Supplementary Information

Stibine-catalyzed selective conversion of nitroarenes to hydroxylanilines through deoxygenation and hydroboration processes

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This document includes:

1. Materials and Methods

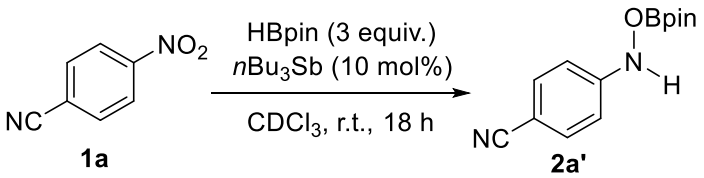
General Remarks

Unless otherwise noted, all syntheses were carried out in an argon-filled glove box or using standard Schlenk techniques under an inert atmosphere of anhydrous argon. Solvents were dried by refluxing under argon over Na (Et_2O, hexane, THF) or CaH (DCM, $CHCl_3$, MeCN) and stored under argon atmosphere over 4 Å molecular sieves. Dry deuterated benzene (C_6D_6), deuterated chloroform ($CDCl_3$), and deuterated dimethyl sulfoxide (DMSO-d_6) purchased from J&K Scientific Ltd. were degassed and stored over molecular sieves (4 Å) for at least two days prior to use. Me_3Sb, Et_3Sb, $n$$Pr_3Sb$, $n$$Bu_3Sb$ and [$n$$Bu_3Sb$($\mu$-O)]$_2$ were synthesized according to literature procedures.[S1] 4-(2-oxa-3-azabicyclo[2.2.2]oct-5-en-3-yl)benzonitrile (**3a**) was synthesized according to literature procedures.[S2] 4-Nitrosobenzonitrile (**4a**) was synthesized according to literature procedures.[S3] Commercial reagents were used without further purification unless indicated otherwise. NMR spectra were obtained on Bruker Avance II 400 spectrometer. ^{1}H and ^{13}C{^{1}H} NMR chemical shifts (δ/ppm) are referenced to the residual solvent resonance of the deuterated solvent. ^{19}F and ^{11}B NMR chemical shifts (δ/ppm) are referenced to $CFCl_3$ and $BF_3{\cdot}OEt_2$, respectively. Mass spectroscopy (MS) studies were performed on an LCMS-IT-TOF (ESI).

2. Syntheses and Spectroscopic Data

2.1 Optimization of Reaction Conditions

The reduction of **1a** with HBpin (3 equiv.) catalyzed by nBu$_3$Sb in CDCl$_3$



4-Nitrobenzonitrile (**1a**) (29.6 mg, 0.20 mmol), mesitylene (24.0 mg, 0.20 mmol) and HBpin (79.6 mg, 0.62 mmol) were combined in 0.6 mL of CDCl$_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. Then nBu$_3$Sb (6.0 mg, 0.02 mmol) was added to the reaction solution. The progress of the reaction solution was monitored by NMR spectroscopy analysis. After 18 h, the reaction finished. The yield of 4-(((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)amino)benzonitrile (**2a′**) (93%) was calculated by ^{1}H NMR using mesitylene as internal standard as shown in Figure S1.

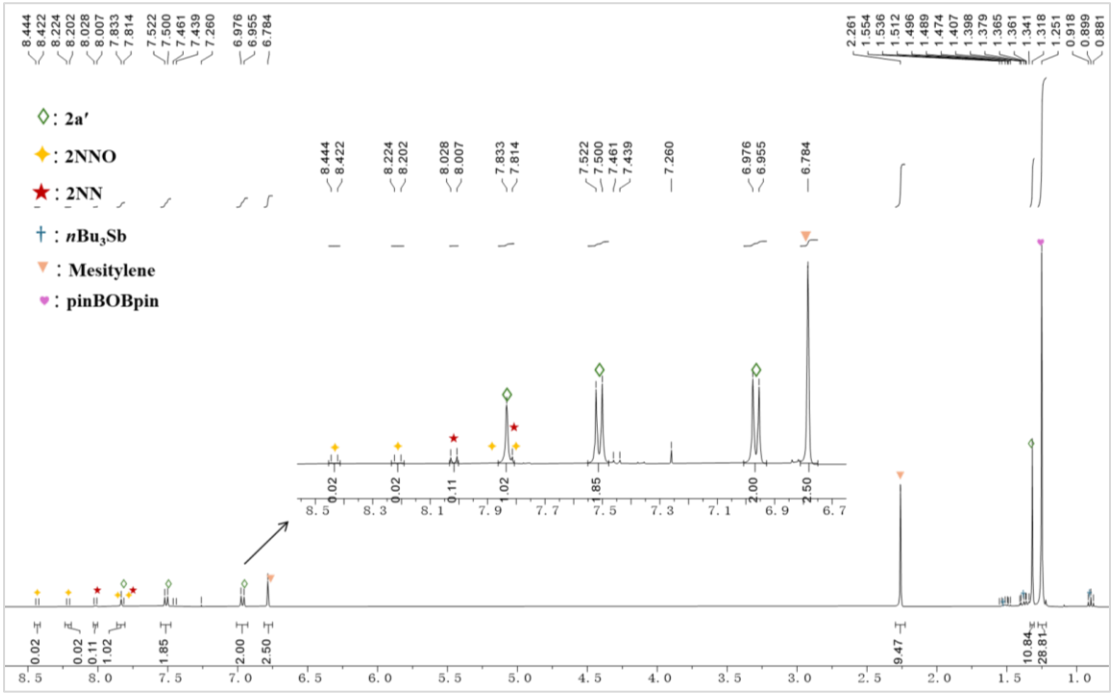


Figure S1: ^{1}H NMR spectrum of reaction solution of **1a** and HBpin (3 equiv.) catalyzed by nBu$_3$Sb with mesitylene as initial standard at r.t. for 18 h (400 MHz, CDCl$_3$).

The characterization of **2a′**

1a (14.8 mg, 0.10 mmol), HBpin (38.4 mg, 0.30 mmol) and *n*Bu_3Sb (3.0 mg, 0.01 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and monitored by NMR spectroscopy. After 18 h, **1a** was consumed. The predominant product **2a′** was characterized by NMR spectroscopy. **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C):δ (ppm) 7.69 (s, 1H, Ar-N*H*), 7.50 (d, $^3J_{H\text{-}H}$ = 8.7 Hz, 1H, NCAr-*m*-*H*), 6.94 (d, $^3J_{H\text{-}H}$ = 8.7 Hz, 1H, NCAr-*o*-*H*), 1.29 (s, 12H, NOBpin-CH_3). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): **2a′:** δ (ppm) 152.3 (s), 133.2 (s), 119.3 (s), 113.9 (s), 104.8 (s), 84.5 (s), 24.5 (s). **^{11}B{^{1}H} NMR** (128 MHz, $CDCl_3$, 25 °C): **2a′:** δ (ppm) 23.7 (s). **HRMS** (ESI) [M+H] $C_{13}H_{18}BN_2O_3$ calc. 261.1405 m/z; found 261.1407 m/z.

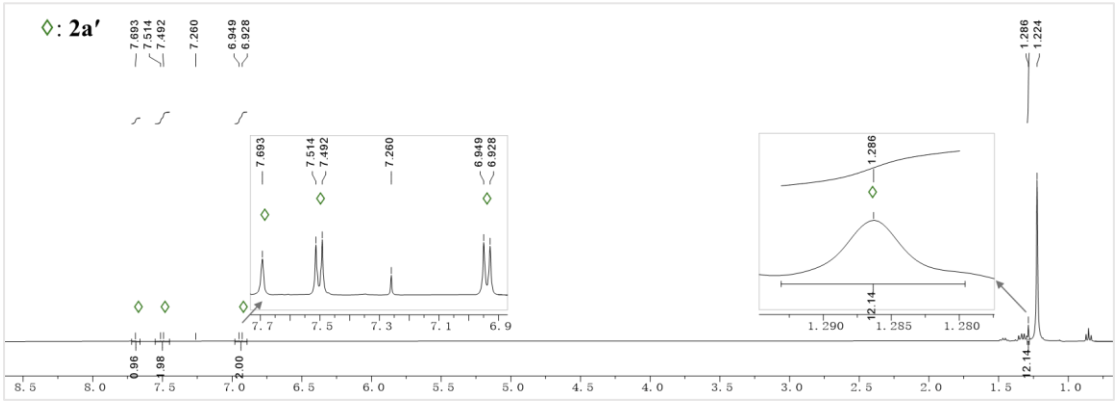


Figure S2: ^{1}H NMR spectrum of **2a′** (400 MHz, $CDCl_3$).

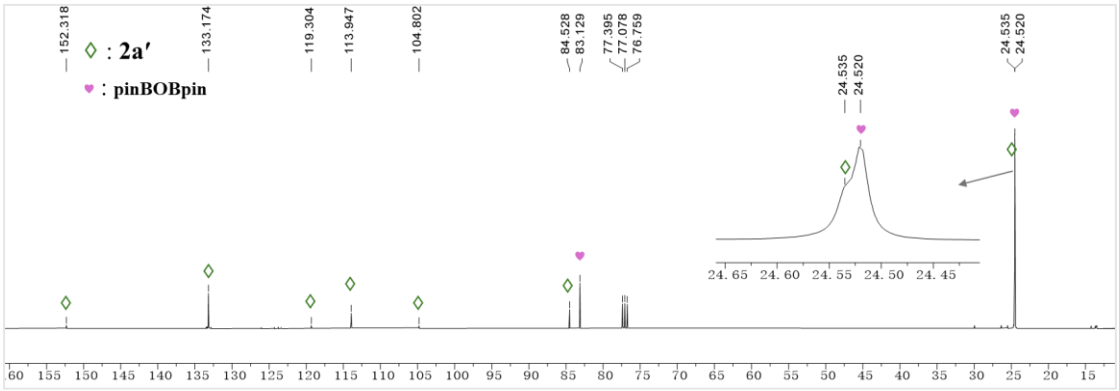


Figure S3: ^{13}C{^{1}H} NMR spectrum of **2a′** (100 MHz, $CDCl_3$).

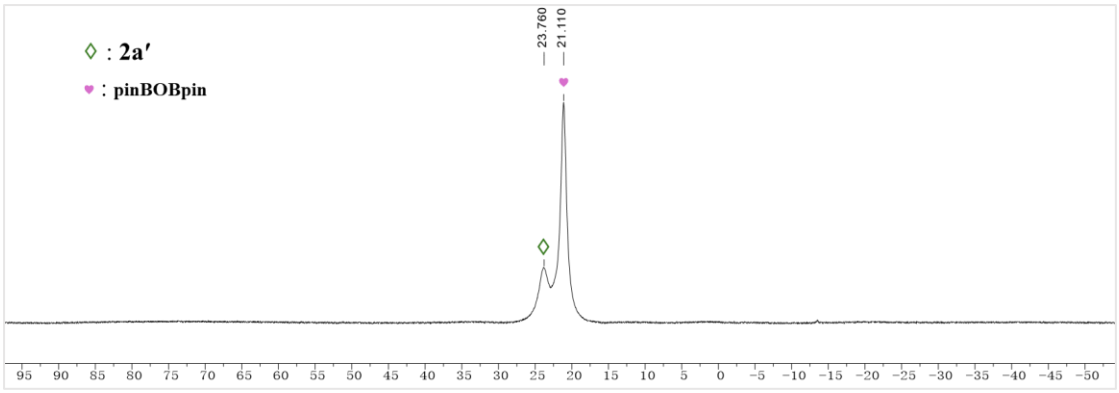


Figure S4: $^{11}B\{^{1}H\}$ NMR spectrum of **2a′** (128 MHz, $CDCl_3$).

The reduction of **1a** with $(MeO)_3SiH$ (3 equiv.) catalyzed by nBu$_3$Sb in $CDCl_3$

1a (14.8 mg, 0.10 mmol), mesitylene (12.0 mg, 0.10 mmol) and $(MeO)_3SiH$ (36.7 mg, 0.3 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. Then nBu$_3$Sb (3.0 mg, 0.01 mmol) was added to the reaction solution. The progress of the reaction was monitored by NMR spectroscopy analysis. After 36 h, the color of the reaction solution changed from colorless to orange and the conversion of **1a** was 94%. The yield of **2Si** (30%) was calculated by ^{1}H NMR using mesitylene as internal standard as shown in Figure S5.

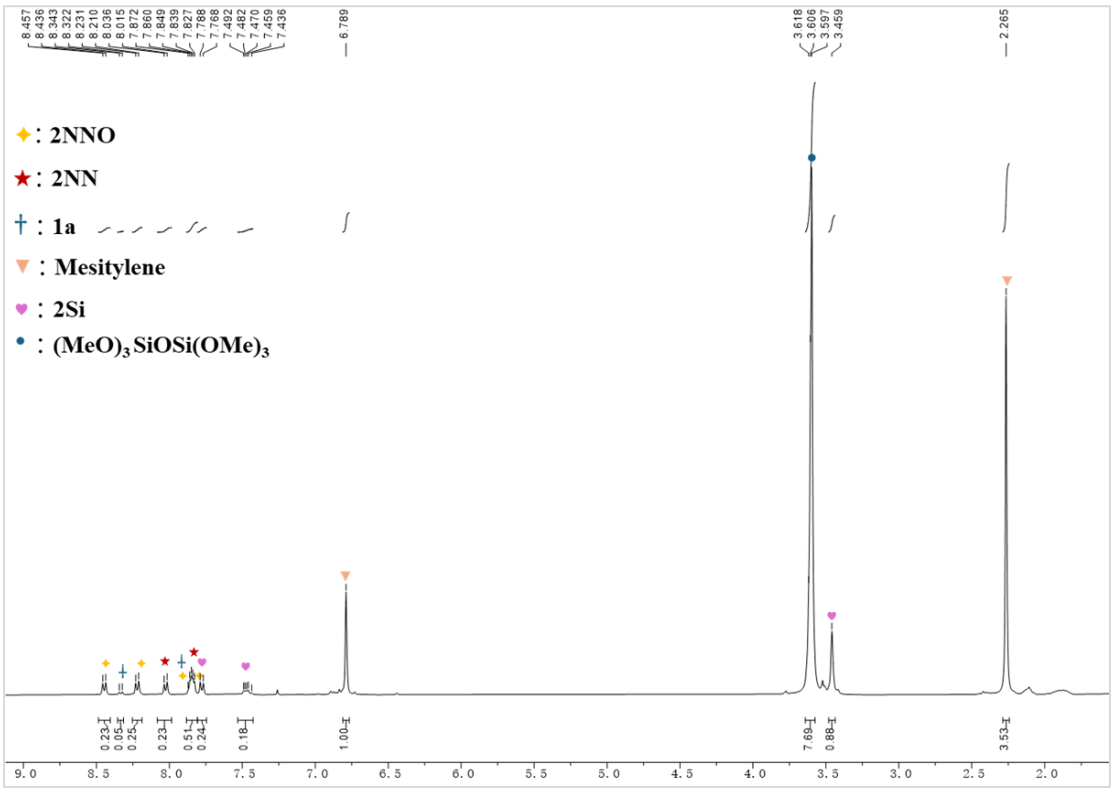


Figure S5: ^{1}H NMR spectrum of reaction solution of **1a** and $(MeO)_3SiH$ (3 equiv.) catalyzed by nBu$_3$Sb with mesitylene as initial standard at r.t. for 36 h (400 MHz, $CDCl_3$).

<u>The reduction of **1a** with H_3NBH_3 (2 equiv.) catalyzed by nBu$_3$Sb in $CDCl_3$</u>

1a (29.6 mg, 0.20 mmol), mesitylene (24.0 mg, 0.20 mmol) and H_3NBH_3 (12.0 mg, 0.4 mmol) were combined in 1.2 mL of $CDCl_3$. The resulting reaction mixture was stirred and analyzed by NMR spectroscopy analysis. Then nBu$_3$Sb (6.0 mg, 0.02 mmol) was added to the reaction solution under stirring. After 18 h, the reaction solution turned red with the formation of a white precipitate. The precipitate was separated by filtration, and the reaction solution was transformed into an NMR tube. The progress of the reaction solution was analyzed by NMR spectroscopy. **1a** was fully consumed as shown in Figure S6.

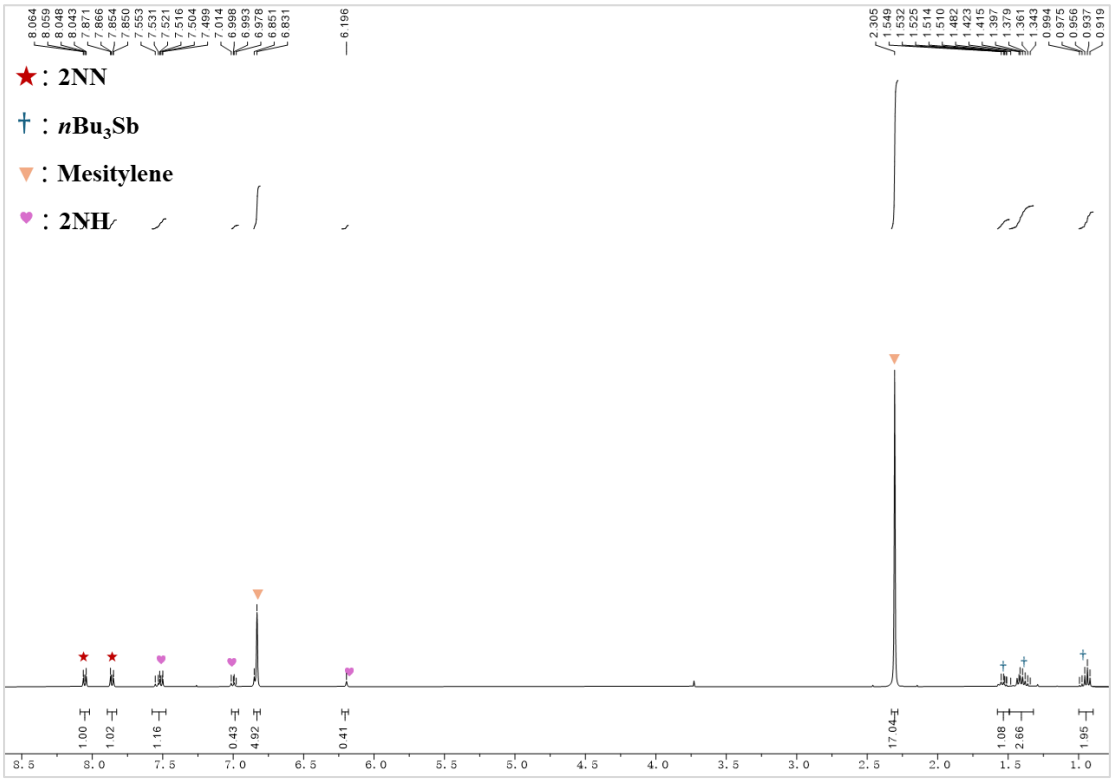


Figure S6: ^{1}H NMR spectrum of reaction solution of **1a** and H_3NBH_3 (2 equiv.) catalyzed by nBu$_3$Sb with mesitylene as initial standard at r.t. for 18 h (400 MHz, $CDCl_3$).

<u>The reduction of **1a** with Et_2SiH_2 (2 equiv.) catalyzed by nBu$_3$Sb in $CDCl_3$</u>

1a (14.8 mg, 0.10 mmol), mesitylene (12.0 mg, 0.10 mmol) and Et_2SiH_2 (26.5 mg, 0.2 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. Then nBu$_3$Sb (3.0 mg, 0.01 mmol) was added to the reaction solution. The NMR tube was placed into an oil bath heated at 60 °C. The progress of the reaction was monitored by NMR spectroscopy analysis. After 36 h, the conversion of **1a** was 15% as shown in Figure S7.

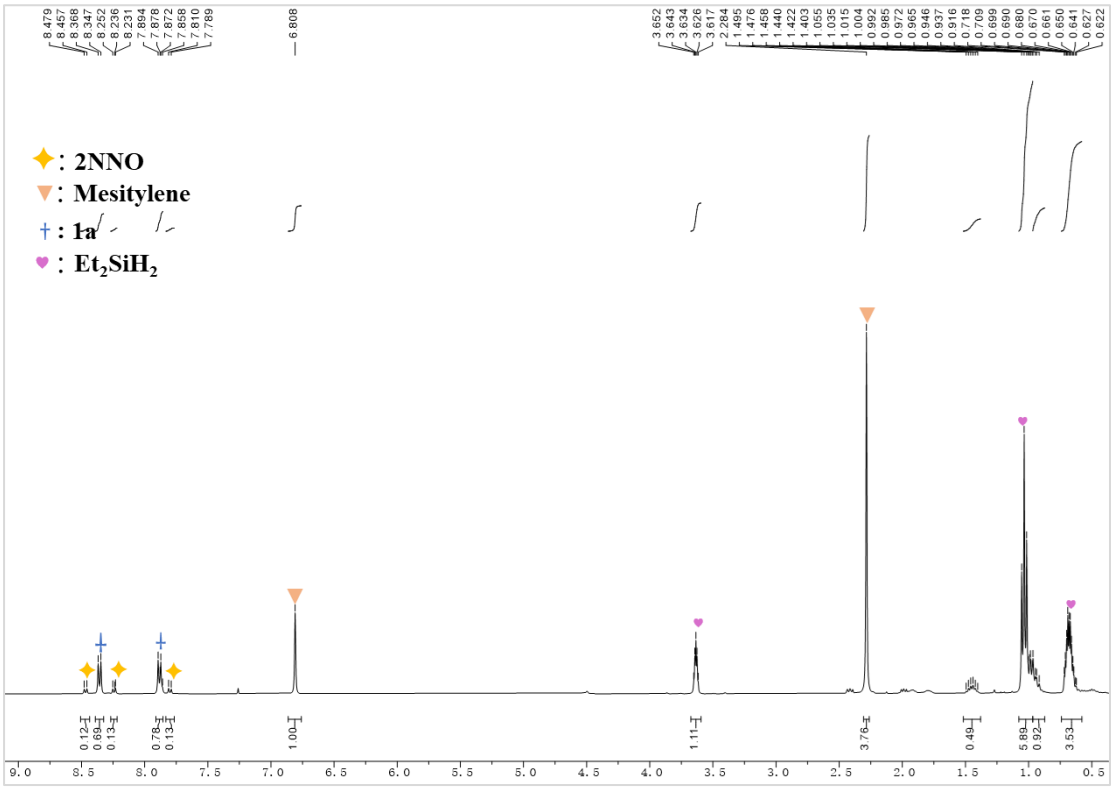


Figure S7: ^{1}H NMR spectrum of reaction solution of **1a** and Et_2SiH_2 (2 equiv.) catalyzed by nBu$_3$Sb with mesitylene as initial standard at 60°C for 36 h (400 MHz, $CDCl_3$).

The reduction of **1a** with HBpin catalyzed by Me_3Sb in $CDCl_3$

1a (14.8 mg, 0.10 mmol), mesitylene (12.0 mg, 0.10 mmol) and HBpin (38.4 mg, 0.30 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. Then Me_3Sb·46.7Et_2O (33.9 mg, 0.01 mmol) was added to the reaction solution. The progress of the reaction was monitored by NMR spectroscopy analysis. After 18 h, the conversion of **1a** was 13%, and the yield of **2a′** was 13% calculated by ^{1}H NMR using mesitylene as internal standard as shown in Figure S8.

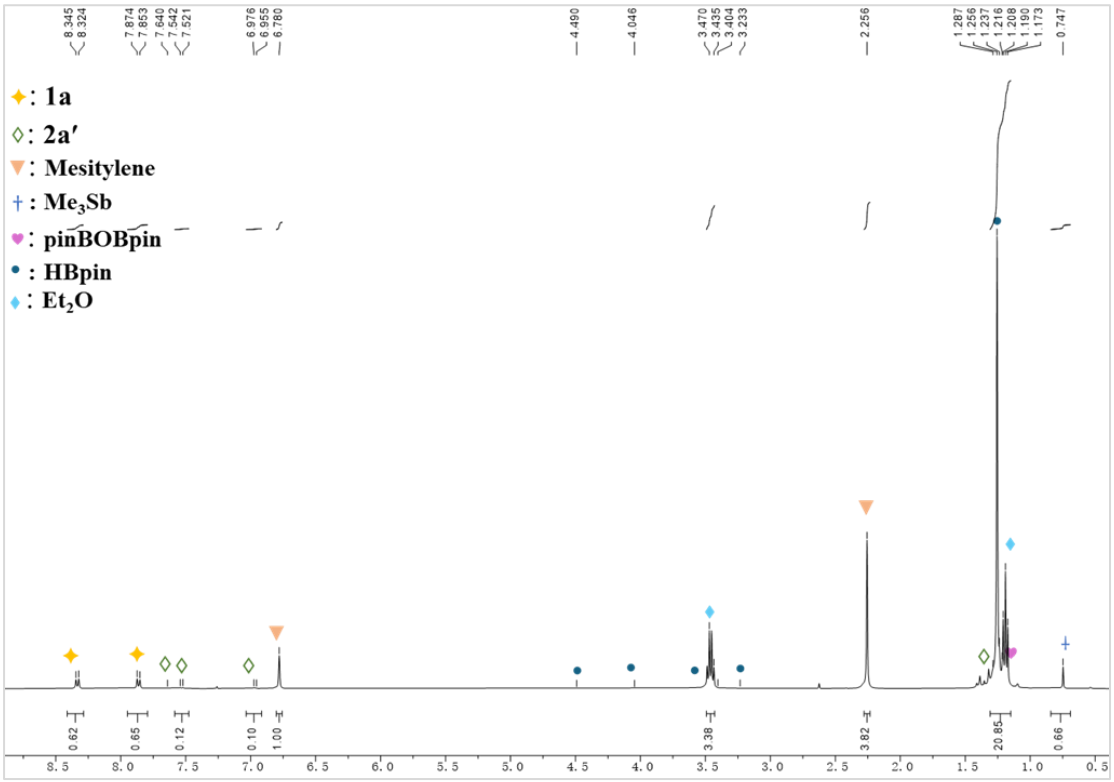


Figure S8: ^{1}H NMR spectrum of reaction solution of **1a** and HBpin (3 equiv.) catalyzed by Me_3Sb with mesitylene as initial standard at r.t. for 18 h (400 MHz, $CDCl_3$).

The reduction of **1a** with HBpin catalyzed by Et_3Sb in $CDCl_3$

1a (14.8 mg, 0.10 mmol), mesitylene (12.0 mg, 0.10 mmol) and HBpin (38.4 mg, 0.30 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. Then Et_3Sb (2.1 mg, 0.01 mmol) was added to the reaction solution. The progress of the reaction was monitored by NMR spectroscopy analysis. After 18 h, the conversion of **1a** was 84%, and the yield of **2a′**was 84% calculated by ^{1}H NMR using mesitylene as internal standard as shown in Figure S9.

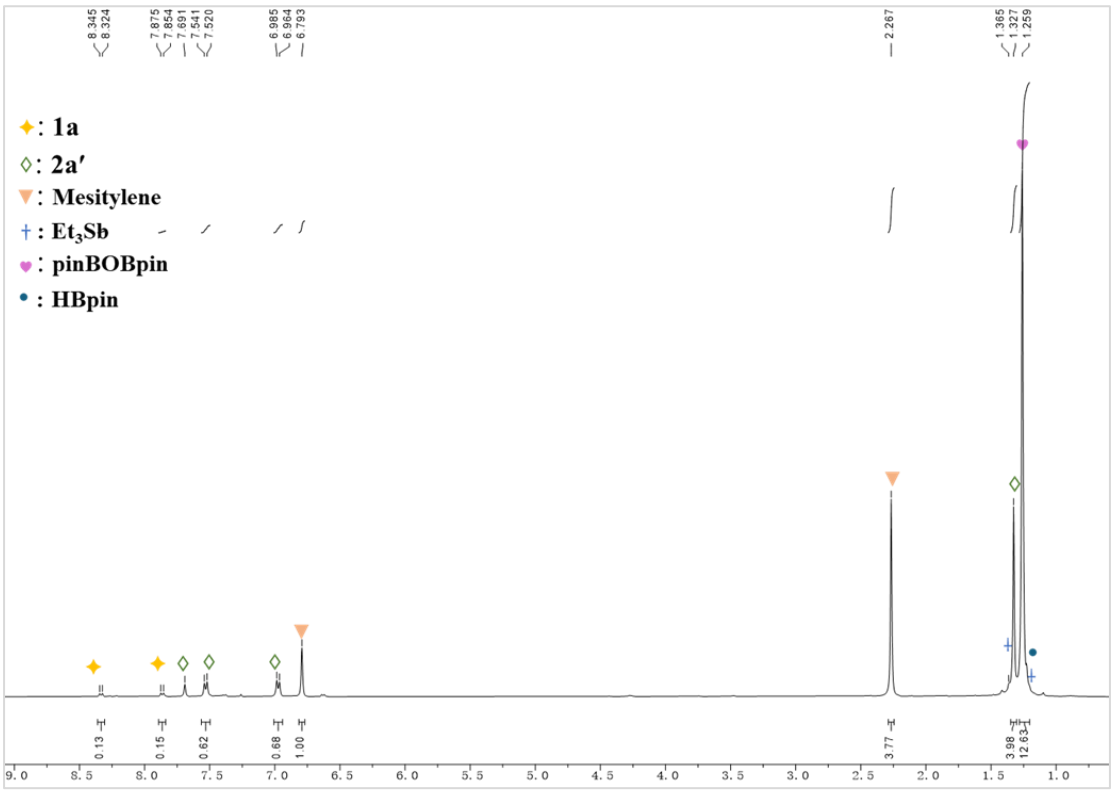


Figure S9: ^{1}H NMR spectrum of reaction solution of **1a** and HBpin (3 equiv.) catalyzed by Et_3Sb with mesitylene as initial standard at r.t. for 18 h (400 MHz, $CDCl_3$).

The reduction of **1a** with HBpin catalyzed by *n*Pr_3Sb in $CDCl_3$

1a (14.8 mg, 0.10 mmol), mesitylene (12.0 mg, 0.10 mmol) and HBpin (38.4 mg, 0.30 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. Then *n*Pr_3Sb (2.5 mg, 0.01 mmol) was added to the reaction solution. The progress of the reaction was monitored by NMR spectroscopy analysis. After 18 h, the conversion of **1a** was 66%. The yield of **2a′** (66%) was calculated by ^{1}H NMR using mesitylene as internal standard as shown in Figure S10.

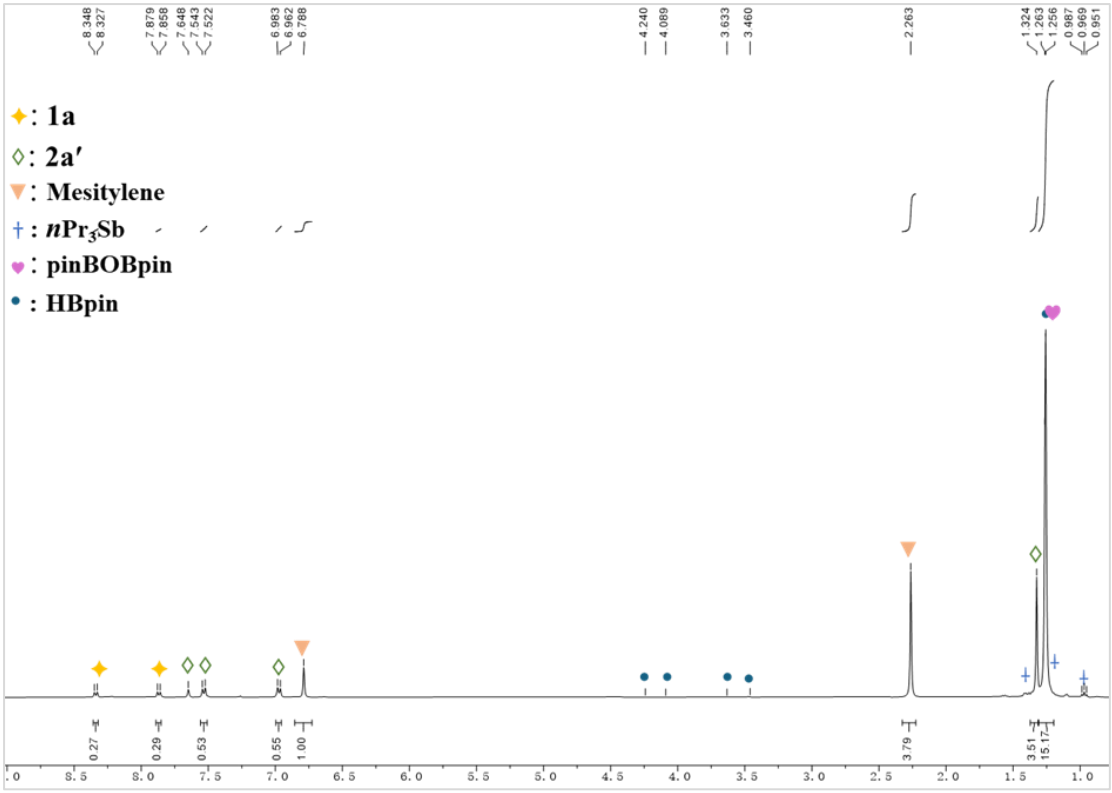


Figure S10: ^{1}H NMR spectrum of reaction solution of **1a** and HBpin (3 equiv.) catalyzed by *n*Pr$_3$Sb with mesitylene as initial standard at r.t. for 18 h (400 MHz, $CDCl_3$).

The reduction of **1a** with HBpin catalyzed by Ph_3Sb in $CDCl_3$

1a (14.8 mg, 0.10 mmol), mesitylene (12.0 mg, 0.10 mmol) and HBpin (38.4 mg, 0.30 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. Then Ph_3Sb (3.5 mg, 0.01 mmol) was added to the reaction solution. The progress of the reaction was monitored by NMR spectroscopy analysis. After 18 h, no reaction was observed as shown in Figure S11.

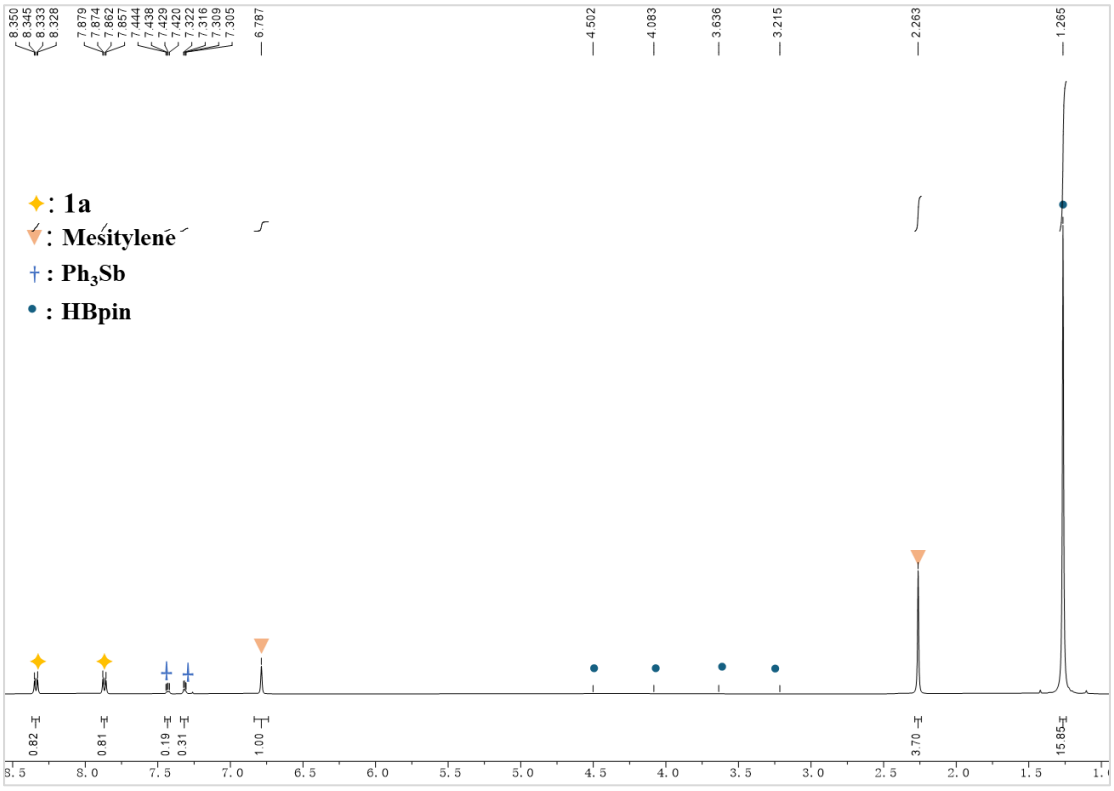


Figure S11: ^{1}H NMR spectrum of reaction solution of **1a** and HBpin (3 equiv.) catalyzed by Ph_3Sb with mesitylene as initial standard at r.t. for 18 h (400 MHz, $CDCl_3$).

The reaction of **1a** and HBpin

1a (14.8 mg, 0.10 mmol), mesitylene (12.0 mg, 0.10 mmol) and HBpin (38.4 mg, 0.30 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy analysis. The NMR tube was placed into an oil bath heated at 60 °C. The progress of the reaction was monitored by NMR spectroscopy analysis. After 18 h, no reaction was observed as shown in Figure S12.

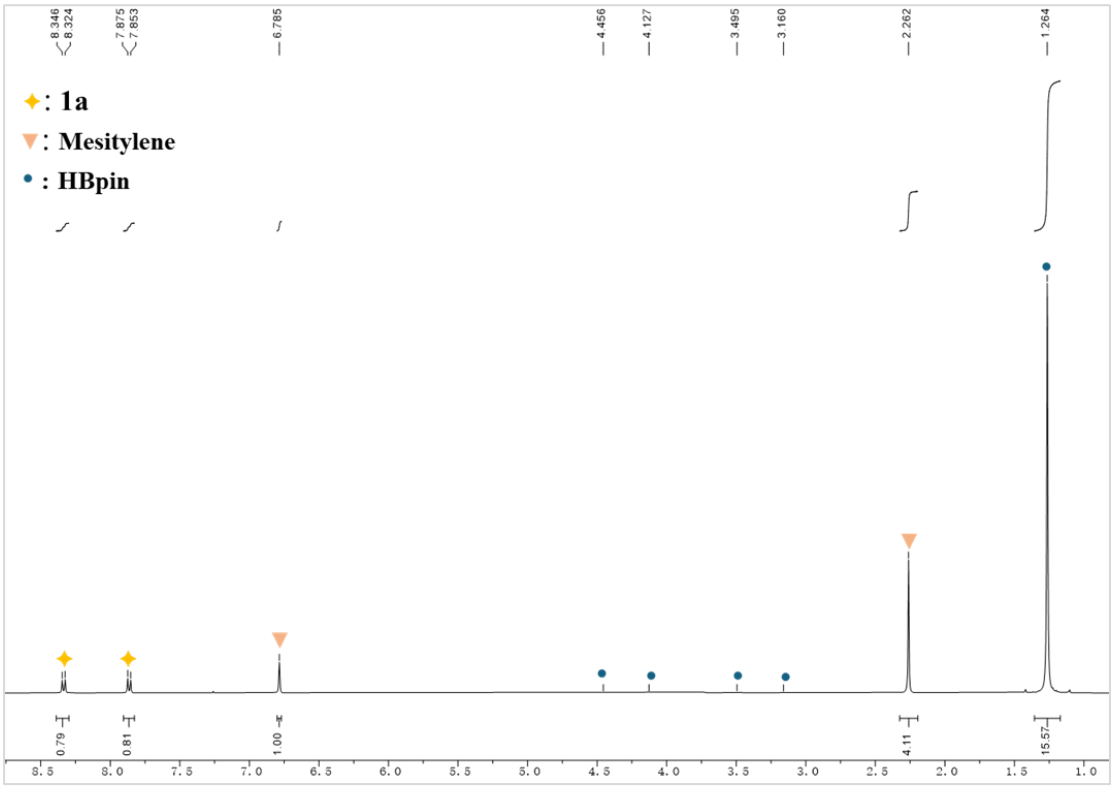
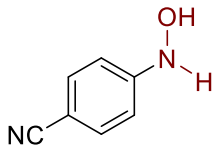


Figure S12: ^{1}H NMR spectrum of reaction solution of **1a** and HBpin (3 equiv.) with mesitylene as initial standard at 60°C for 18 h (400 MHz, $CDCl_3$).

The reduction of **1a** with 3 equiv. of HBpin catalyzed by *n*Bu_3Sb in $CHCl_3$



1a (148.4 mg, 1.0 mmol), HBpin (385.3 mg, 3.0 mmol) and *n*Bu_3Sb (29.8 mg, 0.10 mmol) were combined in 5 mL of $CHCl_3$ in a Schlenk tube. The tube was sealed and placed into an oil bath heated at 25 °C. The reaction solution was stirred at 25 °C for 18 h. All volatiles were removed under reduced pressure using a rotary evaporator. 4-(Hydroxyamino)benzonitrile (**2a**) was obtained as a white solid (125 mg, yield 93%) after purification by column chromatography on silica gel (hexane/DCM = 100:15, v/v). **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.54 (d, $^{3}J_{H\text{-}H}$ = 8.7 Hz, 2H, NHAr-*H*), 7.00 (d, $^{3}J_{H\text{-}H}$ = 8.7 Hz, 2H, CNAr-*H*), 7.00 (s, 1H, ArNO*H*), 5.54 (s, 1H, ArN*H*). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 153.6 (s), 133.4 (s), 119.5 (s), 113.6 (s), 104.1 (s).

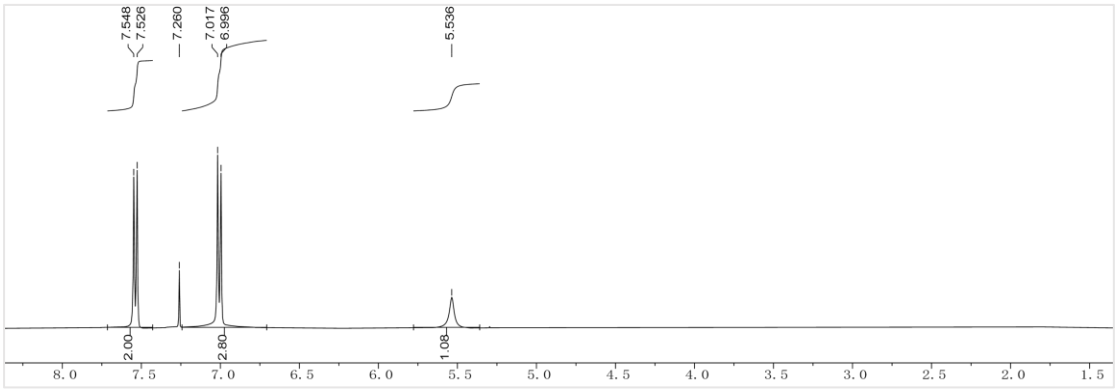


Figure S13: ^{1}H NMR spectrum of **2a** (400 MHz, $CDCl_3$).

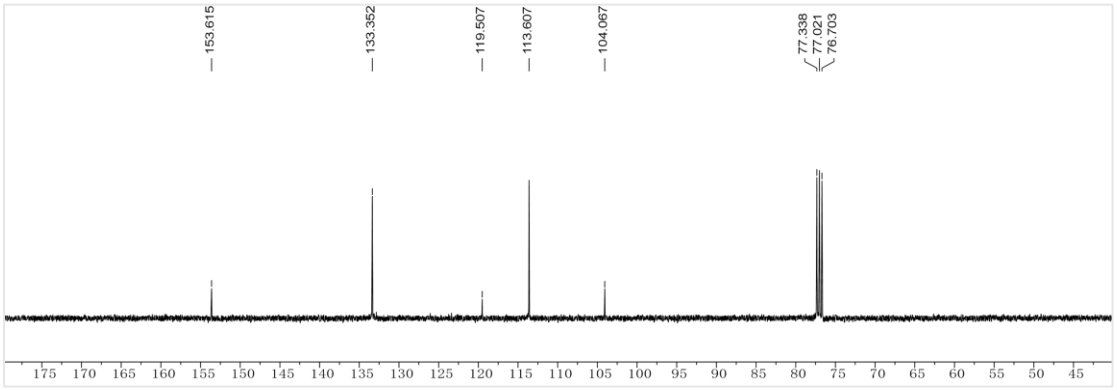


Figure S14: $^{13}C\{^{1}H\}$ NMR spectrum of **2a** (100 MHz, $CDCl_3$).

The reduction of **1a** with 3 equiv. of HBpin catalyzed by nBu$_3$Sb in DCM

1a (147.8 mg, 1.0 mmol), HBpin (386.0 mg, 3.0 mmol) and nBu$_3$Sb (29.6 mg, 0.10 mmol) were combined in 5 mL of DCM in a Schlenk tube. The tube was sealed and placed into an oil bath heated at 25 °C. The reaction solution was stirred at 25 °C for 18 h. All volatiles were removed under reduced pressure using a rotary evaporator. **2a** was obtained as a white solid (118 mg, yield 88%) after purification by column chromatography on silica gel (hexane/DCM = 100:15, v/v).

The reduction of **1a** with 3 equiv. of HBpin catalyzed by nBu$_3$Sb in THF

1a (148.1 mg, 1.0 mmol), HBpin (384.8 mg, 3.0 mmol) and nBu$_3$Sb (29.3 mg, 0.10 mmol) were combined in 5 mL of THF in a Schlenk tube. The tube was sealed and placed into an oil bath heated at 25 °C. The reaction solution was stirred at 25 °C for 18 h. All volatiles were removed under reduced pressure using a rotary evaporator. **2a**

was obtained as a white solid (81 mg, yield 60%) after purification by column chromatography on silica gel (hexane/DCM = 100:15, v/v).

The reduction of **1a** with 3 equiv. of HBpin catalyzed by nBu$_3$Sb in MeCN

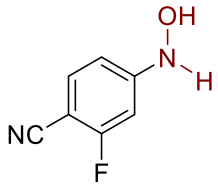
1a (148.0 mg, 1.0 mmol), HBpin (384.8 mg, 3.0 mmol) and nBu$_3$Sb (30.1 mg, 0.10 mmol) were combined in 5 mL of MeCN in a Schlenk tube. The tube was sealed and placed into an oil bath heated at 25 °C. The reaction solution was stirred at 25 °C for 18 h. All volatiles were removed under reduced pressure using a rotary evaporator. **2a** was obtained as a white solid (62 mg, yield 46%) after purification by column chromatography on silica gel (hexane/DCM = 100:15, v/v).

The reduction of **1a** with 3 equiv. of HBpin catalyzed by Me$_3$Sb in CHCl$_3$

1a (148.4 mg, 1.0 mmol), HBpin (385.3 mg, 3.0 mmol) and Me$_3$Sb (33.6 mg, 0.20 mmol) were combined in 5 mL of CHCl$_3$ in a Schlenk tube. The tube was sealed and placed into an oil bath heated at 40 °C. The reaction solution was stirred at 40 °C for 24 h. All volatiles were removed under reduced pressure using a rotary evaporator. **2a** was obtained as a white solid (104 mg, yield 77%) after purification by column chromatography on silica gel (hexane/DCM = 1:1, v/v).

2.2 The transformations of nitroarenes to hydroxylanilines

Synthesis of **2b**



2-Fluoro-4-(hydroxyamino)benzonitrile (**2b**) was synthesized as white solid (147 mg, yield 97%) following the synthetic protocol for **2a**. The reaction involved the use of nBu$_3$Sb (29.5 mg, 0.10 mmol), 2-fluoro-4-nitrobenzonitrile (**1b**) (166.3 mg, 1.0 mmol), and HBpin (387.0 mg, 3.0 mmol). The reaction solution was stirred at 25 °C for 18 h. **2b** was purified by column chromatography on silica gel (hexane/EtOAc = 100:5, v/v). **^{1}H NMR** (400 MHz, DMSO-d_6, 25 °C): δ (ppm) 9.51 (s, 1H, ArNO*H*), 9.04 (s, 1H, ArN*H*), 7.55 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H,F-Ar-*o*-*H*), 6.63 (m, 2H, NCAr-*o*-*H*, NCAr-*m*-*H*). **^{13}C{^{1}H}**

NMR (100 MHz, DMSO-d_6, 25 °C): δ (ppm) 165.8 163.3 (d, $J_{C\text{-}F}$ = 251.1 Hz), 158.0 (d, $J_{C\text{-}F}$ = 11.4 Hz), 134.2 (d, $J_{C\text{-}F}$ = 2.5 Hz), 115.9 (s), 108.3 (s), 97.7 (d, $J_{C\text{-}F}$ = 24.1 Hz), 87.2 (d, $J_{C\text{-}F}$ = 15.9 Hz). **^{19}F{^{1}H} NMR** (376 MHz, DMSO-d_6, 25 °C): δ (ppm) 108.3 (s). **HRMS** (ESI) [M+H] $C_7H_6FN_2O$ calc. 153.0459 m/z; found 153.0460 m/z.

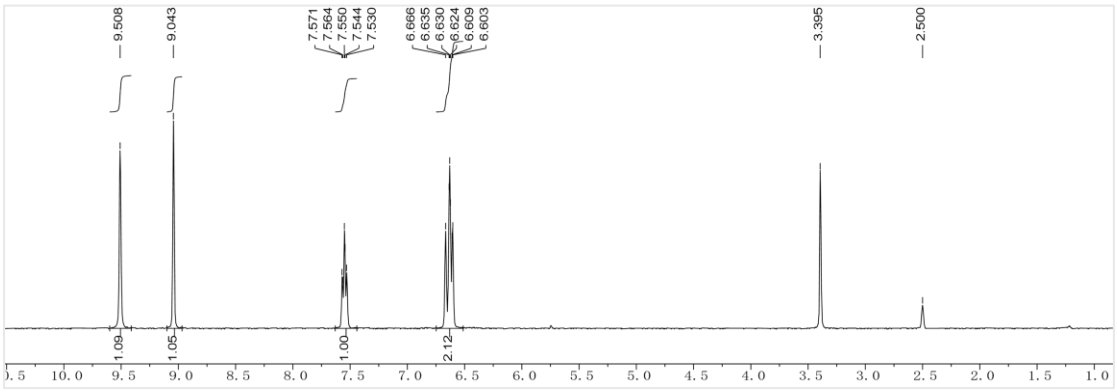


Figure S15: ^{1}H NMR spectrum of **2b** (400 MHz, DMSO-d_6).

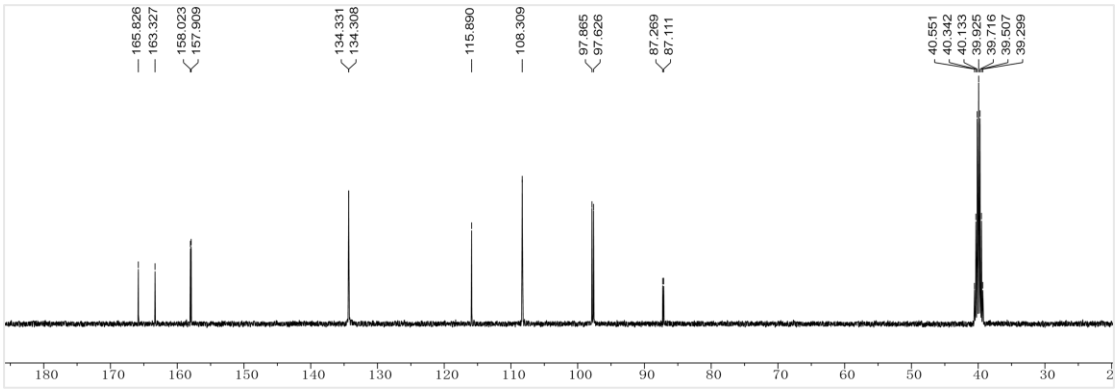


Figure S16: ^{13}C{^{1}H} NMR spectrum of **2b** (100 MHz, DMSO-d_6).

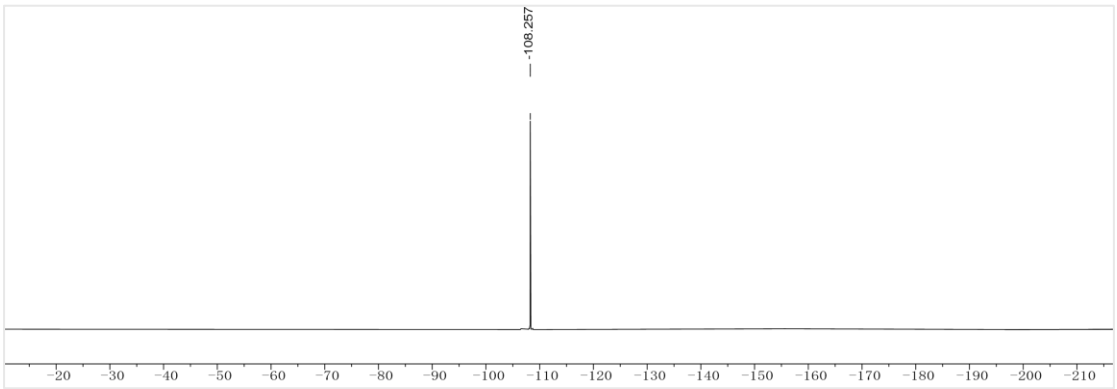
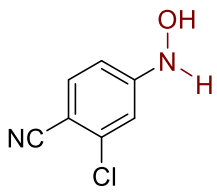


Figure S17: ^{19}F{^{1}H} NMR spectrum of **2b** (376 MHz, DMSO-d_6).

Synthesis of **2c**



2-Chloro-4-(hydroxyamino)benzonitrile (**2c**) was synthesized as white solid (153 mg, yield 91%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu_3Sb (29.5 mg, 0.10 mmol), 2-chloro-4-nitrobenzonitrile (**1c**) (182.3 mg, 1.0 mmol), and HBpin (386.0 mg, 3.0 mmol). The reaction solution was stirred at 25 °C for 13 h. **2c** was purified by column chromatography on silica gel (hexane/DCM = 2:3, v/v). **^{1}H NMR** (400 MHz, DMSO-d_6, 25 °C): δ (ppm) 9.45 (s, 1H, ArNO*H*), 9.02 (s, 1H, ArN*H*), 7.62 (d, $^3J_{H\text{-}H}$ = 8.7 Hz, 1H,NCAr-*o*-*H*), 6.90 (d, $^4J_{H\text{-}H}$ = 2.1 Hz, 1H, ClAr-*o*-*H*), 6.75 (dd, $^3J_{H\text{-}H}$ = 8.7 Hz, $^4J_{H\text{-}H}$ = 2.1 Hz, 1H, NCAr-*m*-*H*). **^{13}C{^{1}H} NMR** (100 MHz, DMSO-d_6, 25 °C): δ (ppm) 156.5 (s), 136.9 (s), 135.3 (s), 117.8 (s), 111.4 (s), 110.6 (s), 99.3 (s). **HRMS** (ESI) [M+H] $C_7H_6ClN_2O$ calc. 169.0163 m/z; found 169.0164 m/z.

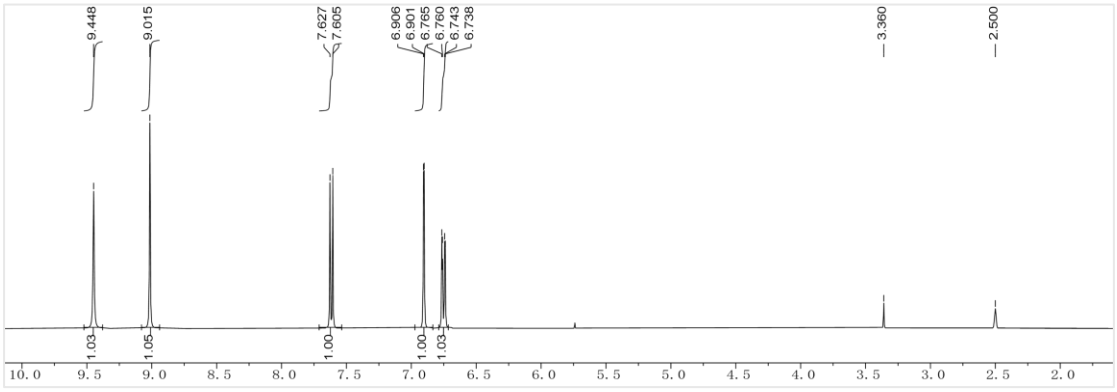


Figure S18: ^{1}H NMR spectrum of **2c** (400 MHz, DMSO-d_6).

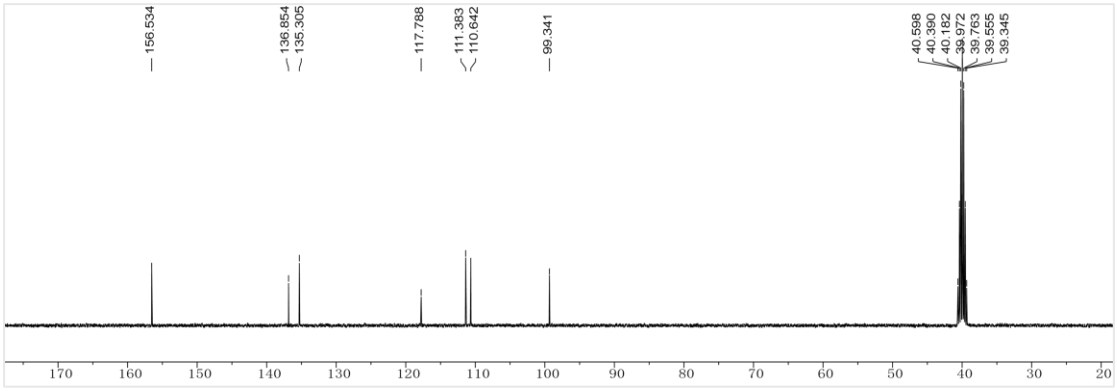
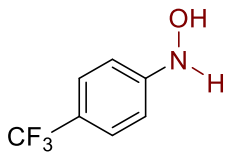


Figure S19: ^{13}C{^{1}H} NMR spectrum of **2c** (100 MHz, DMSO-d_6).

Synthesis of **2d**



(4-(Trifluoromethyl)phenyl)hydroxylamine (**2d**) was synthesized as white solid (76 mg, yield 45%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu$_3$Sb (29.3 mg, 0.10 mmol), 1-nitro-4-(trifluoromethyl)benzene (**1d**) (191.2 mg, 1.0 mmol), and HBpin (384.6 mg, 3.0 mmol). The reaction took 20 h at 25 °C, **2d** was purified by column chromatography on silica gel (hexane/DCM = 1:5, v/v). **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.53 (d, $^3J_{H\text{-}H}$ = 8.5 Hz, 2H, NAr-*o*-*H*), 7.04 (d, $^3J_{H\text{-}H}$ = 8.5 Hz, 2H, NAr-*m*-*H*), 6.95 (s, 1H, ArNHO*H*), 5.53 (s, 1H, ArN*H*). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 152.5 (s), 126.3 (q, $J_{C\text{-}F}$ = 3.8 Hz), 125.7 (s), 123.7 (m), 113.6 (s). **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$, 25 °C): δ (ppm) 61.7 (s).

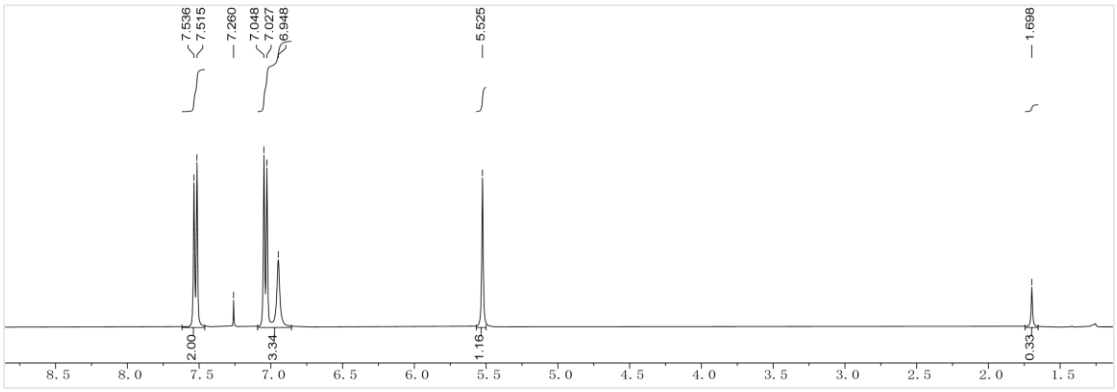


Figure S20: ^{1}H NMR spectrum of **2d** (400 MHz, $CDCl_3$).

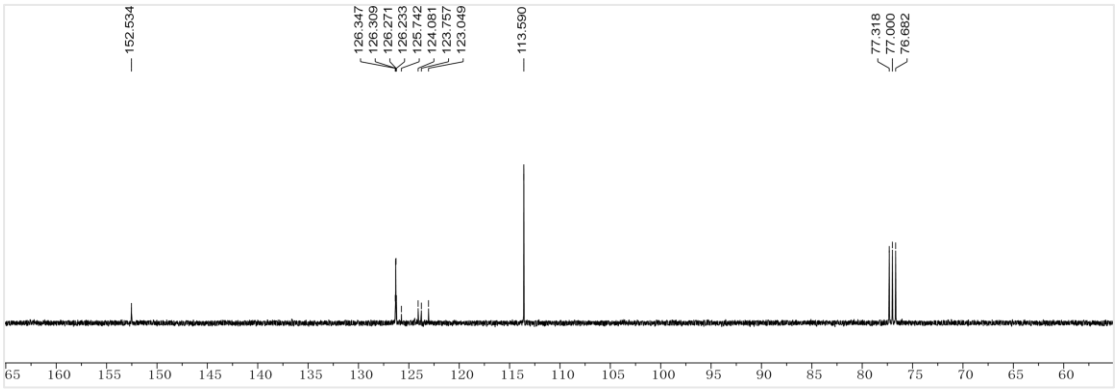


Figure S21: ^{13}C{^{1}H} NMR spectrum of **2d** (100 MHz, $CDCl_3$).

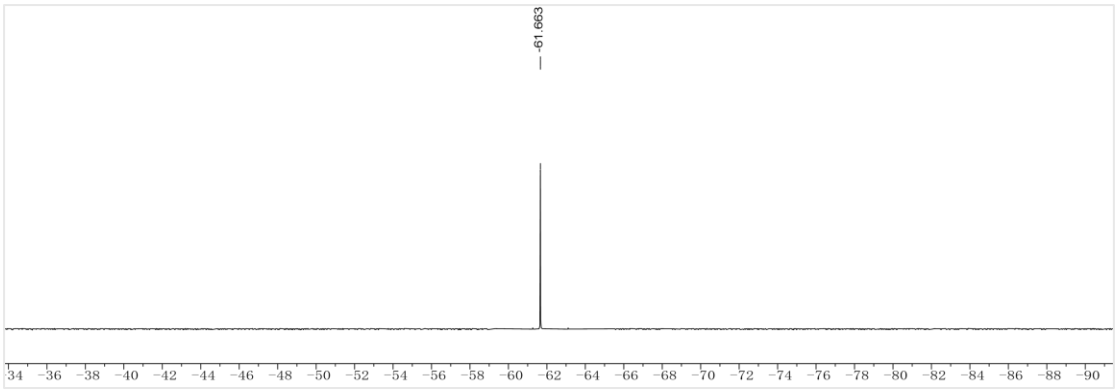
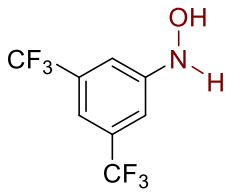


Figure S22: $^{19}F\{^{1}H\}$ NMR spectrum of **2d** (376 MHz, $CDCl_3$).

Synthesis of **2e**



(3,5-Bis(trifluoromethyl)phenyl)hydroxylamine (**2e**) was synthesized as white solid (144 mg, yield 59%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu_3Sb (29.3 mg, 0.10 mmol), 1-nitro-3,5-bis(trifluoromethyl)benzene (**1e**) (191.2 mg, 1.0 mmol), and HBpin (384.6 mg, 3.0 mmzol). The reaction took 20 h at 25 °C, **2e** was purified by column chromatography on silica gel (hexane/DCM = 1:5, v/v). **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.44 (s, 1H, NHAr-*p*-*H*), 7.40 (s, 2H, NHAr-*o*-*H*), 7.04 (s, 1H, ArNHO*H*), 5.55 (s, 1H, ArN*H*). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 150.9 (s), 132.3 (q, $J_{C\text{-}F}$ = 33.3 Hz), 123.1 (q, $J_{C\text{-}F}$ = 273.1 Hz), 115.3 (p, $J_{C\text{-}F}$ = 3.9 Hz), 113.8 (d, $J_{C\text{-}F}$ = 15.1 Hz). **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$, 25 °C): δ (ppm) 63.2 (s).

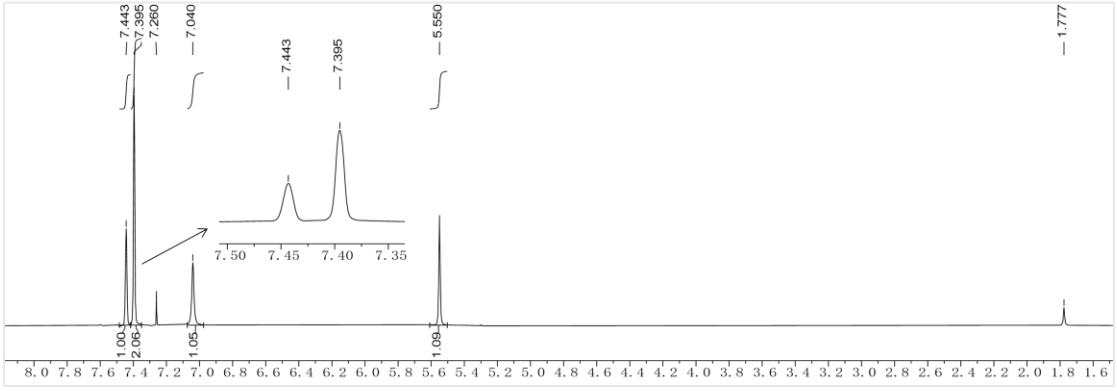


Figure S23: ^{1}H NMR spectrum of **2e** (400 MHz, $CDCl_3$).

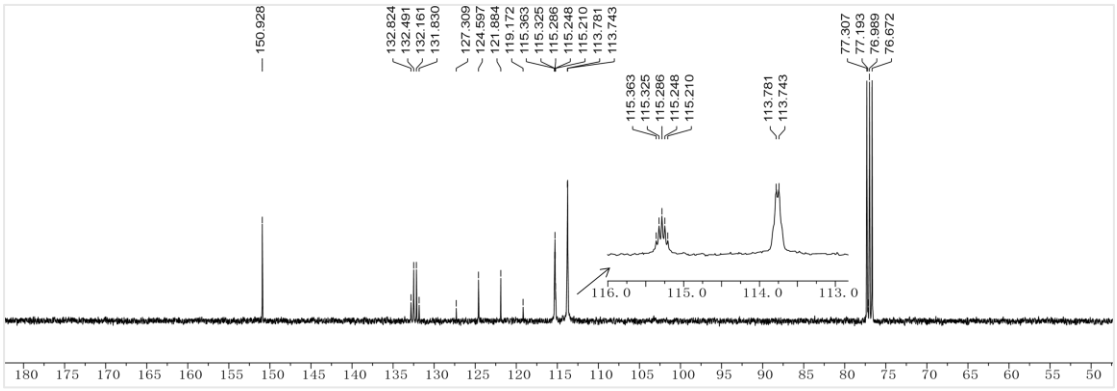


Figure S24: $^{13}C\{^{1}H\}$ NMR spectrum of **2e** (100 MHz, $CDCl_3$).

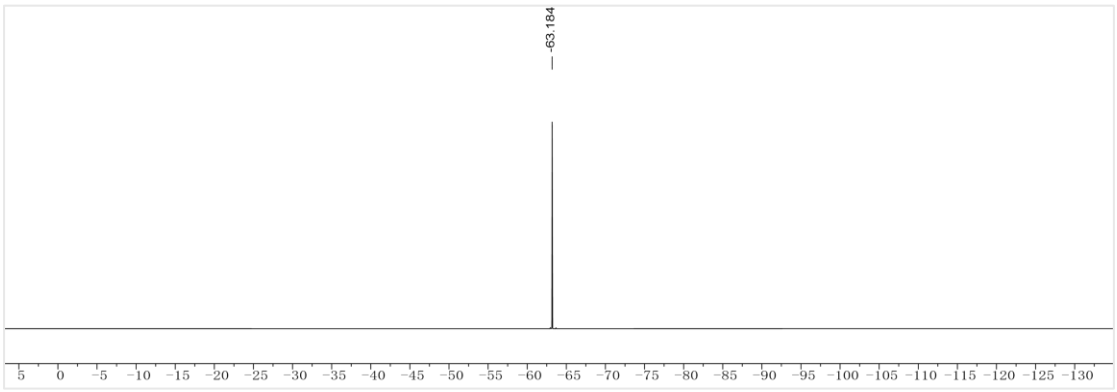
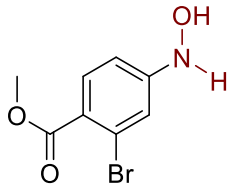


Figure S25: $^{19}F\{^{1}H\}$ NMR spectrum of **2e** (376 MHz, $CDCl_3$).

Synthesis of **2f**



Methyl-2-bromo-4-(hydroxyamino)benzoate (**2f**) was synthesized as white solid (170 mg, yield 69%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu_3Sb (29.2 mg, 0.10 mmol), methyl 2-bromo-4-nitrobenzoate (**1f**) (260.2 mg, 1.0 mmol), and HBpin (388.0 mg, 3.0 mmol). The reaction took 20 h at 25 °C, **2f** was purified by column chromatography on silica gel (DCM/EtOAc= 10:1, v/v). **^{1}H NMR** (400 MHz, DMSO-d_6, 25 °C): δ (ppm) 9.12 (s, 1H, ArNO*H*), 8.82 (s, 1H, ArN*H*), 7.72 (d, $^{3}J_{H\text{-}H}$ = 8.6 Hz, 1H, OCAr-*o*-*H*), 7.06 (d, $^{3}J_{H\text{-}H}$ = 2.2 Hz, 1H, BrAr-*o*-*H*), 6.78 (dd, $^{3}J_{H\text{-}H}$ = 8.7 Hz, $^{4}J_{H\text{-}H}$ = 2.2 Hz, 1H, BrAr-*p*-*H*), 3.76 (s, 3H, O-C*H*$_3$) **^{13}C{^{1}H} NMR** (100 MHz, DMSO-d_6, 25 °C): δ (ppm) 165.6 (s), 155.9 (s), 133.3 (s), 123.0 (s), 119.6 (s), 116.7 (s), 110.8 (s), 52.2 (s). **HRMS** (ESI) [M+H] $C_8H_9BrNO_3$ calc. 245.9760 m/z; found 245.9759 m/z.

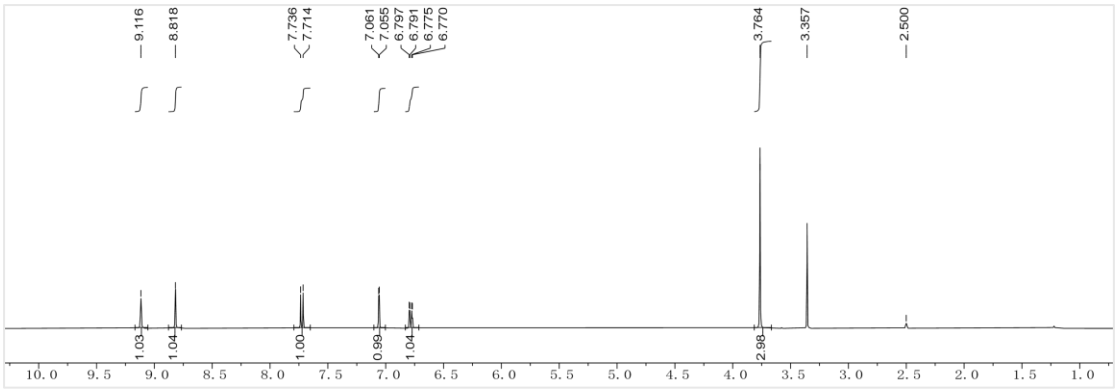


Figure S26: ^{1}H NMR spectrum of **2f** (400 MHz, DMSO-d_6).

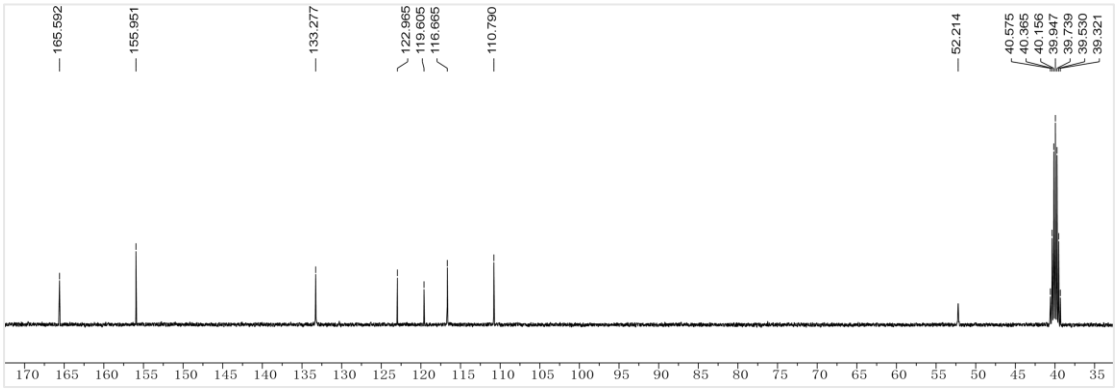
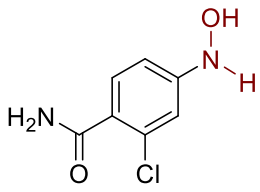


Figure S27: ^{13}C{^{1}H} NMR spectrum of **2f** (100 MHz, DMSO-d_6).

Synthesis of **2g**



2-Chloro-4-(hydroxyamino)benzamide (**2g**) was synthesized as white solid (120 mg, yield 65%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu$_3$Sb (29.6 mg, 0.10 mmol), 2-chloro-4-nitrobenzamide (**1g**) (200.2 mg, 1.0 mmol), and HBpin (514.0 mg, 4.0 mmol). The reaction took 20 h at 25 °C, **2g** was purified by column chromatography on silica gel (hexane/EtOAc = 1:1, v/v). **^{1}H NMR** (400 MHz, DMSO-d_6, 25 °C): δ (ppm) 8.72 (s, 1H, ArNO*H*), 8.61 (s, 1H, ArN*H*), 7.59 (s, 1H, OC-NH_2), 7.32 (d, $^{3}J_{H\text{-}H}$ = 8.4 Hz, 1H, ClAr-*m*-*H*), 7.32 (s, 1H, OC-NH_2) 6.82 (d, $^{4}J_{H\text{-}H}$ = 1.9 Hz, 1H, ClAr-*o*-*H*), 6.72(dd, $^{2}J_{H\text{-}H}$ = 8.4 Hz, $^{4}J_{H\text{-}H}$ = 1.9 Hz, 1H, ClAr-*p*-*H*). **^{13}C{^{1}H} NMR** (100 MHz, DMSO-d_6, 25 °C): δ (ppm) 168.6 (s), 154.4 (s), 131.2 (s), 130.3 (s), 126.8 (s), 113.1 (s), 111.0 (s). **HRMS** (ESI) [M+H] $C_7H_8ClN_2O_2$ calc. 187.0269 m/z; found 187.0270 m/z.

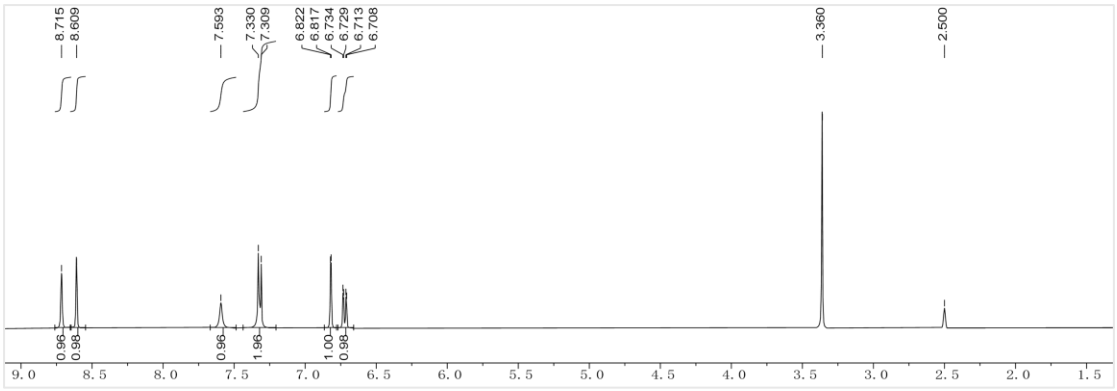


Figure S28: ^{1}H NMR spectrum of **2g** (400 MHz, DMSO-d_6).

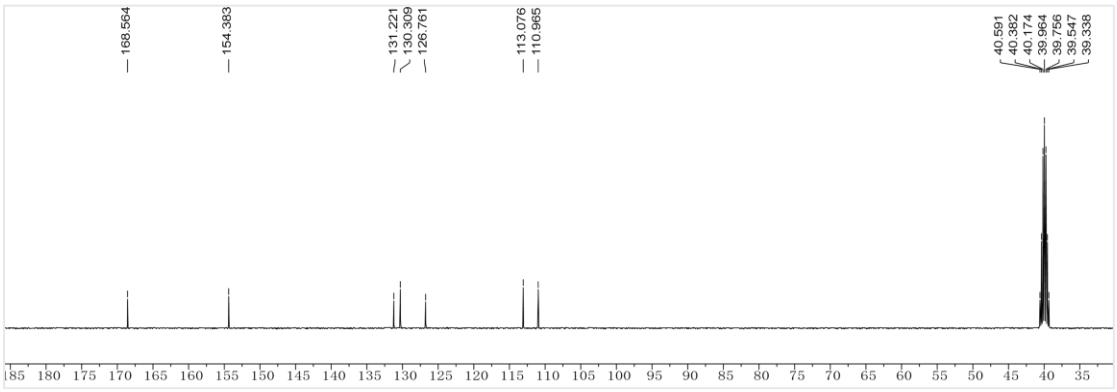
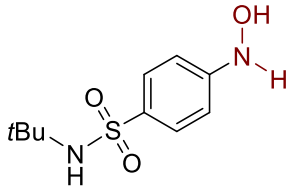


Figure S29: ^{13}C{^{1}H} NMR spectrum of **2g** (100 MHz, DMSO-d_6).

Synthesis of **2h**



(Tert-butyl)-4-(hydroxyamino)benzenesulfonamide (**2h**) was synthesized as white solid (178 mg, yield 73%) following the synthetic protocol for **2a**. The reaction involved the use of nBu$_3$Sb (29.3 mg, 0.10 mmol), n-(tert-butyl)-4-nitrobenzenesulfonamide (**1h**) (258.1 mg, 1.0 mmol), and HBpin (512.3 mg, 4.0 mmol). The reaction took 64 h at 25 °C, **2h** was purified by column chromatography on silica gel (hexane/EtOAc = 1:1, v/v). **^{1}H NMR** (400 MHz, DMSO-d_6, 25 °C): δ (ppm) 8.88 (s, 1H, ArNO*H*), 8.63 (s, 1H, ArN*H*), 7.58 (d, $^{3}J_{H\text{-}H}$ = 8.6 Hz, 2H, SAr-*o*-*H*), 7.17 (s, 1H, S-N*H*), 6.86 (d, $^{3}J_{H\text{-}H}$ = 8.6 Hz, 2H, SAr-*m*-*H*). **^{13}C{^{1}H} NMR** (100 MHz, DMSO-d_6, 25 °C): δ (ppm) 155.1 (s), 133.6 (s), 128.1 (s), 111.8 (s), 53.3 (s), 30.2 (s). **HRMS** (ESI) [M+H] $C_{10}H_{17}N_2O_3S$: calc. 245.0954 m/z; found 245.0958 m/z.

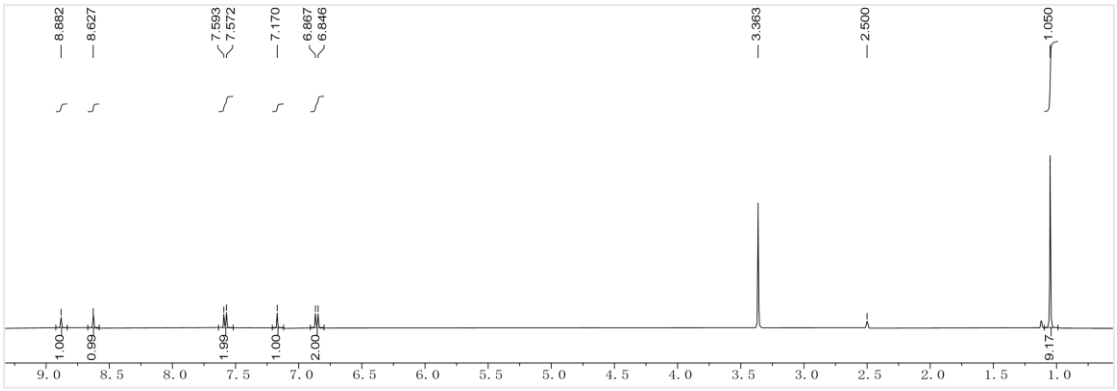


Figure S30: ^{1}H NMR spectrum of **2h** (400 MHz, DMSO-d_6).

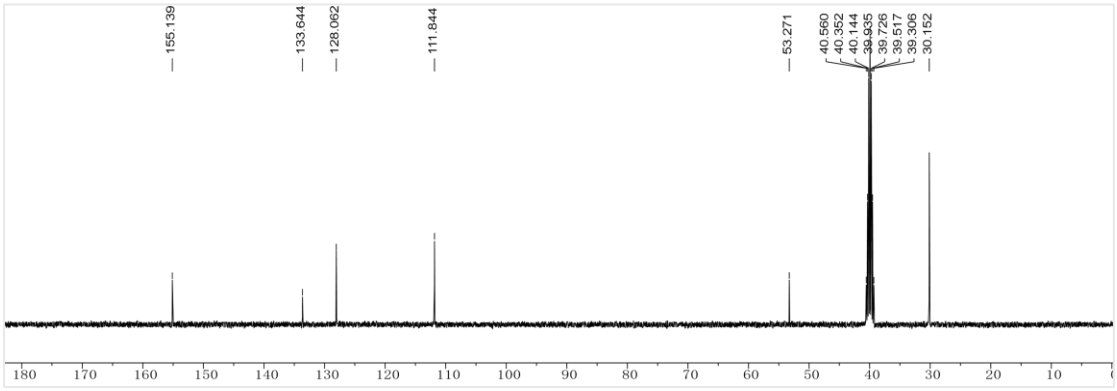
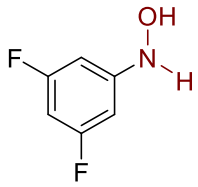


Figure S31: ^{13}C{^{1}H} NMR spectrum of **2h** (100 MHz, DMSO-d_6).

Synthesis of **2i**



(3,5-Difluorophenyl)hydroxylamine **(2i)** was synthesized as white solid (55 mg, yield 38%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu$_3$Sb (29.4 mg, 0.10 mmol), 1,3-difluoro-5-nitrobenzene (**1i**) (161.1 mg, 1.0 mmol), and HBpin (386.5 mg, 3.0 mmol). The reaction took 24 h at 25 °C, **2i** was purified by column chromatography on silica gel (hexane/DCM = 1:1, v/v). **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 6.86 (s, 1H, NHO*H*), 6.50 (m, 2H, NHAr-*o*-*H*), 6.39 (tt, $^{3}J_{H\text{-}F}$ = 8.9 Hz, $^{4}J_{H\text{-}H}$ = 2.3 Hz, 1H, NHAr-*p*-*H*), 5.55 (s, 1H, ArN*H*). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 163.5 (dd, $J_{C\text{-}F}$ = 246.5 Hz, $J_{C\text{-}F}$ = 14.7 Hz), 152.5 (t, $J_{C\text{-}F}$ = 12.3 Hz), 97.1 (dd, $J_{C\text{-}F}$ = 23.0 Hz, $J_{C\text{-}F}$ = 8.8 Hz), 97.0 (t, $J_{C\text{-}F}$ = 26.0 Hz). **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$, 25 °C): δ (ppm) 109.3 (t, $^{4}J_{F\text{-}F}$ = 8.8 Hz).

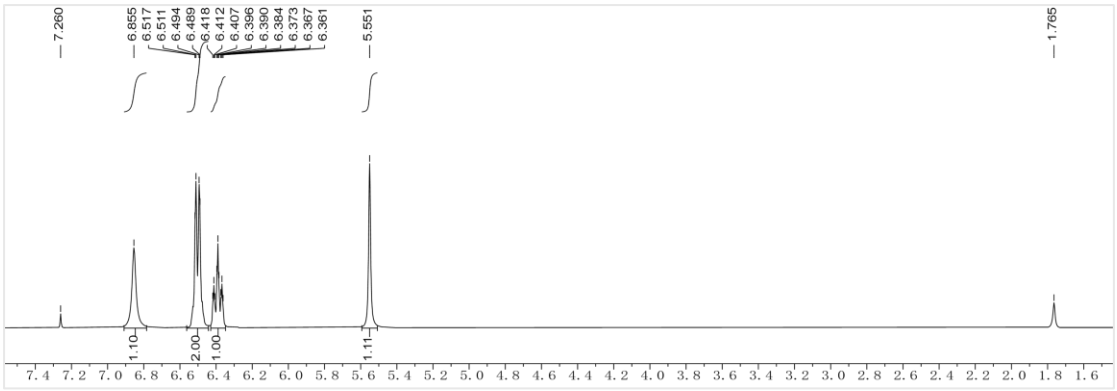


Figure S32: ^{1}H NMR spectrum of **2i** (400 MHz, $CDCl_3$).

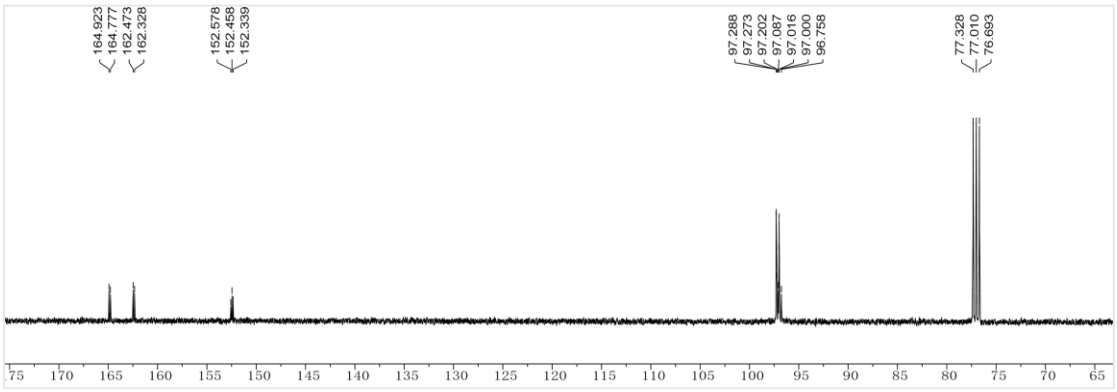


Figure S33: $^{13}C\{^{1}H\}$ NMR spectrum of (**2i**) (100 MHz, $CDCl_3$).

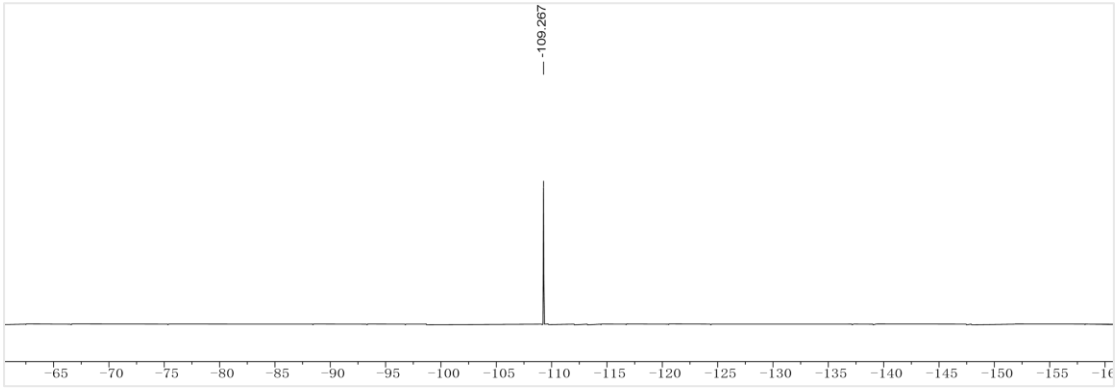
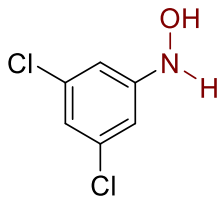


Figure S34: $^{19}F\{^{1}H\}$ NMR spectrum of (**2i**) (376 MHz, $CDCl_3$).

Synthesis of **2j**



(3,5-Dichlorophenyl)hydroxylamine (**2j**) was synthesized as white solid (59 mg, yield 33%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu_3Sb (29.4 mg, 0.10 mmol), 1,3-dichloro-5-nitrobenzene (**1j**) (161.1 mg, 1.0 mmol), and HBpin (386.5 mg, 3.0 mmol). The reaction took 24 h at 25 °C, **2j** was purified by column

chromatography on silica gel (hexane/DCM = 1:1, v/v). **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 6.93 (s, 1H, NHAr-*p*-*H*), 6.88 (s, 2H, NHAr-*o*-*H*), 6.80 (s, 1H, ArNHO*H*), 5.29 (s, 1H, ArN*H*). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 151.7 (s), 135.4 (s), 121.8 (s), 112.5 (s).

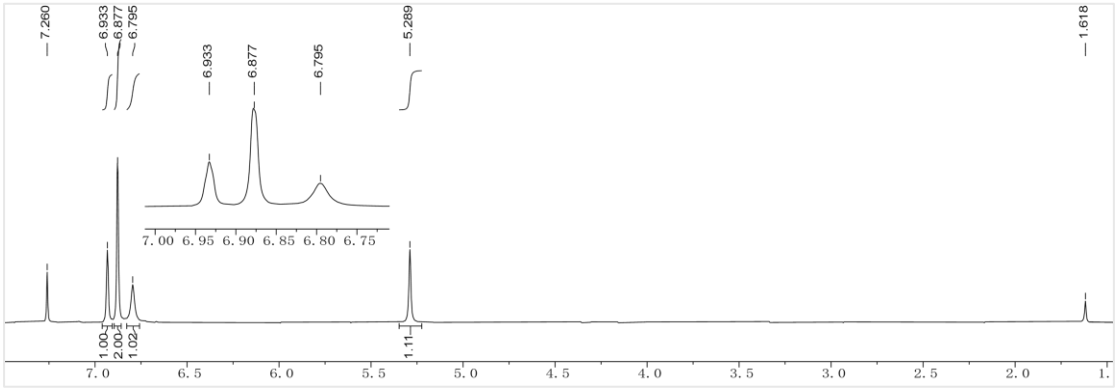


Figure S35: ^{1}H NMR spectrum of **2j** (400 MHz, $CDCl_3$).

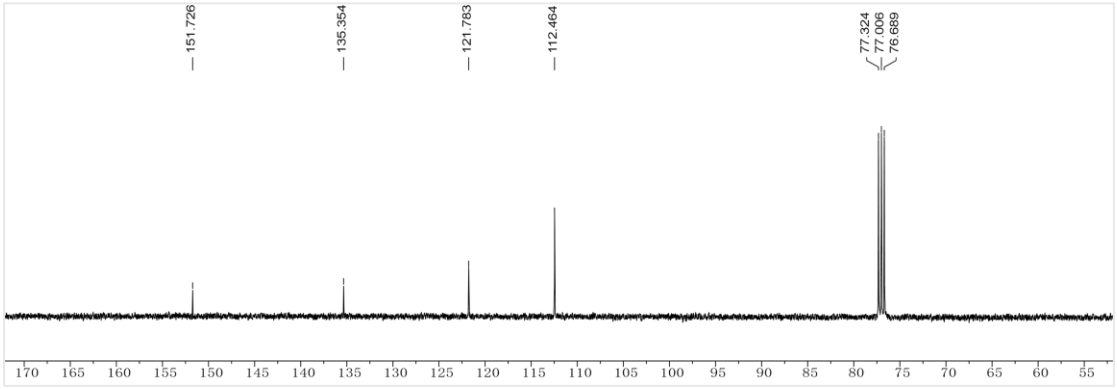
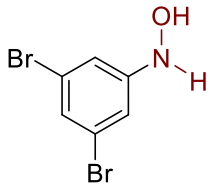


Figure S36: ^{13}C{^{1}H} NMR spectrum of **2j** (100 MHz, $CDCl_3$).

Synthesis of **2k**



N-(3,5-dibromophenyl)hydroxylamine (**2k**) was synthesized as white solid (123 mg, yield 46%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu_3Sb (29.5 mg, 0.10 mmol), 1,3-dibromo-5-nitrobenzene (**1k**) (280.2 mg, 1.0 mmol), and HBpin (387.2 mg, 3.0 mmol). The reaction took 24 h at 25 °C, **2k** was purified by column chromatography on silica gel (hexane/DCM = 1:1, v/v). **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.23 (t, $^4J_{H\text{-}H}$ = 1.7 Hz, 1H, NHAr-*p*-*H*), 7.07 (d, $^4J_{H\text{-}H}$ = 1.7 Hz, 2H,

NHAr-*o*-*H*), 6.78 (s, 1H, ArNHO*H*), 5.43 (s, 1H, ArN*H*). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 149.7 (s), 135.9 (s), 120.4 (s), 110.6 (s).

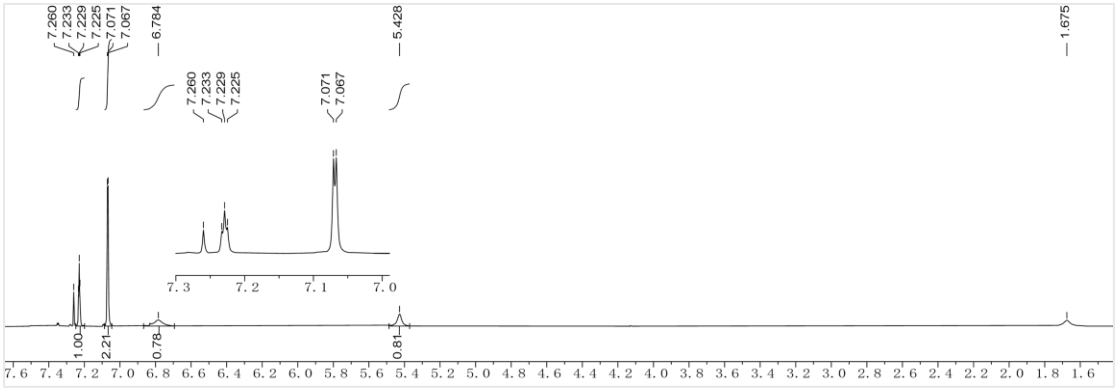


Figure S37: ^{1}H NMR spectrum of **2k** (400 MHz, $CDCl_3$).

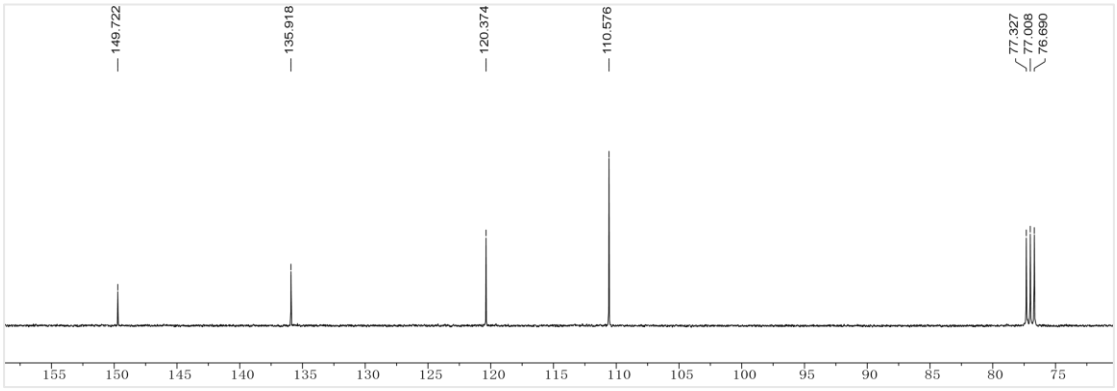
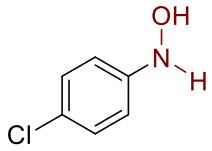


Figure S38: ^{13}C{^{1}H} NMR spectrum of **2k** (100 MHz, $CDCl_3$).

Synthesis of **2l**



(4-Chlorophenyl)hydroxylamine (**2l**) was synthesized as white solid (38 mg, yield 27%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu_3Sb (59.5 mg, 0.2 mmol), 1-chloro-4-nitrobenzene (**1l**) (157.2 mg, 1.0 mmol), and HBpin (386.6 mg, 3.0 mmol). The reaction took 18 h at 25 °C, **2l** was purified by column chromatography on silica gel (hexane/DCM = 5:1, v/v). The product of **2l** was not stable at room temperature, the impurity composition was marked in the NMR spectrum. **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.24 (d, $^{3}J_{H\text{-}H}$ = 8.8 Hz, 2H, NHAr-*o*-*H*), 6.93 (d, $^{3}J_{H\text{-}H}$ = 8.8 Hz, 2H, NHAr-*m*-*H*), 5.52 (s, 1H, ArN*H*). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 149.7 (s), 135.9 (s), 120.4 (s), 110.6 (s).

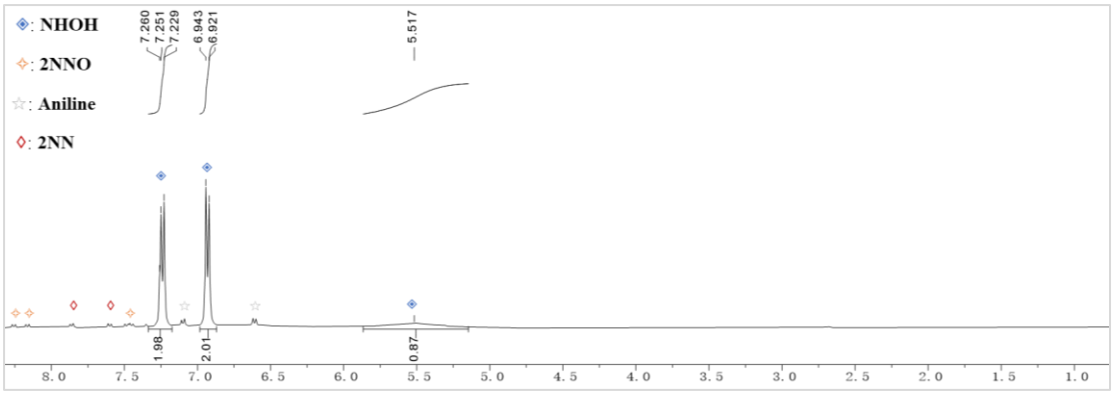


Figure S39: ^{1}H NMR spectrum of **2l** (400 MHz, $CDCl_3$).

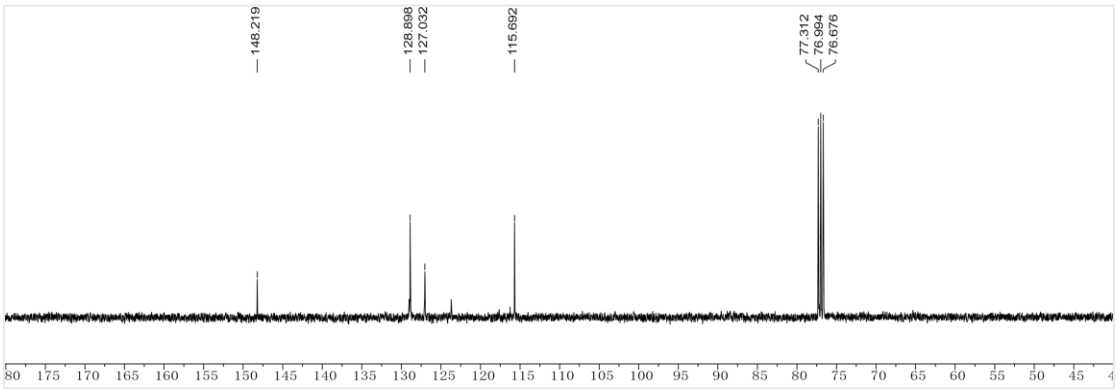
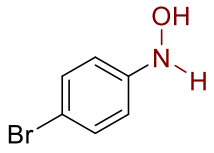


Figure S40: $^{13}C\{^{1}H\}$ NMR spectrum of **2l** (100 MHz, $CDCl_3$).

Synthesis of **2m**



(4-Bromophenyl)hydroxylamine (**2m**) was synthesized as white solid (42 mg, yield 30%) following the synthetic protocol for **2a**. The reaction involved the use of *n*Bu_3Sb (59.5 mg, 0.2 mmol), 1-bromo-4-nitrobenzene (**1m**) (157.2 mg, 1.0 mmol), and HBpin (386.6 mg, 3.0 mmol). The reaction took 18 h at 25 °C, **2m** was purified by column chromatography on silica gel (hexane/DCM = 5:1, v/v). **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.38 (d, $^{3}J_{H\text{-}H}$ = 8.5 Hz, 2H, NHAr-*o*-*H*), 6.87 (d, $^{3}J_{H\text{-}H}$ = 8.5 Hz, 2H, NHAr-*m*-*H*), 6.77 (s, 1H, ArN*H*), 5.77 (s, 1H, ArNO*H*). **$^{13}C\{^{1}H\}$ NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) 148.6 (s), 131.8 (s), 116.2 (s), 114.5 (s).

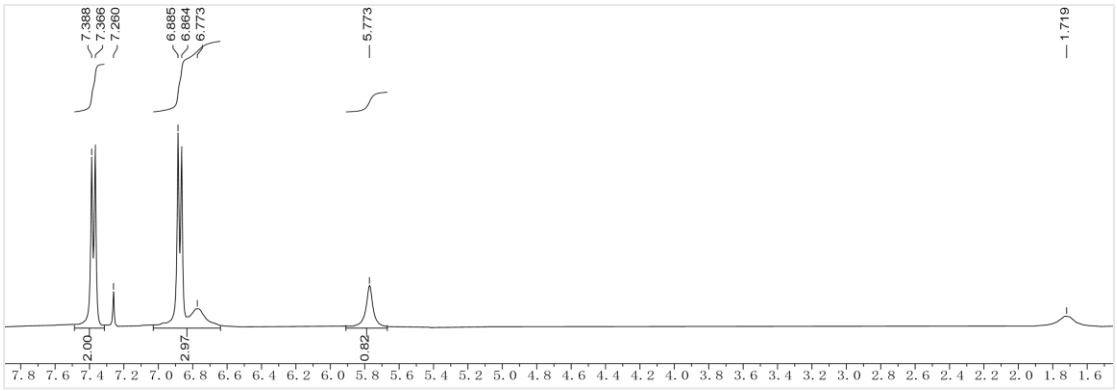


Figure S41: ^{1}H NMR spectrum of **2m** (400 MHz, $CDCl_3$).

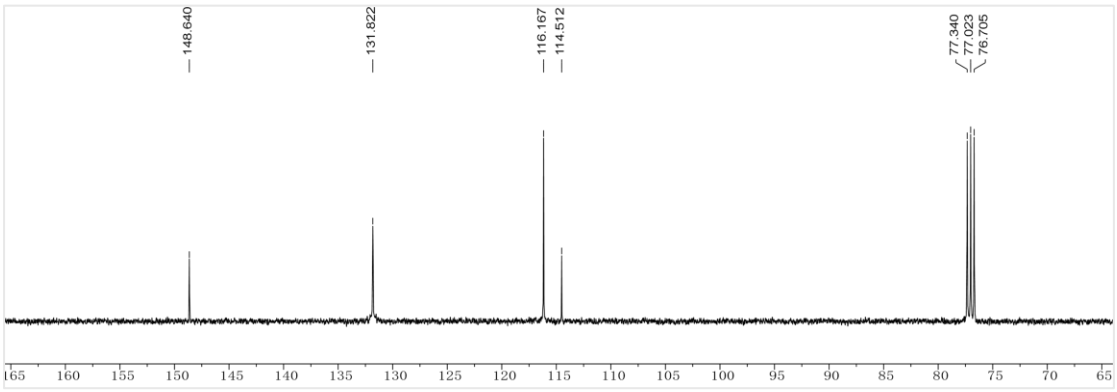


Figure S42: $^{13}C\{^{1}H\}$ NMR spectrum of **2m** (100 MHz, $CDCl_3$).

2.3 Stoichiometric reaction studies

The reduction of **1a** with *n*Bu_3Sb in the presence of 1,3-cyclohexadiene

1a (7.4 mg, 0.05 mmol) and mesitylene (6.0 mg, 0.050 mmol) were combined in 0.6 mL of $CDCl_3$. The resulting reaction mixture was transferred into an NMR tube and analyzed by NMR spectroscopy. Then *n*Bu_3Sb (44.0 mg, 0.15 mmol) and 1,3-cyclohexadiene (20.0 mg, 0.25 mmol) were added to the reaction solution at 25 °C. The progress of the reaction was monitored by NMR spectroscopy analysis, **1a** was completely consumed after 24 h. The yield of **3a** (55%) was calculated by **^{1}H NMR** spectrum as shown in Figure S43.

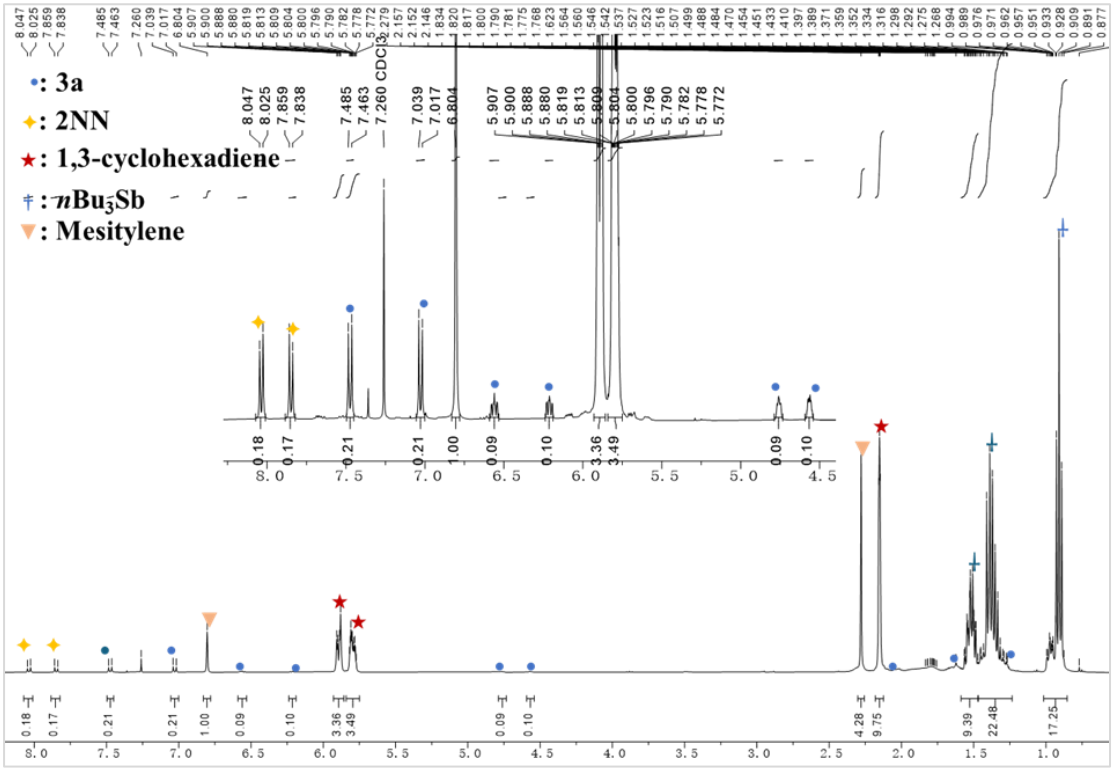


Figure S43: ^{1}H NMR spectrum of reaction solution of **1a**, nBu$_3$Sb and 1,3-cyclohexadiene at r.t. for 24 h (400 MHz, $CDCl_3$).

<u>The reduction of [nBu$_3$Sb(μ-O)]$_2$ with HBpin in C_6D_6</u>

[nBu$_3$Sb(μ-O)]$_2$ (10.3 mg, 0.017 mmol) and HBpin (9.1 mg, 0.071 mmol) were combined in 0.6 mL of C_6D_6. Effervescence was observed immediately. The resulting reaction mixture was immediately transferred into a J. Young NMR tube. The progress of the reaction was monitored by NMR spectroscopy analysis. After 15 minutes, the reaction was completed. The NMR spectrum of the reaction solution confirmed the formation of nBu$_3$Sb, H_2, pinBOBpin, and residual HBpin as shown in Figure S44. **^{1}H NMR** (400 MHz, C_6D_6, 25 °C): nBu$_3$Sb: δ (ppm) 1.53 (m, 6H, Sb-CH_2), 1.37 (m, 12H, CH$_2$-CH_2-CH_2), 0.90 (t, $^{3}J_{C\text{-}H}$ = 7.3 Hz, 9H, CH$_2$-CH_3); **pinBOBpin**: δ (ppm) 1.01 (s, 18H, CH_3); **HBpin**: δ (ppm) 0.99 (s, 18H, CH_3); **H$_2$**: δ (ppm) 4.47 (s, 2H, H_2); **^{11}B{^{1}H} NMR** (128 MHz, C_6D_6, 25 °C): **pinBOBpin**: δ (ppm) 21.8 (s); **HBpin**: δ (ppm) 28.5 (s).

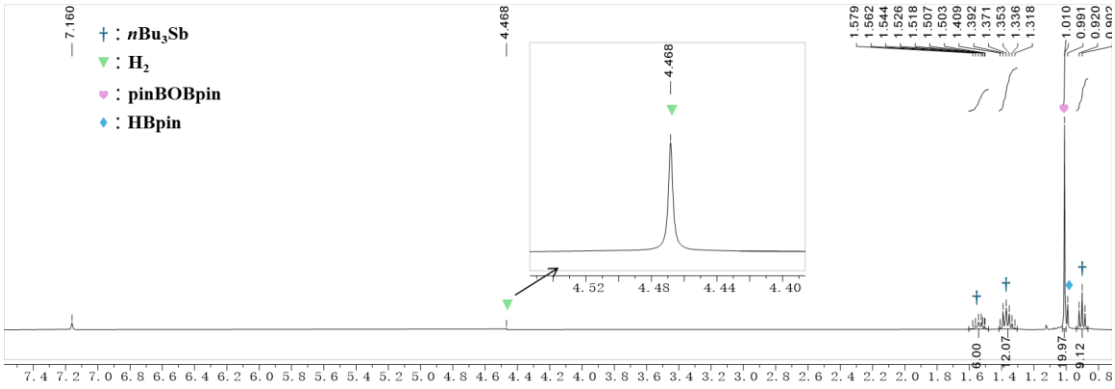


Figure S44: ^{1}H NMR spectrum of reaction solution of [nBu$_3$Sb(μ-O)]$_2$ with HBpin at r.t. for 15 min (400 MHz, C_6D_6).

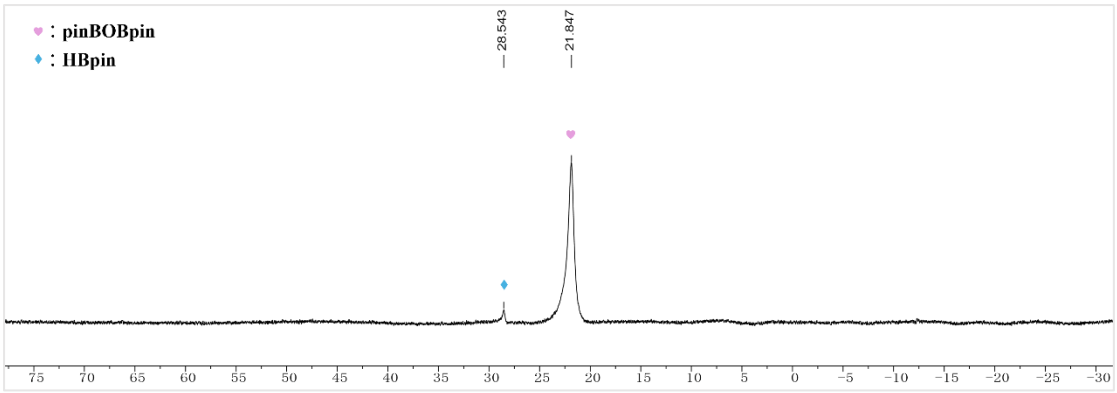


Figure S45: ^{11}B{^{1}H} NMR spectrum of reaction solution of [nBu$_3$Sb(μ-O)]$_2$ with HBpin at r.t. for 15 min (128 MHz, C_6D_6).

<u>The reaction of **4a** and HBpin</u>

4a (6.6 mg, 0.05 mmol) and HBpin (64.0 mg, 0.5 mmol) were combined in 0.6 mL of $CDCl_3$ at -35 °C. The resulting reaction mixture was then transferred into an NMR tube and kept at -35 °C. Once returning the solution to room temperature, the progress of the reaction was immediately monitored by NMR spectroscopy analysis. At room temperature, **4a** was completely consumed after 3.5 h. The ratio of **2NNO/2a′** (88:12) was calculated by ^{1}H NMR spectrum as shown in Figure S46.

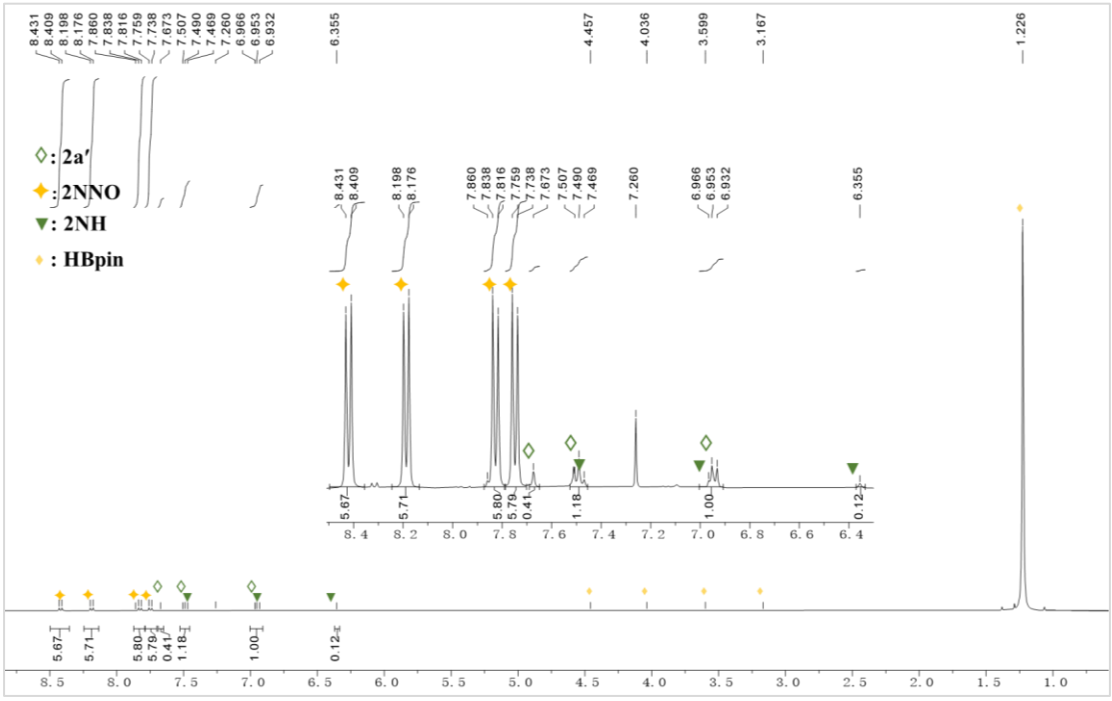


Figure S46: ^{1}H NMR spectrum of reaction solution of **4a** with HBpin at r.t. for 3.5 h (400 MHz, $CDCl_3$).

<u>The reaction of **4a** and HBpin in presence of *n*Bu_3Sb</u>

The solution of *n*Bu_3Sb (15.0 mg, 0.5 mmol) and HBpin (64.2 mg, 0.5 mmol) in 0.3 mL of $CDCl_3$ was added to the solution of **4a** (6.6 mg, 0.05 mmol) in 0.3 mL of $CDCl_3$ at -35 °C. The resulting reaction mixture was then transferred into an NMR tube and kept at -35 °C. Once returning the solution to room temperature, the progress of the reaction was immediately monitored by NMR spectroscopy analysis. **4a** was consumed within 5 min. The ratio of **2NNO/2a′** (7:93) was calculated by ^{1}H NMR spectrum as shown in Figure S47.

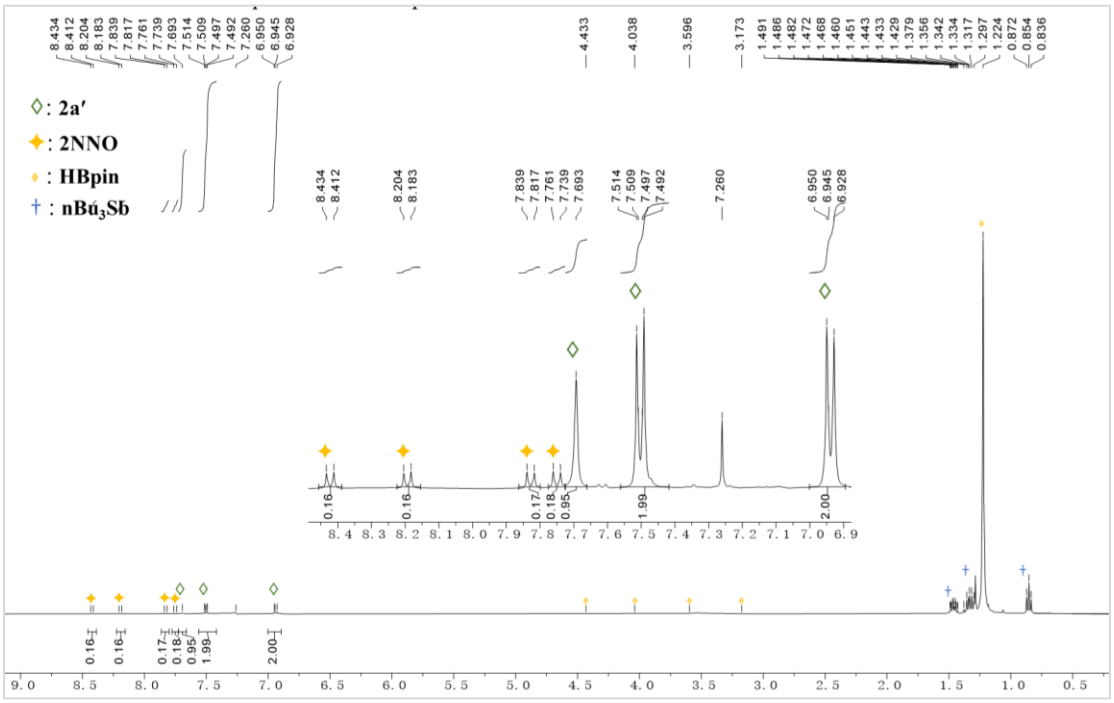


Figure S47: ^{1}H NMR spectrum of reaction solution of **4a** with HBpin catalyzed by *n*Bu$_3$Sb at r.t. for 5 min (400 MHz, CDCl$_3$).

3. Computational Details

Calculations were carried out with the Gaussian 16 package.[S2] Geometry optimizations were performed with the M06-2X functional.[S3] The Def2-SVP basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states). Transition states were submitted to intrinsic reaction coordinate (IRC) calculations to determine two corresponding minima. The single-point energy calculations were performed at the M06-2X-D3/Def2-TZVP level of theory in solution-phase (benzene for optimized structures of **1** and **2**, chloroform for the mechanism considerations). The SMD method was used with the corresponding solvent, while Bondi radii[S4] were chosen as the atomic radii to define the molecular cavity. The Gibbs energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energies in solution. All the solution-phase free energies reported in the paper correspond to the reference state of 1 mol/L, 298K. Optimized structures were visualized by the Avogadro program[S5].

Table S1. Energy of Intermediates and Transition States.

Species	Thermal Corrections of Gibbs Free Energies (Hartree)	Solvation Energies (Hartree)
Me_3Sb	0.075774	-359.879520060
1a	0.068928	-528.999204802
TS1	0.163044	-888.854239892
IN1	0.164480	-888.886899546
TS2	0.161525	-888.857604110
4a	0.064155	-453.781778472
$[Me_3Sb(\mu\text{-}O)]_2$	0.177498	-870.231777194
TS3′	0.242103	-865.577001891
TS3″	0.421881	-1277.46728352
TS3	0.161514	-813.651141352
IN2	0.160896	-813.666228950
HBpin	0.15864	-411.858031135
IN3	0.347621	-1225.56355858
TS4	0.346484	-1225.55081010
IN4	0.343666	-1225.589403
IN5	0.343449	-1225.58600
TS5	0.341616	-1225.572043
2a′	0.247074	-865.743220080

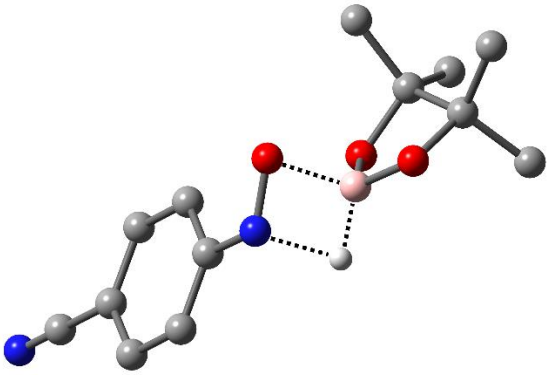


Figure S48: Optimized structure of **TS3′**.

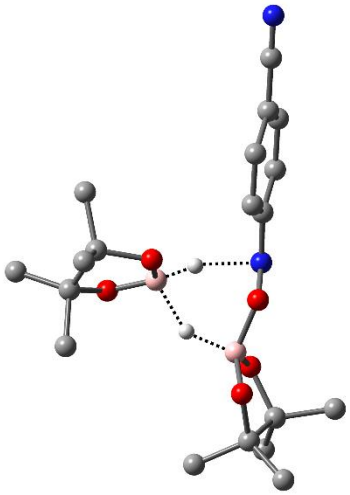


Figure S49: Optimized structure of **TS3′′**.

Cartesian Coordinates:

Me_3Sb:

Sb	-0.00009100	0.00002600	-0.42227400
C	0.67921800	-1.71170800	0.73174000
H	0.59717600	-1.49846200	1.80644100
H	0.06945400	-2.59328700	0.49214000
H	1.72607900	-1.93828100	0.48851300
C	-1.82198800	0.26783100	0.73208300
H	-2.54064300	-0.52693500	0.49063200
H	-1.59590200	0.23465500	1.80675000
H	-2.28185500	1.23562500	0.49064400
C	1.14322900	1.44378900	0.73178000
H	1.00099300	1.26492200	1.80647400
H	2.21130300	1.35719600	0.49069000
H	0.81526900	2.46378700	0.49004400

$[Me_3Sb(\mu\text{-}O)]_2$:

Sb	1.58930400	0.00003600	0.04621400
O	-0.14036400	0.00062300	1.25507300
Sb	-1.58922300	-0.00007800	-0.04619000
O	0.14043000	-0.00062700	-1.25502400
C	3.11428300	-0.00057900	-1.49028200
H	2.99559500	-0.89155300	-2.12145200
H	2.99527000	0.88967600	-2.12240500
H	4.11894400	-0.00016600	-1.04310500
C	2.17694400	-1.79684900	1.02901600
H	1.73122500	-1.80453300	2.02968700
H	1.78056000	-2.64270400	0.45001800
H	3.27029500	-1.87918100	1.07625800
C	2.17666000	1.79786400	1.02744600

H	3.26998300	1.88184900	1.07223600
H	1.77765100	2.64300700	0.44920600
H	1.73310800	1.80523400	2.02908700
C	-2.17699200	-1.79766900	-1.02760000
H	-1.73269400	-1.80546100	-2.02890700
H	-1.77917300	-2.64313400	-0.44901300
H	-3.27035500	-1.88073300	-1.07323700
C	-3.11415400	0.00076900	1.49035600
H	-2.99501400	-0.88914400	2.12292900
H	-2.99556500	0.89207600	2.12108200
H	-4.11882600	0.00003200	1.04320400
C	-2.17717700	1.79664500	-1.02909800
H	-3.27055500	1.87897600	-1.07575800
H	-1.78049200	2.64260700	-0.45045500
H	-1.73200900	1.80422600	-2.03001400

1a:

O	-3.00680300	-1.07255800	-0.00001000
O	-3.00680400	1.07255800	-0.00001000
N	-2.45696600	0.00000000	-0.00011900
C	-0.97539600	0.00000000	0.00001500
C	-0.31190800	1.22107600	0.00004000
C	-0.31190800	-1.22107600	0.00004000
C	1.07790100	1.21871800	0.00007800
C	1.07790100	-1.21871800	0.00007900
H	-0.88845900	-2.14462600	-0.00000600
C	1.77100500	0.00000000	0.00008100
H	1.63246400	2.15679800	0.00002800
H	1.63246400	-2.15679800	0.00002800
H	-0.88845900	2.14462600	-0.00000700

C	3.21346800	0.00000000	-0.00004000
N	4.36760500	0.00000000	-0.00011500

TS1:

O	-0.48425000	1.06713000	-1.15945000
O	-0.48429700	-1.06681700	-1.15939800
N	0.21281500	0.00015100	-1.32053700
C	1.52785200	0.00009900	-0.80182000
C	2.16919300	-1.21950400	-0.55973900
C	2.16917800	1.21964700	-0.55942100
C	3.46515000	-1.21561200	-0.06412800
C	3.46513400	1.21563500	-0.06380200
H	1.63531900	2.14603600	-0.76254700
C	4.11982300	-0.00001600	0.18497900
H	3.98087300	-2.15501600	0.13573400
H	3.98084100	2.15499100	0.13632600
C	-3.43914500	0.00157700	-1.31621200
H	-4.46802500	-0.00094400	-0.93455000
H	-3.26460400	0.89466500	-1.92933400
H	-3.26173700	-0.88812600	-1.93341700
H	1.63534900	-2.14584800	-0.76311300
C	-2.75233000	1.65560500	1.45475100
H	-3.83201700	1.54057400	1.62445400
H	-2.22977500	1.68520600	2.41920300
H	-2.55886700	2.59041200	0.91312700
C	-2.75266200	-1.65753500	1.45178700
H	-3.83238700	-1.54281400	1.62145200
H	-2.55906300	-2.59142200	0.90862600
H	-2.23033500	-1.68878600	2.41631300
Sb	-2.02293300	-0.00001300	0.26676500

C	5.46540200	-0.00007200	0.69876300
N	6.54387300	-0.00011300	1.11232700

IN1:

O	0.60104600	-1.09237000	-0.84197600
O	0.60101800	1.09297000	-0.84095000
N	-0.12604800	0.00045100	-1.30595400
C	-1.43885900	0.00023800	-0.78596900
C	-2.09817200	1.21570300	-0.56200900
C	-2.09789100	-1.21534800	-0.56198600
C	-3.41298300	1.21283800	-0.11829100
C	-3.41273100	-1.21275500	-0.11827000
H	-1.55973500	-2.14471900	-0.73824500
C	-4.08042000	-0.00004100	0.10676900
H	-3.93376300	2.15373100	0.06208900
H	-3.93329500	-2.15376500	0.06213200
C	3.63455700	-0.00102100	-1.19036200
H	4.59826400	-0.00098400	-0.66605000
H	3.54579100	-0.89535700	-1.81934900
H	3.54630200	0.89267200	-1.82033100
H	-1.56020900	2.14518800	-0.73826900
C	2.36497300	-1.65002000	1.49722700
H	3.35178900	-1.56025200	1.97035200
H	1.58652900	-1.66186800	2.27074800
H	2.30130300	-2.57637600	0.91310800
C	2.36677000	1.65007000	1.49672300
H	3.35392500	1.55979100	1.96905400
H	2.30312700	2.57647000	0.91267800
H	1.58898800	1.66229600	2.27090500
Sb	2.02995600	0.00000100	0.18227500

C	-5.44277400	-0.00016900	0.57233600
N	-6.53511200	-0.00025700	0.94903300

TS2:

O	-0.53460600	0.96961700	-0.31207000
O	-0.34035000	-1.48841100	-0.54678400
N	0.24307300	-0.52666800	-1.11230500
C	1.57843600	-0.29270400	-0.62818900
C	2.28479100	-1.31863200	-0.00299700
C	2.18441000	0.93691800	-0.90404200
C	3.61429900	-1.11503900	0.35532900
C	3.50414400	1.14487200	-0.53951400
H	1.58524800	1.71478400	-1.37626400
C	4.22616300	0.11561700	0.09084300
H	4.18560700	-1.90644100	0.84142300
H	3.99090200	2.10081100	-0.73380900
C	-3.18071600	-0.73735200	-1.49775900
H	-4.21061500	-1.00110800	-1.22620900
H	-3.18474600	-0.01405300	-2.32288000
H	-2.60359200	-1.62378000	-1.78269100
H	1.77494900	-2.26247300	0.18374200
C	-3.41417700	1.76875700	0.73352400
H	-4.41560400	1.41027900	1.00597100
H	-2.95961700	2.27688800	1.59320900
H	-3.49019900	2.48001200	-0.09831800
C	-2.18229100	-1.13621900	1.83585000
H	-3.20792200	-1.44675800	2.07343700
H	-1.54985100	-1.99841400	1.59934200
H	-1.75724200	-0.58597200	2.68498500
Sb	-2.17804100	0.13756200	0.14518700

C	5.60136900	0.32892700	0.46478600
N	6.70318900	0.50095900	0.76621300

4a:

O	-0.25924500	-1.54480500	-0.82963900
N	0.21997300	-0.47778300	-1.06536100
C	1.60054200	-0.33063000	-0.64489900
C	2.31182500	-1.35543900	-0.01488700
C	2.17979000	0.90769500	-0.91042200
C	3.62892900	-1.13051600	0.35495900
C	3.50081700	1.13838400	-0.54116900
H	1.57671800	1.67022300	-1.40507300
C	4.22170100	0.11706400	0.09120700
H	4.21249900	-1.90804600	0.84822500
H	3.97978600	2.09770400	-0.73610900
H	1.81303800	-2.30701200	0.17028100
C	5.59222800	0.34727400	0.47757800
N	6.68907600	0.53105400	0.78687300

TS3:

O	-0.76808600	-2.05035600	-0.41136500
N	-0.32842000	-0.87533400	-0.87031000
C	0.99062200	-0.51866600	-0.52721000
C	1.84367900	-1.48579300	0.02612100
C	1.50004100	0.75516200	-0.85377600
C	3.17528400	-1.17251700	0.27001500
C	2.82354800	1.06233000	-0.60532300
H	0.84112300	1.49808100	-1.31235800
C	3.67863700	0.09907300	-0.03442300
H	3.84130900	-1.91939800	0.70444200

H	3.21708500	2.04835500	-0.85458800
C	-3.49071900	-0.58200100	-0.89889900
H	-4.34751800	-0.64823400	-0.21784800
H	-3.75152100	0.01862900	-1.77809300
H	-3.14849800	-1.58386600	-1.18985600
H	1.42012100	-2.46552300	0.23804400
C	-2.05878100	2.37183900	0.12953700
H	-2.96275900	2.61732800	0.70332500
H	-1.18192400	2.82687500	0.60695900
H	-2.15845300	2.75114800	-0.89515700
C	-1.71272700	-0.48737900	2.07446200
H	-1.24480200	0.25553500	2.72997800
H	-2.71017900	-0.75324700	2.44397900
H	-1.09695600	-1.39224100	1.97349400
Sb	-1.80789700	0.22870800	0.08340400
C	5.05403800	0.42273700	0.22988400
N	6.15823000	0.68913600	0.44497900

TS3′:

C	-0.60680600	1.37453100	3.06313600
C	-0.69360800	-0.19308500	3.00990200
O	-1.75878000	1.75845100	2.29156200
O	-2.11122100	-0.42856300	3.00379500
C	-0.76980800	1.91232400	4.48429900
H	0.12546900	1.71533500	5.09053400
H	-0.92117900	3.00028300	4.43485600
H	-1.63965800	1.46216600	4.98210600
C	0.63085100	1.96299700	2.40883700
H	0.61391700	3.05744700	2.50702800
H	1.54267600	1.58688300	2.89624500

H	0.66754800	1.71585800	1.34114700
C	-0.08434500	-0.89892300	4.20943200
H	-0.18104900	-1.98590200	4.08180000
H	0.98467600	-0.65482400	4.30228600
H	-0.59925500	-0.61773500	5.13582200
C	-0.12508900	-0.75614700	1.70969800
H	0.97175200	-0.69029800	1.68239600
H	-0.41732800	-1.81191900	1.62925800
H	-0.53435100	-0.21622900	0.84377300
B	-2.68882600	0.74438900	2.53704200
H	-3.55730700	0.64217500	1.59556000
O	-3.78145700	1.35006100	3.71946100
N	-4.59207700	1.26075900	2.73827300
C	-4.89853900	2.52244300	2.12976000
C	-4.20708100	3.69515500	2.44844900
C	-5.97053800	2.51184400	1.23540100
C	-4.60896600	4.88406600	1.85781700
C	-6.37296300	3.70226800	0.64533500
H	-6.47395500	1.56709600	1.02655900
C	-5.68935200	4.88614000	0.95972300
H	-4.09302300	5.81827000	2.07893700
H	-7.20976000	3.72867300	-0.05209300
H	-3.36582500	3.63875200	3.13776200
C	-6.10335600	6.12668200	0.35140300
N	-6.43491100	7.11928300	-0.13567600

TS3′′:

C	-3.71069500	-1.55563900	-0.54187400
C	-3.89248700	-0.72252600	0.77387800
O	-2.44382400	-1.08750600	-1.01983800

O	-2.54457100	-0.60228200	1.23841400
C	-3.57833600	-3.05193700	-0.26118600
H	-4.53846700	-3.49828700	0.03426800
H	-3.22436800	-3.54852900	-1.17495600
H	-2.84497400	-3.23361900	0.53827200
C	-4.76688500	-1.30357700	-1.60434300
H	-4.56530200	-1.93670800	-2.47956100
H	-5.76951100	-1.54883100	-1.22286000
H	-4.75367400	-0.25700100	-1.93171800
C	-4.72832800	-1.40252200	1.84507200
H	-4.80836000	-0.74359600	2.72082800
H	-5.74314800	-1.60947700	1.47354400
H	-4.26620600	-2.34334400	2.16775400
C	-4.42129200	0.68429000	0.49450200
H	-5.48108300	0.67190100	0.20372200
H	-4.31337600	1.28569500	1.40785200
H	-3.84025400	1.16452500	-0.30691400
B	-1.74170900	-0.64312700	0.09932800
H	-1.14334000	0.52103400	-0.18862400
O	-0.39007500	-1.29512500	0.38010500
N	0.31063500	-1.55393500	-0.62690900
C	1.68215700	-1.66782400	-0.31430800
C	2.22316900	-1.31035800	0.92902700
C	2.48560400	-2.17239900	-1.34366100
C	3.58356400	-1.47728000	1.13912100
C	3.84602900	-2.33721000	-1.13211000
H	2.01719700	-2.42765600	-2.29473600
C	4.39371600	-1.98893100	0.11213200
H	4.03411400	-1.20867500	2.09458200
H	4.49116400	-2.73184600	-1.91655800

H	1.57100700	-0.89562000	1.69527000
C	5.80753100	-2.15623400	0.33914300
N	6.93990400	-2.28888200	0.52102500
C	0.19936400	3.35031000	-0.45803800
C	1.34740200	2.66598600	0.35963800
O	-0.16791700	2.31153600	-1.38203200
O	0.94343500	1.28734600	0.34284400
C	-1.02894000	3.64809400	0.40069200
H	-0.84732700	4.48337700	1.09128700
H	-1.86285300	3.91415000	-0.26325500
H	-1.32325500	2.76217600	0.98316400
C	0.62243600	4.58338400	-1.23645400
H	-0.24525500	4.99447100	-1.77027800
H	1.00859800	5.35679300	-0.55588500
H	1.39445200	4.34032000	-1.97645500
C	1.46392500	3.13366400	1.80031500
H	2.29864900	2.61277500	2.29028700
H	1.66290300	4.21494600	1.84128900
H	0.54728400	2.91741900	2.36208500
C	2.69950500	2.75278900	-0.34503800
H	3.11299000	3.77024700	-0.30564100
H	3.40072500	2.06886800	0.15348400
H	2.60954600	2.44806100	-1.39762600
B	0.12428800	1.11767400	-0.76625400
H	0.21443900	0.03920400	-1.41180300

IN2:

O	-0.95476700	-1.55448400	-0.79471800
N	-0.30815600	-0.26259800	-1.14596200
C	1.01449800	-0.18765900	-0.75668900

C	1.71692600	-1.31293000	-0.28057900
C	1.69023000	1.04842000	-0.87091500
C	3.05304900	-1.19587100	0.07473400
C	3.01819700	1.15768400	-0.50099900
H	1.15191000	1.90958400	-1.27094900
C	3.71764000	0.03580000	-0.02114400
H	3.59849600	-2.06834700	0.43748000
H	3.53530000	2.11402600	-0.58862300
C	-3.75890400	-0.25822300	-0.73124500
H	-4.51981700	0.37440800	-0.25862200
H	-3.67137900	-0.00820100	-1.79660100
H	-4.01184900	-1.32019800	-0.63575500
H	1.18284900	-2.25863900	-0.21517300
C	-1.79307500	2.19470500	0.42015800
H	-2.57373500	2.50374800	1.12883600
H	-0.80604800	2.46933800	0.81604100
H	-1.94757200	2.69672300	-0.54374500
C	-1.52951100	-0.69878600	2.07888900
H	-1.96272700	-0.04246000	2.84293600
H	-1.94594100	-1.71024200	2.14453900
H	-0.43910700	-0.75648100	2.20416500
Sb	-1.85475900	0.05917100	0.13143300
C	5.09729000	0.15203700	0.36435700
N	6.20564200	0.24886100	0.67892300

HBpin:

C	0.09856600	-0.64986300	0.05967400
C	1.66095300	-0.65009400	-0.07568500
O	1.92816100	0.69568100	-0.51273900
O	-0.18223500	0.73534900	0.33489800

B	0.86913700	1.46643500	-0.13354500
H	0.86322300	2.66060900	-0.20410000
C	2.36950500	-0.83048900	1.26449600
H	2.26861900	-1.85844800	1.63913700
H	3.43628100	-0.60607100	1.13058600
H	1.96499600	-0.13904900	2.01734500
C	2.21094800	-1.62673600	-1.10095200
H	3.30685400	-1.55414700	-1.12359600
H	1.93755400	-2.65887300	-0.83604000
H	1.83345100	-1.40505500	-2.10624300
C	-0.44252500	-1.50413600	1.19322400
H	-1.53915600	-1.44079300	1.20715400
H	-0.15820200	-2.55747400	1.05228300
H	-0.06869400	-1.16125400	2.16528100
C	-0.60719600	-0.99431800	-1.24953100
H	-0.49582700	-2.05828200	-1.50024900
H	-1.67622600	-0.76620000	-1.14258800
H	-0.20909500	-0.39261300	-2.07897600

IN3:

C	0.06873900	0.39286100	2.62655500
C	-0.63745200	-0.70751100	1.76169600
O	-0.48160400	1.58832000	2.12605200
O	-1.95470100	-0.16040400	1.62264500
C	-0.27268400	0.27190600	4.11469800
H	0.18709800	-0.60867800	4.58714100
H	0.09653700	1.17459900	4.61969600
H	-1.36238500	0.24957700	4.25434500
C	1.58108600	0.42906000	2.44551300
H	2.00267700	1.20480600	3.09937300

H	2.04139000	-0.53511100	2.71140100
H	1.84338000	0.68340000	1.41139100
C	-0.67222900	-2.08457800	2.40517300
H	-1.22135900	-2.79646500	1.76748700
H	0.35287100	-2.46746900	2.51596900
H	-1.13385500	-2.06545800	3.39869900
C	-0.03646800	-0.80001400	0.35900300
H	0.96300700	-1.25620700	0.37493300
H	-0.68850200	-1.41857800	-0.27521900
H	0.03363500	0.20189800	-0.08623700
B	-1.81058000	1.38232500	1.65988500
H	-2.07195000	1.87417800	0.56368200
O	-2.86561000	1.75784800	2.65761800
N	-4.08129900	1.39176200	2.11610600
C	-4.71458900	2.36841000	1.35228900
C	-4.40968600	3.72278500	1.59296100
C	-5.67673800	2.05729300	0.37426100
C	-5.07590700	4.72179100	0.90487800
C	-6.34891600	3.06296900	-0.30527700
H	-5.89488200	1.02157800	0.11151900
C	-6.06186200	4.40808900	-0.04469900
H	-4.83485800	5.76716200	1.10077900
H	-7.09097300	2.80672900	-1.06201000
C	-3.79760600	-1.52830100	-0.04290400
H	-4.70927800	-1.94623600	-0.48530300
H	-3.36940900	-0.74149800	-0.67756400
H	-3.03939600	-2.30586300	0.11013500
H	-3.64061900	3.95659100	2.32556400
C	-6.36335400	-0.81513500	1.92267800
H	-6.60260100	-1.76739600	2.41705900

H	-6.77236000	0.01314700	2.51751000
H	-6.82716000	-0.80703200	0.92851500
C	-3.75529200	-1.58268300	3.64619800
H	-3.35777600	-2.58550000	3.45015600
H	-3.00302000	-0.97828000	4.16416800
H	-4.67416000	-1.64846900	4.24043000
Sb	-4.21968000	-0.61695300	1.82752600
C	-6.75662500	5.44847800	-0.75359100
N	-7.31974300	6.28159900	-1.32323600

TS4:

C	0.48431300	0.51890500	2.66995300
C	-0.44973300	-0.74288100	2.79162600
O	0.00560200	1.16418500	1.49809800
O	-1.68367400	-0.22659500	2.27957000
C	0.32084600	1.46311500	3.86406200
H	0.76775200	1.04559100	4.77778200
H	0.82834100	2.40720300	3.62357700
H	-0.73941400	1.68757600	4.04264500
C	1.95447800	0.17939400	2.47270700
H	2.53544200	1.11093900	2.43375100
H	2.33561900	-0.43082700	3.30555600
H	2.11296900	-0.35718100	1.52924600
C	-0.65678000	-1.23422200	4.21577200
H	-1.28873300	-2.13493800	4.21699500
H	0.30646000	-1.49751600	4.67781300
H	-1.14495000	-0.46598700	4.82746500
C	0.01737200	-1.88797100	1.89678300
H	0.94640400	-2.33676400	2.27441000
H	-0.75214500	-2.67469900	1.87615900

H	0.19250200	-1.52873200	0.87208900
B	-1.39078700	1.00740000	1.46406000
H	-1.94232500	0.79756200	0.32150200
O	-2.19892800	2.09409000	2.02014700
N	-3.48740600	1.63766700	2.18866100
C	-4.43164800	2.63609400	1.93096900
C	-4.09888100	3.83926700	1.28467100
C	-5.74857700	2.44334400	2.38816200
C	-5.07596900	4.79889300	1.06212800
C	-6.72592000	3.39583200	2.15068200
H	-5.98778300	1.54434700	2.96045800
C	-6.39851000	4.58314900	1.47801100
H	-4.82060300	5.72972400	0.55441900
H	-7.74550500	3.24115700	2.50496300
C	-3.03938000	-1.68617500	-0.04913800
H	-3.13453500	-1.26231900	-1.05622800
H	-1.98719500	-1.86087400	0.18987000
H	-3.62300000	-2.61484100	0.02586400
H	-3.06800400	3.99562500	0.97434600
C	-5.68011200	0.10513300	0.29454100
H	-5.82354600	-0.72506700	-0.41064100
H	-6.53812800	0.16060200	0.97379300
H	-5.61066000	1.05051400	-0.26029500
C	-4.40668400	-1.36818100	3.06770100
H	-3.79425700	-2.27569500	3.13821500
H	-4.20284400	-0.72435100	3.93212700
H	-5.47060800	-1.63311600	3.03024200
Sb	-3.83361900	-0.27801400	1.34220800
C	-7.40950000	5.57786400	1.23546000
N	-8.22494100	6.37227700	1.03747700

IN4:

C	0.46025100	0.97982800	2.71613900
C	-0.59320000	-0.13812500	3.03807800
O	0.01455200	1.45730000	1.43444500
O	-1.76711600	0.35765300	2.36706700
C	0.37363700	2.15369600	3.68812800
H	0.76134000	1.88748000	4.68098600
H	0.97013000	2.98418900	3.28745200
H	-0.66623400	2.49680500	3.79480400
C	1.89089100	0.48646400	2.59497200
H	2.55203000	1.33602600	2.37698100
H	2.22116500	0.02389700	3.53678700
H	1.99404200	-0.24247300	1.78219900
C	-0.89916200	-0.31660100	4.51443500
H	-1.63043100	-1.12641800	4.64645800
H	0.01307100	-0.58501000	5.06722500
H	-1.32164600	0.59874300	4.94541900
C	-0.23942300	-1.47598500	2.39351700
H	0.61454600	-1.95286900	2.89371700
H	-1.10564000	-2.14994700	2.47275400
H	0.00511600	-1.34666800	1.32880400
B	-1.32362300	1.19601800	1.36694800
H	-2.33477300	-0.73970600	-0.15789600
O	-2.12663100	1.69789200	0.39154600
N	-3.49202000	1.40341900	0.53290500
C	-4.15980500	2.34385900	1.25100100
C	-3.54771400	3.50646400	1.78775500
C	-5.55251000	2.17113400	1.48454900
C	-4.28349100	4.41756500	2.52683800

C	-6.27359500	3.08549800	2.22683000
H	-6.06839700	1.30459000	1.06740600
C	-5.65228000	4.22474000	2.76760900
H	-3.79265600	5.30556800	2.92812500
H	-7.33990800	2.92754800	2.39416200
C	-4.06517900	-2.98759700	0.15006700
H	-3.84677700	-3.27165500	-0.88943800
H	-3.33367200	-3.48284400	0.80535100
H	-5.07007200	-3.34900700	0.41224500
H	-2.49334500	3.69317400	1.59391500
C	-5.46175500	-0.36115500	-1.02390300
H	-5.26978100	-0.92245900	-1.94743800
H	-6.43242000	-0.67523400	-0.61615500
H	-5.45589600	0.71597800	-1.22277400
C	-4.54723200	-0.84638700	2.42713600
H	-3.92770000	-1.59540600	2.93663700
H	-4.40029500	0.13753800	2.88325200
H	-5.60085100	-1.15377900	2.47468500
Sb	-3.93713400	-0.82243900	0.38686500
C	-6.40423400	5.17018100	3.54229100
N	-7.01136300	5.92902300	4.16955500

IN5:

C	-2.51605200	-2.57631700	0.26290100
C	-1.82950100	-1.86173700	-0.95682200
O	-1.67966900	-2.17919400	1.36452400
O	-1.25016500	-0.69910700	-0.32896500
C	-3.91782500	-2.04402600	0.54587000
H	-4.63467200	-2.36173400	-0.22361200
H	-4.24926000	-2.42977500	1.51911900

H	-3.92009600	-0.94540500	0.59745900
C	-2.53130900	-4.09220200	0.17339400
H	-3.03073300	-4.50564900	1.05998100
H	-3.08270000	-4.42039400	-0.72000100
H	-1.51359000	-4.49796800	0.13381800
C	-2.78291500	-1.41209400	-2.04934200
H	-2.21530100	-0.92873500	-2.85687100
H	-3.31520000	-2.27535700	-2.47471900
H	-3.52190000	-0.69610800	-1.66770800
C	-0.67567200	-2.66949100	-1.54235600
H	-1.03762000	-3.54784600	-2.09405100
H	-0.10773800	-2.02758600	-2.22959800
H	0.01071400	-3.00345700	-0.75082900
B	-1.05079500	-1.02646500	0.99691600
H	0.45677800	1.26252300	-1.31444000
O	-0.32354300	-0.26443200	1.85552300
N	0.56059600	0.65549600	1.24802300
C	1.71361900	0.04266200	0.85075700
C	1.98560100	-1.33777300	1.03854600
C	2.70612600	0.81950200	0.19426200
C	3.16162600	-1.89990100	0.57030800
C	3.87348500	0.24571000	-0.27460400
H	2.56613900	1.89505900	0.08551100
C	4.11876600	-1.12624000	-0.10361700
H	3.35243200	-2.96202100	0.73136700
H	4.61908100	0.86484200	-0.77509900
C	-1.52272900	3.25367800	-1.71589700
H	-2.09122600	4.08822300	-1.28164100
H	-0.81456800	3.64736700	-2.45880100
H	-2.22478500	2.58110800	-2.23036600

H	1.27796100	-1.95828200	1.58576500
C	0.70505900	3.75553000	0.61368400
H	1.21828600	3.40736700	1.51770000
H	1.43643900	4.10212600	-0.12811700
H	0.02766700	4.58414700	0.85867500
C	-2.16107800	1.92250700	1.07067500
H	-2.86005000	1.21609300	0.60671600
H	-1.86753600	1.57135700	2.06529600
H	-2.63082700	2.91357900	1.12492700
Sb	-0.44222400	2.15114300	-0.17729100
C	5.32954200	-1.72052700	-0.59602700
N	6.30315300	-2.19882400	-0.99692000

TS5:

C	0.66094200	0.47458300	3.10189900
C	-0.06760500	-0.52403100	2.14218300
O	0.23106400	1.73905100	2.59509900
O	-1.28789500	0.18739900	1.84483800
C	0.16217400	0.36184300	4.54162700
H	0.52366000	-0.55331400	5.03077100
H	0.52635200	1.23072800	5.10569700
H	-0.93772400	0.37064900	4.57363400
C	2.17749400	0.40361300	3.05393700
H	2.59835600	1.12815100	3.76422100
H	2.53114200	-0.60006300	3.33325600
H	2.55310900	0.65164200	2.05404400
C	-0.37221800	-1.87051800	2.77474400
H	-0.77608200	-2.56345900	2.02283200
H	0.55150100	-2.31695000	3.17127300
H	-1.09132300	-1.77434800	3.59896100

C	0.67842500	-0.71313700	0.82398900
H	1.58901500	-1.31309700	0.95861700
H	0.01791900	-1.22973100	0.11402300
H	0.95593100	0.25806600	0.39032700
B	-0.97298100	1.54444400	1.96571000
H	-3.48073500	0.18627300	0.08731200
O	-1.74715000	2.57174600	1.58069800
N	-2.75789200	2.23345200	0.63951700
C	-3.86833800	2.90923600	0.88886000
C	-4.08616200	3.83367600	1.97073600
C	-5.00473500	2.63586000	0.04317500
C	-5.34195800	4.33078000	2.23379200
C	-6.25369800	3.15006000	0.32985500
H	-4.84357800	2.05592300	-0.86842600
C	-6.46620100	3.97796600	1.44963300
H	-5.48269500	5.01760500	3.07105400
H	-7.09529400	2.92690400	-0.33047200
C	-3.92099600	-2.32231500	1.86557500
H	-4.60104100	-2.67344000	2.65261300
H	-4.03107200	-2.96002900	0.97934400
H	-2.88765100	-2.36513000	2.22321000
H	-3.23628500	4.12252600	2.58584200
C	-6.47855000	-0.47386600	0.90469600
H	-6.92491400	0.52644700	0.95864700
H	-6.59816200	-0.87519900	-0.10954800
H	-6.96076300	-1.14658800	1.62581800
C	-4.25504600	0.79295900	3.16444800
H	-3.31717600	1.35920700	3.13689000
H	-5.09546200	1.49698000	3.21130300
H	-4.27545300	0.09209500	4.00850600

Sb	-4.41059800	-0.31124600	1.37486700
C	-7.77113900	4.47513700	1.75725000
N	-8.83338700	4.86096900	2.01227200

2a′:

C	-3.54375300	-0.78222700	0.21199700
C	-3.33056500	0.77024100	0.09363100
O	-2.36703600	-1.30431300	-0.43729100
O	-1.88964900	0.87371800	0.10102700
C	-3.51224500	-1.26758400	1.65829900
H	-4.41696900	-0.96697300	2.20411000
H	-3.44694100	-2.36374700	1.65920300
H	-2.63383800	-0.87047300	2.18742800
C	-4.77682500	-1.30615200	-0.50181700
H	-4.84675100	-2.39298100	-0.35933100
H	-5.68598100	-0.84378100	-0.09010200
H	-4.72940200	-1.10528100	-1.57862200
C	-3.89412400	1.57836400	1.24807300
H	-3.70598500	2.64689500	1.07550300
H	-4.98084500	1.42838400	1.32628900
H	-3.42676900	1.29616700	2.19897400
C	-3.81151000	1.32747800	-1.24229200
H	-4.90840300	1.34252100	-1.29881700
H	-3.43932400	2.35499200	-1.35171900
H	-3.42425700	0.72858600	-2.07908300
B	-1.41887000	-0.33503400	-0.33845700
H	0.26236100	1.33324200	-0.07694800
O	-0.10320000	-0.54694700	-0.62623500
N	0.69386700	0.59506100	-0.63295100
C	2.02723400	0.34046900	-0.34892900

C	2.57334000	-0.94725000	-0.45353600
C	2.85883000	1.42385600	-0.01243600
C	3.92856200	-1.14149000	-0.22322000
C	4.20902800	1.22209300	0.21515500
H	2.43527200	2.42696300	0.06283400
C	4.76006500	-0.06510400	0.11232500
H	4.35387200	-2.14253500	-0.30161600
H	4.85101000	2.06327000	0.47788000
H	1.92568100	-1.78190400	-0.71245400
C	6.16286600	-0.27473900	0.35219900
N	7.28974400	-0.44157200	0.54610100

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