

Supporting Information

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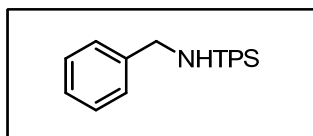
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1. General Information

All reactions and manipulations that are sensitive to moisture or air were performed in an argon-filled glove box or using standard Schlenk techniques. Unless otherwise noted, commercially available reagents were received from commercial sources without further purification. Anhydrous tetrahydrofuran, and toluene were distilled from sodium benzophenone ketyl under nitrogen before use. The other solvents were all purified according to the standard procedures. Melting points were measured on X-4B microscope melting point apparatus and uncorrected. NMR spectra were recorded on Bruker AV 400 spectrometer at 400 MHz (^1H NMR), 100 MHz (^{13}C NMR). Proton and carbon chemical shifts are reported relative to the solvent used as an internal reference (CDCl_3 : $\delta_{\text{H}} = 7.26$ ppm; $\delta_{\text{C}} = 77.16$ ppm). All coupling constants (J values) were reported in Hertz (Hz). High resolution mass spectra (HRMS) were recorded on an Agilent6520 Q-TOF LC/MS with Electron Spray Ionization (ESI) resource. All TPS-protected amines were prepared according to the reported method.¹

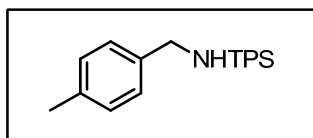
2. Preparation of Amines

General procedure¹: To a solution of benzylamine (5 mmol, 1 equiv) and triethylamine (7.5 mmol, 1.5 equiv) in CH_2Cl_2 (25 mL) was added 2,4,6-triisopropylbenzene-1-sulfonyl chloride (5 mmol, 1 equiv) portionwise. The reaction was allowed to stir at room temperature for 3 hours before being quenched by saturated NaHCO_3 . The aqueous layer was extracted with dichloromethane, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was crystallized (CH_2Cl_2 /hexane) to afford the pure products.



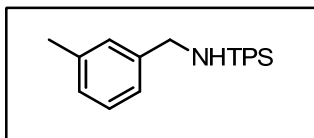
***N*-Benzyl-2,4,6-triisopropylbenzenesulfonamide (1a).²**

White solid (95% yield). m.p. 90-92 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.24 (m, 3H), 7.23-7.14 (m, 4H), 4.55 (t, $J = 6.0$ Hz, 1H), 4.23-4.13 (m, 2H), 4.15 (d, $J = 6.4$ Hz, 2H), 2.99-2.84 (m, 1H), 1.27 (d, $J = 6.0$ Hz, 6H), 1.26 (d, $J = 6.4$ Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.9, 150.4, 136.6, 132.4, 128.7, 128.1, 128.0, 123.9, 47.0, 34.2, 29.8, 25.0, 23.7.



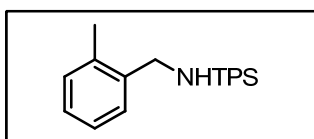
2,4,6-Triisopropyl-*N*-(4-methylbenzyl)benzenesulfonamide (1b).

White solid (83% yield). m.p. 97-98 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.18 (s, 2H), 7.09 (s, 4H), 4.48 (t, $J = 6.0$ Hz, 1H), 4.24-4.13 (m, 2H), 4.10 (d, $J = 6.0$ Hz, 2H), 2.98-2.85 (m, 1H), 2.31 (s, 3H), 1.27 (d, $J = 6.0$ Hz, 6H), 1.26 (d, $J = 6.8$ Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.9, 150.5, 137.8, 133.5, 132.3, 129.5, 128.2, 123.9, 46.9, 34.3, 29.8, 25.0, 23.7, 21.2. HRMS (ESI) calcd. for $\text{C}_{23}\text{H}_{34}\text{NO}_2\text{S}$ ($[\text{M}+\text{H}]^+$) 388.2305, Found 388.2311.



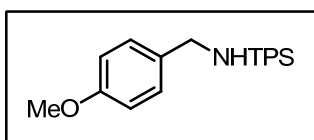
2,4,6-Triisopropyl-N-(3-methylbenzyl)benzenesulfonamide (1c).

White solid (85% yield). m.p. 90-91 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.18 (s, 2H), 7.16 (t, $J = 7.2$ Hz, 1H), 7.06 (d, $J = 7.6$ Hz, 1H), 7.00 (s, 1H), 6.99 (d, $J = 8.8$ Hz, 1H), 4.52 (t, $J = 6.0$ Hz, 1H), 4.23-4.13 (m, 2H), 4.12 (d, $J = 6.0$ Hz, 2H), 2.99-2.86 (m, 1H), 2.28 (s, 3H), 1.28 (d, $J = 5.6$ Hz, 6H), 1.26 (d, $J = 6.8$ Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.9, 150.4, 138.5, 136.5, 132.5, 128.9, 128.8, 128.7, 125.2, 123.9, 47.1, 34.3, 29.8, 25.0, 23.7, 21.4. HRMS (ESI) calcd. for $\text{C}_{23}\text{H}_{34}\text{NO}_2\text{S}$ ($[\text{M}+\text{H}]^+$) 388.2305, Found 388.2311.



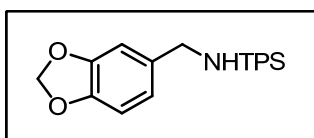
2,4,6-Triisopropyl-N-(2-methylbenzyl)benzenesulfonamide (1d).

White solid (70% yield). m.p. 95-96 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.22-7.17 (m, 1H), 7.19 (s, 2H), 7.17-7.13 (m, 1H), 7.13-7.07 (m, 2H), 4.35 (t, $J = 6.0$ Hz, 1H), 4.24-4.14 (m, 2H), 4.13 (d, $J = 6.0$ Hz, 2H), 2.99-2.86 (m, 1H), 2.28 (s, 3H), 1.27 (d, $J = 6.8$, 6H), 1.26 (d, $J = 6.8$, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.0, 150.5, 136.9, 134.3, 132.1, 130.7, 128.9, 128.3, 126.3, 124.0, 45.0, 34.3, 29.8, 25.0, 23.7, 18.9. HRMS (ESI) calcd. for $\text{C}_{23}\text{H}_{34}\text{NO}_2\text{S}$ ($[\text{M}+\text{H}]^+$) 388.2305, Found 388.2310.



2,4,6-Triisopropyl-N-(4-methoxybenzyl)benzenesulfonamide (1e).³

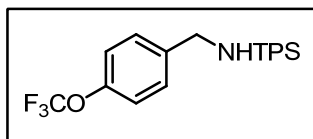
White solid (81% yield). m.p. 99-100 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.18 (s, 2H), 7.11 (d, $J = 8.8$ Hz, 2H), 6.80 (d, $J = 8.8$ Hz, 2H), 4.49 (t, $J = 6.0$ Hz, 1H), 4.23-4.13 (m, 2H), 4.08 (d, $J = 6.0$ Hz, 2H), 3.77 (s, 3H), 2.99-2.85 (m, 1H), 1.28 (d, $J = 6.4$ Hz, 6H), 1.26 (d, $J = 6.4$ Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 159.4, 152.9, 150.5, 132.4, 129.6, 128.6, 123.9, 114.2, 55.4, 46.6, 34.3, 29.8, 25.0, 23.7.



N-(Benzo[d][1,3]dioxol-5-ylmethyl)-2,4,6-triisopropylbenzenesulfonamide (1f).

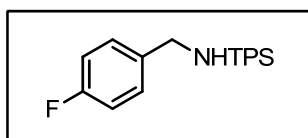
White solid (83% yield). m.p. 126-127 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.18 (s, 2H), 6.72-6.61 (m, 3H), 5.93 (s, 2H), 4.47 (t, $J = 6.0$ Hz, 1H), 4.22-4.10 (m, 2H), 4.05 (d, $J = 6.0$ Hz, 2H), 2.98-2.84 (m, 1H), 1.27 (d, $J = 6.8$ Hz, 6H), 1.26 (d, $J = 6.8$ Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.0, 150.4, 148.0, 147.4, 132.4, 130.3, 123.9, 121.6, 108.8, 108.3,

101.2, 47.0, 34.3, 29.8, 25.0, 23.7. **HRMS** (ESI) calcd. for $C_{23}H_{32}NO_4S$ ($[M+H]^+$) 418.2047, Found 418.2050.



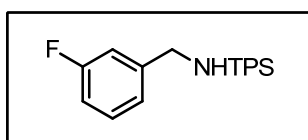
2,4,6-Triisopropyl-N-(4-(trifluoromethoxy)benzyl)benzenesulfonamide (1g).

White solid (85% yield). m.p. 122-123 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, J = 8.8 Hz, 2H), 7.17 (s, 2H), 7.12 (d, J = 8.0 Hz, 2H), 4.61 (t, J = 6.2 Hz, 1H), 4.17 (d, J = 6.4 Hz, 2H), 4.21-4.06 (m, 2H), 2.98-2.84 (m, 1H), 1.26 (d, J = 6.8 Hz, 6H), 1.25 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 150.4, 148.8, 135.6, 132.5, 129.6, 123.9, 121.2, 120.5 (q, J = 255 Hz), 46.2, 34.3, 29.8, 24.9, 23.6. **HRMS** (ESI) calcd. for $C_{23}H_{31}F_3NO_3S$ ($[M+H]^+$) 458.1971, Found 458.1979.



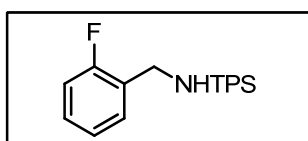
N-(4-Fluorobenzyl)-2,4,6-triisopropylbenzenesulfonamide (1h).

White solid (70% yield). m.p. 126-127 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.22-7.13 (m, 2H), 7.17 (s, 2H), 6.97 (d, J = 8.4 Hz, 1H), 6.95 (d, J = 8.8 Hz, 1H), 4.53 (t, J = 6.0 Hz, 1H), 4.22-4.09 (m, 2H), 4.13 (d, J = 6.0 Hz, 1H), 2.98-2.86 (m, 1H), 1.27 (d, J = 6.4 Hz, 6H), 1.25 (d, J = 6.4 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4 (d, J = 245 Hz), 153.1, 150.4, 132.5 (d, J = 3.2 Hz), 132.4, 129.9 (d, J = 8.3 Hz), 123.9, 115.6 (d, J = 21.3 Hz), 46.4, 34.3, 29.8, 25.0, 23.7. **HRMS** (ESI) calcd. for $C_{22}H_{31}FNO_2S$ ($[M+H]^+$) 392.2054, Found 392.2062.



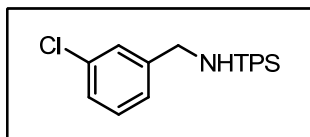
N-(3-Fluorobenzyl)-2,4,6-triisopropylbenzenesulfonamide (1i).

White solid (83% yield). m.p. 113-115 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.26-7.20 (m, 1H), 7.18 (s, 2H), 6.99 (d, J = 7.6 Hz, 1H), 6.96-6.86 (m, 2H), 4.65 (t, J = 6.4 Hz, 1H), 4.23-4.08 (m, 2H), 4.16 (d, J = 6.4 Hz, 2H), 2.99-2.84 (m, 1H), 1.27 (d, J = 6.8 Hz, 6H), 1.26 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, J = 245.2 Hz), 153.1, 150.4, 139.3 (d, J = 7.1 Hz), 132.4, 130.2 (d, J = 8.1 Hz), 123.9, 123.6 (d, J = 2.9 Hz), 115.0 (d, J = 21.8 Hz), 114.8 (d, J = 20.8 Hz), 46.5, 46.4, 34.3, 29.8, 24.9, 23.7. **HRMS** (ESI) calcd. for $C_{22}H_{31}FNO_2S$ ($[M+H]^+$) 392.2054, Found 392.2060.

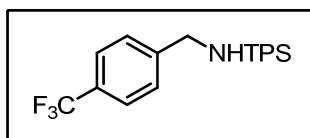


***N*-(2-Fluorobenzyl)-2,4,6-triisopropylbenzenesulfonamide (1j).**

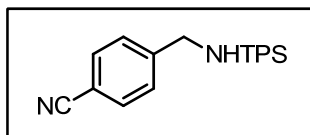
White solid (74% yield). m.p. 102-103 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.25-7.18 (m, 2H), 7.15 (s, 2H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.98 (t, *J* = 9.2 Hz, 1H), 4.68 (t, *J* = 6.4 Hz, 1H), 4.22 (d, *J* = 6.4 Hz, 2H), 4.19-4.09 (m, 2H), 2.96-2.83 (m, 1H), 1.30-1.19 (m, 18H). ¹³C NMR (100 MHz, CDCl₃) δ 160.9 (d, *J* = 244.9 Hz), 153.0, 150.4, 132.4, 130.3 (d, *J* = 3.8 Hz), 129.8 (d, *J* = 8.1 Hz), 124.4 (d, *J* = 3.3 Hz), 124.0, 123.9, 115.5 (d, *J* = 20.9 Hz), 41.0, 40.9, 34.3, 29.9, 24.9, 23.7. HRMS (ESI) calcd. for C₂₂H₃₁FNO₂S ([M+H]⁺) 392.2054, Found 392.2059.

***N*-(3-Chlorobenzyl)-2,4,6-triisopropylbenzenesulfonamide (1k).**

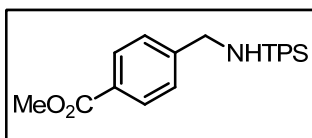
White solid (77% yield). m.p. 112-113 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.25-7.19 (m, 2H), 7.19-7.13 (m, 3H), 7.12-7.05 (m, 1H), 4.60 (t, *J* = 6.0 Hz, 1H), 4.22-4.06 (m, 2H), 4.15 (d, *J* = 6.4 Hz, 1H), 2.98-2.83 (m, 1H), 1.36-1.16 (m, 18H). ¹³C NMR (100 MHz, CDCl₃) δ 153.1, 150.4, 138.8, 134.6, 132.4, 130.0, 128.2, 128.1, 126.2, 124.0, 46.5, 34.3, 29.8, 25.0, 23.7. HRMS (ESI) calcd. for C₂₂H₃₁ClNO₂S ([M+H]⁺) 408.1759, Found 408.1760.

**2,4,6-Triisopropyl-*N*-(4-(trifluoromethyl)benzyl)benzenesulfonamide (1l).**

White solid (90% yield). m.p. 148-150 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.53 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.17 (s, 2H), 4.68 (t, *J* = 6.4 Hz, 1H), 4.23 (d, *J* = 6.4 Hz, 2H), 4.19-4.07 (m, 2H), 2.98-2.85 (m, 1H), 1.27 (d, *J* = 7.2 Hz, 6H), 1.25 (d, *J* = 6.8 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 153.2, 150.4, 140.9, 132.4, 130.1 (q, *J* = 32.2 Hz), 128.3, 125.6 (q, *J* = 3.7 Hz), 124.1 (q, *J* = 270.5 Hz), 124.0, 46.5, 34.3, 29.8, 25.0, 23.7. HRMS (ESI) calcd. for C₂₃H₃₁F₃NO₂S ([M+H]⁺) 442.2022, Found 442.2024.

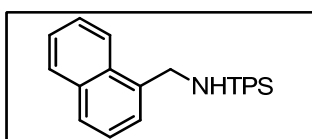
***N*-(4-Cyanobenzyl)-2,4,6-triisopropylbenzenesulfonamide (1m).**

White solid (83% yield). m.p. 188-190 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.17 (s, 2H), 4.73 (t, *J* = 6.4 Hz, 1H), 4.23 (d, *J* = 6.4 Hz, 2H), 4.18-4.05 (m, 2H), 2.98-2.85 (m, 1H), 1.27 (d, *J* = 6.8 Hz, 6H), 1.25 (d, *J* = 6.4 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 153.2, 150.3, 142.5, 132.4, 132.3, 128.6, 123.9, 118.6, 111.5, 46.4, 34.2, 29.8, 24.9, 23.7. HRMS (ESI) calcd. for C₂₃H₃₁N₂O₂S ([M+H]⁺) 399.2101, Found 399.2108.



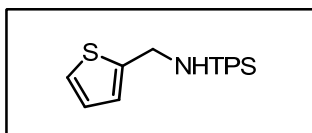
Methyl 4-((2,4,6-triisopropylphenyl)sulfonamido)methyl benzoate (1n).

White solid (87% yield). m.p. 164-165 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.94 (d, J = 8.4 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 7.17 (s, 2H), 4.66 (t, J = 6.2 Hz, 1H), 4.22 (d, J = 6.4 Hz, 2H), 4.19-4.08 (m, 2H), 3.90 (s, 3H), 2.97-2.85 (m, 1H), 1.26 (d, J = 6.8 Hz, 6H), 1.25 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 166.8, 153.1, 150.4, 141.9, 132.3, 130.0, 129.7, 127.9, 123.9, 52.2, 46.6, 34.2, 29.8, 25.0, 23.7. HRMS (ESI) calcd. for $\text{C}_{24}\text{H}_{34}\text{NO}_4\text{S}$ ($[\text{M}+\text{H}]^+$) 432.2203, Found 432.2211.



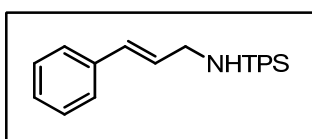
2,4,6-Triisopropyl-N-(naphthalen-1-ylmethyl)benzenesulfonamide (1o).

White solid (85% yield). m.p. 107-108 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.99-7.91 (m, 1H), 7.89-7.83 (m, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.54-7.45 (m, 2H), 7.35 (t, J = 7.6 Hz, 1H), 7.31-7.26 (m, 1H), 7.21 (s, 2H), 4.58 (d, J = 6.0 Hz, 2H), 4.52 (t, J = 6.0 Hz, 1H), 4.26-4.14 (m, 2H), 3.01-2.88 (m, 1H), 1.29 (d, J = 6.8 Hz, 6H), 1.25 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.1, 150.6, 133.9, 132.1, 131.7, 131.4, 129.2, 128.8, 127.1, 126.9, 126.2, 125.3, 124.0, 123.5, 45.1, 34.3, 29.9, 25.0, 23.8. HRMS (ESI) calcd. for $\text{C}_{26}\text{H}_{34}\text{NO}_2\text{S}$ ($[\text{M}+\text{H}]^+$) 424.2305, Found 424.2308.



2,4,6-Triisopropyl-N-(thiophen-2-ylmethyl)benzenesulfonamide (1p).

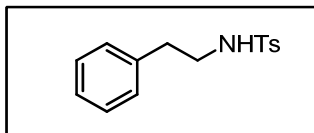
Off-white solid (80% yield). m.p. 109-110 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.19 (dd, J = 4.8, 1.2 Hz, 1H), 7.17 (s, 2H), 6.9-6.87 (m, 1H), 6.86-6.82 (m, 1H), 4.58 (t, J = 6.0 Hz, 1H), 4.36 (d, J = 6.0 Hz, 2H), 4.23-4.09 (m, 2H), 2.98-2.84 (m, 1H), 1.27 (d, J = 6.8 Hz, 6H), 1.26 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.1, 150.5, 139.0, 132.2, 127.0, 126.7, 125.9, 124.0, 41.8, 34.3, 29.8, 25.0, 23.7. HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{30}\text{NO}_2\text{S}_2$ ($[\text{M}+\text{H}]^+$) 380.1712, Found 380.1715.



N-Cinnamyl-2,4,6-triisopropylbenzenesulfonamide (1q).

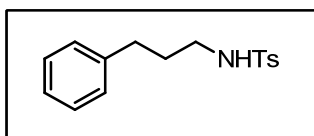
White solid (70% yield). m.p. 103-105 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.31-7.25 (m, 2H), 7.25-7.20 (m, 3H), 7.18 (s, 2H), 6.46 (d, J = 15.6 Hz, 1H), 6.01 (dt, J = 16.0, 6.6 Hz, 1H),

4.44 (t, $J = 6.2$ Hz, 1H), 4.27-4.12 (m, 2H), 3.79 (t, $J = 6.4$ Hz, 2H), 2.96-2.84 (m, 1H), 1.28 (d, $J = 6.8$ Hz, 12H), 1.26 (d, $J = 7.6$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.9, 150.3, 136.2, 133.1, 132.7, 128.7, 128.0, 126.5, 124.5, 123.9, 45.4, 34.2, 29.8, 25.0, 23.7. HRMS (ESI) calcd. for $\text{C}_{24}\text{H}_{34}\text{NO}_2\text{S}$ ($[\text{M}+\text{H}]^+$) 400.2305, Found 400.2300.



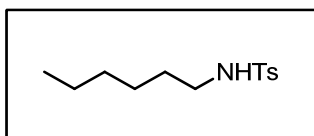
***N*-Cinnamyl-2,4,6-triisopropylbenzenesulfonamide (1r).**⁴

White solid (89% yield). m.p. 64-66 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.69 (d, $J = 8.4$ Hz, 2H), 7.34-7.19 (m, 5H), 7.08 (d, $J = 6.8$ Hz, 2H), 4.40 (t, $J = 6.0$ Hz, 1H), 3.21 (q, $J = 6.8$ Hz, 2H), 2.76 (t, $J = 6.8$ Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 143.4, 137.9, 136.8, 129.7, 128.8, 128.7, 127.1, 126.7, 44.3, 35.8, 21.5.



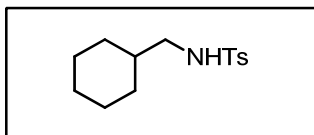
4-Methyl-*N*-(3-phenylpropyl)benzenesulfonamide (1s).⁵

White solid (97% yield). m.p. 65-67 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, $J = 8.4$ Hz, 2H), 7.30 (d, $J = 8.0$ Hz, 2H), 7.28-7.22 (m, 2H), 7.18 (t, $J = 7.2$ Hz, 1H), 7.08 (d, $J = 6.8$ Hz, 2H), 4.59-4.41 (m, 1H), 2.97 (q, $J = 6.4$ Hz, 2H), 2.60 (t, $J = 7.6$ Hz, 2H), 2.43 (s, 3H), 1.86-1.72 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 143.4, 141.0, 137.0, 129.8, 128.5, 128.4, 127.2, 126.1, 42.7, 32.7, 31.2, 21.6.



***N*-Hexyl-4-methylbenzenesulfonamide (1t).**⁶

White solid (84% yield). m.p. 63-65 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, $J = 8.4$ Hz, 2H), 7.31 (d, $J = 8.0$ Hz, 2H), 4.43-4.29 (m, 1H), 2.92 (q, $J = 6.4$ Hz, 2H), 2.43 (s, 3H), 1.51-1.38 (m, 2H), 1.32-1.14 (m, 6H), 0.84 (t, $J = 6.8$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 143.1, 137.0, 129.6, 127.1, 43.2, 31.2, 29.4, 26.1, 22.4, 21.4, 13.9.



***N*-(Cyclohexylmethyl)-4-methylbenzenesulfonamide (1u).**⁵

White solid (74% yield). m.p. 79-81 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, $J = 8.4$ Hz, 2H), 7.30 (d, $J = 8.0$ Hz, 2H), 4.45 (t, $J = 6.4$ Hz, 1H), 2.75 (t, $J = 6.6$ Hz, 2H), 2.43 (s, 3H), 1.74-1.60 (m, 5H), 1.46-1.32 (m, 1H), 1.24-1.02 (m, 3H), 0.91-0.77 (m, 2H). ^{13}C NMR (100

MHz, CDCl₃) δ 143.2, 137.2, 129.7, 127.1, 49.4, 37.8, 30.6, 26.3, 25.7, 21.6.

3. Reaction Optimization

Table S1. Ligand Effects

entry	Ligand	yield (%) ^{a,b}
1	IPr-HCl	19
2	IPr ^{Me} -HCl	8
3	IMes⁺-HCl	29
4	SIPr-HCl	0
5	IPr ^{NQ} -HCl	0
6	IMe-HI	9
7	ICy-HCl	trace
8	I ^t Bu-HBF ₄	20

^aReaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), toluene (2 mL). ^bDetermined by ¹H NMR with TCE as the internal standard.

Table S2. Protecting Group Effects

entry	PG	yield (%) ^{a,b}
1	<i>p</i> -CF ₃ -C ₆ H ₄ SO ₂	42
2	3,5-(CF ₃) ₂ -C ₆ H ₃ SO ₂	40
3	<i>p</i> -NO ₂ -C ₆ H ₄ SO ₂	0
4	<i>p</i> -Me-C ₆ H ₄ SO ₂ (Ts)	29
5	2,4,6-Me ₃ -C ₆ H ₂ SO ₂ (TMS)	22
6	2,4,6- <i>i</i> Pr ₃ -C ₆ H ₂ SO ₂ (TPS)	56
7	<i>p</i> -OMe-C ₆ H ₄ SO ₂	32
8	CH ₃ -SO ₂ (Ms)	35
9	<i>t</i> Bu-SO ₂ (Bs)	15
10	CF ₃ -SO ₂ (Tf)	19
11 ^c	2,4,6-<i>i</i>Pr₃-C₆H₂SO₂ (TPS)	68
12 ^d	2,4,6- <i>i</i> Pr ₃ -C ₆ H ₂ SO ₂ (TPS)	24

^aReaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), toluene (2 mL). ^bDetermined by ¹H NMR with TCE as the internal standard. ^cIPr-HCl (10 mol%). ^dIPr^{Me}-HCl (10 mol%).

Table S3. Phosphine Ligand Effects

entry	P Ligand	yield (%) ^{a,b}
1	0	68
2	PPh ₃	76
3	BINAP	19
4	dppe	26
5	ⁿ Bu ₃ P	38
6	^t Bu ₃ P	70
7	PCy ₃	83
8	PCy ₃	99
9	dcype	23
10 ^c	PCy₃	99

^aReaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), toluene (2 mL). ^bDetermined by ¹H NMR with TCE as the internal standard. ^cNi(cod)₂ (5 mol%), IPrHCl (5 mol%), *t*-BuOK (6 mol%)

Table S4. Temperature Effects

entry	T	yield (%) ^{a,b}
1	50	67
2	60	75
3	70	89
4	80	99
5	90	99
6	100	99

^aReaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), toluene (2 mL). ^bDetermined by ¹H NMR with TCE as the internal standard.

Table S5. Substrate Loading Effects

entry	1a (mmol)	2a (mmol)	yield (%) ^{a,b}
1	0.15	0.1	78
2	0.12	0.1	92
3	0.11	0.1	95
4	0.1	0.1	95
5	0.1	0.11	99
6	0.1	0.12	84
7	0.1	0.15	79

^aReaction conditions: toluene (2 mL). ^bDetermined by ¹H NMR with TCE as the internal standard.

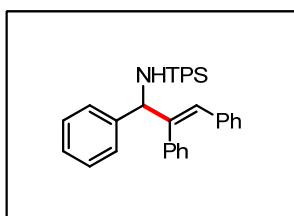
Table S6. Ni Catalyst Effects

$\text{Ph-CH}_2\text{-NHTPS} + \text{Ph-C}\equiv\text{C-Ph} \xrightarrow[\text{PCy}_3 (5 \text{ mol}\%), \text{ 80 }^\circ\text{C, toluene, 12 h}]{\text{Ni catalyst (5 mol}\%), \text{ IPr}\cdot\text{HCl (5 mol}\%), \text{ } t\text{-BuOK (6 mol}\%)}$			
1a	2a		3a
entry	Ni catalyst	additive	yield (%) ^{a,b}
1	Ni(cod) ₂	-	99
2	Ni(OAc) ₂ ·4H ₂ O	-	0
3	Ni(PPh ₃) ₂ Cl ₂	-	0
4	NiBr ₂	-	0
5	NiCl ₂ -glyme	-	0
6	NiCl ₂ -glyme	Mn	0
7	Ni(acac) ₂	-	0

^aReaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), toluene (2 mL). ^bDetermined by ¹H NMR with TCE as the internal standard.

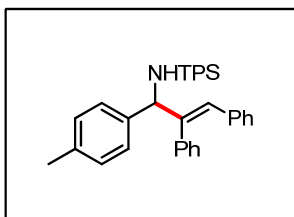
4. General Procedure for Redox-Neutral Coupling Reaction

To a 15 mL pressure tube were added Ni(cod)₂ (2.75 mg, 0.01 mmol), IPr·HCl (4.25 mg, 0.01 mmol), PCy₃ (2.8 mg, 0.01 mmol), KO^tBu (1.34 mg, 0.012 mmol), toluene (2.0 mL), alkynes (0.22 mmol) and amines (0.20 mmol) in a glove box. The tube was sealed with a Teflon cap and the mixture was stirred at 80 °C or 110 °C for 1-12 h. After cooled to room temperature, the crude product was filtered through a short pad of Celite, and the filtrate was concentrated under vacuum. The resulting residue was obtained by chromatography on silica gel column with petroleum ether/ethyl acetate as the eluent. The analytic data for the products are listed below.



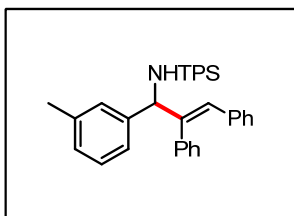
(E)-2,4,6-Triisopropyl-N-(1,2,3-triphenylallyl)benzenesulfonamide (**3a**).

Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (94% yield). m.p. 118-119 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.23-7.13 (m, 6H), 7.13-7.07 (m, 4H), 7.06-6.99 (m, 3H), 6.86-6.81 (m, 2H), 6.79-6.74 (m, 2H), 6.73 (s, 1H), 5.39 (d, *J* = 5.6 Hz, 1H), 4.78 (d, *J* = 5.6 Hz, 1H), 4.17-4.04 (m, 2H), 2.94-2.81 (m, 1H), 1.24 (d, *J* = 6.4 Hz, 12H), 1.12 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 152.8, 150.0, 140.8, 139.2, 138.1, 136.1, 134.0, 129.4, 129.3, 128.8, 128.7, 128.7, 128.0, 127.9, 127.6, 127.6, 127.1, 123.8, 64.5, 34.3, 30.0, 25.1, 24.8, 23.8, 23.7. HRMS (ESI) calcd. for C₃₆H₄₁NNaO₂S ([M+Na]⁺) 574.2750, Found 574.2742.



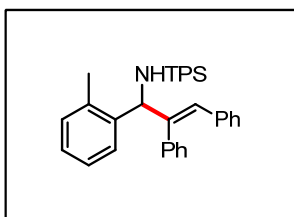
(E)-N-(2,3-Diphenyl-1-(p-tolyl)allyl)-2,4,6-triisopropylbenzenesulfonamide (3b).

Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (89% yield). m.p. 56-58 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.23-7.14 (m, 3H), 7.11 (s, 2H), 7.07-7.02 (m, 3H), 7.00 (s, 4H), 6.86 (d, *J* = 7.2 Hz, 2H), 6.76 (d, *J* = 6.8 Hz, 2H), 6.71 (s, 1H), 5.36 (d, *J* = 5.6 Hz, 1H), 4.75 (d, *J* = 5.6 Hz, 1H), 4.19-4.05 (m, 2H), 2.95-2.81 (m, 1H), 2.28 (s, 3H), 1.25 (d, *J* = 6.4 Hz, 12H), 1.14 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 152.8, 150.0, 141.0, 138.3, 137.7, 136.2, 136.2, 134.1, 129.4, 129.3, 129.3, 128.7, 128.6, 127.9, 127.6, 127.0, 123.8, 64.3, 34.3, 30.0, 25.1, 24.8, 23.8, 23.8, 21.2. HRMS (ESI) calcd. for C₃₇H₄₃NNaO₂S ([M+Na]⁺) 588.2907, Found 588.2899.



(E)-N-(2,3-Diphenyl-1-(m-tolyl)allyl)-2,4,6-triisopropylbenzenesulfonamide (3c).

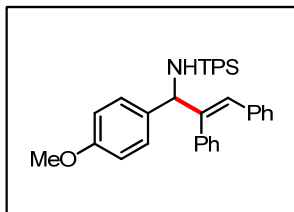
Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (89% yield). m.p. 74-76 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.23-7.15 (m, 3H), 7.14-7.10 (m, 2H), 7.10-6.97 (m, 5H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.89-6.84 (m, 3H), 6.82-6.76 (m, 2H), 6.74 (s, 1H), 5.37 (d, *J* = 5.6 Hz, 1H), 4.77 (d, *J* = 5.6 Hz, 1H), 4.18-4.04 (m, 2H), 2.97-2.80 (m, 1H), 2.20 (s, 3H), 1.30-1.17 (m, 12H), 1.13 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 152.7, 149.9, 140.9, 139.1, 138.3, 138.2, 136.2, 134.0, 129.4, 129.3, 128.9, 128.7, 128.7, 128.5, 128.4, 127.9, 127.6, 127.0, 124.7, 123.8, 64.5, 34.3, 30.0, 25.1, 24.8, 23.7, 21.5. HRMS (ESI) calcd. for C₃₇H₄₃NNaO₂S ([M+Na]⁺) 588.2907, Found 588.2907.



(E)-N-(2,3-Diphenyl-1-(o-tolyl)allyl)-2,4,6-triisopropylbenzenesulfonamide (3d).

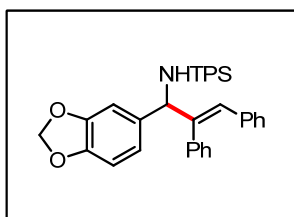
Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (62% yield). m.p. 126-127 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.25-7.20 (m, 1H), 7.20-7.13 (m, 3H), 7.12-7.06 (m, 4H), 7.05-6.96 (m, 4H), 6.92-6.86 (m, 2H), 6.70 (d, *J* = 7.6 Hz, 2H), 6.68 (s, 1H), 5.58 (d, *J* = 4.8 Hz, 1H), 4.77 (d, *J* = 4.4 Hz, 1H), 4.16-4.02 (m, 2H), 2.93-2.78 (m, 1H), 1.90 (s, 3H), 1.25 (d, *J* = 6.4 Hz, 6H), 1.21 (dd, *J* = 6.8, 2.4 Hz, 6H), 1.09 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 152.7, 149.8, 140.5, 138.8, 137.4, 136.2, 136.2, 134.4, 130.7, 129.2, 129.2, 128.6,

128.2, 128.0, 127.9, 127.5, 127.3, 126.9, 126.4, 123.8, 60.3, 34.3, 30.0, 25.1, 24.6, 23.7, 23.7, 19.0. **HRMS** (ESI) calcd. for $C_{37}H_{43}NNaO_2S$ ($[M+Na]^+$) 588.2907, Found 588.2901.



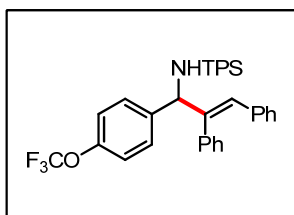
(E)-2,4,6-Triisopropyl-N-(1-(4-methoxyphenyl)-2,3-diphenylallyl)benzenesulfonamide (3e).

Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (85% yield). m.p. 59-61 °C. **¹H NMR** (400 MHz, $CDCl_3$) δ 7.22-7.13 (m, 3H), 7.11 (s, 2H), 7.07-6.97 (m, 5H), 6.88-6.82 (m, 2H), 6.77-6.71 (m, 3H), 6.71-6.67 (m, 2H), 5.34 (d, J = 5.6 Hz, 1H), 4.73 (d, J = 5.2 Hz, 1H), 4.18-4.04 (m, 2H), 3.75 (s, 3H), 2.94-2.81 (m, 1H), 1.29-1.19 (m, 12H), 1.13 (d, J = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, $CDCl_3$) δ 159.3, 152.8, 149.9, 141.0, 138.4, 136.1, 134.0, 131.2, 129.4, 129.3, 128.9, 128.7, 128.4, 127.9, 127.6, 127.0, 123.8, 114.0, 64.0, 55.3, 34.3, 30.0, 25.1, 24.8, 23.8, 23.7. **HRMS** (ESI) calcd. for $C_{37}H_{43}NNaO_3S$ ($[M+Na]^+$) 604.2856, Found 604.2859.



(E)-N-(1-(Benzo[d][1,3]dioxol-5-yl)-2,3-diphenylallyl)-2,4,6-triisopropylbenzenesulfonamide (3f).

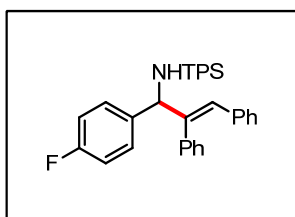
Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (84% yield). m.p. 55-57 °C. **¹H NMR** (400 MHz, $CDCl_3$) δ 7.25-7.15 (m, 3H), 7.11 (s, 2H), 7.09-6.99 (m, 3H), 6.92-6.84 (m, 2H), 6.78-6.71 (m, 2H), 6.68 (s, 1H), 6.64-6.52 (m, 3H), 5.94-5.88 (m, 2H), 5.29 (d, J = 5.2 Hz, 1H), 4.72 (d, J = 5.6 Hz, 1H), 4.17-4.04 (m, 2H), 2.94-2.81 (m, 1H), 1.31-1.19 (m, 12H), 1.14 (d, J = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, $CDCl_3$) δ 152.8, 149.9, 147.9, 147.3, 140.8, 138.2, 136.0, 133.9, 133.1, 129.3, 129.3, 128.7, 128.6, 127.9, 127.6, 127.0, 123.8, 121.3, 108.2, 108.0, 101.2, 64.2, 34.2, 30.0, 25.1, 24.8, 23.7, 23.7. **HRMS** (ESI) calcd. for $C_{37}H_{41}NNaO_4S$ ($[M+Na]^+$) 618.2649, Found 618.2655.



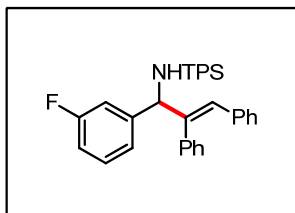
(E)-N-(2,3-Diphenyl-1-(4-(trifluoromethoxy)phenyl)allyl)-2,4,6-triisopropylbenzenesulfonamide (3g).

Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (90% yield). m.p. 124-126 °C. **¹H**

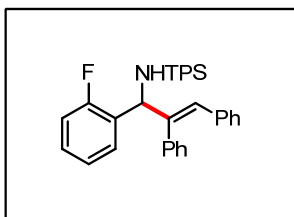
NMR (400 MHz, CDCl₃) δ 7.25-7.15 (m, 3H), 7.14-7.08 (m, 4H), 7.08-6.97 (m, 5H), 6.85-6.80 (m, 2H), 6.79-6.74 (m, 2H), 6.67 (s, 1H), 5.45 (d, J = 5.6 Hz, 1H), 4.78 (d, J = 6.0 Hz, 1H), 4.12-3.98 (m, 2H), 2.94-2.81 (m, 1H), 1.23 (dd, J = 7.2, 1.2 Hz, 6H), 1.20 (d, J = 6.8 Hz, 6H), 1.13 (d, J = 6.4 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 153.1, 150.0, 148.8, 140.5, 138.0, 137.7, 135.8, 133.8, 129.5, 129.3, 129.1, 128.9, 128.0, 127.9, 127.3, 123.8, 120.9, 120.5 (q, J = 255.7 Hz), 63.9, 34.3, 30.0, 25.0, 24.8, 23.7, 23.7. **HRMS** (ESI) calcd. for C₃₇H₄₀F₃NNaO₃S ([M+Na]⁺) 658.2573, Found 658.2568.



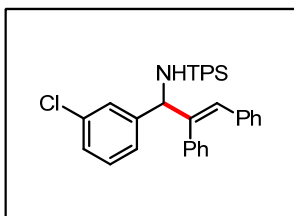
(E)-N-(1-(4-Fluorophenyl)-2,3-diphenylallyl)-2,4,6-triisopropylbenzenesulfonamide (3h). Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (89% yield). m.p. 54-56 °C. **¹H NMR** (400 MHz, CDCl₃) δ 7.24-7.15 (m, 3H), 7.12 (s, 2H), 7.10-7.00 (m, 5H), 6.92-6.81 (m, 4H), 6.80-6.73 (m, 2H), 6.70 (s, 1H), 5.41 (d, J = 5.6 Hz, 1H), 4.79 (d, J = 5.6 Hz, 1H), 4.18-4.02 (m, 2H), 2.95-2.82 (m, 1H), 1.32-1.20 (m, 12H), 1.15 (d, J = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 162.3 (d, J = 245.6 Hz), 153.0, 150.0, 140.7, 137.9, 135.9, 135.0 (d, J = 2.9 Hz), 133.8, 129.4, 129.3, 129.3, 129.0, 128.8, 128.0, 127.8, 127.2, 123.8, 115.4 (d, J = 21.5 Hz), 63.9, 34.3, 30.0, 25.0, 24.8, 23.7. **HRMS** (ESI) calcd. for C₃₆H₄₀FNNaO₂S ([M+Na]⁺) 592.2656, Found 592.2652.



(E)-N-(1-(3-Fluorophenyl)-2,3-diphenylallyl)-2,4,6-triisopropylbenzenesulfonamide (3i). Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (94% yield). m.p. 139-141 °C. **¹H NMR** (400 MHz, CDCl₃) δ 7.24-7.15 (m, 4H), 7.12 (s, 2H), 7.10-7.00 (m, 3H), 6.97-6.88 (m, 2H), 6.85 (d, J = 6.8 Hz, 2H), 6.82-6.74 (m, 3H), 6.70 (s, 1H), 5.43 (d, J = 6.0 Hz, 1H), 4.80 (d, J = 6.0 Hz, 1H), 4.17-4.01 (m, 2H), 2.95-2.82 (m, 1H), 1.30-1.19 (m, 12H), 1.16 (d, J = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 162.9 (d, J = 245.5 Hz), 153.1, 150.0, 142.0 (d, J = 6.7 Hz), 140.4, 137.6, 135.8, 133.7, 130.2, 130.1, 129.6, 129.4, 128.9, 128.0, 127.9, 127.3, 123.9, 123.3 (d, J = 2.3 Hz), 114.9 (d, J = 20.9 Hz), 114.6 (d, J = 22.3 Hz), 64.0, 34.3, 30.0, 25.1, 24.8, 23.7. **HRMS** (ESI) calcd. for C₃₆H₄₀FNNaO₂S ([M+Na]⁺) 592.2656, Found 592.2651.

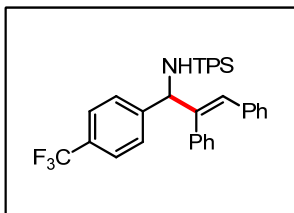


(E)-N-(1-(2-Fluorophenyl)-2,3-diphenylallyl)-2,4,6-triisopropylbenzenesulfonamide (3j). Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (82% yield). m.p. 97-99 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.12 (m, 4H), 7.08 (s, 2H), 7.06-6.95 (m, 4H), 6.94-6.85 (m, 4H), 6.79-6.73 (m, 2H), 6.63 (s, 1H), 5.67 (d, J = 6.8 Hz, 1H), 5.00 (d, J = 6.8 Hz, 1H), 4.16-4.00 (m, 2H), 2.93-2.78 (m, 1H), 1.26-1.18 (m, 12H), 1.15 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 160.3 (d, J = 246.0 Hz), 152.8, 150.0, 139.9, 137.8, 136.0, 133.6, 129.5 (d, J = 8.3 Hz), 129.3, 129.3, 129.1, 128.8, 127.9, 127.7, 127.1, 126.8, 126.7, 124.0 (d, J = 3.2 Hz), 123.7, 115.7 (d, J = 21.5 Hz), 58.6, 34.3, 30.1, 25.0, 24.8, 23.7. HRMS (ESI) calcd. for $\text{C}_{36}\text{H}_{40}\text{FNNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 592.2656, Found 592.2656.



(E)-N-(1-(3-Chlorophenyl)-2,3-diphenylallyl)-2,4,6-triisopropylbenzenesulfonamide (3k).

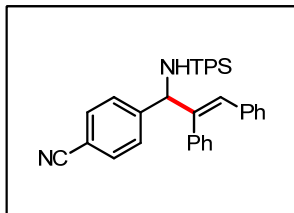
Purified by column (PE/EtOAc = 50:1 to 20:1), white solid (93% yield). m.p. 111-113 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.13 (m, 4H), 7.12-7.09 (m, 3H), 7.09-6.98 (m, 5H), 6.88-6.82 (m, 2H), 6.82-6.76 (m, 2H), 6.68 (s, 1H), 5.41 (d, J = 6.0 Hz, 1H), 4.77 (d, J = 6.0 Hz, 1H), 4.13-3.97 (m, 2H), 2.94-2.79 (m, 1H), 1.24 (dd, J = 6.8, 1.2 Hz, 6H), 1.21 (d, J = 6.8 Hz, 6H), 1.15 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.0, 150.0, 141.4, 140.3, 137.5, 135.8, 134.5, 133.6, 129.8, 129.7, 129.4, 128.9, 128.1, 128.0, 128.0, 127.7, 127.3, 125.8, 123.9, 64.0, 34.3, 30.0, 25.0, 24.9, 23.7, 23.7. HRMS (ESI) calcd. for $\text{C}_{36}\text{H}_{40}\text{ClNNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 608.2360, Found 608.2356.



(E)-N-(2,3-Diphenyl-1-(4-(trifluoromethyl)phenyl)allyl)-2,4,6-triisopropylbenzenesulfonamide (3l).

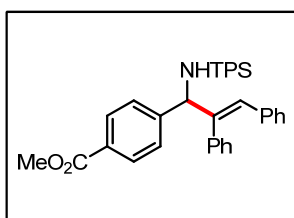
Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (88% yield). m.p. 155-156 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.43 (d, J = 8.4 Hz, 2H), 7.26-7.16 (m, 5H), 7.10 (s, 2H), 7.09-7.02 (m, 3H), 6.86-6.74 (m, 4H), 6.66 (s, 1H), 5.52 (d, J = 5.6 Hz, 1H), 4.84 (d, J = 6.0 Hz, 1H), 4.11-3.96 (m, 2H), 2.96-2.81 (m, 1H), 1.24 (dd, J = 6.8, 1.6 Hz, 6H), 1.19 (d, J = 6.8

Hz, 6H), 1.16 (d, $J = 6.8$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.2, 150.0, 143.4, 140.3, 137.4, 135.7, 133.7, 130.0 (q, $J = 32.3$ Hz), 130.0, 129.3, 129.0, 128.1, 128.0, 127.5, 125.4 (q, $J = 3.3$ Hz), 123.8, 121.4 (q, $J = 270.3$ Hz), 64.2, 34.3, 30.0, 24.9, 24.9, 23.7. HRMS (ESI) calcd. for $\text{C}_{37}\text{H}_{40}\text{F}_3\text{NNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 642.2624, Found 642.2621.



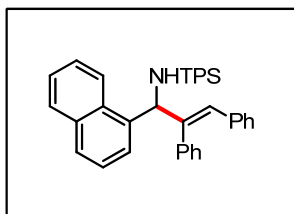
(E)-N-(1-(4-Cyanophenyl)-2,3-diphenylallyl)-2,4,6-triisopropylbenzenesulfonamide (3m).

Purified by column (PE/EtOAc = 50:1 to 10:1), white solid (84% yield). m.p. 96-98 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.48 (d, $J = 8.4$ Hz, 2H), 7.26 (s, 1H), 7.24 (s, 1H), 7.23-7.16 (m, 3H), 7.11 (s, 2H), 7.09-7.02 (m, 3H), 6.81-6.73 (m, 4H), 6.63 (s, 1H), 5.50 (d, $J = 5.6$ Hz, 1H), 4.87 (d, $J = 6.0$ Hz, 1H), 4.10-3.95 (m, 2H), 2.96-2.81 (m, 1H), 1.25 (dd, $J = 6.8, 1.6$ Hz, 6H), 1.18 (d, $J = 6.0$ Hz, 6H), 1.17 (d, $J = 6.4$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.3, 150.1, 144.9, 139.9, 137.0, 135.4, 133.4, 132.2, 130.3, 129.3, 129.3, 129.1, 128.3, 128.2, 128.1, 127.6, 123.9, 118.6, 111.7, 64.2, 34.3, 30.0, 24.9, 23.8, 23.7. HRMS (ESI) calcd. for $\text{C}_{37}\text{H}_{40}\text{N}_2\text{NaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 599.2703, Found 599.2700.



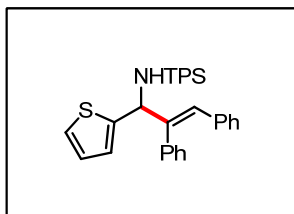
(E)-Methyl 4-(2,3-diphenyl-1-(2,4,6-triisopropylphenylsulfonamido)allyl)benzoate (3n).

Purified by column (PE/EtOAc = 50:1 to 15:1), white solid (92% yield). m.p. 121-123 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, $J = 8.4$ Hz, 2H), 7.25-7.14 (m, 5H), 7.10 (s, 2H), 7.08-7.01 (m, 3H), 6.85-6.75 (m, 4H), 6.69 (s, 1H), 5.49 (d, $J = 6.0$ Hz, 1H), 4.84 (d, $J = 6.0$ Hz, 1H), 4.14-4.02 (m, 2H), 3.89 (s, 3H), 2.94-2.81 (m, 1H), 1.24 (dd, $J = 6.8, 1.2$ Hz, 6H), 1.20 (d, $J = 6.8$ Hz, 6H), 1.15 (d, $J = 6.8$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 166.7, 153.1, 150.0, 144.4, 140.3, 137.5, 135.7, 133.6, 129.8, 129.7, 129.6, 129.3, 129.3, 128.9, 128.0, 127.9, 127.6, 127.3, 123.8, 64.3, 52.2, 34.3, 30.0, 25.0, 24.9, 23.7, 23.7. HRMS (ESI) calcd. for $\text{C}_{38}\text{H}_{43}\text{NNaO}_4\text{S}$ ($[\text{M}+\text{Na}]^+$) 632.2805, Found 632.2806.

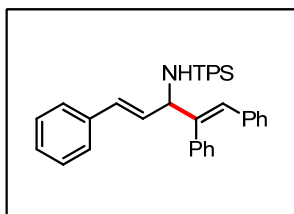


(E)-2,4,6-Triisopropyl-N-(1-(naphthalen-1-yl)-2,3-diphenylallyl)benzenesulfonamide (3o).

Purified by column (PE/EtOAc = 50:1 to 20:1), white solid (86% yield). m.p. 60-62 °C. **¹H NMR** (400 MHz, CDCl₃) δ 8.03 (d, J = 8.0 Hz, 1H), 7.81 (d, J = 7.6 Hz, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.48-7.36 (m, 3H), 7.28 (t, J = 8.0 Hz, 1H), 7.18-7.09 (m, 3H), 7.07 (s, 2H), 7.05-6.95 (m, 5H), 6.75-6.65 (m, 3H), 6.29 (d, J = 4.8 Hz, 1H), 4.92 (d, J = 4.8 Hz, 1H), 4.15-3.99 (m, 2H), 2.91-2.77 (m, 1H), 1.24-1.15 (m, 12H), 1.07 (d, J = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 152.7, 149.6, 140.0, 138.7, 136.2, 134.7, 134.4, 134.1, 131.1, 129.8, 129.2, 129.2, 129.1, 128.9, 128.6, 127.9, 127.6, 127.0, 126.8, 126.4, 125.9, 125.1, 123.8, 122.9, 60.7, 34.2, 30.1, 25.0, 24.7, 23.8, 23.7. **HRMS** (ESI) calcd. for C₄₀H₄₃NNaO₂S ([M+Na]⁺) 624.2907, Found 624.2900.

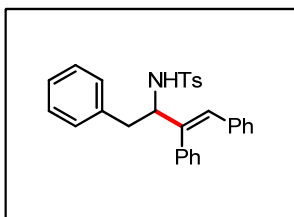


(E)-N-(2,3-Diphenyl-1-(thiophen-2-yl)allyl)-2,4,6-triisopropylbenzenesulfonamide(3p). Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (86% yield). m.p. 115-117 °C. **¹H NMR** (400 MHz, CDCl₃) δ 7.24-7.16 (m, 4H), 7.12 (s, 2H), 7.09-7.01 (m, 3H), 6.99-6.93 (m, 2H), 6.88-6.83 (m, 1H), 6.83-6.77 (m, 2H), 6.77-6.74 (m, 1H), 6.73 (s, 1H), 5.67 (d, J = 6.8 Hz, 1H), 4.86 (d, J = 6.8 Hz, 1H), 4.19-4.05 (m, 2H), 2.94-2.81 (m, 1H), 1.25 (d, J = 6.8 Hz, 6H), 1.23 (dd, J = 6.8, 2.0 Hz, 6H), 1.16 (d, J = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 152.9, 150.1, 144.0, 140.8, 137.6, 135.9, 133.8, 129.5, 129.4, 128.9, 128.8, 128.0, 127.9, 127.2, 127.1, 126.1, 125.9, 123.9, 60.2, 34.3, 30.0, 25.1, 24.9, 23.7, 23.7. **HRMS** (ESI) calcd. for C₃₄H₃₉NNaO₂S₂ ([M+Na]⁺) 580.2314, Found 580.2322.



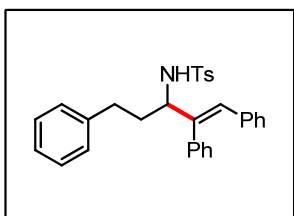
2,4,6-Triisopropyl-N-((1E,4E)-1,2,5-triphenylpenta-1,4-dien-3-yl)benzenesulfonamide (3q).

Purified by column (PE/EtOAc = 50:1 to 20:1), white solid (45% yield). m.p. 118-120 °C. **¹H NMR** (400 MHz, CDCl₃) δ 7.32-7.27 (m, 3H), 7.25-7.17 (m, 3H), 7.17-7.12 (m, 2H), 7.12-7.03 (m, 7H), 6.87-6.81 (m, 2H), 6.62 (s, 1H), 6.36 (d, J = 16.0 Hz, 1H), 6.02-5.92 (m, 1H), 5.04 (t, J = 6.8 Hz, 1H), 4.64 (d, J = 6.8 Hz, 1H), 4.20-4.06 (m, 2H), 2.92-2.77 (m, 1H), 1.28-1.12 (m, 18H). **¹³C NMR** (100 MHz, CDCl₃) δ 152.8, 150.0, 140.6, 137.7, 136.3, 136.0, 134.1, 132.3, 129.5, 129.5, 129.4, 129.0, 128.6, 128.0, 128.0, 127.8, 127.3, 126.6, 123.8, 62.9, 34.2, 30.0, 25.0, 24.9, 23.7, 23.7. **HRMS** (ESI) calcd. for C₃₈H₄₃NNaO₂S ([M+Na]⁺) 600.2907, Found 600.2915.



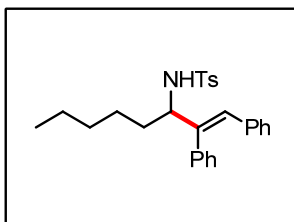
(E)-4-Methyl-N-(1,3,4-triphenylbut-3-en-2-yl)benzenesulfonamide (3r).

Purified by column (PE/EtOAc = 50:1 to 10:1), white solid (54% yield). m.p. 117-119 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.56 (d, J = 7.6 Hz, 2H), 7.36-7.29 (m, 3H), 7.24-7.18 (m, 3H), 7.14-7.07 (m, 4H), 7.06-6.97 (m, 5H), 6.75-6.65 (m, 2H), 6.30 (s, 1H), 4.53 (d, J = 6.4 Hz, 1H), 4.39 (q, J = 6.8 Hz, 1H), 2.93 (dd, J = 6.0, 13.6 Hz, 1H), 2.65 (dd, J = 8.0, 13.6 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 143.2, 140.2, 138.2, 137.5, 136.5, 136.2, 129.6, 129.5, 129.5, 129.2, 129.0, 128.7, 127.9, 127.7, 127.2, 126.9, 61.9, 40.9, 21.5. HRMS (ESI) calcd. for $\text{C}_{29}\text{H}_{26}\text{NO}_2\text{S}$ ($[\text{M}-\text{H}]^+$) 452.1679, Found 452.1685.



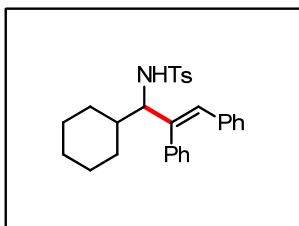
(E)-4-Methyl-N-(1,2,5-triphenylpent-1-en-3-yl)benzenesulfonamide (3s).

Purified by column (PE/EtOAc = 50:1 to 10:1), white semi-solid (41% yield). ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, J = 8.4 Hz, 2H), 7.30-7.23 (m, 5H), 7.23-7.16 (m, 3H), 7.09 (d, J = 7.2 Hz, 2H), 7.07-6.98 (m, 3H), 6.94-6.86 (m, 2H), 6.75-6.64 (m, 2H), 6.31 (s, 1H), 4.50 (d, J = 8.8 Hz, 1H), 4.20 (q, J = 7.6 Hz, 1H), 2.79-2.61 (m, 2H), 2.32 (s, 3H), 1.95-1.84 (m, 1H), 1.84-1.71 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 143.5, 141.1, 139.9, 138.1, 137.4, 136.0, 129.7, 129.4, 129.2, 129.0, 128.6, 127.9, 127.8, 127.4, 127.1, 126.2, 61.3, 36.8, 32.3, 21.6. HRMS (ESI) calcd. for $\text{C}_{30}\text{H}_{33}\text{N}_2\text{O}_2\text{S}$ ($[\text{M}+\text{NH}_4]^+$) 485.2257, Found 485.2259.



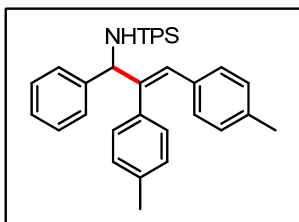
(E)-N-(1,2-Diphenyloct-1-en-3-yl)-4-methylbenzenesulfonamide (3t).

Purified by column (PE/EtOAc = 50:1 to 10:1), white solid (46% yield). m.p. 117-119 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.77 (d, J = 8.0 Hz, 2H), 7.30-7.26 (m, 3H), 7.21 (d, J = 8.0 Hz, 2H), 7.08-6.98 (m, 3H), 6.94-6.86 (m, 2H), 6.74-6.65 (m, 2H), 6.32 (s, 1H), 4.42 (d, J = 8.4 Hz, 1H), 4.14 (q, J = 7.6 Hz, 1H), 2.31 (s, 3H), 1.60-1.12 (m, 8H), 0.83 (t, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 143.4, 140.5, 138.3, 137.6, 136.1, 129.6, 129.5, 129.2, 129.2, 128.9, 127.9, 127.7, 127.4, 126.9, 61.6, 35.2, 31.4, 25.7, 22.6, 21.5, 14.1. HRMS (ESI) calcd. for $\text{C}_{27}\text{H}_{35}\text{N}_2\text{O}_2\text{S}$ ($[\text{M}+\text{NH}_4]^+$) 451.2414, Found 451.2416.



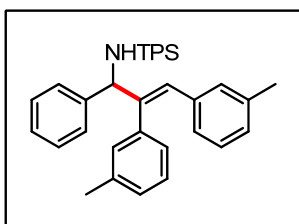
(E)-4-Methyl-N-(1,3,4-triphenylbut-3-en-2-yl)benzenesulfonamide (3u).⁷

Purified by column (PE/EtOAc = 50:1 to 10:1), white solid (45% yield). m.p. 155-157 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.30-7.24 (m, 3H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.09-6.96 (m, 3H), 6.88-6.78 (m, 2H), 6.68-6.59 (m, 2H), 6.19 (s, 1H), 4.43 (d, *J* = 9.6 Hz, 1H), 3.92 (t, *J* = 9.0 Hz, 1H), 2.30 (s, 3H), 1.96 (d, *J* = 12.4 Hz, 1H), 1.86-1.68 (m, 3H), 1.64 (s, 1H), 1.43-1.29 (m, 1H), 1.24-1.02 (m, 4H), 1.01-0.84 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 143.3, 138.8, 138.4, 137.7, 136.1, 130.1, 129.6, 129.4, 129.1, 128.9, 127.8, 127.7, 127.4, 126.8, 66.8, 40.1, 31.0, 28.9, 26.4, 26.1, 21.5.



(E)-2,4,6-Triisopropyl-N-(1-phenyl-2,3-di-p-tolylallyl)benzenesulfonamide (4a).

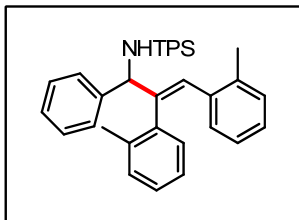
Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (86% yield). m.p. 63-65 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.21-7.16 (m, 3H), 7.13-7.07 (m, 4H), 6.96 (d, *J* = 7.6 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, 2H), 6.71 (d, *J* = 8.0 Hz, 2H), 6.67 (d, *J* = 8.0 Hz, 2H), 6.63 (s, 1H), 5.37 (d, *J* = 6.0 Hz, 1H), 4.76 (d, *J* = 6.0 Hz, 1H), 4.16-4.02 (m, 2H), 2.94-2.80 (m, 1H), 2.27 (s, 3H), 2.21 (s, 3H), 1.29-1.18 (m, 12H), 1.13 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 152.8, 150.0, 139.9, 139.6, 137.2, 136.8, 135.1, 134.0, 133.4, 129.5, 129.3, 129.2, 128.7, 128.7, 128.6, 127.8, 127.6, 123.8, 64.5, 34.3, 30.0, 25.1, 24.8, 23.8, 21.3, 21.2. HRMS (ESI) calcd. for C₃₈H₄₅NNaO₂S ([M+Na]⁺) 602.3063, Found 602.3063.



(E)-2,4,6-Triisopropyl-N-(1-phenyl-2,3-di-m-tolylallyl)benzenesulfonamide (4b).

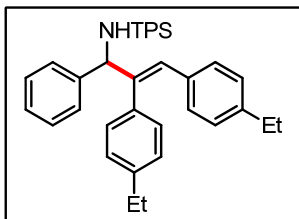
Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (84% yield). m.p. 50-52 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.21-7.14 (m, 3H), 7.10 (s, 2H), 7.09-7.05 (m, 2H), 7.04-6.98 (m, 2H), 6.94-6.85 (m, 2H), 6.68 (d, *J* = 7.6 Hz, 2H), 6.67 (s, 1H), 6.60-6.52 (m, 2H), 5.36 (d, *J* = 6.0 Hz, 1H), 4.78 (d, *J* = 6.0 Hz, 1H), 4.17-4.03 (m, 2H), 2.94-2.81 (m, 1H), 2.18 (s, 3H), 2.13 (s, 3H), 1.30-1.19 (m, 12H), 1.13 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 152.8, 150.0, 140.8, 139.4, 138.2, 138.0, 137.3, 136.1, 133.9, 130.3, 129.9, 128.9, 128.5, 128.5, 128.4, 127.9, 127.8, 127.8, 127.6, 126.5, 126.2, 123.8, 64.5, 34.3, 30.0, 25.1, 24.8,

23.8, 23.7, 21.5, 21.4. **HRMS** (ESI) calcd. for $C_{38}H_{45}NNaO_2S$ ($[M+Na]^+$) 602.3063, Found 602.3061.



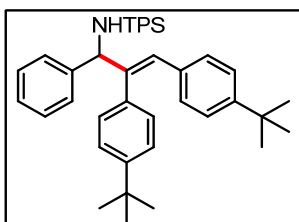
(E)-2,4,6-Triisopropyl-N-(1-phenyl-2,3-di-o-tolylallyl)benzenesulfonamide (4c).

Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (79% yield, $Z/E = 1:1$). **1H NMR** (400 MHz, $CDCl_3$) δ 7.20-7.09 (m, 9H), 7.09-7.06 (m, 6H), 7.06-7.00 (m, 5H), 7.00-6.92 (m, 2H), 6.92-6.80 (m, 5H), 6.77-6.66 (m, 2H), 6.63 (d, $J = 7.6$ Hz, 1H), 6.59 (d, $J = 7.6$ Hz, 1H), 6.49 (d, $J = 8.0$ Hz, 1H), 5.40 (d, $J = 4.8$ Hz, 1H), 5.12 (d, $J = 5.2$ Hz, 1H), 4.94 (d, $J = 4.8$ Hz, 1H), 4.91 (d, $J = 5.6$ Hz, 1H), 4.20-4.00 (m, 4H), 2.95-2.77 (m, 2H), 2.35 (s, 3H), 2.27 (s, 3H), 1.89 (s, 3H), 1.40 (s, 3H), 1.25 (d, $J = 6.4$ Hz, 6H), 1.24 (d, $J = 6.8$ Hz, 6H), 1.20 (d, $J = 6.8$ Hz, 6H), 1.17 (d, $J = 6.8$ Hz, 6H), 1.14 (d, $J = 6.8$ Hz, 6H), 1.05 (d, $J = 6.8$ Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.8, 152.8, 150.0, 149.8, 140.7, 140.3, 139.3, 139.2, 137.2, 137.0, 136.5, 136.5, 136.4, 135.9, 135.7, 135.5, 134.0, 133.5, 130.4, 130.3, 130.2, 129.7, 129.6, 128.6, 128.5, 128.4, 128.0, 127.8, 127.7, 127.6, 127.5, 127.4, 127.3, 127.0, 127.0, 126.7, 125.7, 125.3, 125.2, 125.2, 123.7, 65.0, 64.2, 34.3, 30.0, 29.9, 25.0, 24.8, 24.6, 23.8, 23.7, 23.7, 20.2, 20.1, 19.2, 18.9. **HRMS** (ESI) calcd. for $C_{38}H_{45}NNaO_2S$ ($[M+Na]^+$) 602.3063, Found 602.3074.



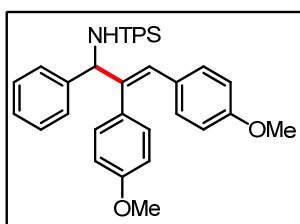
(E)-N-(2,3-Bis(4-ethylphenyl)-1-phenylallyl)-2,4,6-triisopropylbenzenesulfonamide (4d).

Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (92% yield). m.p. 54-56 °C. **1H NMR** (400 MHz, $CDCl_3$) δ 7.22-7.16 (m, 3H), 7.16-7.11 (m, 2H), 7.10 (s, 2H), 7.00 (d, $J = 8.0$ Hz, 2H), 6.88 (d, $J = 8.0$ Hz, 2H), 6.74 (d, $J = 8.0$ Hz, 2H), 6.70 (d, $J = 8.0$ Hz, 2H), 6.63 (s, 1H), 5.39 (d, $J = 6.0$ Hz, 1H), 4.77 (d, $J = 6.0$ Hz, 1H), 4.17-4.03 (m, 2H), 2.95-2.80 (m, 1H), 2.59 (q, $J = 7.6$ Hz, 2H), 2.51 (q, $J = 7.6$ Hz, 2H), 1.28-1.09 (m, 24H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.7, 150.0, 143.6, 143.2, 139.8, 139.6, 135.2, 134.0, 133.6, 129.3, 128.9, 128.5, 128.2, 127.8, 127.6, 127.5, 123.8, 64.6, 34.3, 30.0, 28.6, 28.6, 25.1, 24.8, 23.8, 23.8, 15.4, 15.4. **HRMS** (ESI) calcd. for $C_{40}H_{49}NNaO_2S$ ($[M+Na]^+$) 630.3376, Found 630.3372.



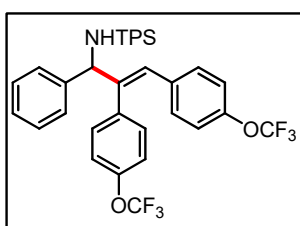
(E)-N-(2,3-Bis(4-(tert-butyl)phenyl)-1-phenylallyl)-2,4,6-triisopropylbenzenesulfonamide (4e).

Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (88% yield). m.p. 140-142 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.23-7.16 (m, 5H), 7.17-7.12 (m, 2H), 7.10 (s, 2H), 7.06 (d, *J* = 8.4 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 2H), 6.72 (d, *J* = 8.4 Hz, 2H), 6.62 (s, 1H), 5.40 (d, *J* = 6.4 Hz, 1H), 4.77 (d, *J* = 6.4 Hz, 1H), 4.15-4.02 (m, 2H), 2.94-2.81 (m, 1H), 1.28 (s, 9H), 1.24 (dd, *J* = 6.8, 1.6 Hz, 6H), 1.22 (s, 9H), 1.20 (d, *J* = 6.8 Hz, 6H), 1.13 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 152.7, 150.6, 150.1, 150.0, 139.8, 139.7, 134.8, 134.1, 133.3, 129.1, 129.0, 128.9, 128.5, 127.8, 127.6, 125.7, 124.9, 123.8, 64.6, 34.6, 34.6, 34.3, 31.4, 31.3, 30.0, 25.1, 24.9, 23.8, 23.8. HRMS (ESI) calcd. for C₄₄H₅₇NNaO₂S ([M+Na]⁺) 686.4002, Found 686.4003.



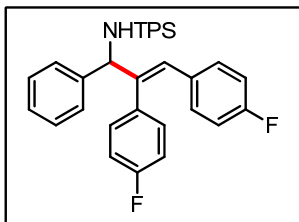
(E)-N-(2,3-Bis(4-methoxyphenyl)-1-phenylallyl)-2,4,6-triisopropylbenzenesulfonamide (4f).

Purified by column (PE/EtOAc = 50:1 to 10:1), white solid (92% yield). m.p. 64-66 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.23-7.15 (m, 3H), 7.14-7.07 (m, 4H), 6.78-6.67 (m, 6H), 6.63-6.56 (m, 3H), 5.36 (d, *J* = 6.0 Hz, 1H), 4.76 (d, *J* = 6.0 Hz, 1H), 4.17-4.01 (m, 2H), 3.75 (s, 3H), 3.71 (s, 3H), 2.96-2.81 (m, 1H), 1.28-1.18 (m, 12H), 1.13 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 158.9, 158.5, 152.7, 150.0, 139.6, 138.3, 134.0, 130.7, 130.5, 130.2, 128.9, 128.5, 128.3, 127.8, 127.5, 123.8, 114.2, 113.4, 64.6, 55.2, 34.3, 30.0, 25.1, 24.8, 23.8, 23.7. HRMS (ESI) calcd. for C₃₈H₄₅NNaO₄S ([M+Na]⁺) 634.2962, Found 634.2965.



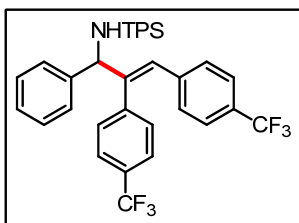
(E)-2,4,6-Triisopropyl-N-(1-phenyl-2,3-bis(4-(trifluoromethoxy)phenyl)allyl)benzenesulfonamide (4g).

Purified by column (PE/EtOAc = 50:1 to 20:1), white solid (60% yield). m.p. 122-124 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.25-7.18 (m, 3H), 7.11 (s, 2H), 7.06-6.99 (m, 4H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 6.80 (s, 1H), 6.75 (d, *J* = 8.8 Hz, 2H), 5.32 (d, *J* = 5.2 Hz, 1H), 4.75 (d, *J* = 5.6 Hz, 1H), 4.16-4.01 (m, 2H), 2.94-2.81 (m, 1H), 1.29-1.19 (m, 12H), 1.09 (d, *J* = 6.4 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 153.1, 150.0, 148.9, 148.2, 140.5, 138.6, 136.6, 134.5, 133.8, 130.9, 130.6, 129.0, 128.5, 128.0, 127.6, 123.9, 121.2, 120.5 (q, *J* = 255.6 Hz), 120.5, 64.4, 34.3, 30.0, 25.1, 24.7, 23.8, 23.7. HRMS (ESI) calcd. for C₃₈H₃₉F₆NNaO₄S ([M+Na]⁺) 742.2396, Found 742.2388.



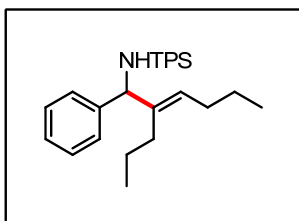
(E)-N-(2,3-Bis(4-fluorophenyl)-1-phenylallyl)-2,4,6-triisopropylbenzenesulfonamide (4h).

Purified by column (PE/EtOAc = 50:1 to 25:1), colorless semi-solid (87% yield). ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.16 (m, 3H), 7.11 (s, 2H), 7.07-6.99 (m, 2H), 6.87 (t, $J = 8.8$ Hz, 2H), 6.83-6.76 (m, 2H), 6.76-6.68 (m, 5H), 5.31 (d, $J = 5.6$ Hz, 1H), 4.75 (d, $J = 5.6$ Hz, 1H), 4.18-4.01 (m, 2H), 2.95-2.80 (m, 1H), 1.30-1.18 (m, 12H), 1.10 (d, $J = 6.4$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 162.2 (d, $J = 245.8$ Hz), 161.8 (d, $J = 246.1$ Hz), 153.0, 150.0, 139.7, 138.9, 133.9 (d, $J = 3.4$ Hz), 133.8, 132.0 (d, $J = 3.3$ Hz), 131.2 (d, $J = 7.8$ Hz), 130.9 (d, $J = 7.8$ Hz), 128.8, 128.3, 128.0, 127.6, 123.9, 115.8 (d, $J = 21.2$ Hz), 115.0 (d, $J = 21.3$ Hz), 64.5, 34.3, 30.0, 25.1, 24.7, 23.8, 23.7. HRMS (ESI) calcd. for $\text{C}_{36}\text{H}_{39}\text{F}_2\text{NNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 610.2562, Found 610.2571.



(E)-2,4,6-Triisopropyl-N-(1-phenyl-2,3-bis(4-(trifluoromethyl)phenyl)allyl)benzenesulfonamide (4i).

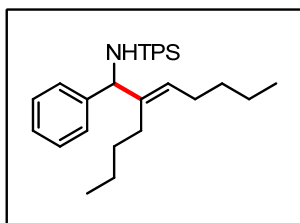
Purified by column (PE/EtOAc = 50:1 to 30:1), white solid (65% yield). m.p. 127-128 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.43 (d, $J = 8.0$ Hz, 2H), 7.31 (d, $J = 8.4$ Hz, 2H), 7.25-7.17 (m, 3H), 7.11 (s, 2H), 7.04-6.98 (m, 3H), 6.97 (s, 1H), 6.93-6.89 (m, 1H), 6.84 (d, $J = 8.0$ Hz, 2H), 5.33 (d, $J = 5.2$ Hz, 1H), 4.77 (d, $J = 5.2$ Hz, 1H), 4.18-4.03 (m, 2H), 2.94-2.80 (m, 1H), 1.26 (d, $J = 6.8$ Hz, 6H), 1.22 (dd, $J = 6.8, 2.8$ Hz, 6H), 1.09 (d, $J = 6.8$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.2, 150.0, 142.2, 141.9, 139.3, 138.2, 133.6, 131.3, 130.0 (q, $J = 32.4$ Hz), 129.7, 129.4, 129.1, 129.1 (q, $J = 32.2$ Hz), 128.6, 128.2, 127.6, 125.8 (q, $J = 3.3$ Hz), 125.0 (q, $J = 3.6$ Hz), 124.1 (q, $J = 270.3$ Hz), 124.0, 124.0 (q, $J = 270.5$ Hz), 64.3, 34.3, 30.0, 25.1, 24.6, 23.7, 23.6. HRMS (ESI) calcd. for $\text{C}_{38}\text{H}_{39}\text{F}_6\text{NNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 710.2498, Found 710.2491.



(E)-2,4,6-Triisopropyl-N-(1-phenyl-2-propylhex-2-en-1-yl)benzenesulfonamide (4j).

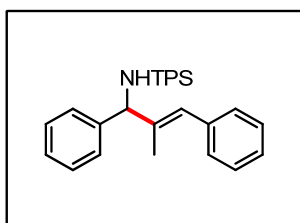
Purified by column (PE/EtOAc = 50:1 to 40:1), white solid (91% yield). m.p. 66-68 °C. ^1H

NMR (400 MHz, CDCl₃) δ 7.19-7.13 (m, 3H), 7.10 (s, 2H), 7.04-6.98 (m, 2H), 5.40 (t, J = 7.2 Hz, 1H), 4.90 (d, J = 6.0 Hz, 1H), 4.59 (d, J = 6.0 Hz, 1H), 4.11-3.95 (m, 2H), 2.86-2.82 (m, 1H), 2.01-1.84 (m, 3H), 1.74-1.61 (m, 1H), 1.33-1.18 (m, 4H), 1.25 (d, J = 6.8 Hz, 6H), 1.21 (d, J = 6.8 Hz, 6H), 1.15 (d, J = 6.8 Hz, 6H), 0.84 (t, J = 7.2 Hz, 3H), 0.77 (t, J = 7.2 Hz, 3H). **¹³C NMR** (100 MHz, CDCl₃) δ 152.6, 149.8, 140.4, 138.5, 134.0, 128.5, 128.4, 127.6, 127.4, 123.6, 61.9, 34.3, 31.3, 29.9, 29.8, 25.0, 24.8, 23.8, 23.7, 22.8, 21.9, 14.2, 14.0. **HRMS** (ESI) calcd. for C₃₀H₄₅NNaO₂S ([M+Na]⁺) 506.3063, Found 506.3069.



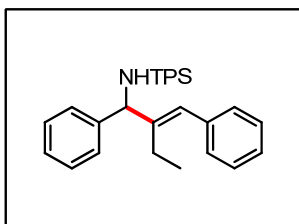
(E)-N-(2-Butyl-1-phenylhept-2-en-1-yl)-2,4,6-triisopropylbenzenesulfonamide (4k).

Purified by column (PE/EtOAc = 50:1 to 40:1), colorless semi-solid (84% yield). **¹H NMR** (400 MHz, CDCl₃) δ 7.19-7.13 (m, 3H), 7.10 (s, 2H), 7.03-6.97 (m, 2H), 5.38 (t, J = 7.2 Hz, 1H), 4.89 (d, J = 6.0 Hz, 1H), 4.58 (d, J = 6.0 Hz, 1H), 4.08-3.95 (m, 2H), 2.95-2.82 (m, 1H), 2.03-1.85 (m, 3H), 1.75-1.62 (m, 1H), 1.32-1.23 (m, 4H), 1.25 (d, J = 6.8 Hz, 6H), 1.20 (d, J = 6.8 Hz, 6H), 1.18-1.09 (m, 4H), 1.14 (d, J = 6.8 Hz, 6H), 0.86 (t, J = 6.8 Hz, 3H), 0.78 (t, J = 7.0 Hz, 3H). **¹³C NMR** (100 MHz, CDCl₃) δ 152.6, 149.8, 140.4, 138.5, 134.0, 128.4, 128.4, 127.5, 127.4, 123.6, 61.8, 34.2, 31.8, 30.9, 29.9, 28.9, 27.4, 25.0, 24.8, 23.8, 23.7, 22.9, 22.5, 14.0, 13.9. **HRMS** (ESI) calcd. for C₃₂H₄₉NNaO₂S ([M+Na]⁺) 534.3376, Found 534.3378.



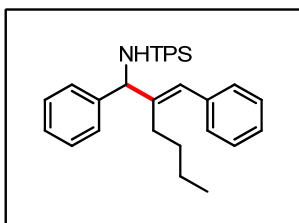
(E)-2,4,6-Triisopropyl-N-(2-methyl-1,3-diphenylallyl)benzenesulfonamide and (E)-N-(1,2-diphenylbut-2-en-1-yl)-2,4,6-triisopropylbenzenesulfonamide (8.1 : 1 mixture) (4l).

Purified by column (PE/EtOAc = 50:1 to 30:1), colorless semi-solid (67% yield). **¹H NMR** (400 MHz, CDCl₃) δ 7.29-7.23 (m, 4H), 7.23-7.16 (m, 4H), 7.14 (s, 2H), 6.96 (d, J = 6.8 Hz, 2H), 6.51 (s, 1H), 5.10 (d, J = 5.6 Hz, 1H), 4.76 (d, J = 5.6 Hz, 1H), 4.14-3.99 (m, 2H), 2.98-2.83 (m, 1H), 1.65 (d, J = 0.8 Hz, 3H), 1.30-1.22 (m, 12H), 1.14 (d, J = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 152.8, 150.0, 139.6, 137.1, 135.9, 134.1, 129.0, 128.9, 128.1, 127.6, 127.4, 126.7, 123.8, 64.6, 34.3, 30.1, 25.1, 24.8, 23.8, 23.8, 15.9. **HRMS** (ESI) calcd. for C₃₁H₃₉NNaO₂S ([M+Na]⁺) 512.2594, Found 512.2586.



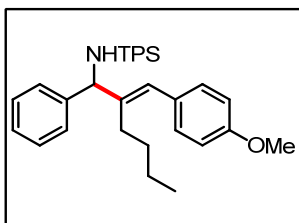
(E)-N-(2-Benzylidene-1-phenylbutyl)-2,4,6-triisopropylbenzenesulfonamide and (E)-N-(1,2-diphenylpent-2-en-1-yl)-2,4,6-triisopropylbenzenesulfonamide (20 : 1 mixture) (4m).

Purified by column (PE/EtOAc = 50:1 to 30:1), colorless semi-solid (67% yield). ^1H NMR (400 MHz, CDCl_3) δ 7.30-7.26 (m, 1H), 7.25-7.16 (m, 5H), 7.16-7.09 (m, 4H), 7.01 (d, J = 7.6 Hz, 2H), 6.54 (s, 1H), 5.18 (d, J = 5.6 Hz, 1H), 4.69 (d, J = 5.6 Hz, 1H), 4.15-3.98 (m, 2H), 2.98-2.83 (m, 1H), 2.38-2.24 (m, 1H), 1.99-1.84 (m, 1H), 1.31-1.22 (m, 12H), 1.12 (d, J = 6.8 Hz, 6H), 0.92 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.7, 149.8, 142.3, 139.9, 137.2, 134.3, 128.8, 128.7, 128.2, 128.1, 127.7, 127.1, 126.7, 123.8, 61.8, 34.3, 30.1, 25.1, 24.7, 23.8, 23.8, 22.9, 13.0. HRMS (ESI) calcd. for $\text{C}_{32}\text{H}_{41}\text{NNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 526.2750, Found 526.2755.



(E)-N-(2-Benzylidene-1-phenylhexyl)-2,4,6-triisopropylbenzenesulfonamide (4n).

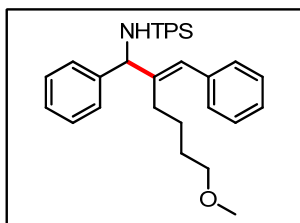
Purified by column (PE/EtOAc = 50:1 to 30:1), colorless semi-solid (70% yield). ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.26 (m, 1H), 7.25-7.16 (m, 5H), 7.16-7.09 (m, 4H), 7.02 (d, J = 7.2 Hz, 2H), 6.55 (s, 1H), 5.13 (d, J = 5.6 Hz, 1H), 4.69 (d, J = 6.0 Hz, 1H), 4.13-3.99 (m, 2H), 2.98-2.83 (m, 1H), 2.29-2.16 (m, 1H), 1.90-1.78 (m, 1H), 1.35-1.28 (m, 2H), 1.27 (d, J = 6.4 Hz, 6H), 1.25 (d, J = 6.4 Hz, 6H), 1.20-1.14 (m, 2H), 1.12 (d, J = 6.8 Hz, 6H), 0.76 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.7, 149.8, 141.4, 140.0, 137.3, 134.2, 128.8, 128.7, 128.1, 128.0, 127.6, 127.4, 126.6, 123.8, 62.0, 34.3, 30.4, 30.0, 29.6, 25.1, 24.7, 23.8, 23.8, 22.8, 13.8. HRMS (ESI) calcd. for $\text{C}_{34}\text{H}_{45}\text{NNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$) 554.3063, Found 554.3057.



(E)-2,4,6-Triisopropyl-N-(2-(4-methoxybenzylidene)-1-phenylhexyl)benzenesulfonamide (4o).

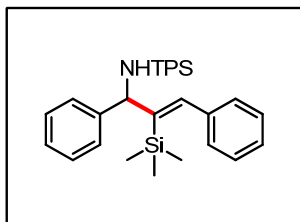
Purified by column (PE/EtOAc = 50:1 to 10:1), white solid (88% yield). m.p. 87-89 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.25-7.19 (m, 3H), 7.17-7.09 (m, 4H), 6.96 (d, J = 8.8 Hz, 2H),

6.80 (d, $J = 8.8$ Hz, 2H), 6.45 (s, 1H), 5.12 (d, $J = 5.6$ Hz, 1H), 4.68 (d, $J = 6.0$ Hz, 1H), 4.13-4.00 (m, 2H), 3.79 (s, 3H), 2.97-2.83 (m, 1H), 2.26-2.12 (m, 1H), 1.93-1.80 (m, 1H), 1.35-1.22 (m, 2H), 1.27 (d, $J = 6.8$ Hz, 6H), 1.24 (d, $J = 6.4$ Hz, 6H), 1.21-1.15 (m, 2H), 1.13 (d, $J = 6.4$ Hz, 6H), 0.77 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 158.3, 152.7, 149.9, 140.2, 139.9, 134.3, 129.9, 129.8, 128.7, 128.0, 127.6, 127.0, 123.8, 113.6, 62.2, 55.3, 34.3, 30.4, 30.0, 29.7, 25.1, 24.7, 23.8, 23.8, 22.9, 13.9. HRMS (ESI) calcd. for $\text{C}_{35}\text{H}_{47}\text{NNaO}_3\text{S}$ ($[\text{M}+\text{Na}]^+$) 584.3169, Found 584.3174.



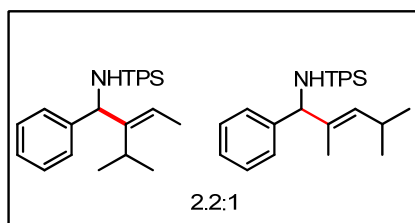
(E)-N-(2-Benzylidene-6-methoxy-1-phenylhexyl)-2,4,6-triisopropylbenzenesulfonamide (4p).

Purified by column (PE/EtOAc = 50:1 to 20:1), colorless semi-solid (50% yield). ^1H NMR (400 MHz, CDCl_3) δ 7.30-7.16 (m, 6H), 7.15-7.08 (m, 4H), 7.02 (d, $J = 7.6$ Hz, 2H), 6.57 (s, 1H), 5.14 (d, $J = 5.6$ Hz, 1H), 4.74 (d, $J = 6.0$ Hz, 1H), 4.13-3.98 (m, 2H), 3.25 (s, 3H), 3.20 (t, $J = 6.0$ Hz, 2H), 2.97-2.82 (m, 1H), 2.33-2.19 (m, 1H), 1.96-1.81 (m, 1H), 1.49-1.35 (m, 4H), 1.26 (d, $J = 6.8$ Hz, 6H), 1.24 (d, $J = 6.8$ Hz, 6H), 1.12 (d, $J = 6.4$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.8, 149.9, 141.1, 139.9, 137.3, 134.3, 128.8, 128.7, 128.2, 128.1, 127.8, 127.6, 126.7, 123.8, 72.2, 62.0, 58.6, 34.3, 30.0, 29.5, 29.4, 25.1, 24.7, 23.8, 23.8. HRMS (ESI) calcd. for $\text{C}_{35}\text{H}_{47}\text{NNaO}_3\text{S}$ ($[\text{M}+\text{Na}]^+$) 584.3169, Found 584.3170.



(Z)-N-(1,3-Diphenyl-2-(trimethylsilyl)allyl)-2,4,6-triisopropylbenzenesulfonamide (4q).

Purified by column (PE/EtOAc = 50:1 to 40:1), white solid (55% yield). m.p. 105-107 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.48 (s, 1H), 7.26-7.20 (m, 6H), 7.17 (s, 2H), 7.10-7.04 (m, 2H), 6.96-6.89 (m, 2H), 5.42 (d, $J = 6.4$ Hz, 1H), 4.58 (d, $J = 6.4$ Hz, 1H), 4.15-3.97 (m, 2H), 3.02-2.86 (m, 1H), 1.30 (dd, $J = 6.8, 1.6$ Hz, 6H), 1.27 (d, $J = 6.8$ Hz, 6H), 1.10 (d, $J = 6.8$ Hz, 6H), -0.29 (s, 9H). ^{13}C NMR (100 MHz, CDCl_3) δ 152.7, 149.7, 141.9, 141.8, 140.5, 139.7, 134.9, 128.9, 128.6, 128.5, 128.2, 127.9, 127.2, 123.9, 62.2, 34.4, 30.1, 25.1, 24.8, 23.9, 23.9, 0.4. HRMS (ESI) calcd. for $\text{C}_{33}\text{H}_{45}\text{NNaO}_2\text{SSi}$ ($[\text{M}+\text{Na}]^+$) 570.2832, Found 570.2837.



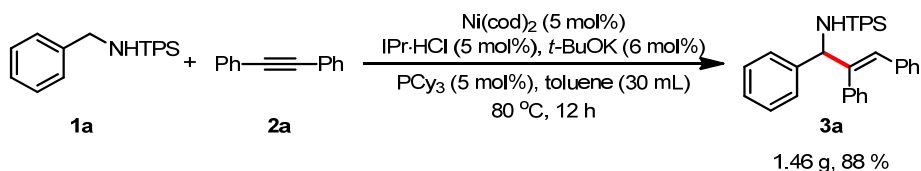
(E)-2,4,6-Triisopropyl-N-(2-isopropyl-1-phenylbut-2-en-1-yl)benzenesulfonamide

(E)-N-(2,4-dimethyl-1-phenylpent-2-en-1-yl)-2,4,6-triisopropylbenzenesulfonamide (2.2 : 1 mixture) (4r).

Purified by column (PE/EtOAc = 50:1 to 40:1), colorless oil (69% yield). ¹H NMR (400 MHz, CDCl₃) δ 7.23-7.18 (m, 1.38H), 7.15-7.09 (m, 4.92H), 7.08 (s, 2H), 7.01-6.94 (m, 1.92H), 5.46 (q, *J* = 6.8 Hz, 1H), 5.21 (d, *J* = 9.2 Hz, 0.46H), 5.05 (d, *J* = 5.6 Hz, 1H), 4.88 (d, *J* = 6.0 Hz, 0.46H), 4.64 (d, *J* = 6.4 Hz, 0.46H), 4.52 (d, *J* = 5.6 Hz, 1H), 4.10-3.93 (m, 2.92H), 2.96-2.81 (m, 1.46H), 2.76-2.62 (m, 1H), 2.47-2.34 (m, 0.46H), 1.60 (d, *J* = 6.8 Hz, 3H), 1.42 (s, 1.38H), 1.30-1.21 (m, 12H), 1.21-1.15 (m, 8.52H), 1.13 (d, *J* = 6.8 Hz, 6H), 1.02 (d, *J* = 7.2 Hz, 3H), 0.82 (d, *J* = 6.4 Hz, 1.38H), 0.78 (d, *J* = 7.2 Hz, 2.76H), 0.75 (d, *J* = 6.8 Hz, 1.38H). ¹³C NMR (100 MHz, CDCl₃) δ 152.6, 152.6, 149.9, 149.7, 144.3, 141.1, 140.0, 135.6, 134.4, 134.1, 130.8, 128.6, 128.4, 127.7, 127.5, 127.5, 127.3, 123.8, 123.6, 122.7, 63.9, 59.3, 34.3, 30.0, 30.0, 28.9, 27.0, 25.0, 24.9, 24.7, 23.8, 23.8, 22.8, 22.6, 21.5, 20.8, 13.9, 13.3. HRMS (ESI) calcd. for C₂₈H₄₁NNaO₂S ([M+Na]⁺) 478.2750, Found 478.2746.

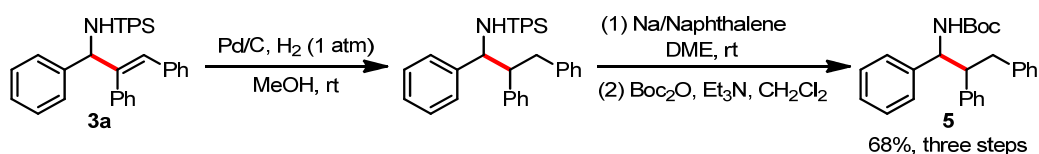
5. Gram-Scale Reaction and Product Transformation

5.1 Gram-Scale Reaction

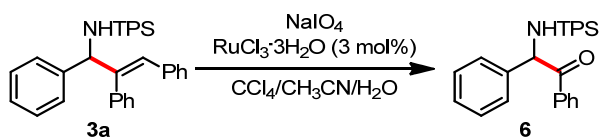


To a 48 mL pressure tube were added Ni(cod)₂ (41.3 mg, 0.15 mmol), IPr·HCl (63.8 mg, 0.15 mmol), PCy₃ (42.1 mg, 0.15 mmol), KO^tBu (20.2 mg, 0.18 mmol), toluene (30 mL), **1a** (3 mmol, 1.12 g) and **2a** (3.3 mmol, 588.2 mg) in a glove box. The tube was sealed with a Teflon cap and the mixture was stirred at 80 °C for 12 h. After cooled to room temperature, the crude product was filtered through a short pad of Celite, and the filtrate was concentrated under vacuum. The resulting residue was obtained by chromatography on silica gel column with petroleum ether/ethyl acetate as the eluent to afford pure product **3a** (88% yield, 1.46 g).

5.2 Transformation of Product 3a



The solution of compound **3a** (0.21 mmol) and Pd/C (contain 10% Pd) (5 mol%) in CH₃OH (5 mL) was stirred under 1 atm pressure of hydrogen at room temperature for 4 hours. The mixture was filtered through a short pad of Silica gel, and the filtrate was concentrated under vacuum to obtain a crude product, which was pure enough for next step without further purification. To a solution of the crude product in DME (2 mL), sodium-naphthalene (8 equiv) was added dropwise. The reaction was stirred at room temperature for 5 h then quenched with water. The aqueous and organic layers were separated and the aqueous layer was extracted using CH₂Cl₂. The combined organic layers were dried over anhydrous Na₂SO₄, filtered, and concentrated *in vacuo*. Then Boc₂O (59.6 mg, 1.3 equiv), Et₃N (88 μ L, 3 equiv) and CH₂Cl₂ (2 mL) were added and stirred for 12 h at room temperature. The mixture was washed with saturated NH₄Cl, dried over anhydrous Na₂SO₄ and concentrated *in vacuo*. The residue was purified by silica column chromatography with petroleum ether/ethyl acetate to give compound **5** in 68% yield (55 mg, three steps). White solid. m.p. 178-179 °C. **¹H NMR** (400 MHz, CDCl₃) δ 7.26 (s, 1H), 7.22-7.15 (m, 3H), 7.15-7.04 (m, 5H), 6.98 (d, *J* = 7.2 Hz, 4H), 6.88 (d, *J* = 7.6 Hz, 2H), 4.99 (s, 2H), 3.38-3.28 (m, 1H), 3.24 (d, *J* = 16.4 Hz, 1H), 2.93 (dd, *J* = 13.6, 10.4 Hz, 1H), 1.43 (s, 9H). **¹³C NMR** (100 MHz, CDCl₃) δ 155.4, 140.6, 140.1, 129.2, 129.1, 128.2, 128.1, 128.0, 127.5, 127.2, 126.6, 125.9, 79.7, 59.4, 53.5, 38.8, 28.5. **HRMS** (ESI) calcd. for C₂₆H₃₀NO₂ ([M+H]⁺) 388.2271, Found 388.2269. Note: For sodium-naphthalene preparation, a flame-dried 50 mL round bottom flask was charged with a stir bar, naphthalene (790 mg, 6.16 mmol), DME (6 mL), and small pieces of sodium metal (118 mg, 5.13 mmol). The mixture was allowed to vigorously stir overnight for approximately 12 h, resulting into a dark green solution.

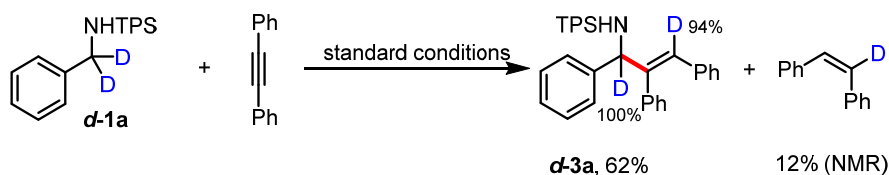


To a solution of **3a** (105 mg, 0.19 mmol) in a mixed solvent CCl₄/CH₃CN/H₂O (1:1:1.6, v/v/v, 1.1 mL) was added NaIO₄ (165 mg, 0.77 mmol), and the mixture was stirred for 5 min before the addition of RuCl₃·3H₂O (1.5 mg, 0.0056 mmol). The resulting brown mixture was stirred for 24 h and quenched with 1N HCl. The mixture was extracted with CH₂Cl₂ and the extract was concentrated. The residue was purified by silica column chromatography with petroleum ether/ethyl acetate to give product **6** in 90% yield (82 mg). White solid. m.p. 115-117 °C. **¹H NMR** (400 MHz, CDCl₃) δ 7.82 (d, *J* = 7.6 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.19-7.08 (m, 5H), 7.03 (s, 2H), 6.25 (d, *J* = 6.8 Hz, 1H), 6.04 (d, *J* = 7.2 Hz, 1H), 4.20-4.02 (m, 2H), 2.91-2.75 (m, 1H), 1.23 (d, *J* = 6.8 Hz, 6H), 1.20 (d, *J* = 7.2 Hz, 6H), 1.16 (d, *J* = 6.8 Hz, 6H). **¹³C NMR** (100 MHz, CDCl₃) δ 194.9, 152.9, 150.1, 136.2, 134.0, 133.2, 129.1, 128.8, 128.5, 128.1, 123.6, 61.3, 34.2, 29.9, 24.9, 24.9, 23.7, 23.7. **HRMS** (ESI) calcd. for C₂₉H₃₆NO₃S ([M+H]⁺) 478.2410, Found 478.2407.

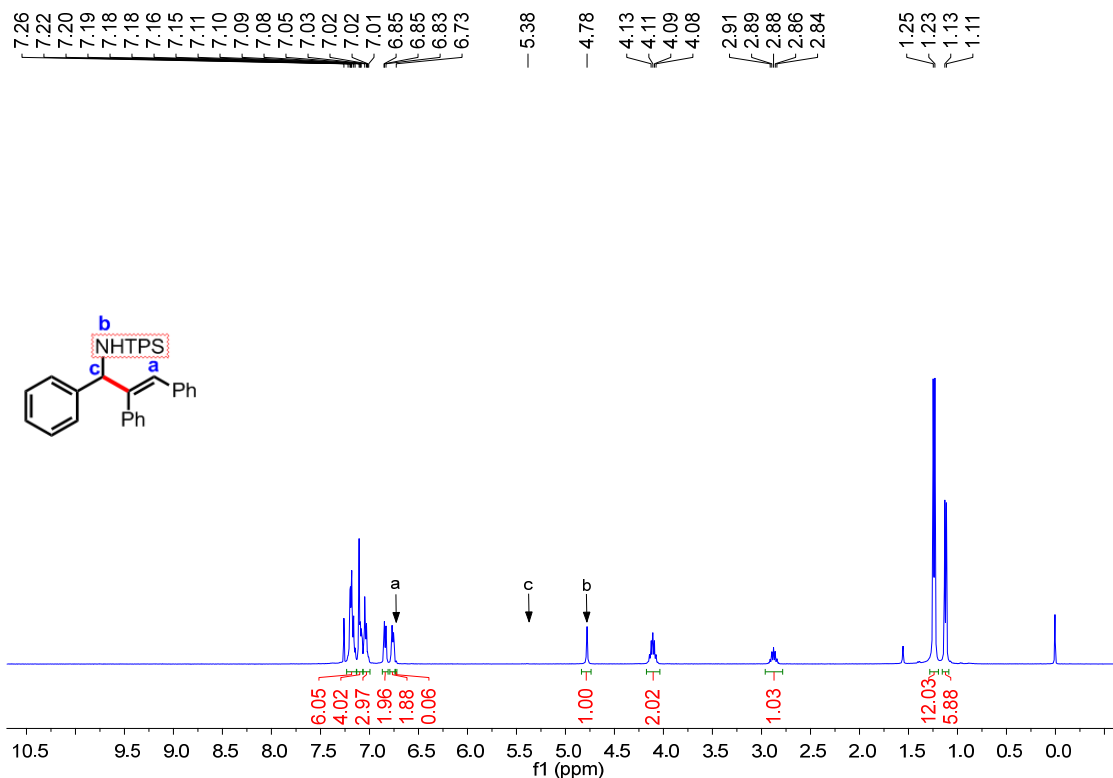
6. Mechanistic Experiments

6.1 Deuterium Labeling Experiments

Scheme S1. Deuterium Labeling Experiments

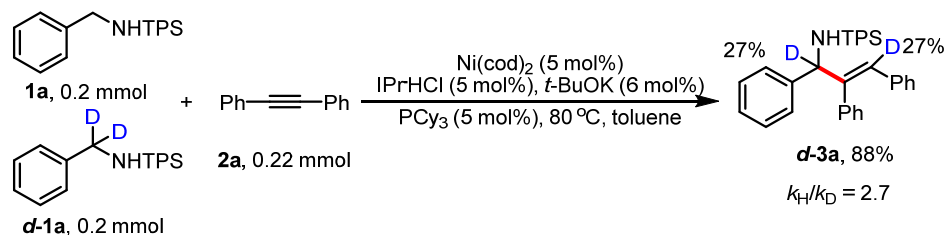


To a 15 mL pressure tube were added $\text{Ni}(\text{cod})_2$ (2.75 mg, 0.01 mmol), $\text{IPr}\cdot\text{HCl}$ (4.3 mg, 0.01 mmol), PCy_3 (2.8 mg, 0.01 mmol), KO^tBu (1.4 mg, 0.012 mmol), toluene (2 mL), **d-1a** (0.20 mmol, 75.1 mg) and **2a** (0.22 mmol, 39.2 mg) in a glove box. The tube was sealed with a Teflon cap and the mixture was stirred at 80 °C for 12 h. After cooled to room temperature, the crude product was filtered through a short pad of Celite, and the filtrate was concentrated under vacuum. The resulting residue was obtained by chromatography on silica gel column with petroleum ether/ethyl acetate as the eluent to afford pure product **d-3a** (62% yield, 68.1 mg).

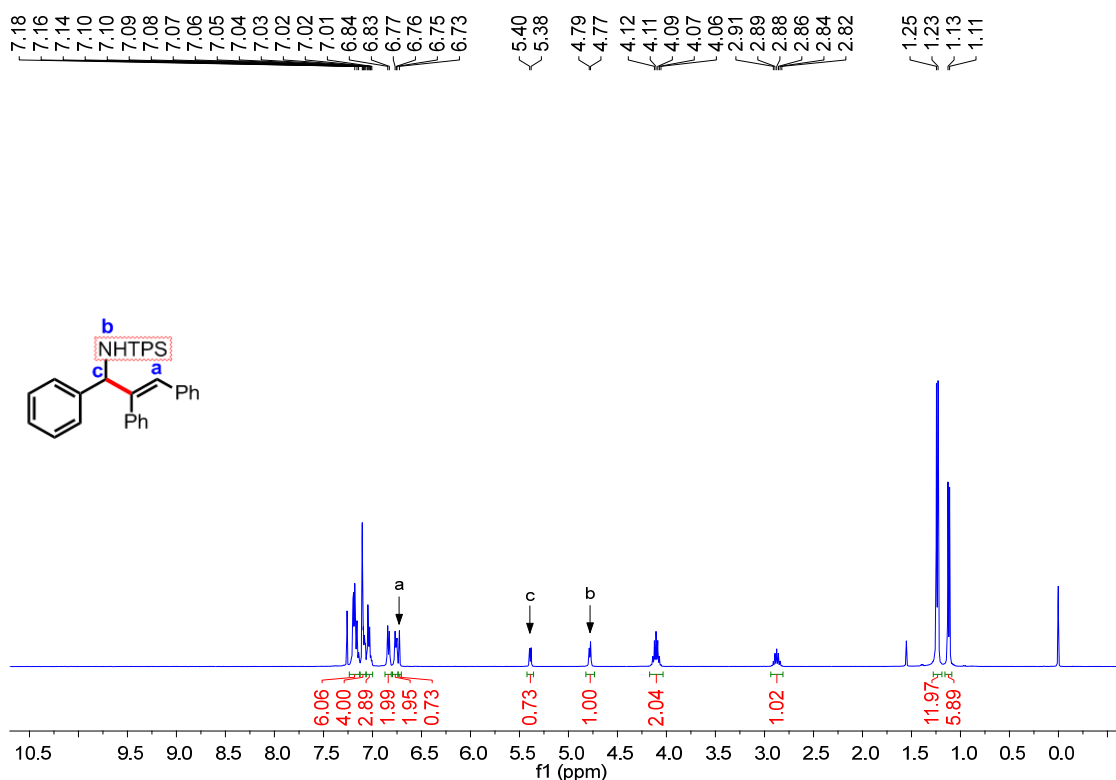


6.2 KIE Determination

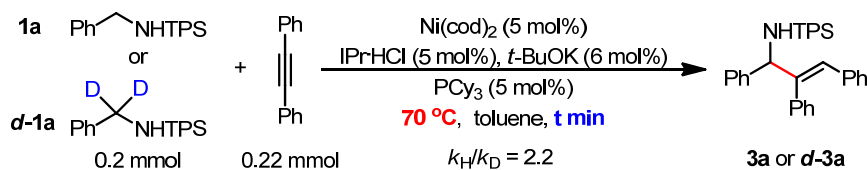
Scheme S2. Competitive Experiment



To a 15 mL pressure tube were added Ni(cod)_2 (2.75 mg, 0.01 mmol), $\text{IPr}\cdot\text{HCl}$ (4.3 mg, 0.01 mmol), PCy_3 (2.8 mg, 0.01 mmol), KO^tBu (1.4 mg, 0.012 mmol), toluene (2 mL), **d-1a** (0.20 mmol, 75.1 mg), **1a** (0.20 mmol, 74.7 mg) and **2a** (0.22 mmol, 39.2 mg) in a glove box. The tube was sealed with a Teflon cap and the mixture was stirred at 80°C for 12 h. After cooled to room temperature, the crude product was filtered through a short pad of Celite, and the filtrate was concentrated under vacuum. The resulting residue was obtained by chromatography on silica gel column with petroleum ether/ethyl acetate as the eluent to afford pure product **d-3a** (88% yield, 97.6 mg).

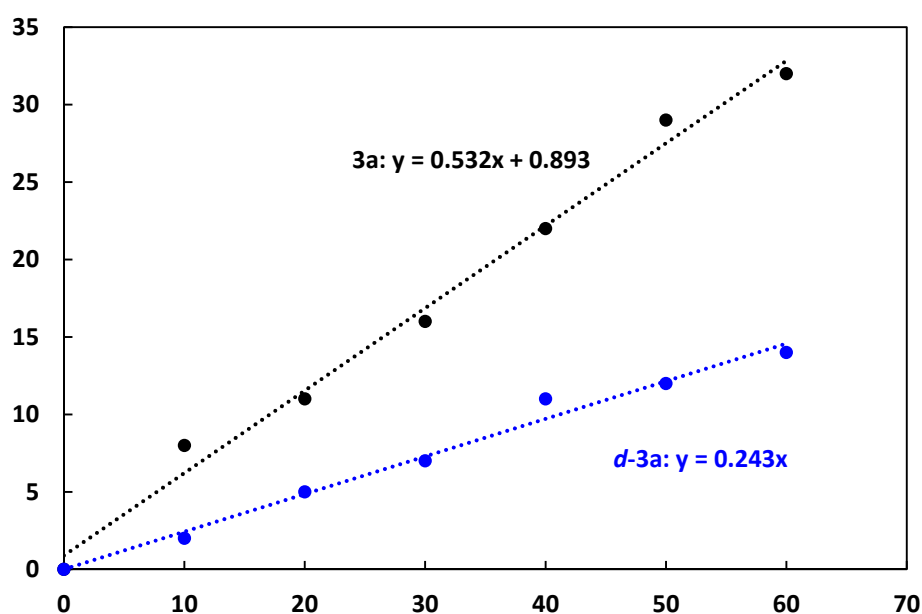


Scheme S3. Parallel Experiments



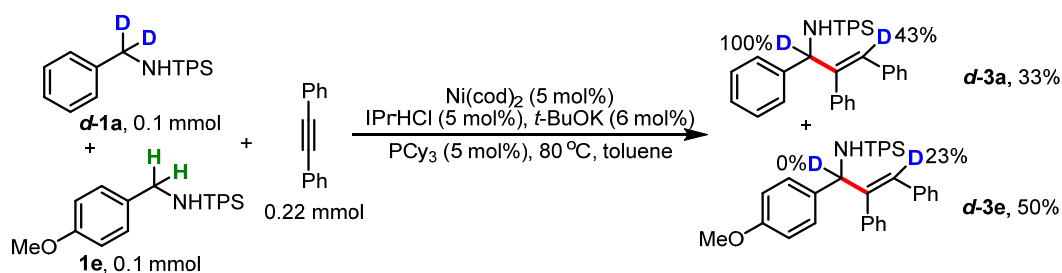
Six side-by-side reactions were conducted following the general procedure for the redox-neutral coupling of alkynes with **1a** (0.2 mmol) and **d-1a** (0.2 mmol), respectively. Aliquots were taken at 10 minute intervals in the first hour. Product yields were determined by ^1H NMR using $\text{Cl}_2\text{CHCHCl}_2$ as the internal standard. Data points represent the average of two runs.

time/min	0	10	20	30	40	50	60
yield of 3a /%	0	8	11	16	22	29	32
yield of d-3a /%	0	2	5	7	11	12	14

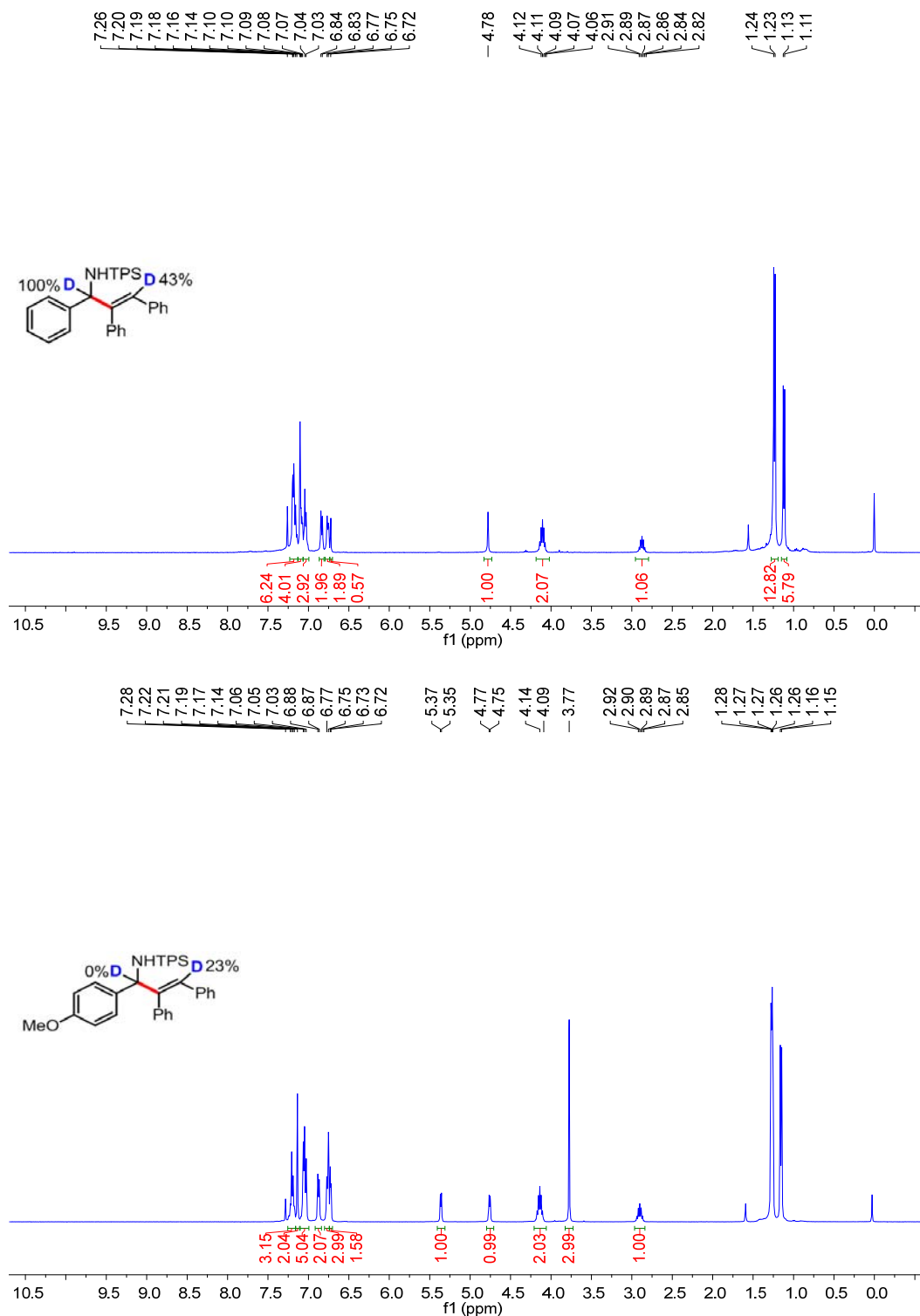


6.3 Competitive Experiments

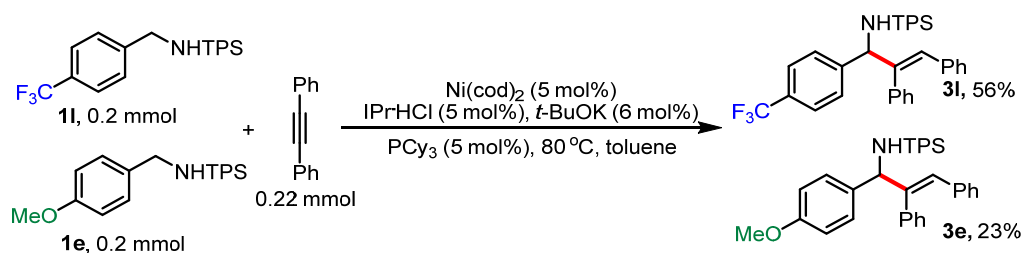
Scheme S4. Crossover Experiments



To a 15 mL pressure tube were added Ni(cod)₂ (2.75 mg, 0.01 mmol), IPr·HCl (4.3 mg, 0.01 mmol), PCy₃ (2.8 mg, 0.01 mmol), KO^tBu (1.4 mg, 0.012 mmol), toluene (2 mL), **d-1a** (0.1 mmol, 37.6 mg), **1e** (0.1 mmol, 40.4 mg) and **2a** (0.22 mmol, 39.2 mg) in a glove box. The tube was sealed with a Teflon cap and the mixture was stirred at 80 °C for 12 h. After cooled to room temperature, the crude product was filtered through a short pad of Celite, and the filtrate was concentrated under vacuum. The resulting residue was obtained by chromatography on silica gel column with petroleum ether/ethyl acetate as the eluent to afford pure product **d-3a** (33% yield, 36.6 mg) and **d-3e** (50% yield, 57.7 mg).



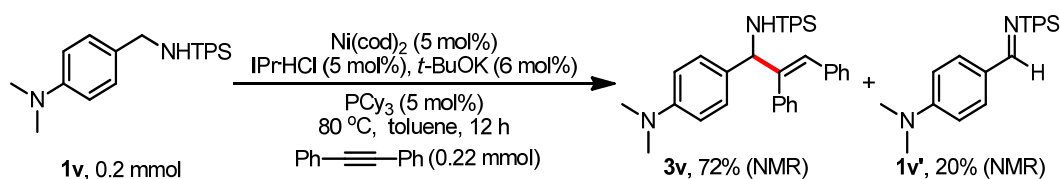
Scheme S5. Electronic Effect



To a 15 mL pressure tube were added $\text{Ni}(\text{cod})_2$ (2.75 mg, 0.01 mmol), $\text{IPr}\cdot\text{HCl}$ (4.3 mg, 0.01 mmol), PCy_3 (2.8 mg, 0.01 mmol), KO^tBu (1.4 mg, 0.012 mmol), toluene (2 mL), **1f** (0.20 mmol, 88.3 mg), **1e** (0.2 mmol, 80.7 mg) and **2a** (0.22 mmol, 39.2 mg) in a glove box. The tube was sealed with a Teflon cap and the mixture was stirred at 80 °C for 12 h. After cooled to room temperature, the crude product was filtered through a short pad of Celite, and the filtrate was concentrated under vacuum. The resulting residue was obtained by chromatography on silica gel column with petroleum ether/ethyl acetate as the eluent to afford pure product **3f** (56% yield, 69.7 mg) and **3e** (23% yield, 26.5 mg). This experiment suggested electron-deficient group on the amide had a positive effect to the reaction rate.

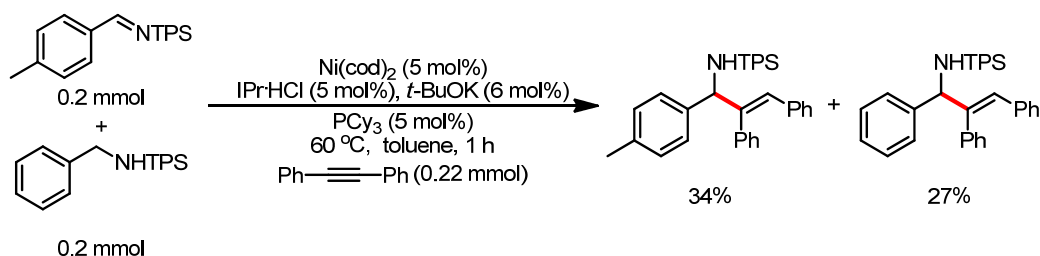
6.4 Role of Imine

Scheme S6. Detection of Imine



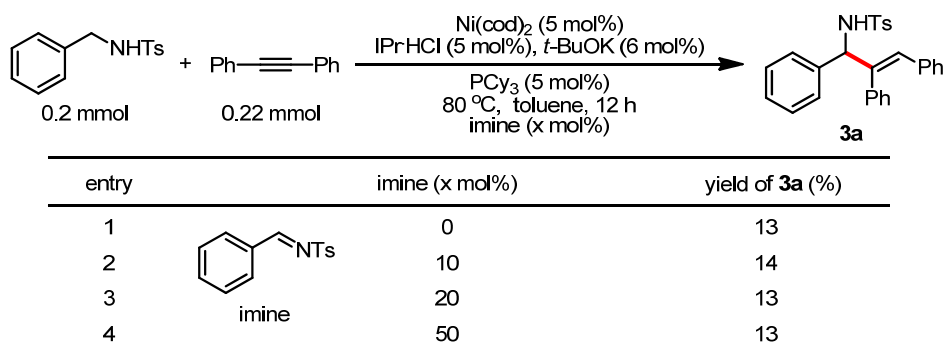
Under the standard conditions, the reaction of substrate **1v** with diphenylethyne gave the desired product **3v** along with small amounts of imine **1v'** that was confirmed by ^1H NMR using $\text{Cl}_2\text{CHCHCl}_2$ as the internal standard. In all other examined reactions, the crude NMR also showed the presence of imines, but which were trace amounts and cannot be isolated.

Scheme S7. Competitive Experiment of Imine and Amide



The reaction of 1:1 of the imine and the amide with alkyne was run for 1 h under the standard conditions but at 60 °C (hoping to achieve a lower conversion), and the crude product was detected by ^1H NMR using $\text{Cl}_2\text{CHCHCl}_2$ as the internal standard.

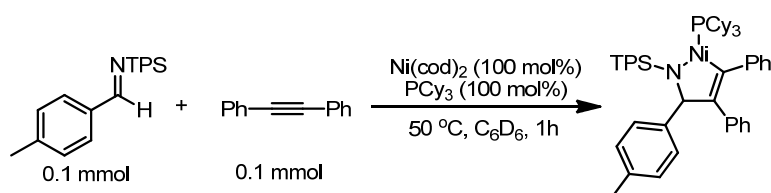
Scheme S8. Effects of Imine as Additive in Reaction of Ts-Protected Amide



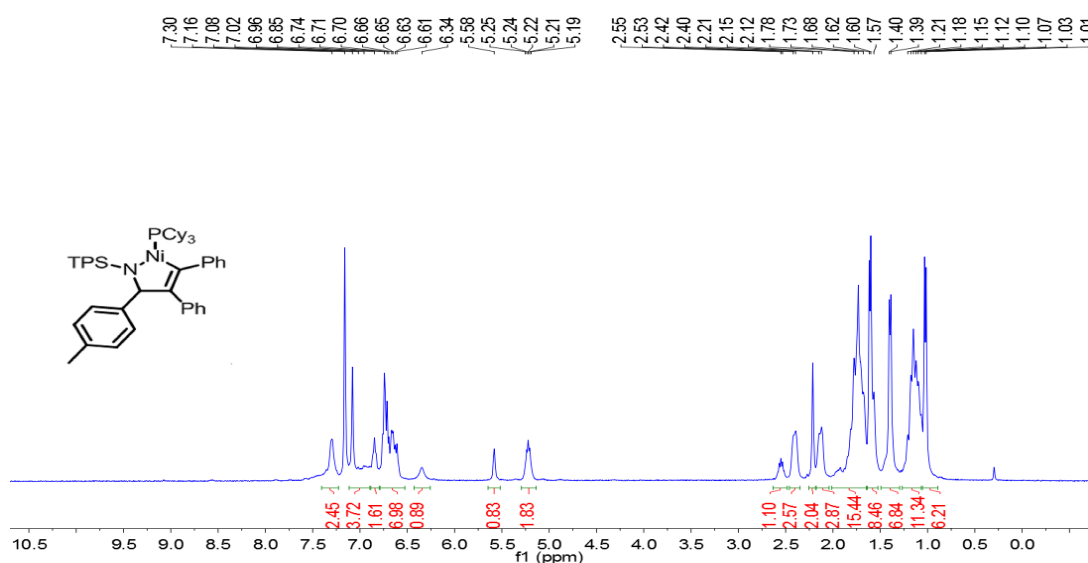
The reaction of Ts-amide and alkyne was selected to detect the effects of imine because the reaction in general gave low yields under the standard conditions. But whatever loading of imine, no acceleration was observed, suggesting the generation of the imine at the induction stage was not the rate-determining step.

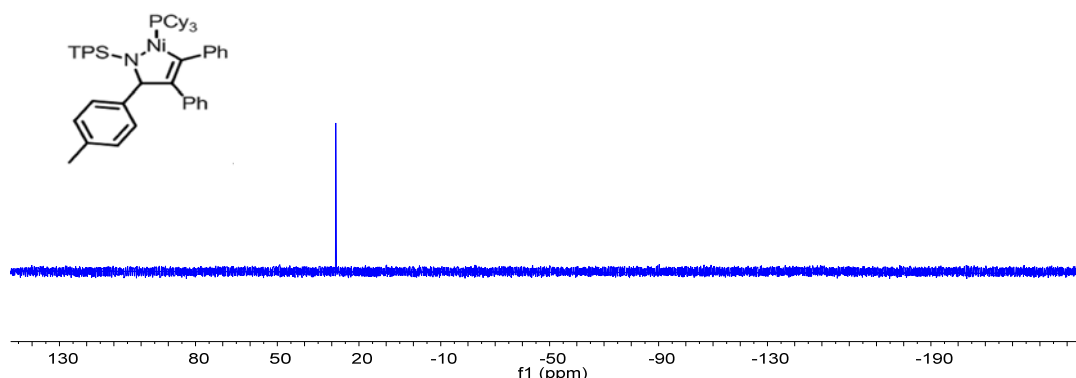
6.5 Reaction of Nickelacycle

Scheme S9. Preparation of Five-Membered Nickelacycle with PCy₃ as a Ligand

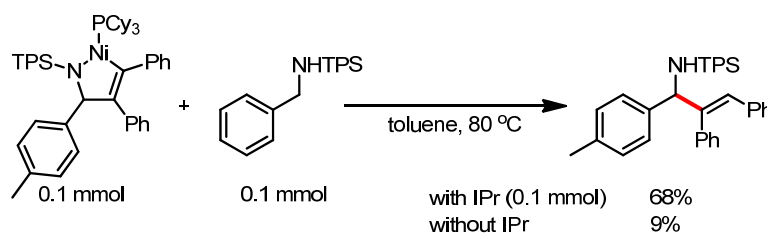


According to the literature,⁸ the nickelacycle was prepared from the imine and alkyne, and the corresponding spectrum of ¹H and ³¹P NMR was shown below.





Scheme S10. Reaction of Five-Membered Nickelacycle with Amide



The reaction of nickelacycle (0.1 mmol) was treated with amide (0.1 mmol) at 80 °C. With the IPr ligand, the desired product was obtained in 68% yield. While without the ligand, only 9% of product was afforded.

7. DFT Calculations

7.1 Computational Methods

All DFT calculations were carried out with Gaussian 09.⁹ Geometry optimizations were performed at the B3LYP-D3/LANL2DZ(Ni)-6-31G(d) level (pruned integration grids with 75 radial shells and 302 angular points per shell were used).^{10–13} Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and thermal corrections at 298 K. Quasiharmonic corrections were applied during the entropy calculations by setting all positive frequencies that are less than 100 cm⁻¹ to 100 cm⁻¹.¹⁴ On the basis of the optimized structures, single-point energies were computed at the SMD(toluene)/M06-D3/SDD(Ni)/6-311++G(d,p) level (pruned integration grids with 99 radial shells and 590 angular points per shell were used).^{11,13,15–17} All discussed energy differences were based on Gibbs energies at 298 K unless otherwise specified. Standard states are the hypothetical states at 1 mol/L.

7.2 Gibbs Energy Profiles of the Induction Stage and the Product-Formation Stage

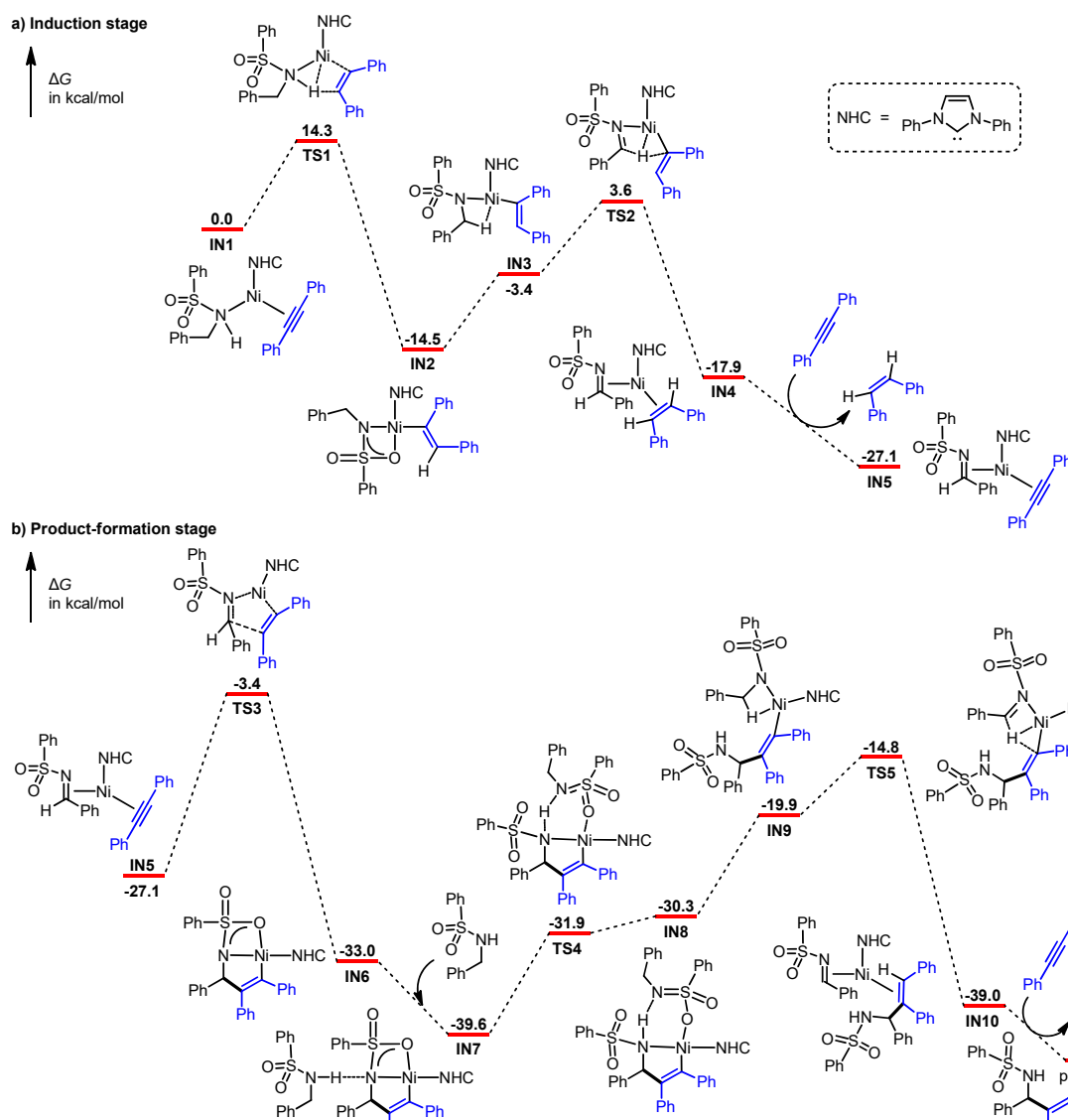


Figure S1. Gibbs energy profiles of (a) the induction stage and (b) the product-formation stage. Computed at the SMD(toluene)/M06-D3/SDD-6-311++G(d,p)//B3LYP-D3/LANL2DZ-6-31G(d) level.

7.3 Two Reaction Pathways of IN5

There are two reaction pathways of Ni-imine-alkyne complex **IN5** (Figure S2). One is the oxidative cyclometallation pathway via **TS3** with an activation Gibbs energy of 23.7 kcal/mol. In the other pathway, **IN5** may first undergo a ligand exchange with the amine substrate. Then, the resulting Ni-amine-alkyne complex **IN1** may proceed through a ligand-to-ligand hydrogen transfer (LLHT) via **TS1** with an overall activation Gibbs energy of 31.7 kcal/mol. Therefore, the oxidative cyclometallation pathway is favored over the ligand exchange/LLHT pathway by 8.0 kcal/mol. As a result, instead of triggering the transfer hydrogenation at the induction stage, **IN5** prefers to initiate a new catalytic cycle for C–C bond formation.

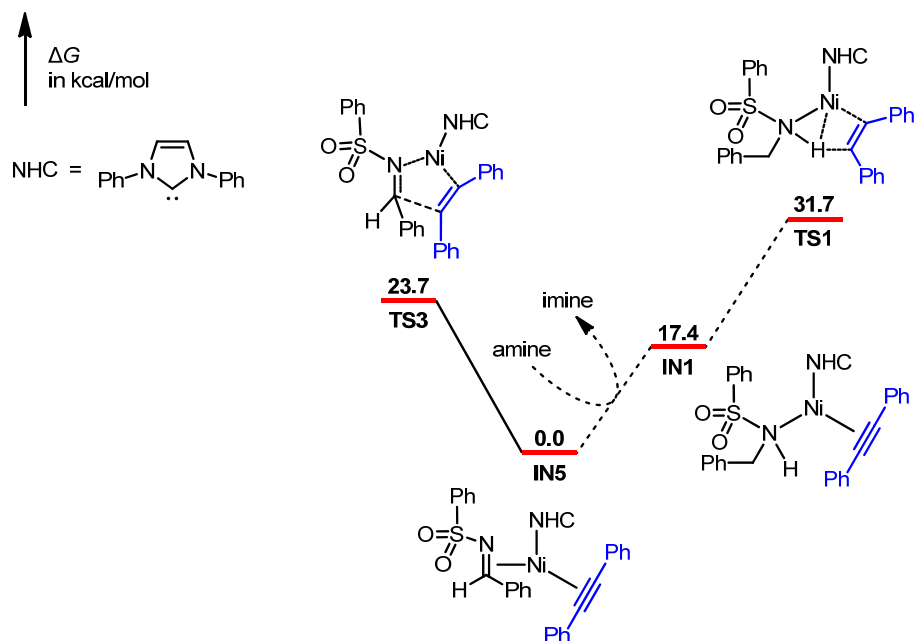


Figure S2. Two reaction pathways of **IN5**. Computed at the SMD(toluene)/M06-D3/SDD-6-311++G(d,p)//B3LYP-D3/LANL2DZ-6-31G(d) level.

7.4 Role of PCy₃

To verify whether the addition of PCy₃ could reduce the overall activation Gibbs energy of the [Ni(NHC)]-catalyzed reaction, we replaced the NHC ligand of the turnover-limiting transition state **TS5** by PCy₃ (Figure S3). DFT calculations indicated that the resulting transition state **TS5-PCy₃** is disfavored over **TS5** by 7.1 kcal/mol. Therefore, PCy₃ could not promote the reaction through accelerating the rate-determining step. Though the actual role of PCy₃ is unclear at the current stage, we proposed that it might act as an auxiliary ligand to facilitate the generation of the catalytic species and/or to inhibit catalyst deactivation.

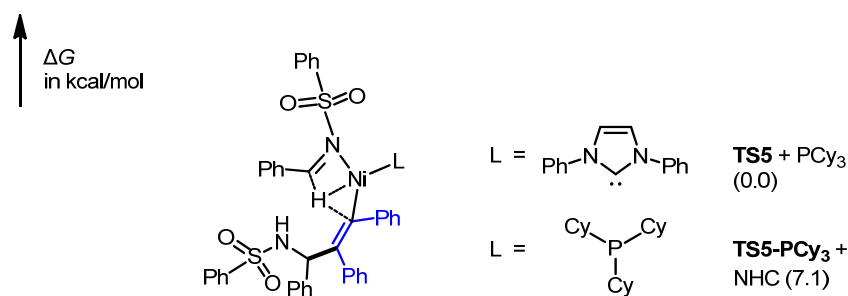


Figure S3. Relative Gibbs energies of **TS5** and **TS5-PCy₃**. Computed at the SMD(toluene)/M06-D3/SDD-6-311++G(d,p)//B3LYP-D3/LANL2DZ-6-31G(d) level.

7.5 Computed Energies of the Stationary Points

Table S7. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs)

	TCG ^{a,b} (a.u.)	SPE ^a (a.u.)	SPE ^c (a.u.)
amine	0.198617	-1106.547590	-1106.241427
imine	0.174178	-1105.329701	-1105.019825
alkyne	0.155379	-539.465171	-539.175397
alkene	0.179651	-540.711203	-540.412250
product	0.383361	-1646.067838	-1645.463652
NHC	0.194303	-688.279819	-687.942622
PCy ₃	0.443264	-1047.215295	-1046.804797
IN1	0.602488	-2503.734395	-2504.437950
IN2	0.603946	-2503.771352	-2504.462442
IN3	0.602064	-2503.751245	-2504.442866
IN4	0.604244	-2503.775136	-2504.468224
IN5	0.579541	-2502.535152	-2503.245552
IN6	0.583612	-2502.560698	-2503.259154
IN7	0.812147	-3609.160464	-3609.537905
IN7-IPr-TPS	1.636291	-4788.678666	-4788.346013
IN7-IPr-Ts	1.193794	-4159.611901	-4159.655958
IN8	0.809755	-3609.144983	-3609.520721
IN9	0.808521	-3609.115343	-3609.502855
IN10	0.812009	-3609.147657	-3609.536770
TS1	0.597775	-2503.710495	-2504.410496
TS2	0.597459	-2503.723919	-2504.427110
TS3	0.580994	-2502.504283	-2503.209243
TS4	0.806132	-3609.143437	-3609.519570
TS5	0.804075	-3609.097931	-3609.490404
TS5-IPr-TPS	1.629842	-4788.626571	-4788.303900
TS5-IPr-Ts	1.188424	-4159.555176	-4159.610960
TS5-PCy₃	1.055456	-3968.013894	-3968.343731

^aComputed at the B3LYP-D3/LANL2DZ-6-31G(d) level. ^bA standard state at 1 atm and 298 K was used. ^cComputed at the SMD(toluene)/M06-D3/SDD-6-311++G(d,p)//B3LYP-D3/LANL2DZ-6-31G(d) level.

7.5 Cartesian Coordinates of the Stationary Points

			amine	H	3.97195000	-1.36562700	2.58314300
S	-1.95641500	-0.56462600	0.29424400	H	4.00405900	-2.39923600	-1.59733900
O	-1.62981000	-1.25892200	1.54738800	O	1.44474400	1.94263100	-1.65660900
H	-2.16494400	-1.90473800	-1.45581100	N	-0.29693700	0.44448400	-0.55683800
C	-0.99013900	0.94191200	0.23405500	C	-1.28231700	0.76174500	0.20601000
C	-0.01522200	1.16877900	1.20318900	C	-2.57946800	0.08972400	0.11863200
C	-1.22944800	1.85033200	-0.79930500	C	-2.82057500	-0.92796600	-0.82242700
C	0.75271100	2.33120900	1.12324200	C	-3.60261700	0.47356300	1.00059600
H	0.14614400	0.43659600	1.98521100	C	-4.06403700	-1.54762900	-0.87235200
C	-0.45690200	3.00787900	-0.86679300	H	-2.02317200	-1.21263700	-1.50118600
H	-2.00614500	1.64854600	-1.52936600	C	-4.84856000	-0.14970300	0.94769400
C	0.53501300	3.24530300	0.09080100	H	-3.41664200	1.26201300	1.72606900
H	1.52536500	2.51586200	1.86352300	C	-5.07926400	-1.16036000	0.01179800
H	-0.62851900	3.72532400	-1.66417800	H	-4.24872200	-2.33289200	-1.59992500
O	-3.34416200	-0.25539400	-0.07000200	H	-5.63613400	0.15149400	1.63232300
N	-1.35789800	-1.44036800	-1.04074800	H	-6.04987300	-1.64701700	-0.03183800
C	-0.22877100	-2.35832600	-0.78029400	H	4.77817300	-2.80451700	0.72726000
H	-0.45139300	-3.04982600	0.04165500	H	-1.18426800	1.54902500	0.96353300
H	-0.11838100	-2.94866700	-1.69780900				
C	1.04924500	-1.60030300	-0.48906700			alkyne	
C	1.74333000	-1.81094000	0.70536000	C	0.60798400	0.00011700	-0.00013200
C	1.53231000	-0.65341700	-1.40178400	C	-0.60798300	0.00001400	-0.00023800
C	2.90965300	-1.09303300	0.98360600	C	-2.03186100	0.00001400	-0.00009800
H	1.35647000	-2.52360000	1.42895800	C	-2.74868300	1.21411300	-0.00007800
C	2.69013600	0.06935600	-1.12381100	C	-2.74865600	-1.21411200	-0.00000200
H	0.97506700	-0.46582500	-2.31537200	C	-4.14118700	1.20913000	0.00003700
C	3.38379200	-0.15056800	0.07057500	H	-2.20040700	2.15123800	-0.00015800
H	3.43910800	-1.26369500	1.91721300	C	-4.14115200	-1.20916400	0.00011100
H	3.04865100	0.80996400	-1.83349100	H	-2.20034500	-2.15121600	-0.00002300
H	4.28595000	0.41488300	0.28854000	C	-4.84253900	-0.00002200	0.00013500
H	1.13808600	4.14719400	0.03051200	H	-4.68173800	2.15183500	0.00005000
				H	-4.68168900	-2.15187800	0.00018200
				H	-5.92906600	-0.00004000	0.00022400
			imine	C	2.03186200	0.00006600	-0.00005100
S	1.13704000	1.37113200	-0.34322400	C	2.74872600	1.21413700	0.00002600
O	1.04647400	2.23414400	0.84729800	C	2.74861200	-1.21408900	-0.00004900
C	2.29613300	0.05230000	0.00182800	C	4.14123100	1.20910100	0.00010600
C	2.72361800	-0.15626500	1.31348500	H	2.20048700	2.15128300	0.00002500
C	2.74589600	-0.74020600	-1.05682400	C	4.14110700	-1.20919300	0.00003100
C	3.62357700	-1.19208400	1.56905800	H	2.20026500	-2.15117100	-0.00010900
H	2.36273900	0.49121200	2.10545700	C	4.84253900	-0.00007500	0.00010800
C	3.64186900	-1.77365800	-0.78662200	H	4.68181500	2.15178800	0.00016700
H	2.40579200	-0.53636100	-2.06655800	H	4.68161100	-2.15192500	0.00003300
C	4.07779200	-1.99932100	0.52295500				

H	5.92906600	-0.00013500	0.00017100	H	1.70770000	-2.23668300	3.98260000
		alkene		H	2.83461900	-3.92309100	2.53891200
C	0.67447800	1.86818700	-0.00462100	S	1.99101600	1.76762900	-1.11979900
C	-0.67446800	1.86820900	0.00453700	C	3.42770100	0.75858300	-0.77416500
C	-1.62322500	0.74111800	0.07821700	C	3.98173800	0.00265100	-1.80853200
C	-1.36547900	-0.42180900	0.82783600	C	3.90835700	0.68418300	0.53295500
C	-2.86681600	0.85056800	-0.56915000	C	5.03883500	-0.85815200	-1.51741900
C	-2.30527300	-1.44732000	0.89835900	H	3.58845800	0.09596100	-2.81546200
H	-0.42424800	-0.51253700	1.35951700	C	4.96165900	-0.18672200	0.81219200
C	-3.80548400	-0.17902300	-0.50474500	H	3.45594900	1.29017900	1.30975500
H	-3.09195300	1.75165200	-1.13533600	C	5.52130000	-0.95810800	-0.20860400
C	-3.52705400	-1.33476600	0.22747300	H	5.48516100	-1.45167400	-2.31018300
H	-2.08694900	-2.33530900	1.48591600	H	5.33912900	-0.26627400	1.82717500
H	-4.75593600	-0.07587300	-1.02180500	O	1.99716800	2.17088700	-2.53012500
H	-4.25852900	-2.13638400	0.28436300	O	1.87791300	2.76367700	-0.04364100
C	1.62321800	0.74108500	-0.07825800	N	0.74081500	0.63215500	-1.00118700
C	1.36541600	-0.42195200	-0.82769400	H	0.02406400	0.86359900	-1.68463600
C	2.86687100	0.85063300	0.56897200	H	-1.02848800	-1.83438300	-0.49148300
C	2.30521100	-1.44746200	-0.89815900	C	-2.12700700	1.23476600	0.69737800
H	0.42414400	-0.51276200	-1.35928600	C	-1.74176000	2.56572600	0.45335000
C	3.80554400	-0.17896000	0.50462700	C	-3.28646800	1.00409000	1.45987300
H	3.09206100	1.75179700	1.13500900	C	-2.51223700	3.62836200	0.92664300
C	3.52705500	-1.33480700	-0.22739900	H	-0.83156600	2.77891800	-0.09963500
H	2.08684400	-2.33553400	-1.48557500	C	-4.05108400	2.06639100	1.93571300
H	4.75604200	-0.07572400	1.02158500	H	-3.58040700	-0.01752100	1.67795700
H	4.25852800	-2.13643100	-0.28424600	C	-3.67139000	3.38423300	1.66505400
H	1.15228700	2.84743300	0.03396300	H	-2.19944900	4.64824900	0.72025400
H	-1.15225300	2.84746500	-0.03406700	H	-4.94111500	1.86524300	2.52612800
		product		H	-4.26803000	4.21274300	2.03708200
C	-1.76465700	-1.05006000	-0.31923900	C	-3.13196100	-1.41620400	-0.72684700
C	-1.29846200	0.09726500	0.22150300	C	-4.05126100	-0.48901000	-1.25250600
C	0.22082100	0.28378300	0.34544600	C	-3.51972100	-2.76601800	-0.64936600
H	0.39277000	1.13070900	1.01746900	C	-5.32015100	-0.89629400	-1.65605000
C	0.95265700	-0.91666900	0.93048800	H	-3.76241400	0.55206000	-1.34809900
C	1.58173000	-1.87133600	0.12525900	C	-4.79386300	-3.17230000	-1.04438200
C	1.00296800	-1.06191600	2.32240500	H	-2.81297300	-3.49816900	-0.26536100
C	2.25590800	-2.94922100	0.70208700	C	-5.70101800	-2.23747200	-1.54704700
H	1.57228100	-1.74134300	-0.95136700	H	-6.01349400	-0.16513800	-2.06326100
C	1.67198600	-2.14027500	2.90061000	H	-5.07534400	-4.21903900	-0.96538300
H	0.51866400	-0.32052800	2.95454900	H	-6.69250500	-2.55148100	-1.86191600
C	2.30391500	-3.08760800	2.09015600	H	6.33891700	-1.63796900	0.01453000
H	2.75424900	-3.67404700	0.06387700			NHC	
				C	0.00001100	0.33823700	-0.09138900

C	-0.67596100	-1.79010800	0.50242600	C	-2.10471900	-1.72420000	-1.17667400
C	0.67593600	-1.79010800	0.50249700	C	-2.69174600	-3.12483200	-0.93350000
H	-1.37446900	-2.56710400	0.76940200	C	-2.84919100	-3.41025900	0.56720800
H	1.37442600	-2.56711200	0.76948400	C	-1.51051400	-3.24600100	1.30072100
N	1.06606900	-0.49616700	0.13963300	C	-0.90243800	-1.85137000	1.06738700
N	-1.06607600	-0.49616300	0.13962200	H	-0.17967700	1.51837500	1.00167600
C	-2.41870900	-0.06654700	0.01158700	H	-2.66352000	1.36300300	-0.78212800
C	-3.42745600	-0.97952100	-0.31287800	H	-2.45617700	0.51094500	0.74294200
C	-2.73296100	1.28238100	0.21443700	H	-3.78867200	2.56780200	1.07834800
C	-4.74986600	-0.54461200	-0.41655100	H	-2.27414900	2.64465000	1.97613100
H	-3.18283200	-2.01838900	-0.51077400	H	-2.84558900	4.00383200	-0.71157600
C	-4.05414500	1.70748600	0.09642900	H	-2.67461600	4.81746300	0.84358400
H	-1.93023400	1.97148300	0.44943800	H	-0.56118200	4.95024100	-0.53425500
C	-5.06998000	0.79795000	-0.21223900	H	-0.29606400	4.10356100	0.98910500
H	-5.52757200	-1.25981000	-0.67018000	H	-0.77857700	2.76843900	-1.73333400
H	-4.29168900	2.75595900	0.25465000	H	0.76902100	2.89377100	-0.92284600
H	-6.09953100	1.13404300	-0.29671600	H	1.51165300	-0.32638900	1.07324400
C	2.41871100	-0.06654800	0.01163300	H	2.84092700	1.33001500	-1.12551400
C	2.73293500	1.28239700	0.21437400	H	2.13110600	1.94912100	0.36417400
C	3.42749100	-0.97953900	-0.31270300	H	4.59939100	1.80289900	0.55445200
C	4.05412500	1.70750900	0.09639400	H	3.79678400	0.77013600	1.73589700
H	1.93019100	1.97151200	0.44927700	H	5.02227900	-0.16533400	-0.91452200
C	4.74989500	-0.54462300	-0.41635500	H	5.68697000	-0.46445300	0.69159200
H	3.18290000	-2.01843000	-0.51051500	H	4.40557900	-2.45833500	-0.16060600
C	5.06998400	0.79796700	-0.21214300	H	3.67955400	-1.80091700	1.30483200
H	4.29163500	2.75600200	0.25453900	H	2.72555000	-1.29610000	-1.56741800
H	5.52762700	-1.25982600	-0.66988600	H	1.93857200	-2.31600200	-0.36673600
H	6.09953600	1.13405800	-0.29660800	H	-0.09220300	-2.31333200	-0.85494200
PCy ₃				H	-2.83009900	-0.97762700	-0.83428400
P	0.13802000	0.04146000	-0.96189900	H	-1.96290500	-1.55247200	-2.25090100
C	-0.64242300	1.48581900	0.00295200	H	-3.65817700	-3.22042700	-1.44523500
C	-2.17121800	1.41567100	0.19990500	H	-2.02431200	-3.87937600	-1.37609700
C	-2.69969400	2.64452800	0.96146500	H	-3.58248800	-2.70870700	0.99287700
C	-2.32783100	3.95643500	0.25789500	H	-3.25008300	-4.41953700	0.72610700
C	-0.81394700	4.03730200	0.02044600	H	-1.63717700	-3.42445500	2.37662100
C	-0.30638800	2.80282800	-0.74088000	H	-0.80585100	-4.00863200	0.93647100
C	1.75689900	-0.17000700	0.01184600	H	-1.54031200	-1.09835000	1.54751000
C	2.64850700	1.08730600	-0.07002600	H	0.07216400	-1.79548700	1.56507900
C	3.98892100	0.89671000	0.65990600	IN1			
C	4.74874200	-0.32919900	0.13844900	Ni	0.52540800	0.06746000	-0.09964600
C	3.87606800	-1.58599200	0.24381600	C	0.51188200	-1.44874100	1.05873500
C	2.53632900	-1.40556900	-0.48935400	S	-2.07825200	0.10497200	-2.03633400
C	-0.76002600	-1.54420400	-0.43685500	O	-1.42229500	-1.07310300	-2.60912200

C	1.69107000	-0.93695300	0.97933300	H	-0.25083200	-2.00508800	3.60730400
C	-3.83873600	-0.23284100	-1.94866700	C	-2.66069700	-4.02121300	2.27788500
C	-4.25512500	-1.48139500	-1.47573000	H	-2.92470200	-4.39303900	0.16779000
C	-4.75040000	0.76616300	-2.29078100	H	-2.13079100	-3.46498100	4.29397000
C	-5.62059100	-1.72720300	-1.34524900	H	-3.48837300	-4.65671900	2.58136800
H	-3.52636000	-2.24041100	-1.20965400	H	-7.61167700	-0.93809000	-1.59028200
C	-6.11587900	0.50154300	-2.16537600	C	1.68011100	1.23859700	-1.07866900
H	-4.38640000	1.72265600	-2.65048300	C	3.65752800	1.79445000	-2.11158000
C	-6.54850500	-0.73912700	-1.69159400	C	3.17531100	2.92597400	-1.54708200
H	-5.95983300	-2.69039300	-0.97555100	H	4.53807200	1.61957600	-2.70893100
H	-6.83922300	1.26577600	-2.43442700	H	3.54282100	3.94001100	-1.54925500
O	-1.88820700	1.45195800	-2.58168700	N	1.96725000	2.57631400	-0.94165700
N	-1.58915900	0.15892300	-0.38018600	N	2.74052700	0.78429300	-1.83614400
C	-2.28992300	1.22316000	0.41192100	C	1.14319500	3.49314200	-0.22678200
H	-1.88953300	2.17376700	0.06948200	C	1.63239900	4.11046500	0.92694500
H	-1.81724200	-0.76277800	0.01227600	C	-0.14222800	3.77029000	-0.69713500
C	-2.05029700	1.02436800	1.88625100	C	0.82167600	5.00887200	1.62290200
C	-2.98735000	0.33683600	2.66402900	H	2.63026700	3.86654500	1.27952400
C	-0.87879500	1.50532700	2.48461300	C	-0.94584700	4.66911200	0.00668500
C	-2.76447200	0.13579300	4.02740400	H	-0.50198600	3.26394400	-1.58733800
H	-3.89273600	-0.04833800	2.19912000	C	-0.46876200	5.28698300	1.16588600
C	-0.65219000	1.30007400	3.84439300	H	1.19477400	5.48164500	2.52694900
H	-0.14238700	2.02018100	1.87593500	H	-1.94857500	4.88403800	-0.35265900
C	-1.59570500	0.61796900	4.61869300	H	-1.10070800	5.98167100	1.71181500
H	-3.49645600	-0.40436400	4.62133800	C	2.93793600	-0.58592000	-2.18709200
H	0.26288100	1.67008400	4.29857200	C	1.86490300	-1.33267200	-2.67818200
H	-1.41772300	0.46037700	5.67937200	C	4.19250300	-1.17123800	-2.00286800
C	3.10743300	-1.05902300	1.24792500	C	2.05486100	-2.67992600	-2.98131300
C	3.94740200	0.06838100	1.17779400	H	0.89396000	-0.86955300	-2.80034500
C	3.69276000	-2.31020600	1.52574200	C	4.37383300	-2.51766600	-2.31949900
C	5.32258100	-0.04945300	1.37123100	H	4.99730300	-0.59671500	-1.55665200
H	3.49923000	1.03125200	0.95184200	C	3.30703100	-3.27559500	-2.80699000
C	5.06857800	-2.42822300	1.70813200	H	1.21595900	-3.26032900	-3.35486900
H	3.05214800	-3.18634500	1.57253000	H	5.34456900	-2.97706200	-2.15642600
C	5.89210000	-1.29979200	1.63028300	H	3.44911000	-4.32682000	-3.04296500
H	5.95336100	0.83478100	1.31217800	H	-3.36740100	1.20025000	0.20472100
H	5.50318500	-3.40461100	1.90927500				
H	6.96563900	-1.39469400	1.77232800			IN2	
C	-0.50345200	-2.36515300	1.49917400	Ni	-0.04385700	0.08048400	-0.31997200
C	-1.29064200	-3.04145400	0.53530000	C	2.55758900	-1.05679300	-0.72629500
C	-0.82754300	-2.54057400	2.86027200	S	-1.91219300	0.51296100	-2.12565200
C	-2.34758100	-3.86554300	0.92485400	O	-0.70900600	-0.42230900	-2.18567300
H	-1.03850800	-2.91883600	-0.51629300	C	1.31208500	-1.24829700	-0.25153800
C	-1.89329200	-3.35314800	3.23858300	C	-3.34615900	-0.56577800	-1.98881000

C	-4.24142900	-0.68311800	-3.05162200	H	7.06609800	-2.02213900	-1.13743900
C	-3.51437300	-1.29371200	-0.80784400	H	4.34308100	-5.33881000	-1.44325300
C	-5.32512900	-1.55611200	-2.92862900	H	6.67517100	-4.46525900	-1.43473900
H	-4.08550400	-0.09449600	-3.94936900	H	-6.34631300	-2.97330300	-1.66654600
C	-4.59725500	-2.16273700	-0.69749900	C	0.39402000	0.75537200	1.36664500
H	-2.81163800	-1.17028100	0.00775500	C	1.35844000	1.95602700	3.04431800
C	-5.50121500	-2.29599400	-1.75686600	C	0.20263800	1.44574500	3.53114800
H	-6.03108300	-1.65645100	-3.74837700	H	2.10436700	2.59295400	3.49157300
H	-4.73502600	-2.72856700	0.21941800	H	-0.25686500	1.51119500	4.50438200
O	-2.16559800	1.40389700	-3.27048100	N	-0.37482900	0.71039400	2.49662000
N	-1.63290600	1.18443300	-0.71140500	N	1.46167300	1.52499000	1.72459300
C	-2.28116900	2.42947500	-0.31222600	C	-1.62427500	0.01861200	2.62910300
H	-3.10858800	2.66824600	-0.99320600	C	-1.67046200	-1.36685500	2.47921700
H	2.83053300	-0.04591400	-1.01846100	C	-2.77458200	0.74686000	2.94288800
C	-1.28847500	3.57402800	-0.29682000	C	-2.89229300	-2.02653200	2.62086000
C	-0.75644300	4.05309000	0.90350500	H	-0.76556200	-1.91437200	2.25437100
C	-0.83068800	4.11369800	-1.50793500	C	-3.99075100	0.07818100	3.08613200
C	0.21562000	5.05780300	0.90243300	H	-2.71448200	1.82495100	3.05825600
H	-1.08937700	3.62515600	1.84674800	C	-4.05182700	-1.30815600	2.92070400
C	0.13068000	5.12401400	-1.51142000	H	-2.92171300	-3.10367200	2.48951200
H	-1.21920800	3.71372700	-2.44140800	H	-4.88953100	0.64184500	3.31851100
C	0.65832800	5.59834800	-0.30525700	H	-5.00136400	-1.82501400	3.02749200
H	0.62838800	5.41242100	1.84357500	C	2.52679800	1.90670200	0.84890100
H	0.47556600	5.53805600	-2.45549100	C	2.22916200	2.45752700	-0.39752000
H	1.41541600	6.37782200	-0.30970000	C	3.84698400	1.72055000	1.26070800
C	0.77511900	-2.50713600	0.29944000	C	3.27529800	2.80593300	-1.25085100
C	-0.38076000	-3.09857700	-0.24954800	H	1.19741600	2.60219900	-0.69085400
C	1.33325600	-3.09010200	1.45472400	C	4.88644500	2.08648400	0.40486500
C	-0.95846200	-4.22268400	0.34023100	H	4.05352400	1.26246900	2.22333600
H	-0.82206400	-2.65118300	-1.13453200	C	4.60227800	2.62305300	-0.85398500
C	0.75160700	-4.21257900	2.04503100	H	3.04526600	3.22792500	-2.22439900
H	2.22958000	-2.64769600	1.88069800	H	5.91597100	1.93360700	0.71535600
C	-0.40131300	-4.78266800	1.49444000	H	5.41328900	2.89552400	-1.52325900
H	-1.85268200	-4.65697800	-0.10087100	H	-2.71455100	2.29321900	0.68529400
H	1.19751200	-4.64337500	2.93839200				
H	-0.85486300	-5.65580600	1.95640400				
C	3.64881700	-2.03358600	-0.92538400	Ni	-0.28930700	-0.20886500	-0.22259000
C	4.97335700	-1.55504900	-0.95256700	C	-2.01093400	0.52878400	-0.43795100
C	3.44699700	-3.41422500	-1.11630100	S	2.17872700	-2.07786200	-0.21725000
C	6.05342000	-2.41890400	-1.12698800	O	1.69432900	-3.06906800	-1.20882400
H	5.14642100	-0.48861300	-0.82757000	C	-3.01250800	-0.16953900	-1.01593900
C	4.52657900	-4.27740900	-1.29417200	C	3.93508700	-1.84956900	-0.54950000
H	2.43724700	-3.80752700	-1.13759000	C	4.64592000	-2.87709400	-1.17130000
C	5.83619700	-3.78853500	-1.29418000	C	4.56336000	-0.66271300	-0.16204600

IN3

C	6.01314200	-2.71428500	-1.40186200	H	-2.01510300	5.51067400	1.60517600
H	4.12295900	-3.77654400	-1.47881800	H	7.71653500	-1.40748700	-1.20632100
C	5.92849900	-0.50878700	-0.40263800	C	-0.61545200	-0.76852000	1.50191100
H	3.98113000	0.13221700	0.28992800	C	-1.28355000	-1.91178800	3.33954900
C	6.65359000	-1.53325800	-1.01801500	C	-0.43333600	-0.94074500	3.75177600
H	6.57572000	-3.50646200	-1.88830700	H	-1.80190100	-2.68800400	3.87887200
H	6.42313400	0.41607700	-0.11842200	H	-0.06722400	-0.67679800	4.73082200
O	2.00054400	-2.41051400	1.21144600	N	-0.03945100	-0.24392400	2.61290400
N	1.56386300	-0.58274600	-0.43306300	N	-1.38655400	-1.79139300	1.95454300
C	1.49917900	-0.07229000	-1.79996400	C	0.92513600	0.82294900	2.60454800
H	1.74874800	-0.82099900	-2.56198700	C	0.48843200	2.14477400	2.54277100
H	0.40868900	0.16572700	-2.03252100	C	2.28256900	0.50033100	2.64427600
C	2.27337100	1.21778600	-1.98476700	C	1.43703100	3.17023300	2.53277300
C	2.94946300	1.48698100	-3.17718800	H	-0.57156900	2.36343600	2.48366700
C	2.29961400	2.16463500	-0.95250400	C	3.21935700	1.53363400	2.64235300
C	3.64447700	2.68869300	-3.34018200	H	2.57740900	-0.54321300	2.62482000
H	2.94273300	0.75076600	-3.97807900	C	2.79891600	2.86662000	2.58903800
C	2.99089800	3.36393100	-1.11441900	H	1.10194400	4.20101900	2.47037800
H	1.79173400	1.94432300	-0.02015300	H	4.27904000	1.29526700	2.66507100
C	3.66559200	3.63054700	-2.30990100	H	3.53439100	3.66649700	2.57981700
H	4.17370600	2.88426300	-4.26914600	C	-2.15815800	-2.65779200	1.11812600
H	3.00483600	4.08541100	-0.30163300	C	-1.54213500	-3.30610800	0.04550400
H	4.20741700	4.56432500	-2.43599600	C	-3.51820200	-2.82379200	1.38240400
C	-4.35480300	0.27327000	-1.43967700	C	-2.31745300	-4.11425400	-0.78705500
C	-5.35148900	-0.70636300	-1.61669100	H	-0.48070400	-3.18084800	-0.13708400
C	-4.69708000	1.61501000	-1.69853800	C	-4.27849500	-3.64939600	0.55375700
C	-6.64531200	-0.36074100	-2.00284600	H	-3.97620400	-2.28535000	2.20668800
H	-5.09892300	-1.74836600	-1.43603700	C	-3.68112700	-4.28928600	-0.53597000
C	-5.98946900	1.95916100	-2.08906200	H	-1.84447500	-4.61369900	-1.62737600
H	-3.94277700	2.38741900	-1.60274200	H	-5.33959500	-3.77504200	0.74864200
C	-6.97280800	0.97655900	-2.23803300	H	-4.27733600	-4.92322600	-1.18629900
H	-7.39768300	-1.13630900	-2.12513300	H	-2.82941300	-1.22691600	-1.20150700
H	-6.22890600	3.00127200	-2.28600600				
H	-7.97941500	1.24989200	-2.54360700			IN4	
C	-2.07441200	1.91484200	0.06325700	Ni	0.02223700	-0.09638500	-0.30841600
C	-1.18764000	2.89680300	-0.41777400	C	-1.32892300	1.44607500	-1.53060200
C	-2.94093100	2.26607200	1.11725600	S	2.32434900	-1.91765500	0.48978500
C	-1.16865000	4.18030100	0.12748500	O	1.81605100	-3.07353900	-0.28201800
H	-0.49885600	2.63951300	-1.21794800	C	-1.54440800	0.19319500	-2.05378000
C	-2.91892900	3.54789500	1.66616000	C	4.11089300	-1.88152000	0.28466100
H	-3.63262000	1.51772500	1.49416400	C	4.75911300	-3.00371300	-0.22942700
C	-2.03131200	4.51264800	1.17542600	C	4.82117800	-0.74092200	0.66954400
H	-0.47043600	4.91669900	-0.26245400	C	6.15010400	-2.98396900	-0.35501600
H	-3.59670800	3.79703600	2.47911000	H	4.17371000	-3.86655300	-0.52855300

C	6.20828800	-0.73096200	0.53601300	C	-0.86752400	-0.04817800	1.43366300
H	4.28582100	0.12544700	1.04326500	C	-2.28326200	-0.30521100	3.21026000
C	6.87263200	-1.85188700	0.02696000	C	-1.57099200	0.82636300	3.42463100
H	6.66705200	-3.85170200	-0.75540900	H	-3.02267600	-0.80867100	3.81202600
H	6.77198400	0.15191700	0.82482100	H	-1.57197600	1.52885800	4.24269600
O	2.01901700	-1.86197700	1.93224000	N	-0.70706800	0.95746000	2.34291100
N	1.88858100	-0.44574400	-0.13889000	N	-1.83591700	-0.83245700	1.99847900
C	1.59937800	-0.34306000	-1.49095100	C	0.29121800	1.97926500	2.23429000
H	1.53577500	-1.25279700	-2.09497000	C	-0.09672800	3.31147800	2.09940500
H	-0.45492300	1.95860200	-1.92678000	C	1.63769200	1.61085100	2.28124200
C	1.89563100	0.91265400	-2.19532500	C	0.88614600	4.29775700	1.99978800
C	1.67653000	1.00372200	-3.58246400	H	-1.15071200	3.56058300	2.04538100
C	2.28215400	2.07835800	-1.50235500	C	2.60966500	2.60687200	2.18467200
C	1.81109000	2.22116300	-4.25052700	H	1.89816700	0.56131600	2.36589800
H	1.39065300	0.11075800	-4.13517600	C	2.23798100	3.94743900	2.04159100
C	2.41449900	3.29085800	-2.17266300	H	0.59245200	5.33690400	1.88085800
H	2.44299700	2.01829900	-0.43219300	H	3.66087600	2.33372000	2.21987100
C	2.17473400	3.37405800	-3.54966900	H	3.00106700	4.71716100	1.96322900
H	1.63260400	2.26876300	-5.32196800	C	-2.25482800	-2.10506200	1.49985200
H	2.70201200	4.17882300	-1.61437500	C	-1.28763700	-3.03101200	1.10503500
H	2.27640200	4.32282400	-4.06968600	C	-3.61320800	-2.42765800	1.47686100
C	-2.72534500	-0.69384300	-2.00992800	C	-1.69144200	-4.29780900	0.68625000
C	-2.52132600	-2.08297500	-2.08327800	H	-0.23922000	-2.76986900	1.15592700
C	-4.04291300	-0.20629900	-2.03229300	C	-4.00384000	-3.70487200	1.07502000
C	-3.60065300	-2.95807100	-2.16809700	H	-4.35232200	-1.68280100	1.75747100
H	-1.50537900	-2.46765700	-2.05526500	C	-3.04511100	-4.64284300	0.68404700
C	-5.12316200	-1.08444700	-2.11171600	H	-0.93492900	-5.01358100	0.37854200
H	-4.21703000	0.86430600	-2.01017200	H	-5.05955100	-3.95895900	1.05122800
C	-4.90667200	-2.46252600	-2.18102000	H	-3.35465900	-5.63611300	0.37030000
H	-3.42192800	-4.02770600	-2.21069600	H	-0.78933600	-0.13305300	-2.76687400
H	-6.13555300	-0.68924100	-2.13585200				
H	-5.74936000	-3.14559400	-2.24825500			IN5	
C	-2.16357200	2.30789200	-0.67245100	S	1.83670900	-0.69846900	-1.77014700
C	-1.96749900	3.69769000	-0.76935100	O	1.55943200	-2.14456200	-1.77295600
C	-3.11061400	1.83492400	0.25474000	O	1.21886300	0.13910900	-2.82487100
C	-2.71476500	4.58737200	0.00214800	Ni	-0.34183200	0.06204800	0.17885800
H	-1.21542200	4.07701900	-1.45676100	C	-1.50232000	1.67632900	0.28805400
C	-3.84086800	2.72120900	1.04161900	C	1.29587100	1.20986500	-0.08027600
H	-3.25769100	0.76802900	0.36493700	C	1.74332900	1.89347600	1.14691600
C	-3.65439900	4.10268700	0.91461900	C	1.66422400	3.29355800	1.23919200
H	-2.55241900	5.65716800	-0.09941800	C	2.25807900	1.17084300	2.23717600
H	-4.55632300	2.33156800	1.76069900	C	2.05818500	3.94893500	2.40536800
H	-4.23182200	4.79146900	1.52544400	H	1.28886300	3.86740500	0.39760500
H	7.95432800	-1.83891600	-0.07637500	C	2.65370700	1.82929000	3.39784400

H	2.34591200	0.09493200	2.15162500	C	6.36266600	-0.13345400	-2.01447600
C	2.54837800	3.22137900	3.49242200	H	6.44076600	-1.22224300	-0.15140400
H	1.98278000	5.03191400	2.46168800	H	5.98140300	0.92710600	-3.85400600
H	3.05141300	1.25478400	4.23142100	H	7.43983500	-0.00140100	-2.07108400
H	2.85657400	3.73407000	4.40001000	C	0.89689600	-2.80892500	1.49531400
H	1.18312600	1.83016700	-0.96941800	C	0.74891200	-2.12341300	2.70063300
C	-2.10404800	0.66773200	0.75829700	C	2.10296100	-3.42775600	1.16192900
N	1.54167600	-0.13385100	-0.22181500	C	1.82155100	-2.06777200	3.59150000
C	-3.34138100	0.04891900	1.18196400	H	-0.18765700	-1.62137100	2.91868600
C	-4.56352300	0.67676200	0.87150600	C	3.16878600	-3.36976100	2.06043700
C	-3.37014100	-1.17895200	1.86352900	H	2.20545900	-3.89632800	0.18933900
C	-5.77373900	0.08275100	1.21826600	C	3.03029300	-2.69258100	3.27582600
H	-4.54526100	1.62105200	0.33578300	H	1.71241700	-1.52654500	4.52683300
C	-4.58327600	-1.77082400	2.21173800	H	4.11242500	-3.84357800	1.80397000
H	-2.43283200	-1.66985200	2.10096800	H	3.86395100	-2.64630700	3.97089400
C	-5.78995200	-1.14616900	1.88586800	C	-2.63484200	-1.61309800	-1.64454300
H	-6.70783000	0.57529200	0.96076100	C	-2.13665700	-0.63177300	-2.50390500
H	-4.58643600	-2.72228400	2.73740500	C	-4.00414500	-1.86891100	-1.55542600
H	-6.73553300	-1.61047400	2.15305300	C	-3.03445300	0.11374500	-3.26813800
C	-1.34940800	3.06519000	-0.05817900	H	-1.06820300	-0.45596200	-2.56839800
C	-0.93000200	3.43512100	-1.35036400	C	-4.89036000	-1.12634800	-2.33504600
C	-1.58775900	4.07036700	0.89654900	H	-4.36902200	-2.60288400	-0.84408500
C	-0.75228500	4.77797200	-1.67492700	C	-4.40800200	-0.13056300	-3.18758100
H	-0.73497700	2.65531100	-2.08106800	H	-2.65309700	0.88304700	-3.93358200
C	-1.40079100	5.41212400	0.56728100	H	-5.95769800	-1.31075200	-2.25501800
H	-1.89534600	3.78356200	1.89730100	H	-5.10070600	0.45431500	-3.78657900
C	-0.98026200	5.77108100	-0.71601800				
H	-0.42684400	5.05117000	-2.67522100			IN6	
H	-1.57582300	6.17874900	1.31755400	S	-1.95766100	0.69062600	-1.94551800
H	-0.82971800	6.81729500	-0.96815100	O	-1.04869200	1.90866600	-1.95694600
C	-0.80798700	-1.80932500	0.01407300	O	-2.26070200	0.03909400	-3.23053600
C	-0.71559100	-4.08423500	0.09503700	Ni	0.33006900	0.78492100	-0.52108100
C	-1.69094300	-3.75228500	-0.78350400	C	0.07745900	-1.88274100	0.11214900
H	-0.34660600	-5.04120100	0.42761100	C	-1.21501500	-1.62259000	-0.65837000
H	-2.33756000	-4.35792500	-1.39783400	C	-2.49624700	-2.05479400	0.04141400
N	-1.73416300	-2.36101200	-0.82127500	C	-3.58594800	-2.49927300	-0.71259800
N	-0.19797900	-2.88689000	0.58199800	C	-2.64684600	-1.88905300	1.42377200
C	3.61544700	-0.46326700	-1.86461500	C	-4.81135500	-2.77163800	-0.09901800
C	4.42096900	-0.99427300	-0.85281600	H	-3.47855900	-2.61097600	-1.78935200
C	4.15811900	0.22841000	-2.94595600	C	-3.86618400	-2.16482700	2.03971600
C	5.80145200	-0.82245100	-0.93378300	H	-1.80045600	-1.53994200	2.00881400
H	3.96674400	-1.51311300	-0.01524700	C	-4.95417900	-2.60506500	1.27892100
C	5.54402700	0.38966400	-3.01719100	H	-5.65240500	-3.11097800	-0.69822100
H	3.49843500	0.63184500	-3.70668000	H	-3.96997700	-2.03784800	3.11459800

H	-5.90574800	-2.81796100	1.75929600	C	0.88254100	3.23612300	1.61815900
H	-1.16808200	-2.11797600	-1.64015600	C	1.15423000	3.39045400	2.97956500
C	0.91700400	-0.82837900	0.29079400	C	-0.41963500	3.37160800	1.12491700
N	-1.21559100	-0.17410400	-0.82942400	C	0.10927700	3.68332000	3.85743700
C	2.24070800	-0.89871400	0.93813100	H	2.16671700	3.25184700	3.34721300
C	3.26167000	-1.71266100	0.41819200	C	-1.45818100	3.64452600	2.01556100
C	2.53463600	-0.09929200	2.05930000	H	-0.61776200	3.26249100	0.06291200
C	4.52955400	-1.72973200	1.00021500	C	-1.19758500	3.80379800	3.37918800
H	3.04862400	-2.32634200	-0.45148300	H	0.31697800	3.79932500	4.91727800
C	3.80105000	-0.11517200	2.63990600	H	-2.47095100	3.73195100	1.63330000
H	1.75333000	0.53935700	2.46288200	H	-2.00968800	4.02076400	4.06726800
C	4.80823700	-0.92984100	2.11102900	C	3.41541300	0.98421800	-1.86326100
H	5.30408000	-2.36655200	0.57950000	C	2.50795300	0.75202900	-2.90096300
H	4.00436200	0.50748200	3.50831000	C	4.65140100	0.33648800	-1.82931700
H	5.79711500	-0.94193200	2.56213400	C	2.84440200	-0.15589600	-3.90514000
C	0.29963000	-3.26295900	0.61690000	H	1.55355800	1.26924100	-2.91718800
C	-0.03881400	-4.37512300	-0.17489200	C	4.98459800	-0.55281700	-2.85076600
C	0.81191500	-3.50347400	1.90442600	H	5.31574400	0.48662400	-0.98466100
C	0.14837200	-5.67572100	0.29229000	C	4.08145900	-0.80500100	-3.88603900
H	-0.44666000	-4.22170000	-1.16974700	H	2.13656900	-0.34626000	-4.70634900
C	0.99899100	-4.80247700	2.37239300	H	5.94170800	-1.06571300	-2.82215300
H	1.05906800	-2.65978200	2.53998300	H	4.33952300	-1.50733400	-4.67354300
C	0.67086900	-5.89677200	1.56800000				
H	-0.11673200	-6.51778500	-0.34219200			IN7	
H	1.39507200	-4.96035700	3.37247800	Ni	1.32179400	-0.03092100	-1.08307300
H	0.81409500	-6.91000100	1.93426000	C	1.54499200	-0.68169300	0.68484500
C	1.84050000	1.90688500	-0.21231400	S	-2.02669100	2.48585000	-0.80098000
C	3.21950500	3.44931400	0.73527400	O	-3.24234000	3.22241700	-1.17284200
C	3.92530300	2.81187700	-0.23078900	C	0.68277100	-1.68808100	0.97647000
H	3.48619500	4.26159500	1.39210100	C	-0.24322100	-2.15966300	-0.14171300
H	4.93275700	2.95620500	-0.58611300	H	0.27514500	-2.97550000	-0.66519200
N	3.06442900	1.88290400	-0.80863500	C	-1.60832300	-2.67639200	0.27640600
N	1.94218600	2.89560000	0.72293300	C	-2.13931400	-3.81119400	-0.34836200
C	-3.52584000	1.22037000	-1.24549800	C	-2.37002200	-2.02262000	1.25135000
C	-3.63469400	1.36524600	0.14010100	C	-3.41304900	-4.27749600	-0.01392200
C	-4.60207500	1.48462800	-2.09282900	H	-1.55190400	-4.31939100	-1.10970700
C	-4.84714800	1.79055500	0.68149600	C	-3.63891700	-2.48797200	1.59517600
H	-2.78989300	1.11489000	0.77172200	H	-1.96793800	-1.14178700	1.74131200
C	-5.80959800	1.91398100	-1.53932000	C	-4.16528100	-3.61580500	0.95921600
H	-4.49129500	1.33703300	-3.16195200	H	-3.81409800	-5.15806500	-0.50983200
C	-5.93173300	2.06818100	-0.15617700	H	-4.21850300	-1.95965700	2.34600100
H	-4.94901300	1.88937300	1.75881200	H	-5.15550700	-3.97735200	1.22406300
H	-6.65665300	2.11936200	-2.18797000	S	-0.44121100	-1.28963000	-2.67982700
H	-6.87659700	2.39366500	0.27079000	C	-2.08833600	-0.84953600	-3.22723100

C	-2.34913400	0.45487400	-3.64715900	C	0.49652800	-2.41573500	4.69864000
C	-3.09666700	-1.81430600	-3.14661100	H	0.53262200	-0.64172600	3.47449300
C	-3.65955800	0.80287400	-3.97888700	C	0.51691600	-3.81285800	4.71466100
H	-1.54815000	1.18148800	-3.67713200	H	0.60003200	-5.60098400	3.51003100
C	-4.39970800	-1.45374000	-3.48757600	H	0.43169700	-1.86078200	5.63111300
H	-2.86290500	-2.81995500	-2.81798000	H	0.47073400	-4.35033200	5.65812800
C	-4.68111800	-0.14692100	-3.89862600	C	2.64078900	-0.23422000	1.57056800
H	-3.87961500	1.82127500	-4.28380000	C	3.50274300	-1.15293900	2.20150700
H	-5.19415100	-2.19211400	-3.42702900	C	2.89524000	1.13489200	1.76035600
O	0.50602800	-0.24774700	-3.21824500	C	4.55556700	-0.71567500	3.00449000
O	-0.22065300	-2.70095900	-3.05287500	H	3.33610700	-2.21415600	2.05505400
N	-0.34366300	-0.99196600	-1.05987200	C	3.93933500	1.57484700	2.57279900
H	-1.69538400	0.25887300	-0.60743100	H	2.27443800	1.85629200	1.24384300
C	-1.36418000	3.23155900	0.69045300	C	4.77722000	0.65038500	3.20162300
C	-1.81945900	4.48777600	1.08316600	H	5.20400800	-1.44650600	3.48199700
C	-0.37272000	2.55163800	1.40294000	H	4.09952800	2.64232400	2.70369400
C	-1.26371800	5.08165800	2.21968000	H	5.59586700	0.98852400	3.83159200
H	-2.60026300	4.97687200	0.51063500	H	-5.69985600	0.13186200	-4.15422000
C	0.16643400	3.15049600	2.53994500	H	0.15042800	4.87671500	3.83207200
H	-0.03917000	1.56903800	1.07809100	C	3.14016400	0.56192900	-1.29856700
C	-0.27514500	4.41506400	2.94515100	C	5.38892700	0.28607500	-1.53113300
H	-1.61087500	6.06010700	2.53997100	C	5.15326300	1.61549300	-1.42221000
H	0.93676200	2.63219800	3.10284300	H	6.30177600	-0.26679700	-1.68437900
O	-0.90441200	2.39221500	-1.75255200	H	5.81997800	2.46112700	-1.46825700
N	-2.42069000	0.95038300	-0.34660500	N	3.77570600	1.76934700	-1.28741900
C	-3.81535200	0.51411100	-0.32852300	N	4.15169100	-0.34292000	-1.46426000
H	-4.38928300	1.04716900	-1.09267400	C	3.13532500	3.01774200	-1.01338300
H	-3.80247400	-0.53936400	-0.62363800	C	3.74170300	3.91588700	-0.12735600
C	-4.50064500	0.64456500	1.01813400	C	1.89475600	3.29875700	-1.58104100
C	-5.85985300	0.31825000	1.11195900	C	3.08906100	5.10528000	0.19261800
C	-3.81649600	1.02094800	2.17644300	H	4.68564700	3.65904400	0.34238800
C	-6.51862300	0.35044200	2.34004900	C	1.24505100	4.48645300	-1.24134300
H	-6.40065000	0.02330800	0.21458500	H	1.42380500	2.58743600	-2.24837500
C	-4.47406800	1.05693500	3.40914300	C	1.83683800	5.39018100	-0.35915500
H	-2.76472800	1.27622200	2.11127200	H	3.55087900	5.79765400	0.89094300
C	-5.82497500	0.71794400	3.49757200	H	0.26472000	4.67834700	-1.66076300
H	-7.57230200	0.08869100	2.39609000	H	1.31767600	6.30477900	-0.08843100
H	-3.92541000	1.34887500	4.30106700	C	3.96410600	-1.76276900	-1.43145100
H	-6.33555900	0.74253200	4.45664900	C	2.99320800	-2.35113400	-2.24375200
C	0.63251900	-2.41966900	2.26896800	C	4.71491900	-2.52672600	-0.53633800
C	0.64104700	-3.82416100	2.29777400	C	2.73827600	-3.71735100	-2.12252700
C	0.55152200	-1.72753000	3.48820500	H	2.43500500	-1.74583000	-2.94772500
C	0.58847000	-4.51394400	3.50872600	C	4.47166800	-3.89780200	-0.44207900
H	0.69570600	-4.37660600	1.36375000	H	5.43509400	-2.04132600	0.11419100

C	3.47597800	-4.49110900	-1.22265400	H	-5.72698600	-3.80370000	1.54476800
H	1.95168400	-4.15495300	-2.72789100	O	-1.86075700	-0.62949700	2.52161900
H	5.04392500	-4.49561400	0.26168900	N	-2.24193400	-0.18204700	0.06308400
H	3.27661700	-5.55509000	-1.12951000	C	-2.77178600	0.71705700	-0.97978900
IN7-IPr-TPS				H	-2.69325200	1.76324300	-0.67278300
Ni	2.21472600	0.17947500	0.12913000	H	-2.09193500	0.57320700	-1.82273000
C	1.67186000	-1.62608600	0.44005800	C	-4.18741400	0.41380400	-1.42109800
S	-2.76987400	0.11840000	1.64045500	C	-5.01948900	1.46122800	-1.83125900
O	-2.89236100	1.56701600	1.87058600	C	-4.67808500	-0.89446200	-1.48111300
C	1.14101200	-2.11942700	-0.70808300	C	-6.31773200	1.20877000	-2.28255000
C	0.97169500	-1.08568200	-1.84021300	H	-4.64196900	2.47877000	-1.80202500
H	1.93030300	-0.99240700	-2.36668400	C	-5.97798400	-1.15094200	-1.91104700
C	-0.07530200	-1.39777300	-2.89539900	H	-4.04081600	-1.70437800	-1.15376500
C	0.24167900	-1.20091700	-4.24519600	C	-6.80550400	-0.09877500	-2.31380500
C	-1.34608300	-1.88613500	-2.56660500	H	-6.94981300	2.03611900	-2.59476800
C	-0.69095800	-1.47439600	-5.24765700	H	-6.34683600	-2.17318100	-1.92614000
H	1.22121900	-0.80957100	-4.50396000	H	-7.82094700	-0.29764400	-2.64593800
C	-2.28022300	-2.16121500	-3.56567700	C	0.90490500	-3.55345300	-1.03008200
H	-1.59993900	-2.05544300	-1.52549600	C	1.37375000	-4.05723000	-2.26024200
C	-1.95690600	-1.95542000	-4.90925300	C	0.27476300	-4.45906000	-0.15953700
H	-0.42840900	-1.31005900	-6.28973500	C	1.24220200	-5.40336800	-2.59215700
H	-3.26353200	-2.53402000	-3.29648800	H	1.86221500	-3.38667400	-2.95739100
H	-2.68770300	-2.16901100	-5.68481700	C	0.14570400	-5.80941700	-0.48924400
S	1.15560500	1.60259700	-1.79386000	H	-0.11714100	-4.10883000	0.78464100
C	-0.22948800	2.77929700	-1.62405100	C	0.62982200	-6.29244400	-1.70531800
C	-0.44190900	3.46610600	-0.39382800	H	1.62002200	-5.75831000	-3.54802900
C	-1.13571000	2.92036300	-2.71254800	H	-0.34462600	-6.48208500	0.21026400
C	-1.55700100	4.30533900	-0.31204200	H	0.52586300	-7.34339000	-1.96181800
C	-2.20337500	3.81306300	-2.55283100	C	1.77716600	-2.32077600	1.73758600
C	-2.44378800	4.50277900	-1.36813800	C	3.00221100	-2.67148300	2.33135300
H	-1.73529100	4.82769500	0.61917400	C	0.60775800	-2.59362500	2.47297000
H	-2.89383500	3.94565700	-3.37873500	C	3.05995100	-3.32331600	3.56183000
O	2.28391300	2.05262000	-0.87884800	H	3.92035800	-2.42487700	1.82384000
O	1.54560100	1.49643800	-3.21061600	C	0.66027600	-3.23350000	3.71113500
N	0.69104600	0.18909100	-1.07837900	H	-0.34429400	-2.25403200	2.08756000
H	-1.21107900	-0.15990500	0.05194800	C	1.88610100	-3.61607200	4.25938500
C	-4.40524400	-0.67819600	1.66829900	H	4.02716100	-3.59397000	3.97837900
C	-5.60196100	0.08399300	1.76471700	H	-0.26350600	-3.42092200	4.25065900
C	-4.43509300	-2.09355500	1.56228800	H	1.92752900	-4.11915000	5.22181900
C	-6.80675600	-0.62463200	1.79763600	C	3.98190800	0.02796700	0.85925000
C	-5.68377300	-2.72128400	1.61290100	C	6.10521100	-0.76263100	1.10223700
C	-6.87654500	-2.01454300	1.72707800	C	5.85052000	0.05199900	2.15471800
H	-7.73120700	-0.06493300	1.86541900	H	6.98117000	-1.33201400	0.83607700
				H	6.46297500	0.35508500	2.98872200

N	4.55974000	0.55006800	1.97927100	H	4.39504100	-5.49172700	0.84735800
N	4.96245100	-0.76005100	0.30458600	H	3.14686100	-4.42094200	0.19031100
C	4.10244200	1.73213400	2.68728700	C	6.59615400	-4.33119200	-0.38041900
C	3.12638400	1.63806800	3.69232000	H	6.86471100	-5.02054000	0.42874000
C	4.72007400	2.95650300	2.34650900	H	6.62286800	-4.88985300	-1.32287300
C	2.81243100	2.80739800	4.40035300	H	7.36554700	-3.55136500	-0.43842900
C	4.37740700	4.08821200	3.09417900	C	5.19375600	1.06445200	-1.95106200
C	3.43890300	4.01624800	4.12022300	H	4.66162700	1.44326600	-1.07720000
H	2.06202400	2.76035300	5.18353600	C	4.79114700	1.95666300	-3.13240300
H	4.84120100	5.04090500	2.85601600	H	4.96227000	3.00371000	-2.86040400
H	3.18286800	4.90708800	4.68742500	H	5.39818600	1.74718400	-4.02241800
C	4.88429000	-1.32158900	-1.03235200	H	3.73641500	1.84314400	-3.38420600
C	4.84648800	-0.41360300	-2.12181900	C	6.71621700	1.19678000	-1.71493300
C	4.87878800	-2.71621500	-1.22416000	H	7.26770900	0.81098400	-2.58081800
C	4.62187100	-0.94363500	-3.39613000	H	6.99001500	2.24953100	-1.58287100
C	4.67469500	-3.18962700	-2.52860500	H	7.05382700	0.65052700	-0.82977500
C	4.50706600	-2.31833900	-3.59659400	C	-3.21647000	-3.00899400	1.39140400
H	4.54925800	-0.27434700	-4.24488100	H	-2.37314900	-2.41914600	1.03945400
H	4.63760100	-4.26055600	-2.69903200	C	-5.68935200	1.61168400	1.85154400
H	4.32096900	-2.70827800	-4.59388500	H	-4.87094400	2.03313600	1.27180800
C	2.38504300	0.35375700	4.01115600	C	-8.21662300	-2.73192700	1.72395800
H	2.77500000	-0.43674200	3.37053100	H	-8.01292400	-3.81138500	1.71046300
C	0.88840600	0.51279400	3.68901700	C	-9.03609400	-2.42696200	2.99063800
H	0.34081500	-0.39932100	3.92643200	H	-9.29101500	-1.36246500	3.05103800
H	0.43697100	1.33614800	4.25339700	H	-9.97417600	-2.99450700	2.98859900
H	0.73624800	0.71194600	2.62303200	H	-8.47706000	-2.68885100	3.89556400
C	2.60539600	-0.08944700	5.46831600	C	-9.01419300	-2.39036000	0.45042800
H	2.18980000	0.63384700	6.18029500	H	-9.95911200	-2.94596700	0.42329600
H	2.11465900	-1.05324800	5.63636200	H	-9.24875800	-1.32021100	0.41017200
H	3.67271400	-0.20654300	5.69167200	H	-8.44066300	-2.63618600	-0.44983100
C	5.70797000	3.10261300	1.19405600	C	-5.51477100	2.07391300	3.31208700
H	5.84168500	2.12883700	0.72255300	H	-4.55995600	1.73912800	3.72258300
C	7.09400400	3.55564200	1.68675500	H	-5.54142400	3.16898900	3.36739700
H	7.79977100	3.59454200	0.84882100	H	-6.32616700	1.68053300	3.93767800
H	7.05469400	4.55369100	2.13814400	C	-6.98926600	2.19241400	1.26664300
H	7.49412900	2.86489000	2.43805000	H	-7.19216900	1.79644300	0.26704100
C	5.15576100	4.04786600	0.11070500	H	-7.86221500	2.00134000	1.90233000
H	4.22129600	3.66017600	-0.30331400	H	-6.88592700	3.28072100	1.18879700
H	4.96290800	5.04992200	0.50983900	C	-2.82915500	-3.62814400	2.74707800
H	5.87949000	4.14863800	-0.70645200	H	-2.58762400	-2.84437600	3.46943300
C	5.19706600	-3.72966200	-0.13042800	H	-3.65113100	-4.23513400	3.14622200
H	5.24907300	-3.20812700	0.82612900	H	-1.95258400	-4.27644000	2.63256300
C	4.13858300	-4.83625600	0.00718300	C	-3.43599000	-4.11465000	0.33887600
H	4.07774000	-5.45569900	-0.89382000	H	-2.48279700	-4.60854200	0.12670000

H	-4.13665900	-4.88502500	0.67982800	C	2.61170100	-0.47780100	-5.54095700
H	-3.81601600	-3.71161500	-0.60579200	H	0.48269500	-0.53345800	-5.20256500
C	0.48540200	3.45530000	0.82503700	C	3.94417100	0.36964400	-3.71463500
H	1.00750000	2.50117300	0.87528900	H	2.84987200	0.99563900	-1.97856200
C	1.53726200	4.56886900	0.64858700	C	3.86184000	-0.16414200	-5.00375300
H	1.04934900	5.55209000	0.66654100	H	2.53694700	-0.89391600	-6.54249600
H	2.26759200	4.53043100	1.46207400	H	4.90729200	0.62140700	-3.27815400
H	2.06961300	4.46369400	-0.29822500	H	4.76480900	-0.33164600	-5.58539600
C	-0.23548800	3.62525100	2.17390800	S	-0.29899000	-2.19893900	-2.13442000
H	0.48825700	3.44176800	2.97359100	C	1.02759300	-3.27121400	-1.61114400
H	-0.61617900	4.64381400	2.31827500	C	1.14082200	-3.58522300	-0.25381600
H	-1.06590800	2.92434900	2.28526500	C	1.97699200	-3.69682000	-2.53938000
C	-1.06557800	2.17384000	-4.05053600	C	2.22013700	-4.35267300	0.17049100
H	-0.51978800	1.24543600	-3.90952800	H	0.40743000	-3.22157400	0.45738600
C	-0.29483600	3.01349900	-5.08719700	C	3.05133100	-4.46760900	-2.09330200
H	0.71290000	3.24235000	-4.73423300	H	1.87172300	-3.42530400	-3.58473800
H	-0.21158000	2.46123400	-6.03106800	C	3.18987300	-4.80320000	-0.73927400
H	-0.82155300	3.95496200	-5.28929000	H	2.32592500	-4.56688200	1.22958800
C	-2.44336300	1.76949300	-4.60915900	H	3.79703800	-4.80611000	-2.80823500
H	-3.01418700	2.62312200	-4.99292800	O	-1.43442000	-2.45873800	-1.17409200
H	-2.29000700	1.07737100	-5.44345000	O	-0.52942600	-2.39772900	-3.57326500
H	-3.05815800	1.25548700	-3.86506000	N	0.14323900	-0.69160300	-1.67150400
C	-3.63756000	5.43308600	-1.22018300	H	1.62328800	-0.67453800	-0.47011700
H	-4.22278300	5.36941000	-2.14811200	C	2.86157400	0.62683600	2.51600900
C	-3.18076300	6.89487900	-1.05373600	C	4.07571600	0.44627900	3.17564200
H	-4.04555500	7.56620900	-0.99318000	C	2.31178600	1.89773100	2.34657200
H	-2.59418600	7.01780000	-0.13566000	C	4.75545900	1.56477700	3.65399700
H	-2.55563700	7.21217700	-1.89554900	H	4.48313700	-0.55206000	3.28782200
C	-4.55358000	5.00678700	-0.05648700	C	3.00202000	3.00410000	2.83439500
H	-4.90879900	3.97952800	-0.18115100	H	1.35740200	2.01704200	1.84787100
H	-4.02883800	5.05708300	0.90416900	C	4.23901900	2.85643000	3.47980000
H	-5.42742500	5.66649100	0.00328900	H	5.71059700	1.43370100	4.15632400
				H	2.57178000	3.99456800	2.70731400
				O	0.59589100	-0.55672400	1.80147500
				N	2.45599100	-0.59920100	0.14298600
				C	3.71073300	-1.18776500	-0.32864800
				H	3.86092800	-2.18334700	0.10110900
				H	3.58581500	-1.32477800	-1.40691300
				C	4.92374000	-0.31752200	-0.04993000
				C	6.15506100	-0.91481300	0.24120600
				C	4.84703100	1.08098400	-0.08245700
				C	7.28827800	-0.13627600	0.48775000
				H	6.22396600	-2.00005100	0.28602600
				C	5.97492100	1.86198600	0.16510400

H	3.89014400	1.55907700	-0.25714700	C	-4.57194700	0.23547300	-2.02374800
C	7.20148400	1.25688200	0.45071800	C	-4.72975900	2.40046800	-0.82766500
H	8.23515700	-0.61809300	0.71816700	C	-4.98928200	0.87912100	-3.19406700
H	5.88986600	2.94550400	0.14487700	C	-5.16250700	2.98078000	-2.02900700
H	8.08014100	1.86505000	0.64952500	C	-5.28510200	2.23737000	-3.19805300
C	0.86535600	2.86027800	-2.13340900	H	-5.09644000	0.30510100	-4.10791200
C	0.77241900	3.43220400	-3.41095400	H	-5.40073800	4.03718700	-2.05584100
C	1.77100500	3.42260500	-1.21631600	H	-5.61655300	2.71977000	-4.11400300
C	1.54648400	4.54159500	-3.75649400	C	-1.75864000	-0.14306600	4.24094400
H	0.09193100	2.99856100	-4.13913100	H	-2.20417600	0.52533400	3.49864700
C	2.54732400	4.52635800	-1.56022600	C	-0.47205500	0.51998900	4.75995000
H	1.86399600	2.97530900	-0.23222000	H	-0.69905100	1.51164500	5.16684700
C	2.43675700	5.09364900	-2.83337300	H	-0.01797600	-0.05787300	5.57256800
H	1.45788100	4.97062400	-4.75138100	H	0.26616500	0.62670200	3.96375300
H	3.24501700	4.93950400	-0.83553400	C	-2.77596600	-0.29930600	5.39131600
H	3.04411200	5.95292200	-3.10531200	H	-2.38230200	-0.96947300	6.16482000
C	-0.98681000	2.56866200	0.28375200	H	-2.98555800	0.67211800	5.85503000
C	-1.13173900	3.91856500	-0.09675900	H	-3.72489400	-0.71829000	5.03958800
C	-1.08200600	2.26967800	1.65563500	C	-3.11448600	-3.77486400	0.88768400
C	-1.29133000	4.92232500	0.85567000	H	-3.34752000	-2.96298100	0.19742000
H	-1.10285400	4.18047700	-1.14802400	C	-4.43188400	-4.24075000	1.54706500
C	-1.27004400	3.27123900	2.60814400	H	-5.12336100	-4.61462100	0.78230600
H	-0.96453700	1.23692800	1.95425300	H	-4.23774800	-5.05317500	2.25769200
C	-1.36270900	4.60806900	2.21514200	H	-4.93666400	-3.43524900	2.08596600
H	-1.38414500	5.95539500	0.53054000	C	-2.54172800	-4.93573900	0.05666600
H	-1.33063800	3.00725900	3.65937900	H	-1.54527300	-4.70834300	-0.32239800
H	-1.49780400	5.39265400	2.95519500	H	-2.49992700	-5.86501600	0.63829200
C	-2.87446900	-0.24218100	0.67082800	H	-3.19367100	-5.12030500	-0.80420900
C	-5.06564200	-0.06373900	1.27556900	C	-4.60504000	3.27095700	0.42615000
C	-4.46690200	-0.87035200	2.17972600	H	-3.72167800	2.93432300	0.97948900
H	-6.09203500	0.24076600	1.16506800	C	-4.41466000	4.76267900	0.09245800
H	-4.85273300	-1.37808700	3.04760600	H	-5.35124200	5.21626400	-0.25531900
N	-3.13491300	-0.98459900	1.79728700	H	-4.10333400	5.29694200	0.99428400
N	-4.08367500	0.33131100	0.37080100	H	-3.64825400	4.92042000	-0.66925800
C	-2.23218100	-1.91732500	2.44665100	C	-5.83364800	3.16327400	1.35842900
C	-1.51994000	-1.49768600	3.58433300	H	-5.76185200	3.91763800	2.15062700
C	-2.15826900	-3.23904400	1.94991500	H	-6.75931500	3.34903600	0.79995700
C	-0.62930500	-2.40802700	4.16434000	H	-5.91337500	2.19178700	1.84656300
C	-1.23530400	-4.09888200	2.55709500	C	-4.36633700	-1.27501400	-2.02517600
C	-0.46064800	-3.68180500	3.63689400	H	-3.63626200	-1.52272800	-1.25685700
H	-0.04454100	-2.10905700	5.02712500	C	-3.78870300	-1.81617300	-3.34002500
H	-1.12713200	-5.11162700	2.18495400	H	-3.49179200	-2.85991700	-3.20398500
H	0.26133300	-4.36110100	4.08169000	H	-4.51700300	-1.77771500	-4.15935500
C	-4.43397700	1.01988600	-0.85631700	H	-2.89327200	-1.26639800	-3.64105800

C	-5.68283400	-1.99671200	-1.67121400	N	0.10736900	-1.45818200	-0.86023600
H	-6.45112300	-1.79808200	-2.42864100	H	-0.91109500	-1.21430000	-0.56415000
H	-5.51860900	-3.08013900	-1.62627200	C	-2.20455200	2.13405600	0.45285700
H	-6.07285400	-1.67535500	-0.69978400	C	-3.23948300	3.04281800	0.65806100
C	4.37991100	-5.59243800	-0.24825100	C	-1.18464900	1.98505900	1.39440700
H	5.06611700	-4.94763500	0.31691100	C	-3.24251900	3.82397900	1.81582300
H	4.07244400	-6.40021600	0.42566100	H	-4.03502000	3.11205900	-0.07460100
H	4.94352200	-6.03432700	-1.07597900	C	-1.17946100	2.78421500	2.53509500
C	5.01847200	4.06254600	3.94630200	H	-0.41613100	1.23269000	1.24610400
H	4.36947600	4.93272200	4.08896700	C	-2.21193300	3.70340900	2.74907200
H	5.53886000	3.86545700	4.89002500	H	-4.05666200	4.52237600	1.98934500
H	5.78198600	4.33793800	3.20643500	H	-0.37518700	2.67948900	3.25895800
IN8				O	-0.94100700	1.09262600	-1.65160600
Ni	0.89449400	0.38097300	-0.92370900	N	-2.33403300	-0.47338800	-0.32169800
C	1.91082600	-0.14617900	0.58803300	C	-3.65577100	-1.00556200	0.02994500
S	-2.27830100	0.98349600	-0.94134500	H	-4.29570600	-1.07659700	-0.85834100
O	-3.42908400	1.40291700	-1.77050500	H	-3.46951400	-2.02879200	0.37238700
C	1.62426200	-1.39410100	1.03281300	C	-4.39221200	-0.22975200	1.10938500
C	0.80537200	-2.32322600	0.14772500	C	-5.61101400	0.39594500	0.82984800
H	1.50019500	-2.96120600	-0.40510700	C	-3.83999900	-0.07845300	2.38873200
C	-0.19357000	-3.21032600	0.86753800	C	-6.27220200	1.14691700	1.80581800
C	-0.27307200	-4.57470400	0.57373000	H	-6.03154600	0.31038600	-0.16896200
C	-1.08470200	-2.65833000	1.79509200	C	-4.49074800	0.67355500	3.36426100
C	-1.23912400	-5.37594300	1.18845200	H	-2.87632600	-0.52819400	2.60500200
H	0.41438400	-5.00356800	-0.15108500	C	-5.71366200	1.28814500	3.07636800
C	-2.05328600	-3.45243400	2.40555900	H	-7.21764200	1.62885200	1.56867200
H	-1.01907800	-1.59821500	2.01842200	H	-4.04001900	0.79093700	4.34647300
C	-2.13397900	-4.81510300	2.10124000	H	-6.22059100	1.87847500	3.83545600
H	-1.29224500	-6.43572400	0.95263200	C	2.09159200	-1.96961600	2.32421700
H	-2.74925300	-3.00702600	3.11126100	C	2.70425800	-3.23288100	2.36658900
H	-2.88916300	-5.43515900	2.57685600	C	1.90046100	-1.28126300	3.53309700
S	0.00602900	-2.13867600	-2.48005700	C	3.12983400	-3.78119400	3.57647400
C	-1.72570500	-2.49662500	-2.71960200	H	2.85588900	-3.78695100	1.44403900
C	-2.53454400	-1.51018200	-3.28553900	C	2.32285900	-1.82864400	4.74282900
C	-2.22914600	-3.72973200	-2.30497300	H	1.42041800	-0.30767200	3.51245600
C	-3.89069200	-1.78241400	-3.45742000	C	2.94149000	-3.08126300	4.77010200
H	-2.11274000	-0.55071200	-3.55878500	H	3.60702200	-4.75785700	3.58642500
C	-3.58870100	-3.98565100	-2.48341700	H	2.16425300	-1.27847600	5.66679700
H	-1.57322700	-4.46413900	-1.85277000	H	3.26895100	-3.51006100	5.71346600
C	-4.41390600	-3.01674900	-3.06157700	C	2.81509400	0.77304100	1.31842600
H	-4.53639600	-1.01847000	-3.87849900	C	4.10244300	0.36408400	1.71190000
H	-4.00140600	-4.93976800	-2.16908900	C	2.42360300	2.08883700	1.62705600
O	0.37622500	-1.06442100	-3.41144800	C	4.96007500	1.23252800	2.38670700
O	0.76781800	-3.39823200	-2.48338200	H	4.42230400	-0.64610400	1.48151800

C	3.27518600	2.95506900	2.31083100	C	2.26084700	-0.43194400	0.13092200
H	1.44252500	2.43157400	1.32056100	H	2.22511600	-0.40677200	1.22125500
C	4.55207000	2.53335800	2.69189300	C	3.74482000	-0.42241400	-0.23506600
H	5.94956800	0.88906200	2.67878300	C	4.66212900	0.05637500	0.70785900
H	2.93918200	3.96217600	2.54825300	C	4.22607700	-0.84613500	-1.48075100
H	5.21953000	3.20892400	3.22038700	C	6.02742900	0.10413400	0.42615800
H	-5.47312000	-3.22064400	-3.19316300	H	4.29794000	0.40974600	1.66715200
H	-2.21851500	4.31315000	3.64885400	C	5.59078500	-0.80743700	-1.76405900
C	2.08405300	1.80443300	-1.40825800	H	3.53075900	-1.20160200	-2.22941400
C	4.06023300	2.78653000	-1.98059000	C	6.49743400	-0.33555700	-0.81191200
C	3.15028100	3.77432200	-1.81119800	H	6.71996100	0.48785700	1.17074300
H	5.09505200	2.81315200	-2.28116500	H	5.94499700	-1.14857000	-2.73322100
H	3.22244200	4.84408100	-1.92338300	H	7.56086700	-0.30735500	-1.03557600
N	1.94844000	3.15823000	-1.47781900	S	2.00449500	1.84445500	-1.49601000
N	3.39651900	1.58880700	-1.74606400	C	3.49028600	2.70082600	-0.96764700
C	0.75181300	3.91561700	-1.23960900	C	4.66790400	2.57923000	-1.69801100
C	0.70854400	4.77917100	-0.14438100	C	3.41420900	3.48386700	0.18854700
C	-0.31404700	3.82276800	-2.13271500	C	5.80805700	3.24975300	-1.24987500
C	-0.42810800	5.56087300	0.06148200	H	4.68943700	1.94706200	-2.57755700
H	1.55257700	4.82096400	0.53730700	C	4.55940100	4.14478500	0.62587800
C	-1.44751900	4.60438400	-1.91592500	H	2.47530800	3.56985400	0.72927700
H	-0.26265200	3.12492100	-2.95839500	C	5.75552500	4.02649000	-0.09185600
C	-1.50337600	5.47364800	-0.82439400	H	6.73856700	3.15293700	-1.80162700
H	-0.47986900	6.22054300	0.92219800	H	4.52003200	4.75547100	1.52371000
H	-2.29515300	4.51034800	-2.58726300	O	2.30759100	1.03438000	-2.67881600
H	-2.39475300	6.06942000	-0.65195700	O	0.95542600	2.87427700	-1.55669000
C	4.03800100	0.31065600	-1.82089400	N	1.57160000	0.83644900	-0.24924400
C	3.40887200	-0.73770000	-2.49294500	H	1.09073000	1.35660900	0.49035200
C	5.28014000	0.12853300	-1.21007300	C	-2.31708200	3.95209100	0.64890400
C	4.00179000	-1.99979600	-2.50255700	C	-1.50266900	4.74150300	-0.16678300
H	2.46244100	-0.57090000	-2.99122800	C	-3.62343100	4.32665800	0.96953000
C	5.88156000	-1.13045300	-1.25202900	C	-2.02242000	5.93336600	-0.67617500
H	5.74076000	0.94529700	-0.66461700	H	-0.49112200	4.42329200	-0.39645800
C	5.23808600	-2.19860000	-1.88207200	C	-4.12545100	5.52324300	0.45947700
H	3.48449900	-2.81854100	-2.99323300	H	-4.21875700	3.69359000	1.61918200
H	6.84313000	-1.27897100	-0.76866300	C	-3.32720800	6.32299100	-0.36473800
H	5.70199700	-3.18102800	-1.89336500	H	-1.40390500	6.55736800	-1.31507500
IN9				H	-5.13730200	5.83317600	0.70568700
Ni	-1.04504200	-0.28032800	0.23892200	O	-2.37353300	2.05417600	2.52318300
C	0.11046900	-1.69541500	-0.28452400	N	-2.20858400	1.26668700	0.15479800
S	-1.69668900	2.38085200	1.25187200	C	-1.62644700	1.33776600	-1.17607300
O	-0.21069600	2.52609400	1.31195400	H	-1.18415800	2.30339000	-1.43276200
C	1.45929700	-1.68060700	-0.31503400	H	-0.66997200	0.69426100	-1.22493000
				C	-2.51046100	0.80454500	-2.28076800

C	-1.94737800	0.65148200	-3.55643000	C	-5.56683000	-2.29759200	-0.26861700
C	-3.82551900	0.40080300	-2.05503900	H	-3.74096800	-3.34689100	0.24708800
C	-2.69568600	0.09464200	-4.59221300	C	-5.89293700	-0.16567100	0.83670300
H	-0.91513900	0.95316200	-3.72557800	H	-4.28610000	0.45053200	2.16507900
C	-4.57392200	-0.15850000	-3.09384300	C	-6.33950200	-1.15609300	-0.04454500
H	-4.24282800	0.50992200	-1.06298400	H	-5.89848100	-3.05661500	-0.97099200
C	-4.01345800	-0.31638100	-4.36181100	H	-6.48289600	0.73313900	0.99166200
H	-2.25032400	-0.02471100	-5.57645800	H	-7.28426600	-1.02983900	-0.56660200
H	-5.59371000	-0.48028300	-2.90104600	C	0.55764100	-1.07408800	3.18952400
H	-4.59580300	-0.75607900	-5.16758000	C	0.77319300	0.29380700	3.36520700
C	2.22696500	-2.92700300	-0.62146300	C	1.58434200	-2.00183600	3.37274100
C	3.14621600	-3.44320500	0.30770700	C	2.04683300	0.73612100	3.72738600
C	2.03231800	-3.63002000	-1.82065100	H	-0.04269200	0.99091800	3.21934300
C	3.84065200	-4.62474700	0.05092000	C	2.84938900	-1.54950000	3.75001500
H	3.32345200	-2.90398700	1.23357200	H	1.39459000	-3.05655400	3.20014700
C	2.72637100	-4.81172800	-2.07977500	C	3.07964200	-0.18246200	3.93288800
H	1.32886700	-3.24055300	-2.54956000	H	2.22249000	1.80021700	3.85332300
C	3.63331500	-5.31608100	-1.14504900	H	3.65663400	-2.26269400	3.88819100
H	4.54776700	-5.00433500	0.78472600	H	4.06668900	0.16465200	4.22505400
H	2.55970100	-5.33763100	-3.01650300				
H	4.17632500	-6.23546400	-1.34813500			IN10	
C	-0.71577800	-2.86741600	-0.66067000	Ni	0.94721300	0.13517700	-0.02215000
C	-1.54229400	-2.80106400	-1.79849200	C	-0.00004100	1.15466000	1.55501800
C	-0.76762800	-4.02979200	0.12924100	S	3.69287800	-1.26869700	0.03585900
C	-2.36358500	-3.87120900	-2.15229900	O	4.27346900	-0.30075700	0.98581300
H	-1.53581100	-1.89914600	-2.40420900	C	-0.69903500	1.39250600	0.35661900
C	-1.59739800	-5.09610800	-0.21803700	C	-1.99643100	0.51362100	0.30318900
H	-0.13248100	-4.09516200	1.00837500	H	-1.73960500	-0.45521000	0.74214800
C	-2.39564900	-5.02609100	-1.36489300	C	-3.05499400	1.13839800	1.19969300
H	-2.98686200	-3.79334600	-3.03946400	C	-3.31962700	0.52325700	2.43113300
H	-1.61358200	-5.98943200	0.40202900	C	-3.70971600	2.33639900	0.88363900
H	-3.03642400	-5.86048000	-1.63814700	C	-4.22459300	1.08803700	3.33096200
H	6.64688000	4.54194500	0.25559300	H	-2.82887800	-0.41469600	2.67787900
H	-3.72393000	7.25311400	-0.76279700	C	-4.61864600	2.89693200	1.78050900
C	-1.51918400	-1.15237100	1.81997200	H	-3.53227600	2.80822500	-0.07375700
C	-1.50440000	-2.30892600	3.77894700	C	-4.87869400	2.27794900	3.00636600
C	-2.75009100	-2.40591700	3.25969900	H	-4.42192600	0.59390500	4.27890200
H	-1.07620600	-2.67811600	4.69685100	H	-5.12898200	3.81908500	1.51641600
H	-3.64103200	-2.89697500	3.61640200	H	-5.58850200	2.71954800	3.70113500
N	-2.74379700	-1.68627900	2.06872000	S	-3.97622400	-0.14045800	-1.586353

H	-5.60712600	-0.17515100	0.79447600	H	-1.06845800	6.04052200	0.38926500
C	-4.67803100	-3.84547700	-0.08474800	H	-1.49100500	6.16146700	-2.06532800
H	-3.60480700	-2.99388600	-1.75934200	C	0.95796600	1.96463500	2.33259300
C	-5.45722300	-3.57341300	1.04343400	C	1.86918200	2.88223700	1.78502800
H	-6.39732300	-2.04392600	2.24279900	C	0.96848800	1.77206900	3.72830900
H	-4.43049000	-4.87161700	-0.34264900	C	2.74996900	3.58269900	2.60550200
O	-4.86810000	0.99382700	-1.35828600	H	1.88286300	3.04163900	0.71681700
O	-3.78360900	-0.67766800	-2.94101400	C	1.84915400	2.47396500	4.54886700
N	-2.41988900	0.27595600	-1.09406800	H	0.26142800	1.07459200	4.17013400
C	4.26181700	-2.90700900	0.50837900	C	2.74760100	3.38378000	3.98848200
C	4.60335700	-3.15097600	1.83891900	H	3.44543600	4.28286900	2.15500900
C	4.30858600	-3.91509400	-0.45625100	H	1.83214800	2.31075000	5.62340700
C	4.99078700	-4.43923800	2.21070900	H	3.43986000	3.93191600	4.62200300
H	4.57791400	-2.33891900	2.55804400	H	-5.81431700	-4.39089600	1.66410100
C	4.69951700	-5.19798600	-0.07333000	H	5.33778600	-6.46192800	1.55234800
H	4.06056600	-3.68412600	-1.48694400	C	1.25634800	0.58138300	-1.90997200
C	5.03499000	-5.46067500	1.25825800	C	1.73662100	1.72201500	-3.83242200
H	5.26248100	-4.64355500	3.24251900	C	1.07416200	0.60010400	-4.19313200
H	4.74688700	-5.99135300	-0.81416800	H	2.16267400	2.52257400	-4.41539200
O	3.95665900	-1.10687900	-1.40700900	H	0.79597800	0.20749100	-5.15791400
N	2.04363900	-1.44879600	0.19915200	N	0.80196100	-0.09182300	-3.01381500
C	1.48069500	-1.18520100	1.42260600	N	1.85056800	1.68973800	-2.44552900
H	2.07188600	-0.68597100	2.19338700	C	0.23235400	-1.40631300	-3.01979100
H	-0.46409200	0.40176900	2.18413300	C	-1.03129600	-1.60258600	-3.57652300
C	0.33634800	-1.99577700	1.87221900	C	0.98056800	-2.47928500	-2.52833300
C	-0.11510800	-1.89480600	3.19975600	C	-1.57198800	-2.89081200	-3.60919100
C	-0.37701100	-2.81865900	0.98033300	H	-1.60558300	-0.76188000	-3.94822700
C	-1.26980800	-2.56151100	3.61432400	C	0.42919800	-3.75925500	-2.56023400
H	0.44172600	-1.28139900	3.90367000	H	1.96356800	-2.28867500	-2.12149500
C	-1.52360900	-3.48562600	1.39886700	C	-0.84660200	-3.96785000	-3.09660100
H	-0.02762000	-2.90667600	-0.04174200	H	-2.56522600	-3.03168400	-4.02338600
C	-1.98765000	-3.35010600	2.71204100	H	1.00106800	-4.59420900	-2.16484900
H	-1.60826500	-2.46244800	4.64267700	H	-1.26955600	-4.96863300	-3.11916400
H	-2.06895000	-4.10334900	0.69352200	C	2.62461300	2.66693400	-1.73529700
H	-2.89799700	-3.85440700	3.02316200	C	3.80276400	2.26730100	-1.10370700
C	-0.79769300	2.71273000	-0.34480100	C	2.22562700	4.00492200	-1.74760100
C	-1.03033700	2.80114400	-1.72886700	C	4.58514300	3.22575400	-0.45993100
C	-0.82690000	3.90505500	0.39951200	H	4.09712800	1.22705200	-1.12498400
C	-1.28746800	4.02771500	-2.34072300	C	3.02175800	4.95604800	-1.10862600
H	-1.02660400	1.90329800	-2.32991300	H	1.29344000	4.28648700	-2.22185400
C	-1.05406300	5.13677100	-0.21437300	C	4.20247400	4.56928900	-0.46864100
H	-0.69078500	3.86368700	1.47361100	H	5.49202100	2.91279000	0.04818600
C	-1.29382600	5.20506900	-1.58808100	H	2.70897100	5.99618000	-1.10271400
H	-1.47970900	4.06041900	-3.41000200	H	4.81849400	5.31371200	0.02899100

H	-1.75668800	-0.32915800	-1.57583600	H	6.22110900	-2.91778100	1.49367900
		TS1		C	-0.83756700	-2.53457100	1.10757800
Ni	0.45699700	0.36084800	-0.11845200	C	-2.16387700	-2.70180100	0.67004200
C	-0.01212000	-1.44039300	0.60148400	C	-0.33440100	-3.43538000	2.06720600
S	-2.23736300	0.93828000	-1.77560500	C	-2.95876800	-3.73508600	1.16352400
O	-1.21545900	0.38324200	-2.68147700	H	-2.57387000	-2.01355900	-0.06047400
C	1.26414800	-1.13069400	0.58492600	C	-1.13169400	-4.46293400	2.56423600
C	-3.70405300	-0.08951400	-1.94341200	H	0.68257100	-3.30766300	2.42534200
C	-3.55731200	-1.41524000	-2.36003900	C	-2.44828900	-4.62005500	2.11589500
C	-4.95154200	0.42315400	-1.58044600	H	-3.97859600	-3.84315900	0.80205300
C	-4.67956600	-2.24289400	-2.39864300	H	-0.72681000	-5.14380300	3.30905900
H	-2.57715300	-1.77813900	-2.65115200	H	-3.06691600	-5.42384200	2.50624800
C	-6.06778600	-0.41495000	-1.62036000	H	-6.80275400	-2.39443800	-2.05287700
H	-5.03907800	1.46550300	-1.29285000	C	1.80479000	1.51849300	-0.76279200
C	-5.93154000	-1.74572800	-2.02306300	C	3.75873700	2.21461700	-1.72114600
H	-4.57674600	-3.27445200	-2.72349600	C	3.22192600	3.28388200	-1.08638500
H	-7.04338900	-0.02665500	-1.34142500	H	4.64880400	2.11625600	-2.32158700
O	-2.67615300	2.33998700	-1.93637100	H	3.54489900	4.31021200	-1.01418500
N	-1.69769500	0.68627700	-0.24437300	N	2.02741400	2.84646000	-0.51834400
C	-2.51247200	1.25751800	0.85129700	N	2.88213400	1.15049900	-1.52737000
H	-2.59195100	2.34071000	0.71410700	C	1.09526700	3.70590400	0.14235400
H	-1.01420000	-0.43774800	0.08379100	C	1.48712500	4.42347100	1.27429700
C	-1.87008700	0.93982700	2.18290600	C	-0.19717100	3.81978200	-0.37186500
C	-2.28969500	-0.16163300	2.93463800	C	0.56478100	5.26328000	1.90178900
C	-0.79537100	1.70958700	2.64716700	H	2.49375600	4.30557700	1.66487200
C	-1.63644100	-0.50382400	4.12022600	C	-1.11410200	4.65380100	0.26737200
H	-3.11050200	-0.77565100	2.57489500	H	-0.48924600	3.25359300	-1.24722100
C	-0.14431800	1.37433100	3.83329800	C	-0.73582100	5.37680800	1.40194600
H	-0.46445400	2.56398100	2.06965200	H	0.85965100	5.81761700	2.78816100
C	-0.55934400	0.26149000	4.57028300	H	-2.12070600	4.72599200	-0.13285500
H	-1.96140000	-1.37616600	4.68043300	H	-1.45230200	6.02415200	1.89952000
H	0.68911400	1.98064800	4.17916100	C	3.07494000	-0.15021400	-2.09104900
H	-0.04712600	-0.00578600	5.49101500	C	2.00510800	-0.79388700	-2.71791600
C	2.59364600	-1.63148700	0.85705200	C	4.32787500	-0.75854200	-1.99511600
C	3.60034100	-0.75365800	1.29995300	C	2.20044500	-2.07422300	-3.23641700
C	2.92315400	-2.98404300	0.64574800	H	1.03808400	-0.30562900	-2.78085600
C	4.89314900	-1.21467900	1.53647700	C	4.51286800	-2.03273200	-2.52952800
H	3.34384800	0.29217600	1.44274100	H	5.13094400	-0.26126900	-1.46122700
C	4.22065100	-3.43930900	0.87023300	C	3.44882200	-2.69452400	-3.14626000
H	2.15395600	-3.66241000	0.28939000	H	1.36959200	-2.58288500	-3.71689200
C	5.21039700	-2.55894100	1.31747800	H	5.48070800	-2.51632800	-2.43707000
H	5.65785200	-0.52495800	1.88559000	H	3.59167000	-3.69245100	-3.55164400
H	4.46225100	-4.48427300	0.69269900	H	-3.52879300	0.83789000	0.82333300

TS2				C	-1.29121700	2.90044500	-0.35411400
Ni	-0.07036800	-0.18297200	-0.23316900	C	-2.75886100	1.84277300	1.24663300
C	-1.84699500	0.45464500	-0.61857900	C	-1.37145700	4.09412700	0.36480400
S	2.37516000	-1.94005400	-0.43017900	H	-0.67801100	2.84967200	-1.24751100
O	1.75954200	-2.78245700	-1.48027600	C	-2.83901400	3.03561500	1.96310100
C	-2.84164300	-0.25662900	-1.19080000	H	-3.29629200	0.96045100	1.58269400
C	4.10818800	-1.72704800	-0.85542000	C	-2.14241900	4.16923000	1.52749300
C	4.66831200	-2.52076500	-1.85502900	H	-0.82011400	4.96294100	0.01437200
C	4.86600700	-0.78120800	-0.15832300	H	-3.44267900	3.08180500	2.86625200
C	6.02246800	-2.36495300	-2.16147700	H	-2.20033700	5.09724400	2.09007600
H	4.04566300	-3.23810900	-2.37888100	H	7.84438700	-1.30316000	-1.71965300
C	6.21443700	-0.63275400	-0.47653600	C	-0.37385700	-0.85455300	1.52110900
H	4.39648700	-0.16605900	0.60213500	C	-1.03503900	-2.06652500	3.32830600
C	6.79261000	-1.42435100	-1.47489700	C	-0.15758800	-1.13170000	3.76730500
H	6.47241700	-2.97614400	-2.93883200	H	-1.55932500	-2.85477200	3.84422400
H	6.81507000	0.10318500	0.05098100	H	0.22352800	-0.91384600	4.75219200
O	2.29062200	-2.38722900	0.97005500	N	0.22880600	-0.39729000	2.65021900
N	1.84163300	-0.36238100	-0.46018400	N	-1.15678900	-1.88132900	1.95148100
C	1.35468000	0.15618200	-1.65034000	C	1.18694000	0.67069500	2.66648800
H	1.31176500	-0.49605500	-2.52704200	C	0.75153000	1.98395200	2.49923300
H	-0.38502400	0.31350000	-1.61974100	C	2.53867700	0.36513100	2.83067700
C	1.63144000	1.59765100	-1.91692300	C	1.69096800	3.01655400	2.51281800
C	1.24965400	2.16713300	-3.13932400	H	-0.30177600	2.18713100	2.34767900
C	2.21589000	2.40828700	-0.93549400	C	3.46821400	1.40582500	2.84977200
C	1.43517300	3.52951800	-3.37218900	H	2.84274400	-0.67445800	2.88954100
H	0.78624700	1.54254700	-3.90039400	C	3.04584300	2.73086200	2.69475400
C	2.39869300	3.77027200	-1.16897000	H	1.35544000	4.03934300	2.37043100
H	2.50184000	1.96222100	0.00909100	H	4.52393300	1.18091600	2.97585400
C	2.00641500	4.33779000	-2.38408100	H	3.77487200	3.53670700	2.70601400
H	1.13133300	3.96141700	-4.32197300	C	-1.94133800	-2.71409800	1.09414900
H	2.84315200	4.38956600	-0.39407600	C	-1.35255500	-3.28888700	-0.03434400
H	2.14641300	5.40047000	-2.56344500	C	-3.28161100	-2.94683200	1.40646900
C	-4.26796000	0.08526300	-1.34127500	C	-2.13014500	-4.09508100	-0.86582800
C	-5.19324400	-0.96620700	-1.49230700	H	-0.30723100	-3.10928000	-0.25680200
C	-4.76380000	1.40394200	-1.37161000	C	-4.04447700	-3.76970600	0.57741100
C	-6.55737000	-0.71700100	-1.63279700	H	-3.72412000	-2.46776300	2.27491200
H	-4.82763400	-1.98930000	-1.48650500	C	-3.47165900	-4.34233400	-0.56127500
C	-6.12720200	1.65232900	-1.51598700	H	-1.67582100	-4.53839900	-1.74709100
H	-4.07461400	2.23665800	-1.29319100	H	-5.09035900	-3.94530000	0.81181800
C	-7.03409200	0.59577600	-1.64083600	H	-4.06966000	-4.97712400	-1.20926500
H	-7.24902200	-1.54934300	-1.74039300	H	-2.58093500	-1.24385600	-1.56872700
H	-6.48319200	2.67947900	-1.53864700	TS3			
H	-8.09675200	0.79446200	-1.75336400	S	1.78585800	-0.52569300	-2.10184100
C	-1.98618600	1.75526700	0.07157100				

O	1.63659800	-1.90513500	-2.60516500	H	-2.89533400	-4.95348600	-0.03081500
O	1.05886600	0.55523200	-2.81712900	H	-4.41949200	-3.21133400	-1.57524800
Ni	-0.39844400	-0.62455000	-0.06493500	N	-2.80529700	-1.85677600	-1.08450200
C	-0.15250800	1.42826800	0.58057600	N	-1.61830700	-3.21155100	0.10667200
C	1.37952800	0.71581900	0.18060100	C	3.52863300	-0.06048300	-2.16457500
C	2.14107600	0.66143200	1.49098600	C	4.39855800	-0.49465900	-1.16061500
C	2.98344900	1.71178700	1.86639600	C	3.98484200	0.71579400	-3.23155100
C	2.02093600	-0.45287500	2.33290900	C	5.74718200	-0.14485900	-1.23271700
C	3.69711000	1.65222000	3.06648900	H	4.00929500	-1.07038100	-0.32762300
H	3.07780700	2.58076700	1.22127300	C	5.33706500	1.05531000	-3.29694200
C	2.73204400	-0.51281300	3.52923000	H	3.27965100	1.05518500	-3.98294400
H	1.38125600	-1.27749500	2.03332300	C	6.21702300	0.62548700	-2.30015000
C	3.57302000	0.54150900	3.90154500	H	6.42925500	-0.46801300	-0.45103500
H	4.35032300	2.47519500	3.34470800	H	5.70175400	1.66128500	-4.12199200
H	2.63278600	-1.38654700	4.16848600	H	7.26806700	0.89746200	-2.35096000
H	4.12869200	0.49431300	4.83456100	C	-0.54198000	-3.73710800	0.89327200
H	1.75547000	1.51372900	-0.46166000	C	-0.81541400	-4.30435000	2.13932900
C	-1.31104300	0.77198600	0.63861600	C	0.76470200	-3.64301300	0.40638300
N	1.47491600	-0.58587800	-0.49675800	C	0.24075700	-4.78032400	2.91768900
C	-2.68309200	1.13380800	0.95941900	H	-1.83959400	-4.34932000	2.49880600
C	-3.22624900	2.37607200	0.58350800	C	1.81206000	-4.10589400	1.20363000
C	-3.51432400	0.20300300	1.60802100	H	0.95770100	-3.18919200	-0.56044800
C	-4.56046500	2.67367900	0.85278900	C	1.55484800	-4.67426600	2.45404200
H	-2.59780400	3.09312500	0.06628700	H	0.03668000	-5.21881500	3.89034200
C	-4.84428500	0.50921400	1.88834900	H	2.83110600	-4.01732500	0.83960500
H	-3.09926300	-0.76417300	1.87753400	H	2.37641700	-5.03380900	3.06736000
C	-5.37445500	1.74524400	1.50744700	C	-3.24459100	-0.68926500	-1.78722000
H	-4.96771600	3.63381600	0.54661300	C	-2.33402900	0.03151400	-2.56342600
H	-5.47065700	-0.21946300	2.39707100	C	-4.57132000	-0.27403900	-1.65761800
H	-6.41448100	1.98175900	1.71646500	C	-2.76287800	1.19660200	-3.19900000
C	0.06684300	2.85209000	0.92703900	H	-1.30350000	-0.29231500	-2.66050000
C	0.52495200	3.75613300	-0.04478100	C	-4.99128700	0.88251200	-2.31246000
C	-0.19789800	3.31660800	2.22322400	H	-5.24871500	-0.82005200	-1.00923500
C	0.71482800	5.10041500	0.27830400	C	-4.08759500	1.62229100	-3.07937900
H	0.71291400	3.40215900	-1.05555600	H	-2.04908100	1.76277800	-3.78968700
C	-0.00512400	4.66013300	2.54313000	H	-6.01738500	1.21886600	-2.19762600
H	-0.54610000	2.61318600	2.97307100	H	-4.41497500	2.53090600	-3.57706300
C	0.45362600	5.55529700	1.57335300				
H	1.06323400	5.79283000	-0.48357000			TS4	
H	-0.20735600	5.00710000	3.55302600	Ni	0.92199600	0.34300000	-0.95156200
H	0.60588800	6.60150200	1.82485600	C	1.87877400	-0.20349700	0.58906200
C	-1.64793700	-1.93251100	-0.36615200	S	-2.25509100	1.07175800	-0.90996800
C	-2.75191000	-3.91651400	-0.28922700	O	-3.44574100	1.45301200	-1.69394600
C	-3.49586800	-3.06576800	-1.03868100	C	1.54327700	-1.43910600	1.03174800

C	0.67405300	-2.32233900	0.15104300	C	-5.56146500	0.39978300	0.79119500
H	1.33616700	-3.00138400	-0.39494700	C	-3.81951100	-0.03724100	2.39474500
C	-0.36188600	-3.15923700	0.88201400	C	-6.24753200	1.16167500	1.74107900
C	-0.59569500	-4.48297100	0.49562700	H	-5.95885300	0.29703800	-0.21519500
C	-1.12663400	-2.60872200	1.91667900	C	-4.49594200	0.72543900	3.34420400
C	-1.58974800	-5.24012700	1.12078000	H	-2.85797500	-0.47680900	2.63721200
H	-0.00038100	-4.91254000	-0.30619000	C	-5.71633800	1.32689400	3.02053900
C	-2.11875200	-3.36055200	2.54401200	H	-7.19076100	1.63337700	1.47660700
H	-0.93817800	-1.58405500	2.22133000	H	-4.06680400	0.86166000	4.33358000
C	-2.35611200	-4.67907800	2.14389900	H	-6.24293700	1.92589800	3.75914800
H	-1.76253700	-6.26746300	0.81019900	C	2.00983700	-2.04002600	2.31239800
H	-2.71284800	-2.91549800	3.33746600	C	2.56825000	-3.32868400	2.33684400
H	-3.13033800	-5.26544000	2.63148500	C	1.87378300	-1.35057300	3.52826300
S	-0.06178400	-2.06662600	-2.45729400	C	2.99476900	-3.90080800	3.53539200
C	-1.79934600	-2.35163100	-2.77695300	H	2.67557900	-3.88397000	1.40890700
C	-2.55557600	-1.31107900	-3.31811200	C	2.29649200	-1.92178400	4.72675900
C	-2.36324900	-3.58582600	-2.45172000	H	1.43633600	-0.35683300	3.52197200
C	-3.91642400	-1.51855100	-3.53956800	C	2.86128100	-3.19981900	4.73581900
H	-2.08880500	-0.35859000	-3.53649700	H	3.42935200	-4.89722100	3.53127900
C	-3.72490400	-3.78080700	-2.68424000	H	2.18085000	-1.37002700	5.65619800
H	-1.74852000	-4.37250000	-2.03145800	H	3.18936000	-3.64721000	5.67032000
C	-4.49810300	-2.75050500	-3.22700300	C	2.82298200	0.67827200	1.31469400
H	-4.51897900	-0.70806100	-3.93696000	C	4.09900500	0.22290800	1.69348200
H	-4.18021300	-4.73610900	-2.43959600	C	2.47917100	2.00388100	1.63669800
O	0.36600000	-0.98311800	-3.36195600	C	4.99111700	1.05679500	2.36730100
O	0.64106700	-3.36240700	-2.49926700	H	4.38203400	-0.79595500	1.45378700
N	0.01817600	-1.42645300	-0.85605800	C	3.36512300	2.83584600	2.31936900
H	-1.10895700	-1.05361700	-0.53753700	H	1.50776100	2.38095500	1.34033300
C	-2.17155300	2.19584600	0.49749700	C	4.63011500	2.36825000	2.68606800
C	-3.18842000	3.12175100	0.71174400	H	5.97088100	0.67781300	2.64808600
C	-1.13886300	2.02723600	1.42125400	H	3.06563100	3.85179000	2.56808900
C	-3.16159500	3.90254200	1.86950400	H	5.32448800	3.01658200	3.21401600
H	-3.99345500	3.20212600	-0.00947700	H	-5.55968700	-2.90618500	-3.39934500
C	-1.10727300	2.82411100	2.56278100	H	-2.10575100	4.37008400	3.68942800
H	-0.38536600	1.26318100	1.25572300	C	2.17221800	1.72488800	-1.41577500
C	-2.12141700	3.76105100	2.78932200	C	4.18582800	2.64243100	-1.96499600
H	-3.96010700	4.61580900	2.05426500	C	3.31116500	3.66059400	-1.78970000
H	-0.29626300	2.70528200	3.27668700	H	5.22275900	2.63575400	-2.25924700
O	-0.94066800	1.19072500	-1.63926300	H	3.42320800	4.72823200	-1.88892700
N	-2.27469800	-0.40273000	-0.29030300	N	2.08610400	3.08430300	-1.47043600
C	-3.57608600	-0.98976400	0.05284600	N	3.47849000	1.46661300	-1.74726400
H	-4.19835400	-1.10083200	-0.84279500	C	0.91781700	3.87985200	-1.21630900
H	-3.34809200	-1.99546100	0.41748600	C	0.90169300	4.71636200	-0.09920700
C	-4.34474400	-0.21225100	1.10708700	C	-0.14900100	3.84934600	-2.11229000

C	-0.21141100	5.52447700	0.13149800	H	4.75743700	1.68341000	-2.61975400
H	1.74764100	4.71617800	0.58097400	C	4.97418100	3.95791300	0.52477400
C	-1.25834500	4.65867000	-1.87228500	H	2.87077800	3.51680900	0.77536100
H	-0.11760900	3.17619500	-2.95940300	C	6.11288400	3.74136600	-0.26017000
C	-1.29022200	5.49426400	-0.75388600	H	6.92836400	2.76131800	-1.99964800
H	-0.24200000	6.16115200	1.01034800	H	5.03109600	4.59101400	1.40590600
H	-2.10620800	4.61498200	-2.54877400	O	2.33647600	0.93888000	-2.55932400
H	-2.16380900	6.11019600	-0.56257700	O	1.16736100	2.89688100	-1.42639700
C	4.07834800	0.16767000	-1.81724000	N	1.71181200	0.86848600	-0.08835700
C	3.41174600	-0.86523300	-2.47643400	H	1.07397600	1.34040800	0.55756900
C	5.31628600	-0.05082200	-1.20907100	C	-2.17441900	4.06872200	0.77456300
C	3.96125400	-2.14686100	-2.47535400	C	-1.32999900	4.77382400	-0.08710800
H	2.47078800	-0.67199100	-2.97507800	C	-3.41862100	4.56682900	1.16348800
C	5.87515000	-1.32942500	-1.24229300	C	-1.75815100	6.01053100	-0.57213100
H	5.80626200	0.75374800	-0.67104700	H	-0.36577400	4.36320400	-0.36890900
C	5.19299600	-2.38148900	-1.85883500	C	-3.82883900	5.80693300	0.67403800
H	3.41203700	-2.95156300	-2.95444600	H	-4.03659000	3.99286700	1.84591400
H	6.83341700	-1.50563300	-0.76162600	C	-3.00154300	6.52493100	-0.19436600
H	5.62326300	-3.37918000	-1.86184500	H	-1.11613400	6.57259000	-1.24439300
				H	-4.79180900	6.21284900	0.97122900
		TS5		O	-2.40710600	2.13277700	2.58952900
Ni	-1.21087500	-0.23635800	0.29659800	N	-2.24609000	1.41266300	0.17933800
C	0.01374600	-1.53638300	-0.44166100	C	-1.49360800	1.31799200	-0.99432000
S	-1.67240800	2.44814100	1.35192500	H	-0.66622100	2.00972000	-1.14180800
O	-0.18368100	2.47439700	1.42558100	H	-0.45142300	0.05278200	-0.98747800
C	1.35779200	-1.63037400	-0.34395500	C	-2.20958100	0.93550000	-2.24417500
C	2.22426500	-0.48247800	0.22702400	C	-1.50587100	0.98269900	-3.45720600
H	2.12464300	-0.53270800	1.31473500	C	-3.52397200	0.45628600	-2.22342000
C	3.72466600	-0.56429100	-0.06229700	C	-2.11202200	0.54363500	-4.63388500
C	4.61386500	-0.12778100	0.92712100	H	-0.47710000	1.33575500	-3.46607700
C	4.24602100	-0.99873800	-1.28705500	C	-4.12592600	0.01782900	-3.40186900
C	5.99152800	-0.13469200	0.71089000	H	-4.05274700	0.41547000	-1.28003900
H	4.21641200	0.23451600	1.87040200	C	-3.42309800	0.05622300	-4.60910800
C	5.62384300	-1.01778100	-1.50339900	H	-1.55983500	0.57726800	-5.56930200
H	3.57326400	-1.31377100	-2.07355600	H	-5.14345600	-0.36287000	-3.37122700
C	6.50202300	-0.58837100	-0.50648200	H	-3.89226200	-0.29051200	-5.52631400
H	6.66318100	0.21639400	1.48993100	C	2.04285900	-2.93294600	-0.60323400
H	6.00991900	-1.36658000	-2.45764600	C	2.83373300	-3.53357600	0.39054000
H	7.57517100	-0.60208000	-0.67892500	C	1.90398100	-3.59818700	-1.83197700
S	2.14352800	1.79176600	-1.38124300	C	3.45376000	-4.76282900	0.16892000
C	3.71488900	2.54896300	-0.95831100	H	2.96844200	-3.02625800	1.34073900
C	4.83441900	2.33130200	-1.75506500	C	2.52496600	-4.82629900	-2.05581000
C	3.76467000	3.36176000	0.17799300	H	1.30143500	-3.14274400	-2.61124700
C	6.04237400	2.93348800	-1.39540900	C	3.30147300	-5.41650200	-1.05586300

H	4.06071300	-5.20865900	0.95333400	H	3.80051700	-0.16858500	4.38701600
H	2.40363300	-5.32175200	-3.01576500				
H	3.78701800	-6.37296700	-1.23117800				
C	-0.85332600	-2.65156600	-0.90603000	Ni	-0.99348000	-1.20853600	-0.19538500
C	-1.59568700	-2.54420600	-2.09428500	C	0.69358200	-2.08444900	-0.76613200
C	-0.99396500	-3.82208000	-0.13743800	S	-1.96328000	1.53459200	0.62913000
C	-2.42948100	-3.58180900	-2.51268500	O	-0.54792600	2.00697100	0.72730400
H	-1.51264300	-1.64343700	-2.69306800	C	1.92705000	-1.81340300	-0.27411300
C	-1.82491800	-4.85955600	-0.55665700	C	2.16063800	-0.54029400	0.57449700
H	-0.42475900	-3.91521200	0.78275800	H	1.41281500	-0.56018700	1.37465700
C	-2.54655000	-4.74673700	-1.75039900	C	3.52451700	-0.34352300	1.23455700
H	-2.99004400	-3.47195800	-3.43740000	C	3.56981900	0.03562500	2.58052600
H	-1.90582100	-5.76102300	0.04621800	C	4.73143100	-0.40944700	0.52398800
H	-3.19323600	-5.55642700	-2.07871500	C	4.77982200	0.33406800	3.20991000
H	7.05602500	4.20441400	0.01732600	H	2.64563400	0.10502200	3.14052000
H	-3.32619300	7.48937500	-0.57567000	C	5.94154200	-0.10639500	1.14544400
C	-1.74831800	-1.20562000	1.84399100	H	4.72619600	-0.70257600	-0.51745100
C	-1.81781300	-2.57226800	3.66802300	C	5.97357800	0.26432200	2.49153100
C	-3.04199600	-2.60701800	3.08911400	H	4.78499400	0.62654200	4.25705300
H	-1.43196200	-3.04161400	4.55877200	H	6.86223400	-0.15372000	0.57078200
H	-3.94653300	-3.12965500	3.35620500	H	6.92007200	0.49614300	2.97305500
N	-2.98274000	-1.75925100	1.98716000	S	2.46968700	1.25226800	-1.55563100
N	-1.04200600	-1.70401500	2.89943400	C	3.90479100	2.26603700	-1.06924900
C	-4.11107700	-1.45511800	1.15076100	C	5.20530700	2.02677100	-1.59384500
C	-4.52956600	-2.38043200	0.19684300	C	3.67065300	3.27831700	-0.10983100
C	-4.77118100	-0.23835600	1.33222700	C	6.25668400	2.76540000	-1.04557400
C	-5.65392500	-2.09038500	-0.57811600	C	4.78106400	3.96198000	0.39929600
H	-3.96553600	-3.29490400	0.05102000	C	6.07804400	3.70605600	-0.02907500
C	-5.89835900	0.03609300	0.55737500	H	7.26078600	2.58758400	-1.40977200
H	-4.37680400	0.48166600	2.04169400	H	4.62089200	4.71956000	1.16129000
C	-6.34476200	-0.89091800	-0.39039000	O	2.90883400	0.08040800	-2.32386900
H	-5.97907900	-2.79972100	-1.33355400	O	1.47828000	2.16117100	-2.16745200
H	-6.41846000	0.98116900	0.68358000	N	1.78369800	0.68580400	-0.16895300
H	-7.22077800	-0.66889300	-0.99392000	H	1.00227700	1.23418000	0.19313000
C	0.27697000	-1.29347300	3.26098000	C	-2.93829800	3.05084300	0.25536500
C	0.53671100	0.06699800	3.43964300	C	-3.73379600	3.25942400	-0.89715700
C	1.26899500	-2.25274400	3.47327800	C	-2.87316600	4.02919900	1.28530900
C	1.81352200	0.46793500	3.83508700	C	-4.42750200	4.47261200	-0.99640300
H	-0.25002900	0.79179700	3.27218900	C	-3.61788600	5.20079800	1.11977000
C	2.53812700	-1.84180300	3.88419200	C	-4.39332800	5.45276800	-0.00954300
H	1.05126600	-3.30163000	3.29641600	H	-5.02126100	4.64627800	-1.88794000
C	2.81054400	-0.48318200	4.06925700	H	-3.59302400	5.94777700	1.90771200
H	2.01943400	1.52640100	3.96253800	O	-2.56144800	0.97771400	1.85695900
H	3.31645700	-2.58189500	4.04588400	N	-2.12519200	0.37719800	-0.54800700

TS5-IPr-TPS

C	-1.12105400	0.36091500	-1.53784200	C	-4.12245300	-3.12921200	-1.01877500
H	-0.39396900	1.16933200	-1.52540700	C	-5.19857100	-1.37324600	0.35547400
H	-0.00292100	-0.67023600	-1.26614300	C	-5.14819600	-2.97061900	-1.95928400
C	-1.53288200	-0.03727500	-2.91542000	C	-6.18885200	-1.25270400	-0.62890900
C	-0.72548200	0.33762200	-3.99907700	C	-6.16695300	-2.03939700	-1.77343400
C	-2.70453600	-0.76553800	-3.14653200	H	-5.14810700	-3.57476100	-2.85819100
C	-1.08853700	-0.02305100	-5.29711800	H	-6.99135600	-0.53574300	-0.48861200
H	0.17912700	0.91064200	-3.81650000	H	-6.94634400	-1.93158700	-2.52325500
C	-3.06703400	-1.12056800	-4.44450700	C	-0.12598800	-2.71567300	3.01245500
H	-3.32953100	-1.03629700	-2.30592300	C	0.22231400	-1.60886900	3.81178200
C	-2.25784000	-0.75494200	-5.52443300	C	0.66080000	-3.88685800	2.95141000
H	-0.45972100	0.27312800	-6.13248500	C	1.42191400	-1.68275900	4.53048400
H	-3.98226400	-1.68364700	-4.60694100	C	1.86303800	-3.89060000	3.67018800
H	-2.53947800	-1.03290900	-6.53668400	C	2.24459200	-2.80058500	4.44789000
C	3.08887300	-2.71494100	-0.54067300	H	1.70973900	-0.85388600	5.16928400
C	3.71002600	-3.38300400	0.52610300	H	2.50447000	-4.76412800	3.63225900
C	3.59476000	-2.90597700	-1.83569300	H	3.18092400	-2.82786300	4.99813000
C	4.79816600	-4.22818900	0.30706400	C	0.20663900	-5.14780400	2.21953500
H	3.34283200	-3.22268000	1.53474800	H	-0.44064600	-4.83882900	1.39141200
C	4.68625200	-3.74676000	-2.05419200	C	-0.70813600	-0.41768200	3.99440700
H	3.13499800	-2.37806900	-2.66125200	H	-1.45236300	-0.42631100	3.19869200
C	5.29172400	-4.41338800	-0.98597500	C	1.37520100	-5.97308000	1.64681500
H	5.26333300	-4.73555800	1.14876200	H	1.92527500	-6.48672100	2.44409500
H	5.06532600	-3.87963900	-3.06442100	H	0.98476000	-6.74915500	0.97869900
H	6.14204300	-5.06798300	-1.15949100	H	2.08747900	-5.36345200	1.08586300
C	0.52142200	-3.17411900	-1.76845300	C	-0.62208600	-6.06370000	3.14744900
C	0.41141600	-2.86510100	-3.13396100	H	-0.02971600	-6.35654200	4.02263000
C	0.57208700	-4.52685200	-1.40514600	H	-1.53692800	-5.58366600	3.49934100
C	0.39946100	-3.87158200	-4.09960200	H	-0.91090700	-6.97564100	2.61171700
H	0.38643900	-1.82827800	-3.44457700	C	0.01126900	0.93505200	3.89365600
C	0.57358400	-5.53630200	-2.36723500	H	0.43848400	1.08560600	2.89996500
H	0.65776600	-4.77712400	-0.36035600	H	-0.71080600	1.73971000	4.05608900
C	0.49568600	-5.21351700	-3.72437000	H	0.80500600	1.04829600	4.64165700
H	0.32819800	-3.59893600	-5.14947200	C	-1.45661600	-0.53487000	5.33754800
H	0.64575000	-6.57538000	-2.05423400	H	-0.75908900	-0.50000100	6.18374800
H	0.49989000	-5.99709800	-4.47746800	H	-2.16734100	0.29275300	5.44408700
C	-1.85391200	-2.24793700	1.19422500	H	-2.01838900	-1.47332500	5.40401800
C	-2.50512200	-3.25252800	3.14176000	C	-3.00147300	-4.13970900	-1.25027800
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H	-2.36844900	-3.63711500	4.13815200	C	-5.31341300	-0.53198600	1.62292300
H	-4.62018200	-3.45811600	2.51945900	H	-4.35380800	-0.55532700	2.14144700
N	-3.19959700	-2.53189100	1.18382900	C	-5.61560200	0.94444100	1.31663000
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C	-4.16792800	-2.30906200	0.13091200	H	-4.93702400	1.33735500	0.56230500

H	-6.64377600	1.08749600	0.96269800	H	1.50971800	3.16893600	-0.08468000
C	-6.40769900	-1.08942100	2.55719300	C	5.51587300	1.06858300	-2.74841500
H	-7.38628900	-1.06499100	2.06264100	H	4.95764900	0.14800300	-2.59075800
H	-6.21948100	-2.12409500	2.85984200	C	7.26524600	4.41140600	0.60471500
H	-6.47353200	-0.48093800	3.46685300	H	6.86840500	5.13709900	1.32785900
C	-3.11287200	-5.36376600	-0.31739200	C	8.13648900	3.40626500	1.38287500
H	-3.10587500	-5.08946300	0.74070900	H	8.57781000	2.66650700	0.70408000
H	-4.03662400	-5.92045900	-0.51842500	H	8.95540600	3.91944900	1.90127600
H	-2.26501100	-6.03563200	-0.49457700	H	7.53955500	2.86218600	2.12261000
C	-2.90437800	-4.61335000	-2.70599600	C	8.10126100	5.19072200	-0.42581100
H	-2.80431500	-3.77197900	-3.39777300	H	7.48414100	5.91439000	-0.96946900
H	-2.02003800	-5.24108600	-2.82206400	H	8.91402700	5.73467500	0.07004000
H	-3.77750400	-5.21052600	-2.99782200	H	8.55461600	4.51688700	-1.16232200
C	-2.09742300	3.89448000	2.60045400	C	2.16327800	3.45249100	1.92491700
H	-1.37729600	3.08774900	2.51214000	H	2.83986600	4.08646800	2.51052300
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H	-1.90503000	6.01069800	3.20088000	H	1.01838600	5.46584000	0.38489700
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C	-3.05677600	3.53236400	3.74906000	C	5.02052200	1.67925500	-4.07598600
H	-3.81576700	4.31107600	3.89307600	H	5.19396600	0.98149600	-4.90383500
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H	-5.23360700	8.51565700	-1.43266000	Ni	1.02772400	-0.13929700	0.04889900
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H	-3.45247800	3.78358000	-3.61645100	C	-1.69227800	-1.21252400	0.63390900
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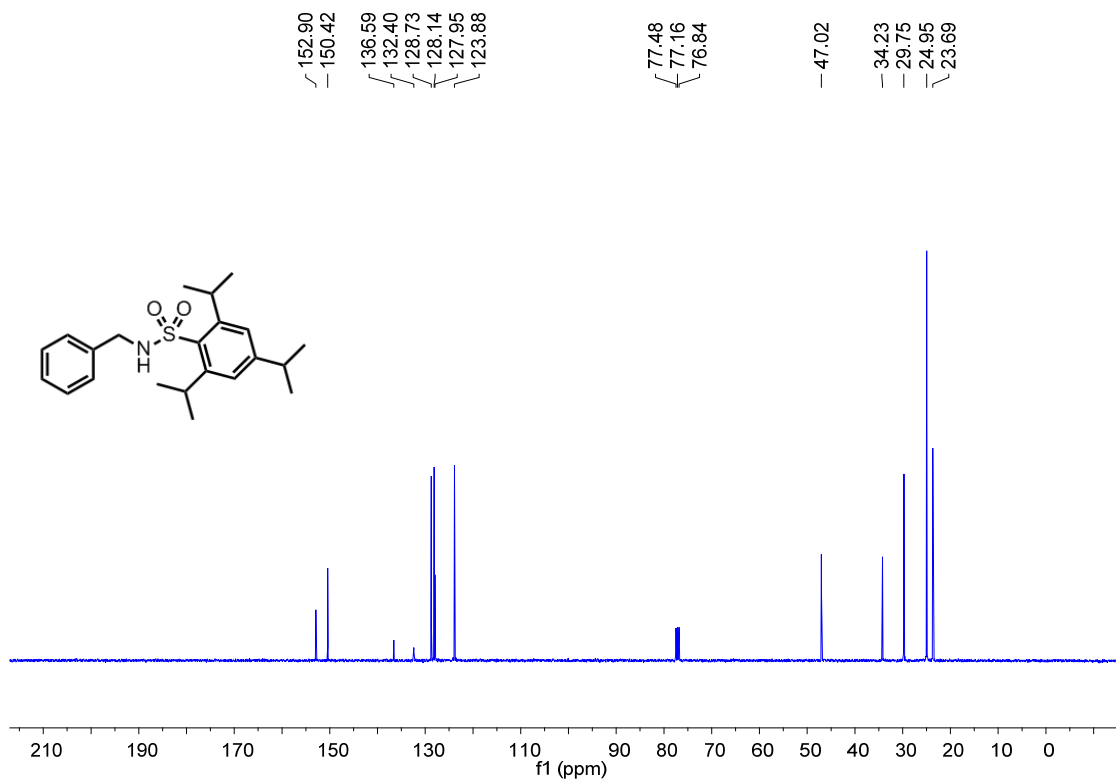
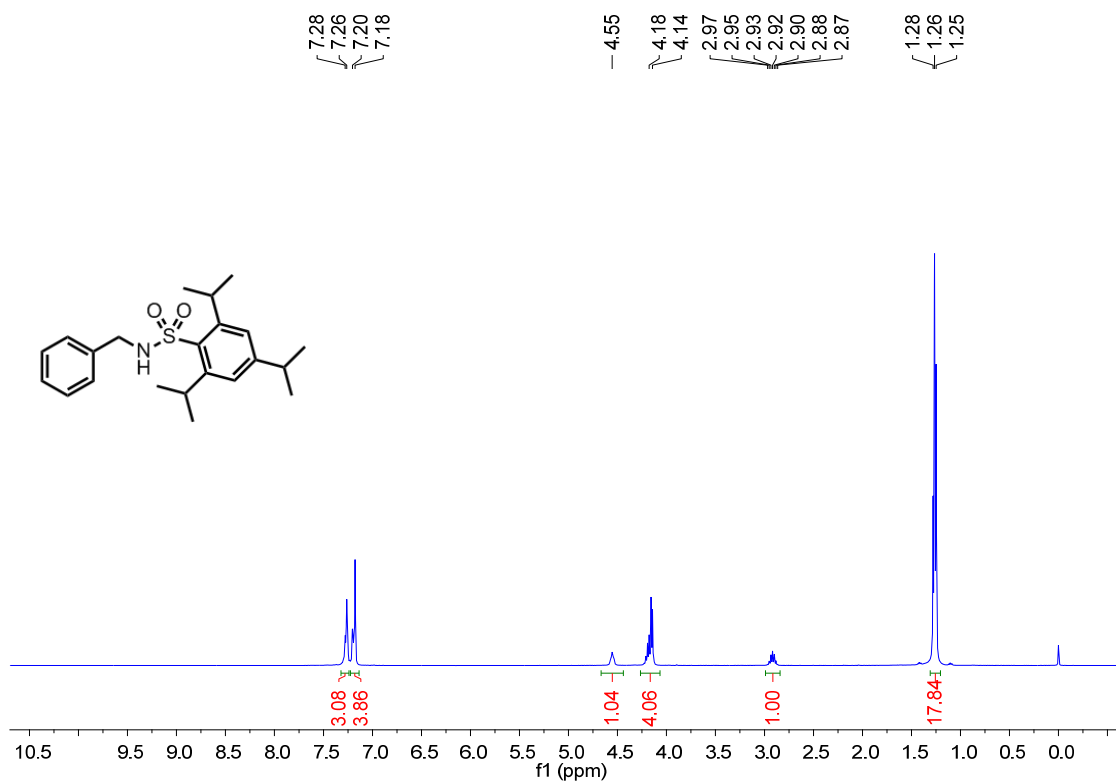
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H	-7.56234700	2.38239600	2.17303900	C	0.05829300	-1.44262200	3.45160800
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O	-2.84295700	0.99139000	2.43525400	C	0.34202100	-2.26792200	4.53983200
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N	-2.10448300	1.16737100	0.00181200	C	0.77940600	-4.10358500	3.03773500
H	-1.53501700	1.76642300	-0.60211400	H	0.58062900	-3.64861600	0.94147700
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C	0.74137500	6.24098000	0.13662800	H	0.88469300	-4.25562000	5.19035900
H	-0.39714400	4.41381200	0.10525600	C	2.00297800	-1.47774200	-0.93442500
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C	1.63254100	1.77938600	2.21484800	C	6.05679000	0.81446500	-0.06971200
C	0.86021800	1.99858200	3.36650500	C	6.40454000	0.43327100	1.22232900
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C	1.46973900	2.05522700	4.61829200	H	6.60806000	1.61434700	-0.55100300
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C	3.62650500	1.70444400	3.58290800	C	0.32446200	-2.72134100	-2.37559800
H	3.61150100	1.49344500	1.43164600	C	-0.23122000	-1.76968800	-3.26451700
C	2.85551400	1.90413700	4.73048700	C	-0.28037700	-3.97388900	-2.13659000
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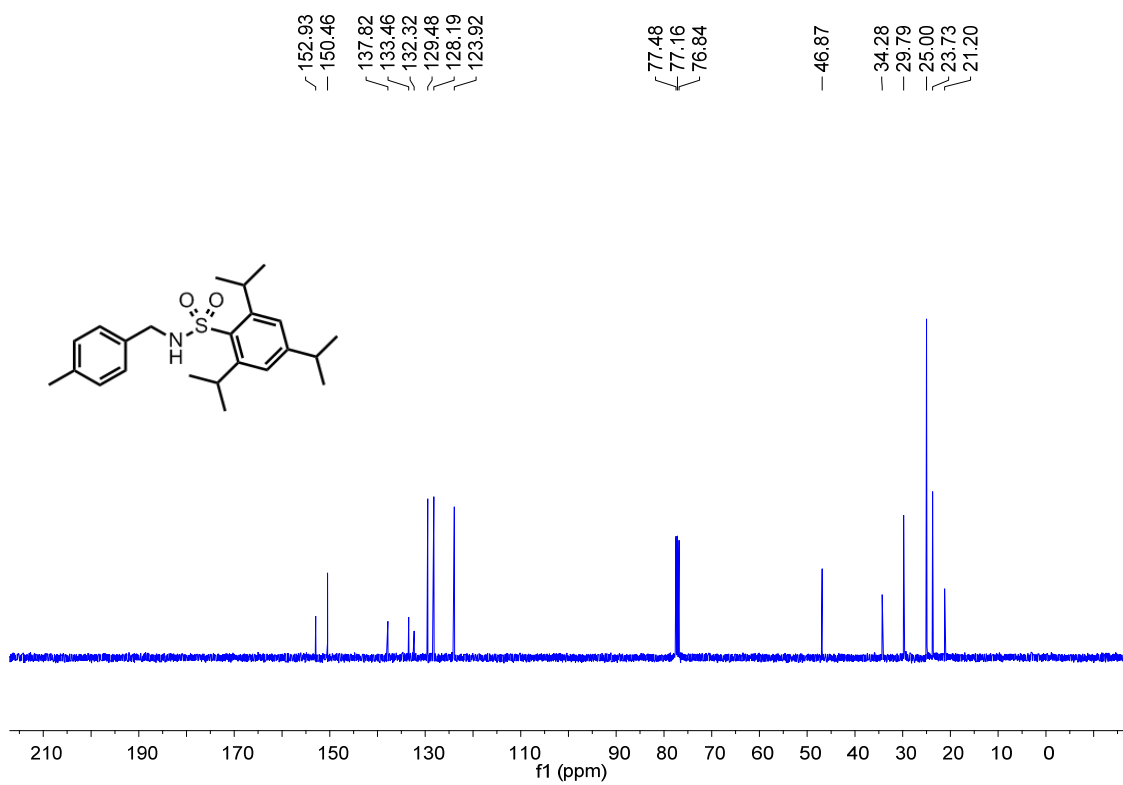
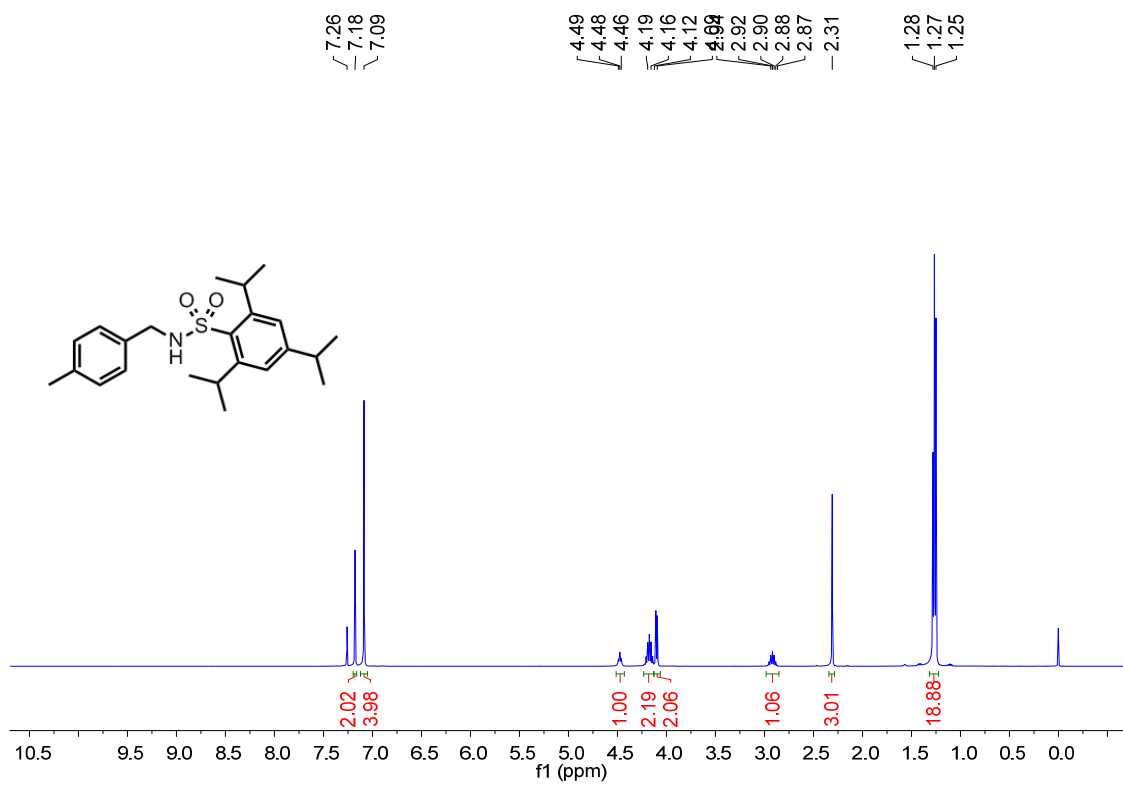
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C	1.70806400	-0.71306500	-4.52013300	Ni	-0.00954800	-0.77826500	-0.21321600
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H	-1.08545100	-4.96175800	0.35276300	C	0.40700400	-4.02820000	0.24628500
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C	4.90249300	2.12447600	-2.39352600	H	5.38144400	-1.04458800	-0.84357500
H	4.42291900	2.43937700	-3.32351900	H	6.72087600	-1.94016700	-0.12557900
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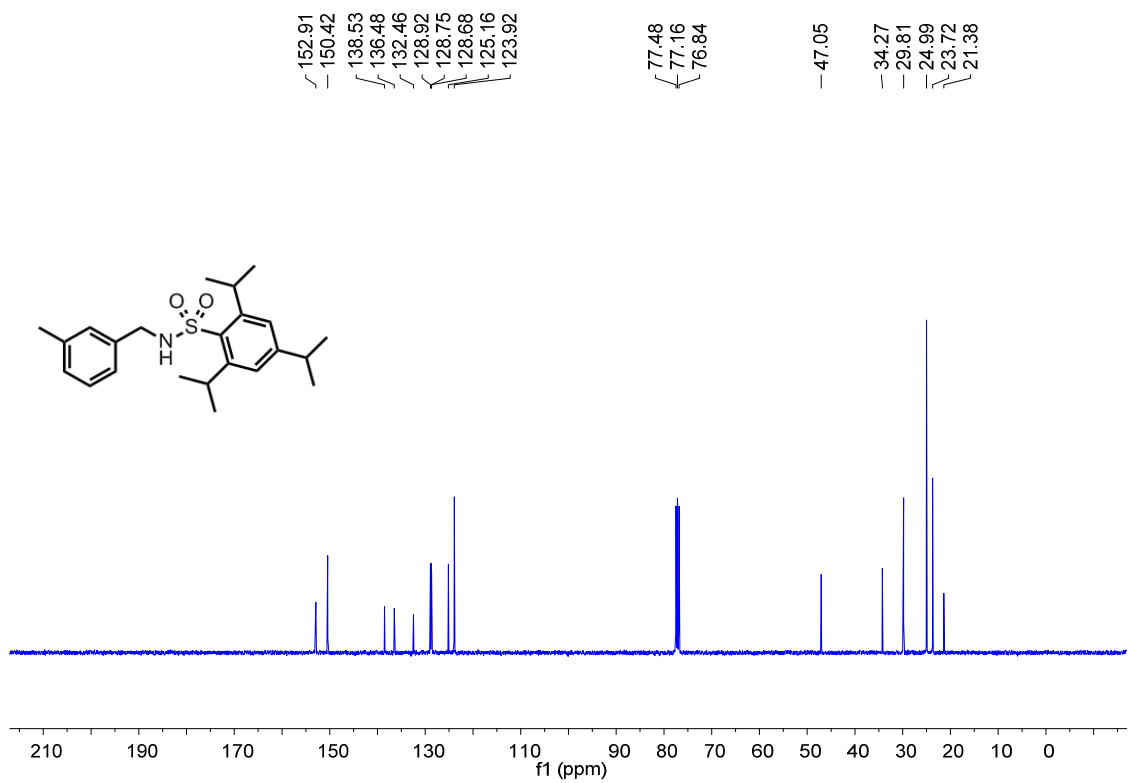
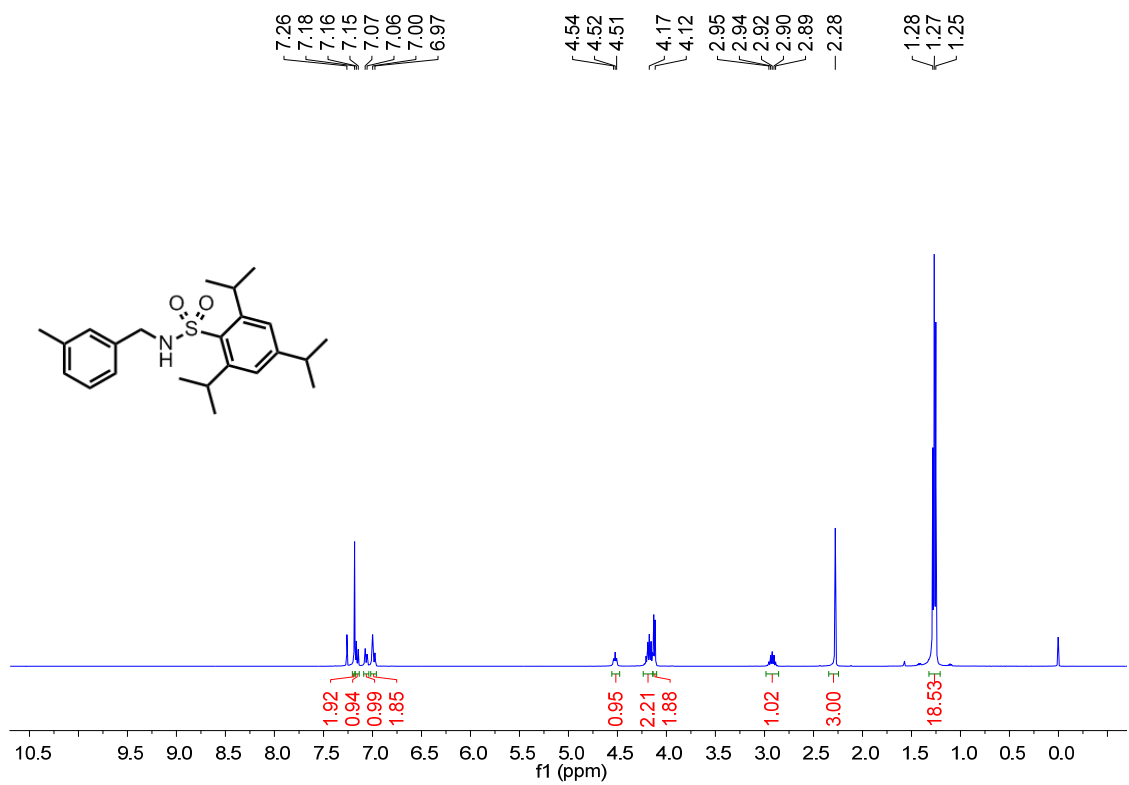
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H	-2.39942500	-4.96674200	-1.41948400	O	0.02389800	4.72119400	-0.71070100
H	-1.92678800	-6.65017900	-1.65115700	O	-0.96328700	2.72815400	-1.87438100
H	-2.32783100	-6.13077900	0.77884100	N	-0.29272100	2.60050900	0.67465000
H	-0.66146900	-6.62257700	0.48602600	H	-1.02626900	1.94901600	0.97172200
H	-1.66126700	-3.73695300	0.82986500	C	-4.32324400	-0.41485400	1.01465000
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H	-0.44733800	-2.69156600	2.71218700	C	-5.07373100	-1.55924900	0.73138600
H	1.64791200	-0.62286700	3.46322900	C	-6.20624300	0.99654100	0.54336300
H	0.05280800	-0.29511500	2.78495900	H	-4.26428400	1.73289700	1.16004400
H	0.05146700	-0.07834400	5.26787300	C	-6.40521900	-1.41207900	0.34843900
H	-1.04386800	-1.34417700	4.71013700	H	-4.61855900	-2.54053800	0.81822200
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H	0.27652700	-2.16391400	6.66760000	H	-6.64293400	1.98783300	0.47221700
H	1.33873400	-4.19609700	5.62825600	H	-7.00310800	-2.29103100	0.12514700
H	-0.25465500	-3.87231800	4.94326300	O	-2.48506900	-1.71137400	2.42931200
H	2.43050800	-3.11237100	3.67884400	N	-1.92256100	-1.14331900	0.03430300
H	1.36821500	-4.41105700	3.13659500	C	-1.83139100	-0.18225500	-0.98007000
S	-2.59709000	-0.61442700	1.45802900	H	-2.15591600	0.83579300	-0.76507000
O	-2.10567600	0.73257900	1.86016800	H	-0.29902800	0.38478300	-1.18342000
C	1.72010100	1.56366400	-0.52305600	C	-2.17228100	-0.65424900	-2.35698400
C	1.06435400	1.98883800	0.80628800	C	-2.01873200	0.20300300	-3.45814000
H	0.84194700	1.05604400	1.33124900	C	-2.64963300	-1.95596000	-2.56410000
C	1.95880800	2.80244300	1.72829400	C	-2.31136800	-0.24962700	-4.74316700
C	2.79036000	2.11522100	2.62150300	H	-1.63801300	1.20552000	-3.29981800
C	2.01812800	4.20020100	1.69034900	C	-2.93576300	-2.40706200	-3.85287900
C	3.67764300	2.80207900	3.45110400	H	-2.79651200	-2.59920100	-1.70439300
H	2.75224100	1.03247100	2.65650100	C	-2.76152000	-1.55789100	-4.94768600
C	2.90034000	4.88877800	2.52436000	H	-2.17749400	0.41842400	-5.58971200
H	1.38955700	4.74480300	0.99637600	H	-3.29875500	-3.42125300	-3.99852900
C	3.73611600	4.19610300	3.40339500	H	-2.98091900	-1.90909400	-5.95248200
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H	2.93999600	5.97407100	2.47865900	C	3.92942500	2.81925500	-0.62434500
H	4.42356200	4.73765600	4.04804800	C	2.32709400	3.07708400	-2.41331300
S	-0.79602600	3.50686700	-0.62797700	C	4.80998200	3.66989100	-1.29280800
C	-2.45640100	3.88713300	-0.04761900	H	4.22097700	2.38437600	0.32545700
C	-2.65538200	4.35156500	1.25565900	C	3.20493800	3.93339100	-3.07581400
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C	-3.94852100	4.67860500	1.66273400	C	4.45115600	4.23079700	-2.52051100
H	-1.81397400	4.43324000	1.93521100	H	5.77771300	3.89413500	-0.85130500
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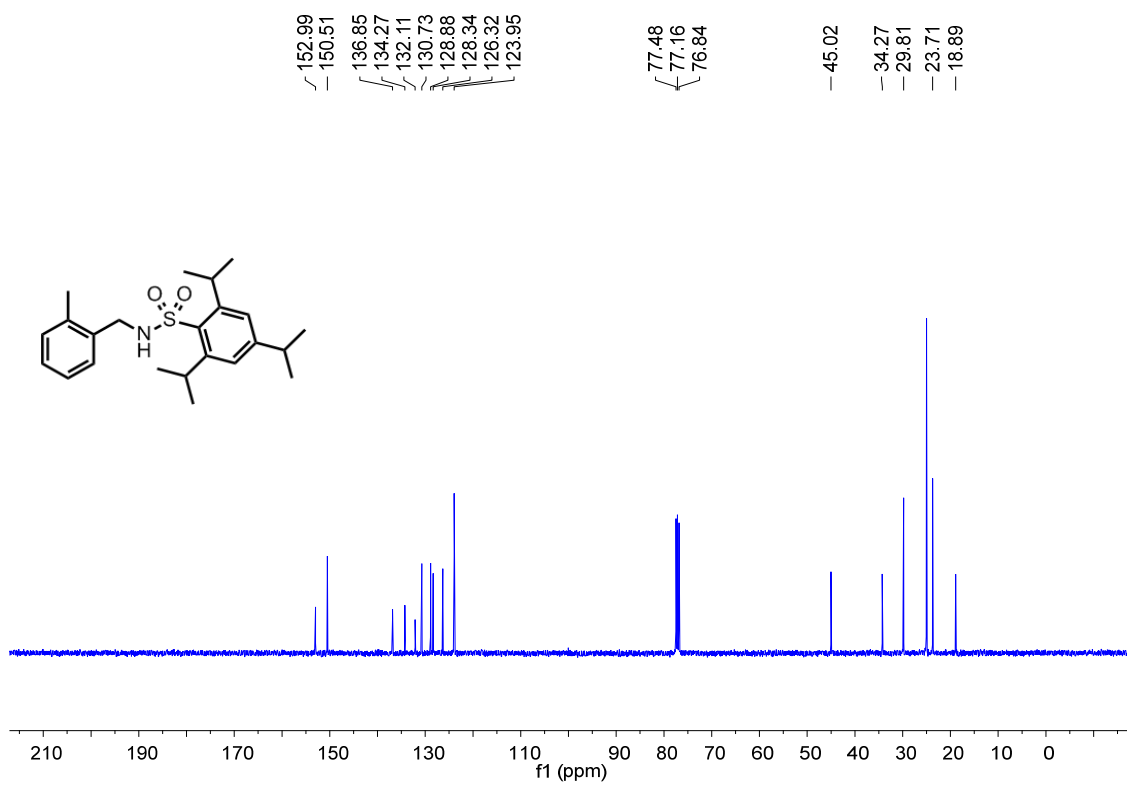
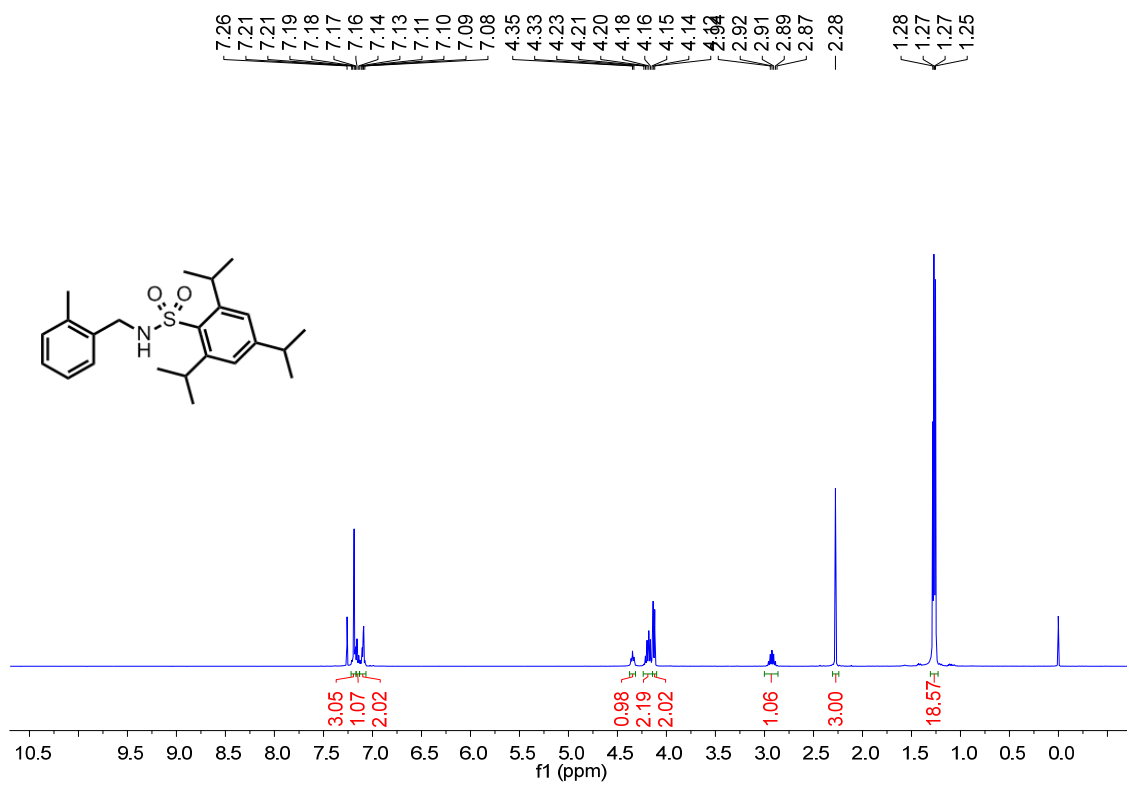
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C	1.20979600	-1.05935100	-3.13608600
C	3.33991000	-0.09693600	-2.57461300
C	1.79051200	-1.72685600	-4.21408000
H	0.15589100	-1.20504700	-2.94314700
C	3.92442700	-0.77182100	-3.64365000
H	3.96116800	0.52282300	-1.94175200
C	3.15499300	-1.59217400	-4.47354100
H	1.16898500	-2.35902900	-4.84310100
H	4.99059200	-0.65925900	-3.82372800
H	3.61375100	-2.11952100	-5.30567000
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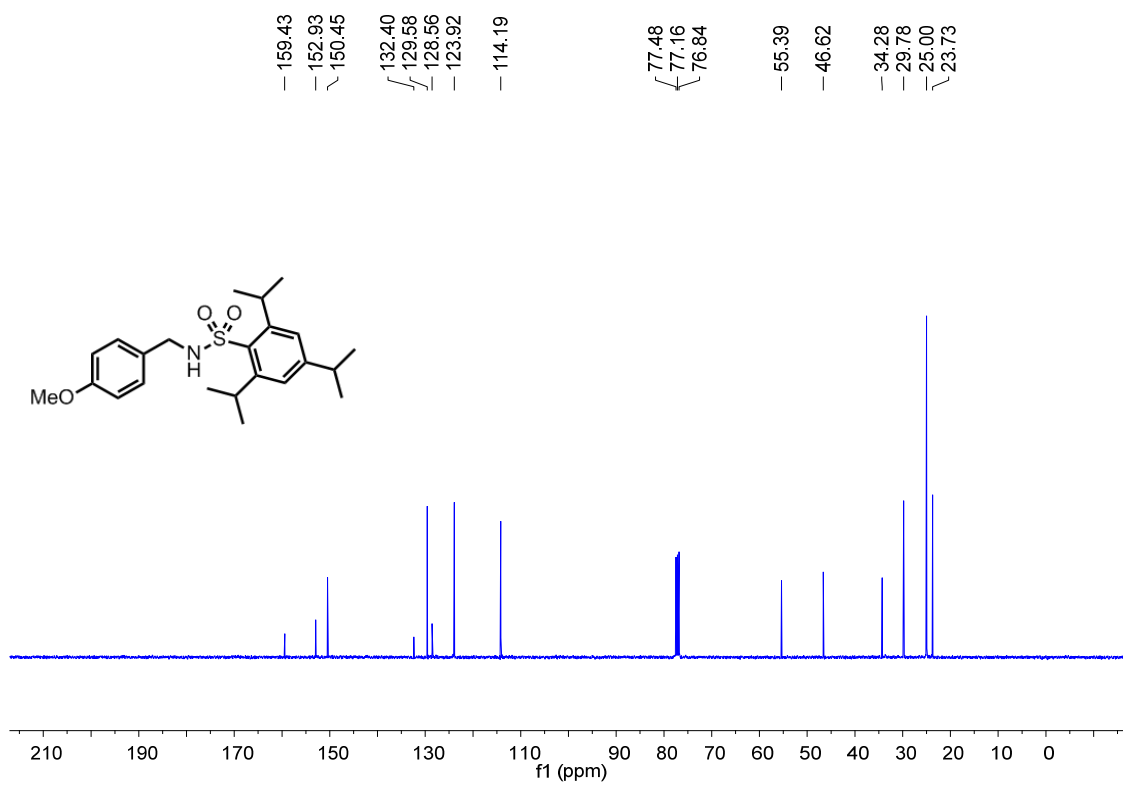
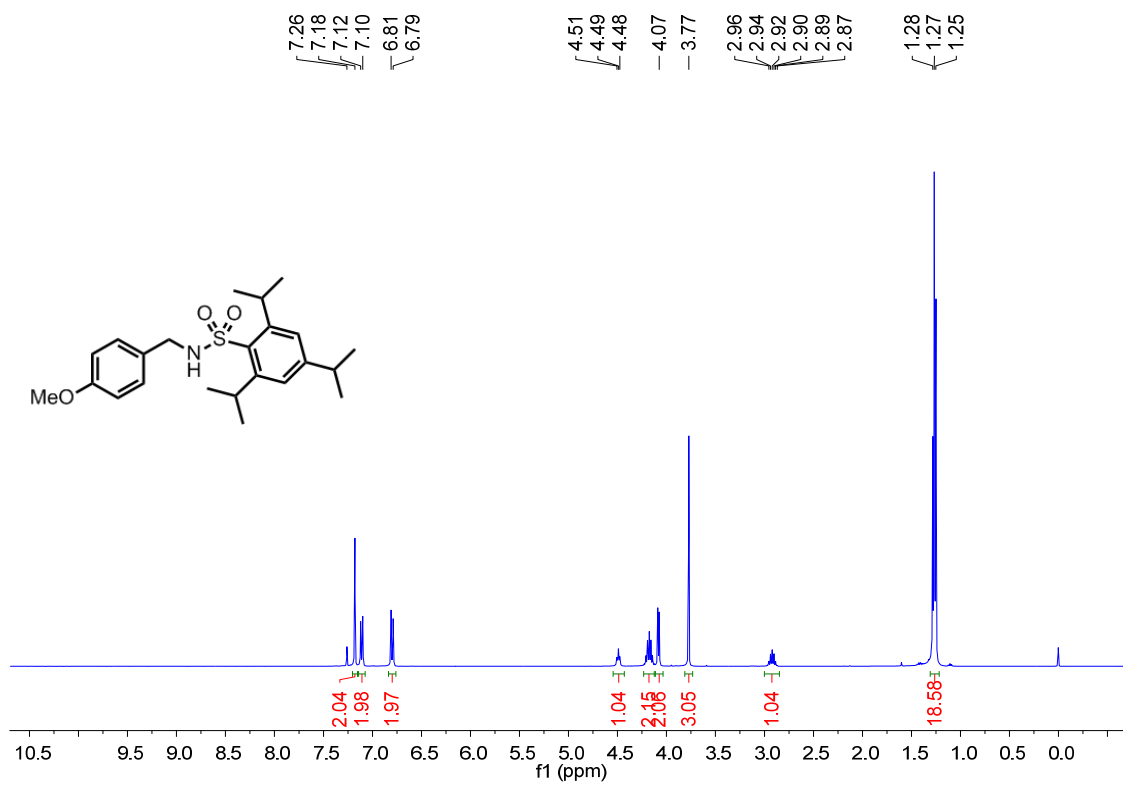
8. NMR Spectra

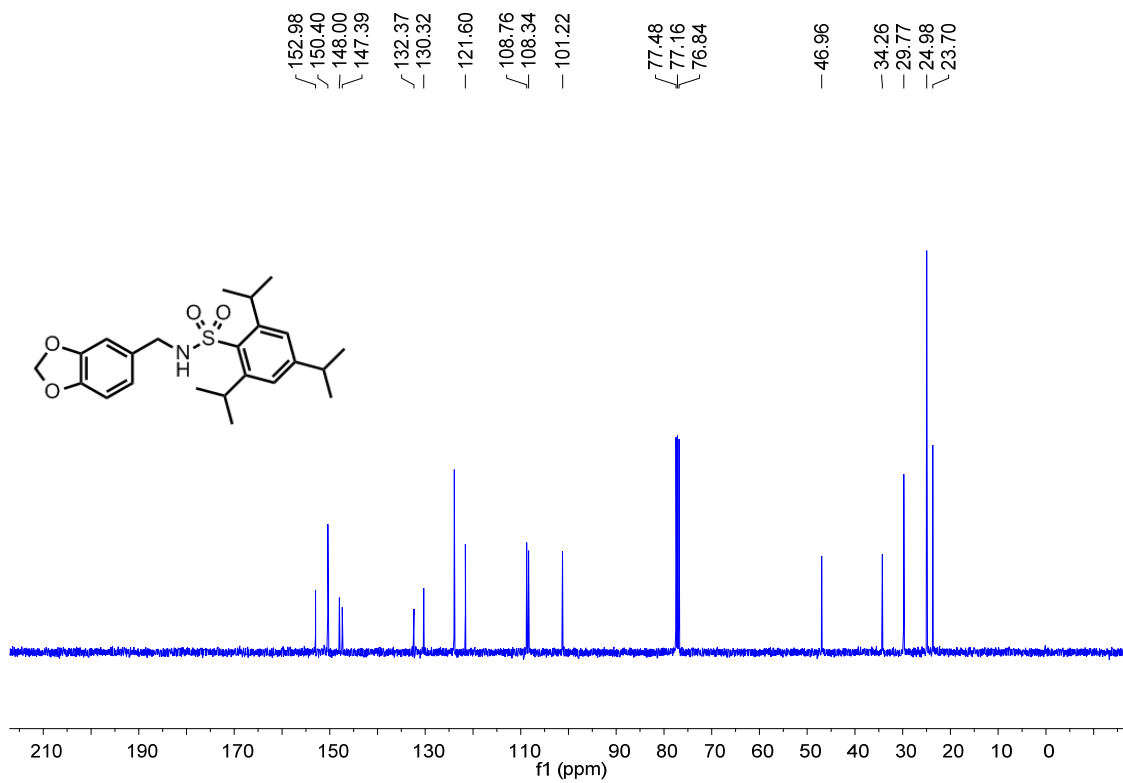
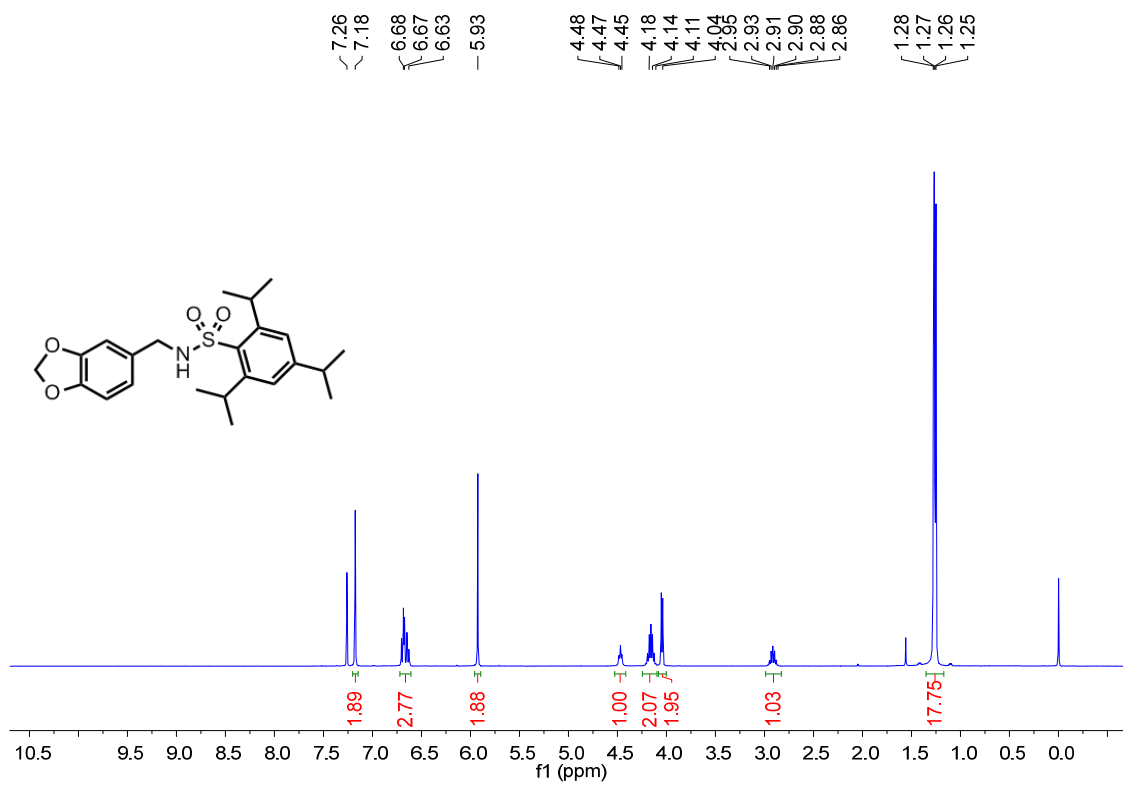


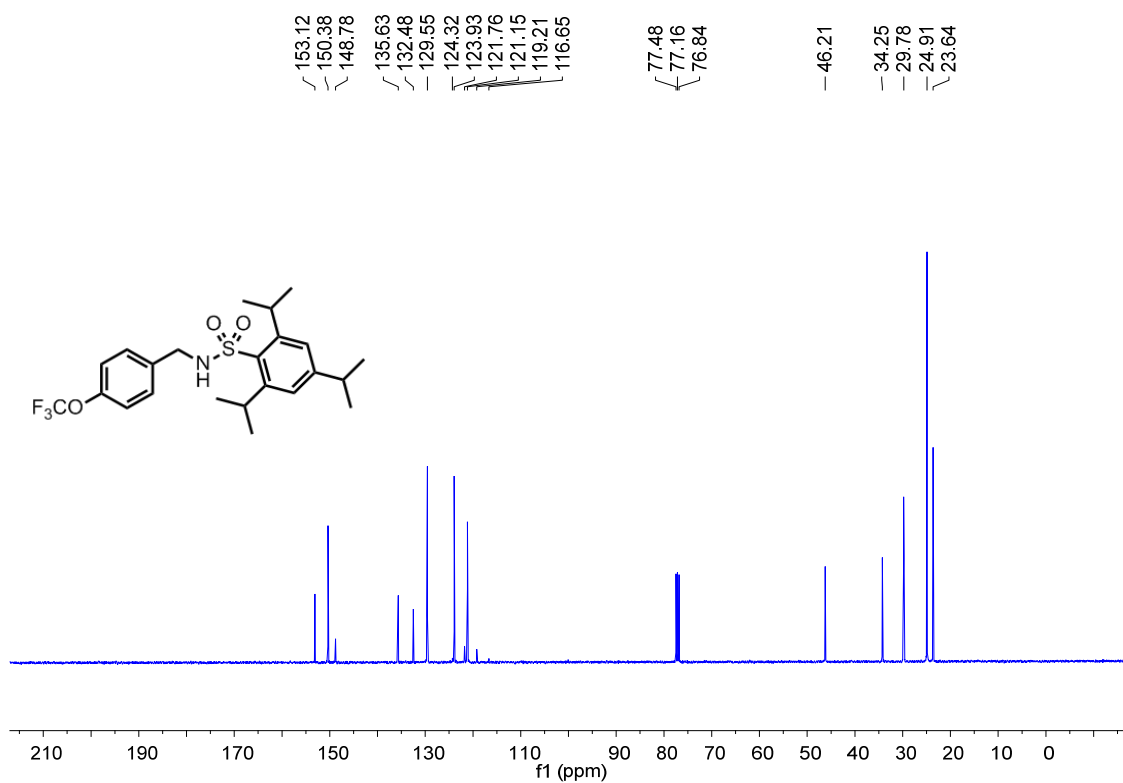
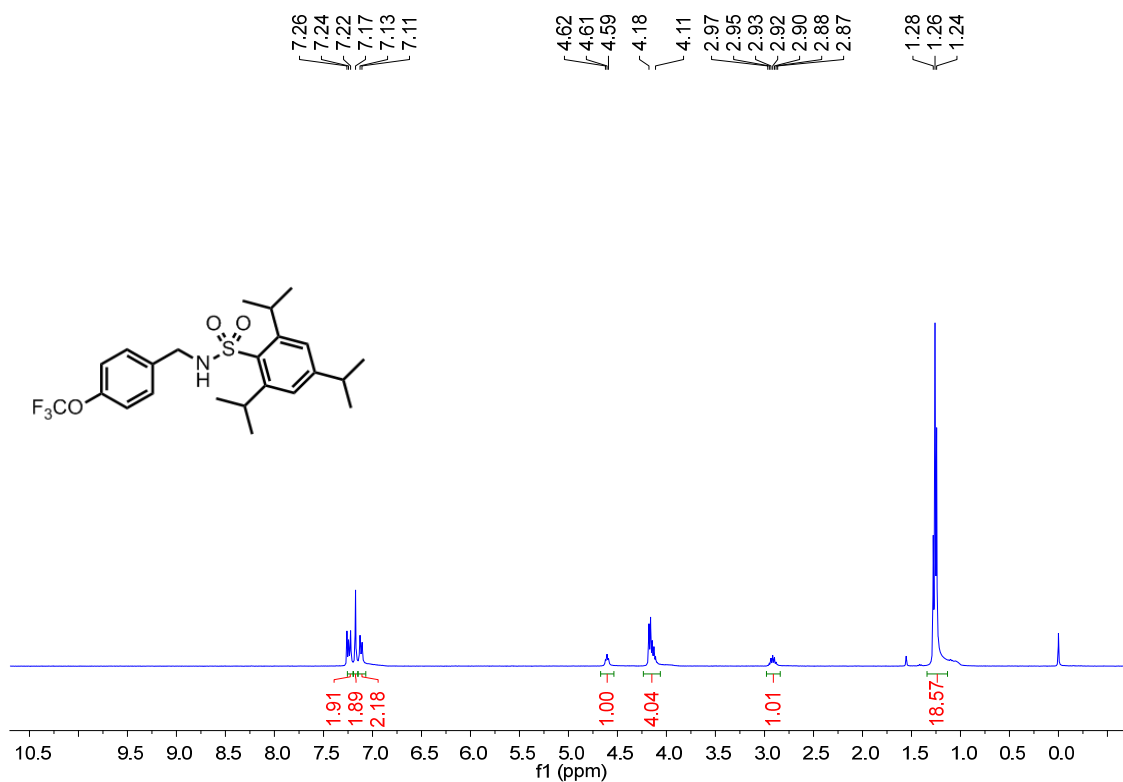


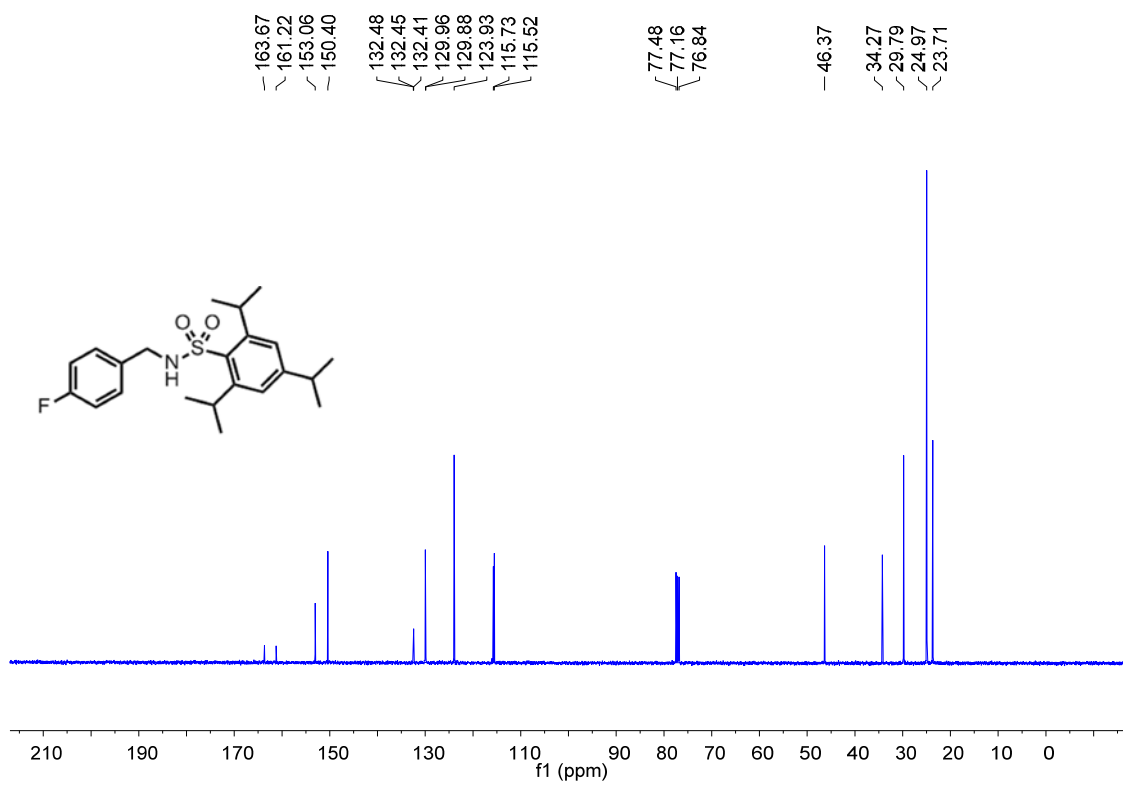
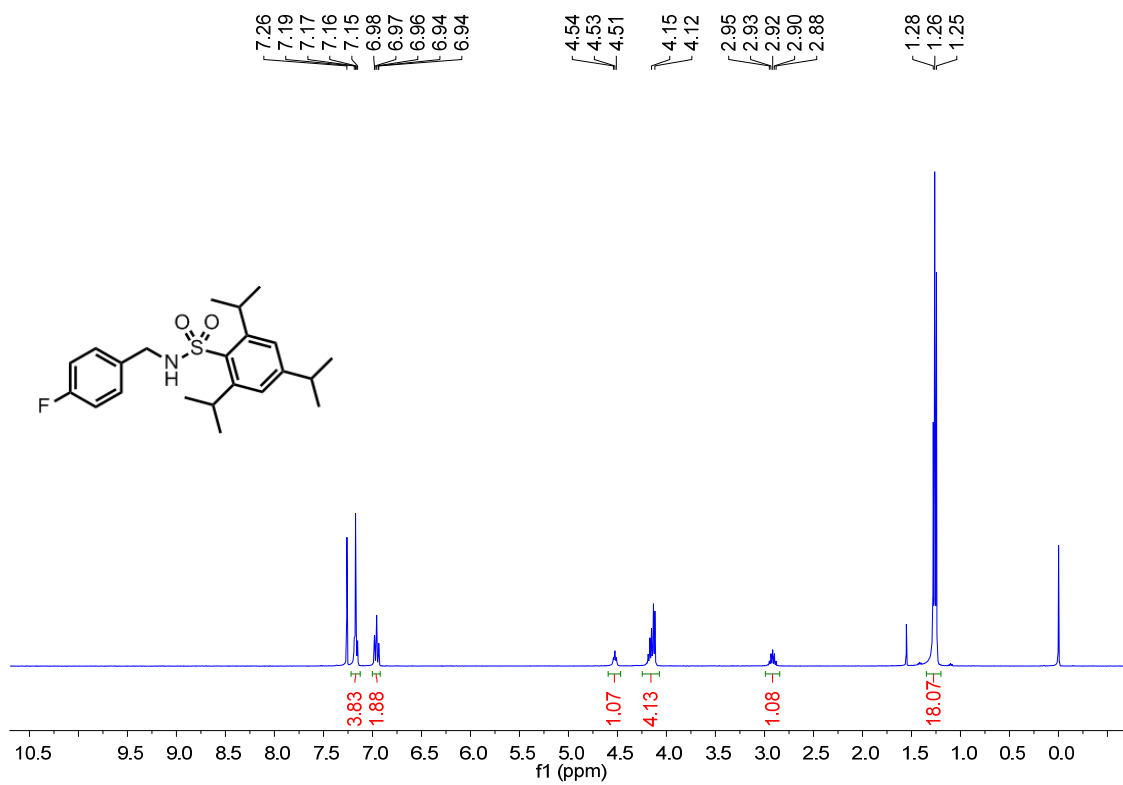


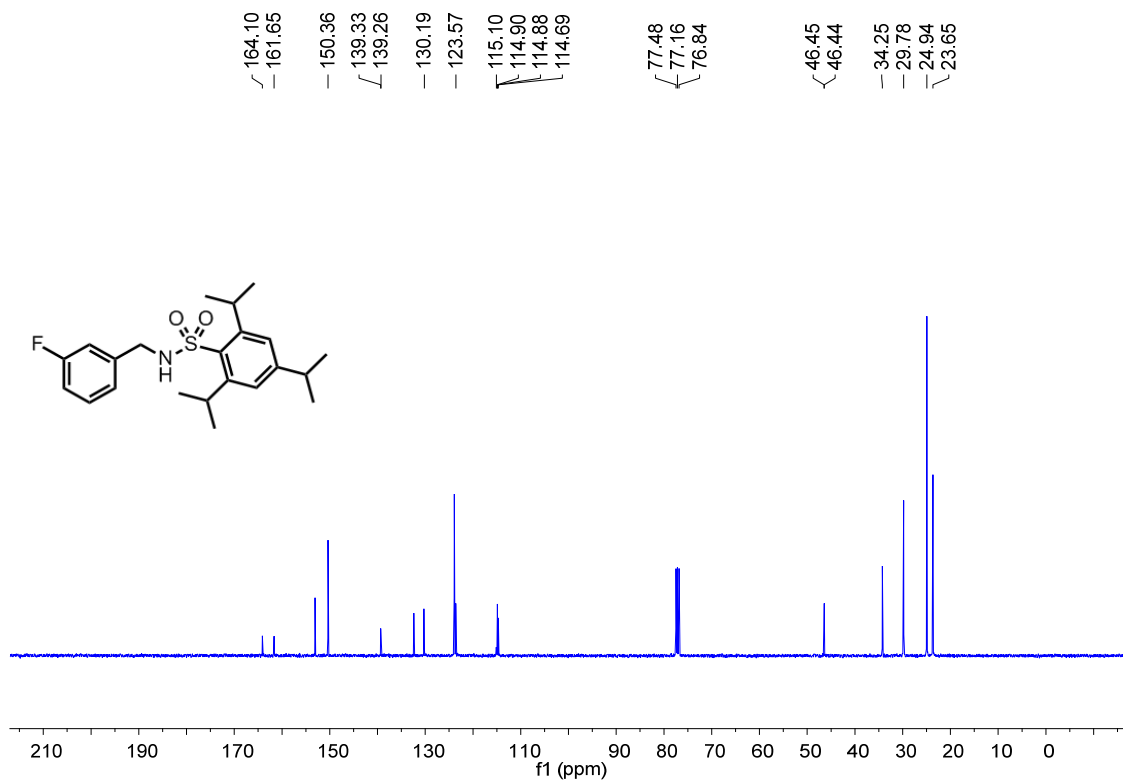
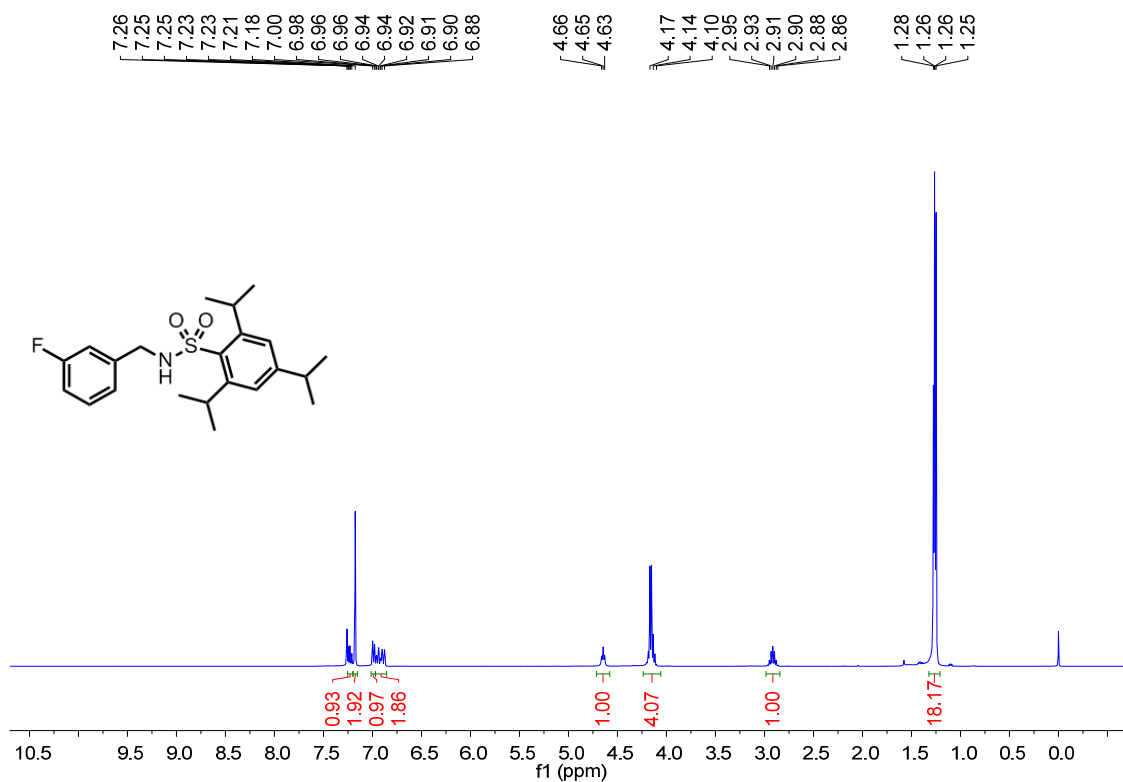


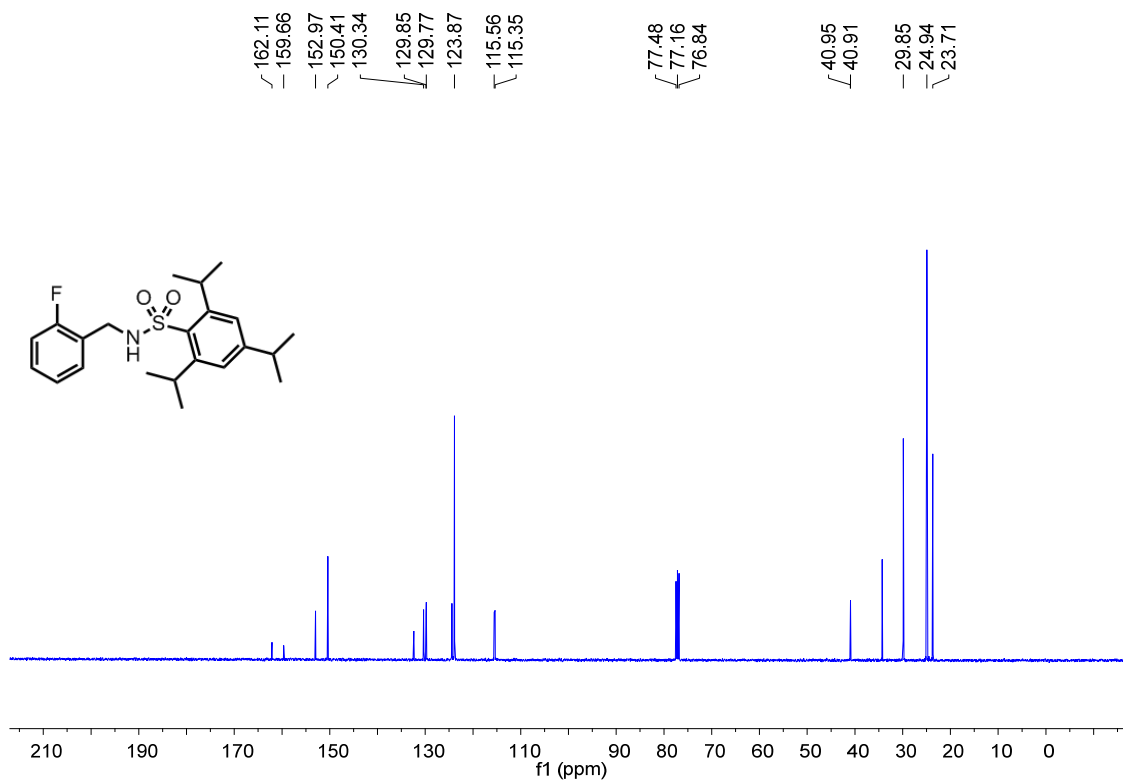
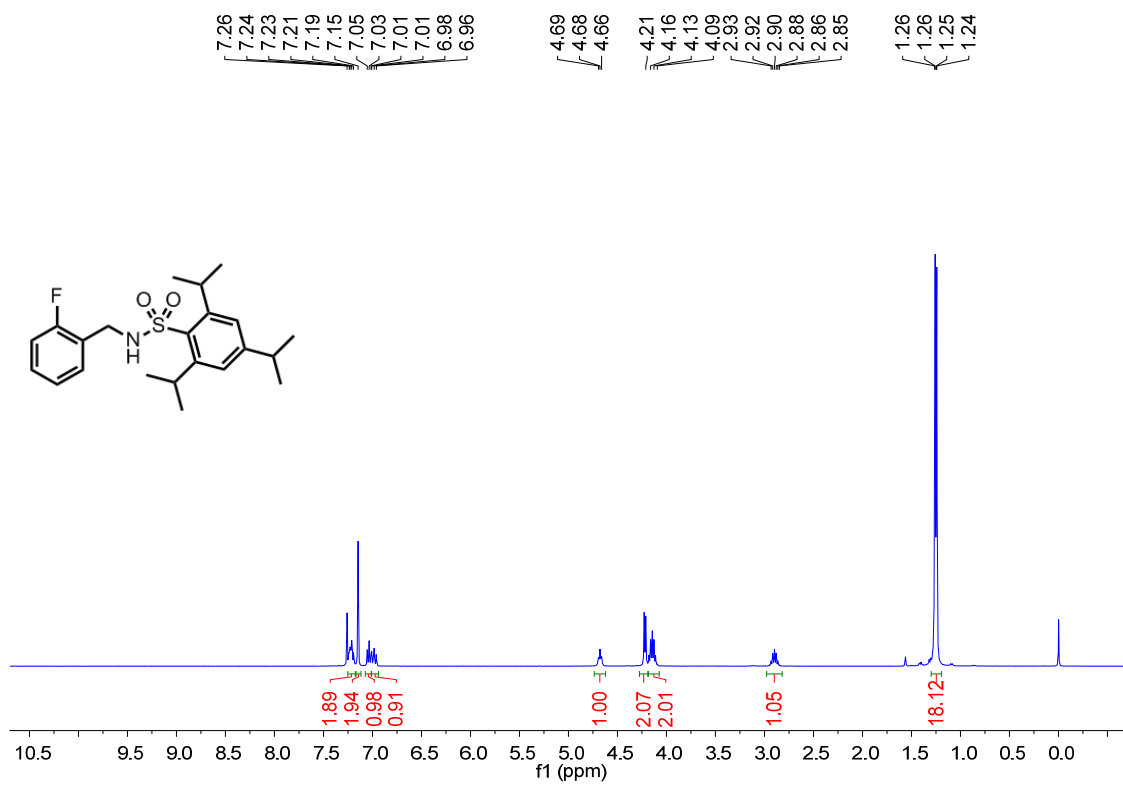


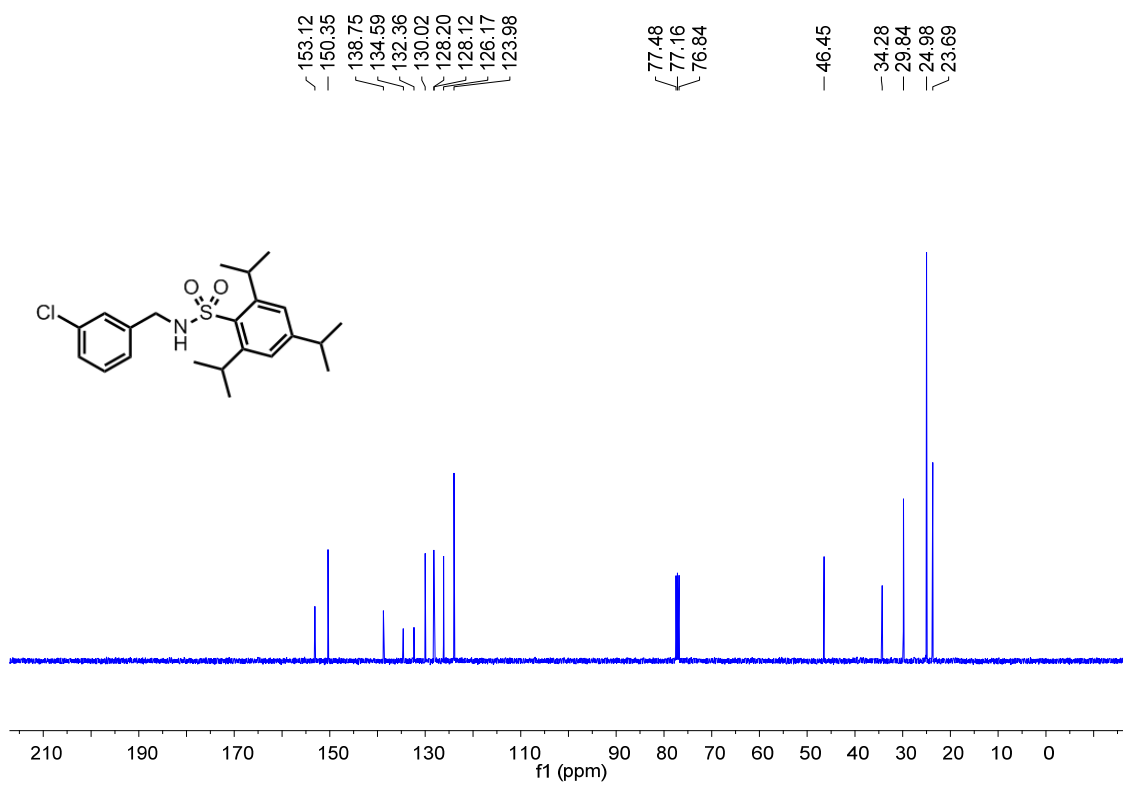
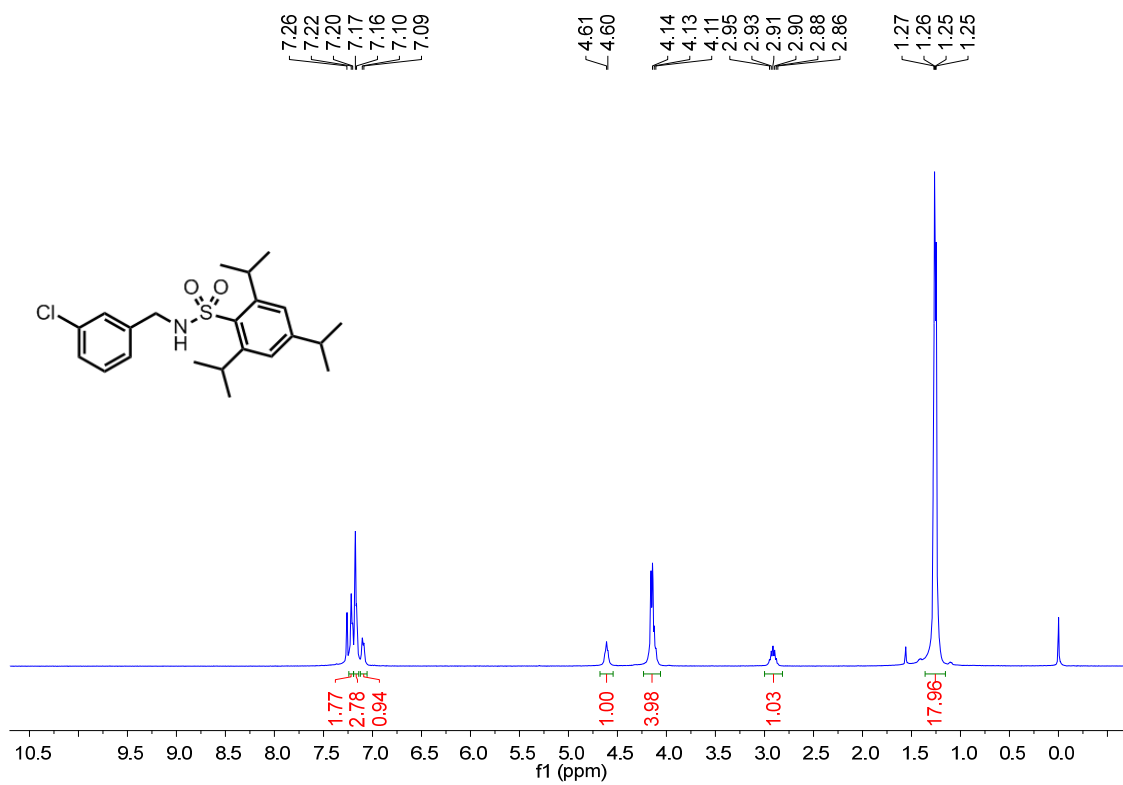


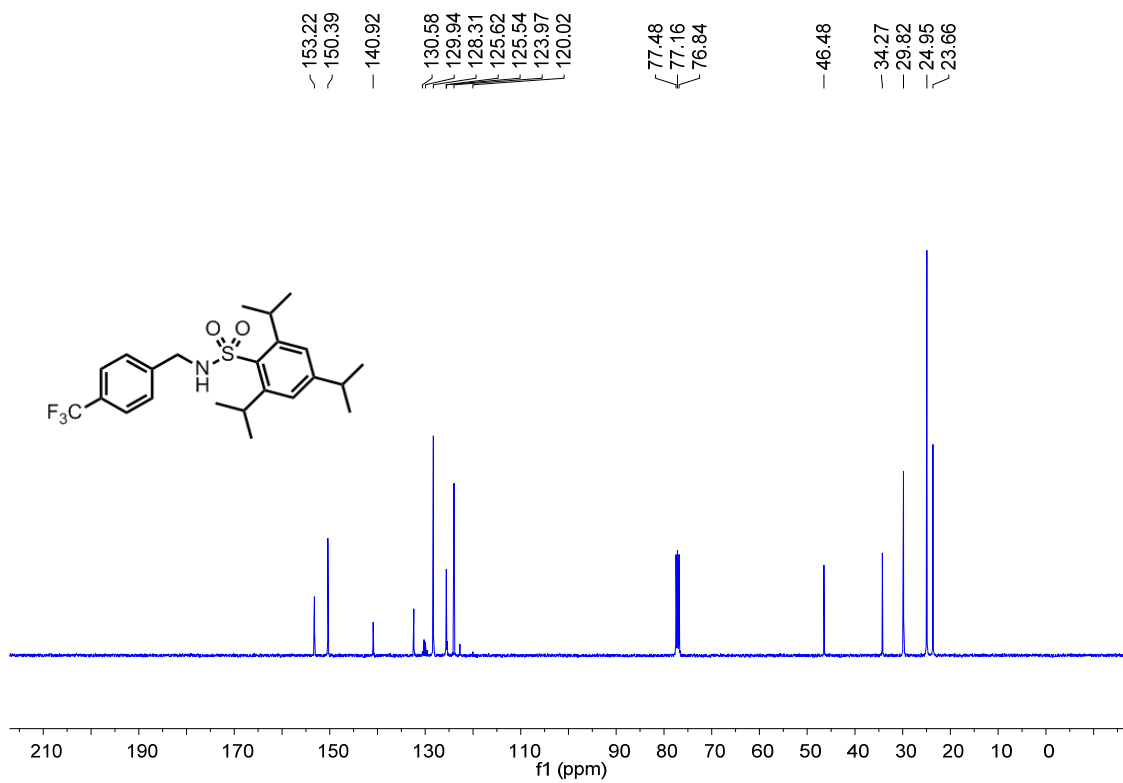
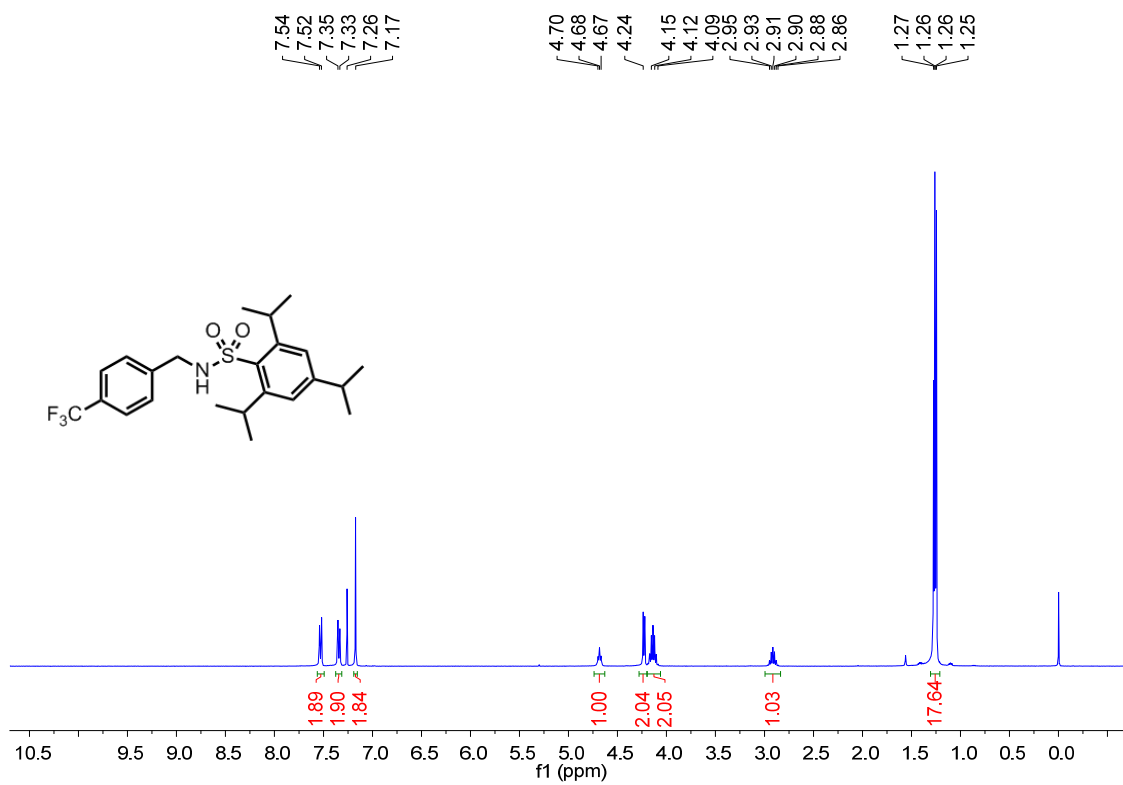


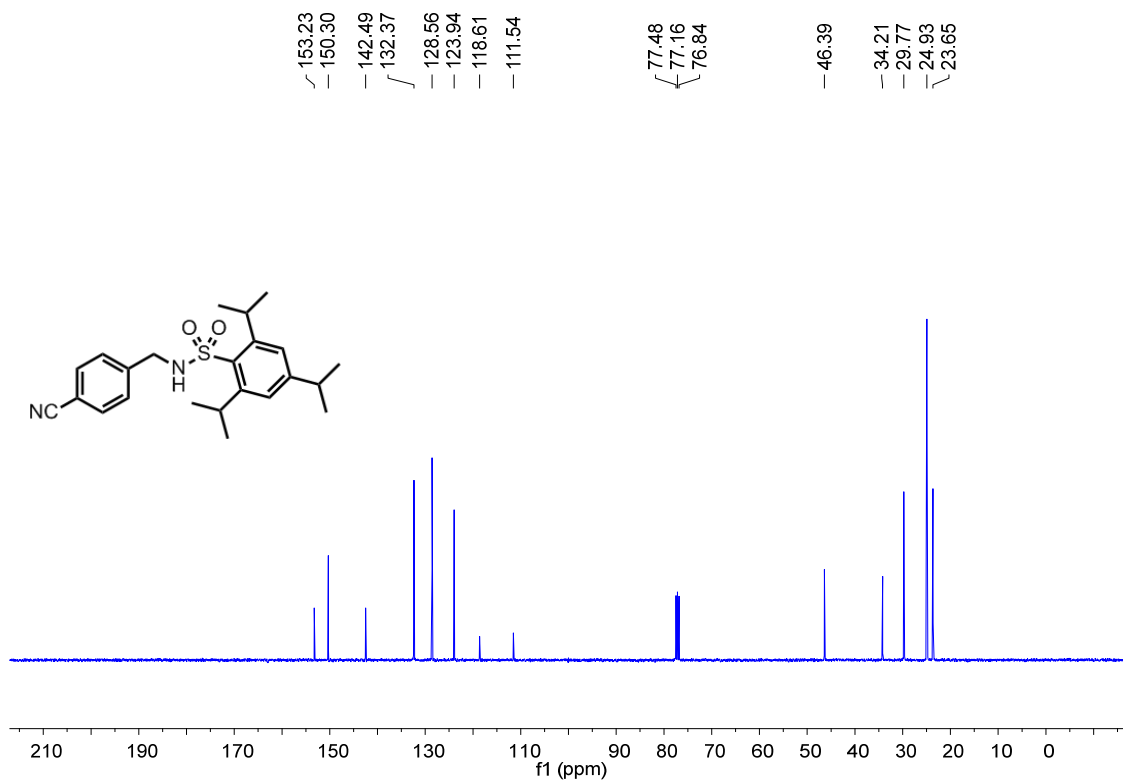
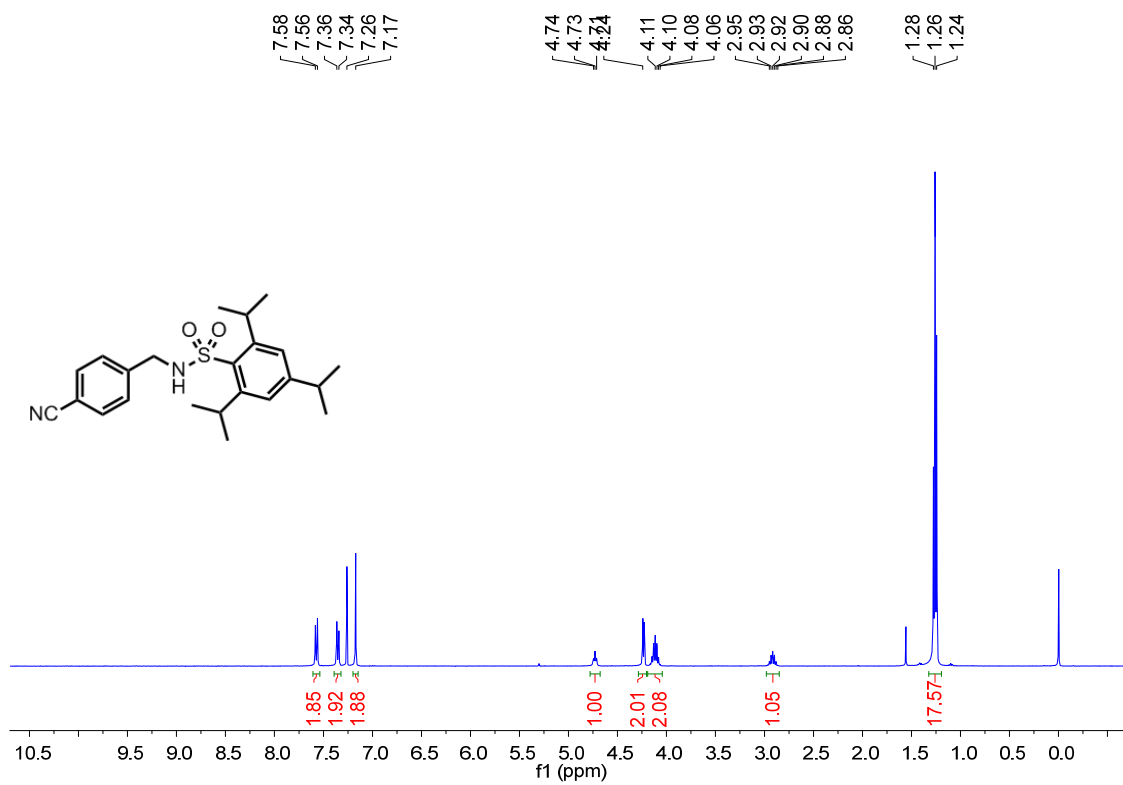


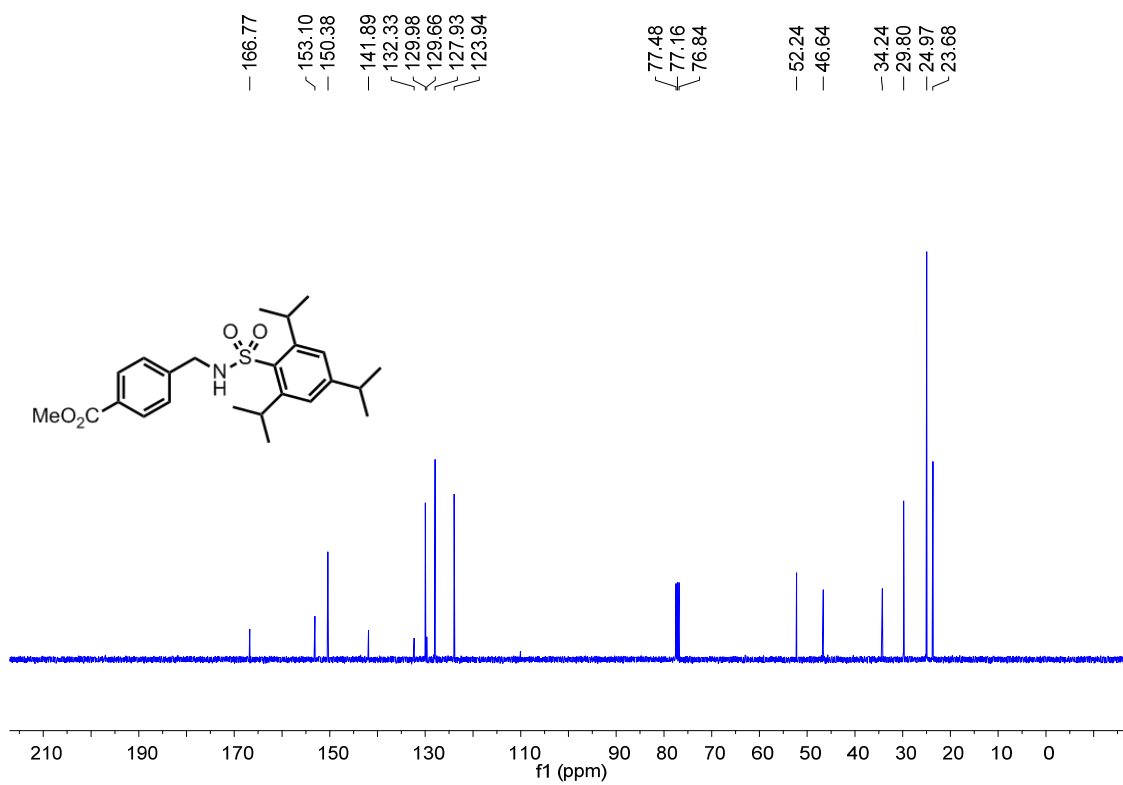
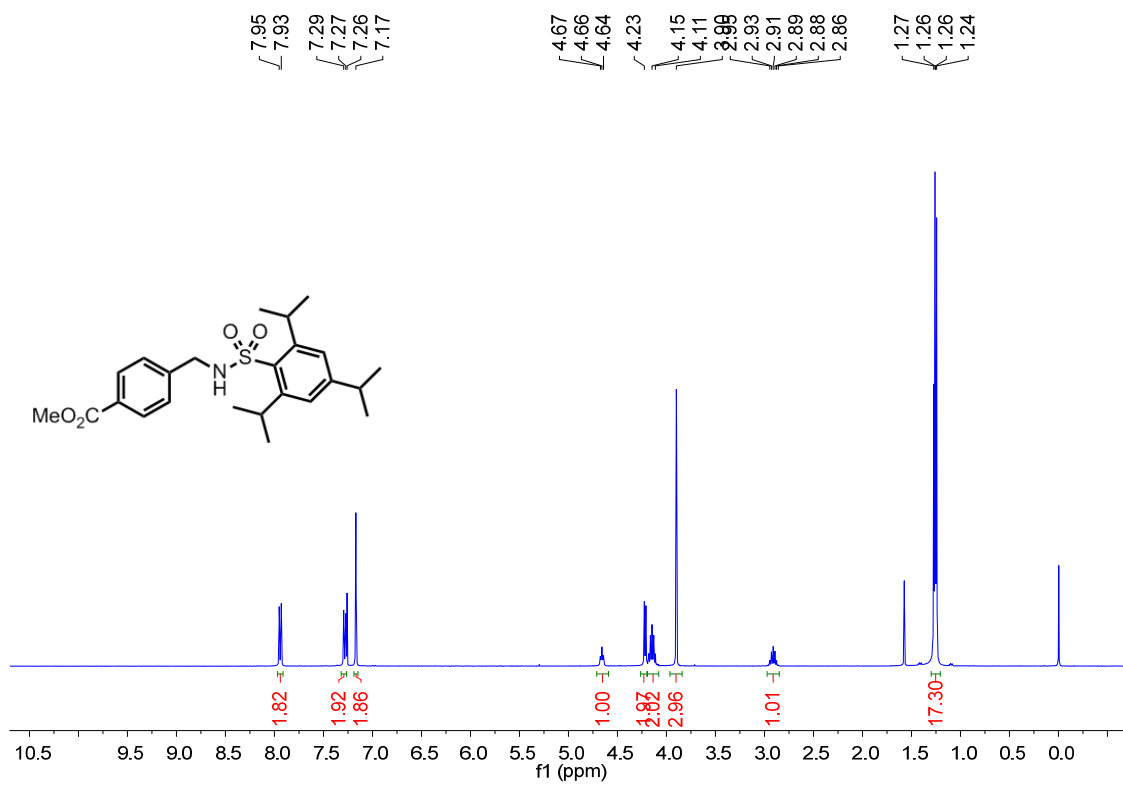


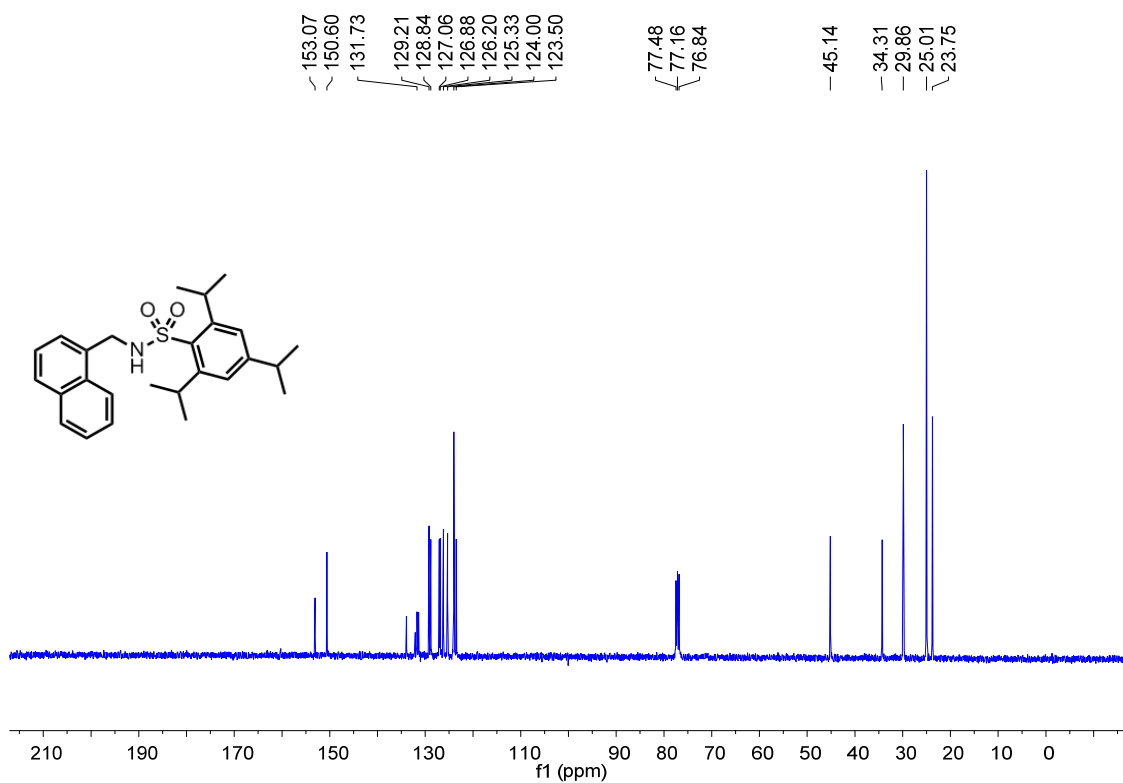
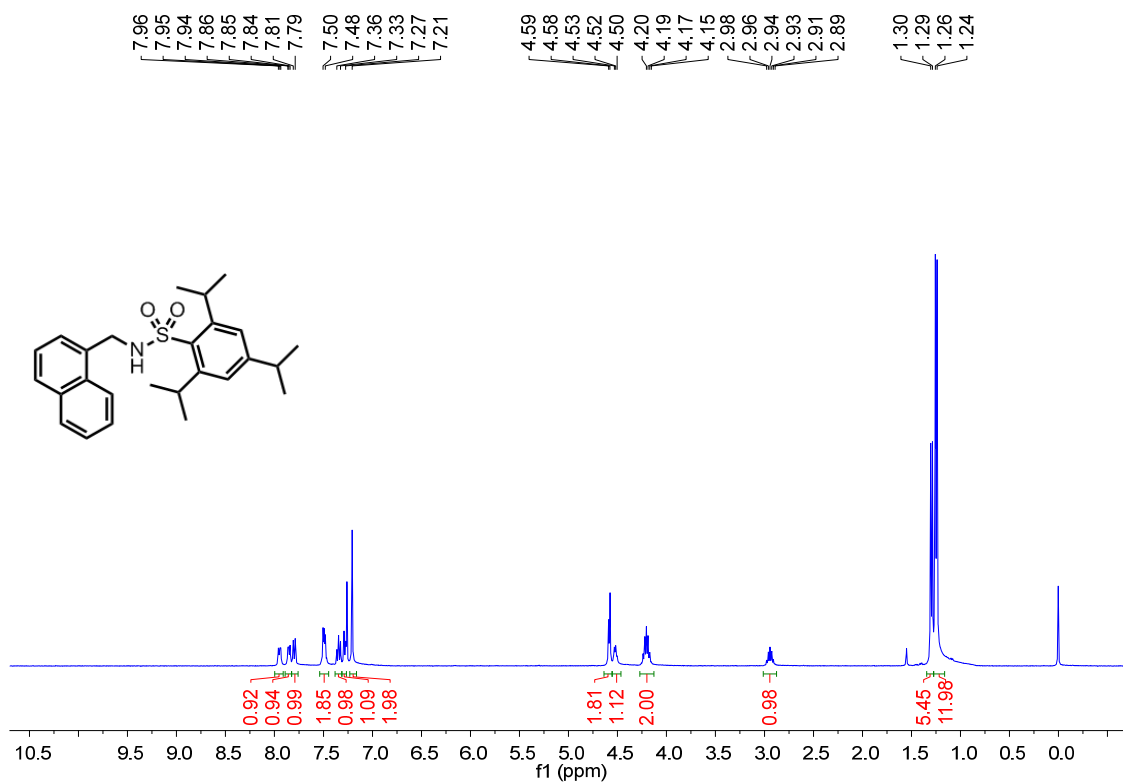


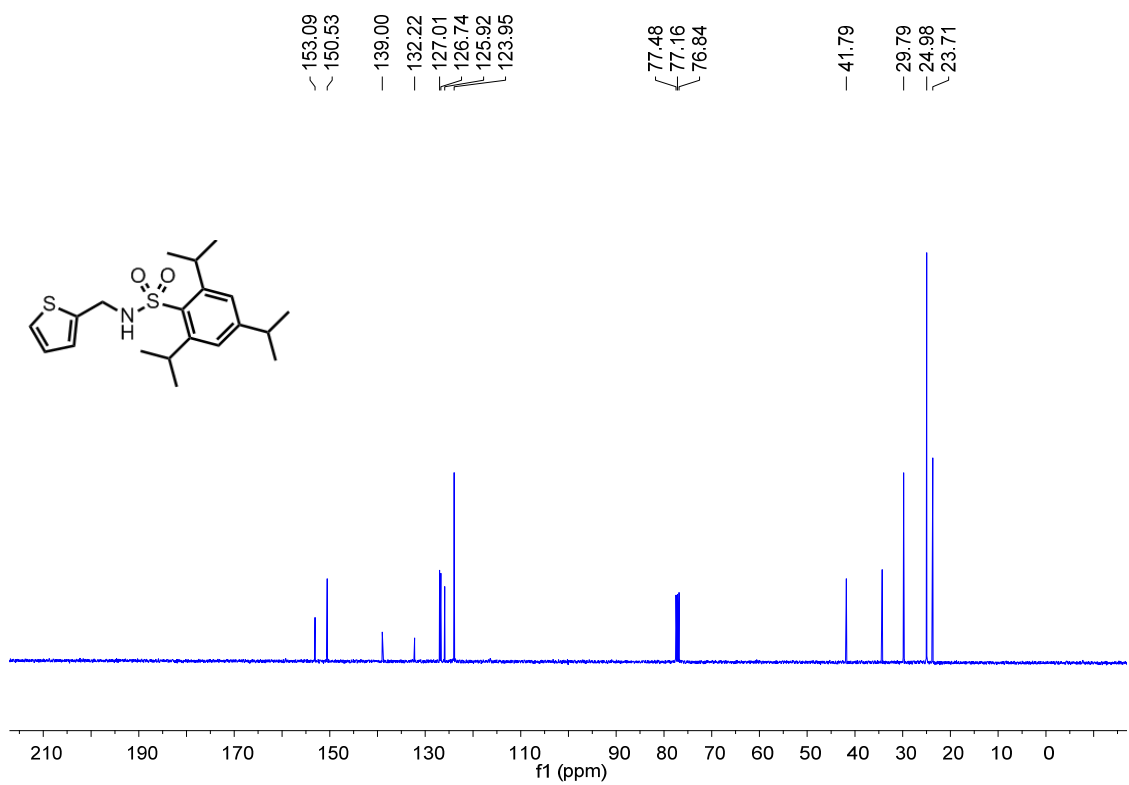
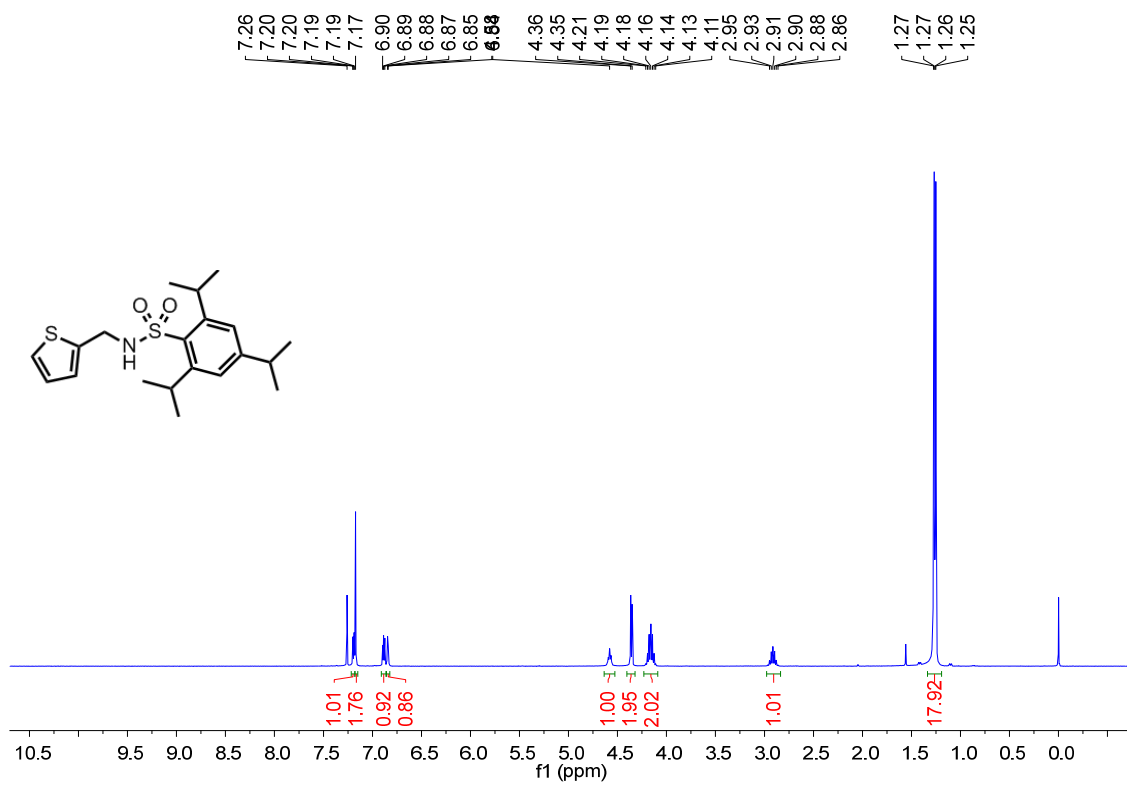


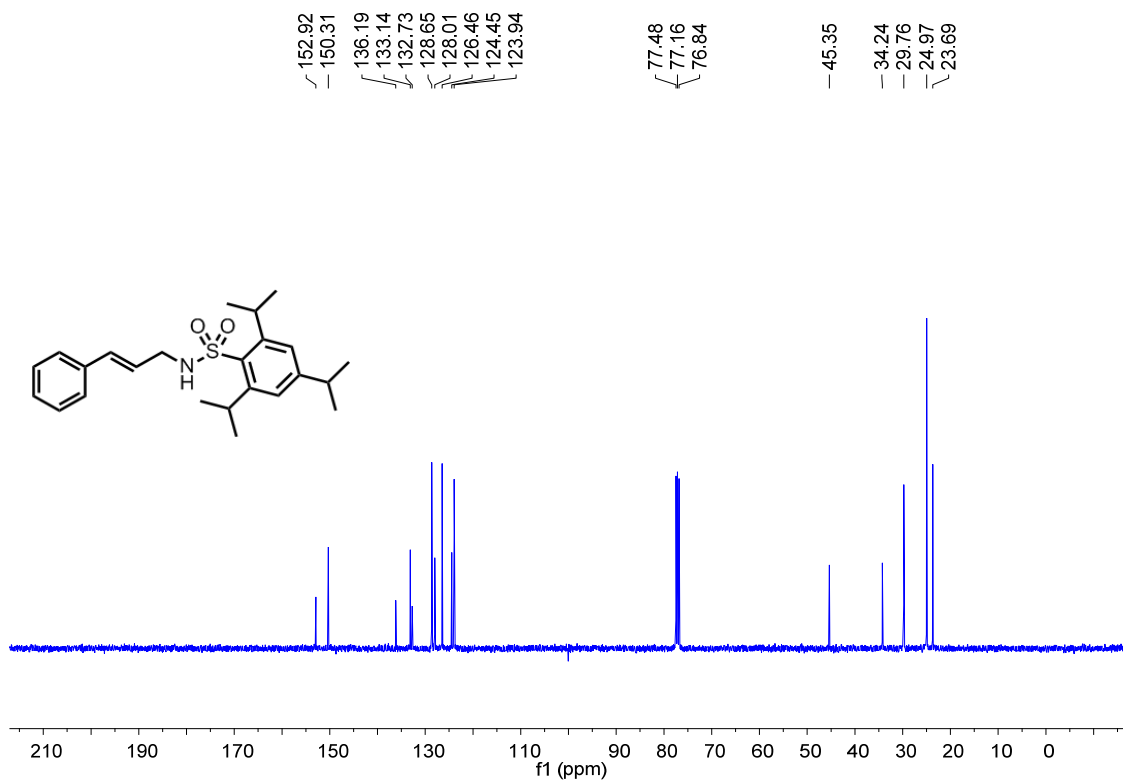
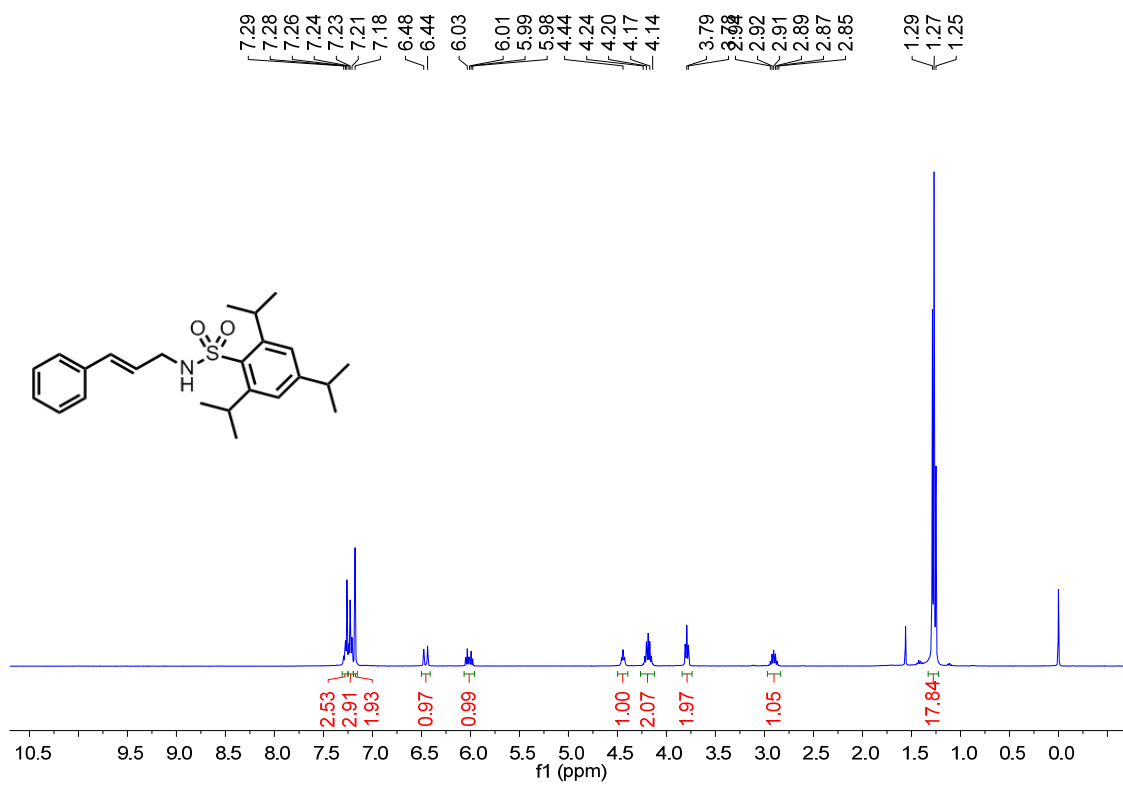


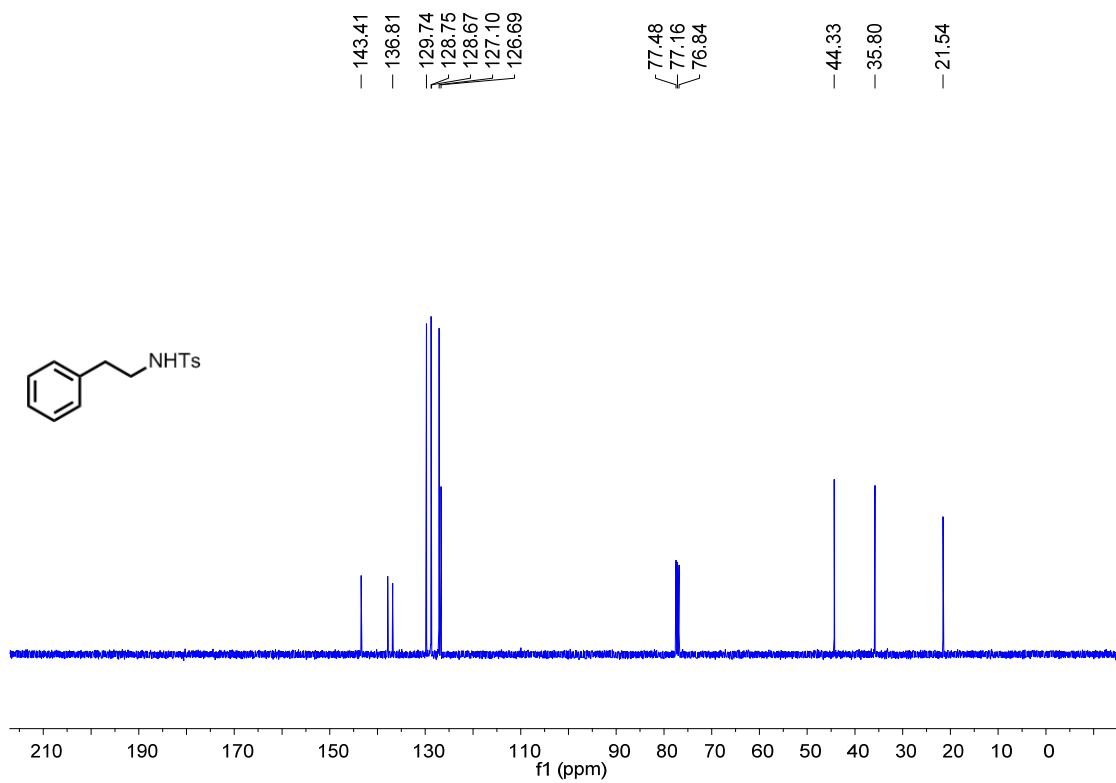
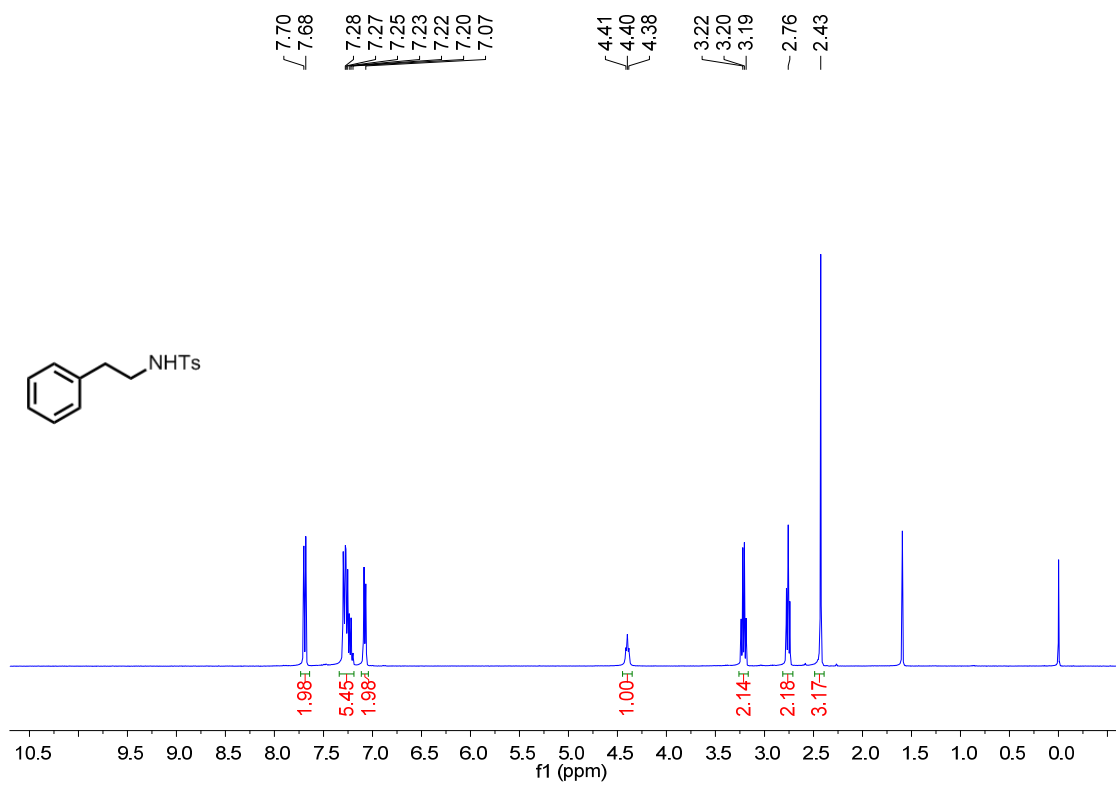


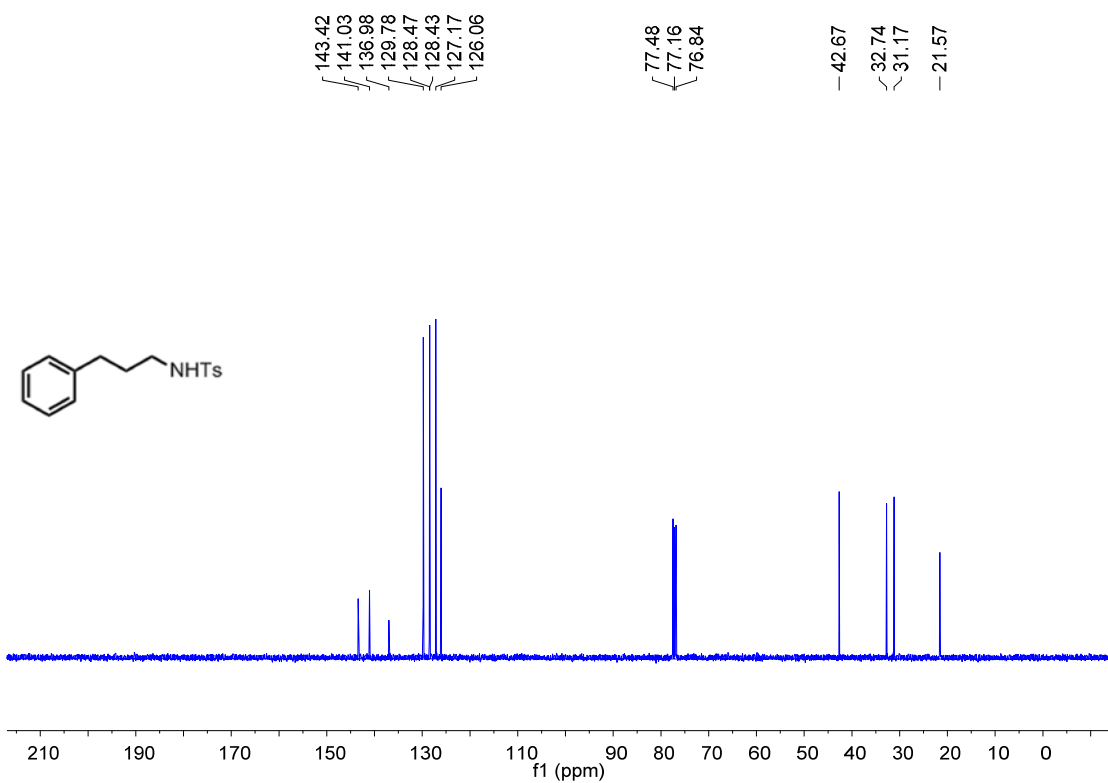
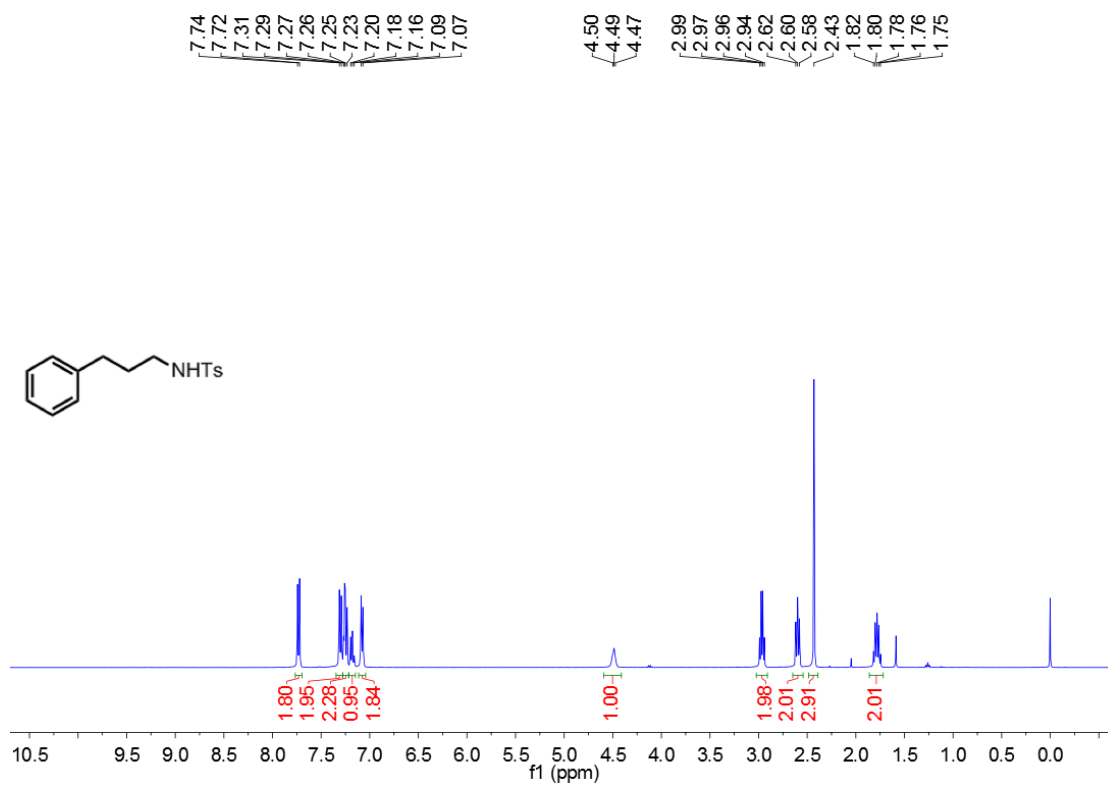


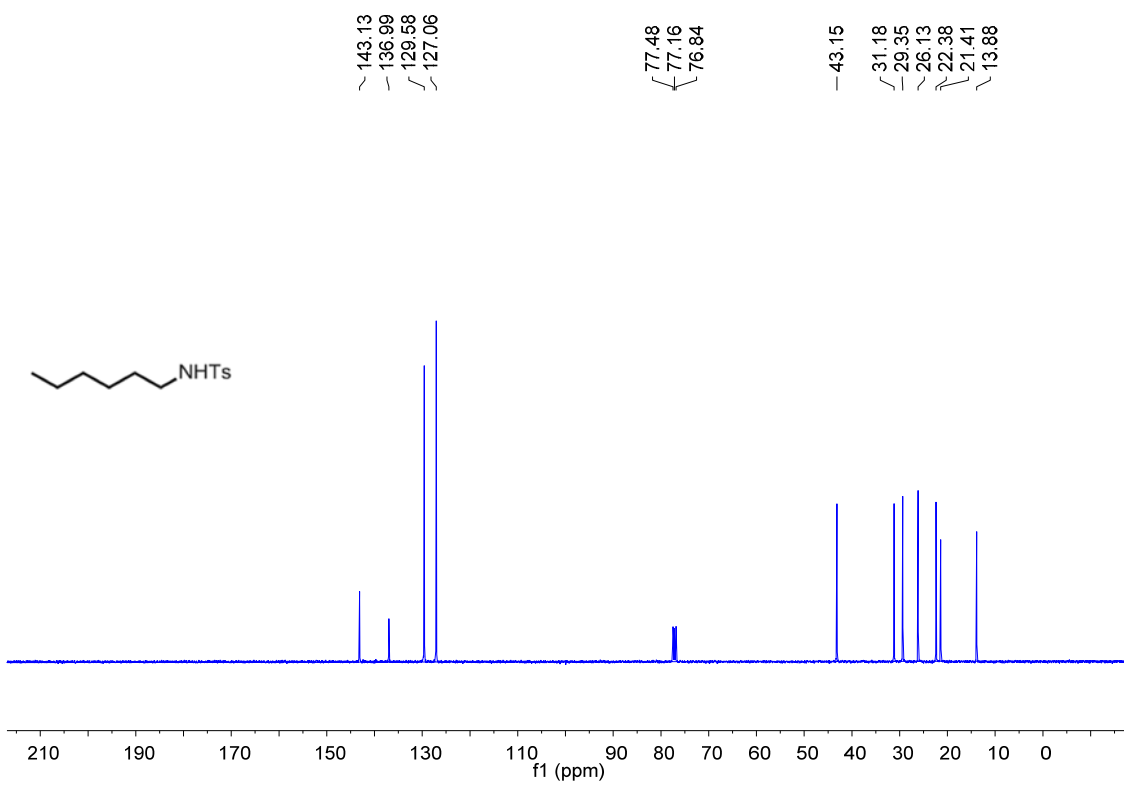
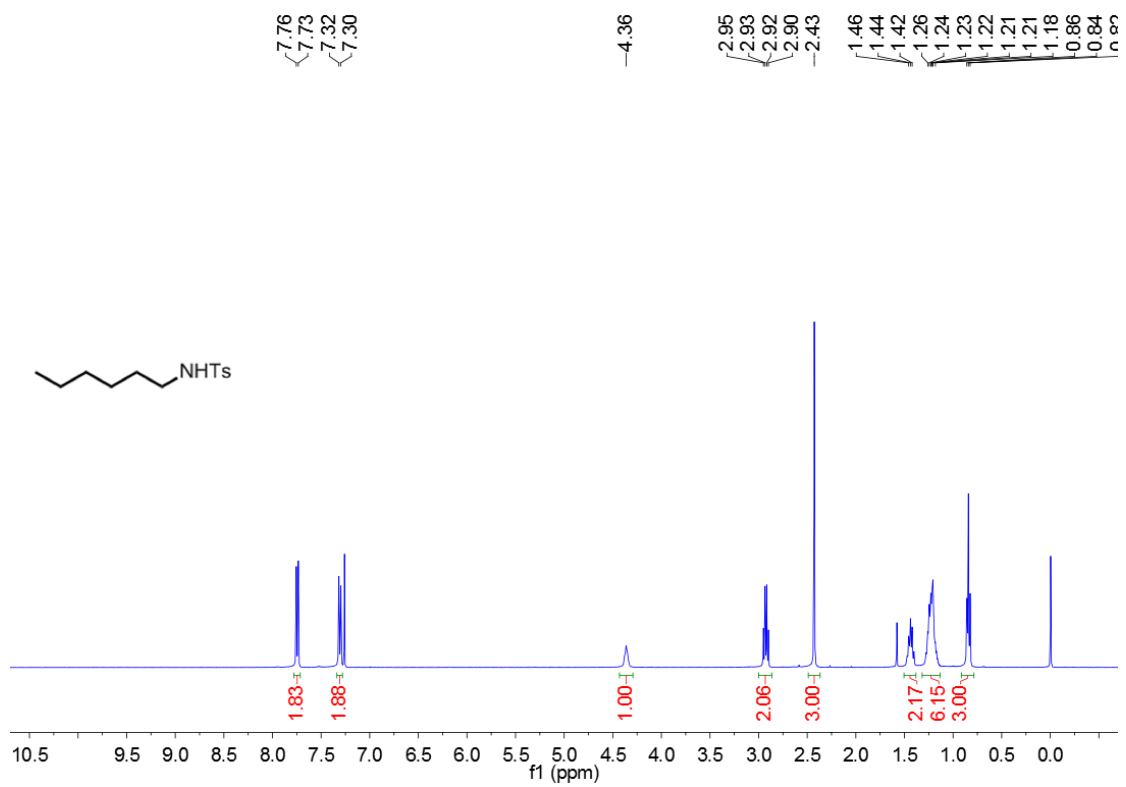


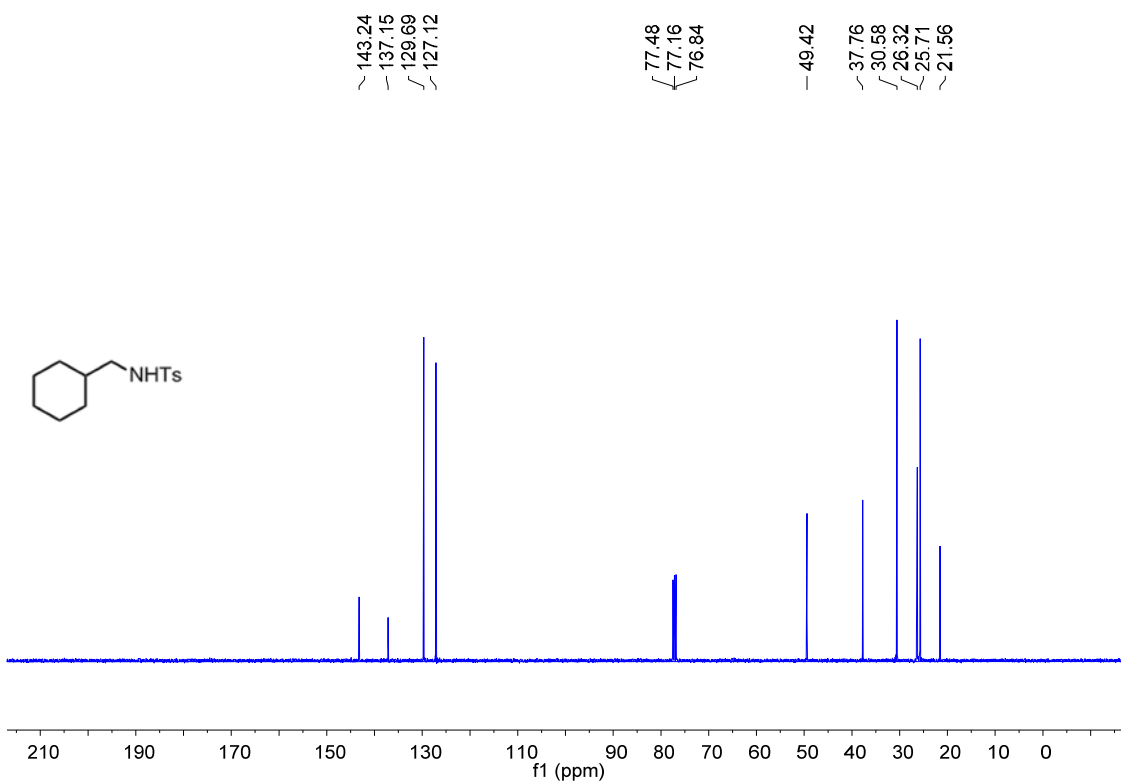
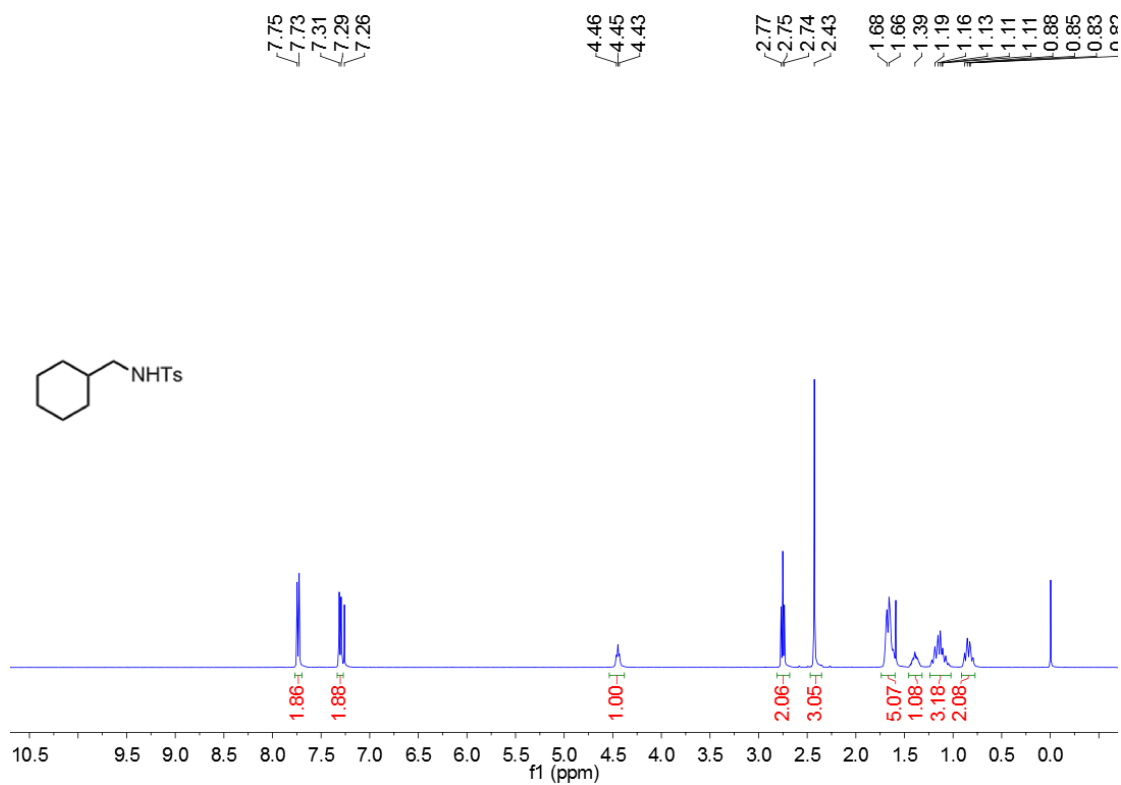


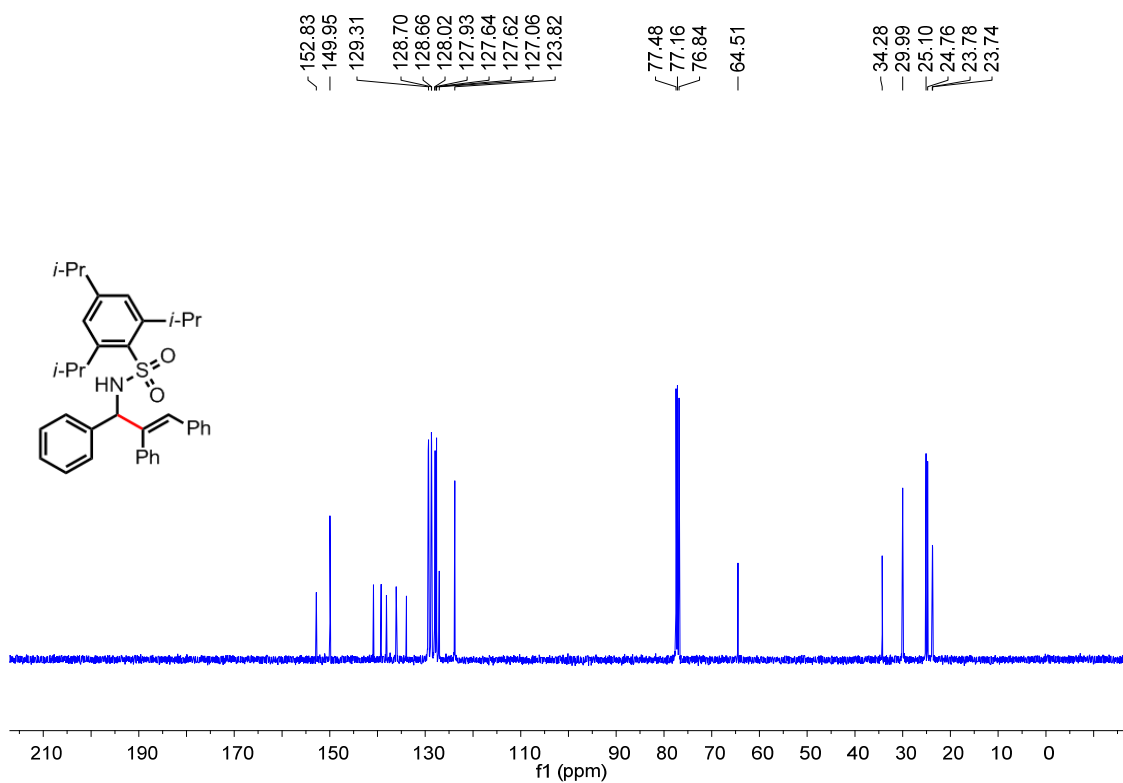
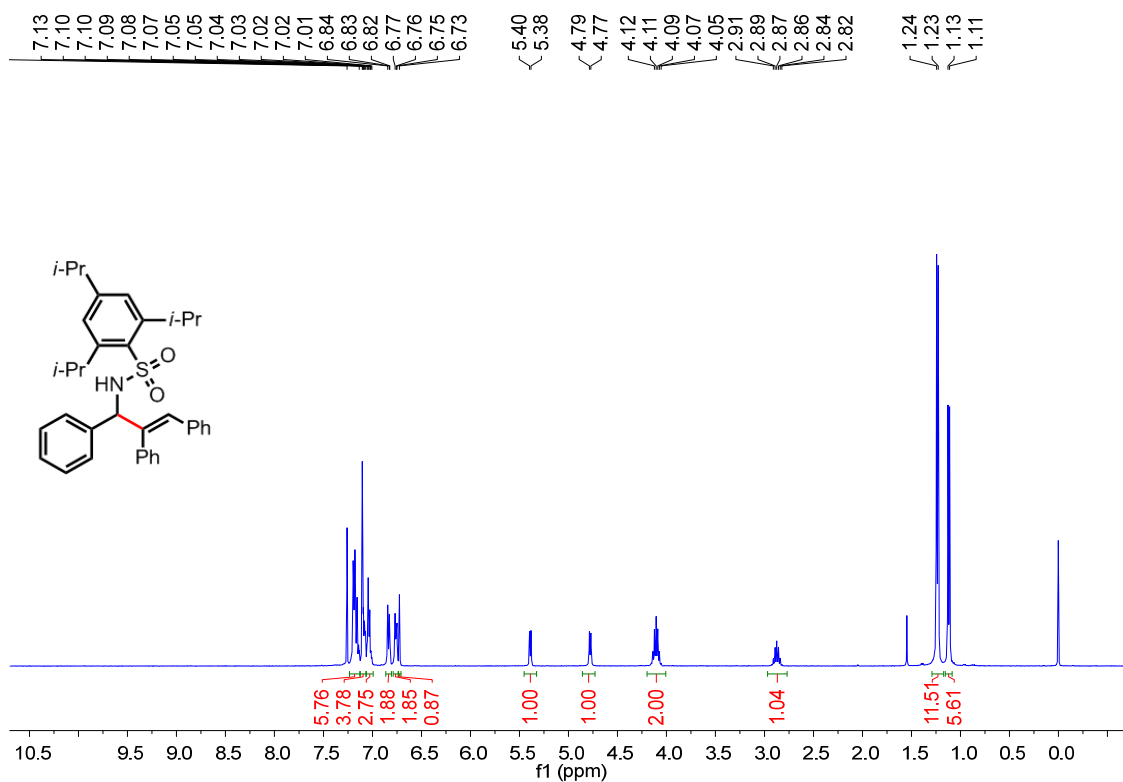


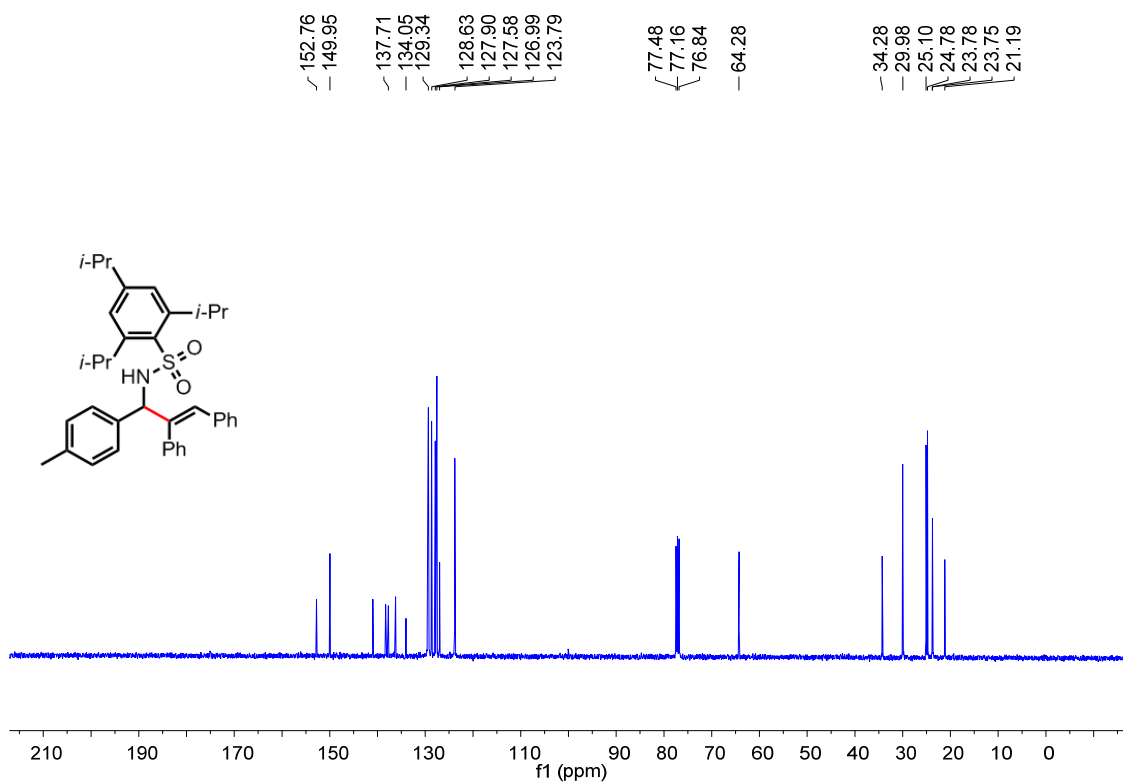
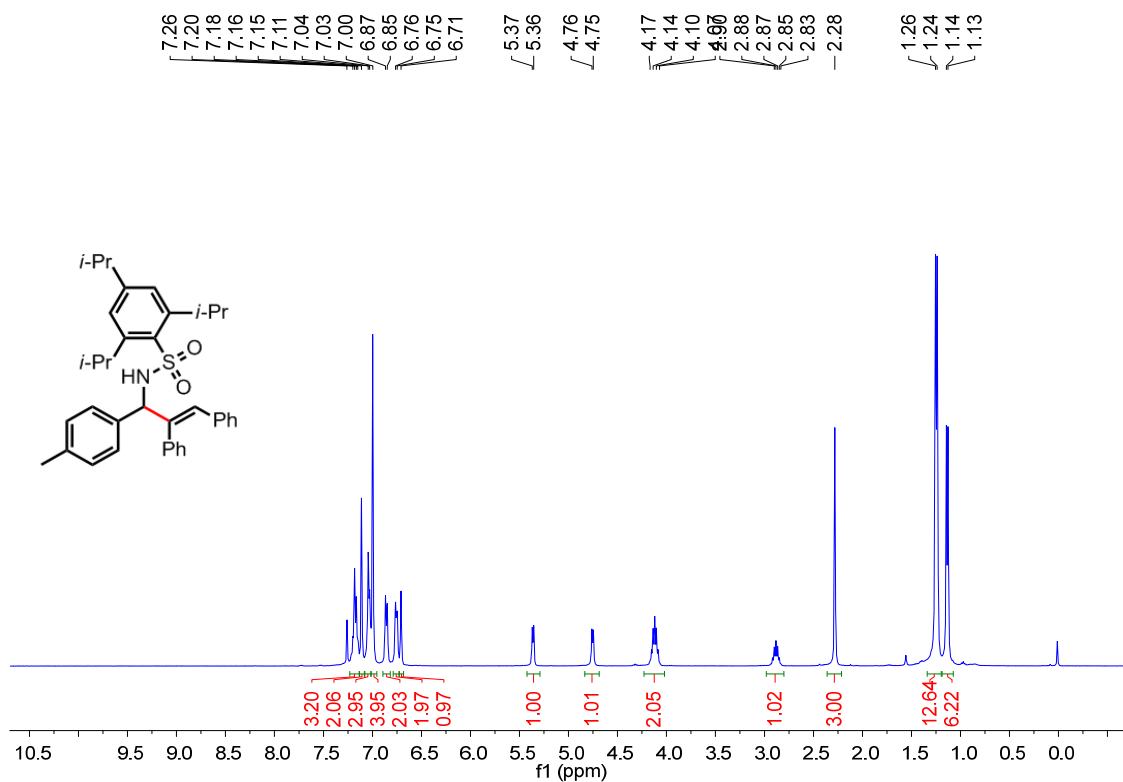


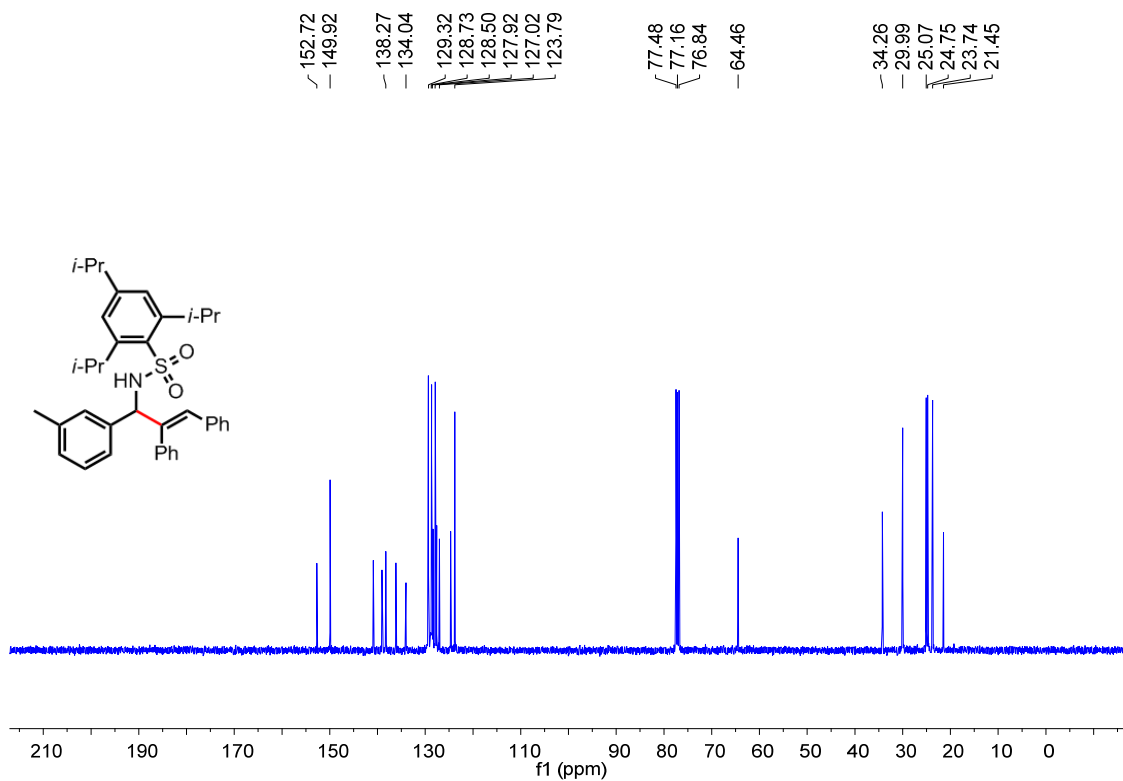
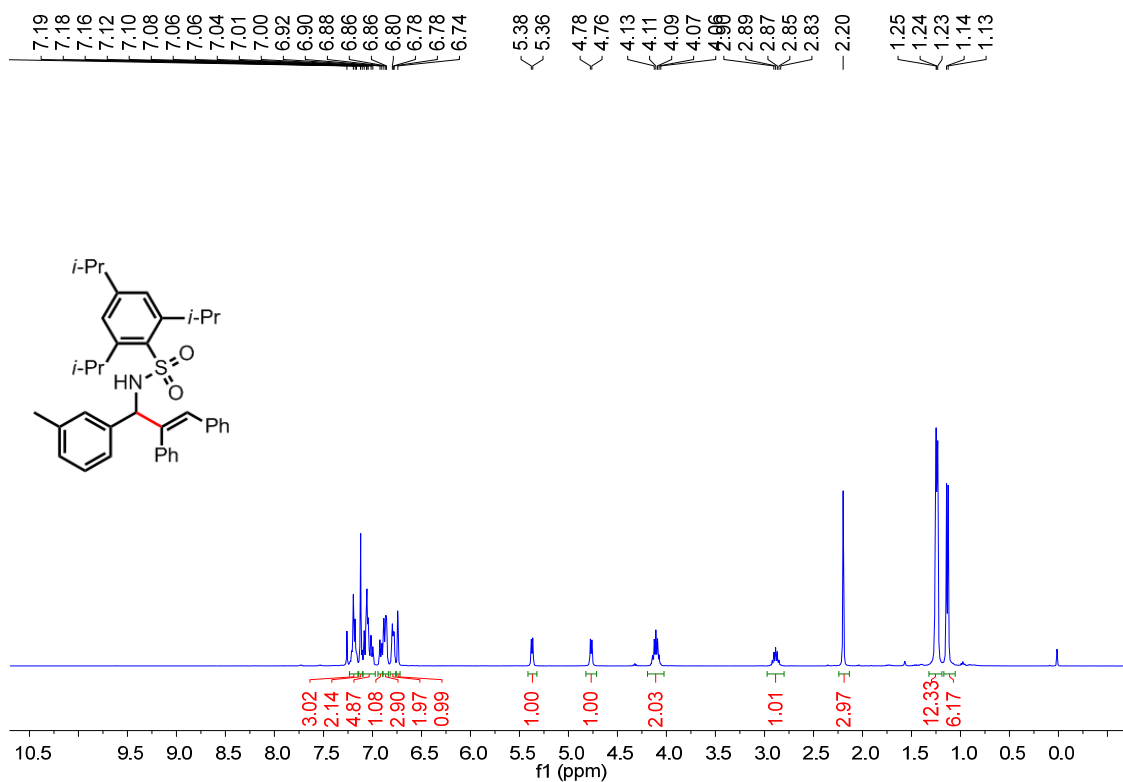


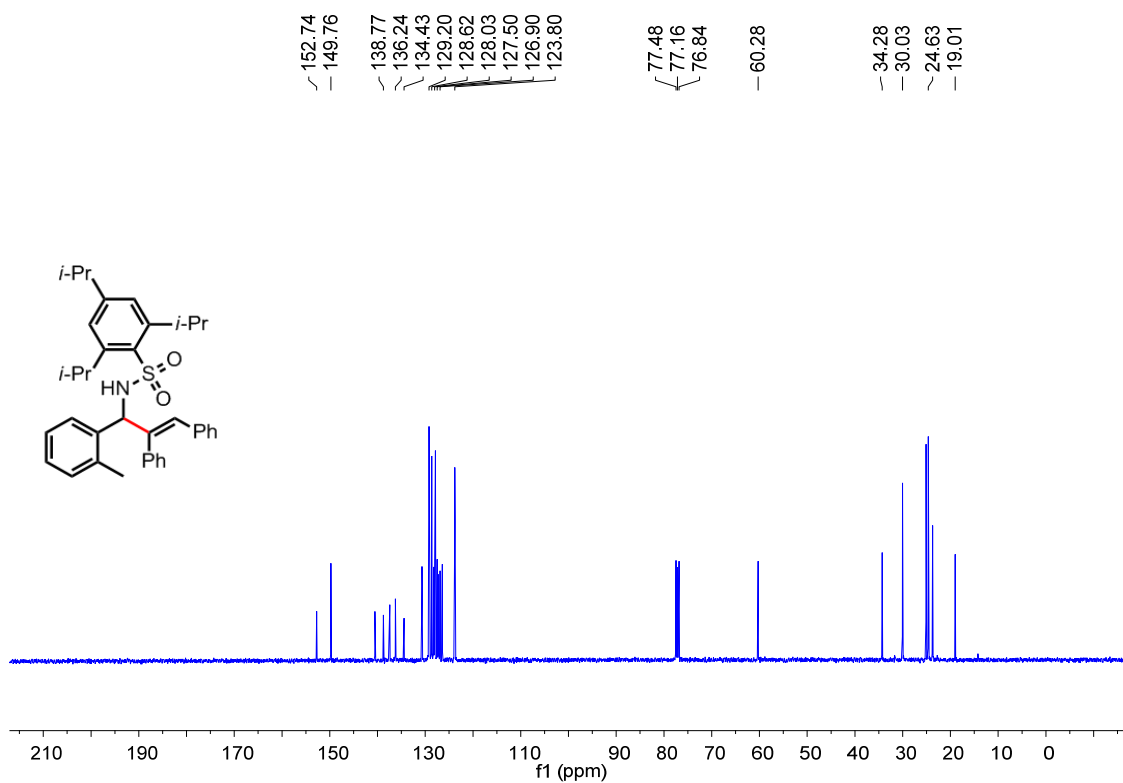
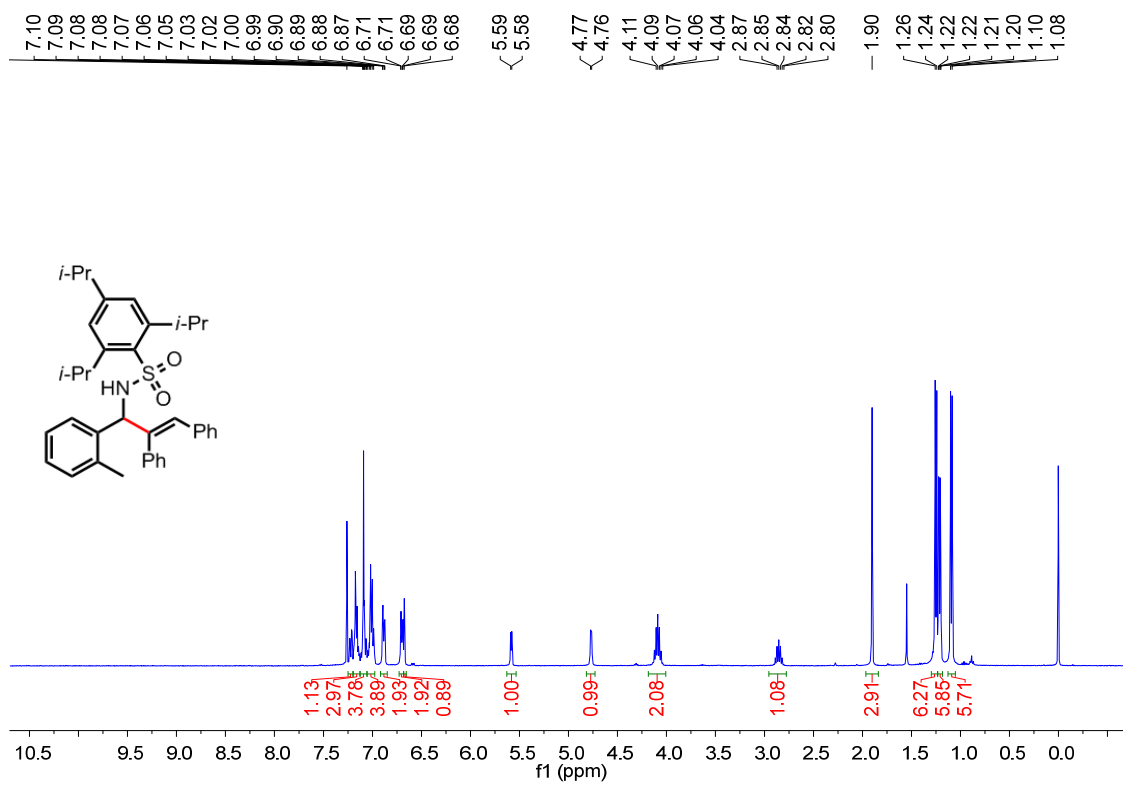


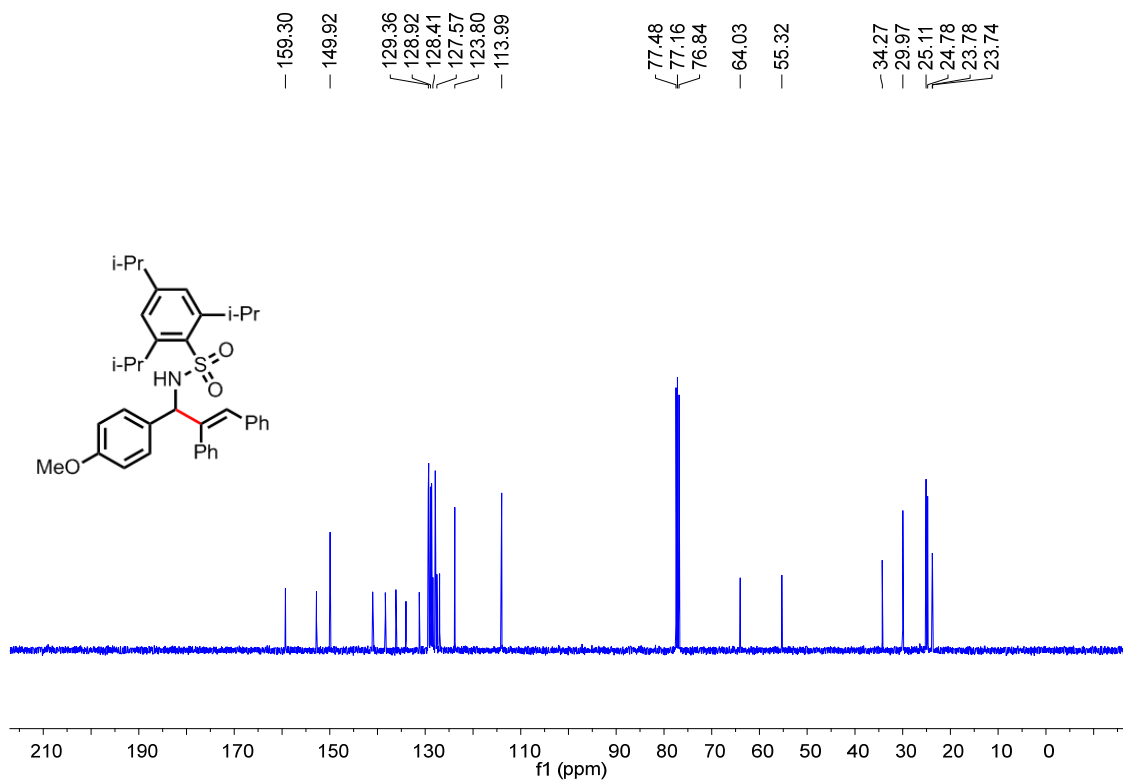
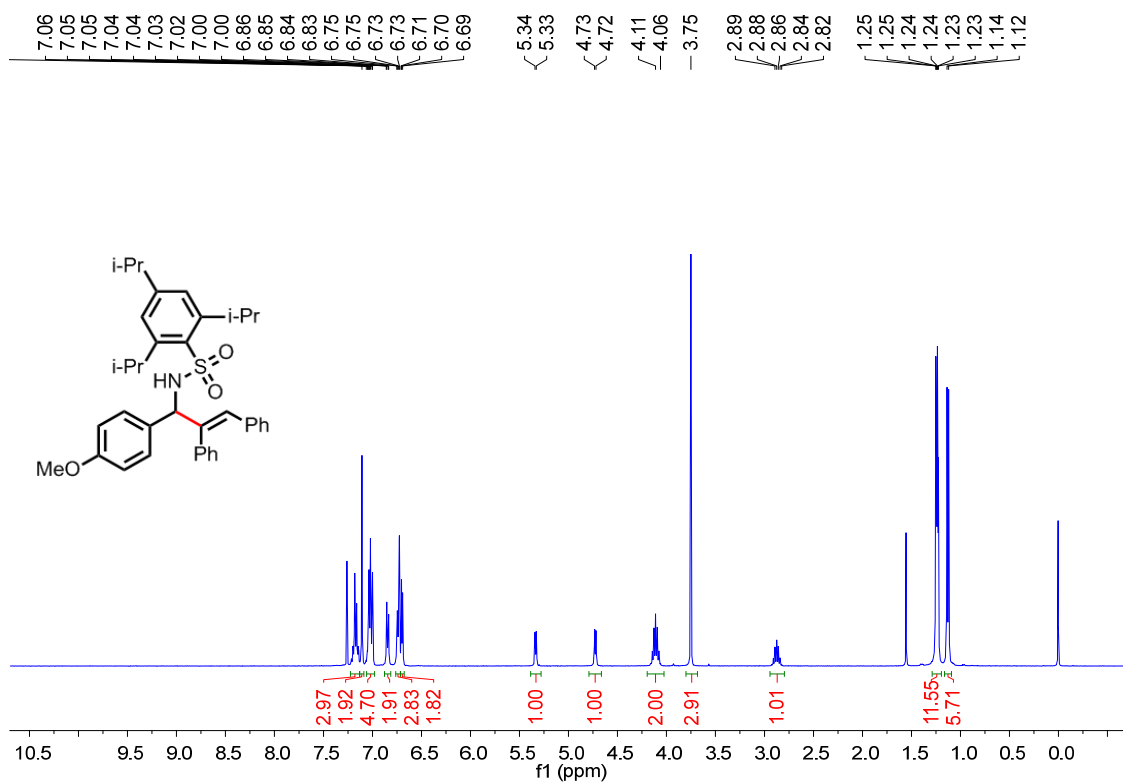


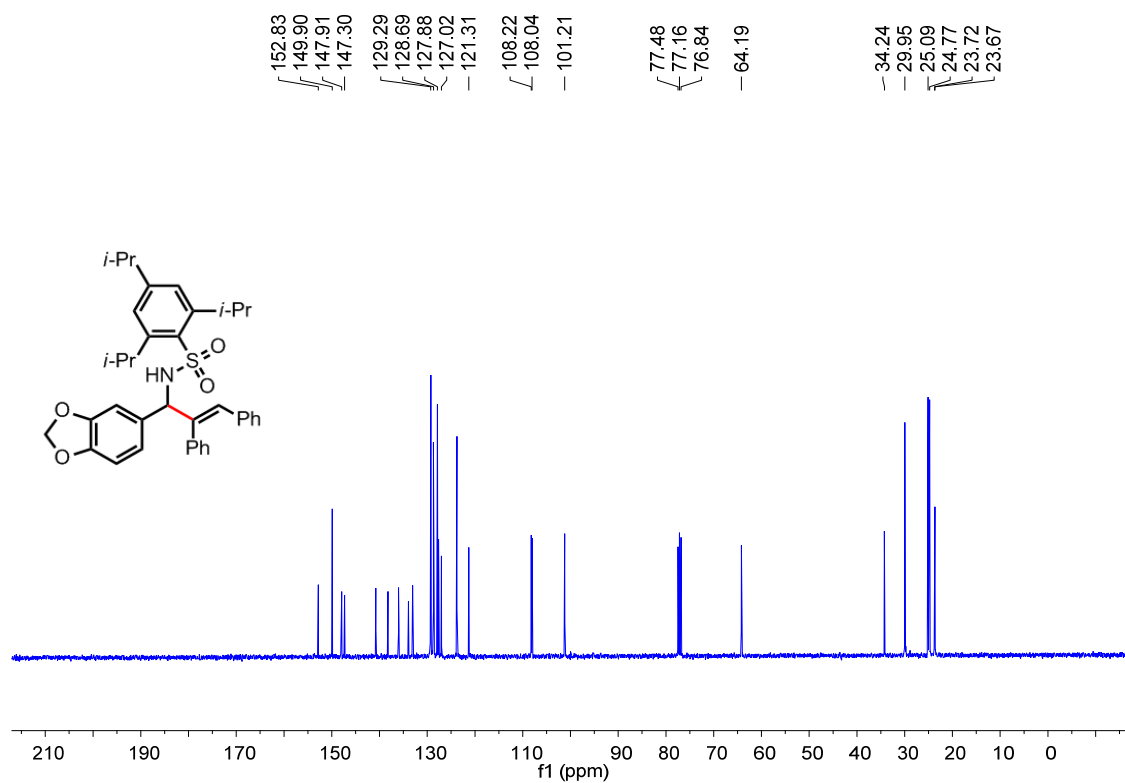
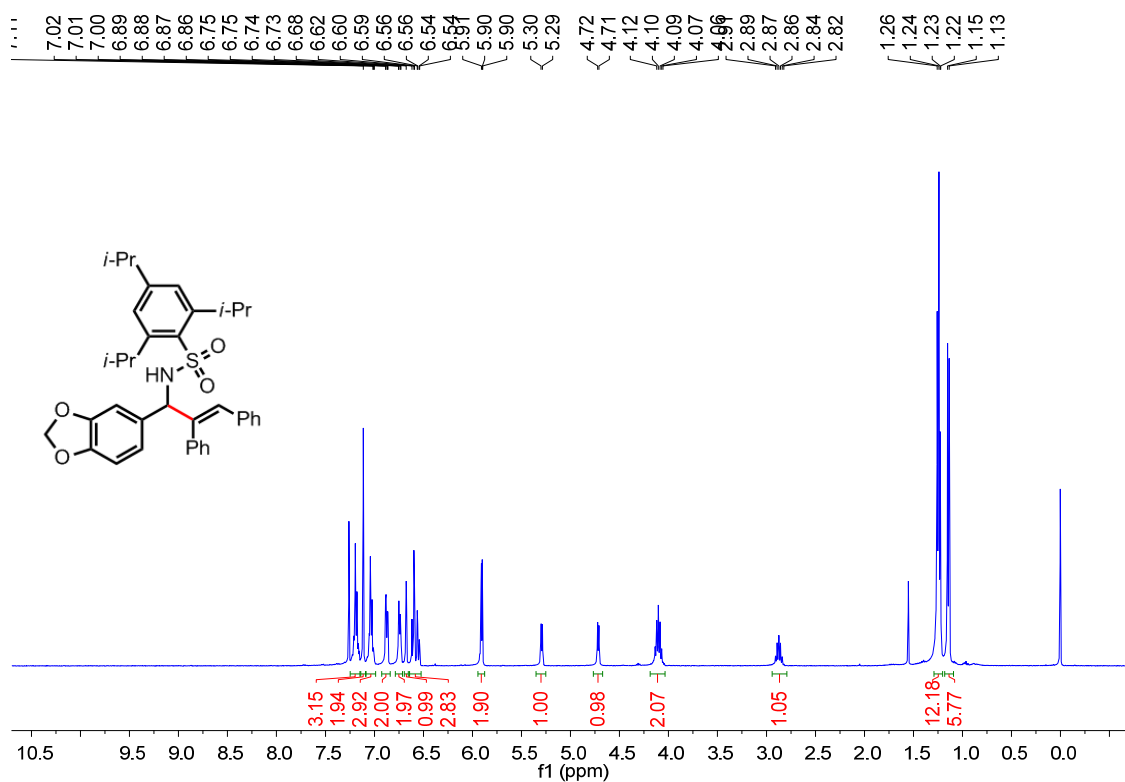


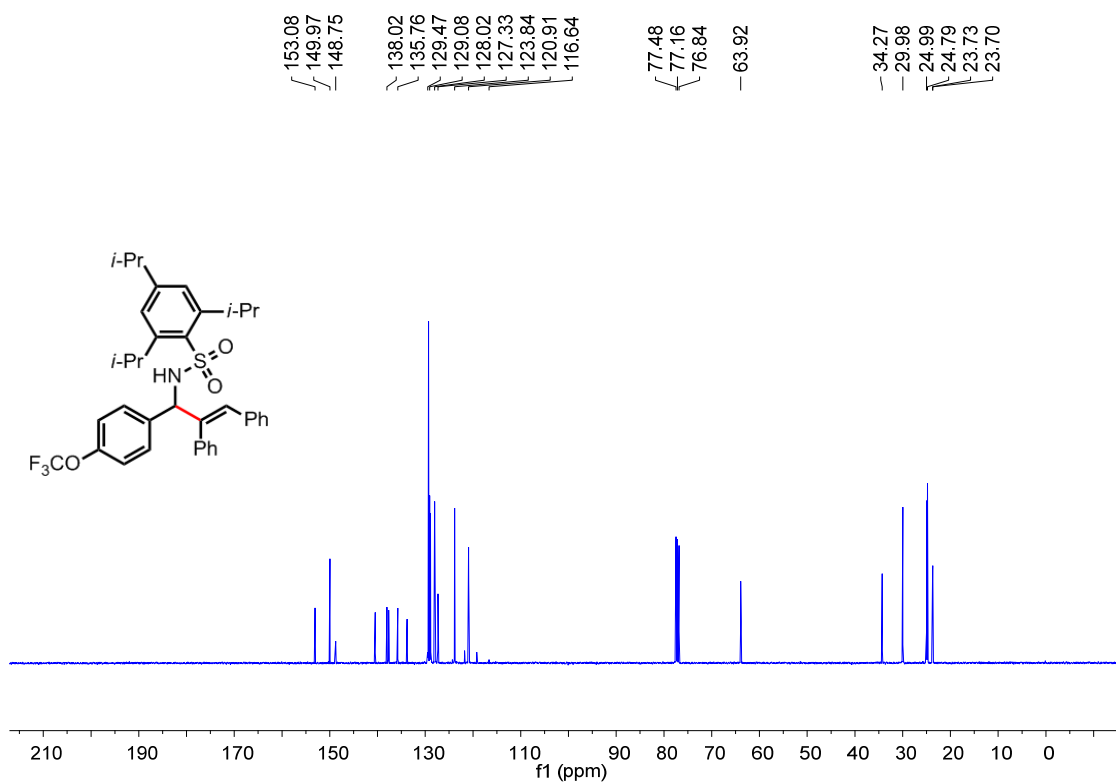
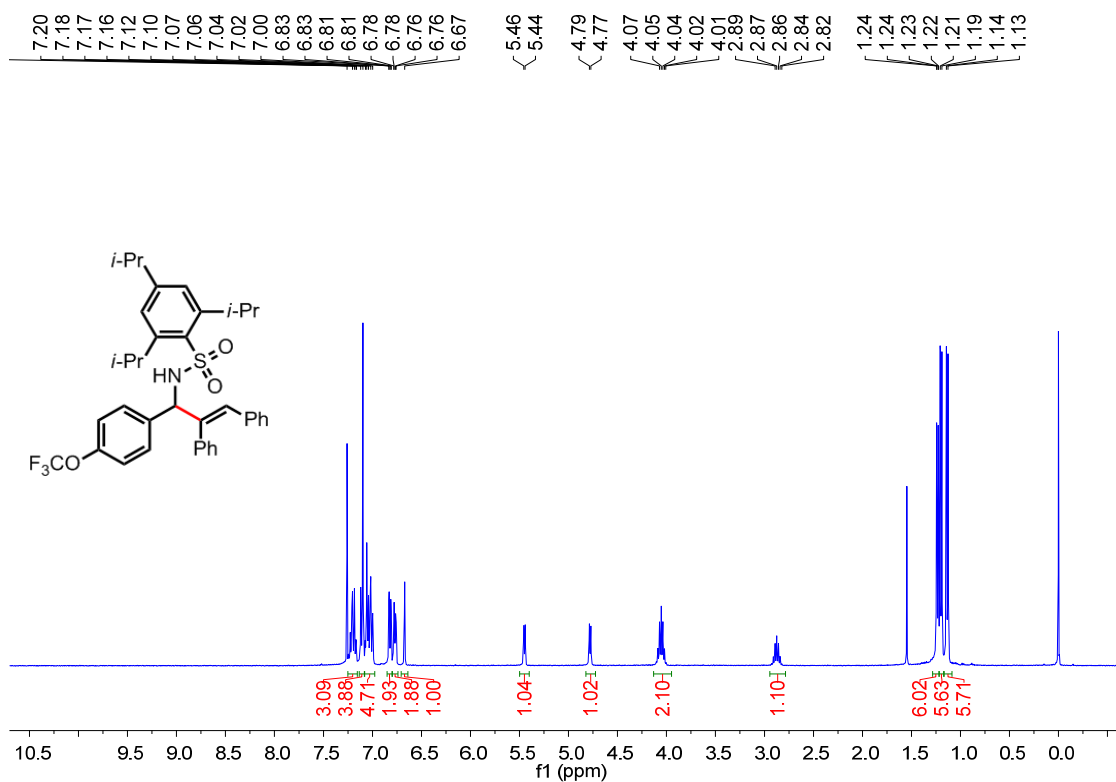


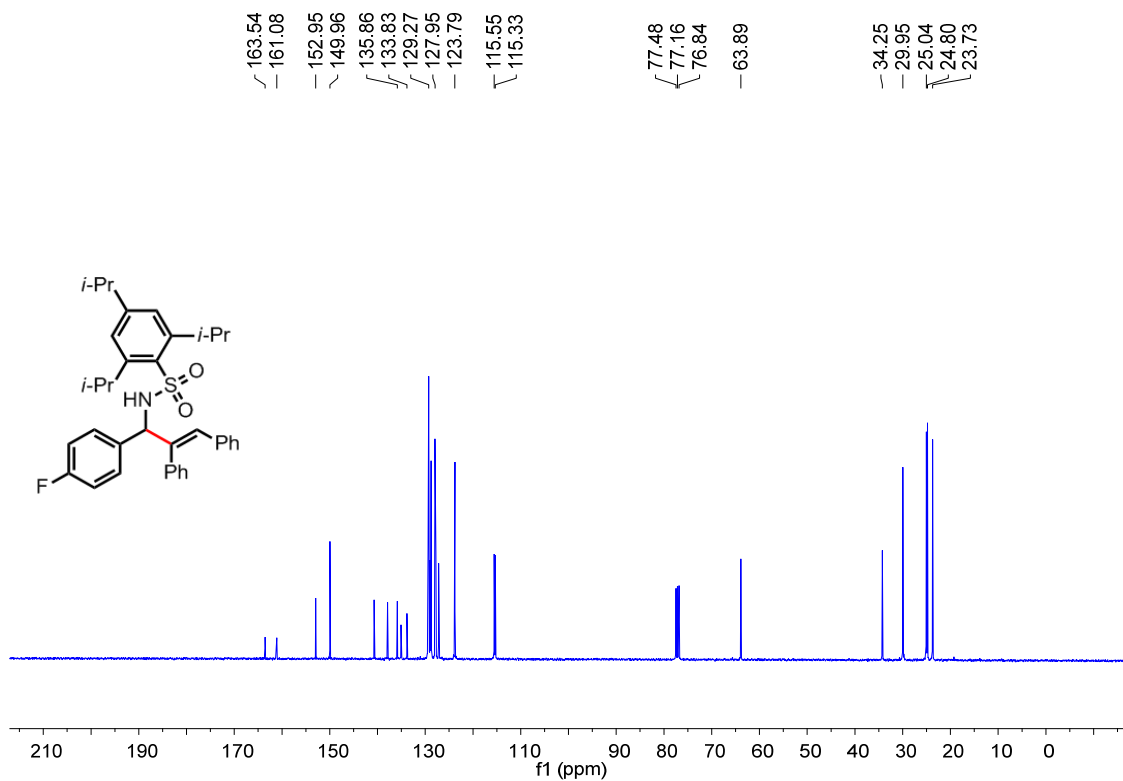
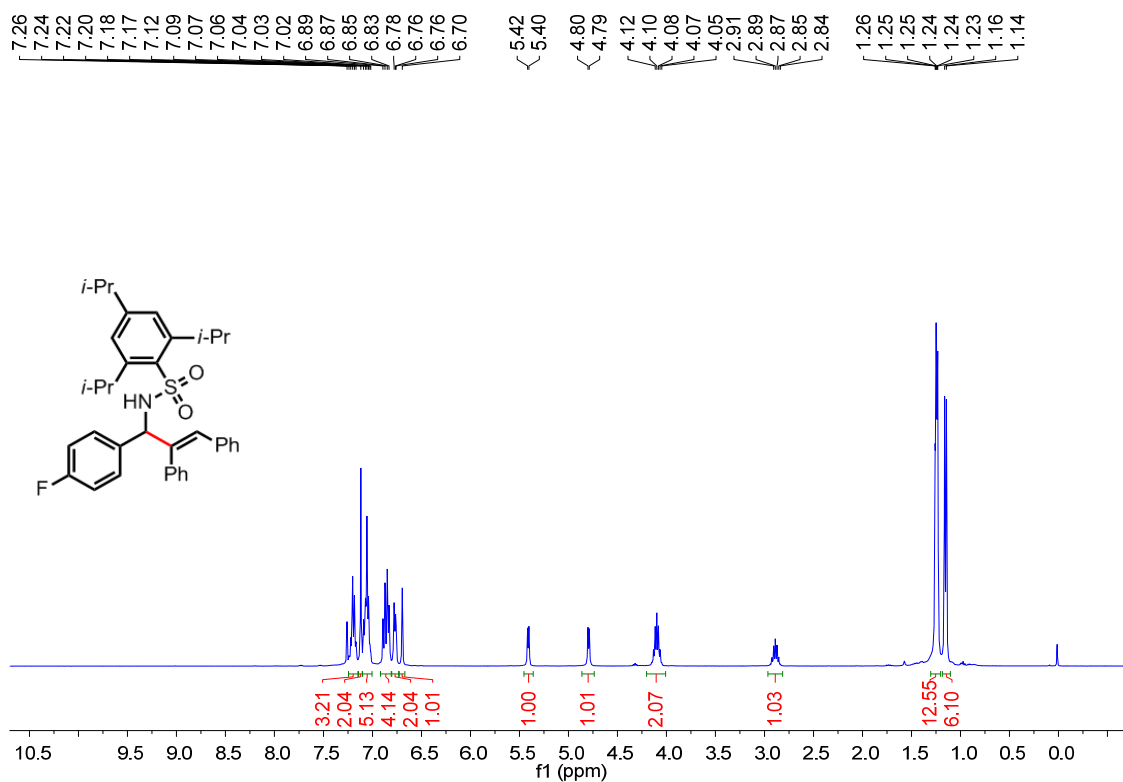


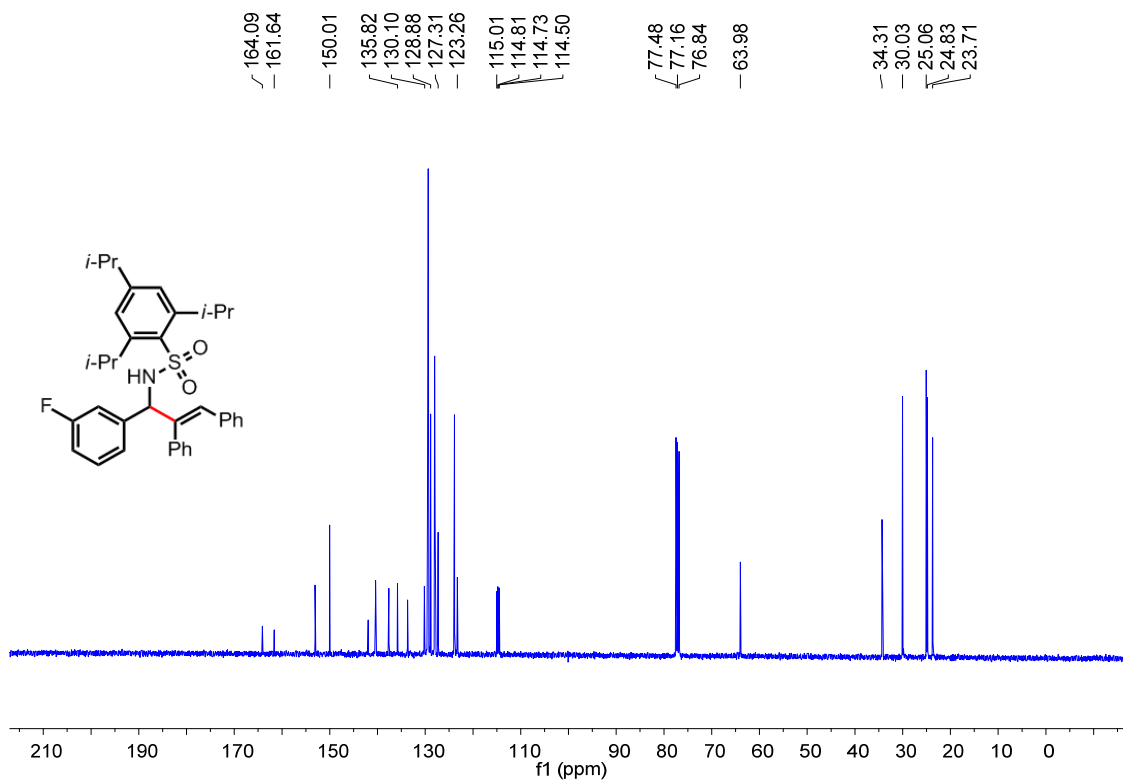
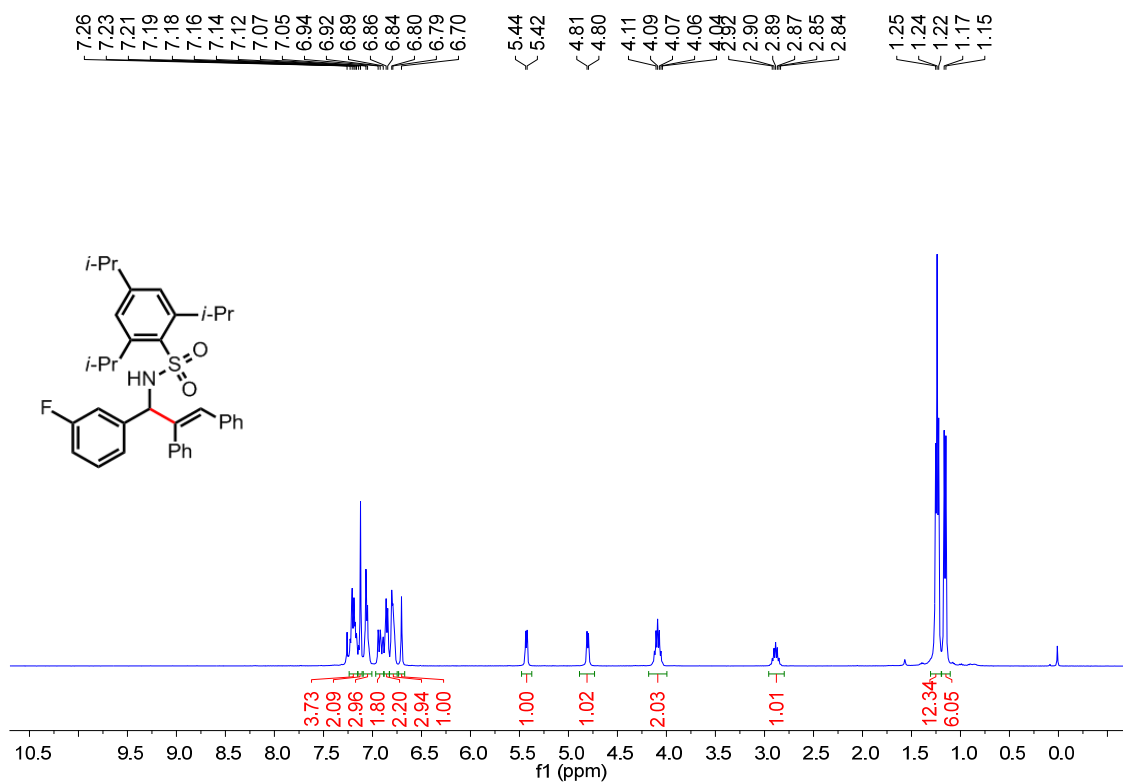


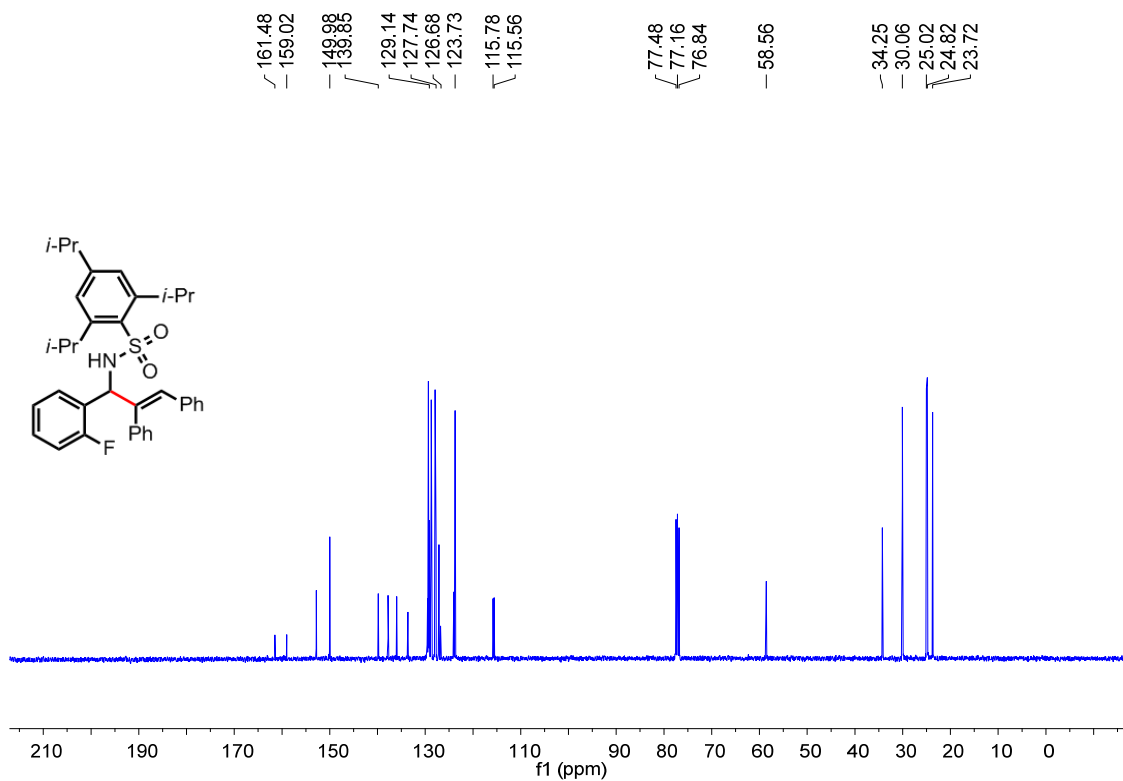
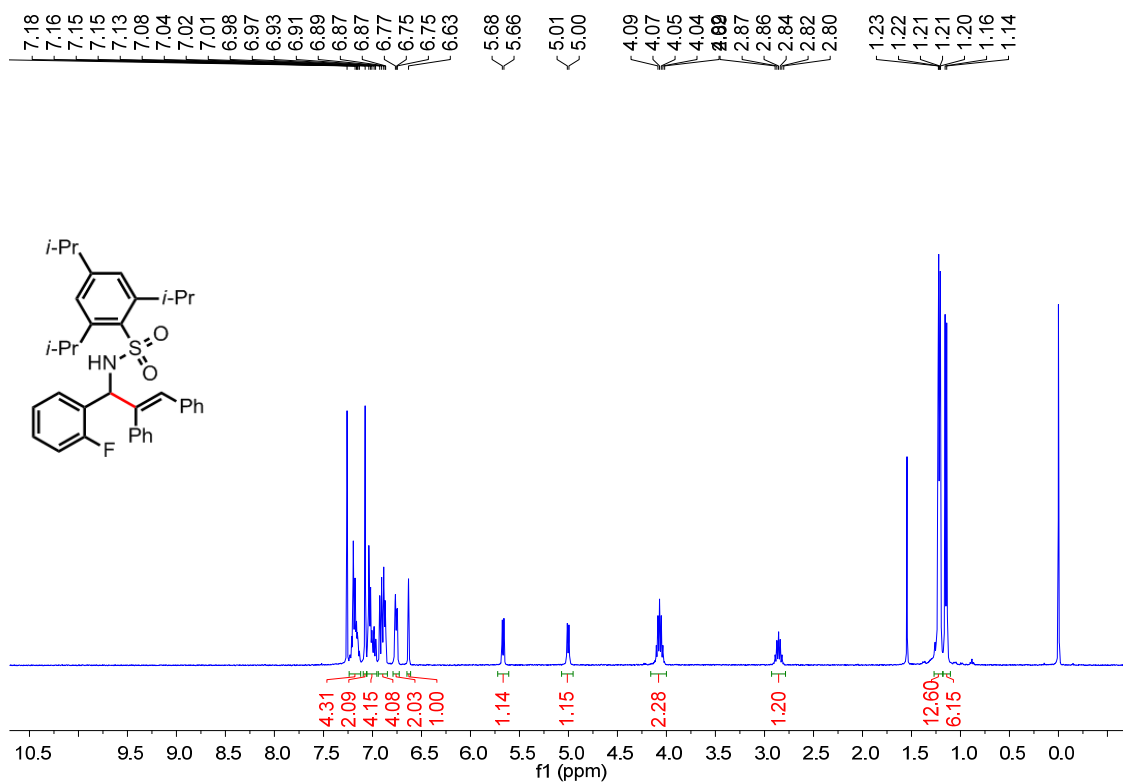


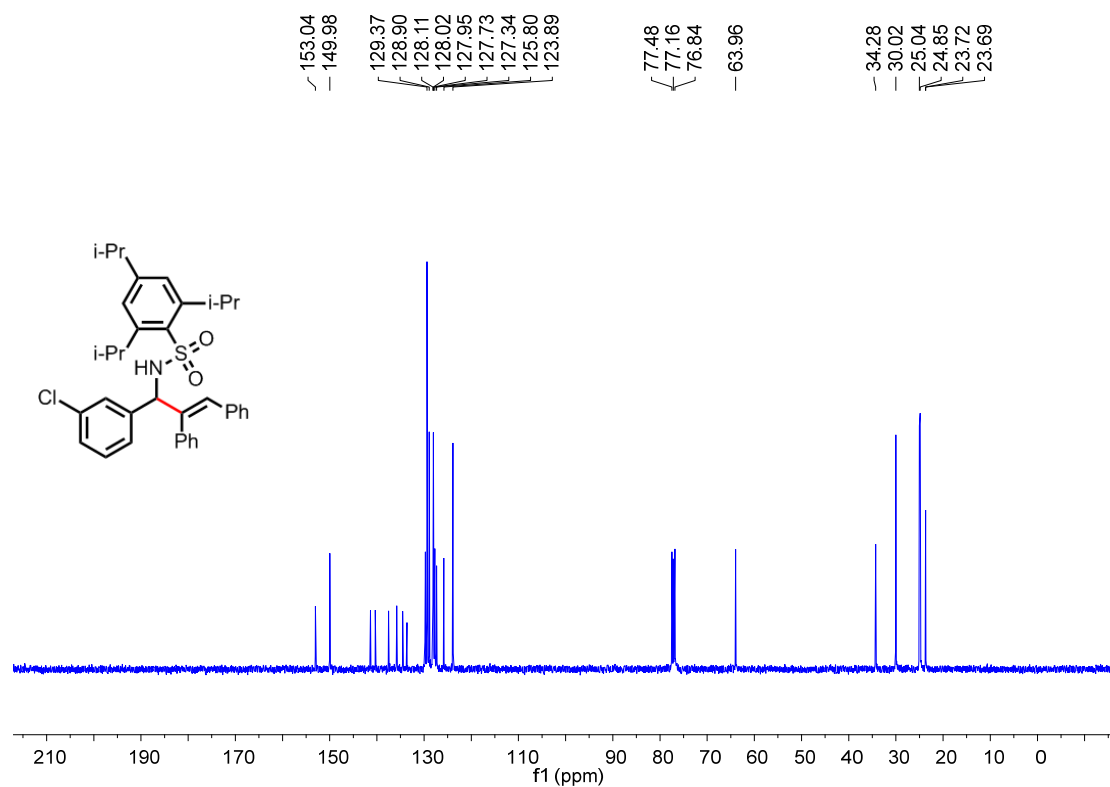
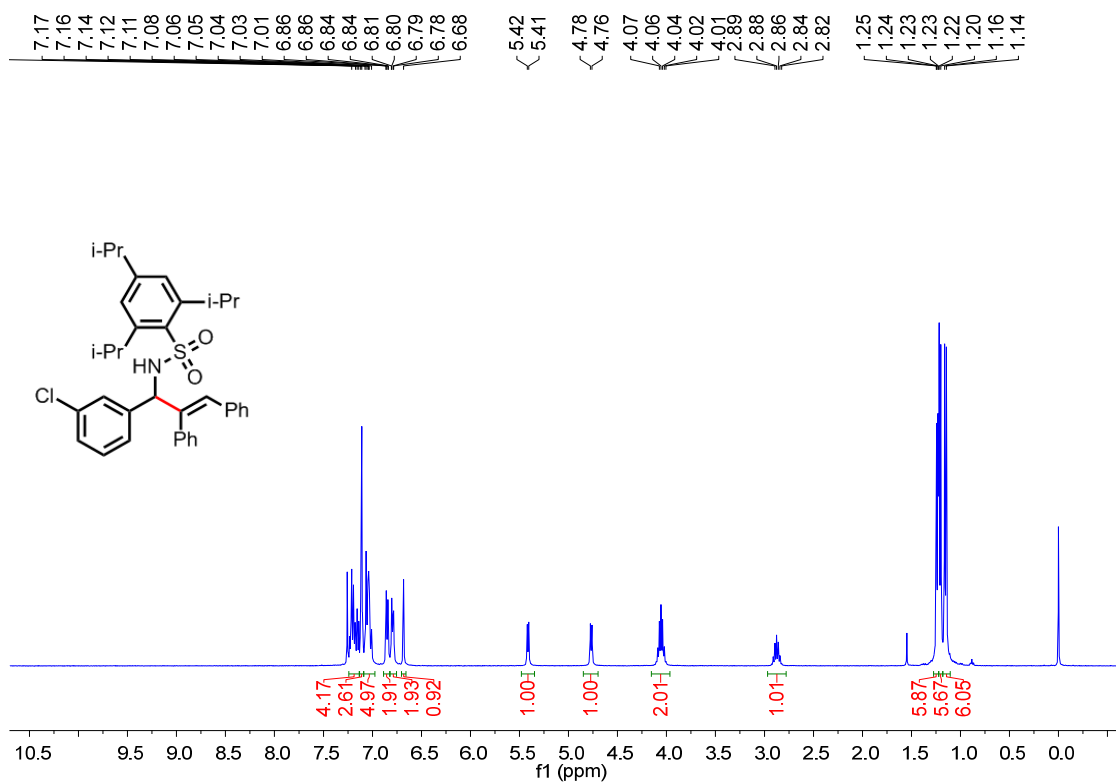


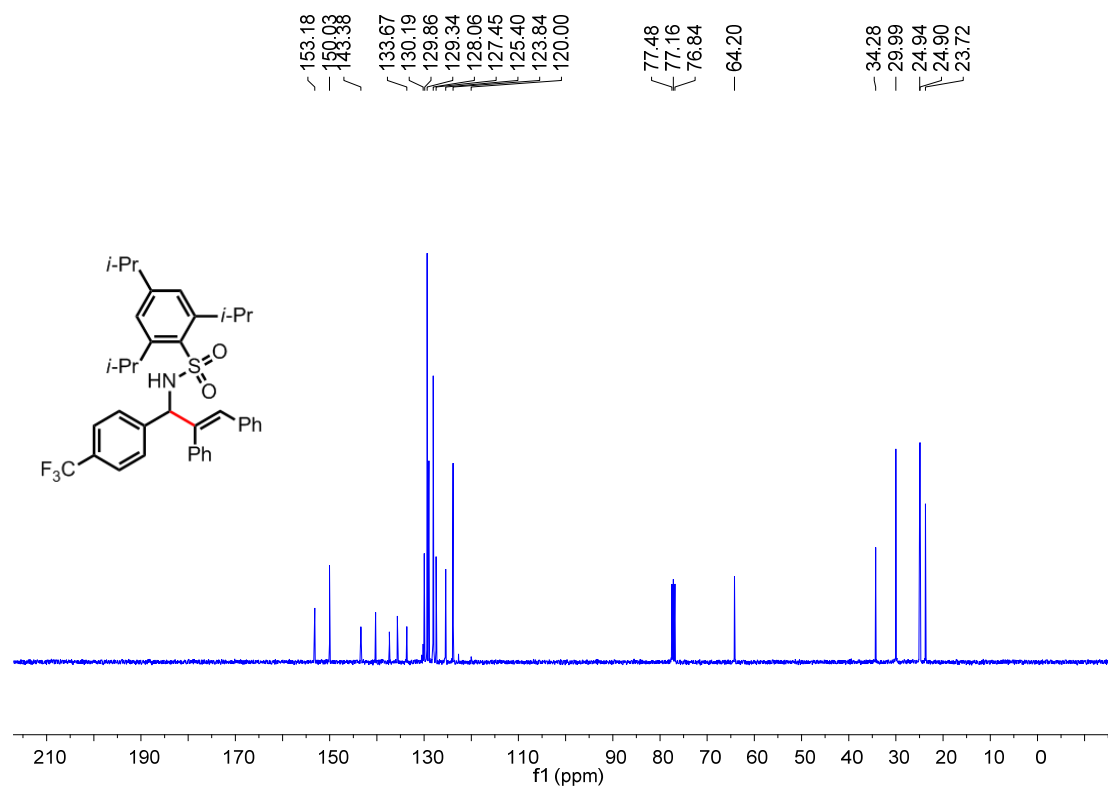
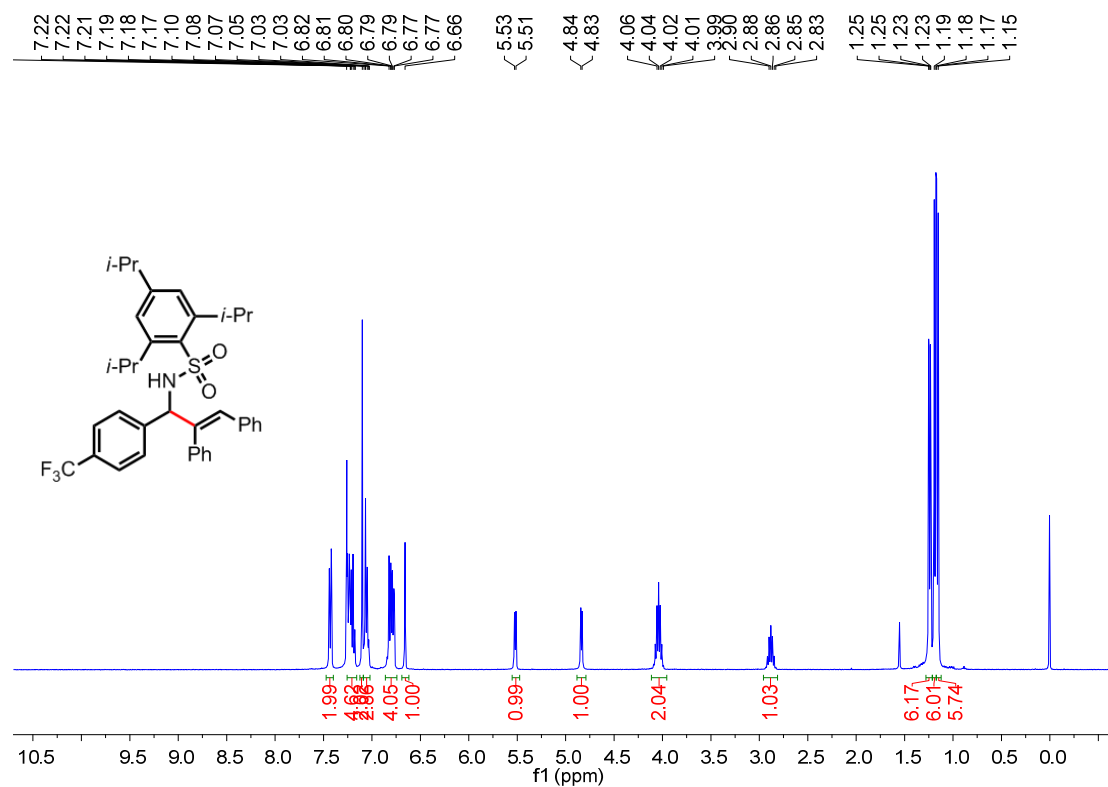


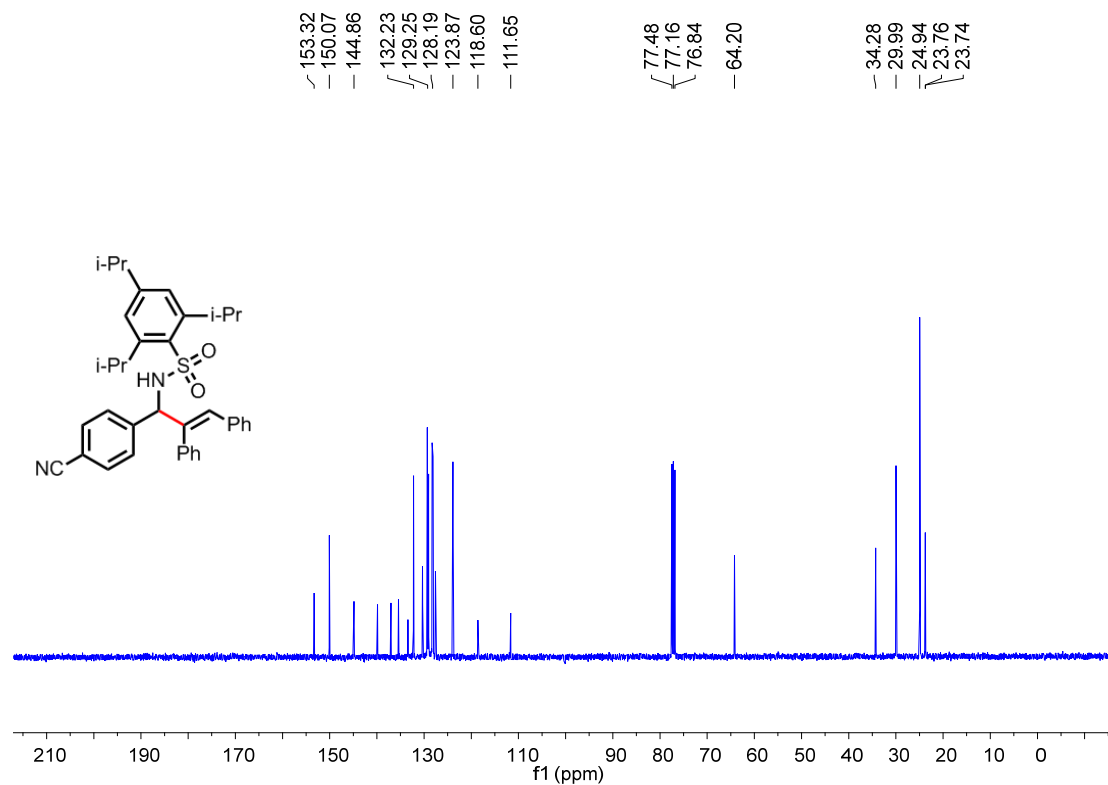
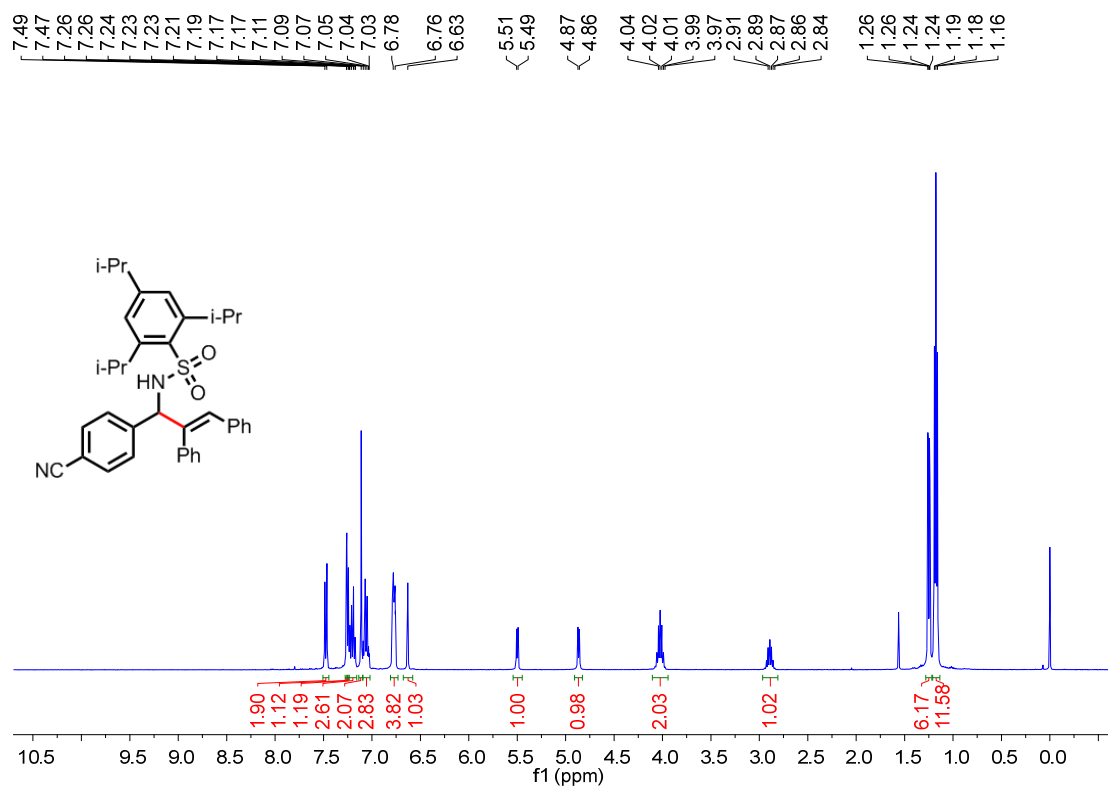


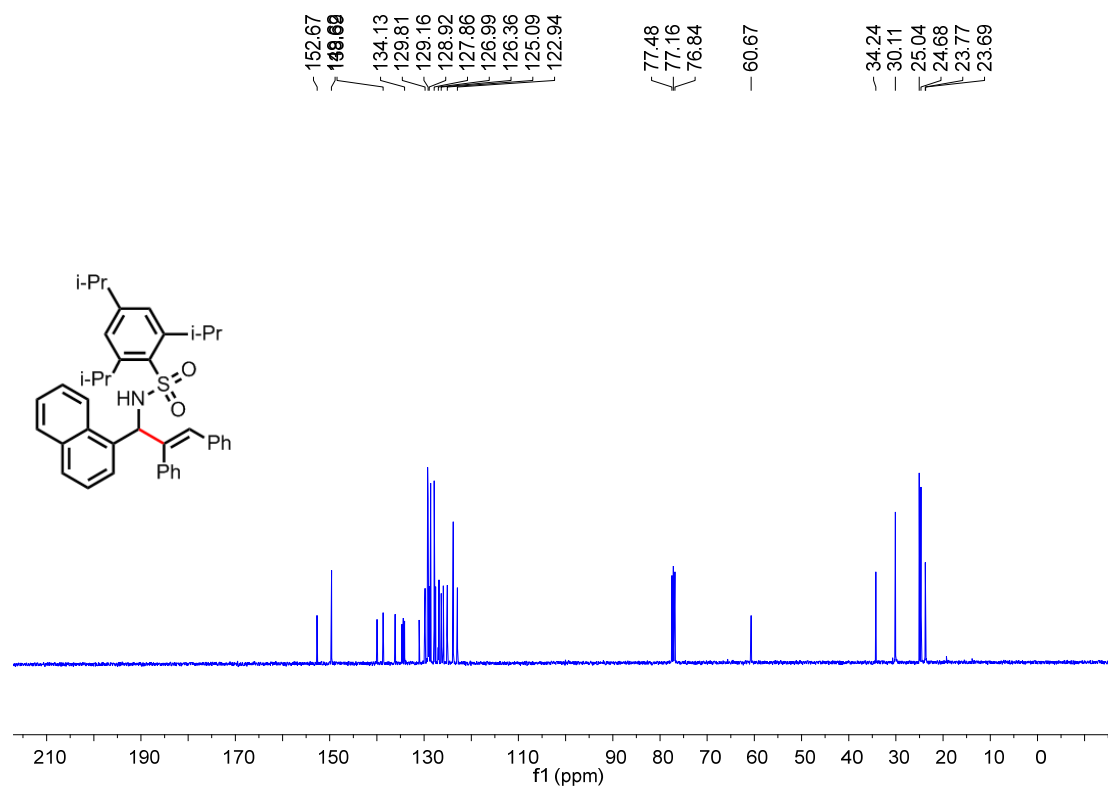
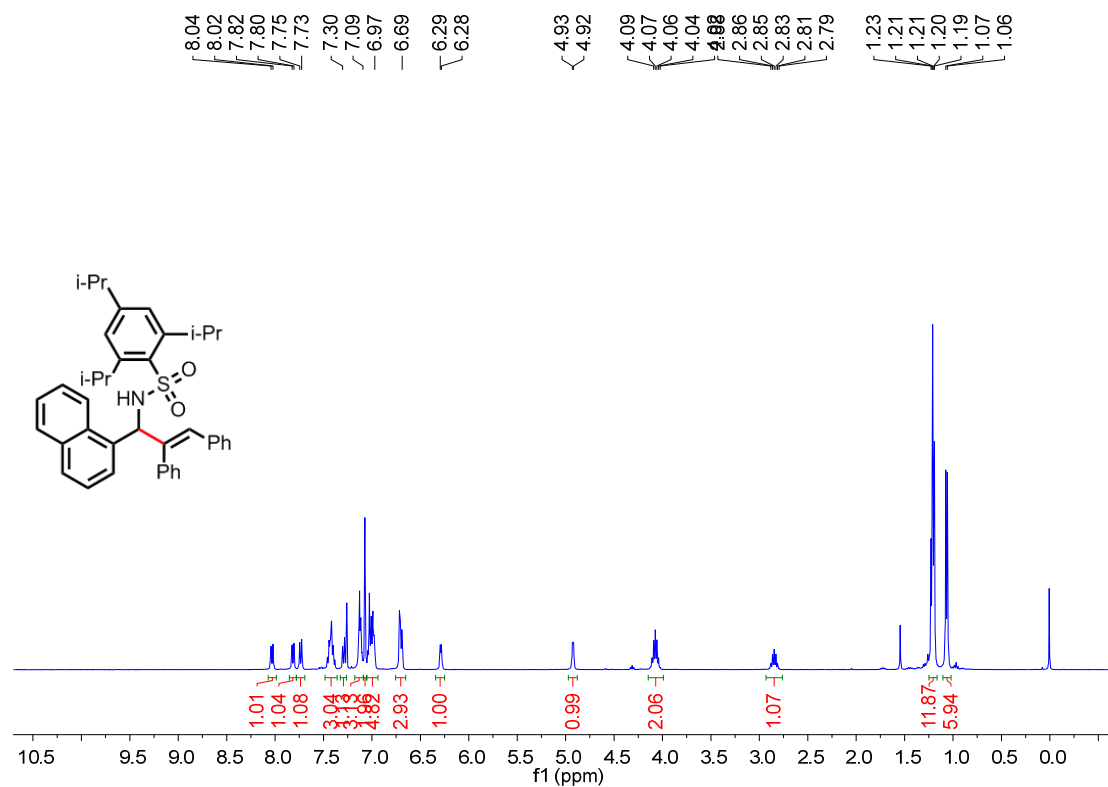


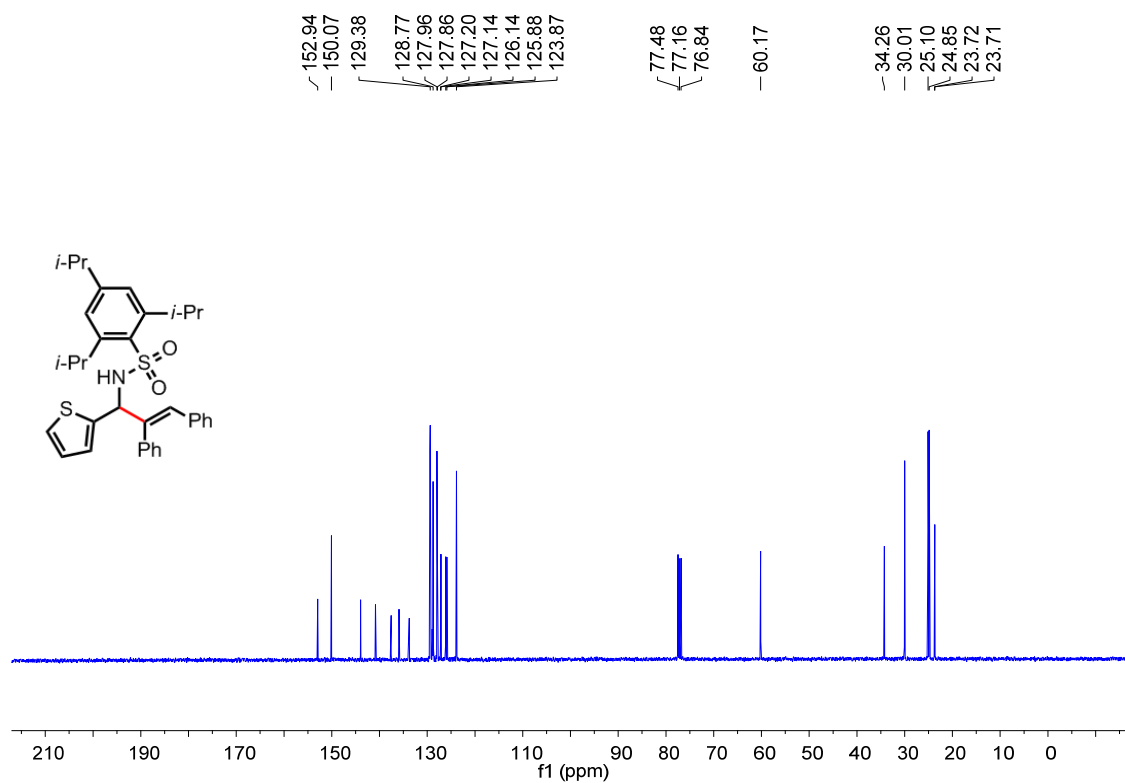
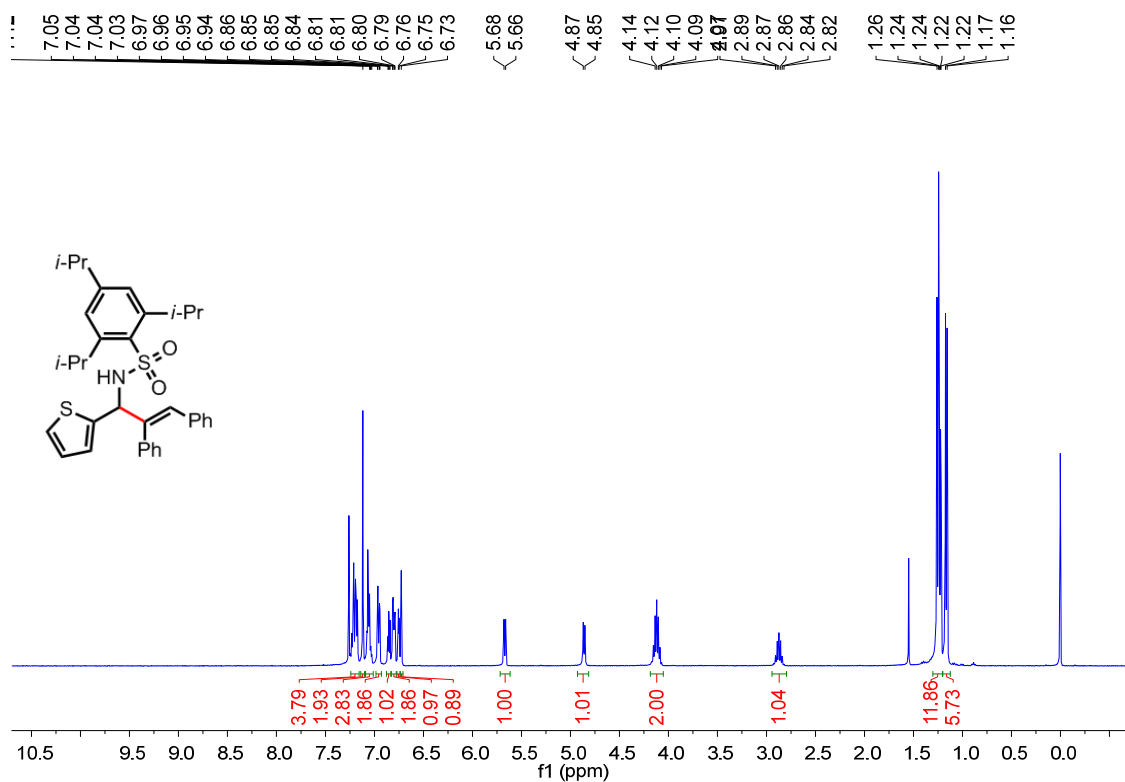


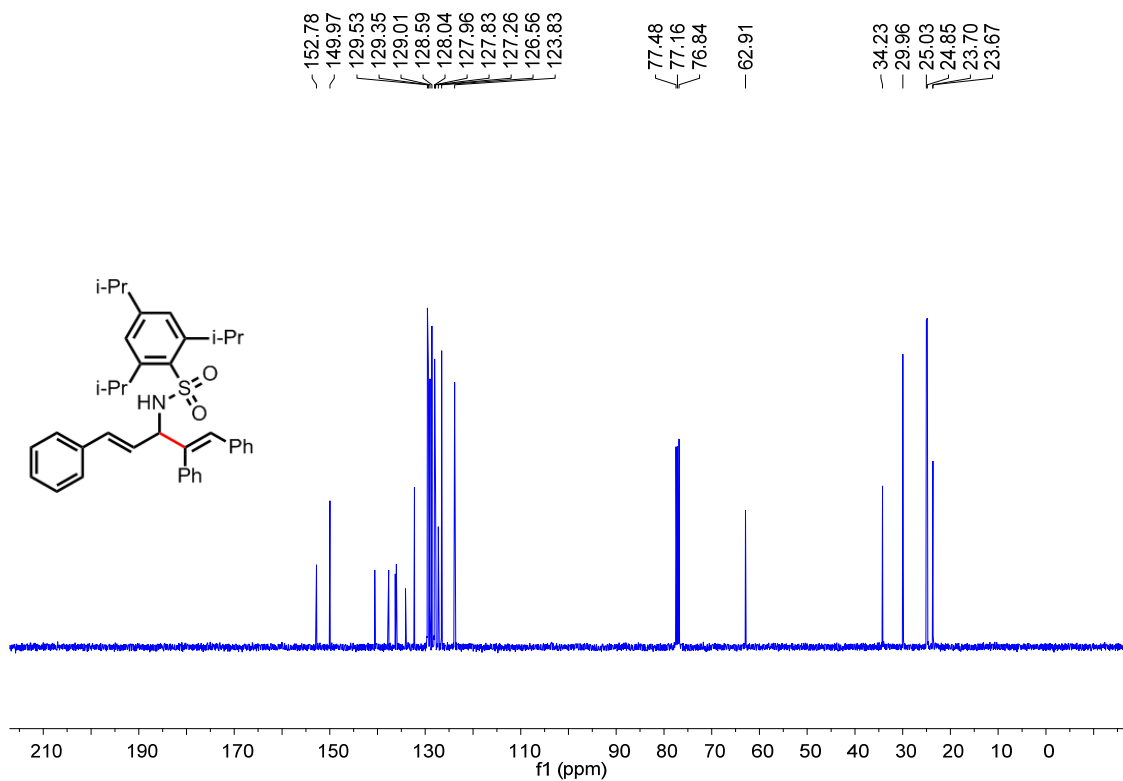
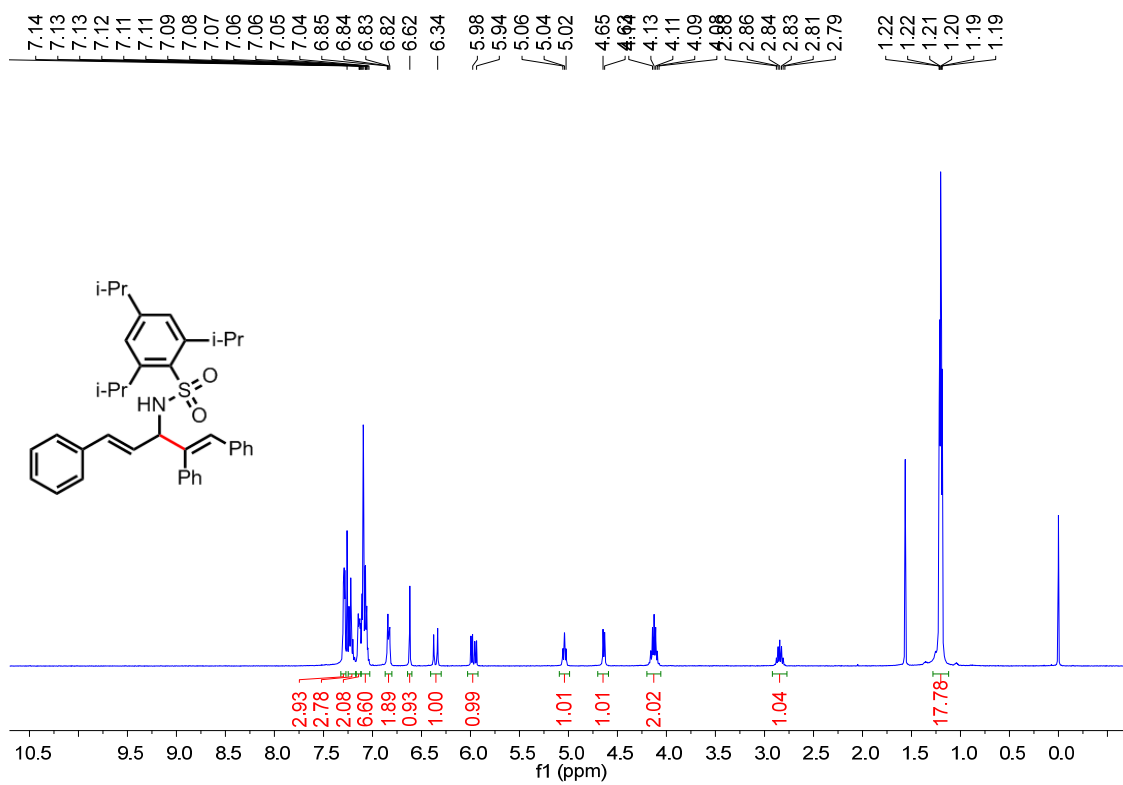


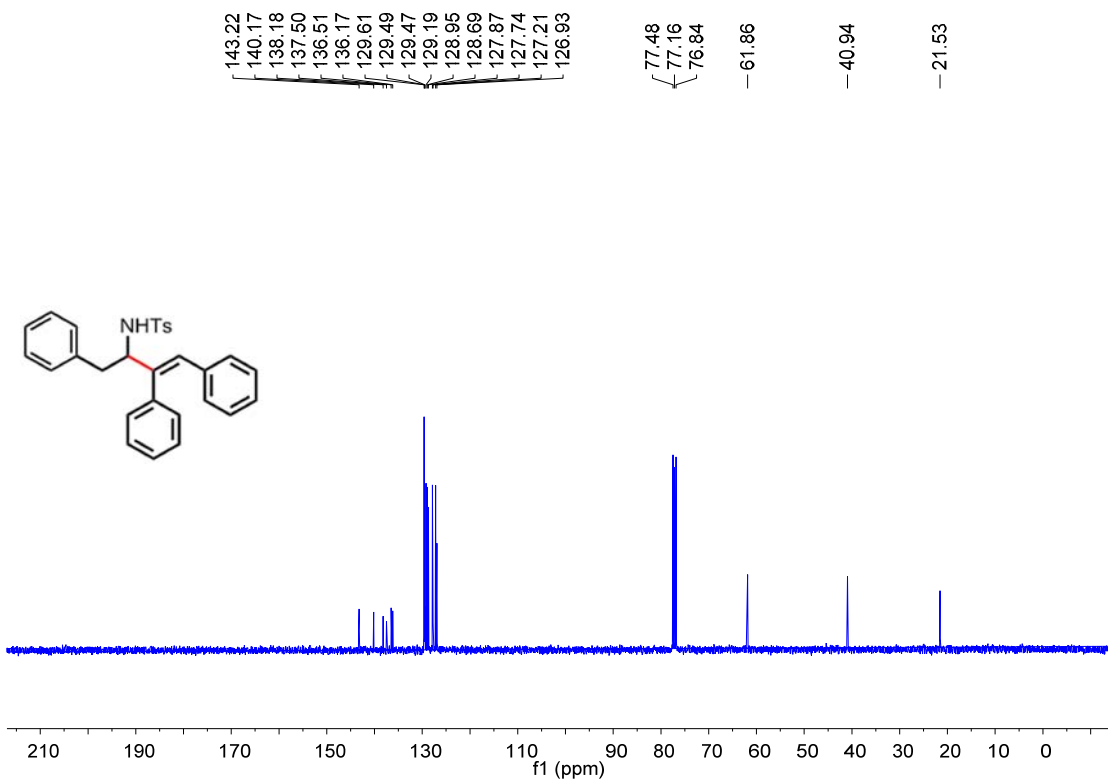
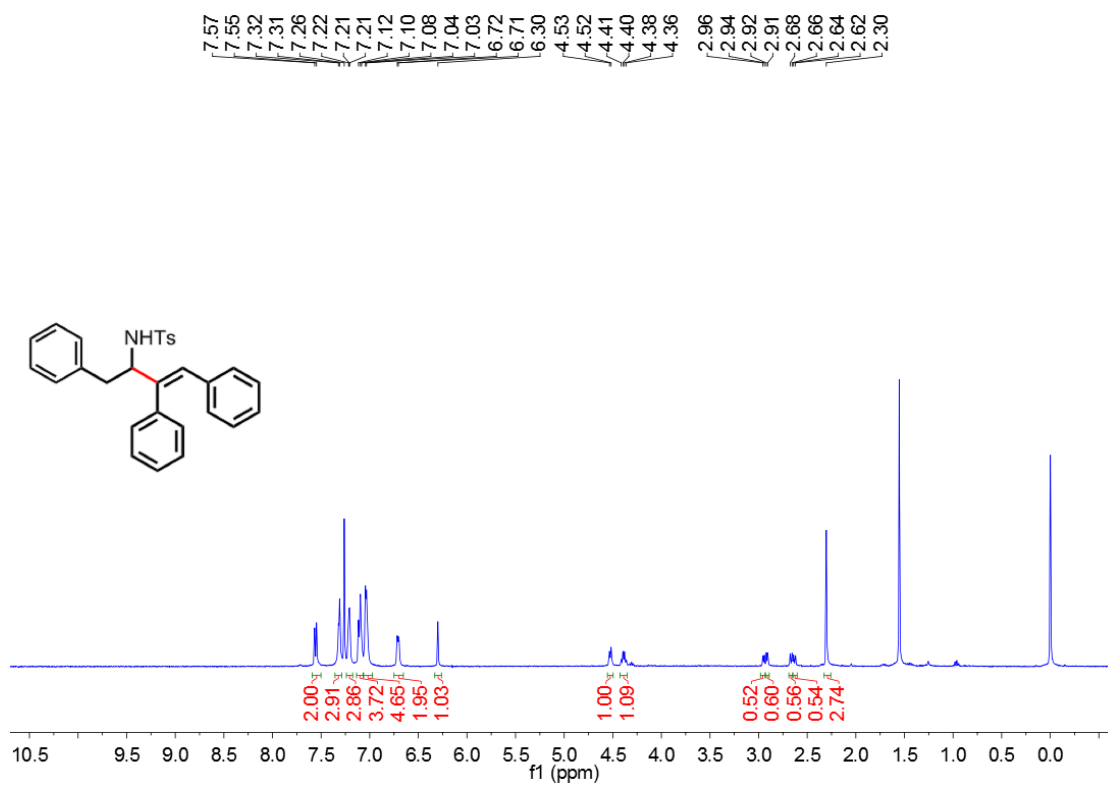


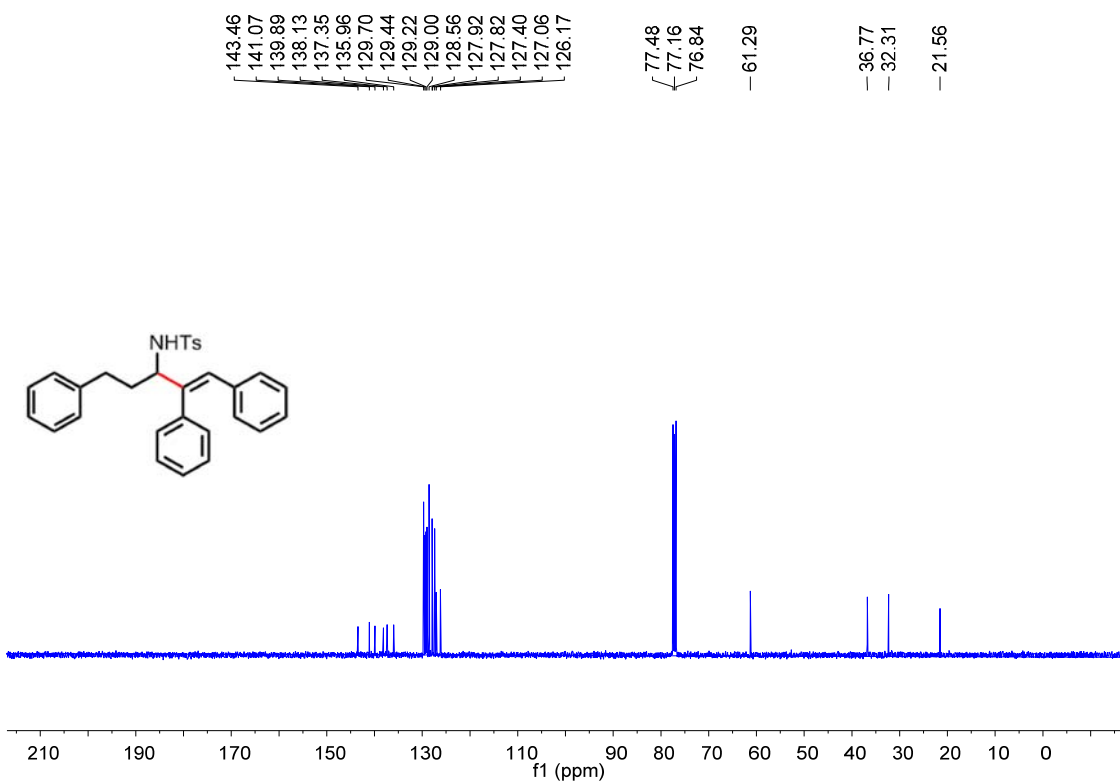
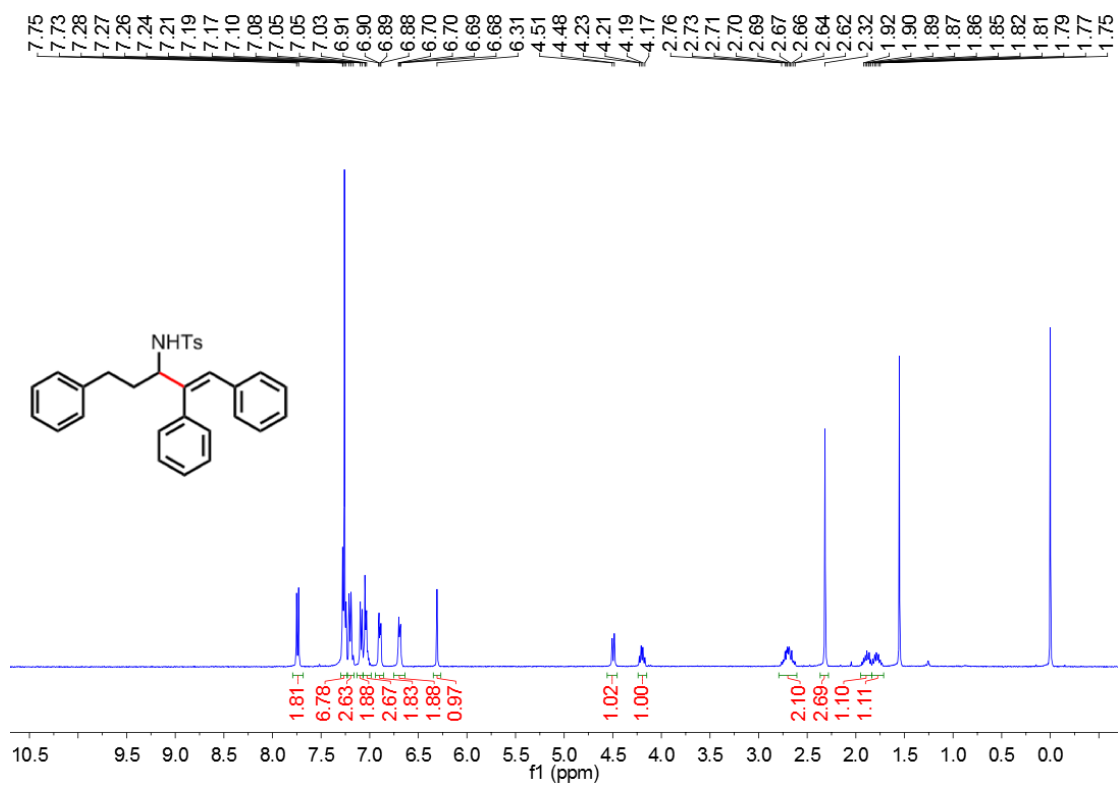


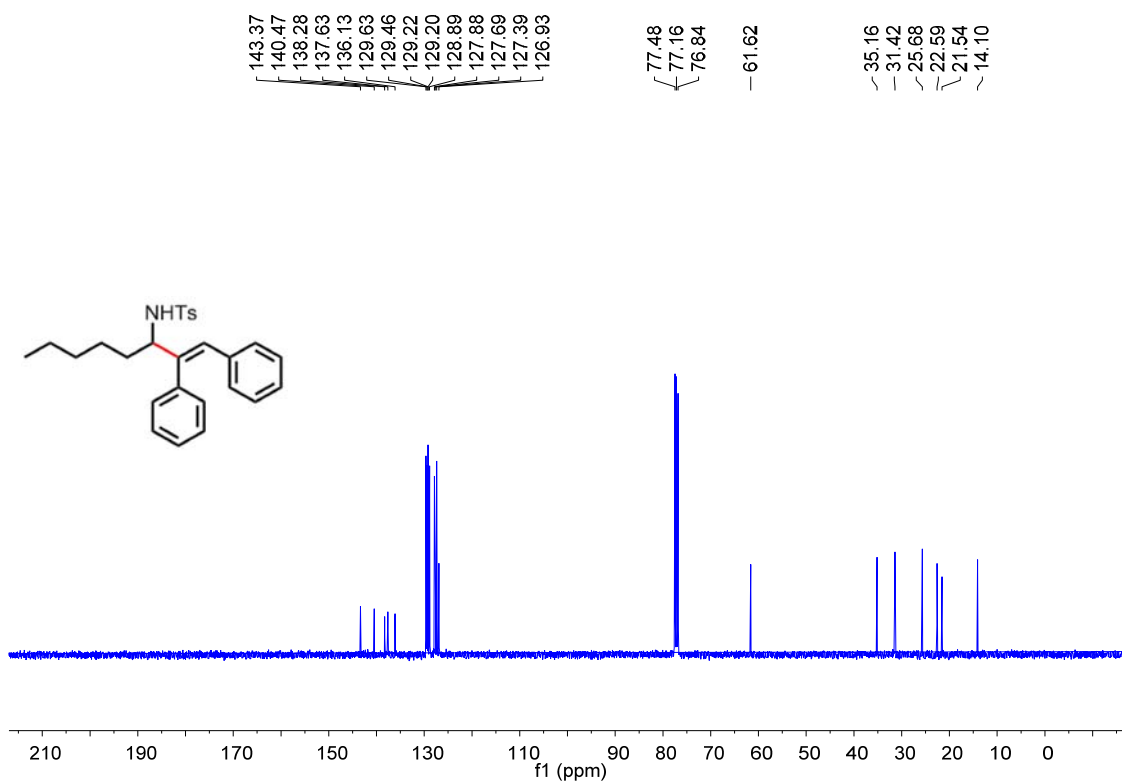
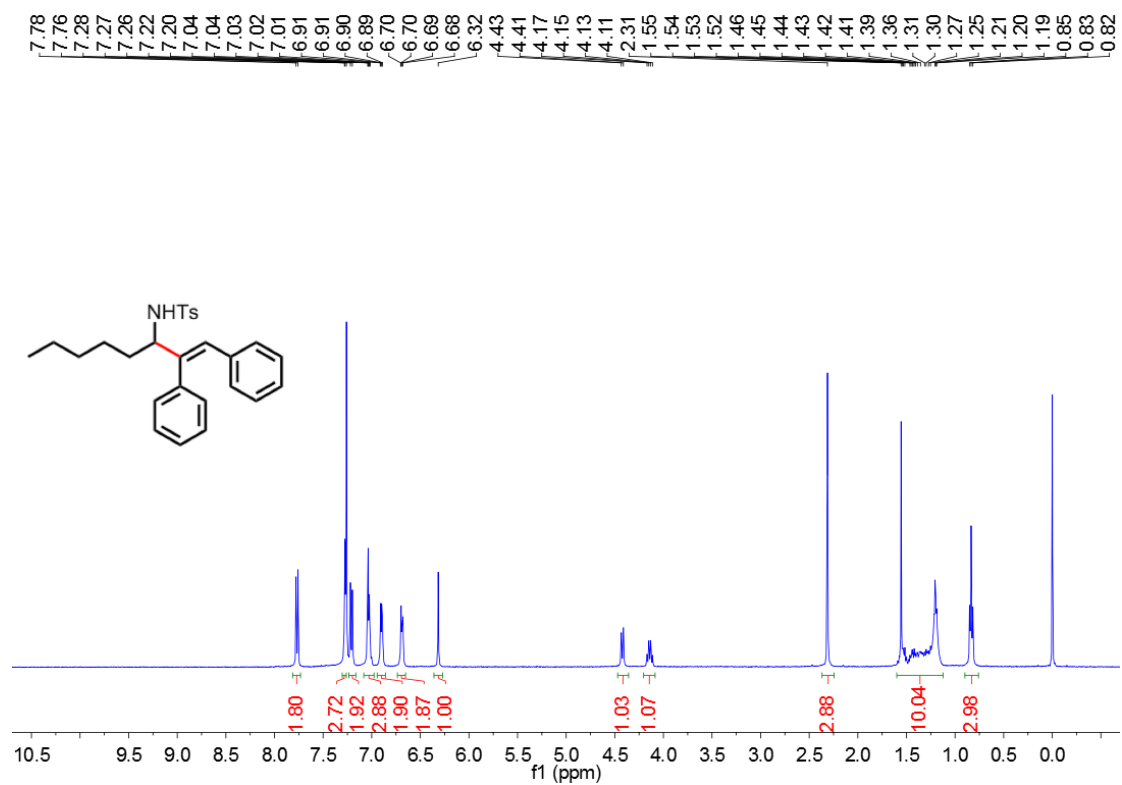


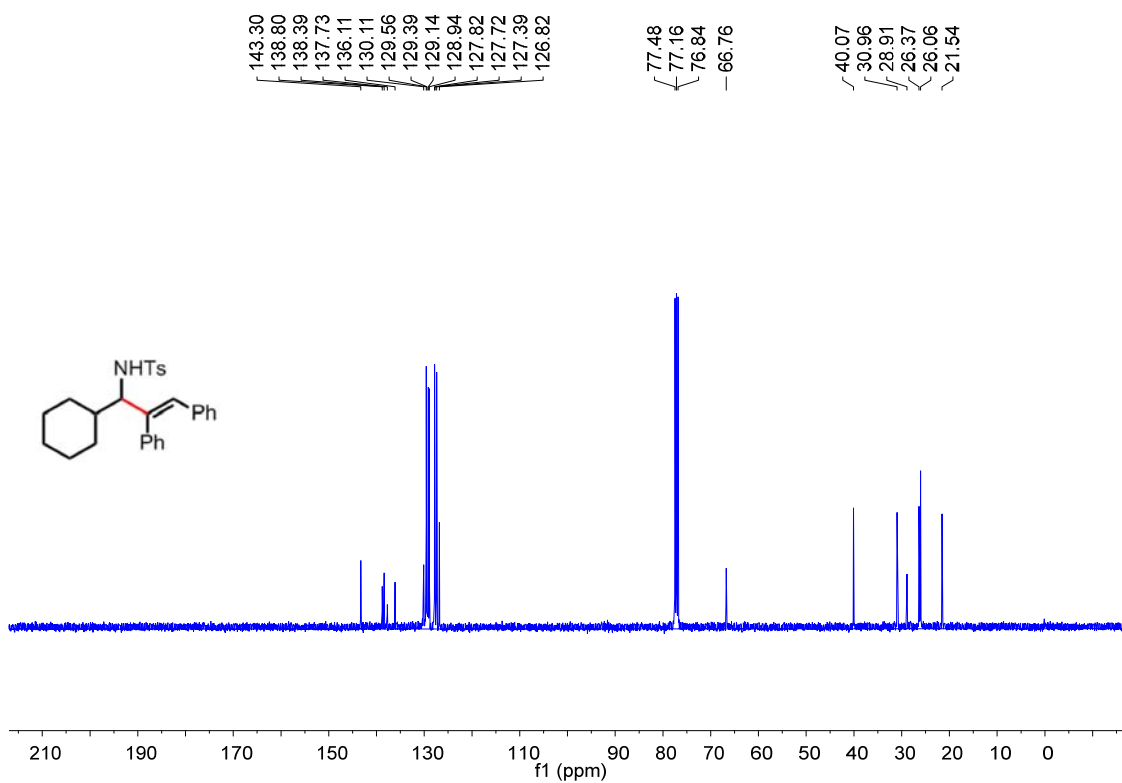
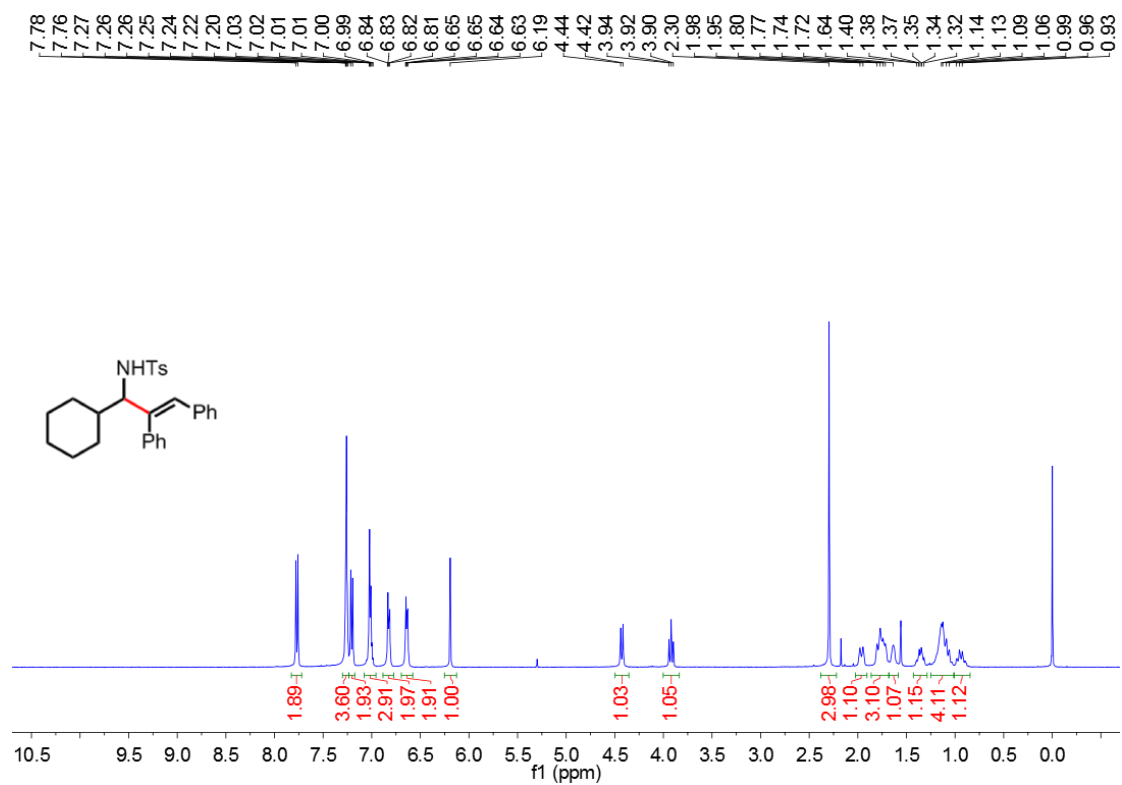


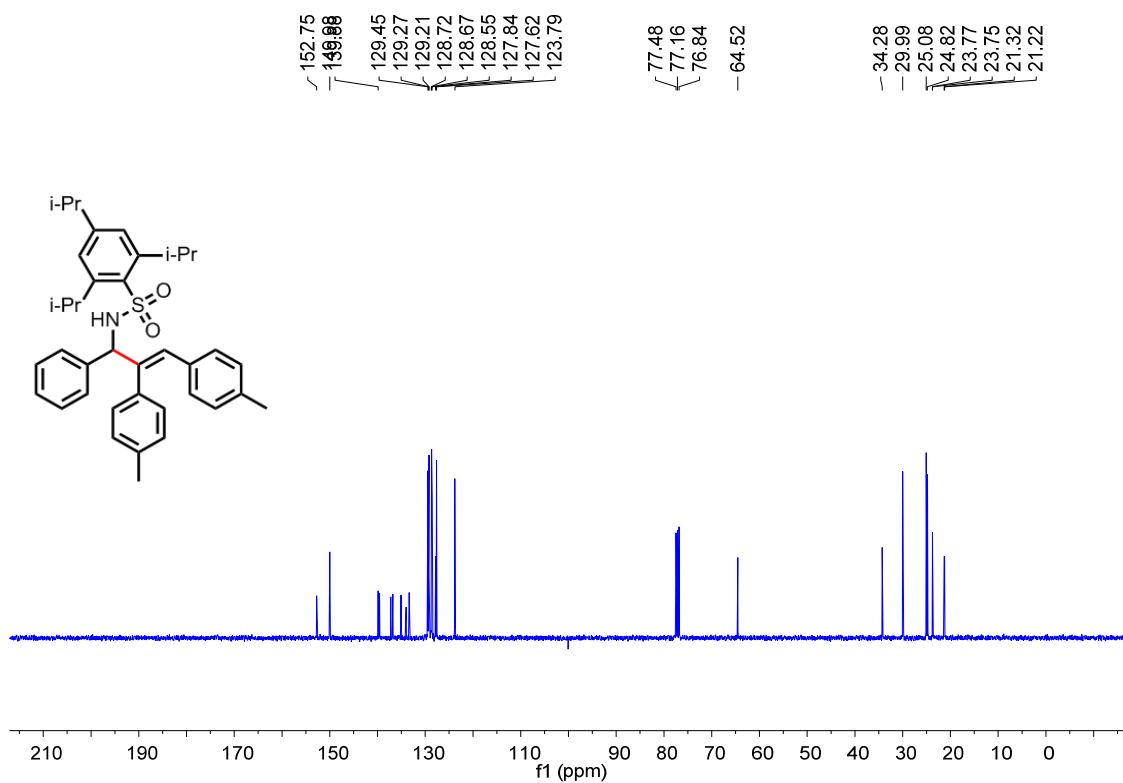


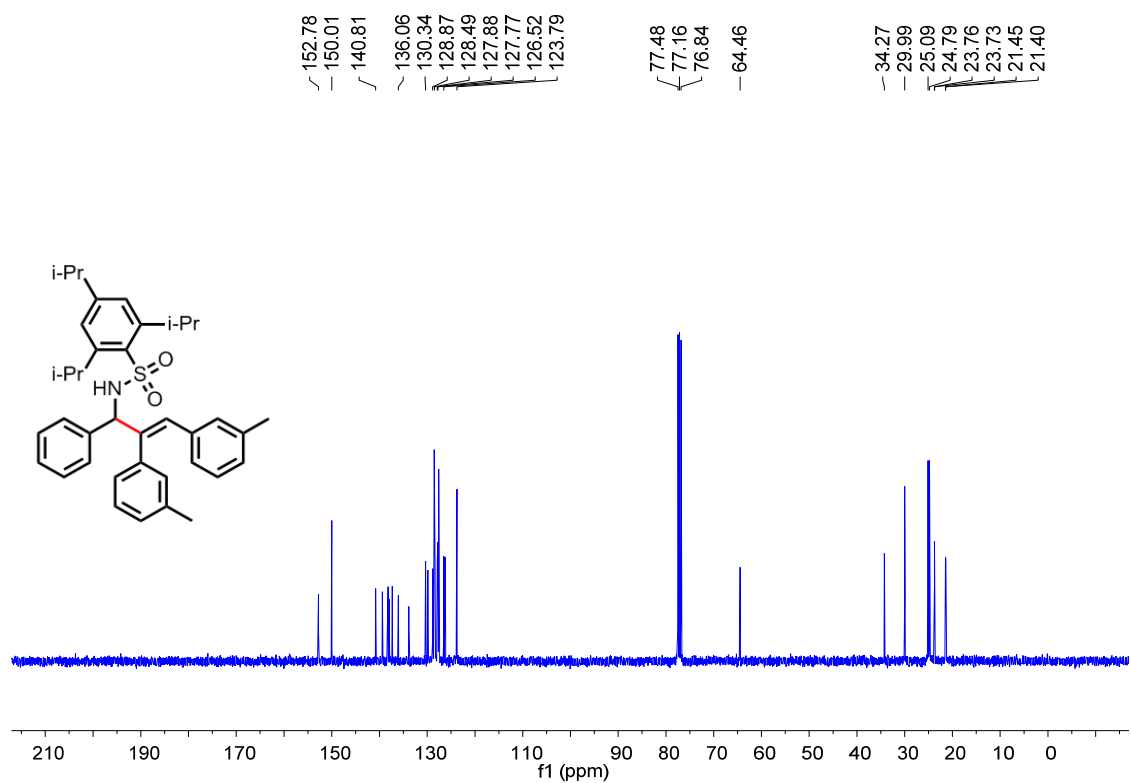
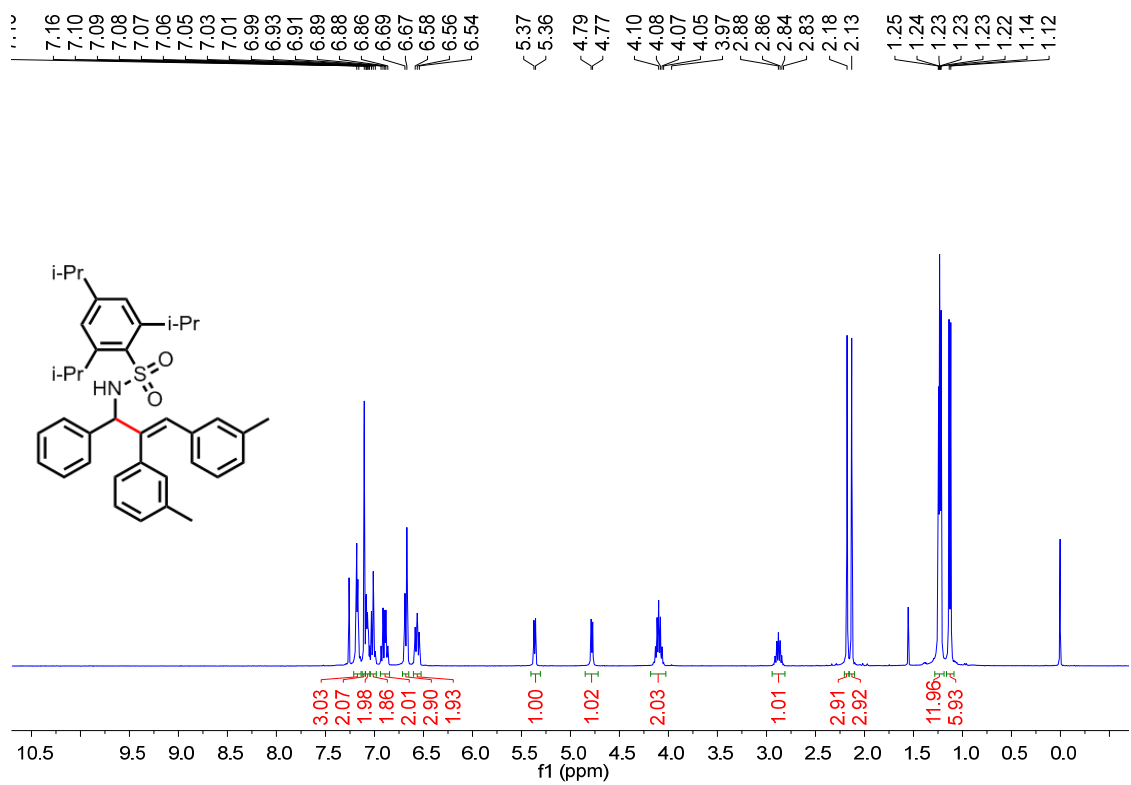


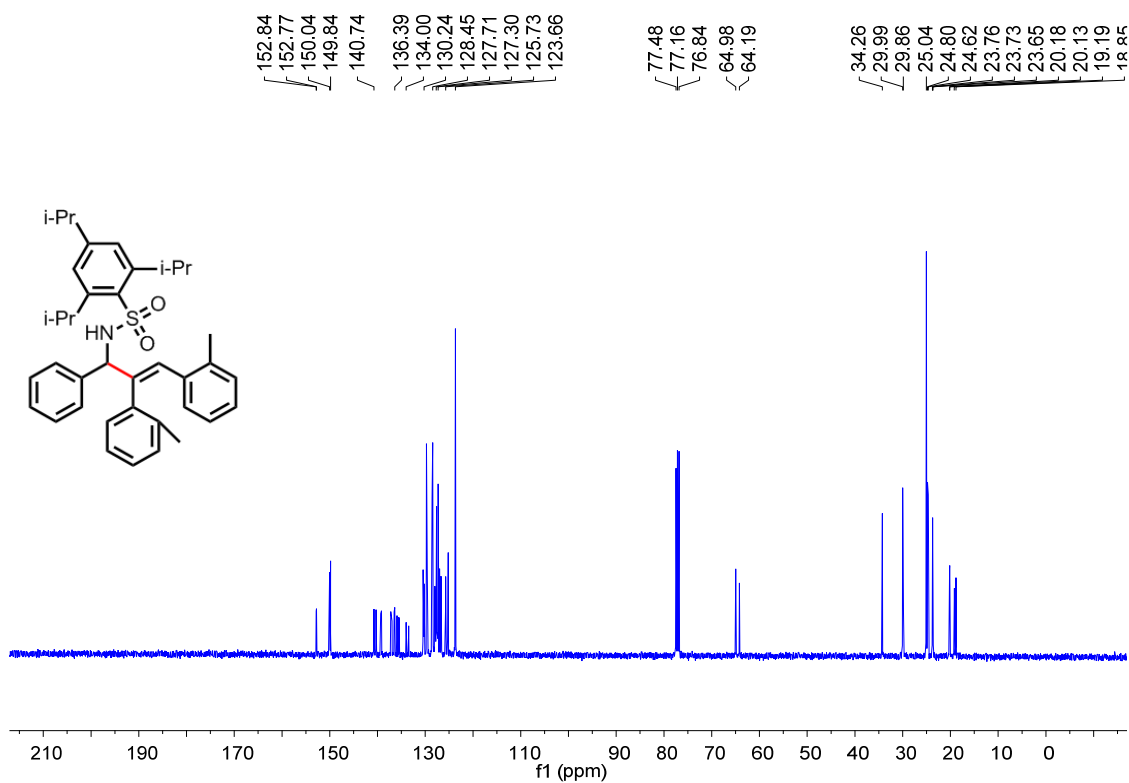
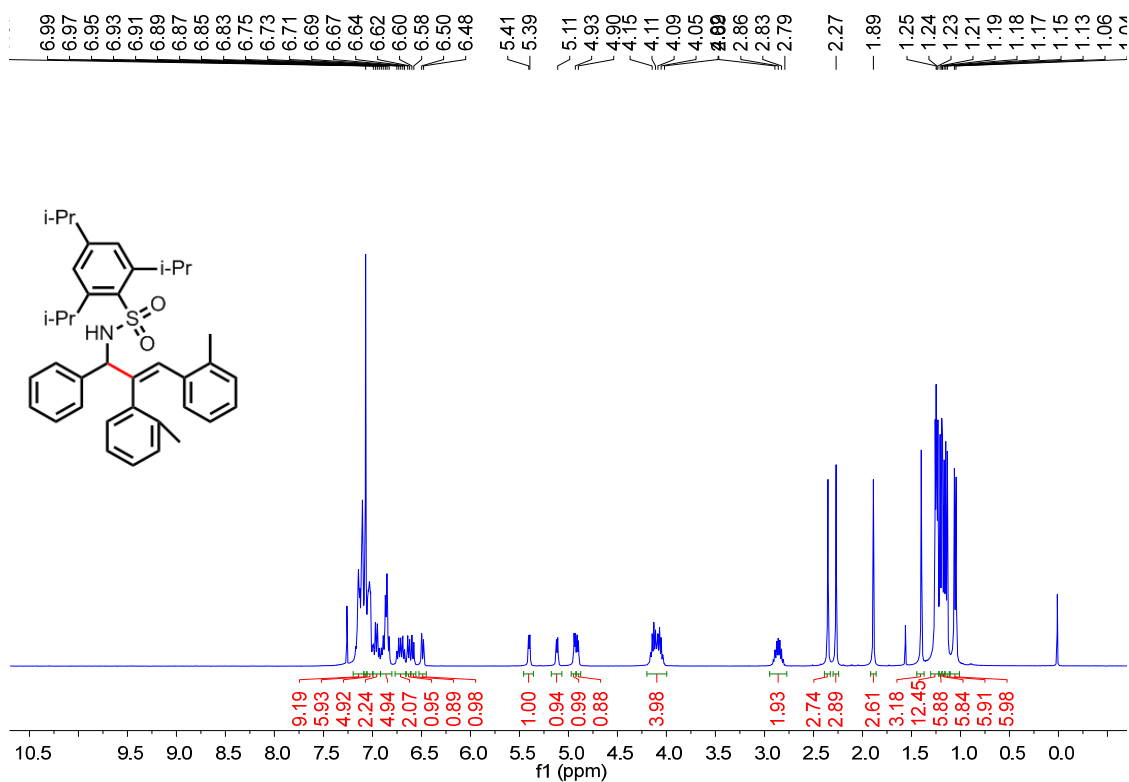


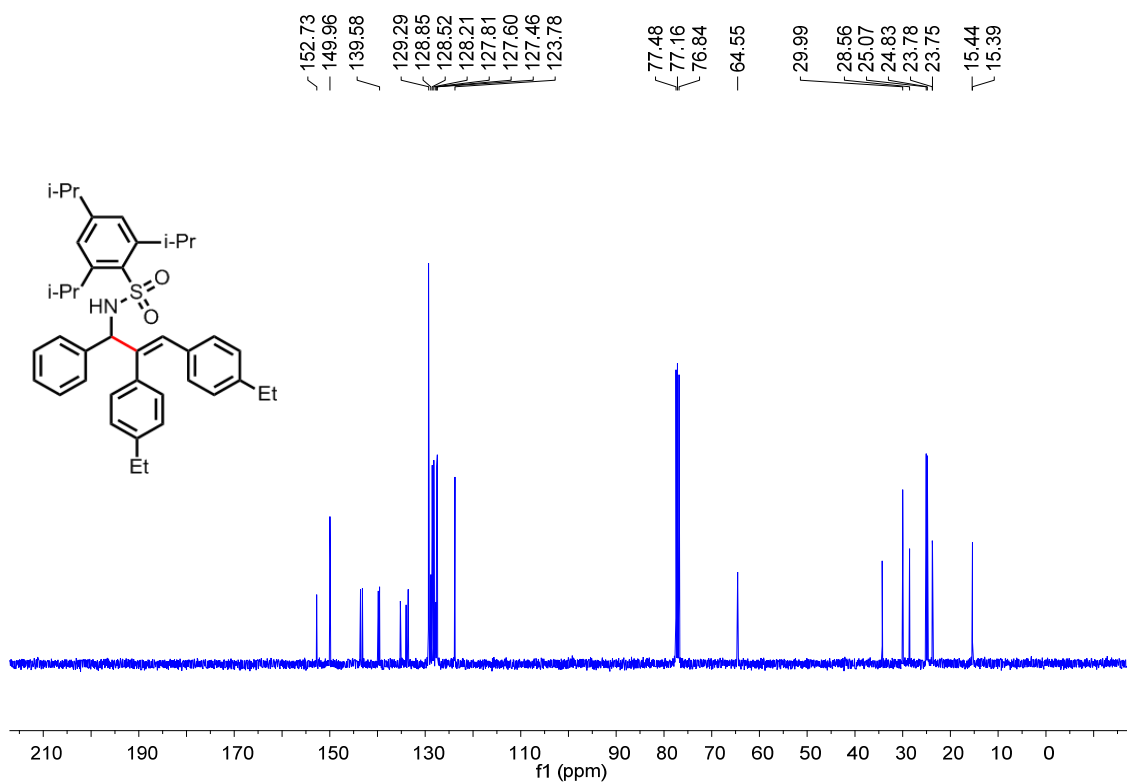
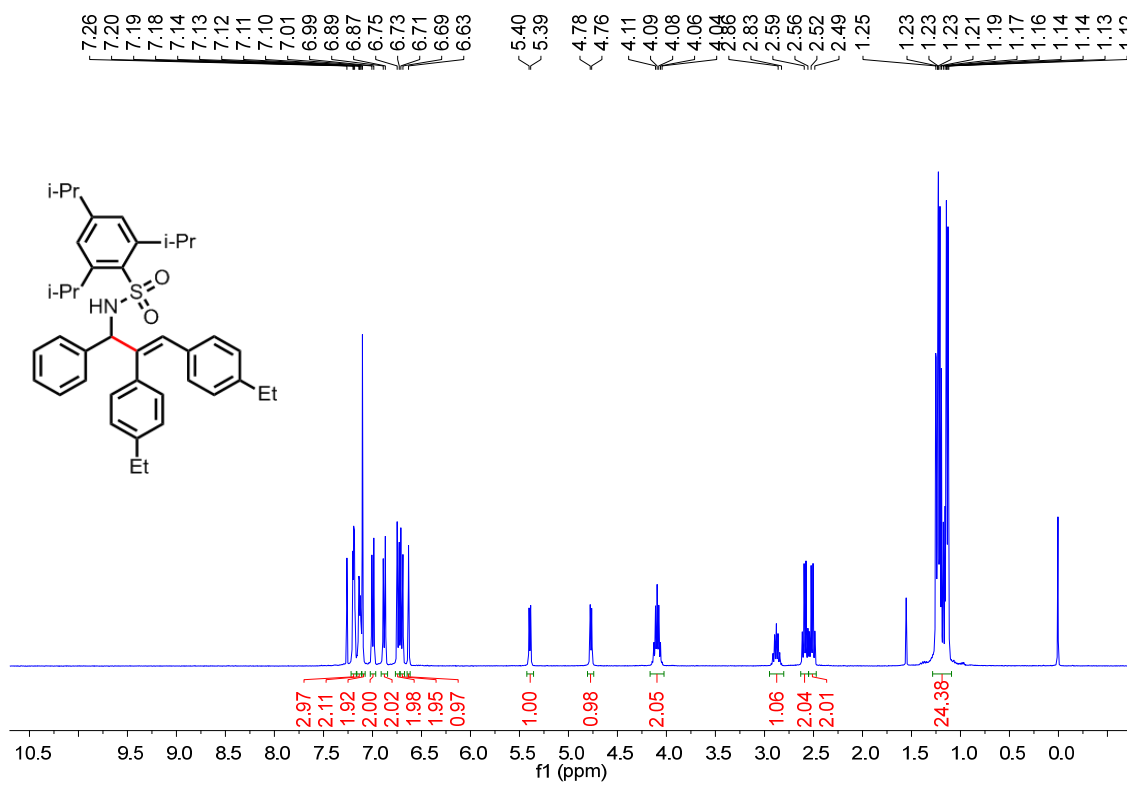


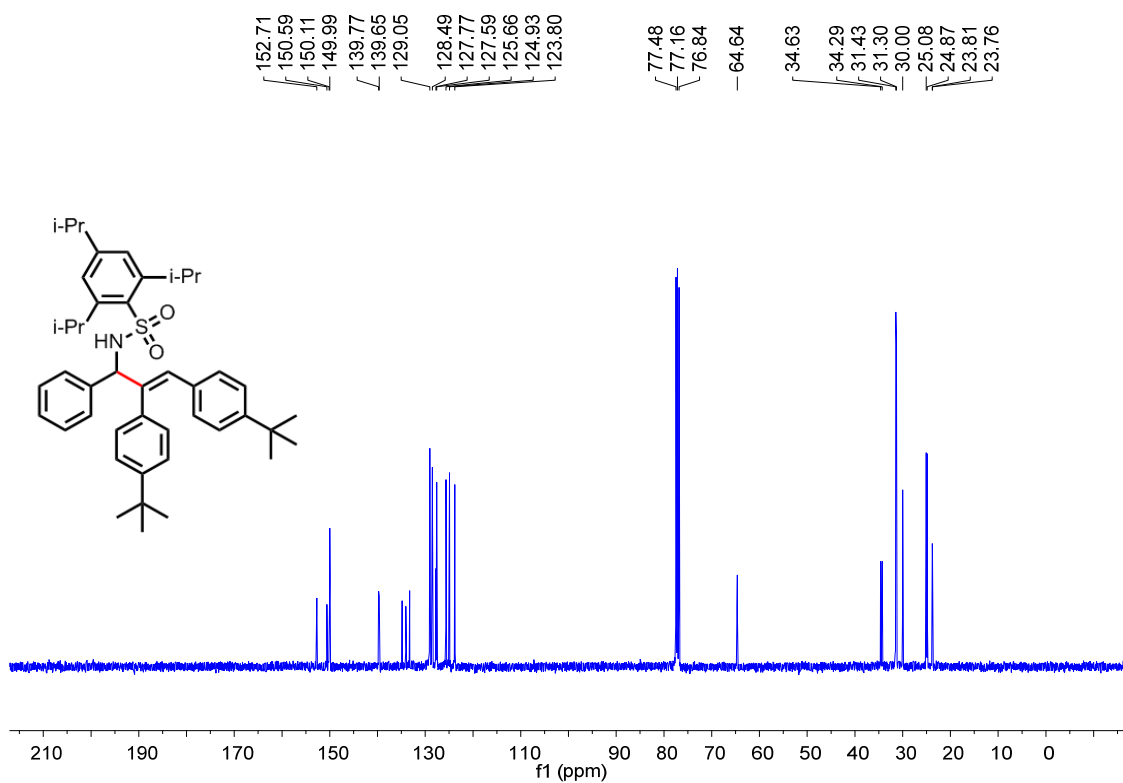
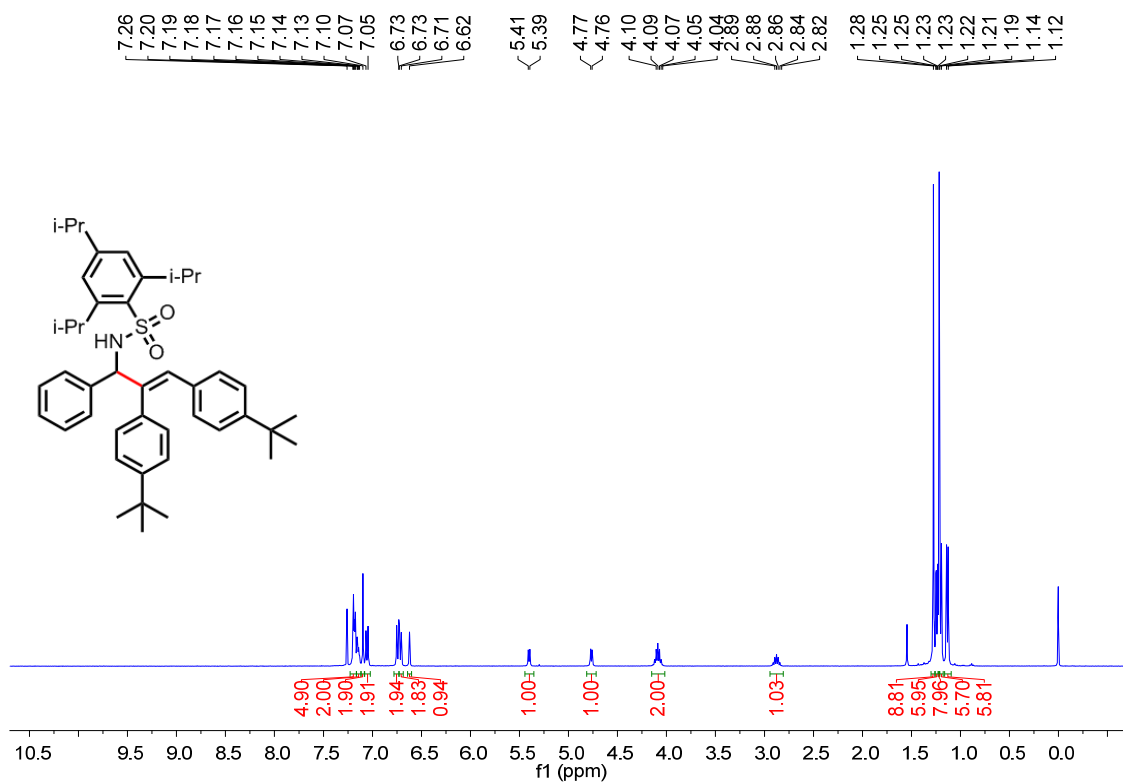


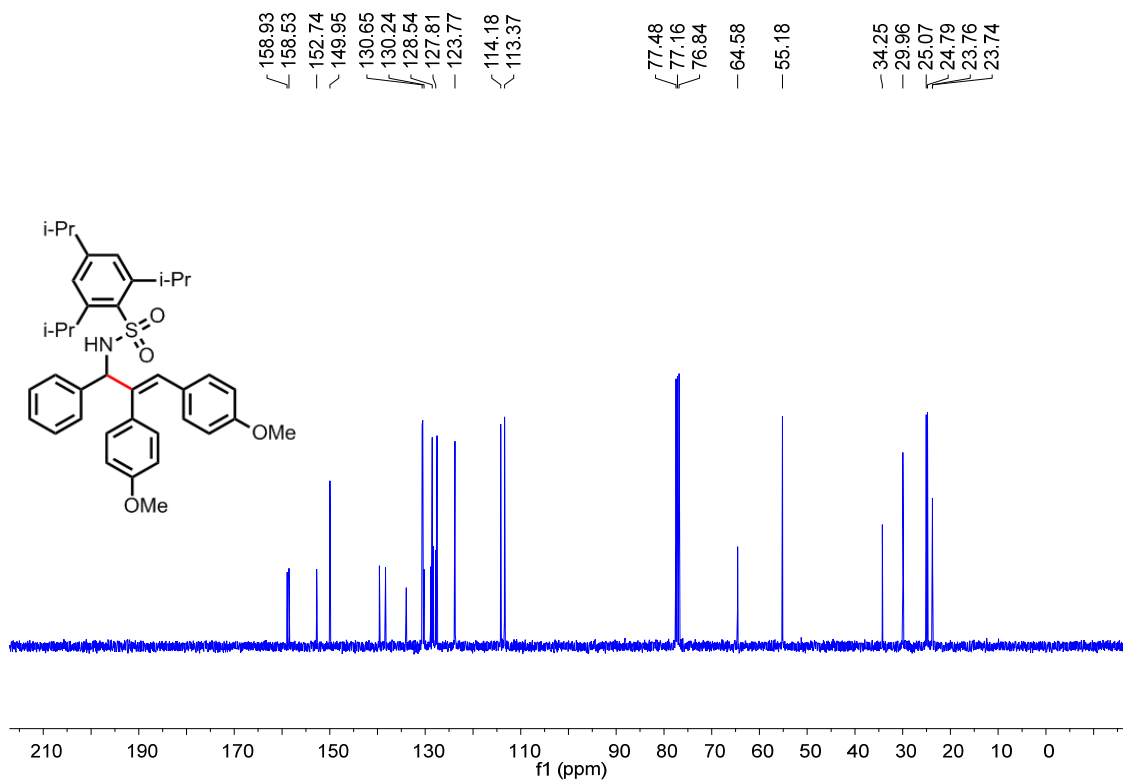
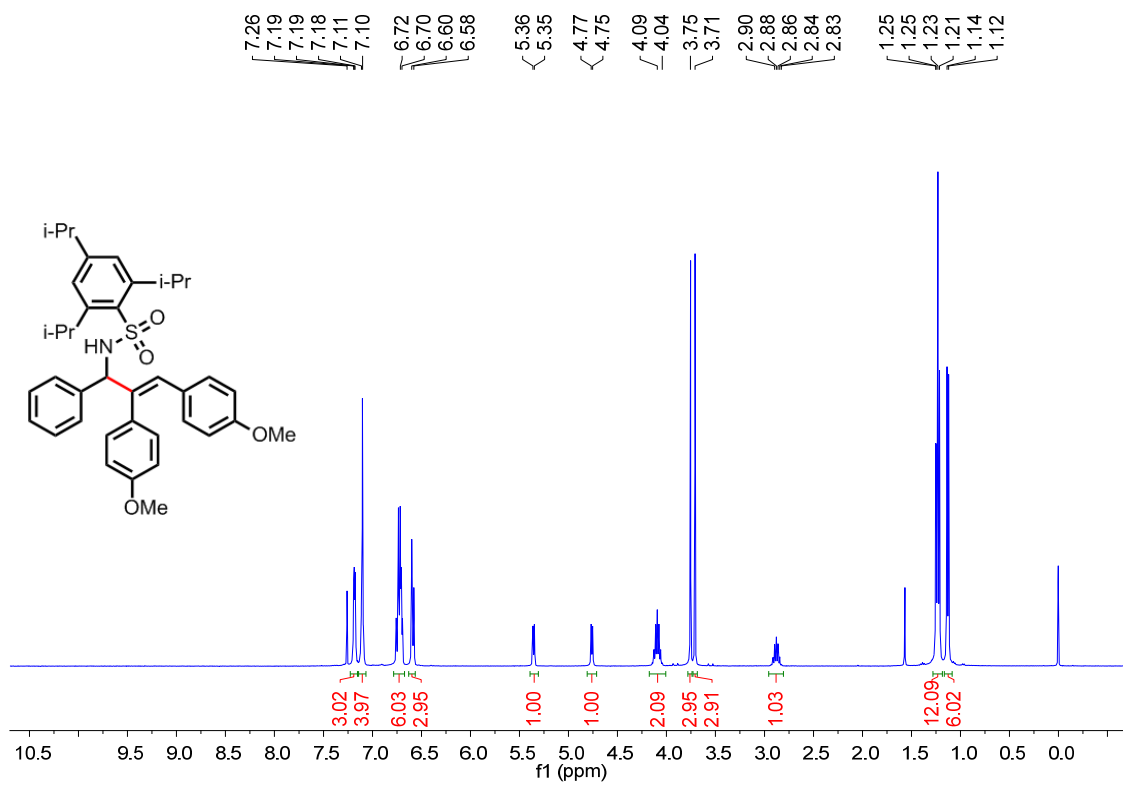


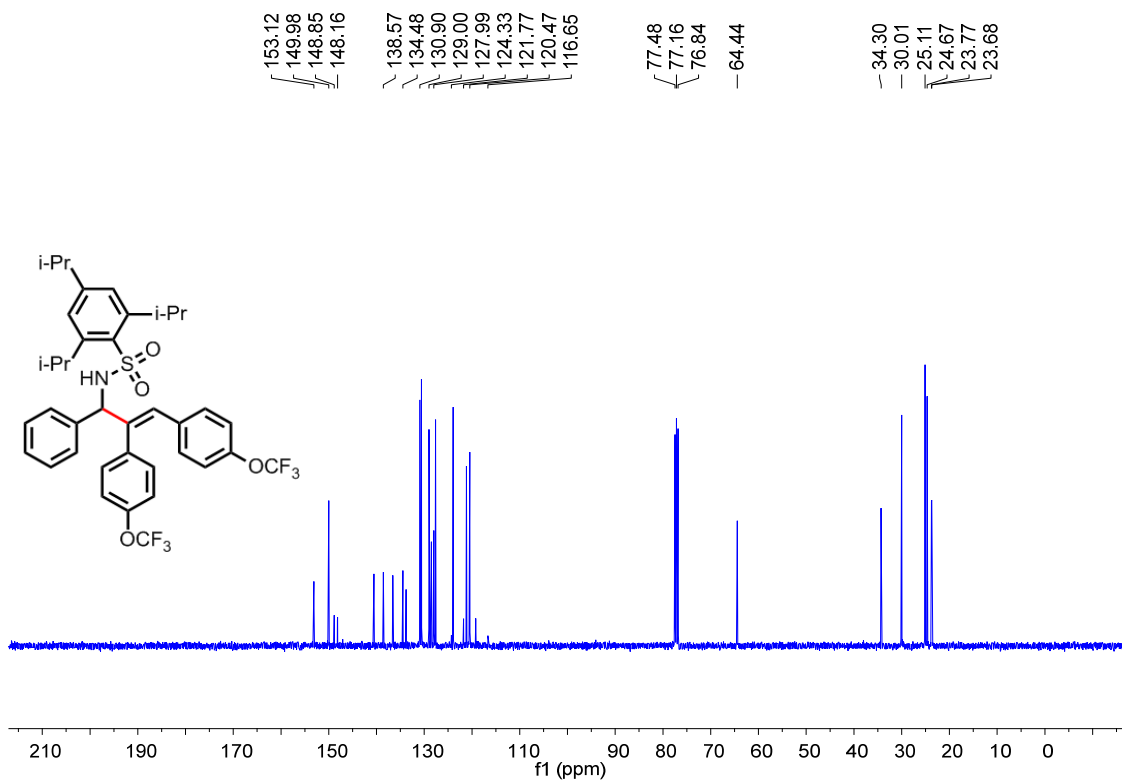
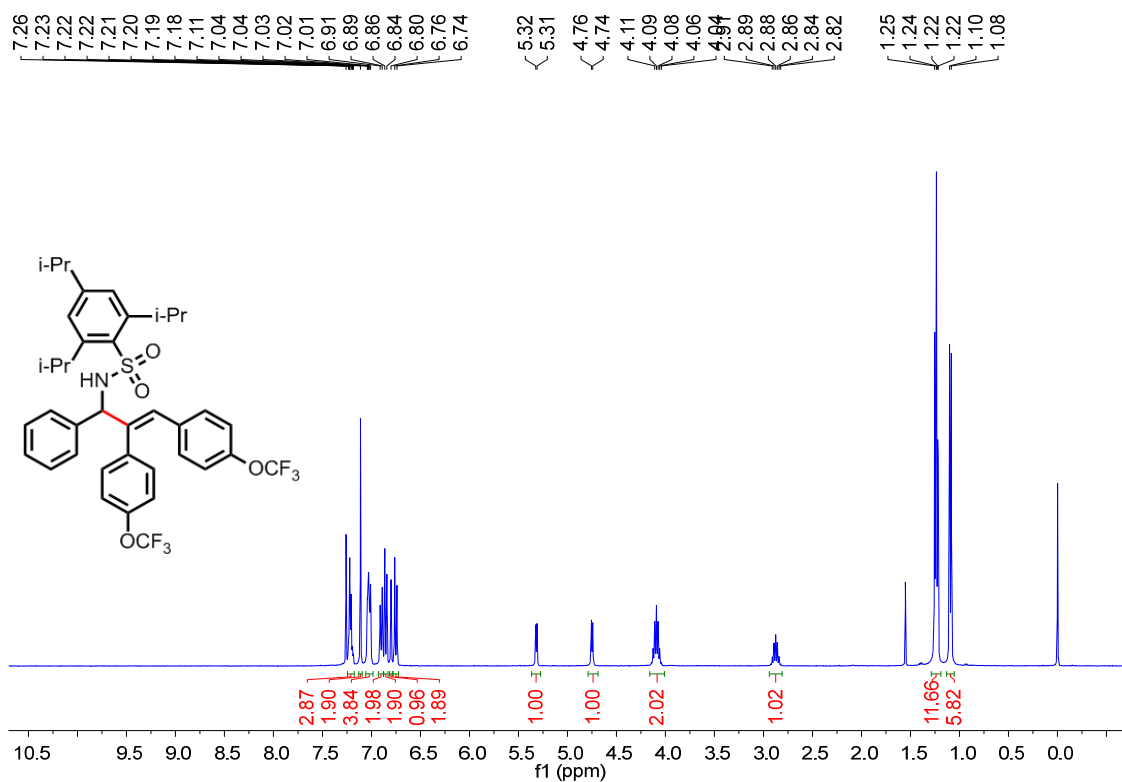


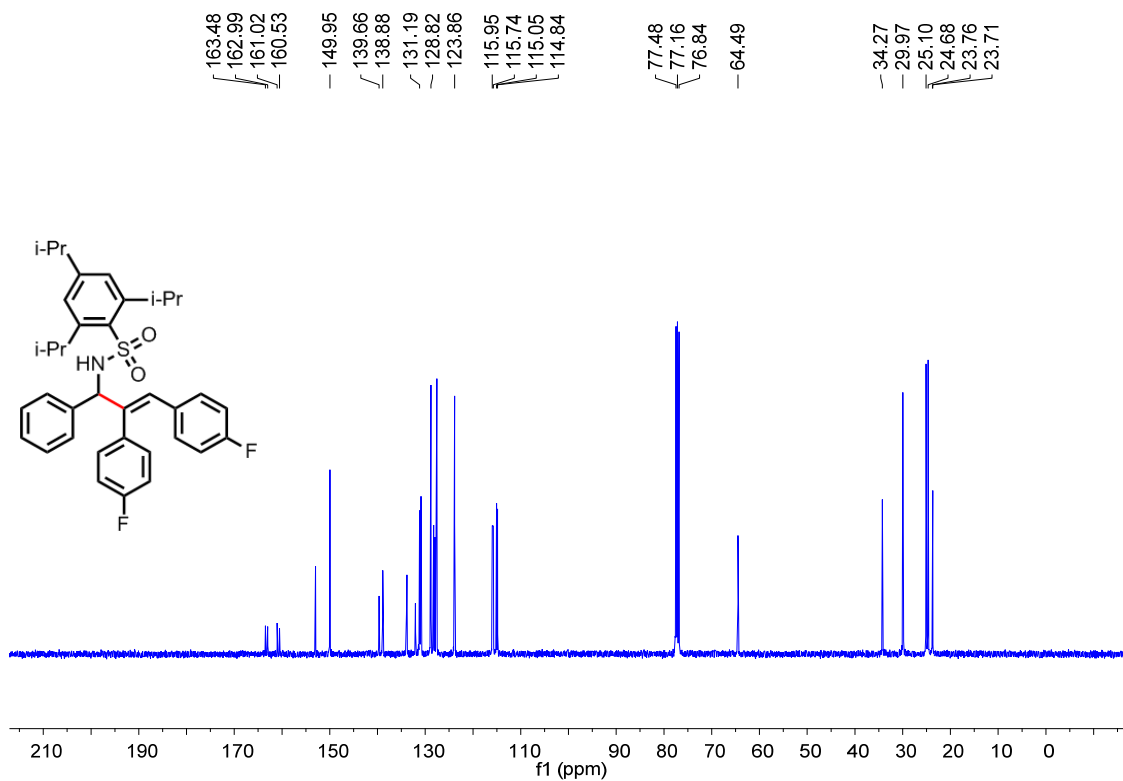
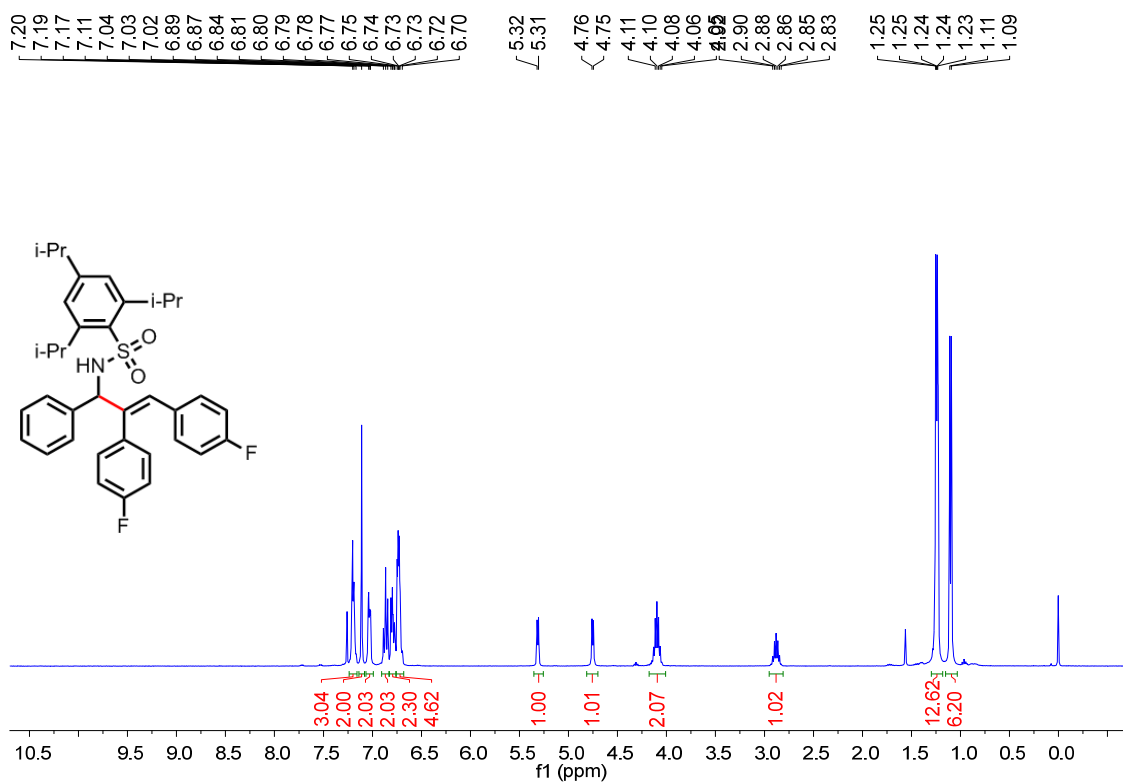


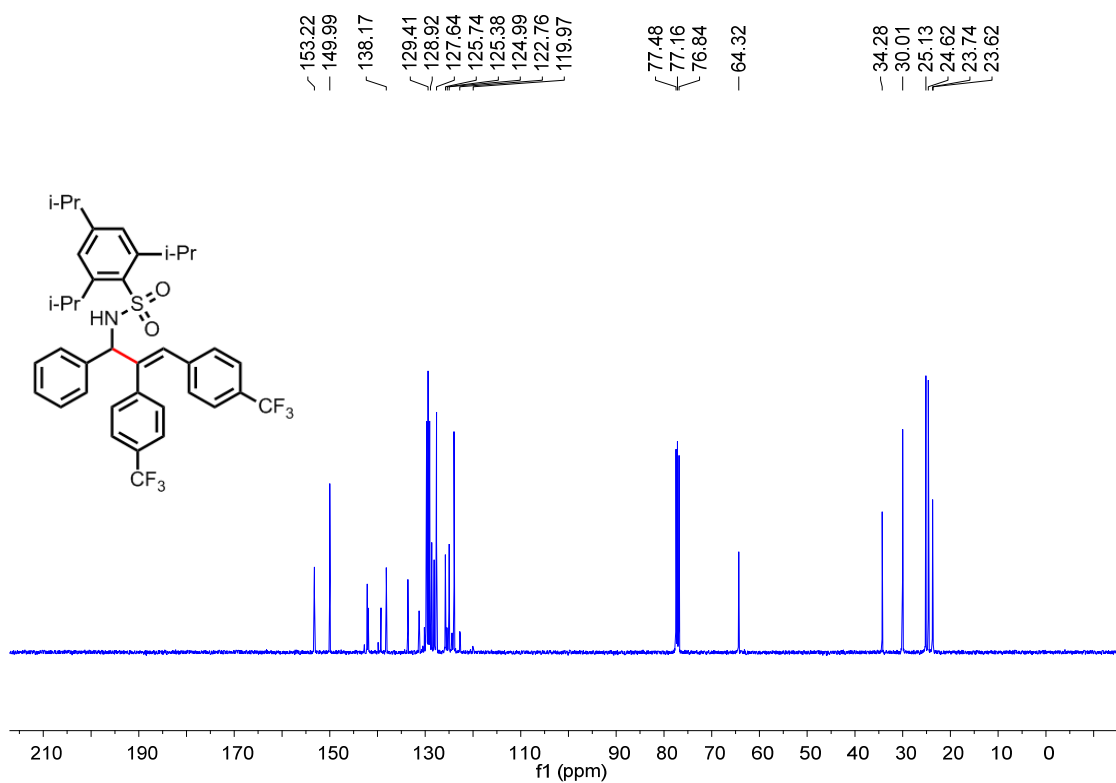
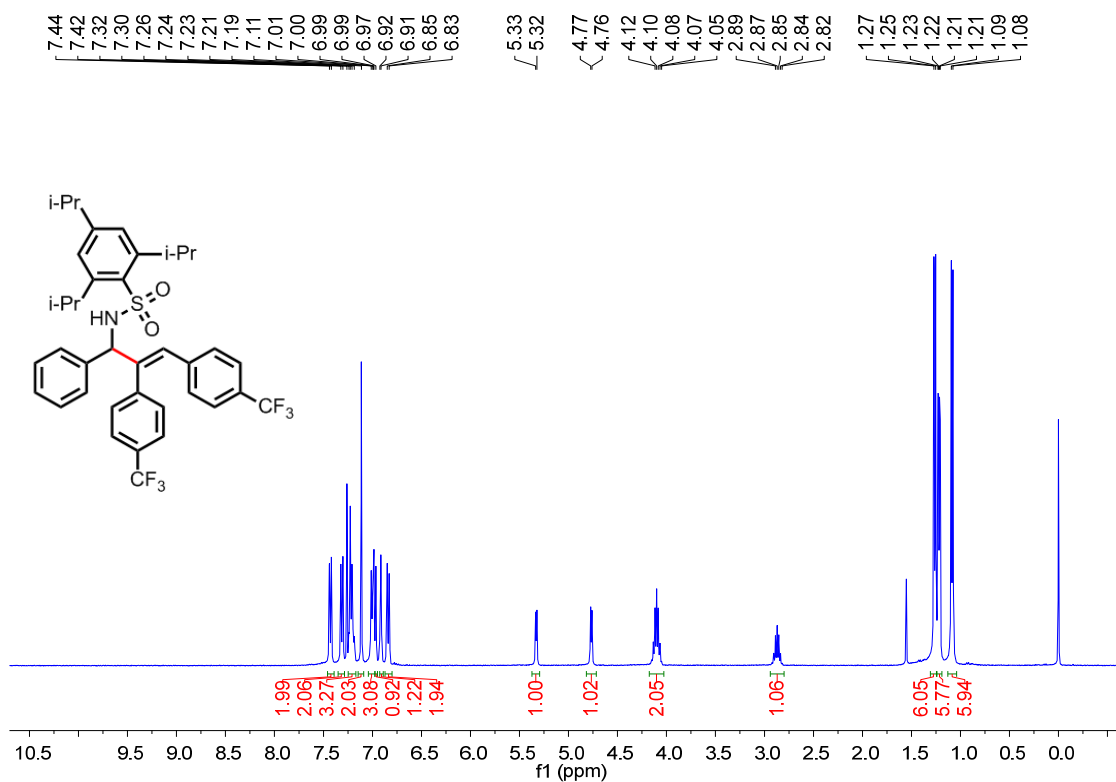


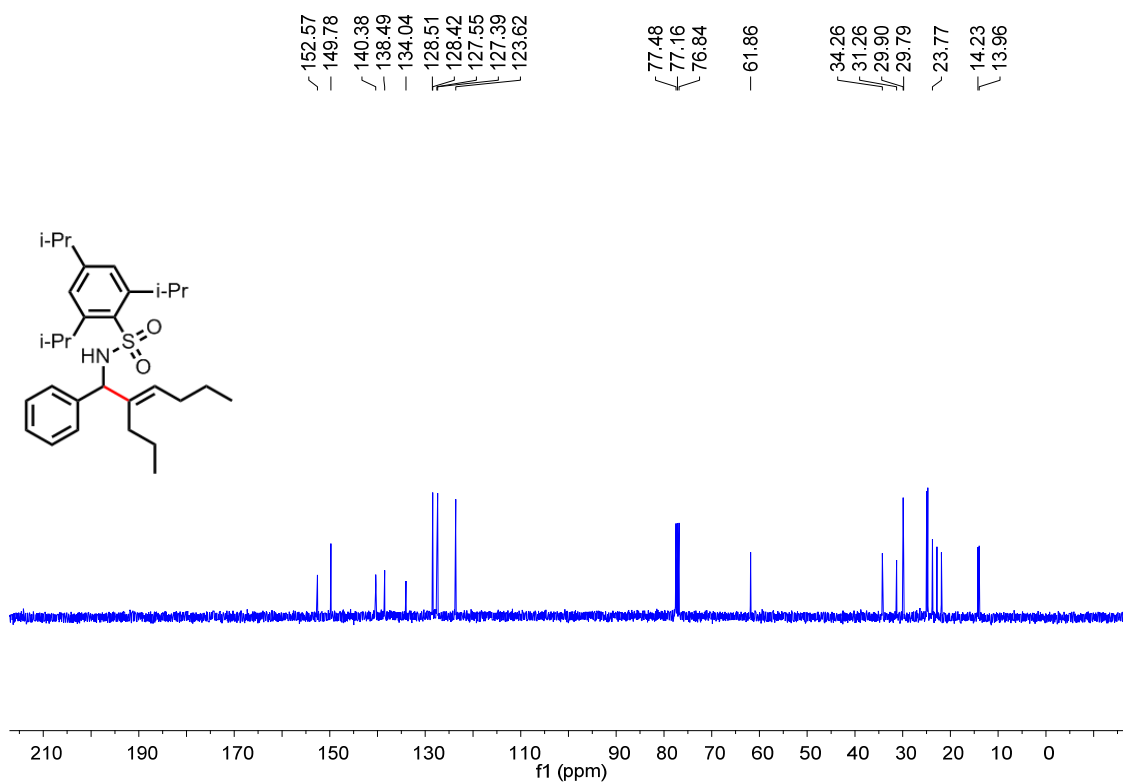
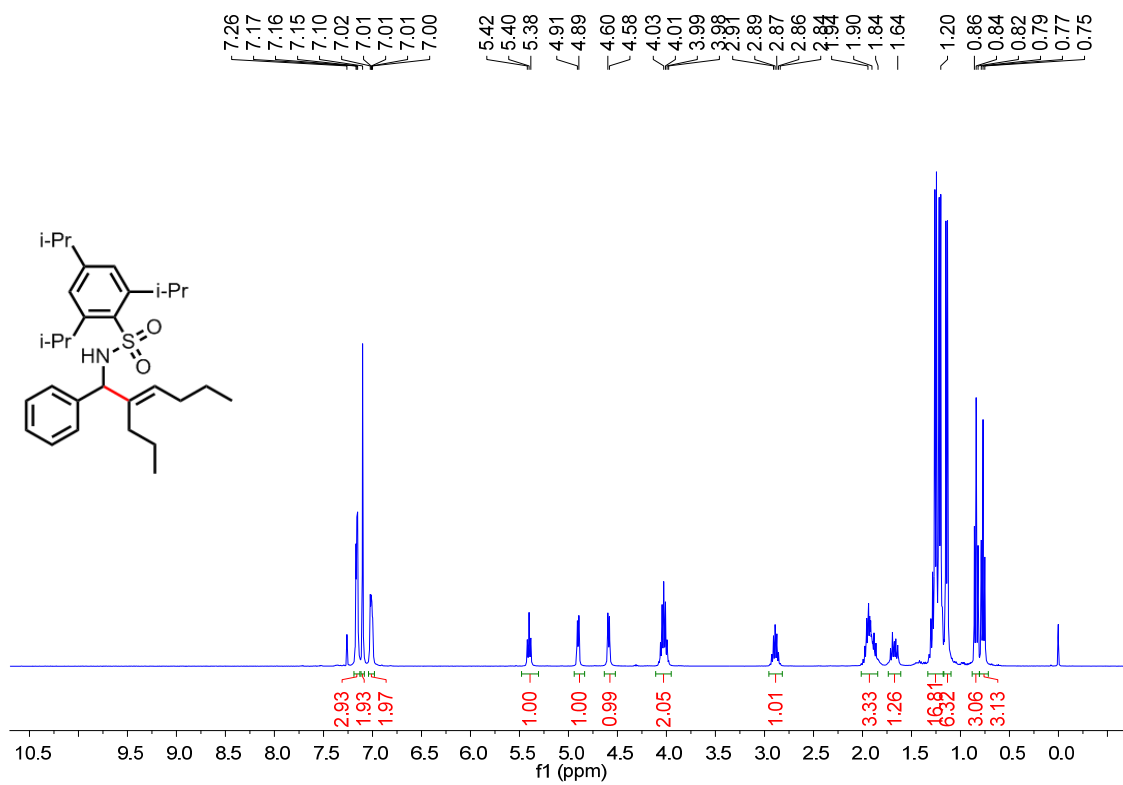


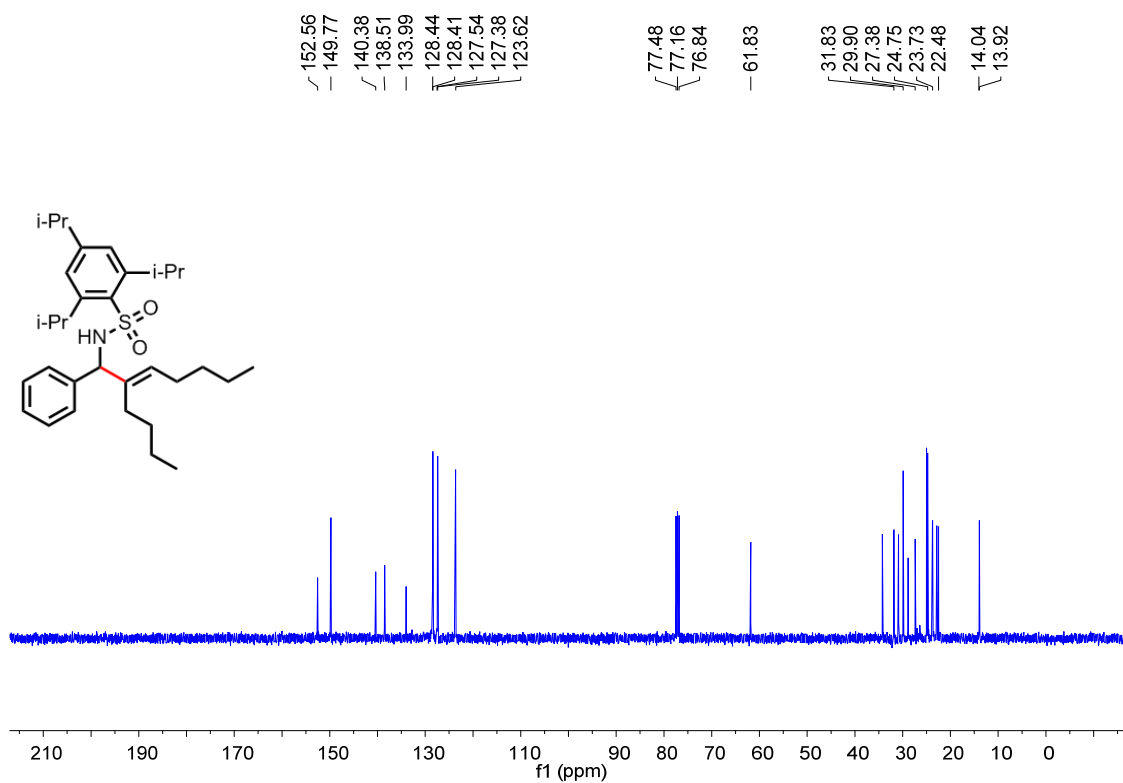
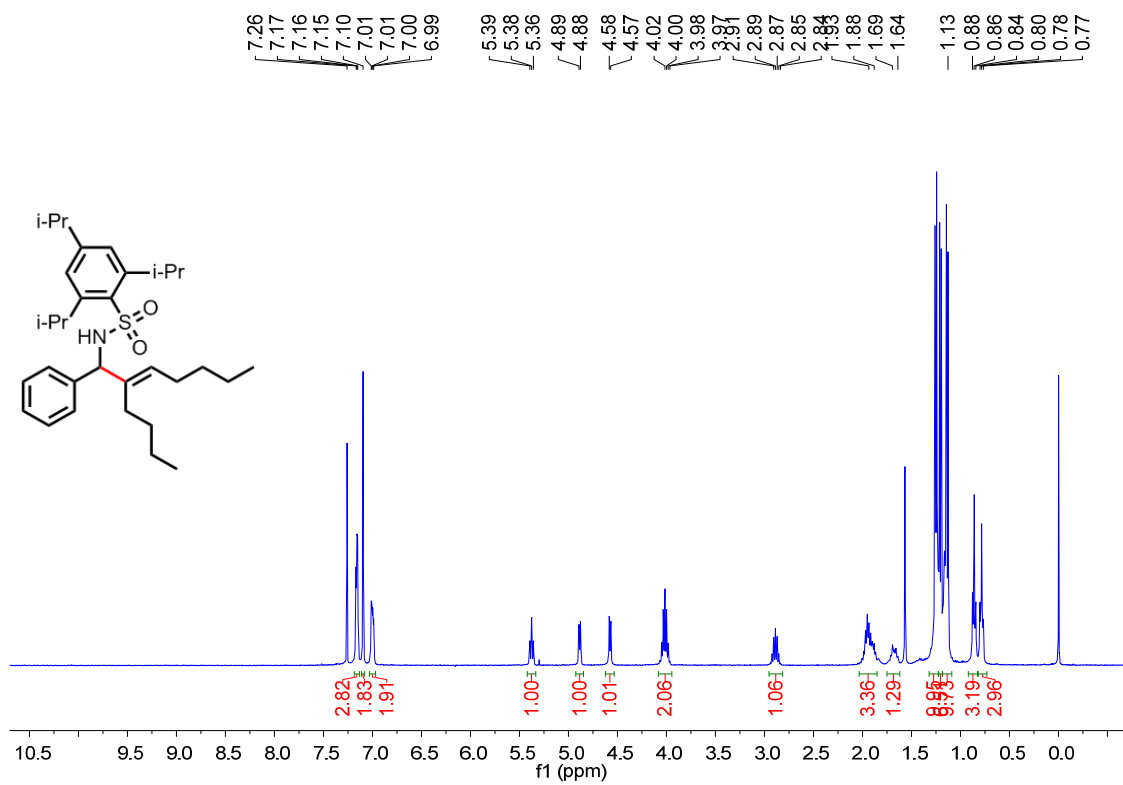


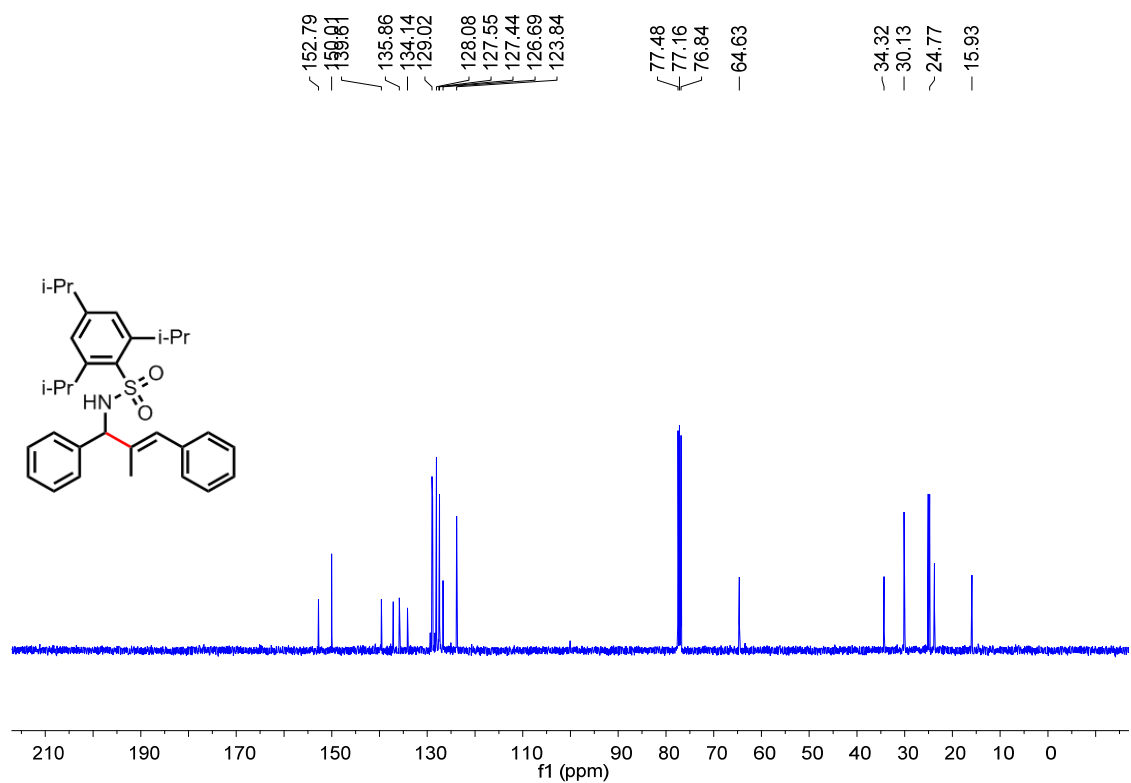
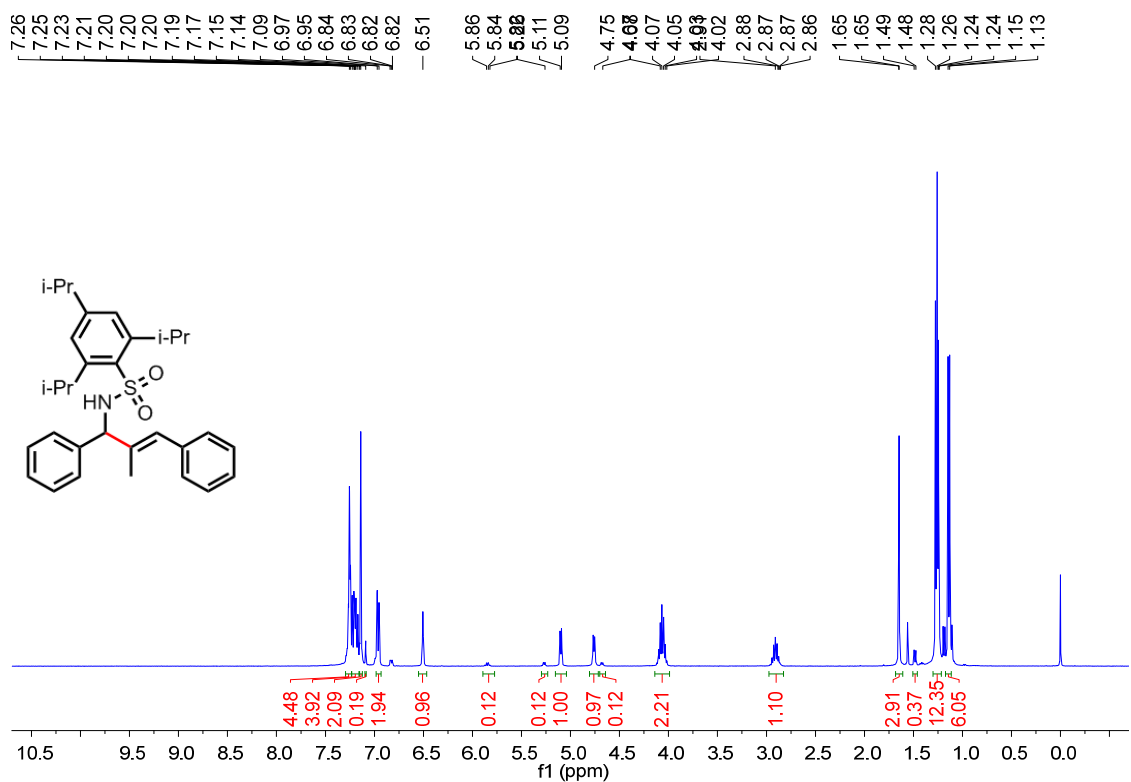


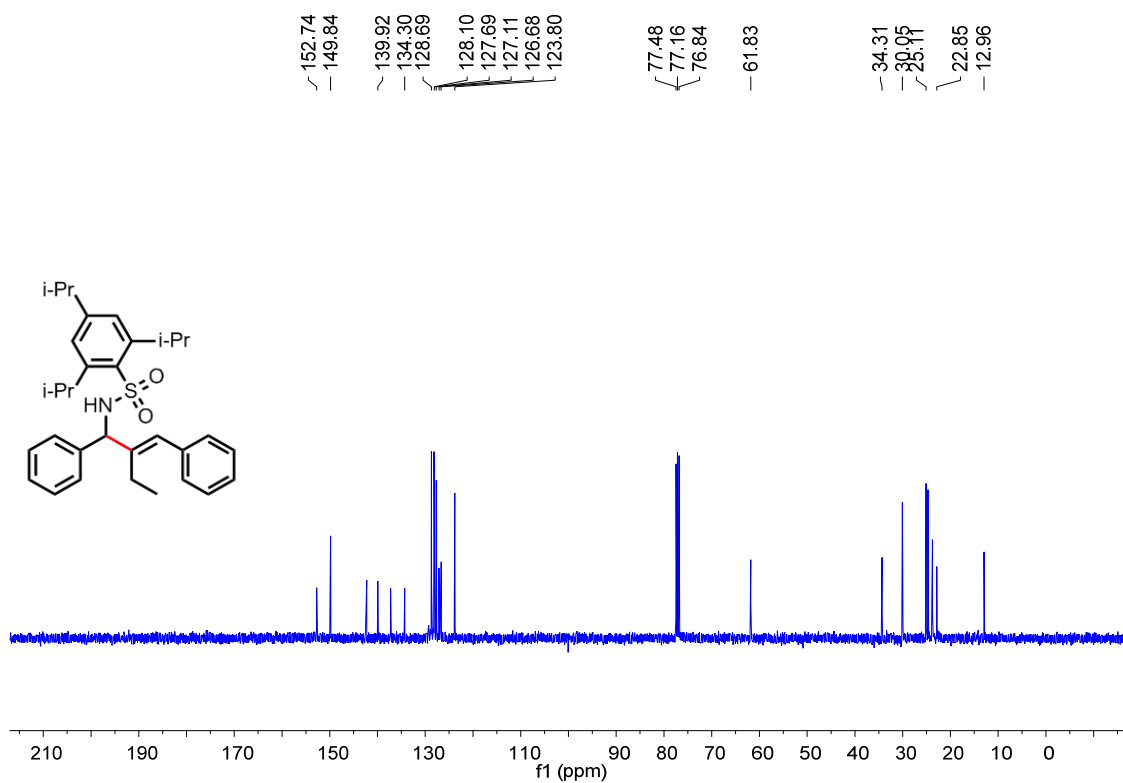
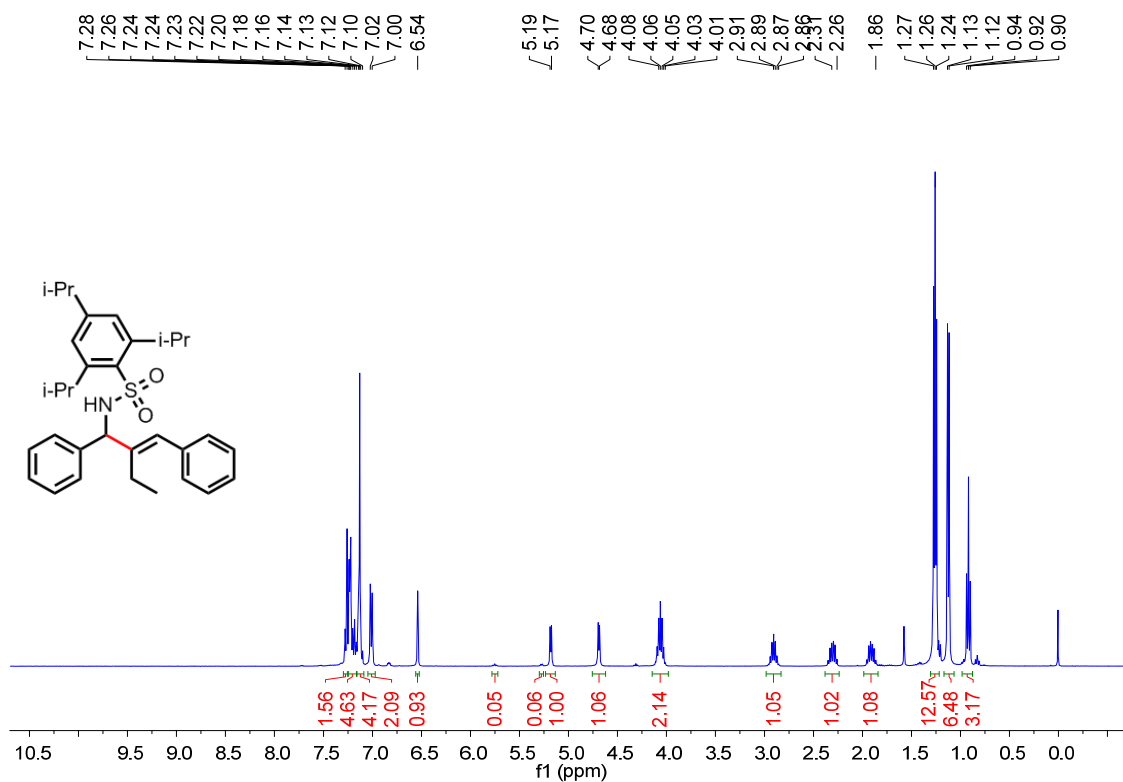


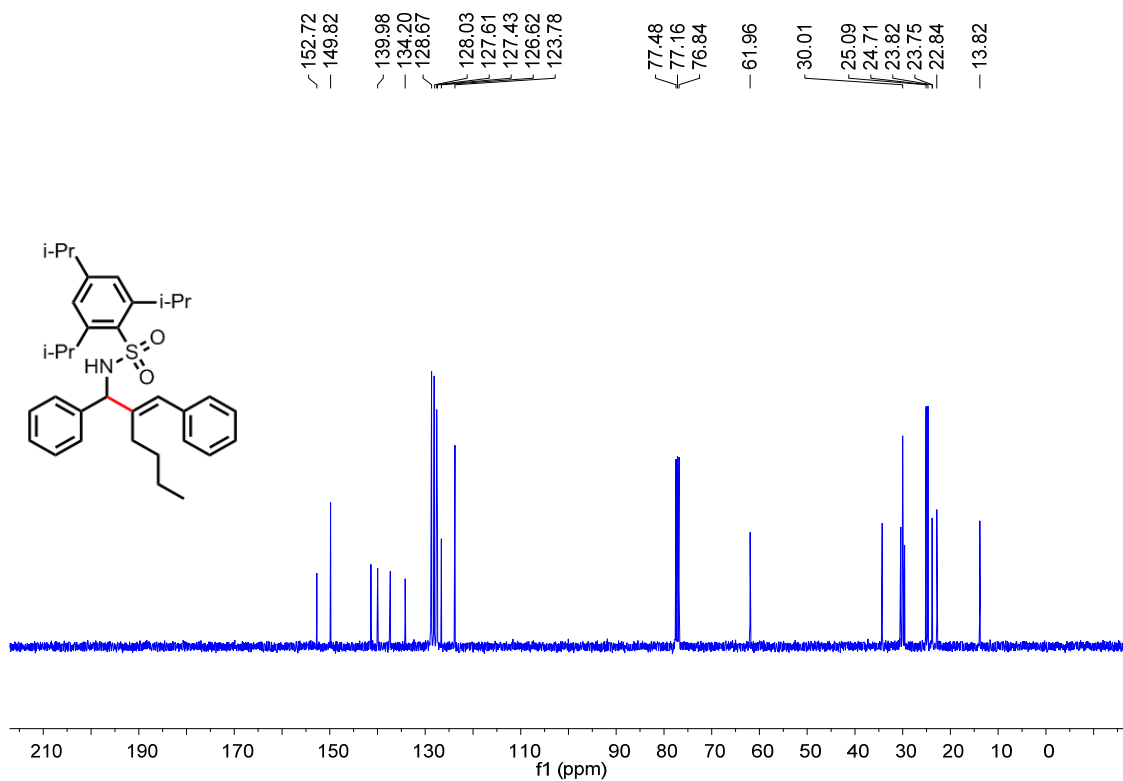
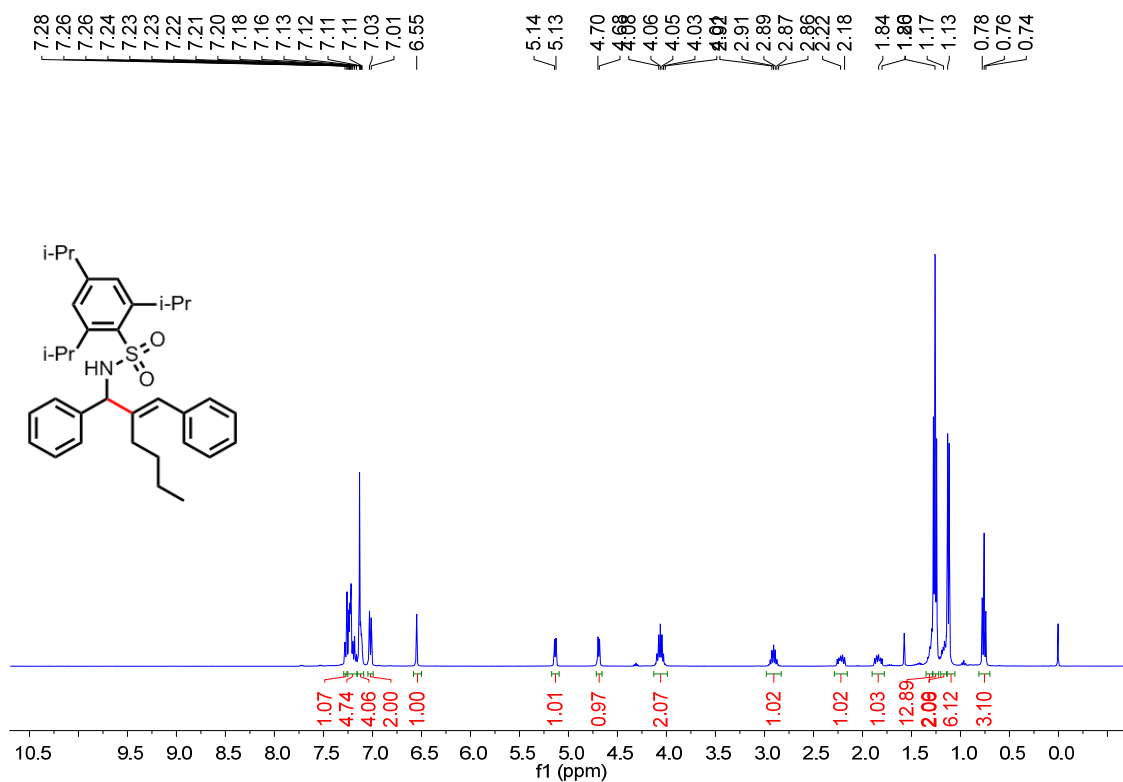


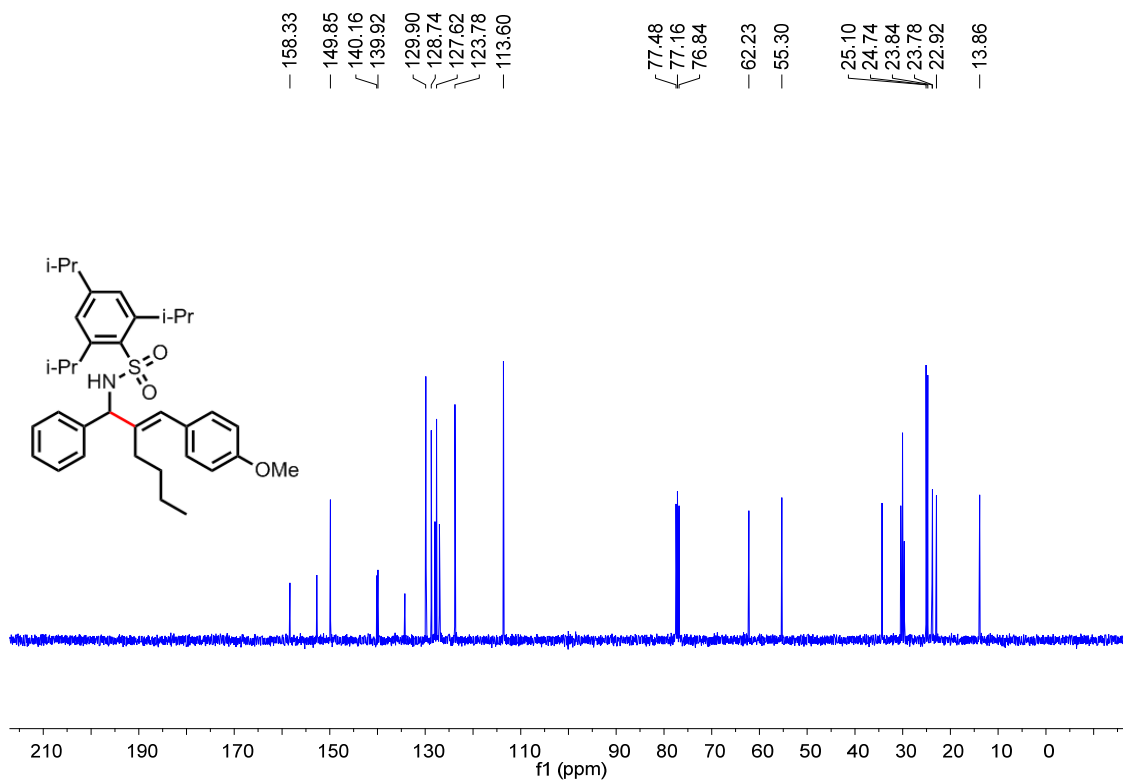
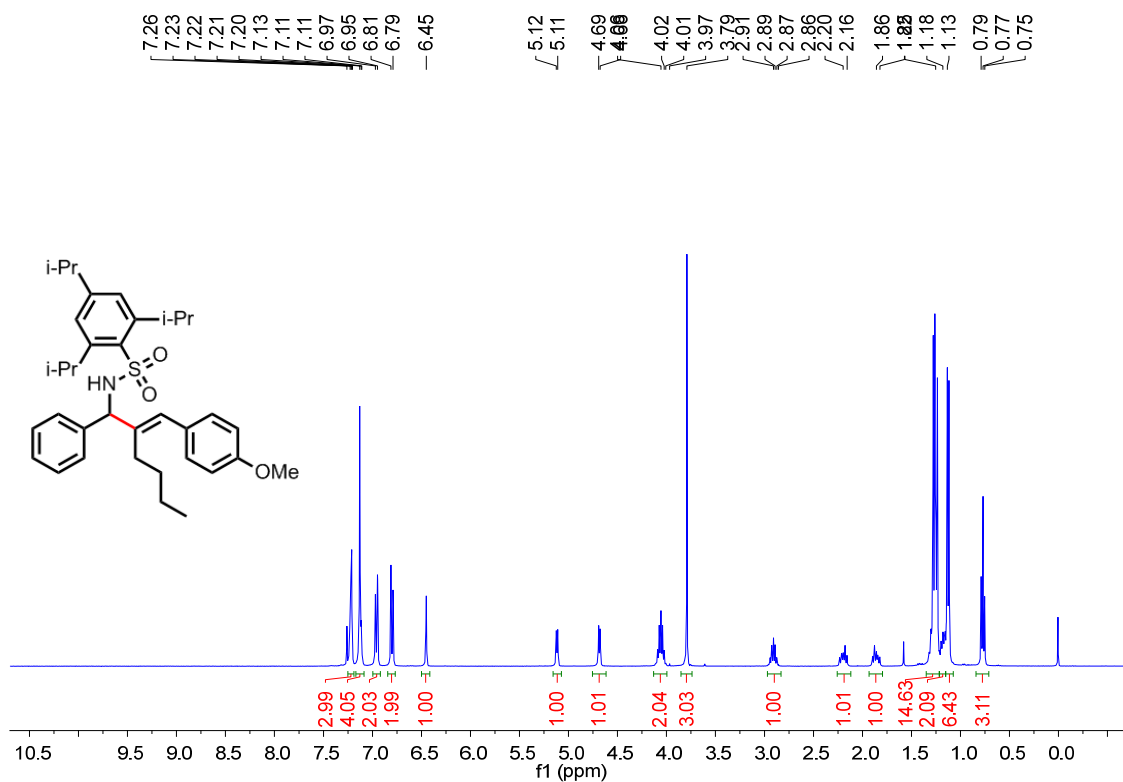


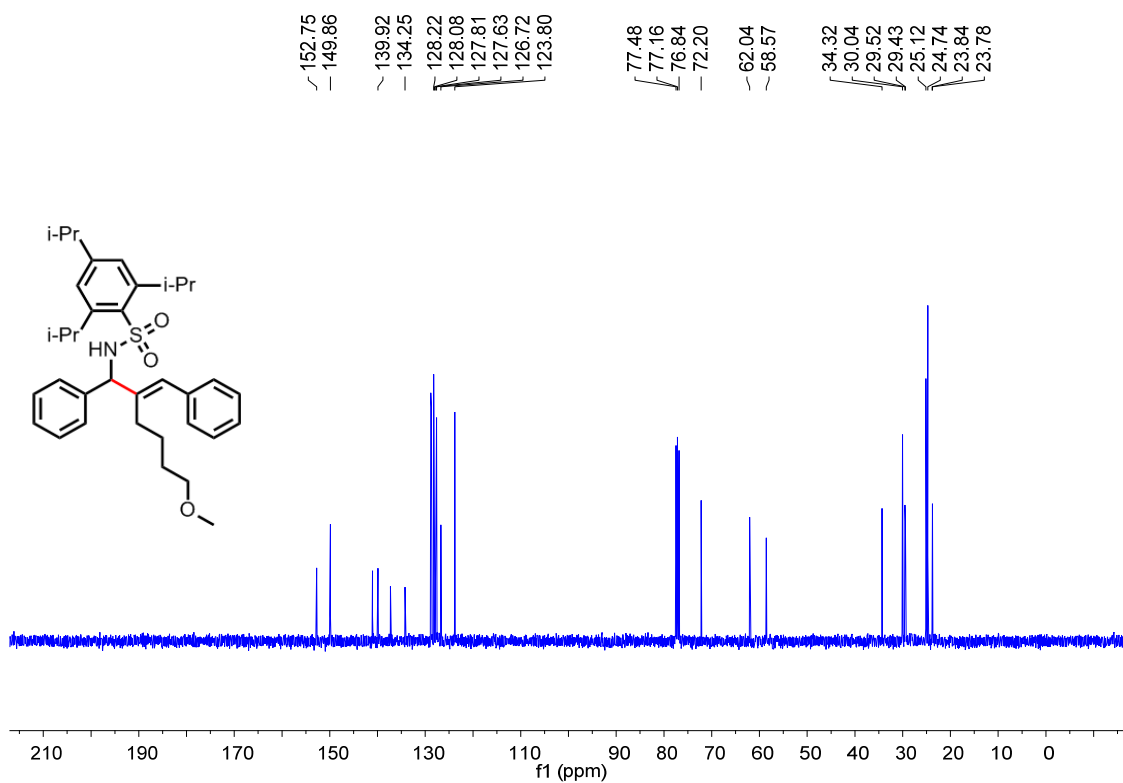
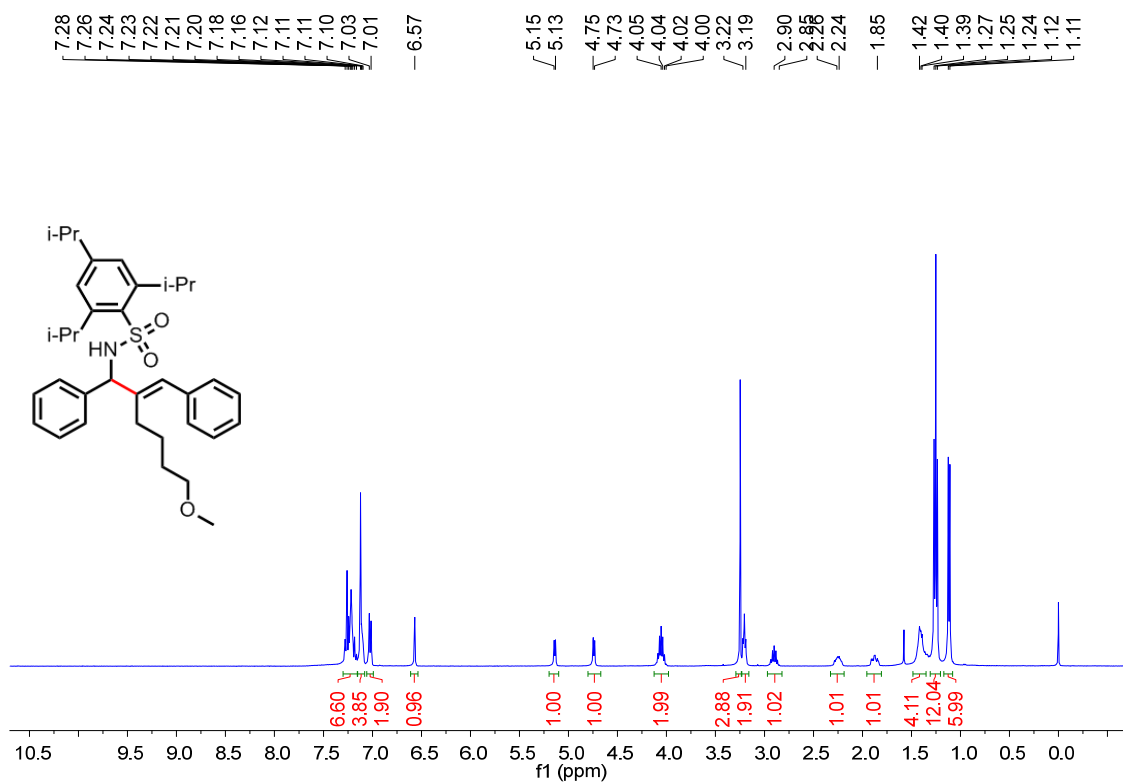


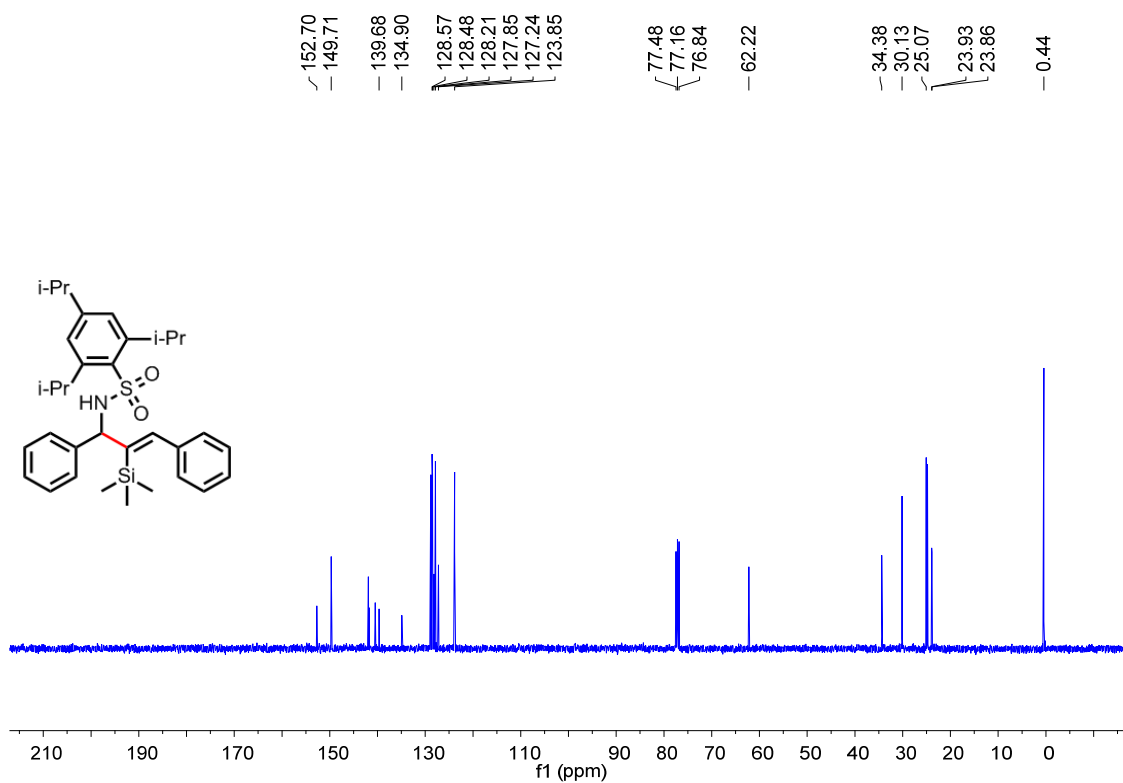
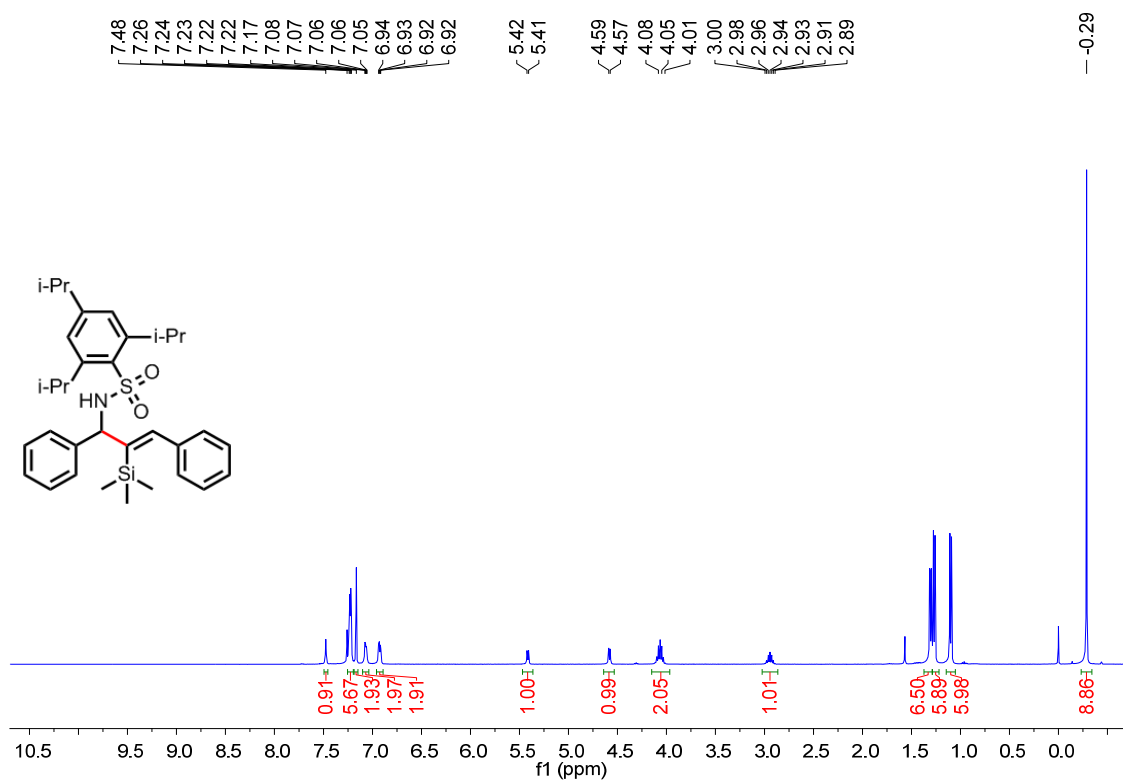


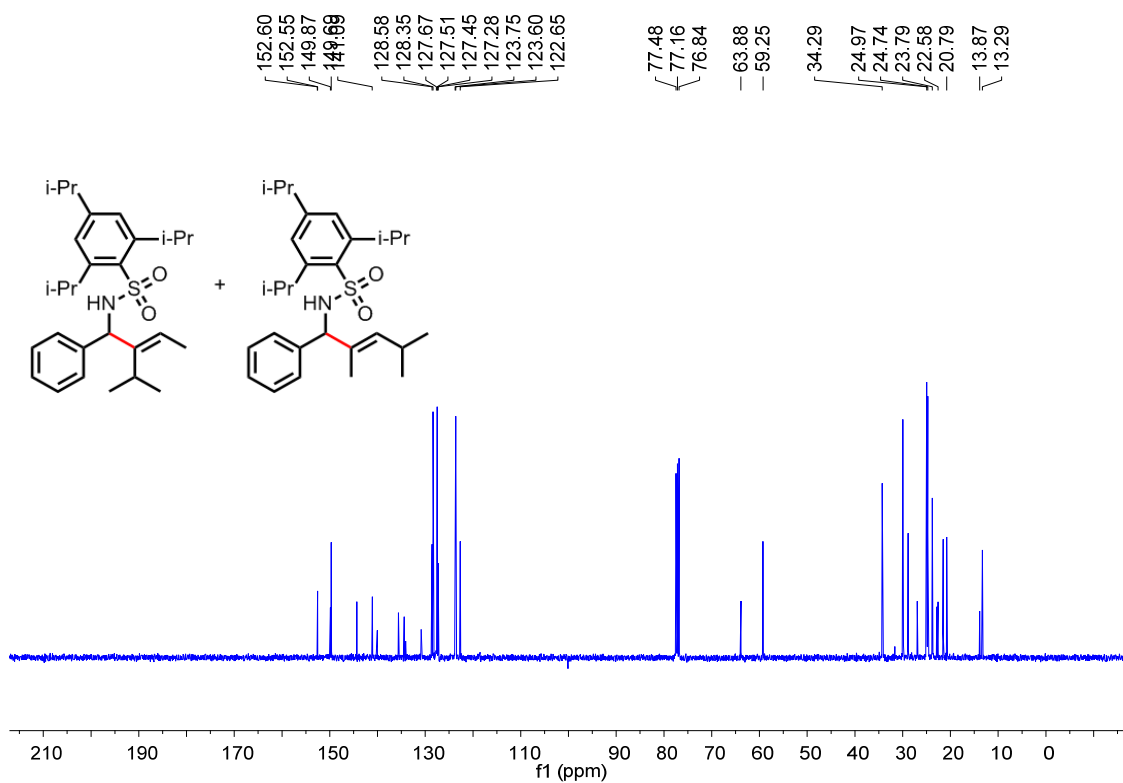
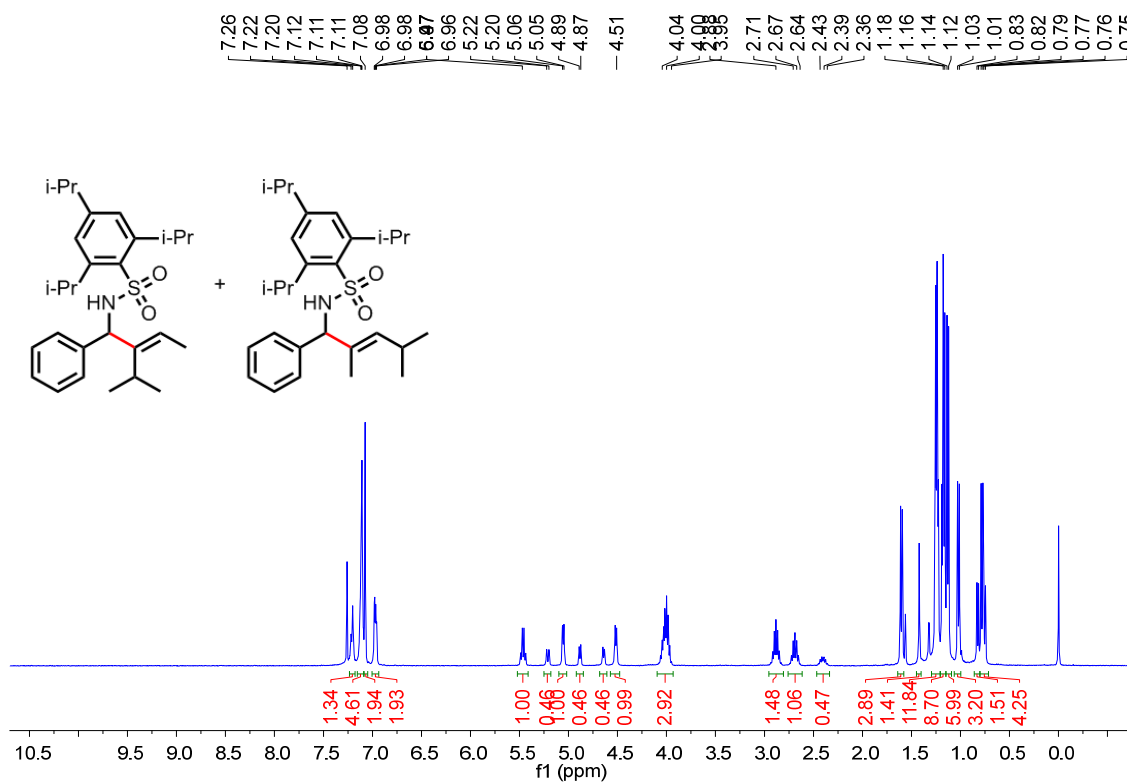


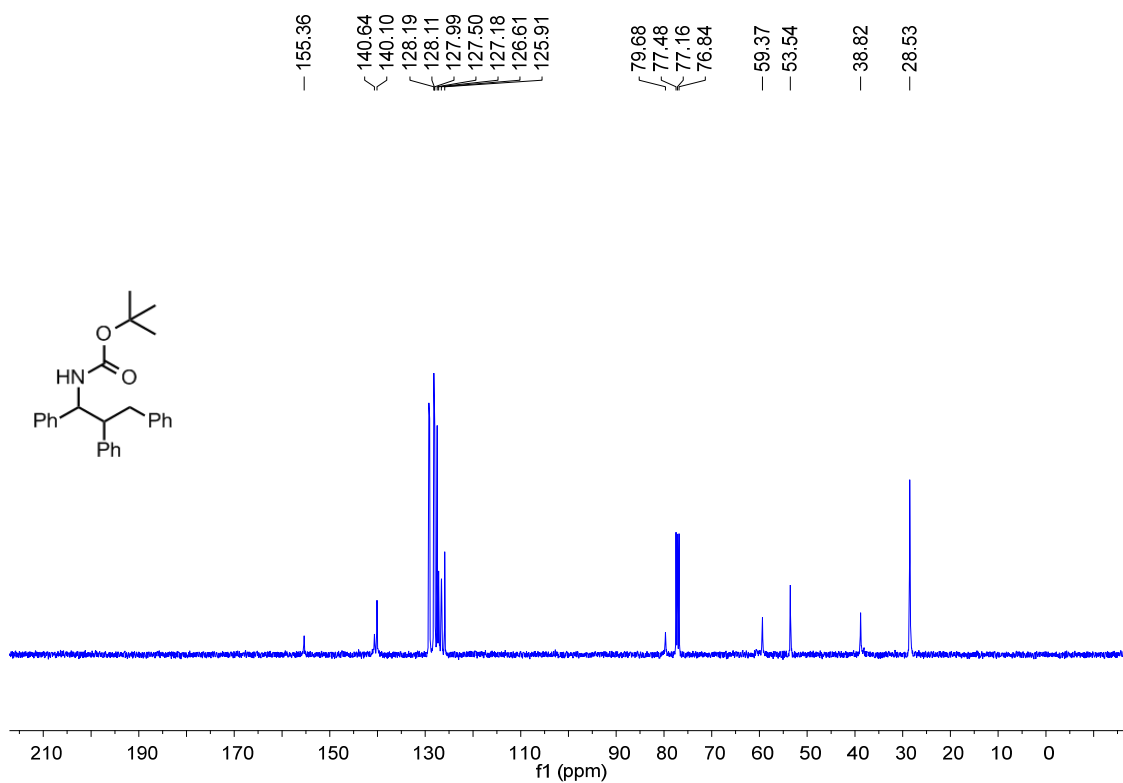
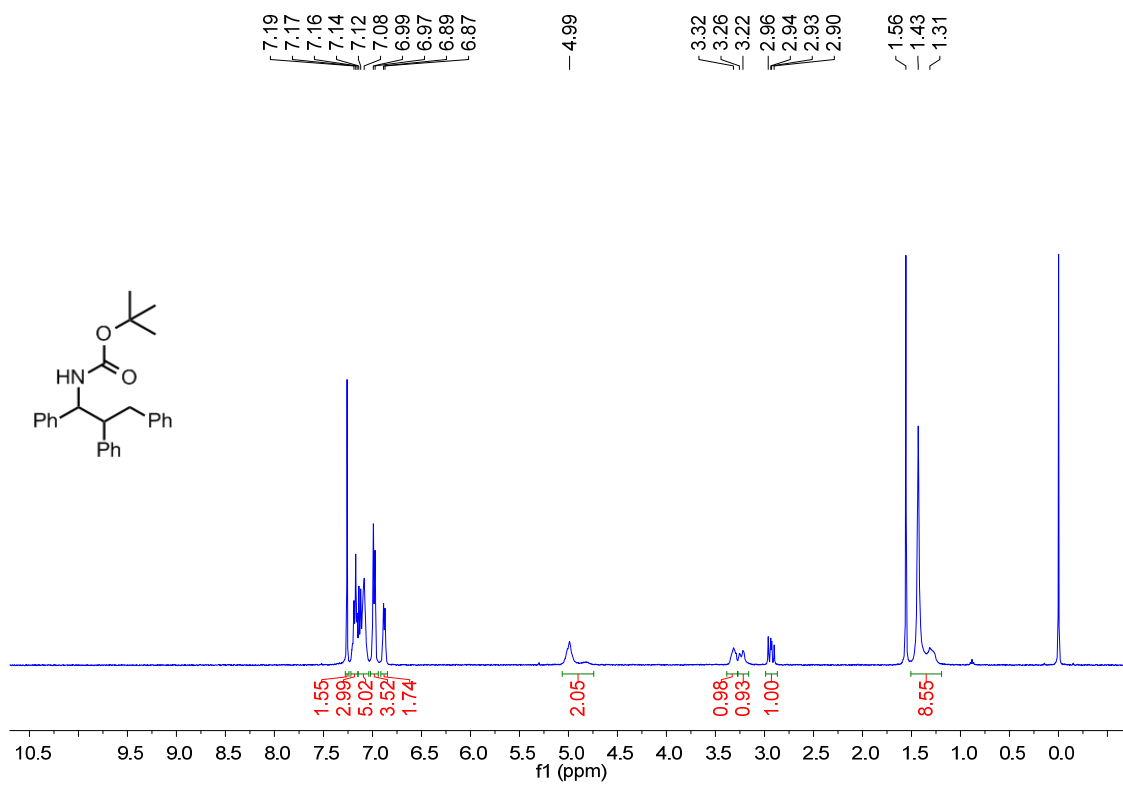


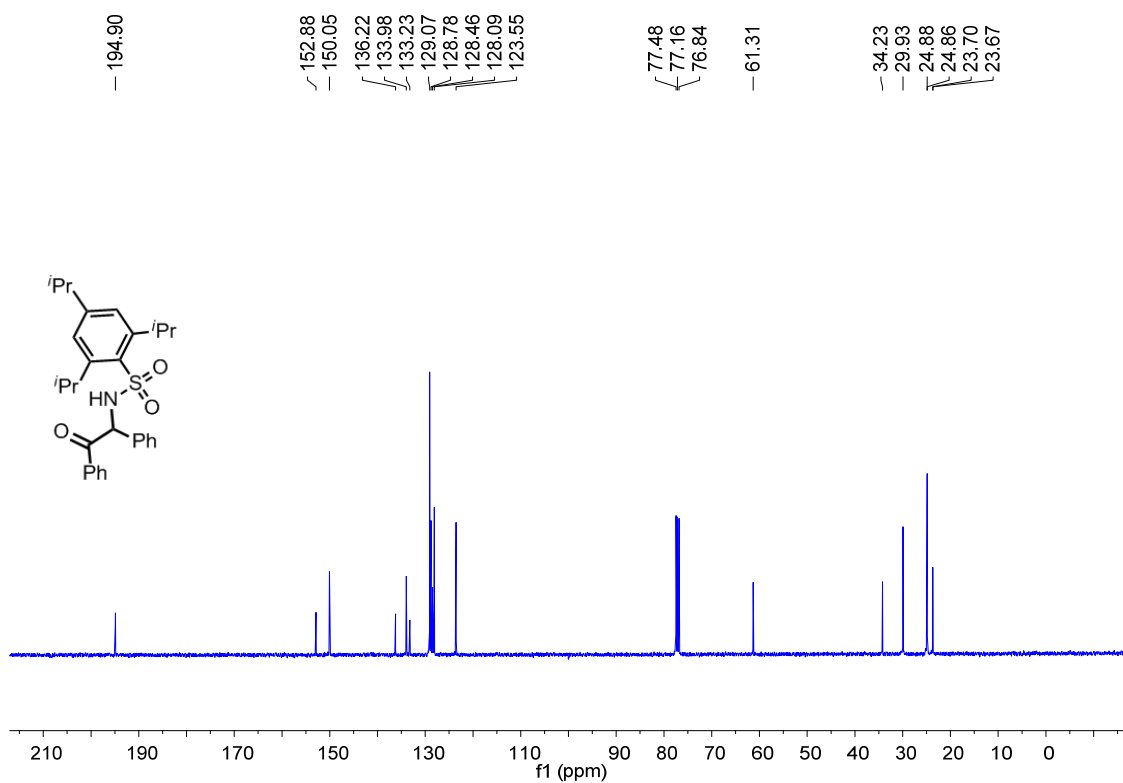
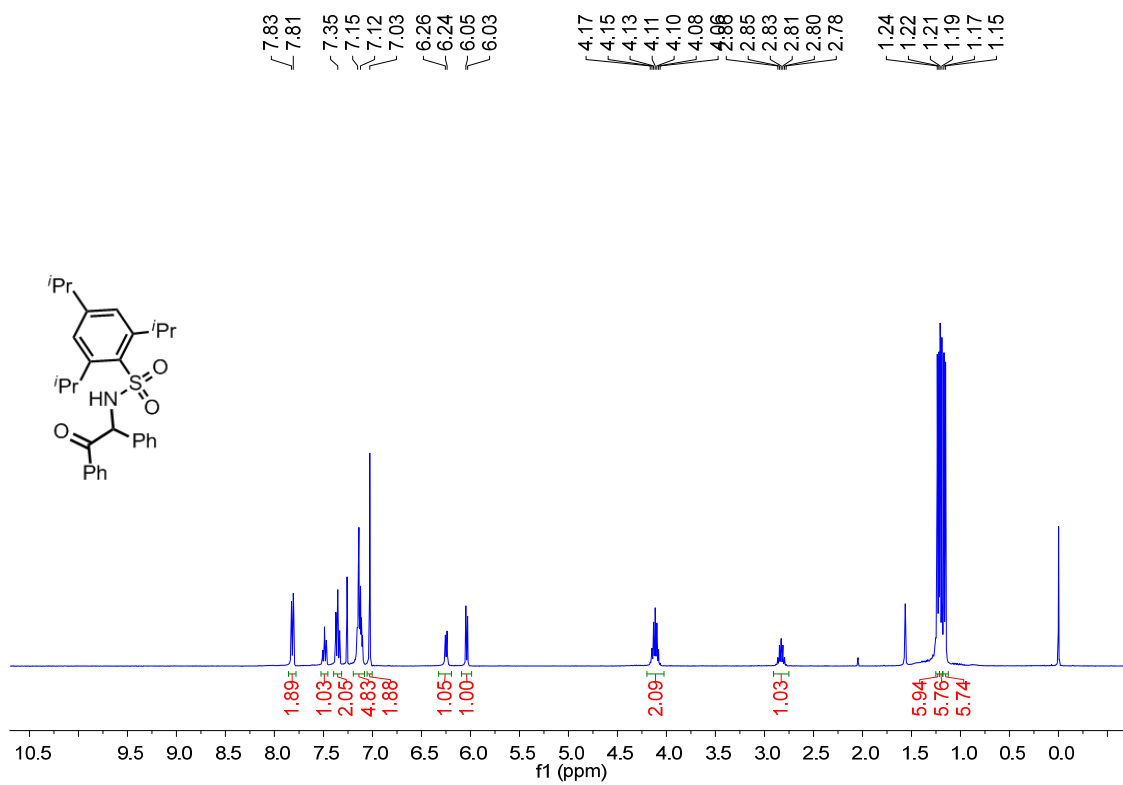


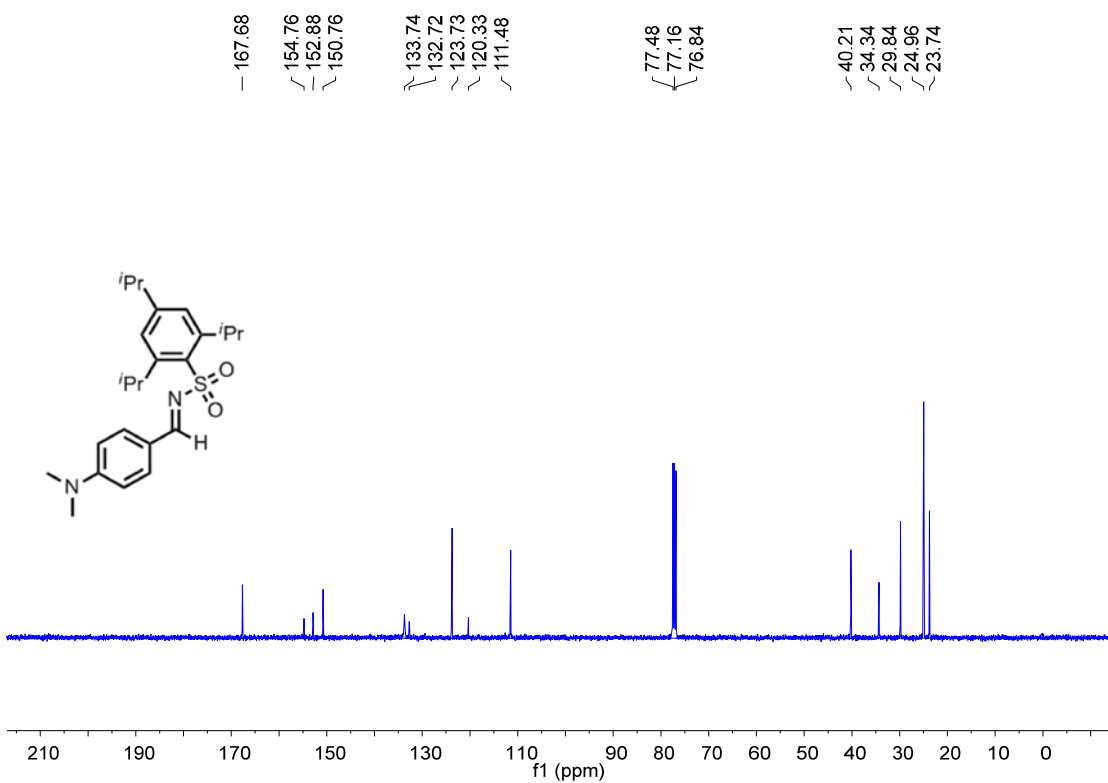
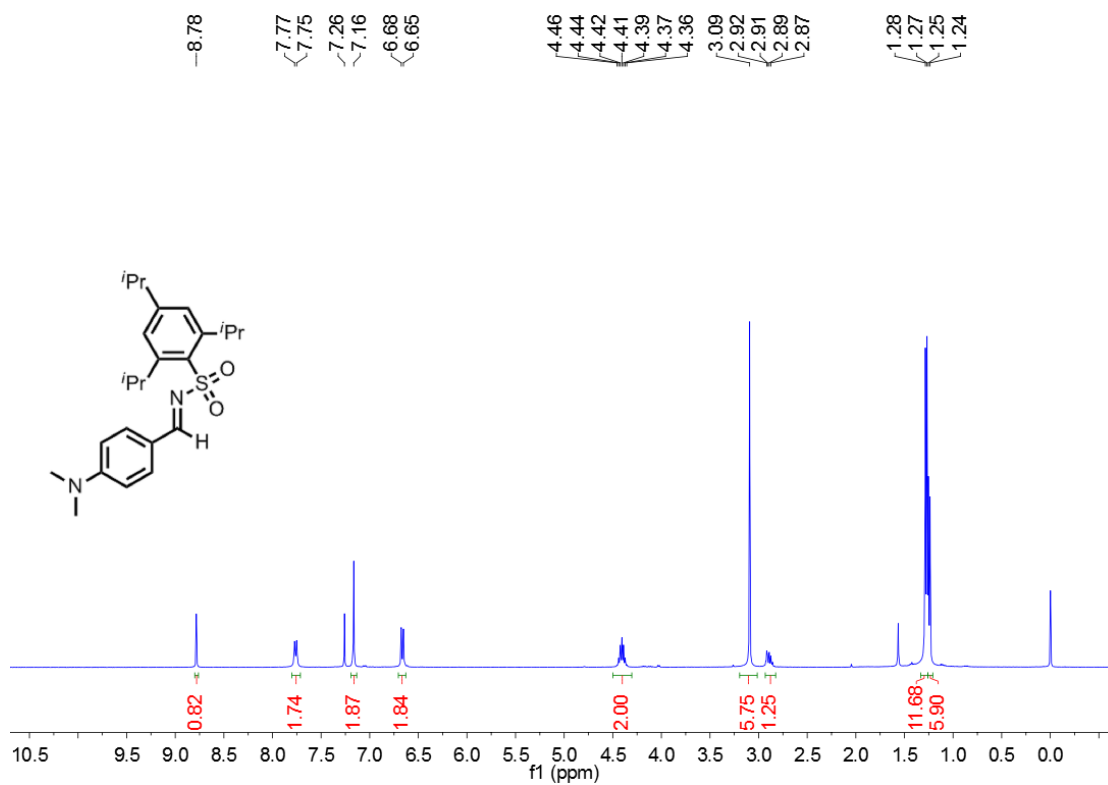












9. References

1. S. J. Heffernan, J. M. Beddoes, M. F. Mahon, A. J. Hennessy, D. R. Carbery, *Chem. Commun.* **2013**, 49, 2314.
2. B. G. Reed-Berendt, L. C. Morrill, *J. Org. Chem.* **2019**, 84, 3715.
3. G. A. Molander, N. Fleury-Brégeot, M.-A. Hiebel, *Org. Lett.* **2011**, 13, 1694.
4. M. K. Ghorai, A. Kumar, D. P. Tiwari, *J. Org. Chem.* **2010**, 75, 137.
5. M. Zhu, K.-i. Fujita, R. Yamaguchi, *Org. Lett.* **2010**, 12, 1336.
6. S. Y. Chow, M. Y. Stevens, L. R. Odell, *J. Org. Chem.* **2016**, 81, 2681.
7. W.-W. Yao, R. Li, J.-F. Li, J. Sun, M. Ye, *Green Chem.* **2019**, 21, 2240.
8. S. Ogoshi, H. Ikeda, H. Kurosawa, *Angew. Chem., Int. Ed.* **2007**, 46, 4930.
9. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford CT, 2009.
10. a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, 37, 785; b) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648.
11. S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, 132, 154104.
12. P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, 82, 299.
13. W. J. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople, *Ab Initio Molecular Orbital Theory*, Wiley: New York, 1986.
14. a) Y. Zhao, D. G. Truhlar, *Phys. Chem. Chem. Phys.* **2008**, 10, 2813; b) R. F. Ribeiro, A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2011**, 115, 14556.
15. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, 113, 6378.
16. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, 120, 215.
17. M. Dolg, U. Wedig, H. Stoll, H. Preuss, *J. Chem. Phys.* **1987**, 86, 866.