Electronic Supplementary Material (ESI) for Chemical Science

Supporting Information

Rhodium (III)-catalyzed intramolecular annulations involving amide-directed C-H activations: synthetic scope and mechanistic studies

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Contents

1. General experimental procedures

Reactions were conducted in dry solvents under Argon atmosphere unless otherwise stated. Dry solvents were freshly distilled under Argon from an appropriate drying agent before use. Toluene was distilled from Na, THF from Na / benzophenone. Dried dichloromethane and *tert*-amyl alcohol (2-methylbutan-2-ol) were purchased from Aldrich and used without further purification. $[RhCp^*Cl_2]_2$ (99%) [12354-85-7] was purchased from Strem, $[Ru(p\text{-cymene})Cl_2]_2$ was purchased from TCI [52562-29-0] (>95%) and CsOAc (99%) [3396-11-0] was purchased from Alfa Aesar, All other chemicals were purchased from Aldrich and used without further purification.

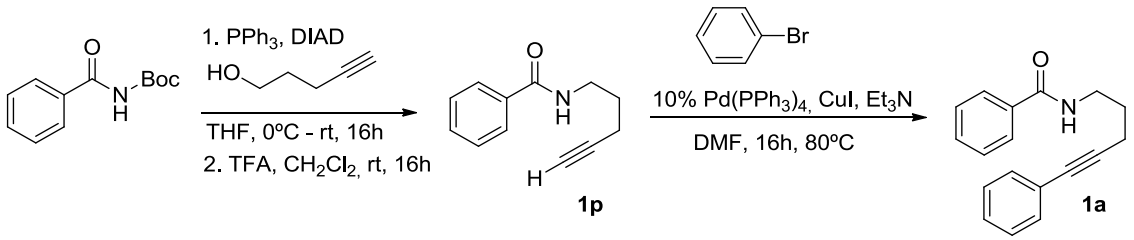
The abbreviation "*rt*" refers to reactions carried out at a temperature between 21-25 ºC. Reaction mixtures were stirred using Teflon-coated magnetic stir bars. High reaction temperatures were maintained using Thermowatch-controlled silicone oil baths. Thin-layer chromatography (TLC) was performed on silica gel plates and components were visualized by observation under UV light, and / or by treating the plates with *p*-anisaldehyde or cerium nitrate solutions, followed by heating. Flash chromatography was carried out on silica gel. Dryings were performed with anhydrous Na_2SO_4. Concentration refers to the removal of volatile solvents via distillation using a Büchi rotary evaporator followed by high vacuum.

All Rhodium-catalyzed reactions were carried out without any particular precautions to extrude moisture or oxygen.

^1H NMR (300MHz) spectra were recorded at room temperature on a Varian 300MHz spectrometer in CD Cl3 [using $(CH_3)_4Si$ (for 1H, δ = 0.00) as internal standard]. ^{13}C NMR (75 MHz) spectra on a Varian spectrometer in $CDCl_3$ [using $CDCl_3$ (for ^{13}C, δ = 77.160) as internal standard]. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br s = broad singlet (typically NH). Carbon types and structure assignments were determined from DEPT-NMR and two dimensional experiments (HMQC and HMBC, COSY and NOESY). NMR spectra were analyzed using MestReNova© NMR data processing software (www.mestrelab.com). Mass spectra were acquired using electronic impact (EI) and were recorded at the CACTUS facility of the University of Santiago de Compostela.

2. Experimental data

General procedure for the synthesis of alkynylbenzamides (1a-1n), exemplified for 1a.

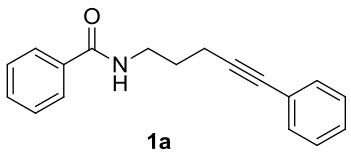


To a solution of *tert*-butyl benzoylcarbamate**7a** (4 g, 17.8 mmol)**,** triphenylphosphine (5.60 g, 21.4mmol) and 4-pentyn-1-ol (10.0 g, 202 mmol) in THF (90 mL) at 0 °C was added diisopropylazodicarboxylate (DIAD, 4.16 mL, 21.4 mmol) dropwise, very slowly. After complete addition, the yellow solution was stirred at r.t. overnight. The reaction was concentrated, water (40 mL) was added and the mixture was extracted with Et_2O (3x20 mL). The combined organic layers were dried over sodium sulfate and the solvent was evaporated *in vacuo* to afford a viscous oil that was purified by flash chromatography (hexanes:diethylether 1:3) to obtain the *tert*-butyl benzoyl(pent-4-yn-1-yl)carbamate (3.58 g, 70%).

To a solution of *tert*-butyl benzoyl(pent-4-yn-1-yl)carbamate (2.9 g, 10.1 mmol) in CH_2Cl_2 (40 mL) at 0 °C was added trifluoroacetic acid (0.78 mL, 1 eq) dropwise. After complete addition, the solution was stirred at r.t. overnight. Water (15 mL) was added and the mixture was extracted with CH_2Cl_2 (3x10 mL). The combined organic layers were dried over sodium sulfate and the solvent was evaporated *in vacuo* to afford a yellow oil that was purified by flash chromatography (hexanes:diethylether 1:1) to obtain the corresponding *N*-(pent-4-yn-1-yl)benzamide **1p** (1.10 g, 58%). Amorfous white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 11.3, 4.3 Hz, 2H), 7.52 – 7.30 (m, 3H), 6.91 (s, 1H), 3.51 (dd, *J* = 12.8, 6.7 Hz, 2H), 2.25 (td, *J* = 6.9, 2.6 Hz, 2H), 1.97 (dd, *J* = 3.5, 1.8 Hz, 1H), 1.90 – 1.73 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.8 (C), 134.6 (C), 131.4 (CH), 128.5 (CH), 127.0 (CH), 83.7 (C), 69.2 (CH), 39.3 (CH_2), 28.1 (CH_2), 16.3 (CH_2).

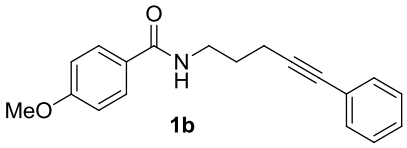
To a solution of benzamide **1p** (100 mg, 0.53 mmol), $Pd(PPh_3)_4$ (48 mg, 10 mol%) and CuI (10.17 mg, 10 mol%) in DMF (8 mL), bromobenzene (125 mg, 0.795 mmol) was added Et_3N (0.75 mL, 5.34 mmol). After complete addition, the solution was stirred at 80 °C overnight. The reaction mixture was diluted with EtOAc (30 mL) and washed with water (10 mL) and brine (10mL). The combined organic layers were dried over anhidrous sodium sulfate and the solvents were evaporated *in vacuo* to afford a yellow oil that was purified by flash chromatography hexanes:ethyl acetate 1:3) to obtain the corresponding arene **1a** (112 mg, 80%).

***N*-(5-Phenylpent-4-yn-1-yl)benzamide (1a):** white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.86 – 7.60 (m, 2H), 7.51 – 7.13 (m, 8H), 6.53 (br s, 1H), 3.57 (dd, *J* = 12.6, 6.4 Hz, 2H), 2.48 (t, *J* = 6.7 Hz, 2H), 1.99 – 1.77 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.5 (C), 134.5 (C), 131.5 (CH), 131.3 (CH), 128.5 (CH), 128.2 (CH), 127.8 (CH), 126.8 (CH), 123.4 (C), 89.2 (C), 81.6 (C), 39.7 (CH_2), 28.2



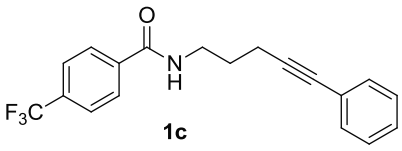
(CH_2), 17.5 (CH_2).**LRMS** (*m/z, I*) 263 (87), 262 (43) 235 (27) **HRMS** calculated for $C_{18}H_{17}NO$ 263.1310, found 263.1318.

4-Methoxy-*N*-(5-phenylpent-4-yn-1-yl)benzamide (1b): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.74 – 7.54 (m, 2H), 7.42 – 7.09 (m, 5H), 6.83 – 6.66 (m, 2H), 6.51 (br s, 1H), 3.73 (s, 3H), 3.53 (dt, *J* = 13.9, 6.9 Hz, 2H), 2.46 (t, *J* = 6.8 Hz, 2H), 1.92 – 1.80 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.2 (C), 162.1 (C), 131.7 (CH), 128.8 (CH), 128.4 (CH), 127.9 (CH), 126.9 (C), 123.6 (C), 113.72 (CH), 89.5 (C), 81.7 (C), 55.4 (CH_3), 39.8 (CH_2), 28.4 (CH_2), 17.6 (CH_2). **LRMS** (*m/z, I*) 293 (16), 292 (25), 291 (291), 277 (4).



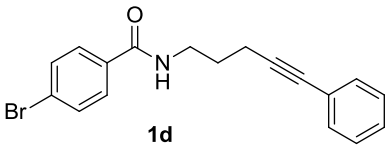
1b

***N*-(5-Phenylpent-4-yn-1-yl)-4-(trifluoromethyl)benzamide (1c):** yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.6 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.40 – 7.22 (m, 5H), 6.90 (br s, 1H), 3.65 (dd, *J* = 12.5, 6.3 Hz, 2H), 2.55 (t, *J* = 6.7 Hz, 2H), 2.08 – 1.83 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 166.4 (C), 137.9 (C), 133.1 (q, *J* = 32.8 Hz, C), 131.6 (CH), 128.4 (CH), 128.1 (CH), 127.5 (CH), 125.6 (q, *J* = 3.5 Hz, CH), 123.4 (C), 120.1 (q, *J* = 272.4 Hz, C), 89.4 (C), 81.9 (C), 40.2 (CH_2), 28.1 (CH_2), 17.7 (CH_2). **LRMS** (*m/z, I*) 331 (74), 330 (27), 312 (13), 302 (23), 277 (15). **HRMS** calculated for $C_{19}H_{16}NOF_3$ 331.1184, found 331.1187



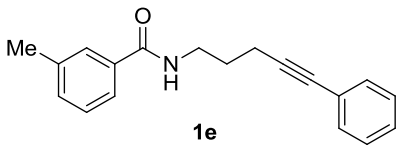
1c

4-Bromo-*N*-(5-phenylpent-4-yn-1-yl)benzamide (1d): white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.66 – 7.06 (m, 8H), 6.80 (br s, 1H), 3.53 (dd, *J* = 12.5, 6.3 Hz, 2H), 2.46 (t, *J* = 6.7 Hz, 2H), 2.03 – 1.64 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δδ 166.7 (C), 133.5 (C), 131.7 (CH), 131.6 (CH), 128.6 (CH), 128.4 (CH), 128.0 (CH), 126.1 (C), 123.4 (C), 89.4 (C), 81.8 (C), 40.0 (CH_2), 28.2(CH_2), 17.6 (CH_2).**LRMS** (*m/z, I*) 341 (28), 313 (9). **HRMS** calculated for $C_{18}H_{16}NOBr$ 341.0415, found 341.0428.



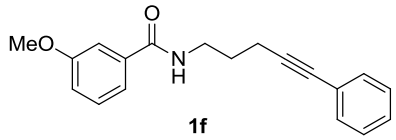
1d

3-methyl-N-(5-phenylpent-4-yn-1-yl)benzamide (1e): white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.60 – 7.47 (m, 1H), 7.40 – 7.30 (m, *J* = 6.7, 3.1 Hz, 1H), 7.30 – 7.17 (m, 2H), 6.49 (s, 1H), 3.63 (dd, *J* = 12.6, 6.4 Hz, 1H), 2.54 (t, *J* = 6.8 Hz, 1H), 2.30 (s, 1H), 2.01 – 1.86 (m, *J* = 6.7 Hz, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.9 (C), 138.5 (C), 134.7 (C), 132.2 (CH), 131.7 (CH), 128.4 (CH), 128.4 (CH), 127.9 (CH), 127.7 (CH), 124.0 (CH), 123.6 (C), 89.4 (C), 81.7 (C), 39.8 (CH_2), 28.4 (CH_2), 21.3 (CH_3), 17.6 (CH_2).



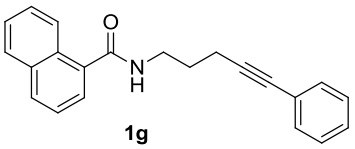
1e

3-methoxy-N-(5-phenylpent-4-yn-1-yl)benzamide (1f): white solid . **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.40 – 7.30 (m, 3H), 7.30 – 7.15 (m, 5H), 7.02 – 6.95 (m, 1H), 6.61 (s, 1H), 3.79 (s, 3H), 3.62 (dd, *J* = 12.6, 6.5 Hz, 2H), 2.53 (t, *J* = 6.8 Hz, 2H), 1.99 – 1.86 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.6 (C), 159.9 (C), 136.2 (C), 131.7 (CH), 129.6 (CH), 128.3 (CH), 127.9 (CH), 123.6 (C), 118.7 (CH), 117.7 (CH), 112.4 (CH), 89.3 (C), 81.7 (C), 55.5 (CH_3), 39.8 (CH_2), 28.4 (CH_2), 17.5 (CH_2).



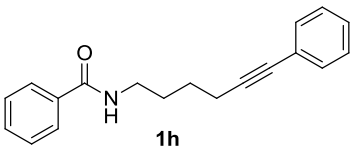
1f

***N*-(5-Phenylpent-4-yn-1-yl)-1-naphthamide (1g):** white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.34 – 8.13 (m, 1H), 7.90 – 7.69 (m, 2H), 7.61 – 7.11 (m, 9H), 6.60 (br s, 1H), 3.59 (dd, *J* = 12.6, 6.4 Hz, 2H), 2.50 (t, *J* = 6.9 Hz, 2H), 2.00 – 1.75 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 170.1 (C), 134.9 (C), 134.0 (C), 131.9 (CH), 130.8 (CH), 130.5 (C), 128.7 (CH), 128.2 (CH), 127.4 (CH), 126.8 (CH), 125.8 (CH), 125.3 (CH), 125.1 (CH),124.0 (C), 89.6 (C), 82.0 (C), 39.9 (CH_2), 28.8(CH_2), 17.8 (CH_2). **LRMS** (*m/z, I*) 313 (57), 312 (90), 285 (40).



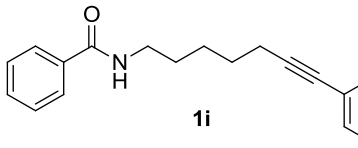
1g

***N*-(6-Phenylhex-5-yn-1-yl)benzamide (1h):** white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.76 – 7.61 (m, 2H), 7.53 – 7.01 (m, 8H), 6.48 (br s, 1H), 3.39 (dt, *J* = 6.7, 3.8 Hz, 2H), 2.35 (dd, *J* = 9.3, 4.2 Hz, 2H), 1.80 – 1.44 (m, 4H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.7 (C), 134.8 (C), 131.7 (CH), 131.5 (CH), 128.7 (CH), 128.3 (CH), 127.8 (CH), 127.0 (CH), 123.9 (C), 89.8 (C), 81.3 (C), 39.7 (CH_2), 29.0 (CH_2), 26.2 (CH_2), 19.2 (CH_2). **LRMS** (*m/z, I*) 277 (32), 261 (50), 249 (12). **HRMS** calculated for $C_{19}H_{17}NO$ 275.1310, found 275.1312



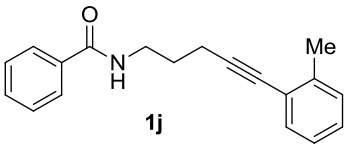
1h

N-(7-Phenylhept-6-yn-1-yl)benzamide (1i): yellow oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.79 – 7.54 (m, 2H), 7.47 – 7.22 (m, 5H), 7.23 – 7.12 (m, 3H), 6.31 (br s, 1H), 3.47 – 3.26 (m, 2H), 2.34 (t, *J* = 6.7 Hz, 2H), 1.70 – 1.36 (m, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.7 (C), 134.9 (C), 131.6 (CH), 131.4 (CH), 128.6 (CH), 128.3 (CH), 127.6 (CH), 126.9 (CH), 124.0 (C), 90.0 (C), 80.1(C), 40.0 (CH_2), 29.3 (CH_2), 28.4 (CH_2), 26.2 (CH_2), 19.4 (CH_2). **LRMS** (*m/z, I*) 291 (36), 277 (16). **HRMS** calculated for $C_{20}H_{19}NO$ 291.1623, found 291.1624.



1i

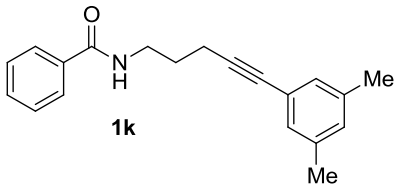
***N*-(5-(*o*-Tolyl)pent-4-yn-1-yl)benzamide (1j):** brown oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.77 – 7.52 (m, 2H), 7.48 – 6.89 (m, 8H), 6.53 (br s, 1H), 3.58 (dd, *J* = 12.5, 6.7 Hz, 2H), 2.61 – 2.40 (m, 2H), 2.32 (s, 3H), 1.97 – 1.77 (m 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.7 (C), 140.1 (C), 134.6 (C), 132.0 (CH), 131.5 (CH), 129.5 (CH), 128.6 (CH), 127.9 (CH), 127.0 (CH), 125.6 (CH), 123.3 (C), 93.2



1j

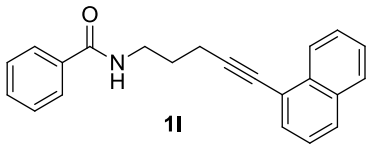
(C), 80.6 (C), 39.8 (CH_2), 28.6 (CH_2), 20.9 (CH_3), 17.7 (CH_2). **LRMS** (*m/z, I*) 277 (59), 259 (28). **HRMS** calculated for $C_{19}H_{19}NO$ 277.1467, found 277.1455.

***N*-(5-(3,5-Dimethylphenyl)pent-4-yn-1-yl)benzamide (1k):** brown solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.9, 6.7 Hz, 2H), 7.42 – 7.32 (m, 1H), 7.31 – 7.20 (m, 2H), 6.92 (s, 2H), 6.84 (s, 1H), 6.59 (brs, 1H), 3.56 (dd, *J* = 12.6, 6.3 Hz, 2H), 2.46 (dd, *J* = 8.4, 5.0 Hz, 2H), 2.18 (s, 3H), 1.92 – 1.78 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 168.0 (C), 138.3 (C), 135.1 (C), 131.8 (CH), 130.3 (CH), 129.8 (CH), 129.0 (CH), 127.4 (CH), 123.6 (C), 89.0 (C), 82.5 (C), 40.3 (CH_2), 28.8 (CH_3), 21.6 (CH_2), 18.1 (CH_2). **LRMS** (*m/z, I*) 291 (55), 263 (20). **HRMS** calculated for $C_{20}H_{21}NO$ 291.1623, found 291.1622.



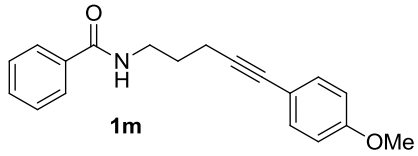
1k

***N*-(5-(Naphthalen-1-yl)pent-4-yn-1-yl)benzamide (1l):** brown solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.96 – 7.00 (m, 11H), 6.64 (brs, 1H), 3.72 – 3.46 (m, 2H), 2.56 (dt, *J* = 31.6, 6.8 Hz, 2H), 2.15 – 1.80 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.7 (C),134.5 (C), 133.4 (C), 133.2 (C), 131.4 (CH), 130.3 (CH), 128.5 (CH), 128.3 (CH), 127.0 (CH), 126.8 (CH), 126.5 (CH), 126.4 (CH), 126.2 (CH), 125.3 (CH), 121.2 (C), 94.4 (C), 79.7 (C), 39.9 (CH_2), 28.6(CH_2), 17.9(CH_2). **LRMS** (*m/z, I*) 313 (47), 262 (7). **HRMS** calculated for $C_{22}H_{19}NO$ 313.1467, found 313.1470.



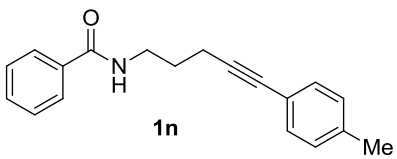
1l

***N*-(5-(4-Methoxyphenyl)pent-4-yn-1-yl)benzamide (1m):** brown solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.47 – 7.11 (m, 5H), 6.82 – 6.67 (m, 2H), 6.56 (brs, 1H), 3.69 (d, *J* = 23.8 Hz, 3H), 3.55 (dt, *J* = 22.2, 10.9 Hz, 2H), 2.48 (dd, *J* = 12.6, 6.0 Hz, 2H), 2.03 – 1.77 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.6 (C), 159.3 (C), 134.7 (C), 133.1 (CH), 131.7 (C), 131.5 (CH), 128.6 (CH), 127.0 (CH), 114.0 (CH), 87.8 (C), 81.5 (C), 55.4 (CH_3), 39.9 (CH_2), 28.4 (CH_2), 17.6 (CH_2). **LRMS** (*m/z, I*) 293 (45), 262 (6). **HRMS** calculated for $C_{19}H_{19}NO_2$ 293.1416, found 293.1420.



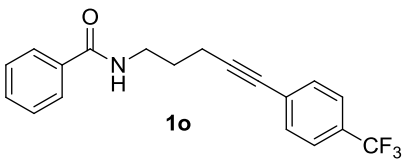
1m

***N*-(5-(*p*-Tolyl)pent-4-yn-1-yl)benzamide (1n):** brown solid. **^{1}H NMR** (300 MHz, $CDCl_3$) 7.66 (dd, *J* = 6.2, 5.2 Hz, 2H), 7.37 (dd, *J* = 10.6, 4.1 Hz, 1H), 7.31 – 7.16 (m, 4H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.54 (brs, 1H), 3.56 (q, *J* = 6.3 Hz, 2H), 2.53 – 2.39 (m, 2H), 2.26 (s, 3H), 1.95 – 1.78 (m, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 168.1 (C), 138.4 (C), 135.1 (C), 132.0 (CH), 131.9 (CH), 129.6 (CH), 129.0 (CH), 127.4 (CH), 120.9 (C), 89.0 (C), 82.3 (C), 40.3 (CH_2), 28.8 (CH_2), 22.0 (CH_3), 18.0 (CH_2). **LRMS** (*m/z, I*) 277 (33), 262 (6) 249 (6) **HRMS** calculated for $C_{19}H_{19}NO$ 277.1467, found 277.1455.



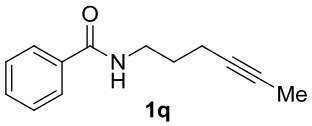
1n

***N*-(5-(4-(Trifluoromethyl)phenyl)pent-4-yn-1-yl)benzamide (1o):** white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.87 – 7.04 (m, 9H), 6.85 (s, 1H), 3.52 (dd, *J* = 12.7, 6.7 Hz, 2H), 2.44 (t, *J* = 6.9 Hz, 2H), 2.00 – 1.70 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.8 (C), 134.5 (C), 131.8 (CH), 131.4 (CH), 129.4 (q, *J* = 32.6 Hz, C), 128.5 (CH), 127.5 (C), 127.0 (CH), 125.2 (q, *J* = 3.8 Hz, CH), 124.0 (q, *J* = 272.3 Hz, C), 92.1 (C), 80.3 (C), 39.6 (CH_2), 28.3 (CH_2), 17.4 (CH_2). **LRMS** (*m/z, I*) 331 (44), 330 (33), 303 (8), 262 (9). **HRMS** calculated for $C_{19}H_{16}NOF_3$ 331.1184, found 331.1182.



1o

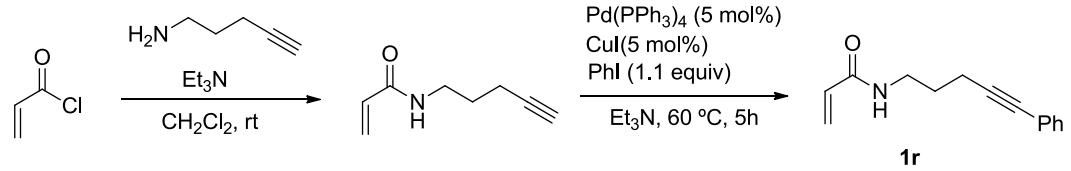
***N*-(Hex-4-yn-1-yl)benzamide (1q)[1]:** white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.88 – 7.65 (m, 2H), 7.55 – 7.30 (m, 3H), 6.55 (d, *J* = 35.7 Hz, 1H), 3.56 (dd, *J* = 12.6, 6.5 Hz, 2H), 2.37 – 2.13 (m, 2H), 1.85-1.70 (m, 5H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 167.5(C), 134.7(C), 131.3 (CH), 128.5 (CH), 126.9 (CH), 78.4 (C), 76.6 (C), 39.7 (CH_2), 28.3 (CH_3), 16.7 (CH_2), 3.5(CH_2). **LRMS** (*m/z, I*) 201 (24), 200 (93) 173 (38). **HRMS** calculated for $C_{13}H_{15}NO$201.1154, found 201.1114.



1q

[1] This substrate was prepared using 4-hexyn-1-ol as starting material for the Mitsunobu reaction following the general procedure for the synthesis of benzamides.

General procedure for the synthesis of alkynylbenzamides (1p-r), exemplified for 1r.

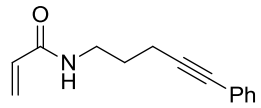


1r

Acryloyl chloride (0.2 mL, 2.4 mmol) was stirred in CH_2Cl_2 (10 mL) with triethylamine (0.46 mL, 0.36 mmol) at rt for 10 min. Addition of commercial available 4-pentynamine (200 mg, 2.40 mmol) was followed by stirring for 5 h. The CH_2Cl_2 was removed in *vacuo*, and the remaining residue was dissolved in ethyl acetate. The solution was washed with 10% HCl and brine, dried over magnesium sulfate and filtered. The solvent was removed and the product was purified by column chromatography (hexanes:EtOAc; 1:1) to afford *N*-(pent-4-yn-1-yl)acrylamide (208 mg, 63%).

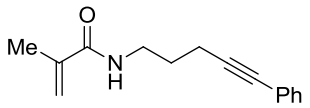
In a Schlenk flask containing $Pd(PPh_3)_4$ (87 mg, 5 mol %) and CuI (14 mg, 5 mol%) at rt, *N*-(pent-4-yn-1-yl)acrylamide (206 mg, 1.5 mmol) and Et_3N (10 mL) were added with stirring. Then iodobenzene (0.16 mL, 1 equiv.) was added and the mixture was heated to 60 ºC. After 5 hours the solvent was removed and the product was purified by column chromatography (hexanes:ethyl acetate; 1:1) to afford the product **1r** (262 mg, 82%).

***N*-(5-Phenylpent-4-yn-1-yl)acrylamide (1r):** yellow oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.42 – 7.21 (m, 5H), 6.48 (s, 1H), 6.25 (d, *J* = 17.0 Hz, 1H), 6.11 (dd, *J* = 17.0, 10 Hz, 1H), 5.57 (d, *J* = 10.0 Hz, 1H), 3.47 (q, *J* = 6.4 Hz, 2H), 2.45 (t, *J* = 6.9 Hz, 2H), 1.83 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 165.7 (C), 131.4 (CH), 130.8 (CH), 128.1 (CH), 127.6 (CH), 126.1 (CH_2), 123.5 (C), 88.9 (C), 81.3 (C), 38.8 (CH_2), 28.2 (CH_2), 17.0 (CH_2). **LRMS** (*m/z, I*) 157 (50), 140 (69).



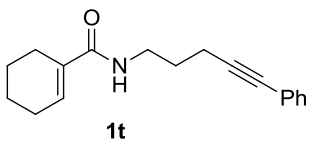
1r

***N*-(5-Phenylpent-4-yn-1-yl)methacrylamide (1r):** yellow solid **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.44 – 7.34 (m, 2H), 7.33 – 7.22 (m, 3H), 6.14 (s, 1H), 5.71 – 5.64 (m, 1H), 5.33 – 5.26 (m, 1H), 3.49 (dd, *J* = 12.7, 6.7 Hz, 2H), 2.49 (t, *J* = 6.9 Hz, 2H), 1.99 – 1.92 (m, 3H), 1.86 (p, *J* = 6.9 Hz, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 168.5 (C), 140.1 (C), 131.5 (CH), 128.2 (CH), 127.8 (CH), 123.5 (C), 119.3 (CH_2), 89.0 (C), 81.5 (C), 39.1 (CH_2), 28.2 (CH_2), 18.6 (CH_3), 17.3 (CH_2). **LRMS** (*m/z, I*) 212 (7), 199 (40). **HRMS** calculated for $C_{15}H_{17}NO$ 227.1310, found 227.1312.



1s

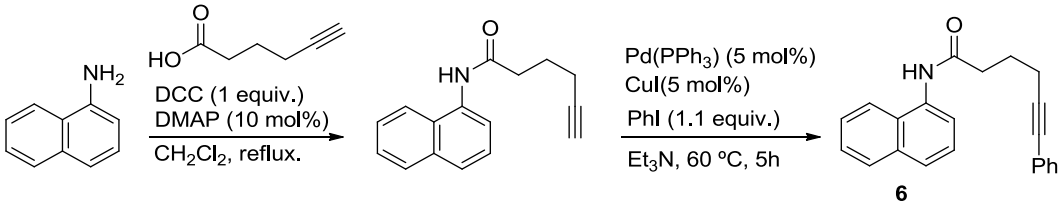
***N*-(5-Phenylpent-4-yn-1-yl)cyclohex-1-enecarboxamide (1t):** yellow oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 2H), 7.31 – 7.24 (m, 3H), 6.66 – 6.54 (m, 1H), 6.03 (s, 1H), 3.49 (dd, *J* = 12.6, 6.5 Hz, 2H), 2.49 (t, *J* = 6.8 Hz, 2H), 2.23 – 2.16 (m, 2H), 2.08 (dd, *J* = 6.1, 2.4 Hz, 2H), 1.85 (p, *J* = 6.7 Hz, 2H), 1.67 – 1.50 (m, 4H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 168.6 (C), 133.3 (CH), 133.1 (C), 131.5 (CH), 128.2



1t

(CH), 127.7 (CH), 123.5 (C), 89.2 (C), 81.5 (C), 39.1 (CH_2), 28.3 (CH_2), 25.3 (CH_2), 24.3 (CH_2), 22.1 (CH_2), 21.5 (CH_2), 17.4 (CH_2). **LRMS** (*m/z, I*) 250 (11), 239 (30).

General procedure C: synthesis of hexynamides 5 and 6 (exemplified for compound 6).

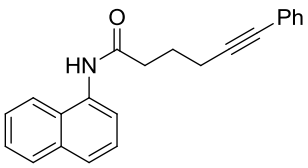


6

To a solution of hex-5-ynoic acid (1.1 mL, 10 mmol) in CH_2Cl_2 (50 mL) at room temperature under argon were added dimethylaminopyridine (DMAP, 12 mg, 0.10 mmol), *N,N'*-Dicyclohexylcarbodiimide (DCC, 2.06 g, 10 mmol) and naphthalen-1-amine (1.43 g, 10.0 mmol). The mixture was stirred 10 min. at this temperature and then heated at reflux for 5 hours. CH_2Cl_2 (20 ml) was added and the precipitate filtered off. The resulting homogeneous solution was washed with 10% HCl (20 ml) and saturated $NaHCO_3$ (20 ml). The solvent was evaporated and the crude product purified by flash chromatography (Hexanes:EtOAc; 3:1) to give N-(naphthalen-1-yl)hex-5-ynamide (1.28 g, 54 %) as a white solid.

In a Schlenk flask containing $Pd(PPh_3)_4$ (232 mg, 5 mol %) and CuI (37 mg, 5 mol%), N-(naphthalen-1-yl)hex-5-ynamide (744 mg, 4 mmol) and Et_3N (20 mL) were stirred at room temperature. Then iodobenzene (0.43 mL, 1 equiv.) was added and the mixture was heated to 60 ºC. After 5 hours the solvent was removed and the crude product was purified by column chromatography (hexanes:diethylether; 1:1) to afford the product **6** (511 mg, 59%).

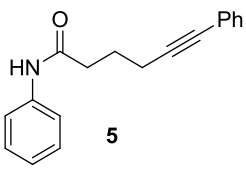
N-(Naphthalen-1-yl)-6-phenylhex-5-ynamide (6): ^{1}**H NMR** (300 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.89 – 7.79 (m, 2H), 7.71 (dd, *J* = 33.9, 7.8 Hz, 2H), 7.53 – 7.21 (m, 8H), 2.59 (t, *J* = 7.2 Hz, 2H), 2.50 (t, *J* = 6.9 Hz, 2H), 2.07 – 1.95 (m, 2H).^{13}**C NMR** (75 MHz, $CDCl_3$) δ 171.5 (C), 133.9 (C), 132.2 (C), 131.5 (CH), 128.4 (CH), 128.2 (CH), 127.7 (CH), 127.4 (C), 126.0 (CH), 125.8 (CH), 125.4 (CH), 123.6 (C), 121.3 (CH), 121.0 (CH), 89.0 (C), 81.7 (C), 35.8 (CH_2), 24.4 (CH_2), 18.7 (CH_2).



6

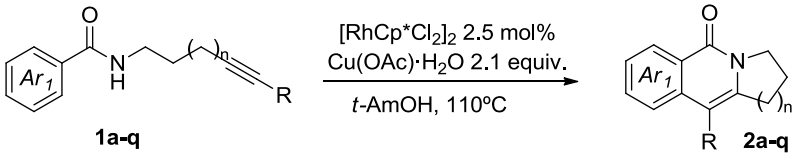
LRMS (*m/z, I*) 183 (19), 128 (27). **HRMS** calculated for $C_{27}H_{19}NO$ 313.1467, found 313.1465.

***N*,6-Diphenylhex-5-ynamide (5):** ^{1}**H NMR** (300 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.60 – 7.21 (m, 9H), 7.16 – 6.96 (m, 1H), 2.68 – 2.41 (m, 4H), 2.09 – 1.95 (m, 2H).^{13}**C NMR** (75 MHz, $CDCl_3$) δ 170.8 (C), 137.9 (C), 131.5 (CH), 128.9 (CH), 128.2 (CH), 127.7 (CH), 124.1 (CH), 123.6 (C), 119.9 (CH), 88.9 (C), 81.6 (C), 36.2(CH_2), 24.2 (CH_2), 18.8 (CH_2).**LRMS** (*m/z, I*) 220 (18), 159 (34). **HRMS** calculated for $C_{18}H_{17}NO$ 263.1310, found 263.1309.



5

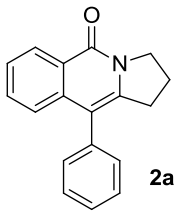
General procedure for catalytic reactions of alkynylbenzamides 1a-q.



1a-q **2a-q**

In a Schlenk flask equipped with a stir bar were added**1a-q** (0.25 mmol), $[Cp^*RhCl_2]_2$ (3.9 mg, 2.5% mol) and $Cu(OAc)_2$ (91 mg, 0.52 mmol) without any particular precautions to extrude oxygen or moisture. *t*-AmOH (2.0 mL) was then added and the flask sealed and placed in a pre-heated (110 °C) block. The reaction was stirred for 16 hours, cooled to room temperature and checked by TLC. The solvent was removed *in vacuo* and the remaining residue was purified by flash column chromatography on silica gel (hexanes:ethyl acetate) to afford the corresponding product **2a-q**.

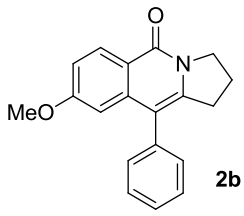
10-Phenyl-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2a): white solid. **^{1}H NMR** (300 MHz, $CDCl_3$)



2a

δ 8.48 (ddd, *J* = 7.9, 1.5, 0.5 Hz, 1H), 7.58 – 7.34 (m, 5H), 7.34 – 7.22 (m, 3H), 4.31 – 4.20 (m, 2H), 2.93 (t, *J* = 7.6 Hz, 2H), 2.14 (dt, *J* = 14.8, 7.5 Hz, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.0 (C), 141.2 (C), 138.0 (C), 136.3 (C), 131.8 (CH), 130.5 (CH), 128.6 (CH), 127.5 (CH), 127.3 (CH), 125.5 (CH), 124.9 (C), 124.2 (CH), 113.6 (C), 48.5 (CH_2), 31.0 (CH_2), 21.8 (CH_2) .**LRMS** (*m/z, I*) 261 (100), 260 (75) **HRMS** calculated for $C_{18}H_{15}NO$ 261.1154, found 275.1160.

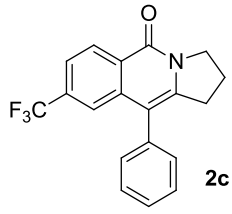
8-Methoxy-10-phenyl-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2b): brown solid. **^{1}H NMR** (300



2b

MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.9 Hz, 1H), 7.66 – 7.12 (m, 6H), 7.04 – 6.82 (m, 1H), 6.55 (d, *J* = 2.5 Hz, 1H), 4.28 – 4.02 (m, 2H), 3.63 (s, 3H), 2.82 (t, *J* = 7.6 Hz, 2H), 2.04 (dt, *J* = 14.9, 7.5 Hz, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 162.6 (C), 160.9 (C), 142.1 (C), 140.3 (C), 136.5 (C), 130.6 (CH), 129.5 (CH), 128.8 (CH), 127.6 (CH), 119.1 (C), 114.5 (CH), 113.4 (C), 106.0 (CH), 55.3 (CH_3), 48.4 (CH_2), 31.2 (CH_2), 21.9 (CH_2).**LRMS** (*m/z, I*) 291 (100), 277 (30). **LRMS** (*m/z, I*) 341 (28), 313 (9), 212 (38). **HRMS** calculated for $C_{19}H_{17}NO_2$ 291.1259, found 291.1266

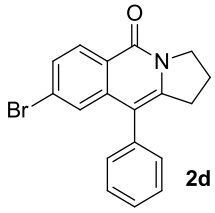
10-Phenyl-8-(trifluoromethyl)-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2c): green solid. **^{1}H**



2c

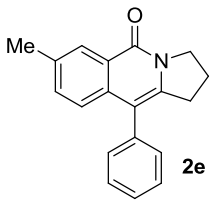
NMR (300 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.4 Hz, 1H), 7.63 – 7.31 (m, 5H), 7.31 – 7.15 (m, 2H), 4.23 (t, *J* = 7.2 Hz, 2H), 2.89 (t, *J* = 7.6 Hz, 2H), 2.25 – 2.03 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.3 (C), 143.2 (C), 138.1 (C), 135.3 (C), 133.53 (q, *J* = 32.1 Hz, C), 130.4 (CH), 129.1 (CH), 128.6 (CH), 128.1 (CH), 127.0 (C), 123.9 (q, *J* = 273.0 Hz, C), 121.6 (q, *J* = 3.4 Hz, CH), 113.6 (C), 48.8 (CH_2) , 31.3 (CH_2), 21.8 (CH_2). **LRMS** (*m/z, I*) 329 ([M] 100), 328 (38) **HRMS** calculated for $C_{19}H_{14}NOF_3$ 329.1027, found 329.1019.

8-Bromo-10-phenyl-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2d): green solid **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.6 Hz, 1H), 7.32 (ddd, *J* = 46.4, 25.7, 6.7 Hz, 7H), 4.16 (t, *J* = 7.2 Hz, 2H), 2.84 (t, *J* = 7.6 Hz, 2H), 2.29 – 1.92 (m, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.6 (C), 143.0 (C), 139.7 (C), 135.6 (C), 130.5 (CH), 129.3 (CH), 129.0 (CH), 128.9 (CH), 127.9 (CH), 127.4 (C), 126.8 (CH), 123.7 (C), 112.8 (C), 48.7 (CH_2), 31.3 (CH_2), 21.8 (CH_2).**LRMS** (*m/z, I*) 341 (28), 313 (9), 212 (38) **HRMS** calculated for $C_{18}H_{14}NOBr$ 339.0259, found 339.0259.



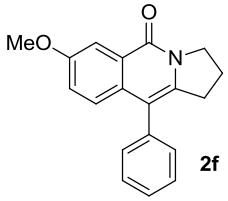
2d

7-methyl-10-phenyl-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2e): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.53 – 7.22 (m, 6H), 7.18 (d, *J* = 8.3 Hz, 1H), 4.30 – 4.22 (m, 2H), 2.92 (t, *J* = 7.6 Hz, 2H), 2.46 (s, 3H), 2.20 – 2.07 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.1 (C), 140.4 (C), 136.6 (C), 135.9 (C), 135.7 (C), 133.5 (CH), 130.7 (CH), 128.8 (CH), 127.5 (CH), 127.1 (CH), 125.0 (C), 124.3 (CH), 113.7 (CH), 48.6 (CH_2), 31.03 (CH_2), 22.1 (CH_2), 21.3 (CH_3).



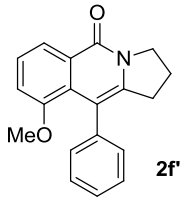
2e

7-methoxy-10-phenyl-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2f): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.88 (d, *J* = 2.7 Hz, 1H), 7.58 – 7.33 (m, 3H), 7.33 – 7.10 (m, 4H), 4.32 – 4.23 (m, 2H), 3.93 (s, 3H), 2.92 (t, *J* = 7.6 Hz, 2H), 2.21 – 2.09 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.7 (C), 157.9 (C), 138.8 (C), 136.4 (C), 132.2 (C), 130.5 (CH), 128.6 (CH), 127.4 (C), 126.1 (C), 125.9 (CH), 122.3 (CH), 113.7 (C), 107.1 (CH), 55.6 (CH_3), 48.6 (CH_2), 30.7 (CH_2), 22.0 (CH_2).



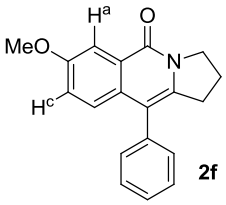
2f

9-methoxy-10-phenyl-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2f'): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.47 – 7.12 (m, 6H), 6.97 (dd, *J* = 7.8, 0.7 Hz, 1H), 4.37 – 4.11 (m, 2H), 3.35 (s, 3H), 2.79 (t, *J* = 7.7 Hz, 2H), 2.22 – 1.98 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.8 (C), 155.9 (C), 141.9 (C), 141.0 (C), 129.5 (CH), 128.5 (C), 127.5 (CH), 126.9 (C), 126.3 (CH), 126.2 (CH), 120.0 (CH), 114.1 (CH), 112.1 (C), 55.9 (CH_3), 48.9 (CH_2), 31.6 (CH_2), 21.7 (CH_2).

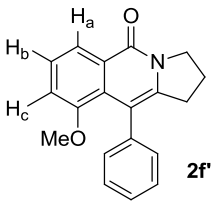


2f'

Assignment of regioisomers by 1H-NMR



2f

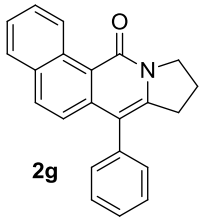


2f'

The two regioisomers were assigned based on the coupling constants. As expected, in the ^{1}H-NMR spectrum of **1f**, H_a appears as a doublet (d) with a small J_{ac} = 2.7 Hz characteristic of this long distant

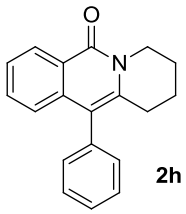
couplings. Meanwhile, in the ^{1}H-NMR spectrum of **2f',** H_a is a double of doublets (dd) with a J_{ab} = 8.1 Hz and a small J_{ac} = 1 Hz, which are also characteristic of these couplings.

7-Phenyl-9,10-dihydrobenzo[h]pyrrolo[1,2-b]isoquinolin-12(8H)-one (2g): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 10.25 (d, *J* = 8.7 Hz, 1H), 8.02 – 6.98 (m, 10H), 4.44 – 4.13 (m, 2H), 2.84 (td, *J* = 7.7, 2.5 Hz, 2H), 2.25 – 1.88 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.6 (C), 143.2 (C), 139.5 (C), 136.8 (C), 133.1 (CH), 132.3 (C), 131.7 (C), 130.9 (CH), 128.8 (CH), 128.2 (CH), 128.0 (CH), 127.6 (CH), 127.4 (CH), 126.0 (CH), 122.8 (CH), 117.9 (C), 114.2 (C), 49.5 (CH_2), 31.6 (CH_2), 21.4 (CH_2). **LRMS** (*m/z, I*) 313(57), 312 (89), 285 (40) **HRMS** calculated for $C_{22}H_{17}NO$311.1309, found 311.1310



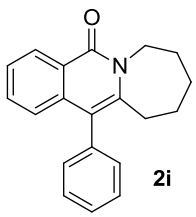
2g

11-Phenyl-3,4-dihydro-1H-pyrido[1,2-b]isoquinolin-6(2H)-one (2h): orange solid **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.78 – 6.78 (m, 8H), 4.40 – 4.04 (m, 2H), 2.73 – 2.38 (m, 2H), 2.11 – 1.84 (m, 2H), 1.84 – 1.59 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 162.5 (C), 138.4 (C), 137.3 (C), 136.9 (C), 131.9 (CH), 131.1 (CH), 128.9 (CH), 127.8 (CH), 127.6 (CH), 125.7 (CH), 124.7 (CH), 124.0 (C), 116.3 (C), 41.2 (CH_2), 26.8 (CH_2), 22.0 (CH_2), 19.1 (CH_2).**LRMS (EI)** m/z 275 (100), 260 (13) 246 (8) **LRMS** (*m/z, I*) 341 (28), 313 (9), 212 (38). **HRMS** calculated for $C_{19}H_{17}NO$275.1310, found 275.1312.



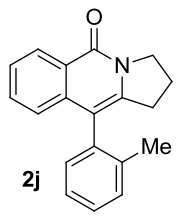
2h

12-Phenyl-8,9,10,11-tetrahydroazepino[1,2-b]isoquinolin-5(7H)-one (2i): white solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.60 – 8.25 (m, 1H), 7.58 – 7.02 (m, 7H), 7.02 – 6.77 (m, 1H), 4.62 – 4.25 (m, 2H), 2.77 – 2.44 (m, 2H), 1.66 (ddd, *J* = 17.1, 15.4, 11.8 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 162.5 (C), 142.9(C), 137.8 (C), 137.6 (C), 132.0 (CH), 131.1 (CH), 128.9 (CH), 128.1 (CH), 127.5 (CH), 125.9 (CH), 125.2 (CH), 124.3 (C), 116.8 (C), 43.8 (CH_2), 30.9 (CH_2), 29.3 (CH_2), 28.6 (CH_2), 27.8 (CH_2). **LRMS** (*m/z, I*) 289 (100), 274 (9), 260 (25), 234 (26) **LRMS** (*m/z, I*) 341 (28), 313 (9), 212 (38). **HRMS** calculated for $C_{20}H_{19}NO$289.1467, found 289.1466.



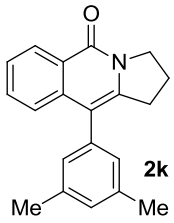
2i

10-(*o*-Tolyl)-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2j): pale yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.54 – 8.38 (m, 1H), 7.71 – 7.20 (m, 5H), 7.16 (d, *J* = 7.0 Hz, 1H), 6.99 (dd, *J* = 8.1, 0.9 Hz, 1H), 4.38 – 4.17 (m, 2H), 2.98 – 2.60 (m, 2H), 2.28 – 2.06 (m, 2H), 2.04 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.4 (C), 141.2 (C), 138.1 (C), 137.8 (C), 135.6 (C), 132.1 (CH), 131.0 (CH), 130.4 (CH), 128.2 (CH), 127.6 (CH), 126.4 (CH), 125.7 (CH), 125.0 (C), 124.2 (CH), 113.0 (C), 48.6 (CH_2), 30.8 (CH_2), 21.9 (CH_2), 19.8 (CH_3). **LRMS** (*m/z, I*) 275 (100), 260 (3), 246 (7). **HRMS** calculated for $C_{19}H_{17}NO$275.1310, found 275.1316.

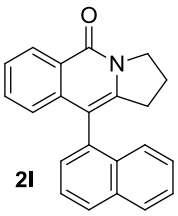


2j

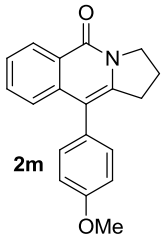
10-(3,5-Dimethylphenyl)-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2k): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.0 Hz, 1H), 7.72 – 7.11 (m, 3H), 6.93 (d, *J* = 21.7 Hz, 1H), 6.84 (s, 2H), 4.35 – 4.08 (m, 2H), 2.87 (t, *J* = 7.6 Hz, 2H), 2.54 – 2.17 (m, 6H), 2.07 (dt, *J* = 15.2, 7.5 Hz, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.2 (C), 141.1 (C), 138.3 (2xC), 136.2 (C), 131.9 (CH), 130.7 (C), 129.2 (CH), 128.3 (2xCH), 127.4 (CH), 125.6 (CH), 125.0 (C), 124.5 (CH), 114.1 (C), 48.6 (CH_2), 31.2 (CH_2), 22.0 (CH_2), 21.5 (CH_3).**LRMS** (*m/z, I*) 289 (100), 274 (7). **HRMS** calculated for $C_{20}H_{19}NO$289.1467, found 289.1467.



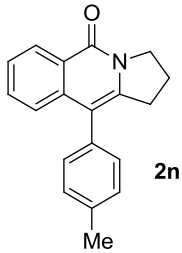
10-(Naphthalen-1-yl)-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2l): brown oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.58 – 8.47 (m, 1H), 7.95 (d, *J* = 7.8 Hz, 2H), 7.63 – 7.32 (m, 7H), 6.98 – 6.88 (m, 1H), 4.42 – 4.24 (m, 2H), 2.94 – 2.78 (m, 1H), 2.63 (ddd, *J* = 17.0, 8.2, 6.8 Hz, 1H), 2.23 – 2.03 (m, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.9 (C), 142.8 (C), 139.2 (C), 134.4 (C), 134.2 (C), 133.2 (C), 132.5 (CH), 129.2 (CH), 129.0 (CH), 128.9 (CH), 127.9 (CH), 126.9 (CH), 126.6(CH), 126.3 (CH), 126.2 (CH), 126.1 (CH), 125.3 (C), 125.1 (CH), 111.9 (C), 49.1 (CH_2), 31.3 (CH_2), 22.2 (CH_2). **LRMS** (*m/z, I*) 311 (100) 282 (5) **HRMS** calculated for $C_{22}H_{17}NO$ 311.1310, found 311.1310



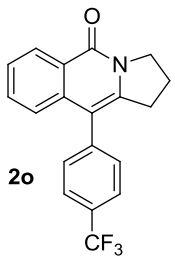
10-(4-Methoxyphenyl)-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2m): yellow oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.40 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.50 – 7.09 (m, 5H), 7.03 – 6.88 (m, 2H), 4.29 – 4.12 (m, 2H), 3.80 (s, 3H), 2.86 (t, *J* = 7.6 Hz, 2H), 2.07 (dt, *J* = 15.3, 7.6 Hz, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.2 (C), 159.1 (C), 141.5 (C), 138.5 (C), 131.9 (CH), 131.7 (CH), 128.5 (C), 127.5 (CH), 125.6 (CH), 125.0 (C), 124.4 (CH), 114.2 (CH), 113.42 (C), 55.4 (CH_3), 48.6 (CH_2), 31.2 (CH_2), 22.0 (CH_2). **LRMS** (*m/z, I*) 275 (100), 261 (24) **HRMS** calculated for $C_{19}H_{17}NO_2$ 291.1250, found 291.1260.



10-(*p*-Tolyl)-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2n): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.9 Hz, 1H), 7.48 – 7.27 (m, 3H), 7.21 (dd, *J* = 8.1, 4.3 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 4.19 (t, *J* = 7.2 Hz, 2H), 2.85 (t, *J* = 7.6 Hz, 2H), 2.35 (s, 3H), 2.13-1.98 (m 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.2 (C), 141.3 (C), 138.4 (C), 137.3 (C), 133.4 (C), 131.9 (CH), 130.5 (CH), 129.5 (CH), 127.5 (CH), 125.6 (CH), 125.1 (C), 124.4 (CH), 113.8 (C), 48.6 (CH_2), 31.2 (CH_2), 22.0 (CH_2), 21.4 (CH_3).**LRMS** (*m/z, I*) 275 (100), 261 (24) **HRMS** calculated for $C_{19}H_{17}NO$275.1310, found 275.1304.

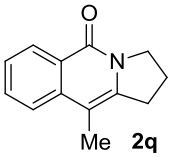


10-(4-(Trifluoromethyl)phenyl)-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2o): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.51 – 7.32 (m, 4H), 7.13 (d, *J* = 8.0 Hz, 1H), 4.24 – 4.16 (m, 2H), 2.85 (t, *J* = 7.6 Hz, 2H), 2.17 – 2.03 (m, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.1 (C), 141.8(C), 140.4 (C), 137.6 (C), 132.2 (CH), 131.2 (2xCH), 129.9 (q, *J* = 33.0 Hz) (C), 127.7 (CH), 126.0 (CH), 125.8 (q, *J* = 3.6



Hz) (2xCH), 125.1 (C), 120.7 (q, *J* = 271.7 Hz) (C), 112.4 (C), 48.7 (CH_2), 31.2 (CH_2), 22.0 (CH_2). **LRMS** (*m/z, I*) 329 (100), 328 (48), 310 (7) **HRMS** calculated for $C_{19}H_{14}NOF_3$ 329.1027, found 329.1028.

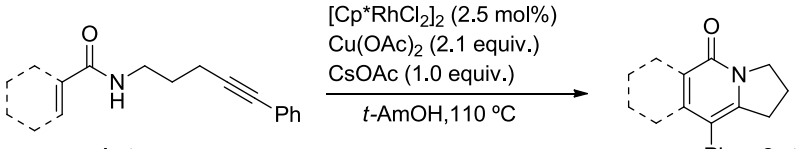
10-methyl-2,3-dihydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2q): white solid **^{1}H NMR** (300 MHz, $CDCl_3$) δ



2q

8.37 (d, *J* = 8.0 Hz, 1H), 7.57 (ddd, *J* = 12.8, 9.8, 4.7 Hz, 2H), 7.45 – 7.28 (m, 1H), 4.26 – 4.04 (m, 2H), 3.03 (t, *J* = 7.6 Hz, 2H), 2.41 – 2.02 (m, 5H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.5 (C), 140.6 (C), 138.9 (C), 132.4 (CH), 128.1 (CH), 125.9 (CH), 125.7 (C), 122.9 (CH), 106.2 (C), 48.9 (CH_2), 30.7 (CH_2), 22.1 (CH_2), 13.9 (CH_3).**LRMS** (*m/z, I*) 199 (100), 184 (8), 170 (9) **HRMS** calculated for $C_{13}H_{13}NO$199.0097, found 199.0098.

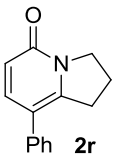
General procedure for catalytic reactions of acrylamides 1r-t.



1r-t **2r-t**

$[Cp^*RhCl_2]_2$ (3.9 mg, 2.5 mol%), $Cu(OAc)_2 \cdot H_2O$ (91 mg, 0.52 equiv.) and CsOAc (58 mg, 0.30mmol) were added to a Schlenk flask followed by the addition of *t*-AmOH (2.0 mL) and acrylamide **1r-t** (0.25 mmol). The reaction was sealed and placed in a pre-heated (110°C) block. The reaction was stirred for 14 hours, cooled to room temperature and checked by TLC. The solvent was removed and the compound purified by flash column chromatography on silica gel (hexanes:ethyl acetate; 1:1) to afford the product **2r-t**.

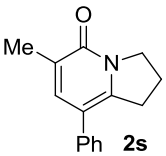
8-Phenyl-2,3-dihydroindolizin-5(1*H*)-one (1r): yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.47 – 7.08 (m,



2r

6H), 6.44 (d, *J* = 9.2 Hz, 1H), 4.25 – 4.02 (m, 2H), 3.09 (t, *J* = 7.6 Hz, 2H), 2.09 (dt, *J* = 14.8, 7.6 Hz, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.6 (C), 147.4 (C), 141.6 (CH), 137.6 (C), 128.6 (CH), 128.0 (CH), 127.0 (CH), 117.7 (CH), 116.2 (C), 49.0 (CH_2), 32.0 (CH_2), 21.6 (CH_2).**LRMS** (*m/z, I*) 210 (100), 181 (25) .**HRMS** calculated for $C_{14}H_{13}NO$ 211.0997, found 211.0997.

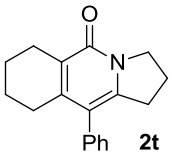
6-Methyl-8-phenyl-2,3-dihydroindolizin-5(1*H*)-one (2s): yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.38



2s

– 7.28 (m, 2H), 7.28 – 7.17 (m, 4H), 4.19 – 4.09 (m, 2H), 3.07 (t, *J* = 7.6 Hz, 2H), 2.12 (s, 3H), 2.11 – 2.05 (m, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.7 (C), 144.3 (C), 139.0 (CH), 137.9 (C), 128.5 (CH), 128.0 (CH), 126.7 (CH), 126.6 (C), 115.5 (C), 49.0 (CH_2), 31.7 (CH_2), 22.0 (CH_2), 16.4 (CH_3). **LRMS** (*m/z, I*) 212 (8), 271 (3). **HRMS** calculated for $C_{15}H_{15}NO$ 225.1154, found 225.1149.

10-Phenyl-2,3,6,7,8,9-hexahydropyrrolo[1,2-b]isoquinolin-5(1H)-one (2t): yellow liquid. **^{1}H NMR** (300

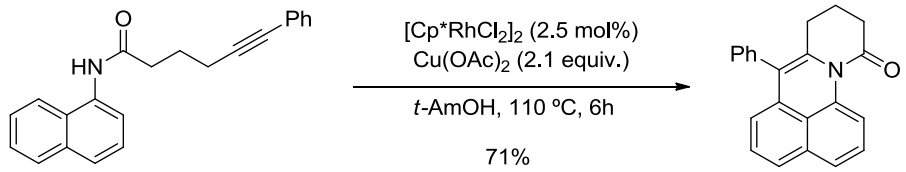


2t

MHz, $CDCl_3$) δ 7.48 – 7.29 (m, 3H), 7.22 – 7.11 (m, 2H), 4.19 (t, *J* = 7.2 Hz, 2H), 2.78 (t, *J* = 7.7 Hz, 2H), 2.69 – 2.56 (m, 2H), 2.22 (t, *J* = 6.1 Hz, 2H), 2.17 – 2.01 (m, 2H), 1.82 – 1.66 (m, 2H), 1.66 – 1.53 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 161.2 (C), 146.7 (C),

143.1 (C), 137.0 (C), 130.0 (CH), 128.4 (CH), 127.2 (CH), 124.4 (C), 117.0 (C), 48.9 (CH_2), 31.1 (CH_2), 28.3 (CH_2), 23.8 (CH_2), 22.3 (CH_2), 22.0 (CH_2), 21.4 (CH_2). **LRMS** (*m/z, I*) 250 (21), 236 (5). **HRMS** calculated for $C_{18}H_{19}NO$ 265.1467, found 265.1461.

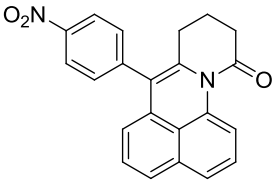
General procedure for annulation of hexynamides 5 and 6. (Exemplified for the synthesis of 7-phenyl-9,10-dihydrobenzo[de]pyrido[1,2-a]quinolin-11(8H)-one(7).)



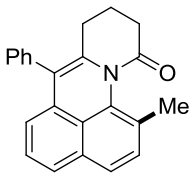
6 **7**

In a Schlenk flask, under argon atmosphere, $[Cp^*RhCl_2]_2$ (2.5 mg, 2.5 mol%), and $Cu(OAc)_2 \cdot H_2O$ (64 mg, 2.1 equiv.) were added with stirring followed by the addition of *t*-AmOH (1.12 mL) and hexynamide **6** (0.15 mmol, 47 mg) .The reaction was sealed and placed in a pre-heated (110°C) block. The reaction was stirred for 6 hours and then cooled to room temperature and checked by TLC. The solvent was removed and the remaining residue was purified by flash column chromatography on silica gel (hexanes:ethyl acetate; 3:1) to afford the product **7** (33 mg, 71%). Yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.4 Hz, 1H), 7.37 (ddd, *J* = 14.9, 11.3, 4.7 Hz, 6H), 7.16 (dd, *J* = 6.5, 5.1 Hz, 2H), 7.09 – 6.99 (m, 1H), 6.25 (d, *J* = 7.2 Hz, 1H), 2.71 (t, *J* = 6.6 Hz, 2H), 2.44 – 2.36 (m, 2H), 1.82 – 1.72 (m, 2H).**^{13}C NMR** (75 MHz, $CDCl_3$) δ 170.2 (C), 137.3 (C), 134.9 (C), 134.2 (C), 133.8 (C), 131.5 (C), 130.2 (CH), 129.2 (CH), 127.5 (CH), 126.3 (CH), 126.2 (CH), 124.3 (CH), 122.8 (CH), 122.2 (C), 118.3 (CH), 118.0 (CH), 35.2 (CH_2), 28.2 (CH_2), 18.6 (CH_2). **LRMS** (*m/z, I*) 282 (57), 253 (69). **HRMS** calculated for $C_{27}H_{17}NO$ 311.1310, found 311.1307.

To fully confirm the regiochemistry of the cycloaddition we have compared the NMR spectra of **7** (1H, 13C, COSY, COSY, HMBC and HMQC) with those of the analogs **8** and **9**.



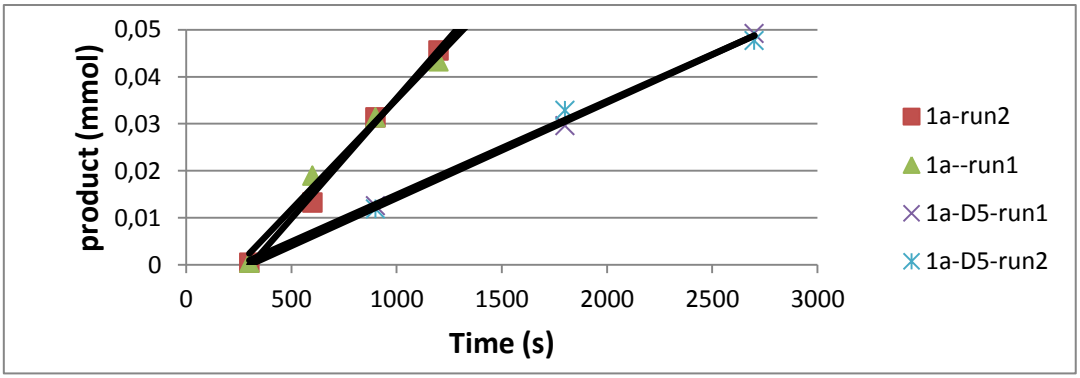
8



9

KINETIC STUDIES.

In a Schlenk flask equipped with a stir bar were added **1a** (120 mg, 0.456 mmol) or **1a-D5** (122 mg, 0,456 mmol), $[Cp^*RhCl_2]_2$ (7.0 mg, 0.011 mmol), and $Cu(OAc)_2$ (91 mg, 0.52 mmol) without any particular precautions to extrude oxygen or moisture. *t*-AmOH (2.0 mL) was then added and the flask sealed and placed in a pre-heated (110 °C) block. Both reactions were set at the same time in the same heater. Aliquots (0.1 mL) were taken every 5 min for **1a** and every 15 min for **1a-D5.** The aliquots were diluted in 1 mL of CH_2Cl_2 and immediately filtered through a florisil pad. Volatiles were removed and ^{1}H NMR of the crude residues were taken. The yield was found by integrating the methylene peaks of the benzamide and the isoquinolone.



DATA FOR 1a

Time	Run 1	Run 2
300	0,0004	0,0004
600	0,013	0,019
900	0,031	0,031
1200	0,046	0,043

Slope = 4.96 x 10^{-5} M·s^{-1}

DATA for 1a-D5

Time	Run 1	Run 2
900	0,012	0,012
1800	0,030	0,033
2700	0,049	0,048

Slope = 2.00 x 10^{-5} M·s^{-1}

KIE = 2.48

3. DFT calculations

Methods:

Gas-phase calculations were performed with Gaussian03[2] and Gaussian 09[3] at DFT level. The geometries of all complexes here reported were optimized using the B3LYP hybrid functional. Optimizations were carried out using the standard 6-31G(d) basis set for C, H, O, and N. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt, and employs a split valence (double-zeta) basis set, was used for Rh. Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). The starting approximate geometries for the transition states (TS) were located graphically. Intrinsic reaction coordinate (IRC) studies were performed to confirm that all transition state structures connect the proposed reactants and products. Single-point PCM calculations (methanol) were performed with Gaussian 09 using the 6-311+G- (2df,2p) basis set for C, H, O, and N, and SDD for Rh. Electronic energy values calculated with the smaller basis set have been corrected using the residual energy at the zero point vibrational energy (ZPE). The evaluation of enthalpy (H) and Gibbs free energy (G) implies the use of the harmonic oscillator / rigid rotor approximation, which introduces some uncertainty in the calculation of the vibrational entropy. Unless otherwise stated, the energy values included in the main text refer to the single point calculations in methanol performed with the higher quality base on previously optimized structures.

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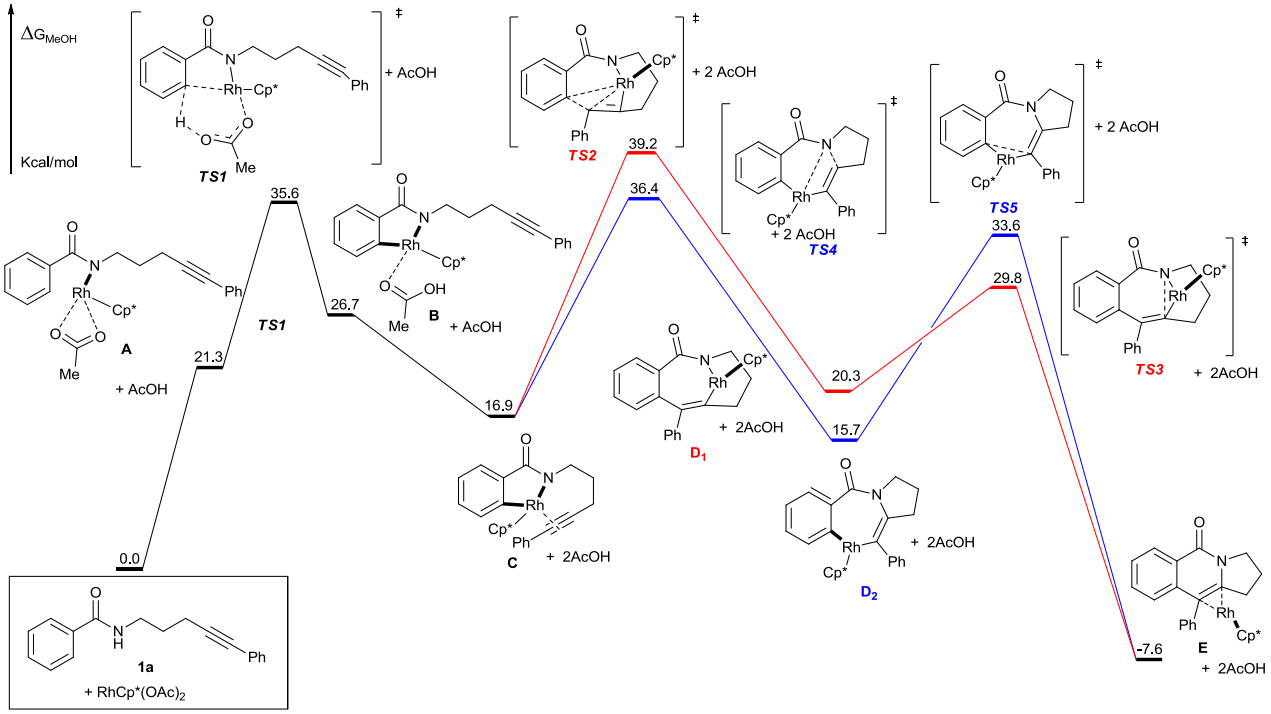
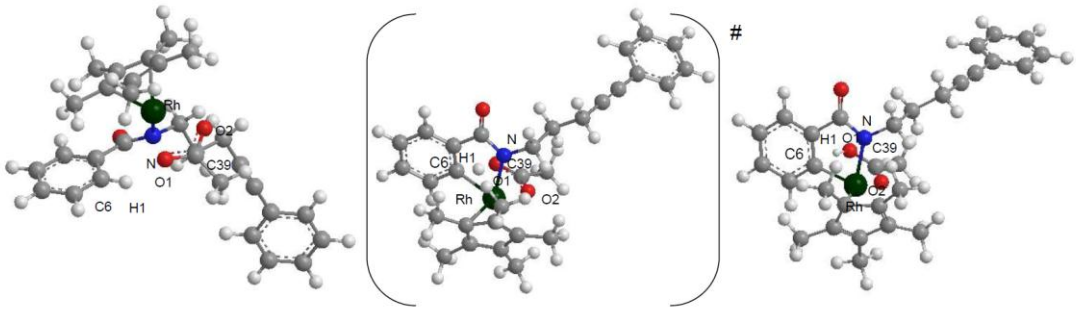
[2] Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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

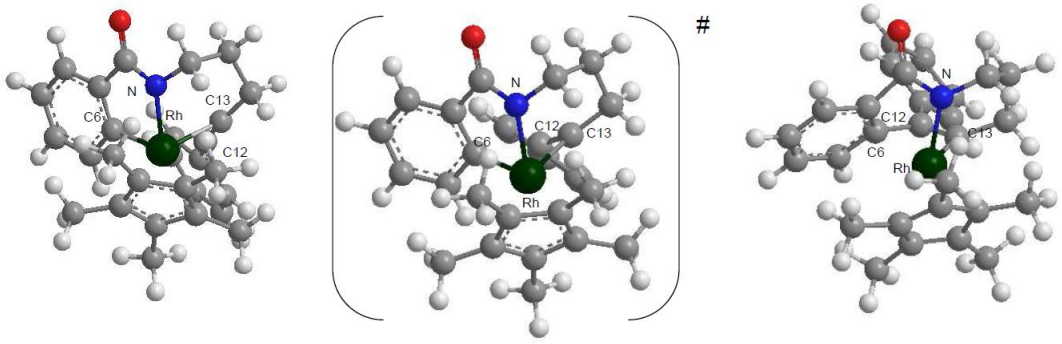
MECHANISTIC PATHWAYS INVESTIGATED BY DFT CALCULATIONS OF THE INTRAMOLECULAR REACTION FOR STANDARD SUBSTRATE 1a.





A	TS1	B
Rh-C6: 3.511	Rh-C6: 2.219	Rh-C6: 2.055
Rh-N: 2.108	Rh-N: 2.069	Rh-N: 2.074
Rh-O1: 2.239	Rh-O1: 3.163	Rh-O1: 3.530
Rh-O2: 2.181	Rh-O2: 2.153	Rh-O2: 2.289
C6-H1: 1.083	C6-H1: 1.334	C6-H1: 2.059
O1-H1: 2.224	O1-H1: 1.312	O1-H1: 0.991
C39-O1:1.269	C39-O1:1.268	C39-O1:1.320
C39-O2: 1.276	C39-O2: 1.269	C39-O2: 1.234

Figure S1: Intermediates involved in the C-H bond cleavage via a concerted metallation-deprotonation transition state. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.



C

Rh-C6: 2.051
Rh-N: 2.085
Rh-C12: 2.309
Rh-C13: 2.191
C12-C13: 1.248
N-C13: 2.731

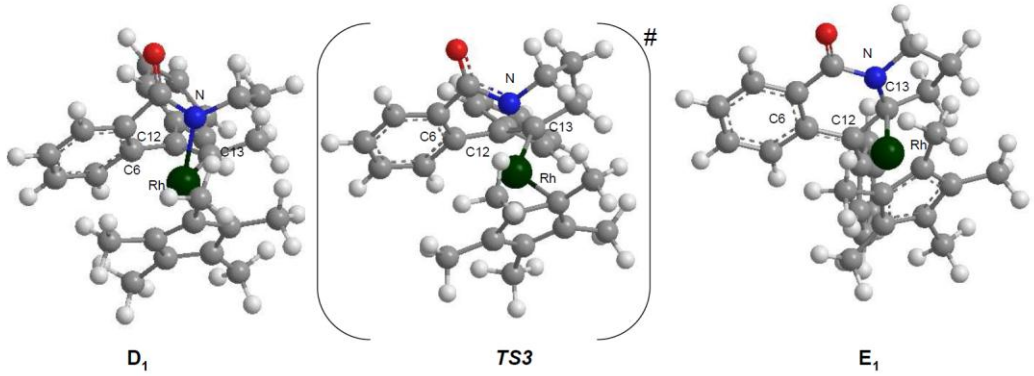
TS2

Rh-C6: 2.141
Rh-N: 2.101
Rh-C12: 2.305
Rh-C13: 2.038
C12-C13: 1.294
N-C13: 2.498
C6-C12: 1.952

D_1

Rh-C6: 2.530
Rh-N: 2.058
Rh-C12: 2.727
Rh-C13: 2.021
C12-C13: 1.348
N-C13: 2.525

Figure S2: Intermediates involved in the carbometallation step. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.[4]



D_1

Rh-C6: 2.530
Rh-N: 2.058
Rh-C12: 2.727
Rh-C13: 2.021
C12-C13: 1.348
N-C13: 2.524

TS3

Rh-C6: 2.721
Rh-N: 2.121
Rh-C12: 2.613
Rh-C13: 1.987
C12-C13: 1.377
N-C13: 2.009

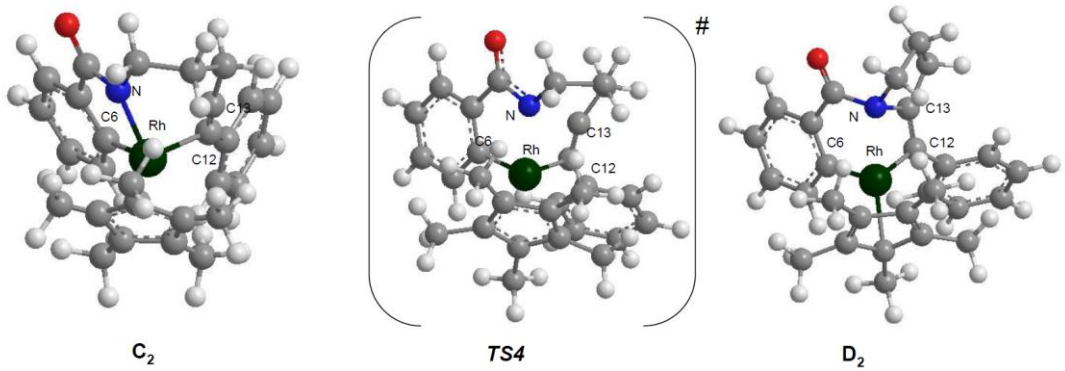
E_1

Rh-C6: 3.033
Rh-N: 2.365
Rh-C12: 2.260
Rh-C13: 2.042
C12-C13: 1.432
N-C13: 1.443

Figure S3: Intermediates involved in the reductive elimination after the carbometallation step. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å. [5]

[4] Two different conformations were found for intermediate **C**: one of them (with a lower energy), showing a "pseudo-chair" conformation, evolving through ***TS2***, and another one with a "pseudo-boat" conformation, reacting through ***TS4***. All intends to find a transition state analogous to ***TS4*** starting with a "pseudo-chair" conformation failed, however, if it would exist, the conclusions presented in this paper would be even more enforced.

[5] Intermediate **E_1** was the one obtained by IRC calculations, and has lower energy than **E,** (figure S5) which is the only one showed in the main text.



C_2

Rh-C6: 2.042
Rh-N: 2.064
Rh-C12: 2.190
Rh-C13: 2.245
C12-C13: 1.242
N-C13: 2.678

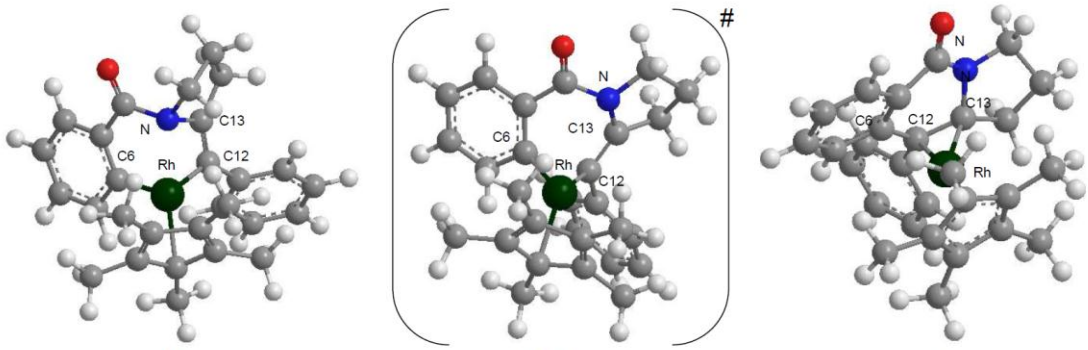
TS4

Rh-C6: 2.035
Rh-N: 2.148
Rh-C12: 2.159
Rh-C13: 2.512
C12-C13: 1.269
N-C13: 2.127

D_2

Rh-C6: 2.024
Rh-N: 2.267
Rh-C12: 2.061
Rh-C13: 2.618
C12-C13: 1.331
N-C13: 1.497

Figure S4: Intermediates involved in the N-metallation step. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.[5]



D_2

Rh-C6: 2.024
Rh-N: 2.267
Rh-C12: 2.061
Rh-C13: 2.618
C12-C13: 1.331
N-C13: 1.497

TS5

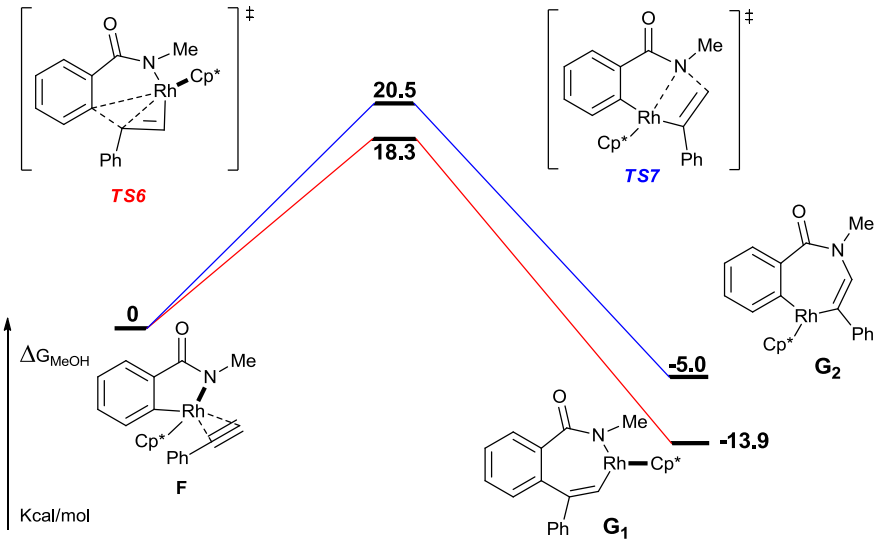
Rh-C6: 2.027
Rh-N: 3.120
Rh-C12: 2.112
Rh-C13: 2.916
C12-C13: 1.360
N-C13: 1.408
C6-C12: 1.981

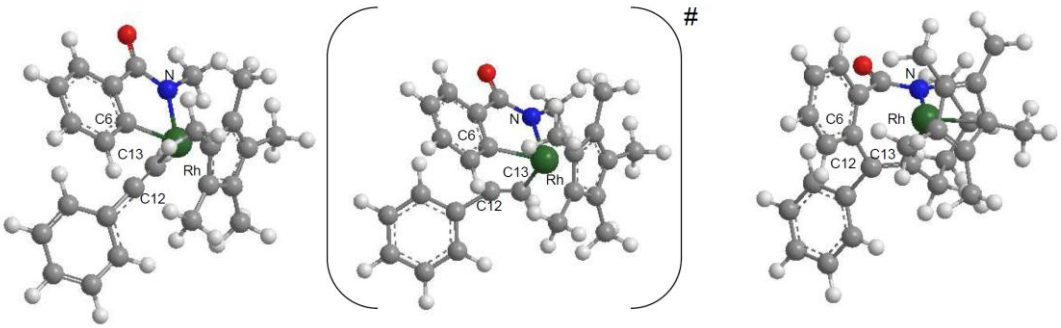
E

Rh-C6: 2.245
Rh-N: 2.948
Rh-C12: 2.136
Rh-C13: 2.152
C12-C13: 1.450
N-C13: 1.443
C6-C12: 1.455

Figure S5: Intermediates involved in the reductive elimination after the N-metallation step. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.[6]

ENERGY PROFILESS FOR THE MIGRATORY INSERTION STEP OF THE INTERMOLECULAR REACTION.





F

Rh-C6: 2.048
Rh-N: 2.088
Rh-C12: 2.404
Rh-C13: 2.154
C12-C13: 1.244
N-C13: 2.730

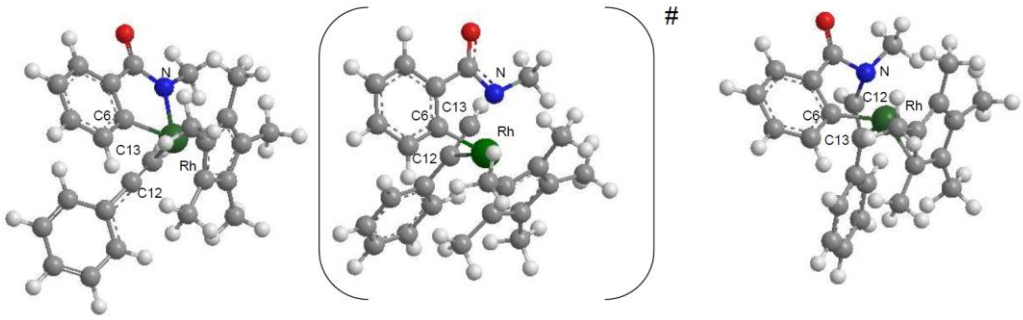
TS6

Rh-C6: 2.146
Rh-N: 2.091
Rh-C12: 2.392
Rh-C13: 2.036
C12-C13: 1.280
N-C13: 2.700
C6-C12: 2.083

G_1

Rh-C6: 2.713
Rh-N: 2.063
Rh-C12: 2.794
Rh-C13: 2.008
C12-C13: 1.342
N-C13: 2.720

Figure S6: Intermediates involved in the carbometallation step for the intermolecular version. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.



F

Rh-C6: 2.048
Rh-N: 2.088
Rh-C12: 2.404
Rh-C13: 2.154
C12-C13: 1.244
N-C13: 2.730

TS7

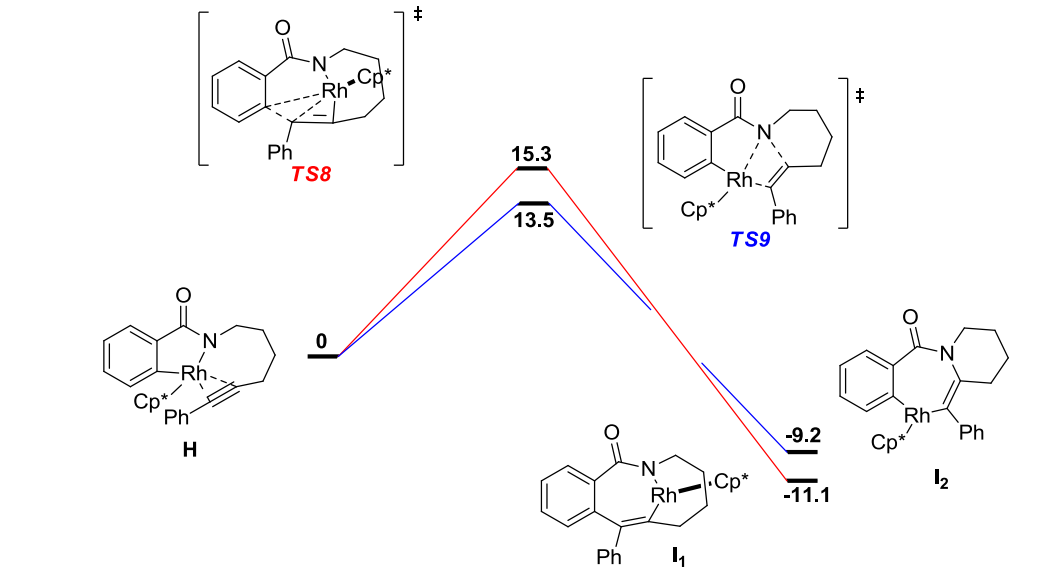
Rh-C6: 2.043
Rh-N: 2.142
Rh-C12: 2.176
Rh-C13: 2.391
C12-C13: 1.263
N-C13: 2.089

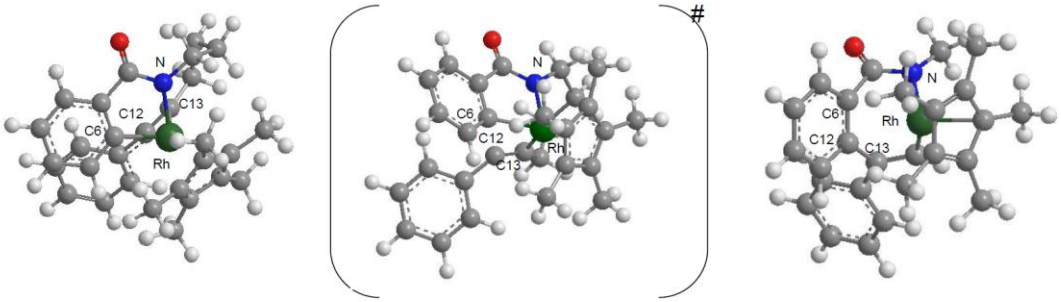
G_2

Rh-C6: 2.031
Rh-N: 2.247
Rh-C12: 2.098
Rh-C13: 2.609
C12-C13: 1.334
N-C13: 1.479

Figure S7: Intermediates involved in the N-metallation step for the intermolecular version. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.

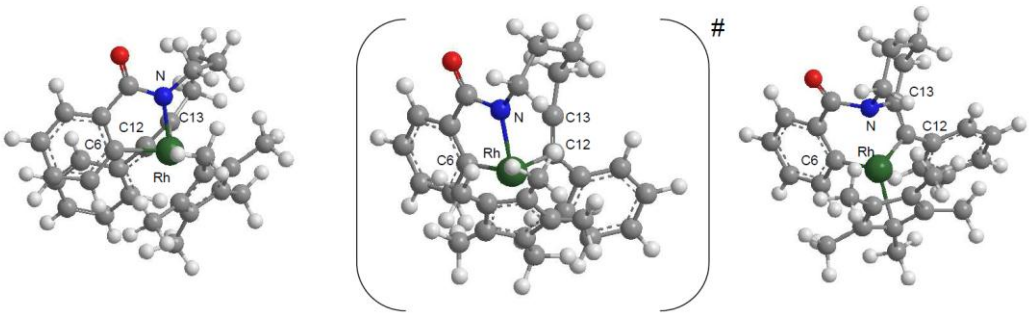
ENERGY PROFILES FOR THE MIGRATORY INSERTION STEP OF THE SUBSTRATE WITH AN ELONGATED CONNECTING CHAIN.





H	TS8	I_1
Rh-C6: 2.053	Rh-C6: 2.136	Rh-C6: 2.595
Rh-N: 2.097	Rh-N: 2.102	Rh-N: 2.070
Rh-C12: 2.303	Rh-C12: 2.308	Rh-C12: 2.743
Rh-C13: 2.206	Rh-C13: 2.056	Rh-C13: 2.031
C12-C13: 1.250	C12-C13: 1.287	C12-C13: 1.346
N-C13: 2.824	N-C13: 2.607	N-C13: 2.617
	C6-C12: 2.008	

Figure S8: Intermediates involved in the carbometallation step for the substrate with an elongated chain. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.



H

Rh-C6: 2.053
Rh-N: 2.097
Rh-C12: 2.303
Rh-C13: 2.206
C12-C13: 1.250
N-C13: 2.824

TS9

Rh-C6: 2.024
Rh-N: 2.109
Rh-C12: 2.119
Rh-C13: 2.685
C12-C13: 1.254
N-C13: 2.386

I_2

Rh-C6: 2.029
Rh-N: 2.264
Rh-C12: 2.048
Rh-C13: 2.631
C12-C13: 1.335
N-C13: 1.496

Figure S9: Intermediates involved in the N-metallation step for the substrate with an elongated chain. Geometries obtained with B3LYP/6-31G(d) and LANL2DZ for Rh. Distances are given in Å.

Atomic Cartesian coordinates and computed energies (atomic units) for the stationary points calculated with basis set [B3LYP/6-31G(d) (C, H, O, N) LANL2DZ (Rh)

1a

Zero-point correction= 0.305399
(Hartree/Particle)
Thermal correction to Energy= 0.323629
Thermal correction to Enthalpy= 0.324574
Thermal correction to Gibbs Free Energy= 0.252629
Sum of electronic and zero-point Energies= -825.773279
Sum of electronic and thermal Energies= -825.755049
Sum of electronic and thermal Enthalpies= -825.754104
Sum of electronic and thermal Free Energies= -825.826049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.444107	-1.392368	-0.312168
2	6	0	-1.237033	-2.127416	0.040854
3	6	0	-3.094706	-0.613775	0.612733
4	6	0	-4.273085	0.172581	0.107850
5	6	0	-4.984456	-0.157260	-1.054988
6	6	0	-4.680287	1.277550	0.867766
7	6	0	-6.071626	0.617970	-1.460341
8	6	0	-5.761059	2.055589	0.458824
9	6	0	-6.457409	1.729419	-0.708249
10	8	0	-2.741425	-0.565953	1.788497
11	6	0	0.042727	-1.285177	-0.062341
12	6	0	1.294157	-2.096823	0.336056
13	6	0	2.534181	-1.331437	0.213376
14	6	0	3.548493	-0.675542	0.102565
15	6	0	4.747679	0.093029	-0.024626
16	6	0	5.902496	-0.468800	-0.603629
17	6	0	7.068021	0.284101	-0.726734
18	6	0	7.104165	1.606592	-0.277287
19	6	0	5.964469	2.173536	0.298844
20	6	0	4.795485	1.426790	0.426403
21	1	0	-2.613271	-1.208752	-1.290916
22	1	0	-1.369675	-2.478101	1.067754
23	1	0	-1.171200	-3.007675	-0.610796
24	1	0	-4.719643	-1.040716	-1.630113
25	1	0	-4.134346	1.504597	1.777526
26	1	0	-6.622002	0.348346	-2.357660
27	1	0	-6.063649	2.915072	1.050862
28	1	0	-7.302862	2.333807	-1.025943
29	1	0	-0.053086	-0.413459	0.593110
30	1	0	0.164232	-0.910845	-1.086779
31	1	0	1.359724	-3.000895	-0.287251
32	1	0	1.179591	-2.450379	1.371132
33	1	0	5.871852	-1.496634	-0.952216
34	1	0	7.951548	-0.162997	-1.174684
35	1	0	8.014653	2.191525	-0.375298
36	1	0	5.986201	3.201440	0.651048

37	1	0	3.908815	1.864306	0.874954

$RhCp^*(OAc)_2$

Zero-point correction= 0.327269
(Hartree/Particle)
Thermal correction to Energy= 0.351481
Thermal correction to Enthalpy= 0.352425
Thermal correction to Gibbs Free Energy= 0.273184
Sum of electronic and zero-point Energies= -956.300144
Sum of electronic and thermal Energies= -956.275931
Sum of electronic and thermal Enthalpies= -956.274987
Sum of electronic and thermal Free Energies= -956.354229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	1.251742	-1.149599	1.088793
3	6	0	0.836594	-1.851442	2.344732
4	6	0	1.155407	-1.681973	-0.242964
5	6	0	0.607803	-3.028057	-0.603774
6	6	0	1.675575	-0.699200	-1.153448
7	6	0	1.797894	-0.830334	-2.641290
8	6	0	2.190771	0.416922	-0.364405
9	6	0	2.849282	1.633225	-0.942241
10	6	0	1.929160	0.140619	1.006467
11	6	0	2.256303	1.004326	2.186865
12	8	0	-1.868965	-0.417690	-0.669726
13	6	0	-2.489647	-1.362380	-0.018612
14	8	0	-2.031410	-2.047908	0.898510
15	6	0	-3.927928	-1.552147	-0.498049
16	1	0	-0.158879	-2.283184	2.215991
17	1	0	0.802771	-1.160326	3.191291
18	1	0	1.549158	-2.650800	2.591527
19	1	0	-0.252177	-3.273242	0.021783
20	1	0	1.385172	-3.791588	-0.462096
21	1	0	0.291048	-3.064219	-1.649444
22	1	0	1.687436	0.139309	-3.135442
23	1	0	1.035701	-1.500145	-3.047161
24	1	0	2.782638	-1.235014	-2.913686
25	1	0	2.267872	2.035015	-1.777675
26	1	0	3.851865	1.385982	-1.315354
27	1	0	2.952830	2.427055	-0.198744
28	1	0	3.088599	0.571453	2.757000
29	1	0	1.397341	1.090730	2.859044
30	1	0	2.545019	2.013320	1.882946
31	1	0	-4.548052	-0.739896	-0.100917
32	1	0	-3.986449	-1.505991	-1.589466
33	1	0	-4.319876	-2.505019	-0.135679
34	6	0	-1.274763	2.405363	0.066718
35	8	0	-0.678756	2.092090	-1.012778
36	8	0	-1.117004	1.669903	1.094411
37	6	0	-2.187996	3.602994	0.118992
38	1	0	-3.201288	3.283292	-0.151144
39	1	0	-2.217896	4.018131	1.129325
40	1	0	-1.865783	4.361651	-0.598367

AcOH

Zero-point correction= 0.062022
(Hartree/Particle)
Thermal correction to Energy= 0.066602
Thermal correction to Enthalpy= 0.067546
Thermal correction to Gibbs Free Energy= 0.034684
Sum of electronic and zero-point Energies= -229.015588
Sum of electronic and thermal Energies= -229.011008
Sum of electronic and thermal Enthalpies= -229.010063
Sum of electronic and thermal Free Energies= -229.042925

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.645495	1.202079	0.000002
2	8	0	0.778870	-1.046544	-0.000004
3	6	0	0.092467	0.125600	-0.000008
4	6	0	-1.397568	-0.110018	0.000000
5	1	0	-1.685280	-0.691964	-0.881887
6	1	0	-1.685359	-0.691357	0.882263
7	1	0	-1.917537	0.848189	-0.000348
8	1	0	1.723861	-0.802641	0.000034

A

Zero-point correction= 0.570386
(Hartree/Particle)
Thermal correction to Energy= 0.608136
Thermal correction to Enthalpy= 0.609080
Thermal correction to Gibbs Free Energy= 0.496621
Sum of electronic and zero-point Energies= -1553.031955
Sum of electronic and thermal Energies= -1552.994205
Sum of electronic and thermal Enthalpies= -1552.993261
Sum of electronic and thermal Free Energies= -1553.105719

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.962382	-0.775810	0.176124
2	7	0	0.270829	0.372899	-0.335589
3	6	0	-0.744023	-0.421177	-1.045293
4	6	0	0.379400	1.654103	-0.802657
5	6	0	1.264199	2.627699	-0.060246
6	6	0	1.547678	2.521952	1.308573
7	6	0	1.737335	3.744660	-0.767720
8	6	0	2.313989	3.501360	1.946555
9	6	0	2.516352	4.712106	-0.134047
10	6	0	2.808454	4.592123	1.228475
11	8	0	-0.259275	2.075622	-1.782953
12	6	0	-2.174136	-0.070278	-0.604839
13	6	0	-3.216567	-0.905986	-1.379886
14	6	0	-4.595572	-0.648346	-0.966415
15	6	0	-5.734431	-0.422655	-0.613781
16	6	0	-9.248562	-0.953072	0.556885
17	6	0	-9.728009	0.358979	0.589001
18	6	0	-8.885345	1.412120	0.223953

19	6	0	-7.573526	1.159584	-0.170919
20	6	0	-7.079127	-0.159455	-0.207144
21	6	0	-7.937830	-1.213396	0.163590
22	1	0	-0.660447	-0.267873	-2.131839
23	1	0	-0.567370	-1.477082	-0.827070
24	1	0	1.164863	1.679472	1.871895
25	1	0	1.462496	3.843675	-1.813204
26	1	0	2.516408	3.413907	3.011362
27	1	0	2.882041	5.567684	-0.696654
28	1	0	3.404529	5.351807	1.728206
29	1	0	-2.358595	0.993485	-0.775996
30	1	0	-2.278681	-0.260193	0.469718
31	1	0	-2.994923	-1.976436	-1.253883
32	1	0	-3.115158	-0.698734	-2.455286
33	1	0	-9.898541	-1.777305	0.839181
34	1	0	-10.751024	0.559315	0.896046
35	1	0	-9.251639	2.435210	0.246456
36	1	0	-6.916864	1.976091	-0.455346
37	1	0	-7.563092	-2.232204	0.137580
38	6	0	3.973138	-0.057229	-0.425002
39	6	0	4.148234	-1.338268	0.261400
40	6	0	3.441583	-2.323857	-0.467833
41	6	0	2.798289	-1.669941	-1.608360
42	6	0	3.206214	-0.288242	-1.613058
43	6	0	4.646981	1.217669	-0.020851
44	6	0	4.938836	-1.516942	1.522416
45	6	0	3.301564	-3.780197	-0.144249
46	6	0	2.024481	-2.366203	-2.686427
47	6	0	2.895960	0.705628	-2.690660
48	1	0	5.685788	1.221885	-0.380552
49	1	0	4.670893	1.326818	1.066648
50	1	0	4.140378	2.094749	-0.427368
51	1	0	4.644998	-0.780479	2.277191
52	1	0	6.011298	-1.385648	1.327322
53	1	0	4.795582	-2.510768	1.953404
54	1	0	3.699655	-4.015711	0.845476
55	1	0	3.841940	-4.389101	-0.880697
56	1	0	2.250502	-4.085583	-0.162260
57	1	0	1.445385	-3.202896	-2.284454
58	1	0	2.703241	-2.767691	-3.451898
59	1	0	1.329417	-1.681760	-3.179614
60	1	0	3.503994	0.485071	-3.578301
61	1	0	3.120697	1.725013	-2.372283
62	1	0	1.843219	0.681853	-2.985997
63	8	0	0.543026	-2.080826	1.194528
64	8	0	1.486095	-0.469912	2.342302
65	6	0	0.640051	-1.413817	2.278504
66	6	0	-0.267009	-1.722747	3.441420
67	1	0	0.207506	-1.436712	4.383031
68	1	0	-1.190470	-1.141791	3.331386
69	1	0	-0.531400	-2.783007	3.452012

TS1

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Zero-point correction=                           0.564943
(Hartree/Particle)
 Thermal correction to Energy=                    0.602174
 Thermal correction to Enthalpy=                  0.603118
 Thermal correction to Gibbs Free Energy=         0.492197
 Sum of electronic and zero-point Energies=          -1553.007949
 Sum of electronic and thermal Energies=             -1552.970719
```

Sum of electronic and thermal Enthalpies= -1552.969774
Sum of electronic and thermal Free Energies= -1553.080695

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.814789	-0.452572	0.135743
2	7	0	0.523278	0.580796	-1.106593
3	6	0	-0.550875	-0.036867	-1.871683
4	6	0	0.757760	1.901639	-1.308472
5	6	0	1.823219	2.433425	-0.394906
6	6	0	2.175037	1.654745	0.730278
7	6	0	2.441677	3.656021	-0.655308
8	6	0	3.189119	2.143857	1.579374
9	6	0	3.451259	4.112022	0.193703
10	6	0	3.823004	3.358940	1.315461
11	8	0	0.171168	2.616791	-2.133364
12	6	0	-1.936474	0.194500	-1.247292
13	6	0	-3.068228	-0.409881	-2.107296
14	6	0	-4.386151	-0.280723	-1.485879
15	6	0	-5.462759	-0.163155	-0.938509
16	6	0	-8.775140	-1.014748	0.579712
17	6	0	-9.227445	0.246424	0.976228
18	6	0	-8.434719	1.371986	0.737264
19	6	0	-7.198941	1.241790	0.107454
20	6	0	-6.732317	-0.025098	-0.296182
21	6	0	-7.540343	-1.152965	-0.050212
22	1	0	-0.543009	0.371330	-2.892006
23	1	0	-0.362234	-1.115210	-1.937081
24	1	0	2.122850	4.225344	-1.523860
25	1	0	3.446223	1.592696	2.481503
26	1	0	3.943132	5.060614	-0.007558
27	1	0	4.591360	3.731573	1.988904
28	1	0	-2.098891	1.271139	-1.135990
29	1	0	-1.958766	-0.254372	-0.249226
30	1	0	-2.859908	-1.474130	-2.295020
31	1	0	-3.075452	0.077309	-3.093051
32	1	0	-9.386841	-1.894562	0.761954
33	1	0	-10.190944	0.351482	1.467710
34	1	0	-8.780469	2.356098	1.042722
35	1	0	-6.581153	2.114883	-0.079252
36	1	0	-7.186735	-2.132076	-0.359067
37	6	0	3.812155	-0.810965	-0.760572
38	6	0	3.883419	-1.325717	0.603345
39	6	0	2.920154	-2.355338	0.726451
40	6	0	2.264428	-2.534916	-0.565226
41	6	0	2.865344	-1.619193	-1.486062
42	6	0	4.734045	0.212458	-1.356088
43	6	0	4.875744	-0.897087	1.643516
44	6	0	2.598727	-3.158466	1.951036
45	6	0	1.249788	-3.598036	-0.865048
46	6	0	2.572278	-1.500796	-2.951244
47	1	0	5.685042	-0.249793	-1.655707
48	1	0	4.957174	1.011845	-0.644584
49	1	0	4.295127	0.675696	-2.243666
50	1	0	5.176265	0.143340	1.504603
51	1	0	5.781335	-1.516394	1.581214
52	1	0	4.475176	-0.998087	2.656475
53	1	0	3.117499	-2.774286	2.833069
54	1	0	2.896495	-4.206612	1.816213
55	1	0	1.523067	-3.138776	2.156130

56	1	0	0.532691	-3.700552	-0.044772
57	1	0	1.733912	-4.574079	-1.009510
58	1	0	0.684959	-3.372939	-1.773996
59	1	0	3.322396	-2.055704	-3.530864
60	1	0	2.595755	-0.458806	-3.280227
61	1	0	1.590286	-1.907662	-3.203447
62	8	0	0.121234	-0.918427	1.380065
63	8	0	0.180426	1.103114	2.352694
64	6	0	-0.312294	-0.056032	2.203952
65	6	0	-1.518290	-0.422968	3.043373
66	1	0	-1.457876	0.055607	4.023503
67	1	0	-2.417940	-0.050294	2.539520
68	1	0	-1.603701	-1.506553	3.146192
69	1	0	1.163048	1.241149	1.494724

B

Zero-point correction= 0.569929
(Hartree/Particle)
Thermal correction to Energy= 0.607018
Thermal correction to Enthalpy= 0.607962
Thermal correction to Gibbs Free Energy= 0.497764
Sum of electronic and zero-point Energies= -1553.022684
Sum of electronic and thermal Energies= -1552.985595
Sum of electronic and thermal Enthalpies= -1552.984651
Sum of electronic and thermal Free Energies= -1553.094848

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.917165	-0.373288	0.131874
2	7	0	0.592945	0.388867	-1.271351
3	6	0	-0.470857	-0.370987	-1.911868
4	6	0	0.758571	1.674650	-1.680417
5	6	0	1.796172	2.375174	-0.858010
6	6	0	2.406500	1.622278	0.163244
7	6	0	2.076313	3.732129	-1.033885
8	6	0	3.277084	2.285696	1.041920
9	6	0	2.972753	4.368999	-0.174995
10	6	0	3.559526	3.648167	0.869398
11	8	0	0.106177	2.236122	-2.572146
12	6	0	-1.853867	-0.077137	-1.305922
13	6	0	-2.986680	-0.824596	-2.042382
14	6	0	-4.298679	-0.618970	-1.429055
15	6	0	-5.373523	-0.431560	-0.897807
16	6	0	-8.245236	1.295376	0.766353
17	6	0	-9.135522	0.234190	0.949786
18	6	0	-8.781188	-1.047467	0.520672
19	6	0	-7.547276	-1.269807	-0.086407
20	6	0	-6.641210	-0.207467	-0.276333
21	6	0	-7.009847	1.081008	0.159216
22	1	0	-0.493927	-0.130370	-2.984064
23	1	0	-0.255861	-1.440308	-1.810754
24	1	0	1.570719	4.262041	-1.836884
25	1	0	3.741054	1.754691	1.869818
26	1	0	3.198723	5.424579	-0.302506
27	1	0	4.238598	4.146195	1.558287
28	1	0	-2.037891	1.000545	-1.355963
29	1	0	-1.854974	-0.371147	-0.249700
30	1	0	-2.762972	-1.901781	-2.068145
31	1	0	-3.014289	-0.495098	-3.090980

32	1	0	-8.514935	2.295156	1.096359
33	1	0	-10.098882	0.405052	1.422597
34	1	0	-9.469471	-1.877280	0.658297
35	1	0	-7.270545	-2.264662	-0.421964
36	1	0	-6.317682	1.904670	0.013300
37	6	0	3.519434	-1.340393	-0.944994
38	6	0	4.029353	-1.141958	0.402870
39	6	0	3.199660	-1.879456	1.280002
40	6	0	2.280963	-2.694957	0.470192
41	6	0	2.516663	-2.408718	-0.880374
42	6	0	4.158969	-0.835671	-2.206032
43	6	0	5.257637	-0.357309	0.754316
44	6	0	3.307706	-1.971928	2.773880
45	6	0	1.288485	-3.656914	1.052224
46	6	0	1.898358	-3.059830	-2.080511
47	1	0	4.925412	-1.536086	-2.567732
48	1	0	4.638422	0.133537	-2.045296
49	1	0	3.418892	-0.707830	-3.000918
50	1	0	5.332536	0.565906	0.174985
51	1	0	6.152412	-0.959803	0.544768
52	1	0	5.284439	-0.091434	1.814530
53	1	0	3.858667	-1.124636	3.191111
54	1	0	3.830115	-2.890442	3.075821
55	1	0	2.317975	-1.988532	3.241611
56	1	0	0.658333	-3.163558	1.800729
57	1	0	1.794952	-4.495858	1.548225
58	1	0	0.629797	-4.072621	0.285010
59	1	0	2.587997	-3.804510	-2.501851
60	1	0	1.684932	-2.333130	-2.869293
61	1	0	0.966166	-3.576371	-1.835929
62	8	0	0.247077	-0.258828	1.693333
63	8	0	-0.086268	1.966368	1.856059
64	6	0	-0.388351	0.708406	2.120330
65	6	0	-1.610644	0.553237	2.983925
66	1	0	0.701411	1.992301	1.255750
67	1	0	-1.625069	1.310929	3.771445
68	1	0	-2.500023	0.701226	2.359841
69	1	0	-1.641562	-0.449865	3.410622

C

Zero-point correction= 0.506868
(Hartree/Particle)
Thermal correction to Energy= 0.538133
Thermal correction to Enthalpy= 0.539077
Thermal correction to Gibbs Free Energy= 0.445450
Sum of electronic and zero-point Energies= -1323.997559
Sum of electronic and thermal Energies= -1323.966294
Sum of electronic and thermal Enthalpies= -1323.965350
Sum of electronic and thermal Free Energies= -1324.058976

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.650891	-0.202761	-0.030164
2	7	0	-1.560665	1.365937	0.999016
3	6	0	-2.375337	1.142801	2.179552
4	6	0	-1.065264	2.624987	0.813596

5	6	0	0.005224	2.640395	-0.222483
6	6	0	0.429611	1.400968	-0.714464
7	6	0	0.606605	3.830267	-0.642555
8	6	0	1.483405	1.362670	-1.632460
9	6	0	1.639691	3.789650	-1.578364
10	6	0	2.076995	2.555087	-2.068646
11	8	0	-1.432191	3.632874	1.432168
12	6	0	0.119531	-0.544372	1.992111
13	6	0	1.176928	-0.576219	1.330134
14	6	0	-1.534727	0.746208	3.402007
15	6	0	-0.752099	-0.565132	3.185641
16	6	0	2.572011	-0.727559	1.004238
17	6	0	3.136171	-2.015308	0.904322
18	6	0	4.493589	-2.174378	0.633394
19	6	0	5.310073	-1.054221	0.458835
20	6	0	4.761189	0.226432	0.561452
21	6	0	3.404063	0.395104	0.829326
22	1	0	-2.911827	2.070973	2.403322
23	1	0	-3.119107	0.361861	1.974241
24	1	0	0.249691	4.764612	-0.217237
25	1	0	1.865038	0.416121	-2.006043
26	1	0	2.110063	4.709084	-1.917743
27	1	0	2.892479	2.514036	-2.788079
28	1	0	-2.182045	0.620548	4.280518
29	1	0	-0.834969	1.560154	3.622341
30	1	0	-1.462363	-1.399568	3.097966
31	1	0	-0.123296	-0.775735	4.062001
32	1	0	2.504618	-2.884854	1.060775
33	1	0	4.915045	-3.173679	0.564476
34	1	0	6.368825	-1.179101	0.248774
35	1	0	5.392187	1.101424	0.432238
36	1	0	2.977620	1.388487	0.906237
37	6	0	-1.273922	-0.800790	-2.174383
38	6	0	-0.462725	-1.858158	-1.646864
39	6	0	-1.191429	-2.461640	-0.549341
40	6	0	-2.416284	-1.768045	-0.376902
41	6	0	-2.447583	-0.696752	-1.350943
42	6	0	-1.021025	-0.021476	-3.431231
43	6	0	0.792666	-2.414672	-2.255441
44	6	0	-0.732306	-3.671698	0.209062
45	6	0	-3.539446	-2.139686	0.548471
46	6	0	-3.595403	0.244928	-1.566395
47	1	0	-1.454677	-0.548062	-4.292948
48	1	0	0.045593	0.113062	-3.623649
49	1	0	-1.472021	0.973119	-3.387257
50	1	0	1.274508	-1.687990	-2.915033
51	1	0	0.574468	-3.307612	-2.858665
52	1	0	1.524180	-2.704063	-1.494302
53	1	0	0.327187	-3.601390	0.474843
54	1	0	-0.854710	-4.578570	-0.398966
55	1	0	-1.300769	-3.814615	1.132102
56	1	0	-3.179480	-2.650493	1.447172
57	1	0	-4.248345	-2.817095	0.051450
58	1	0	-4.106931	-1.261879	0.870808
59	1	0	-4.369674	-0.221989	-2.191191
60	1	0	-3.272747	1.163501	-2.062905
61	1	0	-4.057488	0.533055	-0.618359

TS2

Zero-point correction= 0.506154
(Hartree/Particle)
Thermal correction to Energy= 0.536416
Thermal correction to Enthalpy= 0.537361
Thermal correction to Gibbs Free Energy= 0.446224
Sum of electronic and zero-point Energies= -1323.968903
Sum of electronic and thermal Energies= -1323.938640
Sum of electronic and thermal Enthalpies= -1323.937696
Sum of electronic and thermal Free Energies= -1324.028833

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.862977	-0.124952	0.018270
2	7	0	-0.919370	1.574852	1.251649
3	6	0	-1.418490	1.477837	2.618012
4	6	0	-0.008960	2.558436	1.002855
5	6	0	0.770758	2.284386	-0.242012
6	6	0	0.851607	0.945748	-0.685967
7	6	0	1.400795	3.310103	-0.948993
8	6	0	1.522800	0.678379	-1.895175
9	6	0	2.060415	3.031565	-2.146809
10	6	0	2.105602	1.714983	-2.623838
11	8	0	0.192274	3.555546	1.710039
12	6	0	0.389231	-0.528776	1.574771
13	6	0	1.327612	-0.340733	0.703368
14	6	0	-0.416928	0.754162	3.541184
15	6	0	0.009605	-0.637195	3.001720
16	6	0	3.759421	0.021906	0.197151
17	6	0	5.055558	-0.475674	0.084091
18	6	0	5.302804	-1.843985	0.230287
19	6	0	4.245480	-2.714350	0.500951
20	6	0	2.947444	-2.218633	0.624940
21	6	0	2.687374	-0.844676	0.475257
22	1	0	-1.586629	2.488521	3.006411
23	1	0	-2.379192	0.951289	2.615024
24	1	0	1.335245	4.319446	-0.552092
25	1	0	1.620494	-0.344937	-2.248078
26	1	0	2.533689	3.831418	-2.710196
27	1	0	2.614859	1.492952	-3.558855
28	1	0	-0.841363	0.635733	4.547530
29	1	0	0.474607	1.384337	3.631928
30	1	0	-0.816766	-1.351269	3.115076
31	1	0	0.854853	-1.017949	3.592483
32	1	0	3.569654	1.084124	0.086226
33	1	0	5.876717	0.207011	-0.117071
34	1	0	6.314822	-2.228255	0.134469
35	1	0	4.429580	-3.779234	0.616255
36	1	0	2.121043	-2.890051	0.839659
37	6	0	-2.037571	-0.507339	-1.994192
38	6	0	-1.497206	-1.756082	-1.486193
39	6	0	-2.150828	-2.059443	-0.244679
40	6	0	-2.988568	-0.954796	0.083848
41	6	0	-2.924578	0.004574	-1.021256
42	6	0	-1.707393	0.094318	-3.328564
43	6	0	-0.589071	-2.681180	-2.246418
44	6	0	-1.990101	-3.322601	0.550706
45	6	0	-3.972067	-0.885145	1.216007

46	6	0	-3.738170	1.263502	-1.094876
47	1	0	-2.208946	-0.452660	-4.138849
48	1	0	-0.631551	0.070719	-3.530284
49	1	0	-2.024191	1.138938	-3.387726
50	1	0	0.068751	-2.131767	-2.926432
51	1	0	-1.169454	-3.387925	-2.856853
52	1	0	0.043234	-3.271041	-1.575606
53	1	0	-0.982107	-3.738459	0.453077
54	1	0	-2.694622	-4.094737	0.211173
55	1	0	-2.179009	-3.156061	1.615831
56	1	0	-3.620245	-1.426510	2.099680
57	1	0	-4.933887	-1.329548	0.921712
58	1	0	-4.172165	0.148126	1.513649
59	1	0	-4.797105	1.036571	-1.280621
60	1	0	-3.392601	1.919406	-1.898048
61	1	0	-3.675778	1.830573	-0.160548

D_1

Zero-point correction= 0.508498
(Hartree/Particle)
Thermal correction to Energy= 0.538850
Thermal correction to Enthalpy= 0.539794
Thermal correction to Gibbs Free Energy= 0.448500
Sum of electronic and zero-point Energies= -1324.011068
Sum of electronic and thermal Energies= -1323.980716
Sum of electronic and thermal Enthalpies= -1323.979771
Sum of electronic and thermal Free Energies= -1324.071066

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.986001	-0.183280	0.030688
2	7	0	-0.373250	-0.622464	1.945659
3	6	0	-0.110952	-1.980490	2.403752
4	6	0	0.461667	0.382665	2.298460
5	6	0	0.436887	1.476103	1.224746
6	6	0	1.088501	1.262873	-0.034833
7	6	0	-0.063545	2.760890	1.535550
8	6	0	1.204500	2.358070	-0.924653
9	6	0	0.040762	3.804860	0.630957
10	6	0	0.684000	3.601826	-0.605834
11	8	0	1.173759	0.479361	3.297219
12	6	0	0.809160	-1.071504	-0.239298
13	6	0	1.715223	-0.077822	-0.328678
14	6	0	1.068290	-2.644807	1.657062
15	6	0	1.019460	-2.514499	0.107362
16	6	0	-3.132277	0.820539	-0.537556
17	6	0	-2.340826	0.489877	-1.734652
18	6	0	-2.152247	-0.910040	-1.777791
19	6	0	-2.667584	-1.446025	-0.527829
20	6	0	-3.361494	-0.356754	0.174676
21	6	0	-3.581774	2.211823	-0.202045
22	6	0	-1.974666	1.489223	-2.792269
23	6	0	-1.562704	-1.712483	-2.901239
24	6	0	-2.856921	-2.901474	-0.212420
25	6	0	-4.106161	-0.533132	1.464899
26	6	0	3.182793	-0.184683	-0.519113
27	6	0	3.732972	-1.046873	-1.484339
28	6	0	5.114282	-1.152640	-1.646521

29	6	0	5.975615	-0.388311	-0.856287
30	6	0	5.442598	0.481890	0.098193
31	6	0	4.062325	0.585445	0.264307
32	1	0	0.119143	-1.956334	3.476014
33	1	0	-1.026575	-2.570392	2.275148
34	1	0	-0.505544	2.921012	2.515056
35	1	0	1.734323	2.209249	-1.861666
36	1	0	-0.344859	4.788295	0.886908
37	1	0	0.791517	4.429665	-1.302135
38	1	0	1.121555	-3.706590	1.934877
39	1	0	1.995487	-2.172240	2.000681
40	1	0	0.221603	-3.147426	-0.301267
41	1	0	1.968781	-2.891045	-0.294764
42	1	0	-4.288715	2.588925	-0.953563
43	1	0	-2.736000	2.909430	-0.173261
44	1	0	-4.077204	2.253422	0.771566
45	1	0	-1.544962	2.396211	-2.353800
46	1	0	-2.861107	1.791028	-3.367909
47	1	0	-1.244644	1.082288	-3.497407
48	1	0	-0.856198	-1.122587	-3.492079
49	1	0	-2.350163	-2.067428	-3.580790
50	1	0	-1.028560	-2.592212	-2.530903
51	1	0	-2.881787	-3.080348	0.867035
52	1	0	-2.059091	-3.517705	-0.636722
53	1	0	-3.808443	-3.265375	-0.627152
54	1	0	-4.956169	-1.216767	1.339274
55	1	0	-4.496884	0.417320	1.838027
56	1	0	-3.456230	-0.950106	2.243121
57	1	0	3.065457	-1.621288	-2.121152
58	1	0	5.518138	-1.824349	-2.400038
59	1	0	7.051839	-0.466641	-0.985602
60	1	0	6.104334	1.077727	0.721749
61	1	0	3.656369	1.246939	1.024810

TS3

Zero-point correction= 0.507061
(Hartree/Particle)
Thermal correction to Energy= 0.537165
Thermal correction to Enthalpy= 0.538110
Thermal correction to Gibbs Free Energy= 0.446812
Sum of electronic and zero-point Energies= -1323.991913
Sum of electronic and thermal Energies= -1323.961808
Sum of electronic and thermal Enthalpies= -1323.960864
Sum of electronic and thermal Free Energies= -1324.052162

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.973925	-0.203704	-0.014176
2	7	0	-0.415993	0.493839	1.910014
3	6	0	-0.623980	-0.277921	3.131240
4	6	0	0.122019	1.758122	1.990256
5	6	0	0.628635	2.233799	0.668381
6	6	0	1.261800	1.329489	-0.244332
7	6	0	0.528618	3.594487	0.360137
8	6	0	1.707630	1.863997	-1.476903
9	6	0	0.973516	4.090836	-0.861737
10	6	0	1.558366	3.212185	-1.782967

11	8	0	0.202711	2.426308	3.023986
12	6	0	0.705413	-0.803138	0.863366
13	6	0	1.629753	-0.067447	0.156103
14	6	0	0.544550	-1.272232	3.266732
15	6	0	0.859567	-1.892697	1.877183
16	6	0	-2.686049	0.306699	-1.661930
17	6	0	-1.881378	-0.894770	-1.961185
18	6	0	-2.153138	-1.885928	-0.977919
19	6	0	-2.911549	-1.229755	0.056934
20	6	0	-3.311339	0.107764	-0.438431
21	6	0	-2.723279	1.523654	-2.538242
22	6	0	-1.110379	-1.085665	-3.235674
23	6	0	-1.721999	-3.323445	-0.996339
24	6	0	-3.525417	-1.893312	1.254341
25	6	0	-4.214068	1.043087	0.310711
26	6	0	2.966912	-0.602253	-0.200435
27	6	0	4.114349	0.214362	-0.140673
28	6	0	5.377017	-0.300334	-0.425030
29	6	0	5.531692	-1.643636	-0.780807
30	6	0	4.405143	-2.464171	-0.856656
31	6	0	3.139055	-1.947575	-0.579883
32	1	0	-0.656621	0.409916	3.981424
33	1	0	-1.581538	-0.806368	3.071757
34	1	0	0.087307	4.248578	1.106350
35	1	0	2.199372	1.202665	-2.184400
36	1	0	0.870357	5.146473	-1.096582
37	1	0	1.911682	3.584601	-2.741593
38	1	0	0.334332	-2.051821	4.009618
39	1	0	1.428865	-0.720342	3.606615
40	1	0	0.170775	-2.720168	1.665539
41	1	0	1.879225	-2.294827	1.872549
42	1	0	-3.219661	1.307648	-3.494489
43	1	0	-1.714015	1.882900	-2.772723
44	1	0	-3.262518	2.347047	-2.062295
45	1	0	-0.574229	-0.173743	-3.516881
46	1	0	-1.782753	-1.339805	-4.067813
47	1	0	-0.374714	-1.890291	-3.146541
48	1	0	-0.784154	-3.455537	-1.544880
49	1	0	-2.477762	-3.957755	-1.481227
50	1	0	-1.571179	-3.714082	0.015254
51	1	0	-3.660724	-1.188111	2.080070
52	1	0	-2.913840	-2.725275	1.616271
53	1	0	-4.517663	-2.297292	1.005785
54	1	0	-5.244829	0.663269	0.337885
55	1	0	-4.238468	2.034253	-0.150186
56	1	0	-3.886008	1.171232	1.348351
57	1	0	4.010178	1.256751	0.145354
58	1	0	6.246787	0.348627	-0.359803
59	1	0	6.517680	-2.042279	-1.003788
60	1	0	4.508126	-3.506766	-1.147339
61	1	0	2.264127	-2.585381	-0.673788

E_1

Zero-point correction= 0.509924
(Hartree/Particle)
Thermal correction to Energy= 0.540110
Thermal correction to Enthalpy= 0.541054
Thermal correction to Gibbs Free Energy= 0.450189
Sum of electronic and zero-point Energies= -1324.047336

Sum of electronic and thermal Energies= -1324.017151
Sum of electronic and thermal Enthalpies= -1324.016207
Sum of electronic and thermal Free Energies= -1324.107071

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.857330	-0.059080	-0.034731
2	7	0	-0.218498	1.584712	1.476090
3	6	0	-1.040682	1.755694	2.697408
4	6	0	0.209613	2.741031	0.794400
5	6	0	1.329260	2.545216	-0.147812
6	6	0	1.898221	1.260017	-0.341352
7	6	0	1.820663	3.671127	-0.815059
8	6	0	2.999087	1.178389	-1.215873
9	6	0	2.893537	3.558815	-1.694368
10	6	0	3.478923	2.304027	-1.884119
11	8	0	-0.336880	3.813573	1.023541
12	6	0	0.447202	0.306632	1.482209
13	6	0	1.349502	0.081863	0.379504
14	6	0	-0.992163	0.377206	3.378669
15	6	0	0.330126	-0.246263	2.886343
16	6	0	-1.641164	-1.043044	-2.011120
17	6	0	-1.663147	-1.958892	-0.860774
18	6	0	-2.684367	-1.513419	0.053822
19	6	0	-3.114211	-0.243240	-0.409376
20	6	0	-2.508707	0.017858	-1.720917
21	6	0	-0.874442	-1.263361	-3.282994
22	6	0	-1.012193	-3.311065	-0.823205
23	6	0	-3.189193	-2.266988	1.250321
24	6	0	-4.149470	0.641420	0.224831
25	6	0	-2.833215	1.198156	-2.591266
26	6	0	3.101716	-3.090401	-0.822647
27	6	0	2.296661	-1.952036	-0.789264
28	6	0	2.178973	-1.171081	0.373133
29	6	0	2.921042	-1.566952	1.498264
30	6	0	3.716076	-2.715546	1.475565
31	6	0	3.809439	-3.484424	0.315614
32	1	0	-0.580505	2.541633	3.306345
33	1	0	-2.047794	2.084602	2.435691
34	1	0	1.341635	4.625544	-0.621450
35	1	0	3.488884	0.224472	-1.371829
36	1	0	3.272736	4.432397	-2.216437
37	1	0	4.327639	2.197314	-2.555515
38	1	0	-1.834185	-0.236672	3.048046
39	1	0	-1.038462	0.464958	4.468048
40	1	0	0.333475	-1.337883	2.914197
41	1	0	1.167752	0.107682	3.507957
42	1	0	-1.462243	-1.853719	-4.001329
43	1	0	0.055037	-1.812586	-3.106229
44	1	0	-0.613479	-0.318512	-3.769659
45	1	0	-0.879593	-3.661515	0.205037
46	1	0	-0.026382	-3.305386	-1.293363
47	1	0	-1.628197	-4.054532	-1.350614
48	1	0	-2.388559	-2.822100	1.750457
49	1	0	-3.960305	-2.998682	0.966722
50	1	0	-3.640921	-1.598782	1.990928
51	1	0	-4.257141	0.438142	1.294987
52	1	0	-5.135917	0.494068	-0.237967
53	1	0	-3.896682	1.701342	0.110060

54	1	0	-3.803924	1.069656	-3.092514
55	1	0	-2.078889	1.342851	-3.370391
56	1	0	-2.890984	2.127140	-2.013616
57	1	0	3.172660	-3.673097	-1.737855
58	1	0	1.748143	-1.649186	-1.675542
59	1	0	2.892636	-0.961855	2.398985
60	1	0	4.273850	-2.999537	2.364482
61	1	0	4.431559	-4.375174	0.294668

C_2

Zero-point correction= 0.507267
(Hartree/Particle)
Thermal correction to Energy= 0.538257
Thermal correction to Enthalpy= 0.539201
Thermal correction to Gibbs Free Energy= 0.445987
Sum of electronic and zero-point Energies= -1323.991468
Sum of electronic and thermal Energies= -1323.960478
Sum of electronic and thermal Enthalpies= -1323.959533
Sum of electronic and thermal Free Energies= -1324.052748

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.592862	-0.200204	0.004959
2	7	0	-1.452661	1.351988	1.105769
3	6	0	-2.253820	1.176436	2.313037
4	6	0	-1.050542	2.623377	0.818737
5	6	0	0.005603	2.645421	-0.228850
6	6	0	0.470898	1.412427	-0.700265
7	6	0	0.559352	3.848578	-0.675324
8	6	0	1.530203	1.397119	-1.610789
9	6	0	1.596726	3.829226	-1.605436
10	6	0	2.083440	2.602118	-2.065182
11	8	0	-1.479432	3.637754	1.384285
12	6	0	1.259463	-0.631242	1.209034
13	6	0	0.293999	-0.488558	1.992850
14	6	0	-1.968069	-0.139358	3.043036
15	6	0	-0.466034	-0.375259	3.255406
16	6	0	2.663748	-0.776193	0.898338
17	6	0	3.126257	-1.406892	-0.267958
18	6	0	4.491716	-1.560969	-0.499375
19	6	0	5.421234	-1.083129	0.426715
20	6	0	4.974121	-0.448755	1.588686
21	6	0	3.610426	-0.294639	1.825025
22	1	0	-3.330487	1.229843	2.090678
23	1	0	-2.039733	2.021843	2.979434
24	1	0	0.164121	4.775872	-0.268941
25	1	0	1.949319	0.462912	-1.969765
26	1	0	2.034787	4.758578	-1.960542
27	1	0	2.906547	2.575780	-2.776458
28	1	0	-2.470653	-0.118306	4.018001
29	1	0	-2.381091	-0.989064	2.489297
30	1	0	-0.307735	-1.289418	3.844413
31	1	0	-0.043274	0.454195	3.840560
32	1	0	2.404507	-1.773476	-0.988165
33	1	0	4.830946	-2.053396	-1.406913
34	1	0	6.485692	-1.200113	0.243166
35	1	0	5.689807	-0.068256	2.312476
36	1	0	3.263089	0.204695	2.724302

37	6	0	-0.850527	-1.214682	-2.069603
38	6	0	-0.790925	-2.289760	-1.130564
39	6	0	-1.951674	-2.217124	-0.270490
40	6	0	-2.698526	-1.077523	-0.650051
41	6	0	-1.996400	-0.408172	-1.731398
42	6	0	0.000543	-1.046906	-3.293883
43	6	0	0.163271	-3.450178	-1.136498
44	6	0	-2.318029	-3.265388	0.741544
45	6	0	-4.033211	-0.643275	-0.121641
46	6	0	-2.527113	0.756159	-2.517279
47	1	0	-0.472651	-1.543972	-4.152411
48	1	0	0.994475	-1.486972	-3.170339
49	1	0	0.135491	0.005822	-3.552153
50	1	0	0.989950	-3.298769	-1.834904
51	1	0	-0.358192	-4.367195	-1.444197
52	1	0	0.588166	-3.636537	-0.144391
53	1	0	-1.460687	-3.548304	1.362389
54	1	0	-2.672782	-4.180594	0.246686
55	1	0	-3.116239	-2.928999	1.408993
56	1	0	-4.252977	-1.079240	0.856405
57	1	0	-4.831096	-0.956219	-0.809504
58	1	0	-4.087927	0.444608	-0.029387
59	1	0	-3.263304	0.427002	-3.264399
60	1	0	-1.724951	1.278839	-3.044279
61	1	0	-3.017017	1.484895	-1.864792

TS4

Zero-point correction= 0.506380
(Hartree/Particle)
Thermal correction to Energy= 0.536787
Thermal correction to Enthalpy= 0.537731
Thermal correction to Gibbs Free Energy= 0.446474
Sum of electronic and zero-point Energies= -1323.976009
Sum of electronic and thermal Energies= -1323.945601
Sum of electronic and thermal Enthalpies= -1323.944657
Sum of electronic and thermal Free Energies= -1324.035914

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.457446	-0.371446	-0.177873
2	7	0	-1.658754	0.426571	1.413657
3	6	0	-2.268235	-0.312601	2.511845
4	6	0	-2.038407	1.755099	1.262357
5	6	0	-1.432346	2.373712	0.058726
6	6	0	-0.641226	1.564969	-0.774694
7	6	0	-1.659594	3.725144	-0.231367
8	6	0	-0.071924	2.156285	-1.911859
9	6	0	-1.093530	4.295416	-1.367751
10	6	0	-0.297648	3.505991	-2.205256
11	8	0	-2.792072	2.350092	2.037610
12	6	0	1.146163	0.367352	1.063893
13	6	0	0.365988	0.407343	2.063463
14	6	0	-1.194936	-0.737478	3.539570
15	6	0	-0.074566	0.311931	3.464355
16	6	0	2.575490	0.456131	0.768437
17	6	0	3.503013	-0.275962	1.534559
18	6	0	4.870035	-0.186196	1.273446

19	6	0	5.336849	0.640547	0.249096
20	6	0	4.424861	1.373164	-0.514566
21	6	0	3.055795	1.278418	-0.265466
22	1	0	-2.803393	-1.191233	2.130661
23	1	0	-2.995506	0.353184	2.985127
24	1	0	-2.285794	4.298817	0.446446
25	1	0	0.562326	1.576541	-2.577795
26	1	0	-1.264831	5.342669	-1.602437
27	1	0	0.155054	3.943931	-3.092832
28	1	0	-1.612297	-0.790631	4.550884
29	1	0	-0.782356	-1.724086	3.296628
30	1	0	0.786763	0.025960	4.082566
31	1	0	-0.447941	1.281909	3.817216
32	1	0	3.142389	-0.916079	2.334990
33	1	0	5.570838	-0.759135	1.875168
38	6	0	0.382479	-1.596035	-1.872003
39	6	0	0.417348	-2.515440	-0.745329
40	6	0	-0.904263	-2.733555	-0.302928
41	6	0	-1.792539	-1.958764	-1.155556
42	6	0	-1.534433	-0.608768	-3.371784
43	6	0	1.558203	-1.275165	-2.751198
44	6	0	1.669233	-3.137989	-0.200443
45	6	0	-1.355344	-3.664109	0.785869
46	6	0	-3.292181	-1.981853	-1.087273
47	1	0	-1.657698	-1.313975	-4.205737
48	1	0	-0.864533	0.186432	-3.707062
49	1	0	-2.508131	-0.152015	-3.175058
50	1	0	1.356524	-0.411200	-3.391279
51	1	0	1.797247	-2.120032	-3.413490
52	1	0	2.455811	-1.050244	-2.166627
53	1	0	2.481036	-2.408494	-0.119763
54	1	0	2.019109	-3.943206	-0.861479
55	1	0	1.510733	-3.572581	0.790957
56	1	0	-0.540070	-3.916014	1.470499
57	1	0	-1.732491	-4.607359	0.366155
58	1	0	-2.168079	-3.233501	1.380089
59	1	0	-3.696342	-2.859117	-1.612585
60	1	0	-3.729537	-1.090702	-1.545628
61	1	0	-3.647889	-2.028658	-0.053670

D_2

Zero-point correction= 0.508604
(Hartree/Particle)
Thermal correction to Energy= 0.538964
Thermal correction to Enthalpy= 0.539908
Thermal correction to Gibbs Free Energy= 0.448728
Sum of electronic and zero-point Energies= -1324.011344
Sum of electronic and thermal Energies= -1323.980985
Sum of electronic and thermal Enthalpies= -1323.980040
Sum of electronic and thermal Free Energies= -1324.071220

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.457031	0.495321	-0.077740
2	7	0	-0.840069	-1.300397	-1.407022
3	6	0	-0.981533	-1.405215	-2.879489
4	6	0	-1.748864	-2.178964	-0.667980
5	6	0	-1.656598	-2.016625	0.794162

6	6	0	-1.033740	-0.859265	1.311025
7	6	0	-2.215175	-2.998497	1.628665
8	6	0	-0.943112	-0.755123	2.707582
9	6	0	-2.122554	-2.863798	3.008924
10	6	0	-1.475843	-1.742055	3.542621
11	8	0	-2.504468	-2.931415	-1.256266
12	6	0	1.162335	-0.749579	-0.353768
13	6	0	0.604985	-1.623096	-1.189603
14	6	0	-0.075283	-2.597056	-3.287829
15	6	0	0.992051	-2.719768	-2.154949
16	6	0	3.622521	-0.591412	-0.806997
17	6	0	4.940895	-0.499335	-0.359760
18	6	0	5.220012	-0.472600	1.008312
19	6	0	4.167137	-0.531067	1.925768
20	6	0	2.848273	-0.613301	1.480986
21	6	0	2.551491	-0.658715	0.105019
22	1	0	-0.617040	-0.465729	-3.303880
23	1	0	-2.027726	-1.550651	-3.149084
24	1	0	-2.712492	-3.851627	1.175413
25	1	0	-0.446754	0.099969	3.159217
26	1	0	-2.541419	-3.621018	3.665792
27	1	0	-1.385136	-1.635998	4.621919
28	1	0	-0.674560	-3.508325	-3.351483
29	1	0	0.382673	-2.424079	-4.266576
30	1	0	2.014893	-2.591179	-2.519560
31	1	0	0.941881	-3.709699	-1.683095
32	1	0	3.412215	-0.602359	-1.873158
33	1	0	5.751692	-0.447669	-1.082292
34	1	0	6.247071	-0.402674	1.356470
35	1	0	4.374346	-0.511451	2.992853
36	1	0	2.029594	-0.659635	2.192913
37	6	0	-1.465228	2.395391	0.817007
38	6	0	-0.011574	2.420345	0.898167
39	6	0	0.496799	2.604348	-0.455047
40	6	0	-0.596439	2.534385	-1.339467
41	6	0	-1.818282	2.393926	-0.549189
42	6	0	-2.400757	2.411485	1.990099
43	6	0	0.794681	2.637386	2.147147
44	6	0	1.933980	2.862194	-0.800823
45	6	0	-0.565292	2.679278	-2.833915
46	6	0	-3.204715	2.378933	-1.128191
47	1	0	-2.464922	3.421109	2.419404
48	1	0	-2.072580	1.735037	2.784939
49	1	0	-3.411651	2.108803	1.703198
50	1	0	0.286715	2.233873	3.028325
51	1	0	0.959518	3.709446	2.330614
52	1	0	1.776614	2.158485	2.079019
53	1	0	2.612344	2.243465	-0.206505
54	1	0	2.193828	3.913209	-0.610082
55	1	0	2.141096	2.659432	-1.855766
56	1	0	0.429148	2.473143	-3.240924
57	1	0	-0.840719	3.698414	-3.140460
58	1	0	-1.273050	1.999259	-3.320815
59	1	0	-3.527868	3.391834	-1.408176
60	1	0	-3.937136	1.984280	-0.418497
61	1	0	-3.258977	1.763802	-2.033011

TS5

Zero-point correction= (Hartree/Particle)	0.507423
Thermal correction to Energy=	0.537468
Thermal correction to Enthalpy=	0.538412
Thermal correction to Gibbs Free Energy=	0.447527
Sum of electronic and zero-point Energies=	-1323.987655
Sum of electronic and thermal Energies=	-1323.957610
Sum of electronic and thermal Enthalpies=	-1323.956666
Sum of electronic and thermal Free Energies=	-1324.047551

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.825921	-0.094480	-0.169353
2	7	0	-0.950028	2.184922	-1.346943
3	6	0	-1.447978	2.886836	-2.546731
4	6	0	-0.222544	2.941218	-0.413855
5	6	0	-0.138323	2.373299	0.946628
6	6	0	-0.211285	0.971349	1.207564
7	6	0	-0.063923	3.288283	2.012300
8	6	0	-0.341178	0.560754	2.558852
9	6	0	-0.156064	2.857608	3.328862
10	6	0	-0.319072	1.486995	3.593803
11	8	0	0.190159	4.057668	-0.734144
12	6	0	-1.278879	0.075520	-0.200281
13	6	0	-1.709430	1.033370	-1.064724
14	6	0	-2.508403	1.927394	-3.113870
15	6	0	-2.978379	1.124834	-1.883487
16	6	0	2.676753	-1.013881	0.871965
17	6	0	1.645189	-1.977161	0.500385
18	6	0	1.696386	-2.164114	-0.962314
19	6	0	2.543990	-1.181550	-1.464441
20	6	0	3.129242	-0.438702	-0.326433
21	6	0	3.091309	-0.682138	2.274451
22	6	0	0.963936	-2.918185	1.448715
23	6	0	1.006539	-3.261848	-1.714782
24	6	0	2.890891	-0.920034	-2.900800
25	6	0	4.132257	0.666506	-0.485432
26	6	0	-2.181502	-1.046974	0.168061
27	6	0	-2.329704	-2.145093	-0.700706
28	6	0	-3.193504	-3.198013	-0.396881
29	6	0	-3.926804	-3.183831	0.792319
30	6	0	-3.798664	-2.098557	1.660636
31	6	0	-2.943184	-1.039074	1.349858
32	1	0	-0.625719	3.090328	-3.238025
33	1	0	-1.865335	3.854139	-2.245444
34	1	0	0.035478	4.341415	1.767390
35	1	0	-0.446259	-0.496407	2.783927
36	1	0	-0.123841	3.574411	4.144339
37	1	0	-0.409797	1.142403	4.622010
38	1	0	-3.320218	2.462793	-3.614290
39	1	0	-2.051979	1.249027	-3.844060
40	1	0	-3.398924	0.148161	-2.131690
41	1	0	-3.746889	1.687184	-1.330631
42	1	0	3.637454	-1.517891	2.733274
43	1	0	2.226948	-0.459721	2.910589
44	1	0	3.747332	0.192560	2.299658
45	1	0	-0.040670	-3.181901	1.104782
46	1	0	0.877230	-2.482590	2.448264
47	1	0	1.539851	-3.850577	1.544732
48	1	0	0.029993	-3.498189	-1.283425

49	1	0	1.602933	-4.185762	-1.687250
50	1	0	0.856470	-3.003066	-2.767845
51	1	0	2.907802	0.152720	-3.123407
52	1	0	2.175096	-1.390239	-3.581522
53	1	0	3.888593	-1.311938	-3.145799
54	1	0	5.110809	0.272265	-0.794641
55	1	0	4.273727	1.220568	0.446245
56	1	0	3.818710	1.385169	-1.250821
57	1	0	-1.767653	-2.154375	-1.629905
58	1	0	-3.296249	-4.028521	-1.091253
59	1	0	-4.596241	-4.005045	1.034176
60	1	0	-4.375763	-2.067879	2.581612
61	1	0	-2.866423	-0.192105	2.023678

E

Zero-point correction= 0.509084
(Hartree/Particle)
Thermal correction to Energy= 0.539501
Thermal correction to Enthalpy= 0.540445
Thermal correction to Gibbs Free Energy= 0.448728
Sum of electronic and zero-point Energies= -1324.054768
Sum of electronic and thermal Energies= -1324.024351
Sum of electronic and thermal Enthalpies= -1324.023407
Sum of electronic and thermal Free Energies= -1324.115124

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.602860	-0.246958	-0.064514
2	7	0	-0.163108	2.367867	-1.189780
3	6	0	-0.171307	2.934222	-2.535693
4	6	0	0.665750	2.778534	-0.185550
5	6	0	0.568389	1.904175	1.033357
6	6	0	-0.599226	1.082208	1.286976
7	6	0	1.435879	2.218558	2.120336
8	6	0	-0.857848	0.667389	2.635941
9	6	0	1.179707	1.762388	3.390609
10	6	0	0.010248	0.993864	3.648177
11	8	0	1.396430	3.763693	-0.260255
12	6	0	-1.342651	0.613086	0.127350
13	6	0	-0.749981	1.051220	-1.121651
14	6	0	-0.498363	1.717053	-3.419529
15	6	0	-1.344720	0.812749	-2.501099
16	6	0	-2.979518	-1.256700	-0.402453
17	6	0	-4.262164	-1.801698	-0.334370
18	6	0	-5.271521	-1.144638	0.372048
19	6	0	-4.987041	0.066763	1.004855
20	6	0	-3.706235	0.615040	0.928961
21	6	0	-2.677323	-0.038669	0.226542
22	1	0	0.795674	3.398355	-2.746517
23	1	0	-0.944016	3.710984	-2.619303
24	1	0	2.270253	2.880804	1.913015
25	1	0	-1.747254	0.079403	2.838125
26	1	0	1.844249	2.021506	4.210310
27	1	0	-0.201420	0.665891	4.662788
28	1	0	-1.018919	1.995543	-4.340331
29	1	0	0.428987	1.202686	-3.695482
30	1	0	-1.324445	-0.236456	-2.800991

31	1	0	-2.396782	1.134357	-2.512791
32	1	0	-2.197409	-1.784195	-0.938532
33	1	0	-4.470613	-2.747511	-0.828194
34	1	0	-6.268659	-1.572646	0.429284
35	1	0	-5.763950	0.591051	1.555339
36	1	0	-3.496725	1.565517	1.412528
37	6	0	1.928590	-2.012938	0.927023
38	6	0	0.997875	-2.627639	0.074447
39	6	0	1.169849	-2.051835	-1.256735
40	6	0	2.317724	-1.172684	-1.229926
41	6	0	2.719014	-1.076106	0.133333
42	6	0	2.121516	-2.251903	2.397071
43	6	0	0.018693	-3.707543	0.433565
44	6	0	0.501394	-2.562446	-2.501771
45	6	0	3.005376	-0.554912	-2.414633
46	6	0	3.876421	-0.287431	0.673680
47	1	0	3.042284	-2.819490	2.593882
48	1	0	1.289140	-2.818821	2.824524
49	1	0	2.196466	-1.309765	2.951989
50	1	0	-0.247522	-3.675530	1.494496
51	1	0	0.433938	-4.705195	0.229015
52	1	0	-0.910933	-3.623658	-0.137467
53	1	0	-0.543224	-2.836433	-2.322376
54	1	0	1.010893	-3.460719	-2.879385
55	1	0	0.518817	-1.818480	-3.303924
56	1	0	2.319576	-0.422210	-3.257454
57	1	0	3.834346	-1.185375	-2.768975
58	1	0	3.421246	0.428571	-2.174742
59	1	0	4.746004	-0.937702	0.846203
60	1	0	3.626227	0.184308	1.630108
61	1	0	4.184233	0.503050	-0.016679

2a

Zero-point correction= 0.286555
(Hartree/Particle)
Thermal correction to Energy= 0.301718
Thermal correction to Enthalpy= 0.302662
Thermal correction to Gibbs Free Energy= 0.243386
Sum of electronic and zero-point Energies= -824.663563
Sum of electronic and thermal Energies= -824.648401
Sum of electronic and thermal Enthalpies= -824.647457
Sum of electronic and thermal Free Energies= -824.706732

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.657605	-1.430834	0.084401
2	6	0	-2.093958	-2.830861	0.169651
3	6	0	-2.572002	-0.383593	0.070660
4	6	0	-1.949490	0.948368	-0.014012
5	6	0	-0.537113	1.105510	-0.047541
6	6	0	-2.795245	2.068808	-0.067598
7	6	0	-0.022766	2.418695	-0.149292
8	6	0	-2.265762	3.345965	-0.159364
9	6	0	-0.871200	3.513936	-0.202650
10	8	0	-3.781898	-0.605423	0.119596
11	6	0	0.320884	-0.069125	0.009265
12	6	0	-0.280181	-1.290990	0.072927

13	6	0	-0.826511	-3.606184	-0.226186
14	6	0	0.328580	-2.670800	0.192915
15	6	0	2.564104	-0.315707	-1.115158
16	6	0	3.956980	-0.219956	-1.106973
17	6	0	4.620386	0.250438	0.027830
18	6	0	3.882583	0.624108	1.153332
19	6	0	2.490709	0.522269	1.145161
20	6	0	1.809914	0.047712	0.011869
21	1	0	-2.948553	-2.989284	-0.490989
22	1	0	-2.420093	-3.052810	1.193792
23	1	0	-3.865950	1.894672	-0.036674
24	1	0	1.051625	2.564155	-0.188008
25	1	0	-2.921961	4.210719	-0.200803
26	1	0	-0.449435	4.512850	-0.281059
27	1	0	-0.773837	-4.588900	0.249572
28	1	0	-0.808646	-3.756507	-1.311439
29	1	0	1.228856	-2.789045	-0.413715
30	1	0	0.619930	-2.851773	1.237359
31	1	0	2.048843	-0.667314	-2.005424
32	1	0	4.522663	-0.506601	-1.989753
33	1	0	5.704324	0.327944	0.034549
34	1	0	4.391050	0.991072	2.041154
35	1	0	1.920121	0.808479	2.024854

F

Zero-point correction= 0.467853
(Hartree/Particle)
Thermal correction to Energy= 0.498968
Thermal correction to Enthalpy= 0.499912
Thermal correction to Gibbs Free Energy= 0.405593
Sum of electronic and zero-point Energies= -1246.598040
Sum of electronic and thermal Energies= -1246.566924
Sum of electronic and thermal Enthalpies= -1246.565980
Sum of electronic and thermal Free Energies= -1246.660299

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.683165	-0.240669	-0.217272
2	7	0	1.692371	1.216530	-1.321110
3	6	0	2.698587	0.922775	-2.320364
4	6	0	1.384154	2.522104	-1.092972
5	6	0	0.303205	2.651430	-0.072995
6	6	0	-0.216157	1.468719	0.464699
7	6	0	-0.174021	3.899547	0.335146
8	6	0	-1.235713	1.546060	1.418120
9	6	0	-1.181121	3.974676	1.297576
10	6	0	-1.709244	2.797768	1.836755
11	8	0	1.919182	3.491092	-1.647980
12	6	0	-1.341520	-0.501593	-1.487712
13	6	0	-0.276041	-0.493164	-2.129440
14	6	0	-2.698090	-0.576523	-1.034424
15	6	0	-3.324291	-1.833273	-0.898410
16	6	0	-4.658161	-1.917349	-0.507095
17	6	0	-5.386987	-0.753729	-0.246143
18	6	0	-4.776750	0.495614	-0.385104
19	6	0	-3.443050	0.591529	-0.775722
20	1	0	2.436402	0.020852	-2.889210
21	1	0	3.693661	0.751649	-1.879211

22	1	0	2.787516	1.768974	-3.009486
23	1	0	0.263169	4.787244	-0.114500
24	1	0	-1.682476	0.646491	1.834857
25	1	0	-1.555796	4.940977	1.625805
26	1	0	-2.498812	2.848093	2.584023
27	1	0	0.286800	-0.485178	-3.043343
28	1	0	-2.760102	-2.733295	-1.123479
29	1	0	-5.130917	-2.890934	-0.411155
30	1	0	-6.427802	-0.820483	0.058478
31	1	0	-5.342333	1.402397	-0.189969
32	1	0	-2.966902	1.558672	-0.883883
33	6	0	1.330051	-0.898280	1.896149
34	6	0	0.429218	-1.892665	1.401756
35	6	0	1.068608	-2.538852	0.267852
36	6	0	2.328508	-1.934189	0.046703
37	6	0	2.470866	-0.865099	1.018910
38	6	0	1.186606	-0.105921	3.161661
39	6	0	-0.839749	-2.350806	2.062097
40	6	0	0.502787	-3.704861	-0.488525
41	6	0	3.363617	-2.377105	-0.946608
42	6	0	3.691309	-0.015306	1.220772
43	1	0	1.611899	-0.666159	4.006183
44	1	0	0.141889	0.110368	3.396490
45	1	0	1.711299	0.850708	3.098906
46	1	0	-1.224397	-1.594651	2.751803
47	1	0	-0.671327	-3.268210	2.643690
48	1	0	-1.630620	-2.562974	1.335881
49	1	0	-0.587783	-3.739798	-0.415464
50	1	0	0.887031	-4.651653	-0.084453
51	1	0	0.767095	-3.670001	-1.549892
52	1	0	2.905622	-2.828748	-1.832428
53	1	0	4.032354	-3.129908	-0.505803
54	1	0	3.987243	-1.545377	-1.283836
55	1	0	4.351756	-0.462456	1.976763
56	1	0	3.427721	0.990419	1.558645
57	1	0	4.265631	0.089593	0.297328

TS6

Zero-point correction= 0.467773
(Hartree/Particle)
Thermal correction to Energy= 0.497641
Thermal correction to Enthalpy= 0.498585
Thermal correction to Gibbs Free Energy= 0.408184
Sum of electronic and zero-point Energies= -1246.574583
Sum of electronic and thermal Energies= -1246.544716
Sum of electronic and thermal Enthalpies= -1246.543772
Sum of electronic and thermal Free Energies= -1246.634172

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.904209	-0.147940	-0.244726
2	7	0	0.844405	1.593693	-1.401094
3	6	0	1.645044	1.782742	-2.594384
4	6	0	-0.068020	2.546365	-1.093621
5	6	0	-0.880934	2.160158	0.102916
6	6	0	-0.840501	0.823903	0.539905
7	6	0	-1.607233	3.117819	0.816092

8	6	0	-1.508426	0.472424	1.725124
9	6	0	-2.263322	2.761356	1.994796
10	6	0	-2.199858	1.439712	2.455662
11	8	0	-0.234512	3.623945	-1.684580
12	6	0	-0.350670	-0.807792	-1.705434
13	6	0	-1.348056	-0.542778	-0.948037
14	6	0	-3.741507	0.091554	-0.556881
15	6	0	-5.077393	-0.281226	-0.436079
16	6	0	-5.438105	-1.632313	-0.446011
17	6	0	-4.454657	-2.613529	-0.583728
18	6	0	-3.115605	-2.246036	-0.713212
19	6	0	-2.744579	-0.888933	-0.705074
20	1	0	1.200886	2.569063	-3.213191
21	1	0	2.677117	2.088059	-2.359875
22	1	0	1.698615	0.850848	-3.172238
23	1	0	-1.617398	4.135405	0.435379
24	1	0	-1.520706	-0.561992	2.059882
25	1	0	-2.819582	3.506678	2.557499
26	1	0	-2.707667	1.158863	3.375476
27	1	0	-0.140663	-1.205823	-2.686862
28	1	0	-3.459251	1.138854	-0.544360
29	1	0	-5.840864	0.484978	-0.333791
30	1	0	-6.481848	-1.917848	-0.345875
31	1	0	-4.728530	-3.665141	-0.591431
32	1	0	-2.345286	-3.003061	-0.826945
33	6	0	2.129658	-0.450583	1.740736
34	6	0	1.651838	-1.731352	1.256893
35	6	0	2.275958	-1.991321	-0.009730
36	6	0	3.055048	-0.847454	-0.362625
37	6	0	2.967964	0.105914	0.742596
38	6	0	1.807640	0.139021	3.082651
39	6	0	0.820302	-2.706794	2.040199
40	6	0	2.152409	-3.260344	-0.802864
41	6	0	3.991821	-0.733728	-1.530253
42	6	0	3.721778	1.401756	0.810638
43	1	0	2.356847	-0.382389	3.878611
44	1	0	0.740003	0.065367	3.312900
45	1	0	2.078179	1.196952	3.132015
46	1	0	0.168207	-2.196681	2.754927
47	1	0	1.457114	-3.394920	2.614390
48	1	0	0.188621	-3.315756	1.385961
49	1	0	1.162026	-3.712637	-0.690954
50	1	0	2.890837	-4.002321	-0.469006
51	1	0	2.321291	-3.087593	-1.869870
52	1	0	3.634163	-1.299953	-2.395614
53	1	0	4.986567	-1.123321	-1.270111
54	1	0	4.119350	0.305091	-1.845069
55	1	0	4.777319	1.225400	1.059982
56	1	0	3.307020	2.070622	1.569011
57	1	0	3.689932	1.931919	-0.145490

G_1

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Zero-point correction=                           0.470625
(Hartree/Particle)
 Thermal correction to Energy=                    0.500723
 Thermal correction to Enthalpy=                  0.501667
 Thermal correction to Gibbs Free Energy=         0.409852
 Sum of electronic and zero-point Energies=          -1246.628247
 Sum of electronic and thermal Energies=             -1246.598150
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Sum of electronic and thermal Enthalpies= -1246.597206
Sum of electronic and thermal Free Energies= -1246.689021

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.970149	-0.242097	0.175103
2	7	0	-0.534069	0.424201	2.078738
3	6	0	-0.718817	-0.251044	3.347145
4	6	0	0.338896	1.443297	1.995033
5	6	0	0.574666	1.858010	0.543578
6	6	0	1.342672	1.071474	-0.361409
7	6	0	0.141305	3.140993	0.145285
8	6	0	1.644184	1.610799	-1.632294
9	6	0	0.425925	3.636762	-1.118588
10	6	0	1.190523	2.866527	-2.010900
11	8	0	0.886229	2.061533	2.913200
12	6	0	0.816050	-1.149063	0.317442
13	6	0	1.817356	-0.314624	-0.003762
14	6	0	4.237779	0.331569	0.189388
15	6	0	5.595280	0.013035	0.161832
16	6	0	6.009142	-1.289347	-0.124848
17	6	0	5.050059	-2.271439	-0.386619
18	6	0	3.693913	-1.952922	-0.362804
19	6	0	3.260960	-0.647952	-0.064603
20	1	0	-0.455071	0.431272	4.161842
21	1	0	-1.761517	-0.565923	3.471604
22	1	0	-0.082016	-1.145253	3.428239
23	1	0	-0.396654	3.748124	0.867989
24	1	0	2.256847	1.024741	-2.311992
25	1	0	0.085268	4.627943	-1.406274
26	1	0	1.439646	3.259029	-2.993580
27	1	0	0.956767	-2.180878	0.638021
28	1	0	3.927423	1.344620	0.429199
29	1	0	6.331346	0.785136	0.370991
30	1	0	7.067228	-1.536068	-0.149406
31	1	0	5.360144	-3.286582	-0.622199
32	1	0	2.955200	-2.716513	-0.591511
33	6	0	-3.035767	0.324410	-0.966590
34	6	0	-2.137840	-0.511700	-1.784692
35	6	0	-1.967809	-1.756350	-1.137347
36	6	0	-2.599070	-1.642172	0.172370
37	6	0	-3.350531	-0.375696	0.197258
38	6	0	-3.485623	1.695681	-1.375843
39	6	0	-1.646014	-0.122244	-3.147734
40	6	0	-1.289567	-2.980471	-1.678641
41	6	0	-2.793128	-2.765250	1.147981
42	6	0	-4.232174	0.058578	1.329734
43	1	0	-4.117884	1.649598	-2.272771
44	1	0	-2.630979	2.339992	-1.613780
45	1	0	-4.060947	2.186299	-0.586644
46	1	0	-1.265458	0.904726	-3.159016
47	1	0	-2.457642	-0.179697	-3.886649
48	1	0	-0.839994	-0.778358	-3.486726
49	1	0	-0.531761	-2.725699	-2.424471
50	1	0	-2.021307	-3.645567	-2.157494
51	1	0	-0.795348	-3.550858	-0.886729
52	1	0	-1.943872	-3.454352	1.140813
53	1	0	-3.694069	-3.344740	0.898526
54	1	0	-2.913245	-2.391897	2.169045
55	1	0	-5.116385	-0.588099	1.407983

56	1	0	-4.581207	1.086061	1.198890
57	1	0	-3.703407	0.010453	2.287452

TS7

Zero-point correction= 0.468360
(Hartree/Particle)
Thermal correction to Energy= 0.498208
Thermal correction to Enthalpy= 0.499152
Thermal correction to Gibbs Free Energy= 0.408855
Sum of electronic and zero-point Energies= -1246.575463
Sum of electronic and thermal Energies= -1246.545614
Sum of electronic and thermal Enthalpies= -1246.544670
Sum of electronic and thermal Free Energies= -1246.634967

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.494025	-0.385879	-0.077050
2	7	0	1.639572	0.470306	-1.672304
3	6	0	2.276672	-0.234670	-2.772310
4	6	0	2.018457	1.787354	-1.497513
5	6	0	1.424917	2.382983	-0.275600
6	6	0	0.664894	1.547314	0.559833
7	6	0	1.643501	3.729728	0.038305
8	6	0	0.117287	2.104711	1.723421
9	6	0	1.097454	4.268479	1.200078
10	6	0	0.333526	3.451328	2.040165
11	8	0	2.780810	2.371791	-2.270890
12	6	0	-1.203994	0.371830	-1.206710
13	6	0	-0.386728	0.363920	-2.169935
14	6	0	-2.612778	0.453412	-0.847202
15	6	0	-3.567190	-0.264112	-1.595191
16	6	0	-4.922028	-0.188431	-1.275859
17	6	0	-5.349669	0.610384	-0.212652
18	6	0	-4.411402	1.330045	0.531154
19	6	0	-3.053170	1.248544	0.225222
20	1	0	1.918027	-1.266023	-2.800347
21	1	0	3.366211	-0.233375	-2.652977
22	1	0	2.064375	0.244230	-3.740515
23	1	0	2.247810	4.324842	-0.641196
24	1	0	-0.492288	1.503030	2.392924
25	1	0	1.260799	5.312790	1.452746
26	1	0	-0.101177	3.863794	2.948614
27	1	0	-0.122286	0.374734	-3.212024
28	1	0	-3.234346	-0.878201	-2.426908
29	1	0	-5.644636	-0.749045	-1.863013
30	1	0	-6.406319	0.672747	0.032900
31	1	0	-4.737558	1.958921	1.355349
32	1	0	-2.323933	1.810606	0.797929
33	6	0	1.130451	-1.372374	1.868421
34	6	0	-0.261834	-1.656456	1.621561
35	6	0	-0.327632	-2.548618	0.474380
36	6	0	0.980099	-2.741171	-0.020803
37	6	0	1.888728	-1.976044	0.817276
38	6	0	1.696603	-0.673847	3.069534
39	6	0	-1.408357	-1.369049	2.549504
40	6	0	-1.590114	-3.173073	-0.042388
41	6	0	1.395163	-3.635233	-1.154078
42	6	0	3.384359	-1.964997	0.688568

43	1	0	1.845300	-1.390905	3.889013
44	1	0	1.036813	0.116268	3.435296
45	1	0	2.663884	-0.213826	2.850262
46	1	0	-1.183077	-0.532594	3.217392
47	1	0	-1.627842	-2.240160	3.183687
48	1	0	-2.323488	-1.119226	2.003524
49	1	0	-2.415651	-2.454918	-0.066555
50	1	0	-1.900954	-4.005507	0.604300
51	1	0	-1.462909	-3.572161	-1.052882
52	1	0	0.585603	-3.781175	-1.875758
53	1	0	1.688480	-4.628559	-0.786130
54	1	0	2.255007	-3.230007	-1.696721
55	1	0	3.828376	-2.833052	1.196251
56	1	0	3.819008	-1.064455	1.130744
57	1	0	3.698872	-2.002422	-0.358498

G_2

Zero-point correction= 0.471814
(Hartree/Particle)
Thermal correction to Energy= 0.501193
Thermal correction to Enthalpy= 0.502137
Thermal correction to Gibbs Free Energy= 0.413067
Sum of electronic and zero-point Energies= -1246.628427
Sum of electronic and thermal Energies= -1246.599048
Sum of electronic and thermal Enthalpies= -1246.598104
Sum of electronic and thermal Free Energies= -1246.687174

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.428111	-0.394764	-0.072082
2	7	0	0.835028	0.731993	-1.973383
3	6	0	1.242580	0.054198	-3.215915
4	6	0	1.693786	1.873305	-1.634041
5	6	0	1.546526	2.306160	-0.233071
6	6	0	0.938392	1.419582	0.684403
7	6	0	2.052885	3.555669	0.158912
8	6	0	0.814005	1.865009	2.009126
9	6	0	1.922959	3.967610	1.480062
10	6	0	1.294373	3.119028	2.399588
11	8	0	2.451575	2.341444	-2.461488
12	6	0	-1.186048	0.579373	-0.871131
13	6	0	-0.599536	1.093024	-1.953238
14	6	0	-2.592738	0.678924	-0.479028
15	6	0	-3.623540	0.444549	-1.409516
16	6	0	-4.962776	0.545361	-1.032888
17	6	0	-5.301527	0.883078	0.279369
18	6	0	-4.288977	1.116127	1.214328
19	6	0	-2.949779	1.005607	0.843025
20	1	0	0.601123	-0.818236	-3.351321
21	1	0	2.286713	-0.257927	-3.137459
22	1	0	1.145447	0.722975	-4.078814
23	1	0	2.540629	4.180813	-0.584045
24	1	0	0.330204	1.238467	2.753994
25	1	0	2.300105	4.936488	1.795185
26	1	0	1.175569	3.438879	3.432990
27	1	0	-0.986306	1.711058	-2.765485
28	1	0	-3.362413	0.173345	-2.428900
29	1	0	-5.743546	0.357673	-1.765739
30	1	0	-6.345186	0.960061	0.572326

31	1	0	-4.544027	1.383785	2.236657
32	1	0	-2.160466	1.192523	1.564390
33	6	0	1.461211	-1.772777	1.516069
34	6	0	0.008523	-1.788547	1.594526
35	6	0	-0.484790	-2.485113	0.416396
36	6	0	0.618407	-2.754855	-0.420248
37	6	0	1.828822	-2.304026	0.261596
38	6	0	2.381345	-1.311153	2.607370
39	6	0	-0.801428	-1.521738	2.831862
40	6	0	-1.917022	-2.870068	0.185492
41	6	0	0.600854	-3.486213	-1.732494
42	6	0	3.222378	-2.495589	-0.267151
43	1	0	2.419646	-2.050146	3.419780
44	1	0	2.055375	-0.360578	3.040414
45	1	0	3.401664	-1.169343	2.240685
46	1	0	-0.316619	-0.784259	3.478658
47	1	0	-0.926568	-2.439304	3.425612
48	1	0	-1.801034	-1.148382	2.588686
49	1	0	-2.604505	-2.078451	0.497213
50	1	0	-2.170910	-3.773553	0.757761
51	1	0	-2.115125	-3.082399	-0.869141
52	1	0	-0.382090	-3.439041	-2.210945
53	1	0	0.848856	-4.548689	-1.598035
54	1	0	1.333510	-3.076259	-2.435954
55	1	0	3.567764	-3.526998	-0.107695
56	1	0	3.937859	-1.829038	0.222406
57	1	0	3.278223	-2.303755	-1.344360

H

Zero-point correction= 0.536345
(Hartree/Particle)
Thermal correction to Energy= 0.568566
Thermal correction to Enthalpy= 0.569510
Thermal correction to Gibbs Free Energy= 0.474392
Sum of electronic and zero-point Energies= -1363.269276
Sum of electronic and thermal Energies= -1363.237055
Sum of electronic and thermal Enthalpies= -1363.236111
Sum of electronic and thermal Free Energies= -1363.331229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.603708	-0.195052	-0.143345
2	7	0	-1.557735	1.450262	0.740027
3	6	0	-2.887958	0.421916	2.633449
4	6	0	-1.000961	2.681004	0.549895
5	6	0	0.219971	2.605763	-0.299521
6	6	0	0.610755	1.343666	-0.754545
7	6	0	0.930604	3.754837	-0.659223
8	6	0	1.736640	1.237904	-1.576274
9	6	0	2.043273	3.648466	-1.492938
10	6	0	2.441390	2.389304	-1.952117
11	8	0	-1.440912	3.751290	0.994150
12	6	0	0.096242	-0.507639	1.924885
13	6	0	1.169309	-0.543004	1.284182
14	6	0	-1.659710	0.462634	3.555772
15	6	0	-0.620531	-0.620961	3.219442
16	6	0	-2.823370	1.401310	1.451890
17	6	0	2.586858	-0.699875	1.071374

18	6	0	3.150056	-1.991453	1.035043
19	6	0	4.526372	-2.161848	0.900092
20	6	0	5.363690	-1.047992	0.801602
21	6	0	4.816423	0.236827	0.845688
22	6	0	3.440782	0.416012	0.977360
23	1	0	-3.795237	0.663844	3.203280
24	1	0	-3.024076	-0.606094	2.274927
25	1	0	0.582331	4.711026	-0.277977
26	1	0	2.092066	0.269301	-1.917002
27	1	0	2.599171	4.536446	-1.783326
28	1	0	3.312616	2.295406	-2.597307
29	1	0	-1.967455	0.286643	4.594138
30	1	0	-1.190764	1.452641	3.524865
31	1	0	-1.118802	-1.600816	3.256885
32	1	0	0.155474	-0.639034	3.998219
33	1	0	-3.650328	1.166079	0.760813
34	1	0	-3.005651	2.417245	1.818264
35	1	0	2.500533	-2.855907	1.136833
36	1	0	4.945202	-3.164377	0.878740
37	1	0	6.437177	-1.180647	0.697817
38	1	0	5.463659	1.106896	0.778085
39	1	0	3.016829	1.412700	1.011409
40	6	0	-0.921743	-0.914570	-2.328295
41	6	0	-0.290197	-1.975401	-1.606600
42	6	0	-1.229798	-2.449267	-0.604544
43	6	0	-2.408189	-1.670468	-0.686304
44	6	0	-2.191188	-0.660564	-1.708657
45	6	0	-0.429056	-0.260437	-3.585011
46	6	0	0.997842	-2.658029	-1.966888
47	6	0	-0.977215	-3.621047	0.298097
48	6	0	-3.714513	-1.925114	0.008457
49	6	0	-3.218291	0.315800	-2.203264
50	1	0	-0.830899	-0.789354	-4.460770
51	1	0	0.660075	-0.275344	-3.660160
52	1	0	-0.747566	0.782890	-3.650878
53	1	0	1.639033	-2.013467	-2.574392
54	1	0	0.806994	-3.571398	-2.548362
55	1	0	1.570492	-2.945524	-1.080673
56	1	0	-0.010314	-3.530693	0.805543
57	1	0	-0.960749	-4.559058	-0.273078
58	1	0	-1.748439	-3.714867	1.067414
59	1	0	-3.588022	-2.517774	0.918571
60	1	0	-4.393889	-2.482477	-0.652171
61	1	0	-4.222007	-0.996356	0.281990
62	1	0	-3.818295	-0.128655	-3.010011
63	1	0	-2.751251	1.223174	-2.595248
64	1	0	-3.904521	0.616081	-1.407572

TS8

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Zero-point correction=                           0.535264
(Hartree/Particle)
 Thermal correction to Energy=                    0.566707
 Thermal correction to Enthalpy=                  0.567651
 Thermal correction to Gibbs Free Energy=         0.474529
 Sum of electronic and zero-point Energies=          -1363.250406
 Sum of electronic and thermal Energies=             -1363.218963
 Sum of electronic and thermal Enthalpies=           -1363.218019
 Sum of electronic and thermal Free Energies=        -1363.311141
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.806223	-0.155924	-0.102786
2	7	0	-1.022227	1.661313	0.930359
3	6	0	-2.018597	0.884891	3.131987
4	6	0	-0.148197	2.661672	0.640090
5	6	0	0.804308	2.267934	-0.441597
6	6	0	0.917224	0.906800	-0.782907
7	6	0	1.514145	3.240148	-1.151474
8	6	0	1.714592	0.549422	-1.885736
9	6	0	2.303401	2.875325	-2.242194
10	6	0	2.388730	1.528085	-2.616325
11	8	0	-0.119410	3.788054	1.159461
12	6	0	0.336006	-0.467808	1.578068
13	6	0	1.324912	-0.296339	0.771853
14	6	0	-0.643701	0.505416	3.707376
15	6	0	0.010195	-0.707303	3.004702
16	6	0	-1.996596	1.909159	1.980790
17	6	0	2.719030	-0.731493	0.654811
18	6	0	3.028938	-2.091314	0.836508
19	6	0	4.354812	-2.525658	0.827078
20	6	0	5.388792	-1.606804	0.640692
21	6	0	5.091085	-0.252114	0.462290
22	6	0	3.768492	0.184240	0.460670
23	1	0	-2.639139	1.320999	3.926874
24	1	0	-2.533116	-0.032630	2.821103
25	1	0	1.403449	4.275213	-0.840695
26	1	0	1.844539	-0.497023	-2.148858
27	1	0	2.845660	3.631875	-2.803373
28	1	0	2.999750	1.236400	-3.467499
29	1	0	-0.751024	0.238559	4.766746
30	1	0	0.037583	1.363617	3.663117
31	1	0	-0.667324	-1.568245	3.090633
32	1	0	0.938552	-0.976741	3.530033
33	1	0	-3.012395	1.964854	1.554786
34	1	0	-1.773074	2.902394	2.385487
35	1	0	2.219789	-2.800298	0.987289
36	1	0	4.578366	-3.579996	0.966939
37	1	0	6.422274	-1.942834	0.634990
38	1	0	5.893713	0.467308	0.324545
39	1	0	3.537131	1.234870	0.320855
40	6	0	-1.739717	-0.722915	-2.193029
41	6	0	-1.191462	-1.904335	-1.554908
42	6	0	-1.956804	-2.170879	-0.368765
43	6	0	-2.893980	-1.109819	-0.205194
44	6	0	-2.752315	-0.209515	-1.349373
45	6	0	-1.320002	-0.185758	-3.529634
46	6	0	-0.167339	-2.823368	-2.158321
47	6	0	-1.803646	-3.378100	0.511042
48	6	0	-4.027564	-1.055825	0.778118
49	6	0	-3.625956	0.984527	-1.600476
50	1	0	-1.691613	-0.828561	-4.339498
51	1	0	-0.231076	-0.128793	-3.623813
52	1	0	-1.713632	0.819911	-3.699054
53	1	0	0.492551	-2.290632	-2.848661
54	1	0	-0.651719	-3.628957	-2.728686
55	1	0	0.458291	-3.295368	-1.394204
56	1	0	-0.754820	-3.678831	0.603047
57	1	0	-2.353567	-4.236467	0.100678
58	1	0	-2.186747	-3.195940	1.519386

59	1	0	-3.824359	-1.654109	1.670586
60	1	0	-4.947434	-1.450347	0.322609
61	1	0	-4.240587	-0.032885	1.101581
62	1	0	-4.609244	0.676548	-1.982798
63	1	0	-3.181154	1.664136	-2.331846
64	1	0	-3.791406	1.555294	-0.682017

I_1

Zero-point correction= 0.537209
(Hartree/Particle)
Thermal correction to Energy= 0.568988
Thermal correction to Enthalpy= 0.569933
Thermal correction to Gibbs Free Energy= 0.475371
Sum of electronic and zero-point Energies= -1363.296162
Sum of electronic and thermal Energies= -1363.264383
Sum of electronic and thermal Enthalpies= -1363.263439
Sum of electronic and thermal Free Energies= -1363.358000

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.997637	-0.111832	-0.030169
2	7	0	-0.455526	-0.756779	1.860664
3	6	0	-0.221700	-3.249648	1.558312
4	6	0	0.343937	0.194446	2.371593
5	6	0	0.442593	1.388741	1.423815
6	6	0	1.154446	1.321921	0.187092
7	6	0	-0.025851	2.641977	1.882050
8	6	0	1.367222	2.522337	-0.532815
9	6	0	0.169924	3.795841	1.141696
10	6	0	0.879364	3.734725	-0.073490
11	8	0	0.935127	0.212251	3.456693
12	6	0	0.807813	-0.954199	-0.422436
13	6	0	1.728429	0.020608	-0.300707
14	6	0	1.101226	-3.183790	0.772289
15	6	0	1.054122	-2.424739	-0.580541
16	6	0	-0.523463	-2.064388	2.491549
17	6	0	3.199483	-0.078167	-0.510597
18	6	0	3.742258	-0.588936	-1.701908
19	6	0	5.123694	-0.677701	-1.880172
20	6	0	5.990513	-0.245687	-0.874550
21	6	0	5.464737	0.276124	0.310441
22	6	0	4.084754	0.361860	0.490399
23	1	0	-0.211735	-4.146497	2.193859
24	1	0	-1.049537	-3.393311	0.853741
25	1	0	-0.512755	2.684016	2.852257
26	1	0	1.944763	2.477696	-1.452262
27	1	0	-0.190892	4.751360	1.513386
28	1	0	1.062557	4.643693	-0.641068
29	1	0	1.421974	-4.209825	0.546619
30	1	0	1.887226	-2.742718	1.398515
31	1	0	0.283762	-2.885563	-1.213920
32	1	0	2.014836	-2.588071	-1.086401
33	1	0	-1.521128	-2.221371	2.931592
34	1	0	0.190997	-2.057201	3.324137
35	1	0	3.071071	-0.903324	-2.496946
36	1	0	5.522558	-1.075247	-2.810236
37	1	0	7.066385	-0.311280	-1.013920
38	1	0	6.131479	0.612295	1.100476

39	1	0	3.680930	0.752443	1.421064
40	6	0	-2.193774	0.926117	-1.700063
41	6	0	-2.050350	-0.448842	-1.998505
42	6	0	-2.680091	-1.184888	-0.914841
43	6	0	-3.382998	-0.213308	-0.062506
44	6	0	-3.067242	1.064443	-0.521633
45	6	0	-1.714646	2.086914	-2.520522
46	6	0	-1.413504	-1.050467	-3.217129
47	6	0	-2.975270	-2.656398	-0.928719
48	6	0	-4.250355	-0.587358	1.102800
49	6	0	-3.510312	2.385091	0.035299
50	1	0	-2.545835	2.528253	-3.088309
51	1	0	-0.945812	1.785418	-3.237001
52	1	0	-1.290338	2.875535	-1.890271
53	1	0	-0.645700	-0.394343	-3.636583
54	1	0	-2.164710	-1.227592	-3.999486
55	1	0	-0.939924	-2.010981	-2.993969
56	1	0	-2.154016	-3.235455	-1.360486
57	1	0	-3.872481	-2.856668	-1.533048
58	1	0	-3.166836	-3.040351	0.076979
59	1	0	-3.757041	-1.319922	1.749937
60	1	0	-5.195051	-1.032794	0.761671
61	1	0	-4.495895	0.281727	1.718647
62	1	0	-4.184857	2.898239	-0.663768
63	1	0	-2.659389	3.052304	0.214516
64	1	0	-4.043003	2.265643	0.982499

TS9

Zero-point correction= 0.535093
(Hartree/Particle)
Thermal correction to Energy= 0.566756
Thermal correction to Enthalpy= 0.567700
Thermal correction to Gibbs Free Energy= 0.473558
Sum of electronic and zero-point Energies= -1363.256829
Sum of electronic and thermal Energies= -1363.225166
Sum of electronic and thermal Enthalpies= -1363.224222
Sum of electronic and thermal Free Energies= -1363.318364

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.223965	0.530402	0.067630
2	7	0	-1.865484	-0.456740	-0.880515
3	6	0	-2.642136	-1.181722	-3.170746
4	6	0	-2.653312	-1.204711	-0.042903
5	6	0	-1.997813	-1.441272	1.272608
6	6	0	-0.803601	-0.750267	1.539044
7	6	0	-2.553916	-2.326190	2.203168
8	6	0	-0.162278	-0.989916	2.761736
9	6	0	-1.910271	-2.548999	3.418369
10	6	0	-0.710811	-1.883013	3.690895
11	8	0	-3.771982	-1.642793	-0.345232
12	6	0	0.981995	-1.104180	-0.743863
13	6	0	0.059875	-1.621438	-1.424441
14	6	0	-1.347383	-1.915626	-3.532301
15	6	0	-0.648471	-2.547799	-2.309031
16	6	0	-2.443057	-0.042250	-2.158628
17	6	0	4.274487	-1.833693	0.947956
18	6	0	5.172487	-1.676000	-0.110849

19	6	0	4.691894	-1.321785	-1.373124
20	6	0	3.325149	-1.129185	-1.577512
21	6	0	2.416085	-1.279523	-0.513978
22	6	0	2.908430	-1.629498	0.755121
23	1	0	-3.082374	-0.759722	-4.084870
24	1	0	-3.367605	-1.887784	-2.756112
25	1	0	-3.487690	-2.821143	1.949311
26	1	0	0.772128	-0.490376	3.007632
27	1	0	-2.332140	-3.236372	4.147062
28	1	0	-0.196173	-2.057618	4.633859
29	1	0	-1.572815	-2.722915	-4.240299
30	1	0	-0.643783	-1.239170	-4.036961
31	1	0	0.137422	-3.243142	-2.650048
32	1	0	-1.368137	-3.143544	-1.733421
33	1	0	-1.775180	0.708362	-2.593362
34	1	0	-3.415526	0.438698	-1.977840
35	1	0	4.638502	-2.115743	1.932468
36	1	0	6.236493	-1.829972	0.046073
37	1	0	5.380327	-1.201032	-2.205494
38	1	0	2.951275	-0.862407	-2.561788
39	1	0	2.210749	-1.752233	1.576433
40	6	0	-0.133594	2.341488	1.424303
41	6	0	1.183137	2.116501	0.898556
42	6	0	1.142216	2.423555	-0.525376
43	6	0	-0.180084	2.757575	-0.876692
44	6	0	-0.998937	2.646332	0.320470
45	6	0	-0.522291	2.385918	2.872792
46	6	0	2.440365	1.917847	1.696293
47	6	0	2.344887	2.444214	-1.421633
48	6	0	-0.664179	3.237973	-2.214407
49	6	0	-2.455673	2.999075	0.410514
50	1	0	-1.567511	2.102972	3.022395
51	1	0	-0.392648	3.405789	3.261655
52	1	0	0.087842	1.718187	3.484919
53	1	0	3.144522	1.252103	1.188622
54	1	0	2.226333	1.483395	2.677088
55	1	0	2.954066	2.874923	1.868795
56	1	0	2.065113	2.412091	-2.478812
57	1	0	3.011868	1.599865	-1.223208
58	1	0	2.927148	3.362885	-1.262694
59	1	0	-0.043020	2.863879	-3.034467
60	1	0	-0.644398	4.335917	-2.265308
61	1	0	-1.695314	2.928905	-2.409178
62	1	0	-2.997373	2.696691	-0.490654
63	1	0	-2.593813	4.083160	0.531433
64	1	0	-2.934806	2.506310	1.260825

I_2

Zero-point correction= 0.537935
(Hartree/Particle)
Thermal correction to Energy= 0.569211
Thermal correction to Enthalpy= 0.570155
Thermal correction to Gibbs Free Energy= 0.477334
Sum of electronic and zero-point Energies= -1363.304802
Sum of electronic and thermal Energies= -1363.273526
Sum of electronic and thermal Enthalpies= -1363.272582
Sum of electronic and thermal Free Energies= -1363.365403

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	0.499684	-0.497577	-0.166395
2	7	0	0.726803	1.675808	-0.759561
3	6	0	0.468779	3.492285	-2.482748
4	6	0	1.609440	2.259445	0.245592
5	6	0	1.478484	1.626085	1.572542
6	6	0	0.943299	0.320927	1.636100
7	6	0	1.944135	2.299254	2.712589
8	6	0	0.846476	-0.266325	2.906299
9	6	0	1.837747	1.693000	3.959607
10	6	0	1.280984	0.411419	4.050254
11	8	0	2.398485	3.140618	-0.045617
12	6	0	-1.205151	0.630244	-0.045965
13	6	0	-0.731947	1.809324	-0.457289
14	6	0	-1.034473	3.593497	-2.178782
15	6	0	-1.327964	3.161952	-0.725175
16	6	0	1.026788	2.098280	-2.153160
17	6	0	-4.956959	0.140722	-0.192925
18	6	0	-3.655670	0.496099	-0.550641
19	6	0	-2.576221	0.270444	0.325884
20	6	0	-2.846503	-0.337910	1.567367
21	6	0	-4.148511	-0.683318	1.926202
22	6	0	-5.210182	-0.447853	1.047549
23	1	0	0.659147	3.701820	-3.543390
24	1	0	1.021645	4.237372	-1.901225
25	1	0	2.383436	3.286705	2.599659
26	1	0	0.420227	-1.260046	3.016615
27	1	0	2.180747	2.207244	4.853063
28	1	0	1.184325	-0.065273	5.023788
29	1	0	-1.386729	4.618196	-2.350176
30	1	0	-1.595055	2.941908	-2.864268
31	1	0	-2.404565	3.134717	-0.528941
32	1	0	-0.892625	3.905743	-0.038783
33	1	0	0.570050	1.345311	-2.803760
34	1	0	2.110660	2.070471	-2.289523
35	1	0	-5.774035	0.322425	-0.886781
36	1	0	-3.463168	0.942933	-1.522396
37	1	0	-2.021448	-0.517904	2.249775
38	1	0	-4.336124	-1.139345	2.895146
39	1	0	-6.223469	-0.724924	1.325824
40	6	0	1.698895	-2.501167	0.020468
41	6	0	0.254936	-2.679932	0.077736
42	6	0	-0.270101	-2.418213	-1.254089
43	6	0	0.792336	-1.949478	-2.052998
44	6	0	2.016977	-1.993970	-1.256688
45	6	0	2.657734	-2.839814	1.124272
46	6	0	-0.496143	-3.393380	1.166193
47	6	0	-1.689906	-2.658995	-1.675695
48	6	0	0.733026	-1.578791	-3.507209
49	6	0	3.382977	-1.649324	-1.779261
50	1	0	2.802281	-3.927104	1.192550
51	1	0	2.297847	-2.493065	2.097769
52	1	0	3.638982	-2.386107	0.959010
53	1	0	-0.001460	-3.281505	2.135766
54	1	0	-0.561729	-4.471695	0.958800
55	1	0	-1.517902	-3.013521	1.265554
56	1	0	-2.397188	-2.373669	-0.891926
57	1	0	-1.851784	-3.723811	-1.896029
58	1	0	-1.949380	-2.093619	-2.575643
59	1	0	-0.277415	-1.287146	-3.809618

60	1	0	1.036061	-2.421177	-4.145293
61	1	0	1.404745	-0.745669	-3.741273
62	1	0	3.796583	-2.470807	-2.381478
63	1	0	4.088249	-1.448008	-0.968087
64	1	0	3.358128	-0.762108	-2.421257

Single Point energies (atomic units) in solution (methanol) calculated with PCM and the basis set [B3LYP/6-311+G(2df,2p) (C, H, O, N) SDD (Rh)] for the stationary points calculated with basis set [B3LYP/6-31G(d) (C, H, O, P) LANL2DZ (Rh)]

1a
SCF Done: E(RB3LYP) = -826.383854445

RhCp*(OAc)$_2$
SCF Done: E(RB3LYP) = -958.034208475

AcOH
SCF Done: E(RB3LYP) = -229.184617354

A
SCF Done: E(RB3LYP) = -1555.20491705

TS1
SCF Done: E(RB3LYP) = -1555.17823861

B
SCF Done: E(RB3LYP) = -1555.19747310

C
SCF Done: E(RB3LYP) = -1326.01092398

TS2
SCF Done: E(RB3LYP) = -1325.97607810

D$_1$
SCF Done: E(RB3LYP) = -1326.01578781

TS3
SCF Done: E(RB3LYP) = -1325.99167880

E$_1$
SCF Done: E(RB3LYP) = -1326.04167573

C$_2$

SCF Done: E(RB3LYP) = -1326.00656776

TS4
SCF Done: E(RB3LYP) = -1325.98087699

D_2
SCF Done: E(RB3LYP) = -1326.00869134

TS5
SCF Done: E(RB3LYP) = -1325.98637592

E
SCF Done: E(RB3LYP) = -1326.05323034

2a:
SCF Done: E(RB3LYP) = -825.235899617

F:
SCF Done: E(RB3LYP) = -1248.55309852

***TS6*:**
SCF Done: E(RB3LYP) = -1248.52655976

G_1
SCF Done: E(RB3LYP) = -1248.57956030

***TS7*:**
SCF Done: E(RB3LYP) = -1248.52362053

G_2
SCF Done: E(RB3LYP) = -1248.56847424

H
SCF Done: E(RB3LYP) = -1365.32606176

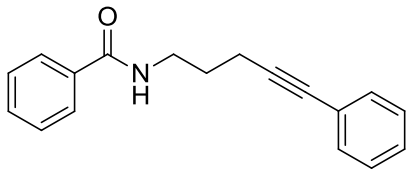
***TS8*:**
SCF Done: E(RB3LYP) = -1365.30182313

I_1
SCF Done: E(RB3LYP) = -1365.34481675

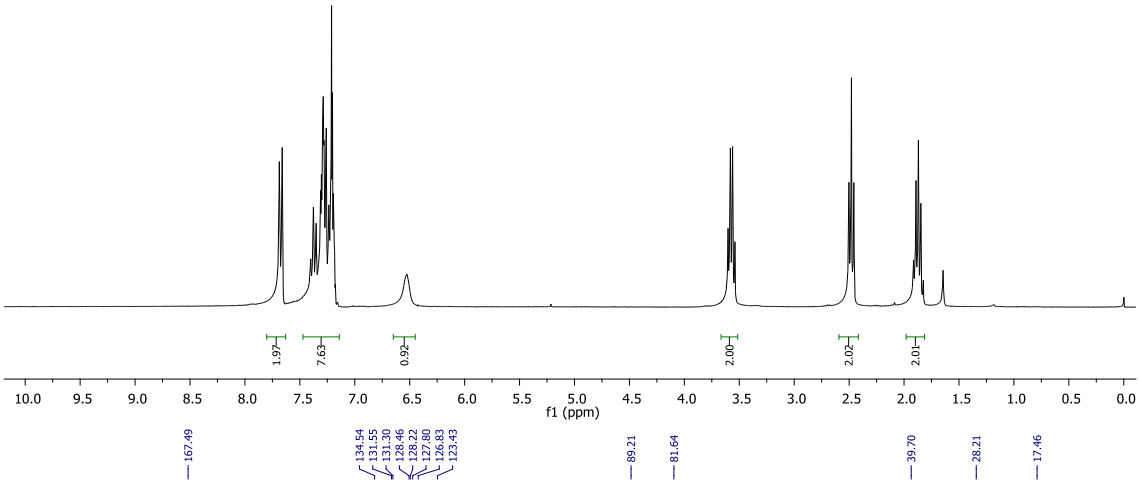
***TS9*:**
SCF Done: E(RB3LYP) = -1365.30375982

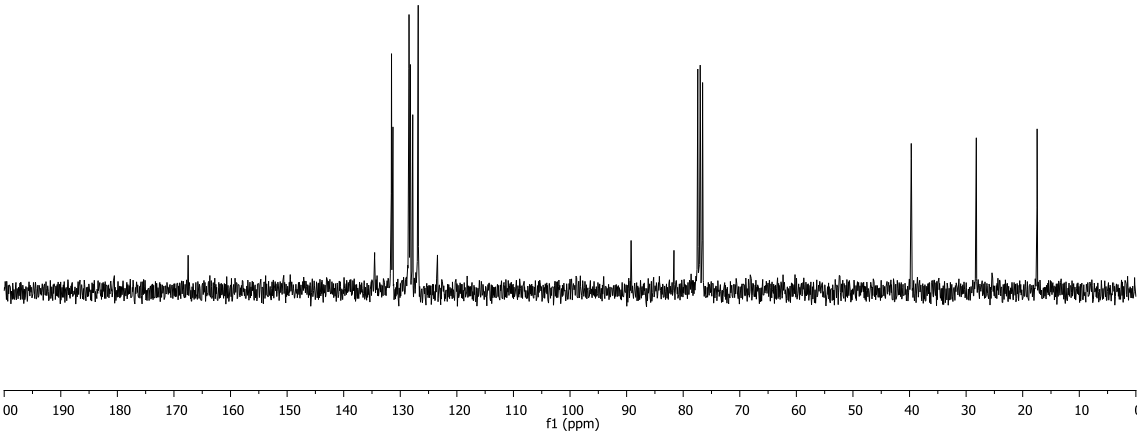
I_2
SCF Done: E(RB3LYP) = -1365.34370592

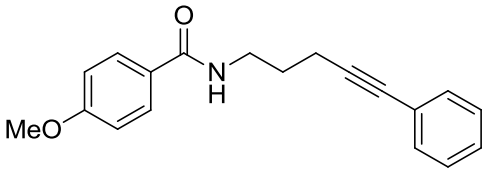
4. NMR-Spectra



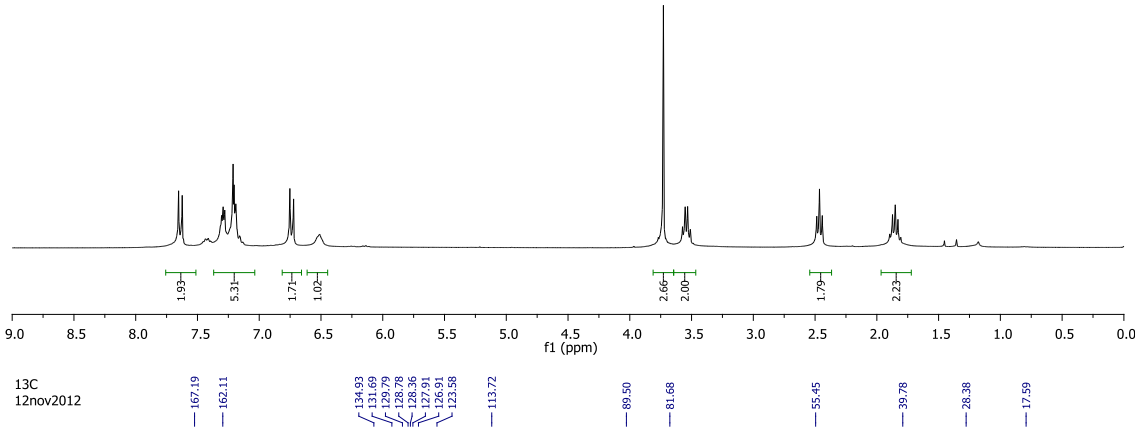
1a



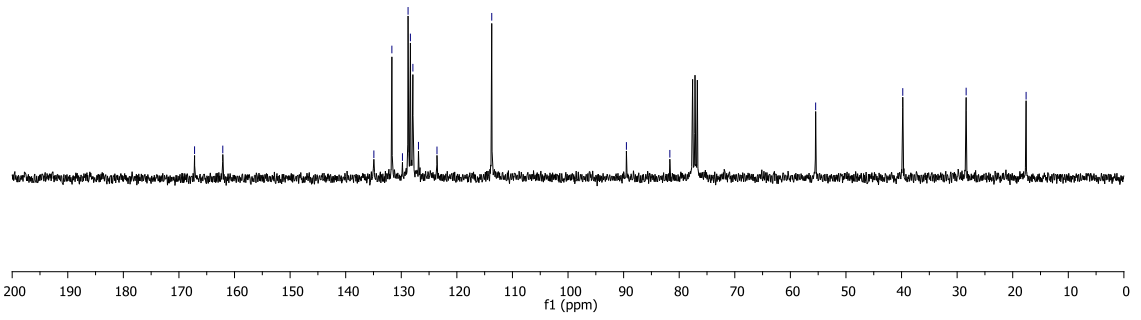


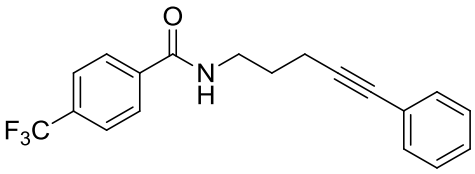

O
N
H
MeO

1b

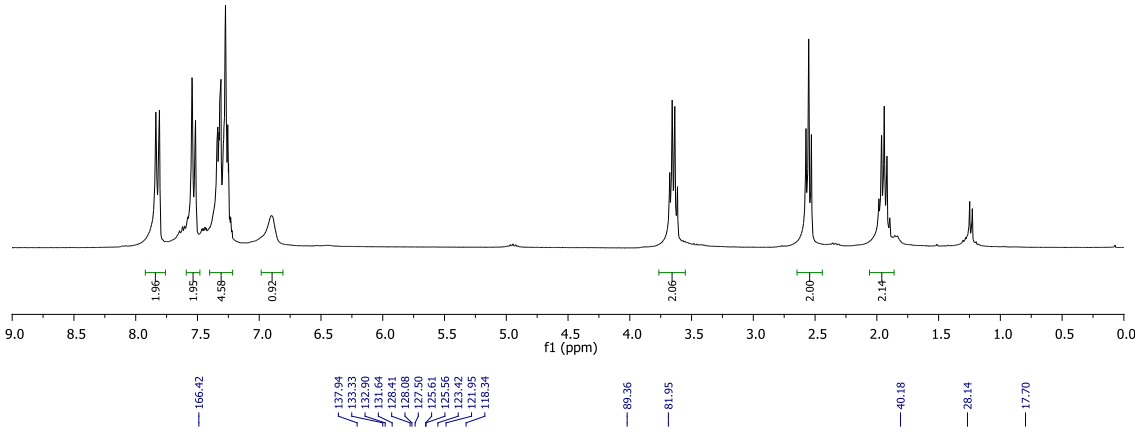

1.93
5.31
1.71
1.02
2.66
2.00
1.79
2.23
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

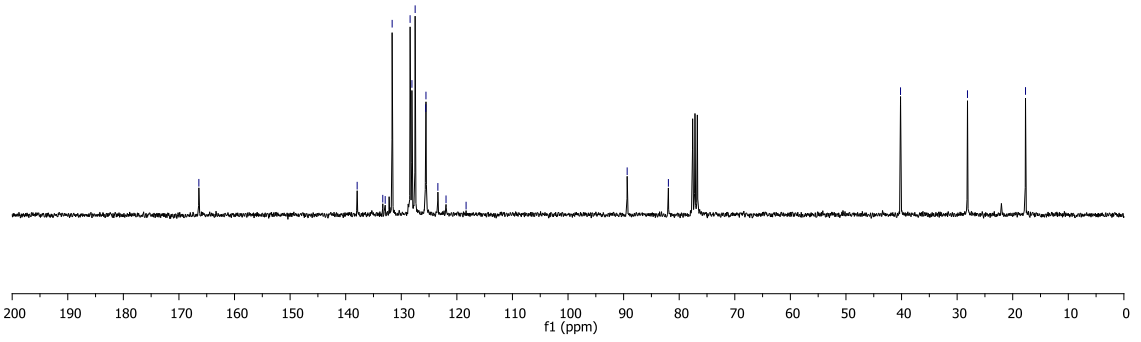
13C
12nov2012
167.19
162.11
134.93
131.69
129.79
128.78
128.36
127.91
126.91
123.58
113.72
89.50
81.68
55.45
39.78
28.38
17.59

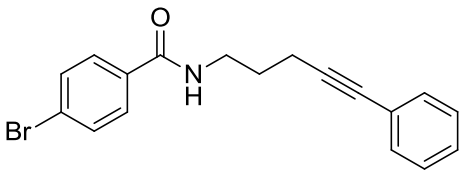

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



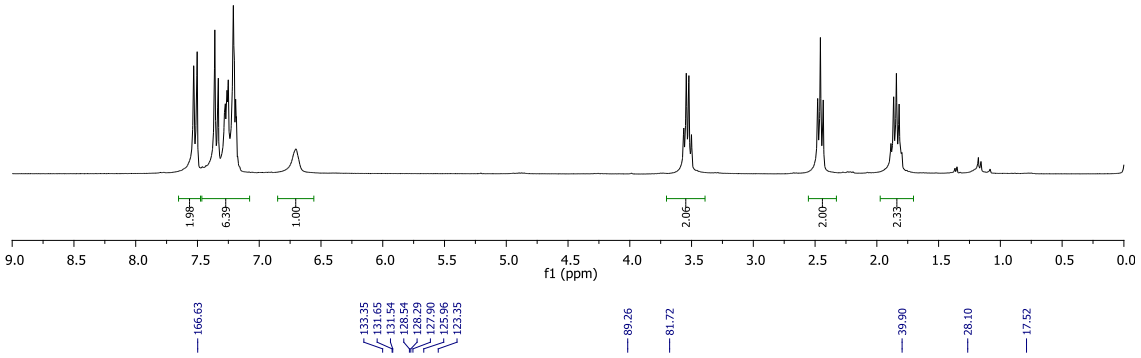
1c

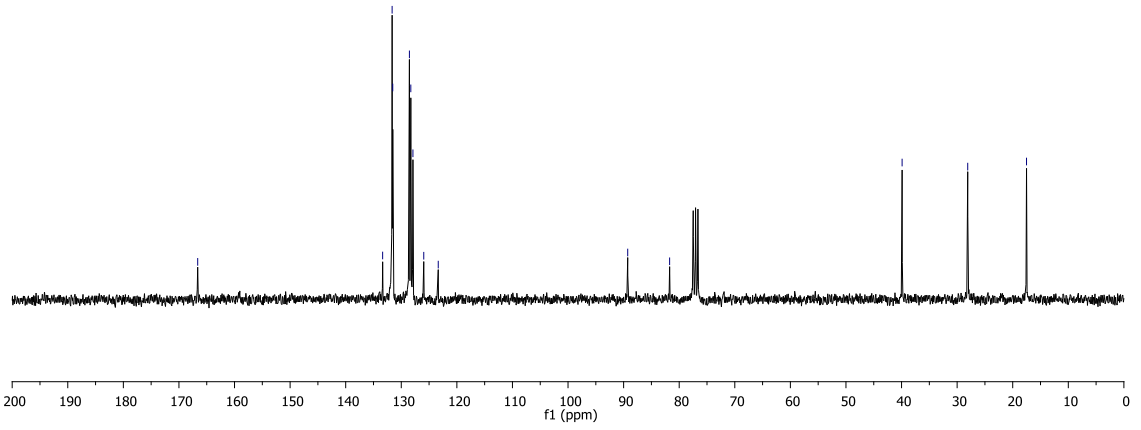


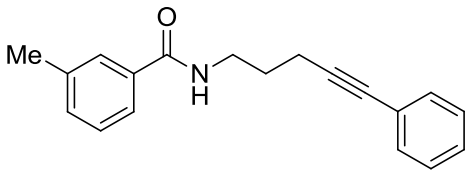




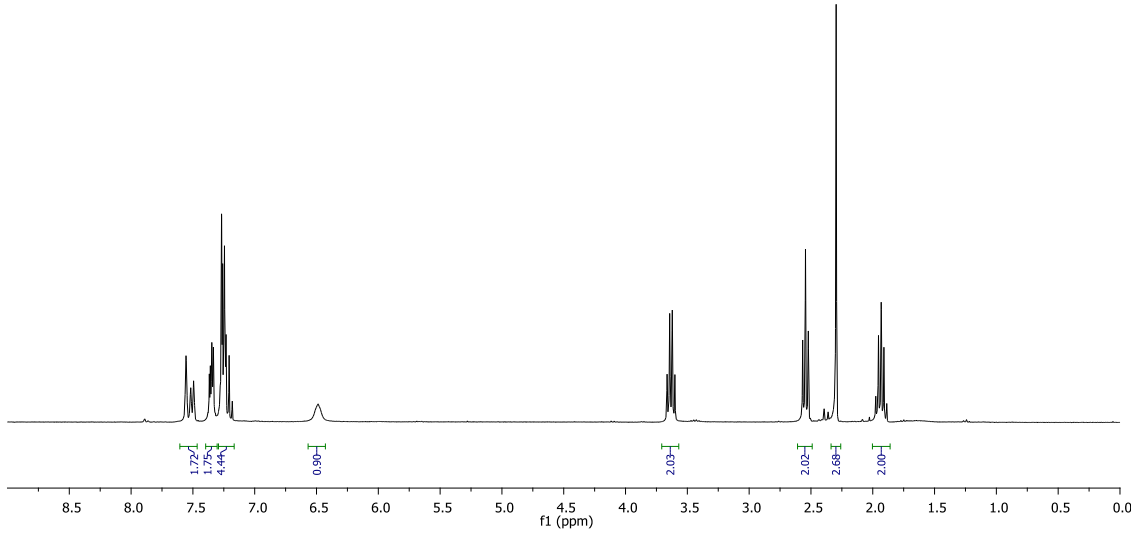
1d

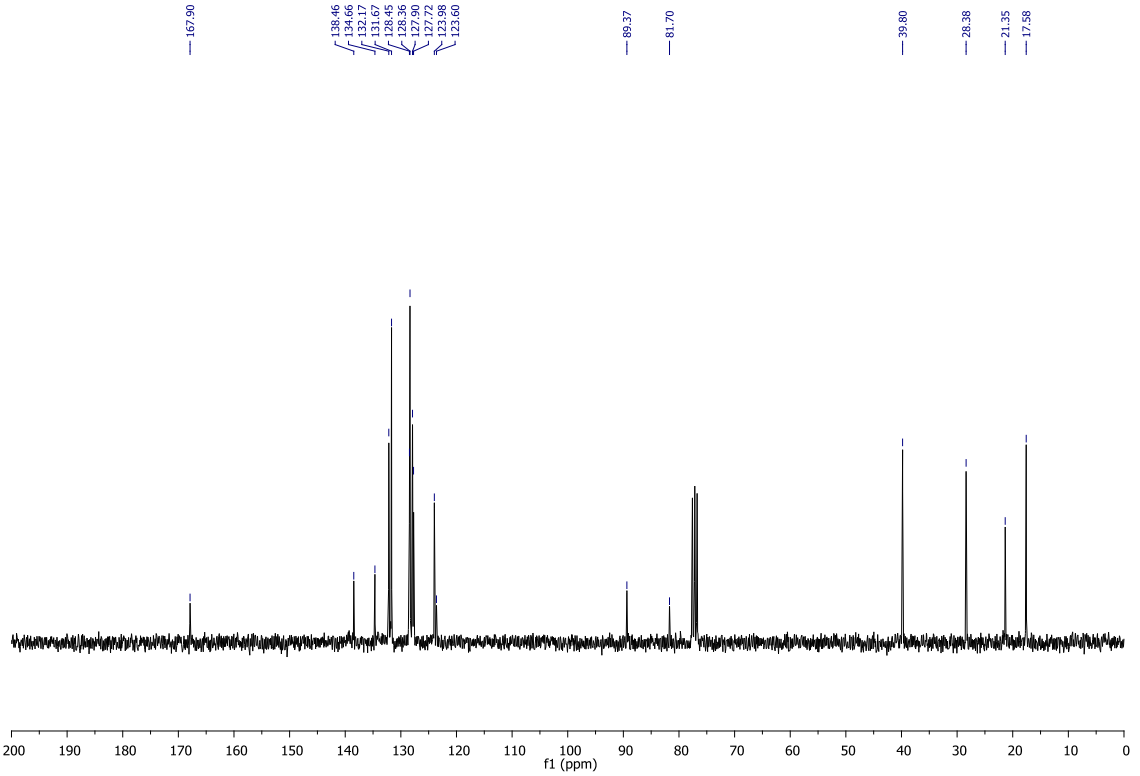


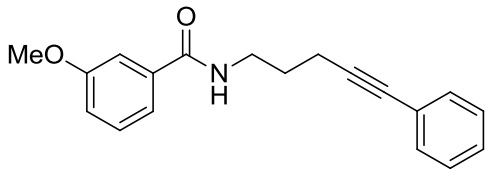



Me
O
N
H

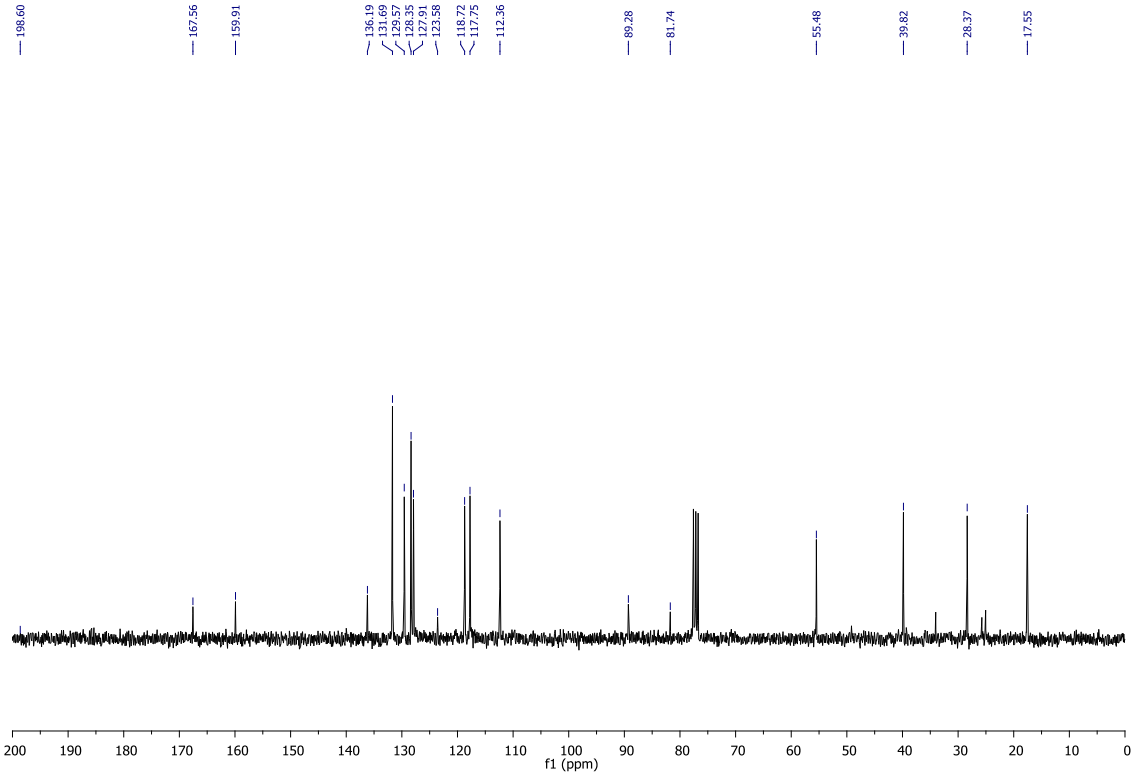
1e

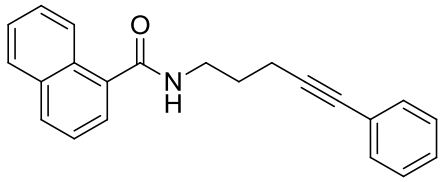

1.72
1.75
4.44
0.90
2.03
2.02
2.68
2.00
f1 (ppm)


167.90
138.46
134.66
131.77
131.67
128.45
128.36
127.90
127.72
123.98
123.60
89.37
81.70
39.80
28.38
21.35
17.58
f1 (ppm)

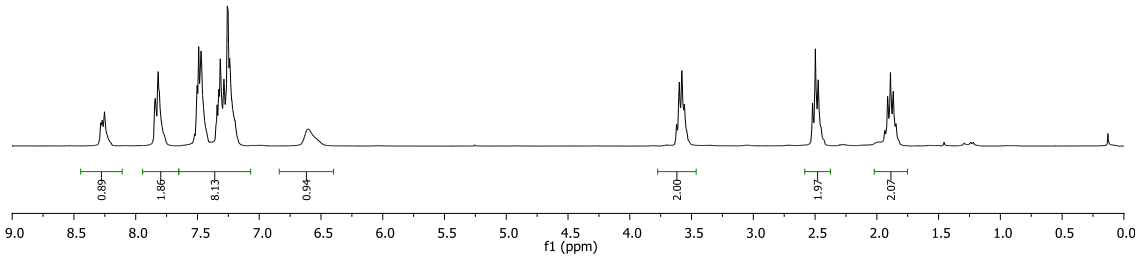


1f

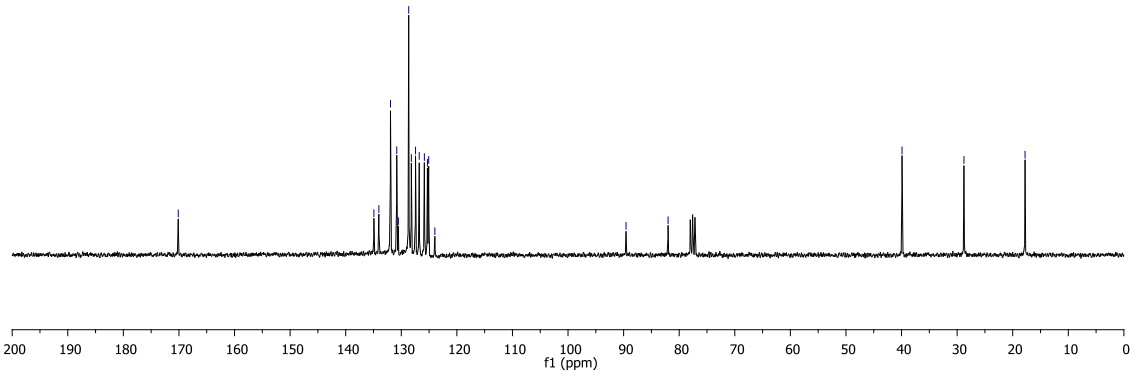


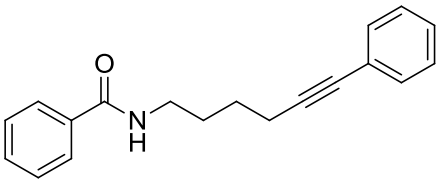

O
N
H

1g

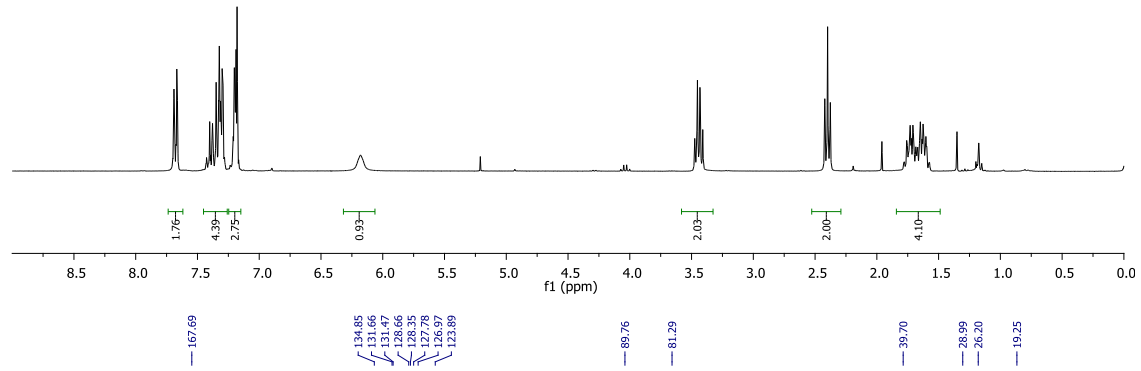

0.89
1.86
8.13
0.94
2.00
1.97
2.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

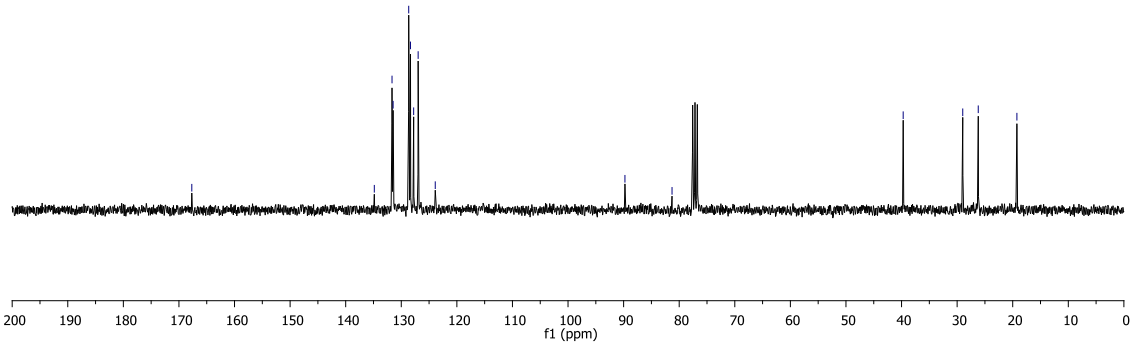

13C
12nov2012
170.12
134.93
134.04
131.94
130.81
130.53
128.66
128.19
127.43
126.77
125.85
125.30
125.07
123.96
89.56
82.00
39.91
28.77
17.78

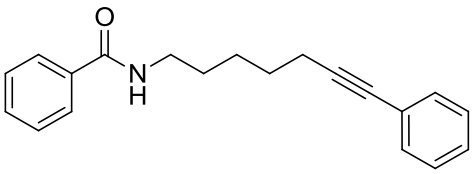

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



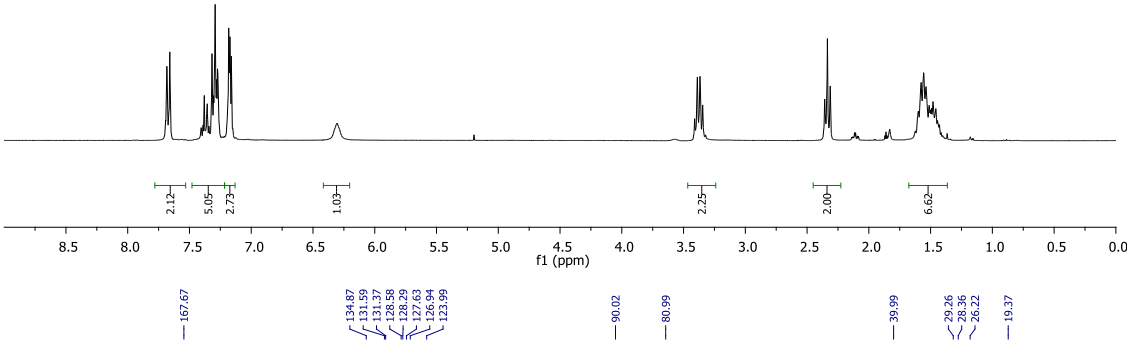
1h

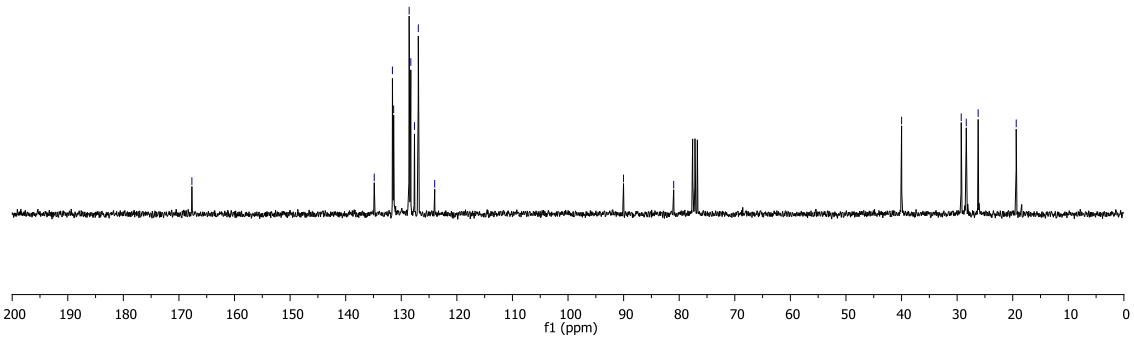


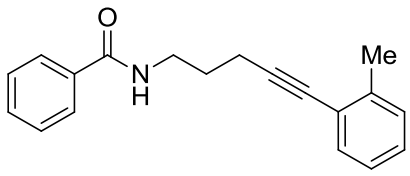




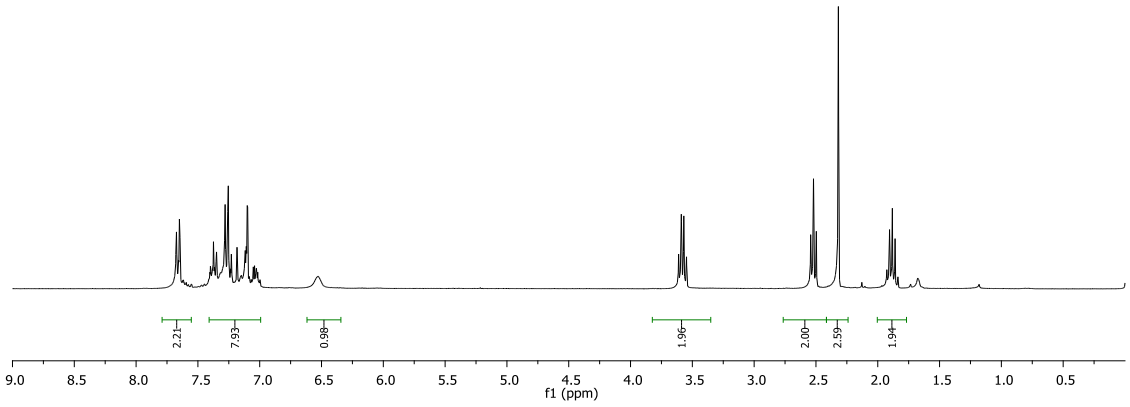
1i



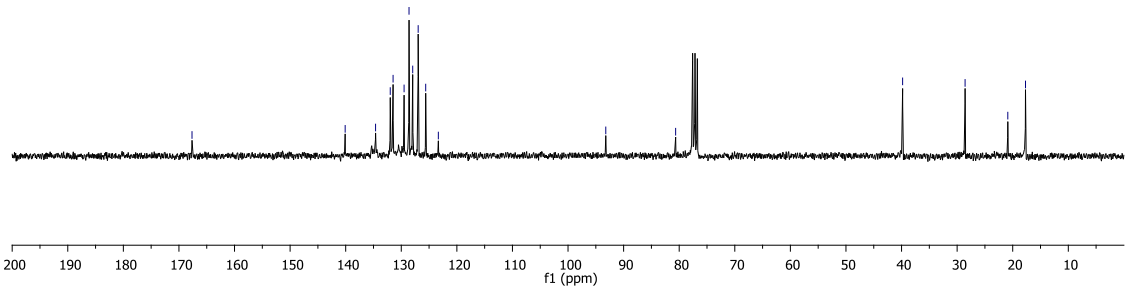


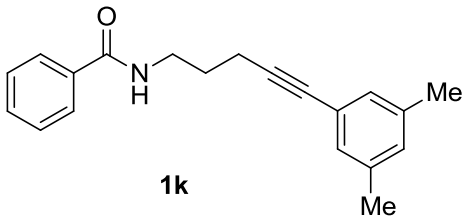

O
N
H
Me

1j

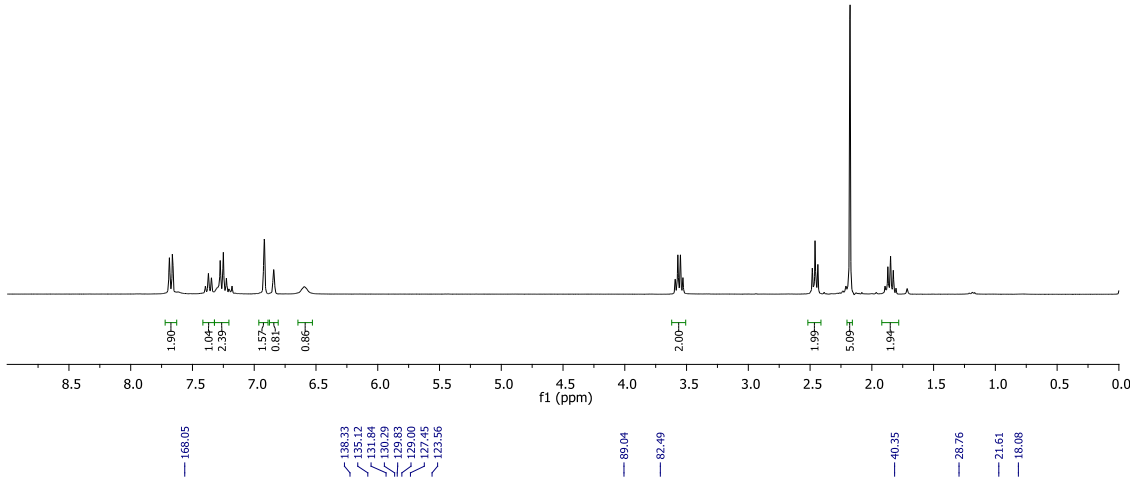

2.21
7.93
0.98
1.96
2.00
2.59
1.94
f1 (ppm)


13C
12nov2012
167.65
140.09
134.63
131.98
131.48
129.49
128.61
127.94
126.96
125.61
123.33
93.21
80.64
39.81
28.57
20.88
17.70

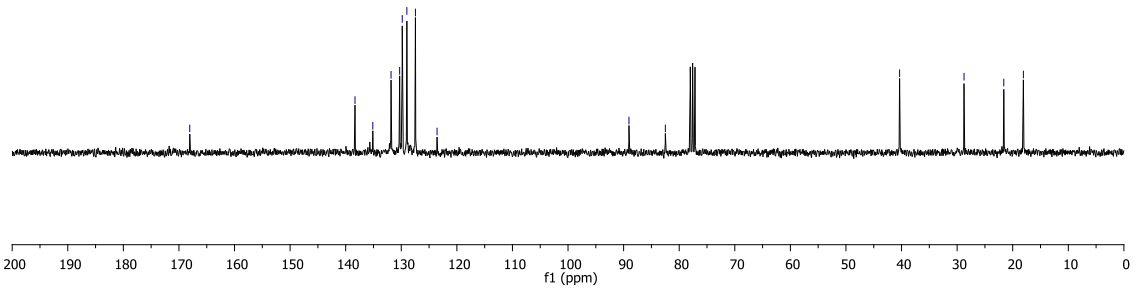

f1 (ppm)

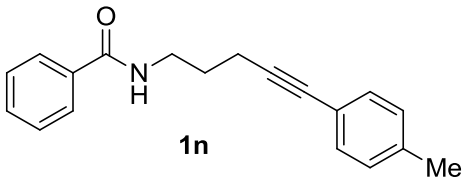

O
N
H
Me
Me

1k

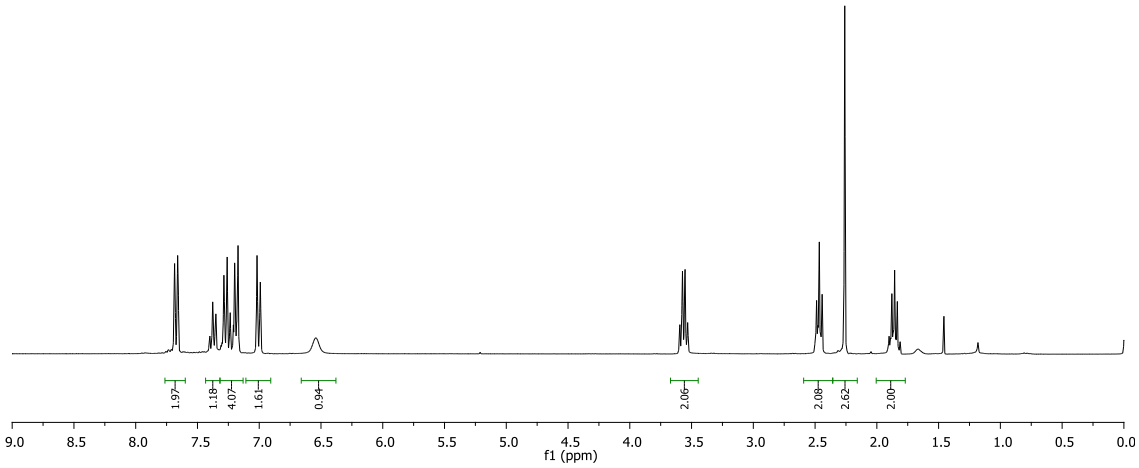

1.90
1.04
2.39
1.57
0.81
0.86
2.00
1.99
5.09
1.94
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

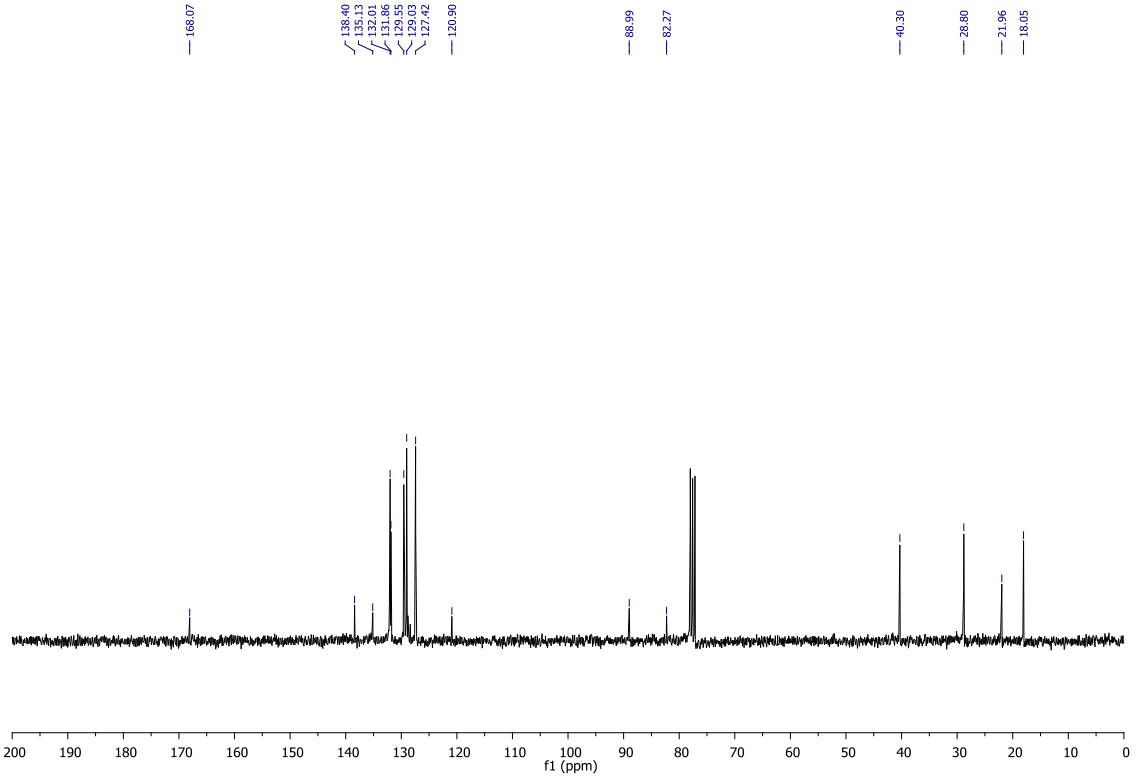
168.05
138.33
135.12
131.84
130.29
129.83
129.00
127.45
123.56
89.04
82.49
40.35
28.76
21.61
18.08

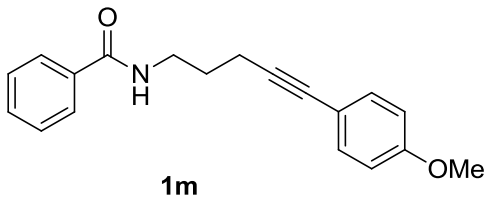

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
H
Me

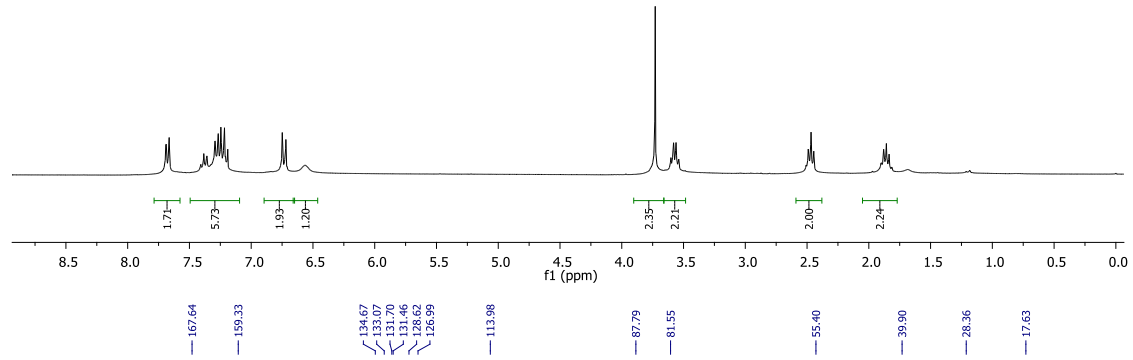
1n

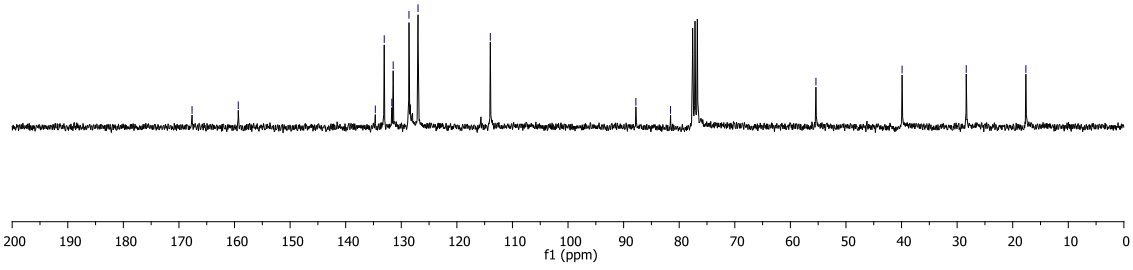

1.97
1.18
4.07
1.61
0.94
2.06
2.08
2.62
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

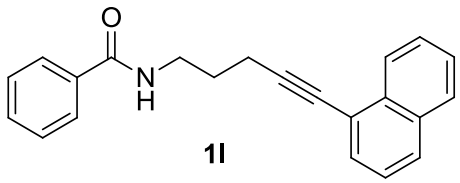

168.07
138.40
135.13
132.01
131.86
129.55
129.03
127.42
120.90
88.99
82.27
40.30
28.80
21.96
18.05
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



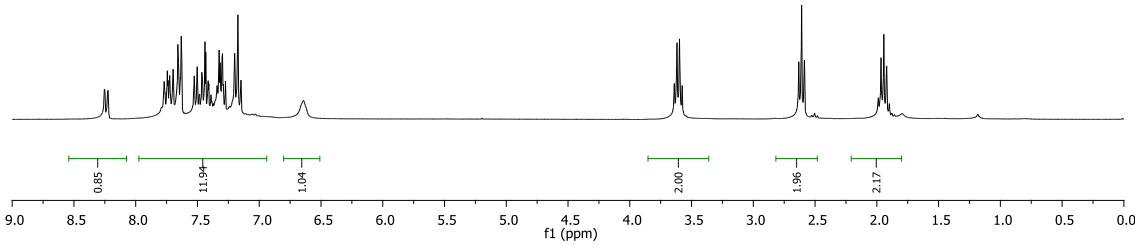
1m



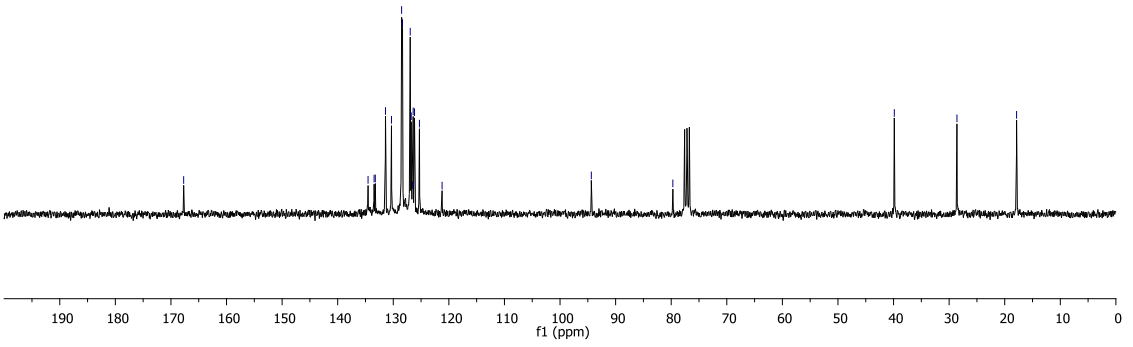


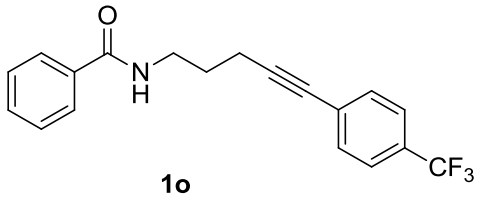

O
N
H

1l

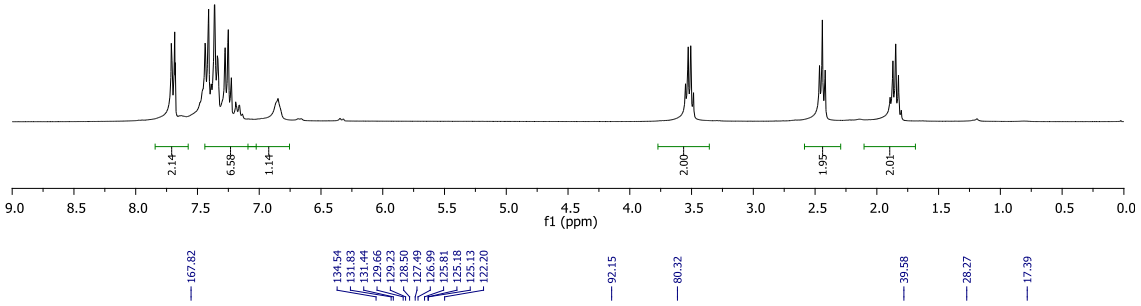

0.85
11.94
1.04
2.00
1.96
2.17
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

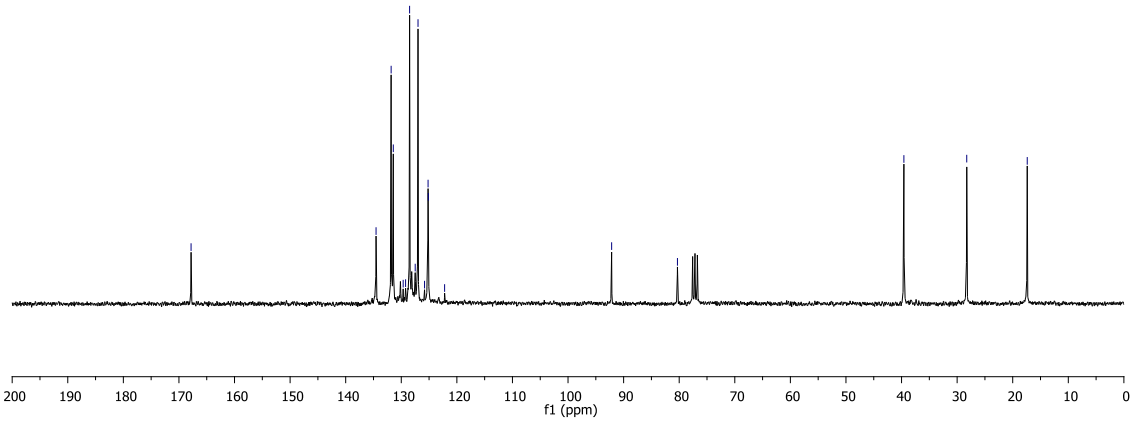

13C
12nov2012
167.71
134.54
133.45
133.23
131.40
130.32
128.50
128.34
126.95
126.77
126.53
126.42
126.18
125.30
121.22
94.37
79.70
39.87
28.59
17.86

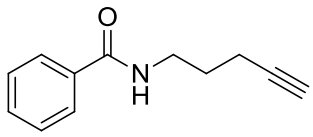

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



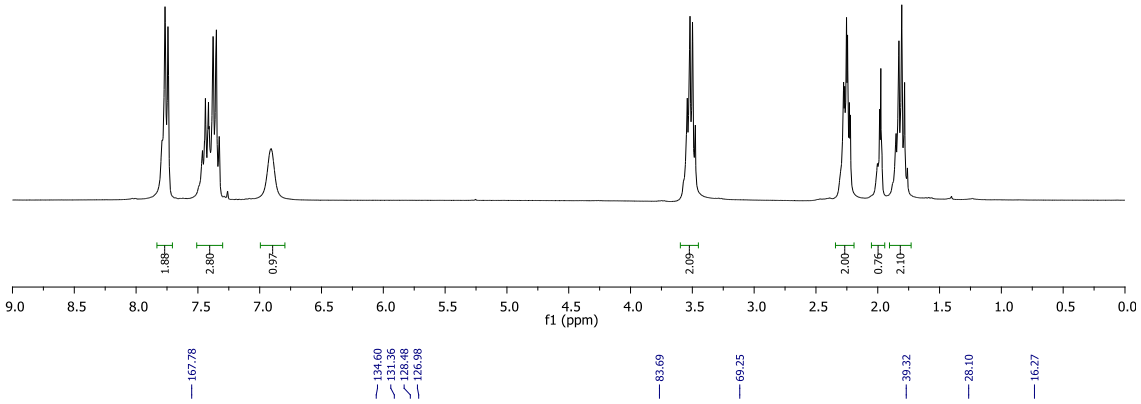
1o



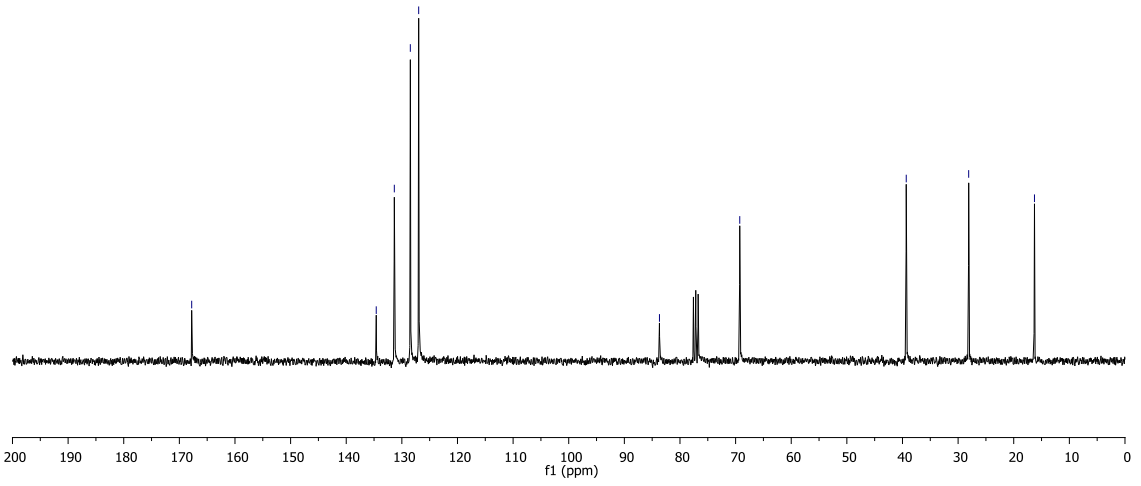


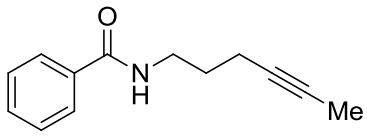


1p

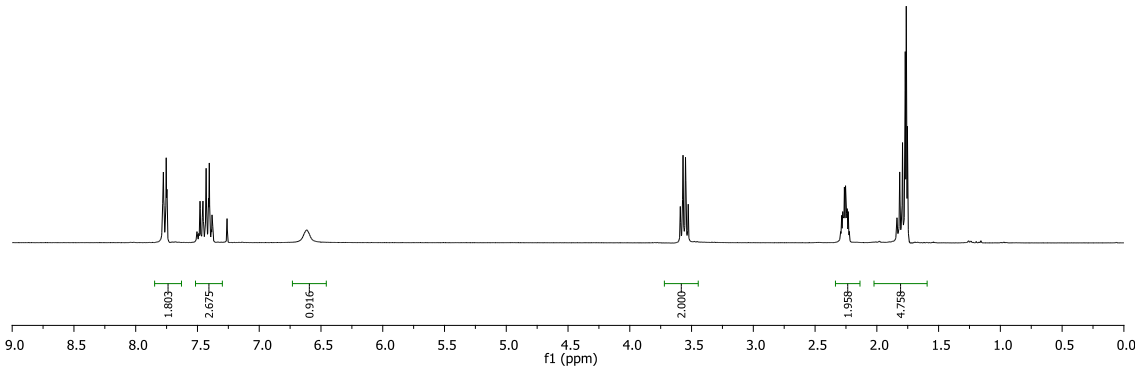

1.88
2.80
0.97
2.09
2.00
0.76
2.10
f1 (ppm)

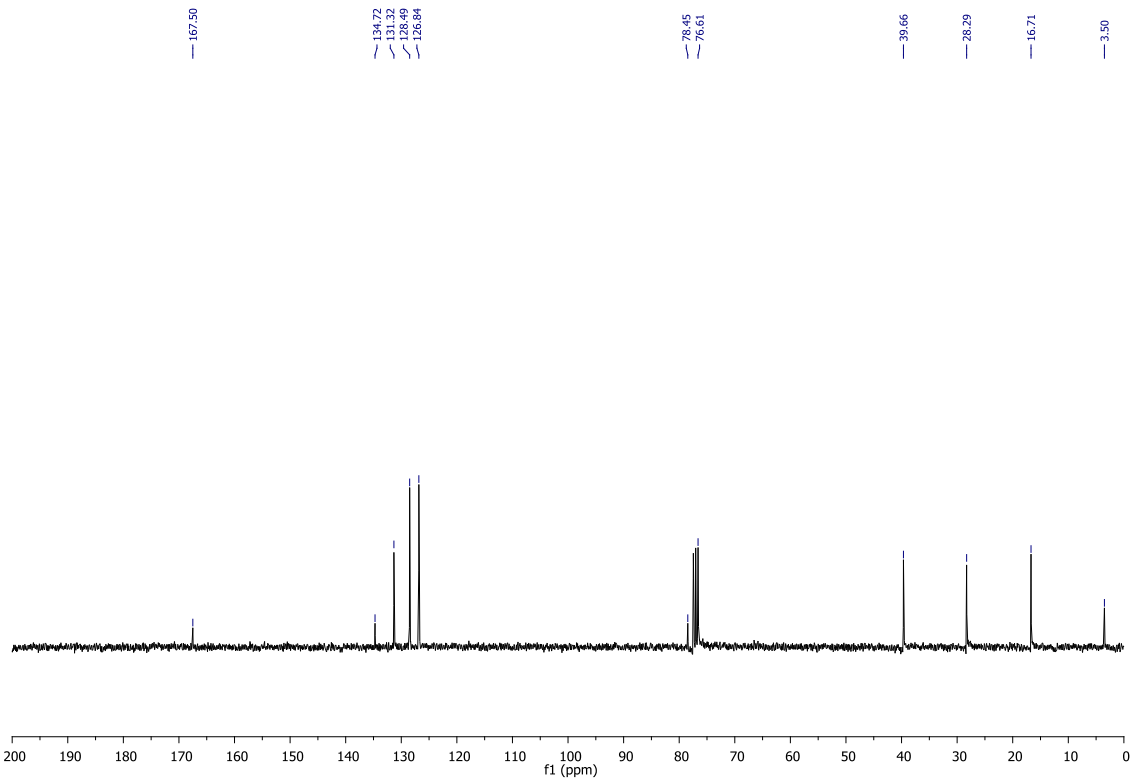
167.78
134.60
131.35
128.48
126.98
83.69
69.25
39.32
28.10
16.27

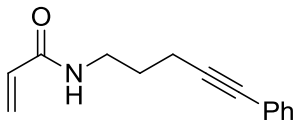

f1 (ppm)



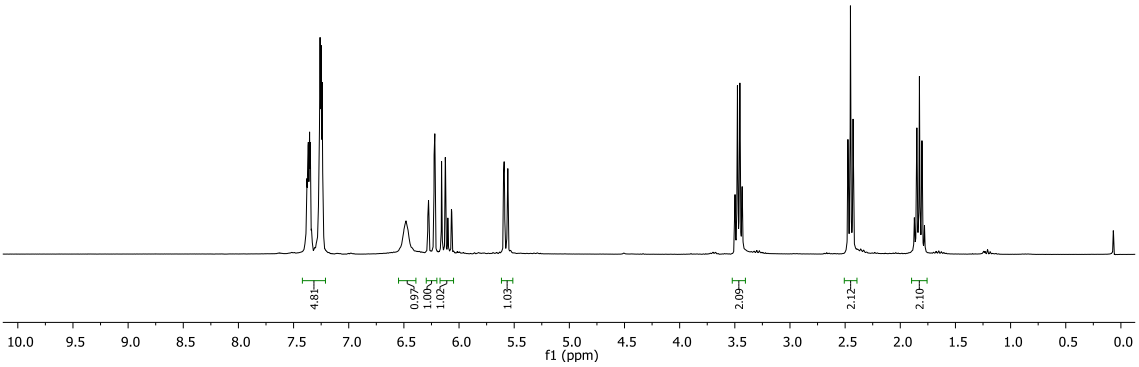
1q

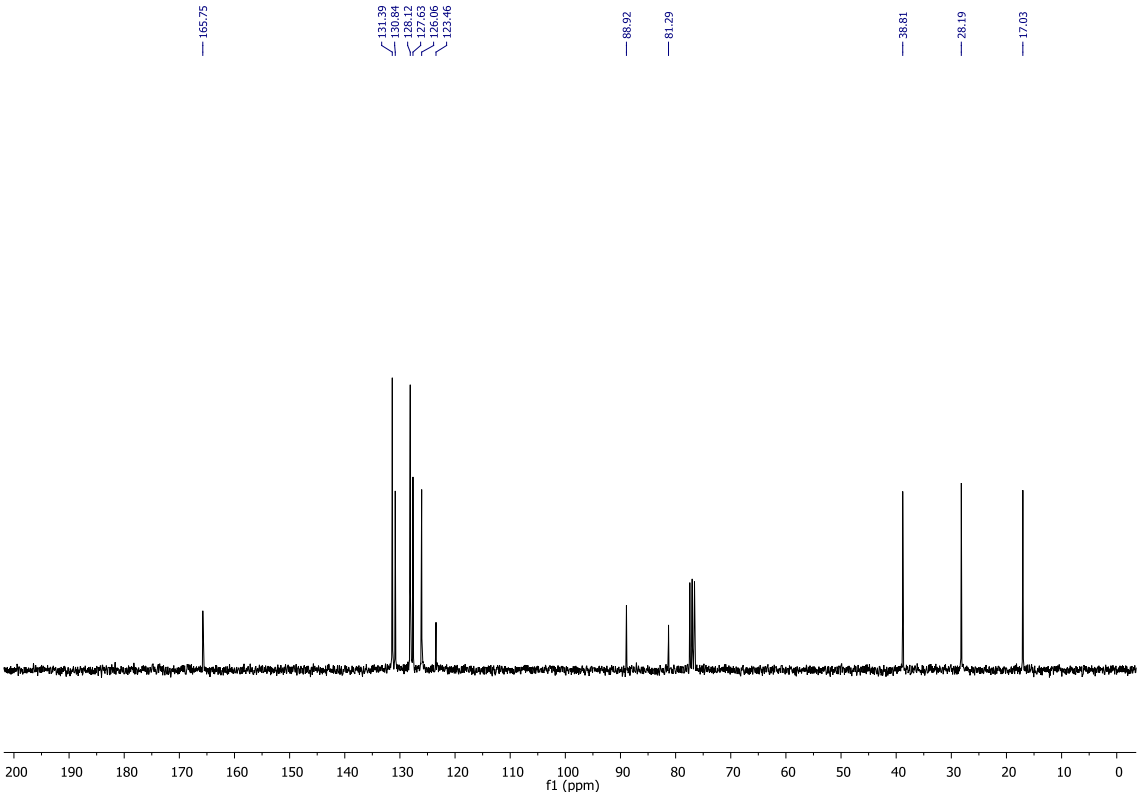


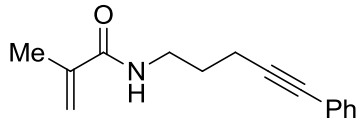




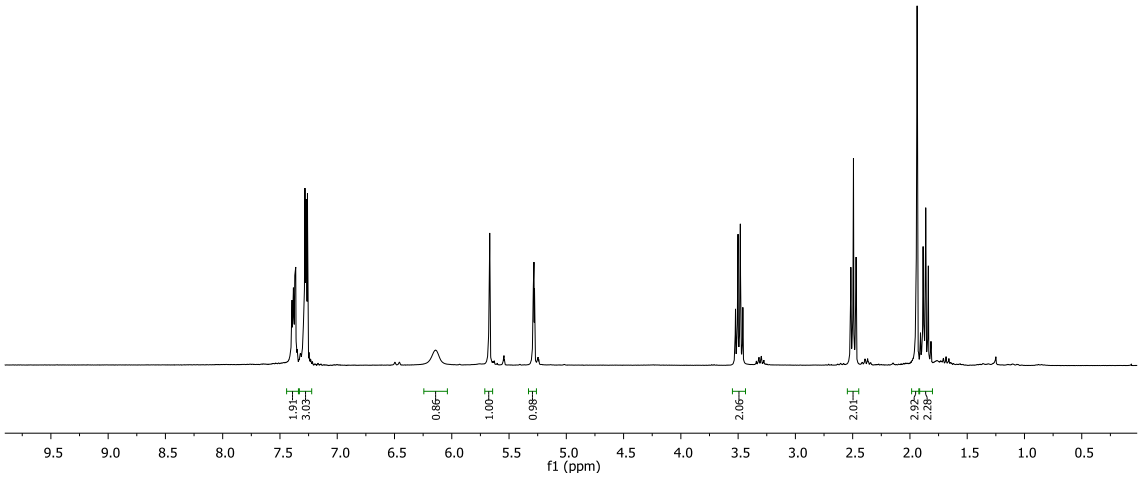
1r

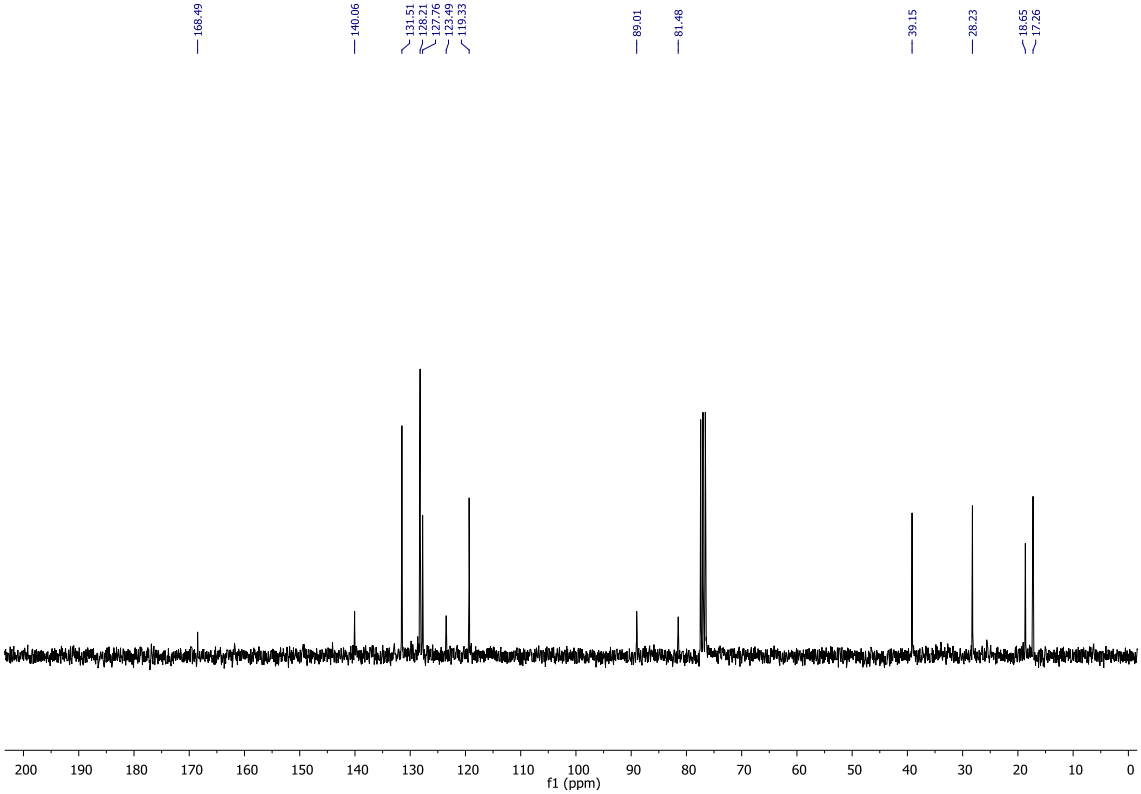


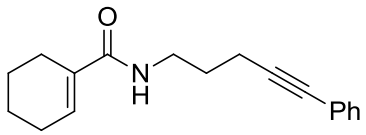




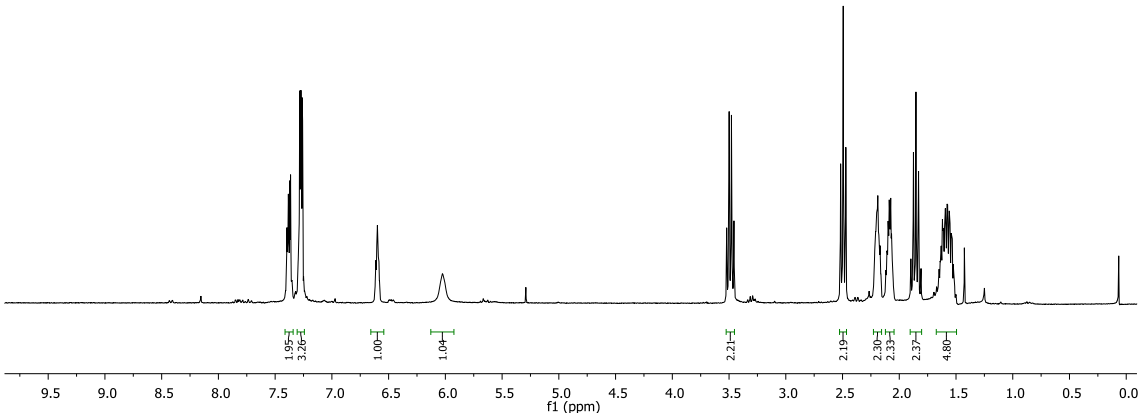
1s

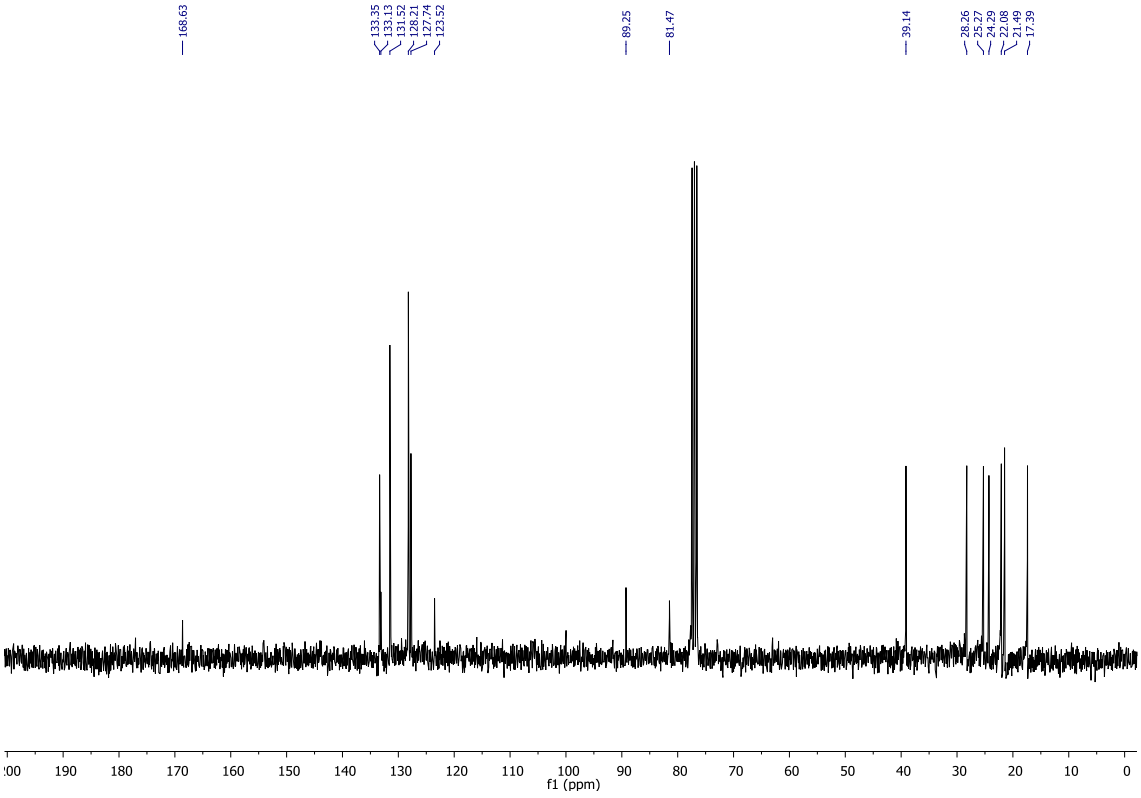


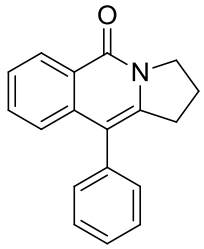



O
N
H
Ph

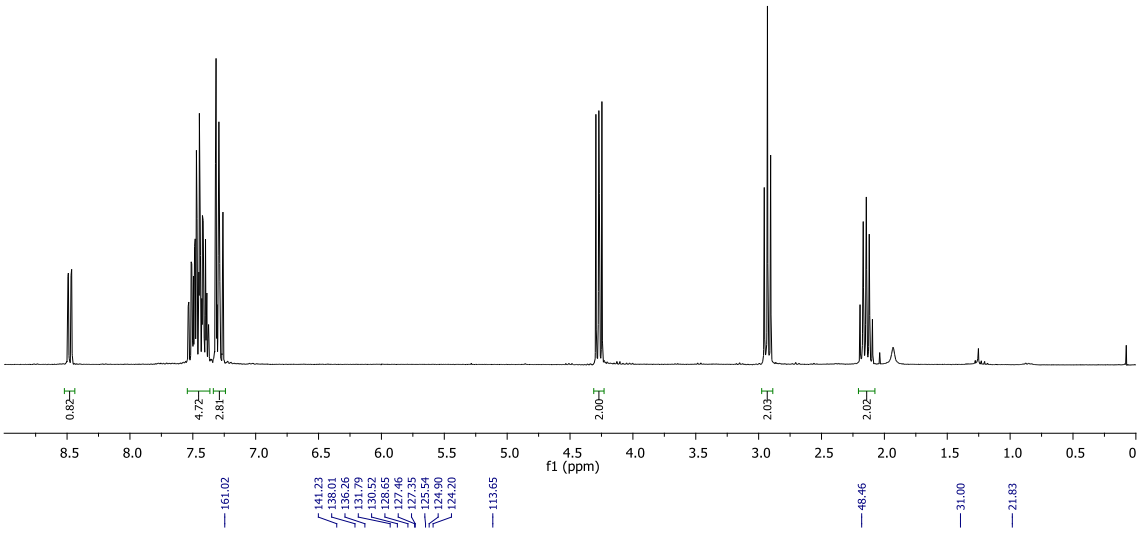
1t


1.95
3.26
1.00
1.04
2.21
2.19
2.30
2.33
2.37
4.80
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

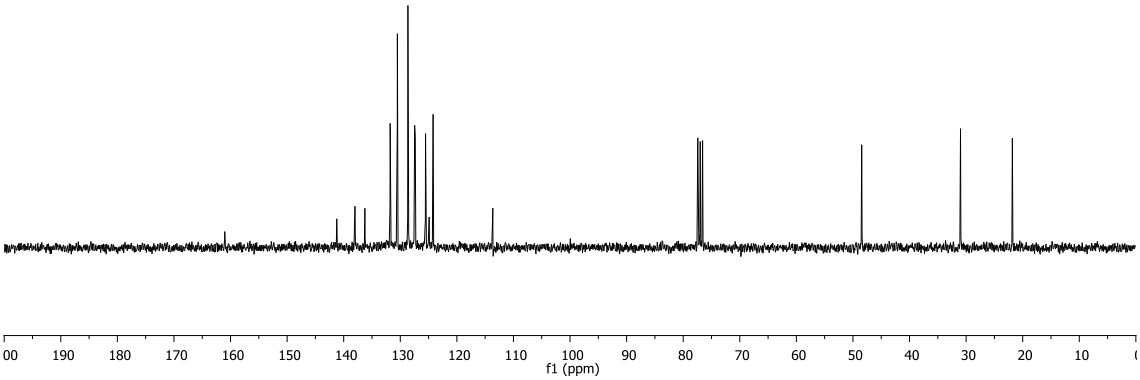

168.63
133.35
133.13
131.52
128.21
127.74
123.52
89.25
81.47
39.14
28.26
25.27
24.29
22.08
21.49
17.39
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

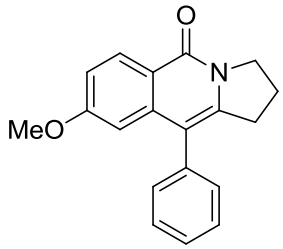

O
N

2a

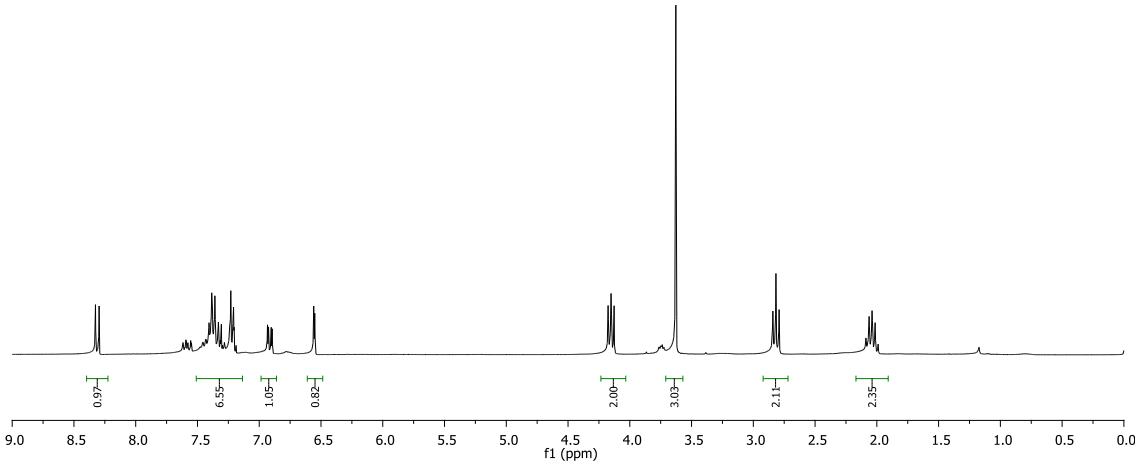

0.82
4.72
2.81
2.00
2.03
2.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

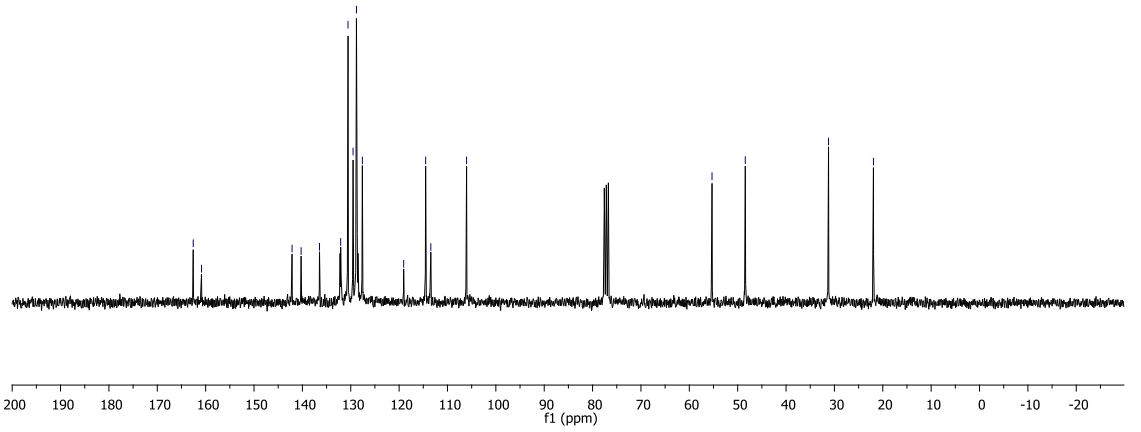
161.02
141.23
138.01
136.26
131.79
130.52
128.65
127.46
127.35
125.54
124.90
124.20
113.65
48.46
31.00
21.83

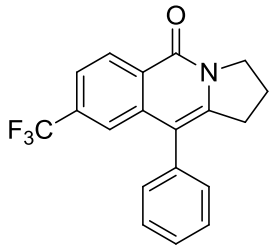

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



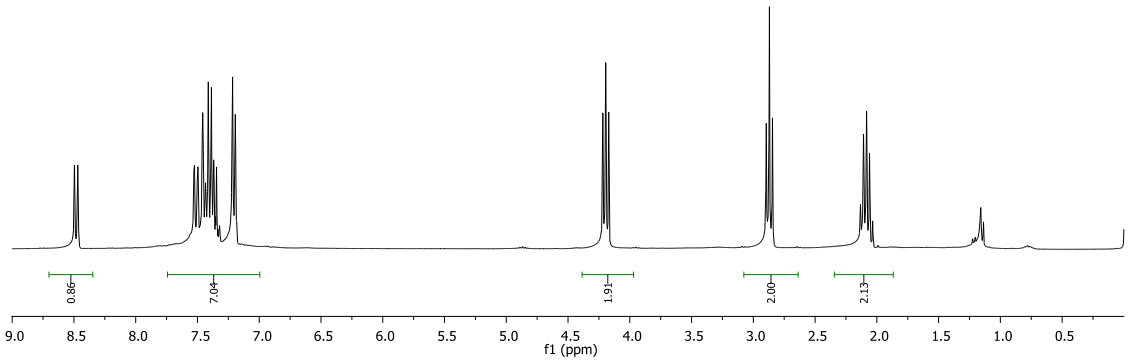
2b



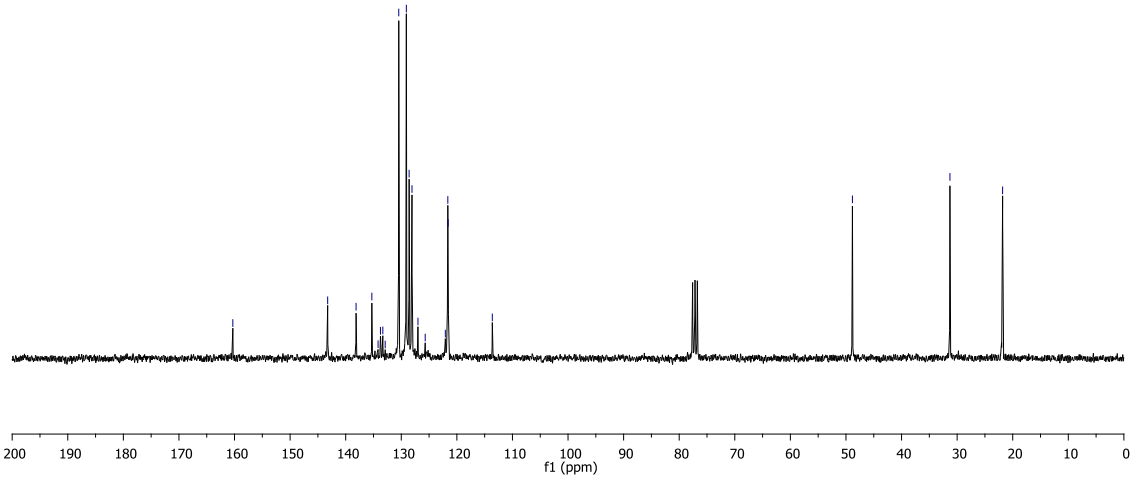


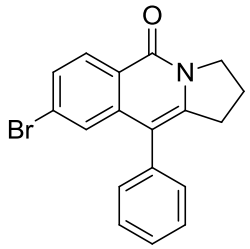

O
N
F3C

2c

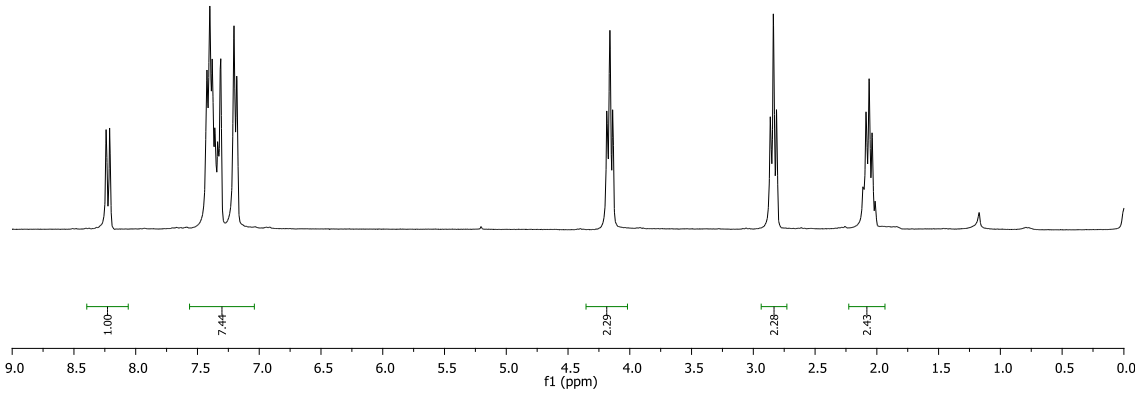

0.86
7.04
1.91
2.00
2.13
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

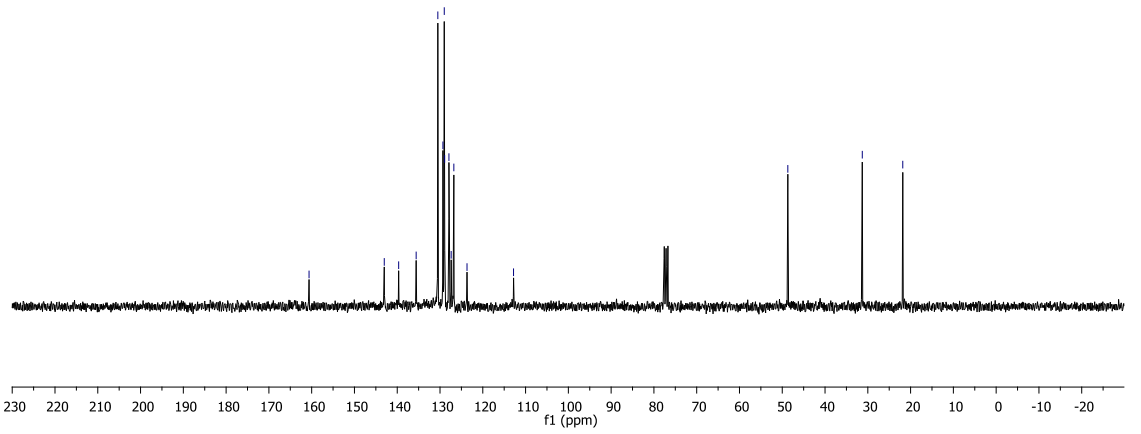

160.30
143.24
138.13
135.29
133.75
133.32
130.45
129.99
129.59
128.07
127.00
121.63
121.58
113.62
48.84
31.29
21.82

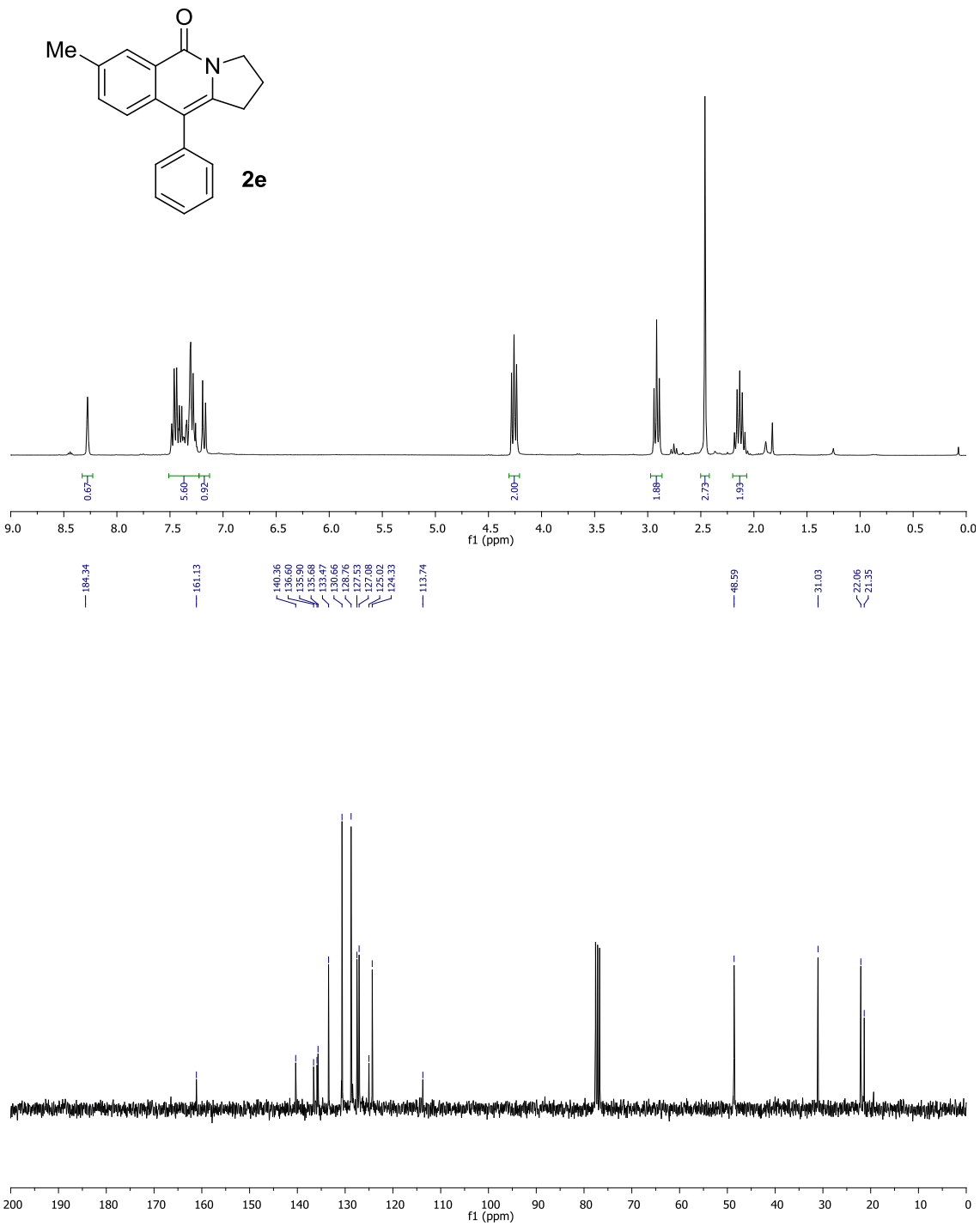

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

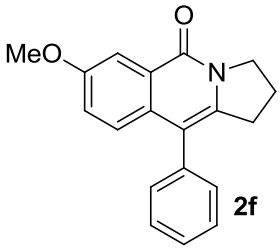


2d

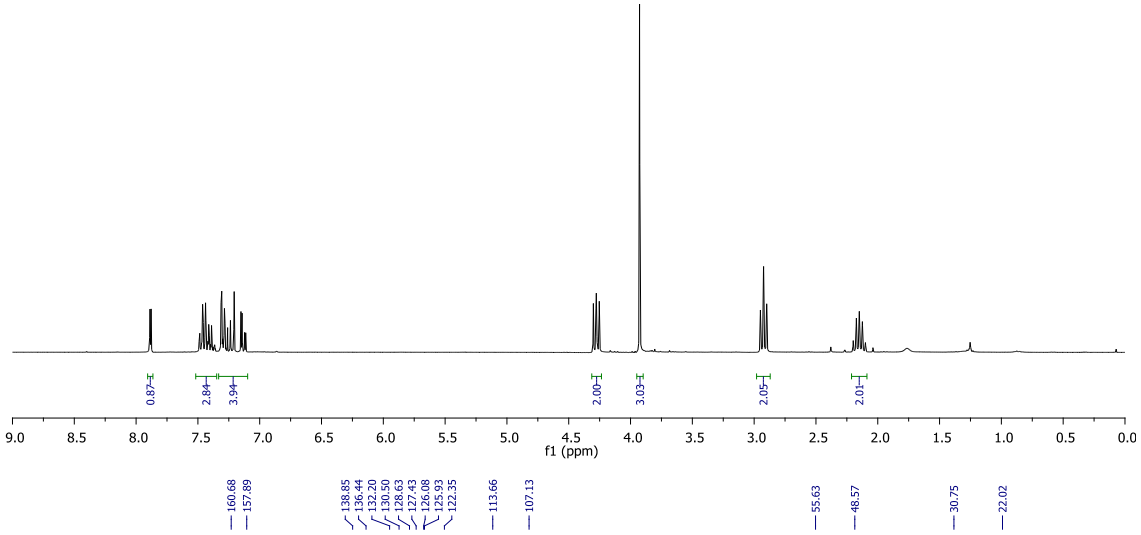




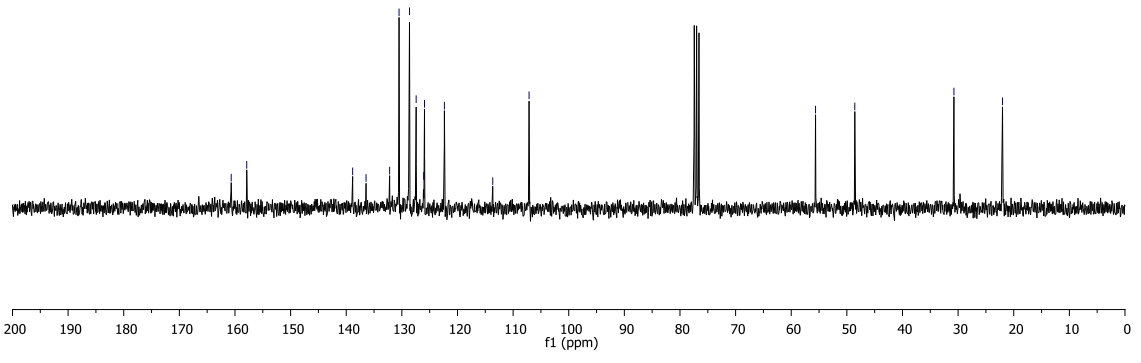


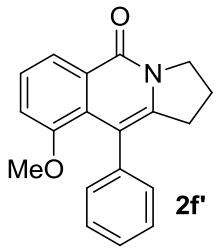

O
MeO
N

2f

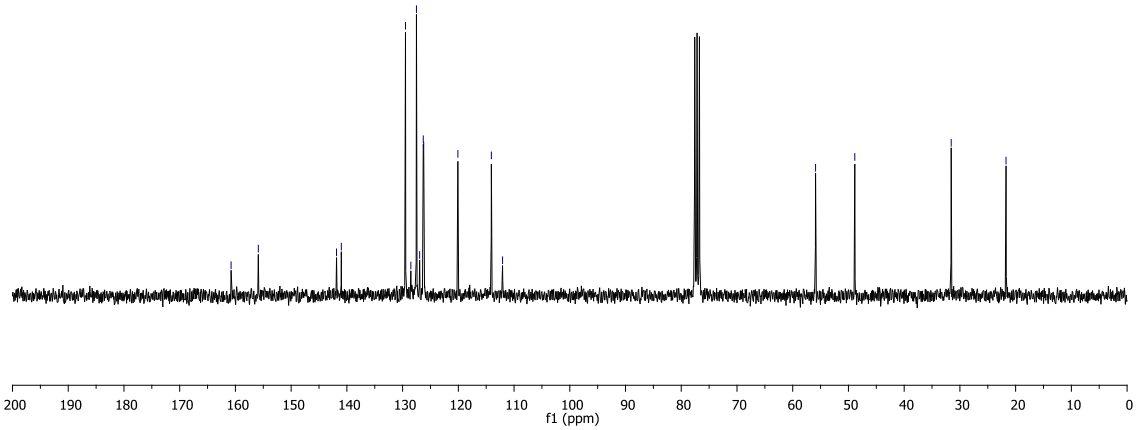

0.87
2.84
3.94
2.00
3.03
2.05
2.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

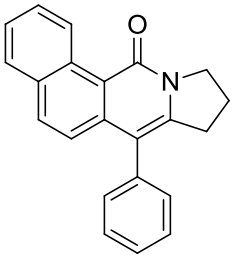
160.68
157.89
138.85
136.44
132.20
130.50
128.63
127.43
126.08
125.93
122.35
113.66
107.13
55.63
48.57
30.75
22.02


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

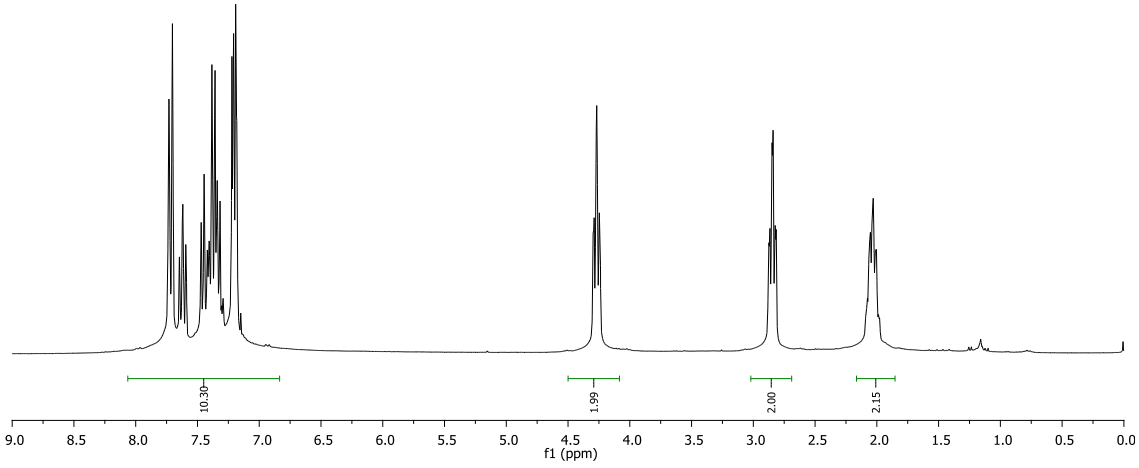


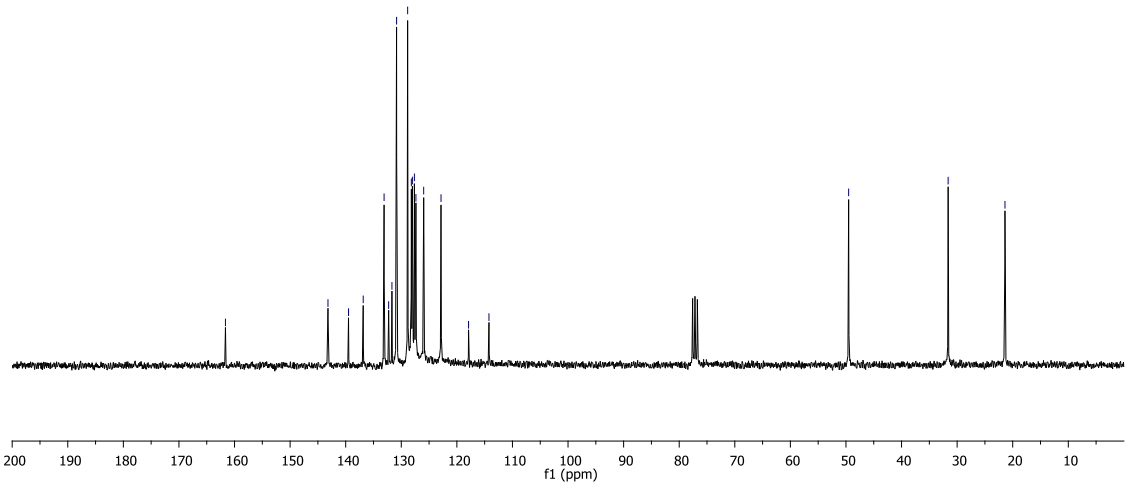
2f'

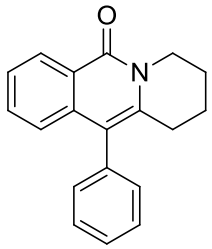




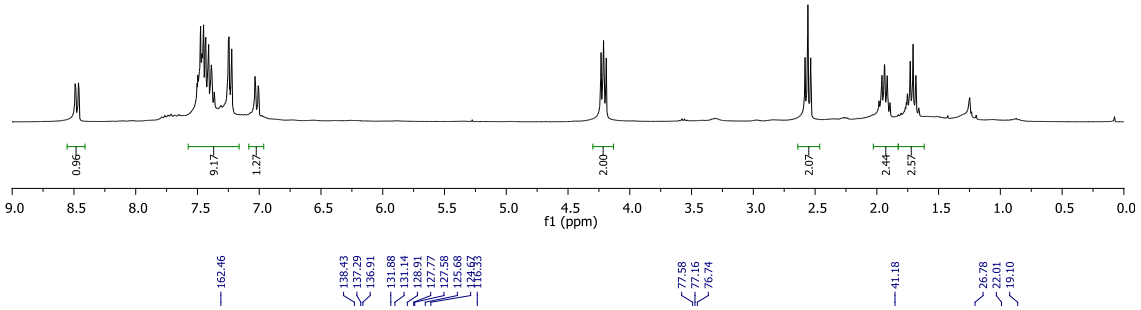
2g

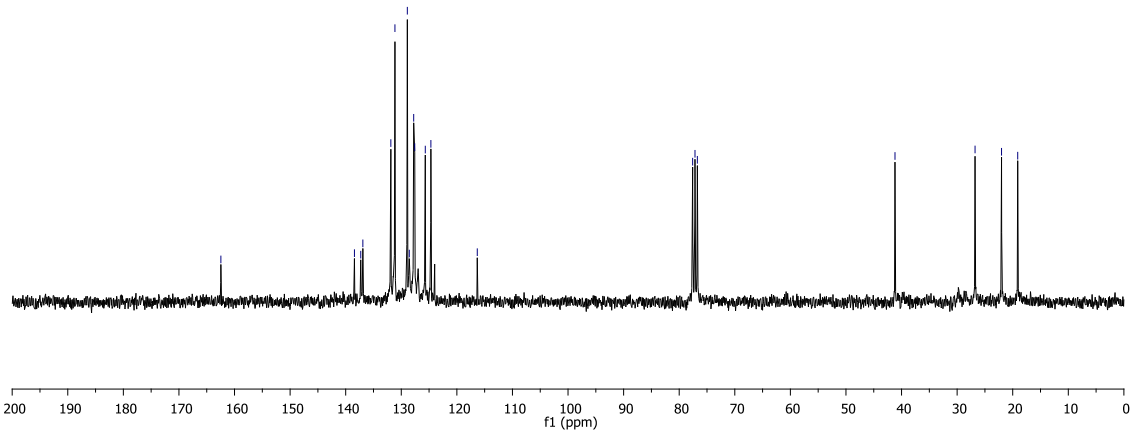


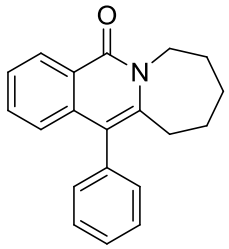




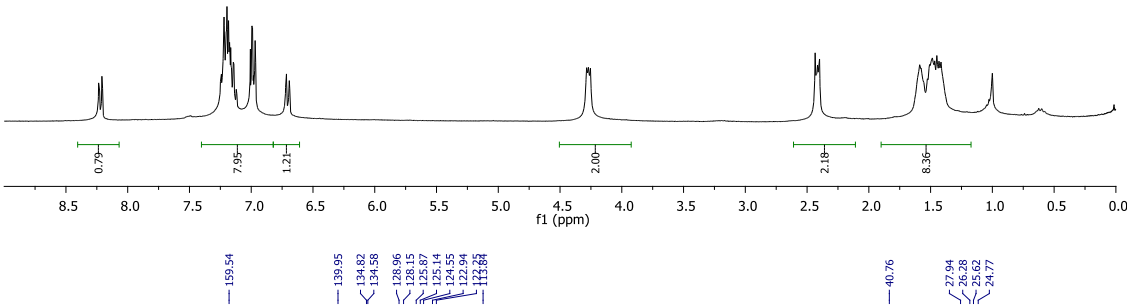
2h



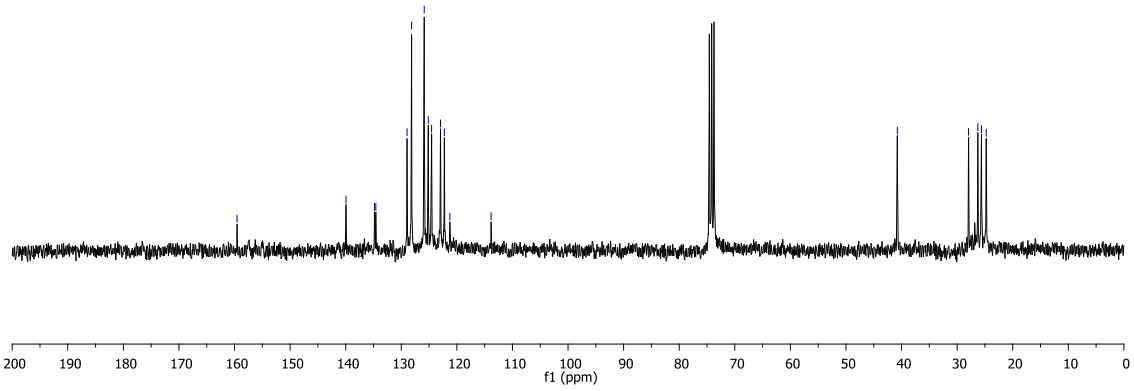


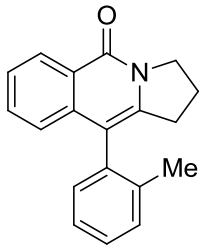


2i

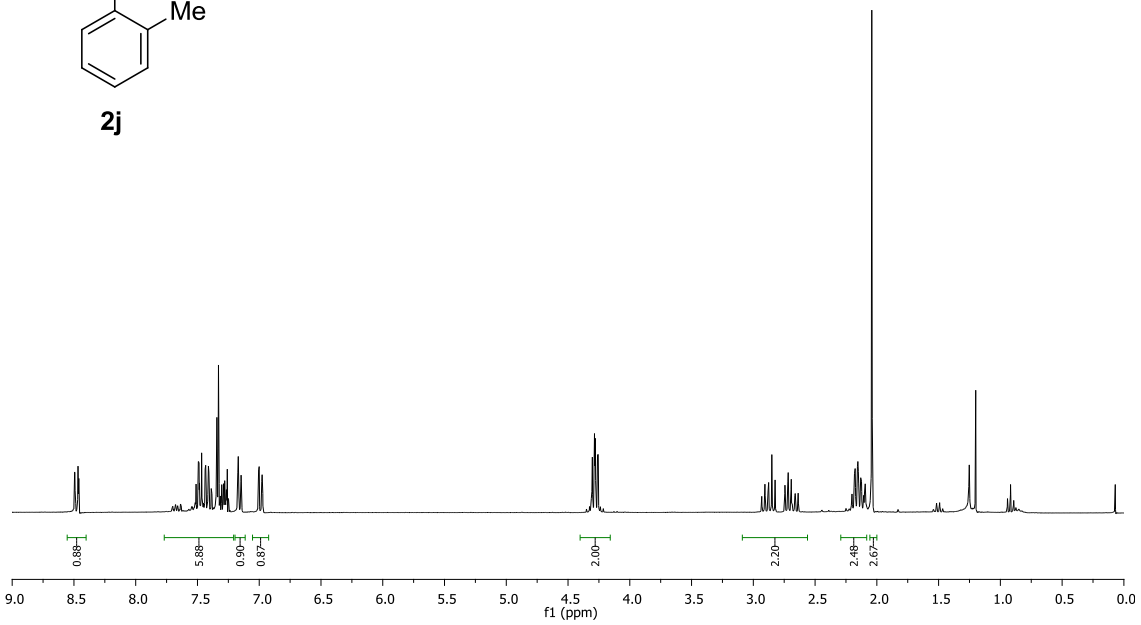

0.79
7.95
1.21
2.00
2.18
8.36
f1 (ppm)

159.54
139.95
134.82
134.58
128.96
128.15
125.87
125.14
124.55
122.94
113.84
40.76
27.94
26.28
25.62
24.77

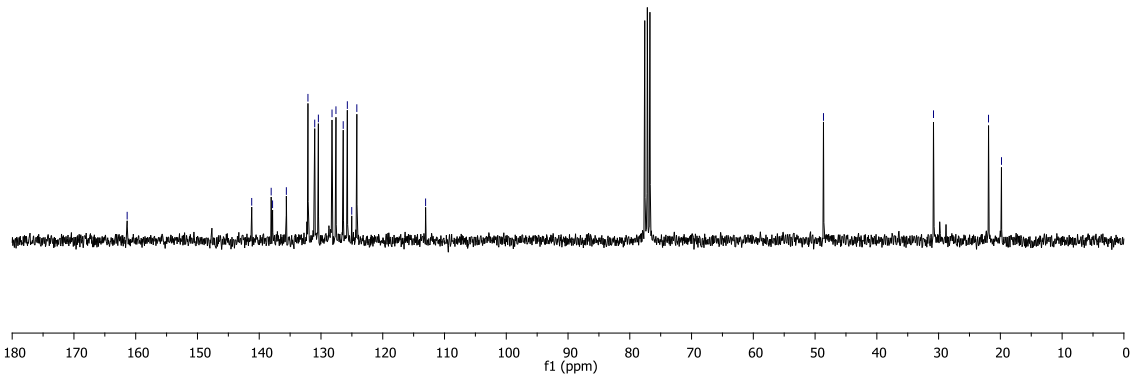

f1 (ppm)

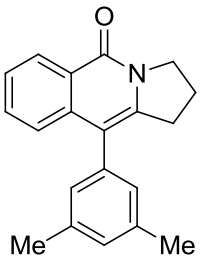

O
N
Me

2j

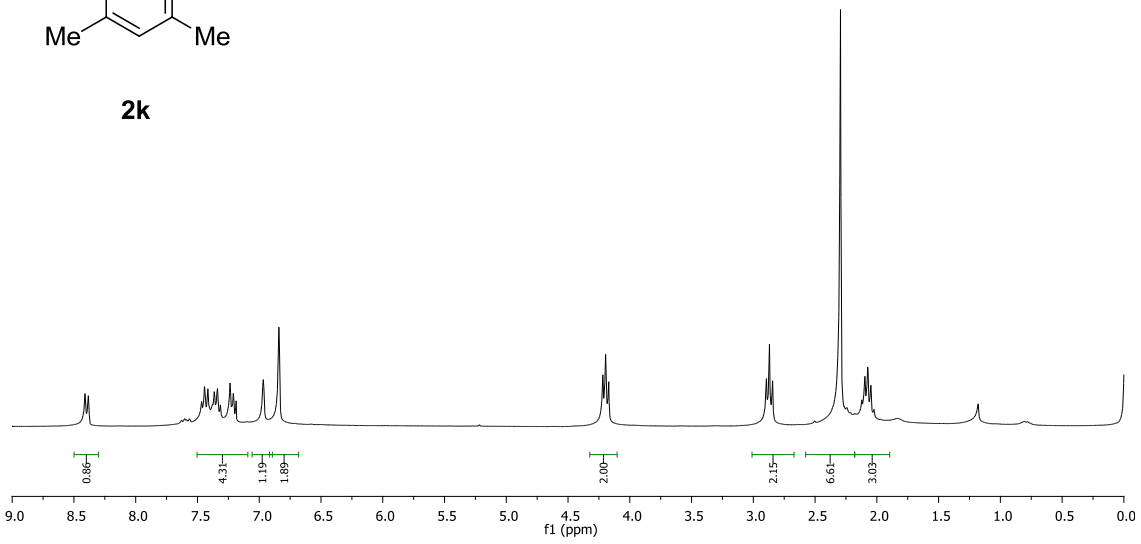

0.88
5.88
0.90
0.87
2.00
2.20
2.48
2.67
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

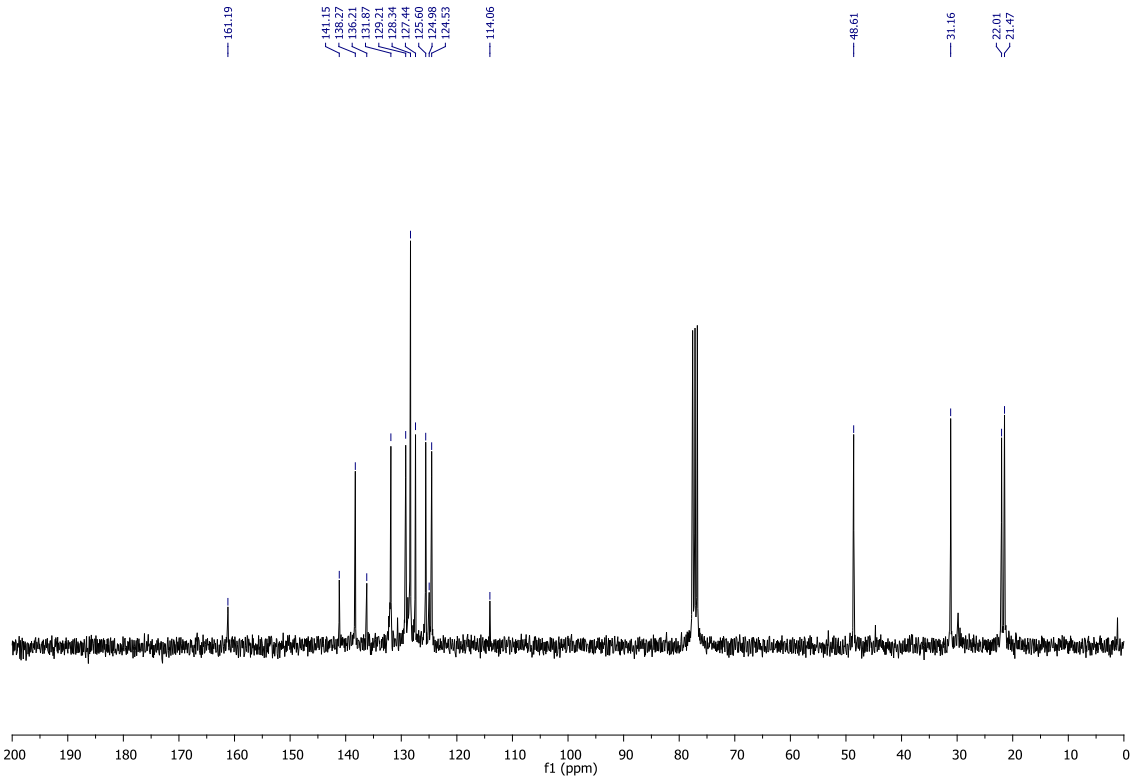

13C
lm1as139
161.38
141.22
138.07
137.84
135.61
132.11
131.02
130.42
128.21
127.58
126.40
125.73
125.02
124.20
113.06
48.64
30.82
21.92
19.82

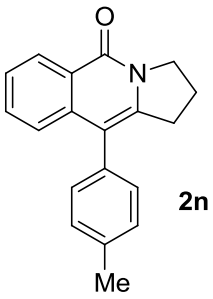

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



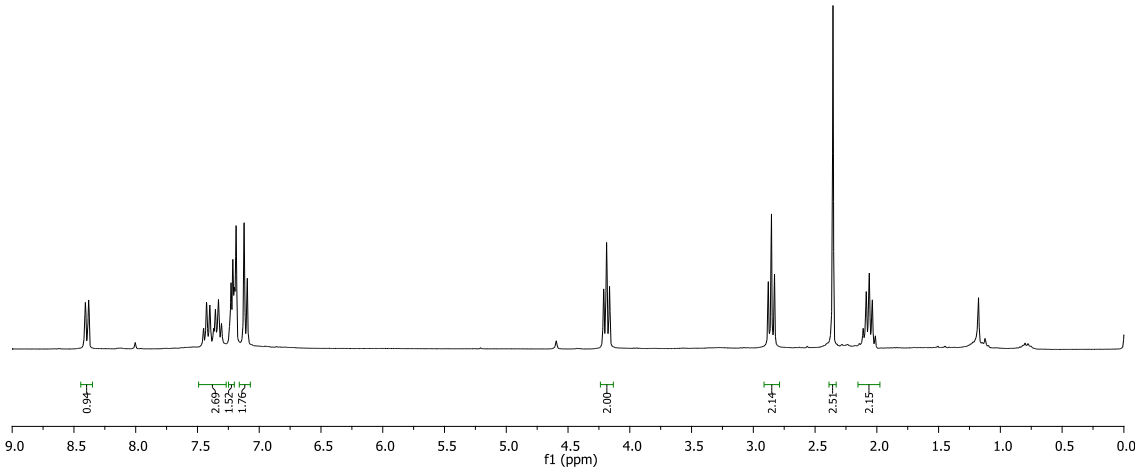
2k

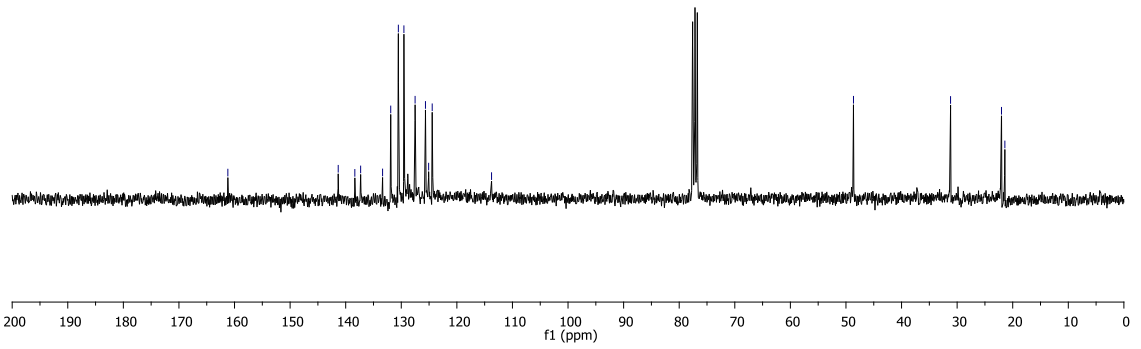


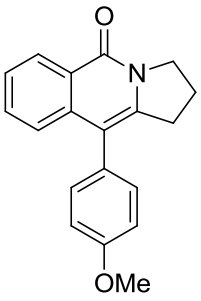




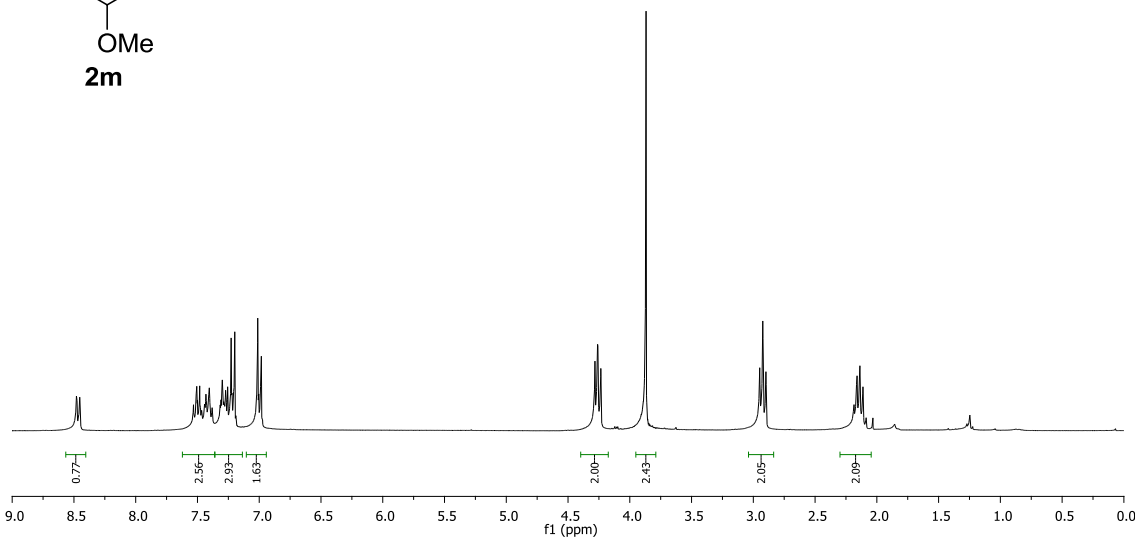
2n



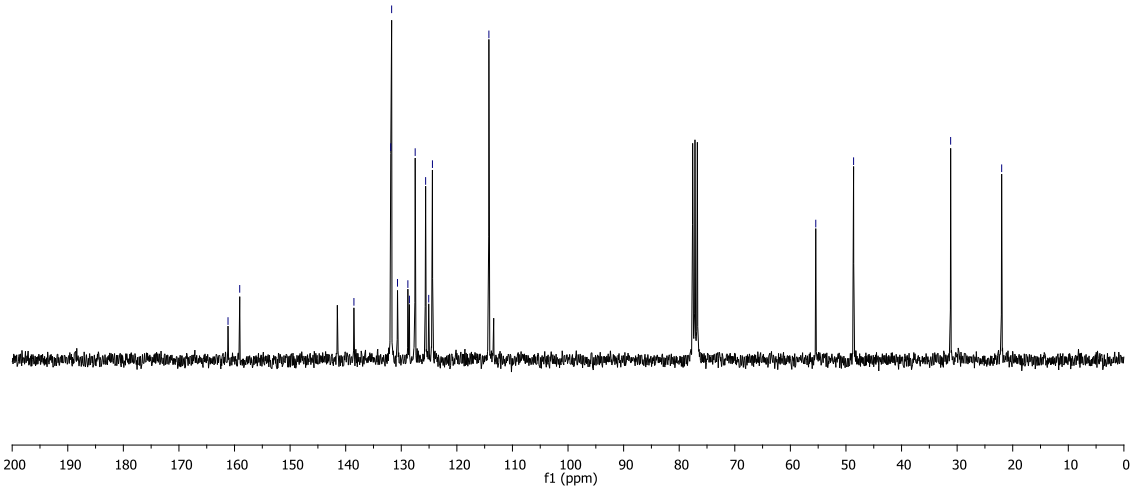


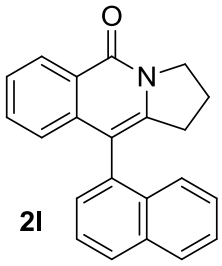

O
N
OMe

2m

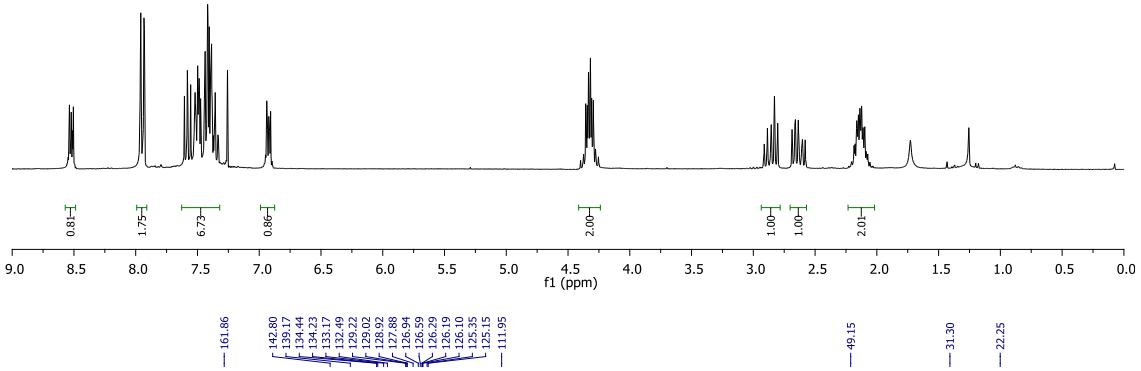

0.77
2.56
2.93
1.63
2.00
2.43
2.05
2.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


13C
lm1as151c2
161.17
159.07
138.52
131.89
131.74
130.68
128.81
128.54
127.50
125.62
125.46
124.40
114.24
55.43
48.63
31.17
21.99

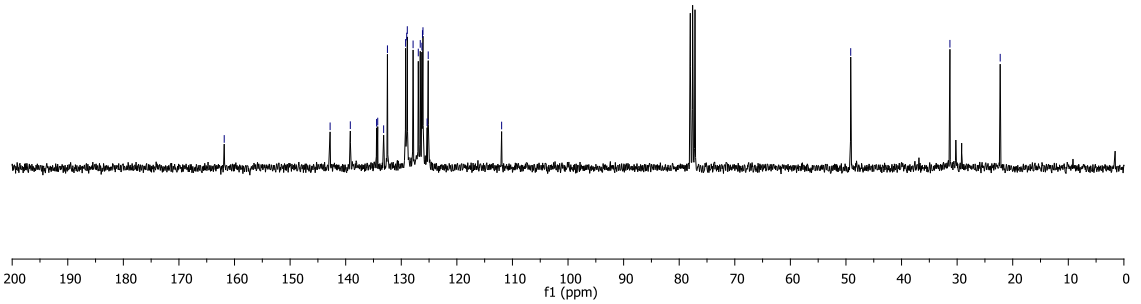

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

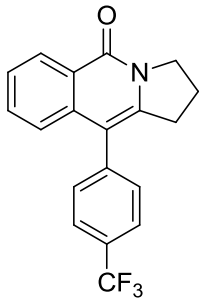

O
N

2l

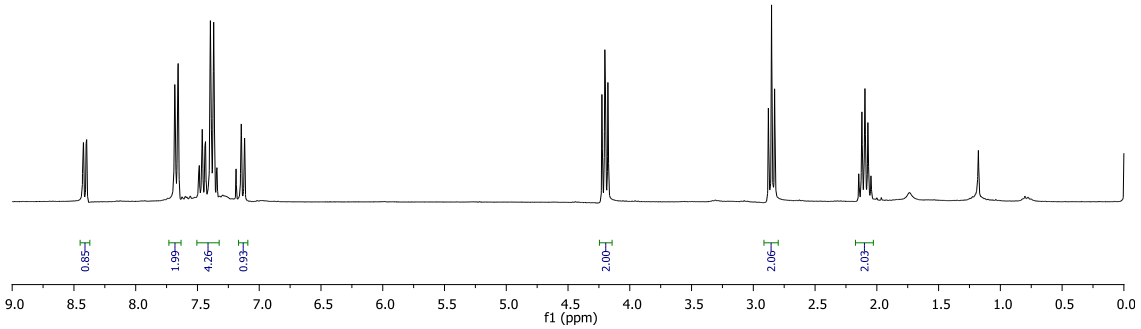

0.81
1.75
6.73
0.86
2.00
1.00
1.00
2.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

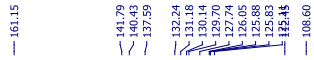
161.86
142.80
139.17
134.44
134.23
133.17
132.49
129.22
129.02
128.92
127.88
126.94
126.59
126.39
126.19
126.10
125.35
125.15
111.95
49.15
31.30
22.25

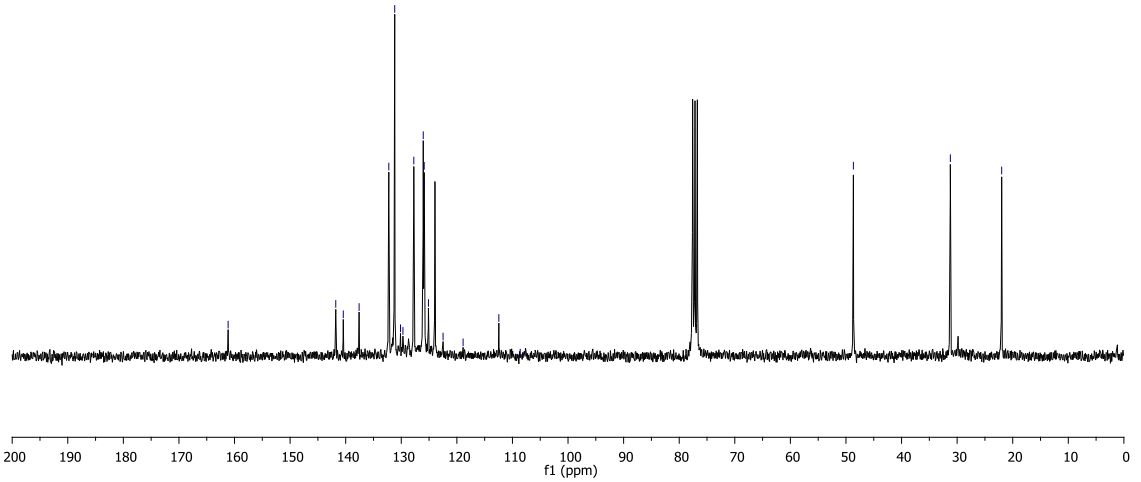

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

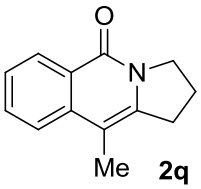


2o

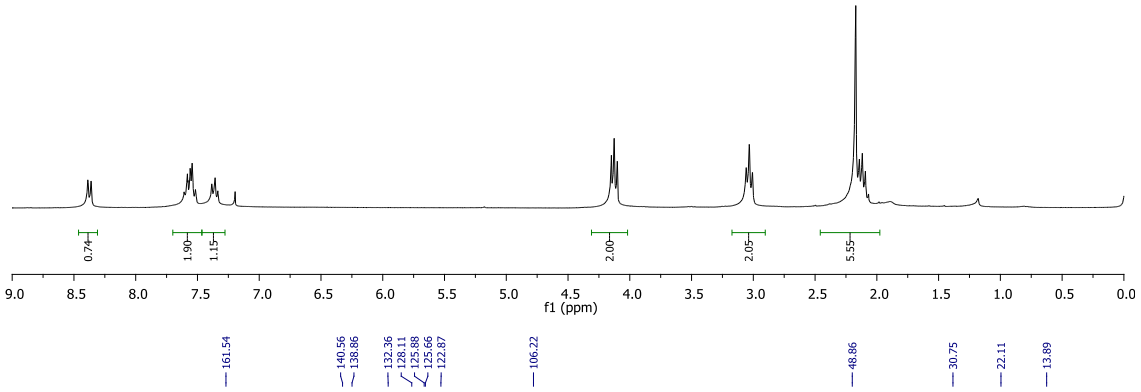


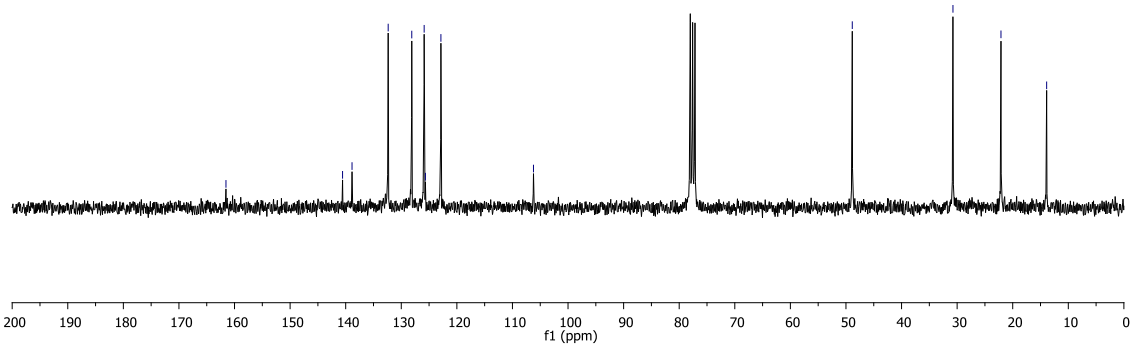


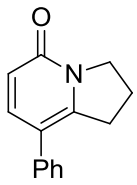




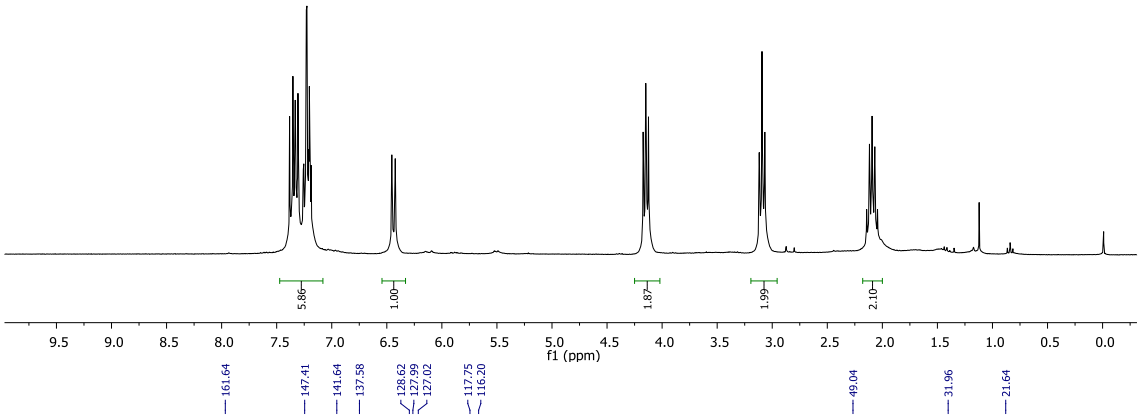
2q

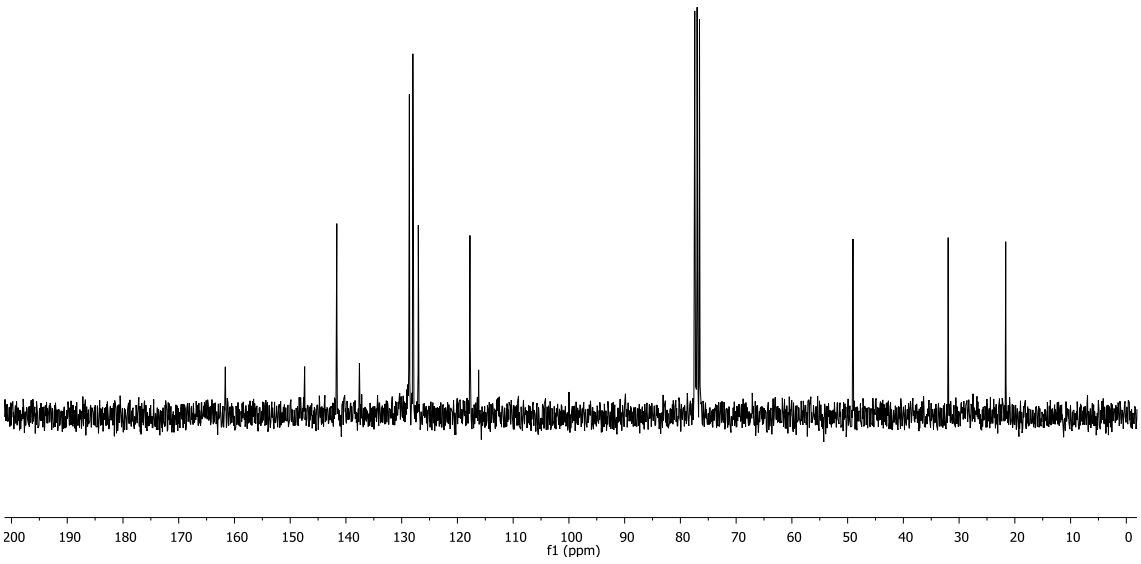


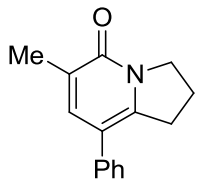




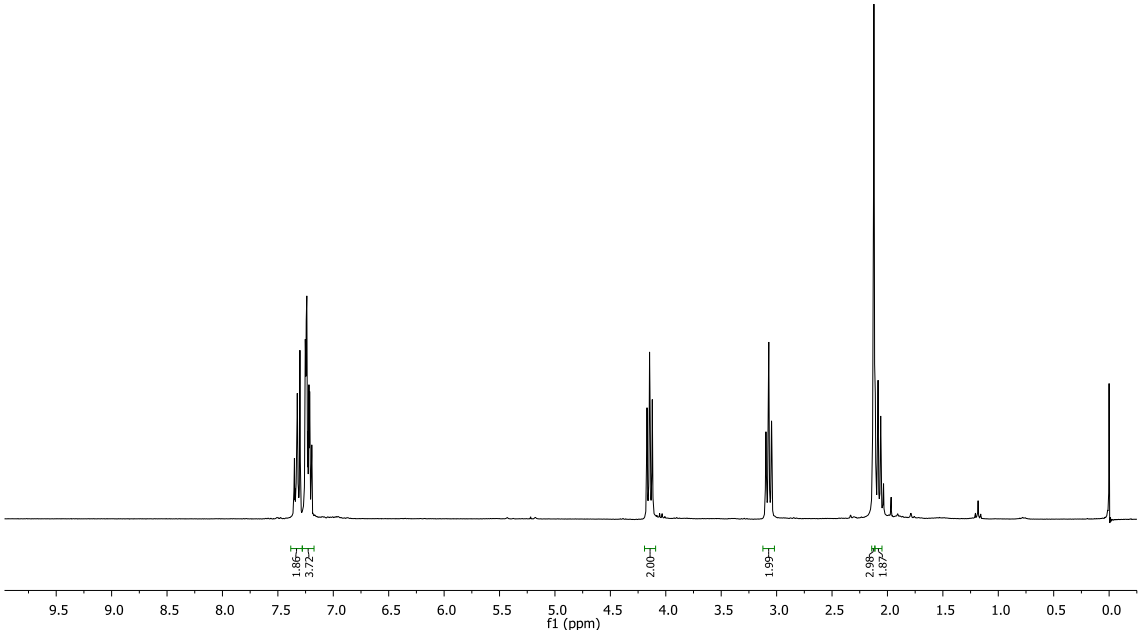
2r

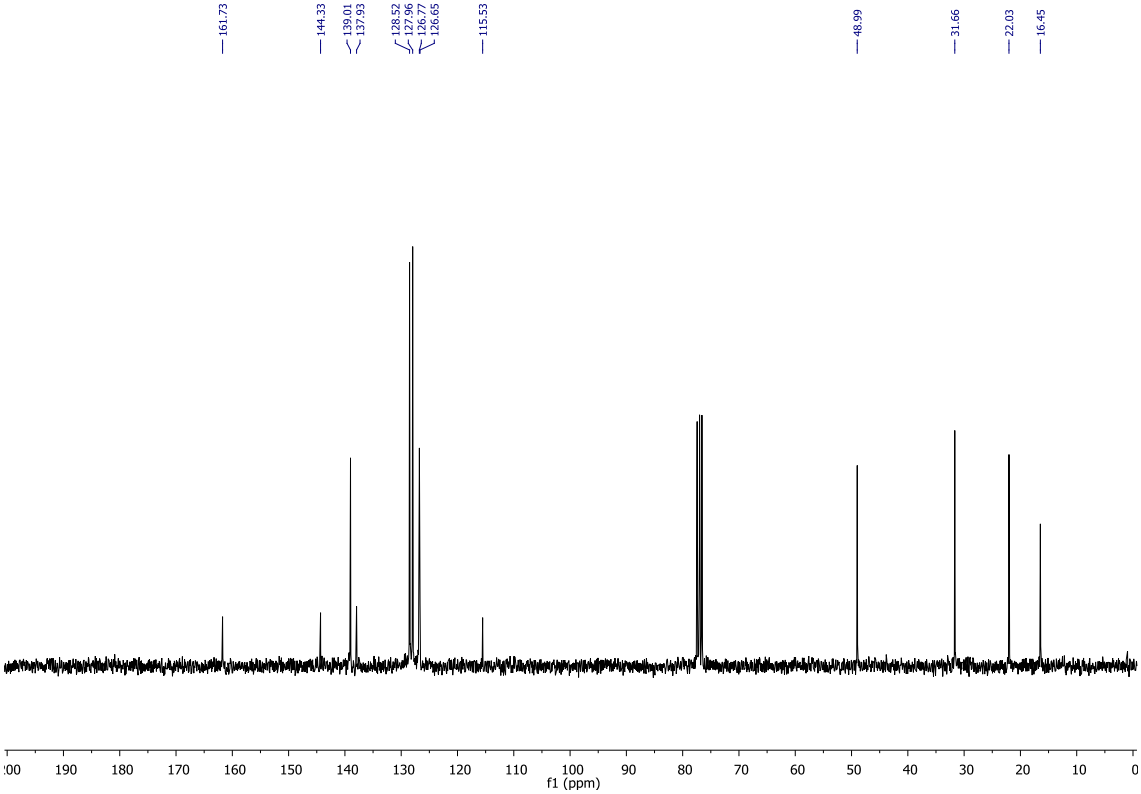


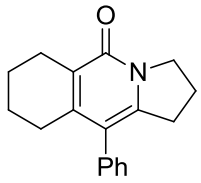




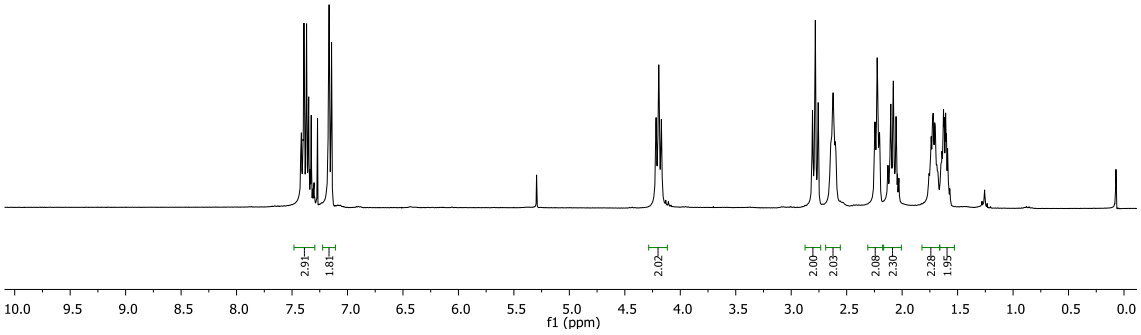
2s



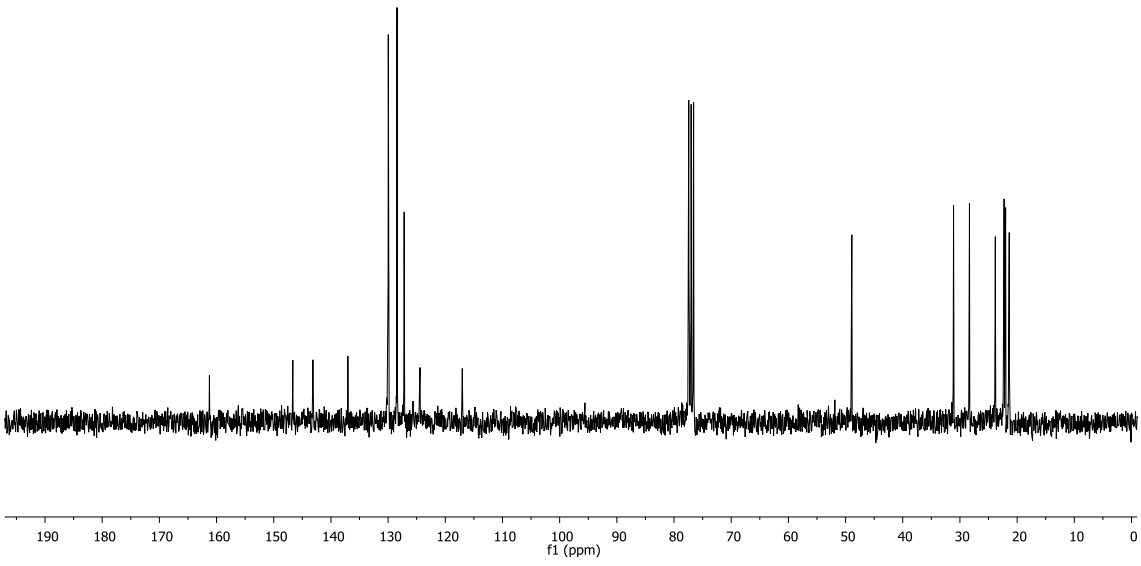


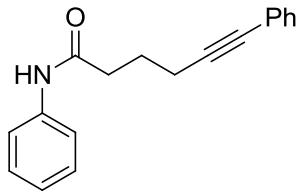

O
N
Ph

2t

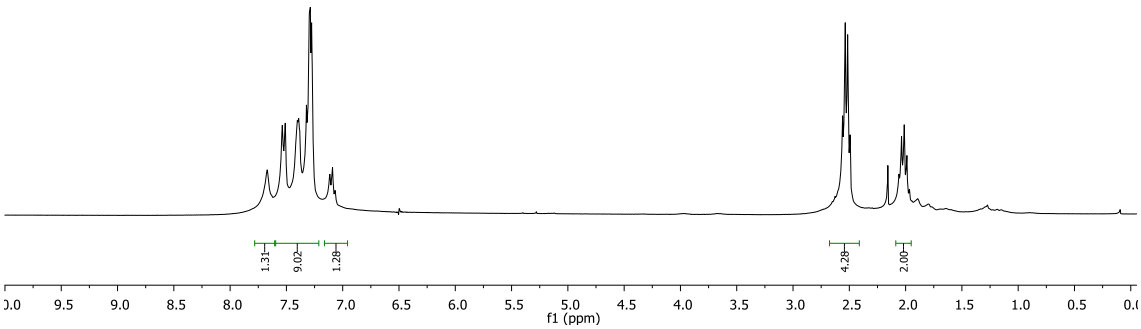

2.91
1.81
2.02
2.00
2.03
2.08
2.30
2.28
1.95
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

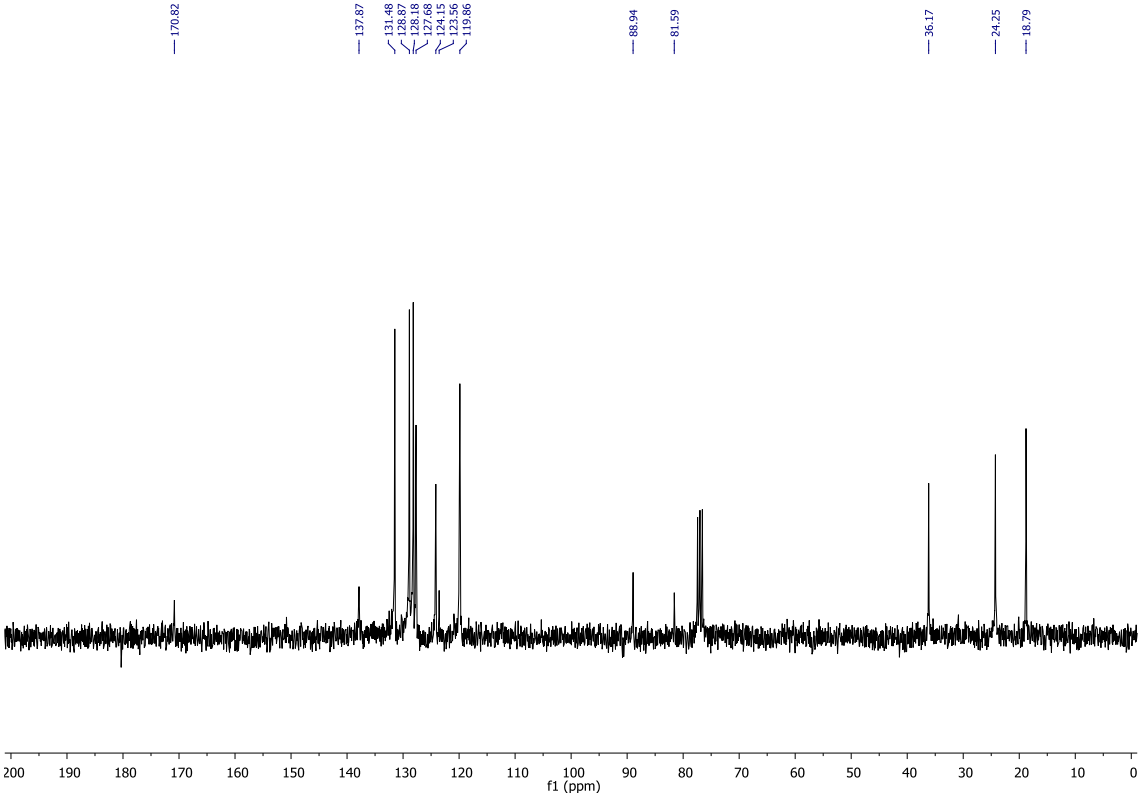

161.25
146.67
143.15
137.04
129.97
128.44
127.20
124.42
117.03
48.91
31.12
28.33
23.82
22.27
22.01
21.38

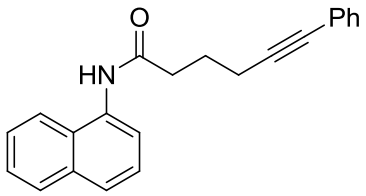

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
Ph
HN

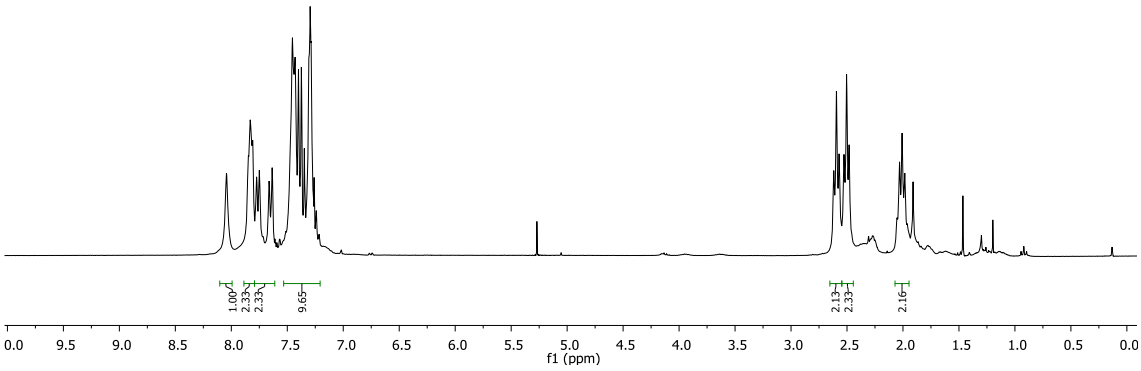
5

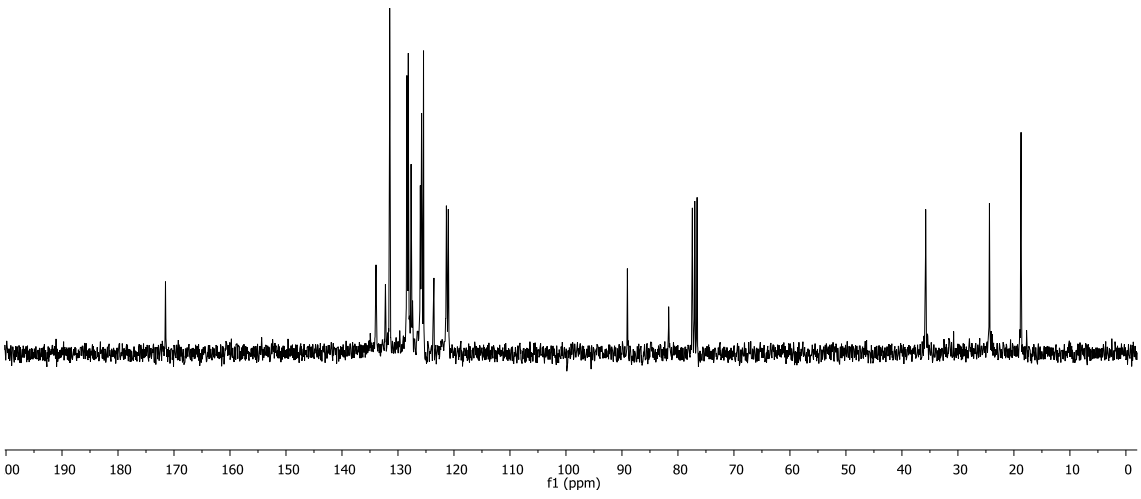

1.31
9.02
1.28
4.28
2.00
f1 (ppm)

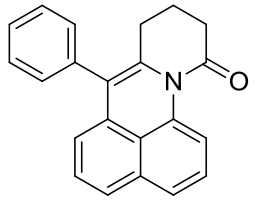

170.82
137.87
131.48
128.87
128.18
127.68
124.15
123.56
119.86
88.94
81.59
36.17
24.25
18.79
f1 (ppm)



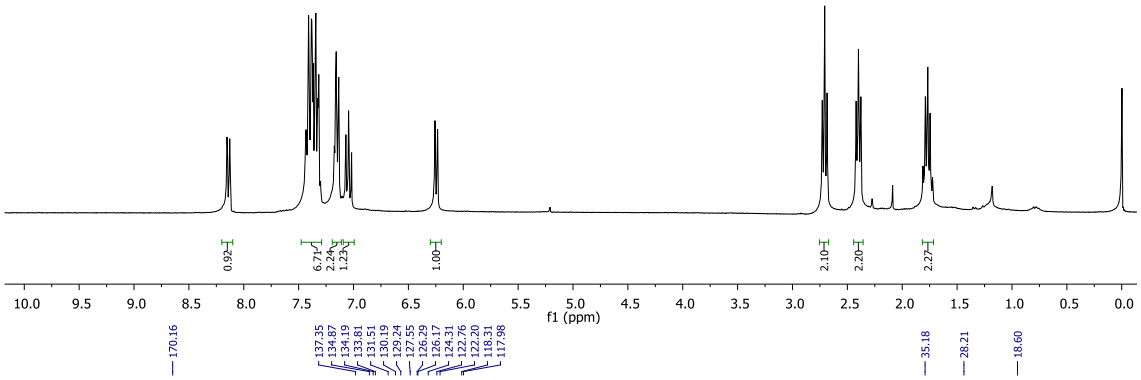
6

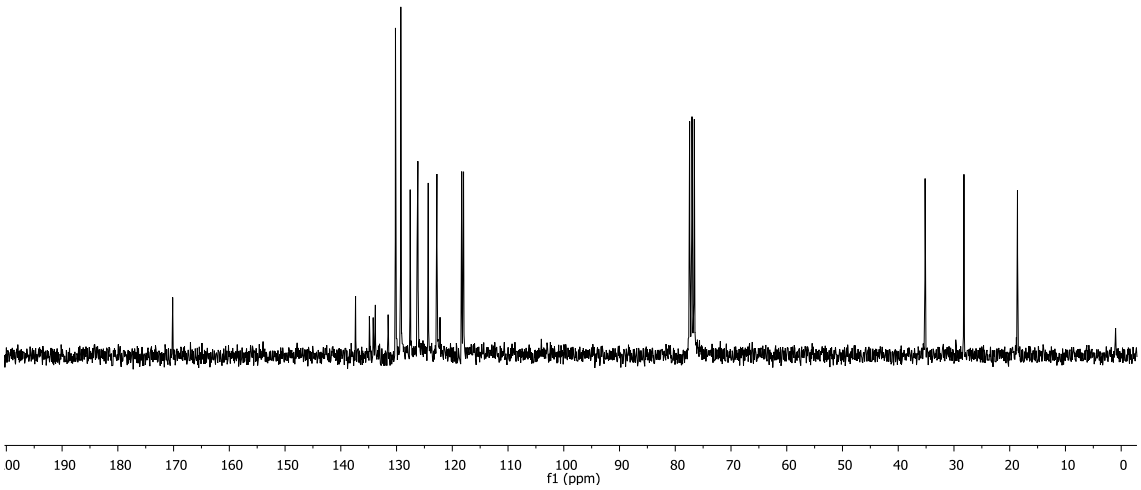





N
O

7


0.92
6.71
2.24
1.23
1.00
2.10
2.20
2.27
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
170.16
137.35
134.87
134.19
133.81
131.51
130.19
129.24
127.55
126.29
126.17
125.71
122.76
122.20
118.31
117.98
35.18
28.21
18.60


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)