



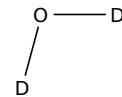
Task History

## Initiating Search

February 22, 2025, 12:19 PM

## Substances:

Filtered By:



Structure Match: As Drawn

## Search Tasks

| Task   | Search Type | View                         |
|--|-------------|------------------------------|
| Returned Substance Results + Filters (1,728)                   | Substances  | <a href="#">View Results</a> |
| Exported: Retrieved Related Reaction Results + Filters (1,028) | Reactions   | <a href="#">View Results</a> |

Filtered By:

| Substance Role: | Reagent, Solvent   |
|-----------------|--|
| Catalyst:       | [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato-κO <sup>2</sup> ,κO <sup>4</sup> )iridium, [(1,2,5,6-η)-1,5-Cyclooctadiene][(1,2,3,3a,7a-η)-1H-inden-1-yl]iridium, [(1,2,5,6-η)-1,5-Cyclooctadiene](2,4-pentanedionato-κO <sup>2</sup> ,κO <sup>4</sup> )iridium, [(1,2,5,6-η)-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato-κO <sup>2</sup> ,κO <sup>4</sup> )iridium, (1-Butyl-1,3-dihydro-3-methyl-2H-imidazol-2-ylidene)chloro[(1,2,5,6-η)-1,5-cyclooctadiene]iridium, [2-[Bis(1-methylethyl)phosphino-κP]-N-[2-[bis(1-methylethyl)phosphino-κP]-4-methylphenyl]-4-methylbenzenaminato-κN]dihydroiridium, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-hydroxydihydroiridium, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydihydroiridium, Chloro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl][2-(2-pyridinyl-κN)phenyl-κC]iridium, Chloro[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](N-phenyl-2-pyridinecarboxamido-κN <sup>1</sup> ,κN <sup>2</sup> )iridium, Chloro[3-[1-[(4-methoxyphenyl)imino-κN]ethyl]-2-naphthalenyl-κC][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium, Chloro[5-(dimethylamino)-2-(2-pyridinyl-κN)phenyl-κC][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium, Chloro(a,a-dimethyl-2-pyridinemethanolato-κN <sup>1</sup> ,κO <sup>2</sup> )[(1,2,3,4,5-η)-1,2,3,4,5- |

pentamethyl-2,4-cyclopentadien-1-yl]iridium,  
Dichloro(1,3-dihydro-1,3,4,5-tetramethyl-2-*H*-imidazol-2-ylidene)[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium, Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]diiridium, Di- $\mu$ -chlorobis[(5,6,11,12- $\eta$ )-dibenzo[*a,e*]cyclooctene]diiridium, Di- $\mu$ -chlorotetrakis[(1,2- $\eta$ )-cyclooctene]diiridium, *fac*-Tris(2-(2-pyridinyl)phenyl)iridium, Iridate(3-), tris[2-(2-pyridinyl- $\kappa N$ )-4-sulfonatophenyl- $\kappa C$ ]-, sodium (1:3), (OC-6-22)-, Iridium, Iridium(1+), [1,1'-(4 *R*)-[4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[1,1-diphenylphosphine- $\kappa P$ ]] [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, 1,1,1-trifluoromethanesulfonate (1:1), Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene][(1,2-dimethyl-1,2-ethanediyl)bis[diphenylphosphine]-*P,P*]-, [*S*(-*R\**,*R\**)]-, salt with trifluoromethanesulfonic acid (1:1), Iridium(1+), [(1,2,5,6- $\eta$ )-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- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1), Iridium(1+), (2,2'-bipyridine- $\kappa N^1,\kappa N^1$ )bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), (2,2'-bipyridine- $\kappa N^1,\kappa N^1$ )bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-(5-methyl-2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[5-(1,1-dimethylethyl)-2-[4-(1,1-dimethylethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-), Iridium(1+), [4,4'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1), Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1), Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, 1,1,1-trifluoromethanesulfonate (1:1), Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1), Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), Iridium(1+), bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]*N*-(2-

pyridinyl- $\kappa M$ -2-pyridinamine- $\kappa N^1$ ]-, chloride, (*OC*-6-33)-, Iridium(1+), bis[3,5-difluoro-2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ](1,10-phenanthroline- $\kappa N^1,\kappa N^{10}$ )-, (*OC*-6-13)-, hexafluorophosphate(1-) (1:1), Iridium(1+), bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ](1,10-phenanthroline- $\kappa N^1,\kappa N^{10}$ )-, (*OC*-6-13)-, hexafluorophosphate(1-) (1:1), Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-4-methoxypyridine- $\kappa M$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1), Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-5-methoxypyridine- $\kappa M$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1), Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-*N,N*-diethyl-4-pyridinamine- $\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1), Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1), Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )pyridine- $\kappa M$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1), Iridium(1+), chloro( $\eta^5$ -2,4-cyclopentadien-1-yl)[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-4-methoxypyridine- $\kappa M$ ]-, chloride (1:1), Iridium(1+), chloro[6-[6-(1,1-dimethylethyl)-1*H*-benzimidazol-2-yl- $\kappa N^3$ ]-2-pyridinol- $\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1), Iridium(1+), peroxytetrakis(trimethylphosphine)-, chloride (1:1), (*OC*-6-22)-, Iridium(1+), trihydro[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl] (trimethylphosphine)-, 1,1,1-trifluoromethanesulfonate (1:1), Iridium(1+), tris[ $\mu$ -(4-(1,1-dimethylethyl)benzenemethanethioato)]bis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, chloride (1:1), Iridium(1+), tris[ $\mu$ -(benzeneethanethiolato)]bis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, chloride (1:1), stereoisomer, Iridium(1+), tris[ $\mu$ -(benzenemethanethiolato)]bis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, chloride (1:1), Iridium(2+), aqua([2,2'-bipyridine]-4,4'-diol- $\kappa N^1,\kappa N^{1'}$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, sulfate (1:1), Iridium(2+), aqua([4,4'-bipyrimidine]-2,2',6,6'(1*H*,1'*H*,3*H*,3'*H*-tetrone- $\kappa N^3,\kappa N^{3'}$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, sulfate (1:1), Iridium(2+), diaquabis[4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^{1'}$ ]bis[ $\mu$ -(4-methylbenzenesulfonato- $\kappa O:\kappa O'$ )]bis(2-methyl-2-phenylpropyl)di-, stereoisomer, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:2), Iridium(2+), triqua[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl], sulfate (1:1), Iridium, aqua([2,2'-bipyridine]-6,6'(1*H*,1'*H*-dionato(2-) $\kappa N^1,\kappa N^{1'}$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, Iridium, compd. with ruthenium (1:2), Iridium, compd. with ruthenium (2:1), Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [*N*-(1*R*,2*R*)-2-(Amino- $\kappa M$ )-1,2-

diphenylethyl]methanesulfonamido(2-)-κΝ]  
[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-  
cyclopentadien-1-yl]iridium, [*N*-(1,5,25)-2-(Amino-κΝ)-  
1,2-diphenylethyl]methanesulfonamido(2-)-κΝ]  
[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-  
cyclopentadien-1-yl]iridium, (*OC*-6-22)-Tris[2-(2-  
pyridinyl-κΝ)-4-(3-pyridinyl)phenyl-κC]iridium, (*OC*-6-  
22)-Tris[2-(2-pyridinyl-κΝ)-4-(4-pyridinyl)phenyl-  
κC]iridium, (*SP*-5-31)-(1-Methylethyl)[5,10,15,20-  
tetrakis(4-methylphenyl)-21*H*,23*H*-porphinato(2-)-  
κΝ<sup>21</sup>,κΝ<sup>22</sup>,κΝ<sup>23</sup>,κΝ<sup>24</sup>]iridium, (7-4)-Oxotris(2,4,6-  
trimethylphenyl)iridium, Tris[2-(2-pyridinyl-  
κΝ)phenyl-κC]iridium, Tris[3,5-difluoro-2-(2-pyridinyl-  
κΝ)phenyl-κC]iridium, Tris[5-methoxy-2-(2-pyridinyl-  
κΝ)phenyl-κC]iridium

Document

Type:

Language: English

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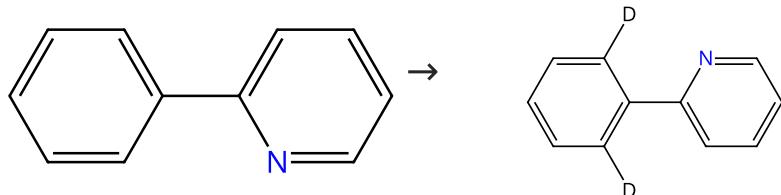


## Reactions (431)

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Scheme 1 (4 Reactions)

Steps: 1 Yield: 97-100%


[Suppliers \(94\)](#)
[Supplier \(1\)](#)

31-116-CAS-3188716

Steps: 1 Yield: 100%

**Hydrogen isotope labelling using iridium(I) dionates**1.1 **Reagents:** Water-*d*<sub>2</sub>**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium**Solvents:** Dimethylacetamide; 2 min, 130 °C

By: Lockley, W. J. S.

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

31-116-CAS-17956528

Steps: 1 Yield: 99%

**Efficient Water Reduction with sp<sup>3</sup>-sp<sup>3</sup> Diboron(4)****Compounds: Application to Hydrogenations, H-D Exchange Reactions, and Carbonyl Reductions**1.1 **Reagents:** Water-*d*<sub>2</sub>, Boron, bis[[2,2'-(imino- $\kappa N$ )bis[ethanolato- $\kappa O$ ]](2-)]di-, (*B-B*)1.2 **Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-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; 72 h, 20 °C

By: Flinker, Mathias; et al

Angewandte Chemie, International Edition (2017), 56(50), 15910-15915.

31-116-CAS-2196951

Steps: 1 Yield: 97%

**Iridium-Catalyzed Phosphoramidation of Arene C-H Bonds with Phosphoryl Azide**1.1 **Reagents:** Silver acetate, Water-*d*<sub>2</sub>**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoro antimonate**Solvents:** Dichloromethane; 12 h, 60 °C

By: Pan, Changduo; et al

Journal of Organic Chemistry (2014), 79(19), 9427-9432.

Experimental Protocols

31-116-CAS-10546863

Steps: 1

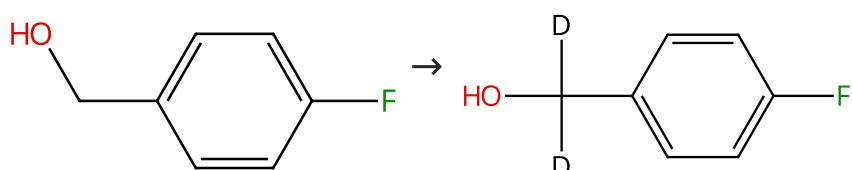
**The scope and limitations of deuteration mediated by Crabtree's catalyst**1.1 **Reagents:** Water-*d*<sub>2</sub>**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**Solvents:** Dichloromethane

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 2 (1 Reaction)

Steps: 1 Yield: 100%


[Suppliers \(80\)](#)
[Supplier \(1\)](#)

|  |  |   |
|--|--|---|
| 31-614-CAS-33408359  | Steps: 1 Yield: 100%   | Iridium-catalyzed $\alpha$ -selective deuteration of alcohols |
| 1.1 <b>Reagents:</b> Methanol- <i>d</i> <sub>4</sub> , Water- <i>d</i> <sub>2</sub> , Sodium hydroxide- <i>d</i><br><b>Catalysts:</b> Iridium, aqua[[2,2'-bipyridine]-6,6'(1 <i>H</i> ,1' <i>H</i> )-dionato(2-)- $\kappa$ N <sup>1</sup> , $\kappa$ N <sup>1</sup> ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-<br><b>Solvents:</b> Isopropanol; 7 h, 80 °C | By: Itoga, Moeko; et al<br>Chemical Science (2022), 13(30), 8744-8751. |   |
| 1.2 <b>Reagents:</b> Sulfuric acid<br><b>Solvents:</b> Water; pH 5   |  |   |
| Experimental Protocols   |  |   |

|                                   |                      |
|-----------------------------------|----------------------|
| Scheme 3 (1 Reaction)             | Steps: 1 Yield: 100% |
|                                   |                      |
| Suppliers (73)       Supplier (1) |                      |

|  |  |   |
|--|--|---|
| 31-614-CAS-33408362  | Steps: 1 Yield: 100%   | Iridium-catalyzed $\alpha$ -selective deuteration of alcohols |
| 1.1 <b>Reagents:</b> Methanol- <i>d</i> <sub>4</sub> , Water- <i>d</i> <sub>2</sub><br><b>Catalysts:</b> Iridium, aqua[[2,2'-bipyridine]-6,6'(1 <i>H</i> ,1' <i>H</i> )-dionato(2-)- $\kappa$ N <sup>1</sup> , $\kappa$ N <sup>1</sup> ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-<br><b>Solvents:</b> Isopropanol; 21 h, 80 °C | By: Itoga, Moeko; et al<br>Chemical Science (2022), 13(30), 8744-8751. |   |
| 1.2 <b>Reagents:</b> Sulfuric acid<br><b>Solvents:</b> Water; pH 5   |  |   |
| Experimental Protocols   |  |   |

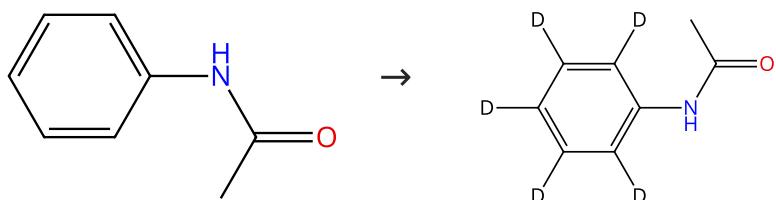
|                                   |                      |
|-----------------------------------|----------------------|
| Scheme 4 (2 Reactions)            | Steps: 1 Yield: 100% |
|                                   |                      |
| Suppliers (74)       Supplier (1) |                      |

|  |   |   |
|--|---|---|
| 31-116-CAS-14496015  | Steps: 1 Yield: 100%  | Cyclocarbopalladation: Sequential Cyclization and C-H Activation/Stille Cross-Coupling in the Pd-5-Exo-Dig Reaction |
| 1.1 <b>Reagents:</b> Water- <i>d</i> <sub>2</sub><br><b>Catalysts:</b> Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)<br><b>Solvents:</b> Dichloromethane; 92 h, rt | By: Bour, Christophe; et al<br>Organic Letters (2005), 7(4), 653-656. |   |
| 1.2 <b>Reagents:</b> Sodium bicarbonate<br><b>Solvents:</b> Water  |   |   |
| Experimental Protocols   |   |   |

|  |   |  |
|--|---|--|
| 31-116-CAS-9449769   | Steps: 1  | The scope and limitations of deuteration mediated by Crabtree's catalyst |
| 1.1 <b>Reagents:</b> Water- <i>d</i> <sub>2</sub><br><b>Catalysts:</b> Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)<br><b>Solvents:</b> Dichloromethane | By: Ellames, George J.; et al<br>Tetrahedron (2001), 57(46), 9487-9497. |  |

**Scheme 5 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (108)

Suppliers (44)

31-116-CAS-20111040

Steps: 1 Yield: 99%

1.1 Reagents: Water- $d_2$   
 Catalysts: Iridium  
 Solvents: Isopropanol; 24 h, rt

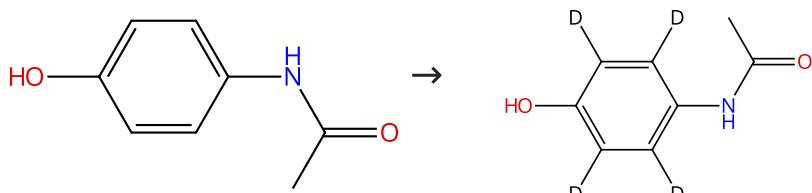
H-D Exchange Deuteration of Arenes at Room Temperature

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

**Scheme 6 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (147)

Suppliers (60)

31-116-CAS-20111042

Steps: 1 Yield: 99%

1.1 Reagents: Water- $d_2$   
 Catalysts: Iridium, Platinum  
 Solvents: Isopropanol; 24 h, rt

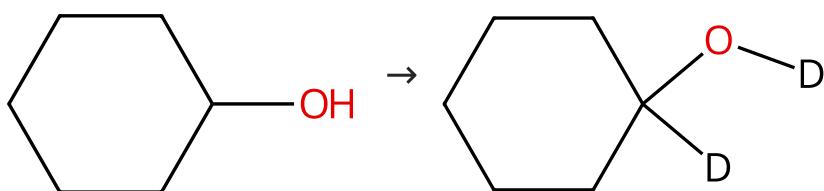
H-D Exchange Deuteration of Arenes at Room Temperature

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

**Scheme 7 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (83)

31-614-CAS-33408360

Steps: 1 Yield: 99%

1.1 Reagents: Methanol- $d_4$ , Water- $d_2$   
 Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1H;1'H)-dionato (2-) $\kappa^N$ ] $\kappa^N$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
 Solvents: Isopropanol; 2 d, 80 °C

1.2 Reagents: Sulfuric acid  
 Solvents: Water; pH 5

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

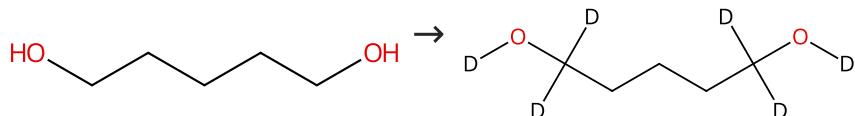
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

Experimental Protocols

**Scheme 8 (1 Reaction)**

Steps: 1 Yield: 99%


[Suppliers \(92\)](#)

31-614-CAS-33408344

Steps: 1 Yield: 99%

**1.1 Reagents:** Water- $d_2$ , Sodium hydroxide- $d$   
**Catalysts:** Iridium, aqua[2,2'-bipyridine]-6,6'(1H,1'H)-dionato(2-)- $\kappa N^1,\kappa N^1'$ [(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol, 1,4-Dioxane; 80 °C

**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**

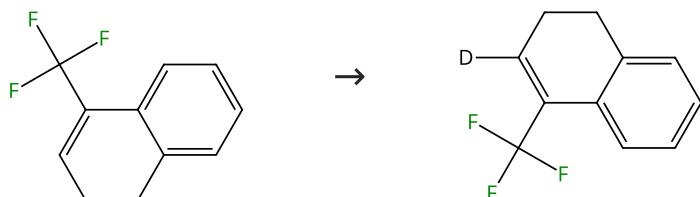
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

Experimental Protocols

**Scheme 9 (1 Reaction)**

Steps: 1 Yield: 99%


[Suppliers \(9\)](#)

31-614-CAS-37018528

Steps: 1 Yield: 99%

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1'$ ]bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )][1-]]( $N,N$ -dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt  
**Solvents:** Acetonitrile; 36 h, rt

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

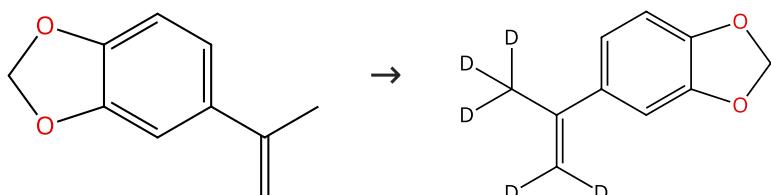
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

**Scheme 10 (1 Reaction)**

Steps: 1 Yield: 99%


[Suppliers \(10\)](#)

31-614-CAS-37018394

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )][1-]] (*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

Experimental Protocols

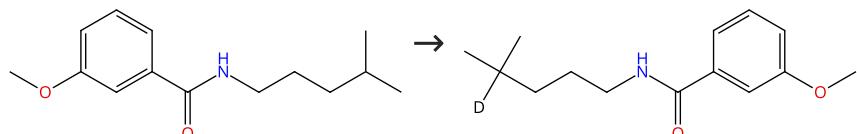
**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 11 (1 Reaction)

Steps: 1 Yield: 99%


🛒 Supplier (1)

31-614-CAS-33530421

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 48 h, rt

Experimental Protocols

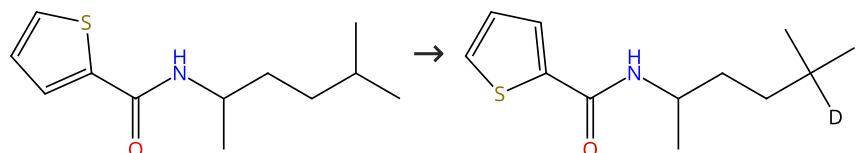
**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 12 (1 Reaction)

Steps: 1 Yield: 99%


🛒 Suppliers (4)

31-614-CAS-33530418

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** 2,4,6-Tris(1-methylethyl)benzenethiol, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Experimental Protocols

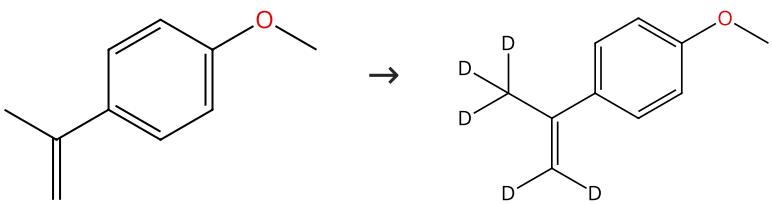
**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

**Scheme 13 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (63)

31-614-CAS-37018415

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa^1,\kappa^1$ ']bis[2-(2-pyridinyl- $\kappa$ M phenyl- $\kappa$ C]-, (OC-6-33), hexafluorophosphate(1-) (1:1), (OC-6-42)Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa$ M)(1-)]( $N,N$ -dimethyl-4-pyridinamine- $\kappa$ N<sup>1</sup>)cobalt

**Solvents:** Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

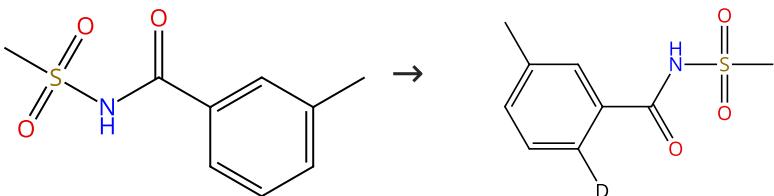
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

**Scheme 14 (2 Reactions)**

Steps: 1 Yield: 99%



Suppliers (2)

31-116-CAS-6695883

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxyd iiridium

**Solvents:** Toluene; 3 h, 70 °C

Asymmetric Alkylation of N-Sulfonylbenzamides with Vinyl Ethers via C-H Bond Activation Catalyzed by Hydroxo iridium /Chiral Diene Complexes

By: Hatano, Miyuki; et al

Journal of the American Chemical Society (2016), 138(12), 4010-4013.

Experimental Protocols

31-116-CAS-9095529

Steps: 1 Yield: 99%

1.1 Reagents: (1*Z*)-1-Ethoxy-1-propene, (1*E*)-1-Ethoxy-1-propene, Water-*d*<sub>2</sub>

**Catalysts:** Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxyd iiridium

**Solvents:** Benzene-*d*<sub>6</sub>; 0.5 h, 70 °C

Asymmetric Alkylation of N-Sulfonylbenzamides with Vinyl Ethers via C-H Bond Activation Catalyzed by Hydroxo iridium /Chiral Diene Complexes

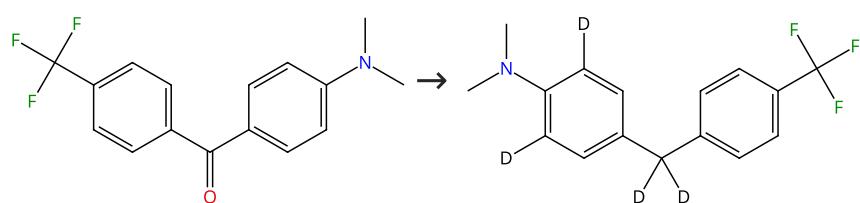
By: Hatano, Miyuki; et al

Journal of the American Chemical Society (2016), 138(12), 4010-4013.

Experimental Protocols

**Scheme 15 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (7)

31-116-CAS-22909006

Steps: 1 Yield: 99%

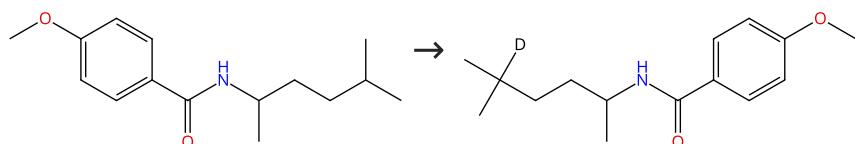
1.1 Reagents: Formic-*d* acid-*d***Catalysts:** Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-*N,N*-diethyl-4-pyridinamine- $\kappa N^1$ ][(1,2,3,4,5-*n*)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1)**Solvents:** 1,1,1,3,3-Hexafluoro-2-propanol, Water-*d*<sub>2</sub>; 2 h, 80 °C**Iridium-Catalysed Reductive Deoxygenation of Ketones with Formic Acid as Traceless Hydride Donor**

By: Yang, Zhiheng; et al

Advanced Synthesis &amp; Catalysis (2020), 362(23), 5496-5505.

Scheme 16 (1 Reaction)

Steps: 1 Yield: 99%



Supplier (1)

31-614-CAS-33530407

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)**Solvents:** Chlorobenzene; 24 h, rt**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

Scheme 17 (1 Reaction)

Steps: 1 Yield: 99%



Suppliers (38)

31-614-CAS-37018410

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximate- $\kappa N^1$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt**Solvents:** Acetonitrile; 36 h, rt**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

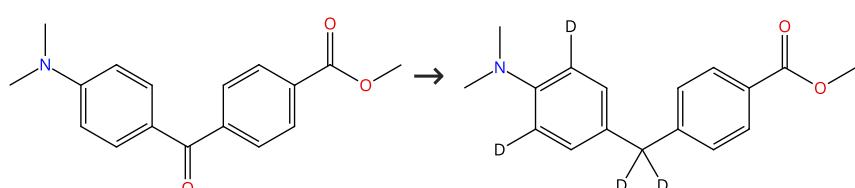
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

Scheme 18 (1 Reaction)

Steps: 1 Yield: 99%



31-116-CAS-22910640

Steps: 1 Yield: 99%

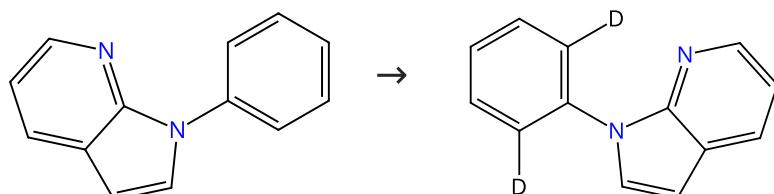
1.1 Reagents: Formic-*d* acid-*d***Catalysts:** Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-*N,N*-diethyl-4-pyridinamine- $\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1)**Solvents:** 1,1,1,3,3-Hexafluoro-2-propanol, Water-*d*<sub>2</sub>; 2 h, 80 °C**Iridium-Catalysed Reductive Deoxygenation of Ketones with Formic Acid as Traceless Hydride Donor**

By: Yang, Zhiheng; et al

Advanced Synthesis &amp; Catalysis (2020), 362(23), 5496-5505.

Scheme 19 (2 Reactions)

Steps: 1 Yield: 99%



Suppliers (6)

31-116-CAS-18932011

Steps: 1 Yield: 99%

1.1 Reagents: Water-*d*<sub>2</sub>, [1,1,1-Trifluoro-*N*-[(trifluoromethyl)sulfonyl- $\kappa O$ ]methanesulfonamido- $\kappa O$ ]silver**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-**Solvents:** 1,2-Dichloroethane; 24 h, 80 °C**Iridium-catalyzed C-H phosphoramidation of N-aryl-7-azaindoles with phosphoryl azides**

By: Pan, Changduo; et al

Organic &amp; Biomolecular Chemistry (2018), 16(20), 3711-3715.

## Experimental Protocols

31-614-CAS-31530285

Steps: 1

**N-Aroyloxycarbamates as switchable nitrogen and oxygen precursor: Ir/Cu controlled divergent C-H functionalization of heteroarenes**

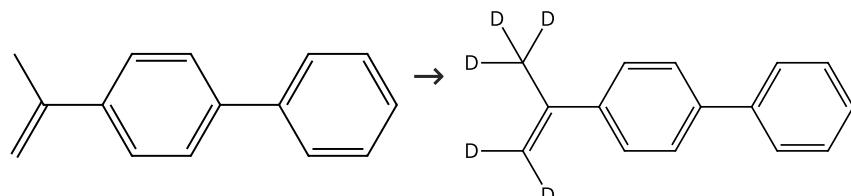
By: Liu, Shanshan; et al

Organic Chemistry Frontiers (2022), 9(8), 2093-2101.

1.1 Catalysts: Silver triflate, Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-**Solvents:** 1-Butyl-3-methylimidazolium tetrafluoroborate; 2 h, rt1.2 Reagents: Water-*d*<sub>2</sub>; 2 h

Scheme 20 (1 Reaction)

Steps: 1 Yield: 99%



Suppliers (33)

31-614-CAS-37018422

Steps: 1 Yield: 99%

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

By: Jia, Zongbin; et al

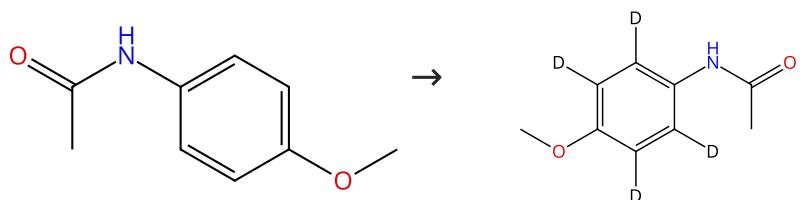
CCS Chemistry (2023), 5(5), 1069-1076.

1.1 Reagents: Water-*d*<sub>2</sub>**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt**Solvents:** Acetonitrile; 36 h, rt

## Experimental Protocols

**Scheme 21 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (84)

31-116-CAS-20111041

Steps: 1 Yield: 99%

1.1 Reagents: Water- $d_2$   
 Catalysts: Iridium, Platinum  
 Solvents: Isopropanol; 24 h, rt

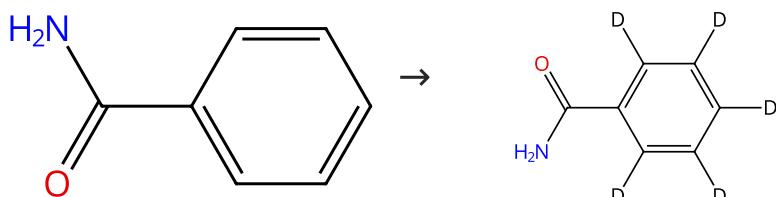
H-D Exchange Deuteration of Arenes at Room Temperature

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

**Scheme 22 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (115)

Suppliers (31)

31-116-CAS-20111039

Steps: 1 Yield: 99%

1.1 Reagents: Water- $d_2$   
 Catalysts: Iridium  
 Solvents: Isopropanol; 24 h, rt

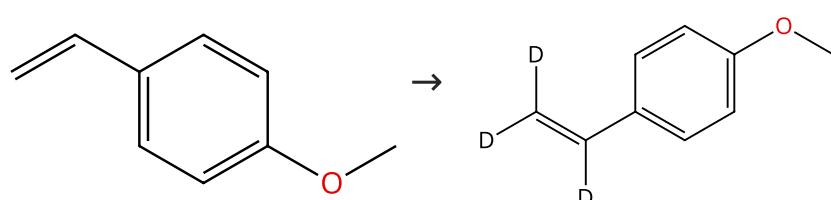
H-D Exchange Deuteration of Arenes at Room Temperature

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

**Scheme 23 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (88)

31-116-CAS-15986847

Steps: 1 Yield: 99%

1.1 Reagents: Water- $d_2$   
 Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium  
 Solvents: Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with  $D_2O$  catalyzed by an iridium complex

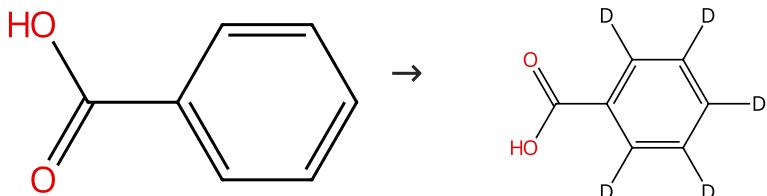
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

**Scheme 24 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (193)

Suppliers (62)

31-116-CAS-20111023

Steps: 1 Yield: 99%

**1.1 Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium  
**Solvents:** Isopropanol; 24 h, rt

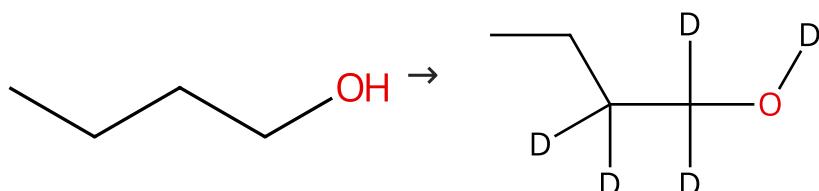
H-D Exchange Deuteration of Arenes at Room Temperature

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

**Scheme 25 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (215)

31-614-CAS-33408341

Steps: 1 Yield: 99%

**1.1 Reagents:** Water-*d*<sub>2</sub>, Sodium hydroxide-*d*  
**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*;1'*H*)-dionato(2-)-κ*N'*,κ*N'*][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol, 1,4-Dioxane; 7 h, 80 °C

Iridium-catalyzed α-selective deuteration of alcohols

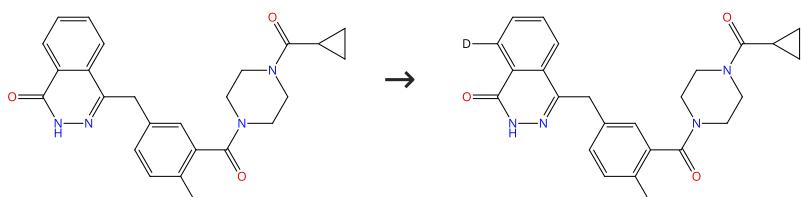
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

## Experimental Protocols

**Scheme 26 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (101)

31-116-CAS-17956527

Steps: 1 Yield: 99%

**1.1 Reagents:** Water-*d*<sub>2</sub>, Boron, bis[[2,2'-(imino-κ*N*)bis[ethanolato-κ*O*]](2-)]di-, (*B*-*B*)  
**1.2 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; 72 h, 20 °C

Efficient Water Reduction with sp<sup>3</sup>-sp<sup>3</sup> Diboron(4)

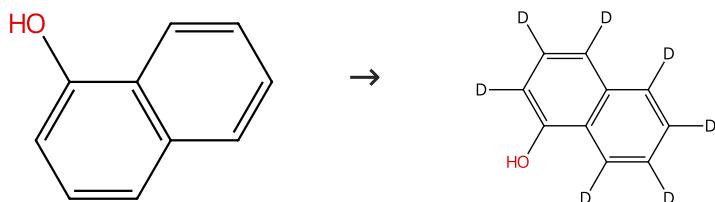
Compounds: Application to Hydrogenations, H-D Exchange Reactions, and Carbonyl Reductions

By: Flinker, Mathias; et al

Angewandte Chemie, International Edition (2017), 56(50), 15910-15915.

**Scheme 27 (1 Reaction)**

Steps: 1 Yield: 99%



Suppliers (133)

Suppliers (33)

31-116-CAS-20111045

Steps: 1 Yield: 99%

**1.1 Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium, Platinum  
**Solvents:** Isopropanol; 24 h, rt

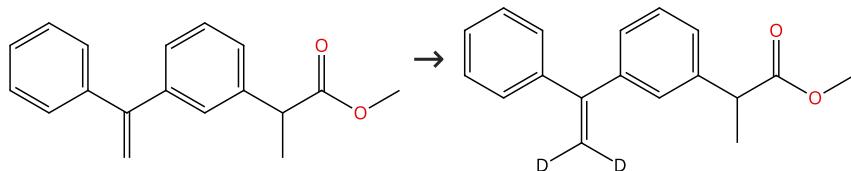
H-D Exchange Deuteration of Arenes at Room Temperature

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

**Scheme 28 (1 Reaction)**

Steps: 1 Yield: 98%



Suppliers (8)

31-614-CAS-37018529

Steps: 1 Yield: 98%

**1.1 Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximate- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

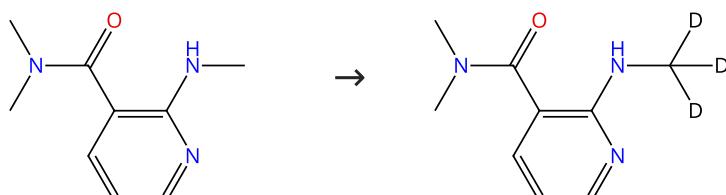
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

**Scheme 29 (1 Reaction)**

Steps: 1 Yield: 98%



Suppliers (3)

31-614-CAS-32010143

Steps: 1 Yield: 98%

**1.1 Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]diiridium, Sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate

**Solvents:** 1,4-Dioxane; 20 h, 80 °C

Ir-Catalyzed cyclization of  $\alpha,\omega$ -dienes with an N-methyl group via two C-H activation steps

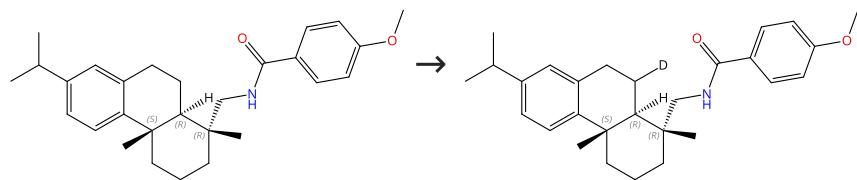
By: Tanaka, Katsumasa; et al

Chemical Communications (Cambridge, United Kingdom) (2022), 58(35), 5371-5374.

Experimental Protocols

**Scheme 30 (1 Reaction)**

Steps: 1 Yield: 98%

Absolute stereochemistry shown,  
Rotation (-)

Absolute stereochemistry shown



Supplier (1)

**31-614-CAS-33530429**

Steps: 1 Yield: 98%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

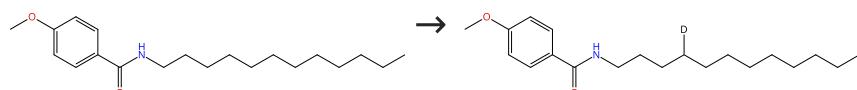
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

**Scheme 31 (1 Reaction)**

Steps: 1 Yield: 98%



Suppliers (16)

**31-614-CAS-33530426**

Steps: 1 Yield: 98%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

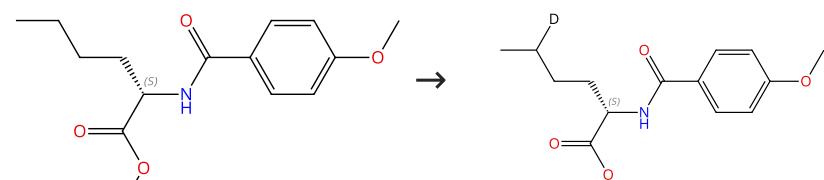
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

**Scheme 32 (1 Reaction)**

Steps: 1 Yield: 98%

Absolute stereochemistry shown,  
Rotation (+)

Absolute stereochemistry shown

31-614-CAS-33530427

Steps: 1 Yield: 98%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

## Experimental Protocols

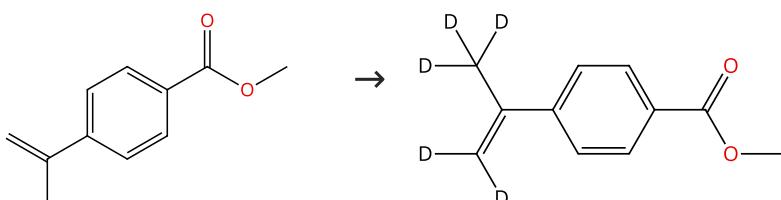
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 33 (1 Reaction)

Steps: 1 Yield: 98%



Suppliers (9)

31-614-CAS-37018444

Steps: 1 Yield: 98%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)] (*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

## Experimental Protocols

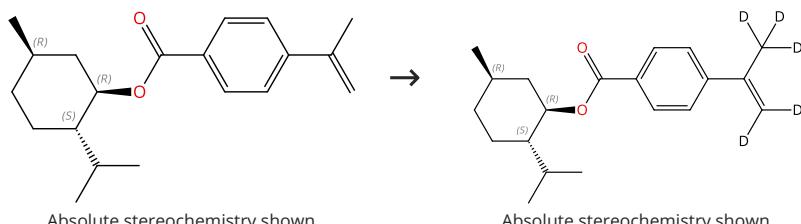
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 34 (1 Reaction)

Steps: 1 Yield: 98%



Absolute stereochemistry shown

Steps: 1 Yield: 98%

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

31-614-CAS-37018499

1.1 Reagents: Water-*d*<sub>2</sub>

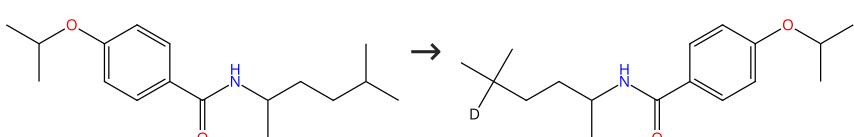
**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)] (*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

## Experimental Protocols

Scheme 35 (1 Reaction)

Steps: 1 Yield: 98%



31-614-CAS-33530417

Steps: 1 Yield: 98%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

## Experimental Protocols

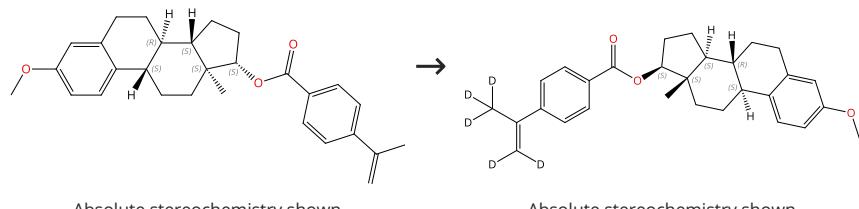
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Scheme 36 (1 Reaction)

Steps: 1 Yield: 98%



31-614-CAS-37018498

Steps: 1 Yield: 98%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )][1-]](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

## Experimental Protocols

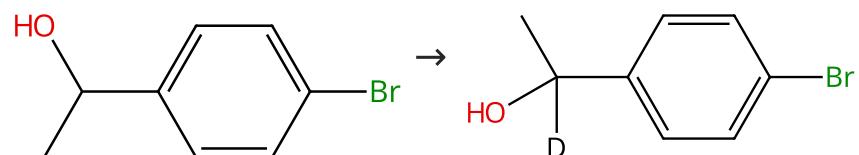
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

## Scheme 37 (1 Reaction)

Steps: 1 Yield: 98%



Suppliers (75)

Supplier (1)

31-614-CAS-33408371

Steps: 1 Yield: 98%

1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>

**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)- $\kappa N^1,\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

**Solvents:** Isopropanol; 21 h, 80 °C

## 1.2 Reagents: Sulfuric acid

**Solvents:** Water; pH 5

## Experimental Protocols

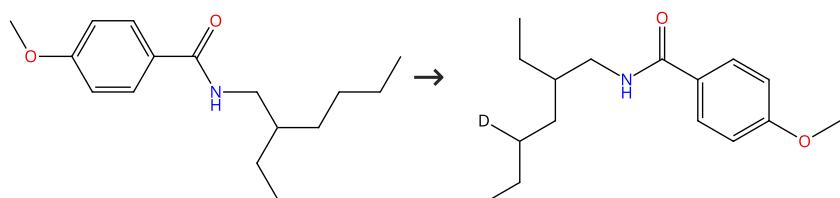
Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 38 (1 Reaction)**

Steps: 1 Yield: 98%



Suppliers (15)

**31-614-CAS-33530425**

Steps: 1 Yield: 98%

**1.1 Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N',N'*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Experimental Protocols**

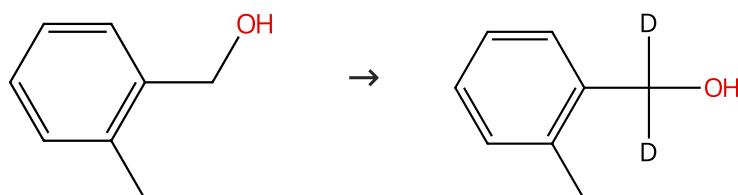
**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

**Scheme 39 (1 Reaction)**

Steps: 1 Yield: 98%



Suppliers (85)

Supplier (1)

**31-614-CAS-33408350**

Steps: 1 Yield: 98%

**1.1 Reagents:** Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*

**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*;1'*H*)-dionato(2-)- $\kappa N^1,\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

**Solvents:** Isopropanol; 3 d, 80 °C

**1.2 Reagents:** Sulfuric acid

**Solvents:** Water; pH 5

**Experimental Protocols**

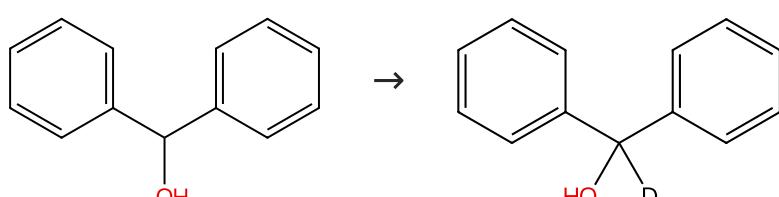
**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 40 (1 Reaction)**

Steps: 1 Yield: 98%



Suppliers (104)

Supplier (1)

31-614-CAS-33408367

Steps: 1 Yield: 98%

1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)-κ*N*<sup>1</sup>,κ*N*'<sup>1</sup>]][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

Solvents: Isopropanol; 2 d, 80 °C

1.2 Reagents: Sulfuric acid

Solvents: Water; pH 5

Experimental Protocols

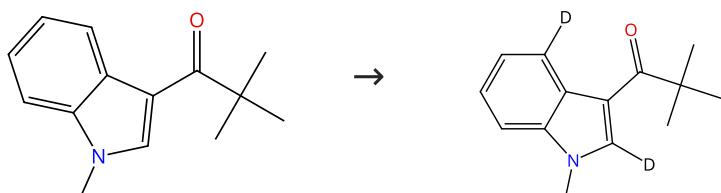
**Iridium-catalyzed α-selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 41 (5 Reactions)**

Steps: 1 Yield: 83-97%



Suppliers (32)

31-614-CAS-33033747

Steps: 1 Yield: 97%

1.1 Reagents: Pivalic acid, Water-*d*<sub>2</sub>

Catalysts: Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoro antimonate

Solvents: 1,2-Dichloroethane; 18 h, 80 °C

Experimental Protocols

**Rh(III)-Catalyzed dienylation and cycloproppylation of indoles at the C4 position with alkylidenecyclopropanes**

By: Liu, Yan-Zhi; et al

Organic Chemistry Frontiers (2022), 9(16), 4287-4293.

31-116-CAS-20471675

Steps: 1 Yield: 91%

1.1 Reagents: Pivalic acid, Water-*d*<sub>2</sub>, Silver oxide (Ag<sub>2</sub>O)

Catalysts: Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoro antimonate

Solvents: 1,2-Dichloroethane; 2 h, 80 °C

**C2/C4 Regioselective Heteroarylation of Indoles by Tuning C-H Metalation Modes**

By: Chen, Shuyou; et al

ACS Catalysis (2019), 9(7), 6372-6379.

31-614-CAS-24624348

Steps: 1 Yield: 83%

1.1 Reagents: Pivalic acid, Water-*d*<sub>2</sub>

Catalysts: Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoro antimonate

Solvents: 1,2-Dichloroethane; 18 h, 0 °C

Experimental Protocols

**Rhodium(III)-Catalyzed Regioselective C-H Allylation and Prenylation of Indoles at C4-Position**

By: Zhang, Shang-Shi; et al

Advanced Synthesis &amp; Catalysis (2022), 364(1), 64-70.

31-614-CAS-36670260

Steps: 1

**Iridium catalyzed C2 site-selective methylation of indoles using a pivaloyl directing group through weak chelation-assistance**

By: Kathiravan, Subban; et al

RSC Advances (2023), 13(17), 11291-11295.

Experimental Protocols

31-116-CAS-23535499

Steps: 1

1.1 Reagents: Silver carbonate, Water-*d*<sub>2</sub>Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-*N*-(trifluoromethyl)sulfonyl- $\kappa O$ ]methanesulfonamidato- $\kappa O$  silver

Solvents: 1,2-Dichloroethane; 120 °C

Tandem Iridium-Catalyzed Decarbonylative C-H Activation of Indole: Sacrificial Electron-Rich Ketone-Assisted Bis-arylsulfonylation

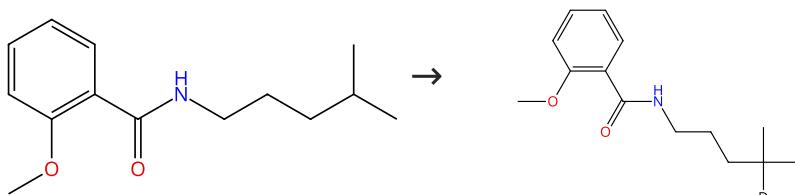
By: Kathiravan, Subban; et al

Organic Letters (2021), 23(9), 3331-3336.

Experimental Protocols

## Scheme 42 (1 Reaction)

Steps: 1 Yield: 97%



Supplier (1)

31-614-CAS-33530545

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]-bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-)(1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

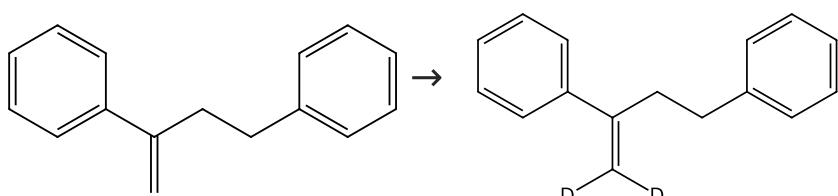
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

## Scheme 43 (1 Reaction)

Steps: 1 Yield: 97%



Supplier (23)

31-116-CAS-15986818

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

Solvents: Tetrahydrofuran; 14 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

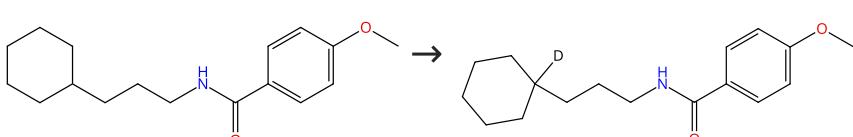
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

## Scheme 44 (1 Reaction)

Steps: 1 Yield: 97%



31-614-CAS-33530413

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

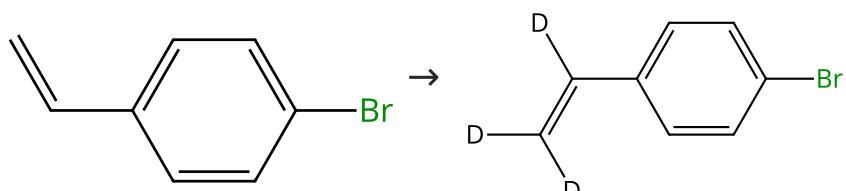
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

Scheme 45 (1 Reaction)

Steps: 1 Yield: 97%



Suppliers (92)

31-116-CAS-15986846

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

**Solvents:** Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

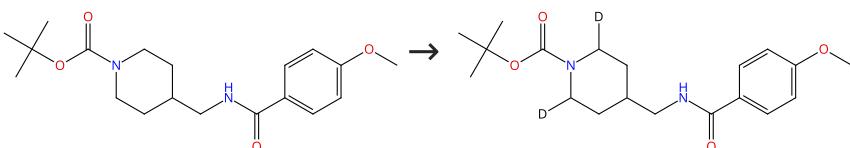
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

## Experimental Protocols

Scheme 46 (1 Reaction)

Steps: 1 Yield: 97%



31-614-CAS-33530445

Steps: 1 Yield: 97%

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

1.1 Reagents: Water-*d*<sub>2</sub>

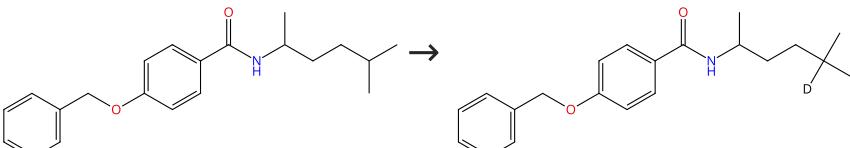
**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

## Experimental Protocols

Scheme 47 (1 Reaction)

Steps: 1 Yield: 97%



31-614-CAS-33530416

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 48 h, rt

## Experimental Protocols

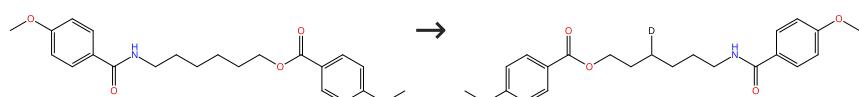
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 48 (1 Reaction)

Steps: 1 Yield: 97%



31-614-CAS-33530422

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

## Experimental Protocols

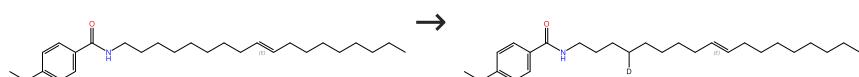
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 49 (1 Reaction)

Steps: 1 Yield: 97%



Double bond geometry shown

Double bond geometry shown

31-614-CAS-33530428

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

## Experimental Protocols

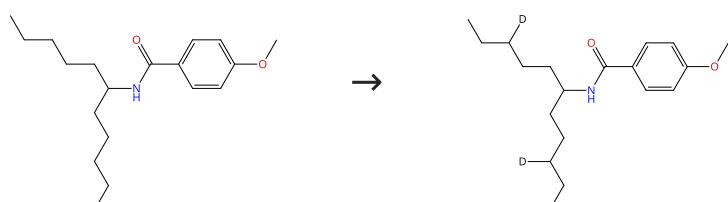
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 50 (1 Reaction)

Steps: 1 Yield: 97%



31-614-CAS-33530450

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-)

(1:1)

**Solvents:** Chlorobenzene; 48 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

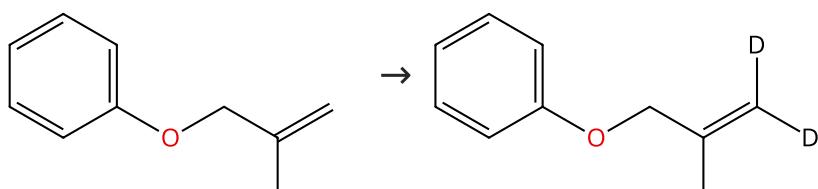
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

Scheme 51 (1 Reaction)

Steps: 1 Yield: 97%



Suppliers (46)

31-116-CAS-15986819

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

**Solvents:** Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

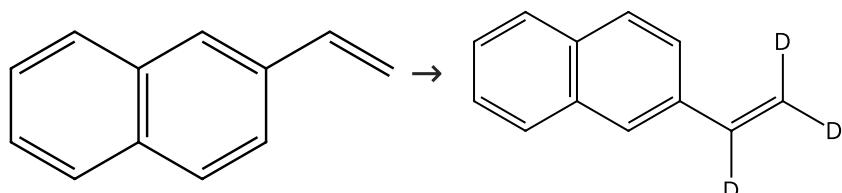
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

## Experimental Protocols

Scheme 52 (1 Reaction)

Steps: 1 Yield: 97%



Suppliers (74)

31-116-CAS-15986811

Steps: 1 Yield: 97%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

**Solvents:** Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

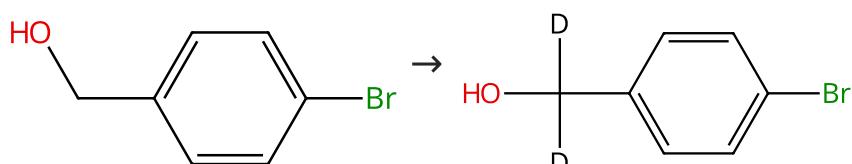
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

## Experimental Protocols

Scheme 53 (1 Reaction)

Steps: 1 Yield: 97%



Suppliers (93)

Suppliers (5)

31-614-CAS-33408357

Steps: 1 Yield: 97%

- 1.1 **Reagents:** Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*  
**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*;1'*H*)-dionato(2-)-κ*N*<sup>1</sup>,κ*N*'][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol; 3 h, 80 °C
- 1.2 **Reagents:** Sulfuric acid  
**Solvents:** Water; pH 5

Experimental Protocols

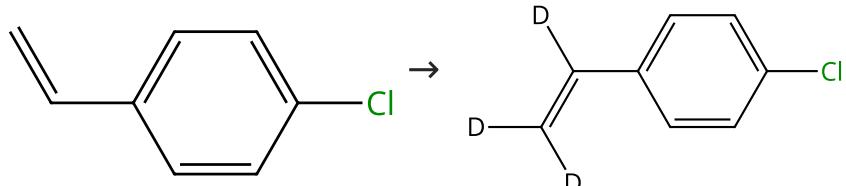
**Iridium-catalyzed α-selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 54 (1 Reaction)**

Steps: 1 Yield: 96%



Suppliers (89)

31-116-CAS-15986852

Steps: 1 Yield: 96%

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-hydroxydiiridium  
**Solvents:** Tetrahydrofuran; 3 h, 70 °C

Experimental Protocols

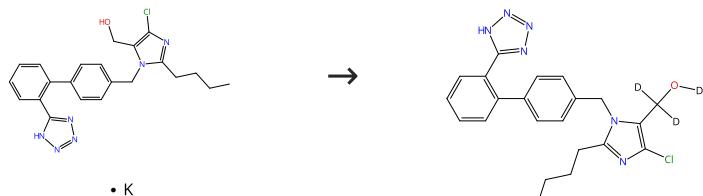
**Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex**

By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

**Scheme 55 (1 Reaction)**

Steps: 1 Yield: 96%



Suppliers (120)

31-614-CAS-33408368

Steps: 1 Yield: 96%

- 1.1 **Reagents:** Water-*d*<sub>2</sub>, Sodium hydroxide-*d*  
**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*;1'*H*)-dionato(2-)-κ*N*<sup>1</sup>,κ*N*'][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol; 24 h, 100 °C
- 1.2 **Reagents:** Sulfuric acid  
**Solvents:** Water; pH 7

Experimental Protocols

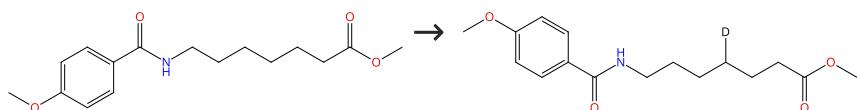
**Iridium-catalyzed α-selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 56 (1 Reaction)**

Steps: 1 Yield: 96%



31-614-CAS-33530430

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

Experimental Protocols

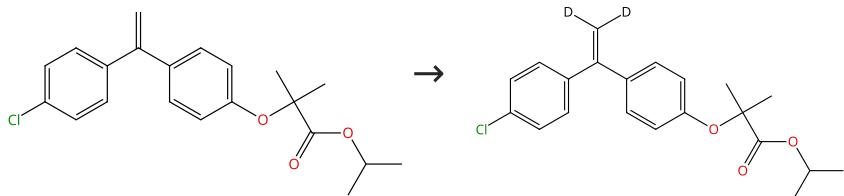
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

**Scheme 57 (1 Reaction)**

Steps: 1 Yield: 96%



31-614-CAS-37018531

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Experimental Protocols

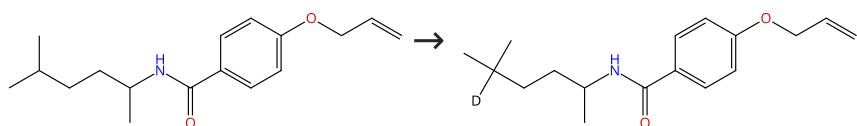
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

**Scheme 58 (1 Reaction)**

Steps: 1 Yield: 96%



31-614-CAS-33530414

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 48 h, rt

Experimental Protocols

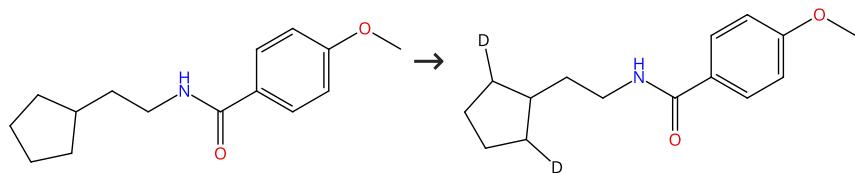
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

**Scheme 59 (1 Reaction)**

Steps: 1 Yield: 96%



31-614-CAS-33530447

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

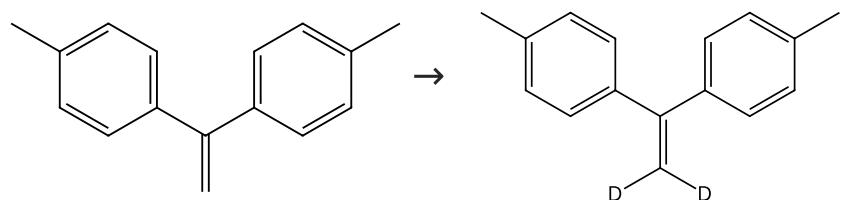
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

**Scheme 60 (1 Reaction)**

Steps: 1 Yield: 96%



🛒 Suppliers (29)

31-614-CAS-37018503

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

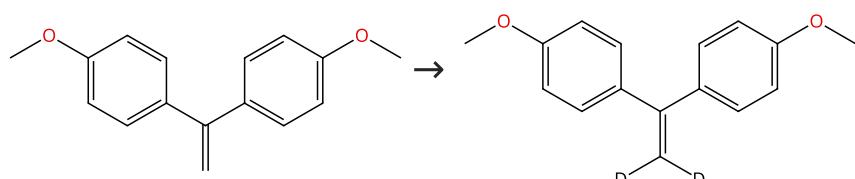
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

## Experimental Protocols

**Scheme 61 (1 Reaction)**

Steps: 1 Yield: 96%



🛒 Suppliers (25)

31-614-CAS-37018514

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )][1-]] (*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

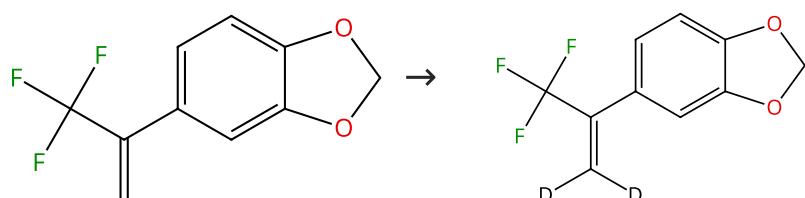
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

Scheme 62 (1 Reaction)

Steps: 1 Yield: 96%



Suppliers (4)

31-614-CAS-37018524

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )][1-]] (*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

Scheme 63 (1 Reaction)

Steps: 1 Yield: 96%



Suppliers (3)

31-614-CAS-37018484

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )][1-]] (*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

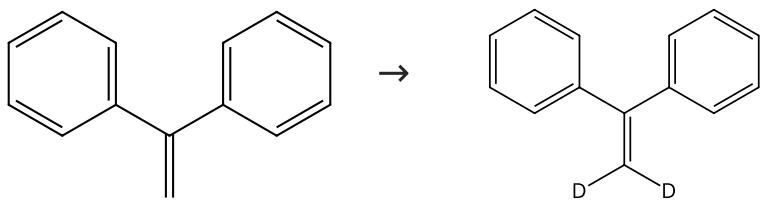
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

**Scheme 64 (1 Reaction)**

Steps: 1 Yield: 96%



Suppliers (77)

Supplier (1)

31-614-CAS-37018501

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33), hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximate- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

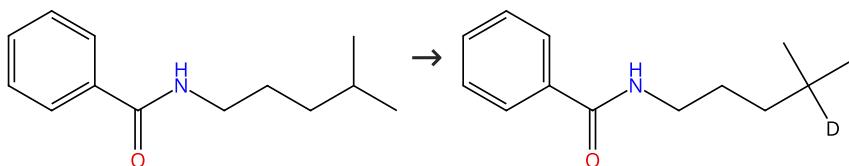
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

**Scheme 65 (1 Reaction)**

Steps: 1 Yield: 96%



Suppliers (6)

31-614-CAS-33530551

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

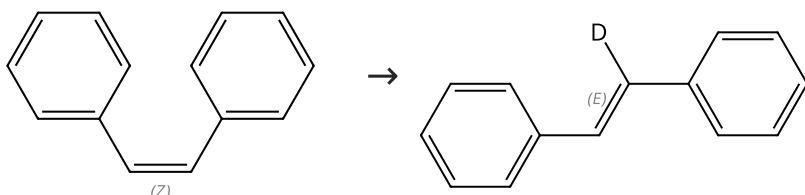
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

**Scheme 66 (1 Reaction)**

Steps: 1 Yield: 96%



Double bond geometry shown

Double bond geometry shown

Suppliers (65)

Supplier (1)

31-116-CAS-15986842

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-hydroxydiiridium

Solvents: Tetrahydrofuran; 20 h, 70 °C

Experimental Protocols

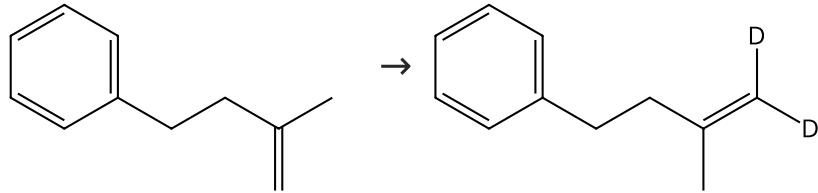
Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Scheme 67 (1 Reaction)

Steps: 1 Yield: 96%



Suppliers (19)

Supplier (1)

31-116-CAS-15986817

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-hydroxydiiridium

Solvents: Tetrahydrofuran; 3 h, 70 °C

Experimental Protocols

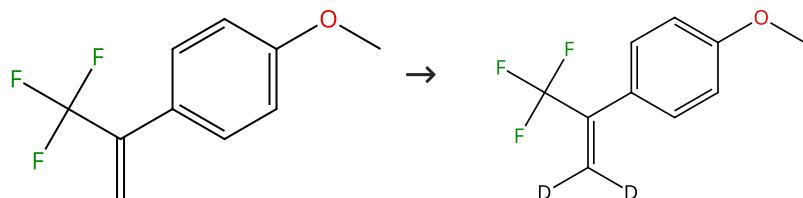
Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Scheme 68 (1 Reaction)

Steps: 1 Yield: 96%



Suppliers (9)

31-614-CAS-37018526

Steps: 1 Yield: 96%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κN<sup>1</sup>,κN<sup>1</sup>]bis[2-(2-pyridinyl-κM phenyl-κC)<sub>2</sub>, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato-κN)](1-)] (*N,N*-dimethyl-4-pyridinamine-κN<sup>1</sup>)cobalt

Solvents: Acetonitrile; 36 h, rt

Experimental Protocols

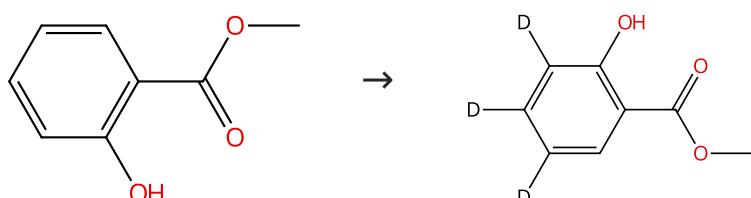
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 69 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (138)

Supplier (1)

31-116-CAS-20111044

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium

Solvents: Isopropanol; 24 h, rt

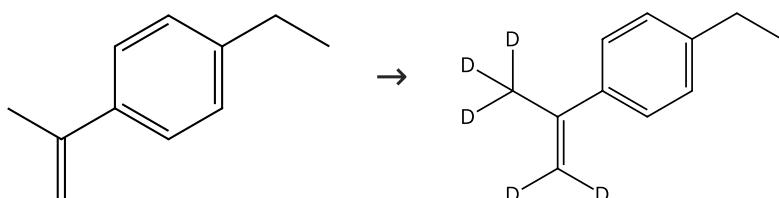
H-D Exchange Deuteration of Arenes at Room Temperature

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

## Scheme 70 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (11)

31-614-CAS-37018398

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ], (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )][1-]](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

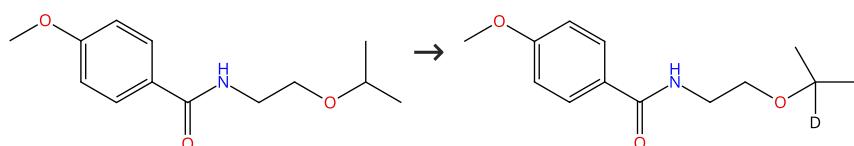
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

## Experimental Protocols

## Scheme 71 (1 Reaction)

Steps: 1 Yield: 95%



Supplier (1)

31-614-CAS-33530409

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

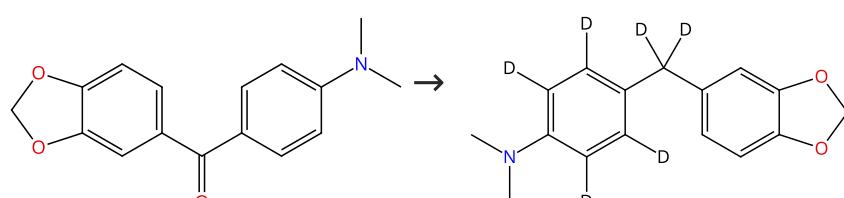
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

## Scheme 72 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (3)

31-116-CAS-22905180

Steps: 1 Yield: 95%

1.1 Reagents: Formic-*d* acid-*d*

**Catalysts:** Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-*N,N*-diethyl-4-pyridinamine- $\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1)

**Solvents:** 1,1,1,3,3-Hexafluoro-2-propanol, Water-*d*<sub>2</sub>; 2 h, 80 °C

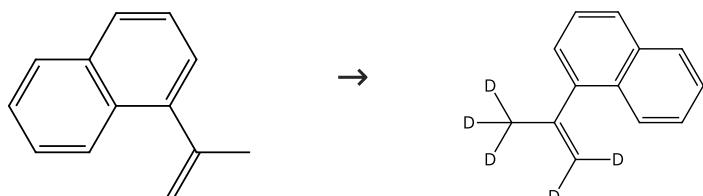
**Iridium-Catalysed Reductive Deoxygenation of Ketones with Formic Acid as Traceless Hydride Donor**

By: Yang, Zhiheng; et al

Advanced Synthesis &amp; Catalysis (2020), 362(23), 5496-5505.

Scheme 73 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (14)

31-614-CAS-37018476

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ], (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )][1-]-(*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

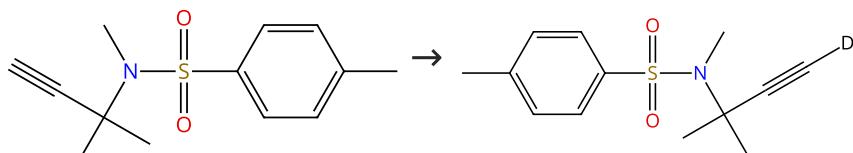
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

Scheme 74 (1 Reaction)

Steps: 1 Yield: 95%



31-614-CAS-40986148

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-

**Solvents:** Toluene; 12 h, 100 °C

**Propargylic Dialkyl Effect for Cyclobutene Formation through Ir(III)-Catalyzed Cycloisomerization of 1,6-Enynes**

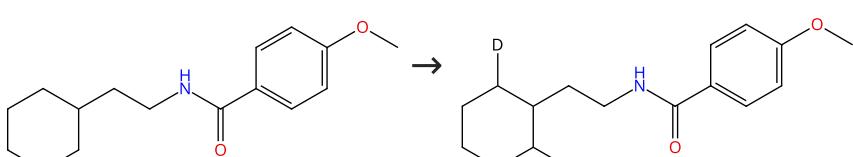
By: Zhu, Xuanyu; et al

Organic Letters (2024), 26(4), 966-970.

Experimental Protocols

Scheme 75 (1 Reaction)

Steps: 1 Yield: 95%



Supplier (1)

31-614-CAS-33530441

Steps: 1 Yield: 95%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

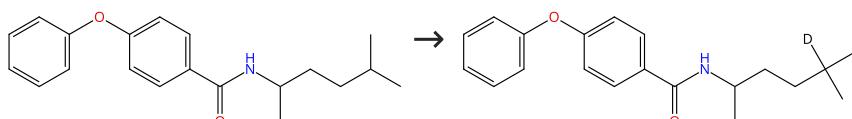
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

Scheme 76 (1 Reaction)

Steps: 1 Yield: 95%



31-614-CAS-33530411

Steps: 1 Yield: 95%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** 2,4,6-Tris(1-methylethyl)benzenethiol, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 48 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

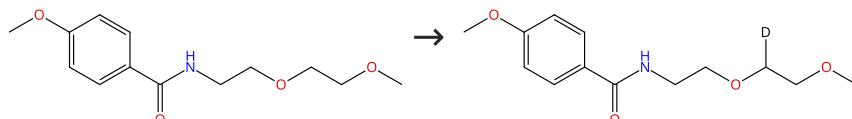
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

Scheme 77 (1 Reaction)

Steps: 1 Yield: 95%



31-614-CAS-33530420

Steps: 1 Yield: 95%

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

1.1 Reagents: Water- $d_2$ 

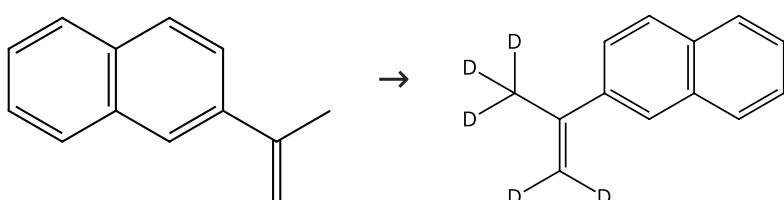
**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

## Experimental Protocols

Scheme 78 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (55)

31-614-CAS-37018472

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

## Experimental Protocols

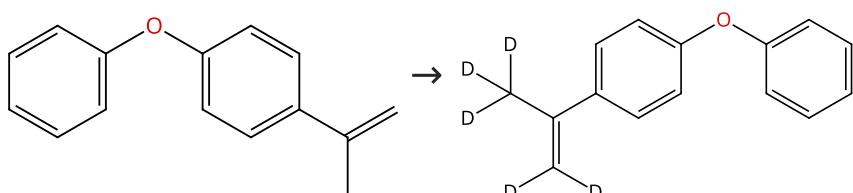
**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 79 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (12)

31-614-CAS-37018430

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

## Experimental Protocols

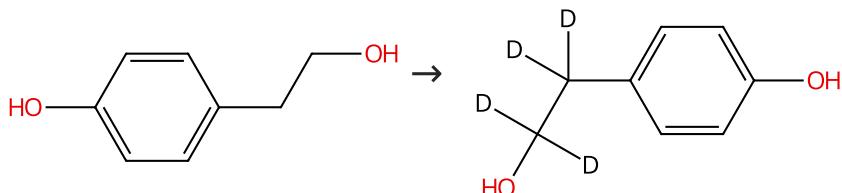
**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 80 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (130)

Suppliers (6)

31-614-CAS-33408348

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>, Sodium hydroxide-*d*

**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)- $\kappa N^1,\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

**Solvents:** Isopropanol, 1,4-Dioxane; 5 h, 80 °C

## Experimental Protocols

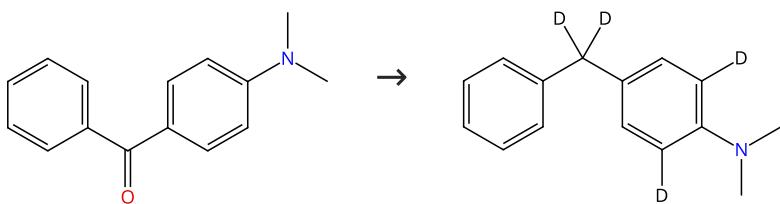
**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 81 (1 Reaction)**

Steps: 1 Yield: 95%



Suppliers (86)

**31-116-CAS-22907525**

Steps: 1 Yield: 95%

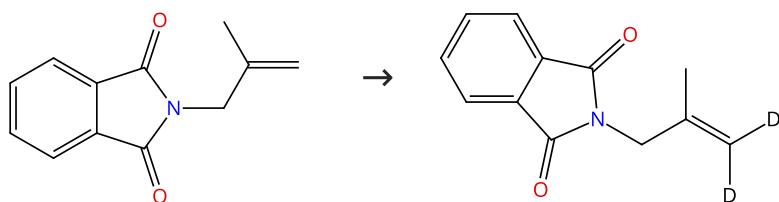
1.1 Reagents: Formic-*d* acid-*d*Catalysts: Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa\lambda^3$ )-*N,N*-diethyl-4-pyridinamine- $\kappa\lambda^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1)Solvents: 1,1,1,3,3-Hexafluoro-2-propanol, Water-*d*<sub>2</sub>; 2 h, 80 °C**Iridium-Catalysed Reductive Deoxygenation of Ketones with Formic Acid as Traceless Hydride Donor**

By: Yang, Zhiheng; et al

Advanced Synthesis &amp; Catalysis (2020), 362(23), 5496-5505.

**Scheme 82 (1 Reaction)**

Steps: 1 Yield: 95%



Suppliers (24)

**31-116-CAS-15986820**

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

Solvents: Tetrahydrofuran; 3 h, 70 °C

**Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex**

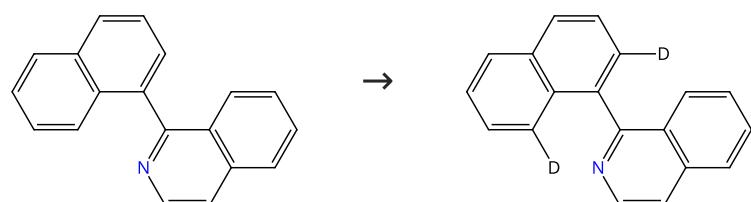
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

## Experimental Protocols

**Scheme 83 (1 Reaction)**

Steps: 1 Yield: 95%



Suppliers (8)

**31-614-CAS-37271938**

Steps: 1 Yield: 95%

1.1 Catalysts: 1,1'-[*(4R*)-[4,4'-Bi-1,3-benzodioxole]-5,5'-diyl]bis[1,1-diphenylphosphine], Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)

Solvents: 1,4-Dioxane; 5 min, rt

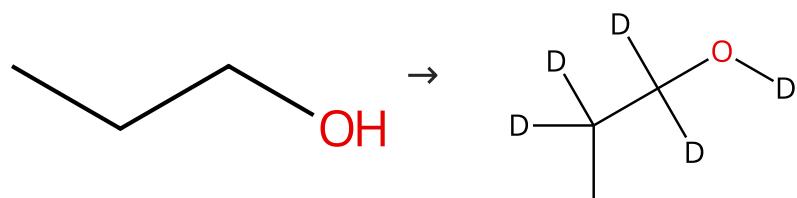
1.2 Reagents: Water-*d*<sub>2</sub>; 24 h, 80 °C**Iridium(I)-Catalyzed Atroposelective Alkenylation of Heterobiaryls with Terminal Alkynes**

By: Xiong, Maoqian; et al

Organic Letters (2023), 25(31), 5703-5708.

## Scheme 84 (1 Reaction)

Steps: 1 Yield: 95%



Suppliers (169)

31-614-CAS-33408340

Steps: 1 Yield: 95%

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols1.1 Reagents: Water-*d*<sub>2</sub>, Sodium hydroxide-*d*Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)- $\kappa N^1,\kappa N^1'][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-$ 

Solvents: Isopropanol, 1,4-Dioxane; 7 h, 80 °C

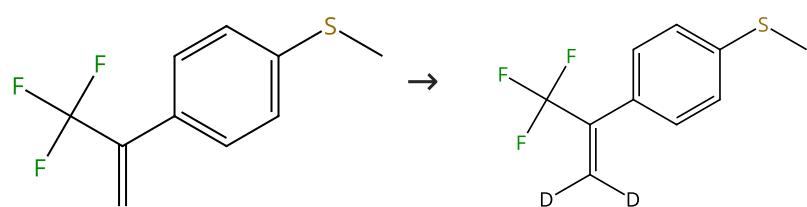
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

Experimental Protocols

## Scheme 85 (1 Reaction)

Steps: 1 Yield: 94%



Suppliers (6)

31-614-CAS-37018518

Steps: 1 Yield: 94%

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1'】bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C】-$ , (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )][1-]] ( $N,N$ -dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt$ 

Solvents: Acetonitrile; 36 h, rt

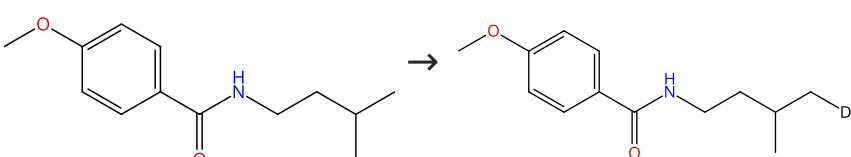
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

## Scheme 86 (1 Reaction)

Steps: 1 Yield: 94%



Suppliers (9)

31-614-CAS-33530440

Steps: 1 Yield: 94%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

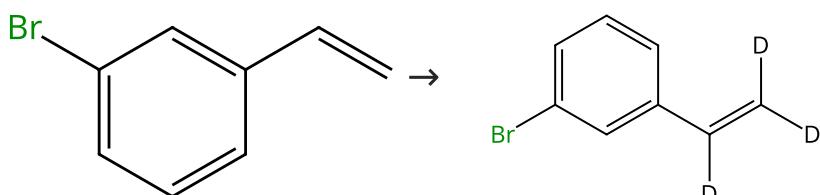
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

Scheme 87 (1 Reaction)

Steps: 1 Yield: 94%



Suppliers (84)

31-116-CAS-15986850

Steps: 1 Yield: 94%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

**Solvents:** Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

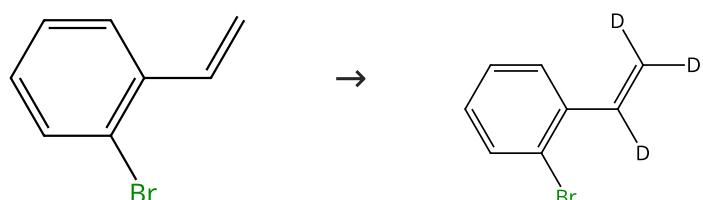
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

Scheme 88 (1 Reaction)

Steps: 1 Yield: 94%



Suppliers (81)

31-116-CAS-15986810

Steps: 1 Yield: 94%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

**Solvents:** Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

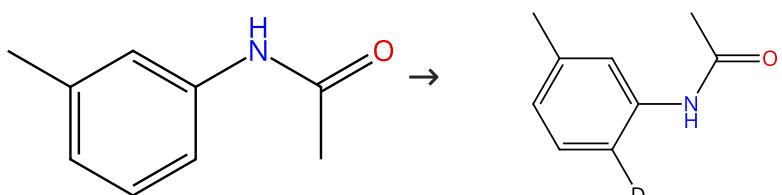
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

Scheme 89 (2 Reactions)

Steps: 1 Yield: 94%



Suppliers (68)

31-116-CAS-19141241

Steps: 1 Yield: 94%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), 1820606-28-7

Solvents: 1,4-Dioxane; 30 min, rt

## 1.2 Reagents: Norbornene; 21 h, 135 °C

## Experimental Protocols

## Iridium-Catalyzed Direct Asymmetric Alkylation of Aniline Derivatives using 2-Norbornene

By: Shirai, Tomohiko; et al

Asian Journal of Organic Chemistry (2018), 7(6), 1054-1056.

31-116-CAS-10629470

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, 1,1, 1-trifluoromethanesulfonate (1:1), 1820981-94-9

Solvents: 1,4-Dioxane; 48 h, 120 °C

## Experimental Protocols

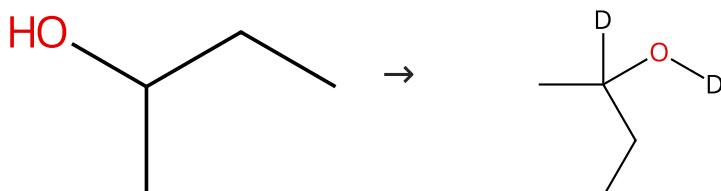
## Branch-selective alkene hydroarylation by cooperative destabilization: iridium-catalyzed ortho-alkylation of acetan ilides

By: Crisenza, Giacomo E. M.; et al

Angewandte Chemie, International Edition (2015), 54(49), 14866-14870.

## Scheme 90 (1 Reaction)

Steps: 1 Yield: 94%



Suppliers (90)

31-614-CAS-33408363

Steps: 1 Yield: 94%

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato (2-) $\kappa$ N<sup>1</sup>, $\kappa$ N<sup>1'</sup>][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

Solvents: Isopropanol; 5 d, 80 °C

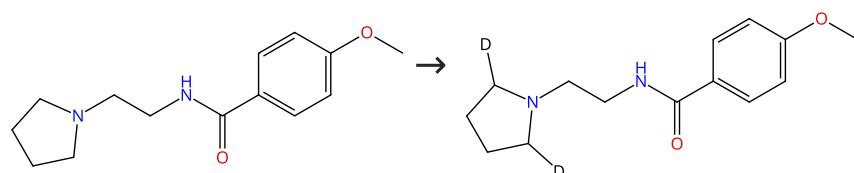
## 1.2 Reagents: Sulfuric acid

Solvents: Water; pH 5

## Experimental Protocols

## Scheme 91 (1 Reaction)

Steps: 1 Yield: 94%



Suppliers (3)

|   |                        |  |
|---|------------------------|--|
| 31-614-CAS-33530449   | Steps: 1 Yield: 94%    | Highly selective single and multiple deuteration of unactivated C(sp <sup>3</sup> )-H bonds<br>By: Li, Nian; et al<br>Nature Communications (2022), 13(1), 4224. |
| 1.1 Reagents: Water-d <sub>2</sub><br>Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, N,N,N-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine-κN <sup>1</sup> ,κN <sup>1</sup> ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κN]phenyl-κC]-, hexafluorophosphate(1-) (1:1)<br>Solvents: Chlorobenzene; 24 h, rt | Experimental Protocols |  |

|                        |                     |
|------------------------|---------------------|
| Scheme 92 (1 Reaction) | Steps: 1 Yield: 94% |
|                        |                     |

Suppliers (2)

|   |                        |  |
|---|------------------------|--|
| 31-614-CAS-33530434   | Steps: 1 Yield: 94%    | Highly selective single and multiple deuteration of unactivated C(sp <sup>3</sup> )-H bonds<br>By: Li, Nian; et al<br>Nature Communications (2022), 13(1), 4224. |
| 1.1 Reagents: Water-d <sub>2</sub><br>Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, N,N,N-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine-κN <sup>1</sup> ,κN <sup>1</sup> ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κN]phenyl-κC]-, hexafluorophosphate(1-) (1:1)<br>Solvents: Chlorobenzene; 24 h, rt | Experimental Protocols |  |

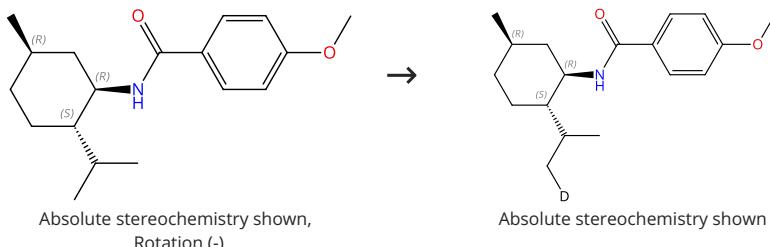
|                        |                     |
|------------------------|---------------------|
| Scheme 93 (1 Reaction) | Steps: 1 Yield: 94% |
|                        |                     |

Suppliers (76)

|   |                        |  |
|---|------------------------|--|
| 31-116-CAS-12032284   | Steps: 1 Yield: 94%    | Harnessing C-H Borylation/Deborylation for Selective Deuteration, Synthesis of Boronate Esters, and Late Stage Functionalization<br>By: Kallepalli, Venkata A.; et al<br>Journal of Organic Chemistry (2015), 80(16), 8341-8353. |
| 1.1 Reagents: Pinacolborane<br>Catalysts: 1,2-Bis(dimethylphosphino)ethane, [(1,2,5,6-η)-1,5-Cyclooctadiene][(1,2,3,3a,7a-η)-1H-inden-1-yl]iridium; rt → 150 °C; 3.25 h, 150 °C; 150 °C → rt<br>1.2 Solvents: Methanol; rt<br>1.3 Reagents: Water-d <sub>2</sub><br>Solvents: Tetrahydrofuran; 60 min, 150 °C | Experimental Protocols |  |

**Scheme 94 (1 Reaction)**

Steps: 1 Yield: 93%



Supplier (1)

**31-614-CAS-33530433**

Steps: 1 Yield: 93%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-)(1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

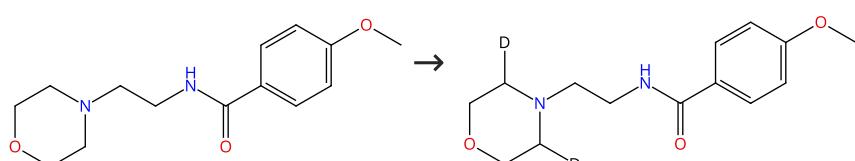
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

**Scheme 95 (1 Reaction)**

Steps: 1 Yield: 93%



Suppliers (5)

**31-614-CAS-33530444**

Steps: 1 Yield: 93%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-)(1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

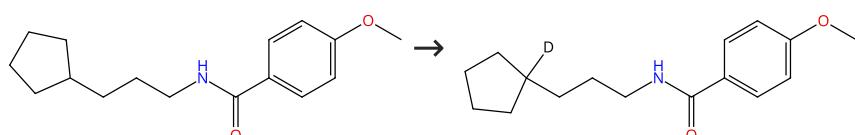
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

**Scheme 96 (1 Reaction)**

Steps: 1 Yield: 93%



31-614-CAS-33530408

Steps: 1 Yield: 93%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

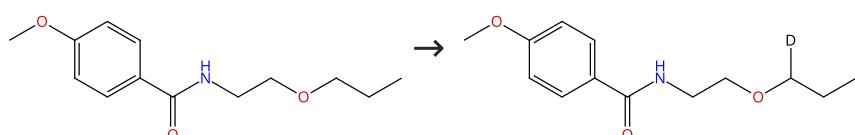
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

Scheme 97 (1 Reaction)

Steps: 1 Yield: 93%



31-614-CAS-33530424

Steps: 1 Yield: 93%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 48 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

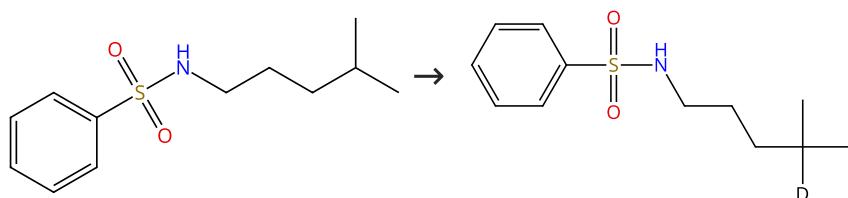
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

Scheme 98 (1 Reaction)

Steps: 1 Yield: 93%



Suppliers (3)

31-614-CAS-33530544

Steps: 1 Yield: 93%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

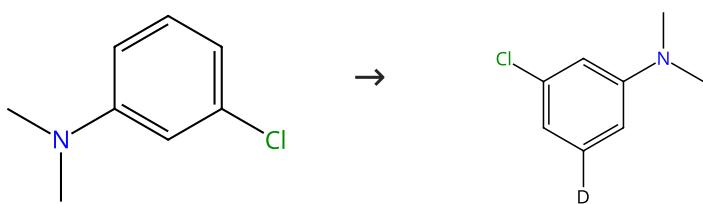
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

**Scheme 99 (1 Reaction)**

Steps: 1 Yield: 93%



Suppliers (59)

31-116-CAS-8970251

Steps: 1 Yield: 93%

## 1.1 Reagents: Pinacolborane

**Catalysts:** 1,2-Bis(dimethylphosphino)ethane, [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene][(1,2,3,3a,7a- $\eta$ )-1H-inden-1-yl]iridium; rt  $\rightarrow$  150 °C; 18 h, 150 °C; 150 °C  $\rightarrow$  rt

1.2 Reagents: Acetic anhydride, Water-*d*<sub>2</sub>

**Solvents:** 1,2-Dimethoxyethane; 2 h, 150 °C; 150 °C  $\rightarrow$  rt

## 1.3 Reagents: Sodium hydroxide

**Solvents:** Water; > pH 10, rt

**Harnessing C-H Borylation/Deborylation for Selective Deuteration, Synthesis of Boronate Esters, and Late Stage Functionalization**

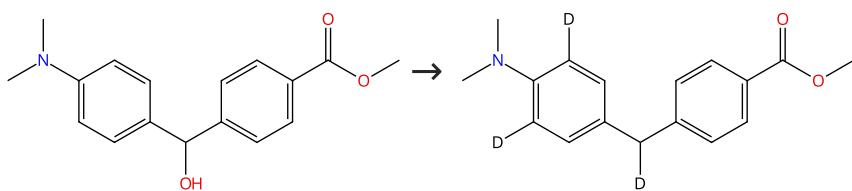
By: Kallepalli, Venkata A.; et al

Journal of Organic Chemistry (2015), 80(16), 8341-8353.

## Experimental Protocols

**Scheme 100 (1 Reaction)**

Steps: 1 Yield: 93%



Suppliers (6)

31-116-CAS-22910654

Steps: 1 Yield: 93%

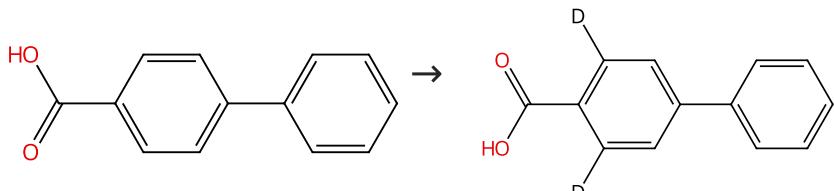
**Iridium-Catalysed Reductive Deoxygenation of Ketones with Formic Acid as Traceless Hydride Donor**

By: Yang, Zhiheng; et al

Advanced Synthesis &amp; Catalysis (2020), 362(23), 5496-5505.

**Scheme 101 (6 Reactions)**

Steps: 1 Yield: 74-93%



Suppliers (111)

31-116-CAS-14455538

Steps: 1 Yield: 93%

**Hydrogen isotope labelling using iridium(I) dionates**

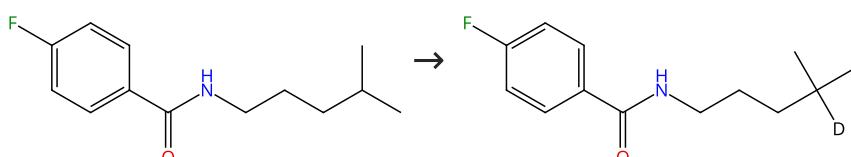
By: Lockley, W. J. S.

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

|                     |                     |   |
|---------------------|---------------------|---|
| 31-116-CAS-6741401  | Steps: 1 Yield: 93% | <p><b>Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates</b></p> <p>By: McAuley, B.; et al<br/>Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.</p>                 |
| 31-116-CAS-9156395  | Steps: 1 Yield: 78% | <p><b>Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates</b></p> <p>By: McAuley, B.; et al<br/>Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.</p>                 |
| 31-116-CAS-5323596  | Steps: 1 Yield: 74% | <p><b>Hydrogen isotope labelling using iridium(I) dionates</b></p> <p>By: Lockley, W. J. S.<br/>Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.</p>  |
| 31-116-CAS-2761266  | Steps: 1 Yield: 74% | <p><b>Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates</b></p> <p>By: McAuley, B.; et al<br/>Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.</p>                 |
| 31-116-CAS-15155638 | Steps: 1 Yield: 74% | <p><b>Parallel chemistry investigations of ortho-directed hydrogen isotope exchange between substituted aromatics and isotopic water: novel catalysis by cyclooctadienyliridium(I)pentan-1,3-dionates</b></p> <p>By: Kingston, Lee P.; et al<br/>Tetrahedron Letters (2000), 41(15), 2705-2708.</p> |

Scheme 102 (1 Reaction)

Steps: 1 Yield: 92%



Suppliers (3)

31-614-CAS-33530549

Steps: 1 Yield: 92%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

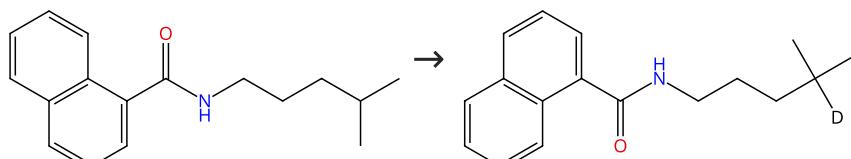
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

Scheme 103 (1 Reaction)

Steps: 1 Yield: 92%


🛒 Supplier (1)

31-614-CAS-33530415

Steps: 1 Yield: 92%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** 2,4,6-Tris(1-methylethyl)benzenethiol, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 48 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

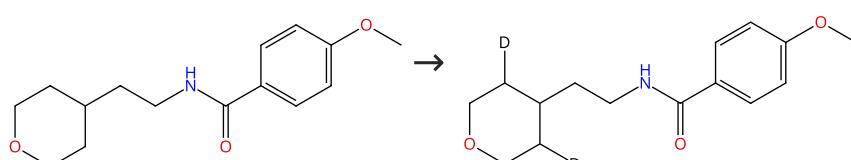
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

Scheme 104 (1 Reaction)

Steps: 1 Yield: 92%


🛒 Supplier (1)

31-614-CAS-33530436

Steps: 1 Yield: 92%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

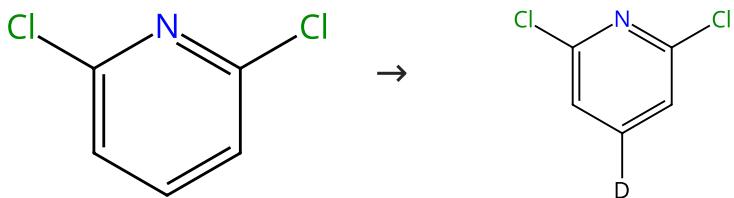
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Experimental Protocols

**Scheme 105 (1 Reaction)**

Steps: 1 Yield: 92%



Suppliers (90)

31-116-CAS-7169544

Steps: 1 Yield: 92%

- 1.1 **Reagents:** Pinacolborane  
**Catalysts:** 1,2-Bis(dimethylphosphino)ethane, [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene][(1,2,3,3a,7a- $\eta$ )-1H-inden-1-yl]iridium  
**Solvents:** Heptane; rt  $\rightarrow$  150 °C; 3.25 h, 150 °C; 150 °C  $\rightarrow$  rt
- 1.2 **Reagents:** Water- $d_2$   
**Solvents:** Tetrahydrofuran; 60 min, 150 °C

**Harnessing C-H Borylation/Deborylation for Selective Deuteration, Synthesis of Boronate Esters, and Late Stage Functionalization**

By: Kallepalli, Venkata A.; et al

Journal of Organic Chemistry (2015), 80(16), 8341-8353.

Experimental Protocols

**Scheme 106 (1 Reaction)**

Steps: 1 Yield: 92%



Suppliers (9)

31-614-CAS-31786827

Steps: 1 Yield: 92%

- 1.1 **Reagents:** Water- $d_2$ , *N*-(Methylsulfonyl)benzamide  
**Catalysts:** Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxyd iridium  
**Solvents:** Tetrahydrofuran; 5 h, 70 °C

**Non-stabilized Vinyl Anion Equivalents from Styrenes by N-Heterocyclic Carbene Catalysis and Its Use in Catalytic Nucleophilic Aromatic Substitution**

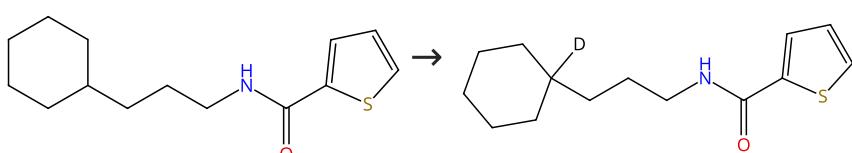
By: Ito, Sora; et al

Journal of the American Chemical Society (2022), 144(15), 6714-6718.

Experimental Protocols

**Scheme 107 (1 Reaction)**

Steps: 1 Yield: 92%



Supplier (1)

31-614-CAS-33530419

Steps: 1 Yield: 92%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** 2,4,6-Tris(1-methylethyl)benzenethiol, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated  $C(sp^3)$ -H bonds

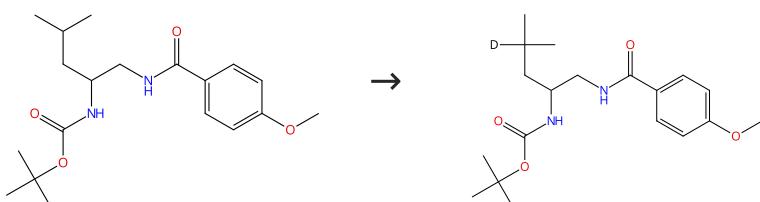
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

Scheme 108 (1 Reaction)

Steps: 1 Yield: 92%



31-614-CAS-33530410

Steps: 1 Yield: 92%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 48 h, rt

Highly selective single and multiple deuteration of unactivated  $C(sp^3)$ -H bonds

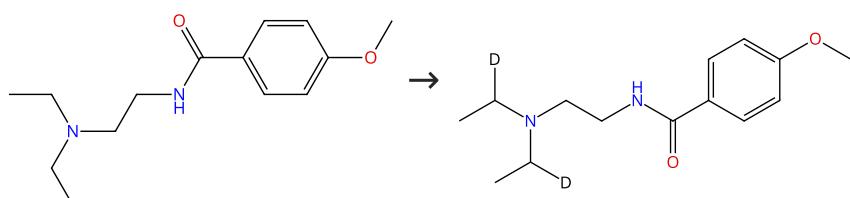
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

Scheme 109 (1 Reaction)

Steps: 1 Yield: 92%



Suppliers (9)

31-614-CAS-33530451

Steps: 1 Yield: 92%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated  $C(sp^3)$ -H bonds

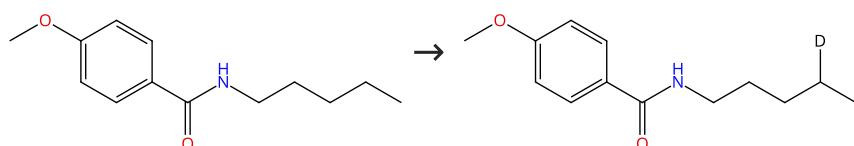
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

## Scheme 110 (1 Reaction)

Steps: 1 Yield: 92%



Suppliers (14)

31-614-CAS-33530423

Steps: 1 Yield: 92%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Experimental Protocols

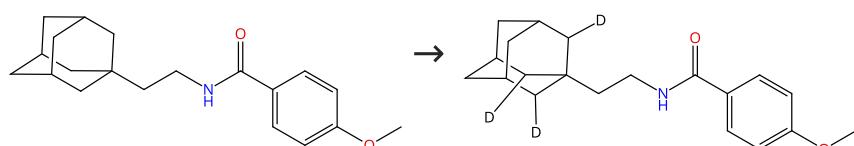
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Scheme 111 (1 Reaction)

Steps: 1 Yield: 92%



Suppliers (5)

31-614-CAS-33530446

Steps: 1 Yield: 92%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Experimental Protocols

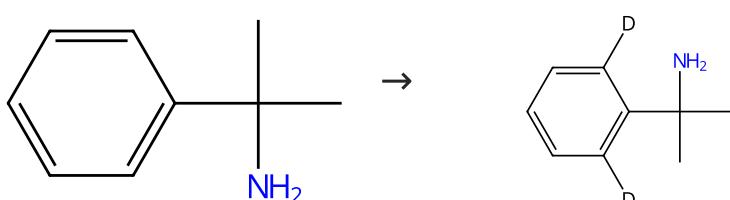
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Scheme 112 (3 Reactions)

Steps: 1 Yield: 48-92%



Suppliers (88)

31-116-CAS-580121

Steps: 1 Yield: 92%

Hydrogen isotope labelling using iridium(I) dionates

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium

**Solvents:** Dimethylacetamide; 2 min, 130 °C

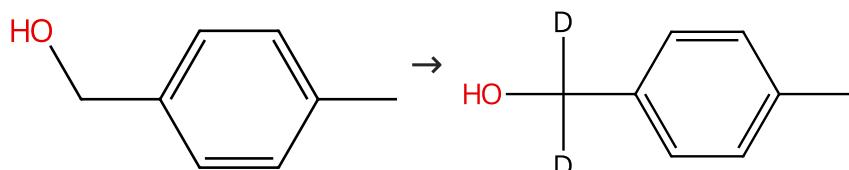
By: Lockley, W. J. S.

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

|                     |                     |  |
|---------------------|---------------------|--|
| 31-116-CAS-3785807  | Steps: 1 Yield: 92% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |
| 31-116-CAS-12226159 | Steps: 1 Yield: 48% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |

Scheme 113 (1 Reaction)

Steps: 1 Yield: 92%



Suppliers (90)

Supplier (1)

31-614-CAS-33408356

Steps: 1 Yield: 92%

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

- 1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*  
Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*;1'*H*)-dionato(2-)*κN*<sup>1</sup>,*κN*<sup>1</sup>][(1,2,3,4,5-*η*)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
Solvents: Isopropanol; 7 h, 80 °C
- 1.2 Reagents: Sulfuric acid  
Solvents: Water; pH 5

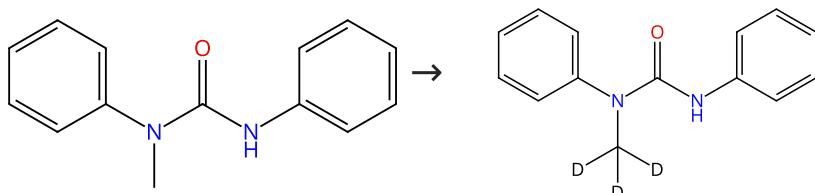
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

## Experimental Protocols

Scheme 114 (1 Reaction)

Steps: 1 Yield: 92%



Suppliers (11)

31-116-CAS-17229536

Steps: 1 Yield: 92%

Hydroxoiridium-Catalyzed Hydroalkylation of Terminal Alkenes with Ureas by C(sp<sup>3</sup>)-H Bond Activation

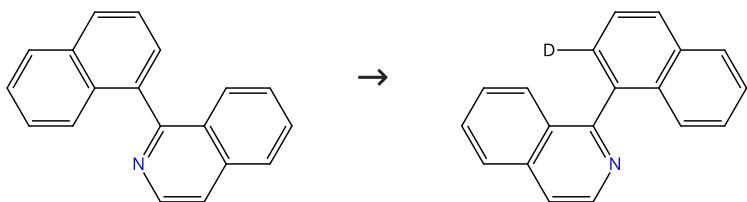
By: Yamauchi, Daisuke; et al

Angewandte Chemie, International Edition (2017), 56(25), 7200-7204.

## Experimental Protocols

**Scheme 115 (1 Reaction)**

Steps: 1 Yield: 92%



Suppliers (8)

31-614-CAS-41473419

Steps: 1 Yield: 92%

- 1.1 **Catalysts:** Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]diiridium, Sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, Ferrocene, 1,1'-bis[(2S,5S)-2,5-diethyl-1-phospholanyl]-
- 
- Solvents:** 1,4-Dioxane; 20 min, rt
- 1.2 **Reagents:** Water- $d_2$ ; 6 h, 130 °C

**Iridium-Catalyzed Asymmetric Hydroarylation of Unactivated Alkenes with Heterobiaryls: Simultaneous Construction of Axial and Central Chirality**

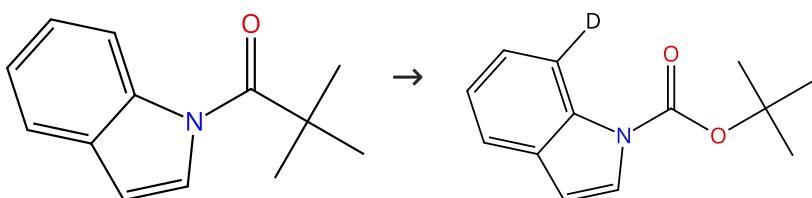
By: Li, Fei; et al

Organic Letters (2024), 26(32), 6835-6840.

Experimental Protocols

**Scheme 116 (1 Reaction)**

Steps: 1 Yield: 92%



Suppliers (8)

31-116-CAS-12476791

Steps: 1 Yield: 92%

- 1.1 **Reagents:** Lithium acetate, Water- $d_2$   
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-N-[trifluoromethyl)sulfonyl- $\kappa O$ ]methanesulfonamido- $\kappa O$  silver  
**Solvents:** 1,2-Dichloroethane; 1 h, rt → 120 °C

**Iridium(III)-catalyzed regioselective C7-sulfonamidation of indoles**

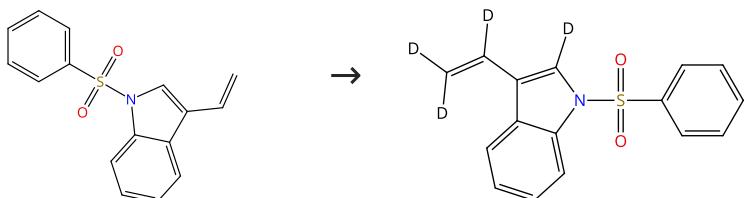
By: Song, Zengqiang; et al

Organic &amp; Biomolecular Chemistry (2016), 14(21), 4804-4808.

Experimental Protocols

**Scheme 117 (1 Reaction)**

Steps: 1 Yield: 92%



Suppliers (3)

31-116-CAS-15986812

Steps: 1 Yield: 92%

- 1.1 **Reagents:** Water- $d_2$   
**Catalysts:** N-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium  
**Solvents:** Tetrahydrofuran; 3 h, 70 °C

**Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex**

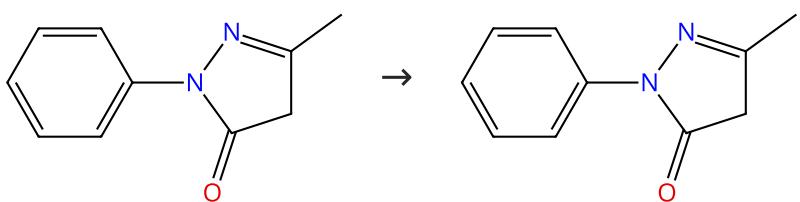
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

## Scheme 118 (1 Reaction)

Steps: 1 Yield: 92%


 Suppliers (132)

31-614-CAS-29334974

Steps: 1 Yield: 92%

1.1 Reagents: *p*-Toluenesulfonic acid, Water-*d*<sub>2</sub>, Silver hexafluoroantimonate, Zinc triflateCatalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-

Solvents: 2,2,2-Trifluoroethanol; 3 h, 120 °C

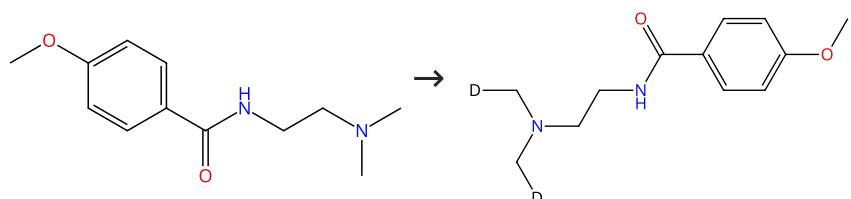
Iridium(III)-Catalyzed Tandem Annulation Synthesis of Pyrazolo[1,2- $\alpha$ ]cinnolines from Pyrazolones and Sulfoxonium Ylides

By: Liu, Chen-Fei; et al

Journal of Organic Chemistry (2019), 84(1), 409-416.

## Scheme 119 (1 Reaction)

Steps: 1 Yield: 92%


 Suppliers (9)

31-614-CAS-33530464

Steps: 1 Yield: 92%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-)

(1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

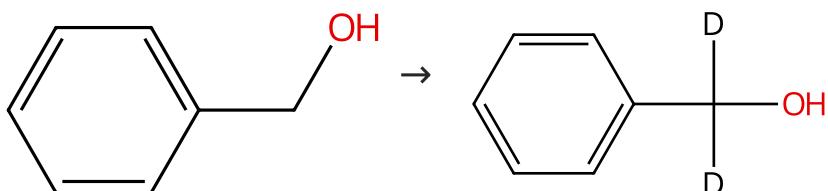
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

## Scheme 120 (1 Reaction)

Steps: 1 Yield: 91%


 Suppliers (161)

 Suppliers (39)

31-614-CAS-33408349

Steps: 1 Yield: 91%

- 1.1 **Reagents:** Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*  
**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)-κ*N*<sup>1</sup>,κ*N*'<sup>1</sup>]][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol; 7 h, 80 °C
- 1.2 **Reagents:** Sulfuric acid  
**Solvents:** Water; pH 5

Experimental Protocols

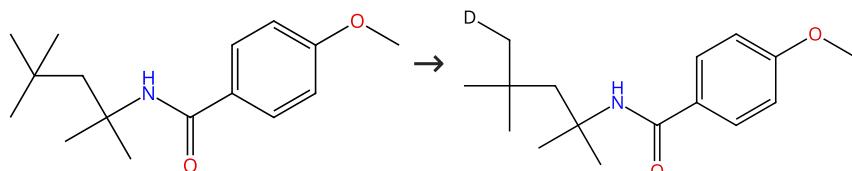
**Iridium-catalyzed α-selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 121** (1 Reaction)

Steps: 1 Yield: 91%



Suppliers (5)

31-614-CAS-33530435

Steps: 1 Yield: 91%

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine-κ*N*<sup>1</sup>,κ*N*'<sup>1</sup>]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κ*N*]phenyl-κ*C*]-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Chlorobenzene; 24 h, rt

Experimental Protocols

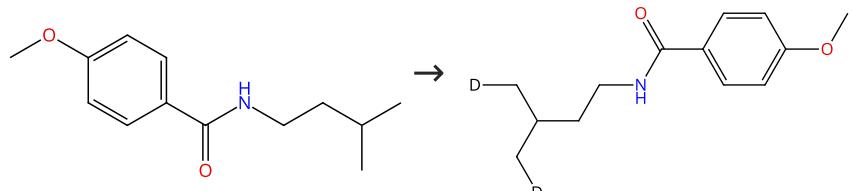
**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

**Scheme 122** (1 Reaction)

Steps: 1 Yield: 91%



Suppliers (9)

31-614-CAS-33530438

Steps: 1 Yield: 91%

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine-κ*N*<sup>1</sup>,κ*N*'<sup>1</sup>]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κ*N*]phenyl-κ*C*]-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Chlorobenzene; 48 h, rt

Experimental Protocols

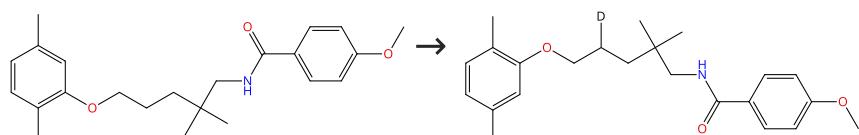
**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Scheme 123 (1 Reaction)

Steps: 1 Yield: 91%



31-614-CAS-33530439

Steps: 1 Yield: 91%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-)

(1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

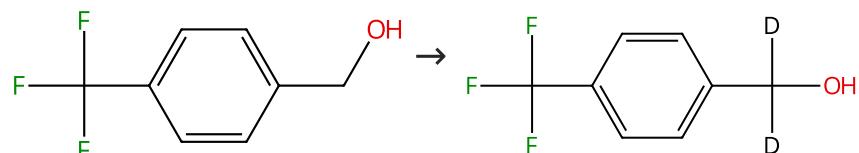
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

## Scheme 124 (1 Reaction)

Steps: 1 Yield: 91%



Suppliers (85)

Suppliers (2)

31-614-CAS-33408366

Steps: 1 Yield: 91%

**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*

**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)- $\kappa N^1,\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

**Solvents:** Isopropanol; 3 h, 80 °C

## 1.2 Reagents: Sulfuric acid

**Solvents:** Water; pH 5

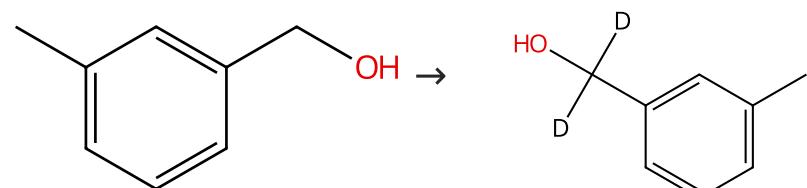
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

## Experimental Protocols

## Scheme 125 (1 Reaction)

Steps: 1 Yield: 91%



Suppliers (72)

31-614-CAS-33408355

Steps: 1 Yield: 91%

- 1.1 **Reagents:** Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*  
**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)-κ*N*<sup>1</sup>,κ*N*<sup>1</sup>][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol; 7 h, 80 °C
- 1.2 **Reagents:** Sulfuric acid  
**Solvents:** Water; pH 5

Experimental Protocols

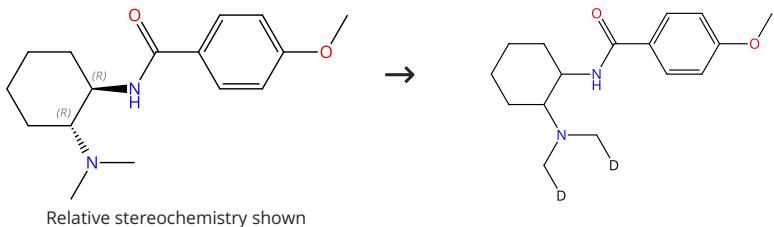
**Iridium-catalyzed α-selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 126 (1 Reaction)**

Steps: 1 Yield: 91%



Suppliers (2)

31-614-CAS-33530461

Steps: 1 Yield: 91%

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine-κ*N*<sup>1</sup>,κ*N*<sup>1</sup>]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κ*N*]phenyl-κ*C*]-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Chlorobenzene; 24 h, rt

Experimental Protocols

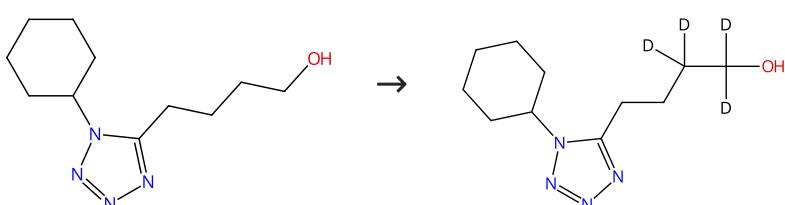
**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

**Scheme 127 (1 Reaction)**

Steps: 1 Yield: 91%



Suppliers (4)

31-614-CAS-33408351

Steps: 1 Yield: 91%

- 1.1 **Reagents:** Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*  
**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)-κ*N*<sup>1</sup>,κ*N*<sup>1</sup>][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol; 2 d, 100 °C

- 1.2 **Reagents:** Sulfuric acid  
**Solvents:** Water; pH 5

Experimental Protocols

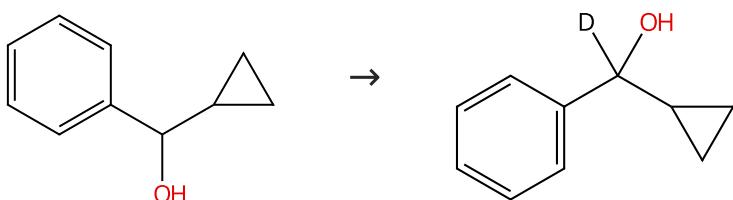
**Iridium-catalyzed α-selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 128 (1 Reaction)**

Steps: 1 Yield: 90%



Suppliers (64)

31-614-CAS-33408364

Steps: 1 Yield: 90%

**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**1.1 Reagents: Methanol- $d_4$ , Water- $d_2$ Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1H,1'H)-dionato(2-)- $\kappa N^1,\kappa N^1'][(1,2,3,4,5-\eta)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-$ 

Solvents: Isopropanol; 1 d, 80 °C

1.2 Reagents: Sulfuric acid

Solvents: Water; pH 5

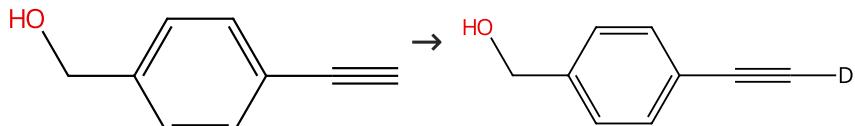
Experimental Protocols

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 129 (1 Reaction)**

Steps: 1 Yield: 90%



Suppliers (75)

31-614-CAS-33408378

Steps: 1 Yield: 90%

**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**1.1 Reagents: Methanol- $d_4$ , Water- $d_2$ Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1H,1'H)-dionato(2-)- $\kappa N^1,\kappa N^1'][(1,2,3,4,5-\eta)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-$ 

Solvents: Isopropanol; 3 h, 80 °C

1.2 Reagents: Sulfuric acid

Solvents: Water; pH 5

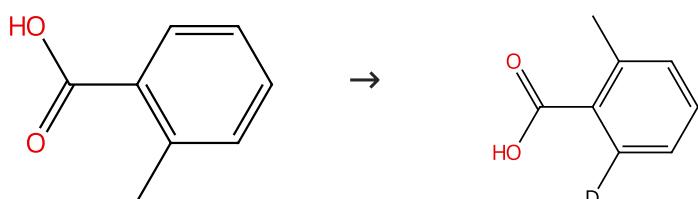
Experimental Protocols

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

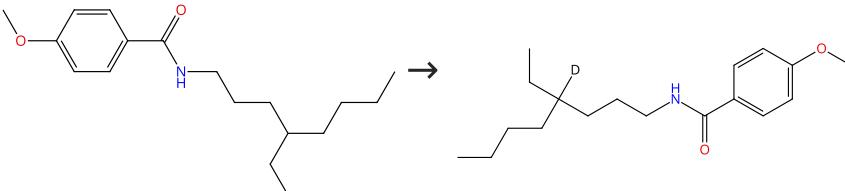
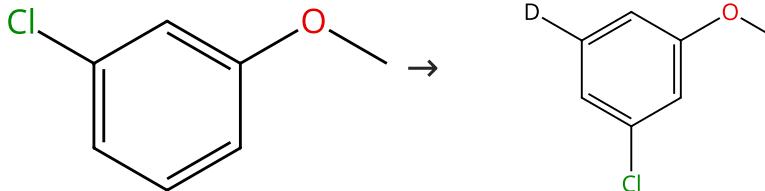
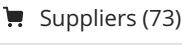
**Scheme 130 (2 Reactions)**

Steps: 1 Yield: 47-90%



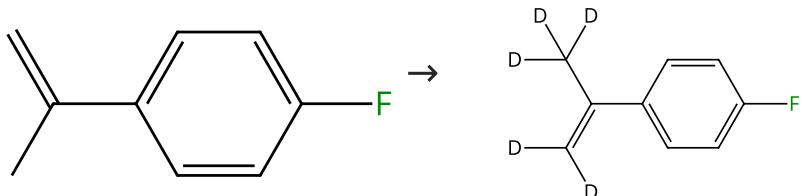
Suppliers (92)

Suppliers (3)

|   |                     |  |
|---|---------------------|--|
| 31-116-CAS-18533492   | Steps: 1 Yield: 90% | Base- and Additive-Free Ir-Catalyzed ortho-Iodination of Benzoic Acids: Scope and Mechanistic Investigations<br>By: Erbing, Elis; et al<br>ACS Catalysis (2018), 8(2), 920-925.  |
| 1.1 Reagents: Water- <i>d</i> <sub>2</sub><br>Catalysts: Iridium(2+), triqua[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, sulfate (1:1)<br>Solvents: 1,1,1,3,3-Hexafluoro-2-propanol; 48 h, 40 °C   |                     |  |
| 1.2 Reagents: Sodium thiosulfate<br>Solvents: Water   |                     |  |
| 1.3 Reagents: Hydrochloric acid<br>Solvents: Water; < pH 2  |                     |  |
| Experimental Protocols  |                     |  |
| 31-116-CAS-20622498   | Steps: 1 Yield: 47% | Iridium-Catalyzed Synthesis of Substituted Indanones from Aromatic Carboxylates and Unsaturated Ketones<br>By: Zhang, Guodong; et al<br>ACS Catalysis (2019), 9(9), 8153-8158.   |
| 1.1 Reagents: Potassium carbonate, Water- <i>d</i> <sub>2</sub><br>Catalysts: Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Indium triflate<br>Solvents: Water; 1 h, 140 °C  |                     |  |
| Scheme 131 (1 Reaction)   | Steps: 1 Yield: 90% |  |
|   |                     |  |
| 31-614-CAS-33530406   | Steps: 1 Yield: 90% | Highly selective single and multiple deuteration of unactivated C(sp <sup>3</sup> )-H bonds<br>By: Li, Nian; et al<br>Nature Communications (2022), 13(1), 4224.   |
| 1.1 Reagents: Water- <i>d</i> <sub>2</sub><br>Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, <i>N,N,N</i> -tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine-κN <sup>1</sup> ,κN <sup>1</sup> ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κN]phenyl-κC]-, hexafluorophosphate(1-) (1:1)<br>Solvents: Chlorobenzene; 24 h, rt |                     |  |
| Experimental Protocols  |                     |  |
| Scheme 132 (1 Reaction)   | Steps: 1 Yield: 90% |  |
|    |                     |  |
|    |                     |  |
| 31-116-CAS-11351433   | Steps: 1 Yield: 90% | Harnessing C-H Borylation/Deborylation for Selective Deuteration, Synthesis of Boronate Esters, and Late Stage Functionalization<br>By: Kallepalli, Venkata A.; et al<br>Journal of Organic Chemistry (2015), 80(16), 8341-8353. |
| 1.1 Reagents: Pinacolborane<br>Catalysts: 1,2-Bis(dimethylphosphino)ethane, [(1,2,5,6-η)-1,5-Cyclooctadiene][(1,2,3,3a,7a-η)-1- <i>H</i> -inden-1-yl]iridium; rt → 150 °C; 12 h, 150 °C; 150 °C → rt  |                     |  |
| 1.2 Reagents: Water- <i>d</i> <sub>2</sub><br>Solvents: Tetrahydrofuran; 1 h, 150 °C  |                     |  |
| Experimental Protocols  |                     |  |

## Scheme 133 (1 Reaction)

Steps: 1 Yield: 90%



Suppliers (71)

31-614-CAS-37018421

Steps: 1 Yield: 90%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

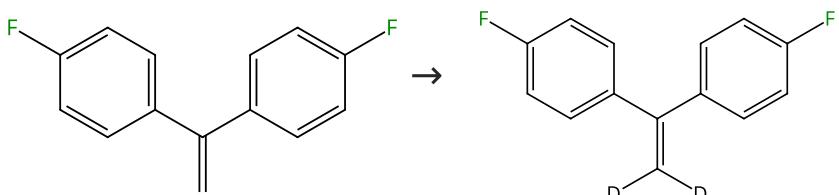
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

## Scheme 134 (1 Reaction)

Steps: 1 Yield: 90%



Suppliers (23)

31-614-CAS-37018510

Steps: 1 Yield: 90%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

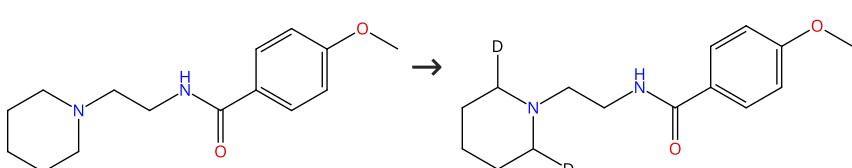
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

## Scheme 135 (1 Reaction)

Steps: 1 Yield: 89%



Suppliers (9)

31-614-CAS-33530442

Steps: 1 Yield: 89%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 12 h, rt

## Experimental Protocols

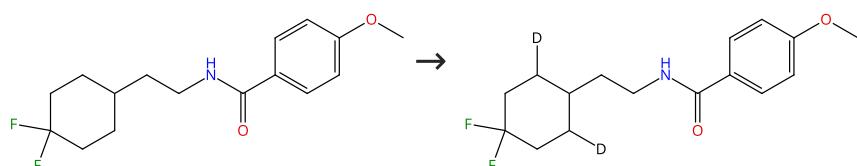
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 136 (1 Reaction)

Steps: 1 Yield: 89%



31-614-CAS-33530443

Steps: 1 Yield: 89%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

## Experimental Protocols

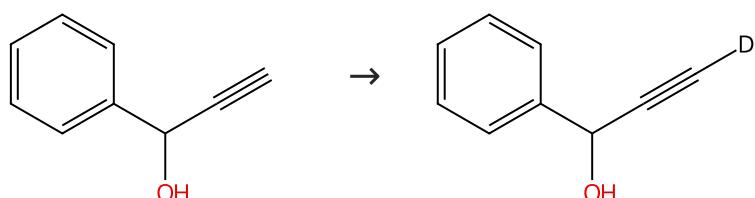
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 137 (1 Reaction)

Steps: 1 Yield: 89%



Suppliers (93)

Supplier (1)

31-614-CAS-33408375

Steps: 1 Yield: 89%

1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>

Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)- $\kappa N^1,\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

Solvents: Isopropanol; 1 d, 80 °C

## 1.2 Reagents: Sulfuric acid

Solvents: Water; pH 5

## Experimental Protocols

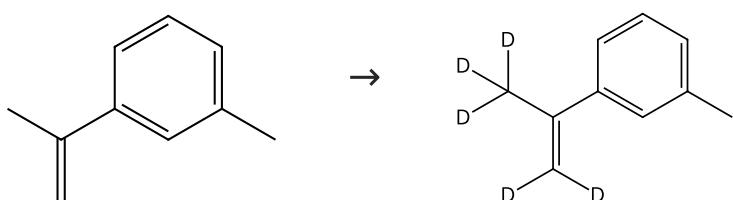
Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

Scheme 138 (1 Reaction)

Steps: 1 Yield: 88%



Suppliers (61)

31-614-CAS-37018449

Steps: 1 Yield: 88%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1'$ ]bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C]$ , (*OC*-6-33), hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

Experimental Protocols

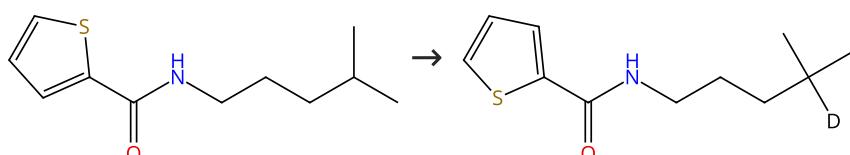
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 139 (1 Reaction)

Steps: 1 Yield: 88%



Suppliers (11)

31-614-CAS-33530412

Steps: 1 Yield: 88%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** 2,4,6-Tris(1-methylethyl)benzenethiol, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1'$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C]$ , hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

Experimental Protocols

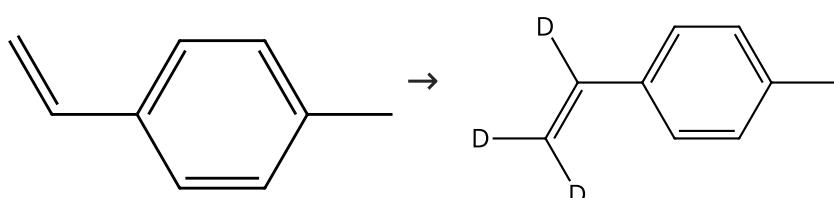
Highly selective single and multiple deuteration of unactivated  $C(sp^3)$ -H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

Scheme 140 (1 Reaction)

Steps: 1 Yield: 88%



Suppliers (70)

31-116-CAS-15986844

Steps: 1 Yield: 88%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

Solvents: Tetrahydrofuran; 3 h, 70 °C

Experimental Protocols

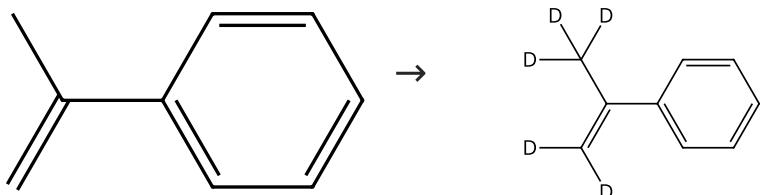
Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Scheme 141 (1 Reaction)

Steps: 1 Yield: 88%



Suppliers (70)

Supplier (1)

31-614-CAS-37018397

Steps: 1 Yield: 88%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C^-$ -, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)] (*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt$ 

Solvents: Acetonitrile; 36 h, rt

Experimental Protocols

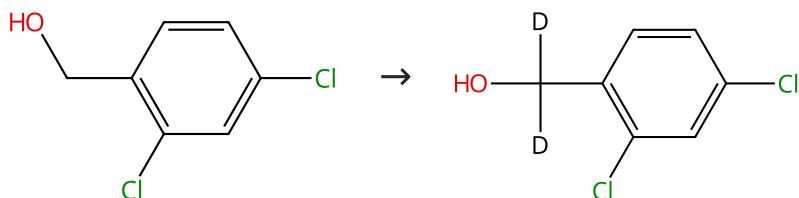
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 142 (1 Reaction)

Steps: 1 Yield: 87%



Suppliers (108)

Supplier (22)

31-614-CAS-33408361

Steps: 1 Yield: 87%

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*;1'*H*)-dionato(2-) $\kappa N^1,\kappa N^1'][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-$ 

Solvents: Isopropanol; 1 d, 80 °C

1.2 Reagents: Sulfuric acid

Solvents: Water; pH 5

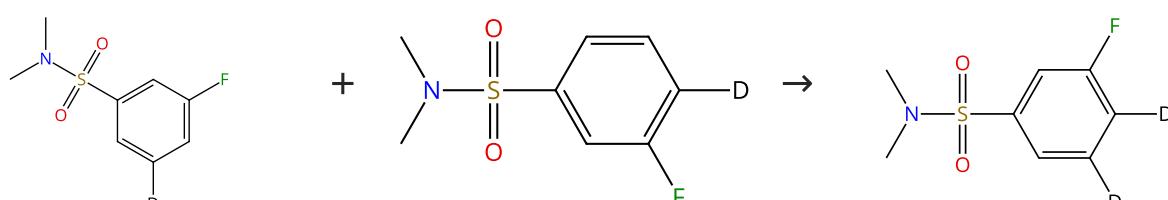
Experimental Protocols

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

Scheme 143 (1 Reaction)

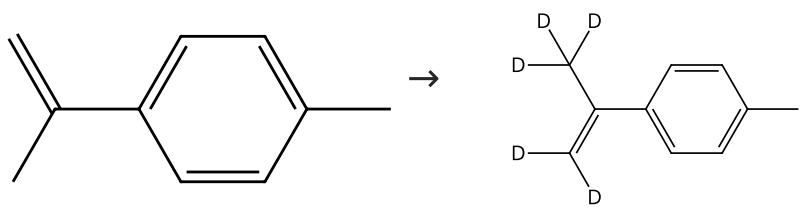
Steps: 1 Yield: 87%



|  |                     |   |
|--|---------------------|---|
| 31-614-CAS-26524545  | Steps: 1 Yield: 87% | Cobalt-Catalyzed Borylation of Fluorinated Arenes: Thermodynamic Control of C(sp <sup>2</sup> )-H Oxidative Addition Results in ortho-to-Fluorine Selectivity<br>By: Pabst, Tyler P.; et al<br>Journal of the American Chemical Society (2019), 141(38), 15378-15389. |
| 1.1 Reagents: Bis(pinacolato)diborane<br>Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-iridium, 4,4'-Bis(1,1-dimethylethyl)-2,2'-bipyridine<br>Solvents: Tetrahydrofuran; 12 h, 50 °C; 50 °C → rt |                     |   |
| 1.2 Reagents: Silver oxide (Ag <sub>2</sub> O)<br>Solvents: Tetrahydrofuran, Water- <i>d</i> <sub>2</sub> ; 12 h, rt → 50 °C; 50 °C → rt   |                     |   |
| 1.3 Reagents: Bis(pinacolato)diborane<br>Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-iridium, 4,4'-Bis(1,1-dimethylethyl)-2,2'-bipyridine<br>Solvents: Tetrahydrofuran; 12 h, 50 °C; 50 °C → rt |                     |   |
| 1.4 Reagents: Silver oxide (Ag <sub>2</sub> O)<br>Solvents: Tetrahydrofuran, Water- <i>d</i> <sub>2</sub> ; 12 h, rt → 50 °C; 50 °C → rt   |                     |   |

Scheme 144 (1 Reaction)

Steps: 1 Yield: 86%



Suppliers (50)

Supplier (1)

31-614-CAS-37018403

Steps: 1 Yield: 86%

- 1.1 Reagents: Water-*d*<sub>2</sub>  
Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κN<sup>1</sup>,κN<sup>1</sup>']bis[2-(2-pyridinyl-κM-phenyl-κC)-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato-κN)(1-)](N,N-dimethyl-4-pyridinamine-κN<sup>1</sup>)cobalt  
Solvents: Acetonitrile; 36 h, rt

Experimental Protocols

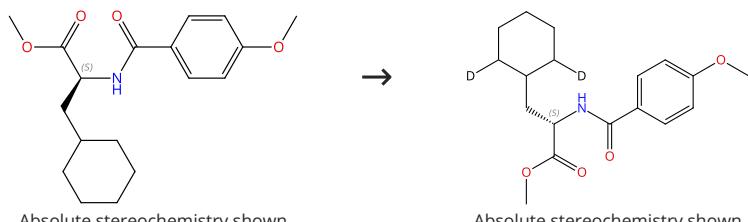
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 145 (1 Reaction)

Steps: 1 Yield: 86%



Absolute stereochemistry shown

Absolute stereochemistry shown

31-614-CAS-33530437

Steps: 1 Yield: 86%

- 1.1 Reagents: Water-*d*<sub>2</sub>  
Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine-κN<sup>1</sup>,κN<sup>1</sup>']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κN]phenyl-κC]-, hexafluorophosphate(1-) (1:1)  
Solvents: Chlorobenzene; 24 h, rt

Experimental Protocols

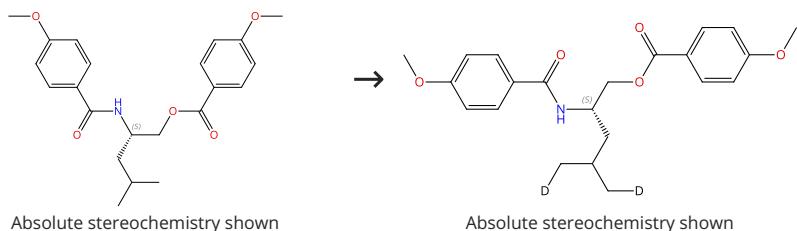
Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

**Scheme 146 (1 Reaction)**

Steps: 1 Yield: 86%



31-614-CAS-33530457

Steps: 1 Yield: 86%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-)

(1:1)

Solvents: Chlorobenzene; 24 h, rt

Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds

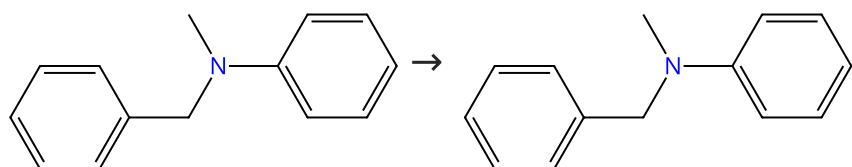
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

**Scheme 147 (1 Reaction)**

Steps: 1 Yield: 86%



Suppliers (56)

31-614-CAS-28305991

Steps: 1 Yield: 86%

Regioselective, Photocatalytic  $\alpha$ -Functionalization of Amines

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

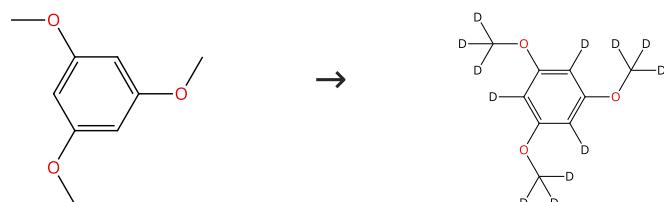
Solvents: Acetonitrile; 24 h, 24 °C

By: Leng, Lingying; et al

Journal of the American Chemical Society (2020), 142(28), 11972-11977.

**Scheme 148 (1 Reaction)**

Steps: 1 Yield: 86%



Suppliers (109)

31-116-CAS-23896486

Steps: 1 Yield: 86%

Gold-Catalyzed Tandem Oxidative Coupling Reaction between  $\beta$ -Ketoallenes and Electron-Rich Arenes to 2-Furylmethylarenes

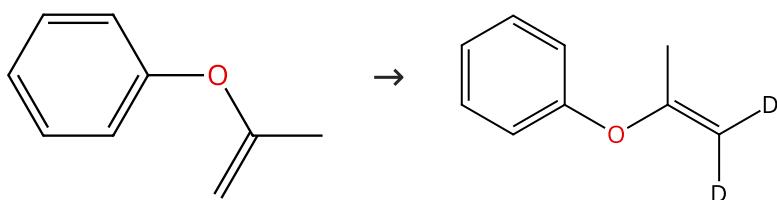
By: Yasukawa, Naoki; et al

Organic Letters (2021), 23(15), 5891-5895.

## Experimental Protocols

## Scheme 149 (1 Reaction)

Steps: 1 Yield: 86%



Suppliers (4)

31-116-CAS-15986821

Steps: 1 Yield: 86%

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

Solvents: Tetrahydrofuran; 3 h, 70 °C

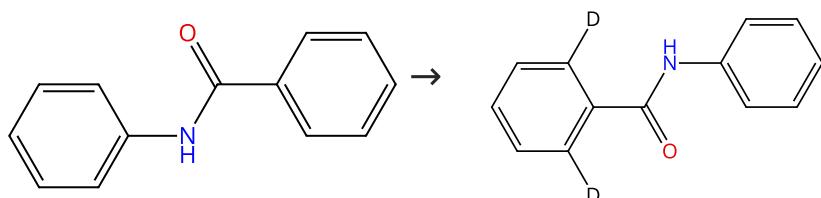
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

## Scheme 150 (3 Reactions)

Steps: 1 Yield: 32-86%



Suppliers (89)

31-116-CAS-15217329

Steps: 1 Yield: 86%

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentaned ionato- $\kappa O^2,\kappa O^4$ )iridium

Solvents: Dimethylformamide; 4 h, 95 °C

By: McAuley, B.; et al  
Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-15485988

Steps: 1 Yield: 58%

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

By: McAuley, B.; et al  
Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-11318553

Steps: 1 Yield: 32%

Hydrogen isotope labelling using iridium(I) dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium

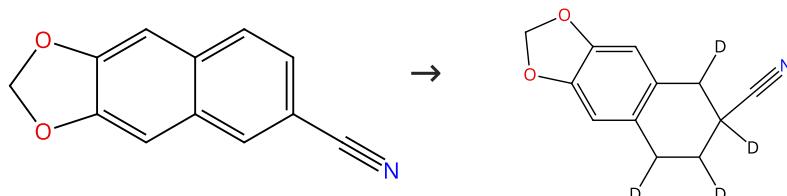
Solvents: Dimethylacetamide; 5 h, 95 °C

By: Lockley, W. J. S.

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

**Scheme 151 (1 Reaction)**

Steps: 1 Yield: 85%



Suppliers (22)

31-614-CAS-37081761

Steps: 1 Yield: 85%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Tris(4-methoxyphenyl)phosphine, 2,4,6-Tris(1-methylethyl)benzenethiol, Iridium(1+), [4,4'-bis(1,1-dimethyl ethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1)

**Solvents:** Acetonitrile; 72 h, 20 °C

Photocatalytic phosphine-mediated water activation for radical hydrogenation

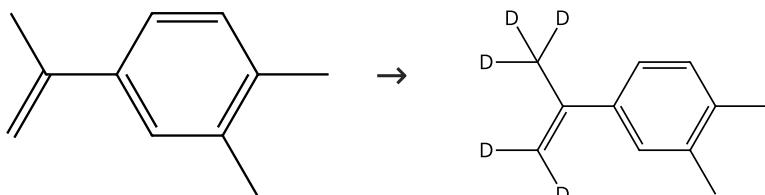
By: Zhang, Jingjing; et al

Nature (London, United Kingdom) (2023), 619(7970), 506-513.

Experimental Protocols

**Scheme 152 (1 Reaction)**

Steps: 1 Yield: 85%



Suppliers (13)

31-614-CAS-37018457

Steps: 1 Yield: 85%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethyl ethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1:) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximate- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

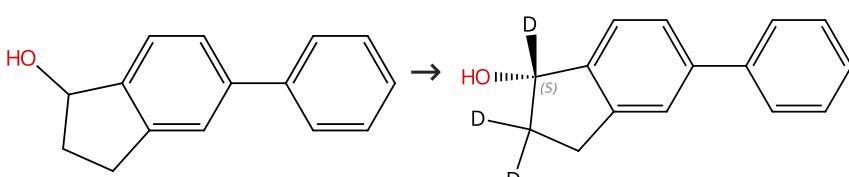
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

**Scheme 153 (1 Reaction)**

Steps: 1 Yield: 85%



Absolute stereochemistry shown

Suppliers (3)

31-614-CAS-41434440

Steps: 1 Yield: 85%

**Electrocatalytic cyclic deracemization enabled by a chemically modified electrode**

By: Zhu, Cheng-Jie; et al

Nature Catalysis (2024), 7(8), 878-888.

1.1 Reagents: Potassium carbonate

Catalysts: [N-[(1R,2R)-2-(Amino- $\kappa N$ )-1,2-diphenylethyl]methanesulfonamido(2-)- $\kappa N$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridiumSolvents: 1,4-Dioxane, Water- $d_2$ ; 24 h

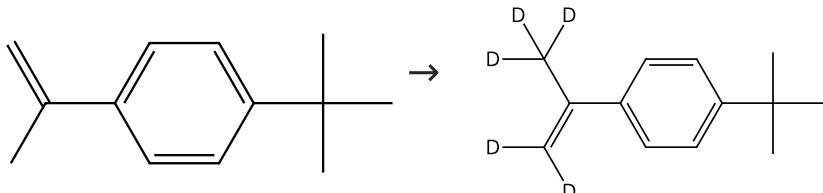
1.2 Reagents: Ammonium chloride

Solvents: Water

Experimental Protocols

**Scheme 154 (1 Reaction)**

Steps: 1 Yield: 85%


🛒 Suppliers (23)

31-614-CAS-37018412

Steps: 1 Yield: 85%

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

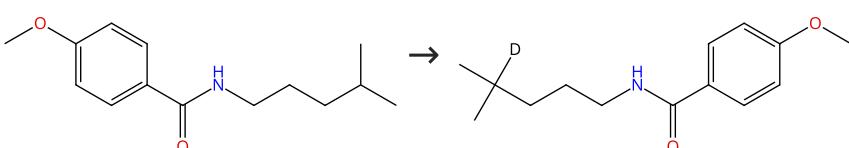
1.1 Reagents: Water- $d_2$ Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)]( $N,N$ -dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Experimental Protocols

**Scheme 155 (1 Reaction)**

Steps: 1 Yield: 85%


🛒 Supplier (1)

31-614-CAS-33530405

Steps: 1 Yield: 85%

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

1.1 Reagents: Water- $d_2$ Catalysts: Bis(4-methoxyphenyl) disulfide, 1-Butanaminium,  $N,N,N$ -tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Chlorobenzene; 24 h, rt

Experimental Protocols

Scheme 156 (1 Reaction)

Steps: 1 Yield: 85%



Suppliers (12)

31-614-CAS-37018474

Steps: 1 Yield: 85%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

Experimental Protocols

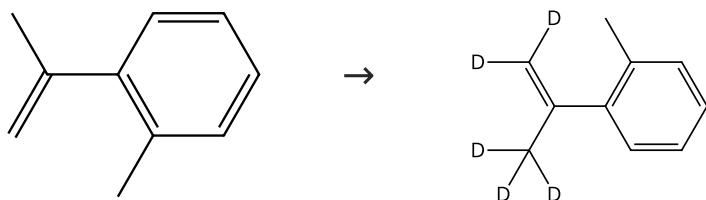
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 157 (1 Reaction)

Steps: 1 Yield: 85%



Suppliers (49)

31-614-CAS-37018467

Steps: 1 Yield: 85%

1.1 Reagents: Water- $d_2$ 

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

Experimental Protocols

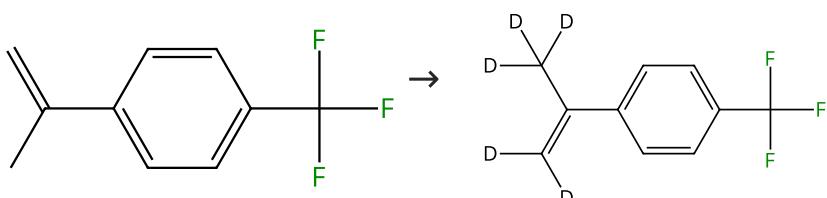
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Scheme 158 (1 Reaction)

Steps: 1 Yield: 84%



Suppliers (33)

31-614-CAS-37018438

Steps: 1 Yield: 84%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[1,2-cyclohexanedione 1,2-di(oximato- $\kappa M$ )](1-)

(*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

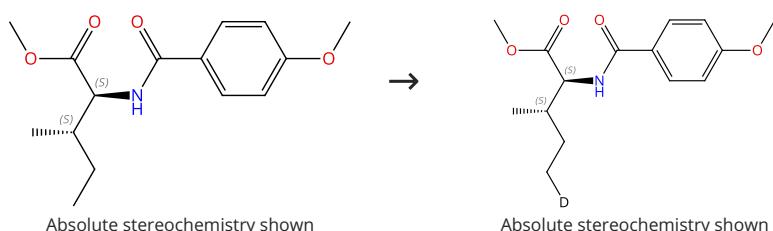
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

## Experimental Protocols

Scheme 159 (1 Reaction)

Steps: 1 Yield: 83%



Supplier (1)

31-614-CAS-33530432

Steps: 1 Yield: 83%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

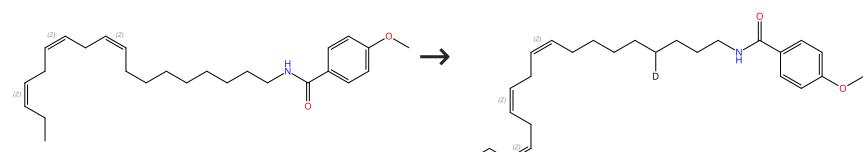
By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

Scheme 160 (1 Reaction)

Steps: 1 Yield: 83%



31-614-CAS-33530431

Steps: 1 Yield: 83%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Bis(4-methoxyphenyl) disulfide, 1-Butanaminium, *N,N,N*-tributyl-, dibutyl phosphate, Iridium(1+), [5,5'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

**Solvents:** Chlorobenzene; 24 h, rt

**Highly selective single and multiple deuteration of unactivated C(sp<sup>3</sup>)-H bonds**

By: Li, Nian; et al

Nature Communications (2022), 13(1), 4224.

## Experimental Protocols

**Scheme 161 (1 Reaction)**

Steps: 1 Yield: 83%



Suppliers (54)

31-116-CAS-15986845

Steps: 1 Yield: 83%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

Solvents: Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

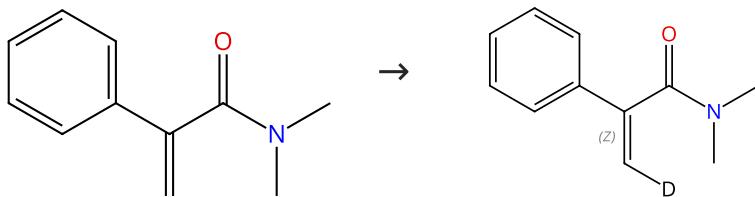
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

**Scheme 162 (1 Reaction)**

Steps: 1 Yield: 83%



Suppliers (8)

Double bond geometry shown

31-116-CAS-20720448

Steps: 1 Yield: 83%

Iridium-Catalyzed Cross-Coupling Reactions of Alkenes by Hydrogen Transfer

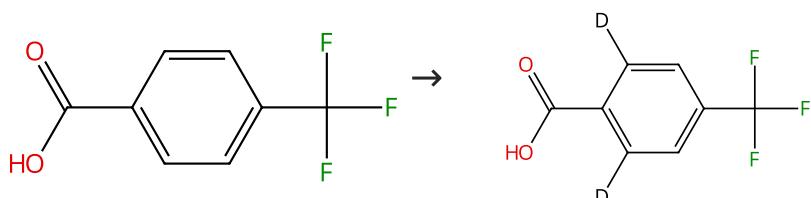
By: Meng, Keke; et al

Organic Letters (2019), 21(20), 8219-8224.

Experimental Protocols

**Scheme 163 (1 Reaction)**

Steps: 1 Yield: 82%



Suppliers (94)

31-116-CAS-22461112

Steps: 1 Yield: 82%

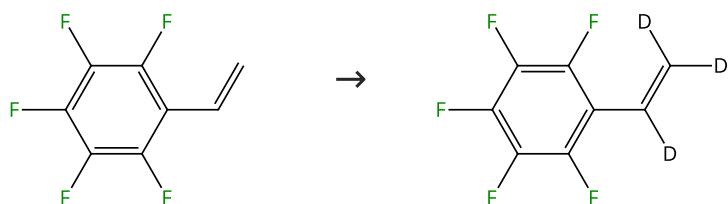
Ir<sup>III</sup>-Catalyzed Selective ortho-Monoiodination of Benzoic Acids with Unbiased C-H Bonds

By: Weis, Erik; et al

Chemistry - A European Journal (2020), 26(45), 10185-10190.

**Scheme 164 (1 Reaction)**

Steps: 1 Yield: 82%



Suppliers (83)

31-116-CAS-15986841

Steps: 1 Yield: 82%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium

Solvents: Tetrahydrofuran; 3 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

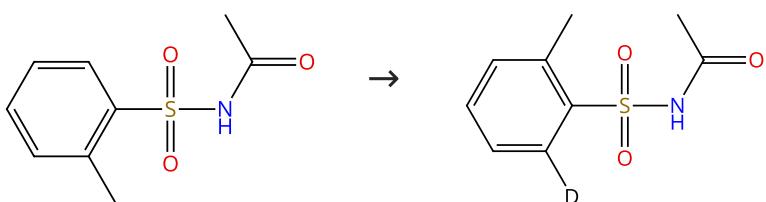
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

Experimental Protocols

**Scheme 165 (1 Reaction)**

Steps: 1 Yield: 81%



Suppliers (5)

31-116-CAS-20579031

Steps: 1 Yield: 81%

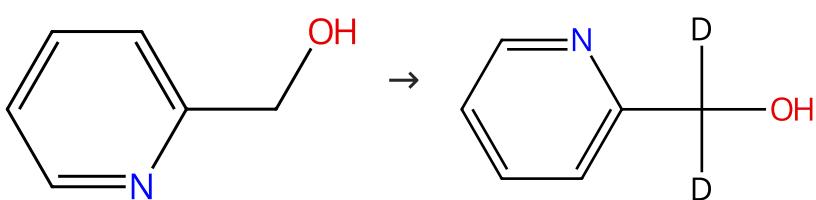
Iridium-Catalyzed ortho-C-H Amidation of Benzenesulfonamides with Sulfonyl Azides

By: Hou, Hongcen; et al

Advanced Synthesis &amp; Catalysis (2019), 361(18), 4393-4398.

**Scheme 166 (1 Reaction)**

Steps: 1 Yield: 81%



Suppliers (94)

31-614-CAS-33408345

Steps: 1 Yield: 81%

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

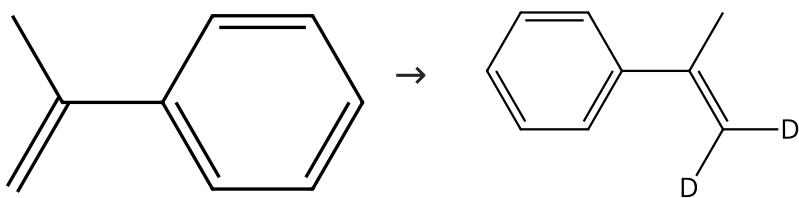
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

Experimental Protocols

**Scheme 167 (1 Reaction)**

Steps: 1 Yield: 81%



Suppliers (70)

Suppliers (2)

31-116-CAS-15986816

Steps: 1 Yield: 81%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-hydroxydiiridium

Solvents: Tetrahydrofuran; 20 h, 70 °C

Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex

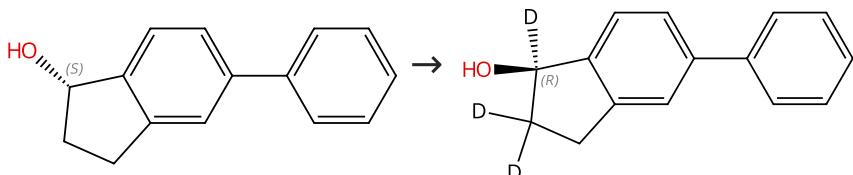
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

## Experimental Protocols

**Scheme 168 (1 Reaction)**

Steps: 1 Yield: 80%

Absolute stereochemistry shown,  
Rotation (+)

Absolute stereochemistry shown

31-614-CAS-41434445

Steps: 1 Yield: 80%

Electrocatalytic cyclic deracemization enabled by a chemically modified electrode

By: Zhu, Cheng-Jie; et al

Nature Catalysis (2024), 7(8), 878-888.

## 1.1 Reagents: Potassium carbonate

Catalysts: [N-[(1S,2S)-2-(Amino-κ*M*)-1,2-diphenylethyl]methanesulfonamido(2-)-κ*M*][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridiumSolvents: 1,4-Dioxane, Water-*d*<sub>2</sub>; 24 h

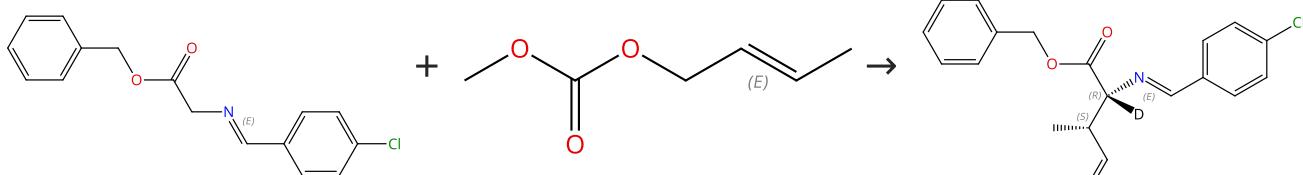
## 1.2 Reagents: Ammonium chloride

Solvents: Water

## Experimental Protocols

**Scheme 169 (1 Reaction)**

Steps: 1 Yield: 79%



Double bond geometry shown

Double bond geometry shown

Absolute stereochemistry shown,  
Rotation (+)  
Double bond geometry shown

Suppliers (2)

|  |                     |  |
|--|---------------------|--|
| 31-614-CAS-36688277  | Steps: 1 Yield: 79% | Stereodivergent synthesis of enantioenriched $\alpha$ -deuterated $\alpha$ -amino acids via cascade Cu(I)-catalyzed H-D exchange and dual Cu- and Ir-catalyzed allylation<br>By: Fu, Cong; et al<br>Organic Letters (2022), 24(30), 5562-5567. |
| 1.1 Reagents: Propylamine<br>Catalysts: Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]diiridium, (11bR)-N,N-Bis[(1R)-1-phenylethyl]dinaphtho[2,1- $\alpha$ :1',2'- $\beta$ ][1,3,2]dioxaphosphhepin-4-amine<br>Solvents: Tetrahydrofuran; 30 min, 50 °C |                     |  |
| 1.2 Catalysts: Tetrakis(acetonitrile)copper(1+) tetrafluoroborate, (2S)-1-[(4R)-4,5-Dihydro-4-(1-methylethyl)-2-oxazolyl]-2-(diphenylphosphino)ferrocene<br>Solvents: Dichloromethane; 0.5 h, rt   |                     |  |
| 1.3 Reagents: Triethylamine, Water- $d_2$<br>Solvents: Dichloromethane; 10 min, rt   |                     |  |
| 1.4 Solvents: Dichloromethane; 14 h, 25 °C   |                     |  |
| Experimental Protocols   |                     |  |

|                          |                        |
|--------------------------|------------------------|
| Scheme 170 (4 Reactions) | Steps: 1 Yield: 50-79% |
|                          |                        |

Suppliers (63)

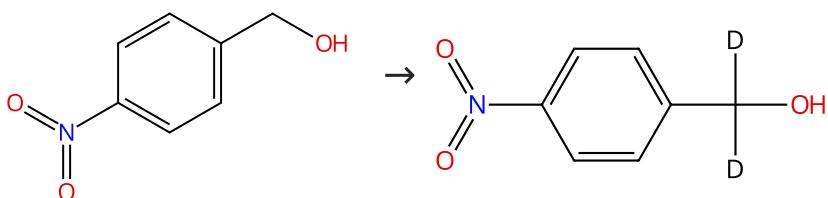
|                    |                     |  |
|--------------------|---------------------|--|
| 31-116-CAS-904     | Steps: 1 Yield: 79% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |
| 31-116-CAS-4250540 | Steps: 1 Yield: 65% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |

|                     |                     |  |
|---------------------|---------------------|--|
| 31-116-CAS-1067127  | Steps: 1 Yield: 50% | Hydrogen isotope labelling using iridium(I) dionates<br>By: Lockley, W. J. S.<br>Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.  |
| 31-116-CAS-13737532 | Steps: 1 Yield: 50% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |

|  |                     |  |
|--|---------------------|--|
| 31-116-CAS-13737532  | Steps: 1 Yield: 50% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |
| 1.1 Reagents: Water- $d_2$<br>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium<br>Solvents: Dimethylacetamide; 2 min, 130 °C |                     |  |

**Scheme 171 (1 Reaction)**

Steps: 1 Yield: 79%



Suppliers (105)

31-614-CAS-33408365

Steps: 1 Yield: 79%

**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**

- 1.1 **Reagents:** Methanol- $d_4$ , Water- $d_2$ , Sodium hydroxide- $d$   
**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1H,1'H)-dionato(2-)- $\kappa N^1,\kappa N^1'][(1,2,3,4,5-\eta)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
**Solvents:** Isopropanol; 13 h, 80 °C$
- 1.2 **Reagents:** Sulfuric acid  
**Solvents:** Water; pH 5

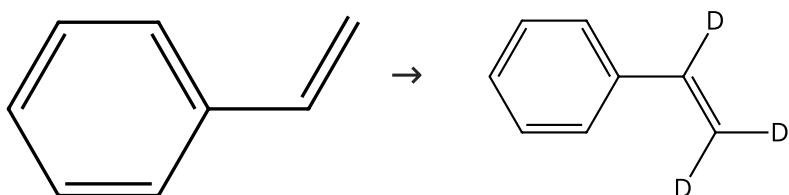
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

## Experimental Protocols

**Scheme 172 (1 Reaction)**

Steps: 1 Yield: 77%



Suppliers (122)

Suppliers (22)

31-116-CAS-15986843

Steps: 1 Yield: 77%

**Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex**

- 1.1 **Reagents:** Water- $d_2$   
**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium  
**Solvents:** Tetrahydrofuran; 3 h, 70 °C

By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

## Experimental Protocols

**Scheme 173 (1 Reaction)**

Steps: 1 Yield: 77%



Suppliers (51)

31-116-CAS-15986814

Steps: 1 Yield: 77%

**Selective H/D exchange at vinyl and methyl idene groups with D<sub>2</sub>O catalyzed by an iridium complex**

- 1.1 **Reagents:** Water- $d_2$   
**Catalysts:** *N*-(Methylsulfonyl)benzamide, Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridium  
**Solvents:** Tetrahydrofuran; 3 h, 70 °C

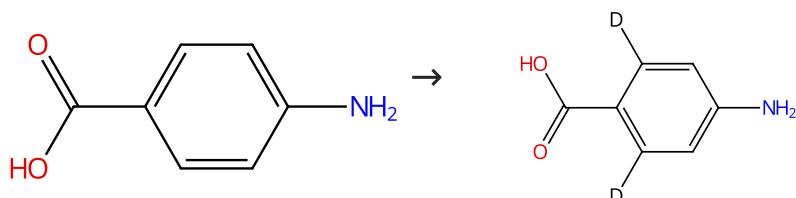
By: Hatano, Miyuki; et al

Organic Letters (2016), 18(15), 3674-3677.

## Experimental Protocols

## Scheme 174 (3 Reactions)

Steps: 1 Yield: 56-77%



Suppliers (137)

Suppliers (12)

31-116-CAS-7458773

Steps: 1 Yield: 77%

Hydrogen isotope labelling using iridium(I) dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato-κO<sup>2</sup>,κO<sup>4</sup>)iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

By: Lockley, W. J. S.

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

31-116-CAS-161178

Steps: 1 Yield: 77%

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato-κO<sup>2</sup>,κO<sup>4</sup>)iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-3120046

Steps: 1 Yield: 56%

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato-κO<sup>2</sup>,κO<sup>4</sup>)iridium

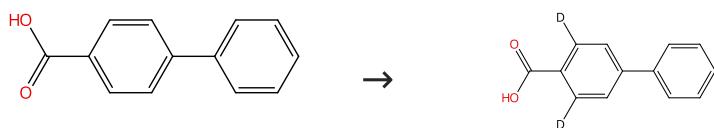
Solvents: Dimethylacetamide; 2.25 h, 90 °C

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

## Scheme 175 (3 Reactions)

Steps: 1 Yield: 27-77%



• Na

• Na

Suppliers (4)

31-116-CAS-2587431

Steps: 1 Yield: 77%

Hydrogen isotope labelling using iridium(I) dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato-κO<sup>2</sup>,κO<sup>4</sup>)iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

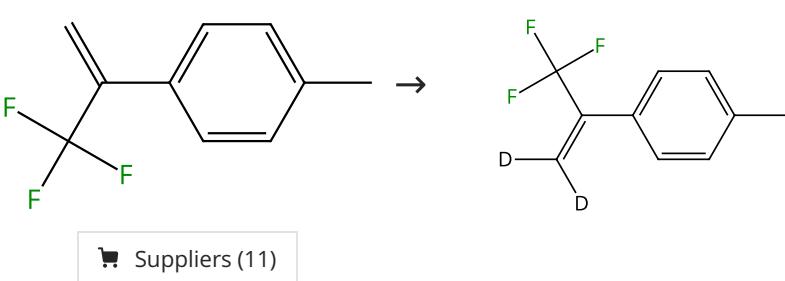
By: Lockley, W. J. S.

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

|                    |                     |   |
|--------------------|---------------------|---|
| 31-116-CAS-8009220 | Steps: 1 Yield: 77% | <b>Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates</b><br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |
| 31-116-CAS-7323401 | Steps: 1 Yield: 27% | <b>Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates</b><br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |

|  |                     |  |
|--|---------------------|--|
| Scheme 176 (1 Reaction)                                    | Steps: 1 Yield: 77% |  |
| Multi-component structure image available in CAS SciFinder | →                   | Multi-component structure image available in CAS SciFinder |

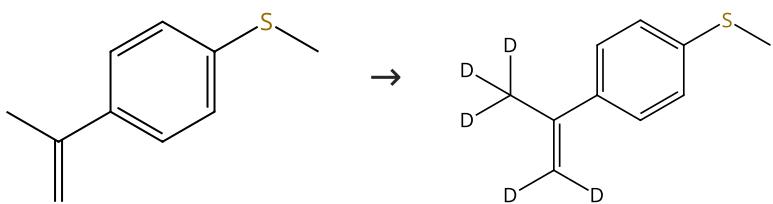
|   |                        |  |
|---|------------------------|--|
| 31-614-CAS-27466901   | Steps: 1 Yield: 77%    | <b>Photoredox-mediated hydrogen isotope exchange reactions of amino acids, peptides, and peptide-derived drugs</b><br>By: Legros, Fabien; et al<br>Chemistry - A European Journal (2020), 26(56), 12738-12742. |
| 1.1 Reagents: Water- <i>d</i> <sub>2</sub> , 2- <i>tert</i> -Butyl-1,1,3,3-tetramethylguanidine, Triisopropylsilanethiol<br>Catalysts: Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κN <sup>1</sup> ,κN <sup>1</sup> ]bis[3,5-difluoro-2-(5-methyl-2-pyridinyl-κN)phenyl-κC]-, ( <i>OC</i> -6-33)-, hexafluorophosphate(1-) (1:1)<br>Solvents: Dimethylformamide, Water- <i>d</i> <sub>2</sub> ; 3 h, rt | Experimental Protocols |  |

|   |                     |
|---|---------------------|
| Scheme 177 (1 Reaction)   | Steps: 1 Yield: 77% |
|  |                     |

|  |                        |  |
|--|------------------------|--|
| 31-614-CAS-37018511  | Steps: 1 Yield: 77%    | <b>Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange</b><br>By: Jia, Zongbin; et al<br>CCS Chemistry (2023), 5(5), 1069-1076. |
| 1.1 Reagents: Water- <i>d</i> <sub>2</sub><br>Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κN <sup>1</sup> ,κN <sup>1</sup> ]bis[2-(2-pyridinyl-κN)phenyl-κC]-, ( <i>OC</i> -6-33)-, hexafluorophosphate(1-) (1:1), ( <i>OC</i> -6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximate-κN)(1-)]( <i>N,N</i> -dimethyl-4-pyridinamine-κN <sup>1</sup> )cobalt<br>Solvents: Acetonitrile; 36 h, rt | Experimental Protocols |  |

**Scheme 178 (1 Reaction)**

Steps: 1 Yield: 77%



Suppliers (8)

31-614-CAS-37018418

Steps: 1 Yield: 77%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa N$ )-phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximate- $\kappa N$ )](1-)](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

**Solvents:** Acetonitrile; 36 h, rt

Experimental Protocols

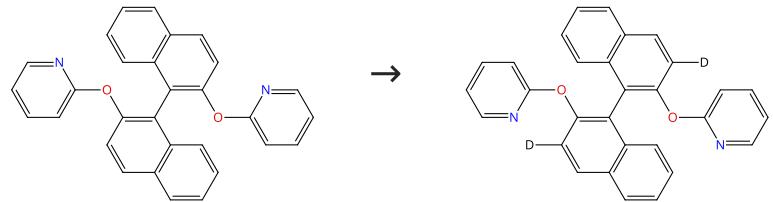
**Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange**

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

**Scheme 179 (1 Reaction)**

Steps: 1 Yield: 76%



31-614-CAS-31118815

Steps: 1 Yield: 76%

## 1.1 Reagents: Sodium acetate, Silver acetate, Silver triflate

**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-

**Solvents:** 2,2,2-Trifluoroethanol, Water-*d*<sub>2</sub>; 3 h, 140 °C

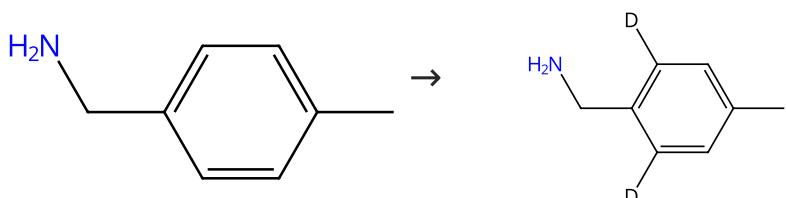
**Iridium(III)-catalyzed two-fold C-H alkylation of BINOLs with allyl alcohols**

By: Liu, Hao; et al

Organic Chemistry Frontiers (2022), 9(2), 471-475.

**Scheme 180 (3 Reactions)**

Steps: 1 Yield: 65-75%



Suppliers (86)

31-116-CAS-12583619

Steps: 1 Yield: 75%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pantanedionato- $\kappa O^2, \kappa O^4$ )iridium

**Solvents:** Dimethylacetamide; 2 min, 130 °C

**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

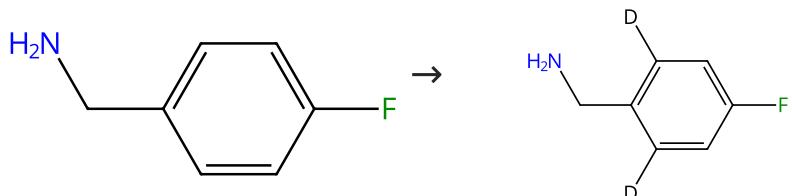
By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

|   |                     |  |
|---|---------------------|--|
| 31-116-CAS-14133067   | Steps: 1 Yield: 70% | Hydrogen isotope labelling using iridium(I) dionates<br>By: Lockley, W. J. S.<br>Journal of Labelled Compounds and Radiopharmaceuticals (2010), 53(11-12), 668-673.  |
| 1.1 Reagents: Water- <i>d</i> <sub>2</sub><br>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pantanenedionato- $\kappa O^2, \kappa O^4$ )iridium<br>Solvents: Dimethylacetamide; 2 min, 130 °C | Steps: 1 Yield: 65% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |

Scheme 181 (1 Reaction)

Steps: 1 Yield: 75%



Suppliers (91)

31-116-CAS-11992848

Steps: 1 Yield: 75%

## Hydrogen isotope labelling using iridium(I) dionates

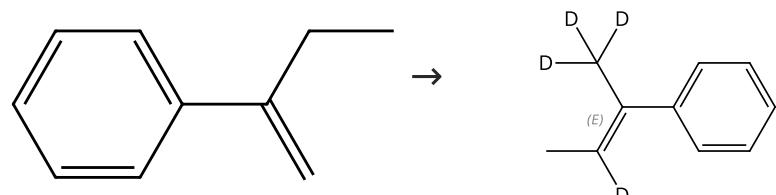
1.1 Reagents: Water-*d*<sub>2</sub>  
Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pantanenedionato- $\kappa O^2, \kappa O^4$ )iridium  
Solvents: Dimethylacetamide; 2 min, 130 °C

By: Lockley, W. J. S.

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

Scheme 182 (1 Reaction)

Steps: 1 Yield: 75%



Suppliers (53)

Double bond geometry shown

31-614-CAS-37018571

Steps: 1 Yield: 75%

## Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>  
Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )](1-)]( $N,N$ -dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt  
Solvents: Acetonitrile; 36 h, rt

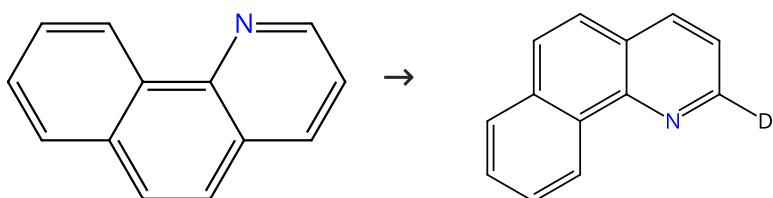
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

Experimental Protocols

## Scheme 183 (2 Reactions)

Steps: 1 Yield: 58-75%



Suppliers (81)

31-116-CAS-10837174

Steps: 1 Yield: 75%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-14673868

Steps: 1 Yield: 58%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

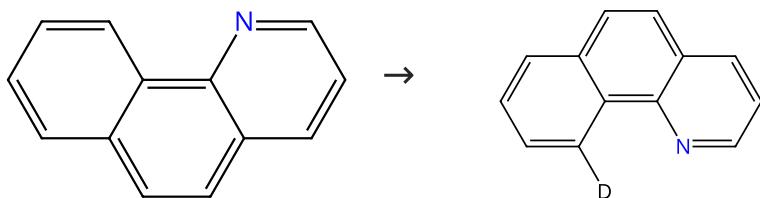
Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

## Scheme 184 (1 Reaction)

Steps: 1 Yield: 75%



Suppliers (81)

31-116-CAS-13844798

Steps: 1 Yield: 75%

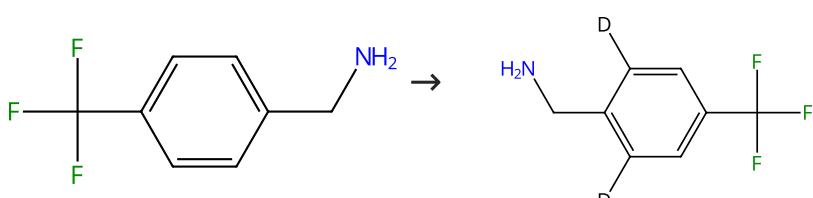
Hydrogen isotope labelling using iridium(I) dionates

By: Lockley, W. J. S.

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

## Scheme 185 (2 Reactions)

Steps: 1 Yield: 28-75%

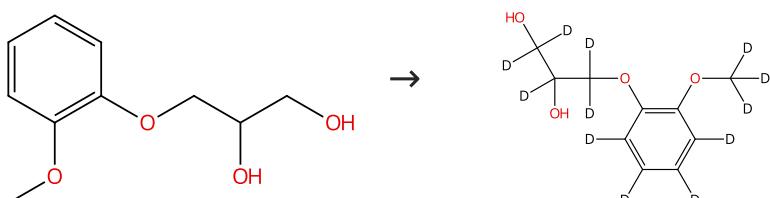


Suppliers (91)

|                     |                     |  |
|---------------------|---------------------|--|
| 31-116-CAS-14404085 | Steps: 1 Yield: 75% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |
| 31-116-CAS-9479178  | Steps: 1 Yield: 28% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |

Scheme 186 (1 Reaction)

Steps: 1 Yield: 75%



Suppliers (101)

31-614-CAS-33408342

Steps: 1 Yield: 75%

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

- 1.1 Reagents: Water- $d_2$ , Sodium hydroxide- $d$   
 Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1H,1'H)-dionato(2-) $\kappa N^1,\kappa N^1'][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-  
 Solvents: Isopropanol, 1,4-Dioxane; 1 d, 80 °C$

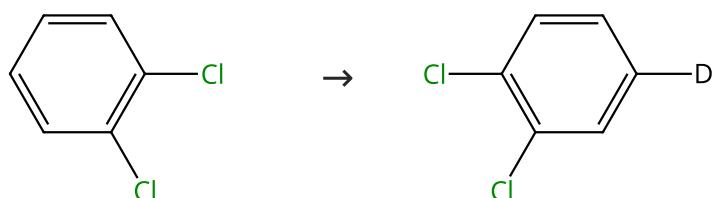
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

## Experimental Protocols

Scheme 187 (1 Reaction)

Steps: 1 Yield: 74%



Suppliers (139)

31-116-CAS-11759455

Steps: 1 Yield: 74%

## Harnessing C-H Borylation/Deborylation for Selective Deuteration, Synthesis of Boronate Esters, and Late Stage Functionalization

- 1.1 Reagents: Pinacolborane  
 Catalysts: 1,2-Bis(dimethylphosphino)ethane, [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene][(1,2,3,3a,7a- $\eta$ )-1H-inden-1-yl]iridium; rt  $\rightarrow$  150 °C; 3.5 h, 150 °C; 150 °C  $\rightarrow$  rt  
 1.2 Solvents: Methanol; rt  
 1.3 Reagents: Water- $d_2$   
 Solvents: Tetrahydrofuran; 30 min, 150 °C

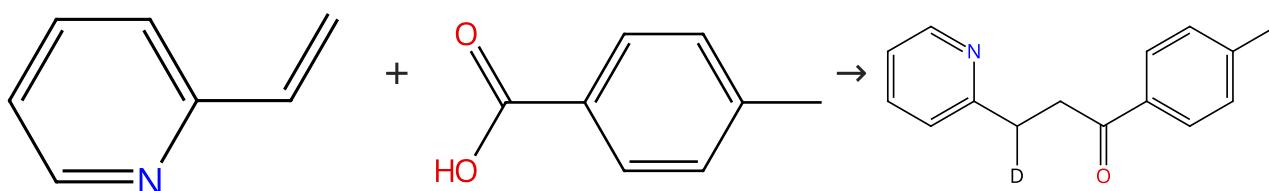
By: Kallepalli, Venkata A.; et al

Journal of Organic Chemistry (2015), 80(16), 8341-8353.

## Experimental Protocols

## Scheme 188 (1 Reaction)

Steps: 1 Yield: 72%



Suppliers (79)

Suppliers (103)

## 31-116-CAS-19898935

Steps: 1 Yield: 72%

## 1.1 Reagents: Triphenylphosphine

**Catalysts:** Dipotassium phosphate, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1)

**Solvents:** Dichloromethane, Water-*d*<sub>2</sub>; 48 h, rt

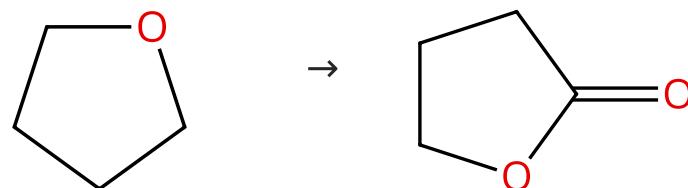
A general deoxygenation approach for synthesis of ketones from aromatic carboxylic acids and alkenes

By: Zhang, Muliang; et al

Nature Communications (2018), 9(1), 1-10.

## Scheme 189 (1 Reaction)

Steps: 1 Yield: 72%



Suppliers (410)

Suppliers (64)

## 31-494-CAS-9657856

Steps: 1 Yield: 72%

## 1.1 Reagents: Ceric ammonium nitrate

**Catalysts:** Iridium(2+), triqua[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, sulfate (1:1)

**Solvents:** Water-*d*<sub>2</sub>; 20 min, rt

## Experimental Protocols

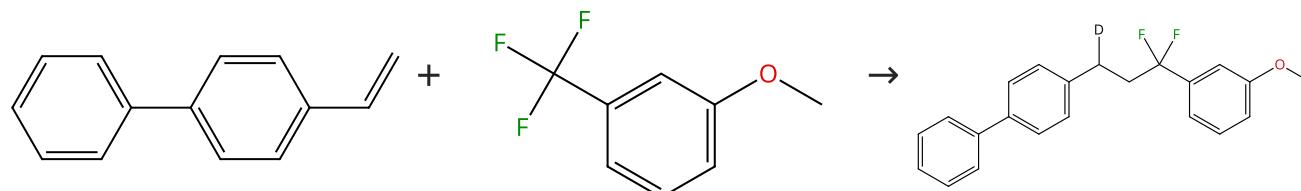
Cp\* Iridium Complexes Give Catalytic Alkane Hydroxylation with Retention of Stereochemistry

By: Zhou, Meng; et al

Journal of the American Chemical Society (2010), 132(36), 12550-12551.

## Scheme 190 (1 Reaction)

Steps: 1 Yield: 72%



Suppliers (74)

Suppliers (75)

## 31-614-CAS-40148871

Steps: 1 Yield: 72%

1.1 Reagents: Diisopropylamine, Water-*d*<sub>2</sub>

**Catalysts:** Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, (*OC*-6-33)-, hexafluorophosphate(1-) (1:1)

**Solvents:** Acetonitrile; 18 h, rt

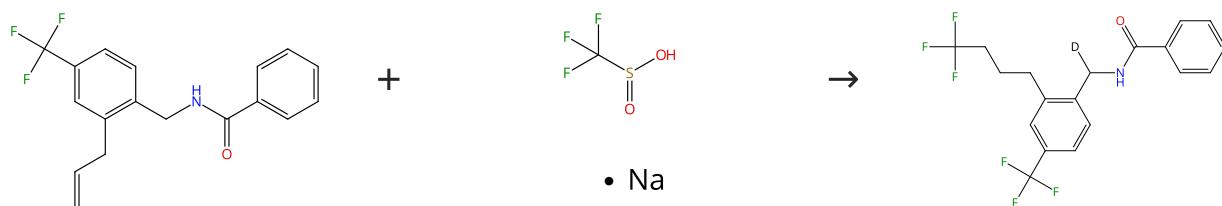
## Experimental Protocols

Selective Mono-Defluorinative Cross-Coupling of Trifluoromethyl arenes via Multiphoton Photoredox Catalysis

By: Jia, Jiaqi; et al

Chemistry - A European Journal (2024), 30(23), e202302927.

Scheme 191 (1 Reaction)



Suppliers (78)

Steps: 1 Yield: 71%

31-116-CAS-22806575

Steps: 1 Yield: 71%

- 1.1 **Reagents:** Carbon dioxide, Cesium carbonate, Water-*d*<sub>2</sub>, Propanoic acid, 2,2-dimethyl-, potassium salt (1:1)  
**Catalysts:** Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa^1,\kappa^1$ ']bis[2-(2-pyridinyl- $\kappa^1$ N)phenyl- $\kappa^1$ Cl]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dimethylacetamide; 24 h, 22 - 25 °C
- 1.2 **Reagents:** Hydrochloric acid  
**Solvents:** Water; 5 min, rt

Visible-Light Photoredox-Catalyzed Remote Difunctionalizing Carboxylation of Unactivated Alkenes with CO<sub>2</sub>

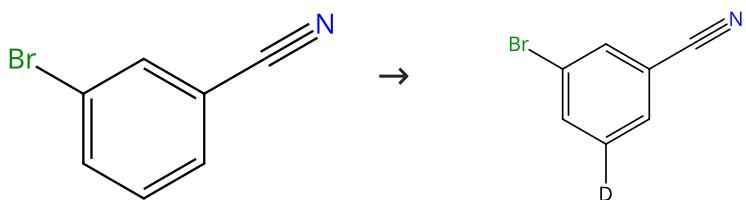
By: Song, Lei; et al

Angewandte Chemie, International Edition (2020), 59(47), 21121-21128.

Experimental Protocols

Scheme 192 (1 Reaction)

Steps: 1 Yield: 70%



Suppliers (88)

31-116-CAS-13839245

Steps: 1 Yield: 70%

- 1.1 **Reagents:** Pinacolborane, 4,4'-Bis(1,1-dimethylethyl)-2,2'-bipyridine  
**Catalysts:** Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydiiridium  
**Solvents:** Heptane; 1 min, rt
- 1.2 6 h, rt
- 1.3 **Reagents:** Water-*d*<sub>2</sub>  
**Solvents:** Tetrahydrofuran; 2 h, 150 °C

Harnessing C-H Borylation/Deborylation for Selective Deuteration, Synthesis of Boronate Esters, and Late Stage Functionalization

By: Kallepalli, Venkata A.; et al

Journal of Organic Chemistry (2015), 80(16), 8341-8353.

Experimental Protocols

Scheme 193 (1 Reaction)

Steps: 1 Yield: 68%



Suppliers (6)

31-614-CAS-36980193

Steps: 1 Yield: 68%

1.1 Reagents: Lithium acetate, Water-*d*<sub>2</sub>Catalysts: Silver acetate, Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate

Solvents: 1,2-Dichloroethane; 24 h, rt

Experimental Protocols

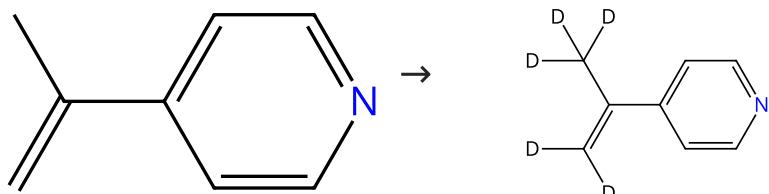
Ir(III)-Catalyzed C(sp<sup>2</sup>)-H Amidation of 2-Aroylimidazoles with 2,2,2-Trichloroethoxycarbonyl Azide (TrocN<sub>3</sub>)

By: Mahato, Sanjit K.; et al

Journal of Organic Chemistry (2022), 87(24), 16390-16398.

## Scheme 194 (1 Reaction)

Steps: 1 Yield: 67%



Suppliers (25)

31-614-CAS-37018482

Steps: 1 Yield: 67%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,N^1'$ ]bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1), (OC-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximate- $\kappa M$ )](1-)]( $N,N$ -dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Experimental Protocols

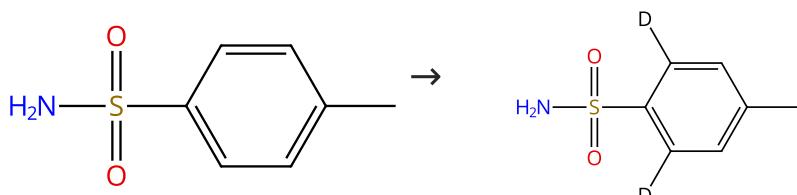
Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

## Scheme 195 (3 Reactions)

Steps: 1 Yield: 50-66%



Suppliers (99)

31-116-CAS-5314601

Steps: 1 Yield: 66%

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-2430088

Steps: 1 Yield: 66%

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-8827576

Steps: 1 Yield: 50%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

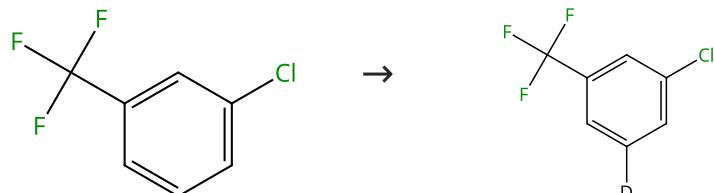
Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

## Scheme 196 (1 Reaction)

Steps: 1 Yield: 66%



Suppliers (62)

31-116-CAS-7433901

Steps: 1 Yield: 66%

1.1 Reagents: Pinacolborane

Catalysts: 1,2-Bis(dimethylphosphino)ethane, [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene][(1,2,3,3a,7a- $\eta$ )-1*H*-inden-1-yl]iridium

Solvents: Cyclohexane; rt → 150 °C; 3.0 h, 150 °C; 150 °C → rt

1.2 Reagents: Water-*d*<sub>2</sub>

Solvents: Tetrahydrofuran; 90 min, 150 °C

Harnessing C-H Borylation/Deborylation for Selective Deuteration, Synthesis of Boronate Esters, and Late Stage Functionalization

By: Kallepalli, Venkata A.; et al

Journal of Organic Chemistry (2015), 80(16), 8341-8353.

## Experimental Protocols

## Scheme 197 (1 Reaction)

Steps: 1 Yield: 62%



Suppliers (4)

31-614-CAS-37018456

Steps: 1 Yield: 62%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Diisopropylethylamine, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ], (*OC*-6-33)-, hexafluorophosphate(1-) (1:1), (*OC*-6-42)-Chlorobis[[1,2-cyclohexanedione 1,2-di(oximato- $\kappa N$ )][1-]](*N,N*-dimethyl-4-pyridinamine- $\kappa N^1$ )cobalt

Solvents: Acetonitrile; 36 h, rt

Visible light promoted direct deuteration of alkenes via Co(III)-H mediated H/D exchange

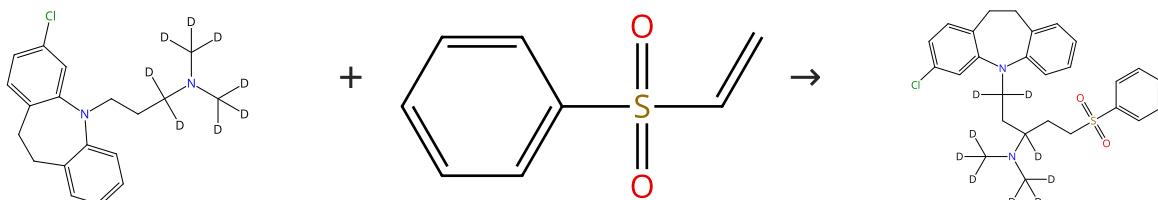
By: Jia, Zongbin; et al

CCS Chemistry (2023), 5(5), 1069-1076.

## Experimental Protocols

Scheme 198 (1 Reaction)

Steps: 1 Yield: 60%



Suppliers (94)

31-614-CAS-24525027

Steps: 1 Yield: 60%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: 1,1,1-Triphenylsilanethiol, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

Solvents: Toluene; 1 min, 28 °C; 8 h, 28 °C

Site-selective  $\alpha$ -C-H Functionalization of Trialkylamines via Reversible HAT-Catalysis

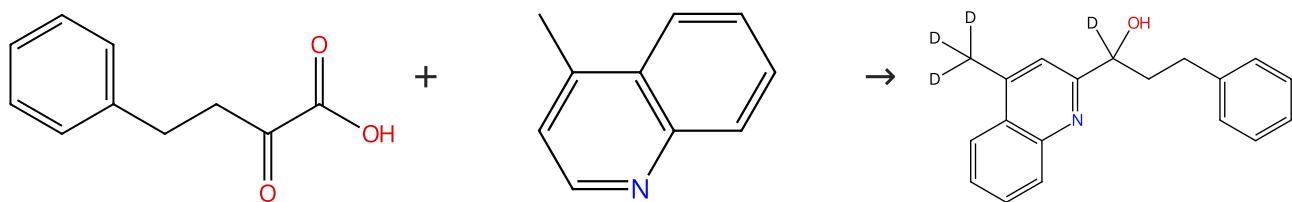
By: Shen, Yangyang; et al

Journal of the American Chemical Society (2021), 143(45), 18952-18959.

## Experimental Protocols

Scheme 199 (1 Reaction)

Steps: 1 Yield: 60%



Suppliers (68)

Suppliers (75)

31-614-CAS-31486606

Steps: 1 Yield: 60%

Photoredox Neutral Decarboxylative Hydroxyalkylations of Heteroarenes with  $\alpha$ -Keto Acids

By: Ji, Xiaochen; et al

Journal of Organic Chemistry (2022), 87(6), 4168-4182.

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa M$ ]phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

Solvents: Methanol; 48 h, 50 °C

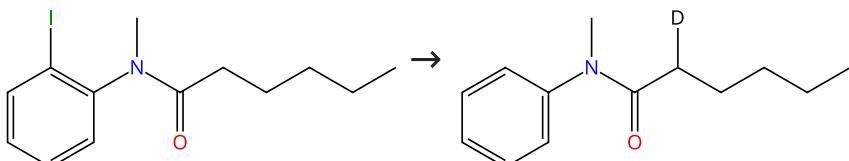
## 1.2 Reagents: Sodium carbonate

Solvents: Water

## Experimental Protocols

Scheme 200 (1 Reaction)

Steps: 1 Yield: 58%



Suppliers (2)

Supplier (1)

31-614-CAS-43333942

Steps: 1 Yield: 58%

1.1 **Reagents:** Cesium carbonate, Diisopropylethylamine, Water-*d*<sub>2</sub>

**Catalysts:** Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-(5-methyl-2-pyridinyl- $\kappa N$ )phenyl- $\kappa Cl$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

**Solvents:** Dimethyl sulfoxide; 16 h, 1 atm, rt

1.2 **Reagents:** Hydrochloric acid

**Solvents:** Water; pH 1

Experimental Protocols

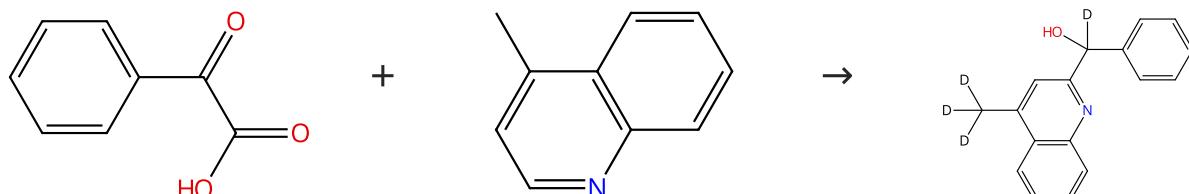
Remote C(sp<sup>3</sup>)-H Carboxylation with CO<sub>2</sub> via Visible-Light-Catalyzed 1,5-Hydrogen Atom Transfer

By: Huang, Haoran; et al

Organic Letters (2024), 26(51), 11195-11200.

## Scheme 201 (1 Reaction)

Steps: 1 Yield: 58%



Suppliers (112)

Suppliers (75)

31-614-CAS-31486604

Steps: 1 Yield: 58%

1.1 **Reagents:** Trifluoroacetic acid, Water-*d*<sub>2</sub>, Zinc triflate

**Catalysts:** Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa Cl$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

**Solvents:** Methanol; 48 h, 50 °C

1.2 **Reagents:** Sodium carbonate

**Solvents:** Water

Experimental Protocols

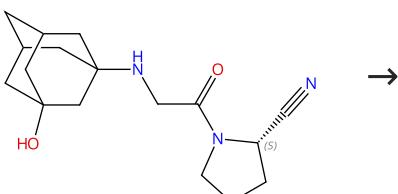
Photoredox Neutral Decarboxylative Hydroxyalkylations of Heteroarenes with  $\alpha$ -Keto Acids

By: Ji, Xiaochen; et al

Journal of Organic Chemistry (2022), 87(6), 4168-4182.

## Scheme 202 (1 Reaction)

Steps: 1 Yield: 56%

Absolute stereochemistry shown,  
Rotation (-)Multi-component  
structure image  
available in CAS  
SciFinder

Suppliers (109)

31-614-CAS-27788809

Steps: 1 Yield: 56%

1.1 **Reagents:** Water-*d*<sub>2</sub>, 2-*tert*-Butyl-1,1,3,3-tetramethylguanidine, Triisopropylsilanethiol

**Catalysts:** Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[3,5-difluoro-2-(5-methyl-2-pyridinyl- $\kappa N$ )phenyl- $\kappa Cl$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

**Solvents:** Dimethylformamide, Water-*d*<sub>2</sub>; 3 h, rt

Experimental Protocols

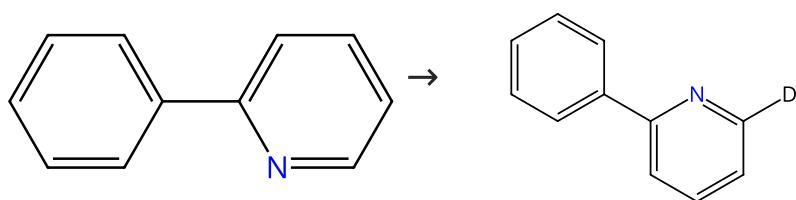
Photoredox-mediated hydrogen isotope exchange reactions of amino acids, peptides, and peptide-derived drugs

By: Legros, Fabien; et al

Chemistry - A European Journal (2020), 26(56), 12738-12742.

Scheme 203 (1 Reaction)

Steps: 1 Yield: 54%



Suppliers (94)

Supplier (1)

31-116-CAS-5201358

Steps: 1 Yield: 54%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

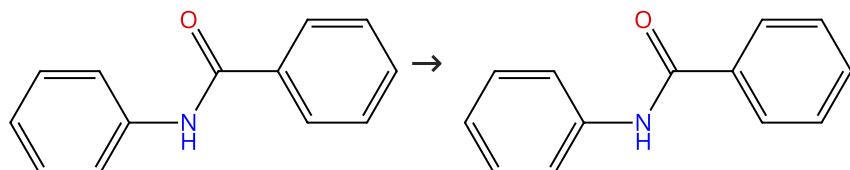
Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

Scheme 204 (1 Reaction)

Steps: 1 Yield: 53%



Suppliers (89)

31-614-CAS-30956872

Steps: 1 Yield: 53%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [1,1'-(4*R*)-[4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[1,1-diphenylphosphine- $\kappa P$ ]][(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, 1,1,1-trifluoromethanesulfonate (1:1)

Solvents: 1,4-Dioxane; 24 h, 120 °C

Ir-Catalyzed Enantioselective Intra- and Intermolecular Formal C-H Conjugate Addition to  $\beta$ -Substituted  $\alpha, \beta$ -Unsaturated Esters

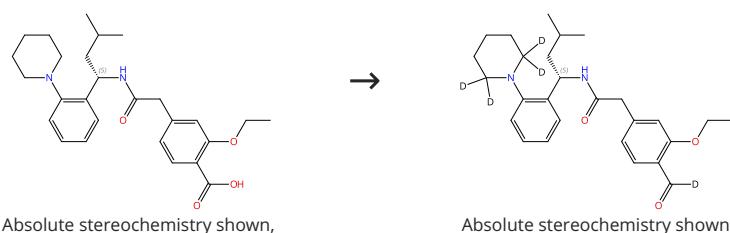
By: Shibata, Takanori; et al

Asian Journal of Organic Chemistry (2018), 7(7), 1411-1418.

## Experimental Protocols

Scheme 205 (1 Reaction)

Steps: 1 Yield: 52%



Suppliers (106)

31-116-CAS-19502689

Steps: 1 Yield: 52%

**1.1 Reagents:** Triphenylphosphine, Dipotassium phosphate, Water-*d*<sub>2</sub>

**Catalysts:** 2,4,6-Tris(1-methylethyl)benzenethiol, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ], (*O*-C-6-33), hexafluorophosphate(1-) (1:1)

**Solvents:** Dichloromethane; 36 h, rt

**1.2 Reagents:** Water; rt

Experimental Protocols

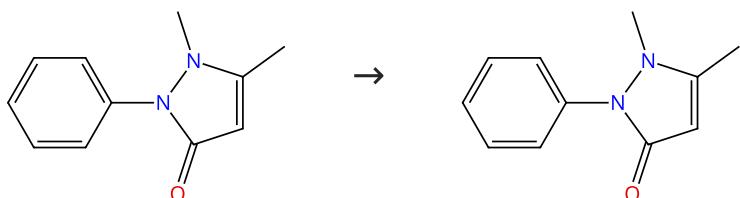
### Deoxygenative Deuteration of Carboxylic Acids with D<sub>2</sub>O

By: Zhang, Muliang; et al

Angewandte Chemie, International Edition (2019), 58(1), 312-316.

### Scheme 206 (2 Reactions)

Steps: 1 Yield: 25-51%



Suppliers (99)

31-116-CAS-4455282

Steps: 1 Yield: 51%

**1.1 Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

**Solvents:** Dimethylacetamide; 2 min, 130 °C

**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

By: McAuley, B.; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-12528949

Steps: 1 Yield: 25%

**1.1 Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

**Solvents:** Dimethylacetamide; 2.25 h, 90 °C

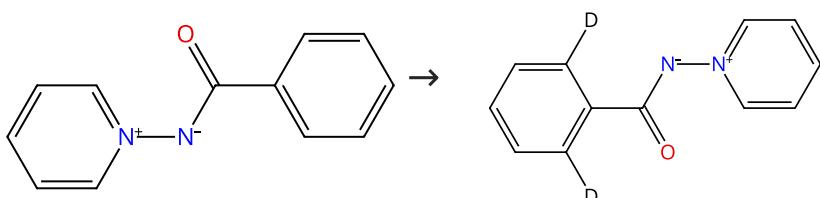
**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

By: McAuley, B.; et al

Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204.

### Scheme 207 (1 Reaction)

Steps: 1 Yield: 50%



Suppliers (5)

31-614-CAS-42421295

Steps: 1 Yield: 50%

**1.1 Reagents:** Potassium acetate, Water-*d*<sub>2</sub>

**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoro antimonate

**Solvents:** 2,2,2-Trifluoroethanol, Water; 24 h, 100 °C

**Ir(III)-catalyzed C-H alkenylation/annulation of N-iminopyridinium ylides with acrylates and alkynes**

By: Chen, Xiaopei; et al

Tetrahedron (2024), 168, 134322.

**Scheme 208 (1 Reaction)**

Steps: 1 Yield: 50%



31-614-CAS-36222321

Steps: 1 Yield: 50%

- 1.1 **Reagents:** Triphenylphosphine, Dipotassium phosphate, Water-*d*<sub>2</sub>

**Catalysts:** Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κN<sup>1</sup>,κN<sup>1</sup>']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κN]phenyl-κCl]-, (OC-6-33)-, hexafluorophosphate(1-)

(1:1)

**Solvents:** Dichloromethane; 48 h, rt

- 1.2 **Reagents:** Water; rt

Experimental Protocols

**Photoredox-Mediated Deoxygenative Radical Additions of Aromatic Acids to Vinyl Boronic Esters and gem-Diboryl alkenes**

By: Nagaraju, Anugula; et al

Chemistry - A European Journal (2023), 29(3), e202202646.

**Scheme 209 (1 Reaction)**

Steps: 1 Yield: 50%



Absolute stereochemistry shown

Absolute stereochemistry shown

31-614-CAS-40118618

Steps: 1 Yield: 50%

- 1.1 **Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene] diiridium, Sodium tetrakis[3,5-bis(trifluoromethyl)phenyl] borate

**Solvents:** Toluene; 12 h, rt → 100 °C

Experimental Protocols

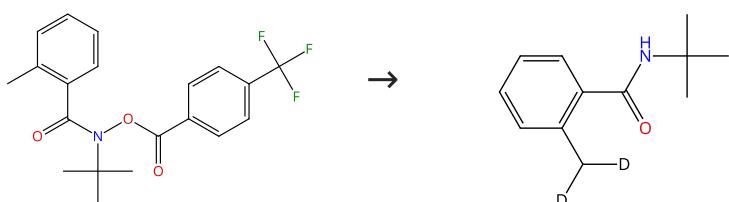
**Reversible-Hydrogen-Transfer-Mediated Anomerization of Azaheterocycl 2-Deoxy-C-glycosides and Mechanistic Studies**

By: Mu, Qiu-Qi; et al

ACS Catalysis (2023), 13(8), 5656-5664.

**Scheme 210 (1 Reaction)**

Steps: 1 Yield: 48%



31-614-CAS-36994349

Steps: 1 Yield: 48%

- 1.1 **Reagents:** Cesium carbonate, Diisopropylethylamine, Water-*d*<sub>2</sub>

**Catalysts:** Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κN<sup>1</sup>,κN<sup>1</sup>']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κN]phenyl-κCl]-, (OC-6-33)-, hexafluorophosphate(1-)

(1:1)

**Solvents:** Dimethylformamide; 48 h, 1 atm, rt

Experimental Protocols

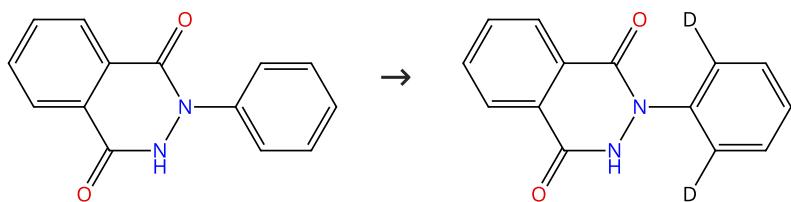
**Photocarboxylation of remote C-H bonds through nitrogen-centred radical 1,5-hydrogen atom transfer**

By: Li, Wenke; et al

Green Chemistry (2023), 25(13), 5030-5034.

**Scheme 211 (1 Reaction)**

Steps: 1 Yield: 46%



Suppliers (38)

31-614-CAS-40822335

Steps: 1 Yield: 46%

1.1 **Reagents:** 1-Adamantanecarboxylic acid, Water-d<sub>2</sub>  
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-  
**Solvents:** 1,2-Dichloroethane; 0.5 h, 100 °C

Experimental Protocols

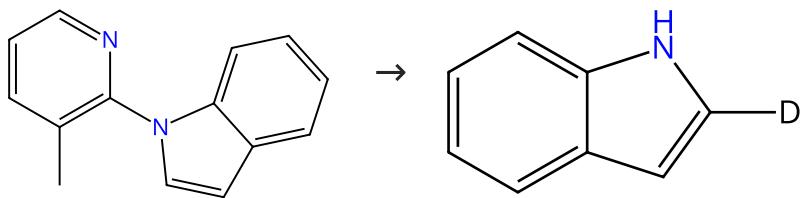
**Synthesis of Phthalazino[2,3-a]cinnoline-6,8,13(5H)-triones via Ir(III)-Catalyzed Dehydrogenative C-H/N-H Functionalization of N-Aryl Phthalazinones**

By: Zhang, Chao; et al

Advanced Synthesis &amp; Catalysis (2024), 366(13), 2996-3000.

**Scheme 212 (1 Reaction)**

Steps: 1 Yield: 43%



Suppliers (3)

Suppliers (12)

31-614-CAS-34491693

Steps: 1 Yield: 43%

1.1 **Reagents:** Norbornene, Water-d<sub>2</sub>  
**Catalysts:** Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-diiridium  
**Solvents:** Toluene; 22 h, 80 °C

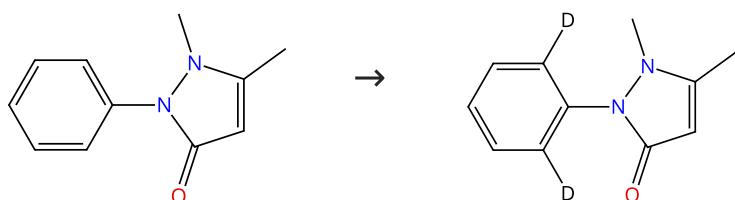
**3-Alkyl-2-pyridyl Directing Group-Enabled C2 Selective C-H Silylation of Indoles and Pyrroles via an Iridium Catalyst**

By: Sun, Hui; et al

Journal of Organic Chemistry (2022), 87(19), 13346-13351.

**Scheme 213 (1 Reaction)**

Steps: 1 Yield: 41%



Suppliers (99)

31-116-CAS-9594461

Steps: 1 Yield: 41%

**Hydrogen isotope labelling using iridium(I) dionates**

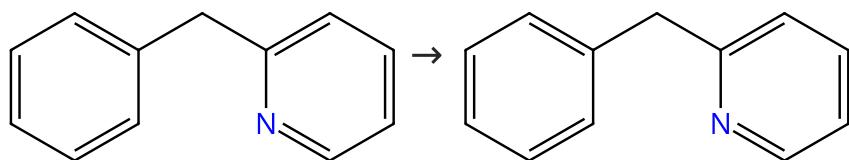
1.1 **Reagents:** Water-d<sub>2</sub>  
**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium  
**Solvents:** Dimethylacetamide; 2 min, 130 °C

By: Lockley, W. J. S.

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

## Scheme 214 (2 Reactions)

Steps: 1 Yield: 4-40%



Suppliers (66)

31-116-CAS-15386002

Steps: 1 Yield: 40%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-5535980

Steps: 1 Yield: 4%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

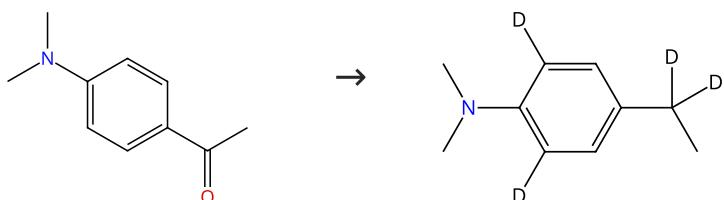
Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

## Scheme 215 (1 Reaction)

Steps: 1 Yield: 40%



Suppliers (83)

31-116-CAS-22909026

Steps: 1 Yield: 40%

1.1 Reagents: Formic-*d* acid-*d*Catalysts: Iridium(1+), chloro[2-(4,5-dihydro-1*H*-imidazol-2-yl- $\kappa N^3$ )-*N,N*-diethyl-4-pyridinamine- $\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, chloride (1:1)Solvents: 1,1,1,3,3-Hexafluoro-2-propanol, Water-*d*<sub>2</sub>; 2 h, 80 °C

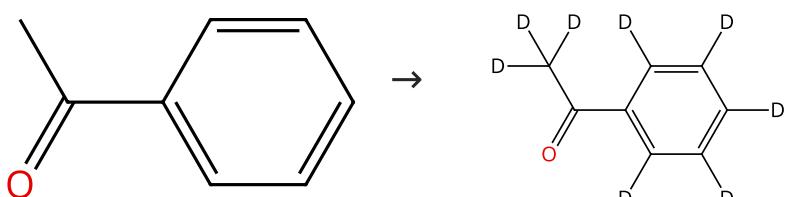
Iridium-Catalysed Reductive Deoxygenation of Ketones with Formic Acid as Traceless Hydride Donor

By: Yang, Zhiheng; et al

Advanced Synthesis &amp; Catalysis (2020), 362(23), 5496-5505.

## Scheme 216 (1 Reaction)

Steps: 1 Yield: 40%



Suppliers (109)

Suppliers (39)

31-116-CAS-20111043

Steps: 1 Yield: 40%

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium

Solvents: Isopropanol; 24 h, rt

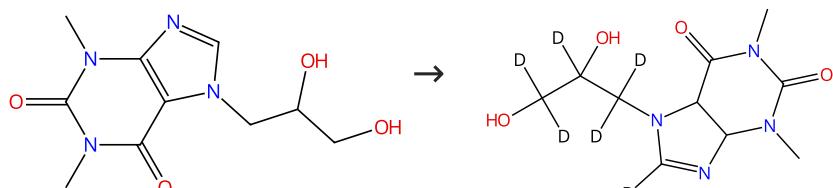
**H-D Exchange Deuteration of Arenes at Room Temperature**

By: Sawama, Yoshinari; et al

Organic Process Research &amp; Development (2019), 23(4), 648-653.

**Scheme 217 (1 Reaction)**

Steps: 1 Yield: 37%



Suppliers (98)

31-614-CAS-33408347

Steps: 1 Yield: 37%

1.1 Reagents: Water-*d*<sub>2</sub>, Sodium hydroxide-*d*Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)·κ*N*<sup>1</sup>,κ*N*'<sup>1</sup>]·[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

Solvents: Isopropanol, 1,4-Dioxane; 80 °C

**Iridium-catalyzed α-selective deuteration of alcohols**

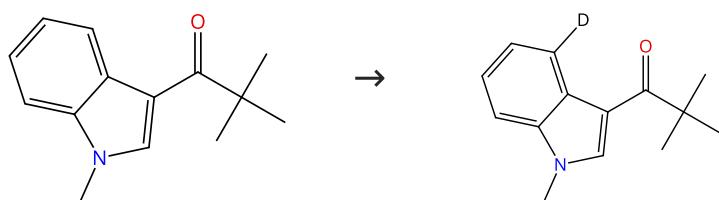
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

## Experimental Protocols

**Scheme 218 (1 Reaction)**

Steps: 1 Yield: 35%



Suppliers (32)

31-116-CAS-20471674

Steps: 1 Yield: 35%

1.1 Reagents: Pivalic acid, Water-*d*<sub>2</sub>, Silver oxide (Ag<sub>2</sub>O)

Catalysts: Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoro antimonate

Solvents: 1,2-Dichloroethane; 2 h, 80 °C

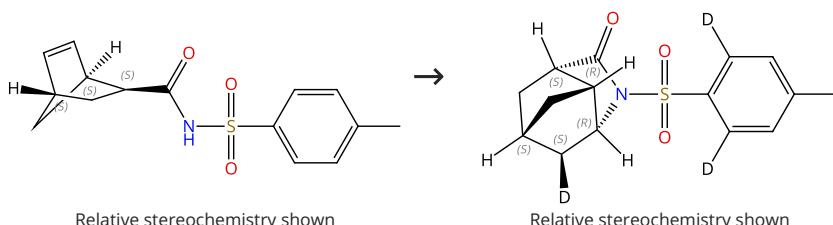
**C2/C4 Regioselective Heteroarylation of Indoles by Tuning C-H Metalation Modes**

By: Chen, Shuyou; et al

ACS Catalysis (2019), 9(7), 6372-6379.

**Scheme 219 (1 Reaction)**

Steps: 1 Yield: 35%



31-116-CAS-16104378

Steps: 1 Yield: 35%

1.1 Reagents: Water-*d*<sub>2</sub>

Solvents: Acetonitrile; 2 h, rt

1.2 Reagents: Water-*d*<sub>2</sub>Catalysts: *N,N*-Dimethylbenzylamine, Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ -1,5-cyclooctadiene]diiridium

Solvents: 1,2-Dichloroethane; 20 h, 80 °C

Experimental Protocols

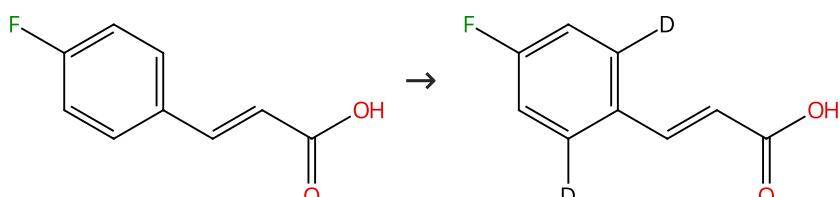
**Asymmetric Cyclization of N-Sulfonyl Alkenyl Amides Catalyzed by Iridium/Chiral Diene Complexes**

By: Nagamoto, Midori; et al

Organic Letters (2016), 18(18), 4474-4477.

Scheme 220 (2 Reactions)

Steps: 1 Yield: 26-30%



Suppliers (83)

31-116-CAS-4081982

Steps: 1 Yield: 30%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ -1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa$ O<sup>2</sup>, $\kappa$ O<sup>4</sup>)iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-14355680

Steps: 1 Yield: 26%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ -1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa$ O<sup>2</sup>, $\kappa$ O<sup>4</sup>)iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

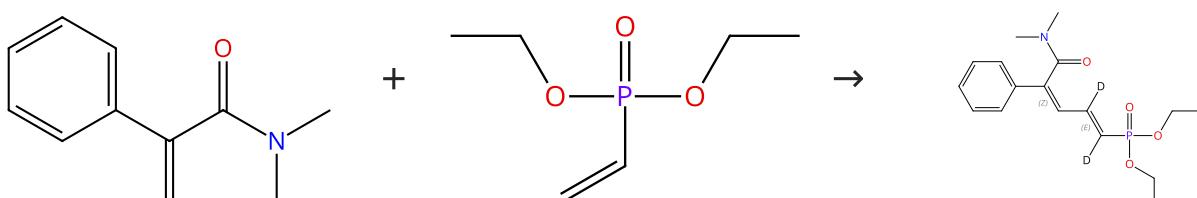
**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

Scheme 221 (1 Reaction)

Steps: 1 Yield: 24%



Suppliers (8)

Suppliers (75)

Double bond geometry shown

31-116-CAS-20720449

Steps: 1 Yield: 24%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ -1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl)di-, Silver tetrafluoroborate

Solvents: Ethyl acetate; 0.5 h, rt → 100 °C

**Iridium-Catalyzed Cross-Coupling Reactions of Alkenes by Hydrogen Transfer**

By: Meng, Keke; et al

Organic Letters (2019), 21(20), 8219-8224.

Experimental Protocols

**Scheme 222 (3 Reactions)**

Steps: 1 Yield: 20%



Suppliers (179)

Suppliers (143)

31-116-CAS-12247537

Steps: 1 Yield: 20%

**Synthesis and spectral analysis of benzene- d<sub>6</sub>****1.1 Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** Iridium(1+), trihydro[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](trimethylphosphine)-, 1,1,1-trifluoromethanesulfonate (1:1); 24 h, 120 °C

**Experimental Protocols**

By: Guo, Yangzhen; et al

Advanced Materials Research (Durten-Zurich, Switzerland) (2015), 1061-1062, 301-306.

31-116-CAS-6784183

Steps: 1

**H/D Exchange Processes Catalyzed by an Iridium-Pincer Complex****1.1 Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** [2-[Bis(1-methylethyl)phosphino- $\kappa P$ ]-*N*-[2-[bis(1-methylethyl)phosphino- $\kappa P$ ]-4-methylphenyl]-4-methylbenzenaminato- $\kappa N$ ]dihydroiridium

**Solvents:** Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °C

**Experimental Protocols**

By: Iluc, Vlad M.; et al

Organometallics (2012), 31(1), 39-41.

31-116-CAS-13663280

Steps: 1

**Effect of Ancillary Ligands and Solvents on H/D Exchange Reactions Catalyzed by Cp\*Ir Complexes****1.1 Reagents:** Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>

**Catalysts:** Dichloro(1,3-dihydro-1,3,4,5-tetramethyl-2-*H*-imidazol-2-ylidene)[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]iridium

**Solvents:** Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>; rt → 150 °C; 24 h, 150 °C; 150 °C → rt

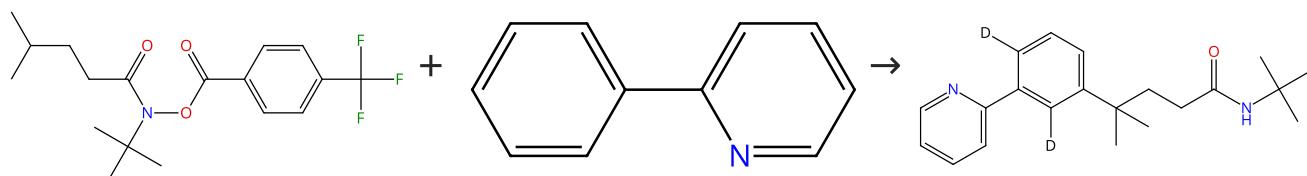
**Experimental Protocols**

By: Feng, Yuee; et al

Organometallics (2010), 29(13), 2857-2867.

**Scheme 223 (1 Reaction)**

Steps: 1 Yield: 19%



Suppliers (94)

31-614-CAS-32015499

Steps: 1 Yield: 19%

**Site-selective coupling of remote C(sp<sup>3</sup>)-H/meta-C(sp<sup>2</sup>)-H bonds enabled by Ru/photoredox dual catalysis and mechanistic studies****1.1 Reagents:** Potassium carbonate, Water-*d*<sub>2</sub>

**Catalysts:** 2,4,6-Trimethylbenzoic acid, Tris[4-(trifluoromethylphenyl)phosphine, Bis(dichloro( $\eta^6$ -*p*-cymene)ruthenium], Tris[2-(2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]iridium

**Solvents:** 1,4-Dioxane; 10 min, rt; 6 h, 60 °C

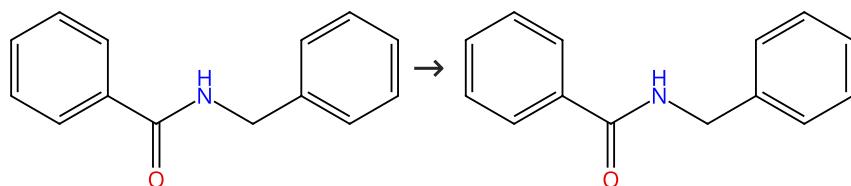
**Experimental Protocols**

By: Liu, Hong-Chao; et al

Chemical Science (2022), 13(18), 5382-5389.

## Scheme 224 (2 Reactions)

Steps: 1 Yield: 7-15%



Suppliers (84)

31-116-CAS-8997677

Steps: 1 Yield: 15%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-3427862

Steps: 1 Yield: 7%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

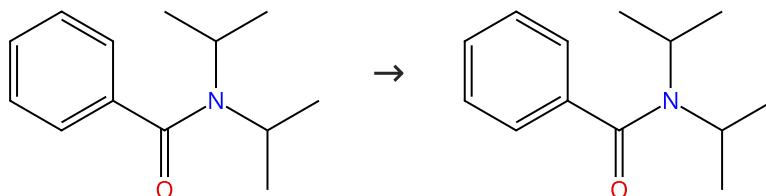
Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

## Scheme 225 (2 Reactions)

Steps: 1 Yield: 9-13%



Suppliers (57)

31-116-CAS-6266359

Steps: 1 Yield: 13%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-9813789

Steps: 1 Yield: 9%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2.25 h, 90 °C

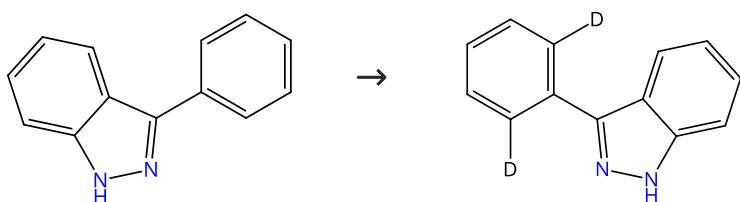
Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

## Scheme 226 (1 Reaction)

Steps: 1 Yield: 12%



Suppliers (59)

31-614-CAS-42619799

Steps: 1 Yield: 12%

1.1 **Reagents:** Acetic acid, Water-*d*<sub>2</sub>, Zinc triflate  
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-  
**Solvents:** 2,2,2-Trifluoroethanol; 4 h, 100 °C

1.2 **Reagents:** Water

Experimental Protocols

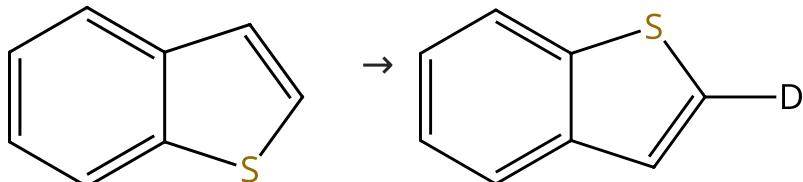
Divergent Synthesis of (CF<sub>3</sub>)-Indazolo[3,2-*a*]Isoquinolines with Potent Photophysical Property and Anticancer Activity from 3-Aryl-1H-Indazoles and Sulfoxonium Ylides

By: Zhou, Qianting; et al

Advanced Synthesis &amp; Catalysis (2024), 366(24), 5190-5196.

## Scheme 227 (2 Reactions)

Steps: 1 Yield: 9%



Suppliers (99)

Supplier (1)

31-116-CAS-20514088

Steps: 1 Yield: 9%

1.1 **Reagents:** Pivalic acid, Water-*d*<sub>2</sub>, Silver oxide (Ag<sub>2</sub>O)  
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver tetrafluoroborate  
**Solvents:** 1,2-Dichloroethane; 2 h, 80 °C

C2/C4 Regioselective Heteroarylation of Indoles by Tuning C-H Metalation Modes

By: Chen, Shuyou; et al

ACS Catalysis (2019), 9(7), 6372-6379.

31-116-CAS-19234896

Steps: 1

Iridium-catalyzed oxidative Ar-H/Ar-H cross-coupling of primary benzamides with thiophenes

1.1 **Reagents:** Water-*d*<sub>2</sub>, Silver oxide (Ag<sub>2</sub>O)  
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-  
**Solvents:** 1,1,1,3,3-Hexafluoro-2-propanol; 1 h, 120 °C

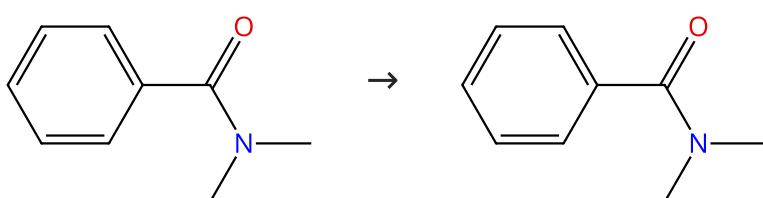
By: Tan, Guangying; et al

Organic Chemistry Frontiers (2018), 5(20), 2930-2933.

Experimental Protocols

## Scheme 228 (1 Reaction)

Steps: 1 Yield: 4%

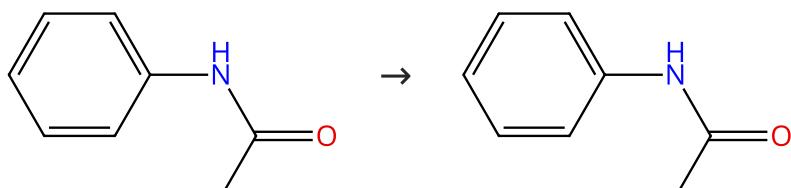


Suppliers (75)

|                    |                    |  |
|--------------------|--------------------|--|
| 31-116-CAS-8674201 | Steps: 1 Yield: 4% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |
|--------------------|--------------------|--|

Scheme 229 (3 Reactions)

Steps: 1 Yield: 3%



Suppliers (108)

|                    |                    |  |
|--------------------|--------------------|--|
| 31-116-CAS-1478152 | Steps: 1 Yield: 3% | Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates<br>By: McAuley, B.; et al<br>Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(13), 1191-1204. |
|--------------------|--------------------|--|

|                        |          |   |
|------------------------|----------|---|
| 31-614-CAS-28995192    | Steps: 1 | Synthesis of oxindole from acetanilide via Ir(III)-catalyzed C-H carbenoid functionalization<br>By: Patel, Pitambar; et al<br>Chemical Communications (Cambridge, United Kingdom) (2017), 53(2), 443-446. |
| Experimental Protocols |          |   |

|                        |          |   |
|------------------------|----------|---|
| 31-614-CAS-28433112    | Steps: 1 | Direct Access to Indoles by Ir <sup>III</sup> -Catalyzed C-H Functionalization of Acetanilides with Diazo Compounds<br>By: Patel, Pitambar; et al<br>European Journal of Organic Chemistry (2017), 2017(16), 2272-2279. |
| Experimental Protocols |          |   |

|   |          |
|---|----------|
| Scheme 230 (1 Reaction)   | Steps: 1 |
| <p>The reaction scheme shows the deuteration of acetanilide. The reactant is acetanilide, which has a benzene ring attached to an acetyl group (-CH<sub>3</sub>-CO-) and an amino group (-NH<sub>2</sub>). An arrow points to the product, which is deuterated acetanilide, where the amino hydrogen has been replaced by a deuterium atom (-NH-D).</p> |          |

Suppliers (103)

31-116-CAS-5571399

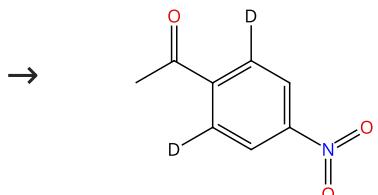
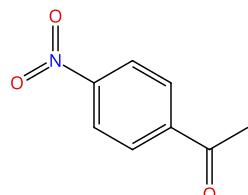
Steps: 1

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
 (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane



Suppliers (83)

Steps: 1

31-116-CAS-1575137

Steps: 1

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

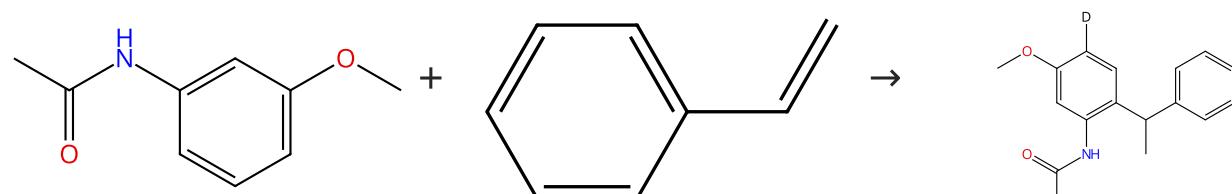
By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
 (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

Scheme 232 (1 Reaction)

Steps: 1



Suppliers (66)

Suppliers (122)

31-085-CAS-8782456

Steps: 1

**Branch-selective alkene hydroarylation by cooperative destabilization: iridium-catalyzed ortho-alkylation of acetan ilides**

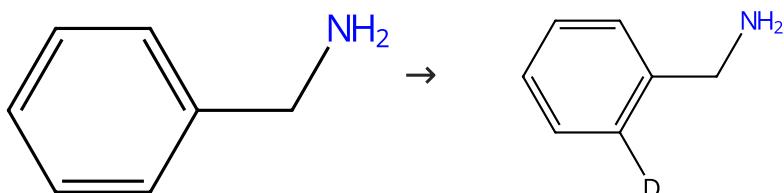
By: Crisenza, Giacomo E. M.; et al

Angewandte Chemie, International Edition (2015), 54(49), 14866-14870.

Experimental Protocols

Scheme 233 (1 Reaction)

Steps: 1



Suppliers (87)

31-116-CAS-1410310

Steps: 1

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

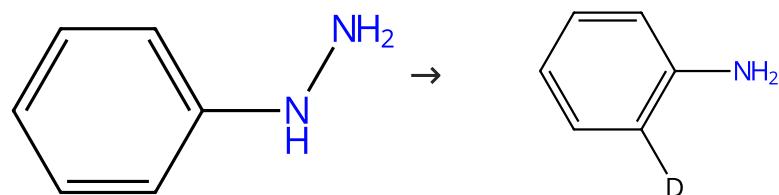
By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
 (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

Scheme 234 (1 Reaction)

Steps: 1



Suppliers (70)

Supplier (1)

31-116-CAS-217772

Steps: 1

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

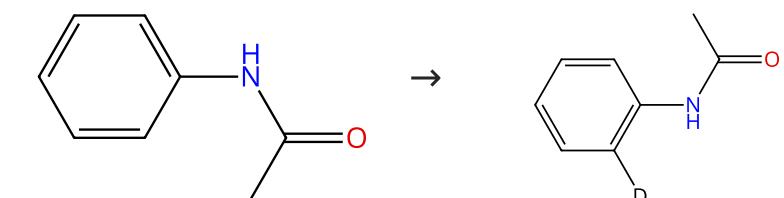
By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
 (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

Scheme 235 (1 Reaction)

Steps: 1



Suppliers (108)

Supplier (2)

31-116-CAS-6981886

Steps: 1

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

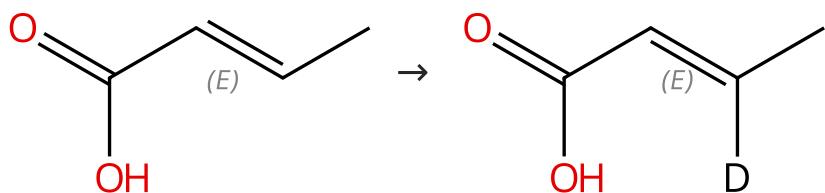
By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
 (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

Scheme 236 (1 Reaction)

Steps: 1



Double bond geometry shown

Double bond geometry shown

Suppliers (81)

31-116-CAS-10385618

Steps: 1

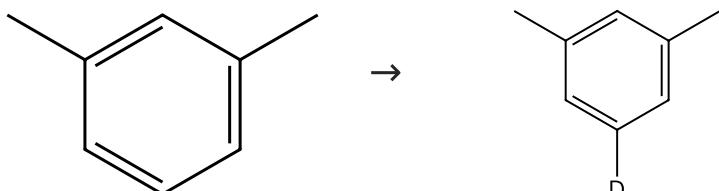
**Iridium-catalyzed H/D exchange**

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

1.1 **Reagents:** Water-*d*<sub>2</sub>**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium**Solvents:** Dimethylacetamide; 4 h, 90 °C; 90 °C → rt1.2 **Reagents:** Hydrochloric acid**Solvents:** Water; acidified, rt**Scheme 237** (1 Reaction)

Steps: 1



Suppliers (104)

31-116-CAS-13175781

Steps: 1

**H/D Exchange Processes Catalyzed by an Iridium-Pincer Complex**

By: Iluc, Vlad M.; et al

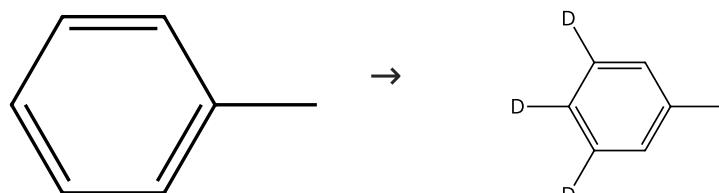
Organometallics (2012), 31(1), 39-41.

1.1 **Reagents:** Water-*d*<sub>2</sub>**Catalysts:** [2-[Bis(1-methylethyl)phosphino- $\kappa P$ ]-*N*-[2-[bis(1-methylethyl)phosphino- $\kappa P$ ]-4-methylphenyl]-4-methylbenzenaminato- $\kappa N$ ]dihydroiridium**Solvents:** Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °C

Experimental Protocols

**Scheme 238** (1 Reaction)

Steps: 1



Suppliers (301)

31-116-CAS-8910311

Steps: 1

**H/D Exchange Processes Catalyzed by an Iridium-Pincer Complex**

By: Iluc, Vlad M.; et al

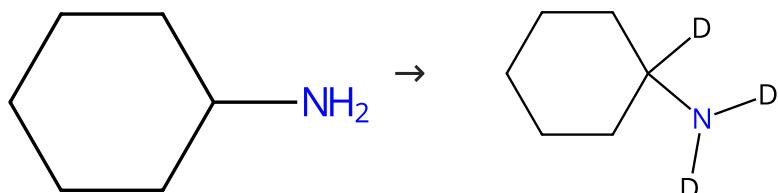
Organometallics (2012), 31(1), 39-41.

1.1 **Reagents:** Water-*d*<sub>2</sub>**Catalysts:** [2-[Bis(1-methylethyl)phosphino- $\kappa P$ ]-*N*-[2-[bis(1-methylethyl)phosphino- $\kappa P$ ]-4-methylphenyl]-4-methylbenzenaminato- $\kappa N$ ]dihydroiridium**Solvents:** Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °C

Experimental Protocols

**Scheme 239** (1 Reaction)

Steps: 1



Suppliers (84)

31-614-CAS-32680407

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: 2,4,6-Tris(1-methylethyl)benzenethiol, Iridium(1+), [4,4'-bis(trifluoromethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl- $\kappa N$ ]phenyl- $\kappa C$ ]-, hexafluorophosphate(1-) (1:1)

Solvents: Acetonitrile-*d*<sub>3</sub>; 20 h, rt

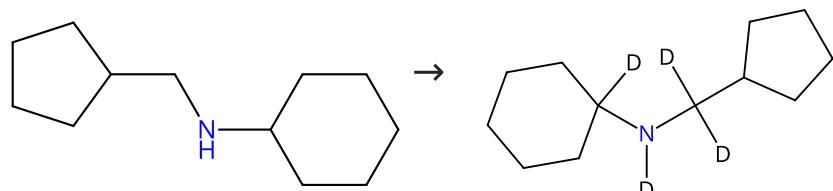
## Mechanistic Investigation and Optimization of Photoredox Anti-Markovnikov Hydroamination

By: Qin, Yangzhong; et al

Journal of the American Chemical Society (2021), 143(27), 10232-10242.

Scheme 240 (1 Reaction)

Steps: 1



Suppliers (4)

31-614-CAS-32680410

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: 2,4,6-Tris(1-methylethyl)benzenethiol, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1, \kappa N^1$ ']bis[3,5-difluoro-2-(5-methyl-2-pyridinyl- $\kappa N$ )phenyl- $\kappa C$ ]-, (OC-6-33), hexafluorophosphate(1-) (1:1)

Solvents: Acetonitrile-*d*<sub>3</sub>; 20 h, rt

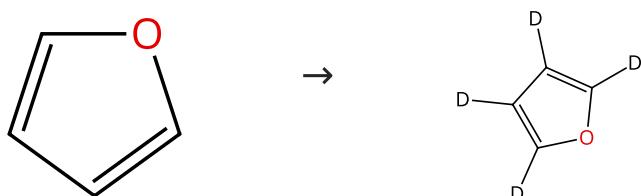
## Mechanistic Investigation and Optimization of Photoredox Anti-Markovnikov Hydroamination

By: Qin, Yangzhong; et al

Journal of the American Chemical Society (2021), 143(27), 10232-10242.

Scheme 241 (1 Reaction)

Steps: 1



Suppliers (44)

Suppliers (30)

31-116-CAS-1913740

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: [2-[Bis(1-methylethyl)phosphino- $\kappa P$ ]-*N*-[2-[bis(1-methylethyl)phosphino- $\kappa P$ ]-4-methylphenyl]-4-methylbenz enaminato- $\kappa N$ ]dihydroiridium

Solvents: Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °C

## H/D Exchange Processes Catalyzed by an Iridium-Pincer Complex

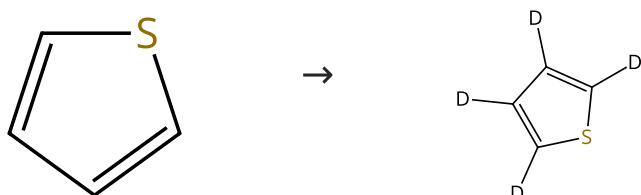
By: Iluc, Vlad M.; et al

Organometallics (2012), 31(1), 39-41.

Experimental Protocols

Scheme 242 (1 Reaction)

Steps: 1



Suppliers (80)

Suppliers (26)

31-116-CAS-4034828

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [2-[Bis(1-methylethyl)phosphino- $\kappa P$ ]-*N*-[2-[bis(1-methylethyl)phosphino- $\kappa P$ ]-4-methylphenyl]-4-methylbenzenaminato- $\kappa N$ ]dihydroiridiumSolvents: Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °C

Experimental Protocols

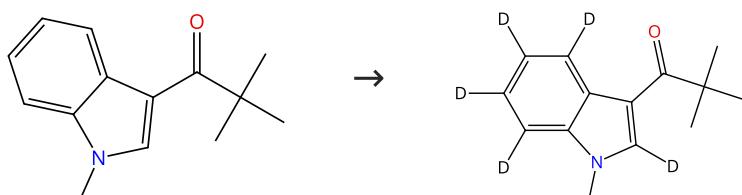
## H/D Exchange Processes Catalyzed by an Iridium-Pincer Complex

By: Iluc, Vlad M.; et al

Organometallics (2012), 31(1), 39-41.

Scheme 243 (1 Reaction)

Steps: 1



Suppliers (32)

31-614-CAS-36670259

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-*N*[(trifluoromethyl)sulfonyl- $\kappa O$ ]methanesulfonamido- $\kappa O$ ]silver

Solvents: 1,2-Dichloroethane; 23 h, rt → 115 °C

Experimental Protocols

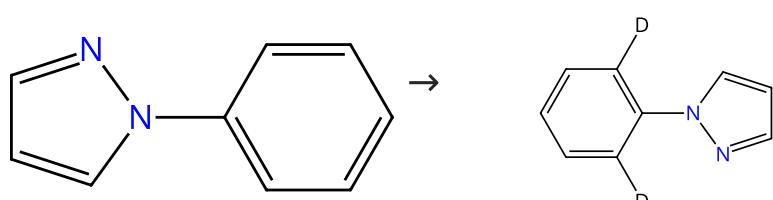
## Iridium catalyzed C2 site-selective methylation of indoles using a pivaloyl directing group through weak chelation-assistance

By: Kathiravan, Subban; et al

RSC Advances (2023), 13(17), 11291-11295.

Scheme 244 (1 Reaction)

Steps: 1



Suppliers (90)

31-116-CAS-6618357

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

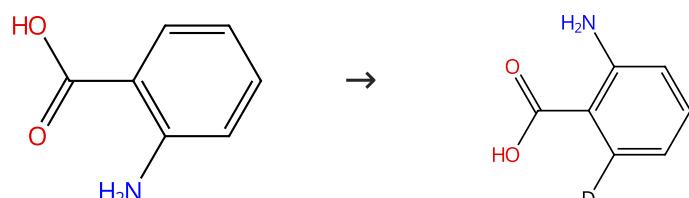
## The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 245 (1 Reaction)

Steps: 1



Suppliers (48)

31-116-CAS-13186142

Steps: 1

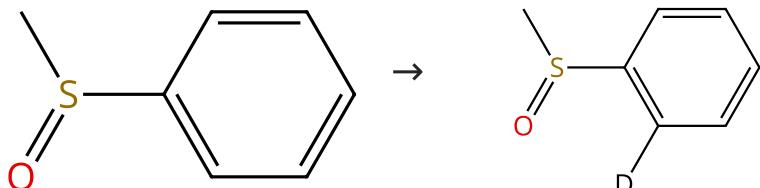
**Hydrogen isotope labelling using iridium(I) dionates**1.1 **Reagents:** Water- $d_2$ **Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium**Solvents:** Dimethylacetamide; 2 min, 130 °C

By: Lockley, W. J. S.

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

**Scheme 246 (1 Reaction)**

Steps: 1



Suppliers (82)

31-116-CAS-10926610

Steps: 1

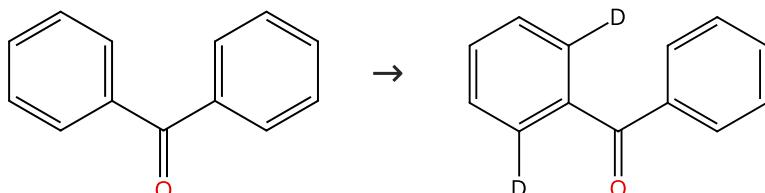
**The scope and limitations of deuteration mediated by Crabtree's catalyst**1.1 **Reagents:** Water- $d_2$ **Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**Solvents:** Dichloromethane

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 247 (1 Reaction)**

Steps: 1



Suppliers (142)

31-116-CAS-5846274

Steps: 1

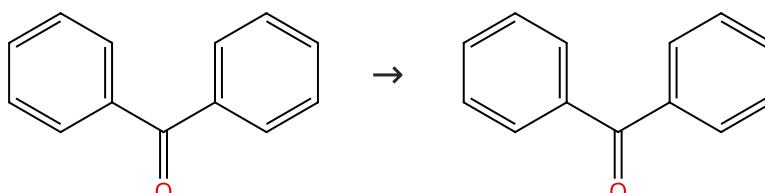
**The scope and limitations of deuteration mediated by Crabtree's catalyst**1.1 **Reagents:** Water- $d_2$ **Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**Solvents:** Dichloromethane

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 248 (1 Reaction)**

Steps: 1



Suppliers (142)

31-614-CAS-25954739

Steps: 1

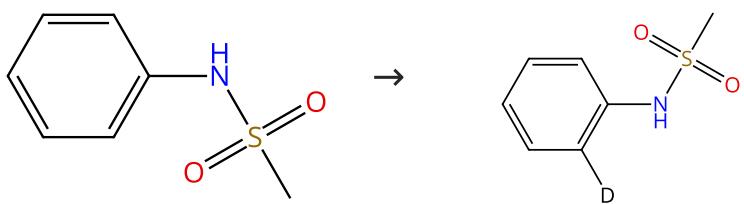
**Iridium-catalyzed H/D exchange**1.1 **Reagents:** Water- $d_2$ **Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentanedionato- $\kappa O^2,\kappa O^4$ )iridium**Solvents:** Dimethylacetamide; 2 h, 90 °C

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

**Scheme 249 (1 Reaction)**

Steps: 1


 Suppliers (75)

31-116-CAS-11529925

Steps: 1

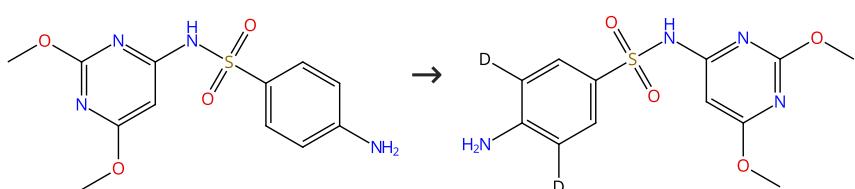
1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)- (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 250 (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*<sub>2</sub>; 3 h, 80 °C**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.

## Experimental Protocols

**Scheme 251 (1 Reaction)**

Steps: 1


 Suppliers (120)
 Suppliers (7)

31-614-CAS-33408376

Steps: 1

**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**

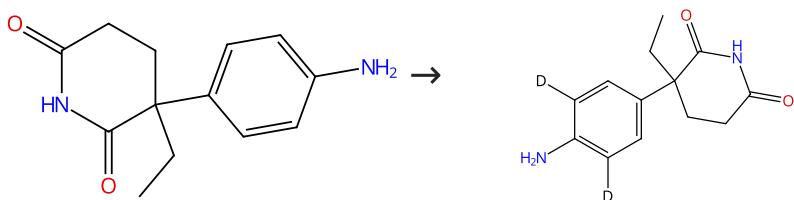
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

## Experimental Protocols

**Scheme 252 (1 Reaction)**

Steps: 1



Suppliers (73)

31-116-CAS-21649683

Steps: 1

1.1 Reagents: Deuterium

Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)

Solvents: Tetrahydrofuran, Water-*d*<sub>2</sub>; 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

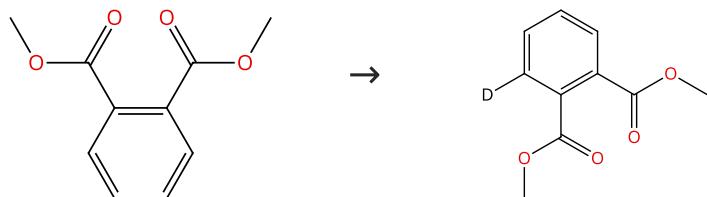
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

**Scheme 253 (1 Reaction)**

Steps: 1



Suppliers (124)

31-116-CAS-10262772

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

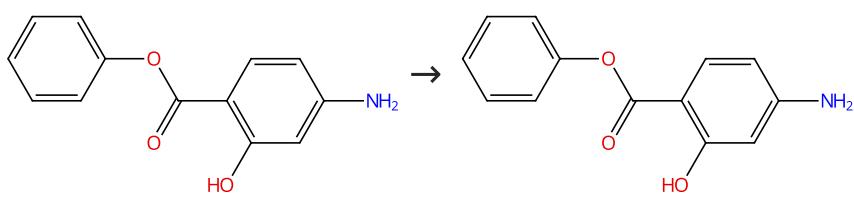
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 254 (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*<sub>2</sub>; 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

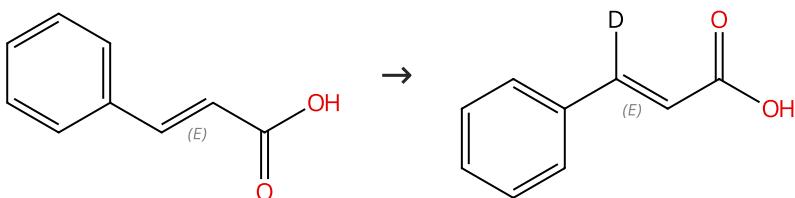
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

Scheme 255 (1 Reaction)

Steps: 1



Double bond geometry shown

Double bond geometry shown

Suppliers (164)

31-116-CAS-12517054

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentaned ionato- $\kappa O^2,\kappa O^4$ )iridium  
**Solvents:** Dimethylacetamide; 2 h, 90 °C; 90 °C → rt
- 1.2 **Reagents:** Hydrochloric acid  
**Solvents:** Water; acidified, rt

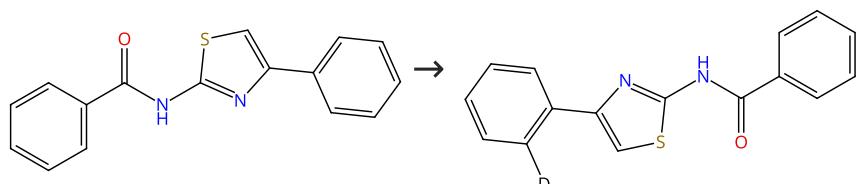
**Iridium-catalyzed H/D exchange**

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

Scheme 256 (1 Reaction)

Steps: 1



Suppliers (15)

31-614-CAS-27554142

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

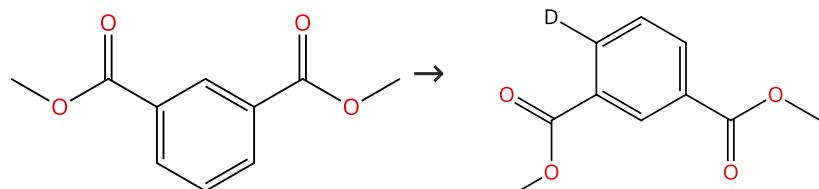
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 257 (1 Reaction)

Steps: 1



Suppliers (87)

31-116-CAS-1142710

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** 1,1-Dichloroacetone

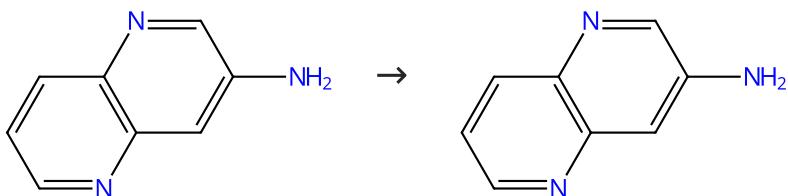
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 258 (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<sub>2</sub>, 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

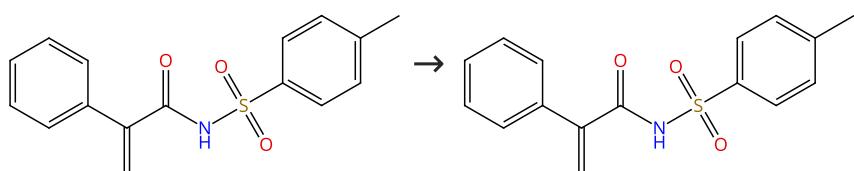
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

## Scheme 259 (1 Reaction)

Steps: 1



31-614-CAS-26575627

Steps: 1

1.1 Catalysts: Bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxyd

iridium

Solvents: Water-d<sub>2</sub>; 2 h, rt → 70 °C**Stereoselective and Atom-Economic Alkenyl C-H Allylation/Alkenylation in Aqueous Media by Iridium Catalysis**

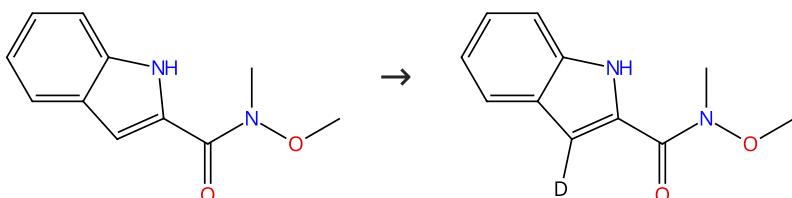
By: Huang, Yinhua; et al

Journal of Organic Chemistry (2020), 85(11), 7225-7237.

Experimental Protocols

## Scheme 260 (1 Reaction)

Steps: 1



Suppliers (53)

31-116-CAS-7653762

Steps: 1

1.1 Reagents: Water-d<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-

(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

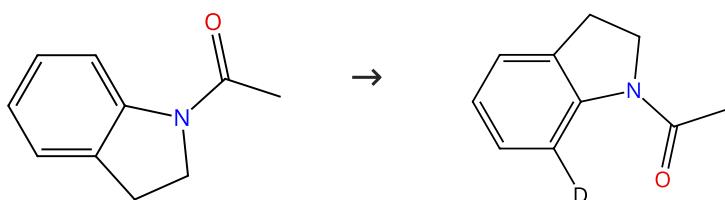
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 261 (1 Reaction)

Steps: 1



Suppliers (79)

31-116-CAS-3544924

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-*N*-[(trifluoromethyl)sulfonyl- $\kappa O$ ]methanesulfonamidato- $\kappa O$ ]silver

**Solvents:** 1,2-Dichloroethane; 8 h, 40 °C

Ir<sup>III</sup>-Catalyzed Direct C-7 Amidation of Indolines with Sulfonyl, Acyl, and Aryl Azides at Room Temperature

By: Hou, Wei; et al

European Journal of Organic Chemistry (2015), 2015(2), 395-400.

## Experimental Protocols

## Scheme 262 (1 Reaction)

Steps: 1



31-614-CAS-24691505

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>, BOC-L-Proline

**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver tetrafluoroborate

**Solvents:** 1,1,1,3,3,3-Hexafluoro-2-propanol; rt → 60 °C; 30 min, 60 °C

## Iridium(III)-catalyzed C(3)-H Alkylation of Isoquinolines via Metal Carbene Migratory Insertion

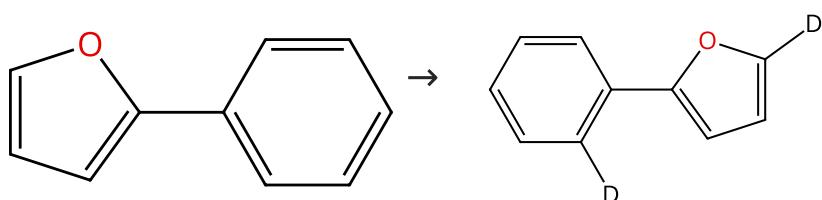
By: Jha, Neha; et al

Organic Letters (2021), 23(22), 8694-8698.

## Experimental Protocols

## Scheme 263 (1 Reaction)

Steps: 1



Suppliers (67)

31-116-CAS-6946480

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

**Solvents:** Dichloromethane

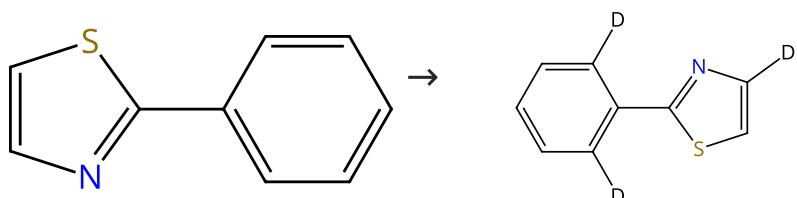
## The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 264 (1 Reaction)

Steps: 1



Suppliers (79)

31-116-CAS-13333593

Steps: 1

1.1 Reagents: Water- $d_2$ Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

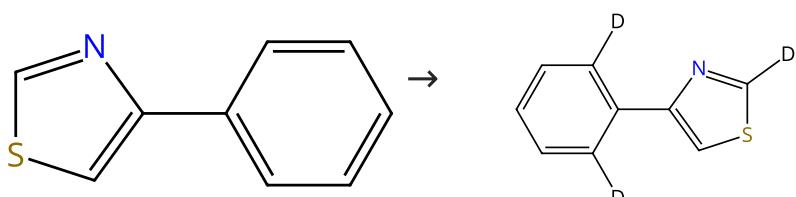
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 265 (1 Reaction)

Steps: 1



Suppliers (62)

31-116-CAS-15464829

Steps: 1

1.1 Reagents: Water- $d_2$ Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

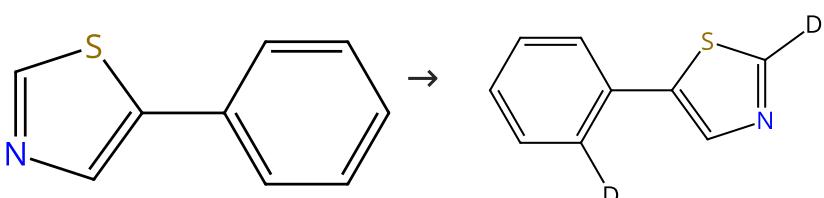
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 266 (1 Reaction)

Steps: 1



Suppliers (62)

31-116-CAS-2072193

Steps: 1

1.1 Reagents: Water- $d_2$ Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 267 (1 Reaction)

Steps: 1



Suppliers (58)

31-116-CAS-23535322

Steps: 1

**1.1 Reagents:** Silver carbonate, Water-*d*<sub>2</sub>  
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-*N*-[(trifluoromethyl)sulfonyl- $\kappa$ O]methanesulfonamido- $\kappa$ O]silver  
**Solvents:** 1,2-Dichloroethane; 120 °C

**Tandem Iridium-Catalyzed Decarbonylative C-H Activation of Indole: Sacrificial Electron-Rich Ketone-Assisted Bis-arylsulfenylation**

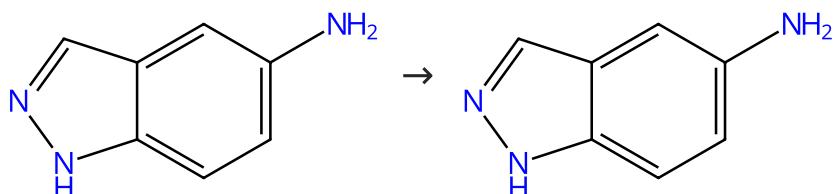
By: Kathiravan, Subban; et al

Organic Letters (2021), 23(9), 3331-3336.

Experimental Protocols

## Scheme 268 (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*<sub>2</sub>; 3 h, 80 °C

**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

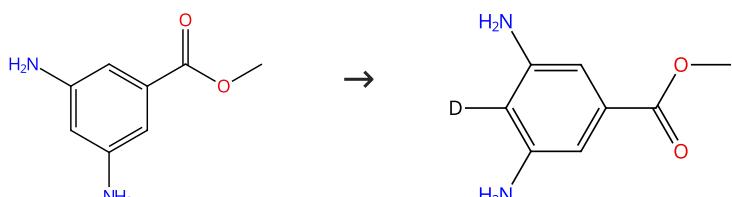
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

## Scheme 269 (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*<sub>2</sub>; 3 h, 80 °C

**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

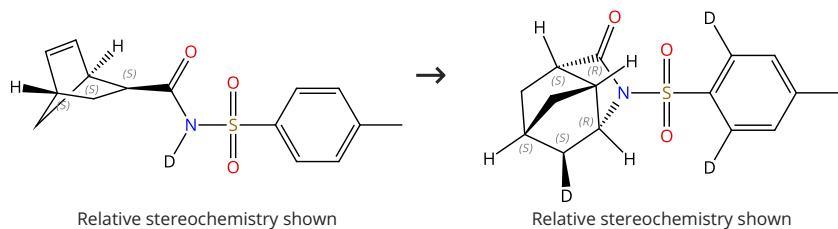
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

**Scheme 270 (1 Reaction)**

Steps: 1



31-116-CAS-16104377

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *N,N*-Dimethylbenzylamine, Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]diiridium

Solvents: 1,2-Dichloroethane; 20 h, 80 °C

**Asymmetric Cyclization of N-Sulfonyl Alkenyl Amides Catalyzed by Iridium/Chiral Diene Complexes**

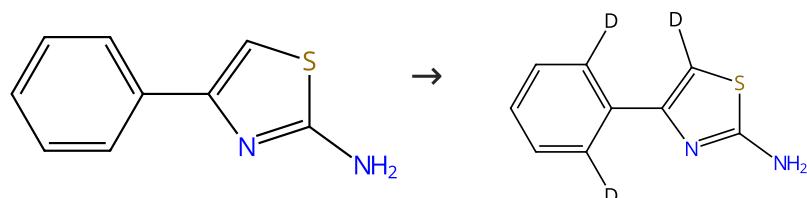
By: Nagamoto, Midori; et al

Organic Letters (2016), 18(18), 4474-4477.

Experimental Protocols

**Scheme 271 (1 Reaction)**

Steps: 1



Suppliers (106)

31-116-CAS-4278585

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

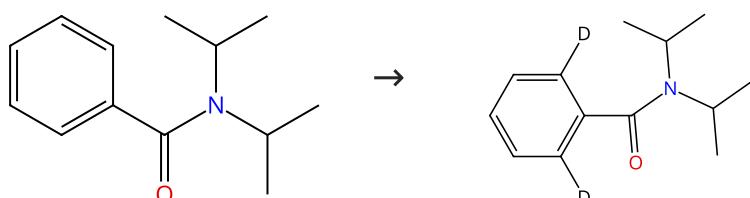
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 272 (1 Reaction)**

Steps: 1



Suppliers (57)

31-614-CAS-29109652

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

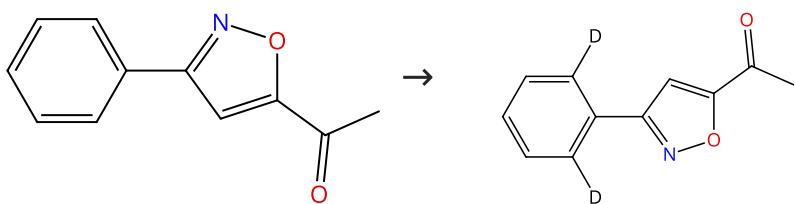
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 273 (1 Reaction)**

Steps: 1


[Suppliers \(53\)](#)
**31-116-CAS-11191551**

Steps: 1

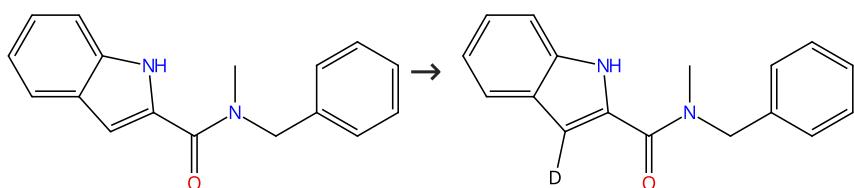
**1.1 Reagents:** Water-*d*<sub>2</sub>**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**Solvents:** Dichloromethane**The scope and limitations of deuteration mediated by  
Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 274 (1 Reaction)**

Steps: 1


[Suppliers \(6\)](#)
**31-116-CAS-11918533**

Steps: 1

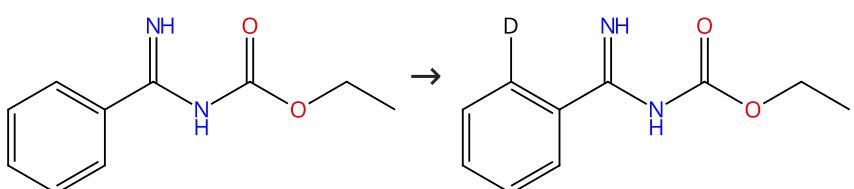
**1.1 Reagents:** Water-*d*<sub>2</sub>**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**Solvents:** Dichloromethane**The scope and limitations of deuteration mediated by  
Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 275 (1 Reaction)**

Steps: 1


[Suppliers \(6\)](#)
**31-116-CAS-14654796**

Steps: 1

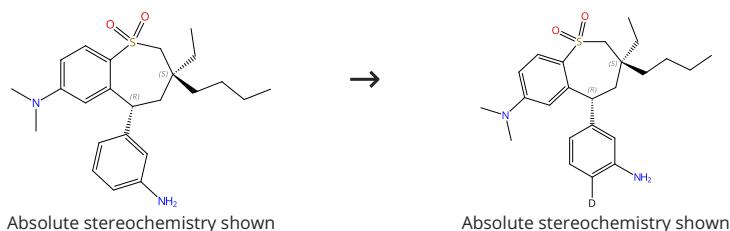
**1.1 Reagents:** Water-*d*<sub>2</sub>**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**Solvents:** Dichloromethane**The scope and limitations of deuteration mediated by  
Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 276 (1 Reaction)**

Steps: 1



31-116-CAS-21649688

Steps: 1

## 1.1 Reagents: Deuterium

Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)

Solvents: Tetrahydrofuran, Water-*d*<sub>2</sub>; 3 h, 80 °C

## Experimental Protocols

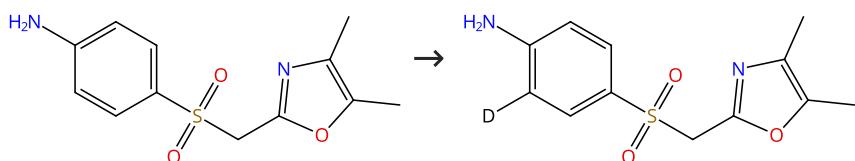
**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

**Scheme 277 (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*<sub>2</sub>; 3 h, 80 °C

## Experimental Protocols

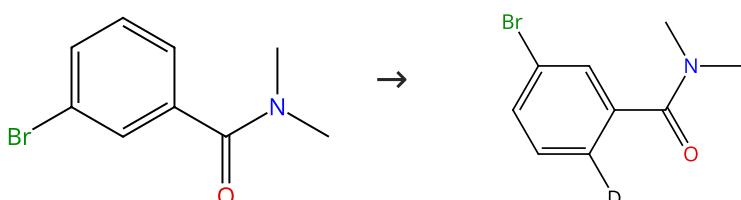
**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

**Scheme 278 (1 Reaction)**

Steps: 1



Suppliers (67)

Supplier (1)

31-116-CAS-5899889

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

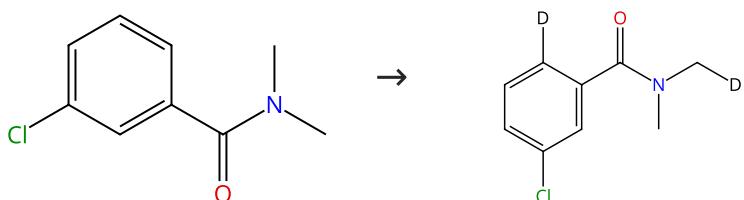
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 279 (1 Reaction)

Steps: 1



Suppliers (49)

31-116-CAS-15033700

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

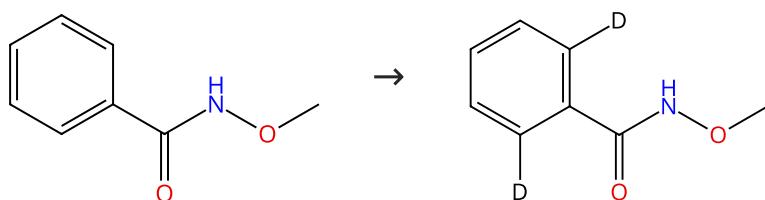
The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 280 (1 Reaction)

Steps: 1



Suppliers (49)

31-116-CAS-15865637

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-*N*-[(trifluoromethyl)sulfonyl]-κ*O*]methanesulfonamido-κ*O*]silver

Solvents: 1,2-Dichloroethane; 12 h, 25 °C

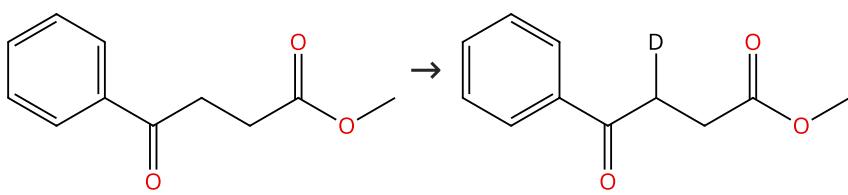
Ir(III)-Catalyzed Carbenoid Functionalization of Benzamides: Synthesis of N-Methoxyisoquinolinediones and N-Methoxyisoquinolinones

By: Phatake, Ravindra S.; et al

Organic Letters (2016), 18(12), 2828-2831.

Scheme 281 (1 Reaction)

Steps: 1



Suppliers (81)

31-116-CAS-22273632

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Quinuclidine, Tetrabutylammonium dihydrogen phosphate, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ<sup>1</sup>,κ<sup>1</sup>]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κ*N*]phenyl-κ*C*]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

Solvents: Acetonitrile; 48 h, 40 °C

Photoredox-Catalyzed Isomerization of Highly Substituted Allylic Alcohols by C-H Bond Activation

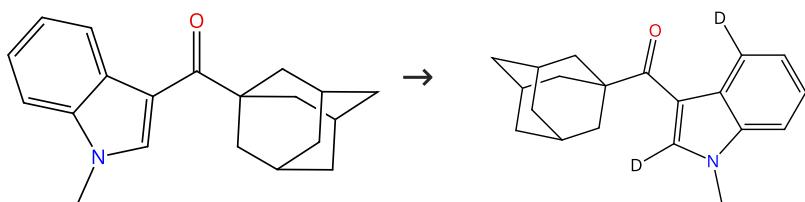
By: Guo, Kai; et al

Angewandte Chemie, International Edition (2020), 59(28), 11660-11668.

Experimental Protocols

**Scheme 282 (1 Reaction)**

Steps: 1



31-116-CAS-23535577

Steps: 1

1.1 Reagents: Silver carbonate, Water-*d*<sub>2</sub>Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-*N*[(trifluoromethyl)sulfonyl- $\kappa O$ ]methanesulfonamidato- $\kappa O$ ]silver

Solvents: 1,2-Dichloroethane; 120 °C

**Tandem Iridium-Catalyzed Decarbonylative C-H Activation of Indole: Sacrificial Electron-Rich Ketone-Assisted Bis-arylsulfonylation**

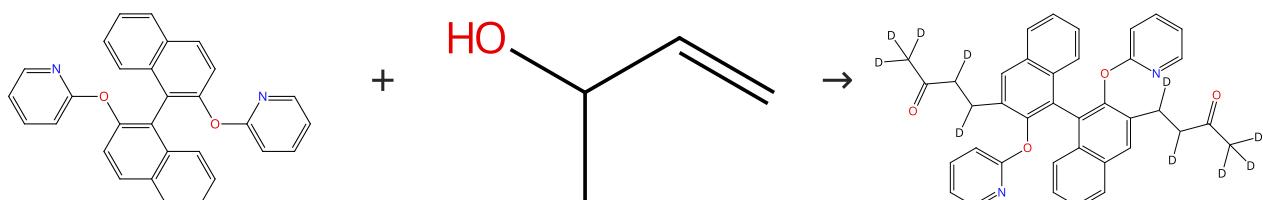
By: Kathiravan, Subban; et al

Organic Letters (2021), 23(9), 3331-3336.

Experimental Protocols

**Scheme 283 (1 Reaction)**

Steps: 1



🛒 Suppliers (70)

31-614-CAS-31118817

Steps: 1

1.1 Reagents: Sodium acetate, Silver acetate, Silver triflate

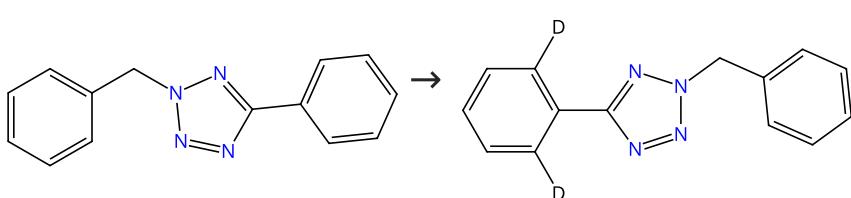
Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-Solvents: 2,2,2-Trifluoroethanol, Water-*d*<sub>2</sub>; 10 h, 140 °C**Iridium(III)-catalyzed two-fold C-H alkylation of BINOLs with allyl alcohols**

By: Liu, Hao; et al

Organic Chemistry Frontiers (2022), 9(2), 471-475.

**Scheme 284 (1 Reaction)**

Steps: 1



🛒 Suppliers (13)

31-116-CAS-6280859

Steps: 1

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

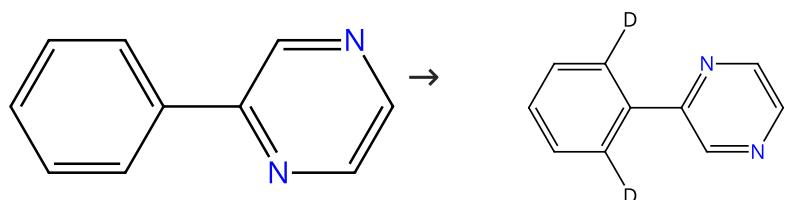
Tetrahedron (2001), 57(46), 9487-9497.

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

## Scheme 285 (1 Reaction)

Steps: 1



Suppliers (34)

31-116-CAS-12670355

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

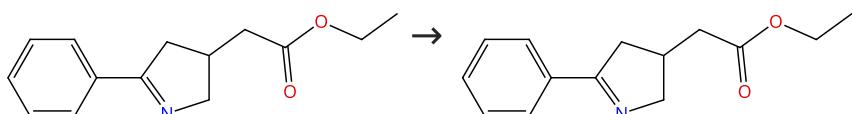
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 286 (1 Reaction)

Steps: 1



31-614-CAS-39390569

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyri-  
dine-κN<sup>1</sup>,κN<sup>1</sup>']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-  
pyridinyl-κN]phenyl-κC]-, (OC-6-33)-, hexafluorophosphate(1-)  
(1:1)

Solvents: 1,2-Dichloroethane; 48 h, rt

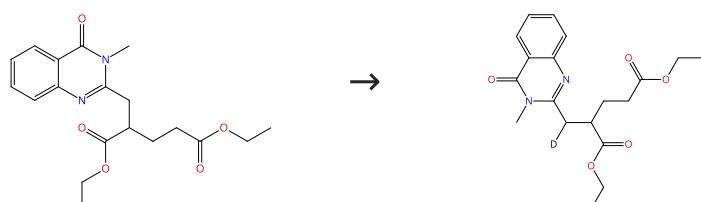
Radical-triggered base-free 1,3-C → C migrations: chemodi-  
vergent synthesis of cyclic imines from N- allyl enamines

By: Zheng, Baihui; et al

Organic Chemistry Frontiers (2024), 11(2), 500-507.

## Scheme 287 (1 Reaction)

Steps: 1



31-614-CAS-41631558

Steps: 1

1.1 Reagents: Boron trifluoride etherate, Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyri-  
dine-κN<sup>1</sup>,κN<sup>1</sup>']bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-  
pyridinyl-κN]phenyl-κC]-, (OC-6-33)-, hexafluorophosphate(1-)  
(1:1)

Solvents: Acetonitrile; 10 h, rt

Chemoselective Hydroheterarylation of Alkenes via Photoredox-Neutral Proton- and BF<sub>3</sub>-Mediated Electron Transfer

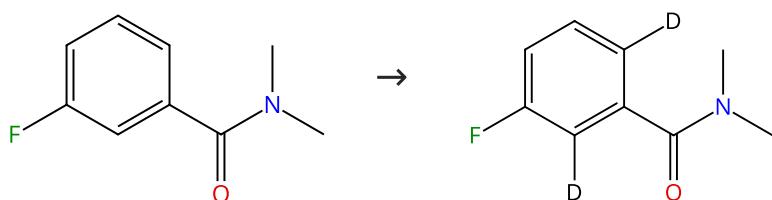
By: Wan, Xiaoyuan; et al

Organic Letters (2024), 26(36), 7707-7712.

## Experimental Protocols

**Scheme 288 (1 Reaction)**

Steps: 1



Suppliers (9)

31-116-CAS-14202444

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

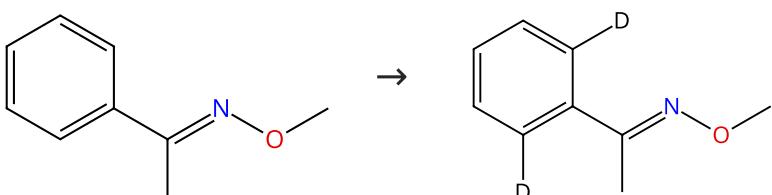
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 289 (1 Reaction)**

Steps: 1



Suppliers (4)

31-116-CAS-10116362

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

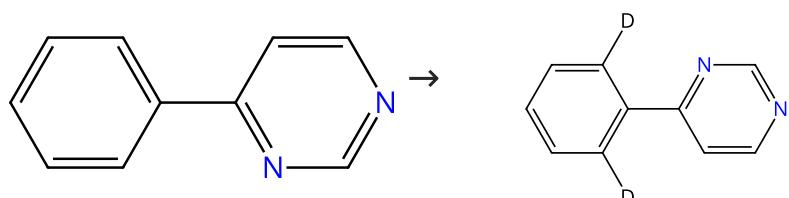
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 290 (1 Reaction)**

Steps: 1



Suppliers (61)

31-116-CAS-14806349

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

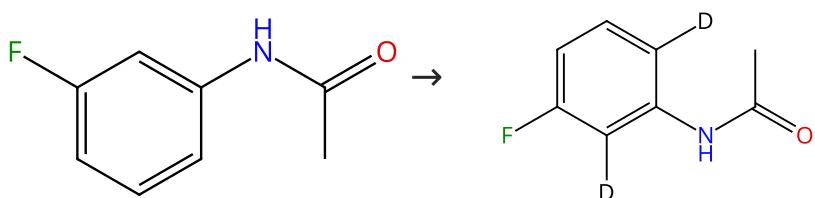
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 291 (1 Reaction)

Steps: 1



Suppliers (71)

31-116-CAS-4522862

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, 1,1,1-trifluoromethanesulfonate (1:1), 1820981-94-9

Solvents: 1,4-Dioxane; 48 h, 120 °C

Experimental Protocols

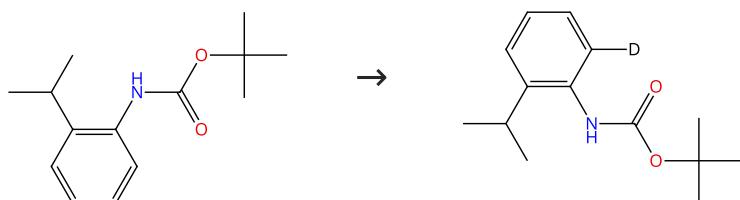
Branch-selective alkene hydroarylation by cooperative destabilization: iridium-catalyzed ortho-alkylation of acetanilides

By: Crisenza, Giacomo E. M.; et al

Angewandte Chemie, International Edition (2015), 54(49), 14866-14870.

Scheme 292 (1 Reaction)

Steps: 1



Suppliers (30)

31-116-CAS-13381149

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)-tricyclohexylphosphine-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

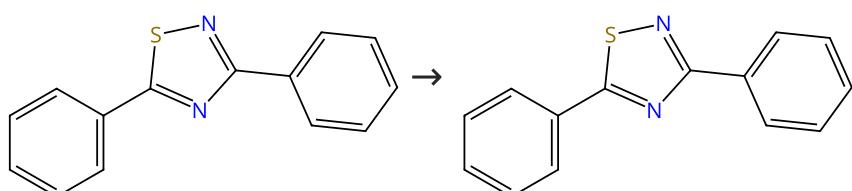
The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 293 (1 Reaction)

Steps: 1



Suppliers (3)

31-614-CAS-30294684

Steps: 1

1.1 Reagents: Acetic acid, Water-*d*<sub>2</sub>Catalysts: Cupric acetate, Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoroantimonate

Solvents: 1,2-Dichloroethane; 3 h, 120 °C

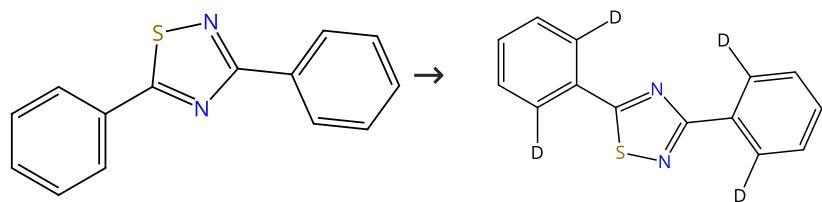
Regioselective C-C cross-coupling of 1,2,4-thiadiazoles with maleimides through iridium-catalyzed C-H activation

By: Tian, Ting; et al

Organic &amp; Biomolecular Chemistry (2019), 17(33), 7664-7668.

Scheme 294 (1 Reaction)

Steps: 1



Suppliers (3)

31-116-CAS-23730184

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Pentafluorobenzoic acid, Iridium, di- $\mu$ -chlorodiclorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoroantimonate; 3 h, 90 °C

Iridium-catalyzed regioselective C-H sulfonamidation of 1,2,4-thiadiazoles with sulfonyl azides in water

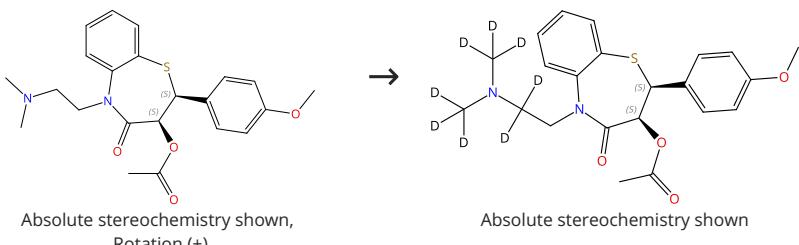
By: Cao, Xian-Ting; et al

RSC Advances (2021), 11(36), 22000-22004.

## Experimental Protocols

Scheme 295 (1 Reaction)

Steps: 1



Suppliers (44)

31-614-CAS-24525050

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: 1,1,1-Triphenylsilanethiol, Iridium(1+), [4,4'-bis(1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)

Solvents: Toluene; 6 h, 28 °C

Site-selective  $\alpha$ -C-H Functionalization of Trialkylamines via Reversible HAT-Catalysis

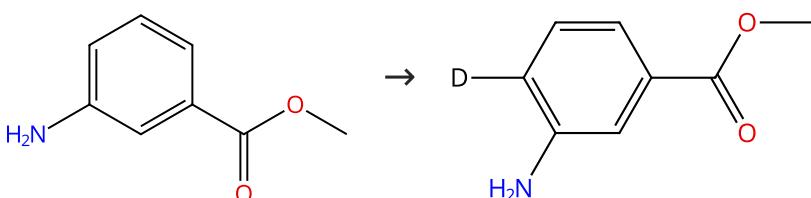
By: Shen, Yangyang; et al

Journal of the American Chemical Society (2021), 143(45), 18952-18959.

## Experimental Protocols

Scheme 296 (1 Reaction)

Steps: 1



Suppliers (101)

31-116-CAS-21649676

Steps: 1

## 1.1 Reagents: Deuterium

Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-stabilized)

Solvents: Tetrahydrofuran, Water-*d*<sub>2</sub>; 3 h, 80 °C

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

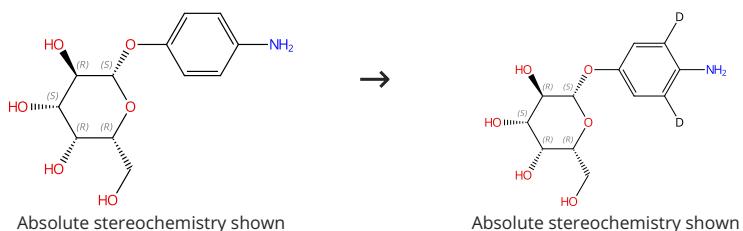
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

## Experimental Protocols

**Scheme 297 (1 Reaction)**

Steps: 1



Suppliers (62)

**31-116-CAS-21649687**

Steps: 1

**1.1 Reagents:** Deuterium**Catalysts:** Iridium (nanoparticles, N-heterocyclic carbene-stabilized)**Solvents:** Tetrahydrofuran, Water-*d*<sub>2</sub>; 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

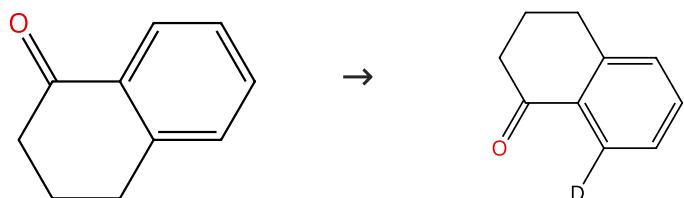
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

**Scheme 298 (1 Reaction)**

Steps: 1



Suppliers (101)

**31-116-CAS-3048868**

Steps: 1

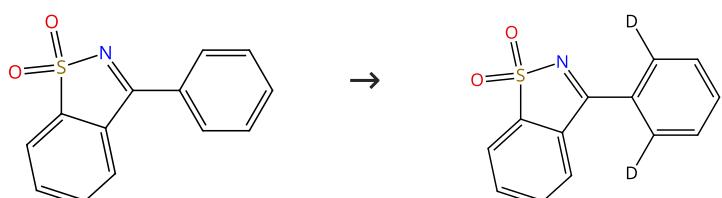
**1.1 Reagents:** Water-*d*<sub>2</sub>**Catalysts:** Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)**Solvents:** Dichloromethane**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 299 (1 Reaction)**

Steps: 1



Suppliers (30)

**31-116-CAS-24356613**

Steps: 1

**1.1 Reagents:** Water-*d*<sub>2</sub>**Catalysts:** 2-Pyridone, Di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]diiridium, Sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate**Solvents:** Toluene; 3 h, 80 °C**Iridium-Catalyzed Direct C-H Allylation of Ketimines**

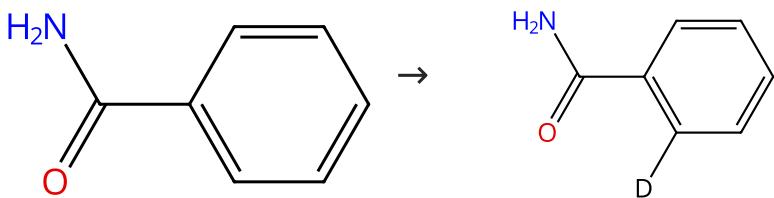
By: Yabe, Ryota; et al

Synthesis (2021), 53(17), 3051-3056.

Experimental Protocols

**Scheme 300 (1 Reaction)**

Steps: 1



Suppliers (115)

31-116-CAS-12672701

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

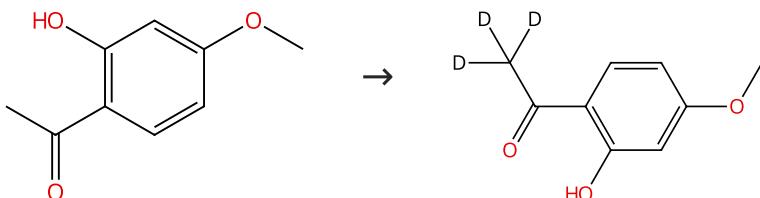
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 301 (1 Reaction)**

Steps: 1



Suppliers (108)

Supplier (1)

31-116-CAS-4134321

Steps: 1

Iridium-catalyzed H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentaned  
ionato- $\kappa O^2,\kappa O^4$ )iridium

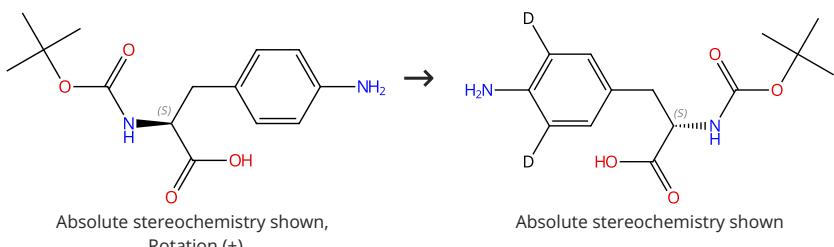
Solvents: Dimethylacetamide; 2 h, 90 °C

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

**Scheme 302 (1 Reaction)**

Steps: 1



Suppliers (90)

31-116-CAS-21649680

Steps: 1

NHC-Stabilized Iridium Nanoparticles as Catalysts in  
Hydrogen Isotope Exchange Reactions of Anilines

1.1 Reagents: Deuterium

Catalysts: Iridium (nanoparticles, N-heterocyclic carbene-  
stabilized)Solvents: Tetrahydrofuran, Water-*d*<sub>2</sub>; 3 h, 80 °C

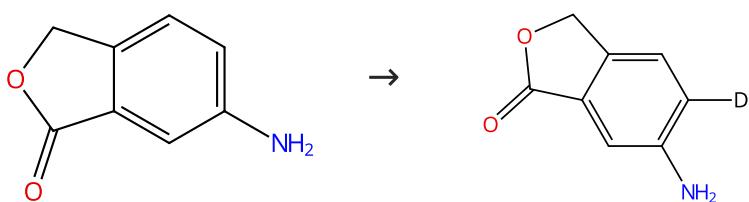
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-  
3522.

Experimental Protocols

## Scheme 303 (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*<sub>2</sub>; 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

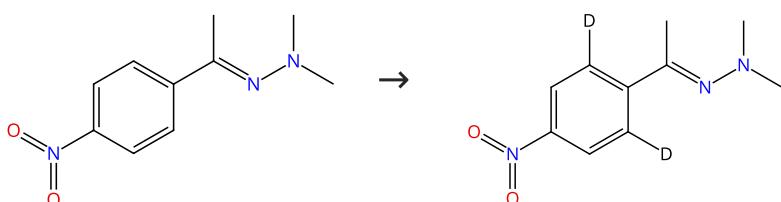
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

## Scheme 304 (1 Reaction)

Steps: 1



Suppliers (3)

31-614-CAS-30587257

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

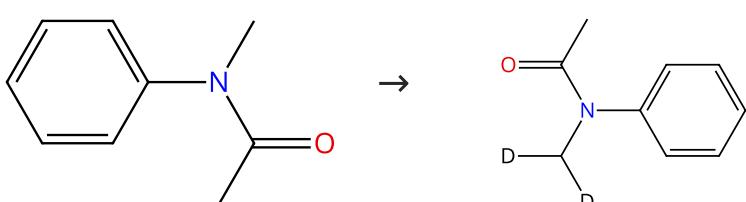
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 305 (1 Reaction)

Steps: 1



Suppliers (58)

31-116-CAS-10902680

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, 1,1'-trifluoromethanesulfonate (1:1), 1820981-94-9

Solvents: 1,4-Dioxane; 48 h, 120 °C

**Branch-selective alkene hydroarylation by cooperative destabilization: iridium-catalyzed ortho-alkylation of acetanilides**

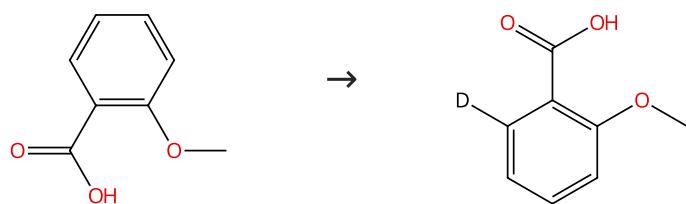
By: Crisenza, Giacomo E. M.; et al

Angewandte Chemie, International Edition (2015), 54(49), 14866-14870.

Experimental Protocols

## Scheme 306 (1 Reaction)

Steps: 1



Suppliers (108)

31-116-CAS-9036340

Steps: 1

Iridium-catalyzed H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](2,4-pentaned ionato-κO<sup>2-</sup>,κO<sup>4-</sup>)iridium

Solvents: Dimethylacetamide; 2 h, 90 °C; 90 °C → rt

1.2 Reagents: Hydrochloric acid

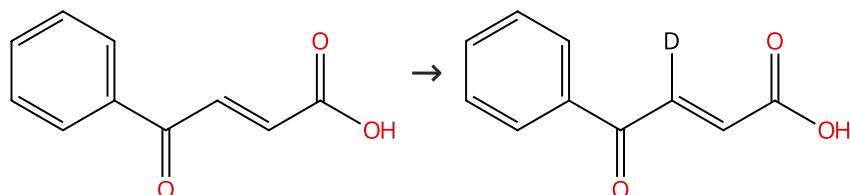
Solvents: Water; acidified, rt

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

## Scheme 307 (1 Reaction)

Steps: 1



Suppliers (61)

31-116-CAS-3380352

Steps: 1

Iridium-catalyzed H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](2,4-pentaned ionato-κO<sup>2-</sup>,κO<sup>4-</sup>)iridium

Solvents: Dimethylacetamide; 2 h, 90 °C; 90 °C → rt

1.2 Reagents: Hydrochloric acid

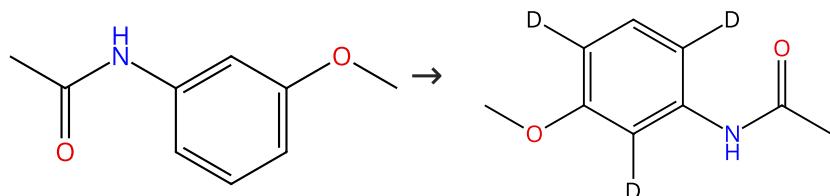
Solvents: Water; acidified, rt

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

## Scheme 308 (1 Reaction)

Steps: 1



Suppliers (66)

31-116-CAS-6655725

Steps: 1

Branch-selective alkene hydroarylation by cooperative

destabilization: iridium-catalyzed ortho-alkylation of acetan ilides

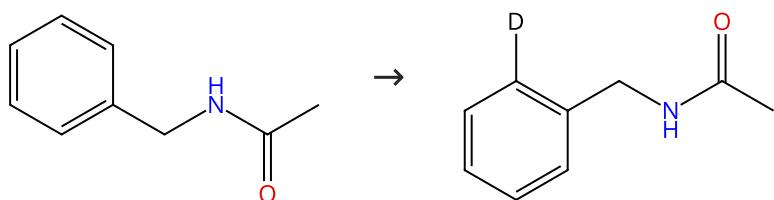
By: Crisenza, Giacomo E. M.; et al

Angewandte Chemie, International Edition (2015), 54(49), 14866-14870.

Experimental Protocols

## Scheme 309 (1 Reaction)

Steps: 1



Suppliers (80)

31-116-CAS-11352096

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

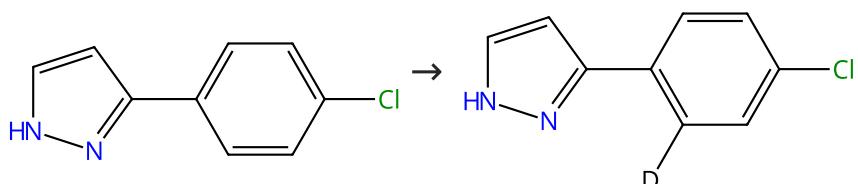
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 310 (1 Reaction)

Steps: 1



Suppliers (65)

31-116-CAS-10869528

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

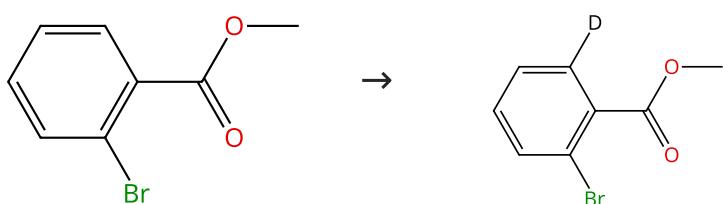
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 311 (1 Reaction)

Steps: 1



Suppliers (92)

Supplier (1)

31-116-CAS-6002270

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

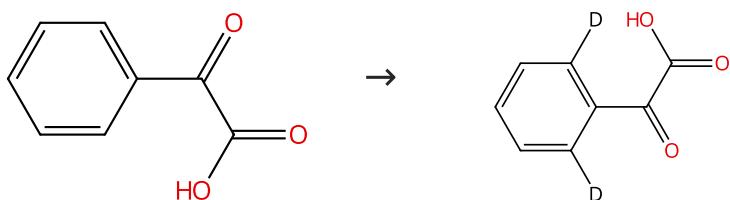
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 312 (1 Reaction)**

Steps: 1



Suppliers (112)

31-116-CAS-18789146

Steps: 1

**1.1 Reagents:** 1-Adamantanecarboxylic acid, Water- $d_2$   
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-N-[trifluoromethyl]sulfonyl- $\kappa O$ ]methanesulfonamidato- $\kappa O$  silver  
**Solvents:** 1,1,1,3,3-Hexafluoro-2-propanol; 3.5 h, 90 °C

**Ir(III)-Catalyzed Oxidative Annulation of Phenylglyoxylic Acids with Benzo[b]thiophenes**

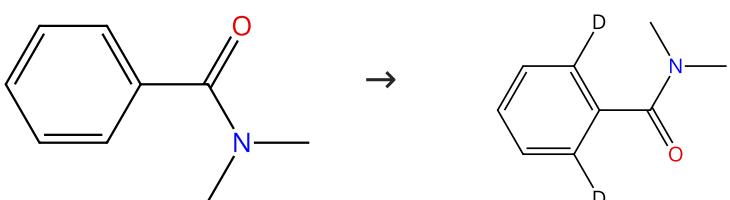
By: Wang, Zhigang; et al

Organic Letters (2018), 20(10), 3001-3005.

## Experimental Protocols

**Scheme 313 (1 Reaction)**

Steps: 1



Suppliers (75)

31-116-CAS-1413191

Steps: 1

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

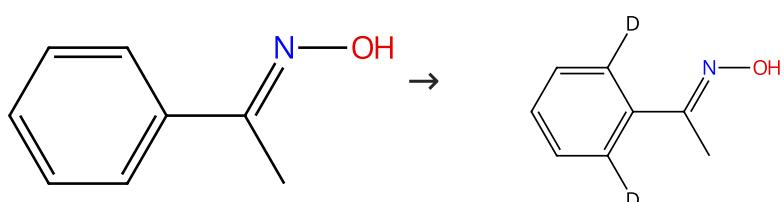
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 314 (1 Reaction)**

Steps: 1



Suppliers (59)

31-116-CAS-6295601

Steps: 1

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentaned ionato- $\kappa O^2,\kappa O^4$ )iridium  
**Solvents:** Dimethylacetamide; 3 h, 90 °C

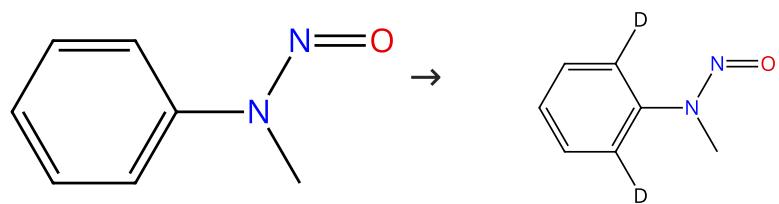
**Iridium-catalyzed H/D exchange**

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

## Scheme 315 (1 Reaction)

Steps: 1



Suppliers (75)

31-116-CAS-23549855

Steps: 1

1.1 **Reagents:** Silver acetate, Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>  
**Catalysts:** Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Silver hexafluoro antimonate  
**Solvents:** Methanol; 1 h, rt

Rh(III)-Catalyzed Olefination and Alkylation of Arenes with Maleimides: A Tunable Strategy for C(sp<sup>2</sup>)-H Functionalization

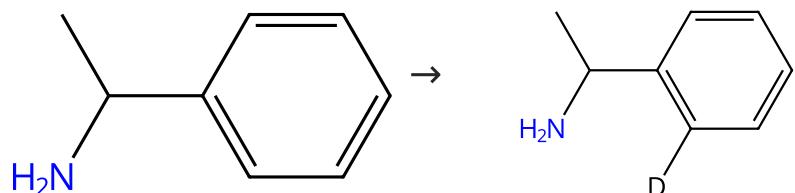
By: Zhang, Wenjie; et al

Synthesis (2021), 53(13), 2229-2239.

Experimental Protocols

## Scheme 316 (1 Reaction)

Steps: 1



Suppliers (87)

31-116-CAS-3548858

Steps: 1

1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

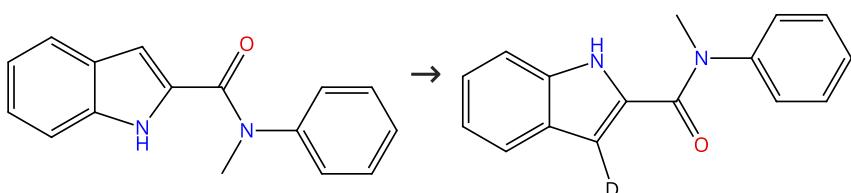
The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 317 (1 Reaction)

Steps: 1



Suppliers (10)

31-116-CAS-3399147

Steps: 1

1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

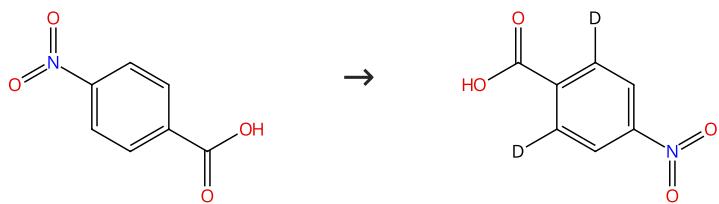
The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 318 (1 Reaction)

Steps: 1



Suppliers (112)

Suppliers (19)

31-116-CAS-13293849

Steps: 1

Iridium-catalyzed H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6-η)-1,5-Cyclooctadiene](2,4-pentaned ionato-κO<sup>2-</sup>,κO<sup>4-</sup>)iridium

Solvents: Dimethylacetamide; 2 h, 90 °C; 90 °C → rt

1.2 Reagents: Hydrochloric acid

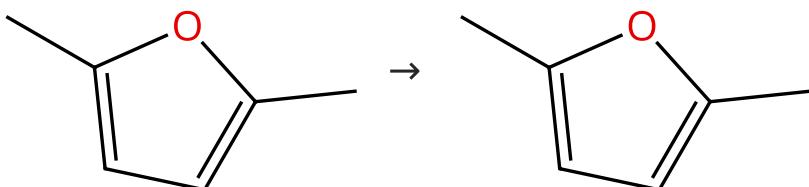
Solvents: Water; acidified, rt

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

## Scheme 319 (1 Reaction)

Steps: 1



Suppliers (72)

31-614-CAS-27493785

Steps: 1

H/D Exchange Processes Catalyzed by an Iridium-Pincer Complex

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: [2-[Bis(1-methylethyl)phosphino-κP]-N-[2-[bis(1-methylethyl)phosphino-κP]-4-methylphenyl]-4-methylbenz enaminato-κN]dihydroiridium

Solvents: Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °C

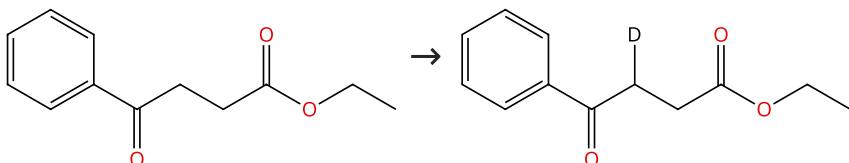
By: Iluc, Vlad M.; et al

Organometallics (2012), 31(1), 39-41.

Experimental Protocols

## Scheme 320 (1 Reaction)

Steps: 1



Suppliers (54)

31-614-CAS-32737281

Steps: 1

Photocatalytic 1,2-oxo-alkylation reaction of styrenes with diazoacetates

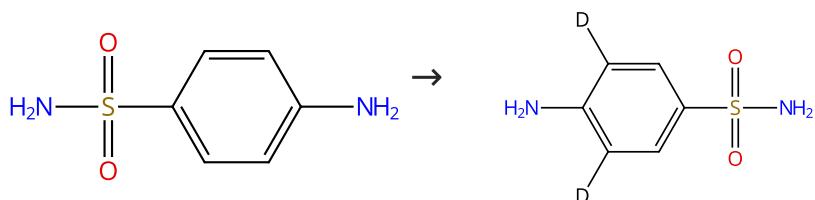
By: Li, Fang; et al

Chemical Communications (Cambridge, United Kingdom) (2022), 58(54), 7526-7529.

Experimental Protocols

## Scheme 321 (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*<sub>2</sub>, 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

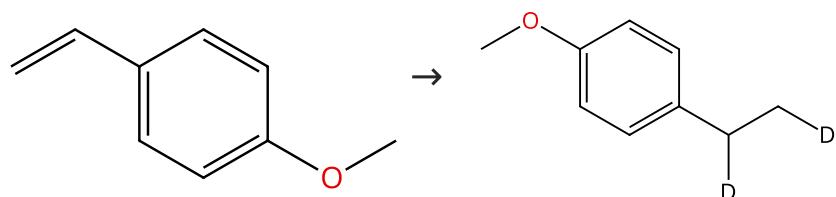
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

## Scheme 322 (1 Reaction)

Steps: 1



Suppliers (88)

31-614-CAS-37081760

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Triphenylphosphine, 2,4,6-Tris(1-methylethyl)benzenethiol, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κN<sup>1</sup>,κN<sup>1</sup>]bis[3,5-difluoro-2-[5-(trifluoromethyl)-2-pyridinyl-κN]phenyl-κCl]<sup>-</sup>, (OC-6-33)-, hexafluorophosphate(1-)

(1:1)

Solvents: Acetonitrile; 72 h, 20 °C

**Photocatalytic phosphine-mediated water activation for radical hydrogenation**

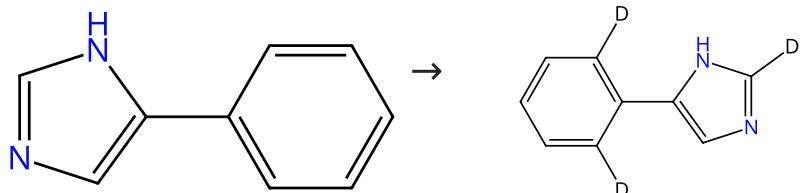
By: Zhang, Jingjing; et al

Nature (London, United Kingdom) (2023), 619(7970), 506-513.

Experimental Protocols

## Scheme 323 (1 Reaction)

Steps: 1



Suppliers (96)

31-116-CAS-2359756

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>

Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)-(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

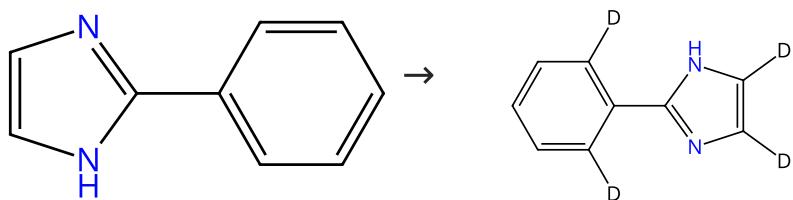
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 324 (1 Reaction)

Steps: 1



Suppliers (94)

31-116-CAS-11723813

Steps: 1

Hydrogen isotope labelling using iridium(I) dionates

1.1 Reagents: Water- $d_2$ Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2 min, 130 °C

By: Lockley, W. J. S.

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

## Scheme 325 (1 Reaction)

Steps: 1



Suppliers (94)

31-116-CAS-8435081

Steps: 1

Iridium-catalyzed H/D exchange

1.1 Reagents: Water- $d_2$ Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

Solvents: Dimethylacetamide; 2 h, 90 °C; 90 °C → rt

By: Krueger, Jens; et al

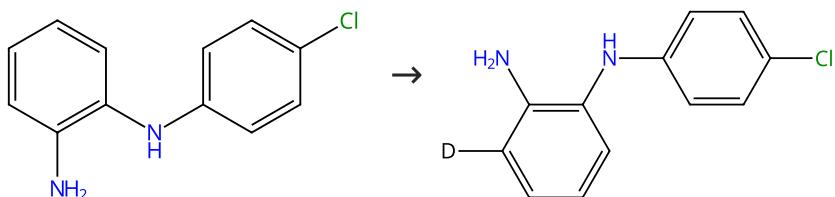
European Journal of Organic Chemistry (2005), (7), 1402-1408.

1.2 Reagents: Ammonia

Solvents: Water; rt

## Scheme 326 (1 Reaction)

Steps: 1



Suppliers (61)

31-116-CAS-21649674

Steps: 1

NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines

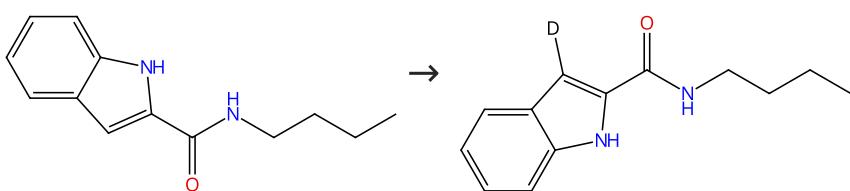
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

## Scheme 327 (1 Reaction)

Steps: 1



Suppliers (6)

31-116-CAS-14048420

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

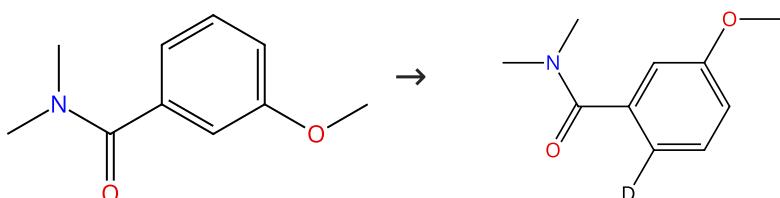
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 328 (1 Reaction)

Steps: 1



Suppliers (14)

31-614-CAS-28429581

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

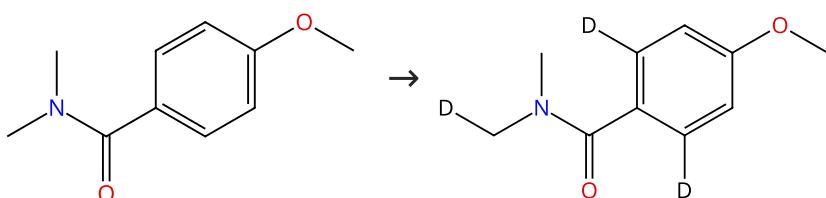
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 329 (1 Reaction)

Steps: 1



Suppliers (24)

31-116-CAS-5701820

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

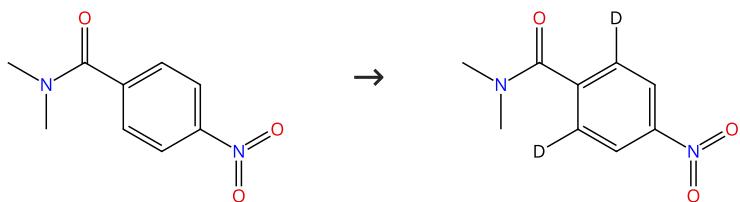
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 330 (1 Reaction)**

Steps: 1



Suppliers (42)

31-116-CAS-9939654

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

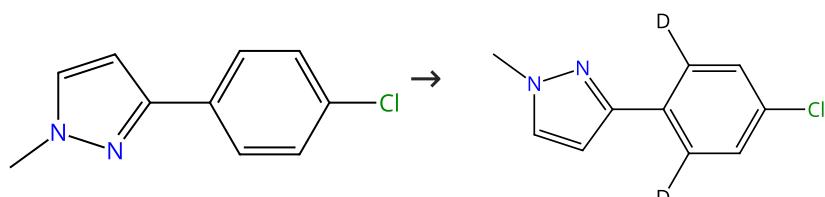
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 331 (1 Reaction)**

Steps: 1



Suppliers (3)

31-116-CAS-15130321

Steps: 1

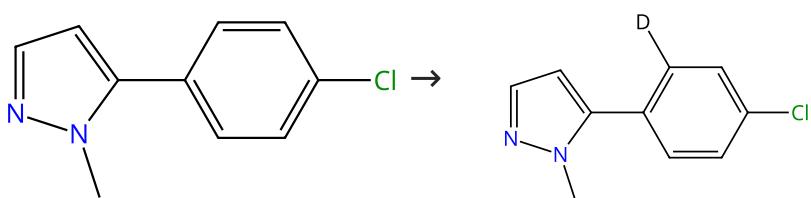
1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 332 (1 Reaction)**

Steps: 1



Suppliers (9)

31-116-CAS-3861506

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

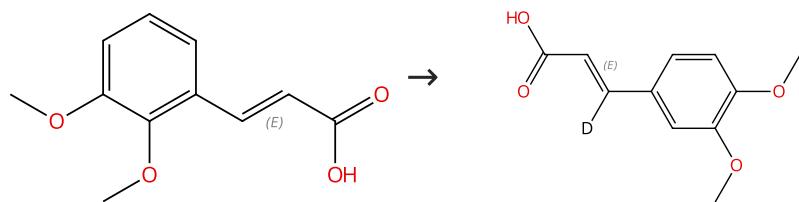
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 333 (1 Reaction)

Steps: 1



Suppliers (72)

31-116-CAS-14653884

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentaned ionato- $\kappa O^2,\kappa O^4$ )iridium  
**Solvents:** Dimethylacetamide; 2 h, 90 °C; 90 °C → rt
- 1.2 **Reagents:** Hydrochloric acid  
**Solvents:** Water; acidified, rt

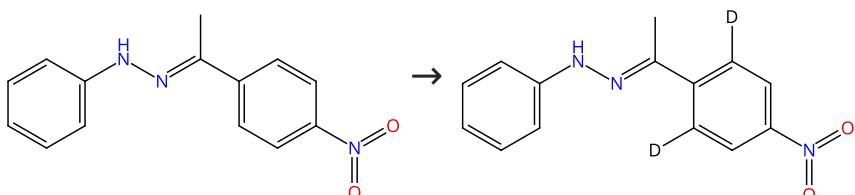
**Iridium-catalyzed H/D exchange**

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

Scheme 334 (1 Reaction)

Steps: 1



Suppliers (20)

31-614-CAS-26358028

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

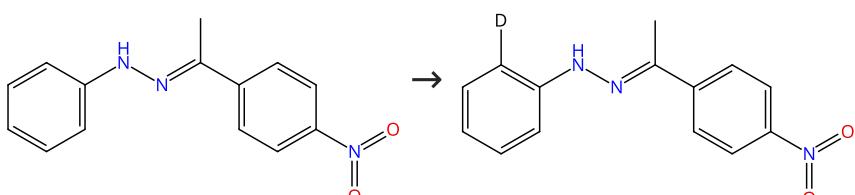
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 335 (1 Reaction)

Steps: 1



Suppliers (20)

31-116-CAS-6659960

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

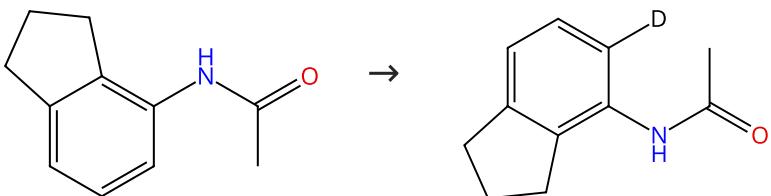
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 336 (1 Reaction)

Steps: 1



Suppliers (27)

31-116-CAS-19083079

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1), 2241328-74-3Solvents: Toluene; 18 h, rt  $\rightarrow$  120 °C

Experimental Protocols

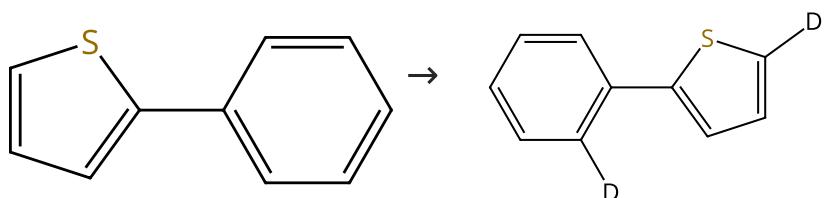
Branch-Selective and Enantioselective Iridium-Catalyzed Alkene Hydroarylation via Anilide-Directed C-H Oxidative Addition

By: Grelaud, Simon; et al

Journal of the American Chemical Society (2018), 140(30), 9351-9356.

## Scheme 337 (1 Reaction)

Steps: 1



Suppliers (78)

31-116-CAS-9068126

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

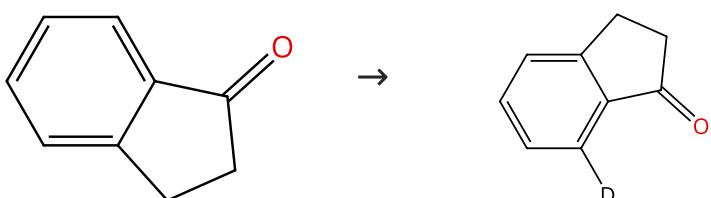
The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 338 (1 Reaction)

Steps: 1



Suppliers (117)

31-116-CAS-12187364

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine) (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

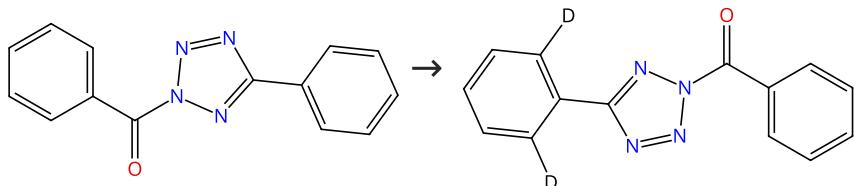
The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 339 (1 Reaction)

Steps: 1



Suppliers (4)

31-614-CAS-30992514

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
 (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 340 (1 Reaction)

Steps: 1



31-116-CAS-13698037

Steps: 1

- 1.1 **Catalysts:** Di- $\mu$ -chlorotetrakis[(1,2- $\eta$ )-cyclooctene]diiridium,  
 Sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, (1*S*,4*R*)-8-Methoxy-1,8-dimethyl-2-(4-methylphenyl)bicyclo[2.2.2]octa-2,5-diene  
**Solvents:** Dichloromethane; 1 h, rt  
 1.2 **Reagents:** Water-*d*<sub>2</sub>  
**Solvents:** Toluene; 7 h, 110 °C

**Iridium-Catalyzed Enantioselective C-H Alkylation of Ferrocenes with Alkenes Using Chiral Diene Ligands**

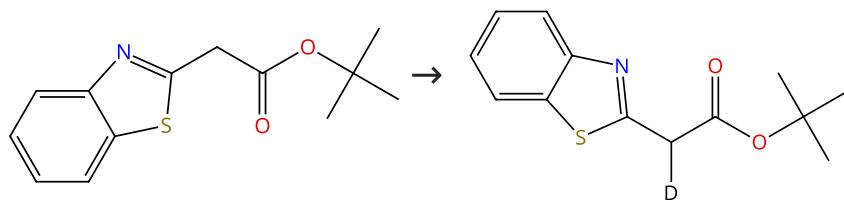
By: Shibata, Takanori; et al

Angewandte Chemie, International Edition (2014), 53(21), 5410-5413.

## Experimental Protocols

## Scheme 341 (1 Reaction)

Steps: 1



Suppliers (6)

31-614-CAS-38220292

Steps: 1

- 1.1 **Reagents:** Water-*d*<sub>2</sub>  
**Catalysts:** BINAP, Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1)  
**Solvents:** Toluene; 48 h, 70 °C

**Iridium-Catalyzed Enantioselective Alkene Hydroalkylation via a Heteroaryl-Directed Enolization-Decarboxylation Sequence**

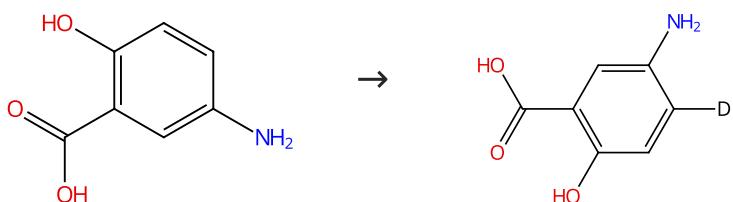
By: Jing, Changcheng; et al

Journal of the American Chemical Society (2023), 145(44), 23918-23924.

## Experimental Protocols

## Scheme 342 (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*<sub>2</sub>, 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

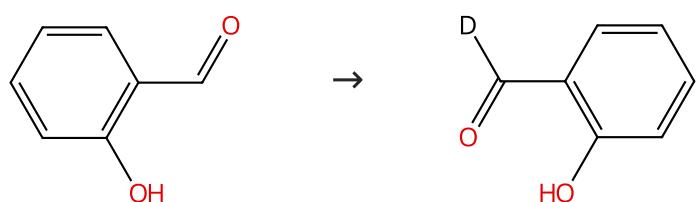
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

Experimental Protocols

## Scheme 343 (1 Reaction)

Steps: 1



Suppliers (102)

31-116-CAS-20076674

Steps: 1

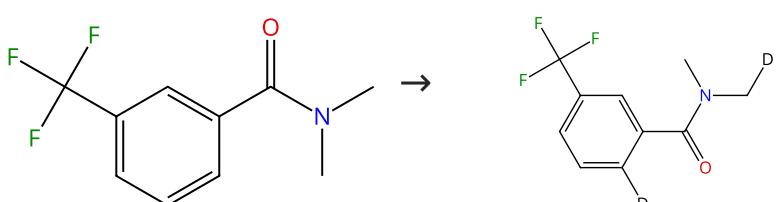
1.1 Reagents: Acetic acid-*d*<sub>4</sub>, Water-*d*<sub>2</sub>Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-; 2 h, 80 °C**On-Water Cp\*Ir(III)-Catalyzed C-H Functionalization for the Synthesis of Chromones through Annulation of Salicyla Idehydes with Diazo-Ketones**

By: Debbarma, Suvankar; et al

Journal of Organic Chemistry (2019), 84(10), 6207-6216.

## Scheme 344 (1 Reaction)

Steps: 1



Suppliers (37)

31-116-CAS-6180044

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)-tricyclohexylphosphine-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

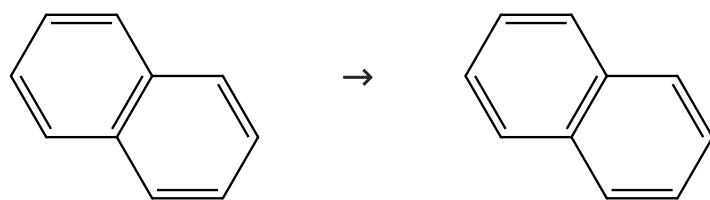
**The scope and limitations of deuteration mediated by Crabtree's catalyst**

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

## Scheme 345 (1 Reaction)

Steps: 1


🛒 Suppliers (137)

31-614-CAS-30950654

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [2-[Bis(1-methylethyl)phosphino- $\kappa P$ ]-*N*-[2-[bis(1-methylethyl)phosphino- $\kappa P$ ]-4-methylphenyl]-4-methylbenz enaminato- $\kappa N$ ]dihydroiridiumSolvents: Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °C

H/D Exchange Processes Catalyzed by an Iridium-Pincer Complex

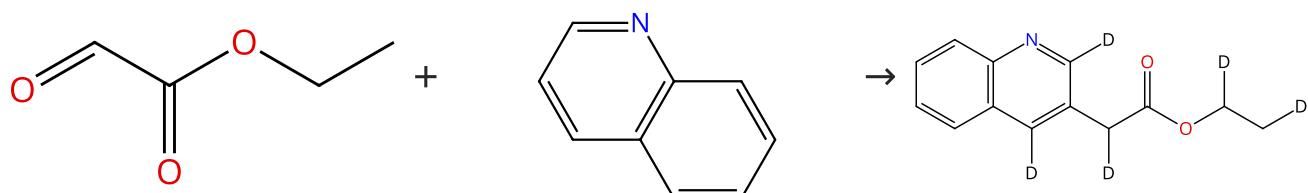
By: Iluc, Vlad M.; et al

Organometallics (2012), 31(1), 39-41.

Experimental Protocols

## Scheme 346 (1 Reaction)

Steps: 1


🛒 Suppliers (47)
🛒 Suppliers (124)

31-614-CAS-42513224

Steps: 1

1.1 Reagents: Formic-*d* acid, Ethanol-*d*<sub>6</sub>, Formic-*d* acid, sodium salt, Water-*d*<sub>2</sub>Catalysts: Iridium (boron-doped ZrO<sub>2</sub>/SiO<sub>2</sub> support); 1 h, 120 °C

Experimental Protocols

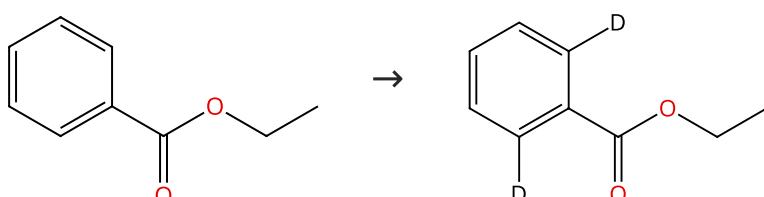
Reductive Coupling of N-Heteroarenes and 1,2-Dicarbonyls for Direct Access to  $\gamma$ -Amino Acids, Esters, and Ketones Using a Heterogeneous Single-Atom Iridium Catalyst

By: Jia, Huanhuan; et al

Journal of the American Chemical Society (2024), 146(46), 31647-31655.

## Scheme 347 (1 Reaction)

Steps: 1


🛒 Suppliers (94)

31-116-CAS-2074064

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)-(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

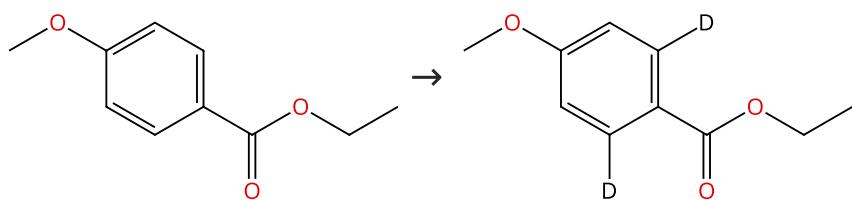
The scope and limitations of deuteration mediated by Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 348 (1 Reaction)**

Steps: 1



Suppliers (66)

31-116-CAS-8463850

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 349 (1 Reaction)**

Steps: 1



Suppliers (119)

31-116-CAS-11042460

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [2-[Bis(1-methylethyl)phosphino- $\kappa P$ ]-*N*-[2-[bis(1-methylethyl)phosphino- $\kappa P$ ]-4-methylphenyl]-4-methylbenz  
enaminato- $\kappa N$ ]dihydroiridiumSolvents: Cyclohexane-*d*<sub>12</sub>, Water-*d*<sub>2</sub>; 72 h, 80 °CH/D Exchange Processes Catalyzed by an Iridium-Pincer  
Complex

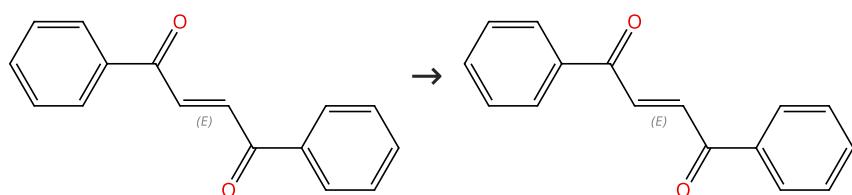
By: Iluc, Vlad M.; et al

Organometallics (2012), 31(1), 39-41.

## Experimental Protocols

**Scheme 350 (1 Reaction)**

Steps: 1



Double bond geometry shown

Double bond geometry shown

Suppliers (69)

31-614-CAS-25639125

Steps: 1

Iridium-catalyzed H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentaned  
ionato- $\kappa O^2,\kappa O^4$ )iridium

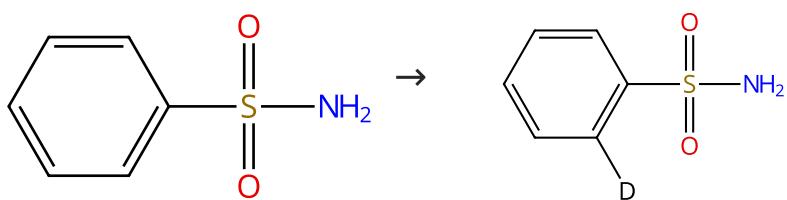
Solvents: Dimethylacetamide; 2 h, 90 °C

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

Scheme 351 (1 Reaction)

Steps: 1



Suppliers (89)

31-116-CAS-4810888

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

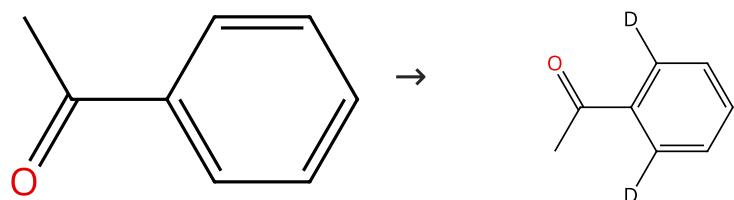
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 352 (1 Reaction)

Steps: 1



Suppliers (109)

Supplier (1)

31-116-CAS-1310281

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

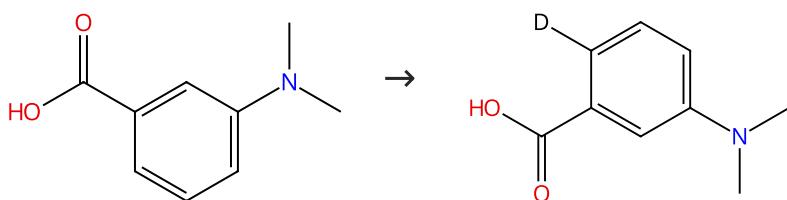
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 353 (1 Reaction)

Steps: 1



Suppliers (97)

31-116-CAS-15431455

Steps: 1

Iridium-catalyzed H/D exchange

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](2,4-pentaned  
ionato- $\kappa^2 O^2, \kappa^4 O^4$ )iridium

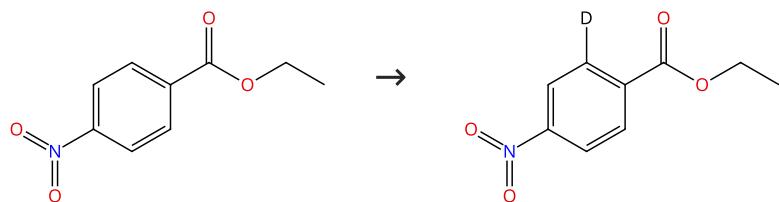
Solvents: Dimethylacetamide; 2 h, 90 °C

By: Krueger, Jens; et al

European Journal of Organic Chemistry (2005), (7), 1402-1408.

**Scheme 354 (1 Reaction)**

Steps: 1



Suppliers (92)

31-116-CAS-14861424

Steps: 1

**The scope and limitations of deuteration mediated by Crabtree's catalyst**

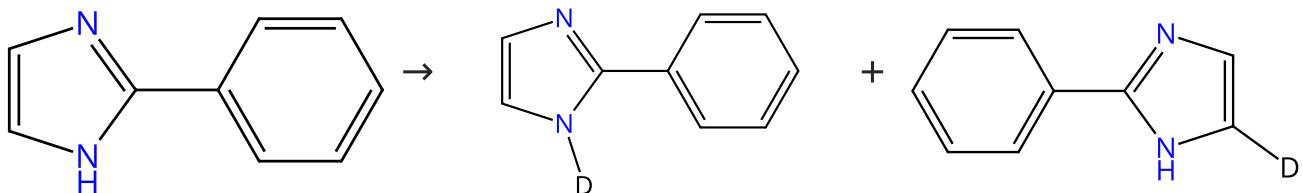
**1.1 Reagents:** Water- $d_2$   
**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
 (tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Dichloromethane

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

**Scheme 355 (3 Reactions)**

Steps: 1 Yield: 68-100%



Suppliers (94)

31-116-CAS-11613813

Steps: 1 Yield: 100%

**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pantanenedionato- $\kappa O^2,\kappa O^4$ )iridium  
**Solvents:** Dimethylacetamide; 2.25 h, 90 °C

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-3481117

Steps: 1 Yield: 100%

**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

**1.1 Reagents:** Water- $d_2$   
**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pantanenedionato- $\kappa O^2,\kappa O^4$ )iridium  
**Solvents:** Dimethylacetamide; 2 min, 130 °C

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

31-116-CAS-3099674

Steps: 1 Yield: 68%

**Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates**

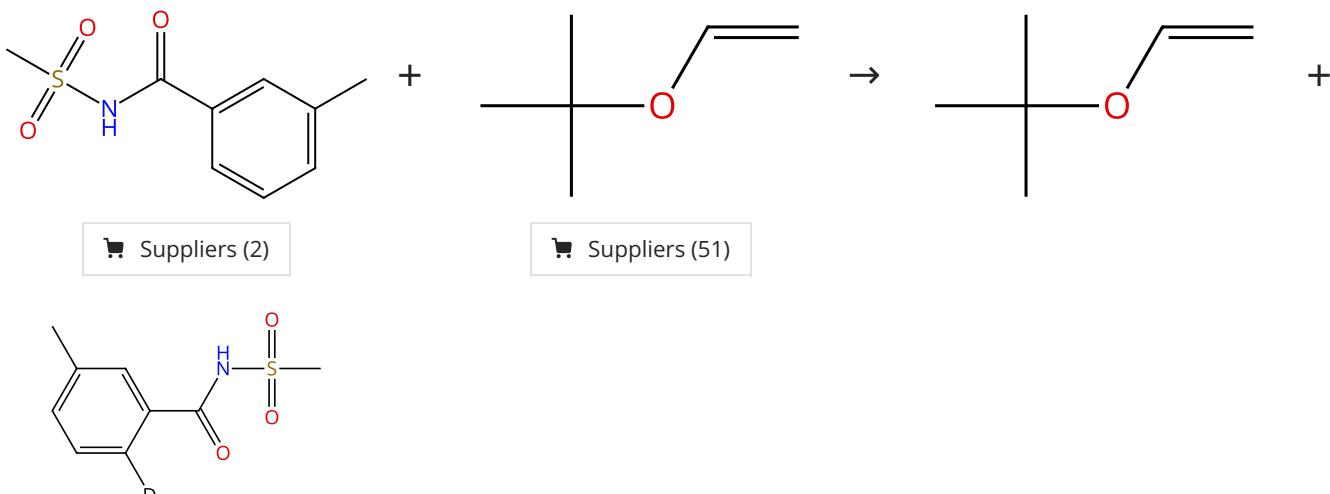
**1.1 Reagents:** Water- $d_2$   
**Catalysts:** [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](3-methyl-2,4-pantanenedionato- $\kappa O^2,\kappa O^4$ )iridium  
**Solvents:** Dimethylacetamide; 2.25 h, 90 °C

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

Scheme 356 (1 Reaction)

Steps: 1 Yield: 95%



31-614-CAS-30917583

Steps: 1 Yield: 95%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxydiiridiumSolvents: Benzene-*d*<sub>6</sub>; 0.5 h, 70 °C

Experimental Protocols

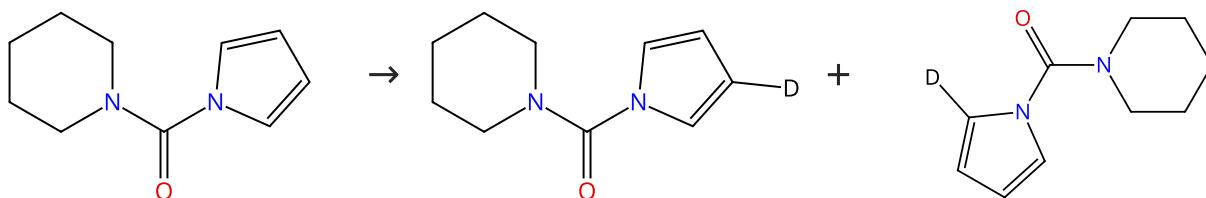
**Asymmetric Alkylation of N-Sulfonylbenzamides with Vinyl Ethers via C-H Bond Activation Catalyzed by Hydroxo iridium /Chiral Diene Complexes**

By: Hatano, Miyuki; et al

Journal of the American Chemical Society (2016), 138(12), 4010-4013.

Scheme 357 (1 Reaction)

Steps: 1 Yield: 91%



31-614-CAS-24681686

Steps: 1 Yield: 91%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]diiridium, *R*-Xyl-BINAP

Solvents: 1,4-Dioxane; 1 h, 100 °C

Experimental Protocols

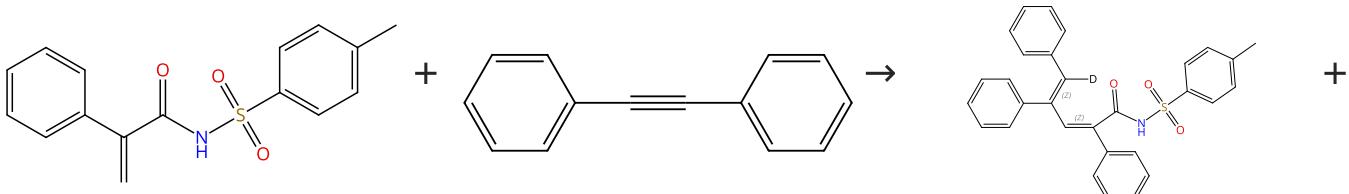
**Ir-Catalyzed Enantioselective Formal C-H Conjugate Addition of Pyrrole and Indoles to  $\alpha,\beta$ -Unsaturated Carbonyl Compounds**

By: Shibata, Takanori; et al

Organic Letters (2021), 23(23), 9078-9082.

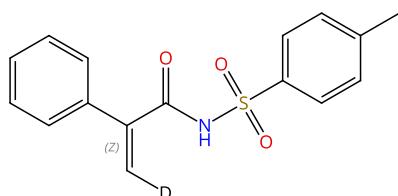
Scheme 358 (1 Reaction)

Steps: 1 Yield: 85%



Suppliers (88)

Double bond geometry shown



Double bond geometry shown

31-116-CAS-21976402

Steps: 1 Yield: 85%

1.1 **Catalysts:** Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -methoxyd iiridium**Solvents:** Water- $d_2$ ; 15 min, 70 °C

Experimental Protocols

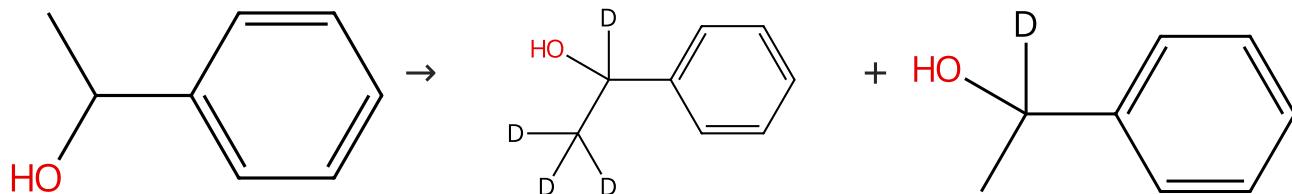
**Stereoselective and Atom-Economic Alkenyl C-H Allylation/Alkenylation in Aqueous Media by Iridium Catalysis**

By: Huang, Yinhua; et al

Journal of Organic Chemistry (2020), 85(11), 7225-7237.

Scheme 359 (1 Reaction)

Steps: 1 Yield: 84%



Suppliers (75)

Suppliers (17)

Suppliers (21)

31-614-CAS-33408369

Steps: 1 Yield: 84%

1.1 **Reagents:** Methanol- $d_4$ , Water- $d_2$ **Catalysts:** Iridium, aqua[2,2'-bipyridine]-6,6'(1H,1'H)-dionato (2-)· $\kappa N^1,\kappa N^1'][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-$ **Solvents:** Isopropanol; 21 h, 80 °C1.2 **Reagents:** Sulfuric acid**Solvents:** Water; pH 5

Experimental Protocols

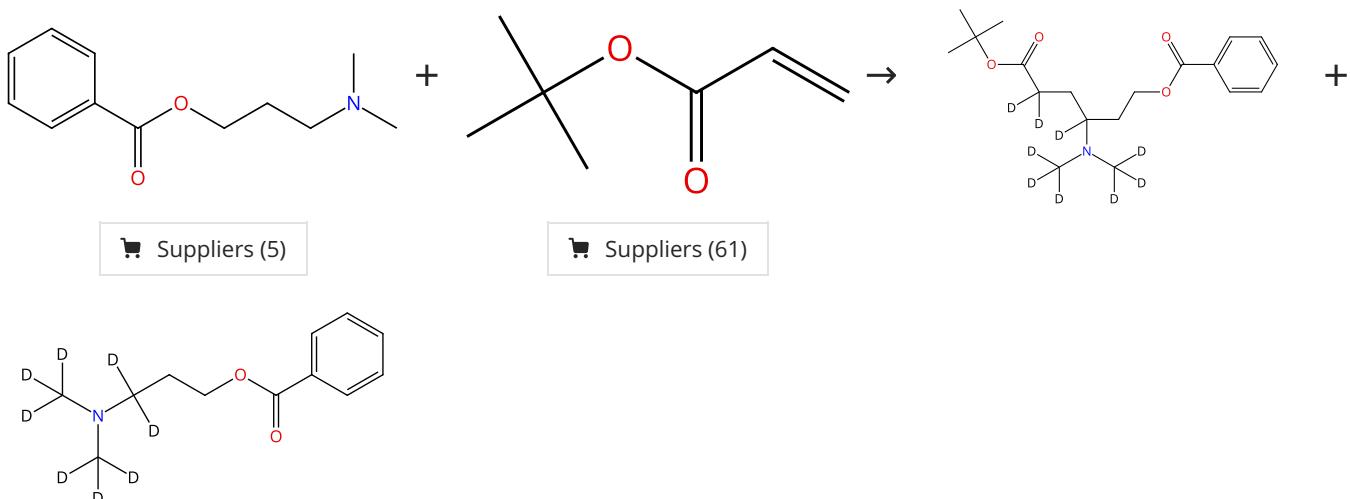
**Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

Scheme 360 (1 Reaction)

Steps: 1 Yield: 83%



31-614-CAS-24525042

Steps: 1 Yield: 83%

1.1 Reagents: Water-*d*<sub>2</sub>

**Catalysts:** 1,1,1-Triphenylsilanethiol, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ']bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa C$ ]-, (*OC*-6-33), hexafluorophosphate(1-) (1:1)

**Solvents:** Toluene; 4 h, 28 °C

Site-selective  $\alpha$ -C-H Functionalization of Trialkylamines via Reversible HAT-Catalysis

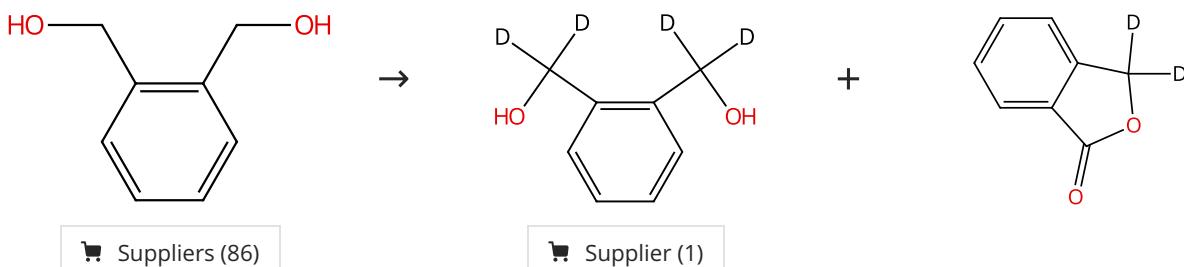
By: Shen, Yangyang; et al

Journal of the American Chemical Society (2021), 143(45), 18952-18959.

## Experimental Protocols

Scheme 361 (1 Reaction)

Steps: 1 Yield: 68%



31-614-CAS-33408370

Steps: 1 Yield: 68%

1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>, Sodium hydroxide-*d*

**Catalysts:** Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)- $\kappa N^1,\kappa N^1$ ][(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

**Solvents:** Isopropanol; 3 d, 80 °C

Iridium-catalyzed  $\alpha$ -selective deuteration of alcohols

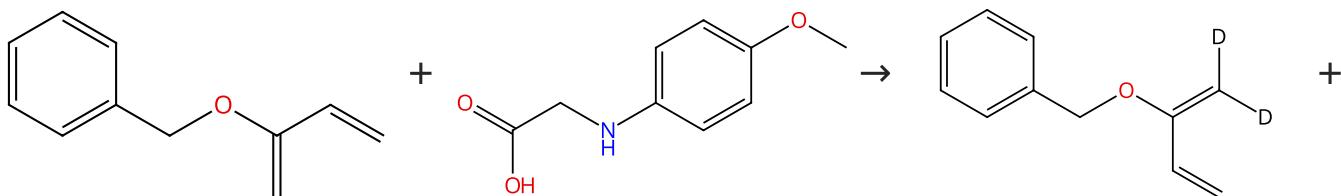
By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

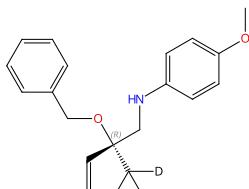
## Experimental Protocols

Scheme 362 (1 Reaction)

Steps: 1 Yield: 65%



Suppliers (43)



Absolute stereochemistry shown

## 31-614-CAS-31760295

Steps: 1 Yield: 65%

- 1.1 **Catalysts:** stereoisomer of ( $\eta^5$ -2,4-Cyclopentadien-1-yl)[(1,2,3- $\eta$ )-1-phenyl-2-propen-1-yl]palladium, (11b*R*)-8,9,10,11,12,13, 14,15-Octahydro-*N,N*-bis[(1*S*)-1-phenylethyl]dinaphtho[2,1-*d*:1',2'-*f*][1,3,2]dioxaphosphhepin-4-amine  
**Solvents:** Dimethylformamide; 30 min, rt

- 1.2 **Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** 3,5-Bis(trifluoromethyl)benzoic acid, Iridium(1+), [4, 4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa N$ phenyl- $\kappa C$ ], (*OC*-6-33)-, hexafluorophosphate(1-)(1:1)  
**Solvents:** *N,N*-Dimethylformamide-*d*<sub>7</sub>; 16 h, rt

## Regio-, Diastereo-, and Enantioselective Decarboxylative Hydro-aminoalkylation of Dienol Ethers Enabled by Dual Palladium/Photoredox Catalysis

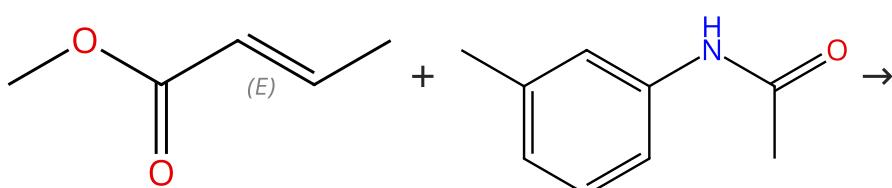
By: Zheng, Jun; et al

Angewandte Chemie, International Edition (2022), 61(20), e202200105.

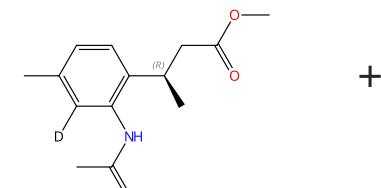
## Experimental Protocols

Scheme 363 (1 Reaction)

Steps: 1 Yield: 65%

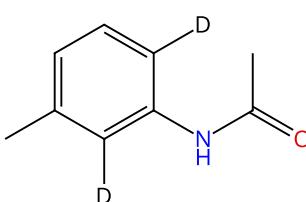


Suppliers (68)



Double bond geometry shown

Suppliers (60)



## 31-614-CAS-29147635

Steps: 1 Yield: 65%

Enantioselective Formal C-H Conjugate Addition of Acetanilides to  $\beta$ -Substituted Acrylates by Chiral Iridium Catalysts

By: Shibata, Takanori; et al

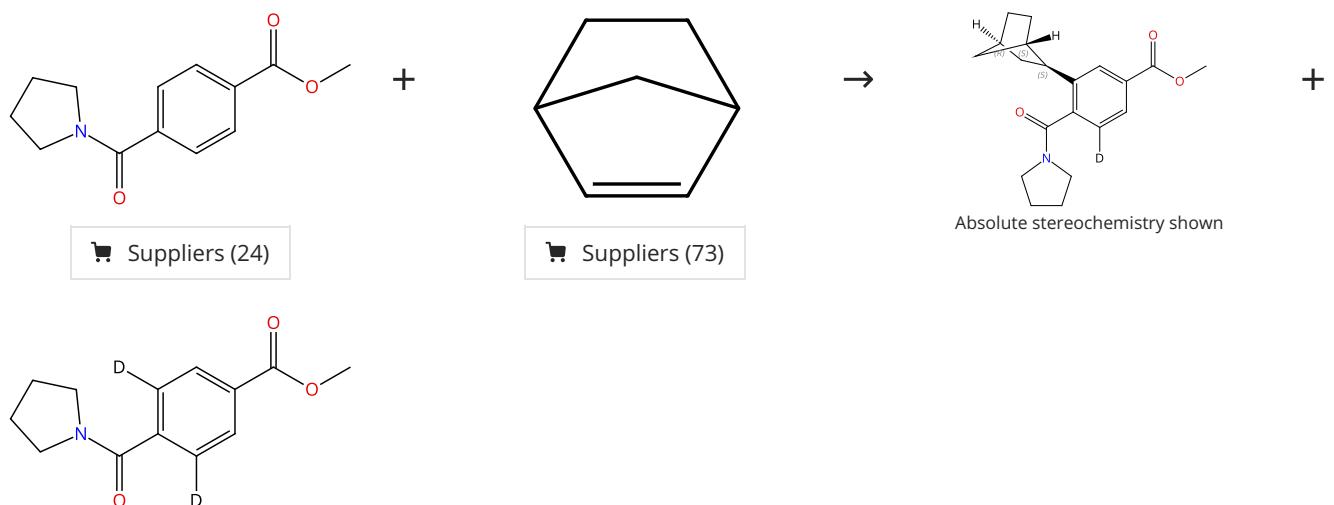
Chemistry - A European Journal (2017), 23(1), 88-91.

- 1.1 **Reagents:** Water-*d*<sub>2</sub>

**Catalysts:** Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene][(1,2-dimethyl-1,2-ethanediyl)bis[diphenylphosphine]-*P,P*]-, [*S*(*R\**), *R\**]-, salt with trifluoromethanesulfonic acid (1:1)

**Solvents:** 1,4-Dioxane; 72 h, 120 °C

Scheme 364 (1 Reaction)



31-085-CAS-6720277

Steps: 1 Yield: 64%

1.1 **Catalysts:** Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), 1820606-28-7**Solvents:** 1,2-Dichloroethane; 30 min, rt1.2 **Reagents:** Water- $d_2$ ; 0.25 h, 135 °C

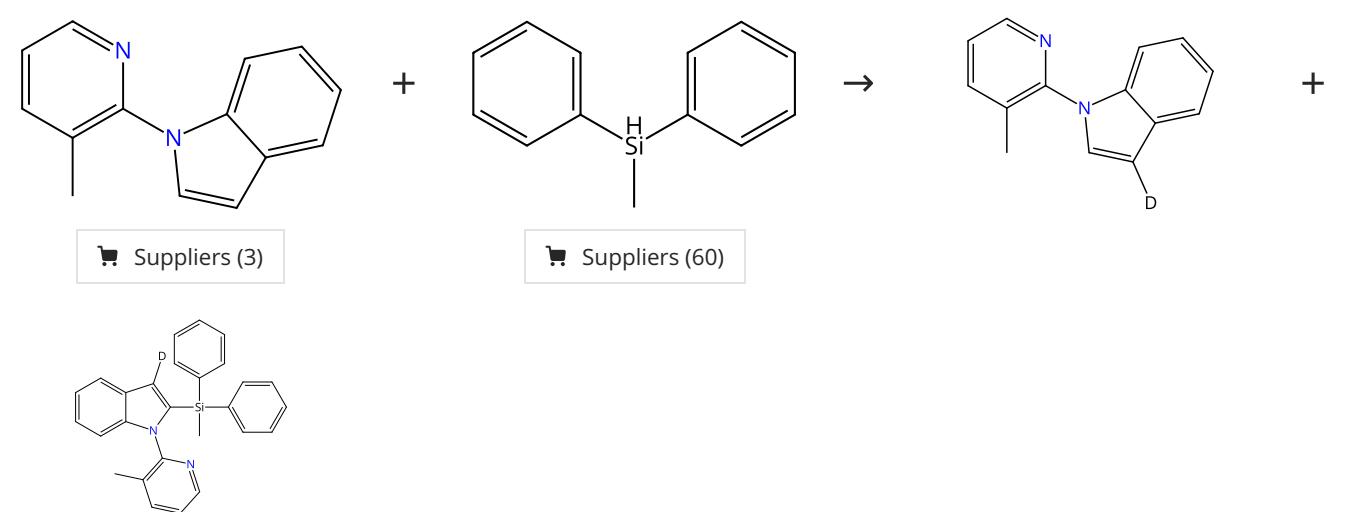
Experimental Protocols

**Cationic Iridium/S-Me-BIPAM-Catalyzed Direct Asymmetric Intermolecular Hydroarylation of Bicycloalkenes**

By: Shirai, Tomohiko; et al

Angewandte Chemie, International Edition (2015), 54(34), 9894-9897.

Scheme 365 (1 Reaction)



31-614-CAS-34491697

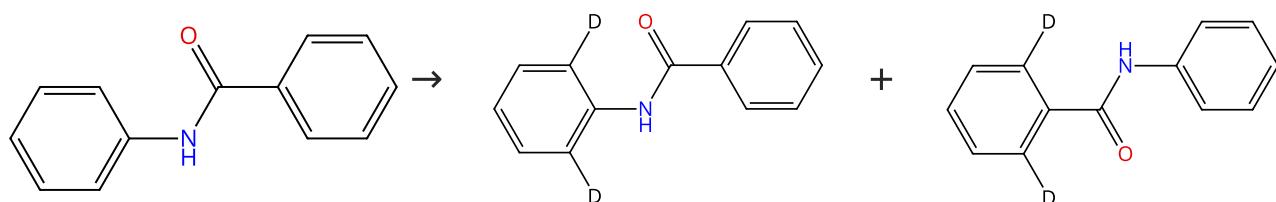
Steps: 1 Yield: 60%

1.1 **Reagents:** Norbornene, Water- $d_2$ **Catalysts:** Di- $\mu$ -chlorobis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]diiridium**Solvents:** Toluene; 4 h, 80 °C**3-Alkyl-2-pyridyl Directing Group-Enabled C2 Selective C-H Silylation of Indoles and Pyrroles via an Iridium Catalyst**

By: Sun, Hui; et al

Journal of Organic Chemistry (2022), 87(19), 13346-13351.

Scheme 366 (1 Reaction)



Suppliers (89)

31-116-CAS-10632806

Steps: 1 Yield: 55%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa O^2, \kappa O^4$ )iridium

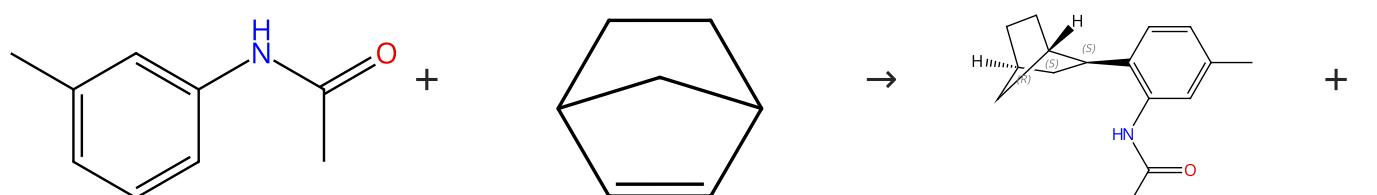
Solvents: Dimethylacetamide; 2 min, 130 °C

Convenient and efficient deuteration of functionalized aromatics with deuterium oxide: Catalysis by cycloocta-1,5-dienyliridium(I) 1,3-dionates

By: McAuley, B.; et al

Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(13), 1191-1204.

Scheme 367 (1 Reaction)



Suppliers (68)

Suppliers (73)

Absolute stereochemistry shown,  
Rotation (+)

31-085-CAS-19141242

Steps: 1 Yield: 54%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:1), 1820606-28-7

Solvents: 1,4-Dioxane; 30 min, rt

1.2 1.5 h, 135 °C

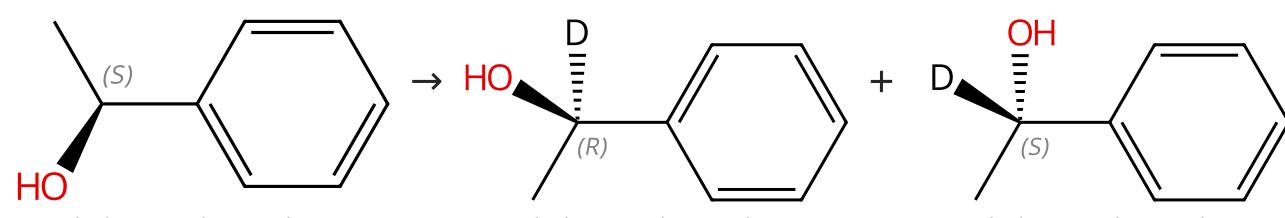
Experimental Protocols

Iridium-Catalyzed Direct Asymmetric Alkylation of Aniline Derivatives using 2-Norbornene

By: Shirai, Tomohiko; et al

Asian Journal of Organic Chemistry (2018), 7(6), 1054-1056.

Scheme 368 (1 Reaction)



Absolute stereochemistry shown,  
Rotation (-)

Absolute stereochemistry shown

Absolute stereochemistry shown

Suppliers (96)

31-614-CAS-33408372

Steps: 1 Yield: 48%

1.1 Reagents: Methanol-*d*<sub>4</sub>, Water-*d*<sub>2</sub>Catalysts: Iridium, aqua[[2,2'-bipyridine]-6,6'(1*H*,1'*H*)-dionato(2-)-κ*N*<sup>1</sup>,κ*N*'][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

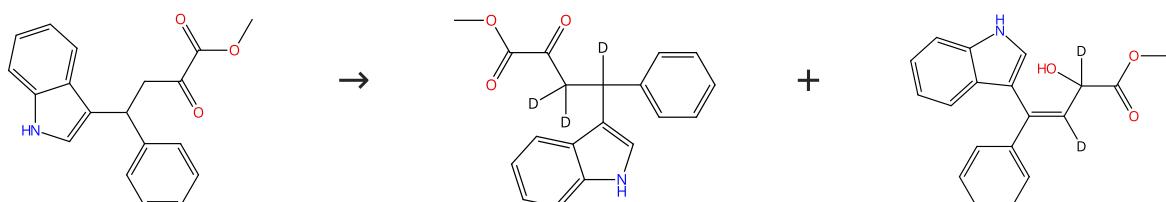
Solvents: Isopropanol; 21 h, 80 °C

Experimental Protocols

**Iridium-catalyzed α-selective deuteration of alcohols**

By: Itoga, Moeko; et al

Chemical Science (2022), 13(30), 8744-8751.

**Scheme 369** (1 Reaction)

31-614-CAS-31490323

Steps: 1 Yield: 38%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Dabco, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ*N*<sup>1</sup>,κ*N*'']bis[3,5-difluoro-2-(5-methyl-2-pyridinyl-κ*M*)phenyl-κ*C*], (*OC*-6-33)-, hexafluorophosphate(1-) (1:1)

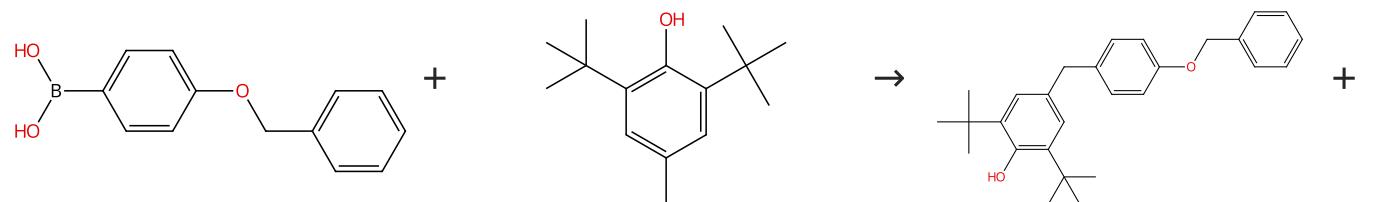
Solvents: Tetrahydrofuran; 4 h, rt

Experimental Protocols

**Photocatalytic redox-neutral reaction of γ-indolyl α-keto esters**

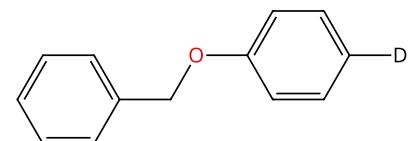
By: Wang, Man; et al

Organic Chemistry Frontiers (2022), 9(7), 1875-1883.

**Scheme 370** (1 Reaction)

Suppliers (98)

Suppliers (154)



Suppliers (3)

31-614-CAS-31585842

Steps: 1 Yield: 29%

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: *tert*-Butyl mercaptan, (±)-3-Quinuclidinol, Iridium (1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine-κ*N*<sup>1</sup>,κ*N*'']bis[2-(2-pyridinyl-κ*M*)phenyl-κ*C*], (*OC*-6-33)-, hexafluorophosphate (1-) (1:1)Solvents: Chloroform-*d*; 24 h, rt

Experimental Protocols

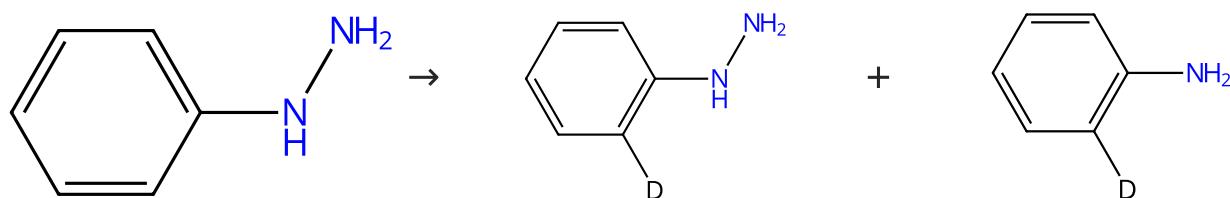
**Arylboronic Acid Deborylation Deuteration via Synergistic Thiol, Lewis Base and Photoredox Catalysis**

By: Dong, Jianyang; et al

Organic Letters (2022), 24(10), 2064-2068.

Scheme 371 (1 Reaction)

Steps: 1



Suppliers (70)

Supplier (1)

31-116-CAS-13984139

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

Solvents: Dichloromethane

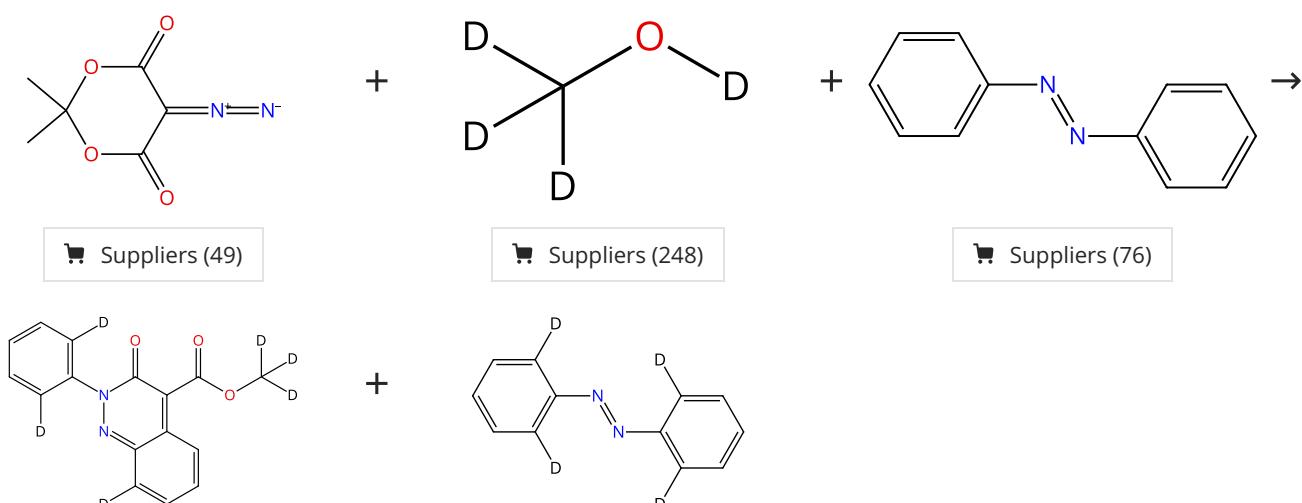
The scope and limitations of deuteration mediated by  
Crabtree's catalyst

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 372 (1 Reaction)

Steps: 1



Suppliers (49)

Suppliers (248)

Suppliers (76)

31-116-CAS-19850307

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium, di-μ-chlorodichlorobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Indium triflate; 6 h,  
80 °C

Experimental Protocols

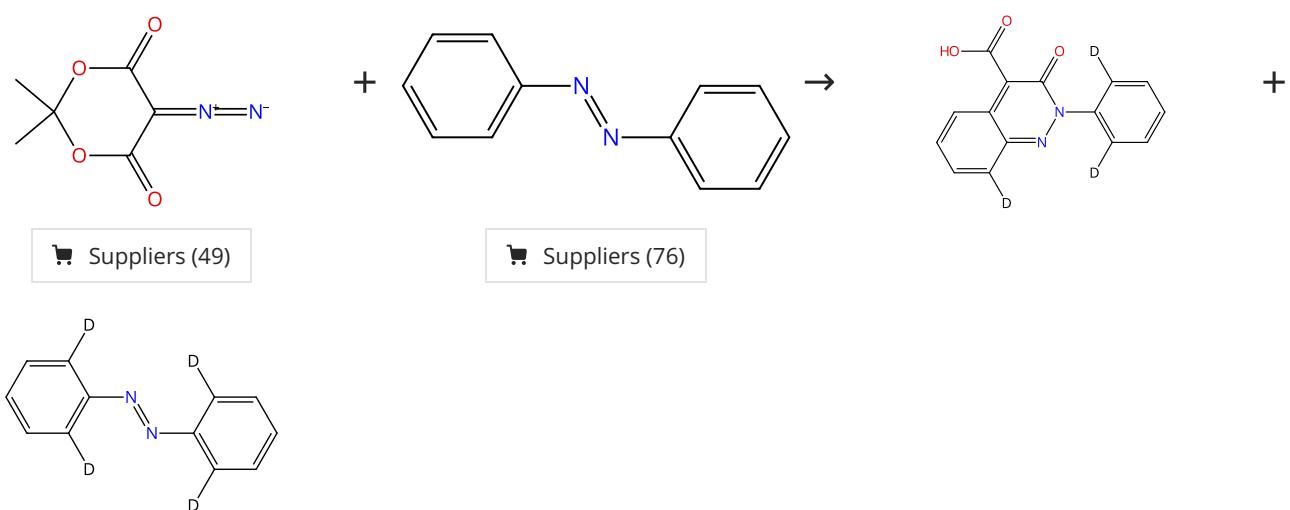
Ir(III)-Catalyzed [4 + 2] cyclization of azobenzene and  
diazotized Meldrum's acid for the synthesis of cinnolin-3(2H)-one

By: Borah, Gongutri; et al

Organic &amp; Biomolecular Chemistry (2019), 17(9), 2554-2563.

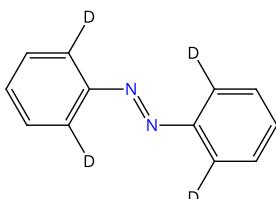
Scheme 373 (1 Reaction)

Steps: 1



Suppliers (49)

Suppliers (76)



31-116-CAS-19850306

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, Indium triflate

Solvents: 1,2-Dichloroethane; 6 h, 80 °C

Experimental Protocols

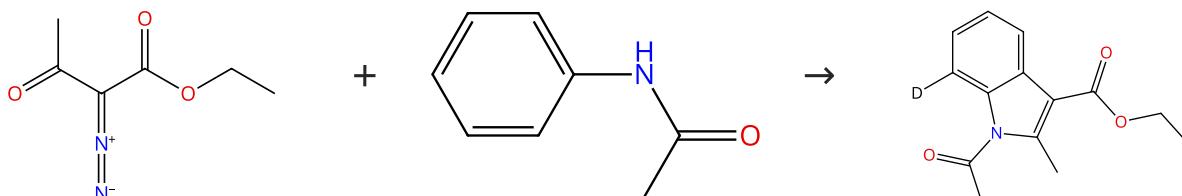
Ir(III)-Catalyzed [4 + 2] cyclization of azobenzene and diazotized Meldrum's acid for the synthesis of cinnolin-3(2H)-one

By: Borah, Gongutri; et al

Organic &amp; Biomolecular Chemistry (2019), 17(9), 2554-2563.

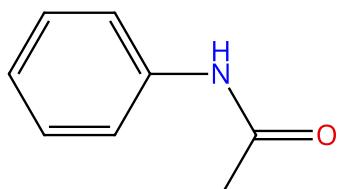
Scheme 374 (1 Reaction)

Steps: 1



Suppliers (41)

Suppliers (108)



31-614-CAS-29235309

Steps: 1

1.1 Reagents: Acetic acid

Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, [1,1,1-Trifluoro-*N*-[(trifluoromethyl)sulfonyl]- $\kappa$ O]methanesulfonamidato- $\kappa$ O silverSolvents: 1,2-Dichloroethane, Water-*d*<sub>2</sub>; 3 h, 60 °C

Experimental Protocols

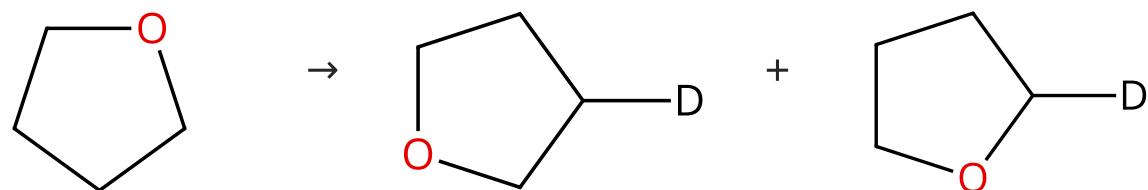
Direct Access to Indoles by Ir III-Catalyzed C-H Functionalization of Acetanilides with Diazo Compounds

By: Patel, Pitambar; et al

European Journal of Organic Chemistry (2017), 2017(16), 2272-2279.

Scheme 375 (1 Reaction)

Steps: 1



Suppliers (410)

31-116-CAS-7123169

Steps: 1

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(2+), diaquaabis[4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa$ N<sup>1</sup>, $\kappa$ N<sup>1</sup>]bis[ $\mu$ -(4-methylbenzenesulfonato- $\kappa$ O- $\kappa$ O')bis(2-methyl-2-phenylpropyl)di-, stereoisomer, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (1:2)

Solvents: Tetrahydrofuran; 40 h, 135 °C

Experimental Protocols

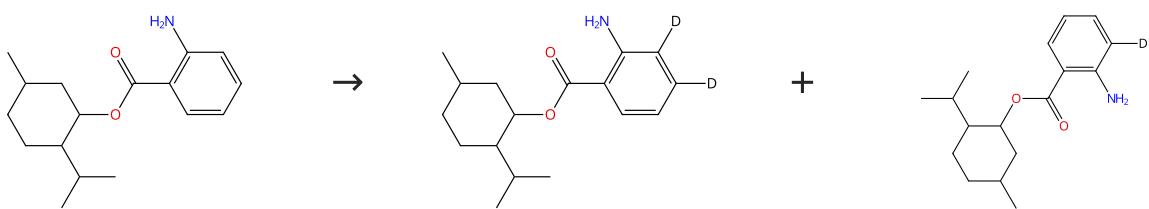
C-H Activation with iridium(III) and rhodium(III) alkyl complexes containing a 2,2'-bipyridyl ligand

By: Yi, Xiao-Yi; et al

European Journal of Inorganic Chemistry (2010), (16), 2369-2375.

**Scheme 376 (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*<sub>2</sub>; 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

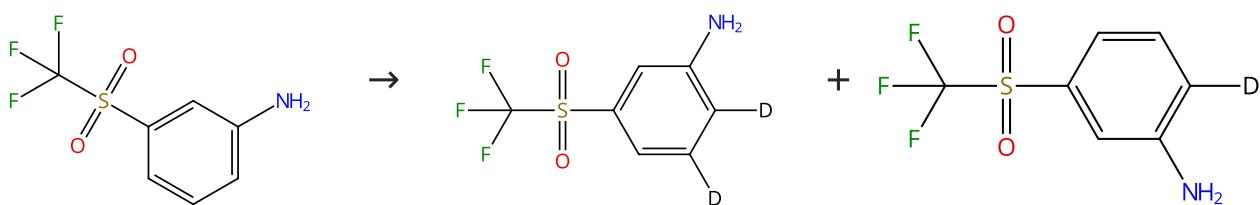
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

## Experimental Protocols

**Scheme 377 (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*<sub>2</sub>; 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

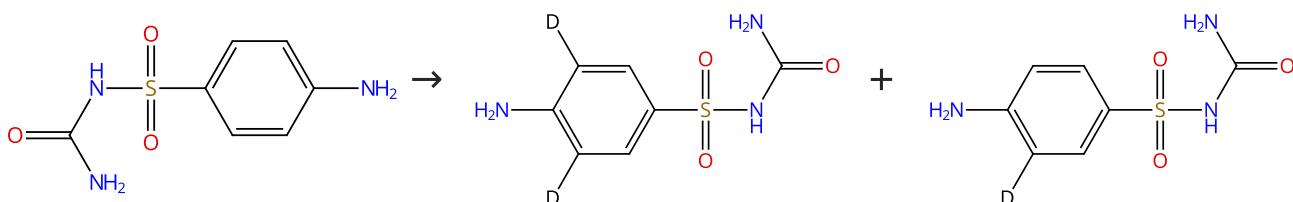
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

## Experimental Protocols

**Scheme 378 (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*<sub>2</sub>; 3 h, 80 °C**NHC-Stabilized Iridium Nanoparticles as Catalysts in Hydrogen Isotope Exchange Reactions of Anilines**

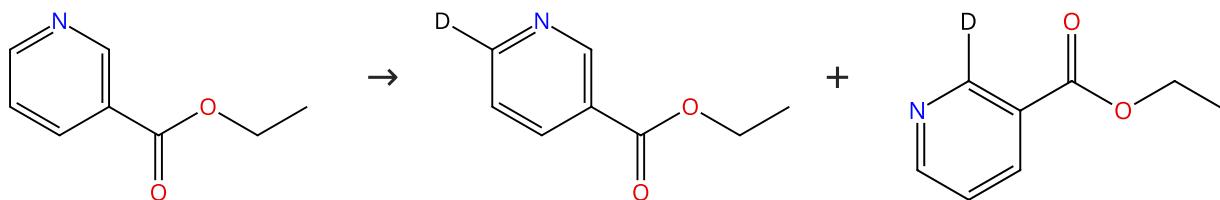
By: Valero, Megane; et al

Angewandte Chemie, International Edition (2020), 59(9), 3517-3522.

## Experimental Protocols

Scheme 379 (1 Reaction)

Steps: 1



Suppliers (109)

31-116-CAS-13000608

Steps: 1

The scope and limitations of deuteration mediated by Crabtree's catalyst

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: Iridium(1+), [(1,2,5,6- $\eta$ )-1,5-cyclooctadiene](pyridine)  
(tricyclohexylphosphine)-, hexafluorophosphate(1-) (1:1)

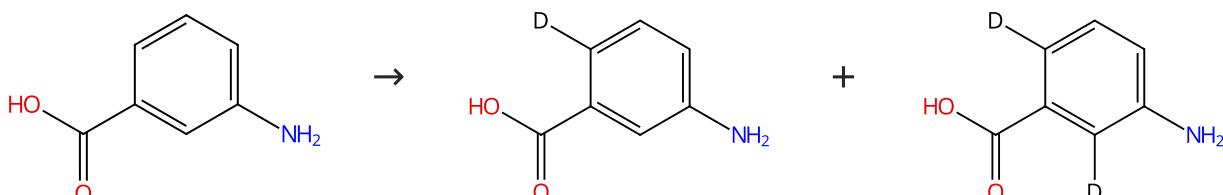
Solvents: Dichloromethane

By: Ellames, George J.; et al

Tetrahedron (2001), 57(46), 9487-9497.

Scheme 380 (1 Reaction)

Steps: 1



Suppliers (105)

31-116-CAS-11056990

Steps: 1

Hydrogen isotope labelling using iridium(I) dionates

1.1 Reagents: Water-*d*<sub>2</sub>Catalysts: [(1,2,5,6- $\eta$ )-1,5-Cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- $\kappa$ O<sup>2-</sup>, $\kappa$ O<sup>4-</sup>)iridium

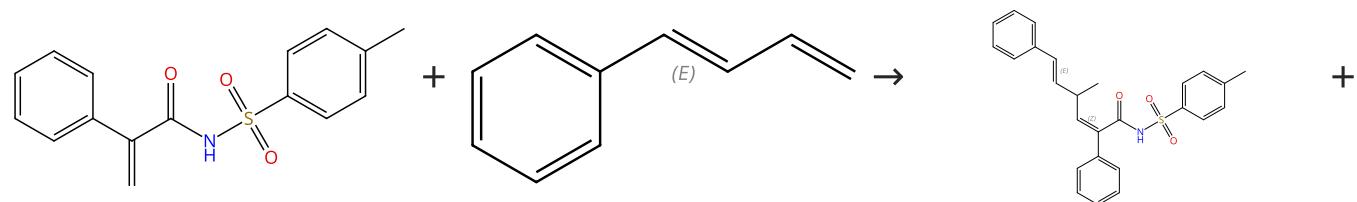
Solvents: Dimethylacetamide; 2 min, 130 °C

By: Lockley, W. J. S.

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

Scheme 381 (1 Reaction)

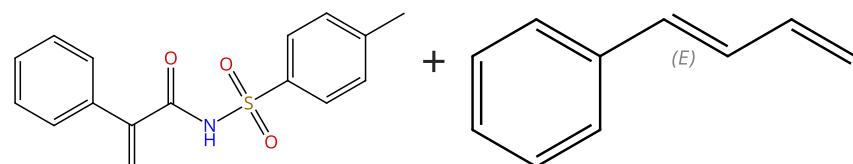
Steps: 1 Yield: 88%



Double bond geometry shown

Double bond geometry shown

Suppliers (57)



Double bond geometry shown

31-614-CAS-27364548

Steps: 1 Yield: 88%

1.1 **Catalysts:** Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -methoxyd  
iiridium  
**Solvents:** Water- $d_2$ ; 10 min, 70 °C

Experimental Protocols

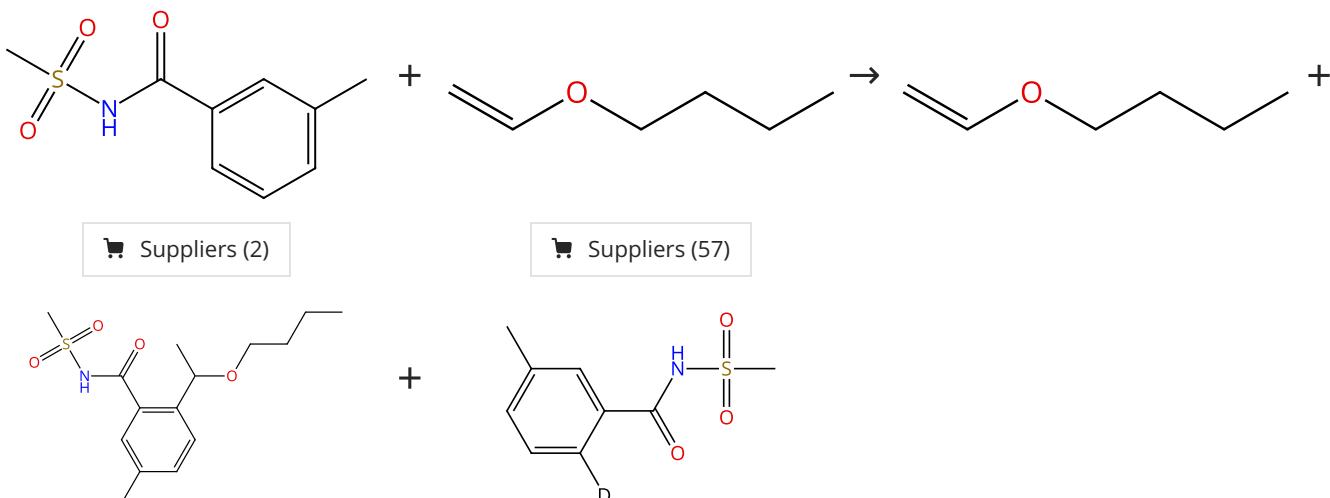
Stereoselective and Atom-Economic Alkenyl C-H Allylation/Alkenylation in Aqueous Media by Iridium Catalysis

By: Huang, Yinhua; et al

Journal of Organic Chemistry (2020), 85(11), 7225-7237.

Scheme 382 (1 Reaction)

Steps: 1 Yield: 67%



31-614-CAS-30110144

Steps: 1 Yield: 67%

1.1 **Reagents:** Water- $d_2$   
**Catalysts:** Bis[(1,2,5,6- $\eta$ )-1,5-cyclooctadiene]di- $\mu$ -hydroxyd  
iiridium  
**Solvents:** Benzene- $d_6$ ; 0.5 h, 70 °C

Experimental Protocols

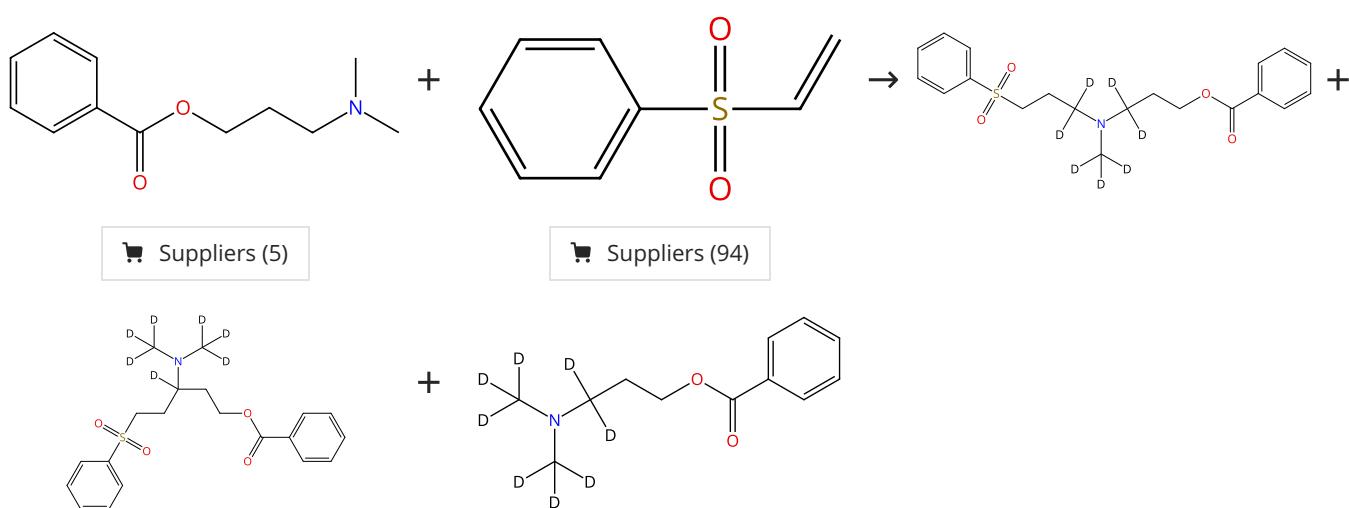
Asymmetric Alkylation of N-Sulfonylbenzamides with Vinyl Ethers via C-H Bond Activation Catalyzed by Hydroxo iridium /Chiral Diene Complexes

By: Hatano, Miyuki; et al

Journal of the American Chemical Society (2016), 138(12), 4010-4013.

Scheme 383 (1 Reaction)

Steps: 1 Yield: 56%



31-614-CAS-24525037

Steps: 1 Yield: 56%

1.1 **Reagents:** Water- $d_2$   
**Catalysts:** 1,1,1-Triphenylsilanethiol, Iridium(1+), [4,4'-bis(1,1-dimethylethyl)-2,2'-bipyridine- $\kappa N^1,\kappa N^1$ ]bis[2-(2-pyridinyl- $\kappa M$ )phenyl- $\kappa Cl$ ]-, (OC-6-33)-, hexafluorophosphate(1-) (1:1)  
**Solvents:** Toluene; 10 min, 28 °C

Experimental Protocols

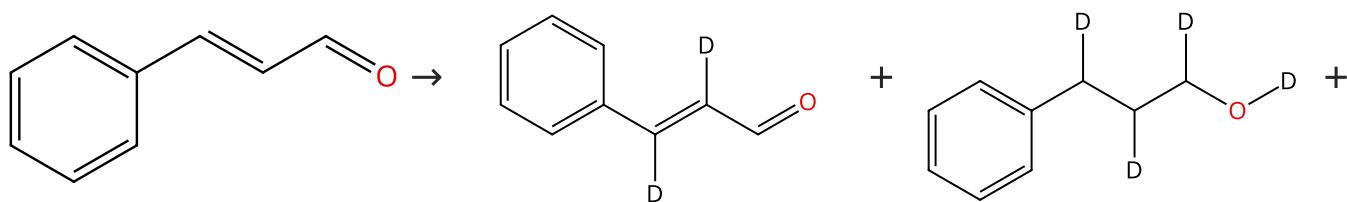
Site-selective  $\alpha$ -C-H Functionalization of Trialkylamines via Reversible HAT-Catalysis

By: Shen, Yangyang; et al

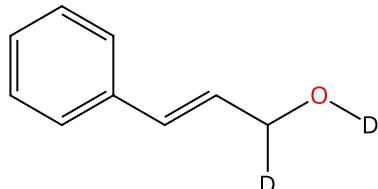
Journal of the American Chemical Society (2021), 143(45), 18952-18959.

Scheme 384 (1 Reaction)

Steps: 1



Suppliers (63)



31-614-CAS-39507452

Steps: 1

**Highly selective hydrogenation of unsaturated aldehydes in aqueous phase**1.1 Reagents: Hydrogen, Water-*d*<sub>2</sub>Catalysts: Tungsten oxide (WO<sub>3</sub>), Iridium (supported on tungsten trioxide nanorods); 1 MPa, rt → 60 °C

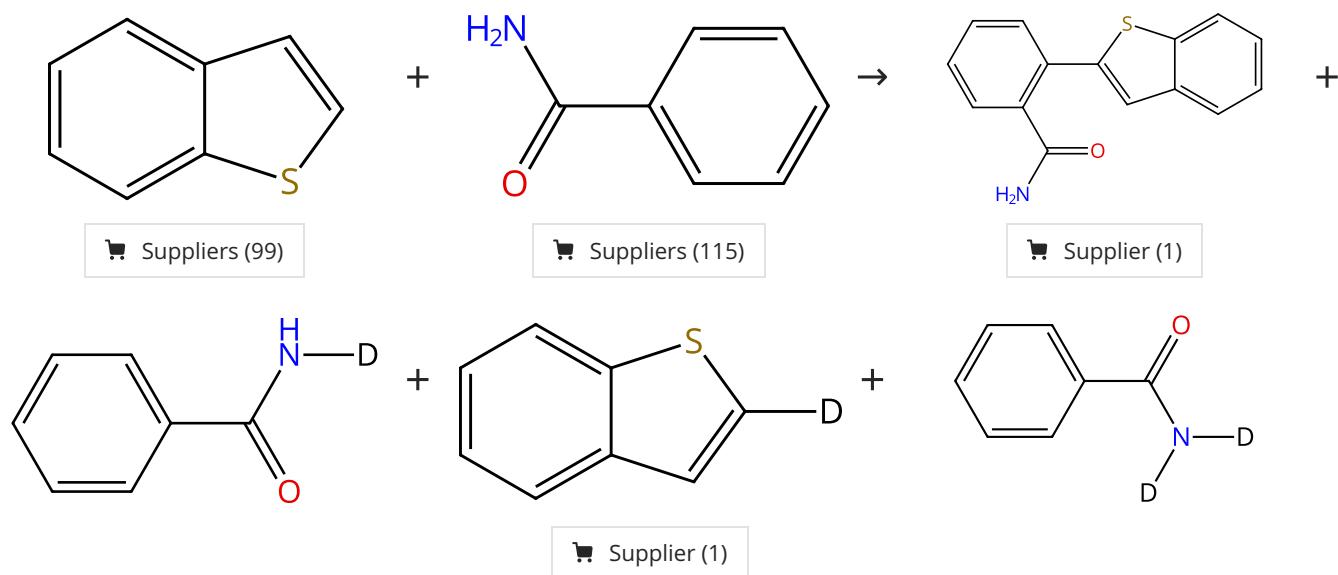
Experimental Protocols

By: Zhou, Shijie; et al

ACS Applied Materials &amp; Interfaces (2024), 16(11), 13685-13696.

Scheme 385 (1 Reaction)

Steps: 1 Yield: 34%



Suppliers (99)

Suppliers (115)

Supplier (1)

Supplier (1)

31-116-CAS-19234897

Steps: 1 Yield: 34%

**Iridium-catalyzed oxidative Ar-H/Ar-H cross-coupling of primary benzamides with thiophenes**1.1 Reagents: Water-*d*<sub>2</sub>, Silver oxide (Ag<sub>2</sub>O)Catalysts: Iridium, di- $\mu$ -chlorodichlorobis[(1,2,3,4,5- $\eta$ )-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-

Solvents: 1,1,1,3,3-Hexafluoro-2-propanol; 1 h, 120 °C

By: Tan, Guangying; et al

Organic Chemistry Frontiers (2018), 5(20), 2930-2933.

Experimental Protocols