Supporting Information

Catalytic Asymmetric Diaziridination

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1. General Methods and Starting Materials

NMR spectra were acquired on a Varian AS 400 spectrometer, running at 400 MHz for ^{1}H and 100 MHz for ^{13}C, respectively. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CDCl_3$: 7.26 ppm for ^{1}H NMR, 77.16 ppm for ^{13}C NMR). The following abbreviations are used to indicate the multiplicity in NMR spectra: s - singlet; d - doublet; t - triplet; q - quartet; dd - double doublet; m - multiplet; bs - broad signal. ^{13}C NMR spectra were acquired on a broad band decoupled mode. Mass spectra were recorded on a Bruker Maxis Impact mass spectrometer using electrospray (ES^+) ionization techniques. Analytical thin layer chromatography (TLC) was performed using pre-coated aluminum-backed plates (Merck Kieselgel 60 F254) and visualized by ultraviolet irradiation or anisaldehyde dip. Optical rotations were measured on a Perkin-Elmer 241 polarimeter. The enantiomeric excess (ee) of the products was determined by chiral stationary phase HPLC (Daicel Chiralcel IA, IB and IC columns). Unless otherwise noted, analytical grade solvents and commercially available reagents were used without further purification. For flash chromatography (FC) silica gel (Silica gel 60, 230-400 mesh, Fluka) was used.

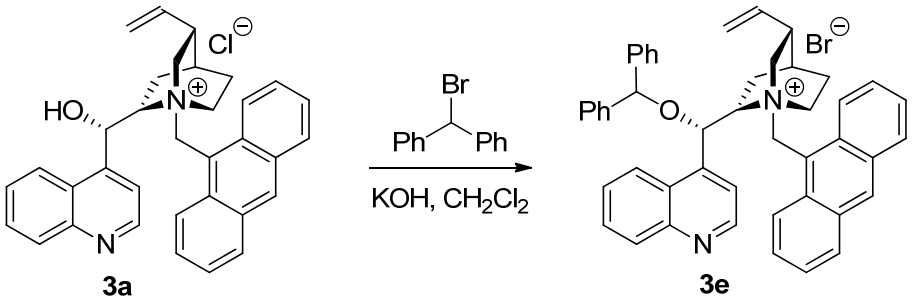
Aromatic[1] and aliphatic[2] imines were prepared following reported procedures. *N*-9-antracenylmethyl cinchoninium chloide **3a** was prepared following a literature procedure[3]

(1) (a) Cheng, L.; Liu, L.; Jia, H.; Wang, D.; Chen, Y.-J. *J. Org. Chem.* **2009**, *74*, 4650. (b) Jia, Y.-X.; Xie, J.-H.; Duan, H.-F.; Wang, L.-X.; Zhou, Q.-L. *Org. Lett.* **2006**, *8*, 1621.

(2) Chemla, F.; Hebbe, V.; Normant, J.-F. *Synthesis* **2000**, 75.

(3) Lygo, B.; Wainwright, P. G. *Tetrahedron*, **1999**, *55*, 6289.

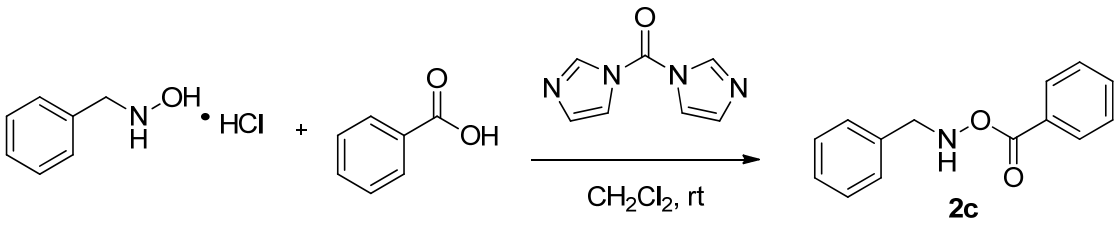
1.1 Synthesis of Catalyst 3e



3a **3e**

To a stirred suspension of *N*-9-antracenylmethyl cinchoninium chloide **3a** (261 mg, 0.5 mmol) in CH_2Cl_2 (5 mL) were sequentially added bromodiphenylmethane (247 mg, 1.0 mmol) and KOH (56 mg, 1.0 mmol). After vigorous stirring overnight at rt, H_2O and CH_2Cl_2 were added. The two phases were separated and the aqueous layer extracted with CH_2Cl_2, the combined organic extracts were dried over $MgSO_4$, filtered and evaporated under reduced pressure. The residue were loaded on a column packed with silica gel and eluted with CH_2Cl_2/MeOH (gradient 98:2 – 90:10). The columned catalyst was dissolved in CH_2Cl_2 (1.5 mL), poured onto Et_2O (15 mL) with stirring. The resulting precipitate was collected by suction filtration, washed several times with Et_2O, giving **3e** as a off-white solid (159 mg, 43% yield). **^{1}H NMR (400 MHz, CD_3OD) δ**: 8.83 (s, 1H), 8.75-8.65 (m, 2H), 8.58 (d, *J* = 8.1 Hz, 1H), 8.25-8.10 (m, 3H), 7.96 (t, *J* = 9.6 Hz, 2H), 7.81 (t, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 4.6 Hz, 1H), 7.73-7.58 (m, 4H), 7.57-7.47 (m, 3H), 7.47-7.28 (m, 3H), 7.22-7.07 (m, 3H), 7.05 (s, 1H), 6.23 (ddd, *J* = 6.7 Hz, *J* = 10.4 Hz, *J* = 17.2 Hz, 1H), 6.08 (s, 1H), 5.95 (d, *J* = 13.7 Hz, 1H), 5.78-5.55 (m, 1H), 5.49-5.34 (m, 1H), 5.14 (d, *J* = 17.2 Hz, 1H), 4.45-4.29 (m, 2H), 4.03 (t, *J* = 11.2 Hz, 1H), 3.39 (bt, *J* = 11.3 Hz, 1H), 2.94 (bt, *J* = 12.4 Hz, 1H), 2.65-2.49 (m, 1H), 2.36 (q, *J* = 8.9 Hz, 1H) 1.98 (bs, 1H), 1.91-1.32 (m, 4H), 0.84 (t, *J* = 7.4 Hz, 1H). **^{13}C NMR (100 MHz, CD_3OD) δ**: 148.9, 147.6, 141.3, 140.3, 140.2, 136.3, 133.2, 132.7, 132.5, 131.6, 131.5, 129.9, 129.8, 129.7, 129.1 (x2), 128.7, 128.1, 128.0 (x2), 127.9 (x2), 127.8, 127.5 (x2), 125.3, 125.0, 123.9, 123.5, 122.8, 121.6, 117.0, 117.0, 84.2, 72.9, 68.5, 57.1, 56.7, 55.4, 37.6, 25.8, 23.3, 22.3. **HRMS** (ESI+) *m/z* calcd. for $C_{47}H_{43}N_2O^+$: 651.3375; found: 651.3372.

1.2 Synthesis of hydroxylamine 2c



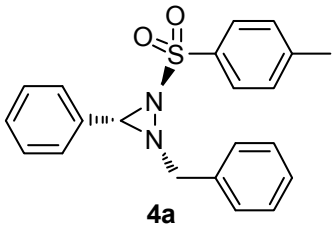
To a stirred solution of benzoic acid (1.22 g, 10 mmol) in CH_2Cl_2 (20 mL) carbonyldiimidazole (1.62 g, 10 mmol) was added. After 15 min gas evolution stopped, and *N*-benzylhydroxylamine hydrogen chloride (1.60 g, 10 mmol) was added. After stirring 1 h at rt the reaction mixture was filtered and the solvent was removed under reduced pressure. The residue were loaded on a column packed with silica gel and eluted with pentane/Et_2O (gradient 90:10 – 70:30), giving **2c** as an colorless oil (1.93 g, 85%). **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.99 (d, *J* = 7.0 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.47-7.41 (m, 4H), 7.40-7.29 (m, 3H), 4.29 (s, 3H) **^{13}C NMR (100 MHz, $CDCl_3$)**: **δ** 166.7, 135.9, 133.3, 129.3 (×2), 128.9 (×2), 128.6 (×2), 128.5 (×2), 128.4, 127.9, 56.7. **HRMS** (ESI+) *m/z* calcd. for $C_{14}H_{13}NO_2$ $[M+H]^+$: 228.1019; found: 228.1021.

2. Catalytic Asymmetric Diaziridinations

2.1. General Procedure

A glass vial equipped with a magnetic stirring bar was charged with anhydrous K_3PO_4 (0.1 mmol), catalyst **3e** (0.005 mmole) and 0.5 mL of anhydrous toluene. After stirring shortly at rt, hydroxylamine **2c** (0.075 mmol) was added, and the mixture was cooled to −30 °C. Then, the corresponding imine **1** (0.05 mmol) was added at once and the stirring was maintained at −12 °C (no fluctuations in temperature is tolerated) for 72 h. The crude mixture was cooled to −30 °C, diluted with 4 mL of a −30 °C pentane/Et_2O (1:1) solution and plugged through a short path of silica (ca. 1 cm) using additional 75 mL of pentane/ Et_2O (1:1) solution. Solvents were evaporated under reduced pressure. The residue was loaded on a column packed with silica gel and eluted with the solvent indicated in each case to furnish pure diaziridines **4a-l**.

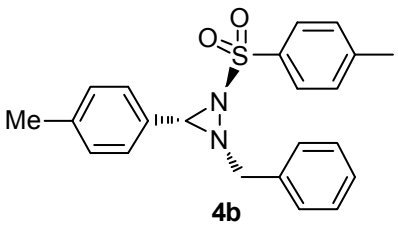
2.2. Characterization Data for Diaziridines 4a-l



4a

Isolated by FC on silica gel using pentane/Et_2O (gradient 95:5 - 90:10) as the eluent.

(1*R*,2*R*,3*S*)-1-Benzyl-3-phenyl-2-tosyldiaziridine (94% ee). Colorless oil. $[\alpha]_D$: +29.2 (c 0.40, $CHCl_3$). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.52-7.47 (m, 2H), 7.44-7.40 (m, 3H), 7.17-7.11 (m, 3H), 7.06 (t, *J* = 7.3 Hz, 2H), 6.91 (d, *J* = 6.9 Hz, 2H), 4.91 (s, 1H), 3.34 (d, *J* =13.2 Hz, 1H), 3.29 (d, *J* = 13.2 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 145.1, 136.0, 132.0, 129.9, 129.6, 129.5 (×2), 129.4 (×2), 129.3 (×4), 128.6 (×2), 128.2 (×2), 127.2, 63.6, 56.2, 21.8. **HRMS** (ESI+) *m/z* calcd. for $C_{21}H_{20}N_2O_2S$ $[M+Na]^+$: 387.1138; found: 387.1142. **HPLC**: Chiralpak IA, Hx/*i*-PrOH 90:10, 1.0 mL·min^{-1}; t_{minor} = 12.3 min; t_{major} = 13.7 min.

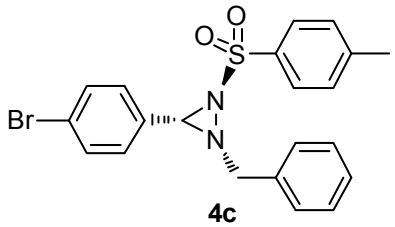


4b

Isolated by FC on silica gel using pentane/Et_2O (gradient 90:10 - 85:15) as the eluent.

(1*R*,2*R*,3*S*)-1-Benzyl-3-(4-tolyl)-2-tosyldiaziridine (84% ee). Colorless oil. $[\alpha]_D$: +23.4 (c 0.50, $CHCl_3$). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.17-7.11 (m, 3H), 7.07 (t, *J* = 7.3 Hz, 2H), 6.93 (d, *J* = 6.8 Hz, 2H), 4.87 (s, 1H), 3.34 (d, *J* =13.3 Hz, 1H), 3.29 (d, *J* = 13.3 Hz, 1H), 2.40 (s, 3H), 2.39 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 145.0, 132.3, 131.6, 130.1, 129.9, 129.5 (×2), 129.3 (×2), 129.3 (×4), 129.2

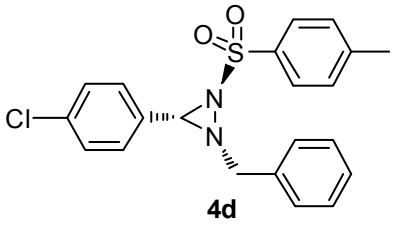
(×2), 128.2, 127.2 (×2), 62.9, 56.3, 21.9. **HRMS** (ESI+) *m/z* calcd. for $C_{22}H_{22}N_2O_2S$ [M+H]$^+$: 379.1475; found: 379.1472. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 20.3 min; t_{major} = 17.3 min.



4c

Isolated by FC on silica gel using CH_2Cl_2/pentane (gradient 1:1 - 1:0) as the eluent.

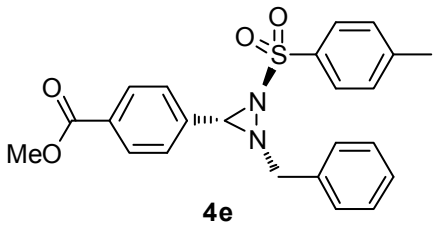
(1*R*,2*R*,3*S*)-1-Benzyl-3-(4-bromophenyl)-2-tosyldiaziridine (75% ee). White solid. **[α]$_D$**: +35.4 (c 0.50, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.18-7.12 (m, 3H), 7.07 (t, *J* = 8.3 Hz, 2H), 6.91 (d, *J* = 6.9 Hz, 2H), 4.85 (s, 1H), 3.31 (d, *J* =13.2 Hz, 1H), 3.26 (d, *J* = 13.2 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 145.2, 135.7, 132.0, 131.9 (×2), 130.9 (×2), 129.6 (×2), 129.3 (×2), 129.2 (×2), 128.7, 128.3 (×2), 127.3, 124.3, 62.9, 56.3, 21.9. **HRMS** (ESI+) *m/z* calcd. for $C_{21}H_{19}N_2O_2SBr$ [M+Na]$^+$: 465.0243; found: 465.0248. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 17.1 min; t_{major} = 20.1 min.



4d

Isolated by FC on silica gel using CH_2Cl_2/pentane (gradient 1:1 - 1:0) as the eluent.

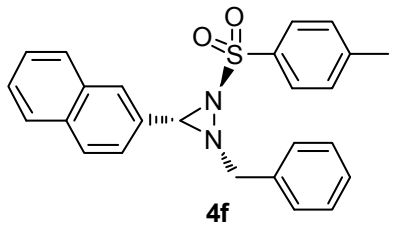
(1*R*,2*R*,3*S*)-1-Benzyl-3-(4-chlorophenyl)-2-tosyldiaziridine (84% ee). White solid. **[α]$_D$**: +28.8 (c 0.50, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.17-7.12 (m, 3H), 7.08 (t, *J* = 7.3 Hz, 2H), 6.91 (d, *J* = 6.8 Hz, 2H), 4.87 (s, 1H), 3.31 (d, *J* =13.2 Hz, 1H), 3.27 (d, *J* = 13.2 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 145.2, 136.1, 135.8, 132.0, 130.6 (×2), 129.6 (×2), 129.3 (×2), 129.2 (×2), 128.9 (×2), 128.3 (×2), 128.1, 127.3, 62.9, 56.3, 21.9. **HRMS** (ESI+) *m/z* calcd. for $C_{21}H_{19}N_2O_2SCl$ [M+H]$^+$: 399.0934; found: 399.0934. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 19.7 min; t_{major} = 16.4 min.



4e

Isolated by FC on silica gel using CH_2Cl_2/pentane (gradient 1:1 - 1:0) as the eluent.

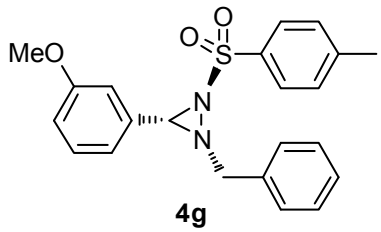
(1*R*,2*R*,3*S*)-1-Benzyl-3-(4-methylbenzoate)-2-tosyldiaziridine (96% ee). Colorless oil. **[α]$_D$**: +40.6 (*c* 0.50, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: **δ** 8.08 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.18-7.12 (m, 3H), 7.07 (t, *J* = 7.3 Hz, 2H), 6.89 (d, *J* = 6.8 Hz, 2H), 4.93 (s, 1H), 3.94 (s, 3H) 3.31 (d, *J* =13.3 Hz, 1H), 3.26 (d, *J* = 13.2 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)**: **δ** 166.5, 145.3, 135.7, 134.5, 131.9, 131.6, 129.8 (×2), 129.6 (×2), 129.4 (×2), 129.3 (×2), 129.2 (×2), 128.3 (×2), 127.3, 63.0, 56.5, 21.9. **HRMS** (ESI+) *m*/*z* calcd. for $C_{23}H_{22}N_2O_4S$ $[M+H]^+$: 423.1379; found: 423.1376. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 42.87 min; t_{major} = 48.53 min.



4f

Isolated by FC on silica gel using CH_2Cl_2/pentane (gradient 1:1 - 1:0) as the eluent.

(1*R*,2*R*,3*S*)-1-Benzyl-3-(naphthalen-2-yl)-2-tosyldiaziridine (80% ee). White solid. **[α]$_D$**: +2.1 (*c* 0.83, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: **δ** 8.03 (2, 1H), 7.92-7.96 (m, 3H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.57-7.53 (m, 3H), 7.17 (d, *J* = 7.9 Hz, 2H), 7.12 (d, *J* = 7.2 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 2H), 6.91 (d, *J* = 7.2 Hz, 2H) 5.07 (s, 1H), 3.38 (d, *J* =13.3 Hz, 1H), 3.29 (d, *J* = 13.3 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)**: **δ** 145.1, 136.0, 133.9, 132.9, 132.1, 129.6 (×2), 129.4 (×2), 129.3 (×2), 129.3, 128.5, 128.4, 128.3 (×2), 128.0, 127.2, 127.2, 127.0, 127.0, 125.9, 63.8, 56.4, 21.9. **HRMS** (ESI+) *m*/*z* calcd. for $C_{25}H_{22}N_2O_2S$ $[M+Na]^+$: 437.1294; found: 437.1299. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 26.8 min; t_{major} = 21.5 min.

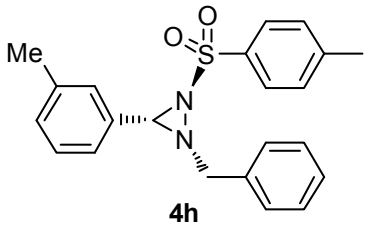


4g

Isolated by FC on silica gel using CH_2Cl_2/Et_2O (gradient 100: - 95:5) as the eluent.

(1*R*,2*R*,3*S*)-1-Benzyl-3-(3-methoxyphenyl)-2-tosyldiaziridine (92% ee). Colorless oil. **[α]$_D$**: +38.4 (*c* 0.24, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: **δ** 7.70 (d, *J* = 8.3 Hz, 2H), 7.32 (t, *J* = 7.9 Hz, 1H), 7.18-7.12 (m, 3H), 7.10-7.05 (m, 3H), 7.01 (s, 1H), 6.98-6.90 (m, 3H), 4.86 (s, 1H), 3.81 (s, 3H), 3.37 (d, *J* =13.2 Hz, 1H), 3.31 (d, *J* = 13.2 Hz, 1H), 2.40 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)**: **δ** 159.7, 145.1, 136.1, 132.1, 131.0, 129.8, 129.5 (×2), 129.4 (×2), 129.3 (×2), 128.2 (×2), 127.2, 121.6, 115.6, 114.6, 63.5, 56.3, 55.5, 21.9. **HRMS** (ESI+) *m*/*z* calcd. for $C_{22}H_{22}N_2O_3S$ $[M+Na]^+$:

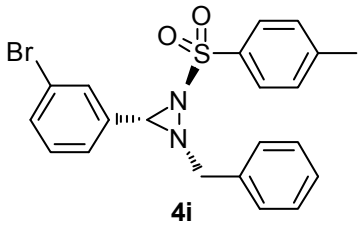
417.1243; found: 417.1244. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 24.7 min; t_{major} = 22.2 min.



4h

Isolated by FC on silica gel using pentane/Et_2O (gradient 90:10 - 85:15) as the eluent.

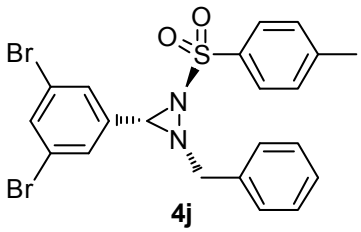
(1*R*,2*R*,3*S*)-1-Benzyl-3-(3-tolyl)-2-tosyldiaziridine (91% ee). Colorless oil. **[α]$_D$**: +36.8 (*c* 0.24, $CHCl_3$). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.72 (d, *J* = 8.3 Hz, 2H), 7.32-7.28 (m, 3H), 7.25-7.31 (m, 1H), 7.17-7.11 (m, 3H), 7.07 (t, *J* = 7.6 Hz, 2H), 7.07 (d, *J* = 6.8 Hz, 2H), 4.86 (s, 1H), 3.35 (d, *J* =13.3 Hz, 1H), 3.30 (d, *J* = 13.3 Hz, 1H), 2.41 (s, 3H), 2.38 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 145.0, 138.4, 136.1, 132.2, 130.6, 129.8 (×2), 129.5 (×2), 129.5 (×2), 129.4 (×2), 129.3, 128.5, 128.2, 127.2, 126.4, 63.6, 56.3, 21.8, 21.5. **HRMS** (ESI+) *m*/*z* calcd. for $C_{22}H_{22}N_2O_2S$ $[M+H]^+$: 379.1480; found: 379.1477. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 16.3 min; t_{major} = 15.2 min.



4i

Isolated by FC on silica gel using pentane/Et_2O (gradient 90:10 - 85:15) as the eluent.

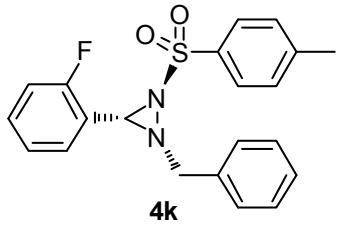
(1*R*,2*R*,3*S*)-1-Benzyl-3-(3-bromophenyl)-2-tosyldiaziridine (92% ee). White solid. **[α]$_D$**: +34.2 (*c* 0.50, $CHCl_3$). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.66 (t, *J* = 2.0 Hz, 1H), 7.57 (ddd, *J* = 1.2 Hz, *J* = 2.0 Hz, *J* = 7.9 Hz, 1H), 7.44 (dd, *J* = 1.3 Hz, *J* = 7.7 Hz, 1H), 7.29 (t, *J* = 7.9 Hz, 1H), 7.18-7.13 (m, 3H), 7.11-7.05 (m, 2H), 6.91 (d, *J* = 7.2 Hz, 2H), 4.86 (s, 1H), 3.34 (d, *J* =13.2 Hz, 1H), 3.27 (d, *J* = 13.2 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 145.2, 135.7, 133.1, 132.1, 131.9, 131.9, 130.2, 129.6 (×2), 129.3 (×2), 129.3 (×2), 128.3 (×2), 127.9, 127.3, 122.8, 62.6, 56.5, 21.9. **HRMS** (ESI+) *m*/*z* calcd. for $C_{21}H_{19}N_2O_2SBr$ $[M+H]^+$: 443.0429; found: 443.0427. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 16.9 min; t_{major} = 14.2 min.



4j

Isolated by FC on silica gel using CH_2Cl_2/pentane (gradient 1:1 - 1:0) as the eluent.

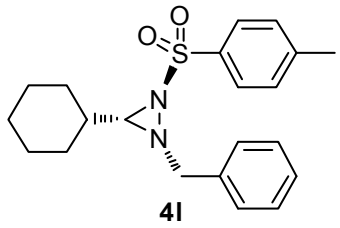
(1*R*,2*R*,3*S*)-1-Benzyl-3-(3,5-dibromophenyl)-2-tosyldiaziridine (84% ee). White solid. **[α]**$_D$: +33.8 (*c* 0.50, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: **δ** 7.74 (t, *J* = 1.8 Hz, 1H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 1.8 Hz, 2H), 7.19-7.13 (m, 3H), 7.09 (t, *J* = 7.6 Hz, 2H), 6.91 (d, *J* = 6.9 Hz, 2H), 4.79 (s, 1H), 3.33 (d, *J* =13.2 Hz, 1H), 3.26 (d, *J* = 13.2 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)**: **δ** 145.4, 135.7, 135.4, 133.6, 131.6, 131.0 (×2), 129.6 (×2), 129.4 (×2), 129.3 (×2), 128.4 (×2), 127.5, 123.3, 61.8, 56.7, 21.9. **HRMS** (ESI+) *m/z* calcd. for $C_{21}H_{18}N_2O_2SBr_2$ $[M+H]^+$: 520.9529; found: 520.9522. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 17.9 min; t_{major} = 15.5 min.



4k

Isolated by FC on silica gel using CH_2Cl_2/pentane (gradient 1:1 - 1:0) as the eluent.

(1*R*,2*R*,3*S*)-1-Benzyl-3-(2-fluorophenyl)-2-tosyldiaziridine (41% ee). Colorless oil. **[α]**$_D$: +15.2 (*c* 0.50, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: **δ** 7.69 (d, *J* = 8.3 Hz, 2H), 7.61 (dt, *J(d)* = 1.8 Hz, *J(t)* = 7.4 Hz, 1H), 7.43 (ddt, *J(d)* = 1.8 Hz, *J(d)* = 5.3 Hz, *J(t)* = 7.5 Hz, 1H), 7.22 (dt, *J(d)* = 1.1 Hz, *J(t)* = 7.5 Hz, 1H), 7.17-7.10 (m, 4H), 7.06 (t, J = 7.5 Hz, 2H), 6.94 (d, *J* = 6.8 Hz, 2H), 5.04 (s, 1H), 3.44 (d, *J* =13.2 Hz, 1H), 3.22 (d, *J* = 13.2 Hz, 1H), 2.40 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)**: **δ** 162.3 (d, *J* = 248.5 Hz), 145.2, 135.8, 131.8, 131.7 (d, *J* = 8.1 Hz), 131.2 (d, *J* = 3.0 Hz), 129.5, 129.3, 129.3, 128.3, 127.2, 124.2 (d, *J* = 3.6 Hz), 117.7 (d, *J* = 13.8 Hz), 115.7 (d, *J* = 20.2 Hz), 59.4 (d, *J* = 4.6 Hz), 56.7, 21.8. **HRMS** (ESI+) *m/z* calcd. for $C_{21}H_{19}N_2O_2SF$ $[M+H]^+$: 383.1230; found: 383.1230. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 90:10, 1.0 mL·min^{-1}; t_{minor} = 29.7 min; t_{major} = 28.4 min.



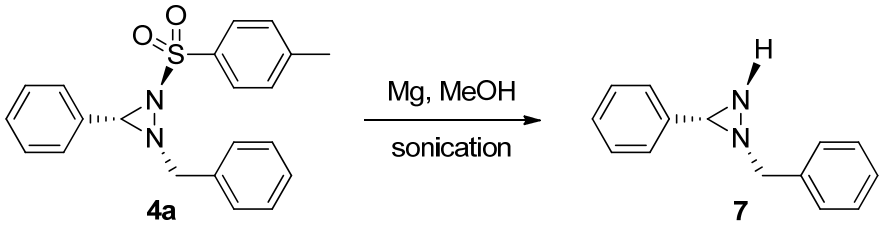
4l

Isolated by FC on silica gel using pentane/Et_2O (gradient 95:5 - 90:10) as the eluent.

(1*R*,2*R*,3*S*)-1-Benzyl-3-cyclohexyl-2-tosyldiaziridine (33% ee). Colorless oil. **[α]**$_D$: +2.5 (*c* 0.40, $CHCl_3$). **^{1}H NMR (400 MHz, CDCl$_3$)**: **δ** 7.57 (d, *J* = 8.3 Hz, 2H), 7.19-7.11 (m, 1H), 7.11-7.08 (m, 4H), 7.05 (d, *J* = 8.1 Hz, 2H), 3.82 (d, *J* = 13.2 Hz, 1H), 3.56 (d, *J* = 9.6 Hz, 1H), 3.55 (d, *J* =13.2 Hz, 1H), 2.37 (s, 3H), 2.98-1.62 (m, 7H), 1.37-1.16 (m, 4H). **^{13}C NMR (100 MHz, CDCl$_3$)**: **δ** 144.7, 136.6, 132.5, 129.4 (×2), 129.2 (×2), 129.1 (×2), 128.3 (×2), 127.1, 67.6, 56.4, 34.6, 30.2,

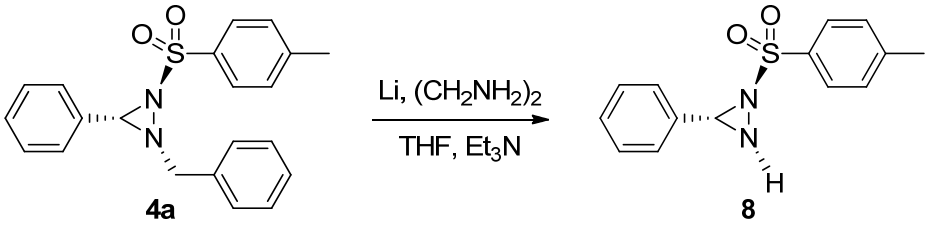
29.5, 26.0, 25.4, 25.2, 21.8. **HRMS** (ESI+) *m/z* calcd. for $C_{21}H_{26}N_2O_2S$ $[M+H]^+$: 371.1793; found: 371.1797. **HPLC**: Chiralpak IC, Hx/*i*-PrOH 80:20, 1.0 mL·min^{-1}; t_{minor} = 27.4 min; t_{major} = 20.6 min.

2.3. Synthesis of 7



To a solution of **4a** (12.4 mg, 0.035 mmol) in dry MeOH (0.5 mL) was added Mg powder (16 mg, 0.35 mmol). The suspension was purged with argon, equipped with a gas outlet and sonicated for 30 min at rt. The solvent was evaporated under a stream of nitrogen, and the residue were loaded on a column packed with silica gel and eluted with CH_2Cl_2/Et_2O (95:5), giving **7** as a white solid (6.1 mg, 84%). **[α]$_D$**: +8.2 (c 0.07, $CHCl_3$). **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.54-7.49 (m, 2H), 7.43-7.37 (m, 3H), 7.30-7.21 (m, 3H), 7.20-7.15 (m, 2H), 4.48 (d, *J* = 7.2 Hz, 1H), 3.31 (s, 2H) 2.69 (d, *J* = 7.2 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)**: **δ** 133.5, 133.4, 129.3 (×2), 128.9, 128.8 (×2), 128.4 (×2), 128.2 (×2), 127.2, 58.0, 56.7. **HRMS** (ESI+) *m/z* calcd. for $C_{14}H_{14}N_2$ $[M+H]^+$: 211.1235; found: 211.1235. **HPLC**: Chiralpak IA, Hx/*i*-PrOH 70:30, 1.0 mL·min^{-1}; t_{minor} = 5.2 min; t_{major} = 7.5 min.

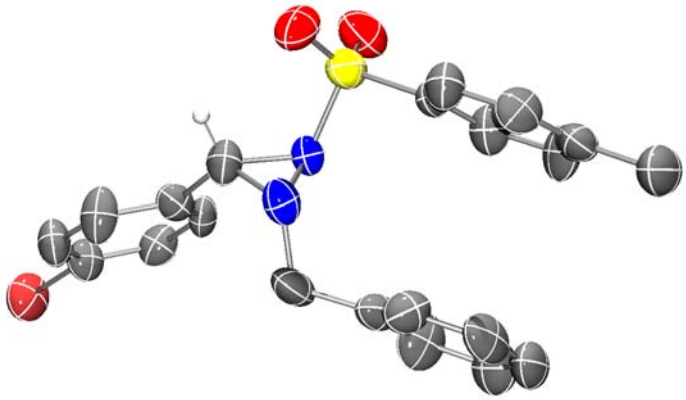
2.4. Synthesis of 8



To a stirring solution of **4a** (15.0 mg, 0.043 mmol) in THF (0.15 mL) and Et_3N (0.3 mL) was added *Li* (12 mg, 1.7 mmol) and ethylenediamine (20 μL, 0.3 mmol). After stirring for 2 h at rt the reaction mixture was added to $CHCl_3$ (2 mL) and loaded on a column packed with silica gel and eluted with pentane/EtOAc (70:30), giving **8** as a white solid (6.3 mg, 53%). **[α]$_D$**: +1.8 (c 0.05, $CHCl_3$). **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.90 (d, *J* = 8.2 Hz, 2H), 7.78 (d, *J* = 7.7 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 4.70 (bs, 1H), 2.44 (s, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)**: **δ** 143.2, 139.5, 132.9, 129.9, 129.5

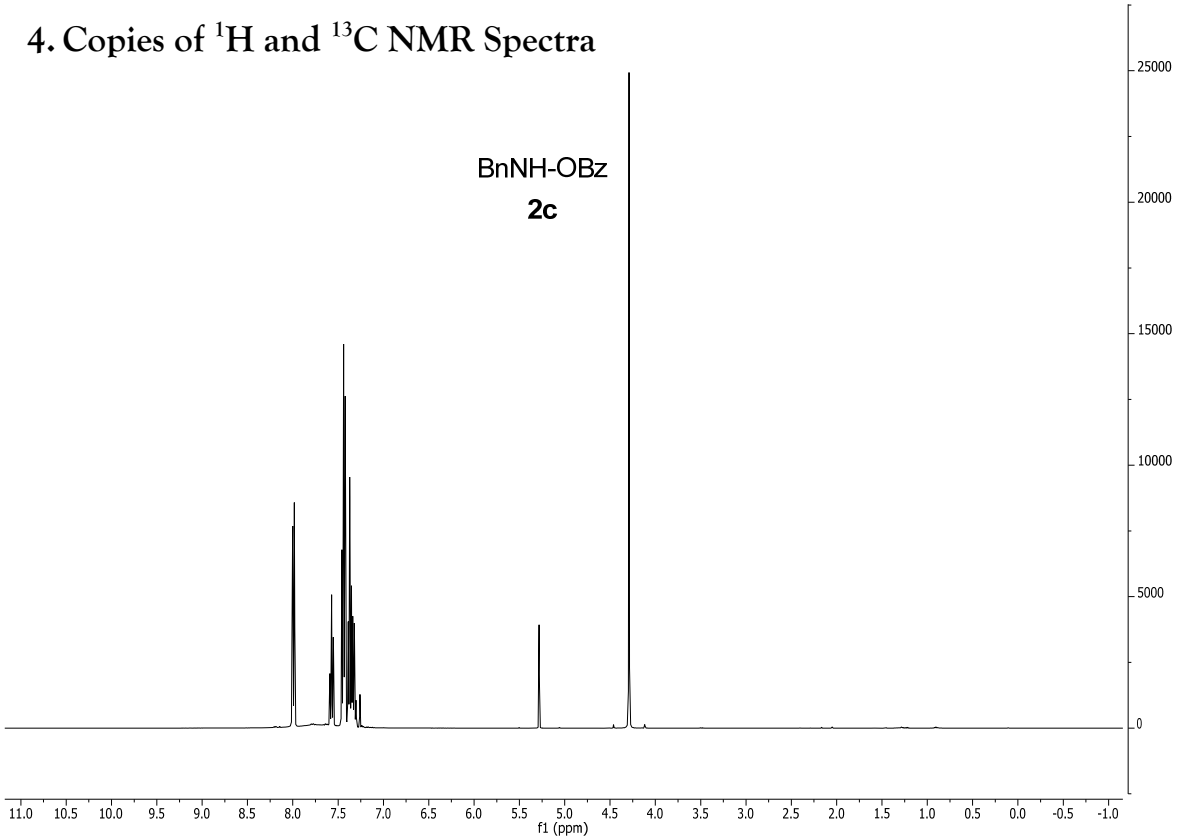
(×2), 129.0 (×2), 127.4 (×2), 126.7 (×2), 31.0, 21.7. **HRMS** (ESI+) *m/z* calcd. for $C_{14}H_{14}N_2O_2S$ $[M+H]^+$: 275.0849; found: 275.0850. **HPLC**: Chiralpak IB, Hx/*i*-PrOH 95:5, 1.0 mL·min^{-1}; t_{minor} = 15.2 min; t_{major} = 16.3 min.

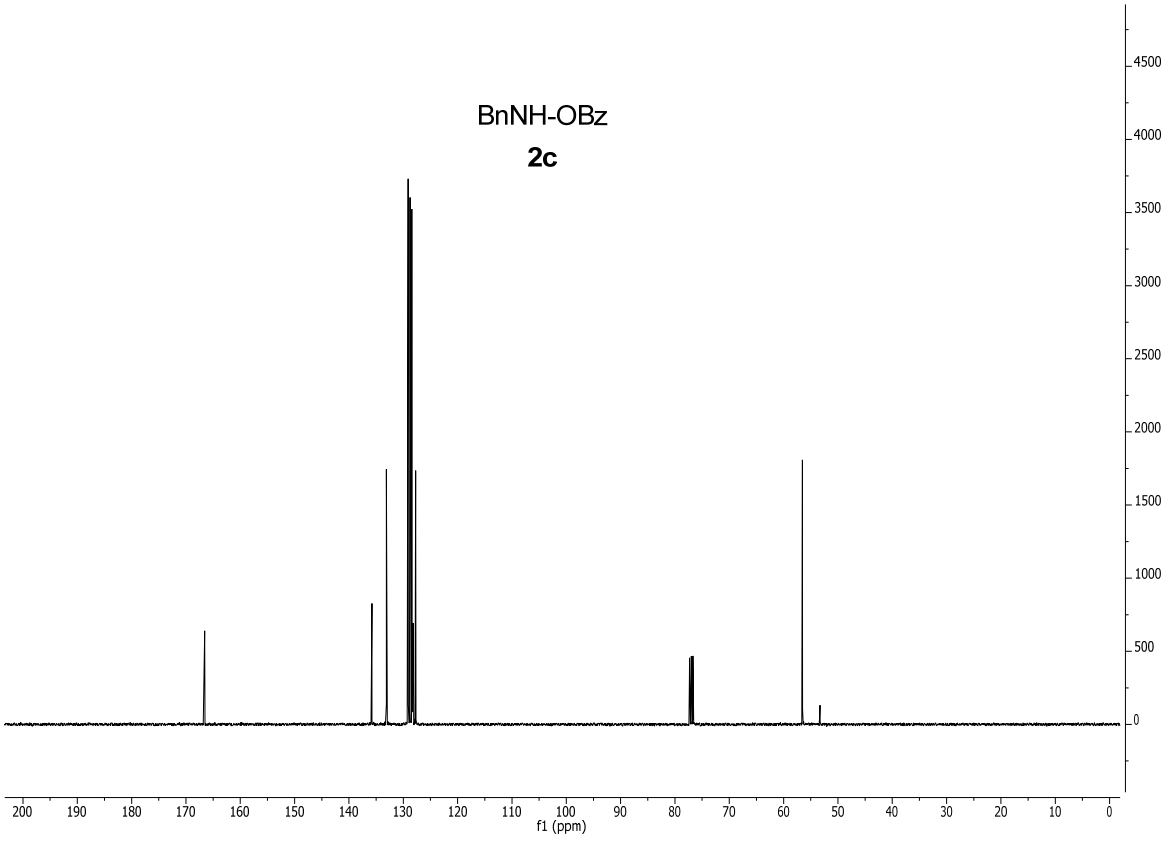
3. X-Ray Structure and Crystal Data for 4c

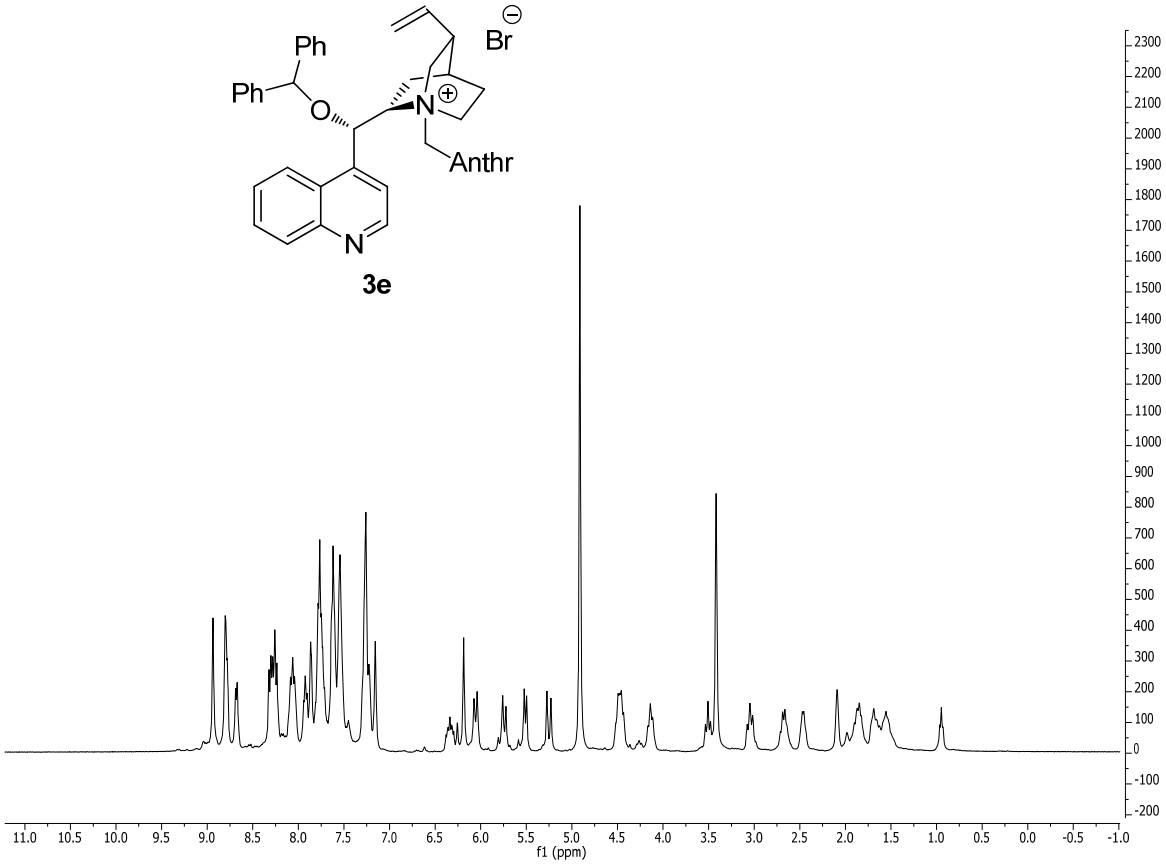


Crystal data for [**4c**]: $C_{21}H_{19}BrN_2O_2S$, M = 443.36, orthorhombic, space group P 21 21 21 (no. 115), *a* = 7.393(10) Å, *b* = 13.6537(19) Å, *c* = 19.656(3) Å, *V* = 1984.1(5) Å^3, *T* = 296 K, *Z* = 4, d_c = 1.488 g cm^{-3}, μ(Mo Kα, λ = 0.71073 Å) = 2.196 mm^{-1}, 11866 reflections collected, 2096 unique [R_{int} = 0.1748], which were used in all calculations. Refinement on F^2, final R(F) = 0.1385, R_w(F2) = 0.1053. CCDC number 902531.

4. Copies of ^{1}H and ^{13}C NMR Spectra



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Br
Anthr
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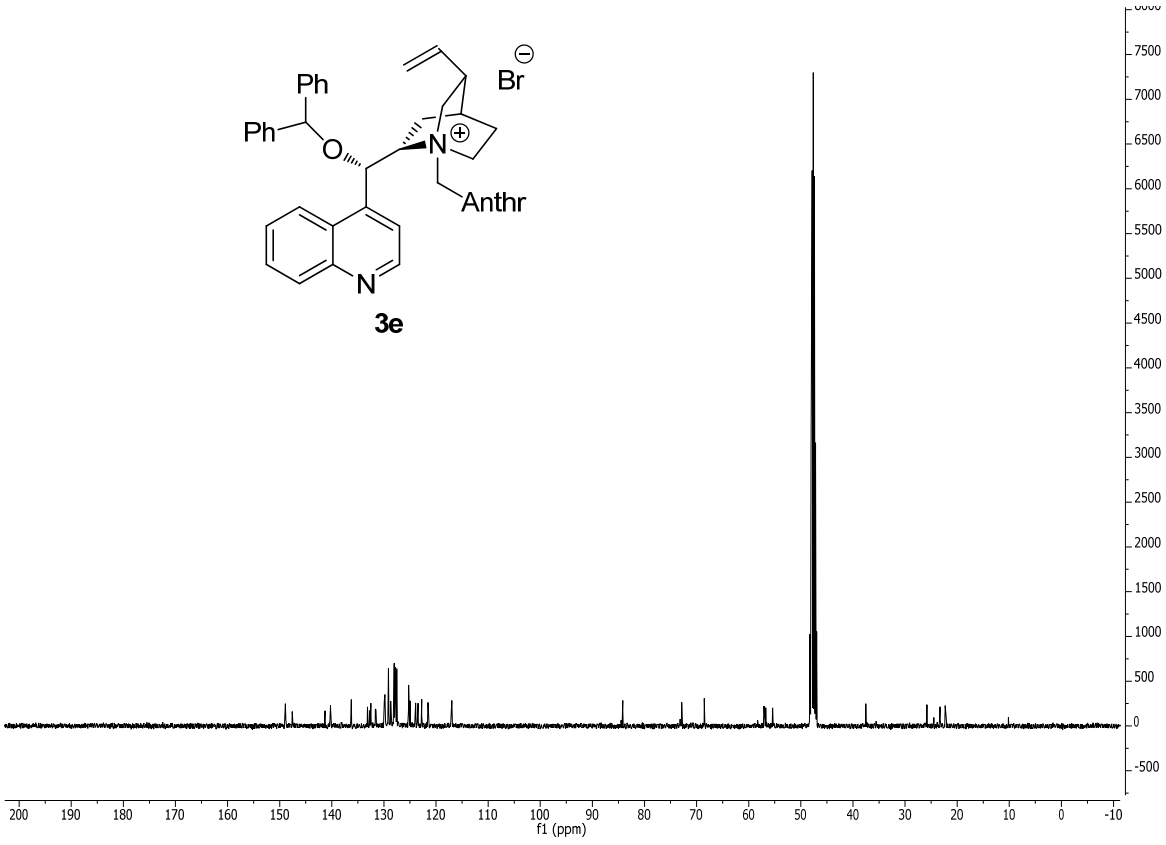
3e
f1 (ppm)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Ph
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Anthr
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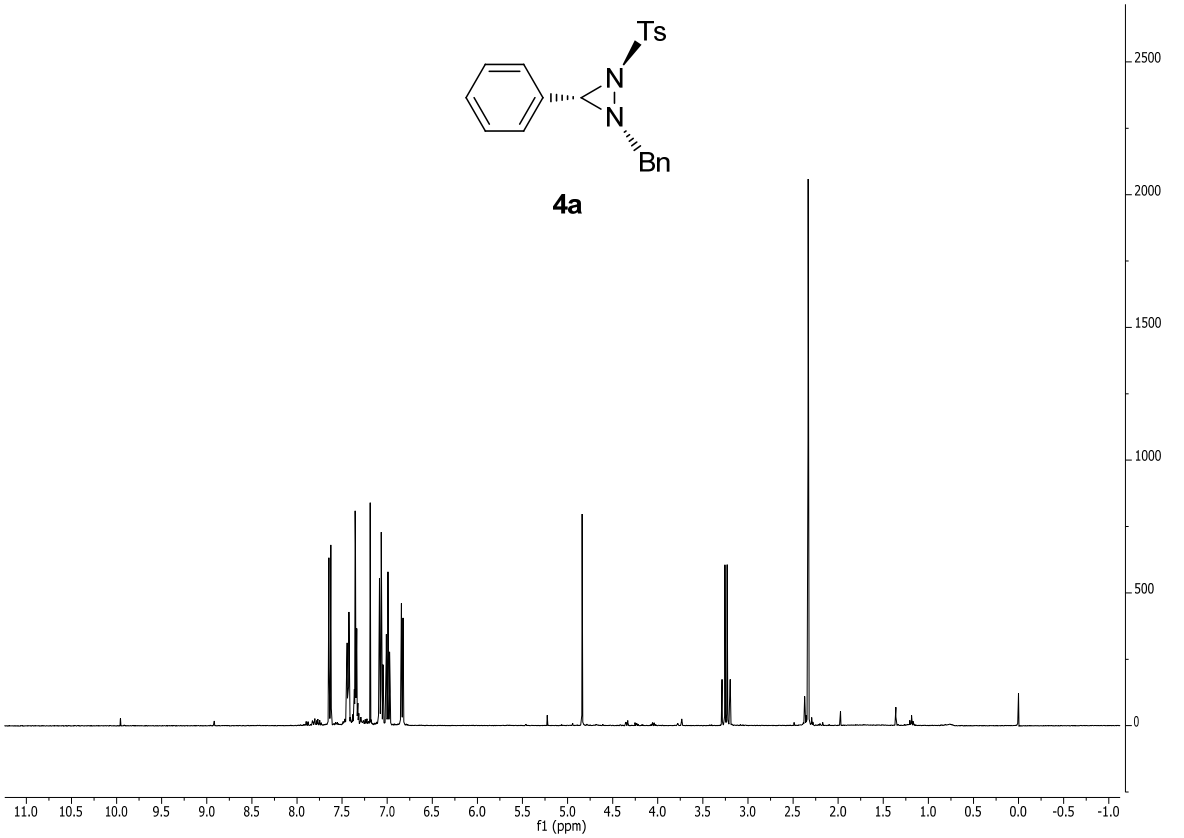
3e
f1 (ppm)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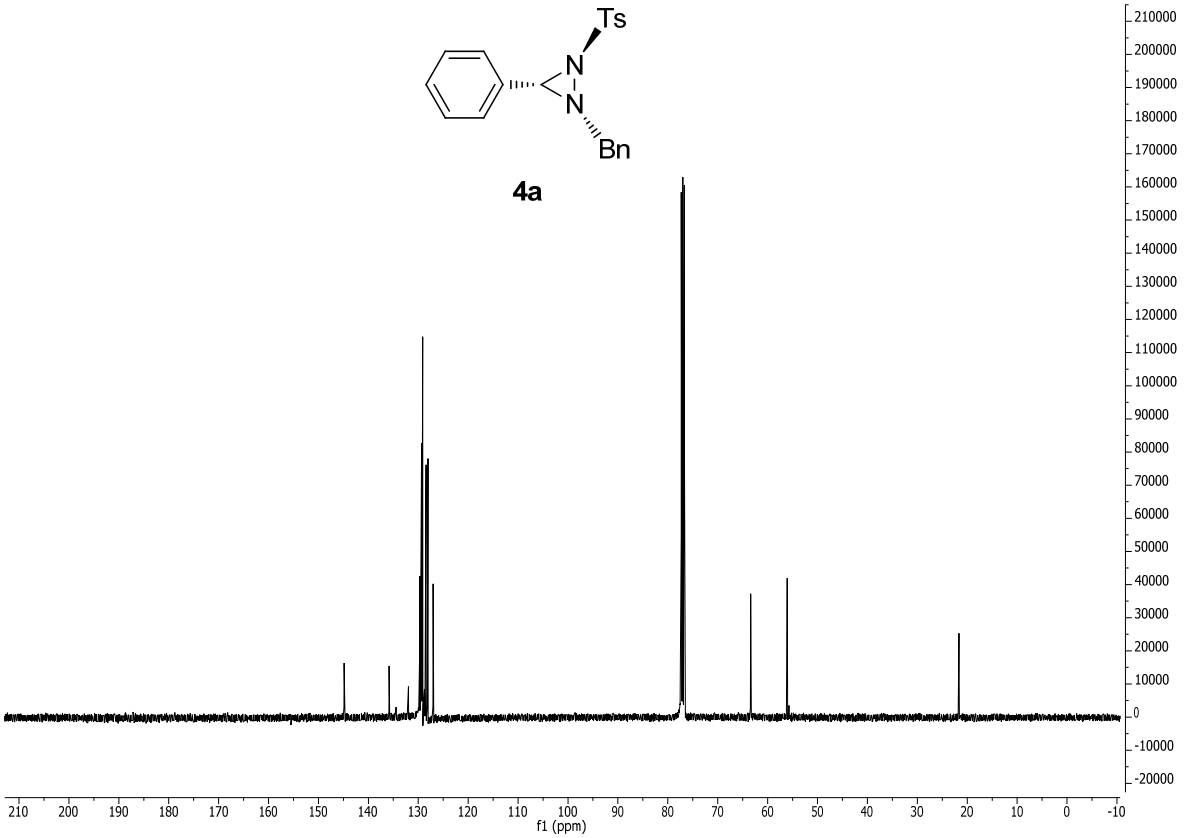
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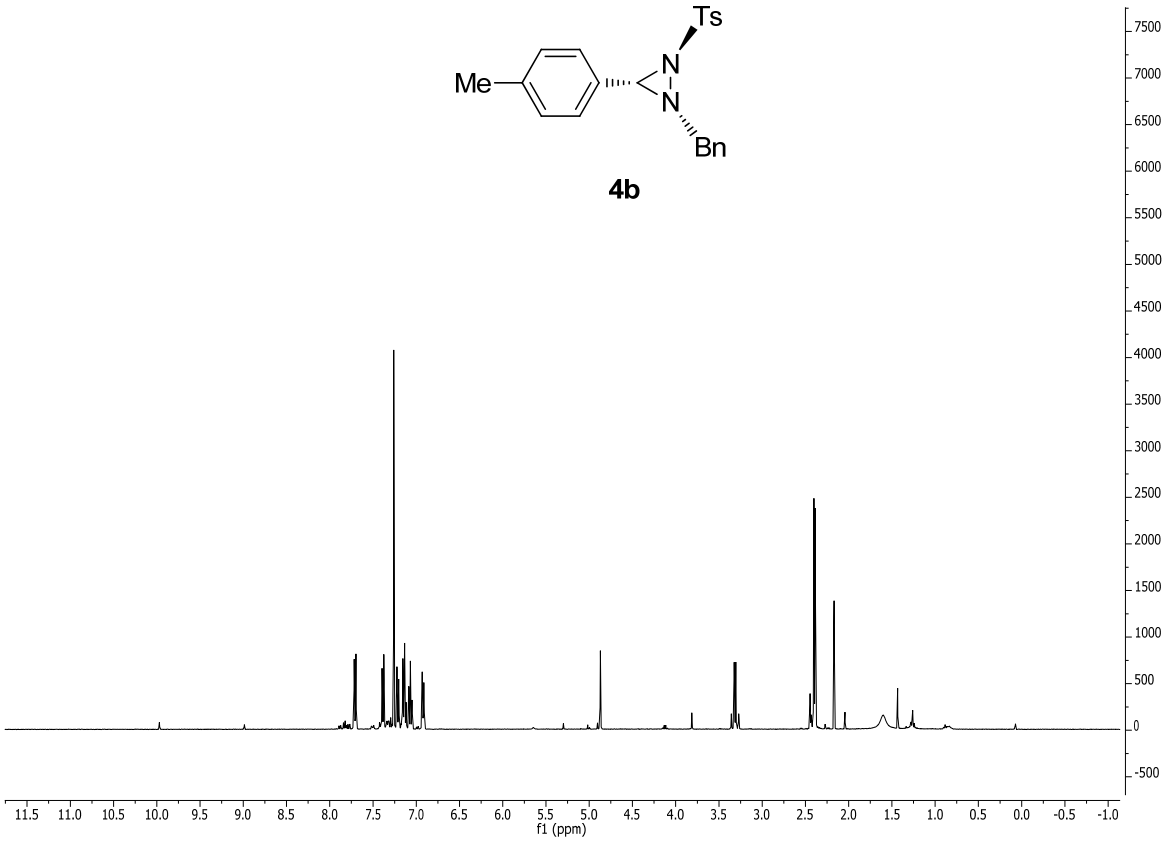
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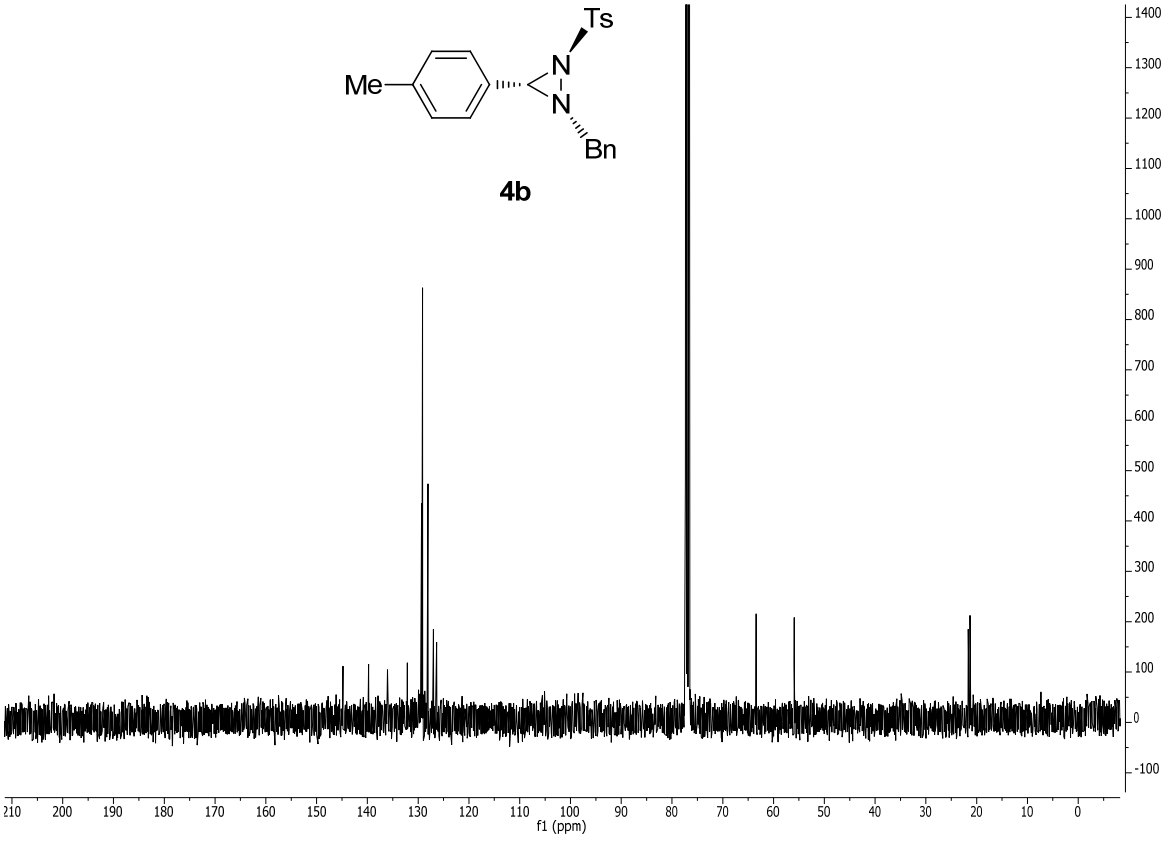
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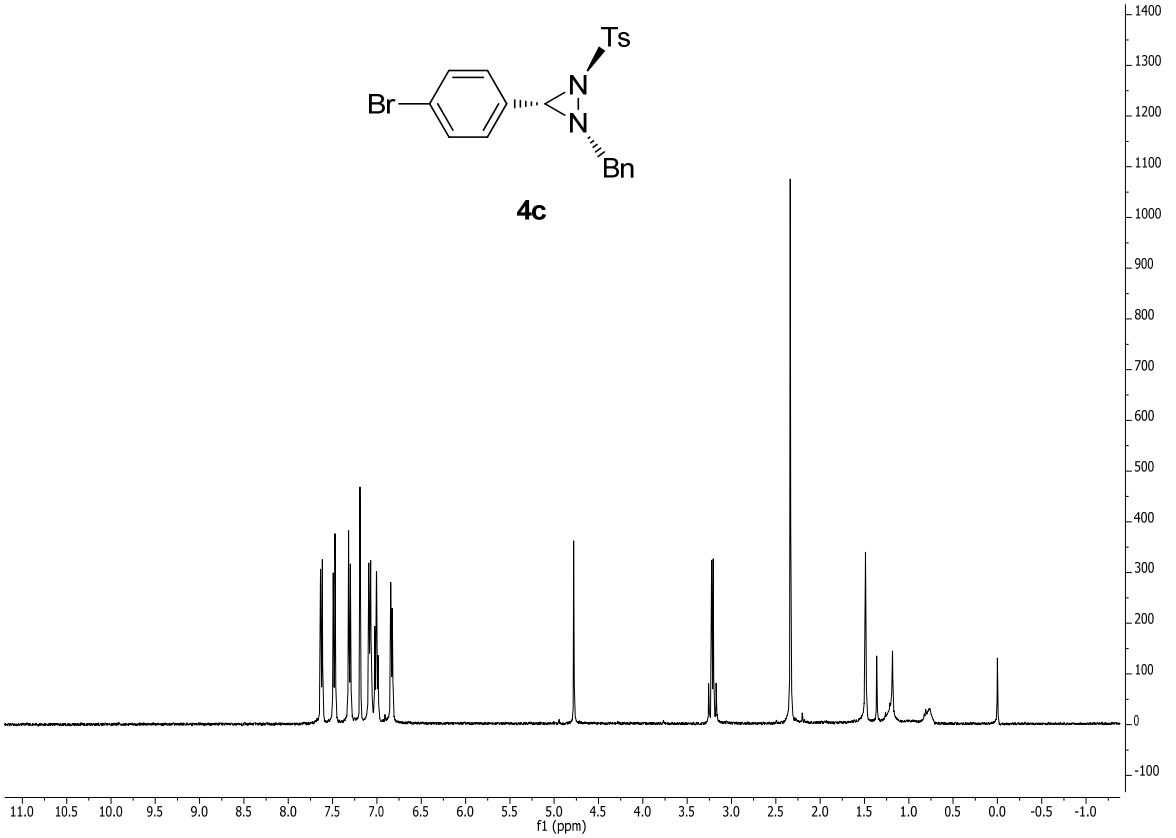
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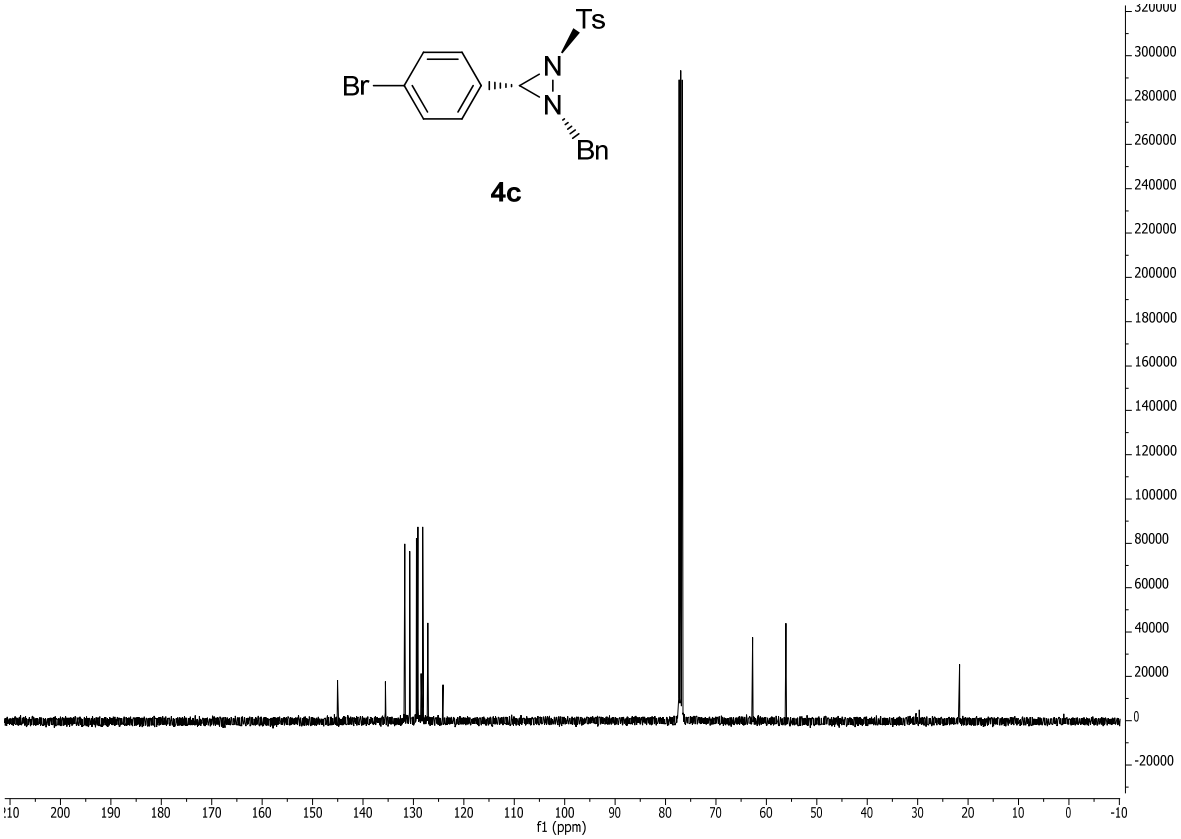
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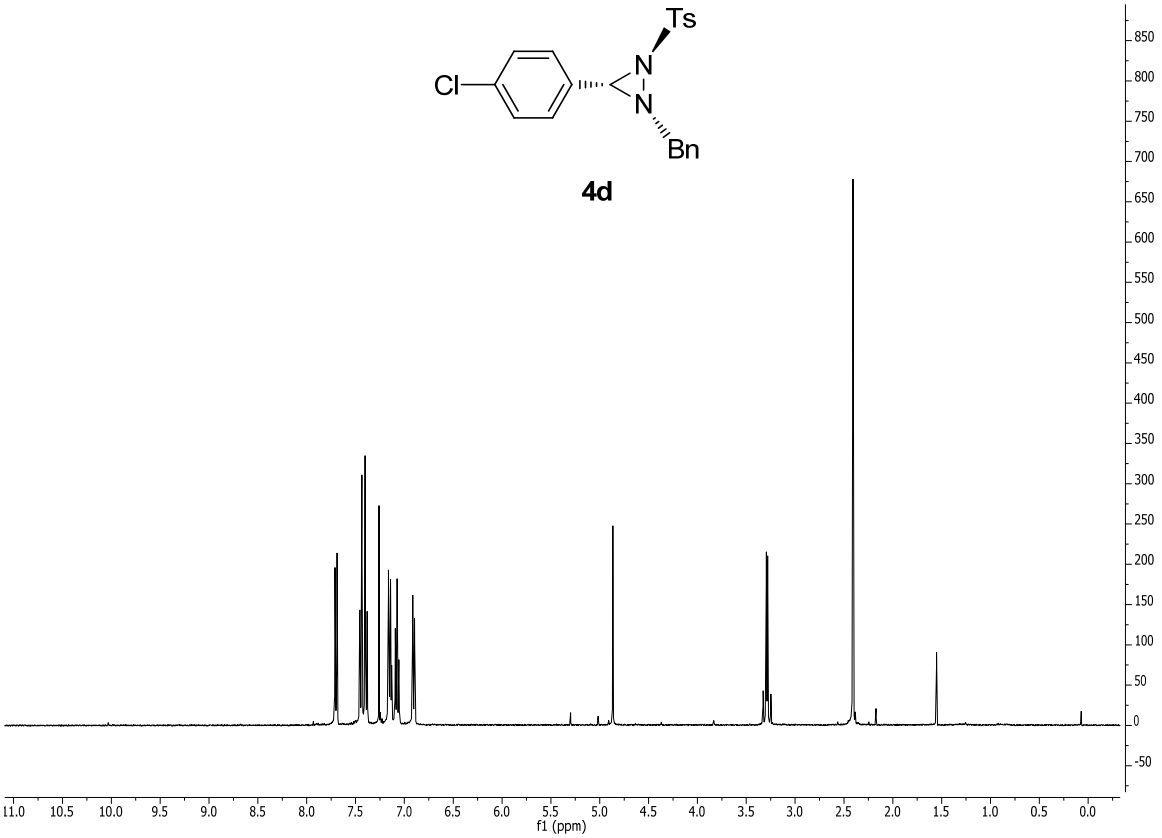
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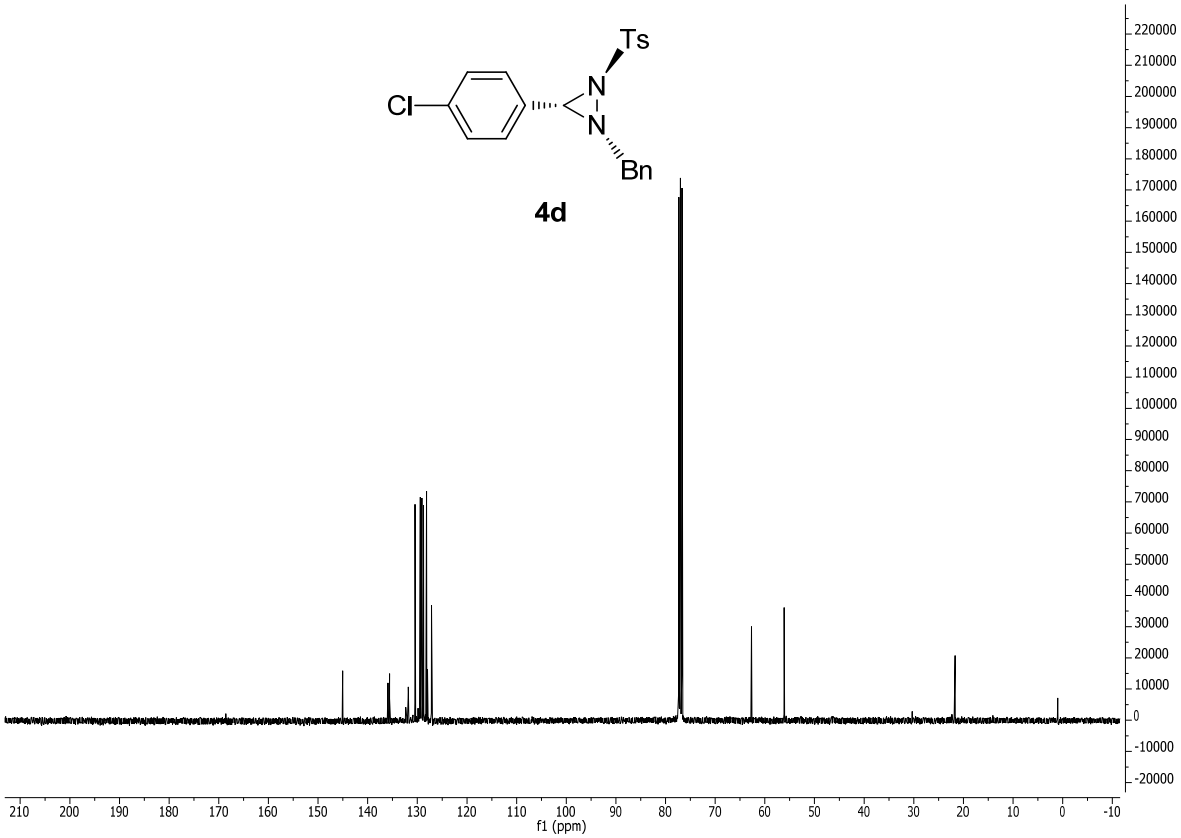
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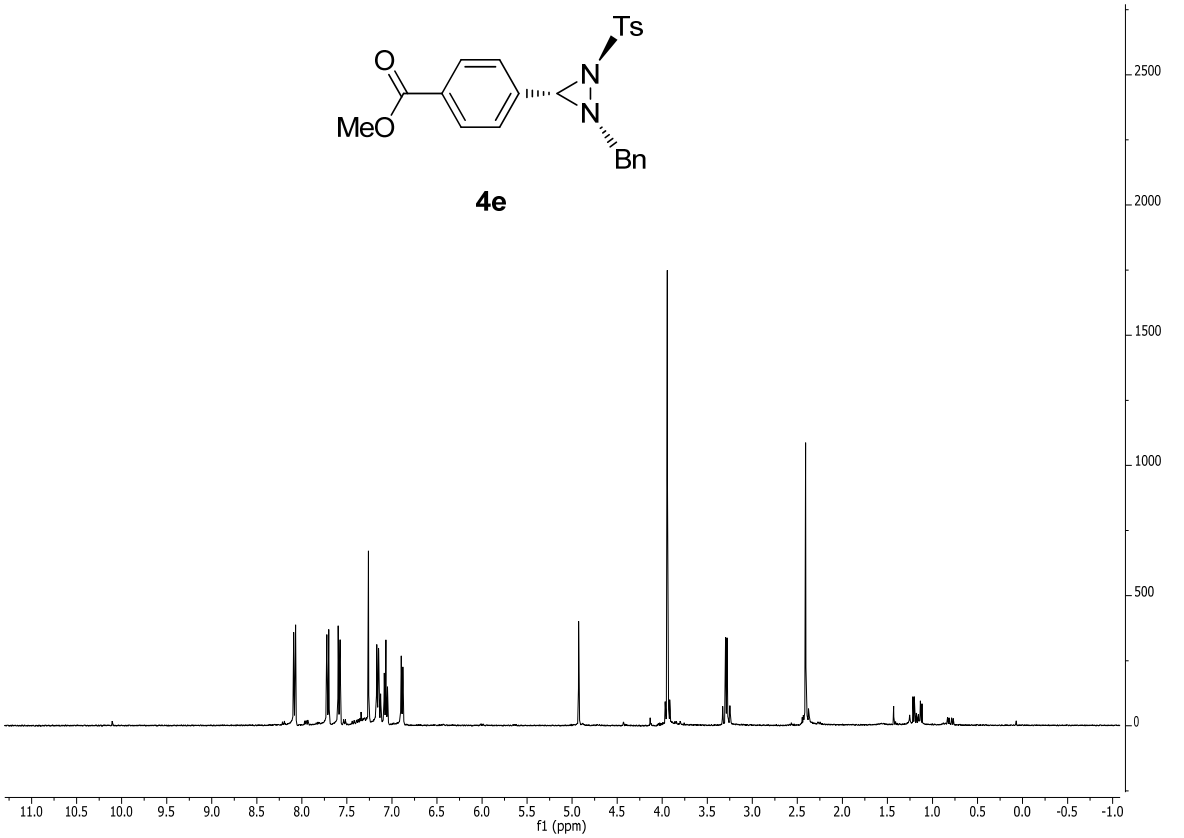
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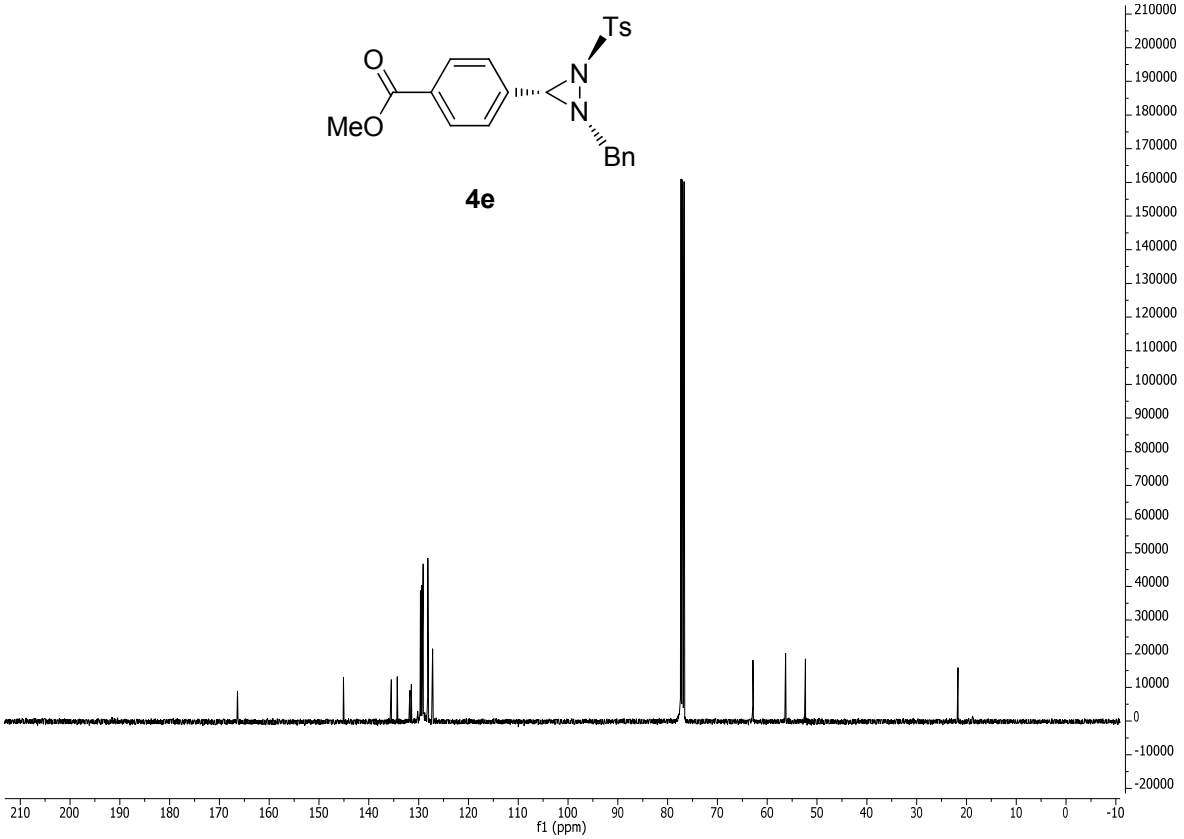
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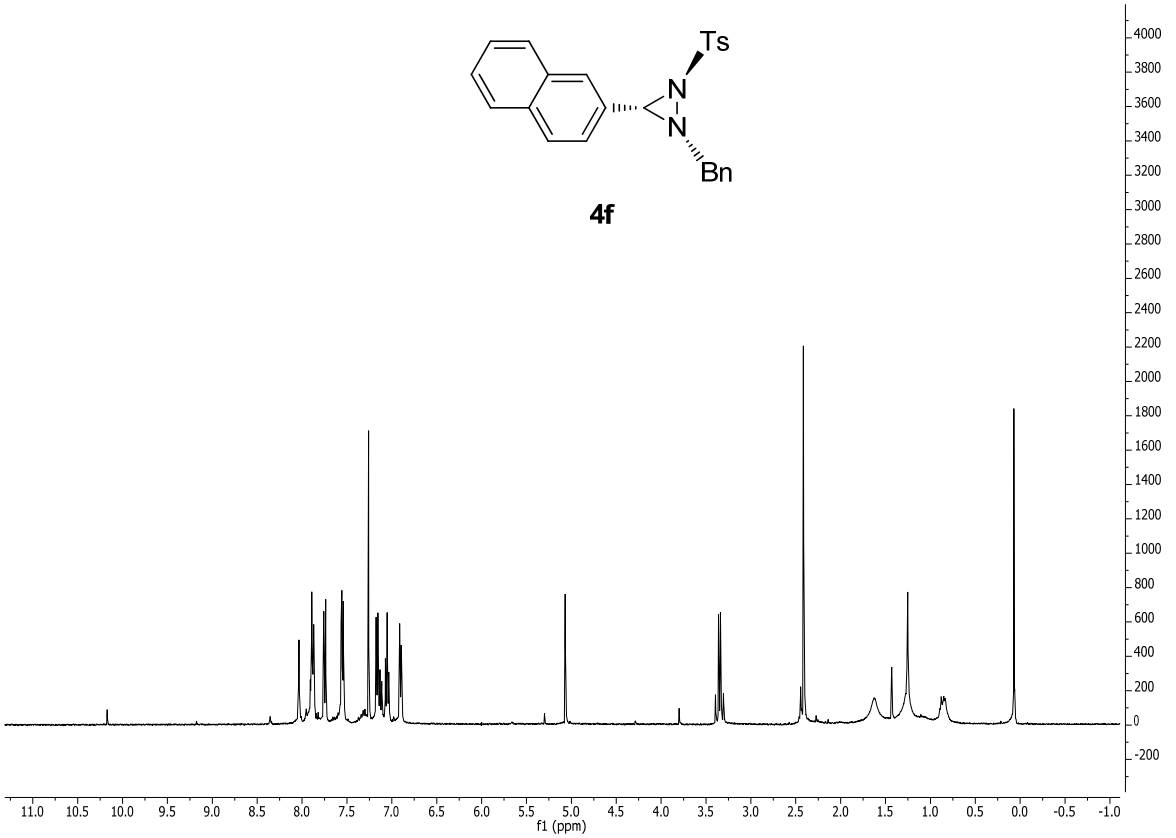
f1 (ppm)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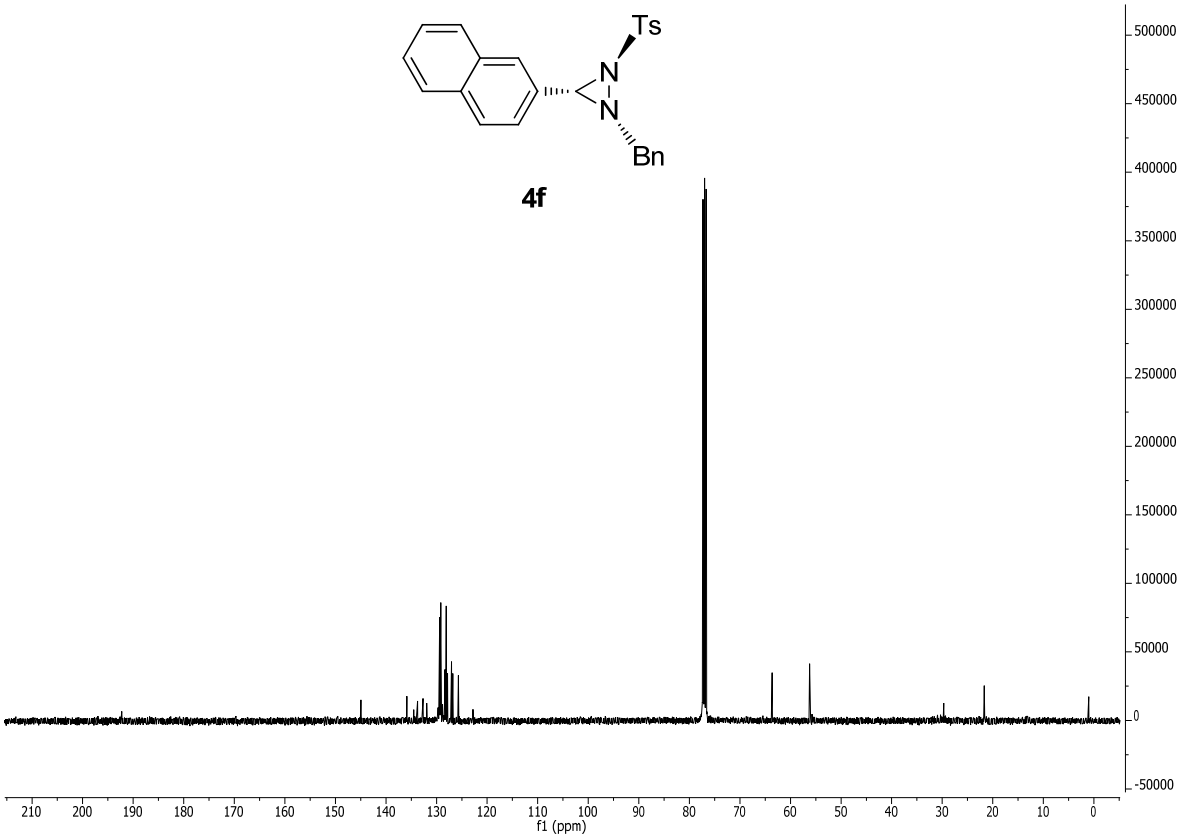
4f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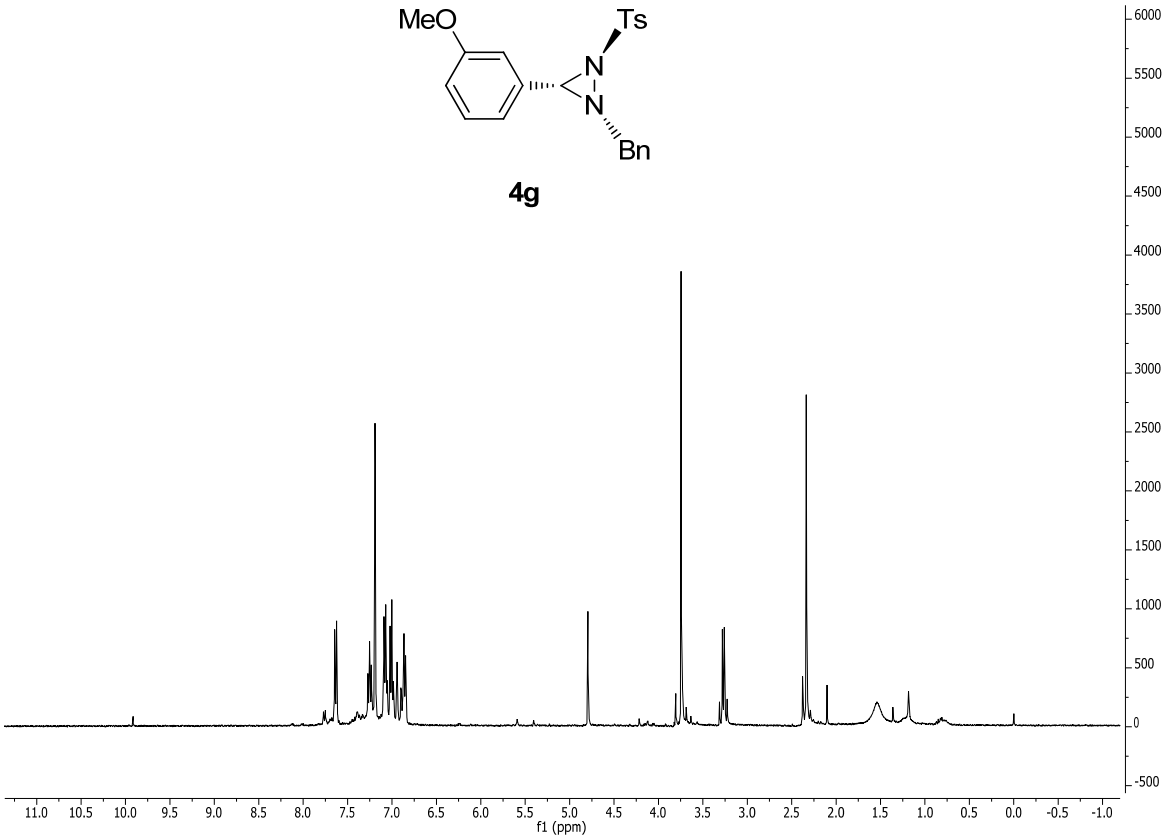
4f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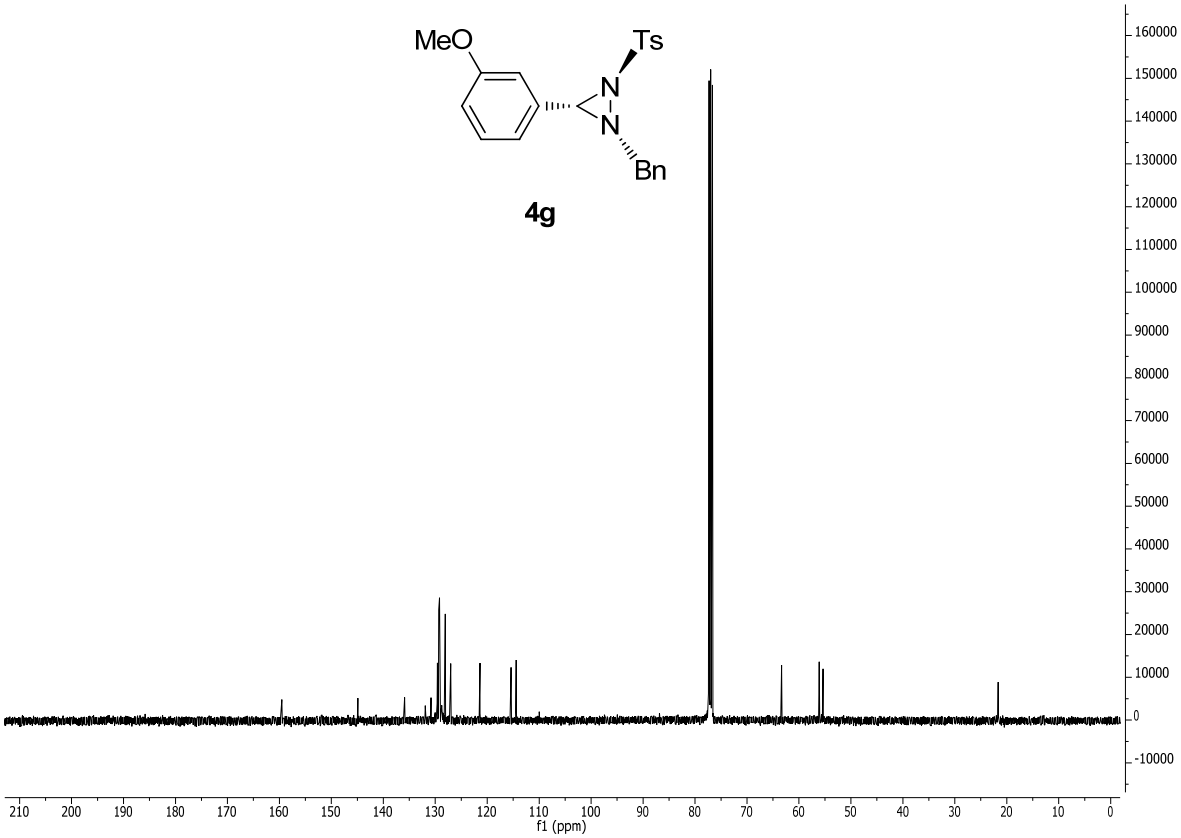
f1 (ppm)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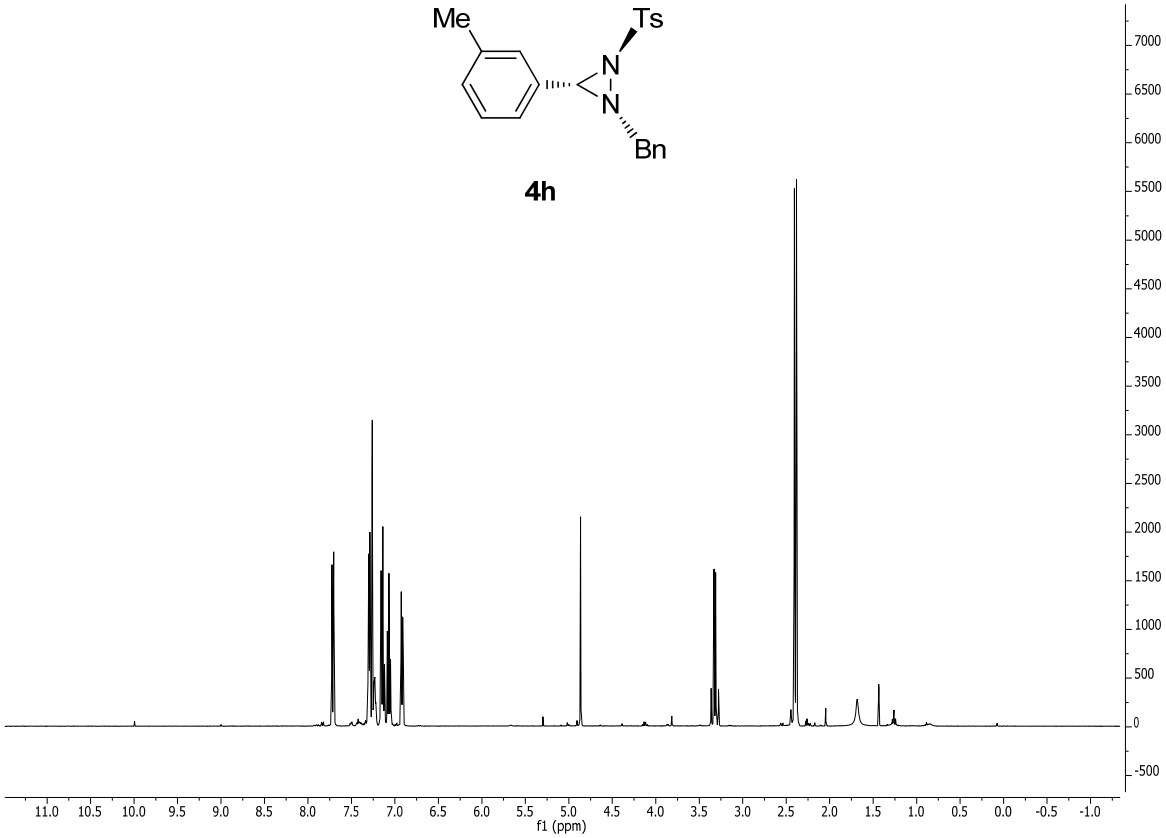
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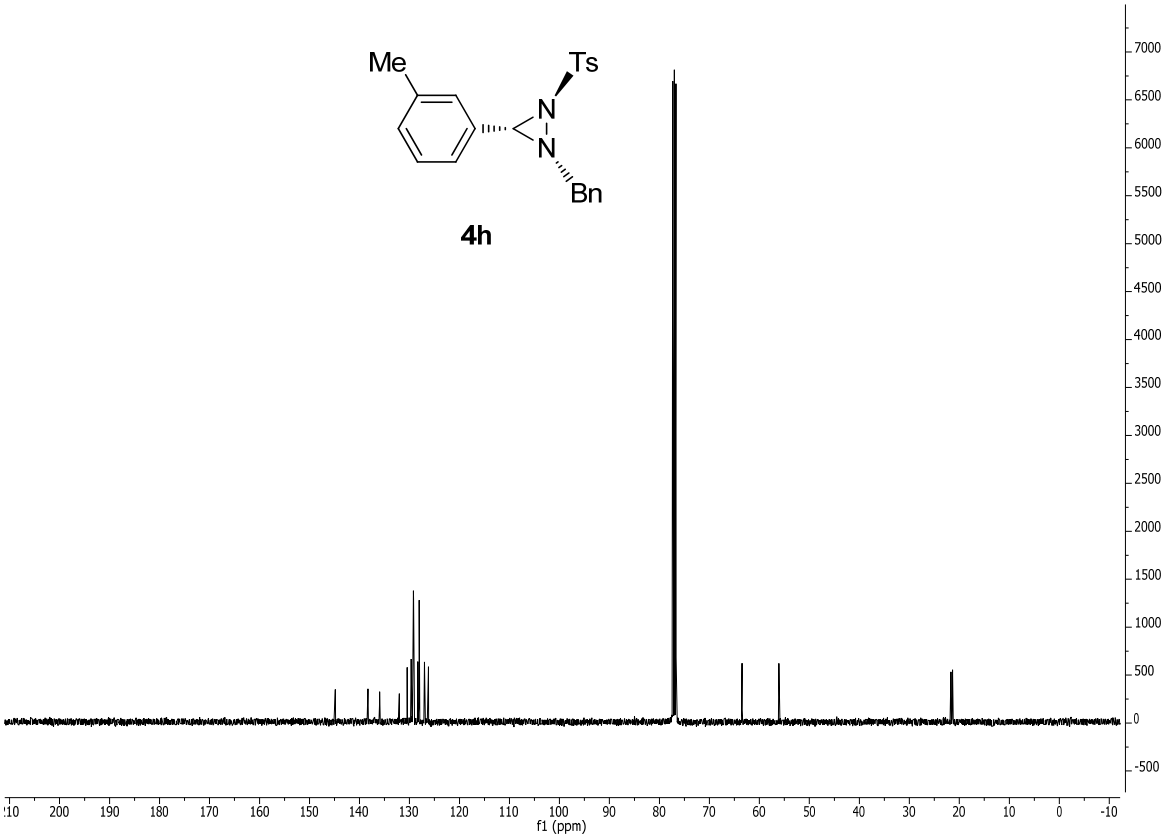
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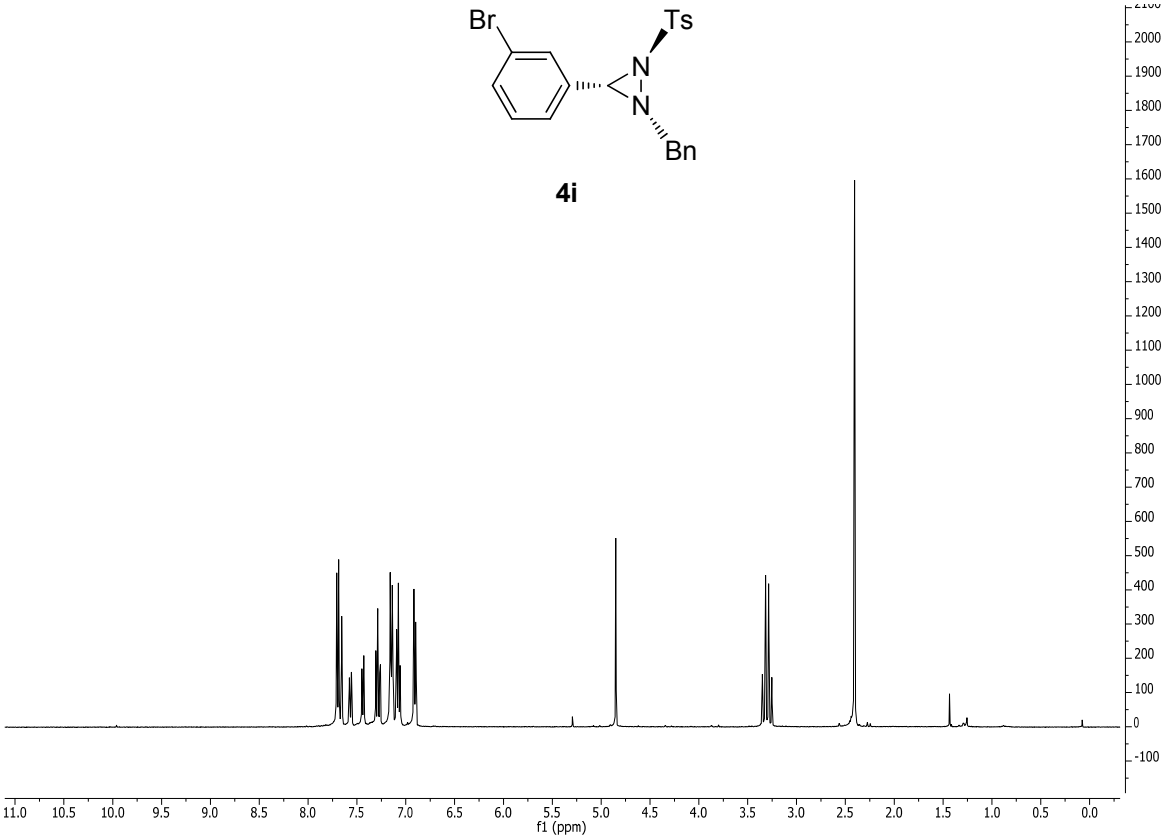
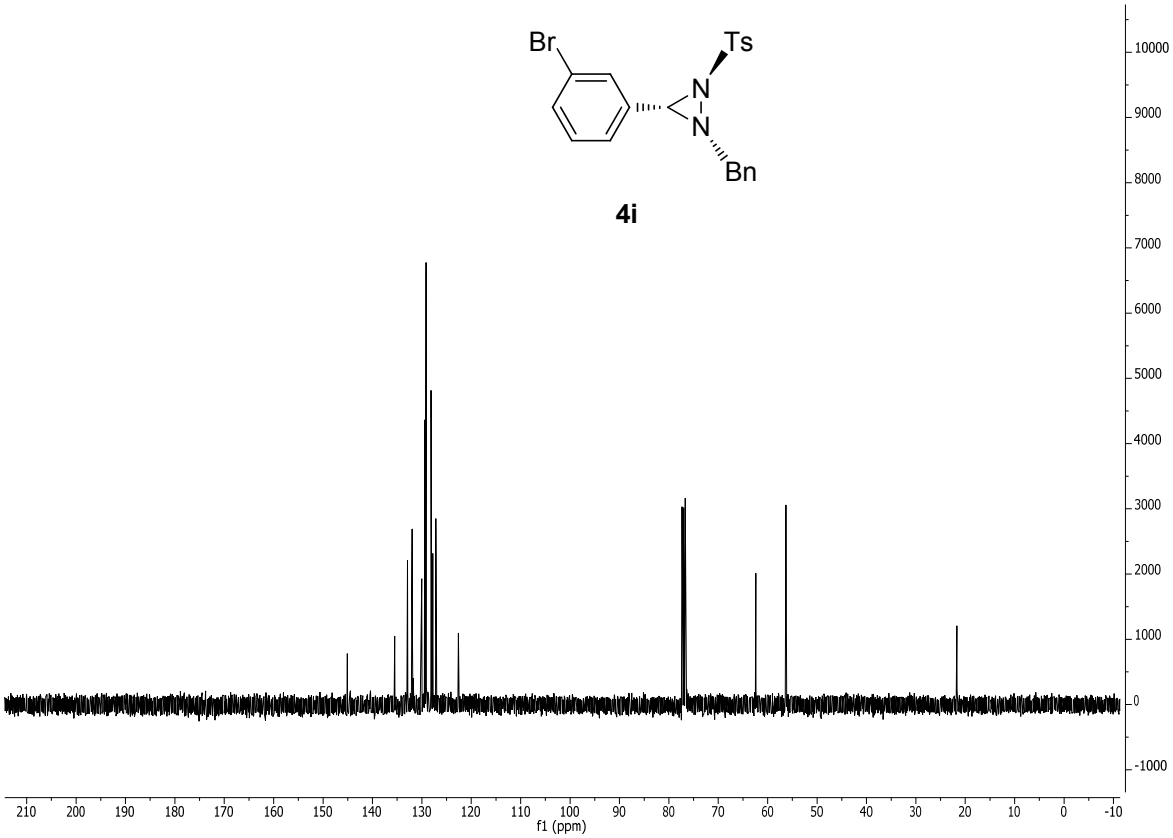
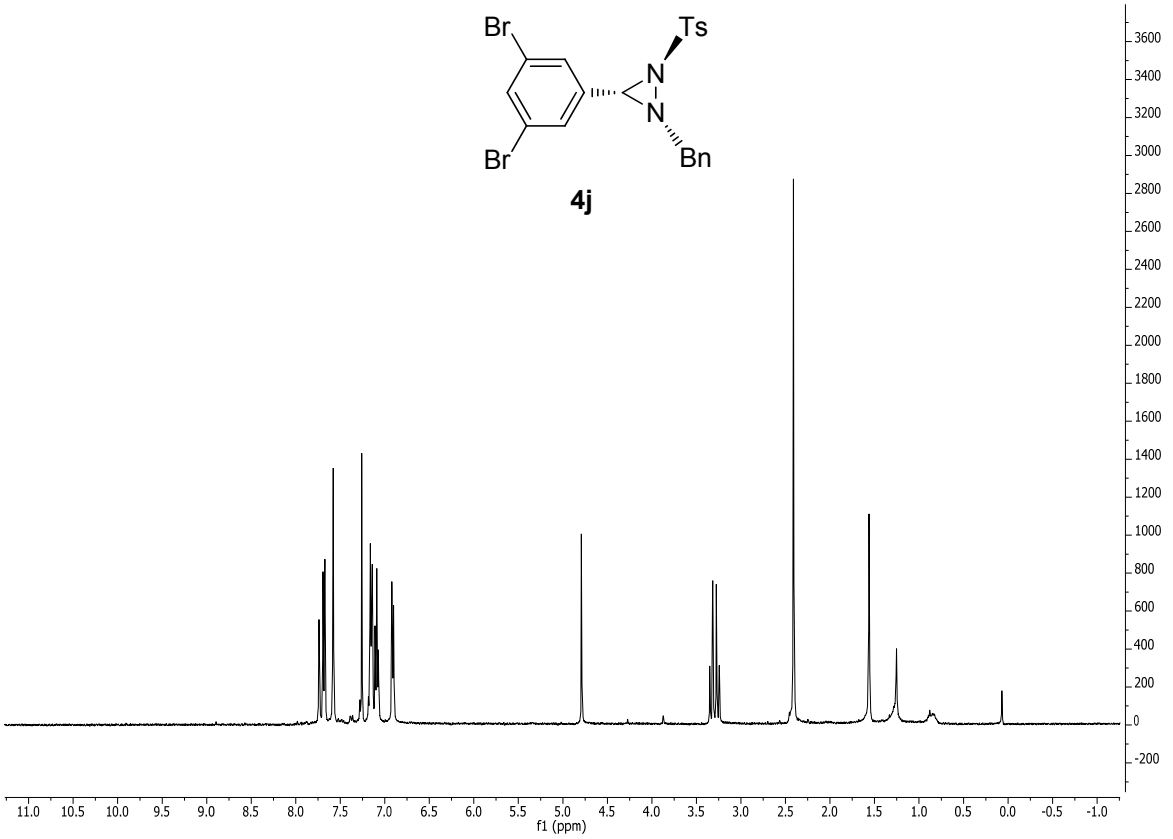
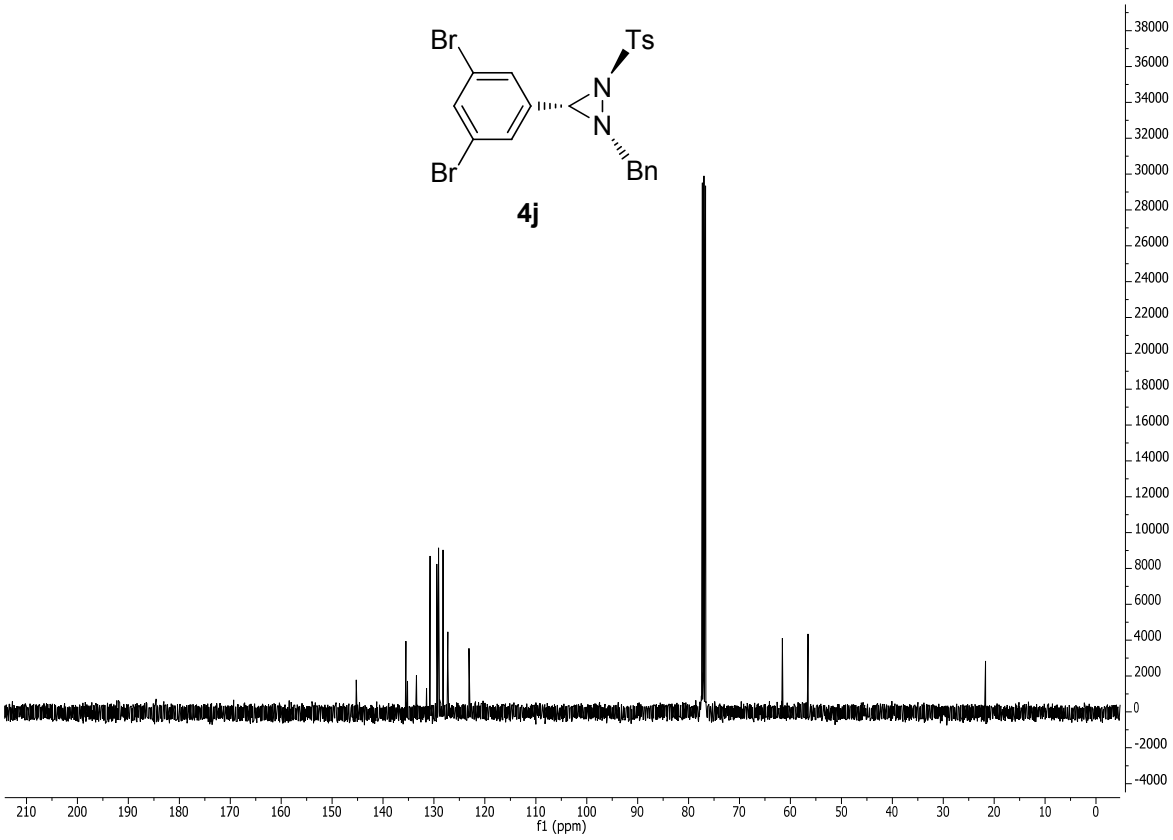
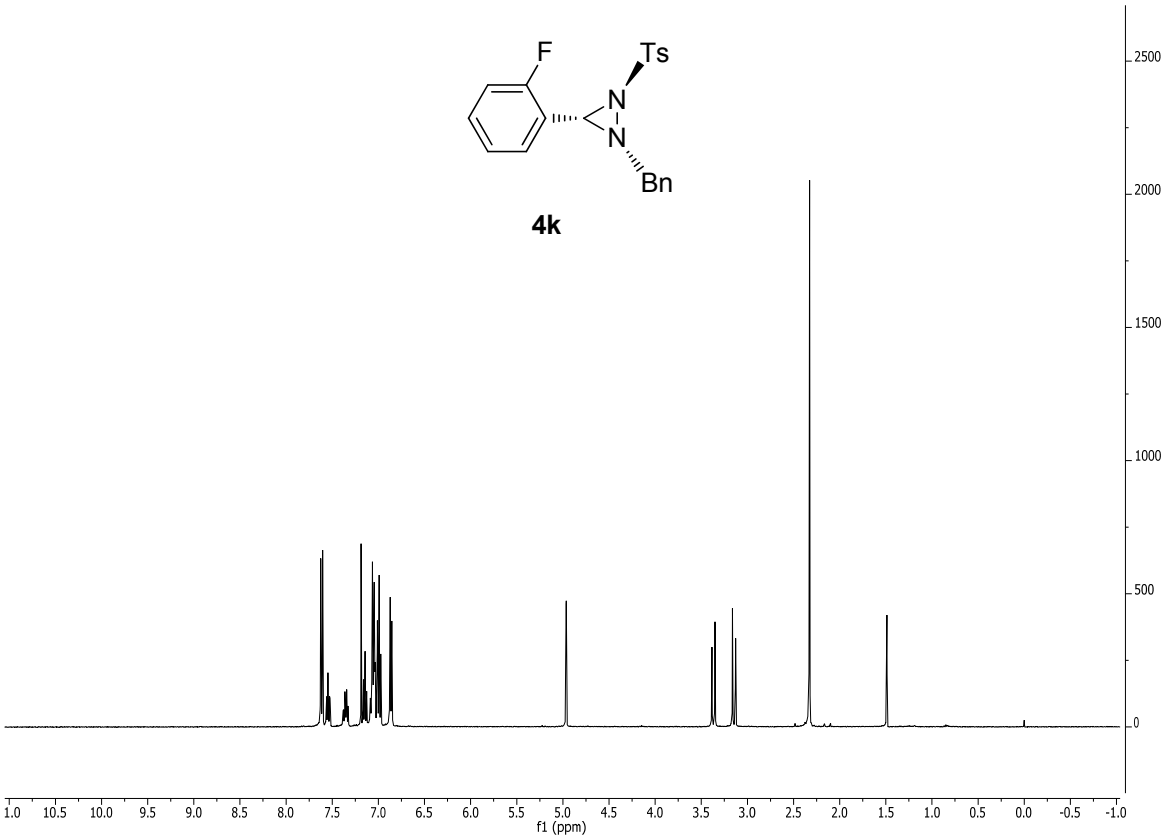
4h
f1 (ppm)


Br
Ts
N
N
Bn
4i
f1 (ppm)

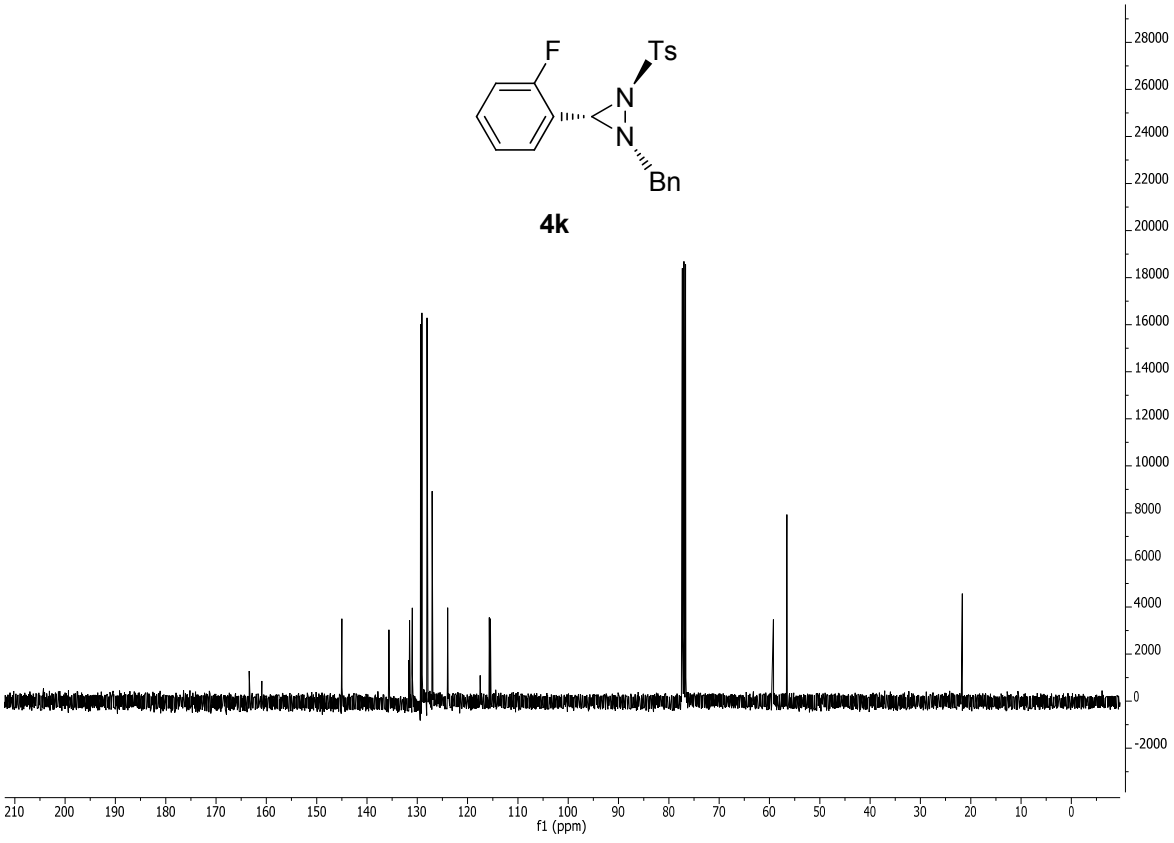

Br
Ts
N
N
Bn
4i
f1 (ppm)


Br
Ts
N
N
Br
Bn
4j
f1 (ppm)

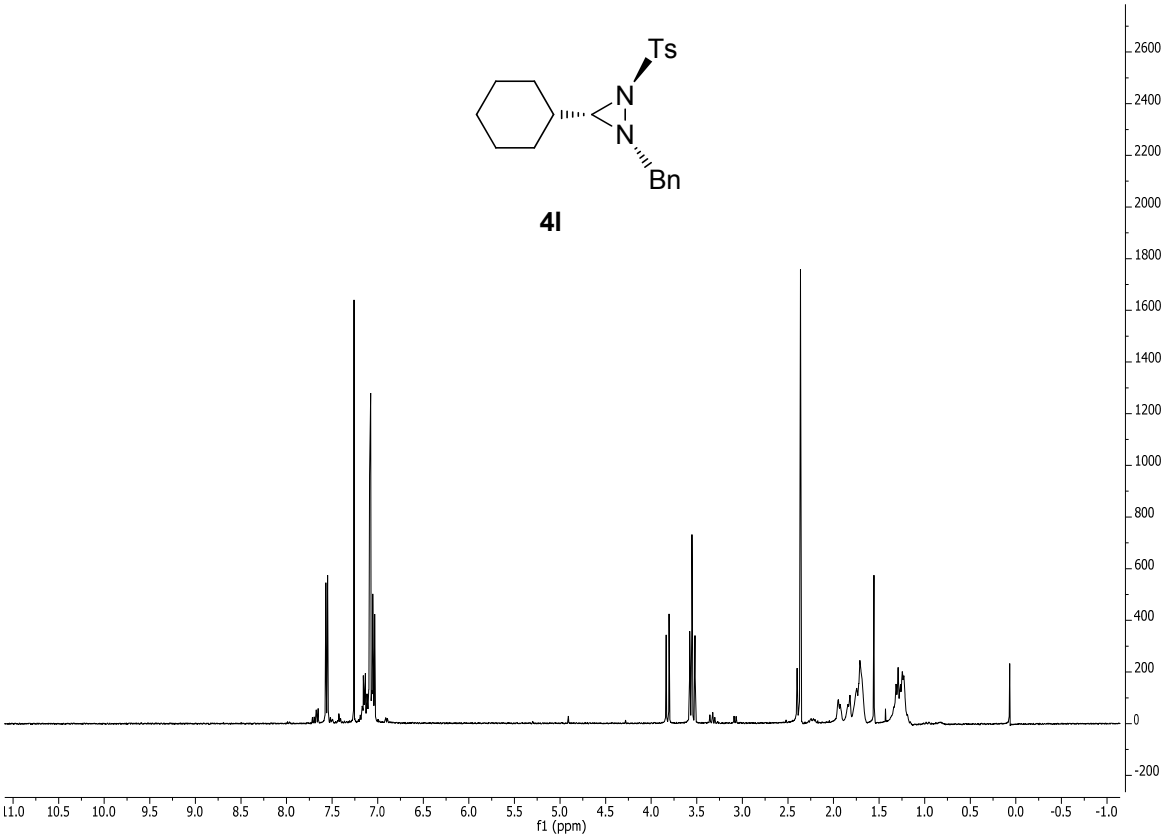

Br
Ts
N
N
Br
Bn
4j
f1 (ppm)

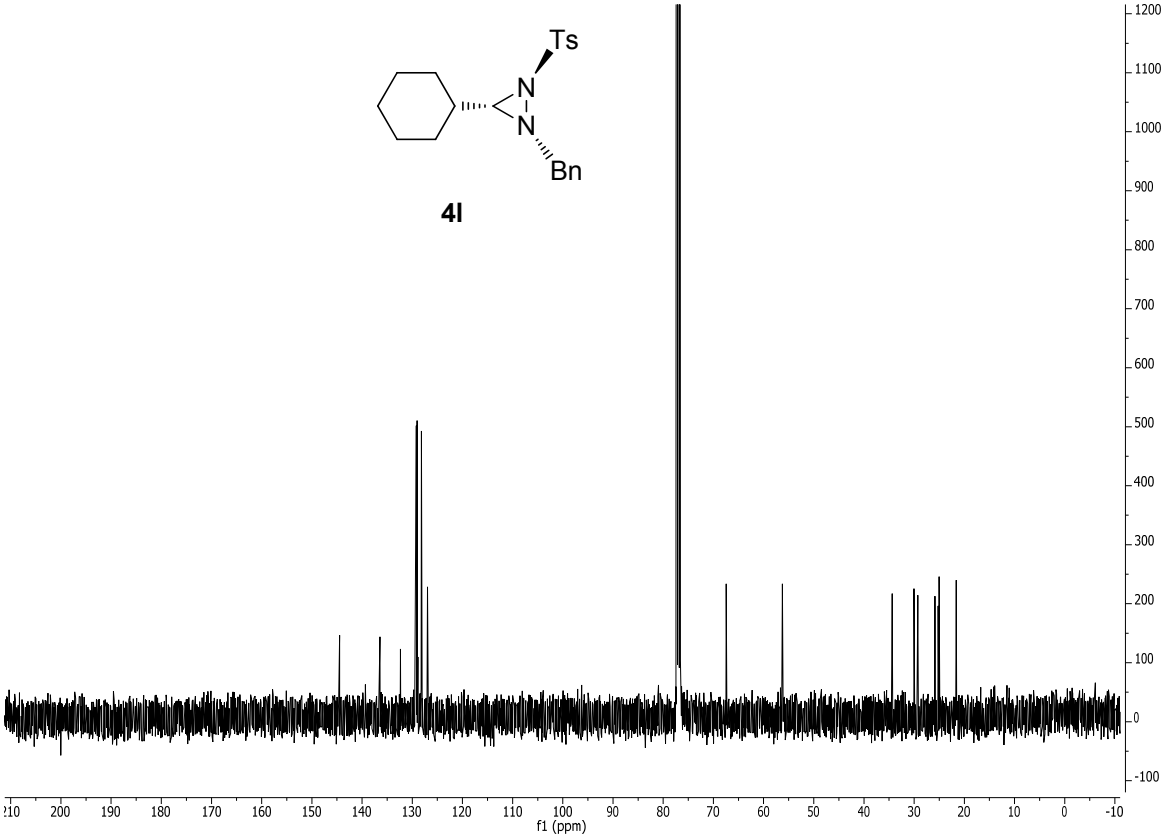

F
Ts
N
N
Bn
2500
2000
1500
1000
500
0
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

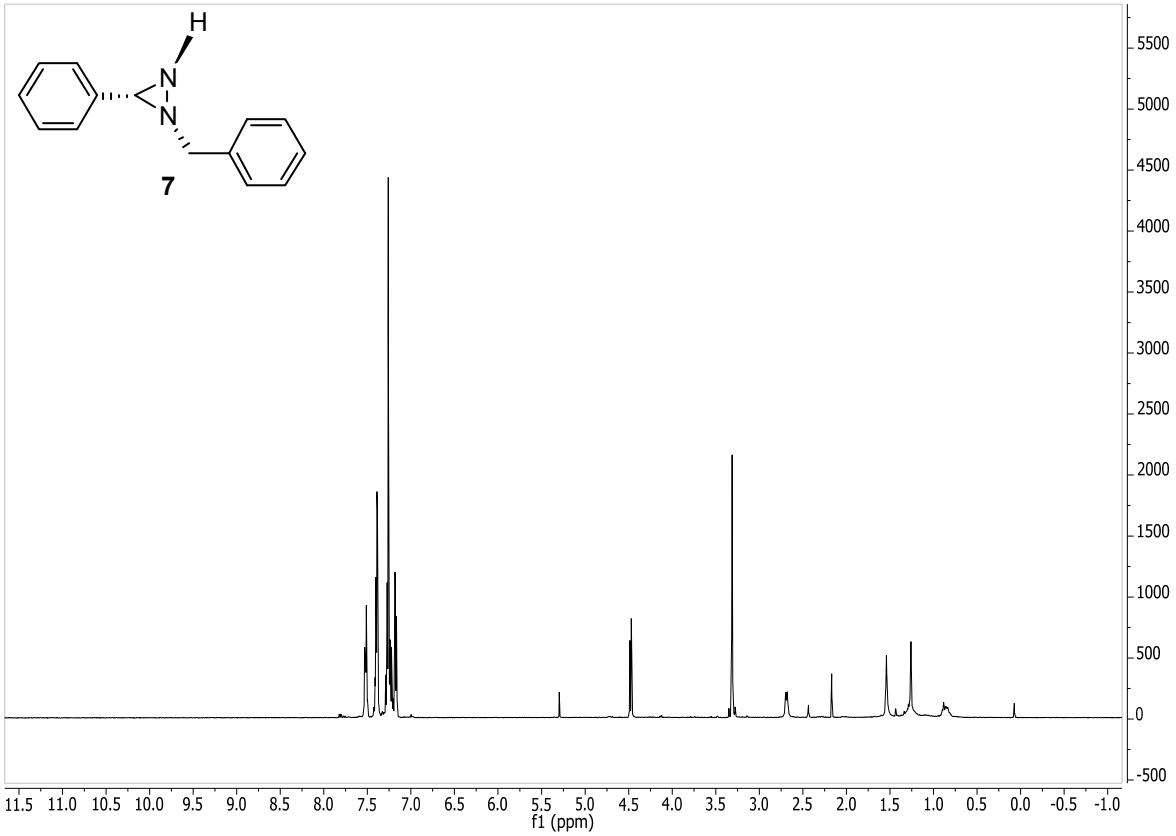
4k

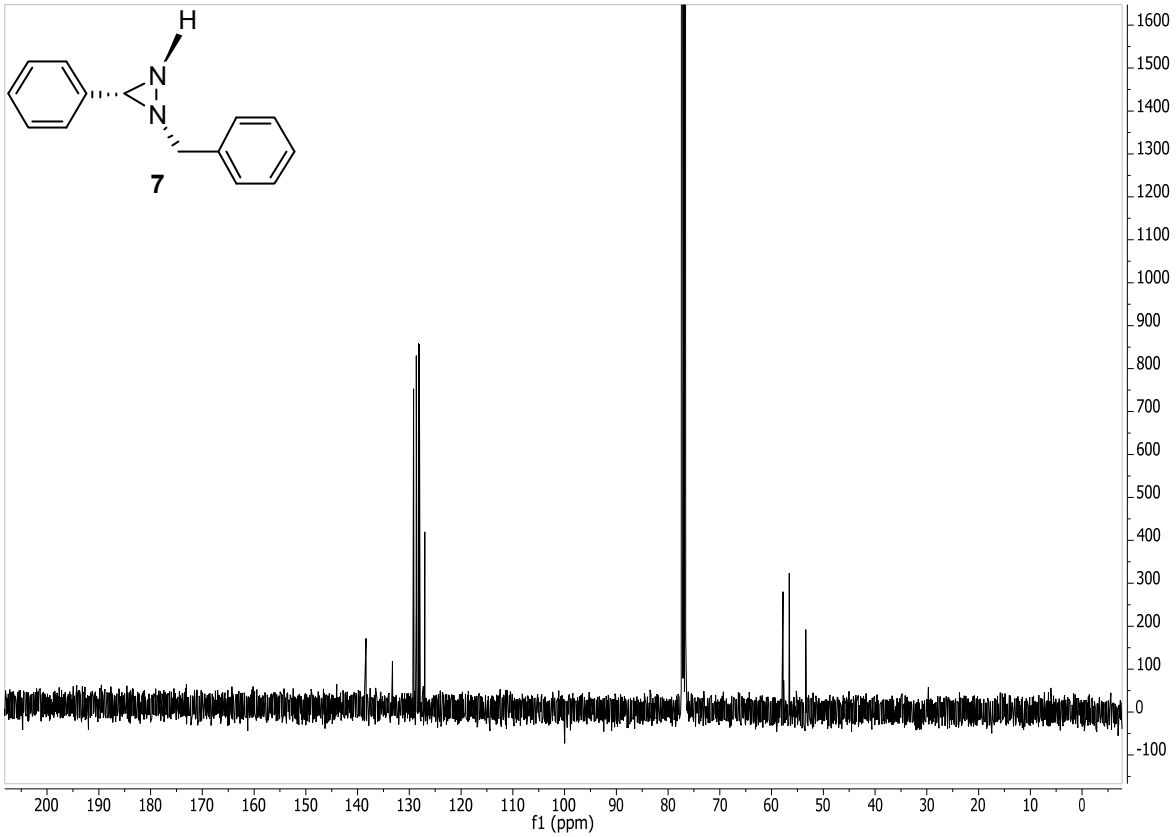

F
Ts
N
N
Bn
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

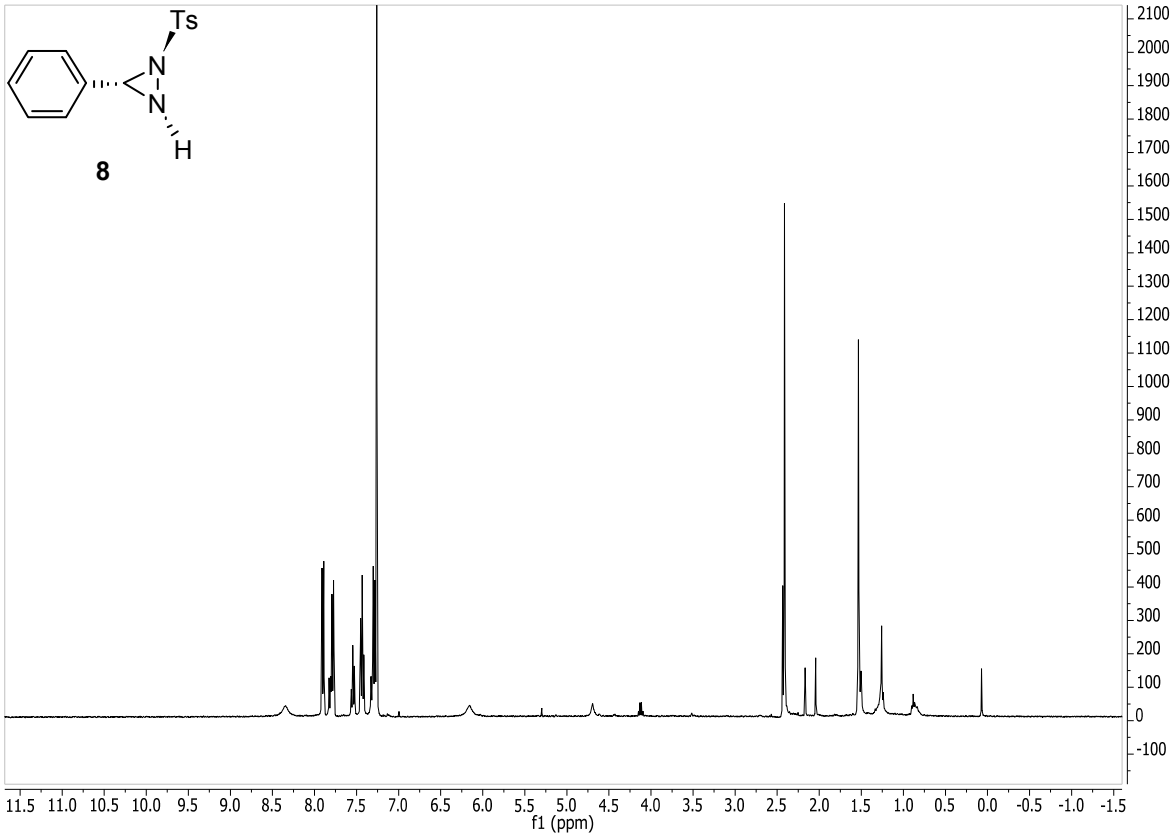
4k

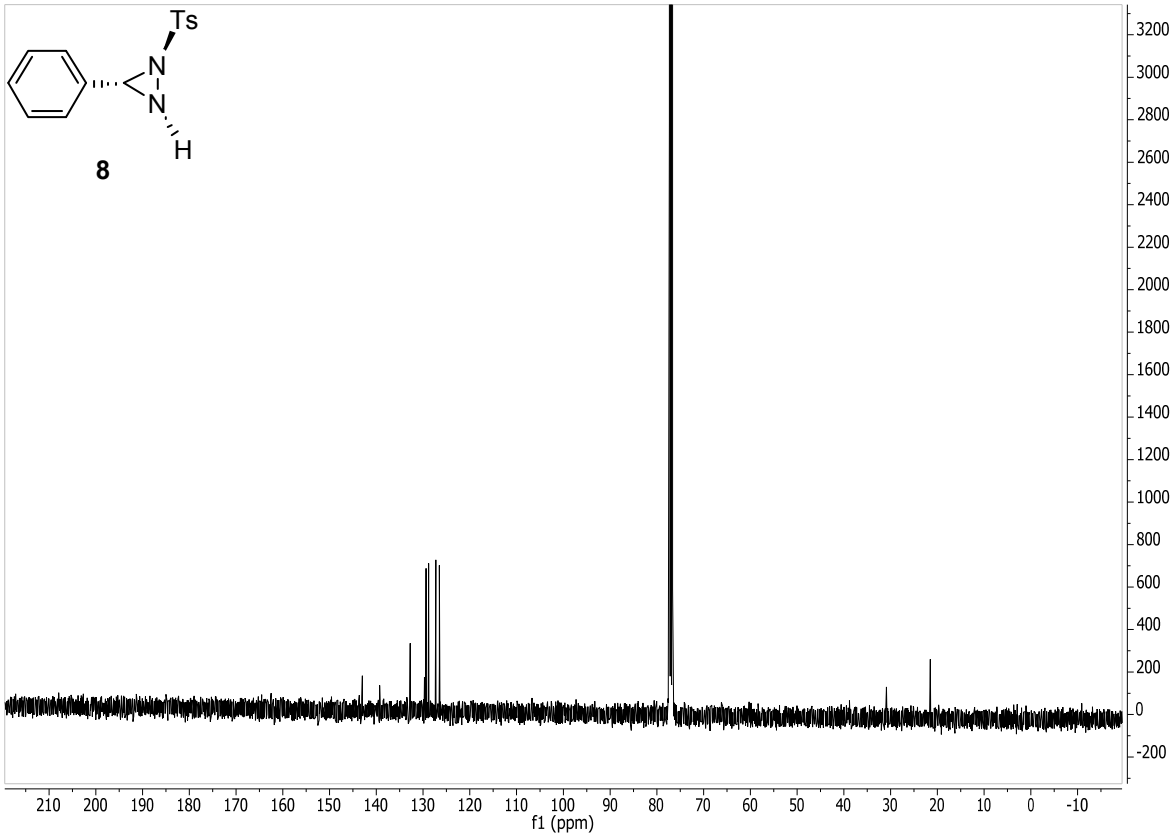

Ts
N
N
Bn
4l
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


Ts
N
N
Bn
4l
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


H
N
N
7
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


H
N
N
7
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Ts
N
N
H
8
f1 (ppm)


Ts
N
N
H
8
f1 (ppm)

5. Computational Data

5.1 Methods

All calculations were run using GAUSSIAN09.[1] All structures were optimized in the gas phase with M06-2x/6-31+G(d,p).[2] Frequency calculations were performed for all stationary points to identify them as local minima or first order saddle points and to obtain the ZPEs and thermochemical corrections for the free energies. The energetics of the system were also examined with the correlated second-order Møller–Plesset perturbation theory (MP2) [3] single point calculations (MP2/cc-pVDZ//M06-2x/6-31+G(d,p)). All of the reported values are free energies at 298 K. Intrinsic reaction coordinate (IRC) calculations were used to characterize transition state structures.[4] Structural images were created using MOLEKEL.[5]

[1] Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

[2] Y. Zhao, D. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215. C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, 37, 785. P. J. Stephens, F. J.Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, 98, 11623.

[3] Møller, C.; Plesset, M. S. *Phys. Rev.* **1934**, *46*, 618.

[4] a) C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.* **1990**, 94, 5523-5527. (b) Fukui, K. Acc. Chem. Res. **1981**, 14, 363-368.

[5] UVaretto, MOLEKEL 5.4.0.8; Swiss National Supercomputing Centre: Manno (Switzerland)

5.2 Energies and Coordinates

A

HF = -1430.5735866 hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.343138 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.291745
Sum of electronic and thermal Free Energies = -1430.281842 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3767604 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.738722	0.209512	-0.988114
2	7	0.785576	-0.775635	0.084569
3	16	-0.174129	-2.169180	-0.297371
4	8	0.153157	-3.129641	0.743896
5	8	-0.014728	-2.508069	-1.704889
6	6	-1.808028	-1.537231	-0.035946
7	6	-2.413170	-0.805301	-1.055924
8	6	-2.440838	-1.800850	1.174329
9	6	-3.700747	-0.323384	-0.846375
10	1	-1.878378	-0.625461	-1.982867
11	6	-3.734519	-1.318873	1.363598
12	1	-1.927269	-2.382755	1.932997
13	6	-4.358186	-0.584258	0.356595
14	1	-4.189484	0.259587	-1.620052
15	1	-4.254036	-1.520335	2.294823
16	1	-5.364063	-0.205023	0.510740
17	6	3.190323	-0.074091	-0.181821
18	6	3.385081	-0.044991	1.199890
19	6	4.199192	0.381041	-1.034829
20	6	4.579350	0.447152	1.723096
21	1	2.599894	-0.415401	1.851630
22	6	5.388593	0.879536	-0.509596
23	1	4.050591	0.343267	-2.111324
24	6	5.579378	0.913592	0.871394
25	1	4.730000	0.462927	2.797907
26	1	6.166930	1.235537	-1.177070
27	1	6.508378	1.296962	1.281549
28	6	1.929372	-0.595983	-0.788635
29	1	2.053563	-1.325337	-1.588714
30	6	0.745791	1.575697	-0.434476
31	1	1.195630	2.206233	-1.208695
32	1	1.365964	1.639059	0.466635
33	6	-0.662260	2.021552	-0.137020
34	6	-1.251395	1.702435	1.089930
35	6	-1.400581	2.738843	-1.079599
36	6	-2.553437	2.105616	1.373210
37	1	-0.681548	1.132599	1.820171
38	6	-2.703422	3.147476	-0.797269
39	1	-0.948796	2.983250	-2.038001
40	6	-3.280126	2.833835	0.431529
41	1	-3.002634	1.848735	2.327969
42	1	-3.264468	3.713881	-1.534596
43	1	-4.293948	3.152835	0.655081

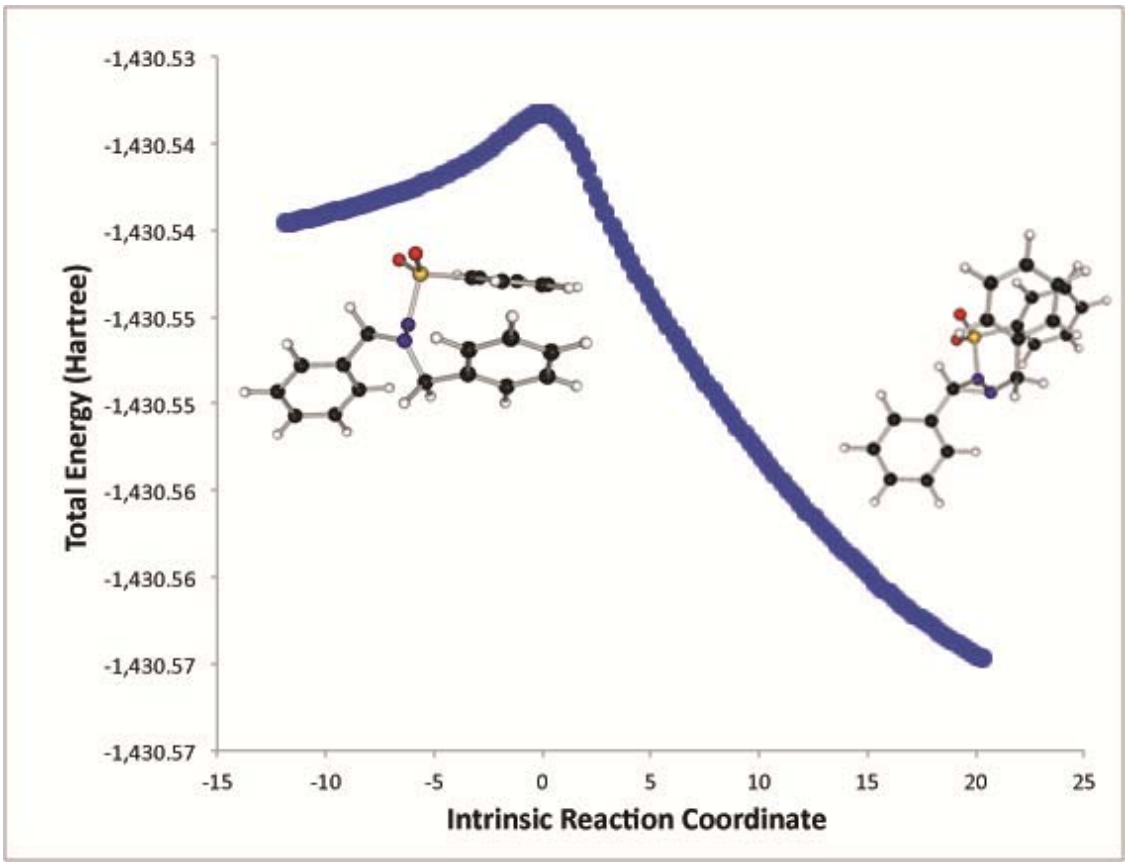
TS-B

HF = -1430.5332646 hartrees
Imaginary Frequencies: 1 (-187.5708 1/cm)
Zero-point correction = 0.341761 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.290001
Sum of electronic and thermal Free Energies = -1430.243263 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3302066 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.882045	-0.610198	-0.520842
2	7	0.944562	0.719251	-0.090138
3	16	-0.167813	1.175116	1.218039
4	8	0.449283	2.364135	1.787919
5	8	-0.512019	0.026754	2.054331
6	6	-1.608071	1.648310	0.293873
7	6	-2.748122	0.854321	0.355738
8	6	-1.552493	2.818568	-0.462874
9	6	-3.871182	1.250107	-0.369596
10	1	-2.747901	-0.050244	0.958098
11	6	-2.677918	3.194086	-1.188526
12	1	-0.646902	3.417122	-0.466690
13	6	-3.833898	2.410973	-1.138994
14	1	-4.771152	0.644716	-0.333021
15	1	-2.658526	4.100037	-1.785244
16	1	-4.711509	2.712153	-1.702803
17	6	3.310012	-0.279464	-0.003986
18	6	3.651144	0.025500	-1.323490
19	6	4.311176	-0.500782	0.940181
20	6	4.988871	0.110379	-1.692384
21	1	2.858041	0.200138	-2.045289
22	6	5.652809	-0.418490	0.569385
23	1	4.041388	-0.733367	1.967328
24	6	5.991966	-0.113386	-0.746352
25	1	5.253333	0.351998	-2.717134
26	1	6.429674	-0.590563	1.307450
27	1	7.035962	-0.048928	-1.036934
28	6	1.880006	-0.364645	0.409659
29	1	1.710663	-0.661074	1.449576
30	6	0.026681	-1.452019	-1.302563
31	1	0.652983	-2.306994	-1.584446
32	1	-0.210692	-0.912944	-2.229010
33	6	-1.261922	-1.946987	-0.670575
34	6	-2.440318	-1.932615	-1.417506
35	6	-1.285973	-2.445459	0.632908
36	6	-3.634102	-2.400500	-0.869631
37	1	-2.429664	-1.533442	-2.429447
38	6	-2.477700	-2.903516	1.188008
39	1	-0.377736	-2.432039	1.227634
40	6	-3.655555	-2.881258	0.437942
41	1	-4.545694	-2.379404	-1.459368
42	1	-2.489762	-3.270504	2.209412
43	1	-4.584325	-3.237742	0.872835

IRC-TS-B


-1,430.53
-1,430.54
-1,430.54
-1,430.55
-1,430.55
-1,430.56
-1,430.56
-1,430.57
-1,430.57
Total Energy (Hartree)
-15
-10
-5
0
5
10
15
20
25
Intrinsic Reaction Coordinate

C

HF = -1430.5566316 hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.342452 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.287659
Sum of electronic and thermal Free Energies = -1430.268973 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3589956 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.245825	0.085602	0.454165
2	7	-0.420009	-1.173072	0.124558
3	16	-1.719249	-1.254980	-1.015982
4	8	-1.996435	-2.675682	-1.116049
5	8	-1.457115	-0.470409	-2.222202
6	6	-3.008996	-0.448707	-0.097789
7	6	-3.568903	0.716803	-0.610719
8	6	-3.436166	-1.015440	1.101254
9	6	-4.586065	1.340319	0.108711
10	1	-3.210020	1.114735	-1.554739
11	6	-4.448183	-0.377167	1.812473
12	1	-2.983240	-1.934710	1.459648
13	6	-5.019376	0.796376	1.316768
14	1	-5.038723	2.248386	-0.275592
15	1	-4.795527	-0.797707	2.750367
16	1	-5.811046	1.286754	1.874475
17	6	2.085283	-1.579885	-0.031007
18	6	2.208133	-2.035314	1.283272
19	6	3.104572	-1.820070	-0.950902
20	6	3.349769	-2.729058	1.669863
21	1	1.403868	-1.841192	1.986730
22	6	4.249846	-2.513013	-0.561180
23	1	3.003057	-1.463742	-1.972890
24	6	4.372172	-2.968214	0.749078
25	1	3.444989	-3.086873	2.690247
26	1	5.041513	-2.696667	-1.280559
27	1	5.261499	-3.510958	1.054156
28	6	0.879232	-0.823997	-0.460148
29	1	0.847750	-0.538957	-1.514643
30	6	-0.224985	1.381466	-0.074271
31	1	-1.041268	1.708839	0.578856
32	1	-0.596236	1.320221	-1.102466
33	6	0.938491	2.339897	-0.003094
34	6	1.442043	2.927134	-1.164129
35	6	1.537178	2.633083	1.226149
36	6	2.522535	3.807611	-1.100304
37	1	0.983980	2.697146	-2.123206
38	6	2.617491	3.507292	1.291185
39	1	1.155203	2.162443	2.127990
40	6	3.111682	4.098206	0.127082
41	1	2.904097	4.260879	-2.009955
42	1	3.076930	3.727576	2.249831
43	1	3.954332	4.780586	0.178669

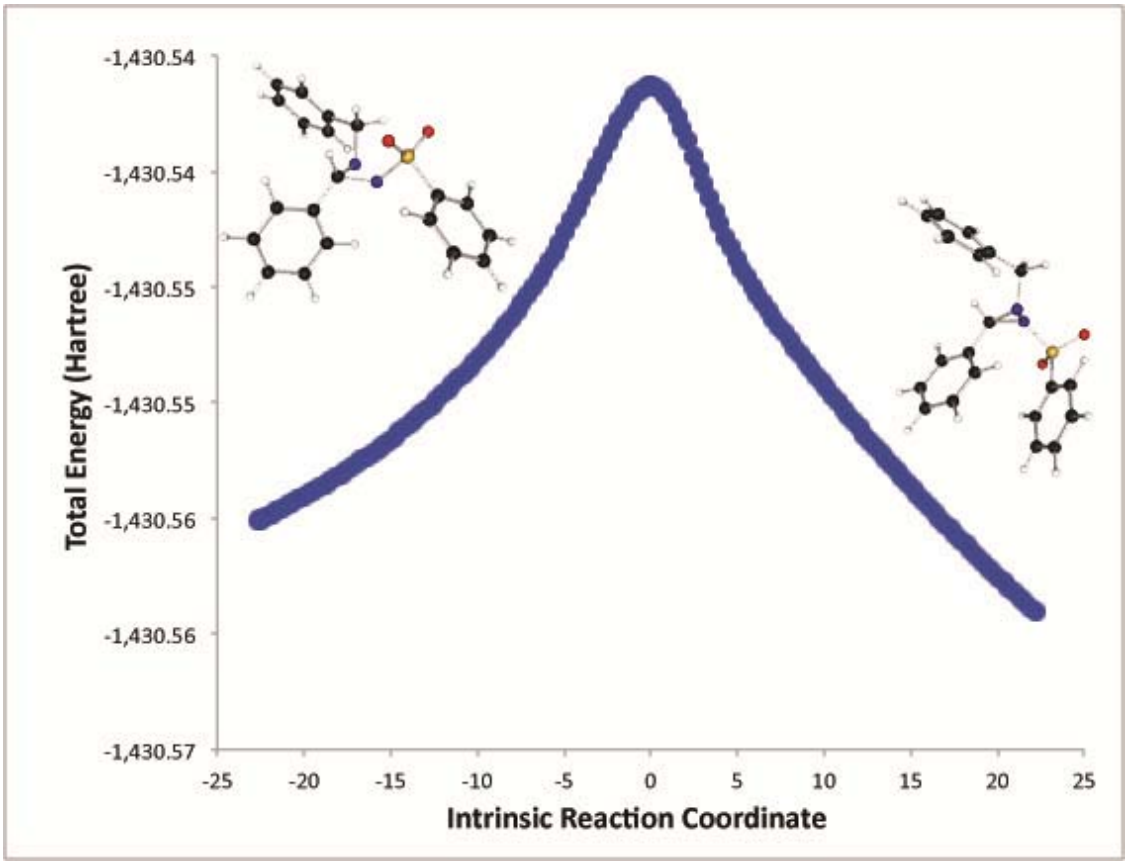
TS-C

HF = -1430.5591487 hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.342665 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.287423
Sum of electronic and thermal Free Energies = -1430.271726 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3314151 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.876738	-0.474053	-0.767091
2	7	-0.565510	-0.331085	-0.584118
3	16	-1.453319	-1.616688	0.151539
4	8	-1.089776	-1.802714	1.556142
5	8	-1.374034	-2.730503	-0.781407
6	6	-3.068174	-0.884154	0.081698
7	6	-3.766839	-0.927686	-1.122019
8	6	-3.587432	-0.287533	1.225600
9	6	-5.028940	-0.345553	-1.176217
10	1	-3.324666	-1.414513	-1.985426
11	6	-4.852597	0.292175	1.155231
12	1	-3.012476	-0.294244	2.145826
13	6	-5.567099	0.263665	-0.041302
14	1	-5.594176	-0.368215	-2.101980
15	1	-5.280461	0.760223	2.035513
16	1	-6.552853	0.715588	-0.091024
17	6	0.479108	1.865089	0.109817
18	6	0.392102	2.444509	-1.158343
19	6	0.671467	2.669416	1.231817
20	6	0.496359	3.824130	-1.296579
21	1	0.245800	1.801641	-2.021461
22	6	0.776994	4.052585	1.091548
23	1	0.744132	2.213636	2.216235
24	6	0.688976	4.630176	-0.172597
25	1	0.428005	4.274522	-2.281934
26	1	0.929771	4.675543	1.967256
27	1	0.771450	5.706892	-0.284702
28	6	0.374057	0.391066	0.270555
29	1	0.455888	0.012009	1.291770
30	6	1.544931	-1.718593	-0.325552
31	1	1.388716	-2.457740	-1.115810
32	1	1.126924	-2.115849	0.607285
33	6	3.006784	-1.397991	-0.143874
34	6	3.583480	-1.405949	1.126677
35	6	3.793237	-1.056402	-1.248393
36	6	4.930899	-1.085437	1.294128
37	1	2.976521	-1.672645	1.988724
38	6	5.136585	-0.734347	-1.083852
39	1	3.340444	-1.037799	-2.236203
40	6	5.708583	-0.749025	0.189167
41	1	5.370437	-1.099889	2.286733
42	1	5.739304	-0.471387	-1.947577
43	1	6.757352	-0.499909	0.317673

IRC-TS-C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Total Energy (Hartree)
-25
-20
-15
-10
-5
0
5
10
15
20
25
Intrinsic Reaction Coordinate

D

HF = -1430.5361817 hartrees
Imaginary Frequencies: 1 (-173.0034 1/cm)
Zero-point correction = 0.341984 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.287846
Sum of electronic and thermal Free Energies = -1430.248336 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3607197 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.802915	-0.631481	0.221147
2	7	0.305019	-0.647700	-0.668040
3	16	1.572598	-1.599780	-1.034677
4	8	1.916908	-1.306633	-2.413375
5	8	1.231815	-2.934374	-0.572636
6	6	2.887266	-0.987156	-0.000251
7	6	3.029799	-1.500038	1.285808
8	6	3.693058	0.041907	-0.480738
9	6	4.007869	-0.956518	2.116242
10	1	2.390713	-2.312594	1.615675
11	6	4.666587	0.574909	0.360236
12	1	3.554359	0.406257	-1.493596
13	6	4.820950	0.078825	1.655335
14	1	4.137386	-1.345513	3.120843
15	1	5.307195	1.374282	0.002463
16	1	5.582446	0.496985	2.305992
17	6	-0.354365	1.764914	-0.550247
18	6	0.609022	2.066503	0.416127
19	6	-1.047443	2.791103	-1.189112
20	6	0.873336	3.393008	0.737701
21	1	1.143004	1.256113	0.906165
22	6	-0.781616	4.121279	-0.864856
23	1	-1.795695	2.550756	-1.940098
24	6	0.178731	4.422185	0.097596
25	1	1.622744	3.627050	1.487252
26	1	-1.322147	4.918479	-1.364820
27	1	0.389450	5.456962	0.348817
28	6	-0.656682	0.347735	-0.892123
29	1	-1.332576	0.193568	-1.736290
30	6	-1.776704	-1.707727	-0.087103
31	1	-1.479604	-2.574319	0.510280
32	1	-1.713121	-1.992357	-1.146437
33	6	-3.159947	-1.231291	0.270190
34	6	-4.145333	-1.104228	-0.710572
35	6	-3.463381	-0.877278	1.589241
36	6	-5.419267	-0.640776	-0.381194
37	1	-3.917123	-1.378151	-1.737960
38	6	-4.731600	-0.408836	1.919165
39	1	-2.695010	-0.964799	2.352459
40	6	-5.713532	-0.291126	0.934202
41	1	-6.178512	-0.552959	-1.152070
42	1	-4.956515	-0.136125	2.945519
43	1	-6.703566	0.070786	1.193108

A-conformer 2

HF = -1430.5695372 hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.343552 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.291648
Sum of electronic and thermal Free Energies = -1430.277889 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3706816 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.110338	0.221741	-0.826112
2	7	0.683447	-1.094379	-0.980735
3	16	2.400725	-1.094306	-1.061106
4	8	2.707084	-0.599424	-2.390784
5	8	2.786826	-2.422270	-0.614760
6	6	2.982994	0.094136	0.129476
7	6	3.412765	-0.359050	1.374822
8	6	3.009635	1.442620	-0.219189
9	6	3.877462	0.572948	2.300259
10	1	3.396072	-1.422532	1.593234
11	6	3.475492	2.362315	0.716148
12	1	2.680691	1.748372	-1.206440
13	6	3.905443	1.927831	1.970616
14	1	4.225741	0.239658	3.272221
15	1	3.508726	3.417165	0.464163
16	1	4.273240	2.649818	2.693043
17	6	-1.245888	-1.488165	0.578314
18	6	-2.000132	-1.063707	1.675095
19	6	-1.692179	-2.559489	-0.197424
20	6	-3.204208	-1.691458	1.981281
21	1	-1.653797	-0.225424	2.274897
22	6	-2.897606	-3.187055	0.110877
23	1	-1.088137	-2.894904	-1.034661
24	6	-3.657109	-2.751567	1.195733
25	1	-3.790153	-1.351988	2.829588
26	1	-3.239741	-4.020962	-0.493868
27	1	-4.595731	-3.242167	1.434130
28	6	0.013387	-0.755699	0.249725
29	1	0.628115	-0.477580	1.106800
30	6	-1.063742	0.410979	-1.698282
31	1	-1.569761	-0.537886	-1.904232
32	1	-0.673691	0.803775	-2.641987
33	6	-2.008723	1.385668	-1.041684
34	6	-1.586528	2.684721	-0.743095
35	6	-3.304353	0.995479	-0.698938
36	6	-2.449258	3.581180	-0.118544
37	1	-0.573696	2.985322	-0.999524
38	6	-4.172187	1.892931	-0.078075
39	1	-3.629973	-0.022197	-0.906104
40	6	-3.746250	3.186887	0.213134
41	1	-2.112677	4.588380	0.107456
42	1	-5.177867	1.578183	0.183244
43	1	-4.420823	3.886873	0.696534

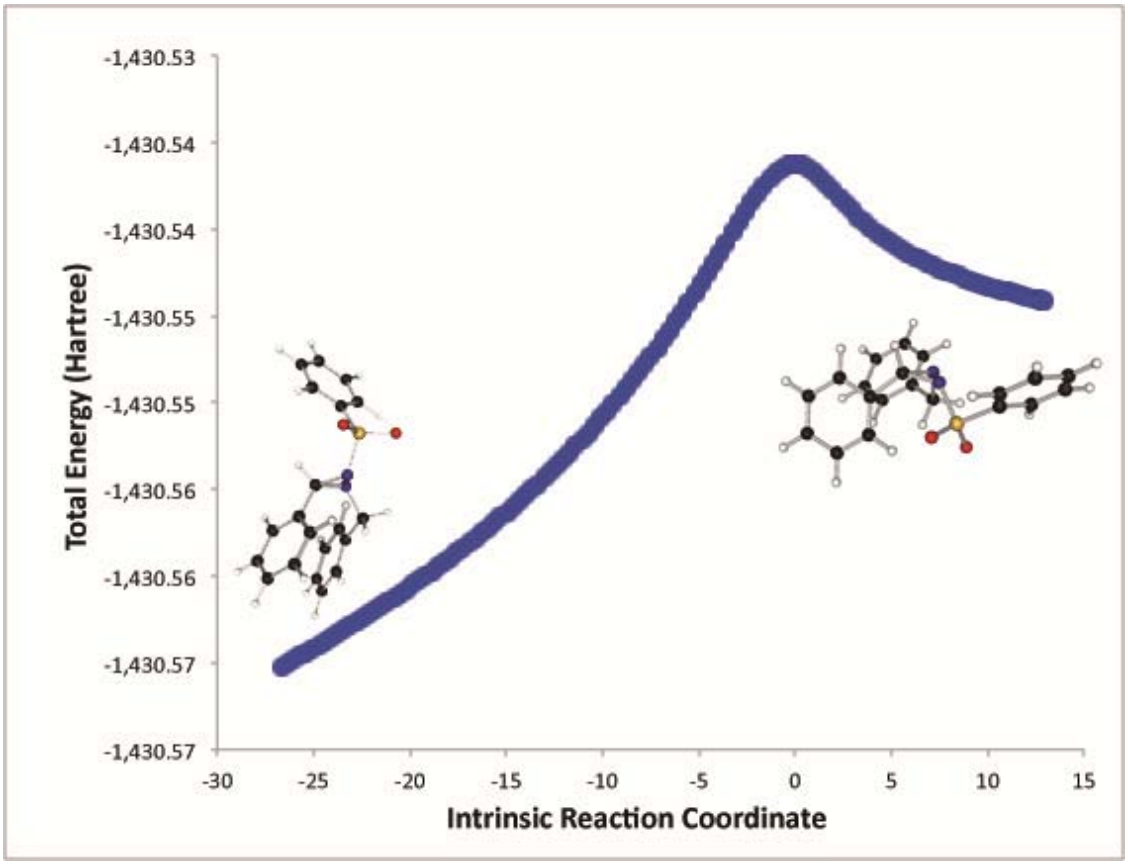
TS-A

HF = -1430.5359951 hartrees
Imaginary Frequencies: 1 (-162.3346 1/cm)
Zero-point correction = 0.342410 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.289548
Sum of electronic and thermal Free Energies = -1430.246447 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3321226 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.123439	-0.891047	-0.201885
2	7	0.803290	0.184760	-0.087023
3	16	2.033121	0.620624	0.881664
4	8	1.833737	-0.079944	2.138899
5	8	2.112336	2.069735	0.799464
6	6	3.498506	-0.049271	0.124341
7	6	4.221206	0.742329	-0.764013
8	6	3.865648	-1.360491	0.414462
9	6	5.342399	0.196063	-1.384062
10	1	3.912087	1.766477	-0.945887
11	6	4.987469	-1.893973	-0.215053
12	1	3.287812	-1.937106	1.129270
13	6	5.721678	-1.118474	-1.112374
14	1	5.923324	0.799649	-2.073634
15	1	5.291787	-2.912780	0.000894
16	1	6.597468	-1.538280	-1.596908
17	6	-1.347288	1.370363	-0.706498
18	6	-2.464668	1.351229	-1.546071
19	6	-1.287603	2.278385	0.352149
20	6	-3.534230	2.208132	-1.307785
21	1	-2.506716	0.641834	-2.369103
22	6	-2.360904	3.136812	0.588207
23	1	-0.397681	2.323476	0.973562
24	6	-3.485716	3.098593	-0.234644
25	1	-4.406160	2.177033	-1.953203
26	1	-2.312037	3.842224	1.411508
27	1	-4.318566	3.769203	-0.047394
28	6	-0.260115	0.385481	-0.977665
29	1	-0.031045	0.236535	-2.033148
30	6	-1.012006	-1.017380	0.978888
31	1	-1.122091	-0.065724	1.509454
32	1	-0.507409	-1.715534	1.652932
33	6	-2.351183	-1.548711	0.535878
34	6	-2.440329	-2.775951	-0.129027
35	6	-3.515364	-0.811357	0.761174
36	6	-3.674647	-3.258105	-0.557831
37	1	-1.534568	-3.347549	-0.312739
38	6	-4.752616	-1.295017	0.338663
39	1	-3.448657	0.156854	1.253787
40	6	-4.834428	-2.518870	-0.322671
41	1	-3.733095	-4.212188	-1.072605
42	1	-5.649823	-0.711019	0.519687
43	1	-5.796959	-2.896128	-0.654037

IRC-TS-A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-1,430.56
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-1,430.57
Total Energy (Hartree)
-30
-25
-20
-15
-10
-5
0
5
10
15
Intrinsic Reaction Coordinate

B

HF = -1430.5456075 hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.342662 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Thermal correction to Gibbs Free Energy = 0.290111
Sum of electronic and thermal Free Energies = -1430.255497 hartrees

Single Point Energy (MP2/cc-pvdz in gas phase) MP2 = -1427.3466895 hartrees

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.891235	-1.094924	-0.781833
2	7	0.569650	-1.027102	-0.723758
3	16	1.346243	-0.956776	0.809058
4	8	1.164469	-2.297322	1.344665
5	8	0.999031	0.200011	1.627157
6	6	3.015203	-0.751699	0.234648
7	6	3.712406	0.393074	0.607374
8	6	3.595044	-1.762968	-0.528980
9	6	5.034784	0.532211	0.187864
10	1	3.220516	1.144580	1.217400
11	6	4.913697	-1.607775	-0.943375
12	1	3.017909	-2.645560	-0.785129
13	6	5.629265	-0.462799	-0.586126
14	1	5.599613	1.414442	0.470292
15	1	5.385371	-2.380584	-1.541023
16	1	6.659080	-0.349737	-0.909956
17	6	-0.289956	1.460757	-0.720137
18	6	-1.521071	2.031962	-0.397999
19	6	0.868024	2.240064	-0.658484
20	6	-1.585408	3.359065	0.026336
21	1	-2.431818	1.445911	-0.481090
22	6	0.802981	3.563233	-0.235950
23	1	1.824297	1.803946	-0.937585
24	6	-0.425405	4.124004	0.115010
25	1	-2.546564	3.793098	0.283053
26	1	1.709411	4.157986	-0.181024
27	1	-0.477373	5.155786	0.447767
28	6	-0.207791	0.075282	-1.286316
29	1	-0.134355	0.068695	-2.374349
30	6	-1.637055	-1.033498	0.490084
31	1	-1.336668	-0.197698	1.131881
32	1	-1.399331	-1.962968	1.018963
33	6	-3.119701	-0.967780	0.201402
34	6	-3.679262	-1.611478	-0.905500
35	6	-3.956512	-0.271713	1.078312
36	6	-5.054514	-1.558017	-1.127744
37	1	-3.029543	-2.148158	-1.589277
38	6	-5.331739	-0.224075	0.859807
39	1	-3.524624	0.239877	1.935511
40	6	-5.884626	-0.866356	-0.247125
41	1	-5.478526	-2.060445	-1.991786
42	1	-5.969349	0.319510	1.550136
43	1	-6.955036	-0.826551	-0.422736