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SUPPORTING INFORMATION FOR:

Synthesis of substituted γ and δ-lactams based on titanocene(III)-catalyzed radical cyclizations of trichloroacetamides

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Experimental Section

General Details. Deoxygenated solvent and reagents were used for all reactions involving Cp_2TiCl. THF was freshly distilled from Na. Drying of organic extracts was performed over anhydrous Na_2SO_4. Me_3SiCl was purchased from Aldrich, and stored at –4 ºC. All product mixtures were analyzed by thin-layer chromatography using TLC silica gel plates with a fluorescent indicator (λ = 254 nm). Analytical thin-layer chromatography was performed on SiO_2 (silica gel 60 F_{254}), and the spots were located by UV light or/and a 1% $KMnO_4$ aqueous solution, or phosphomolybdic acid etanolic solution. Products were purified by flash chromatography on silica gel 60 (240-400 mesh). Yields refer to analytically pure samples. Chemical shifts of ^1H and ^{13}C NMR spectra are reported in ppm downfield (δ) from Me_4Si. Spectroscopic data for compounds **1**,[1] **4**,[2] **6**,[1] **7**,[3] **8**,[1] and **14**[4] matched with previously described.

General procedure for preparation of new trichloroacetamides 9-13 and 15: To a solution of the corresponding amine (1 mmol) in CH_2Cl_2 (15 mL), DMAP (1.5 mmol), Et_3N (1.5 mmol), and trichloroacetyl chloride (1.2 mmol) were added, and the mixture was stirred at room temperature for 3 h. Then, Et_2O was added, and the solution was washed with 2N HCl, dried, and the solvent removed. Compounds **1** and **6-15** were isolated by flash chromatography of the residue (hexane/EtOAc) and characterized by spectroscopic techniques.

Compound **9**: Following the general procedure from (*E*, *Z*)-4-(benzylamino)but-2-en-1-yl ethyl carbonate and after chromatography (hexane/EtOAc 85:15), trichloroacetamide **9** (mixture of isomers) was isolated in 42% yield as a colorless oil. ^1H NMR ($CDCl_3$, 300 MHz): δ 7.41-7.13 (m, 5H), 5.88-5.60 (m, 2H), 5.00-4.88 (m, 1H), 4.70-4.54 (m, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 3.98-3.88 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR

($CDCl_3$, 75 MHz): δ 169.7 (C), 160.9 (C), 155.0 (C), 129.0 (CH), 128.1 (CH), 128.0 (CH), 104.8 (CH), 67.0 (CH_2), 64.3 (CH_2), 14.4 (CH_3). HRMS (ESI-TOF): calcd for [$C_{16}H_{22}Cl_3N_2O_4$] $(M+NH_4)^+$ 411.0640, found 411.0632.

Compound **10**: Following the general procedure from *N*-benzyloct-2-yn-1-amine and after chromatography (hexane/EtOAc 9:1), trichloroacetamide **10** was isolated in 61% yield as a yellowish oil. ^1H NMR ($CDCl_3$, 300 MHz): δ 7.47-7.18 (m, 5H), 5.19–4.72 (m, 2H), 4.50-4.10 (m, 2H), 2.34–2.05 (m, 2H), 1.53 (q, *J* = 6.9 Hz, 2H), 1.48–1.28 (m, 4H), 0.94 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 172.8 (C), 160.4 (C), 128.9 (CH), 128.0 (CH), 93.0 (C), 86.3 (C), 73.3 (C), 65.7 (CH_2), 31.1 (CH_2), 28.3 (CH_2), 22.3 (CH_2), 18.7 (CH_2), 14.1 (CH_3). HRMS (ESI-TOF): calcd for [$C_{17}H_{21}Cl_3NO$] $(M+H)^+$ 360.0683, found 360.0682.

Compound **11**: Following the general procedure from *N*-allyl-1-phenylbut-3-en-1-amine,[5] but without DMAP and only 2 h of reaction time, and after chromatography (hexane/CH_2Cl_2 1:1), trichloroacetamide **11** was isolated in 82% yield as a yellowish oil. ^1H NMR ($CDCl_3$, 400 MHz, rotamer mixture): δ 7.52-7.26 (m, 5H), 5.94-5.74 (m, 2H), 5.22-5.00 (m, 5H), 4.40 and 4.10 (2 m, 1H, major), 3.94 and 3.62 (2 m, 1H, minor), 3.05 (br s, 1H), 2.92 (br s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz, two rotamers): δ 160.3 (C), 138.1 (C, major), 137.2 (C, minor), 134.4 (CH, major), 133.8 (CH, minor), 133.2 (CH, minor), 132.5 (CH, major), 128.5 (CH), 128.2 (CH), 127.8 (CH), 118.6 (CH_2, minor), 118.0 (CH_2, major), 93.7 (C), 62.2 (CH, major), 60.5 (CH, minor), 51.8 (CH_2, major), 49.1 (CH_2, minor), 36.5 (CH_2, minor), 35.4 (CH_2, major). HRMS (ESI-TOF): calcd for [$C_{15}H_{17}Cl_3NO$] $(M+H)^+$ 332.0370, found 332.0370.

Compound **12**: Following the general procedure from *N*-benzyl-1-(4-(prop-1-en-2-yl)cyclohex-1-en-1-yl)methanamine,[6] and after chromatography (hexane/EtOAc 9:1), trichloroacetamide **12** was isolated in 87% yield as a yellowish oil. ^1H NMR ($CDCl_3$,

400 MHz): δ 7.47–6.98 (m, 5H), 5.61 (brs, 1H), 5.43 (brs, 1H), 5.01-4.83 (m, 1H), 4.78-4.64 (m, 2H), 4.12-3.83 (m, 2H), 2.15 (t, *J* = 10.1 Hz, 2H), 2.05-1.91 (m, 3H), 1.87-1.77 (m, 1H), 1.74 (s, 3H), 1.63-1.49 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 174.1 (C), 161.5 (C), 131.6 (C), 129.0 (CH), 128.2 (CH), 128.0 (CH), 127.3 (CH), 109.2 (CH_2), 105.0 (C), 93.6 (C), 65.8 (CH_2), 41.1 (CH), 30.7 (CH_2), 27.5 (CH_2), 26.7 (CH_2), 21.1 (CH_3). HRMS (ESI-TOF): calcd for [$C_{19}H_{23}Cl_3NO$] $(M+H)^+$ 386.0840, found 386.0834.

Compound **13**: Following the general procedure from *N*-benzyl-4-butenylamine,[7] and after chromatography (hexane/EtOAc 95:5), trichloroacetamide **13** was isolated in 87% yield as a 1:1.5 mixture of rotamers: Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.45-7.18 (m), 5.81-5.62 (m), 5.14-4.91 (m), 4.72 (br s), 3.77-3.62 (m), 3.47-3.28 (m, 2H), 2.57-2.26 (m). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 160.8 (2C), 135.4 (C), 134.5 (C),128.9 (CH), 127.9 (CH), 127.6 (CH), 127.2 (CH), 117.7 (CH_2), 117.7 (CH_2), 93.4 (C), 53.4 (CH_2), 50.9 (CH_2), 48.1 (CH_2), 47.4 (CH_2), 32.1 (CH_2), 30.9 (CH_2). HRMS (ESI-TOF): calcd for [$C_{13}H_{14}Cl_3NO$ 305.0141] $(M+H)^+$, found 305.0155.

Compound **15**: Following the general procedure from *N*-benzyl-4-methylcyclohex-3-enamine,[8] but without DMAP and 2 h of reaction time, and after chromatography (hexane/CH_2Cl_2 1:1), trichloroacetamide **15** was isolated in 97% yield as a white solid. mp 76-77 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.34-7.16 (m, 5H), 5.27 (br s, 1H), 4.73 (br s, 1H), 4.66 (d, *J* = 16 Hz, 1H), 4.54 (d, *J* = 16 Hz, 1H), 2.30-2.10 (m, 3H), 2.06-1.88 (m, 2H), 1.81 (m, 1H), 1.64 (s, 3H). ^{13}C NMR ($CDCl_3$,100 MHz): δ 160.8 (C), 137.5 (C), 133.9 (C), 128.5 (CH), 126.9 (CH), 126.1 (CH), 118.7 (CH), 93.7 (C), 56.1 (CH), 47.7 (CH_2), 30.1 (CH_2), 29.0 (CH_2), 27.3 (CH_2), 23.1 (CH_3). HRMS (ESI-TOF): calcd for [$C_{16}H_{19}Cl_3NO$] $(M+H)^+$ 346.0527, found 346.0526.

Cp_2TiCl-mediated cyclization of 1: Strictly deoxygenated THF (20 mL, passing Ar for 15 min) was added to a mixture of Cp_2TiCl_2 (348 mg, 1.4mmol) and Mn dust (204 mg, 3.7mmol) under an Ar atmosphere, and the suspension was stirred at room temperature until it turned lime green (after about 15 min). Then, a solution of trichloroacetamide **1** (150 mg, 0.47 mmol) in THF (2 mL) was added, and the mixture was stirred for 24 h. The reaction was then quenched with 2N HCl, and extracted with EtOAc. The organic layer was washed with brine, dried, and the solvent removed. The residue was purified by flash chromatography (hexane/EtOAc 6:4) to yield **2** (23 mg, 24%), and **3**[9] (18 mg,16%).

Compound **2**: Brown oil.^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.34-7.22 (m, 5H), 4.45 (s, 2H), 2.97 (s, 2H), 2.29 (s, 2H), 1.10 (s, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 174.3 (C), 136.5 (C), 128.7 (CH), 128.2 (CH), 127.6 (CH), 59.7 (CH_2), 46.5 (CH_2), 46.3 (CH_2), 32.6 (C), 27.8 (CH_3). HRMS (ESI-TOF): calcd for $[C_{13}H_{18}NO]$ $(M+H)^+$ 204.1383, found 204.1392.

General procedure for Ti(III)-catalyzed cyclizations of 1, 6-15: Strictly deoxygenated THF (20 mL, passing Ar for 15 min) was added to a mixture of Cp_2TiCl_2 (0.2, 0.4, 0.6 or 0.8 mmol, see Table 1 and SI) and Mn dust (8 mmol) under an Ar atmosphere, and the suspension was stirred at room temperature until it turned lime green (after about 15 min). Then, a solution of the corresponding trichloroacetamide **1**, **6-15** (1 mmol), 2,4,6-collidine (6 mmol) in THF (2 mL), and Me_3SiCl (4 mmol) were added and the mixture was stirred for 72 h. The reaction was then quenched with 2N HCl, and extracted with EtOAc. The organic layer was washed with brine, dried, and the solvent removed. Products **2-3** and **16-27** were isolated by flash chromatography of

the residue (hexane/EtOAc) and characterized by spectroscopic techniques. Results are depicted in Tables 1 and 2.

Compound **16**: Isolated with hexane/EtOAc 6:4.[10]

Compound **18**: Isolated with hexane/EtOAc 6:4.[11]

Compound **19**: Isolated with hexane/EtOAc 6:4 as a 1:1 mixture with **19r**. Yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.42–7.09 (m, 5H), 4.77 (brs, 1H), 4.73 (brs, 1H), 4.56–4.23 (m, 2H), 3.38 (t, *J* = 8.9 Hz, 1H), 3.10 (t, *J* = 8.9 Hz, 1H), 2.62-2.42 (m, 2H), 2.24–1.96 (m, 2H), 1.67 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 174.6 (C), 144.5 (C), 136.4 (C), 128.7 (CH), 128.1 (CH), 127.5 (CH), 111.0 (CH_2), 50.8 (CH_2), 38.5 (CH), 36.0 (CH_2), 20.0 (CH_3). HRMS (ESI-TOF): calcd for $[C_{14}H_{18}NO]$ $(M+H)^+$ 216.1383, found 216.1392.

Compound **19r**: Isolated with hexane/EtOAc 6:4 as a colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.42-7.17 (m, 5H), 4.61–4.28 (m, 2H), 3.31 (t, *J* = 8.9 Hz, 1H), 2.97 (t, *J* = 8.9 Hz, 1H), 2.60-2.44 (m, 2H), 1.60-1.43 (m, 2H), 0.89 (d, *J* = 6.7 Hz, 3H), 0.84 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 174.0 (C), 136.7 (C), 128.7 (CH), 128.2 (CH), 127.6 (CH), 51.1 (CH_2), 46.6 (CH_2), 39.0 (CH), 36.2 (CH_2), 32.64 (CH), 20.6 (CH_3), 20.1 (CH_3). HRMS (ESI-TOF): calcd for $[C_{14}H_{20}NO]$ $(M+H)^+$ 218.1539, found 218.1545.

Compound **20**: Isolated with hexane/EtOAc 1:1.[11]

Compound **21**: Isolated with hexane/EtOAc 6:4, as a 9:1 mixture of isomers. Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.51-7.13 (m, 10H), 5.49-5.30 (m, 2H), 4.54 (s, 2H, major), 4.53 (s, 2H, minor), 3.87 (s, 2H, major), 3.76 (s, 2H, minor), 3.19 (s, 2H, major), 3.12 (s, 2H, minor), 1.97-1.81 (m, 2H), 1.42-1.18 (m, 12H), 0.90 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 173.3 (C), 136.2 (C), 128.8 (CH, major), 128.8 (CH, minor), 128.3 (CH, minor), 128.2 (CH, major), 127.7 (CH), 126.7 (CH, minor),

126.4 (CH), 125.2 (CH, major), 125.1 (CH, minor), 52.1 (CH_2, minor), 50.1 (CH_2, major), 46.5 (CH_2, major), 46.4 (CH_2, minor), 37.2 (CH_2), 31.5 (CH_2), 29.3 (CH_2, minor), 28.8 (CH_2), 28.5 (CH_2), 25.6 (CH_2), 14.1 (CH_3). HRMS (ESI-TOF): calcd for $[C_{17}H_{24}NO]$ $(M+H)^+$ 258.1852, found 258.1853.

Compound **22**: Isolated with hexane/EtOAc1:1, as 7:3 mixture of isomers. Brown oil.^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.48-7.15 (m, 10H), 5.90–5.60 (m, 2H), 5.44 (dd, *J* = 9.7, 6.5 Hz, 1H), 5.38-5.24 (m, 1H), 5.24–4.99 (m, 4H), 3.47–3.33 (m, 1H), 3.26–3.02 (m, 1H), 2.99–2.83 (m, 1H), 2.79–2.48 (m, 6H), 2.44–2.23 (m, 1H), 2.03 (td, *J* = 16.8, 6.8 Hz, 1H), 1.09 (d, *J* = 6.7 Hz, 3H), 0.96 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 175.1 (C, minor), 174.6 (C, major), 139.1 (C, minor), 139.0 (C, major), 134.7 (CH_2, major), 134.7 (CH_2, minor), 128.6 (CH), 127.8 (CH, minor), 127.7 (CH, major), 127.6 (CH), 127.6 (CH, major), 127.4 (CH, minor), 117.6 (CH, minor), 117.5 (CH, major), 53.1 (CH_2, major), 52.9 (CH_2, minor), 49.8 (CH_2, minor), 49.7 (CH_2, major), 39.9 (CH_2, major), 39.8 (CH_2, minor), 34.8 (CH, minor), 34.7 (CH, major), 26.7 (CH, major), 26.6 (CH, minor), 20.1 (CH_3, minor), 19.5 (CH_3, major). HRMS (ESI-TOF): calcd for $[C_{15}H_{20}NO]$ $(M+H)^+$ 230.1539, found 230.1547.

Compound **23**: Isolated with hexane/EtOAc 6:4, as a 2:1 mixture of isomers. Major isomer: Yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.39-7.19 (m, 5H), 4.70 (br s, 2H), 4.46 (s, 2H), 2.99 (s, 2H), 2.38 (s, 2H), 1.72 (s, 3H), 1.72-1.62 (m, 4H), 1.41-1.21 (m, 4H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 173.9 (C), 149.7 (C), 136.6 (C), 128.7 (CH), 128.2 (CH), 127.6 (CH), 108.7 (CH_2), 60.1 (CH_2), 46.5 (CH_2), 44.7 (C), 41.6 (CH_2), 36.9 (CH_2), 36.1 (CH), 28.0 (CH_2), 21.0 (CH_3). HRMS (ESI-TOF): calcd for $[C_{19}H_{26}NO]$ $(M+H)^+$ 284.2009, found 284.2019.

Minor isomer: Yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.35–7.05 (m, 5H), 4.66–4.48 (m, 2H), 4.36 (s, 2H), 2.99 (s, 2H), 2.21 (s, 2H), 1.81-1.52 (m, 4H), 1.60 (s, 3H),

1.44-1.23 (m, 2H), 1.13-0.94 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 174.0 (C), 149.8 (C), 136.7 (C), 128.8 (CH), 128.1 (CH), 127.7 (CH), 108.6 (CH_2), 55.4 (CH_2), 46.7 (CH_2), 46.6 (CH_2), 44.2 (C), 36.9 (CH_2), 35.8 (CH), 28.0 (CH_2), 21.2 (CH_3). HRMS (ESI-TOF): calcd for $[C_{19}H_{26}NO]$ $(M+H)^+$ 284.2009, found 284.2019.

Compound **24**: Isolated with hexane/EtOAc 1:1, as a 1:1 mixture of rotamers. Yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.40–7.15 (m, 10H), 5.84–5.64 (m, 2H), 5.12–4.96 (m, 4H), 4.62 and 4.53 (2s, 2H each), 3.44 and 3.27 (2t, *J* = 7.2 Hz, 2H each), 2.29 (dt, *J* = 14.8, 7.0 Hz, 4H), 2.18 and 2.11 (s, 3H each). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 171.0 (C), 170.6 (C), 137.7 (C), 136.9 (C), 135.5 (CH), 134.3 (CH), 128.9 (CH), 128.6 (CH), 128.0 (CH), 127.8 (CH), 127.3 (CH), 126.2 (CH), 117.6 (CH_2), 116.7 (CH_2), 52.3 (CH_2), 48.1 (CH_2), 47.4 (CH_2), 45.6 (CH_2), 32.8 (CH_2), 32.1 (CH_2), 21.8 (CH_3), 21.6 (CH_3). HRMS (ESI-TOF): calcd for $[C_{13}H_{18}NO]$ $(M+H)^+$ 204.1383, found 204.1391.

Compound **25**: Isolated with hexane/EtOAc 6:4.[12]

Compound **26** and **27**: Isolated with hexane/EtOAc 6:4, as a 1:1 mixture of isomers. Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.44-7.09 (m, 10H), 5.37 and 5.33 (2d, *J* = 15 Hz, 1H each), 4.72 (s, 1H, isomer **26**), 4.67 (s, 1H, isomer **26**), 3.97 and 3.90 (2d, *J* = 15 Hz, 1H each), 3.59-3.52 and 3.49-3.42 (2m, 1H each), 2.86–2.72 (m, 2H), 2.60–2.35 (m, 3H), 2.33–2.15 (m, 3H), 2.02-1.88 (m, 4H), 1.87–1.58 (m, 6H), 1.55-1.39 (m, 2H), 0.95 (d, *J* = 6.9 Hz, 3H, isomer **27**). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 171.4 (2C), 150.3 (C, isomer **26**), 137.9 (C), 137.7 (C), 128.7 (CH), 128.6 (CH), 127.9 (CH), 127.8 (CH), 127.4 (CH), 127.3 (CH), 108.0 (CH_2, isomer **26**), 51.1 (CH), 50.9 (CH), 48.2 (CH_2), 48.0 (CH_2), 38.3 (CH_2), 37.2 (CH), 35.6 (CH), 33.7 (CH_2), 33.6 (CH_2), 33.1 (CH), 31.9 (CH_2), 30.0 (CH_2), 29.0 (CH_2), 26.5 (CH_2), 25.3 (CH_2), 19.8 (CH_3, isomer **27**). For **26**:

HRMS (ESI-TOF): calcd for $[C_{16}H_{20}NO]$ $(M+H)^+$ 242.1539, found 242.1540. For **27**: HRMS (ESI-TOF): calcd for $[C_{16}H_{22}NO]$ $(M+H)^+$ 244.1696, found 244.1693.

Cyclization of compound 1 mediated by Cp_2TiCl in the presence of H_2O or D_2O: Strictly deoxygenated THF (20 mL, passing Ar for 15 min) was added to a mixture of Cp_2TiCl_2 (696 mg, 2.8 mmol) and Mn dust (306 mg, 5.6 mmol) under an Ar atmosphere, and the suspension was stirred at room temperature until it turned lime green (after about 15 min). Then, a solution of trichloroacetamide **1** (150 mg, 0.47 mmol), and H_2O (92 mg, 4.7 mmol) or D_2O (94 mg, 4.7 mmol) in THF (2 mL) were added, and the mixture was stirred for 72 h. The reaction was then quenched with 2N HCl, and extracted with EtOAc. The organic layer was washed with brine, dried, and the solvent removed. The residue was purified by flash chromatography (hexane/EtOAc 6:4) to yield **2** (34 mg, 36%), or **2d** (28 mg, 30%, 46% deuterium incorporation).

Compound **2d**: Colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.40-7.19 (m, 5H), 4.47 (s, 2H), 2.98 (s, 2H), 1.12 (s, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 174.3 (C), 136.7 (C), 128.8 (CH), 128.3 (CH), 127.7 (CH), 59.8 (CH_2), 46.6 (CH_2), 29.8 (C), 27.9 (CH_3). HRMS (ESI-TOF): calcd for $[C_{13}H_{15}D_3NO]$ $(M+H)^+$ 207.1571, found 207.1579.

General procedure for cyclization of 1 catalyzed by Cp_2TiCl in the presence of H_2O: Strictly deoxygenated THF (20 mL, passing Ar for 15 min) was added to a mixture of Cp_2TiCl_2 (0.4, 0.6 or 0.8 mmol, see Table 1), collidine hydrochloride (4 mmol), and Mn dust (8 mmol) under an Ar atmosphere, and the suspension was stirred at room temperature until it turned lime green (after about 15 min). Then, a solution of trichloroacetamide **1** (1 mmol), and H_2O (10 mmol) in THF (2 mL) were added, and the mixture was stirred for 72 h. The reaction was then quenched with 2N HCl, and

extracted with EtOAc. The organic layer was washed with brine, dried, and the solvent removed. The residue was purified by flash chromatography (hexane/EtOAc 6:4) to yield **4** (see Table 1).

Computational General Information.

All reported structures were optimized at DFT level by using the B3LYP[13(1-SI)] hybrid functional as implemented in Gaussian 09.[14(2-SI)] Optimizations were carried out by using the standard 6-31G(d,p) basis set for all atoms. Reported energy values correspond to Enthalpies (H). The critical stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies, and the intrinsic reaction coordinates (IRC)[15(3)] were followed to verify the energy profiles connecting the key transition structures to the correct associated local minima. The structures were also single-point refined at M06-2X/6-31+G(d,p) (iefpcm,solvent=THF) level of theory.

1-rad

E (B3LYP) -1554.35073515

Correction to Enthalpy 0,259492

E (M06-2X) -1554.02172063

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.372821	2.827215	-0.898990
2	6	0	1.136457	-0.607810	-0.821055
3	6	0	0.252624	1.199189	0.657448

4	7	0	0.142097	0.236859	-0.440757
5	6	0	0.831693	2.553978	0.288444
6	6	0	2.276713	-0.804211	0.140304
7	6	0	-1.053310	0.357142	-1.293444
8	6	0	0.748138	3.565701	1.401640
9	1	0	1.783628	3.808094	-1.110876
10	1	0	-0.753150	1.338346	1.066405
11	1	0	1.426029	2.093699	-1.694793
12	1	0	0.838524	0.775585	1.473435
13	1	0	-1.159521	1.401000	-1.597608
14	1	0	-0.865113	-0.230534	-2.191199
15	8	0	1.150945	-1.225839	-1.883890
16	17	0	3.852806	-1.002161	-0.520201
17	17	0	1.987974	-1.556185	1.672804
18	1	0	-0.294902	3.758514	1.676494
19	1	0	1.208555	4.511683	1.113648
20	1	0	1.249788	3.199372	2.304331
21	6	0	-2.323153	-0.112103	-0.607493
22	6	0	-3.454408	0.708060	-0.584740
23	6	0	-2.397713	-1.381590	-0.021770
24	6	0	-4.641852	0.269003	0.003610
25	1	0	-3.408648	1.696392	-1.030716
26	6	0	-3.579761	-1.820569	0.570229
27	1	0	-1.528178	-2.029945	-0.028568
28	6	0	-4.706910	-0.996270	0.583580
29	1	0	-5.510545	0.917782	0.012726
30	1	0	-3.623284	-2.806959	1.018414
31	1	0	-5.626712	-1.338863	1.043903

TS1

E (B3LYP) -1554.33860269

Correction to Enthalpy 0.257593

E (M06-2X) -1554.01432742

Frequency -435.2977

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.126906	2.590892	0.277554
2	6	0	-0.916507	-1.008920	-0.400918
3	6	0	-0.233776	1.306562	-0.710274
4	7	0	0.024358	-0.133929	-0.812798
5	6	0	-1.166373	1.625039	0.447803
6	6	0	-2.187463	-0.295768	0.038879
7	6	0	1.252345	-0.595428	-1.471191
8	6	0	-0.615474	1.360243	1.835462
9	1	0	-2.667301	2.993064	1.126439
10	1	0	0.727712	1.800962	-0.542753
11	1	0	-2.425751	2.926156	-0.708242
12	1	0	-0.643217	1.684245	-1.652853
13	1	0	1.331730	-0.089503	-2.437620
14	1	0	1.122193	-1.661151	-1.660240
15	8	0	-0.806468	-2.230007	-0.379988
16	17	0	-2.959806	-0.964791	1.458731
17	17	0	-3.304762	-0.067841	-1.312281
18	1	0	-0.174356	0.367113	1.932674
19	1	0	-1.392140	1.468055	2.593318
20	1	0	0.174378	2.087381	2.050936
21	6	0	2.505413	-0.349713	-0.653096
22	6	0	3.505265	0.506091	-1.122315
23	6	0	2.686215	-0.990366	0.579413
24	6	0	4.666543	0.720913	-0.377492
25	1	0	3.378143	1.006901	-2.076708
26	6	0	3.842035	-0.775296	1.325859

27	1	0	1.920568	-1.662233	0.952499
28	6	0	4.836321	0.081818	0.848822
29	1	0	5.433556	1.387663	-0.755211
30	1	0	3.970857	-1.279881	2.276897
31	1	0	5.736681	0.247117	1.429650

TS2

E (B3LYP) -1554.33164404

Correction to Enthalpy 0.257719

E (M06-2X) -1554.00573081

Frequency -477.2181

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.333889	0.786378	1.673467
2	6	0	-0.888033	-0.886288	-0.576975
3	6	0	-0.107082	1.522600	-0.356689
4	7	0	0.035522	0.105793	-0.736132
5	6	0	-1.006138	1.798731	0.818385
6	6	0	-2.204929	-0.504086	0.077648
7	6	0	1.264829	-0.201087	-1.488799
8	6	0	-1.657886	3.146097	0.852753
9	1	0	-2.076409	0.950056	2.447278
10	1	0	0.903153	1.892602	-0.146742
11	1	0	-0.677638	-0.060546	1.830728
12	1	0	-0.468035	2.091908	-1.222744
13	1	0	1.367800	0.539751	-2.286811
14	1	0	1.120345	-1.175194	-1.953252
15	8	0	-0.674134	-2.054247	-0.894636

16	17	0	-3.052454	-1.848523	0.826341
17	17	0	-3.255277	0.466987	-0.965657
18	1	0	-0.900944	3.939717	0.865910
19	1	0	-2.286693	3.262463	1.736228
20	1	0	-2.271636	3.314137	-0.040266
21	6	0	2.514856	-0.206936	-0.629713
22	6	0	3.603399	0.605945	-0.957518
23	6	0	2.611139	-1.046243	0.487604
24	6	0	4.769280	0.581627	-0.189630
25	1	0	3.541209	1.262107	-1.819825
26	6	0	3.771384	-1.069455	1.257728
27	1	0	1.776516	-1.686150	0.752186
28	6	0	4.855217	-0.255612	0.920668
29	1	0	5.604326	1.219292	-0.457386
30	1	0	3.832920	-1.725419	2.118961
31	1	0	5.758051	-0.275208	1.520557

TS3

E (B3LYP) -1786.84841981

Correction to Enthalpy 0.377830

E (M06-2X) -1786.41579186

Frequency -1464.5875

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.641720	3.307396	-1.256860
2	6	0	0.176516	0.042990	-0.697563
3	6	0	-1.483979	1.508911	0.495553
4	7	0	-1.074548	0.540477	-0.523534

5	6	0	-1.865463	2.887806	-0.011809
6	6	0	1.352734	0.540218	0.154572
7	6	0	-2.169718	-0.026447	-1.342112
8	6	0	-2.512067	3.753414	1.038283
9	1	0	-1.924003	4.307273	-1.567724
10	1	0	-2.342209	1.080109	1.026534
11	1	0	-1.164696	2.678723	-1.999644
12	1	0	-0.701925	1.611613	1.246650
13	1	0	-2.805184	0.801316	-1.657863
14	1	0	-1.714512	-0.463093	-2.229215
15	8	0	0.440214	-0.833625	-1.519629
16	17	0	1.292761	-0.076990	1.833486
17	1	0	-3.442755	3.302653	1.400429
18	1	0	-2.739316	4.746675	0.648848
19	1	0	-1.857079	3.867768	1.909512
20	6	0	-3.000950	-1.059668	-0.604777
21	6	0	-4.350916	-0.817483	-0.333641
22	6	0	-2.438857	-2.277000	-0.196595
23	6	0	-5.127932	-1.768103	0.331200
24	1	0	-4.800204	0.119475	-0.646753
25	6	0	-3.211056	-3.225102	0.470454
26	1	0	-1.395802	-2.482338	-0.408951
27	6	0	-4.558761	-2.973423	0.736532
28	1	0	-6.173622	-1.564226	0.532857
29	1	0	-2.763620	-4.163651	0.778323
30	1	0	-5.159076	-3.713268	1.253929
31	6	0	3.579275	-0.576751	-0.962908
32	1	0	3.450848	-0.322420	-2.015376
33	6	0	3.665930	-2.056814	-0.583234
34	1	0	3.601392	-2.702060	-1.460990
35	1	0	2.848460	-2.335463	0.086657
36	6	0	5.030192	-2.159837	0.134639
37	1	0	5.022349	-2.871721	0.961018
38	1	0	5.812631	-2.456696	-0.567803

39	6	0	5.267420	-0.725993	0.603185
40	1	0	6.316054	-0.442839	0.688111
41	1	0	4.760147	-0.515244	1.551295
42	8	0	4.686761	0.091756	-0.439215
43	17	0	1.701704	2.282776	0.071876
44	1	0	2.508368	-0.074050	-0.435046

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E (B3LYP) -1554.34716544

Correction to Enthalpy 0.262894

E (M06-2X) -1554.01520511

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.201100	-0.821579	-0.814948
2	6	0	0.253826	1.190165	0.323908
3	7	0	0.168728	0.026244	-0.571443
4	6	0	2.346887	-0.799419	0.159762
5	6	0	-1.032035	-0.059441	-1.422009
6	1	0	-0.755654	1.388493	0.689196
7	1	0	0.856947	0.946147	1.195746
8	1	0	-1.170359	0.894544	-1.936955
9	1	0	-0.831793	-0.814741	-2.180385
10	8	0	1.247412	-1.610470	-1.757888
11	17	0	3.932512	-1.040473	-0.464383
12	17	0	2.086508	-1.288957	1.799757
13	6	0	-2.282800	-0.407530	-0.637422
14	6	0	-3.386175	0.449593	-0.641783
15	6	0	-2.360019	-1.604059	0.086431

16	6	0	-4.547401	0.120927	0.060691
17	1	0	-3.339458	1.380405	-1.197882
18	6	0	-3.515579	-1.933182	0.790569
19	1	0	-1.512823	-2.281630	0.099053
20	6	0	-4.614009	-1.070619	0.779572
21	1	0	-5.394520	0.797540	0.047948
22	1	0	-3.561572	-2.863590	1.345498
23	1	0	-5.513305	-1.327524	1.327830
24	6	0	0.822266	2.443182	-0.372233
25	1	0	0.208777	2.705263	-1.238664
26	1	0	1.825840	2.203376	-0.743186
27	6	0	0.901136	3.610784	0.571162
28	1	0	1.544043	3.478515	1.440295
29	6	0	0.248693	4.762107	0.418152
30	1	0	-0.402770	4.938373	-0.433042
31	1	0	0.347561	5.569606	1.135286

TS4

E (B3LYP) -1554.32617375

Correction to Enthalpy 0.258393

E (M06-2X) -1553.99964144

Frequency -389.7718

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.014780	1.383635	1.324598
2	6	0	-0.685010	-0.660271	-0.673786
3	6	0	0.079071	1.696260	-0.084772
4	7	0	0.155648	0.394547	-0.780550

5	6	0	-2.058077	-0.440010	-0.032737
6	6	0	1.426377	0.179264	-1.504043
7	1	0	0.708112	1.639795	0.811057
8	1	0	-1.383583	0.832584	2.018124
9	1	0	0.550114	2.418794	-0.754162
10	1	0	1.578036	1.041649	-2.156829
11	1	0	1.294280	-0.701900	-2.129185
12	8	0	-0.432733	-1.779311	-1.115497
13	17	0	-2.523274	-1.757983	1.036341
14	17	0	-3.273772	-0.096687	-1.270981
15	6	0	2.630803	0.006180	-0.596208
16	6	0	3.702540	0.900492	-0.664585
17	6	0	2.698883	-1.062325	0.307573
18	6	0	4.824270	0.733591	0.149690
19	1	0	3.662723	1.732805	-1.360027
20	6	0	3.814726	-1.227628	1.124869
21	1	0	1.878456	-1.768766	0.365151
22	6	0	4.881661	-0.329914	1.048079
23	1	0	5.647715	1.435888	0.083430
24	1	0	3.855231	-2.060329	1.818259
25	1	0	5.750361	-0.460929	1.683366
26	6	0	-1.297685	2.222196	0.295900
27	1	0	-1.126648	3.222422	0.710531
28	1	0	-1.924157	2.360967	-0.589649
29	6	0	-3.311485	1.597278	1.681774
30	1	0	-3.754321	1.079462	2.523791
31	1	0	-3.961975	2.237121	1.094730

TS5

E (B3LYP) -1554.32749389

Correction to Enthalpy 0.258641

E (M06-2X) -1554.00194829

Frequency -464.0812

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.934062	-0.299444	0.805897
2	6	0	-0.079098	1.402133	-0.847084
3	7	0	0.036112	0.531913	0.334511
4	6	0	-2.177129	-0.514386	-0.066516
5	6	0	1.239127	0.736526	1.159393
6	1	0	0.935972	1.630684	-1.174531
7	1	0	-0.549976	0.860914	-1.664022
8	1	0	1.054538	0.261008	2.121503
9	1	0	1.358661	1.808262	1.338693
10	8	0	-0.854761	-0.876366	1.886255
11	17	0	-3.506879	-1.258449	0.818555
12	17	0	-1.823994	-1.413110	-1.565216
13	6	0	2.502269	0.179042	0.529207
14	6	0	2.545526	-1.134226	0.046027
15	6	0	3.658347	0.961197	0.459186
16	6	0	3.721306	-1.653004	-0.491590
17	1	0	1.655840	-1.752825	0.089216
18	6	0	4.839146	0.442695	-0.075432
19	1	0	3.637257	1.982850	0.824971
20	6	0	4.873167	-0.866010	-0.552688
21	1	0	3.740332	-2.672417	-0.860655
22	1	0	5.726980	1.063281	-0.123339
23	1	0	5.787768	-1.270675	-0.971153
24	6	0	-0.849285	2.704263	-0.549603
25	1	0	-0.308250	3.303850	0.185927
26	1	0	-0.874927	3.291649	-1.476919

27	6	0	-3.021045	1.455056	-0.668843
28	1	0	-2.836844	1.170105	-1.698795
29	1	0	-4.024613	1.272505	-0.306042
30	6	0	-2.239612	2.405262	-0.064385
31	1	0	-2.564534	2.840228	0.875366

TS6

E (B3LYP) -1786.84505907

Correction to Enthalpy 0.378490

E (M06-2X) -1786.40975062

Frequency -1465.2694

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.212243	-0.125714	-0.769628
2	6	0	-1.517504	1.419767	0.218123
3	7	0	-1.058933	0.339114	-0.667182
4	6	0	1.356204	0.510103	0.032614
5	6	0	-2.109960	-0.347702	-1.445316
6	1	0	-2.383559	1.041102	0.769712
7	1	0	-0.750535	1.636845	0.955427
8	1	0	-2.726382	0.409417	-1.932277
9	1	0	-1.608601	-0.918734	-2.224680
10	8	0	0.524239	-1.078583	-1.483744
11	17	0	1.290469	0.113642	1.774483
12	6	0	-2.986622	-1.256056	-0.603208
13	6	0	-4.367427	-1.048656	-0.542318
14	6	0	-2.433292	-2.328993	0.107728
15	6	0	-5.184319	-1.895470	0.209274

16	1	0	-4.809320	-0.220574	-1.087195
17	6	0	-3.245468	-3.172681	0.861815
18	1	0	-1.364343	-2.506047	0.066483
19	6	0	-4.624586	-2.958794	0.914439
20	1	0	-6.253732	-1.720247	0.245597
21	1	0	-2.803847	-4.000405	1.405583
22	1	0	-5.255714	-3.617010	1.500810
23	6	0	3.634517	-0.656058	-0.917372
24	1	0	3.538210	-0.470904	-1.987760
25	6	0	3.724347	-2.107498	-0.441464
26	1	0	3.680518	-2.808858	-1.276286
27	1	0	2.895977	-2.348272	0.229771
28	6	0	5.074864	-2.151619	0.307035
29	1	0	5.059938	-2.816311	1.171778
30	1	0	5.874991	-2.475725	-0.362756
31	6	0	5.283126	-0.690675	0.698417
32	1	0	6.325830	-0.388502	0.790870
33	1	0	4.751145	-0.433867	1.621241
34	8	0	4.717199	0.058631	-0.402116
35	17	0	1.655583	2.239970	-0.273057
36	1	0	2.540824	-0.133472	-0.460285
37	6	0	-1.901806	2.711396	-0.530425
38	1	0	-1.028719	3.105603	-1.054757
39	1	0	-2.659943	2.478825	-1.286463
40	6	0	-2.456279	3.743212	0.412170
41	1	0	-3.354335	3.456771	0.958039
42	6	0	-1.932756	4.950729	0.618337
43	1	0	-1.038384	5.280158	0.097600
44	1	0	-2.383558	5.652865	1.311140

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E (B3LYP) -1631.7901635

Correction to Enthalpy 0.300403

E (M06-2X) -1631.43475819

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.763342	-1.442097	1.783791
2	1	0	0.587298	-2.718872	0.582700
3	1	0	2.450770	-3.389404	1.941278
4	1	0	3.142907	-1.787114	1.966914
5	1	0	4.327759	-3.469559	0.313760
6	1	0	2.374417	-0.726300	-2.137376
7	1	0	1.295323	-2.096447	-2.012291
8	1	0	3.855190	-2.707941	-1.921717
9	6	0	1.242470	-1.909158	0.920392
10	6	0	2.603666	-2.496980	1.325329
11	6	0	3.459431	-2.841136	0.134296
12	6	0	2.042360	-1.517304	-1.456209
13	6	0	1.416618	-0.877900	-0.201186
14	6	0	3.203851	-2.412833	-1.103530
15	7	0	0.159882	-0.159996	-0.526161
16	6	0	0.101441	1.194232	-0.678763
17	6	0	1.088459	2.027786	0.074441
18	17	0	1.516214	3.561047	-0.572309
19	17	0	1.331409	1.818945	1.773312
20	8	0	-0.747377	1.759323	-1.366368
21	6	0	-0.956959	-0.918540	-1.113566
22	1	0	-0.686181	-1.973948	-1.066071
23	1	0	-1.062618	-0.659771	-2.170211
24	6	0	-2.293683	-0.724813	-0.416994
25	6	0	-4.807842	-0.499281	0.817773

26	6	0	-3.467352	-0.753592	-1.176792
27	6	0	-2.394565	-0.577848	0.969493
28	6	0	-3.642109	-0.463319	1.582619
29	6	0	-4.716225	-0.645713	-0.566221
30	1	0	-3.404304	-0.854192	-2.255606
31	1	0	-1.496653	-0.544499	1.575042
32	1	0	-3.702260	-0.346514	2.659082
33	1	0	-5.615211	-0.667011	-1.172183
34	1	0	-5.777184	-0.408961	1.294813
35	1	0	2.120296	-0.123447	0.148587

TS7

E (B3LYP) -1631.7706594

Correction to Enthalpy 0.295161

E (M06-2X) -1631.42127352

Frequency -355.9628

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.311115	0.776863	1.458179
2	6	0	0.620520	-0.567506	-0.850351
3	6	0	0.049493	1.437839	0.631777
4	7	0	-0.127456	0.501397	-0.499687
5	6	0	1.876949	-0.897713	-0.042110
6	6	0	-1.345642	0.742379	-1.276628
7	1	0	2.931474	0.147619	2.089885
8	1	0	-0.966543	1.637460	0.984014
9	1	0	-1.228369	0.265730	-2.248690

10	1	0	-1.441050	1.817896	-1.438920
11	8	0	0.338345	-1.307638	-1.781320
12	17	0	3.284051	-1.032686	-1.062087
13	17	0	1.628638	-2.308176	0.966606
14	6	0	-2.586614	0.222648	-0.578649
15	6	0	-2.565611	-0.980076	0.128662
16	6	0	-3.778544	0.941506	-0.658633
17	6	0	-3.720089	-1.455902	0.742035
18	1	0	-1.644749	-1.549838	0.199174
19	6	0	-4.936038	0.464265	-0.049901
20	1	0	-3.800927	1.882605	-1.198821
21	6	0	-4.909075	-0.736127	0.652765
22	1	0	-3.691713	-2.390991	1.289098
23	1	0	-5.855335	1.034218	-0.117446
24	1	0	-5.807488	-1.107420	1.131336
25	6	0	0.842506	0.854707	1.791371
26	1	0	0.701554	1.511657	2.655347
27	1	0	0.445659	-0.121217	2.077395
28	6	0	2.909505	1.666447	0.628208
29	1	0	3.986991	1.634472	0.505644
30	6	0	2.130676	2.558822	-0.289729
31	1	0	2.147197	2.106187	-1.293116
32	1	0	2.628464	3.525764	-0.397062
33	6	0	0.686029	2.755038	0.169616
34	1	0	0.659245	3.441620	1.021007
35	1	0	0.094226	3.211089	-0.626971

TS8

E (B3LYP) -1631.76270963

Correction to Enthalpy 0.295989

E (M06-2X) -1631.41356859

Frequency -423.4703

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.362219	2.150694	0.146231
2	6	0	-0.719524	-0.827973	-0.567070
3	6	0	0.070936	1.601945	-0.168849
4	7	0	0.121326	0.225860	-0.751962
5	6	0	-2.136748	-0.597944	-0.015579
6	6	0	1.345365	-0.048970	-1.542375
7	1	0	-3.314904	2.456907	-0.271071
8	1	0	0.972875	2.069653	-0.560180
9	1	0	1.462728	0.773716	-2.251031
10	1	0	1.164048	-0.958708	-2.111322
11	8	0	-0.427765	-1.975705	-0.899447
12	17	0	-2.628431	-1.874956	1.113032
13	17	0	-3.276303	-0.466825	-1.378504
14	6	0	2.609041	-0.196559	-0.715638
15	6	0	3.689792	0.666585	-0.917169
16	6	0	2.727201	-1.213080	0.242067
17	6	0	4.867274	0.521948	-0.180584
18	1	0	3.614747	1.456523	-1.657701
19	6	0	3.899297	-1.356914	0.980427
20	1	0	1.899466	-1.894648	0.401785
21	6	0	4.973892	-0.489308	0.771564
22	1	0	5.695865	1.200393	-0.350459
23	1	0	3.977611	-2.149474	1.716415
24	1	0	5.886032	-0.603587	1.346346
25	6	0	-1.120662	2.458451	-0.630038
26	1	0	-0.842452	3.515158	-0.522068
27	1	0	-1.303092	2.308857	-1.700224

28	6	0	-2.330025	1.287174	1.208973
29	1	0	-3.270679	1.017708	1.679854
30	6	0	-1.087890	1.072650	2.045328
31	1	0	-0.976631	0.015902	2.300175
32	1	0	-1.238562	1.583501	3.002844
33	6	0	0.174565	1.620446	1.363026
34	1	0	0.323776	2.666538	1.648347
35	1	0	1.061097	1.072632	1.687443

TS9

E (B3LYP) -1864.28644552

Correction to Enthalpy 0.415663

E (M06-2X) -1863.82841688

Frequency -1456.3531

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.568028	0.381547	-0.737328
2	1	0	3.410732	0.807603	-1.728321
3	6	0	4.704396	-0.626525	-0.553335
4	1	0	5.215565	-0.836799	-1.494237
5	1	0	4.324196	-1.577325	-0.168362
6	6	0	5.616600	0.057646	0.487158
7	1	0	6.110630	-0.652084	1.151997
8	1	0	6.383412	0.657090	-0.009501
9	6	0	4.639824	0.967963	1.226825
10	1	0	5.087674	1.865294	1.652799
11	1	0	4.094147	0.431186	2.010445
12	1	0	2.438044	-0.216076	-0.534560

13	8	0	3.708101	1.399602	0.206646
14	6	0	-2.289077	4.613926	-0.672986
15	1	0	-1.896124	5.788419	1.091274
16	1	0	-2.535184	5.470795	-1.290324
17	1	0	-1.320348	3.809845	2.478535
18	1	0	-1.387091	1.547615	1.504138
19	1	0	-2.591697	3.204040	-2.265818
20	1	0	-1.987126	0.917836	-2.154384
21	1	0	-3.136219	0.458629	-0.908340
22	1	0	-3.636008	-4.135318	-1.262134
23	1	0	-3.204836	-1.571640	-1.655612
24	1	0	-1.792713	-2.581069	-1.859521
25	1	0	-4.065878	-4.443487	1.088493
26	1	0	-2.250911	-3.020944	2.382915
27	1	0	-3.887403	-2.431628	2.534478
28	1	0	-3.549140	-0.663403	0.941901
29	1	0	-2.115432	-0.650566	1.966730
30	1	0	-0.927245	-2.062813	0.299900
31	6	0	-1.606190	3.681753	1.440291
32	6	0	-1.647140	2.400690	0.889366
33	6	0	-2.322726	3.333105	-1.222153
34	6	0	-1.929356	4.793116	0.662808
35	6	0	-2.005860	2.211923	-0.447810
36	6	0	-2.125078	0.831888	-1.073996
37	8	0	0.495611	0.921513	-1.573115
38	17	0	1.365201	-2.452828	-1.180651
39	17	0	1.184512	-1.138919	1.486690
40	6	0	1.205019	-0.915726	-0.286624
41	6	0	0.113961	-0.000079	-0.856144
42	7	0	-1.197237	-0.182687	-0.542107
43	6	0	-3.279044	-3.398043	-0.548095
44	6	0	-1.766062	-1.447932	-0.015648
45	6	0	-2.513257	-2.228272	-1.114161
46	6	0	-3.524057	-3.562994	0.753370

47	6	0	-3.080598	-2.585264	1.810069
48	6	0	-2.655251	-1.232986	1.216950

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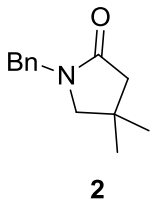
SPECTRA FOR NEW AND DESCRIBED COMPOUNDS



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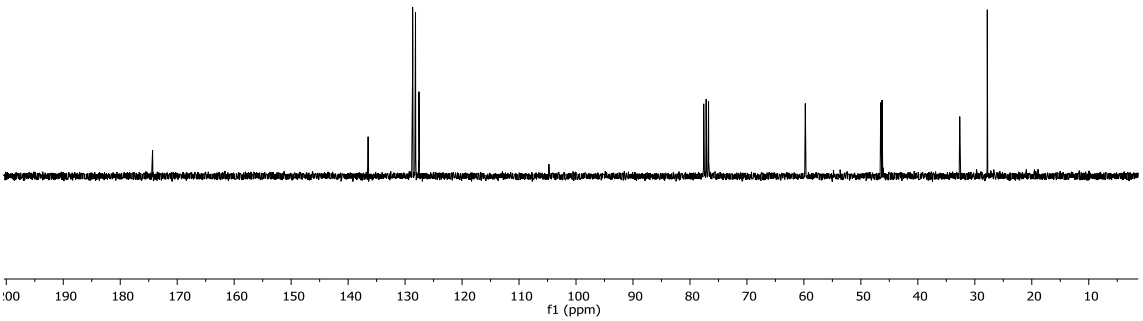

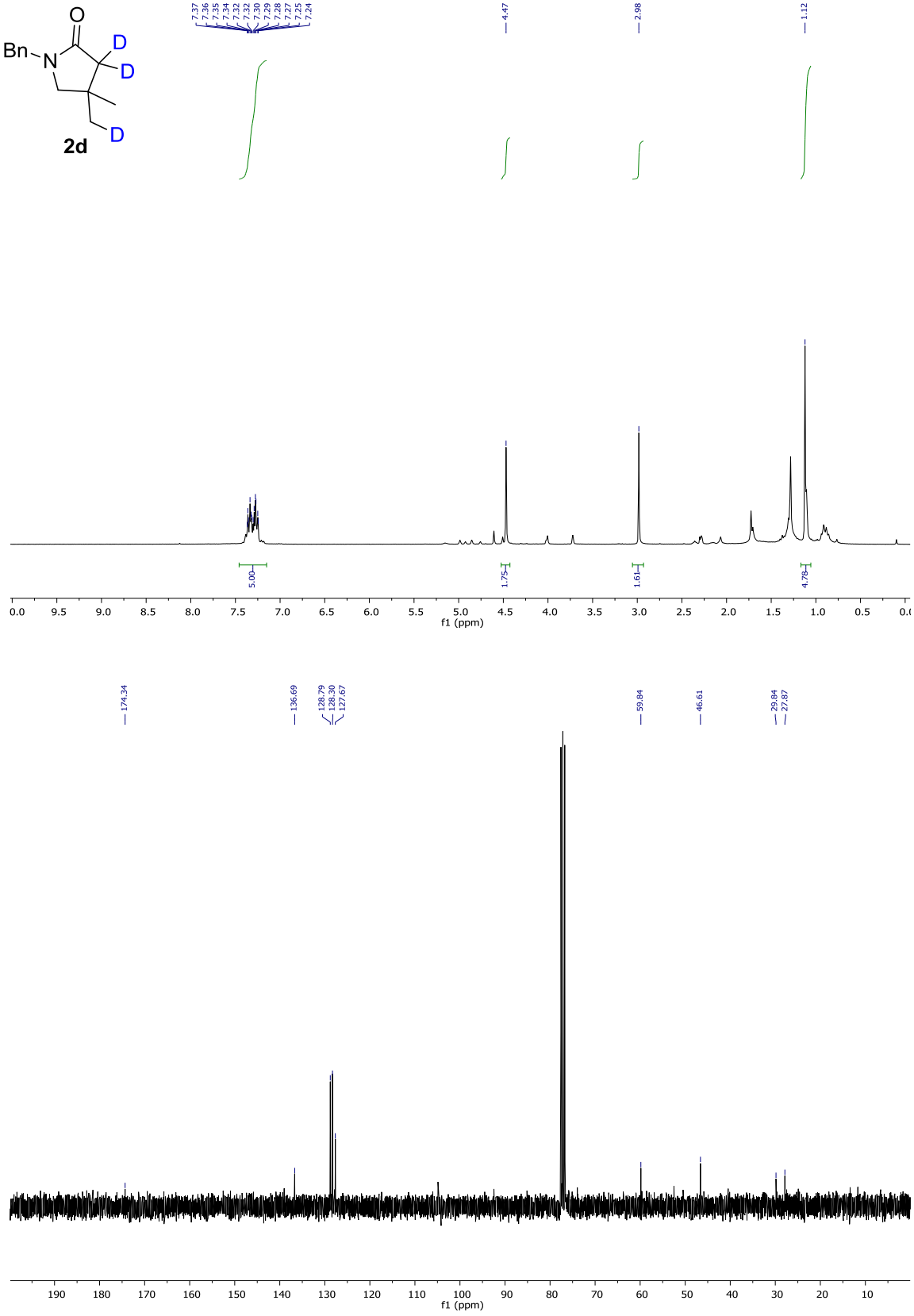
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7.28
7.27
7.25
7.24
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1.12
5.00
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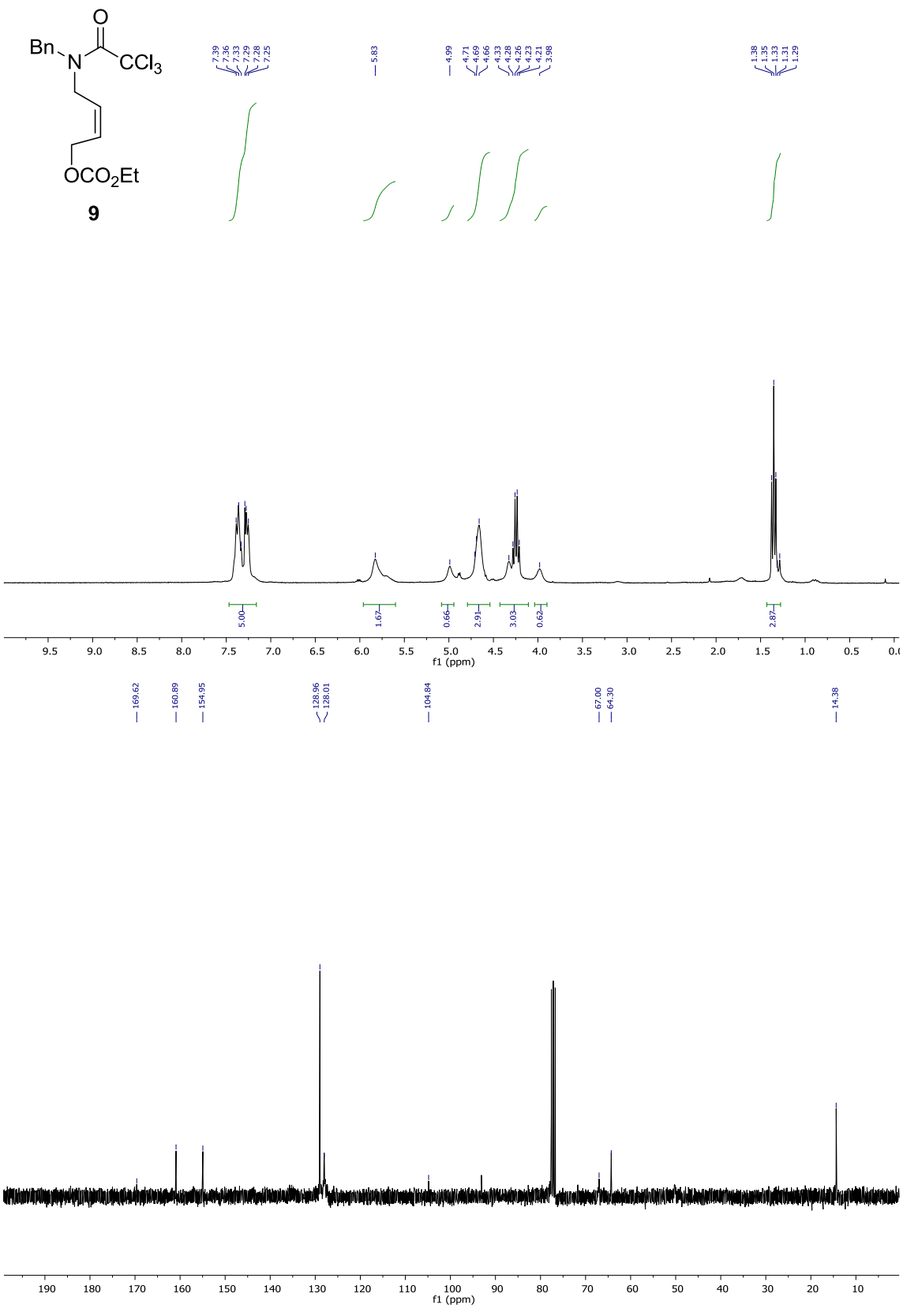
f1 (ppm)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4.28
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4.23
4.21
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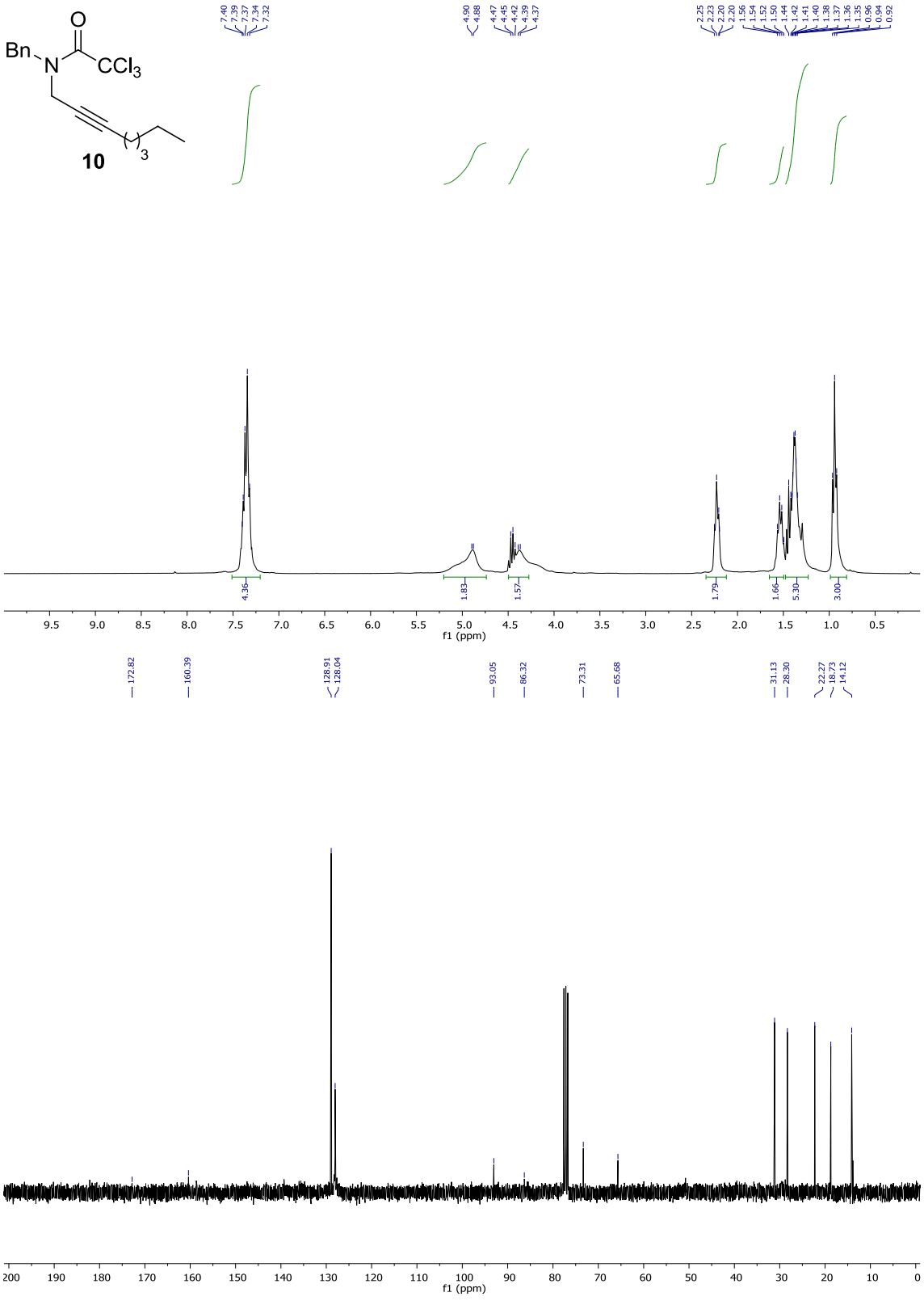
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2.20
2.20
1.56
1.54
1.52
1.50
1.44
1.42
1.41
1.40
1.38
1.37
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1.35
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0.94
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1.79
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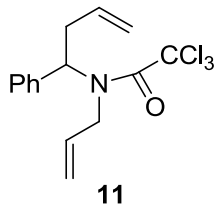
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5.089
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7
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4
3
2
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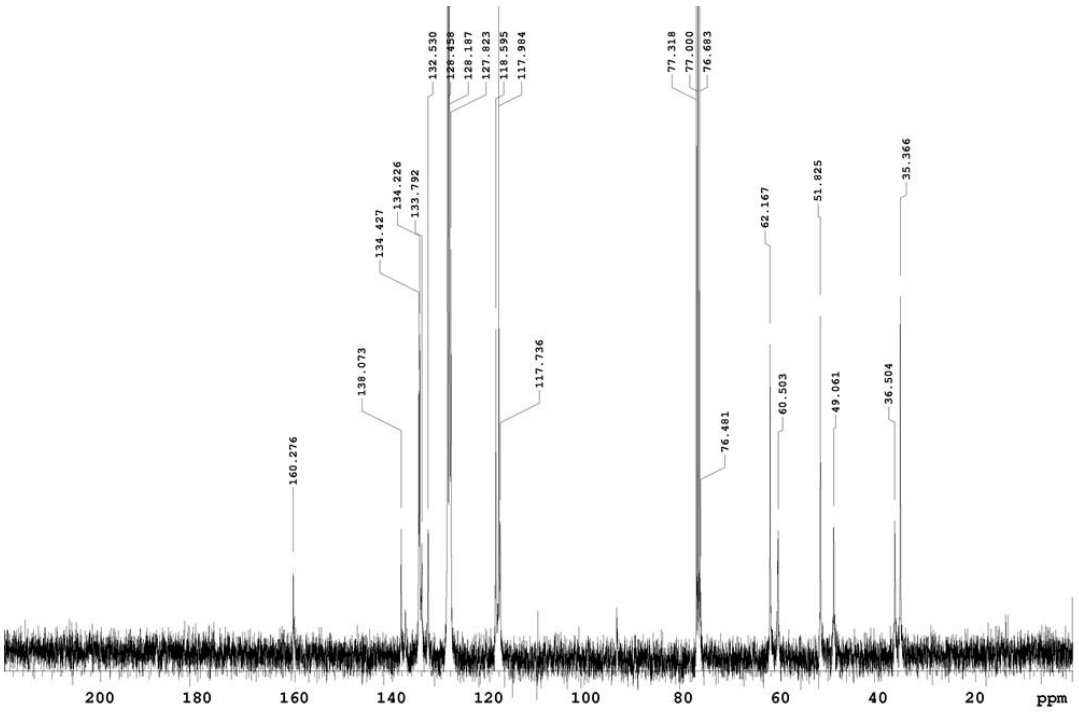
ppm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76.481
62.167
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36.504
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200
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140
120
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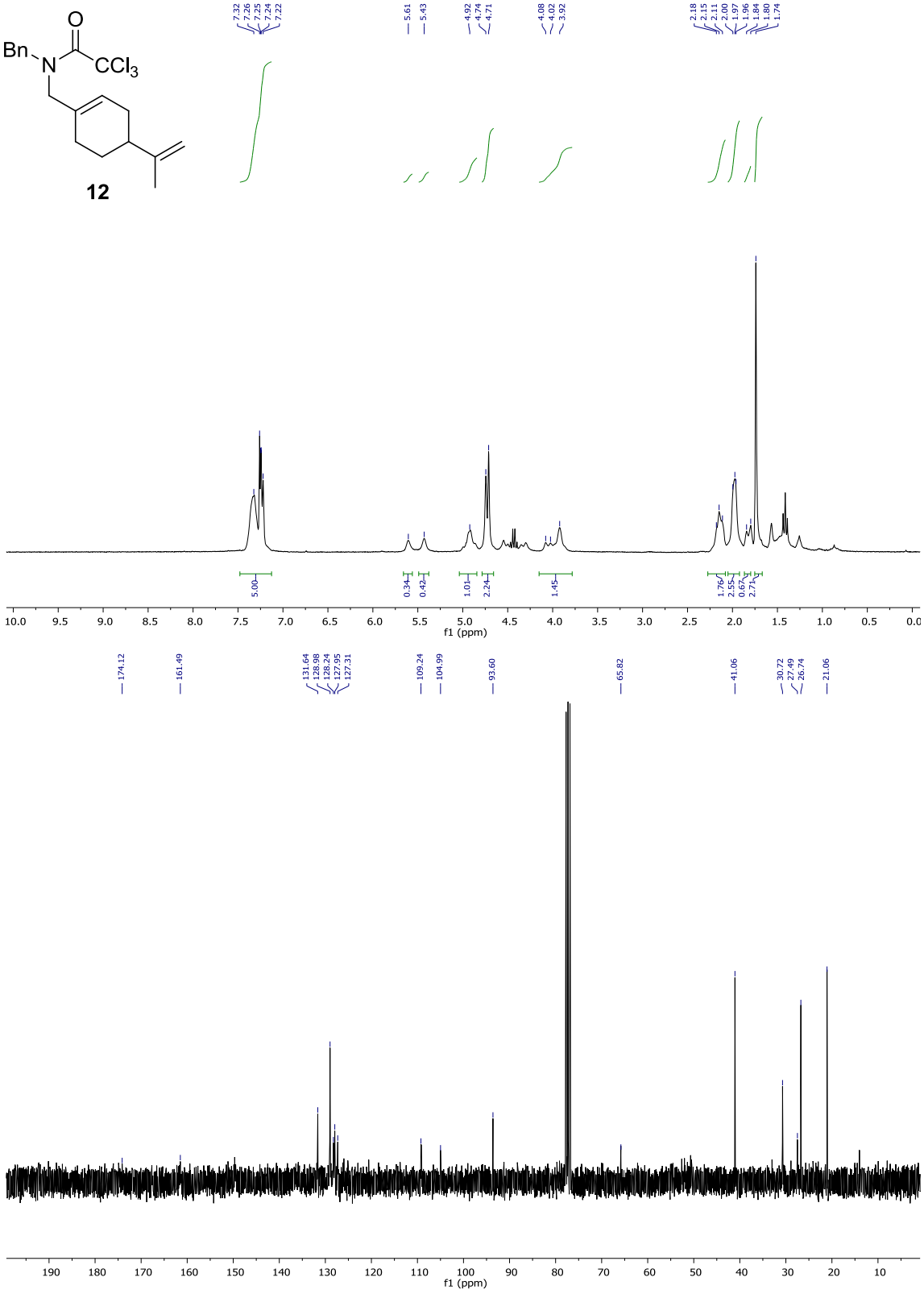
80
60
40
20
ppm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4.71
4.08
4.02
3.92
2.18
2.15
2.11
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1.96
1.84
1.80
1.74
5.00
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0.67
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f1 (ppm)
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161.49
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128.24
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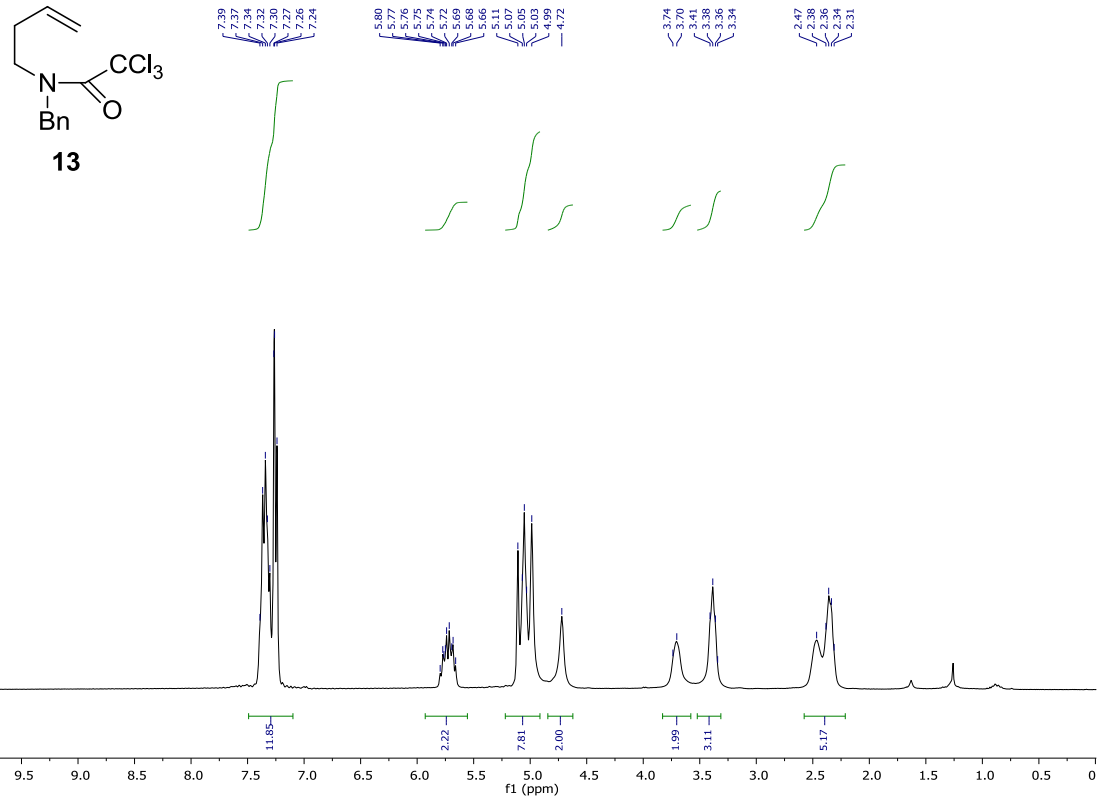
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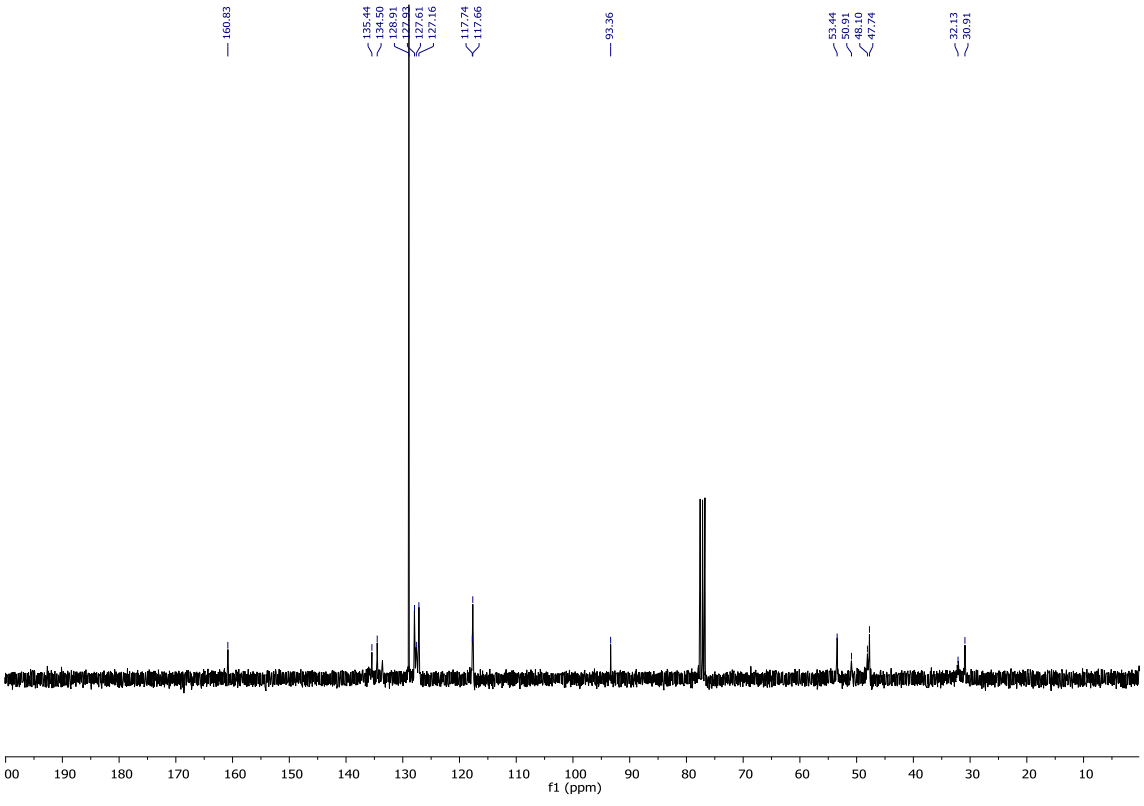
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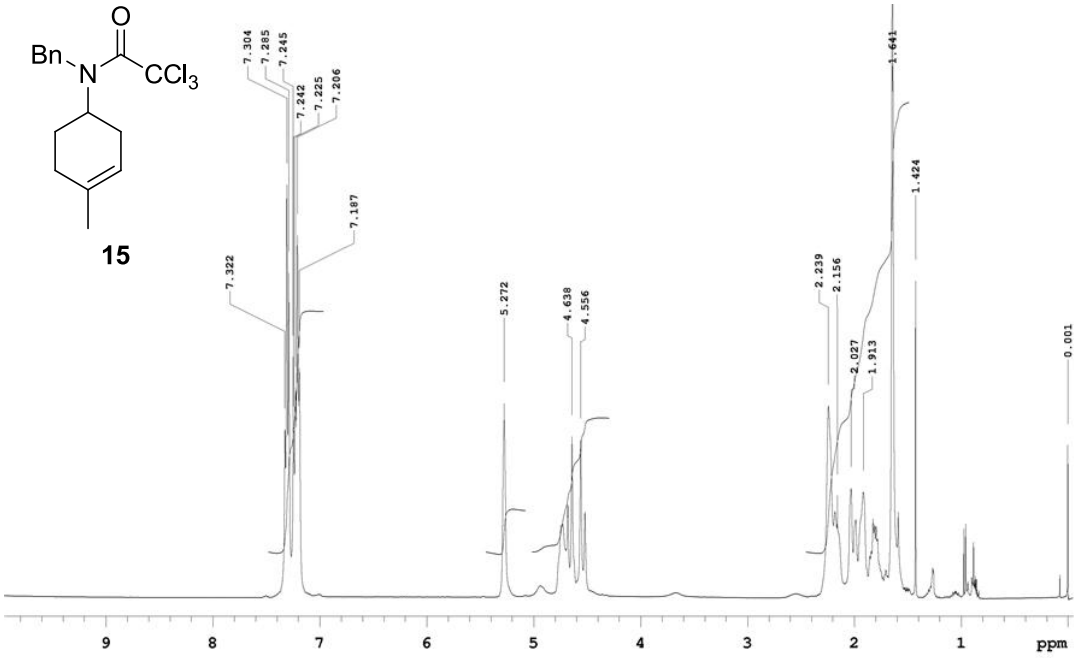
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7
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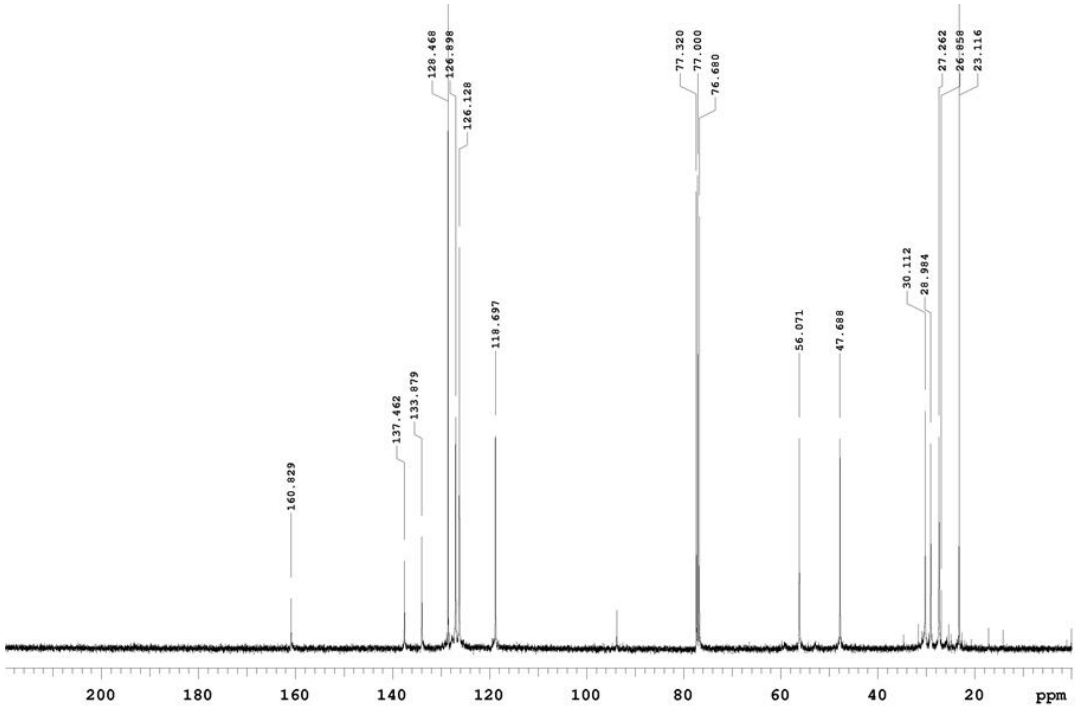
4
3
2
1
ppm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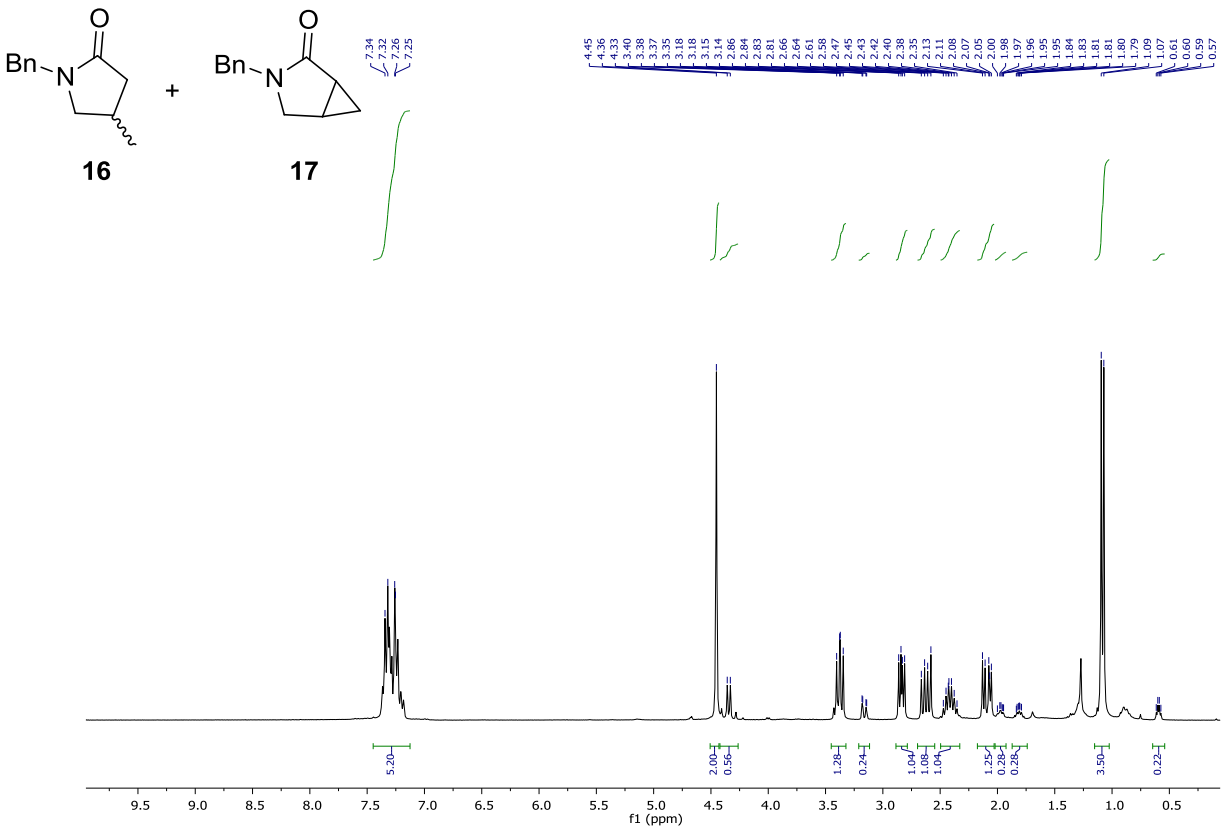
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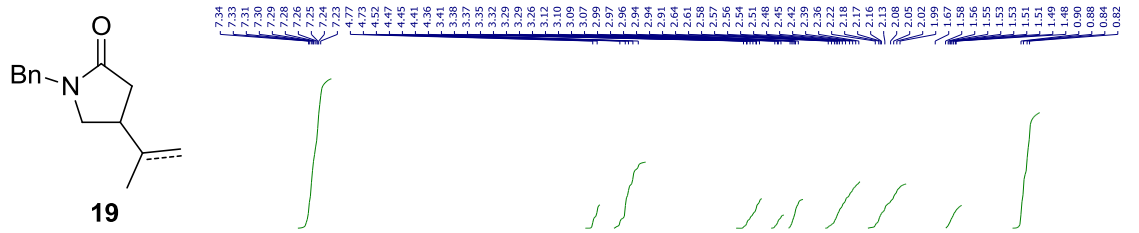
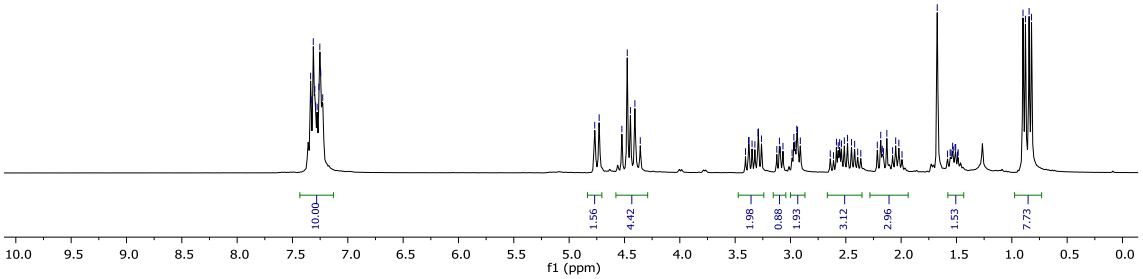
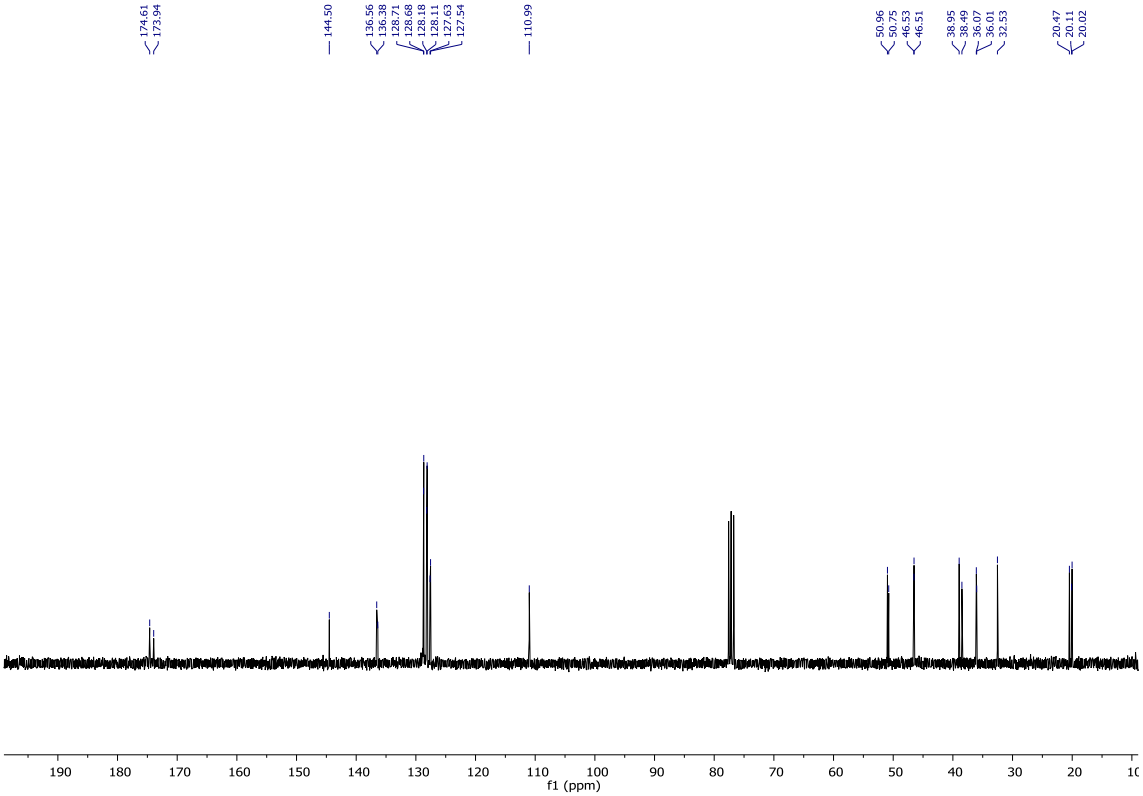
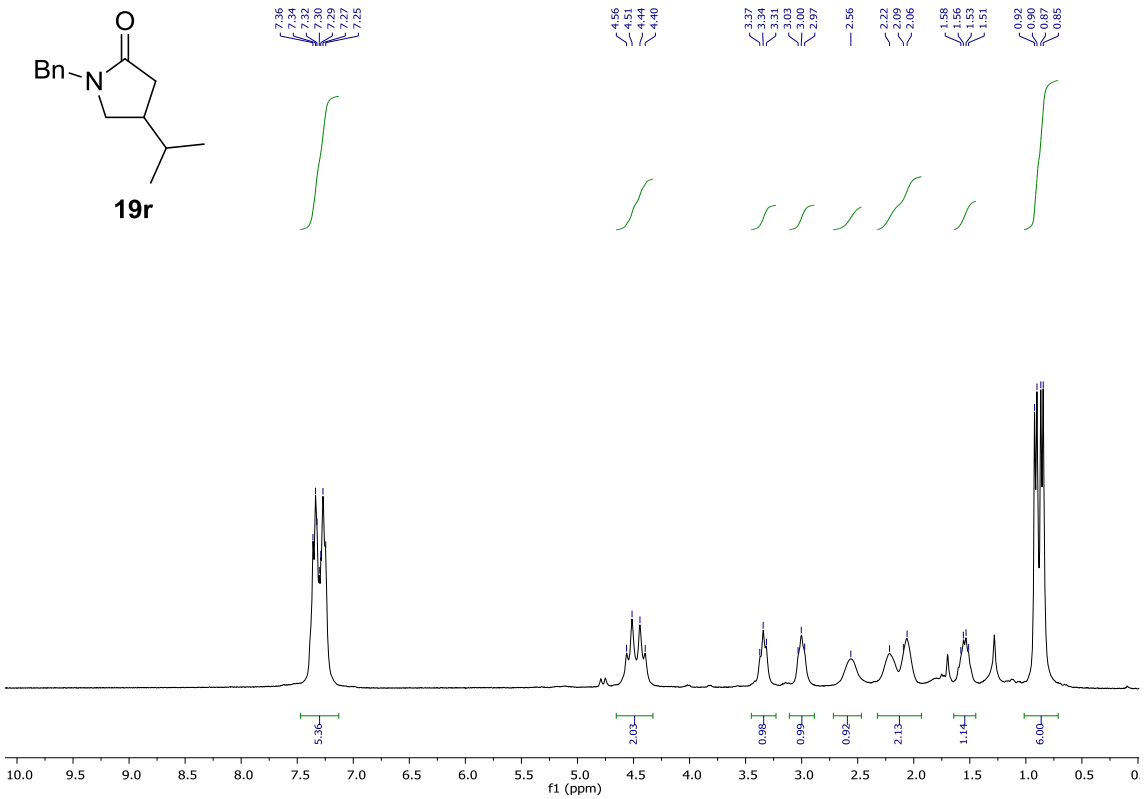
0.28
0.28
3.50
0.22
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

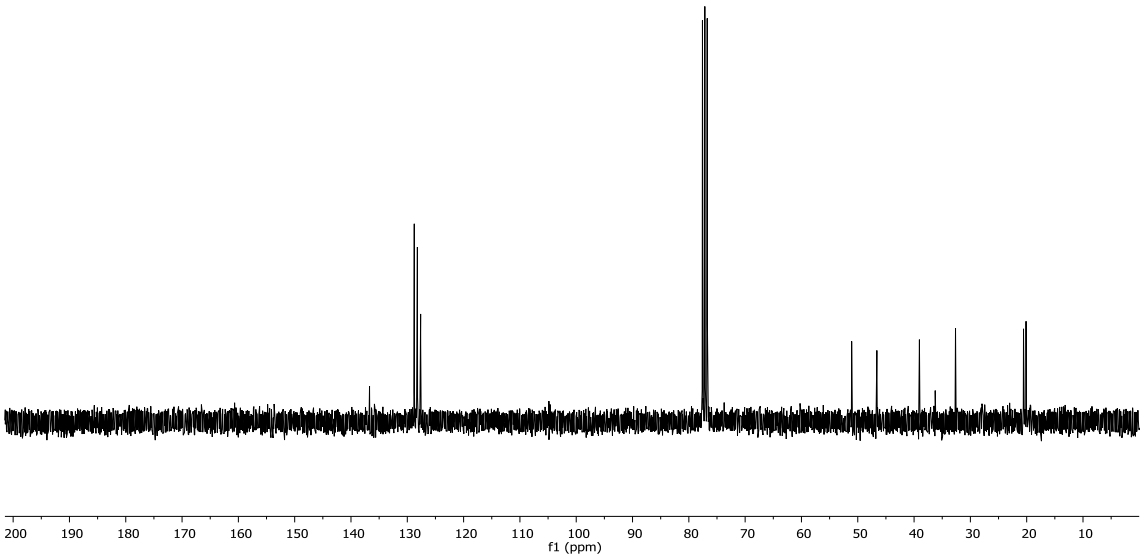

O
Bn
N

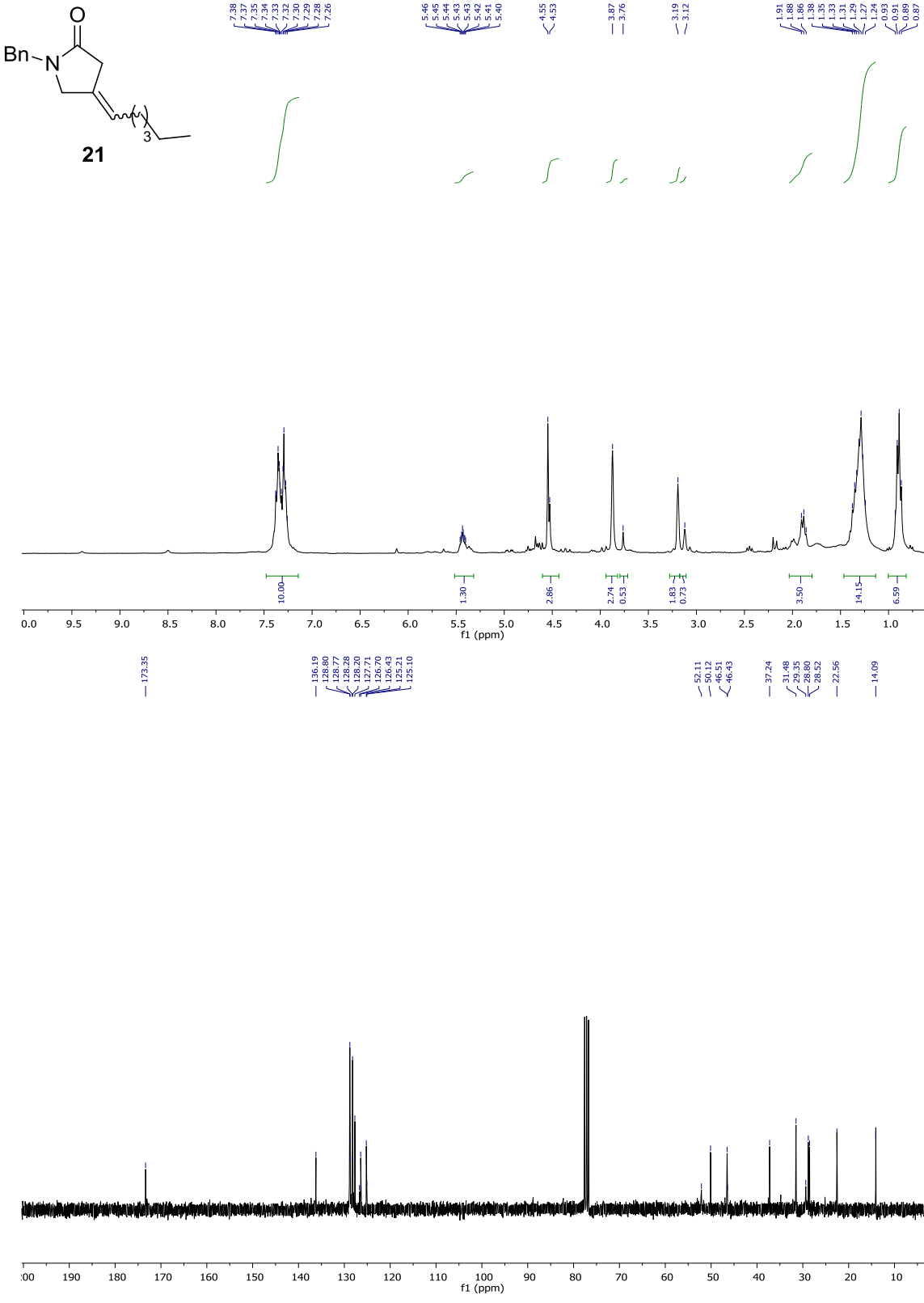
19

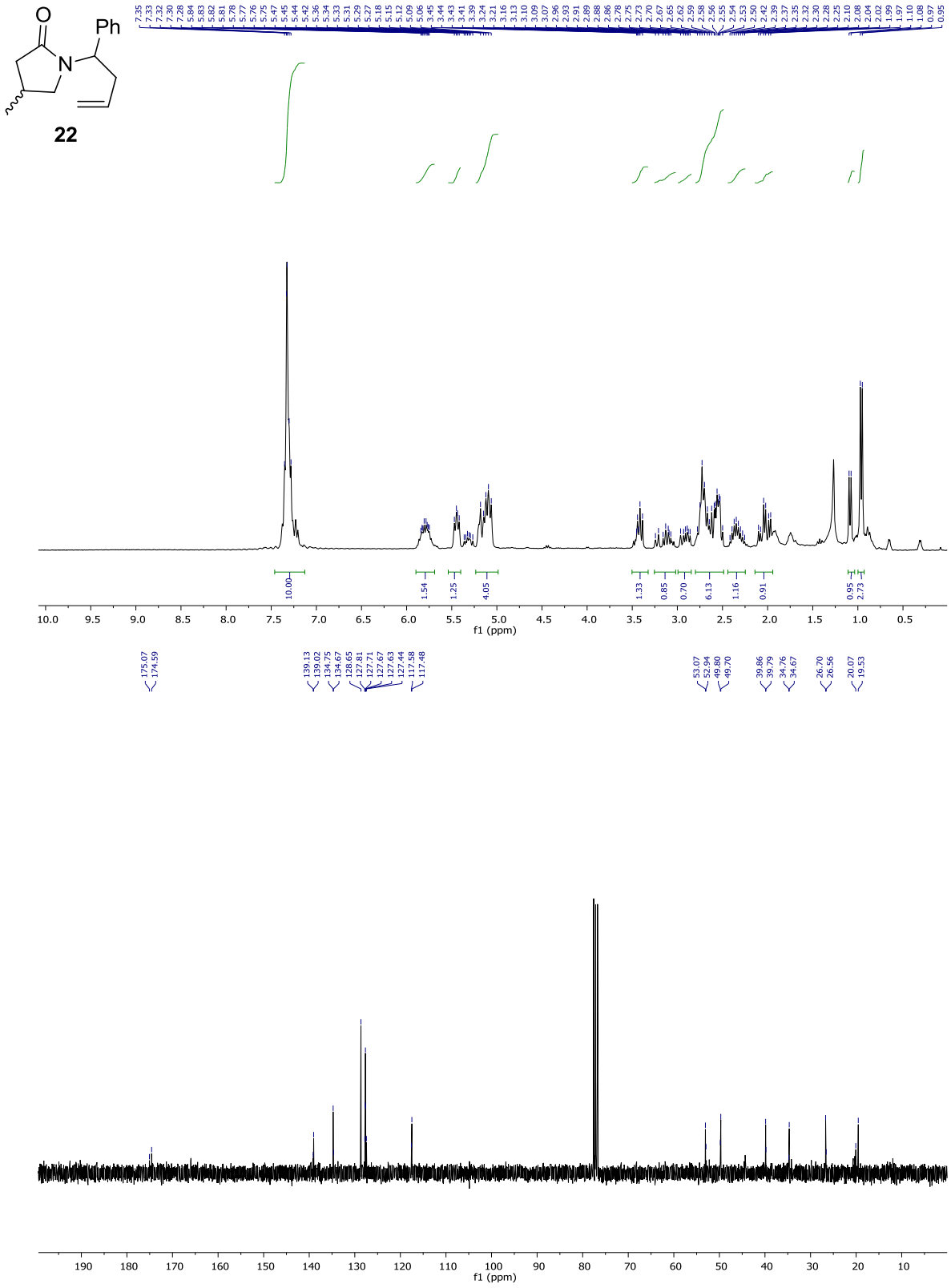

10.00
1.56
4.42
1.98
0.88
1.93
3.12
2.96
1.53
7.73
f1 (ppm)

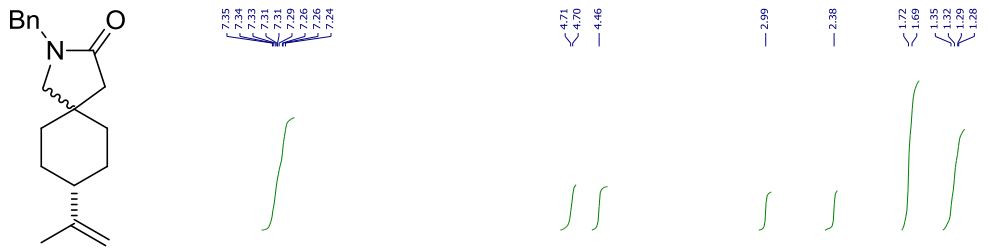

174.61
173.94
144.50
136.56
136.38
128.71
128.68
128.18
128.11
127.63
127.54
110.99
50.96
50.75
46.53
46.51
38.95
38.49
36.07
36.01
32.53
20.47
20.11
20.02
f1 (ppm)


Bn
N
O
19r
7.36
7.34
7.32
7.30
7.29
7.27
7.25
4.56
4.51
4.44
4.40
3.37
3.34
3.31
3.03
3.00
2.97
2.56
2.22
2.09
2.06
1.58
1.56
1.53
1.51
0.92
0.90
0.87
0.85
5.36
2.03
0.98
0.99
0.92
2.13
1.14
6.00
f1 (ppm)

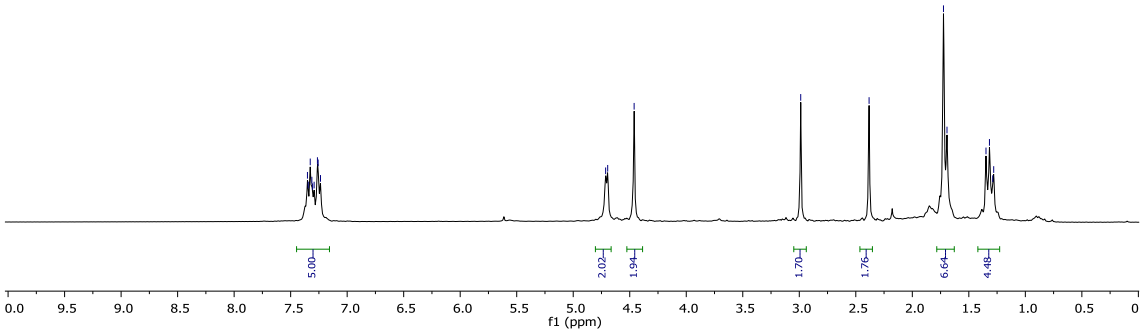

f1 (ppm)

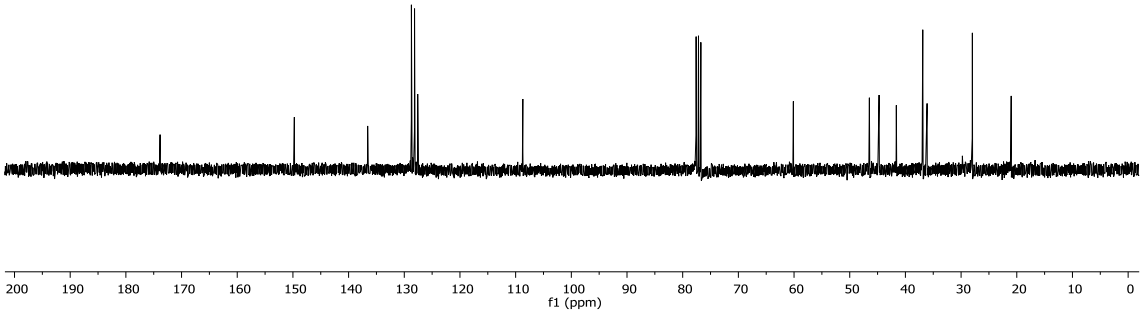

Bn
N
O
3
21
7.38 7.37 7.35 7.34 7.33 7.32 7.30 7.29 7.28 7.26
5.46 5.45 5.44 5.43 5.43 5.42 5.41 5.40
4.55 4.53
3.87 3.76
3.19 3.12
1.91 1.88 1.86 1.86 1.38 1.35 1.33 1.31 1.29 1.27 1.24 0.93 0.91 0.89 0.87
10.00 1.30 2.86 2.74 0.53 1.83 0.73 3.50 14.15 6.59
f1 (ppm)
173.35
136.19 128.80 128.77 128.28 128.20 127.71 126.70 126.43 125.21 125.10
52.11 50.12 46.51 46.43
37.24
31.48 29.35 28.80 28.52
22.56
14.09
f1 (ppm)

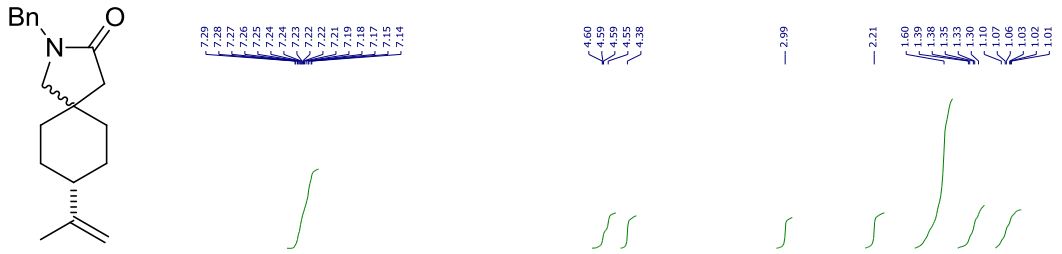

O
Ph
N
22
7.35 7.33 7.32 7.30 7.28 5.84 5.83 5.82 5.81 5.78 5.77 5.76 5.75 5.47 5.45 5.44 5.42 5.36 5.34 5.33 5.31 5.29 5.27 5.18 5.15 5.12 5.09 5.06 3.45 3.44 3.43 3.41 3.39 3.24 3.21 3.16 3.13 3.10 3.09 3.07 2.96 2.93 2.91 2.89 2.88 2.86 2.78 2.75 2.73 2.70 2.67 2.65 2.62 2.59 2.58 2.56 2.55 2.54 2.53 2.50 2.42 2.39 2.37 2.35 2.32 2.30 2.28 2.25 2.10 2.08 2.04 2.02 1.99 1.97 1.10 1.08 0.97 0.95
10.00 1.54 1.25 4.05 1.33 0.85 0.70 6.13 1.16 0.91 0.95 2.73
f1 (ppm)
175.07 174.59 139.13 139.02 134.75 134.67 128.65 127.81 127.71 127.67 127.63 127.44 117.58 117.48 53.07 52.94 49.80 49.70 39.86 39.79 34.76 34.67 26.70 26.56 20.07 19.53
f1 (ppm)



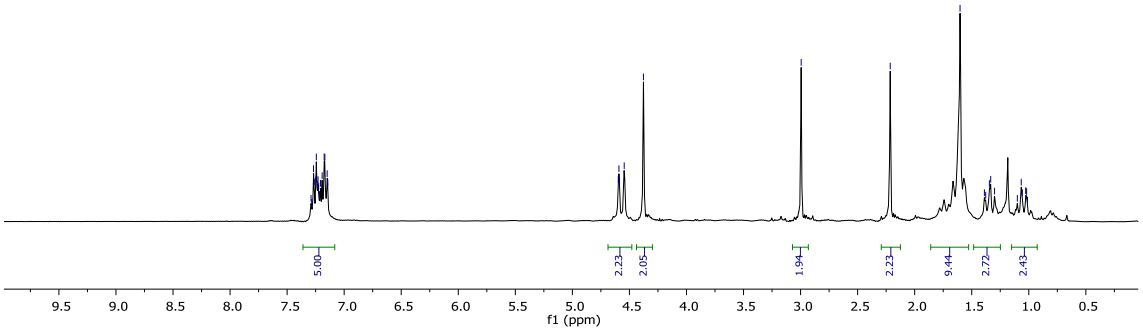
23 (major isomer)

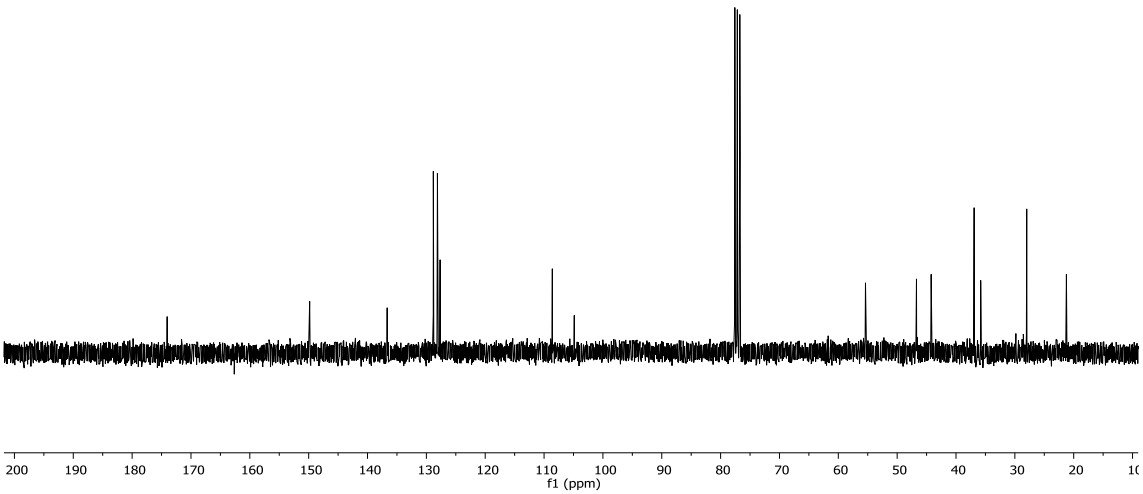


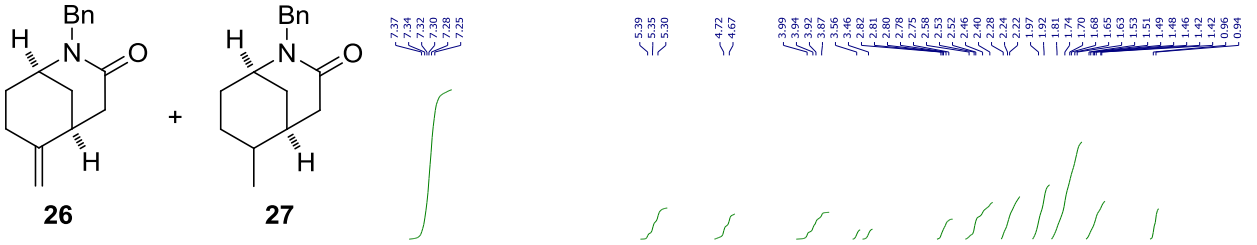




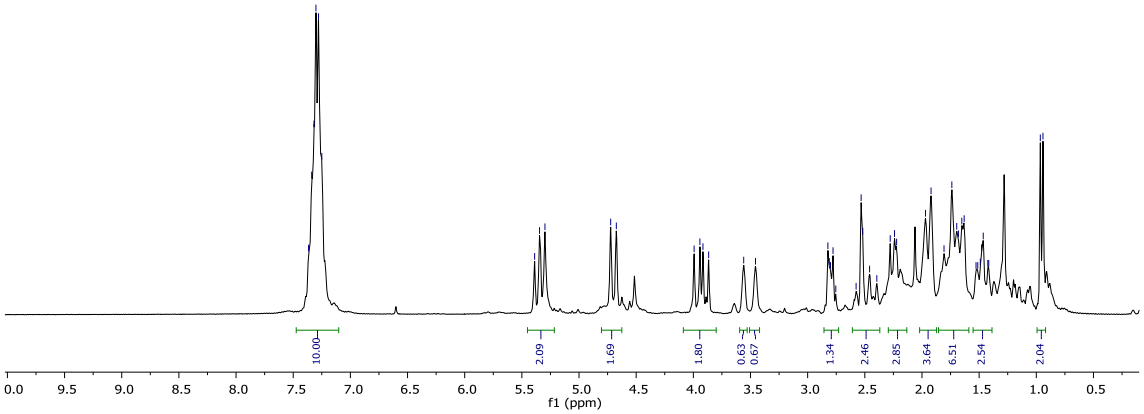
23 (minor isomer)

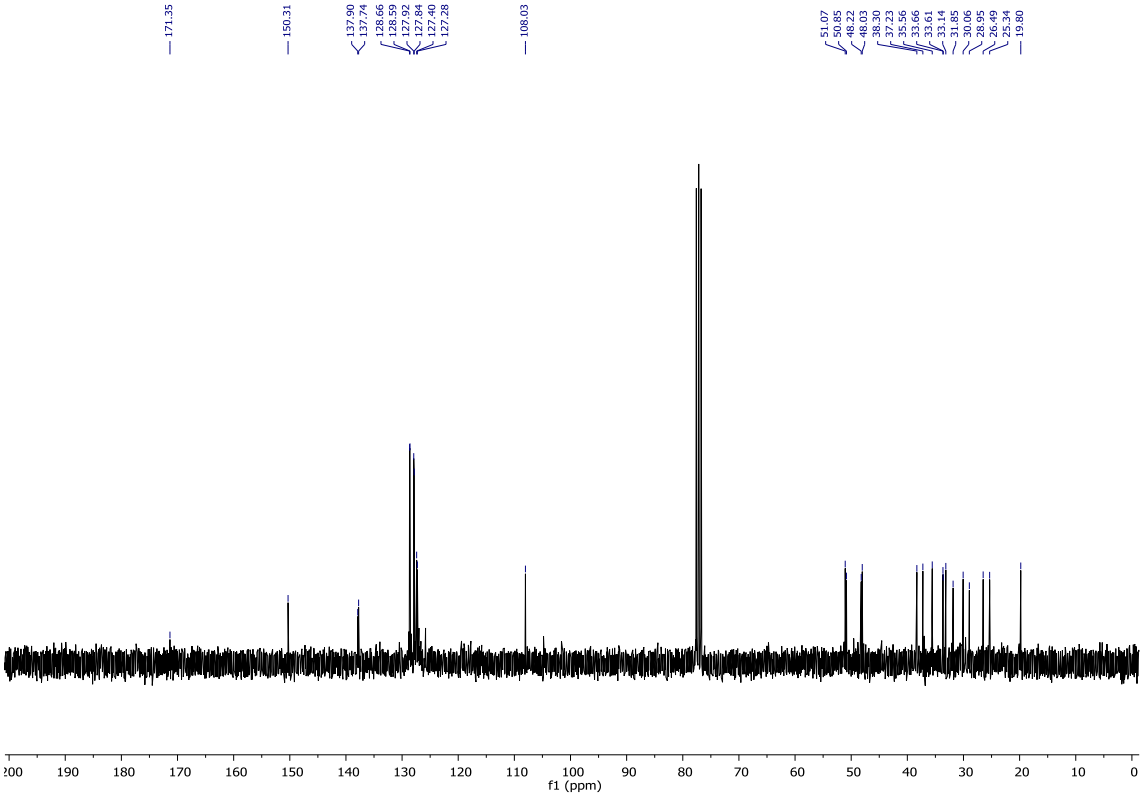





Bn
H
N
O
H
Bn
H
N
O
H
+
7.37
7.34
7.32
7.30
7.28
7.25
5.39
5.35
5.30
4.72
4.67
3.99
3.94
3.92
3.87
3.56
3.46
2.82
2.81
2.80
2.78
2.75
2.58
2.53
2.52
2.46
2.40
2.28
2.24
2.22
1.97
1.92
1.81
1.74
1.70
1.68
1.65
1.63
1.53
1.51
1.49
1.48
1.46
1.42
1.42
0.96
0.94

26 **27**


10.00
2.09
1.69
1.80
0.63
0.67
1.34
2.46
2.85
3.64
6.51
2.54
2.04
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


171.35
150.31
137.90
137.74
128.66
128.59
127.92
127.84
127.40
127.28
108.03
51.07
50.85
48.22
48.03
38.30
37.23
35.56
33.66
33.61
33.14
31.85
31.06
28.95
26.49
25.34
19.80
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)