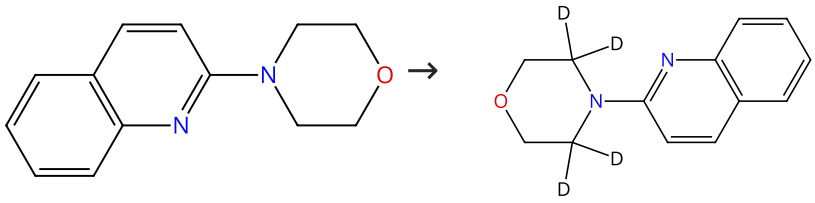
Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 370 (1 Reaction)

Steps: **1**



Suppliers (17)

31-116-CAS-19412269

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

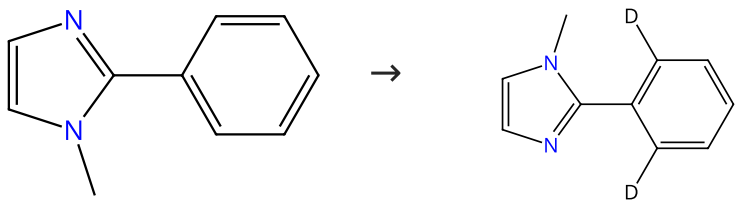
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 371 (1 Reaction)

Steps: **1**



Suppliers (21)

31-614-CAS-23969798 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

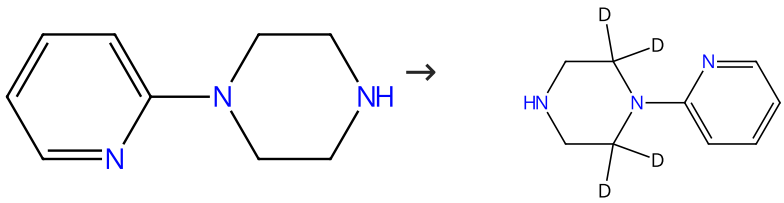
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 372 (1 Reaction) Steps: **1**



Suppliers (108)

31-116-CAS-19412273 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 373 (1 Reaction) Steps: **1**

Suppliers (87)

31-116-CAS-21649661 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 374 (1 Reaction) Steps: **1**

Suppliers (78)

31-116-CAS-21649664 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

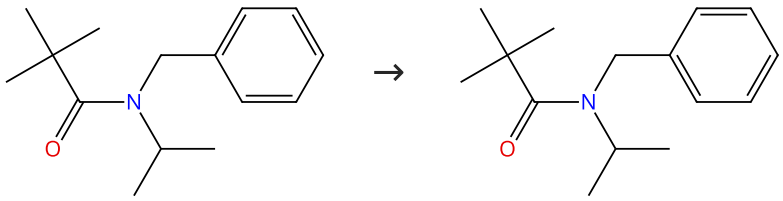
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 375 (1 Reaction) Steps: **1**



Suppliers (40)

31-116-CAS-13734435 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 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)
Solvents: Dichloromethane; 14 h, rt

The development and use of iridium(I) phosphine systems for ortho-directed hydrogen-isotope exchange

By: Salter, Rhys

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 645-657.

CAS SciFinder

Task History

Initiating Search

February 21, 2025, 8:36 PM

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 (880)	Reactions	View Results

Filtered By:

Substance Role: **Reagent**

Catalyst: **[(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium, [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)iridium(1+), [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)iridium(1+), [(1,2,5,6-η)-1,5-Cyclooctadiene][(1*S*)-7'-(diphenylphosphino-κ*P*)-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-indene]-7-carboxylato-κ*O*]iridium, [(1,2,5,6-η)-1,5-Cyclooctadiene](2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium, [μ-[1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2*H*-imidazol-4-yl-2-ylidene-κ*C*^{2}:κ*C*^{4}]][(1,2,5,6-η)-1,5-cyclooctadiene][tris(2,3,4,5,6-pentafluorophenyl)boron]iridium, [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium, Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium, Chloro(1,5-cyclooctadiene)(1,3-**

dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium, Chloro[(2,2-dimethyl-1,2-ethanediyl)[3-(1,1-dimethylethyl)-1*H*-imidazol-1-yl-2(3*H*)-ylidene]][(2,2-dimethyl-1,2-ethanediyl)[3-(1,1-dimethylethyl-κC^2,κH^2)-1*H*-imidazol-1-yl-2(3*H*)-ylidene]]iridium, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Dihydrobis(2-propanone)bis(triphenylphosphine)iridium(1+), Iridium, Iridium(1+), [1,1'-[1,1'-biphenyl]-2,2'-diylbis[1,1-diphenylphosphine-κ*P*]][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(11a*S*)-4,8-bis(1,1-dimethylethyl)-6-[[(1*R*,2*R*)-2-[(2,6-dimethylphenyl)thio-κ*S*]cyclohexyl]oxy]-1,2,10,11-tetramethyldibenzo[*d*,*f*][1,3,2]dioxaphosphepin-κP^6][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,1'-(1,2-ethanediyl)bis[1,1-diphenylphosphine-κ*P*]]-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](pyridine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(pyridine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(tributylphosphine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(tricyclohexylphosphine)-, hexafluorophosphate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1-[(4*S*,5*R*)-4,5-dihydro-5-methyl-2-phenyl-4-oxazolyl-κN^3]-2-phenyl-1-(phenylmethyl)ethyl diphenylphosphinite-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-),

Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1-[(4*S*,5*S*)-4,5-dihydro-5-methyl-2-phenyl-4-oxazolyl-κ*N*^{3}]-2-phenyl-1-(phenylmethyl)ethyl dicyclohexylphosphinite-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(3a*S*,8a*R*)-2-[(1 *S*)-2'-(diphenylphosphino-κ*P*)[1,1'-biphenyl]-2-yl]-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*R*)-2-[2-(diphenylphosphino-κ*P*)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-2-(1,1-dimethylethyl)-4-[2-(diphenylphosphino-κ*P*)ethyl]-4,5-dihydrooxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-2-[(1 *S*)-2'-(diphenylphosphino-κ*P*)[1,1'-biphenyl]-2-yl]-4,5-dihydro-4-(1-methylethyl)oxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-2-[(1 *S*)-2'-(diphenylphosphino-κ*P*)[1,1'-biphenyl]-2-yl]-4,5-dihydro-4-phenyloxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(4*S*)-4-[2-(diphenylphosphino-κ*P*)ethyl]-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yloxazole-κ*N*^{3}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(7*S*)-6,7-dihydro-4-methyl-2-(2,4,6-trimethylphenyl)-5*H*-cyclopenta[*b*]pyridin-7-yl *P*,*P*-dicyclohexylphosphinite-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(8*R*)-8-[(diphenylphosphino-κ*P*)methyl]-5,6,7,8-tetrahydro-2-phenylimidazo[1,2-*a*]pyridine-κ*N*^{1}]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(pyridine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(pyridine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][[*P*(*S*)]-*N*-[(1 *R*)-1-[(4*S*)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κ*N*^{3}]-2-methylpropyl]-*P*-(1,1-dimethylethyl)-*P*-

methylphosphinous amide-κ*P*]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]tris(triphenylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-, Iridium(1+), [1,4-butanediylbis[diphenylphosphine-κ*P*]][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-), Iridium(1+), [(1*R*,3*S*,4*S*)-2-[bis(2-methylphenyl)phosphino-κ*P*]-3-(4-phenyl-2-thiazolyl-κ*N*^{3})-2-azabicyclo[2.2.1]heptane][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(1*S*,3*R*,4*R*)-2-[bis(2-methylphenyl)phosphino-κ*P*]-3-(4,5-dihydro-4,4-diphenyl-2-oxazolyl-κ*N*^{3})-2-azabicyclo[2.2.1]heptane][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [2-[(1*S*)-7'-[bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-4,5-dihydrooxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), 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), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ*N*^{1},κ*N*$^{1'}$]bis[2-(2-pyridinyl-κ*N*)phenyl-κ*C*]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ*N*^{1},κ*N*$^{1'}$]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κ*N*]phenyl-κ*C*]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [(4*S*)-2-[(1*S*)-7'-[bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-4,5-

dihydro-4-methyloxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(4*S*)-2-[(1*S*)-7'-[bis(3,5-dimethylphenyl)phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-4,5-dihydro-4-(1-naphthalenylmethyl)oxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(4*S*)-2-[2-[bis(4-fluorophenyl)phosphino-κ*P*]phenyl]-4-(1,1-dimethylethyl)-4,5-dihydrooxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, stereoisomer, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-), Iridium(1+), [(4*S*)-2-[[bis(1,1-dimethylethyl)phosphino-κ*P*]methyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κ*N*^{3}][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), bis[1,1'-(1*S*)-[1,1'-binaphthalene]-2,2'-diylbis[1,1-diphenylphosphine-κ*P*]]tri-μ-chlorodihydrodi-, chloride (1:1), stereoisomer, Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1), Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), dihydrobis(2-propanone)bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1), Iridium(2+), aqua([4,4'-bipyrimidine]-2,2',6,6'(1*H*,1'*H*,3*H*,3'*H*)-tetrone-κ*N*^{3},κ*N*^{3}')[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, sulfate (1:1), Iridium, chloro[(2,2-dimethyl-1,2-ethanediyl)[3-(1,1-dimethylethyl)-1*H*-imidazol-1-yl-2(3*H*)-ylidene]][1-(1,1-dimethylethyl-κ*C*^{2},κ*H*^{2})-3-(1,1-dimethylethyl)-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*]hydro-, Iridium, compd. with ruthenium (1:2), Iridium, compd. with ruthenium (2:1), Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Iridium trichloride, (*OC*-6-53)-[*N*-[(1'*R*)-7'-[Bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-1,3-dithiane-2-methanamine-κ*N*^{2},κ*S*^{1}]chlorodihydroiridium, (*OC*-6-53)-[*N*-[(1*R*)-7'-[Bis[3,5-bis(1,1-dimethylethyl)phenyl]phosphino-κ*P*]-2,2',3,3'-tetrahydro-1,1'-spirobi[1*H*-inden]-7-yl]-6-methyl-2-pyridinemethanamine-κ*N*^{1},κ*N*^{2}]chlorodihydroiridium, (*SP*-5-43)-[2,6-Bis[[bis(1,1-dimethylethyl)phosphino-κ*P*]oxy]phenyl-κ*C*]chlorohydroiridium, (*SP*-5-43)-[2,6-Bis[[bis(1-methylethyl)phosphino-κ*P*]oxy]phenyl-κ*C*]chlorohydroiridium,

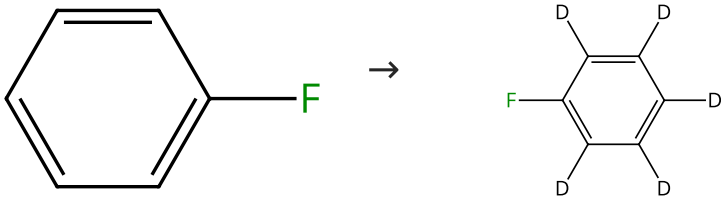
	Stereoisomer of chloro[(1,2-η)-cyclooctene]bis(1,3-dicyclohexyl-1,3-dihydro-2*H*-imidazol-2-ylidene)iridium, Tantalum, [dihydro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium]tris(2,2-dimethylpropyl)-, (*Ir*-*Ta*)
Document Type:	Journal
Language:	English

CAS SciFinder

Reactions (237)

View in CAS SciFinder

Scheme 1 (1 Reaction) Steps: **1**



Suppliers (93) Suppliers (36)

31-116-CAS-20812382 Steps: **1**

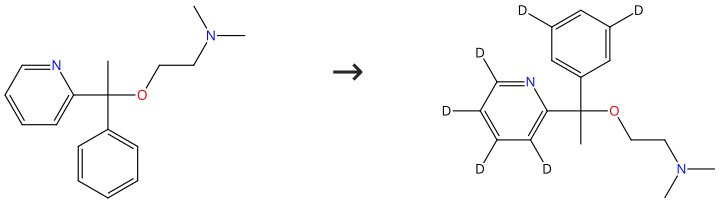
1.1 **Reagents:** Deuterium
Catalysts: Tantalum, [dihydro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium]tris(2,2-dimethylpropyl)-, (*Ir-Ta*) (silica-supported, hydrogenation of)
Solvents: Pentane; 24 h, 800 mbar, 25 °C

Metal-Metal Synergy in Well-Defined Surface Tantalum-Iridium Heterobimetallic Catalysts for H/D Exchange Reactions

By: Lassalle, Sebastien; et al

Journal of the American Chemical Society (2019), 141(49), 19321-19335.

Scheme 2 (1 Reaction) Steps: **1**



Suppliers (30)

31-116-CAS-22794828 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

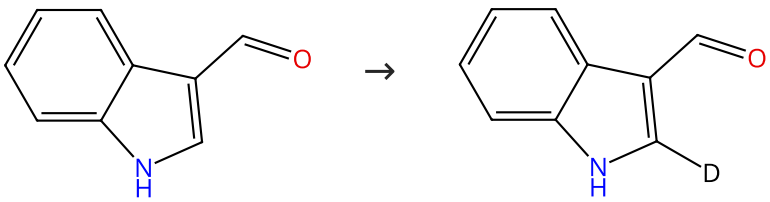
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 3 (1 Reaction) Steps: **1**



Suppliers (123) Supplier (1)

31-116-CAS-18343780 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

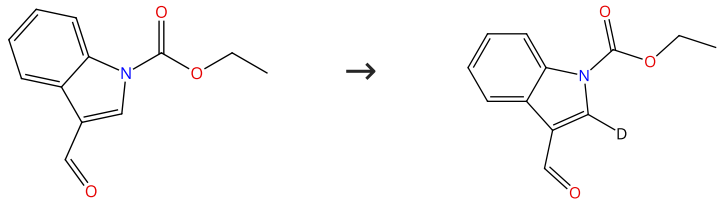
Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 4 (1 Reaction) Steps: **1**



Suppliers (3)

31-116-CAS-18343781 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

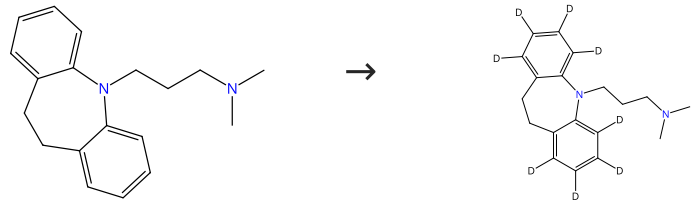
Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 5 (1 Reaction) Steps: **1**



Suppliers (38)

31-116-CAS-22794834 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

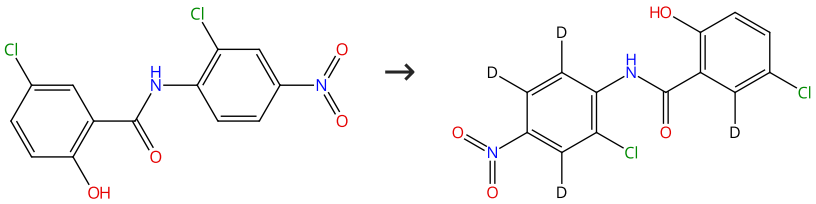
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 6 (3 Reactions) Steps: **1**



Suppliers (92)

31-116-CAS-3051222 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Anion effects to deliver enhanced iridium catalysts for hydrogen isotope exchange processes

By: Kennedy, Alan R.; et al

Organic & Biomolecular Chemistry (2014), 12(40), 7927-7931.

31-116-CAS-9015548 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene][tris(phenylmethyl)phosphine]-, hexafluorophosphate(1-) (1:1)
Solvents: 2-Methyltetrahydrofuran; rt → -78 °C; 1 h, 25 °C

Experimental Protocols

Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes

By: Cochrane, A. R.; et al

Organic & Biomolecular Chemistry (2014), 12(22), 3598-3603.

31-116-CAS-14088015 Steps: **1**

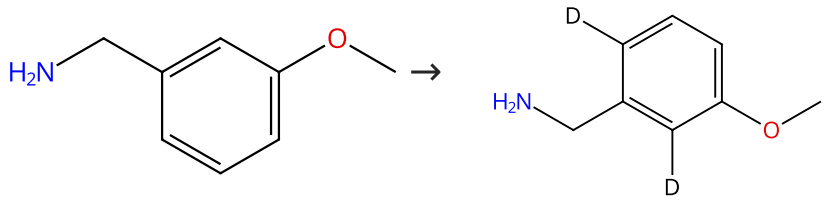
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

The development and use of novel iridium complexes as catalysts for ortho-directed hydrogen isotope exchange reactions

By: Nilsson, Goeran N.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 662-667.

Scheme 7 (2 Reactions) Steps: **1**



Suppliers (89)

31-116-CAS-13804821 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

31-116-CAS-2295326 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylformamide; 4 h, rt

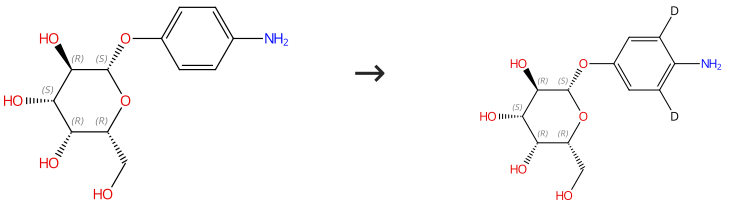
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 8 (1 Reaction)

Steps: **1**



Absolute stereochemistry shown

Absolute stereochemistry shown

Suppliers (62)

31-116-CAS-21649687

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

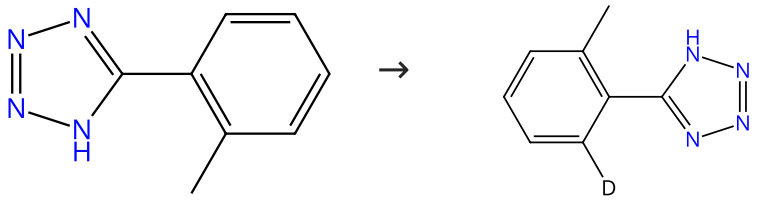
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 9 (1 Reaction)

Steps: **1**



Suppliers (59)

31-116-CAS-15545419

Steps: **1**

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

Experimental Protocols

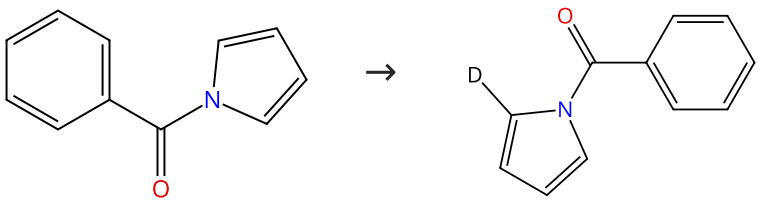
Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 10 (1 Reaction)

Steps: **1**



Suppliers (30)

31-116-CAS-18343786

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

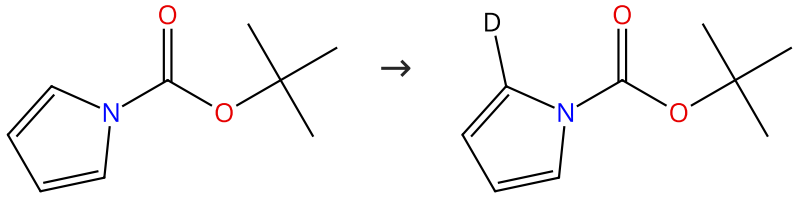
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 11 (1 Reaction)

Steps: **1**



Suppliers (74)

31-116-CAS-18343785

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

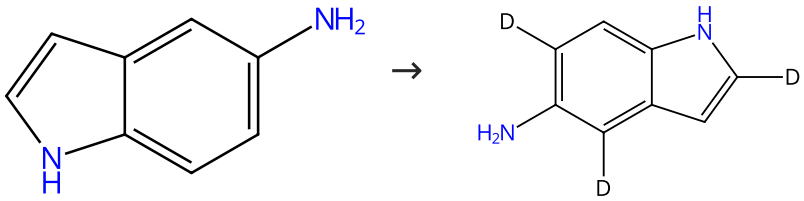
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 12 (1 Reaction)

Steps: **1**



Suppliers (100)

31-116-CAS-21649672

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

Experimental Protocols

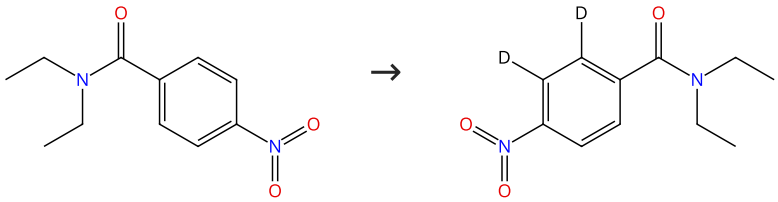
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 13 (1 Reaction)

Steps: **1**



Suppliers (47)

31-116-CAS-15636460

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

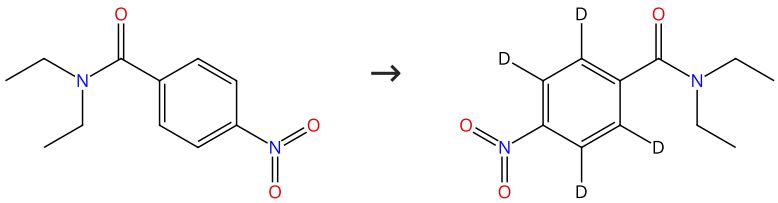
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 14 (1 Reaction)

Steps: **1**



Suppliers (47)

31-116-CAS-16442690

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

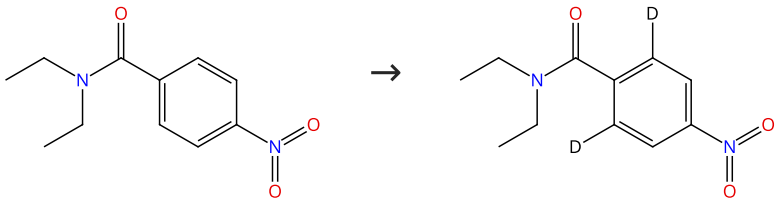
Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

Scheme 15 (1 Reaction)

Steps: **1**



Suppliers (47)

31-116-CAS-16442692

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

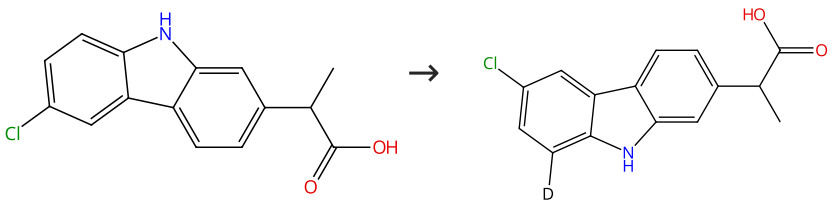
Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

Scheme 16 (1 Reaction)

Steps: **1**



Suppliers (113)

31-116-CAS-22794820

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

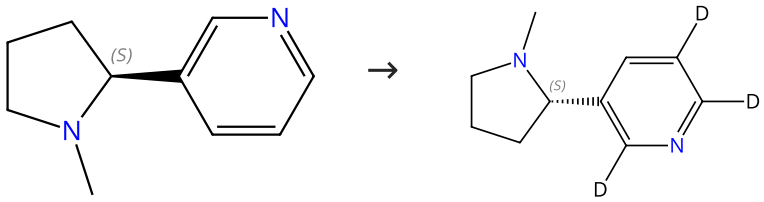
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 17 (1 Reaction)

Steps: **1**



Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (96)

31-116-CAS-22794826

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

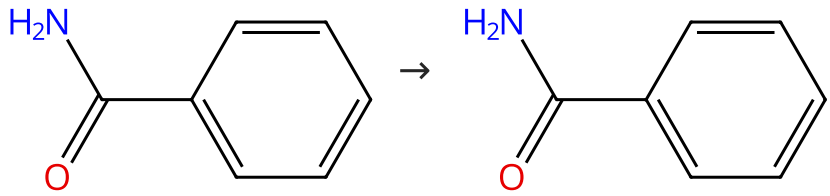
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 18 (1 Reaction)

Steps: **1**



Suppliers (115)

31-614-CAS-29156281

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

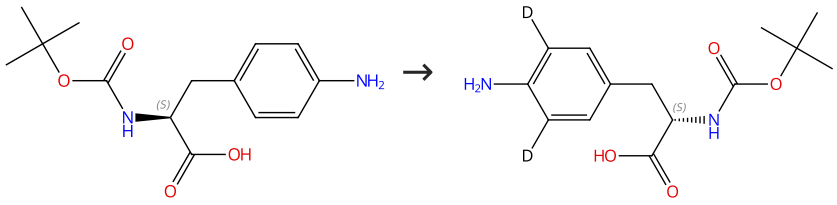
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 19 (1 Reaction)

Steps: **1**



Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown

Suppliers (90)

31-116-CAS-21649680

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

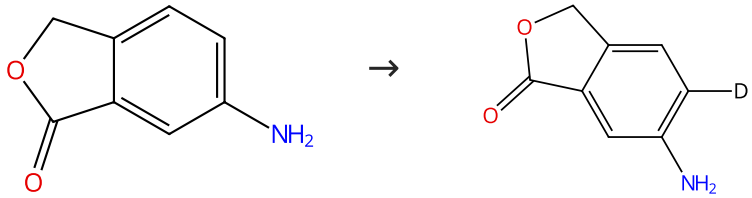
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 20 (1 Reaction)

Steps: **1**



Suppliers (85)

31-116-CAS-21649682

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

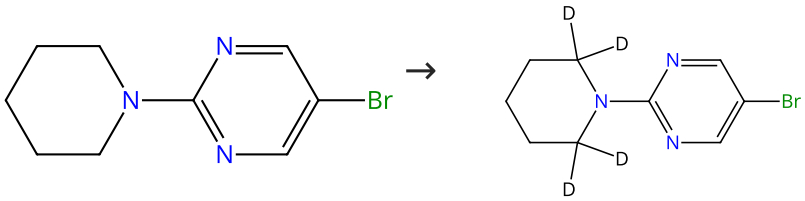
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 21 (1 Reaction)

Steps: **1**



Suppliers (60)

31-116-CAS-19414239

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 22 (1 Reaction)

Steps: **1**

Suppliers (113)

31-614-CAS-27787626

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

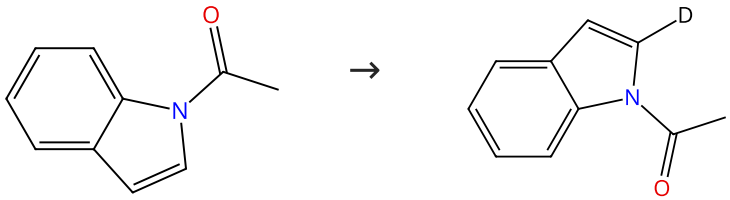
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 23 (1 Reaction)

Steps: **1**



Suppliers (61)

31-116-CAS-18343774

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

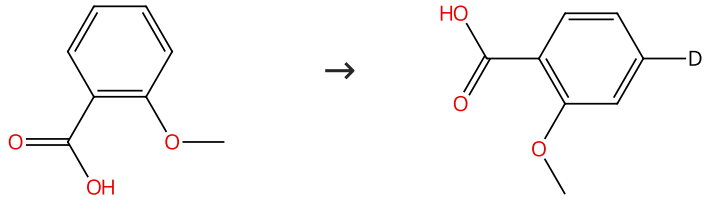
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 24 (1 Reaction)

Steps: **1**



Suppliers (108)

31-116-CAS-11167930

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 2 h, 90 °C; 90 °C → rt

1.2 **Reagents:** Hydrochloric acid
Solvents: Water; acidified, rt

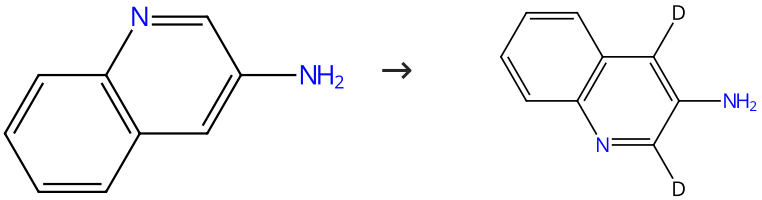
Iridium-catalyzed H/D exchange

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

Scheme 25 (1 Reaction)

Steps: **1**



Suppliers (85)

31-116-CAS-11348113

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

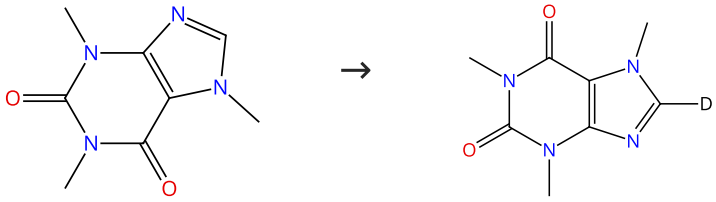
Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 26 (1 Reaction)

Steps: **1**



Suppliers (137)

Suppliers (3)

31-116-CAS-22794817

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

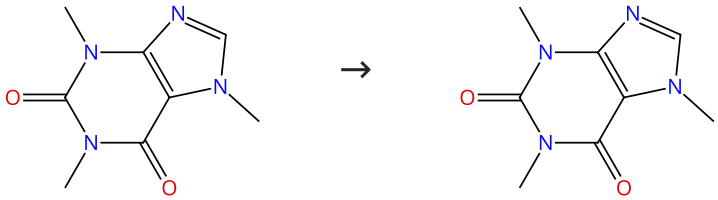
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 27 (1 Reaction)

Steps: **1**



Suppliers (137)

deuterated

31-614-CAS-28183112

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Dihydrobis(2-propanone)bis(triphenylphosphine)iridium(1+)
Solvents: Dichloromethane

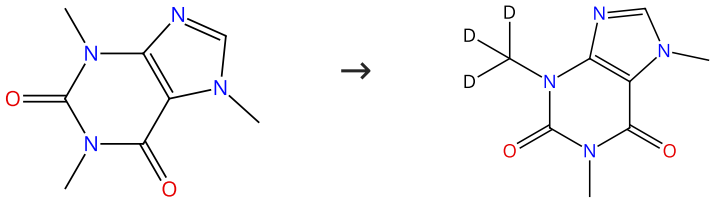
Inter- vs. intramolecular carbon-hydrogen activation: a carbon-hydrogen-iridium bridge in $[IrH_2(mq)L_2]BF_4$ and a C H + M → C M H reaction trajectory

By: Crabtree, Robert H.; et al

Inorganic Chemistry (1985), 24(13), 1986-92.

Scheme 28 (1 Reaction)

Steps: **1**



Suppliers (137)

Suppliers (2)

31-116-CAS-19412285

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

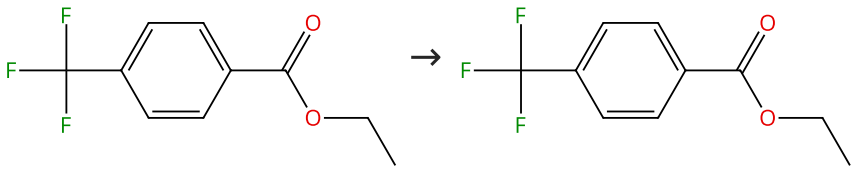
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 29 (1 Reaction)

Steps: **1**



Suppliers (65)

mixture with deuterated analog

31-614-CAS-29811512

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 40 °C; 1 h, 40 °C

Experimental Protocols

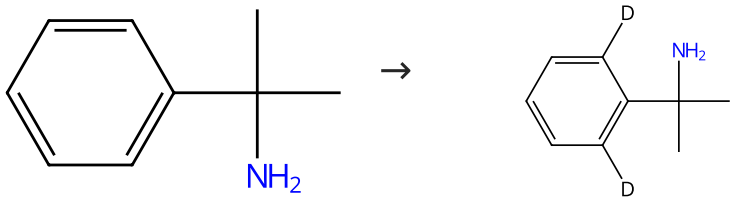
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 30 (1 Reaction)

Steps: **1**



Suppliers (88)

31-116-CAS-12884088

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylformamide; 4 h, rt

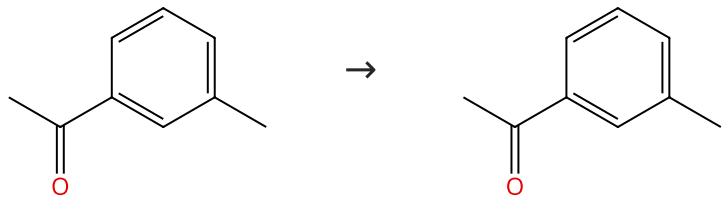
Iridium-catalyzed labeling of anilines, benzylamines and nitrogen heterocycles using deuterium gas and cycloocta-1,5-dienyliridium(I) 1,1,1,5,5,5-hexafluoropentane-2,4-dionate

By: Hickey, Michael J.; et al

Tetrahedron Letters (2003), 44(20), 3959-3961.

Scheme 31 (2 Reactions)

Steps: **1**



Suppliers (86)

31-614-CAS-26532336

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

31-614-CAS-25710176 Steps: 1

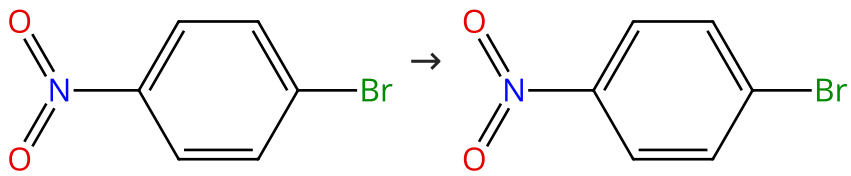
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (polystyrene-supported)
Solvents: Dichloromethane; 1 h, rt

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

Scheme 32 (1 Reaction) Steps: 1



Suppliers (86)

31-614-CAS-25356964 Steps: 1

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

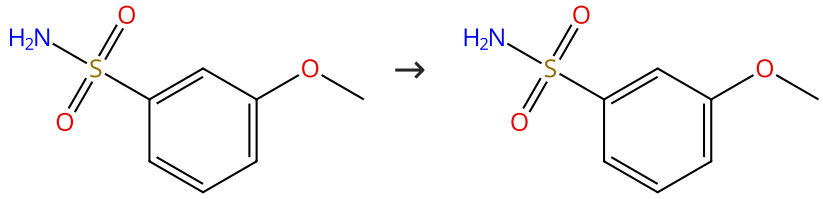
Experimental Protocols

Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 33 (1 Reaction) Steps: 1



Suppliers (54)

31-614-CAS-28540519 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

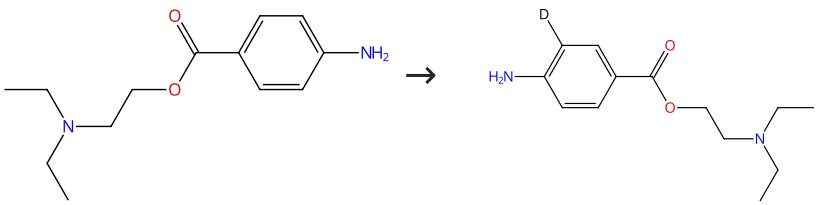
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 34 (1 Reaction) Steps: 1



Suppliers (66)

31-116-CAS-21649673 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

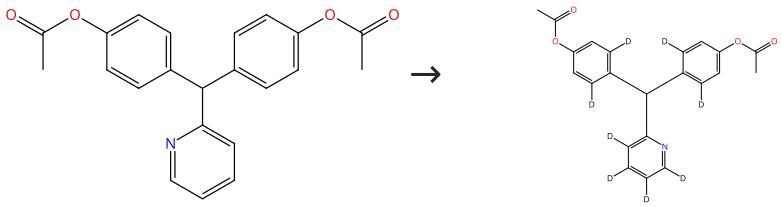
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 35 (1 Reaction) Steps: **1**



Suppliers (95)

31-116-CAS-22794829 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

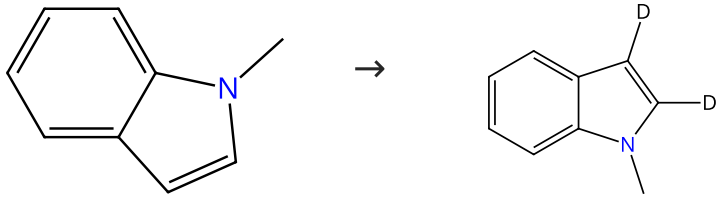
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 36 (1 Reaction) Steps: **1**



Suppliers (107)

31-116-CAS-22794809 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 37 (1 Reaction) Steps: **1**

Suppliers (53)

31-116-CAS-5593896 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 38 (1 Reaction) Steps: **1**

Suppliers (7)

31-116-CAS-18343787 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

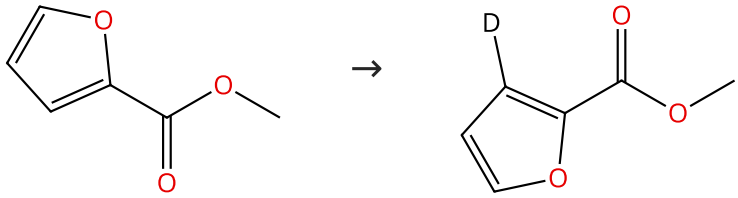
Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 39 (1 Reaction) Steps: **1**



Suppliers (89) Supplier (1)

31-116-CAS-11593800 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 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)
Solvents: Dichloromethane; 2 - 3 h, rt

The development and use of iridium(I) phosphine systems for ortho-directed hydrogen-isotope exchange

By: Salter, Rhys

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 645-657.

Scheme 40 (1 Reaction) Steps: **1**

Suppliers (69) deuterated

31-614-CAS-27372557 Steps: 1

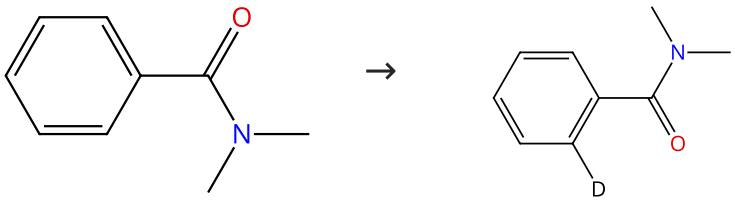
1.1 **Reagents:** Deuterium
Catalysts: Dihydrobis(2-propanone)bis(triphenylphosphine) iridium(1+)
Solvents: Dichloromethane

Inter- vs. intramolecular carbon-hydrogen activation: a carbon-hydrogen-iridium bridge in $[IrH_2(mq)L_2]BF_4$ and a C H + M → CMH reaction trajectory

By: Crabtree, Robert H.; et al

Inorganic Chemistry (1985), 24(13), 1986-92.

Scheme 41 (1 Reaction) Steps: 1



Suppliers (75)

with and without addnl. ortho deuterium

31-116-CAS-6313723 Steps: 1

1.1 **Catalysts:** Methyldiphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η) -1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

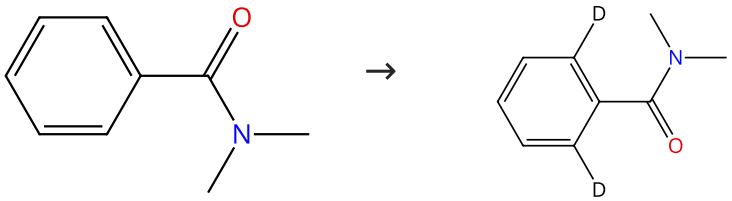
1.2 **Reagents:** Deuterium

Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 42 (3 Reactions) Steps: 1



Suppliers (75)

31-116-CAS-3289937 Steps: 1

1.1 **Catalysts:** Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C

1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the $[(cod)Ir(NHC)(py)]PF_6$ Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

31-116-CAS-6573897 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 4 h, rt

Application of iridium pincer complexes in hydrogen isotope exchange reactions

By: Traeff, Annika; et al

Journal of Organometallic Chemistry (2007), 692(25), 5529-5531.

31-116-CAS-12698213 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1)
Solvents: Methanol; 48 - 72 h, rt

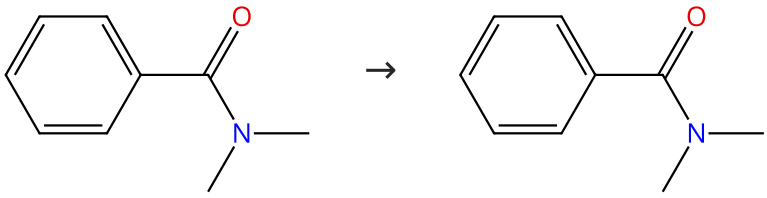
Conditions for deuterium exchange mediated by iridium complexes formed in situ

By: Cross, Paul W. C.; et al

Tetrahedron (2003), 59(18), 3349-3358.

Scheme 43 (1 Reaction)

Steps: **1**



Suppliers (75)

deuterated

31-614-CAS-28680076

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(tricyclohexylphosphine)-, hexafluorophosphate(1-)
Solvents: Dichloromethane; overnight, 500 mbar, rt

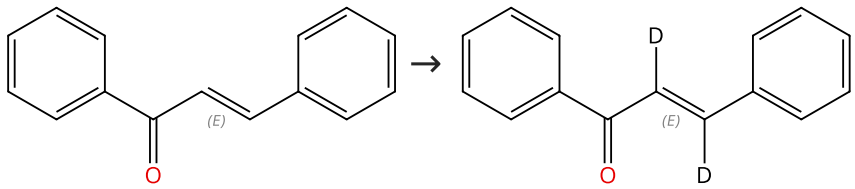
Investigation of isotopic exchange reactions using N-heterocyclic iridium (I) complexes

By: Powell, Mark E.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 523-525.

Scheme 44 (1 Reaction)

Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (78)

31-116-CAS-7574782

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 70 h, rt

Iridium-mediated β-deuteration of enones

By: Gibson, Jennifer S.; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(6), 531-537.

Scheme 45 (1 Reaction)

Steps: **1**

Absolute stereochemistry shown, Rotation (-)

Absolute stereochemistry shown

Suppliers (58)

31-116-CAS-22794835

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

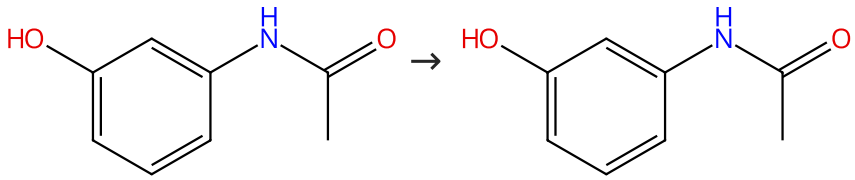
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 46 (1 Reaction)

Steps: **1**



Suppliers (93)

31-614-CAS-30275655

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane

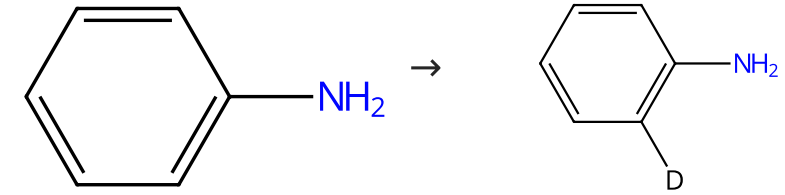
Meta-substituent effects on organoiridium-catalyzed ortho-hydrogen isotope exchange

By: Heys, J. Richard; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(6), 189-200.

Scheme 47 (1 Reaction)

Steps: **1**



Suppliers (120)

Supplier (1)

31-116-CAS-15110414

Steps: **1**

1.1 **Catalysts:** Methyldiphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

1.2 **Reagents:** Deuterium

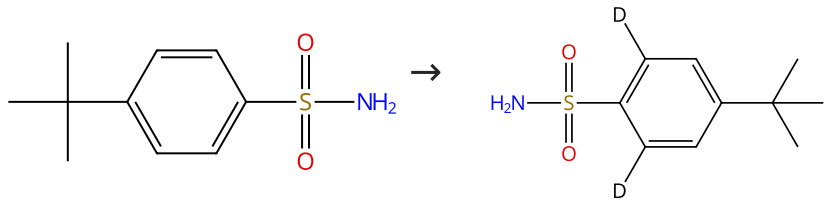
Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 48 (1 Reaction)

Steps: **1**



Suppliers (92)

31-116-CAS-9924694

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

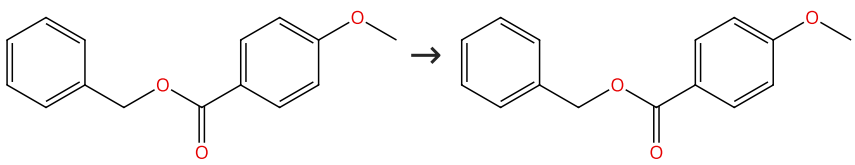
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 49 (1 Reaction)

Steps: **1**



Suppliers (10)

mixture with deuterated analog

31-614-CAS-27454552

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

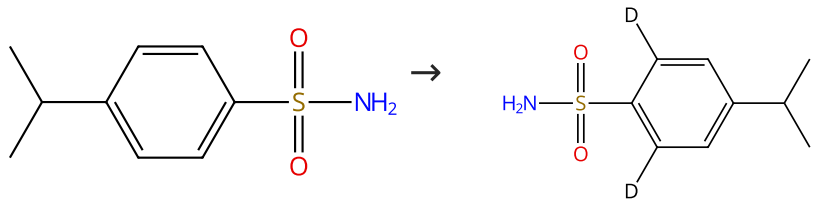
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 50 (1 Reaction)

Steps: **1**



Suppliers (55)

31-116-CAS-14523823

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

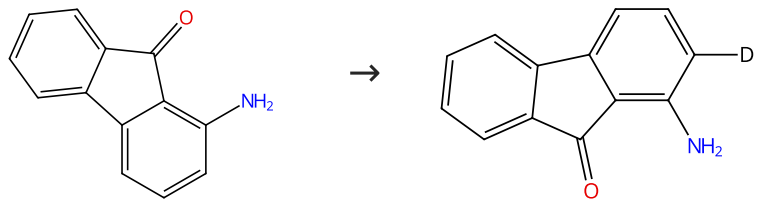
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 51 (1 Reaction)

Steps: **1**



Suppliers (51)

31-116-CAS-21649670

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

Experimental Protocols

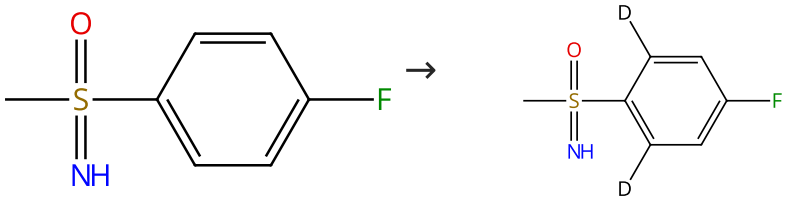
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 52 (1 Reaction)

Steps: **1**



Suppliers (50)

31-614-CAS-42989271

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

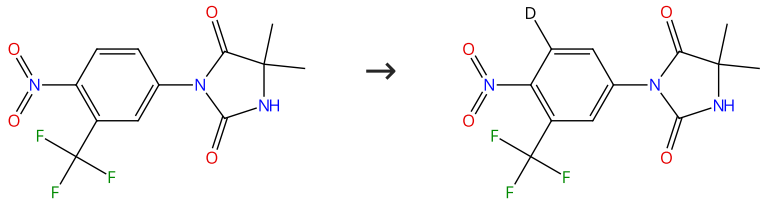
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 53 (2 Reactions)

Steps: **1**



Suppliers (94)

31-116-CAS-16442695

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

31-116-CAS-11956488

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

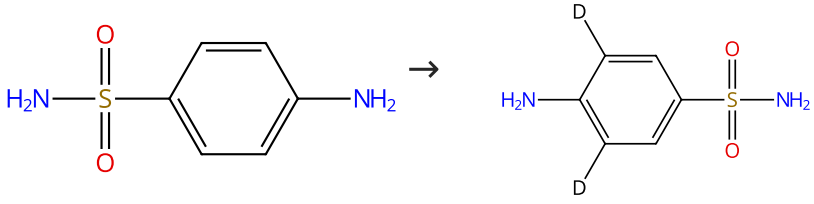
The development and use of novel iridium complexes as catalysts for ortho-directed hydrogen isotope exchange reactions

By: Nilsson, Goeran N.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 662-667.

Scheme 54 (1 Reaction)

Steps: **1**



Suppliers (159)

31-116-CAS-21649675 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

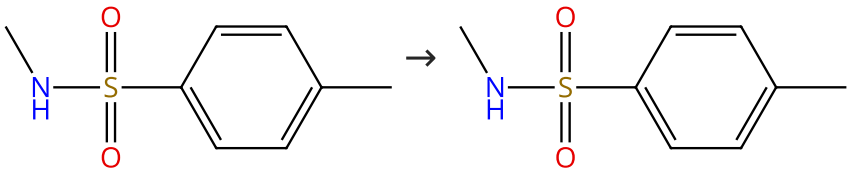
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 55 (1 Reaction) Steps: **1**



Suppliers (81)

31-614-CAS-25590955 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

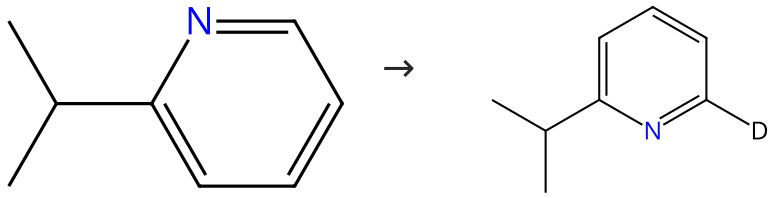
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 56 (1 Reaction) Steps: **1**



Suppliers (64)

Supplier (1)

31-116-CAS-4251612 Steps: **1**

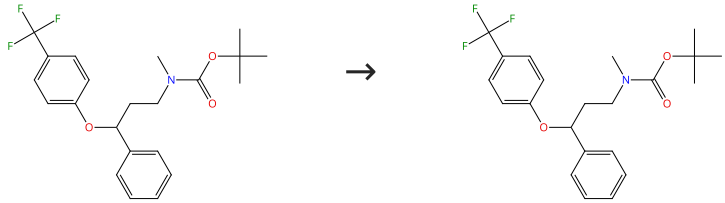
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 57 (1 Reaction) Steps: **1**



31-614-CAS-26187509 Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

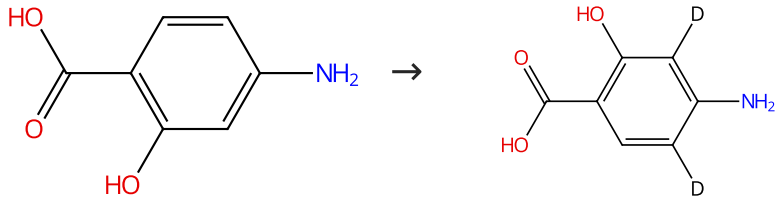
Experimental Protocols

Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 58 (1 Reaction) Steps: **1**



Suppliers (109)

31-116-CAS-9258314 Steps: **1**

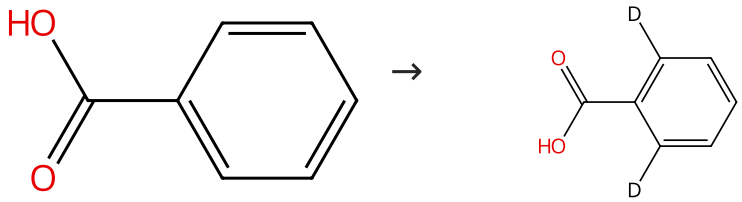
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κ*O*^{2},κ*O*^{4})iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 59 (1 Reaction) Steps: **1**



Suppliers (193)

Suppliers (6)

31-116-CAS-17237229 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

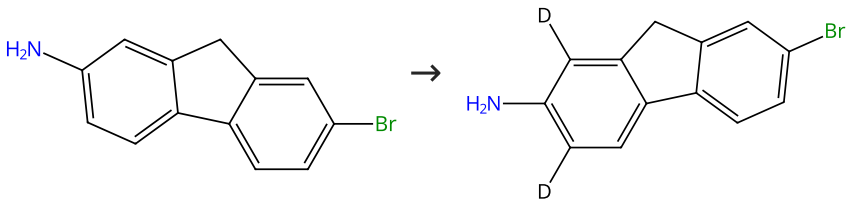
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 60 (1 Reaction) Steps: **1**



Suppliers (76)

31-116-CAS-21649671 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

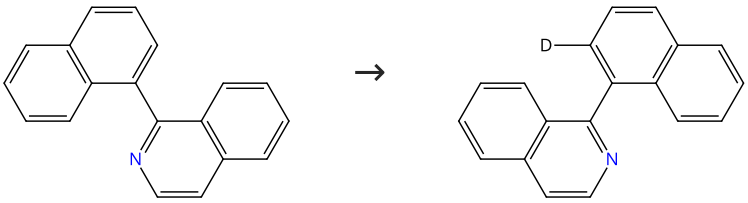
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 61 (1 Reaction) Steps: **1**



Suppliers (8)

31-614-CAS-40147947 Steps: 1

1.1 **Catalysts:** 1,1'-[(4*R*)-[4,4'-Bi-1,3-benzodioxole]-5,5'-diyl]bis[1,1-diphenylphosphine], Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: 1,4-Dioxane; 5 min, rt

1.2 **Reagents:** Deuterium; 24 h, 100 °C

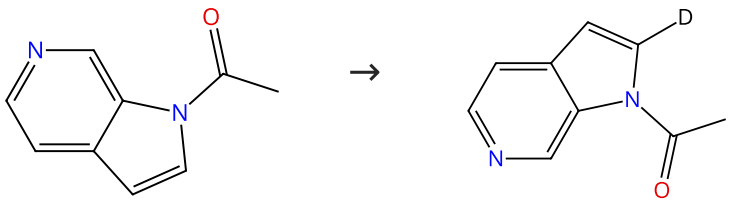
Experimental Protocols

Iridium-Catalyzed Regiodivergent Atroposelective C-H Alkylation of Heterobiaryls with Alkenes

By: Xiong, Maoqian; et al

ACS Catalysis (2024), 14(9), 7243-7255.

Scheme 62 (1 Reaction) Steps: **1**



Suppliers (11) Supplier (1)

31-116-CAS-18343783 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

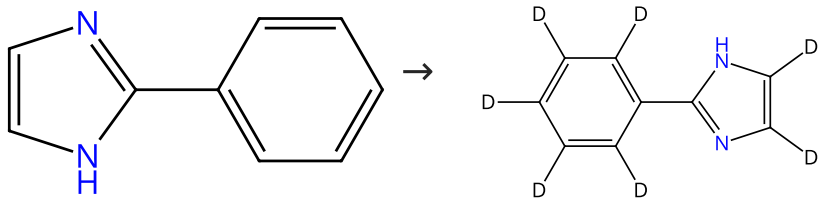
Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 63 (1 Reaction) Steps: **1**



Suppliers (94)

31-116-CAS-22794811 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

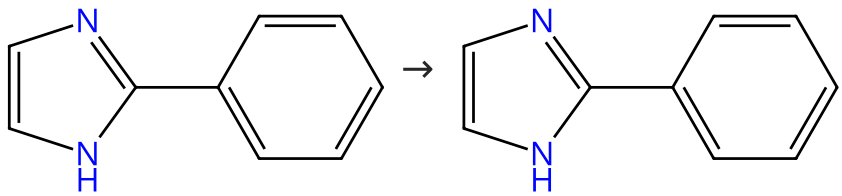
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 64 (1 Reaction) Steps: **1**



Suppliers (94)

deuterated

31-614-CAS-30294169 Steps: 1

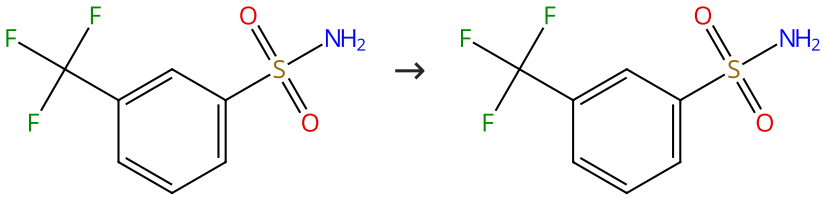
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](1,3-dihydro-1,3-dimethyl-2*H*-imidazol-2-ylidene)(pyridine)-, hexafluorophosphate(1-)
Solvents: Dichloromethane; overnight, 500 mbar, rt

Investigation of isotopic exchange reactions using N-heterocyclic iridium (I) complexes

By: Powell, Mark E.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 523-525.

Scheme 65 (1 Reaction) Steps: **1**



Suppliers (73)

31-614-CAS-26142937 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

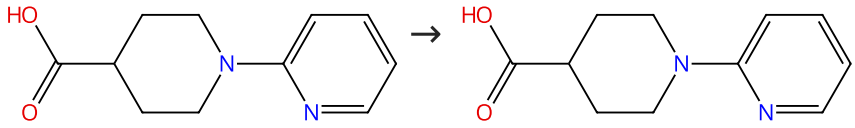
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 66 (1 Reaction) Steps: **1**



Suppliers (62)

31-614-CAS-27104879 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

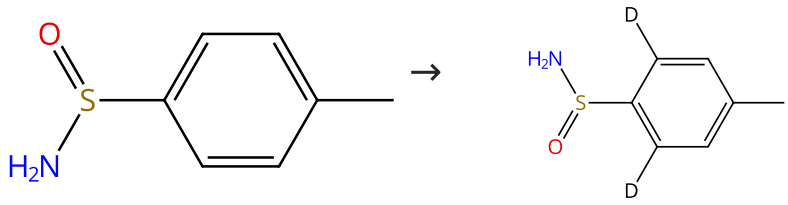
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 67 (1 Reaction) Steps: **1**



Suppliers (49)

31-116-CAS-17237251 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

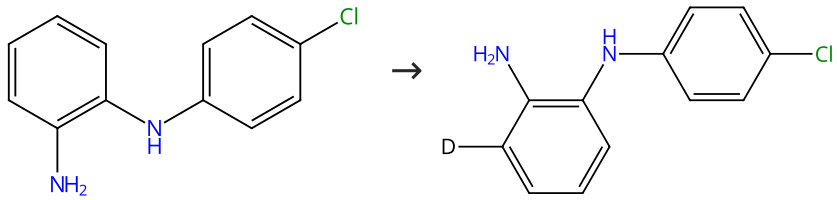
Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 68 (1 Reaction) Steps: **1**



Suppliers (61)

31-116-CAS-21649674 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

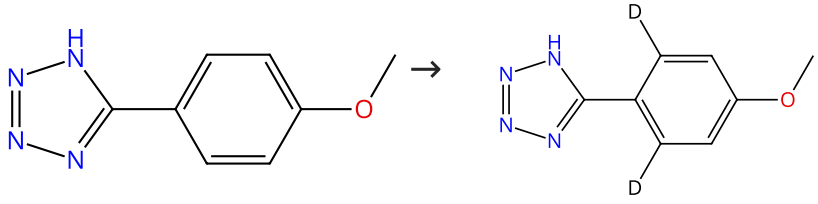
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 69 (1 Reaction) Steps: **1**



Suppliers (61)

31-116-CAS-15674371 Steps: 1

1.1 **Reagents:** Cesium carbonate, Deuterium, Oxygen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Methanol; 3 h, 50 °C

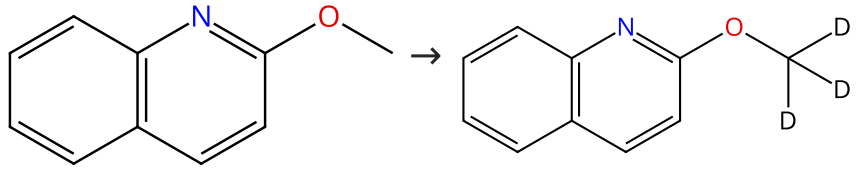
Experimental Protocols

Iridium-catalysed ortho-H/D and -H/T exchange under basic conditions: C-H activation of unprotected tetrazoles

By: Kerr, William J.; et al

Chemical Communications (Cambridge, United Kingdom) (2016), 52(40), 6669-6672.

Scheme 70 (1 Reaction) Steps: **1**



Suppliers (55) Supplier (1)

31-116-CAS-19412282 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

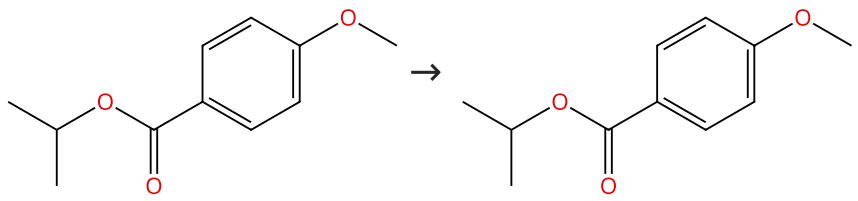
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 71 (1 Reaction) Steps: **1**



Suppliers (8) mixture with deuterated analog

31-614-CAS-26664134 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

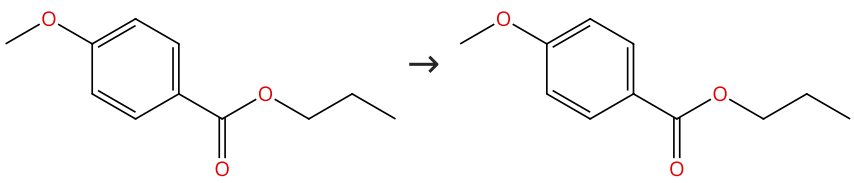
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 72 (1 Reaction)

Steps: **1**



Suppliers (8)

mixture with deuterated analog

31-614-CAS-25990784

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

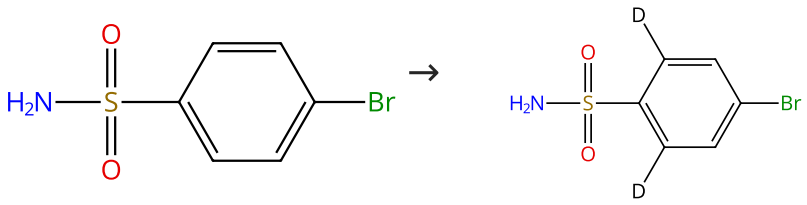
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 73 (1 Reaction)

Steps: **1**



Suppliers (80)

31-116-CAS-9595932

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

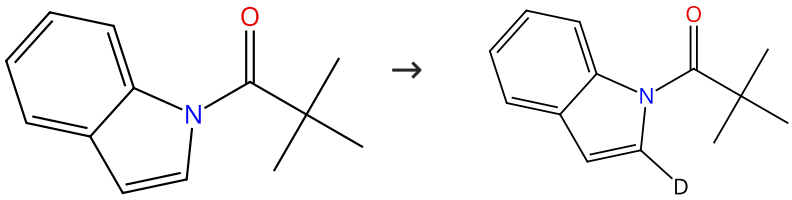
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 74 (1 Reaction)

Steps: **1**



Suppliers (8)

31-116-CAS-18343775

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

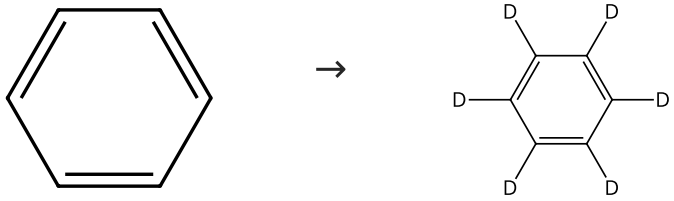
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 75 (1 Reaction)

Steps: **1**



Suppliers (179)

Suppliers (143)

31-116-CAS-20812380

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Tantalum, [dihydro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium]tris(2,2-dimethylpropyl)-, (*Ir-Ta*) (silica-supported, hydrogenation of)
Solvents: Pentane; 24 h, 800 mbar, 25 °C

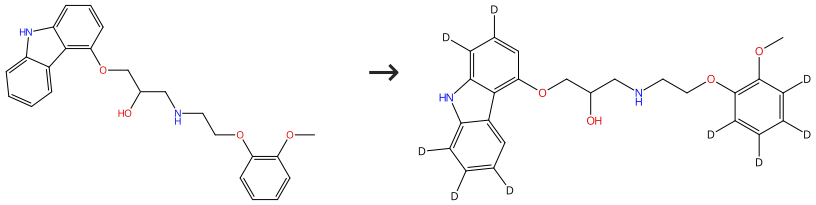
Metal-Metal Synergy in Well-Defined Surface Tantalum-Iridium Heterobimetallic Catalysts for H/D Exchange Reactions

By: Lassalle, Sebastien; et al

Journal of the American Chemical Society (2019), 141(49), 19321-19335.

Scheme 76 (1 Reaction)

Steps: **1**



Suppliers (92)

31-116-CAS-22794819

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

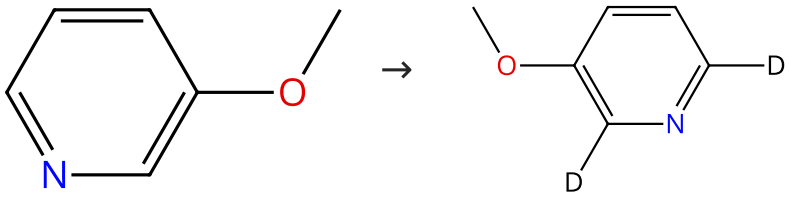
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 77 (1 Reaction)

Steps: **1**



Suppliers (80)

31-116-CAS-8551924

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

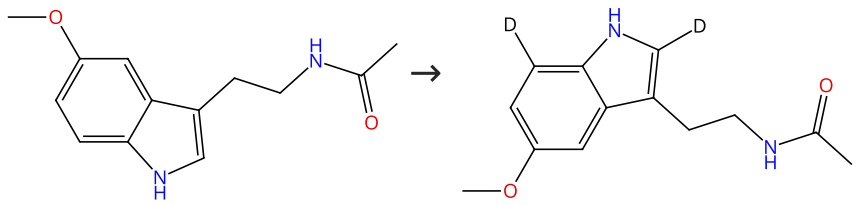
The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 78 (1 Reaction)

Steps: **1**



Suppliers (139)

31-116-CAS-22794821

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

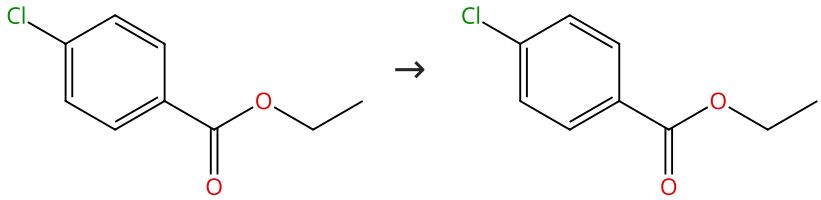
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 79 (1 Reaction)

Steps: **1**



Suppliers (73)

mixture with deuterated analog

31-614-CAS-30489777

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

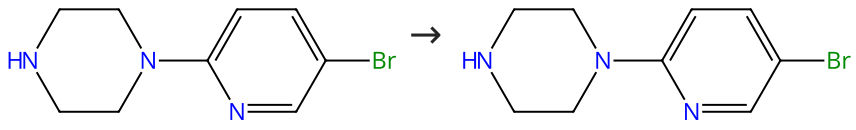
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 80 (1 Reaction)

Steps: **1**



Suppliers (67)

31-614-CAS-26757838

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

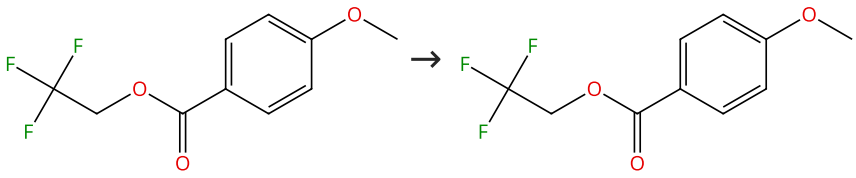
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 81 (1 Reaction)

Steps: **1**



Suppliers (6)

mixture with deuterated analog

31-614-CAS-29989395

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

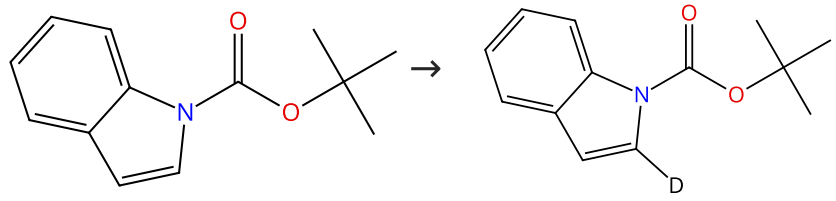
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 82 (1 Reaction)

Steps: **1**



Suppliers (70)

31-116-CAS-18343777

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

Experimental Protocols

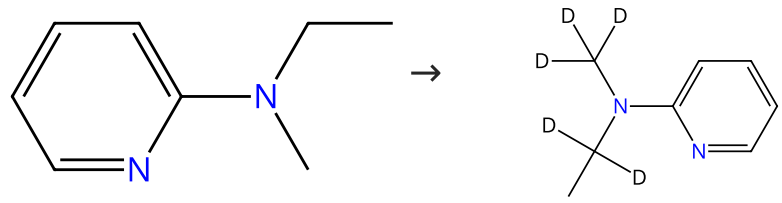
Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 83 (1 Reaction)

Steps: **1**



Suppliers (29)

31-116-CAS-19412280

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

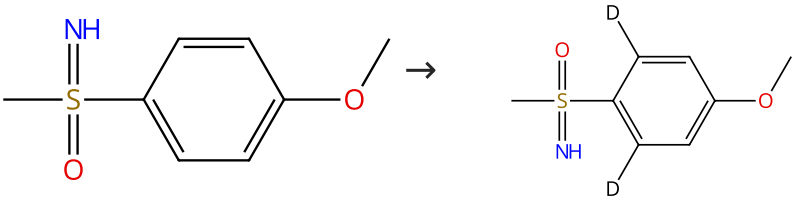
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 84 (1 Reaction)

Steps: **1**



Suppliers (49)

31-614-CAS-42989273

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

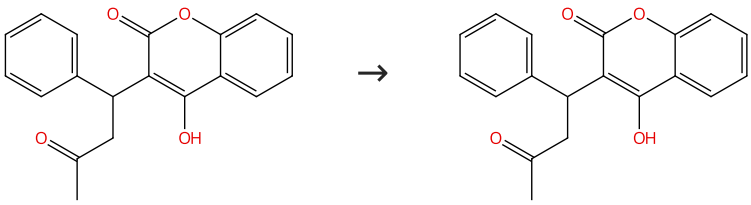
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 85 (1 Reaction)

Steps: **1**



Suppliers (72)

31-614-CAS-26977609

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*C*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

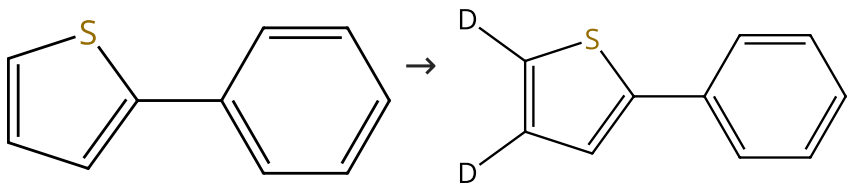
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 86 (1 Reaction)

Steps: **1**



Suppliers (78)

31-116-CAS-22794818 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

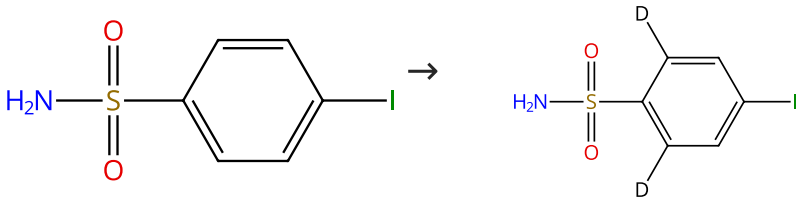
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 87 (1 Reaction) Steps: **1**



Suppliers (59)

31-116-CAS-2601480 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

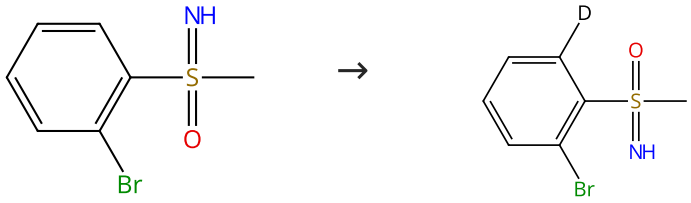
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 88 (1 Reaction) Steps: **1**



Suppliers (36)

31-614-CAS-42989269 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

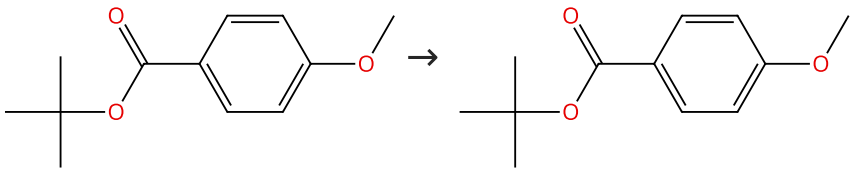
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 89 (1 Reaction) Steps: **1**



Suppliers (19)

mixture with deuterated analog

31-614-CAS-30913106 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

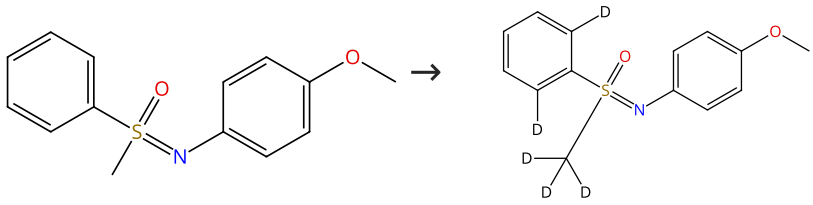
Experimental Protocols

Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 90 (1 Reaction) Steps: **1**



Suppliers (2)

31-614-CAS-42989306 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 4 h, 25 °C

1.2 **Reagents:** Acetonitrile

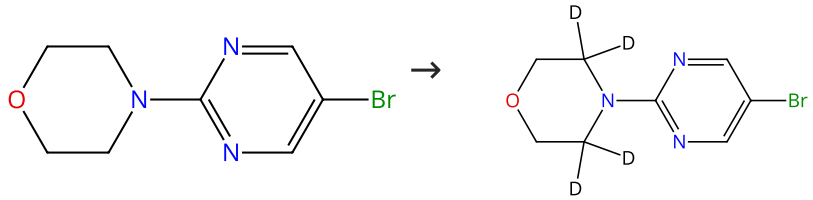
Experimental Protocols

Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 91 (1 Reaction) Steps: **1**



Suppliers (77)

31-116-CAS-19412268 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

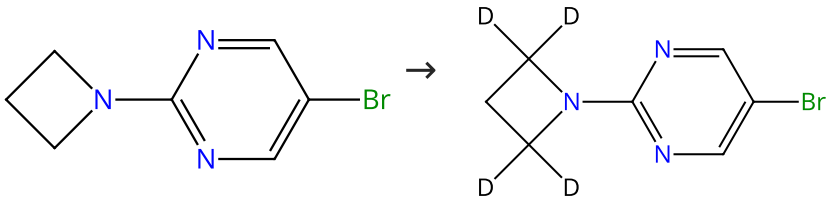
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 92 (1 Reaction)

Steps: **1**



Suppliers (65)

31-116-CAS-19412279

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 93 (1 Reaction)

Steps: **1**

Suppliers (128)

31-116-CAS-19412284

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

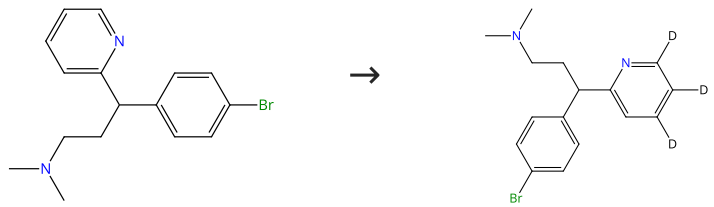
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 94 (1 Reaction)

Steps: **1**



Suppliers (38)

31-116-CAS-22794827

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

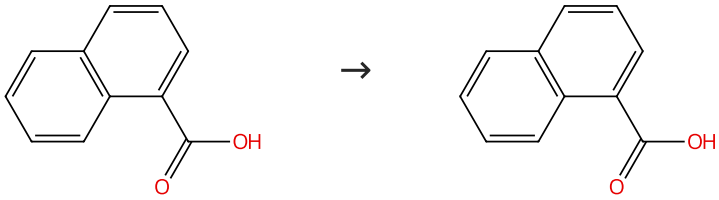
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 95 (1 Reaction)

Steps: **1**



Suppliers (91)

31-614-CAS-28699815

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 96 (1 Reaction)

Steps: **1**

Suppliers (75)

31-614-CAS-25254127

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

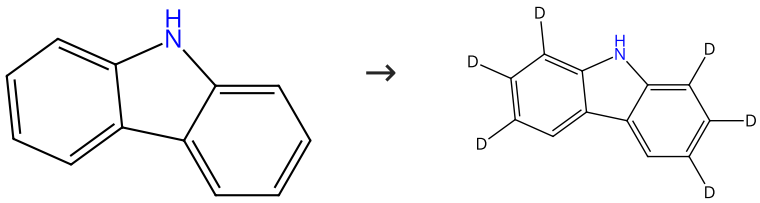
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 97 (1 Reaction)

Steps: **1**



Suppliers (124)

31-116-CAS-22794816

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 98 (1 Reaction)

Steps: **1**

Suppliers (65)

31-614-CAS-29513446

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

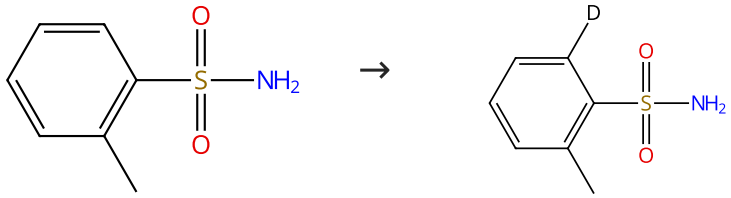
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 99 (1 Reaction)

Steps: **1**



Suppliers (88)

31-116-CAS-7141121

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

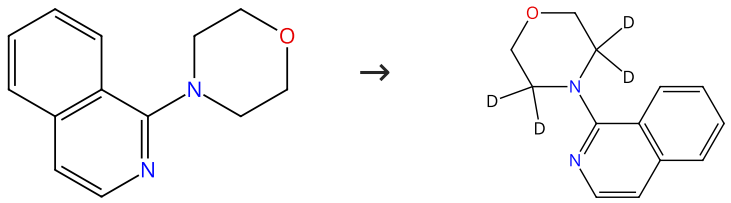
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 100 (1 Reaction)

Steps: **1**



Suppliers (7)

31-116-CAS-19412270

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

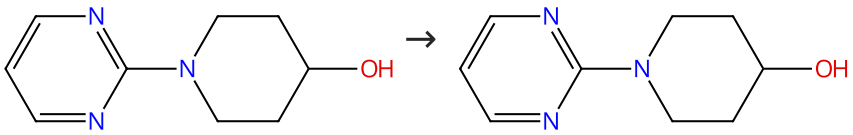
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 101 (1 Reaction)

Steps: **1**



Suppliers (63)

31-614-CAS-30441250

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

Experimental Protocols

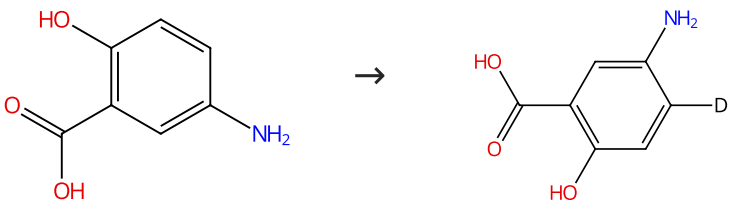
Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 102 (1 Reaction)

Steps: **1**



Suppliers (134)

31-116-CAS-21649678

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

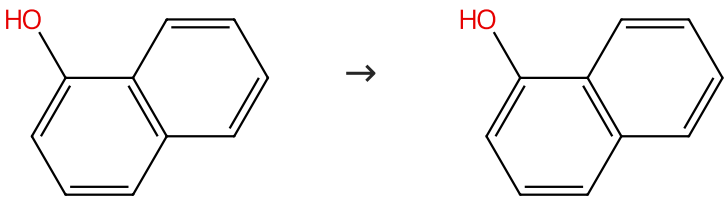
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 103 (1 Reaction)

Steps: **1**



Suppliers (133)

31-614-CAS-24982947

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [(chloro-κ*Cl*)chloromethane]methyl[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 20 min, 25 °C

1.2 **Reagents:** Deuterium; 1 h, 1 atm

Experimental Protocols

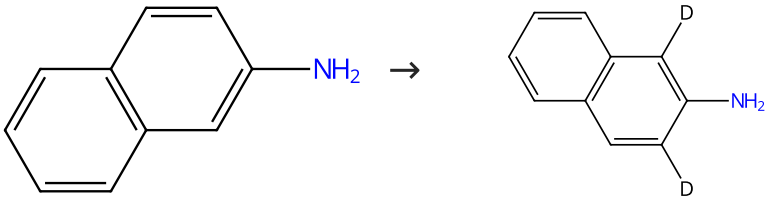
Stoichiometric and Catalytic Deuterium and Tritium Labeling of "Unactivated" Organic Substrates with Cationic Ir(III) Complexes

By: Skaddan, Marc B.; et al

Organic Letters (2004), 6(1), 11-13.

Scheme 104 (1 Reaction)

Steps: **1**



Suppliers (62)

31-116-CAS-21649668

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

Experimental Protocols

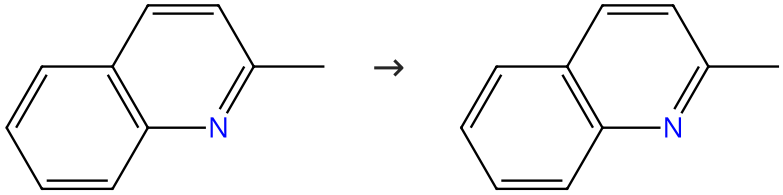
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 105 (1 Reaction)

Steps: **1**



Suppliers (80)

deuterated

31-614-CAS-28987784

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Dihydrobis(2-propanone)bis(triphenylphosphine) iridium(1+)
Solvents: Dichloromethane

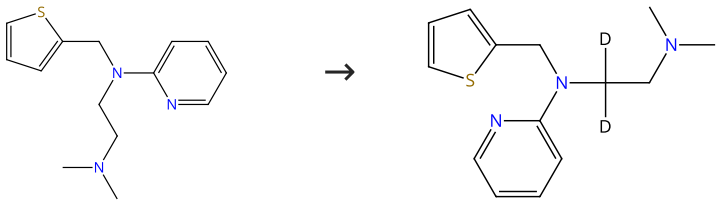
Inter- vs. intramolecular carbon-hydrogen activation: a carbon-hydrogen-iridium bridge in $[IrH_2(mq)L_2]BF_4$ and a C H + M → CMH reaction trajectory

By: Crabtree, Robert H.; et al

Inorganic Chemistry (1985), 24(13), 1986-92.

Scheme 106 (1 Reaction)

Steps: **1**



Suppliers (21)

31-116-CAS-14090853

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 16 h, 0.46 - 1 atm, rt

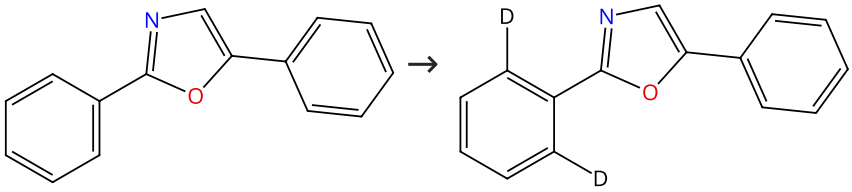
Hydrogen isotope exchange at alkyl positions using Crabtree's catalyst and its application to the tritiation of methapyrilene

By: Bushby, Nick; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 519-520.

Scheme 107 (1 Reaction)

Steps: **1**



Suppliers (91)

31-116-CAS-4846312

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), dihydrobis(2-propanone)bis(triphenyl phosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane

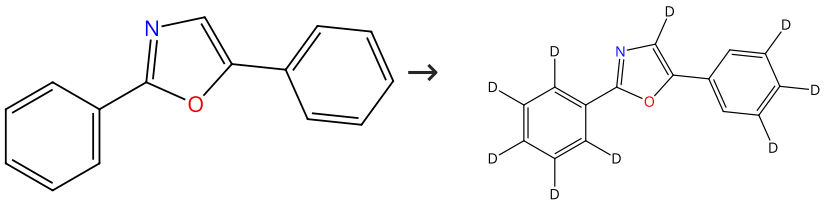
Investigation of iridium hydride complex [$IrH_2(Me_2CO)_2(PPh_3)_2$]BF_4 as a catalyst of hydrogen isotope exchange of substrates in solution

By: Heys, Richard

Journal of the Chemical Society, Chemical Communications (1992), (9), 680-1.

Scheme 108 (1 Reaction)

Steps: **1**



Suppliers (91)

31-116-CAS-22794814

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

Experimental Protocols

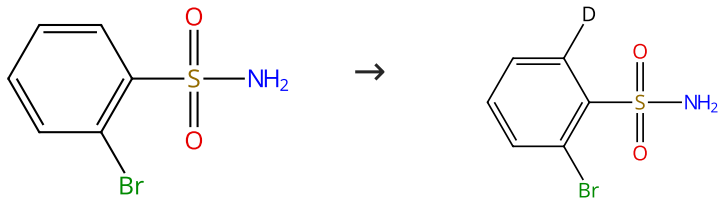
Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 109 (1 Reaction)

Steps: **1**



Suppliers (70)

31-116-CAS-9266297

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 40 °C; 2 h, 40 °C

Experimental Protocols

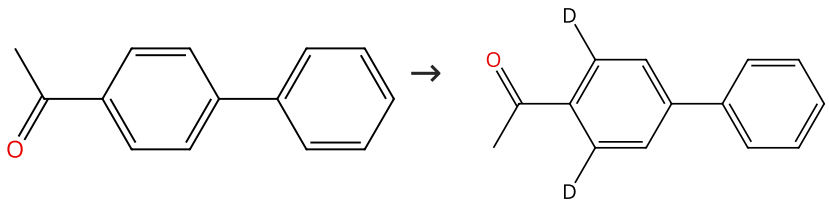
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 110 (2 Reactions)

Steps: **1**



Suppliers (112)

31-116-CAS-17233250

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Toluene; 2 h, 1 atm, rt

Experimental Protocols

Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

31-116-CAS-7717453

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

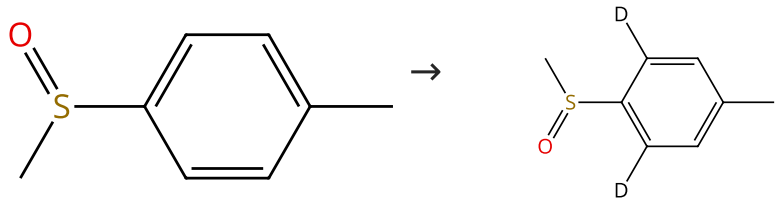
Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 111 (1 Reaction)

Steps: **1**



Suppliers (62)

31-116-CAS-17237234

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1-[2,6-bis(1-methylethyl)phenyl]-3-[2-[(4*S*)-4,5-dihydro-2-tricyclo[3.3.1.1^{3,7}]dec-1-yl-4-oxazolyl-κ*N*^{3}]ethyl]-1,3-dihydro-2*H*-imidazol-2-ylidene-κ*C*][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 2 h, 1 atm, rt

Experimental Protocols

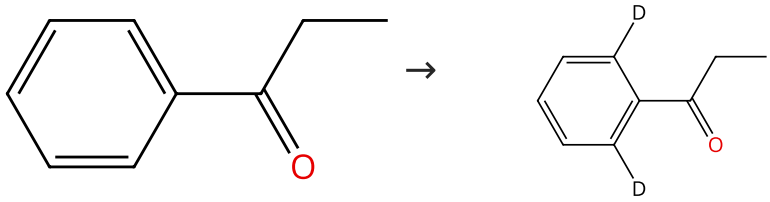
Burgess iridium(I)-catalyst for selective hydrogen isotope exchange

By: Burhop, Annina; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2017), 60(7), 343-348.

Scheme 112 (1 Reaction)

Steps: **1**



Suppliers (72)

31-116-CAS-13108774

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

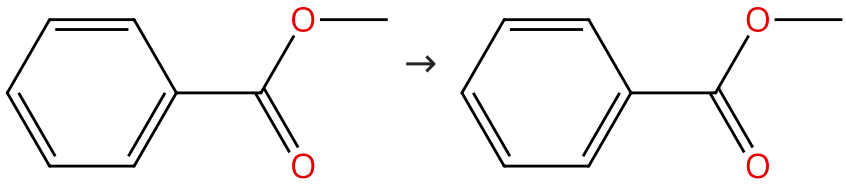
Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 113 (1 Reaction)

Steps: **1**



Suppliers (92)

mixture with deuterated analog

31-614-CAS-25308188

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 40 °C; 1 h, 40 °C

Experimental Protocols

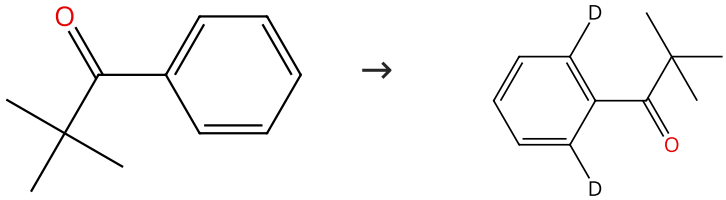
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 114 (1 Reaction)

Steps: **1**



Suppliers (67)

31-116-CAS-1803248

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

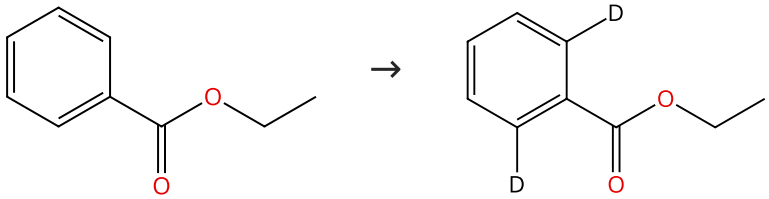
Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 115 (2 Reactions)

Steps: **1**



Suppliers (94)

31-614-CAS-23969787

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

31-116-CAS-6887878

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C

1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

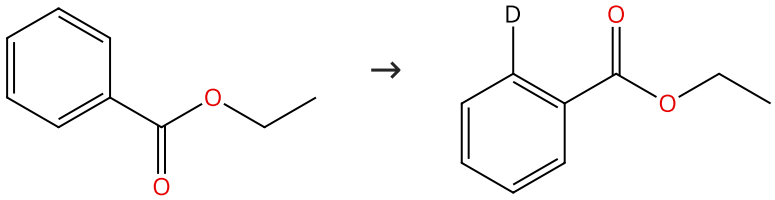
Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

Scheme 116 (1 Reaction)

Steps: **1**



Suppliers (94)

with and without addnl. ortho deuterium

31-116-CAS-2052485

Steps: **1**

1.1 **Catalysts:** Triphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

1.2 **Reagents:** Deuterium

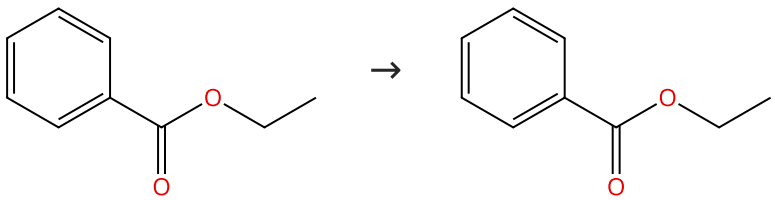
Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 117 (1 Reaction)

Steps: **1**



Suppliers (94)

mixture with deuterated analog

31-614-CAS-26400473 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 40 °C; 1 h, 40 °C

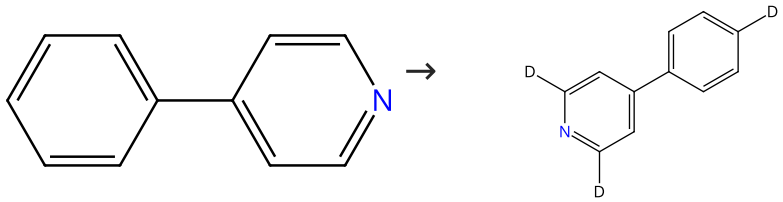
Experimental Protocols

Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 118 (1 Reaction) Steps: **1**



Suppliers (92)

31-116-CAS-22794805 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium
Solvents: Tetrahydrofuran; 22 h, 1 atm, 55 °C

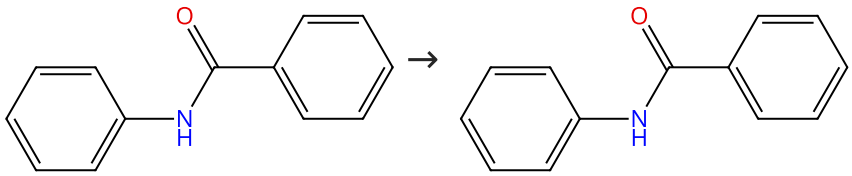
Experimental Protocols

Multiple Site Hydrogen Isotope Labeling of Pharmaceuticals

By: Daniel-Bertrand, Marion; et al

Angewandte Chemie, International Edition (2020), 59(47), 21114-21120.

Scheme 119 (2 Reactions) Steps: **1**



Suppliers (89)

31-614-CAS-29736810 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, rt

Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

31-614-CAS-28936866 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(dicyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (polystyrene-supported)
Solvents: Dichloromethane; 1 h, rt

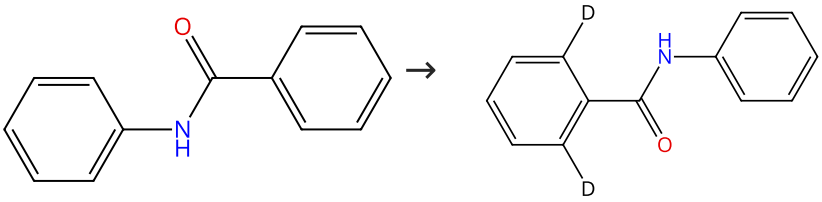
Tritium-labeling via an iridium-based solid-phase catalyst

By: Hickey, Michael J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 286-289.

Scheme 120 (1 Reaction)

Steps: **1**



Suppliers (89)

31-116-CAS-4435518

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Silver hexafluoroantimonate, (*SP*-5-43)-[2,6-Bis[[bis(1,1-dimethylethyl)phosphino-κ*P*]oxy]phenyl-κ*C*]chlorohydroiridium
Solvents: Dichloromethane; 4 h, rt

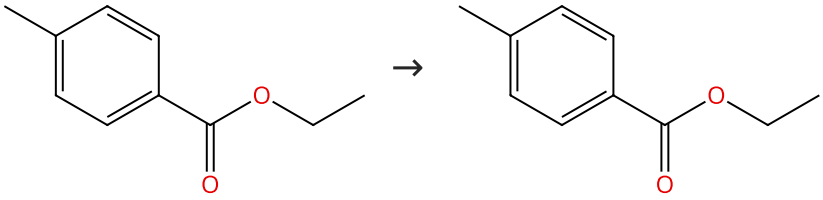
Application of iridium pincer complexes in hydrogen isotope exchange reactions

By: Traeff, Annika; et al

Journal of Organometallic Chemistry (2007), 692(25), 5529-5531.

Scheme 121 (1 Reaction)

Steps: **1**



Suppliers (69)

mixture with deuterated analog

31-614-CAS-28908590

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 40 °C; 1 h, 40 °C

Experimental Protocols

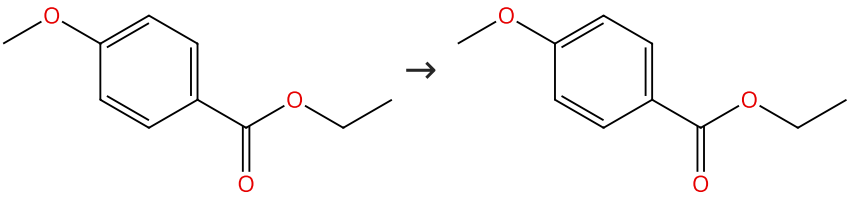
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 122 (1 Reaction)

Steps: **1**



Suppliers (66)

mixture with deuterated analog

31-614-CAS-28753845

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

Experimental Protocols

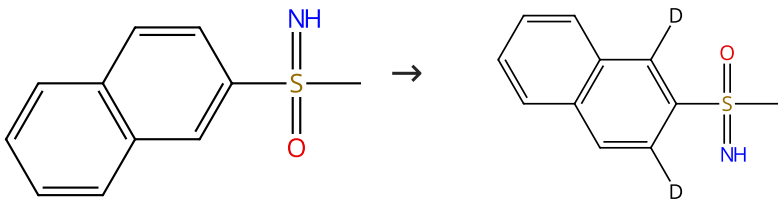
Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 123 (1 Reaction)

Steps: **1**



Suppliers (31)

31-614-CAS-42989279

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 1 h, 25 °C

1.2 **Reagents:** Acetonitrile

Experimental Protocols

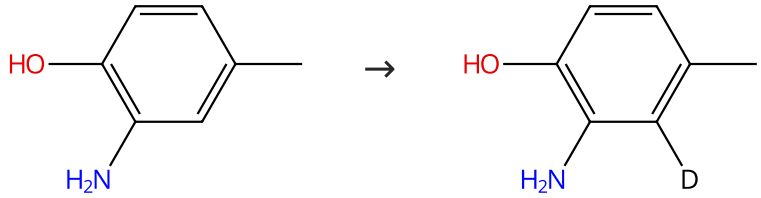
Selective Deuteration and Tritiation of Pharmaceutically Relevant Sulfoximines

By: Smith, Blair I. P.; et al

Angewandte Chemie, International Edition (2025), 64(5), e202417179.

Scheme 124 (1 Reaction)

Steps: **1**



Suppliers (87)

31-116-CAS-21649662

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

Experimental Protocols

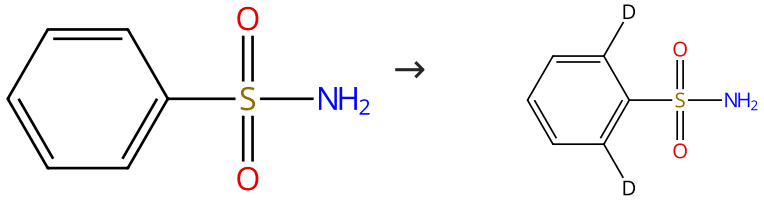
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 125 (2 Reactions)

Steps: **1**



Suppliers (89)

31-116-CAS-13888230

Steps: **1**

1.1 **Catalysts:** Iridium(1+), [1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; rt → -78 °C

1.2 **Reagents:** Deuterium; -78 °C → rt; 16 h, rt

Experimental Protocols

Isotopic Labelling of Functionalised Arenes Catalysed by Iridium(I) Species of the [(cod)Ir(NHC)(py)]PF_6 Complex Class

By: Cross, Paul W. C.; et al

Synlett (2016), 27(1), 111-115.

31-116-CAS-14841634 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

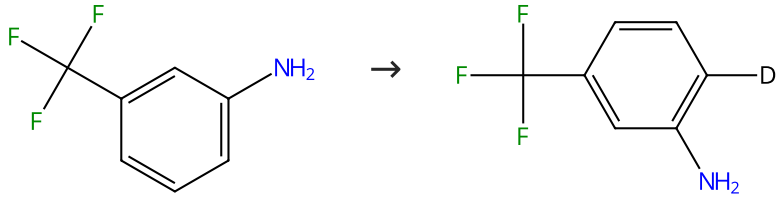
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 126 (1 Reaction) Steps: **1**



Suppliers (73)

31-116-CAS-21649663 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran; 3 h, 55 °C

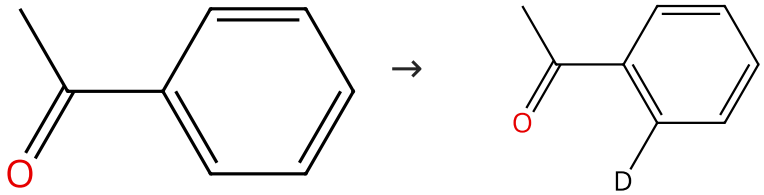
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 127 (1 Reaction) Steps: **1**



Suppliers (109)

with and without addnl. ortho deuterium

31-116-CAS-13317776 Steps: **1**

1.1 **Catalysts:** Triphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

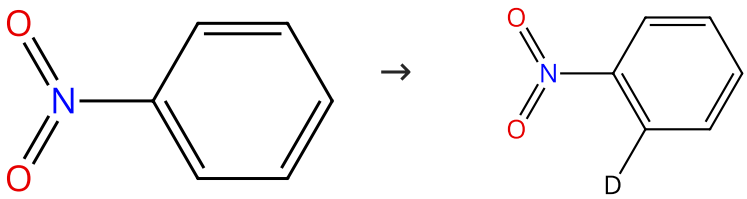
1.2 **Reagents:** Deuterium

Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 128 (1 Reaction) Steps: **1**



Suppliers (107)

31-116-CAS-1732617 Steps: 1

1.1 **Catalysts:** Methyldiphenylphosphine, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Silver tetrafluoroborate
Solvents: Dichloromethane

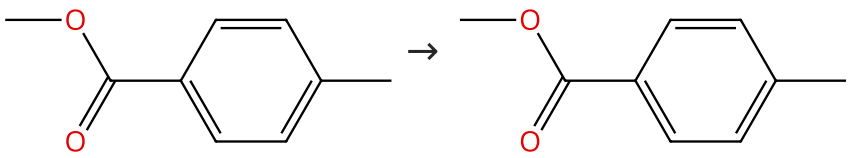
1.2 **Reagents:** Deuterium

Deuterium exchange mediated by an iridium-phosphine complex formed in situ

By: Ellames, George J.; et al

Tetrahedron Letters (2001), 42(36), 6413-6416.

Scheme 129 (1 Reaction) Steps: **1**



Suppliers (93)

mixture with deuterated analog

31-614-CAS-26131427 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 40 °C; 1 h, 40 °C

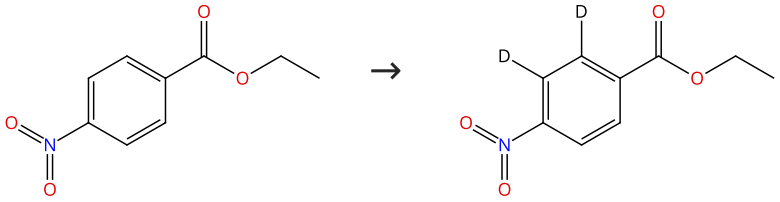
Experimental Protocols

Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 130 (1 Reaction) Steps: **1**



Suppliers (92)

mixture with monodeuterated analog

31-116-CAS-15642666 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 1 h, 25 °C

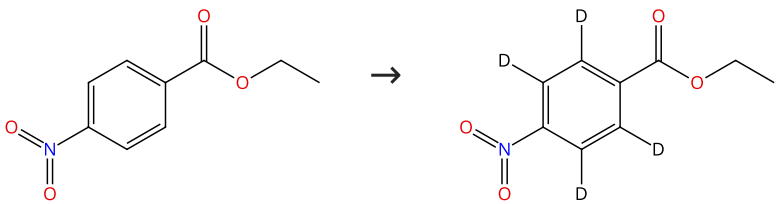
Experimental Protocols

Iridium-catalyzed ortho-directed deuterium labelling of aromatic esters-an experimental and theoretical study on directing group chemoselectivity

By: Devlin, Jennifer; et al

Molecules (2015), 20(7), 11676-11698.

Scheme 131 (1 Reaction) Steps: **1**



Suppliers (92)

31-116-CAS-16442687 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; 1 h, 25 °C

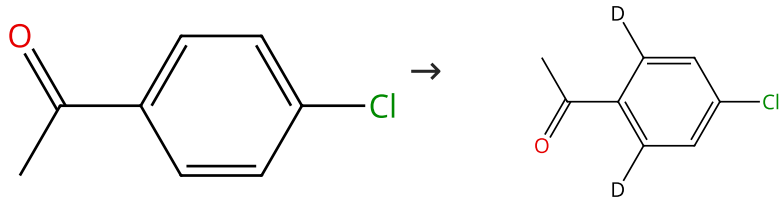
Experimental Protocols

Hydrogen isotope exchange with highly active iridium(I) NHC/phosphine complexes: a comparative counterion study

By: Kerr, William J.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2016), 59(14), 601-603.

Scheme 132 (1 Reaction) Steps: **1**



Suppliers (76)

31-116-CAS-9509608 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 16 h, 25 °C

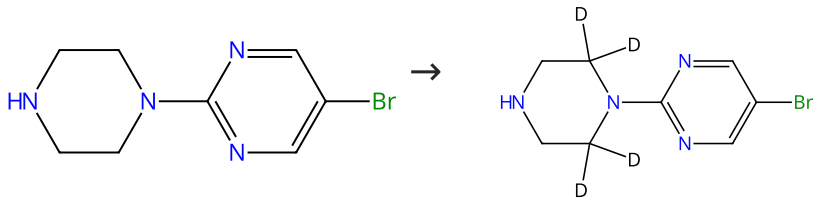
Experimental Protocols

Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

Scheme 133 (1 Reaction) Steps: **1**



Suppliers (71)

31-116-CAS-19412274 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Dichloromethane; 3 h, 25 °C

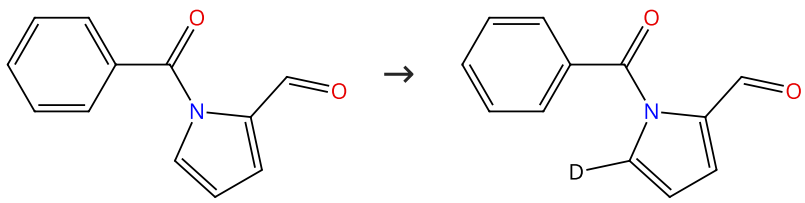
Experimental Protocols

Iridium-Catalyzed Csp^3-H Activation for Mild and Selective Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2018), 8(11), 10895-10900.

Scheme 134 (1 Reaction) Steps: **1**



Suppliers (5)

31-116-CAS-18343788 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 5 min, 1 atm, 25 °C

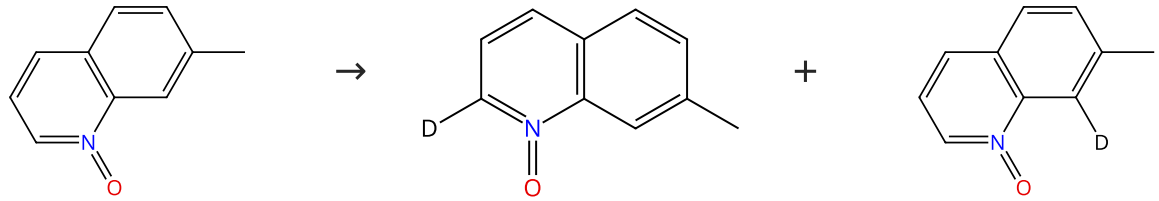
Experimental Protocols

Site-Selective Deuteration of N-Heterocycles via Iridium-Catalyzed Hydrogen Isotope Exchange

By: Kerr, William J.; et al

ACS Catalysis (2017), 7(10), 7182-7186.

Scheme 135 (1 Reaction) Steps: **1** Yield: **96%**



Suppliers (3)

31-614-CAS-36762220 Steps: **1** Yield: **96%**

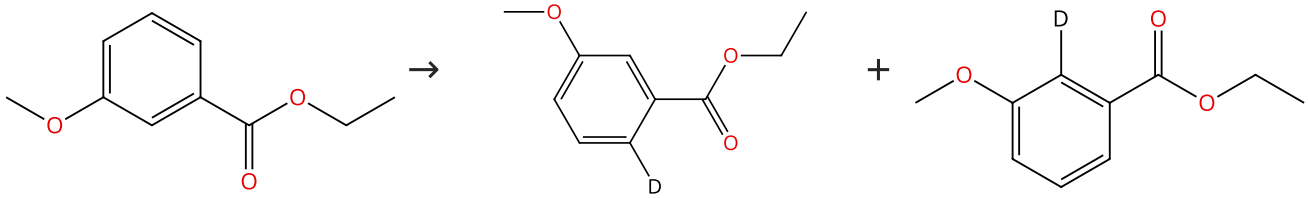
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 136 (1 Reaction) Steps: **1** Yield: **85%**



Suppliers (68)

31-116-CAS-9726709 Steps: **1** Yield: **85%**

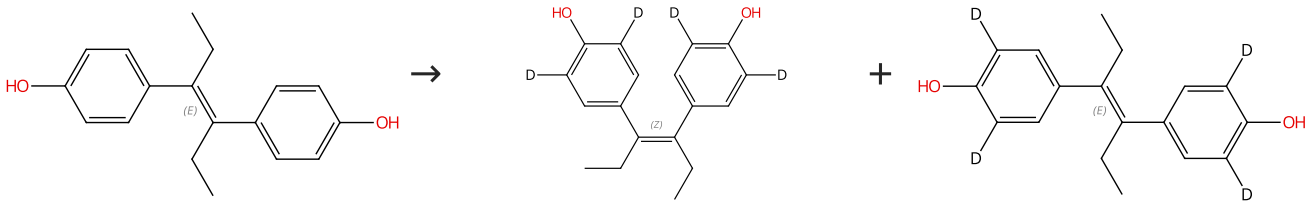
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), dihydrobis(2-propanone)bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane

Investigation of iridium hydride complex [$IrH_2(Me_2CO)_2(PPh_3)_2$]BF_4 as a catalyst of hydrogen isotope exchange of substrates in solution

By: Heys, Richard

Journal of the Chemical Society, Chemical Communications (1992), (9), 680-1.

Scheme 137 (1 Reaction) Steps: **1** Yield: **79%**



Double bond geometry shown

Double bond geometry shown

Double bond geometry shown

Suppliers (102)

31-614-CAS-24835990 Steps: **1** Yield: **79%**

1.1 **Reagents:** Potassium acetate, Deuterium
Catalysts: Iridium(1+), [1,3-bis[2,6-bis(1-methylethyl)phenyl]-1,5-dihydro-5-(2,4,6-trimethylphenyl)-4*H*-1,2,3-triazolium-4-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]-
Solvents: Tetrahydrofuran; 24 h, 1 atm, 70 °C

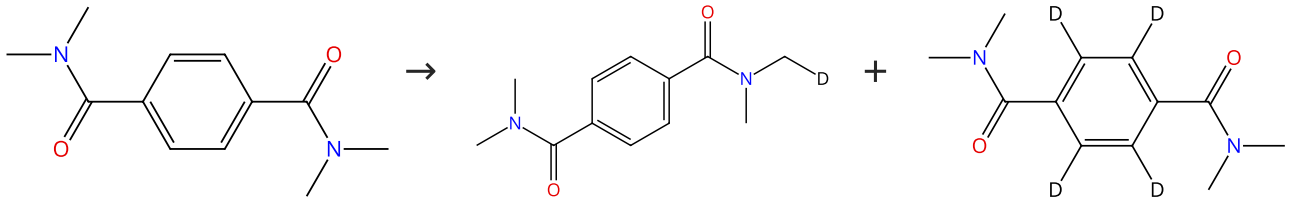
Experimental Protocols

Ortho-Selective Hydrogen Isotope Exchange of Phenols and Benzyl Alcohols by Mesoionic Carbene-Iridium Catalyst

By: Zhao, Liang-Liang; et al

Organic Letters (2021), 23(23), 9297-9302.

Scheme 138 (1 Reaction) Steps: **1** Yield: **55%**



Suppliers (5)

31-116-CAS-11856891 Steps: **1** Yield: **55%**

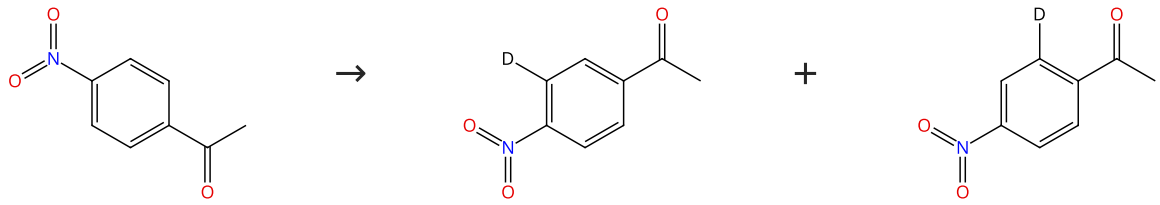
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), dihydrobis(2-propanone)bis(triphenylphosphine)-, tetrafluoroborate(1-) (1:1)
Solvents: Dichloromethane

Investigation of iridium hydride complex $[IrH_2(Me_2CO)_2(PPh_3)_2]BF_4$ as a catalyst of hydrogen isotope exchange of substrates in solution

By: Heys, Richard

Journal of the Chemical Society, Chemical Communications (1992), (9), 680-1.

Scheme 139 (1 Reaction) Steps: **1**



Suppliers (83)

31-614-CAS-23969791 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

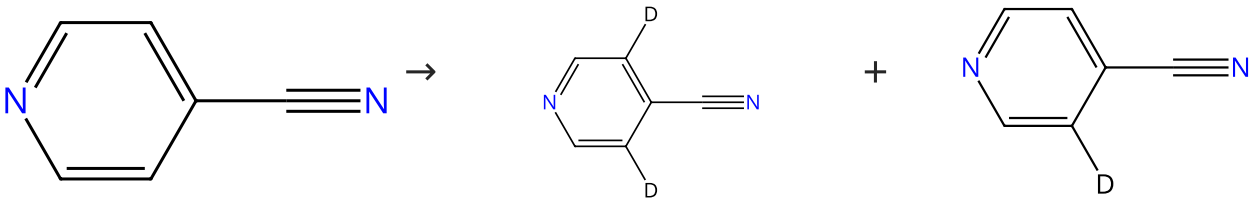
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 140 (1 Reaction) Steps: **1**



Suppliers (103)

31-116-CAS-5497 Steps: **1**

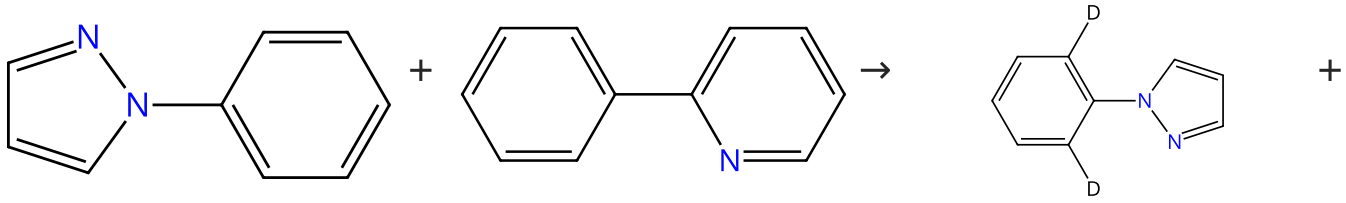
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

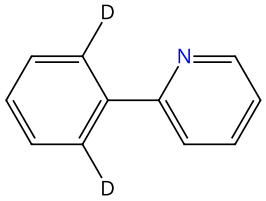
By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 141 (1 Reaction) Steps: **1**



Suppliers (90) Suppliers (94)



Supplier (1)

31-614-CAS-23969796 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

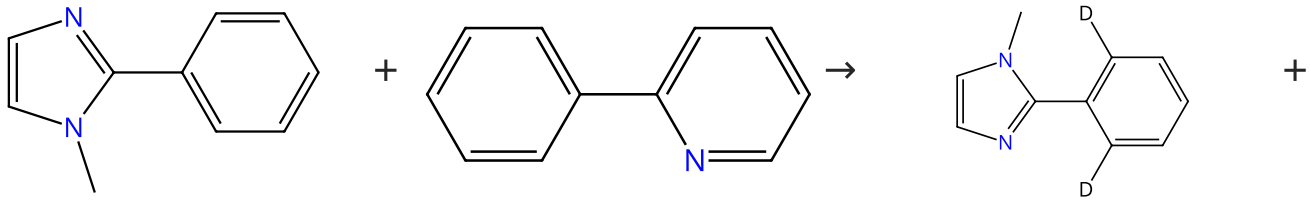
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

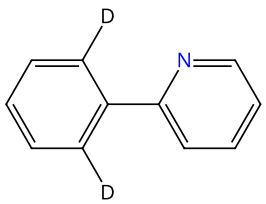
By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 142 (1 Reaction) Steps: **1**



Suppliers (21) Suppliers (94)



Supplier (1)

31-614-CAS-23969804 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

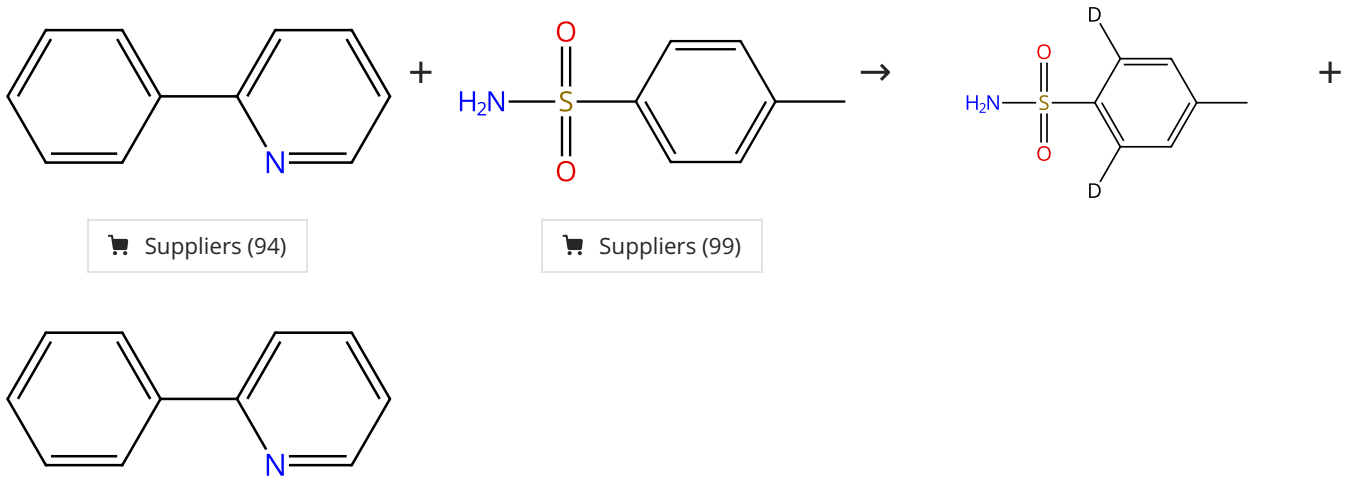
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 143 (1 Reaction) Steps: **1**



Suppliers (94) Suppliers (99)

31-614-CAS-27711752 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

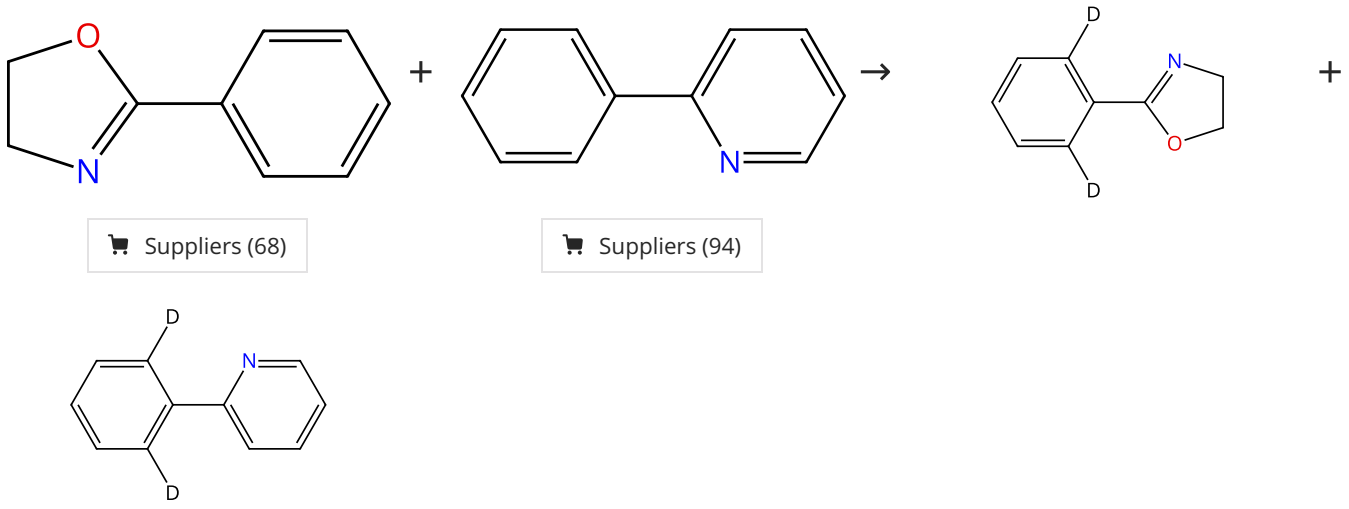
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 144 (1 Reaction) Steps: **1**



Suppliers (68) Suppliers (94) Supplier (1)

31-614-CAS-23969789 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

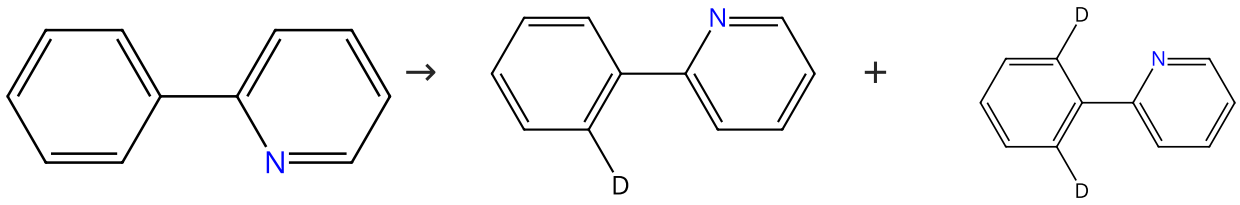
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 145 (1 Reaction) Steps: **1**



Suppliers (94) Suppliers (6) Supplier (1)

31-614-CAS-23969806 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 240 min, 50 °C

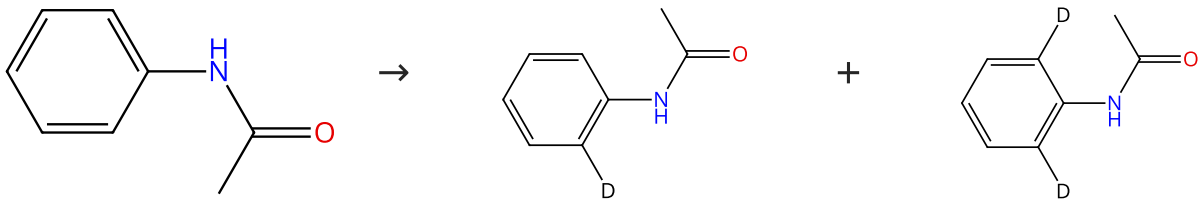
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 146 (1 Reaction) Steps: **1**



Suppliers (108) Suppliers (2)

31-614-CAS-35597993 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

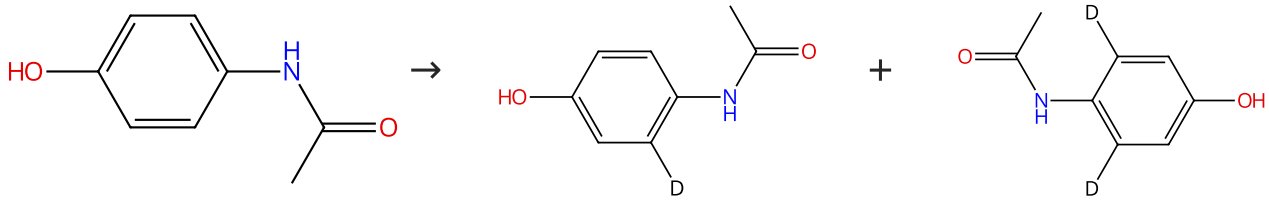
Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 147 (1 Reaction) Steps: **1**



Suppliers (147)

31-614-CAS-35597989 Steps: 1

1.1 **Reagents:** Hydrogen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 1 h, 100 mbar, rt

1.2 **Reagents:** Deuterium; 3 h, 25 mbar, rt

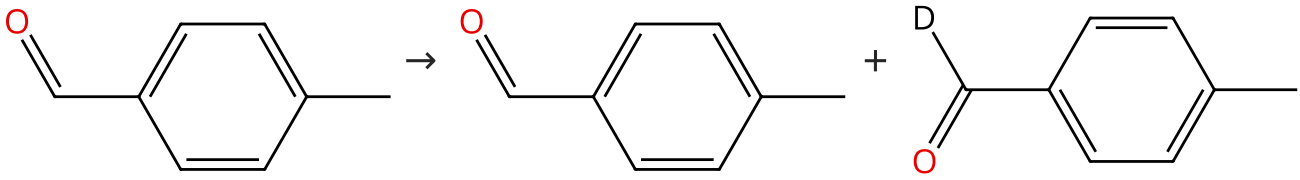
Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 148 (1 Reaction) Steps: 1



Suppliers (107) Supplier (1)

31-614-CAS-25238149 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

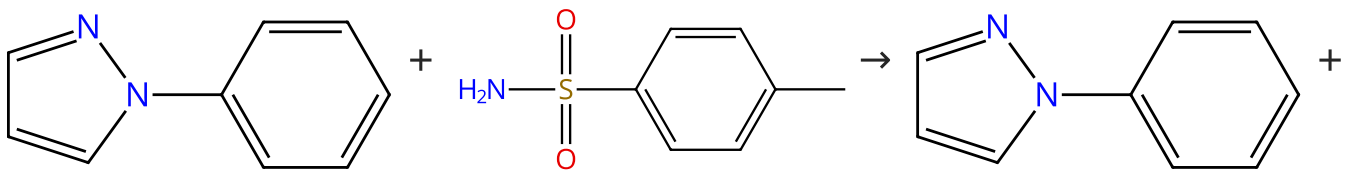
Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

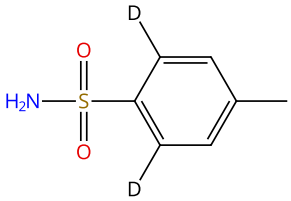
By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 149 (1 Reaction) Steps: 1



Suppliers (90) Suppliers (99)



31-614-CAS-28726680 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

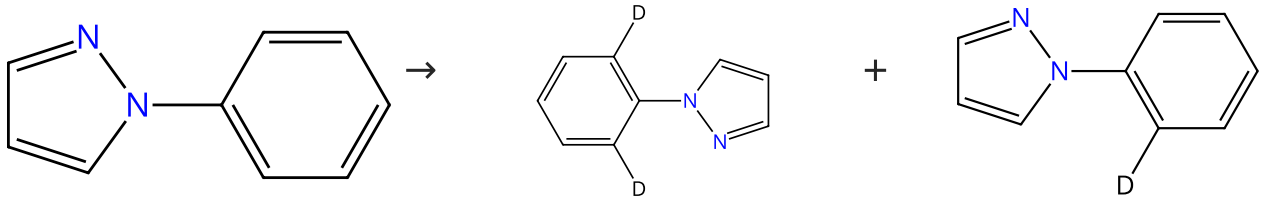
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 150 (1 Reaction)

Steps: **1**



Suppliers (90)

31-614-CAS-35597978

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

Experimental Protocols

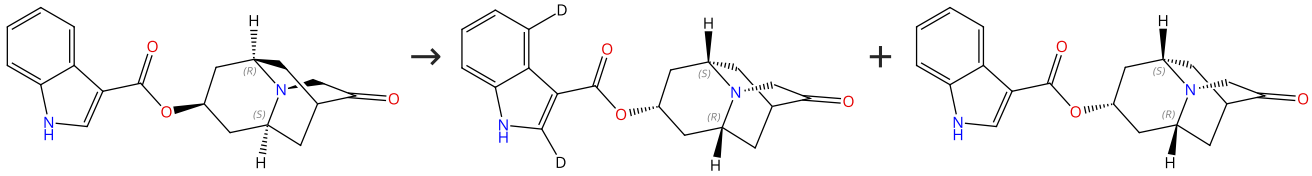
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 151 (1 Reaction)

Steps: **1**



Relative stereochemistry shown

Relative stereochemistry shown

Relative stereochemistry shown

Suppliers (75)

31-614-CAS-35597986

Steps: **1**

1.1 **Reagents:** Hydrogen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 100 mbar, - 196 °C; 1 h, rt

1.2 **Reagents:** Deuterium; 25 mbar, - 196 °C; 3 h, rt

Experimental Protocols

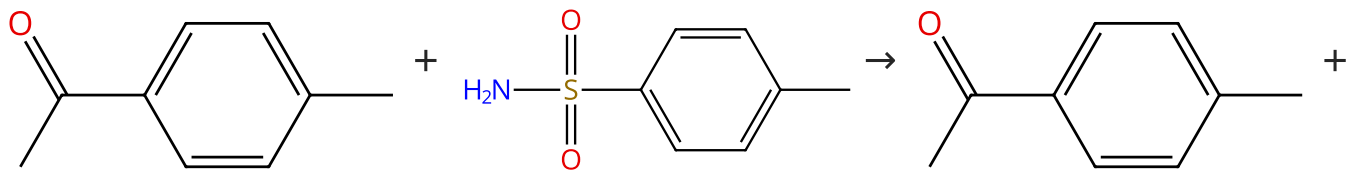
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

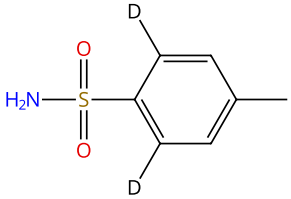
Scheme 152 (1 Reaction)

Steps: **1**



Suppliers (109)

Suppliers (99)



31-614-CAS-27814498 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

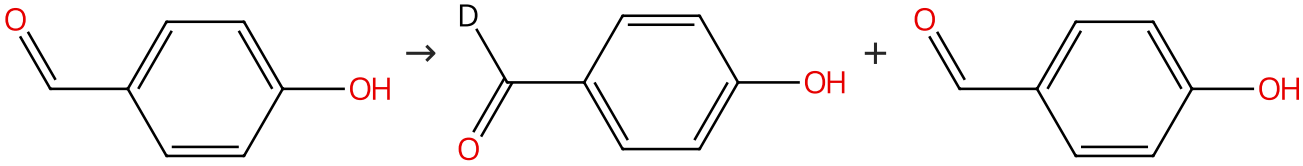
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 153 (1 Reaction) Steps: **1**



Suppliers (132) Suppliers (4)

31-614-CAS-29391315 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

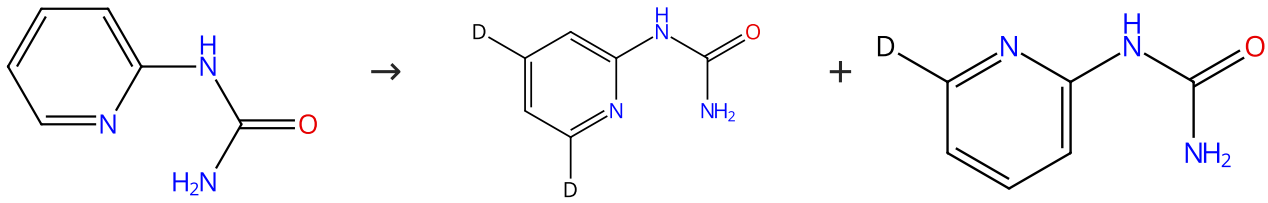
Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 154 (1 Reaction) Steps: **1**



Suppliers (55)

31-116-CAS-6425129 Steps: **1**

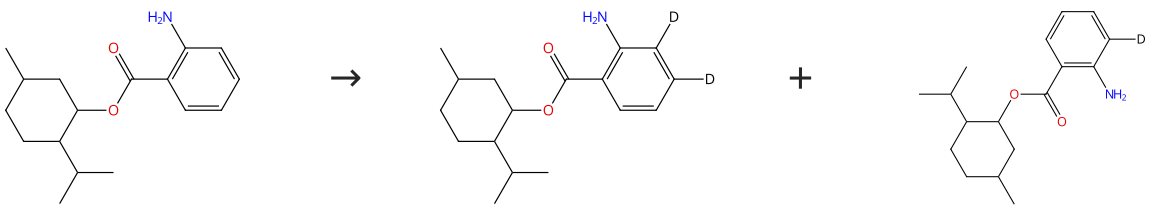
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 155 (1 Reaction) Steps: **1**



Suppliers (32)

31-116-CAS-21649686 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

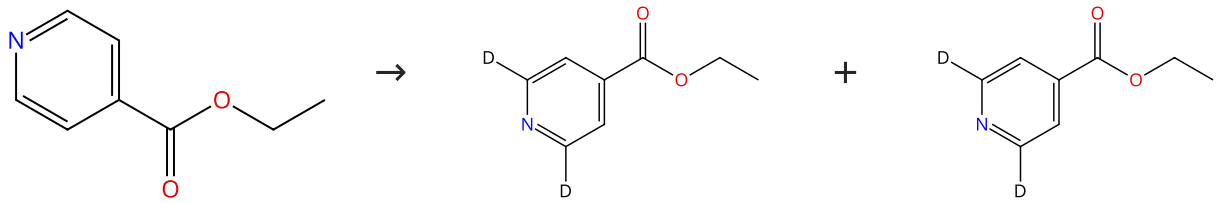
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 156 (1 Reaction) Steps: **1**



Suppliers (95)

31-614-CAS-27728730 Steps: **1**

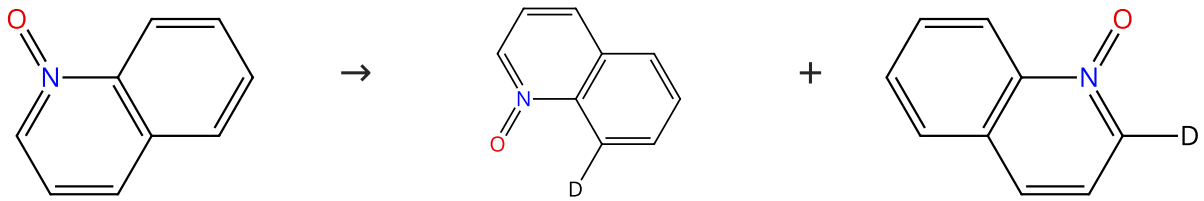
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 157 (1 Reaction) Steps: **1**



Suppliers (57) Supplier (1) Supplier (1)

31-614-CAS-36762226 Steps: **1**

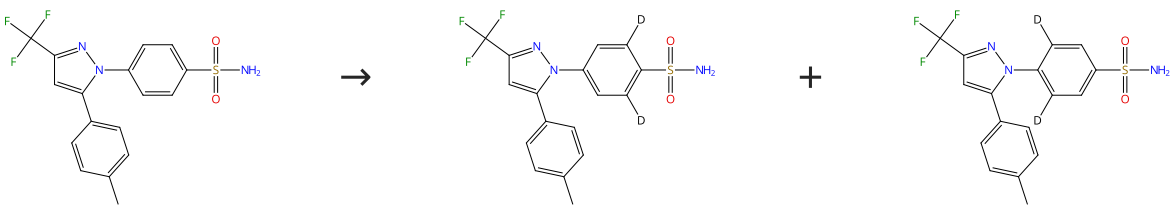
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](dimethylphenylphosphine)iridium(1+)
Solvents: Dichloromethane; -78 °C; -78 °C → 25 °C; 16 h, 25 °C

Selective Deuteration of Heterocycle N -Oxides via Iridium-Catalysed Hydrogen Isotope Exchange

By: Owens, Philippa K.; et al

Synthesis (2023), 55(21), 3644-3651.

Scheme 158 (1 Reaction) Steps: **1**



Suppliers (131)

31-116-CAS-13050608 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

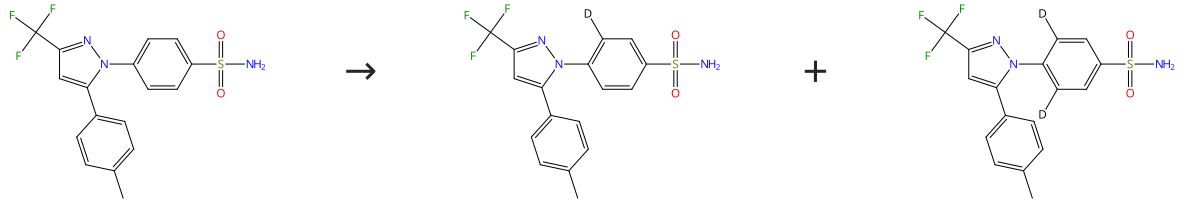
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 159 (1 Reaction) Steps: **1**



Suppliers (131)

31-614-CAS-35597992 Steps: 1

1.1 **Reagents:** Hydrogen
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 1 h, 100 mbar, rt

1.2 **Reagents:** Deuterium; 3 h, 25 mbar, rt

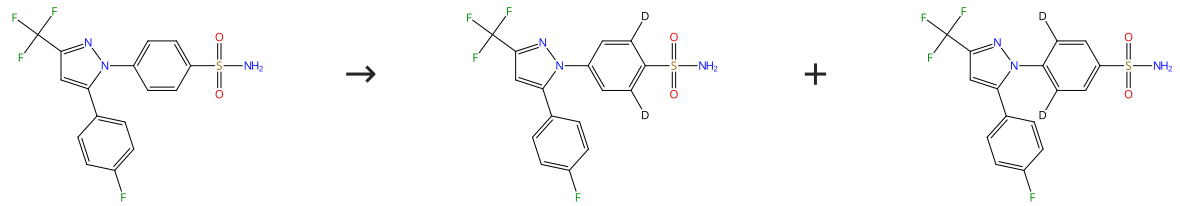
Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 160 (1 Reaction) Steps: **1**



Suppliers (52)

31-116-CAS-15179738 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

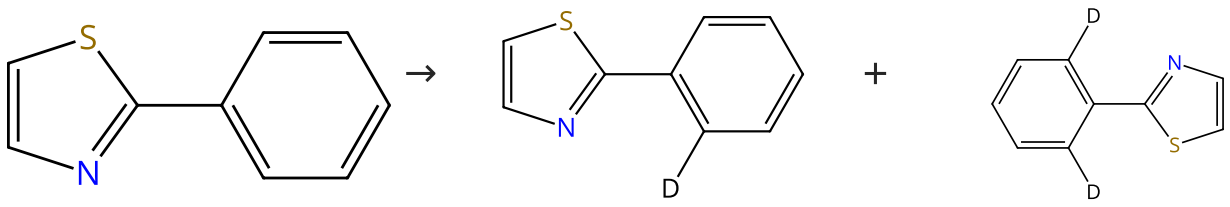
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 161 (1 Reaction) Steps: **1**



Suppliers (79)

31-614-CAS-35597985 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 300 mbar, rt

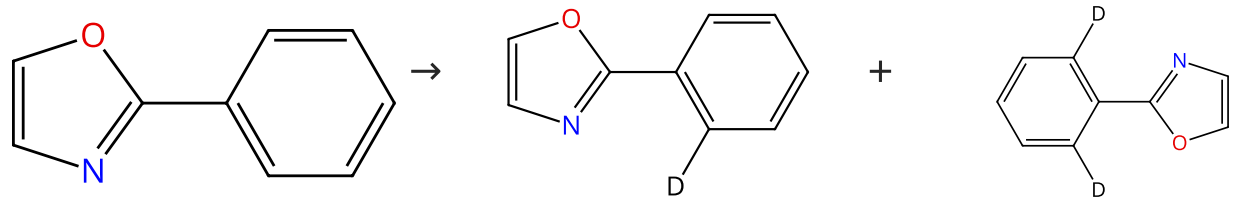
Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 162 (1 Reaction) Steps: **1**



Suppliers (57)

31-614-CAS-35597979 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

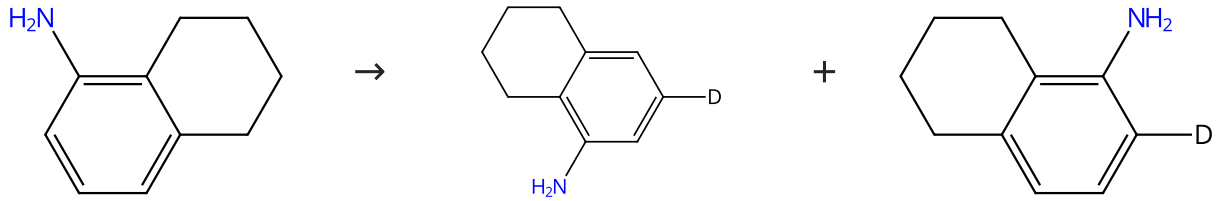
Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 163 (1 Reaction) Steps: **1**



Suppliers (62)

31-614-CAS-34988546 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 1,3-Dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene (Iridium and ruthenium supported), Iridium, compd. with ruthenium (2:1)
Solvents: Tetrahydrofuran; 24 h, 2 bar, 55 °C

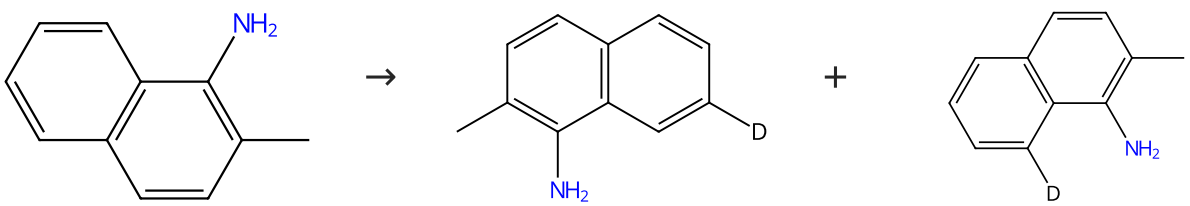
Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

Scheme 164 (3 Reactions) Steps: **1**



Suppliers (79)

31-614-CAS-34988543 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (bound to polyvinylpyrrolidone or IMes N-heterocyclic carbene), 1,3-Dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene (Iridium and ruthenium supported)
Solvents: Tetrahydrofuran; 24 h, 2 bar, 55 °C

Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

31-614-CAS-34988550 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 1,3-Dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene (Iridium and ruthenium supported), Iridium, compd. with ruthenium (1:2)
Solvents: Tetrahydrofuran; 24 h, 2 bar, 55 °C

Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

31-614-CAS-34988544 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 1,3-Dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene (Iridium and ruthenium supported), Iridium, compd. with ruthenium (2:1)
Solvents: Tetrahydrofuran; 24 h, 2 bar, 55 °C

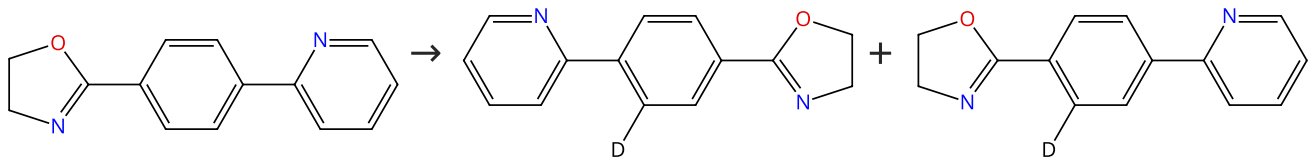
Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

Scheme 165 (1 Reaction) Steps: **1**



31-614-CAS-23969795 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

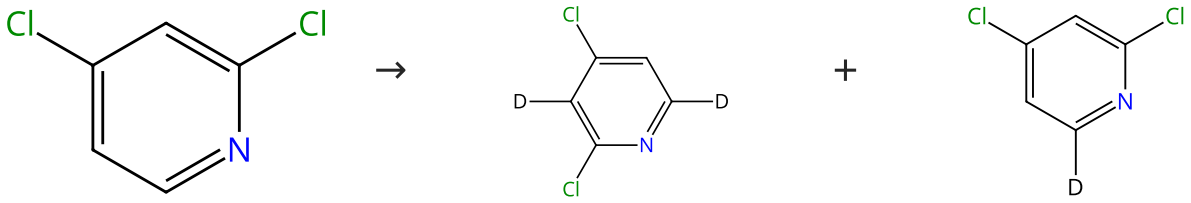
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 166 (1 Reaction) Steps: **1**



Suppliers (107)

31-116-CAS-7045145 Steps: **1**

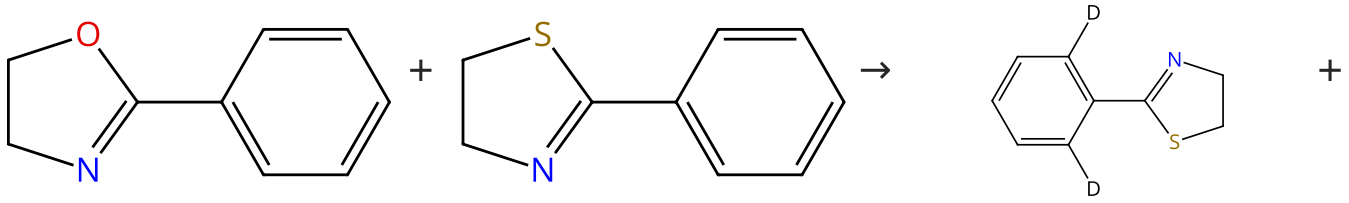
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

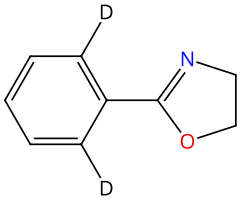
By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 167 (1 Reaction) Steps: **1**



Suppliers (68) Suppliers (8)



31-614-CAS-23969792 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

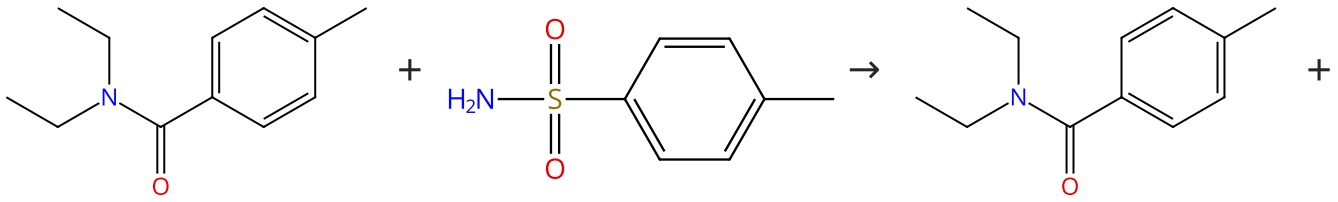
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

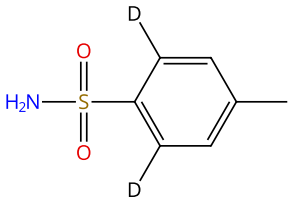
By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 168 (1 Reaction) Steps: **1**



Suppliers (50) Suppliers (99)



31-614-CAS-30322380 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

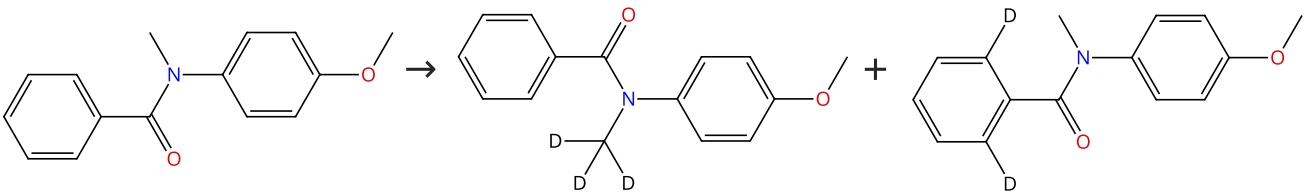
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 169 (2 Reactions) Steps: **1**



Suppliers (9)

31-116-CAS-11409823 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

31-116-CAS-9357029 Steps: **1**

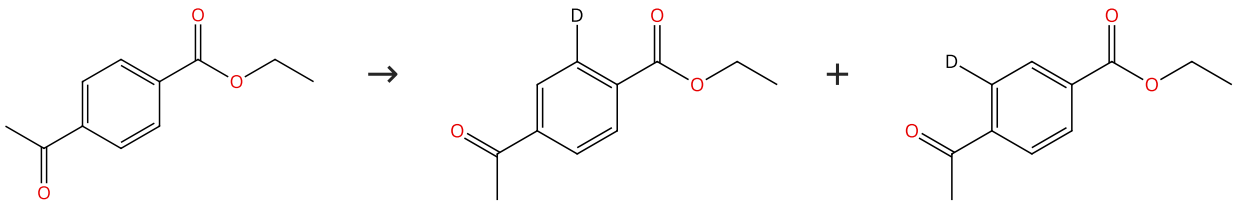
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Ethyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

Scheme 170 (1 Reaction) Steps: **1**



Suppliers (86)

31-614-CAS-23969800 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

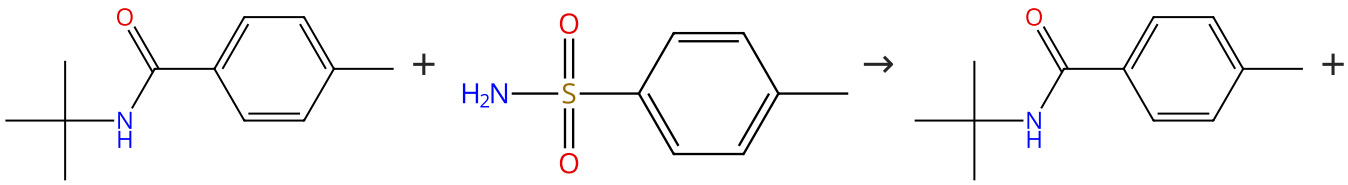
Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

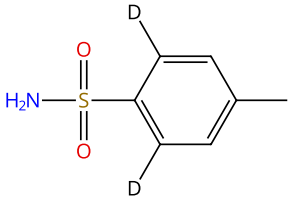
Scheme 171 (1 Reaction)

Steps: **1**



Suppliers (41)

Suppliers (99)



31-614-CAS-25982152

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

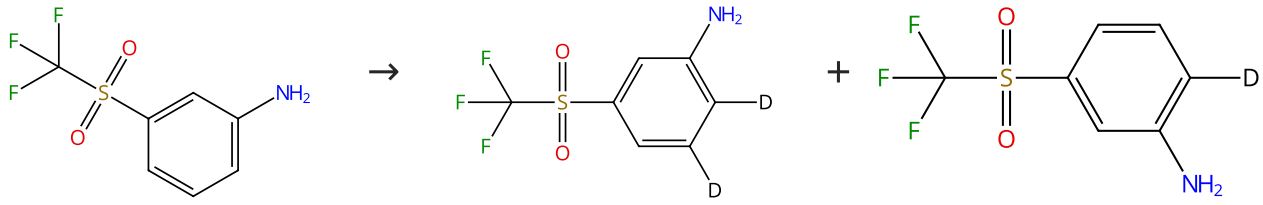
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 172 (1 Reaction)

Steps: **1**



Suppliers (57)

31-116-CAS-21649677

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

Experimental Protocols

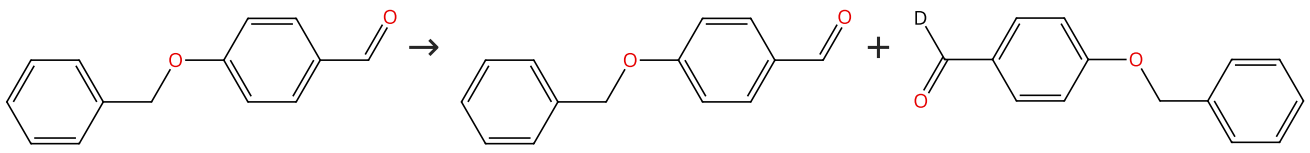
NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 173 (1 Reaction)

Steps: **1**



Suppliers (103)

Suppliers (6)

31-614-CAS-28589057 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

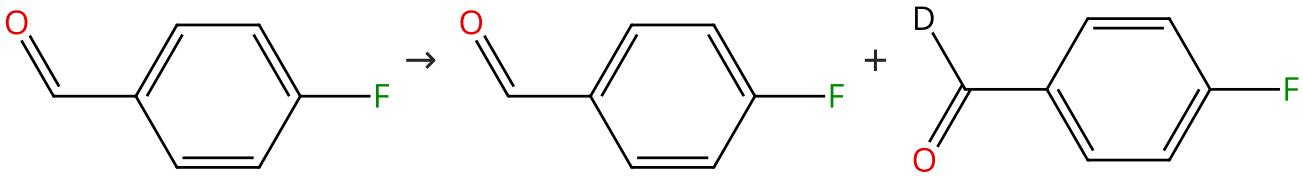
Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 174 (1 Reaction) Steps: **1**



Suppliers (103)

31-614-CAS-30306427 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: [1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene]chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium
Solvents: Dichloromethane; 3 h, 25 °C

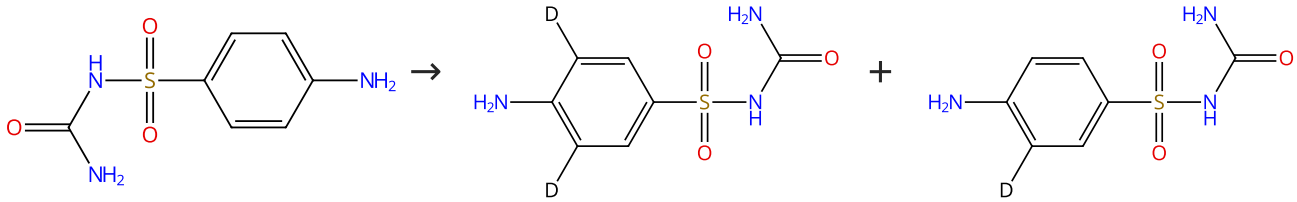
Experimental Protocols

Iridium-Catalyzed Formyl-Selective Deuteration of Aldehydes

By: Kerr, William J.; et al

Angewandte Chemie, International Edition (2017), 56(27), 7808-7812.

Scheme 175 (1 Reaction) Steps: **1**



Suppliers (60)

31-116-CAS-21649681 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)
Solvents: Tetrahydrofuran, Water-d_2; 3 h, 80 °C

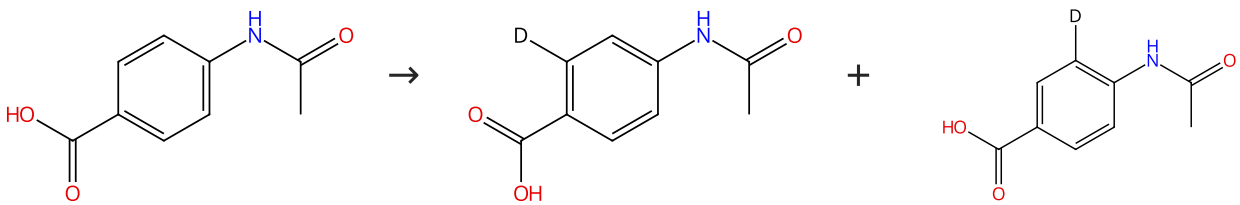
Experimental Protocols

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Scheme 176 (1 Reaction) Steps: **1**



Suppliers (87)

31-116-CAS-15366910 Steps: 1

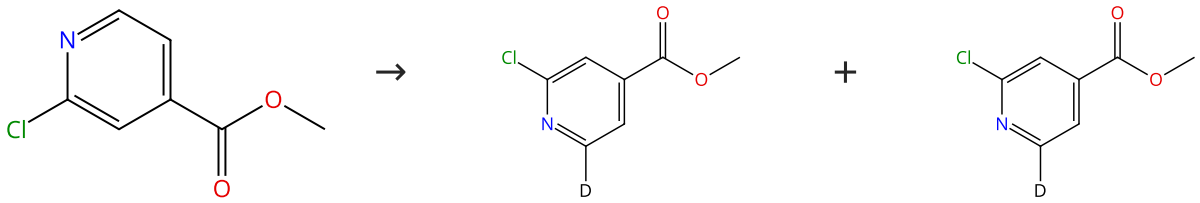
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 6 h, 0.9 atm, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

Scheme 177 (1 Reaction) Steps: 1



Suppliers (79)

31-614-CAS-30235760 Steps: 1

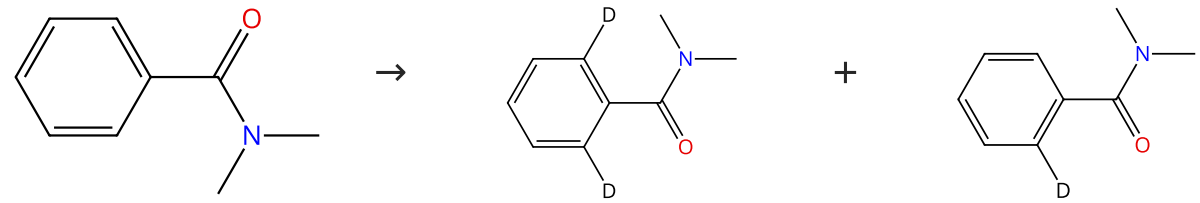
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 178 (1 Reaction) Steps: 1



Suppliers (75)

31-614-CAS-35597983 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

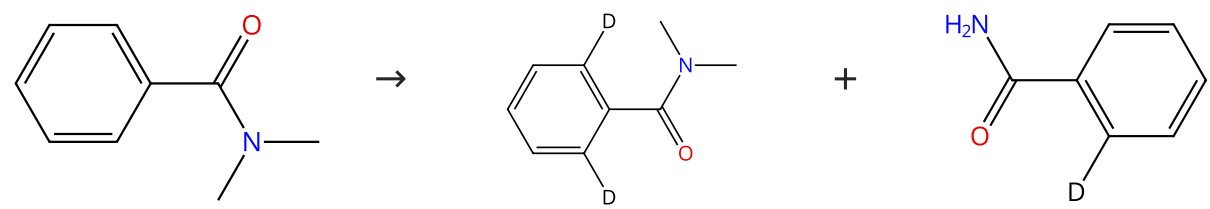
Experimental Protocols

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 179 (2 Reactions) Steps: 1



Suppliers (75)

31-116-CAS-1106219 Steps: **1**

1.1 **Catalysts:** Triphenylphosphine (polystyrene-bound), Iridium (1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 2 h, rt

1.2 **Reagents:** Deuterium
Solvents: Dichloromethane; 4 h, rt; 18 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

31-116-CAS-5638625 Steps: **1**

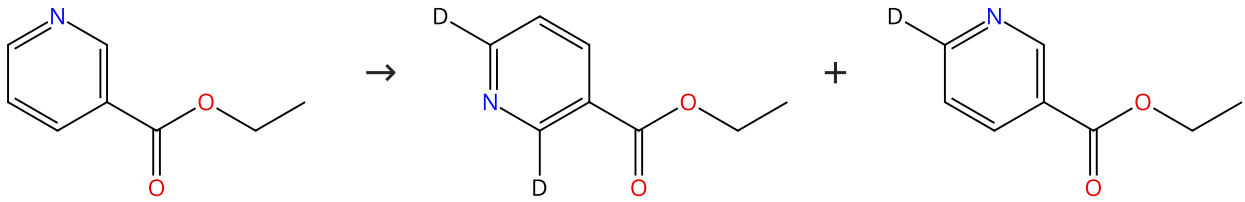
1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1) (complexes with polystyrene-bound triphenylphosphine)
Solvents: Dichloromethane; 1 h, rt

A solid-phase iridium-based ortho-exchange catalyst for the one-step labeling of aromatic substrates with deuterium

By: Hickey, Michael J.; et al

Tetrahedron Letters (2004), 45(47), 8621-8623.

Scheme 180 (1 Reaction) Steps: **1**



Suppliers (109)

31-116-CAS-4626276 Steps: **1**

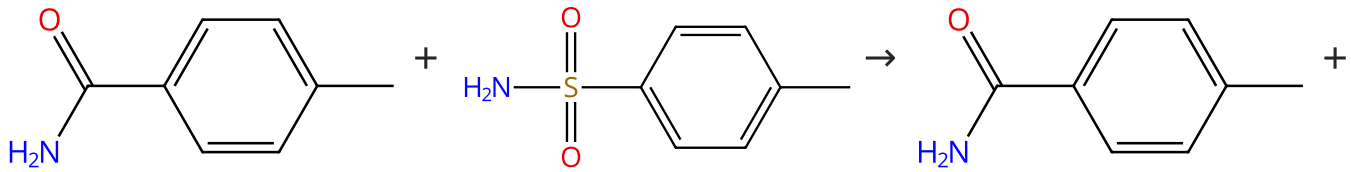
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

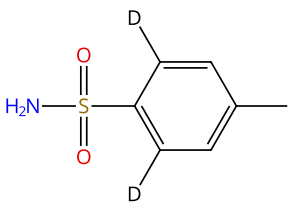
Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 181 (1 Reaction) Steps: **1**



Suppliers (84)

Suppliers (99)



31-614-CAS-31026559 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

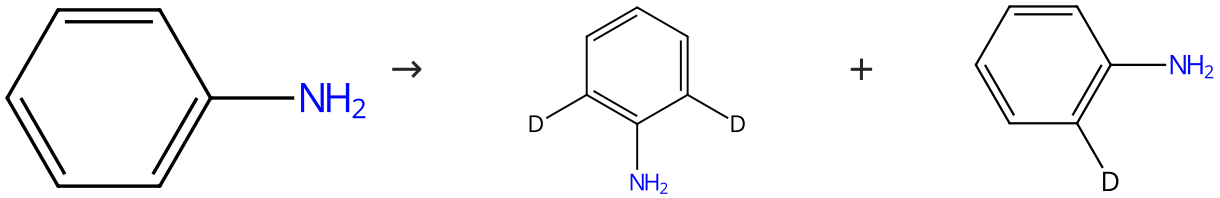
Experimental Protocols

Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 182 (1 Reaction) Steps: **1**



Suppliers (120) Supplier (1) Supplier (1)

31-116-CAS-4572016 Steps: **1**

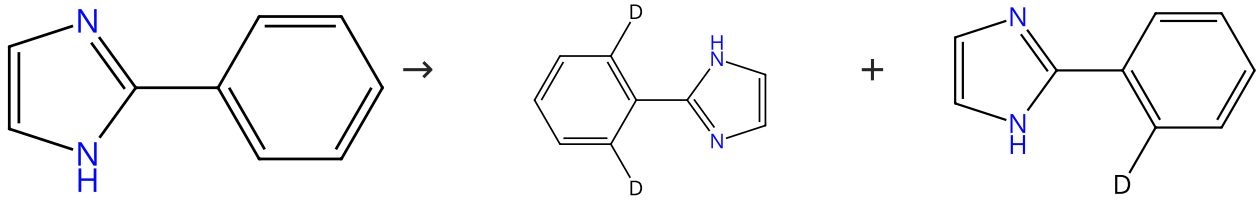
1.1 **Reagents:** Deuterium
Catalysts: Rhodium, Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane, Tetrahydrofuran; cooled; 4 h, 1342 - 1590 mbar, rt

The effect of adding Crabtree's catalyst to rhodium black in direct hydrogen isotope exchange reactions

By: Schou, Soeren Christian

Journal of Labelled Compounds and Radiopharmaceuticals (2009), 52(9), 376-381.

Scheme 183 (1 Reaction) Steps: **1**



Suppliers (94) Suppliers (2)

31-614-CAS-35597977 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 300 mbar, rt

Experimental Protocols

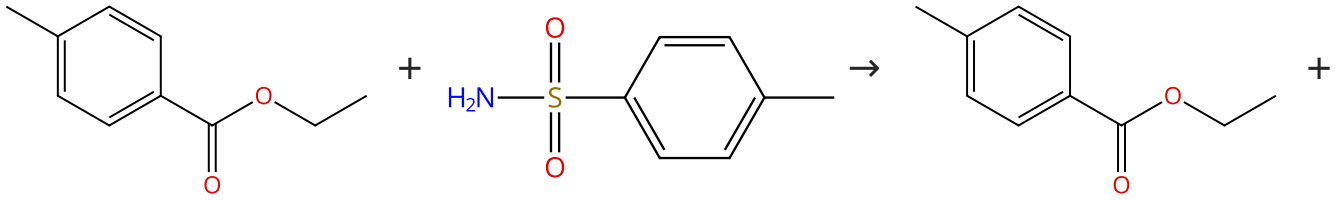
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

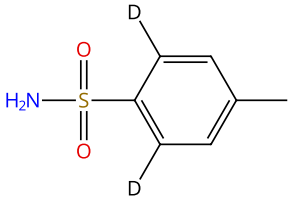
Scheme 184 (1 Reaction)

Steps: **1**



Suppliers (69)

Suppliers (99)



31-614-CAS-28604850

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

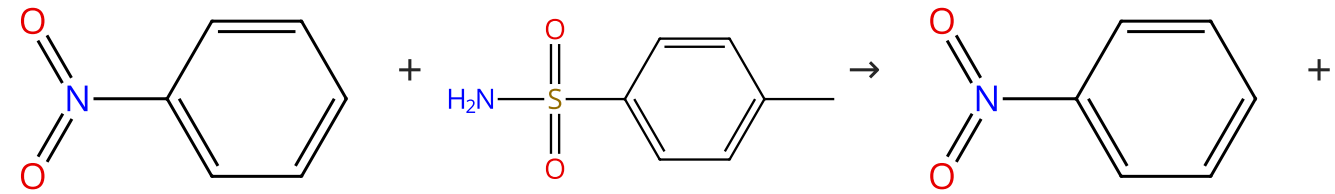
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

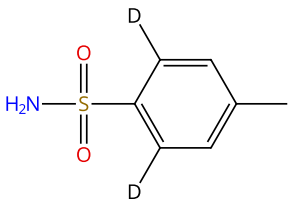
Scheme 185 (1 Reaction)

Steps: **1**



Suppliers (107)

Suppliers (99)



31-614-CAS-26882435

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene]iridium
Solvents: Dichloromethane; -78 °C → 25 °C; 2 h, 25 °C

Experimental Protocols

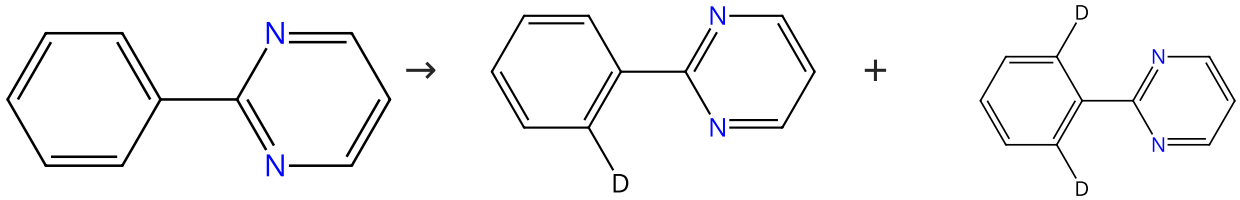
Iridium-Catalyzed C-H Activation and Deuteration of Primary Sulfonamides: An Experimental and Computational Study

By: Kerr, William J.; et al

ACS Catalysis (2015), 5(1), 402-410.

Scheme 186 (1 Reaction)

Steps: **1**



Suppliers (64)

31-614-CAS-35597976

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

Experimental Protocols

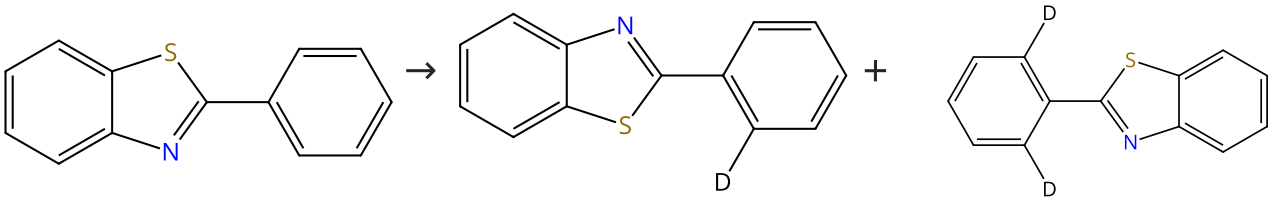
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 187 (1 Reaction)

Steps: **1**



Suppliers (77)

31-614-CAS-35597981

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 25 mbar, rt

Experimental Protocols

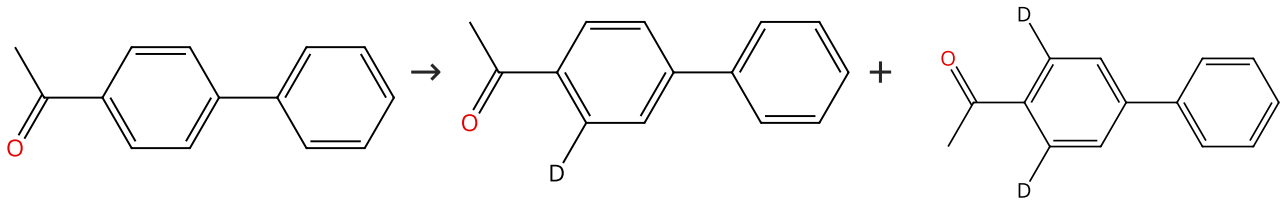
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 188 (1 Reaction)

Steps: **1**



Suppliers (112)

31-614-CAS-35597987

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Isopropyl acetate; 2 h, 300 mbar, rt

Experimental Protocols

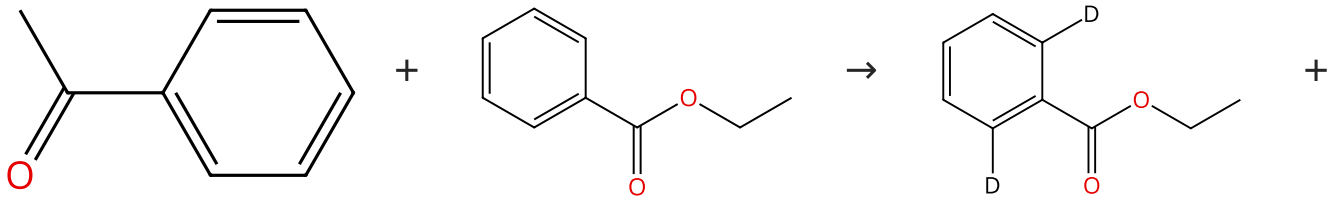
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

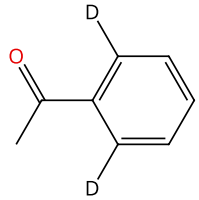
Scheme 189 (1 Reaction)

Steps: **1**



Suppliers (109)

Suppliers (94)



Supplier (1)

31-614-CAS-23969805

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

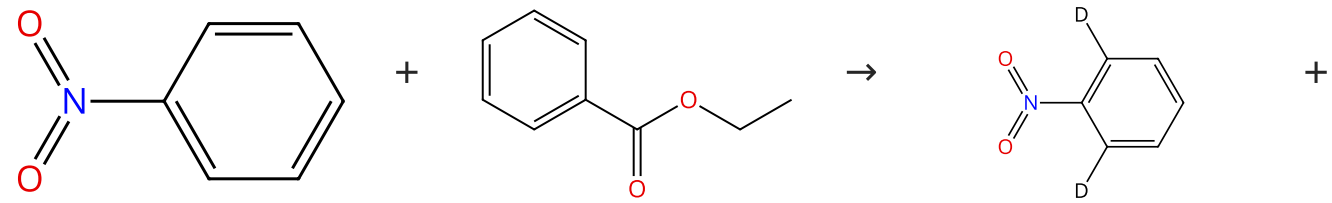
Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

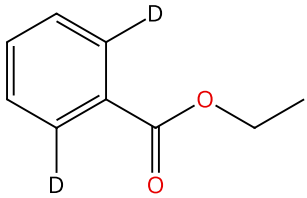
Scheme 190 (1 Reaction)

Steps: **1**



Suppliers (107)

Suppliers (94)



31-614-CAS-23969788

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

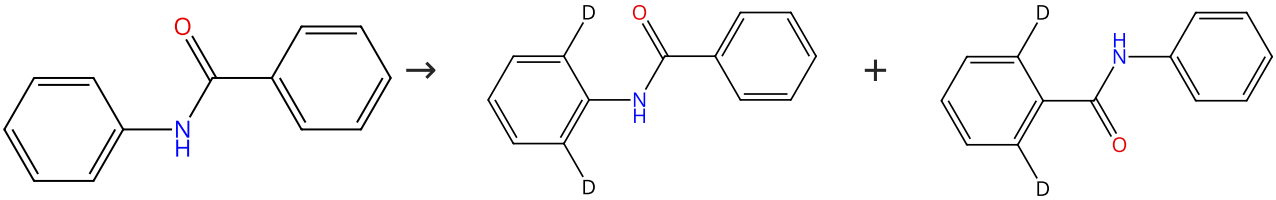
Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 191 (1 Reaction)

Steps: **1**



Suppliers (89)

31-116-CAS-1417334

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Chloro(1,5-cyclooctadiene)(1,3-dihydro-1,3-dimesityl-2*H*-imidazol-2-ylidene)iridium
Solvents: Dichloromethane; 1 atm, -78 °C → 25 °C; 16 h, 25 °C

Experimental Protocols

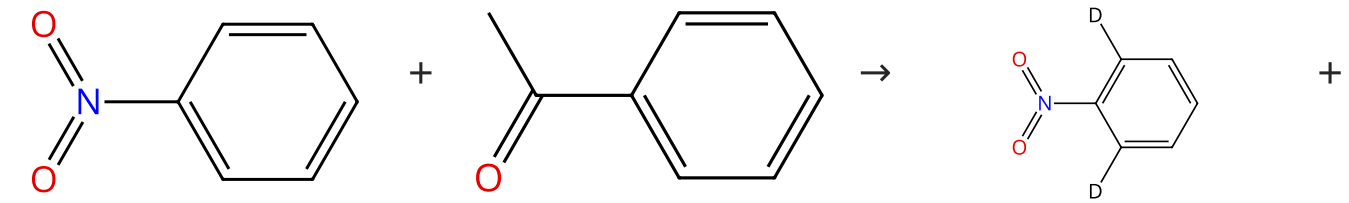
Application of neutral iridium(I) N-heterocyclic carbene complexes in ortho-directed hydrogen isotope exchange

By: Cochrane, Alison R.; et al

Journal of Labelled Compounds and Radiopharmaceuticals (2013), 56(9-10), 451-454.

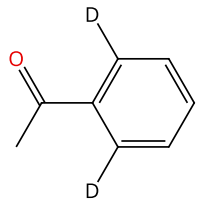
Scheme 192 (1 Reaction)

Steps: **1**



Suppliers (107)

Suppliers (109)



Supplier (1)

31-614-CAS-23969790

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

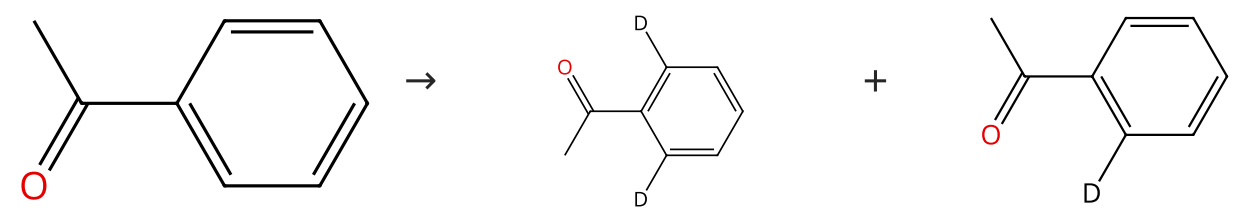
Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 193 (1 Reaction)

Steps: **1**



Suppliers (109)

Supplier (1)

Supplier (1)

31-614-CAS-23969797 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 30 min, 50 °C

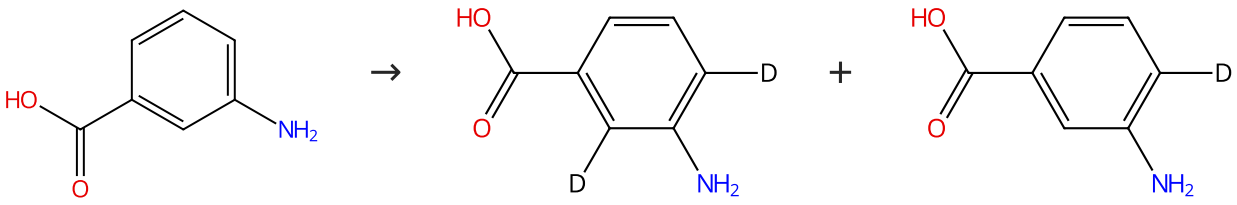
Experimental Protocols

Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 194 (1 Reaction) Steps: **1**



Suppliers (105)

31-116-CAS-7080430 Steps: **1**

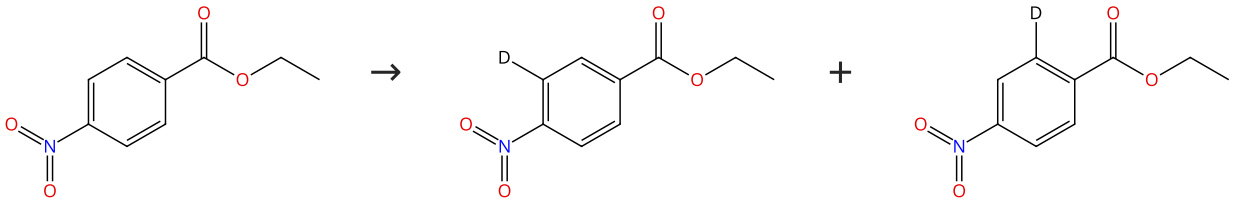
1.1 **Reagents:** Deuterium
Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-κO^2,κO^4)iridium
Solvents: Dimethylacetamide; 34 h, rt

Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.

Scheme 195 (1 Reaction) Steps: **1**



Suppliers (92)

31-614-CAS-23969794 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: Chloroform-*d*; 1 atm, cooled; 50 °C

Experimental Protocols

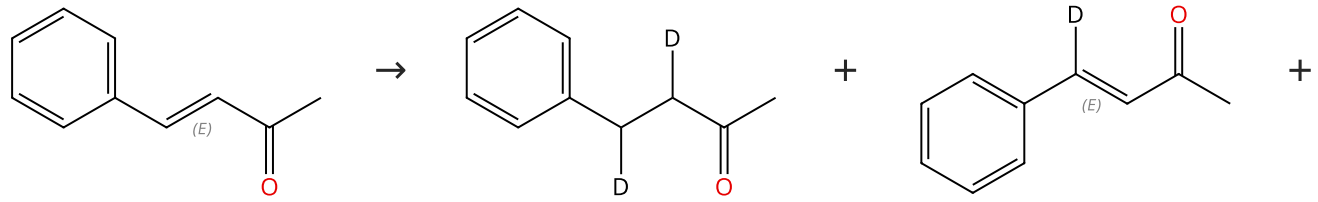
Are rate and selectivity correlated in iridium-catalysed hydrogen isotope exchange reactions?

By: Timofeeva, Daria S.; et al

Catalysis Science & Technology (2021), 11(16), 5498-5504.

Scheme 196 (1 Reaction)

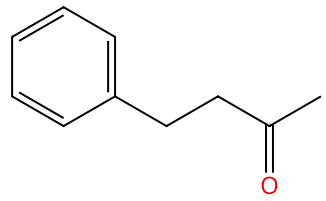
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (84)



Suppliers (85)

31-116-CAS-15514274

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

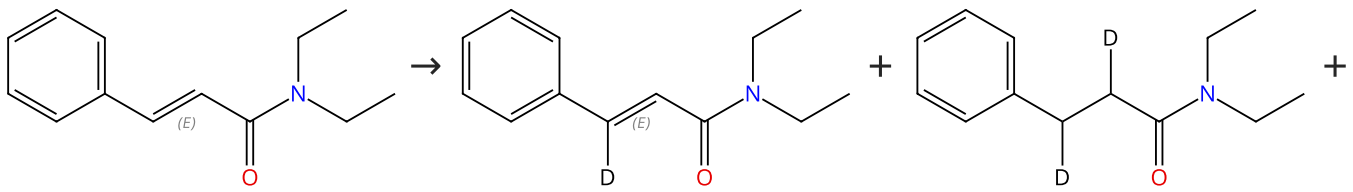
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 197 (1 Reaction)

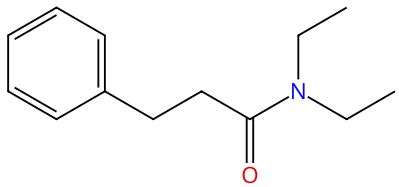
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (22)



Suppliers (12)

31-116-CAS-9157244

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

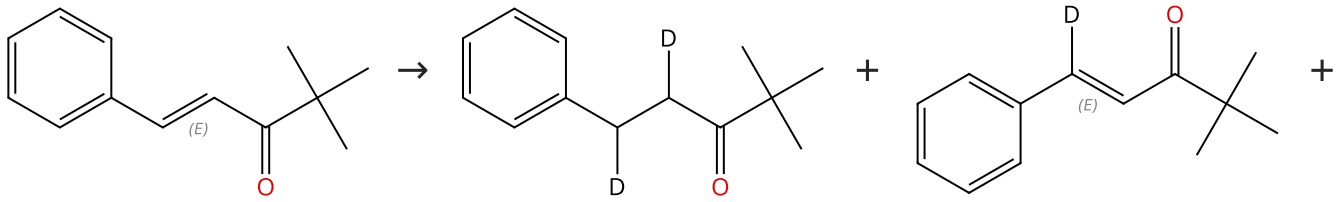
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 198 (1 Reaction)

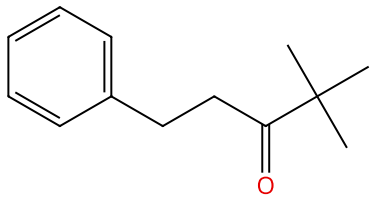
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (24)



Suppliers (43)

31-116-CAS-2815683

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

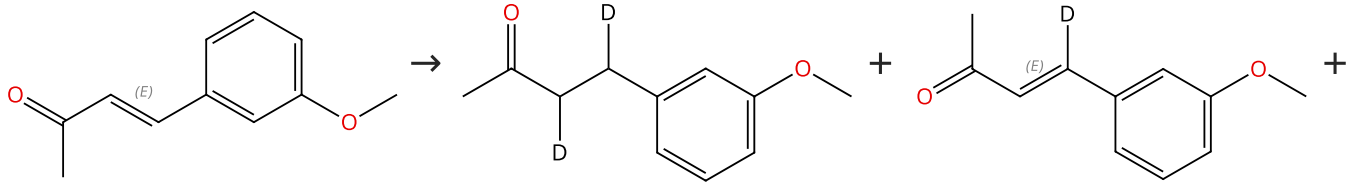
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 199 (1 Reaction)

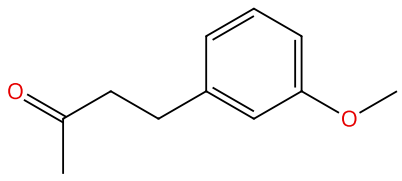
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (17)



Suppliers (24)

31-116-CAS-12067532

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

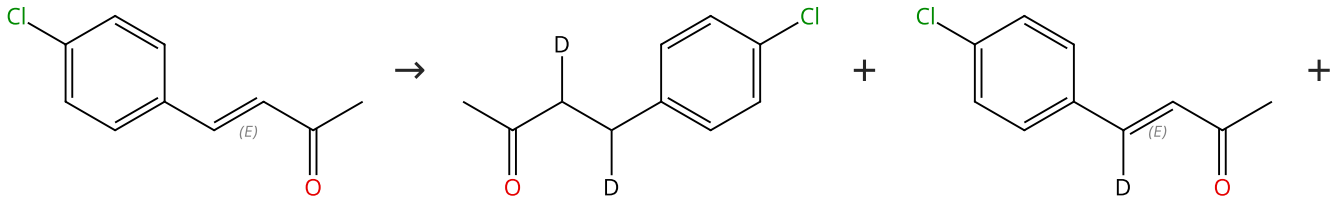
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 200 (1 Reaction)

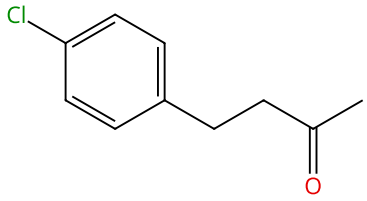
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (31)



Suppliers (52)

31-116-CAS-10931425

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

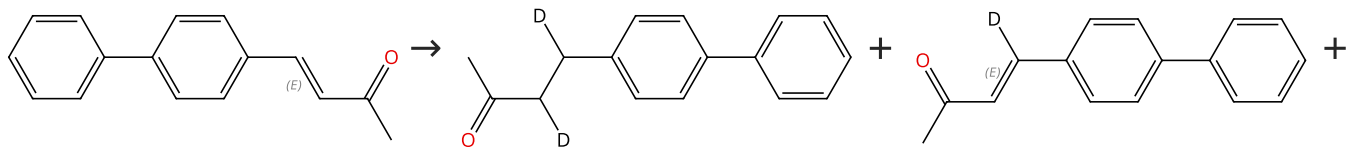
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 201 (1 Reaction)

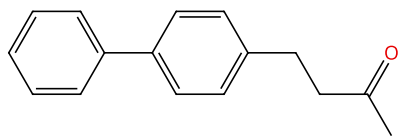
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (11)



Suppliers (15)

31-116-CAS-4546718

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

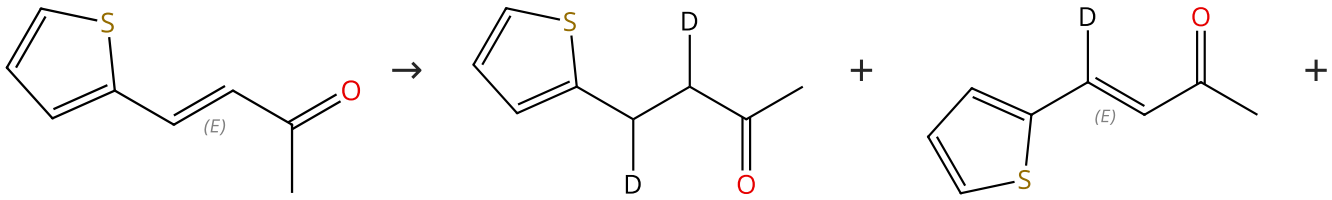
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 202 (1 Reaction)

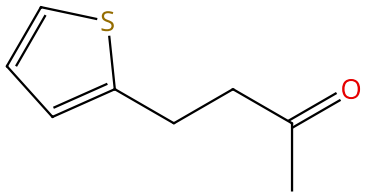
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (51)



Suppliers (12)

31-116-CAS-13815326

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

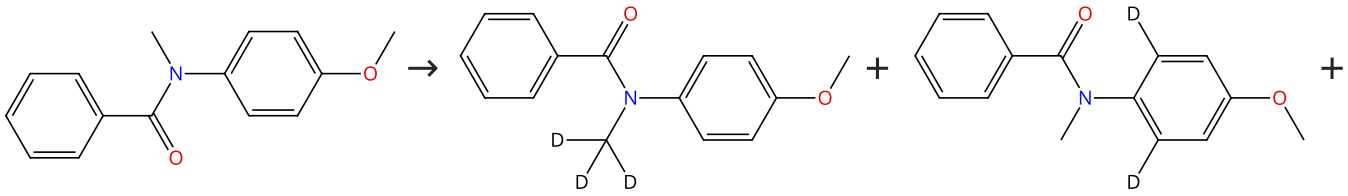
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

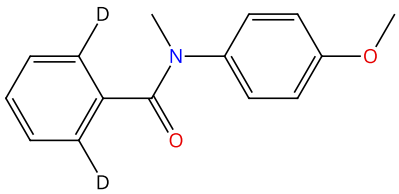
Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 203 (6 Reactions)

Steps: **1**



Suppliers (9)



31-116-CAS-5084032

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

31-116-CAS-13896666 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Hexyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

31-116-CAS-2300600 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(pyridine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

31-116-CAS-783691 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: 1-Octyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

31-116-CAS-4979892 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [1,4-butanediylbis[diphenylphosphine-κ*P*]][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-)
Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

31-116-CAS-4434061 Steps: 1

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(pyridine)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)
Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 6 h, rt

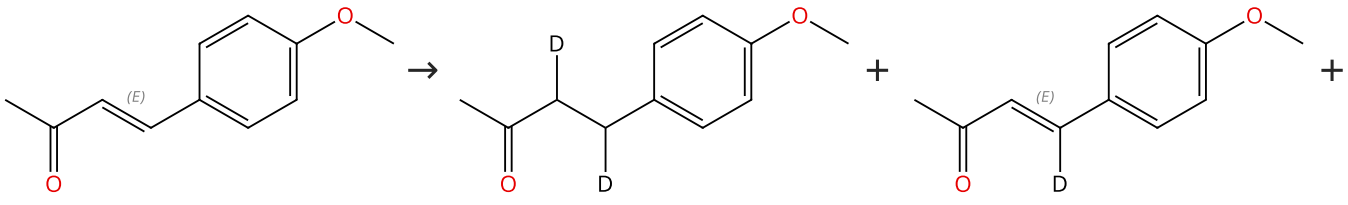
Application of 1-butyl-3-methylimidazolium hexafluoro phosphate to Ir(I)-catalyzed hydrogen isotope exchange labeling of substrates poorly soluble in dichloromethane

By: Salter, Rhys; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(5), 489-498.

Scheme 204 (1 Reaction)

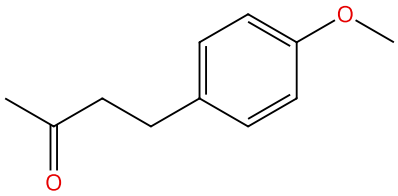
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (42)



Suppliers (77)

31-116-CAS-1408700

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

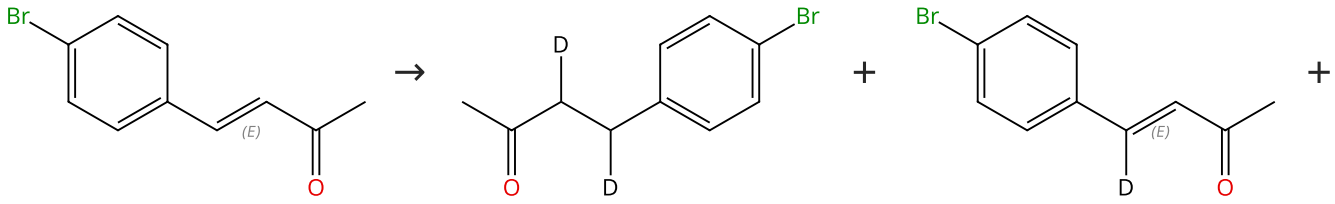
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 205 (1 Reaction)

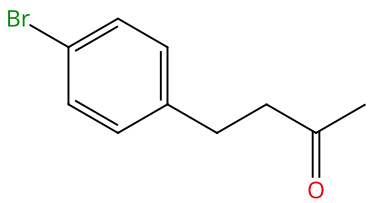
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (60)



Suppliers (41)

31-116-CAS-6345262

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

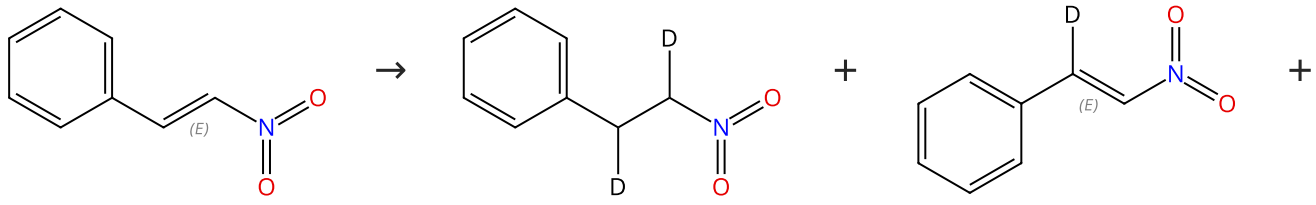
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 206 (1 Reaction)

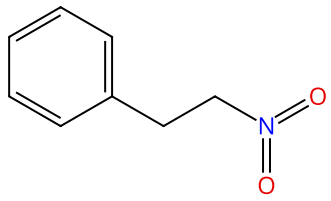
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (97)



Suppliers (65)

31-116-CAS-11273199

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

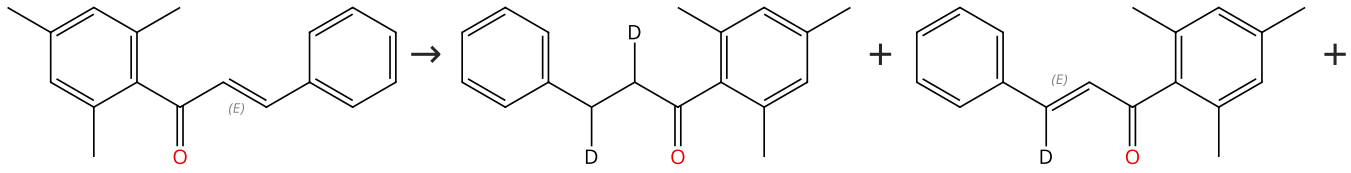
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 207 (1 Reaction)

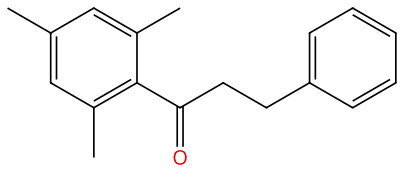
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (10)



Suppliers (6)

31-116-CAS-630364

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

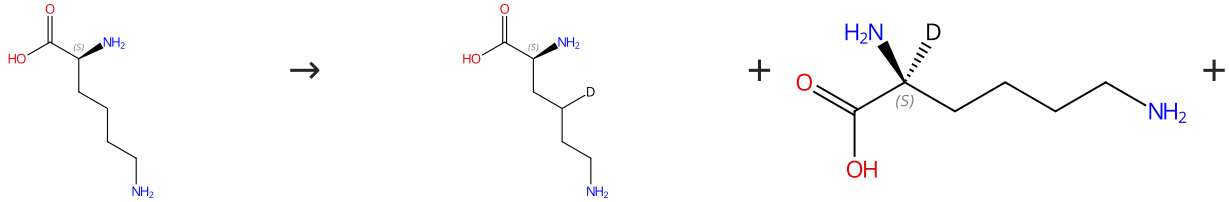
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 208 (3 Reactions)

Steps: **1**

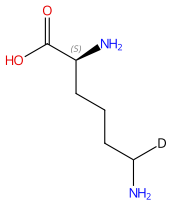


Absolute stereochemistry shown

Absolute stereochemistry shown

Absolute stereochemistry shown

Suppliers (122)



Absolute stereochemistry shown

31-614-CAS-34988556 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (bound to polyvinylpyrrolidone or IMes N-heterocyclic carbene), 1*H*-Imidazolium, 1-(3-sulfopropyl)-3-(2,4,6-trimethylphenyl)-, inner salt (Iridium and ruthenium supported)
Solvents: Water-d_2; 48 h, 2 bar, 55 °C

Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

31-614-CAS-34988549 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 1*H*-Imidazolium, 1-(3-sulfopropyl)-3-(2,4,6-trimethylphenyl)-, inner salt (Iridium and ruthenium supported), Iridium, compd. with ruthenium (2:1)
Solvents: Water-d_2; 48 h, 2 bar, 55 °C

Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

31-614-CAS-34988551 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: 1*H*-Imidazolium, 1-(3-sulfopropyl)-3-(2,4,6-trimethylphenyl)-, inner salt (Iridium and ruthenium supported), Iridium, compd. with ruthenium (1:2)
Solvents: Water-d_2; 48 h, 2 bar, 55 °C

Experimental Protocols

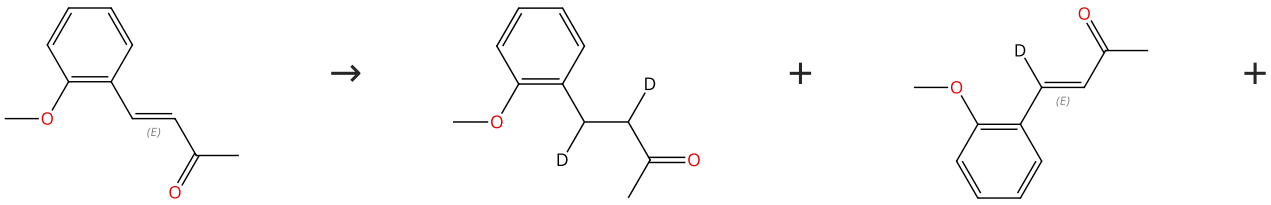
N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

Scheme 209 (1 Reaction)

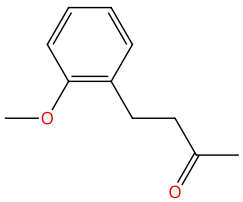
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (15)



Suppliers (16)

31-116-CAS-5337910

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

Experimental Protocols

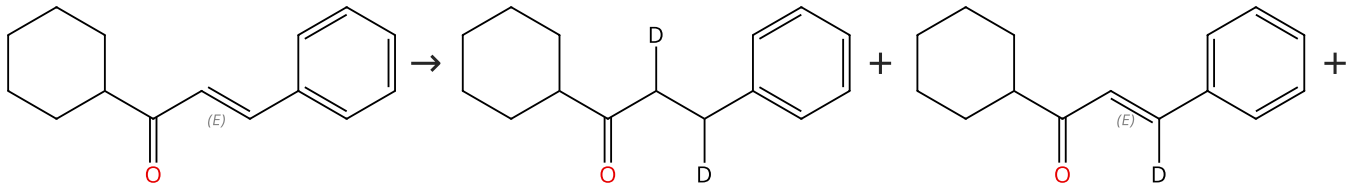
Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 210 (1 Reaction)

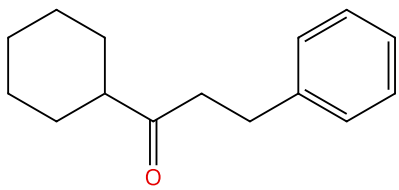
Steps: **1**



Double bond geometry shown

Double bond geometry shown

Suppliers (7)



Suppliers (28)

31-116-CAS-14683609

Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1)
Solvents: Dichloromethane; -78 °C; 1 h, 25 °C

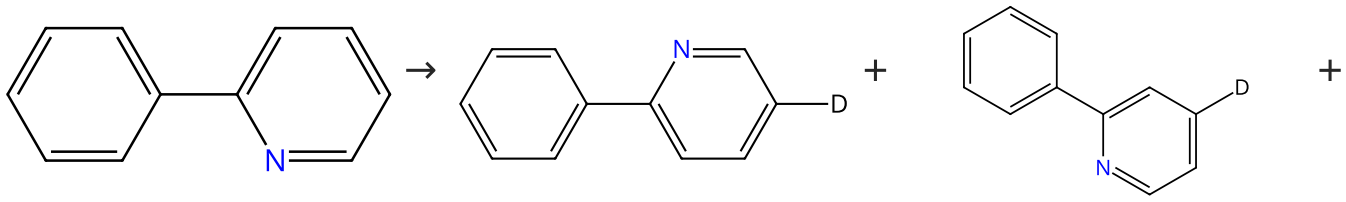
Experimental Protocols

Iridium(I)-Catalyzed Regioselective C-H Activation and Hydrogen-Isotope Exchange of Non-aromatic Unsaturated Functionality

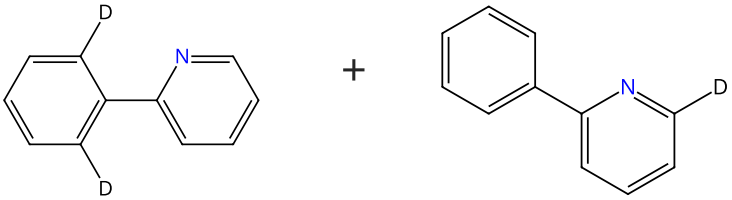
By: Kerr, William J.; et al

Chemistry - A European Journal (2014), 20(45), 14604-14607.

Scheme 211 (3 Reactions) Steps: **1**



Suppliers (94)



Supplier (1)

Supplier (1)

31-614-CAS-34988534 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Poly(vinylpyrrolidone) (Iridium and ruthenium supported), Iridium, compd. with ruthenium (2:1)
Solvents: Tetrahydrofuran; 24 h, 2 bar, 55 °C

Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

31-614-CAS-34988532 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Iridium (bound to polyvinylpyrrolidone or IMes N-heterocyclic carbene), Poly(vinylpyrrolidone) (Iridium and ruthenium supported)
Solvents: Tetrahydrofuran; 24 h, 2 bar, 55 °C

Experimental Protocols

N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

31-614-CAS-34681536 Steps: **1**

1.1 **Reagents:** Deuterium
Catalysts: Poly(vinylpyrrolidone) (Iridium and ruthenium supported), Iridium, compd. with ruthenium (1:2)
Solvents: Tetrahydrofuran; 24 h, 2 bar, 55 °C

Experimental Protocols

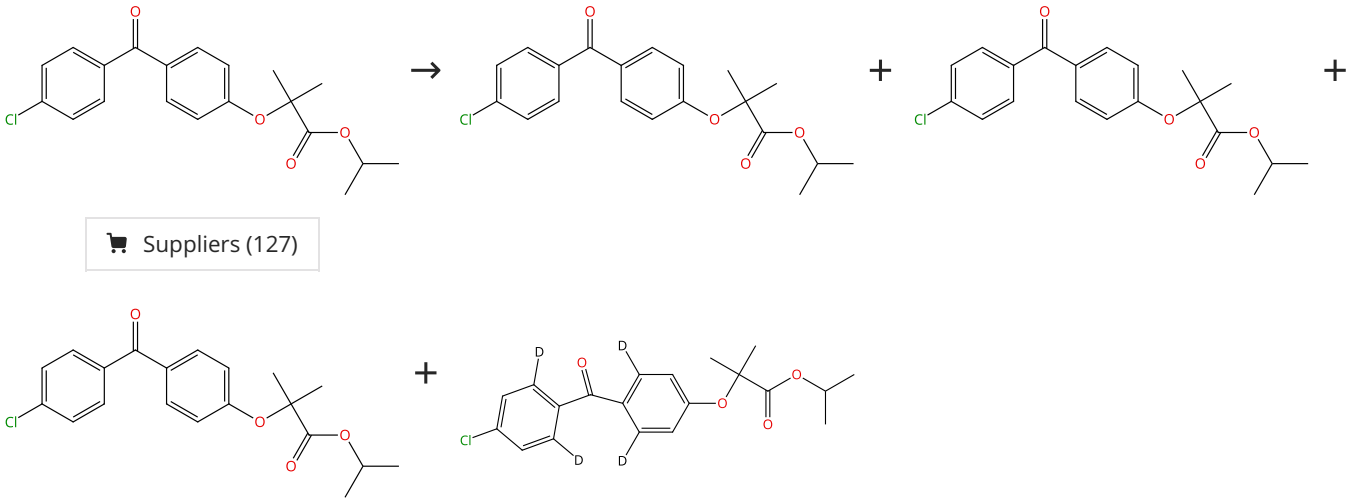
N-Heterocyclic Carbene-Based Iridium and Ruthenium /Iridium Nanoparticles for the Hydrogen Isotope Exchange Reaction through C-H Bond Activations

By: Zuluaga-Villamil, Alejandra; et al

Organometallics (2022), 41(22), 3313-3319.

Scheme 212 (1 Reaction)

Steps: **1**



Suppliers (127)

31-614-CAS-35597988	Steps: **1**
1.1 **Reagents:** Deuterium **Catalysts:** Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1) **Solvents:** Isopropyl acetate; 2 h, 25 mbar, rt	
Experimental Protocols	

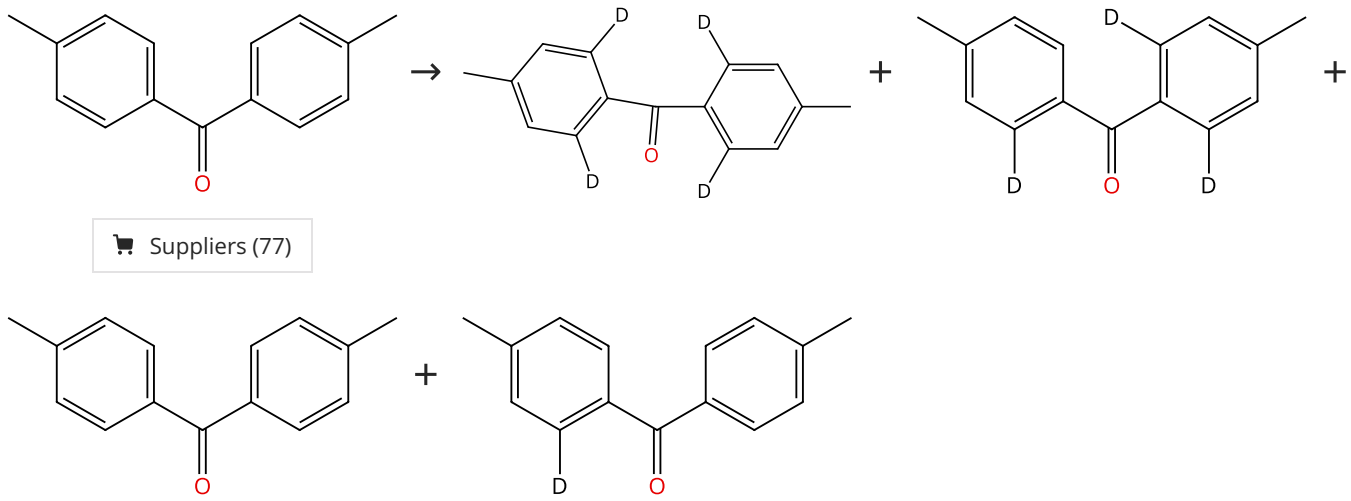
Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.

Scheme 213 (1 Reaction)

Steps: **1**



Suppliers (77)

31-614-CAS-35597984	Steps: **1**
1.1 **Reagents:** Deuterium **Catalysts:** Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene](triphenylphosphine)-, hexafluorophosphate(1-) (1:1) **Solvents:** Isopropyl acetate; 2 h, 25 mbar, rt	
Experimental Protocols	

Significantly improved radiochemical yields in gaseous tritium reactions by iridium(I)-catalyzed hydrogen isotope exchange

By: Morawietz, Patrick; et al

Green Chemistry (2022), 24(12), 4824-4829.