Supporting Information

Gold(III)-Catalyzed Conia-ene Reaction for the Direct Synthesis of Substituted Pyrroles from *β*-ketopropargyl Amines

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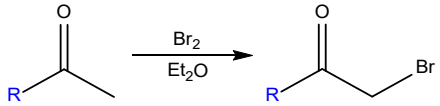
1. General Information

All reagents and solvents were purchased from commercial suppliers (such as Merck, Sigma-Aldrich, Acros Organics, TCI Chemicals) and used without further purification unless otherwise noted. All reactions were carried out in oven-dried glassware under an ambient atmosphere. Thin-layer chromatography (TLC) was performed on silica gel 60 F_{254} aluminum plates and visualized under UV light (254 nm) or by staining with a potassium permanganate solution. Column chromatography was performed on silica gel (230-400 mesh). Nuclear Magnetic Resonance (NMR) spectra (^{1}H and ^{13}C) were recorded on a 400 MHz spectrometer. Chemical shifts (δ) are reported in parts per million (ppm) relative to the residual solvent peak. High-resolution mass spectrometry (HRMS) was performed using an ESI-TOF analyzer.

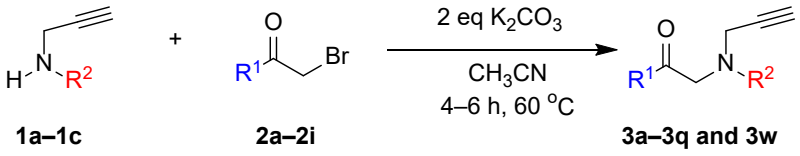
2. General Procedure for the Synthesis of α-Bromoacetophenone Derivatives



Scheme S1. α-Bromination of methyl ketones using Br_2 in diethyl ether.

To a solution of the corresponding acetophenone derivative (1.0 equiv.) in diethyl ether, cooled to 0 °C in an ice bath, was added bromine (1.0 equiv.) dropwise. The reaction mixture was then allowed to warm to room temperature and was stirred for 2–3 hours. The progress of the reaction was monitored by thin-layer chromatography (TLC). Upon completion, the organic layer was washed with a saturated aqueous solution of $NaHCO_3$, dried over anhydrous $MgSO_4$, and filtered. The volatile materials were removed under reduced pressure to afford the crude product. The crude material was then purified by column chromatography to afford the desired products in 80-93% yield.[1]

3. General Procedure for the Synthesis of *N*–Propargyl-α-amino Ketones (3a-3q)

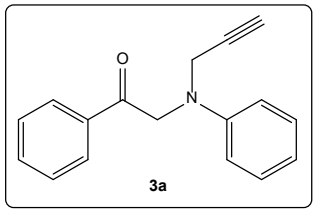


Scheme S2. Synthesis of β-ketopropargyl amine substrates (**3a–3q and 3w**).

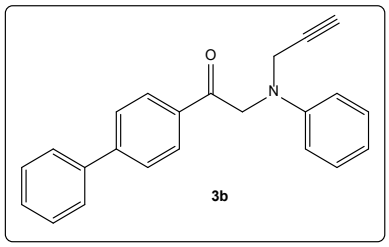
For the synthesis of the target compounds **3a–3q**, the protocol reported by Yi et al.[2] was employed with key modifications and optimizations. While the reference method suggests a 24-hour reaction time for the *N*-alkylation, we found that with our specific substrates, the reaction proceeded remarkably faster, reaching full completion within 4–6 hours.

Optimized Procedure: To a solution of the corresponding α-bromo ketone (**1a–1i**) (1.0 equiv) in acetonitrile (CH_3CN), the respective propargylamine (**2a–2b**) (1.1 equiv) and potassium carbonate (K_2CO_3) (2.0 equiv) were added. The reaction mixture was heated to 60 °C and stirred for 4–6 hours, with its progress carefully monitored by TLC. Upon completion, the solvent was removed under reduced pressure. The residue was diluted with water and extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine, dried over anhydrous $MgSO_4$, filtered, and concentrated. The crude product was purified by column chromatography to afford the final products **3a–3q** in 50% to 88% yields.

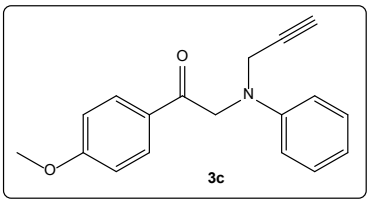
1-Phenyl-2-(phenyl(prop-2-yn-1-yl)amino)ethan-1-one (3a)[2]: White solid (purified by column chromatography, hexane/EtOAc 20:1), 73% yield, m.p.: 112–113 ºC (lit.,[2] 113–114 ºC); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99–7.82 (m, 2H), 7.61–7.45 (m, 1H), 7.45–7.34 (m, 2H), 7.22–7.07 (m, 2H), 6.86–6.51 (m, 3H), 4.75 (s, 2H), 4.09 (d, *J* = 2.5 Hz, 2H), 2.18 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.1, 148.3, 135.3, 133.7, 129.3, 128.9, 128.0, 118.7, 113.9, 79.8, 72.8, 57.0, 41.2.



1-([1,1'-Biphenyl]-4-yl)-2-(phenyl(prop-2-yn-1-yl)amino)ethan-1-one (3b): Orange solid (purified by column chromatography, hexane/EtOAc 20:1), 50% yield, m.p.: 140–141 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02–7.98 (m, 2H), 7.65–7.61 (m, 2H), 7.57–7.52 (m, 2H), 7.42–7.37 (m, 2H), 7.35–7.31 (m, 1H), 7.19–7.12 (m, 2H), 6.76–6.69 (m, 3H), 4.79 (s, 2H), 4.12 (d, *J* = 2.4 Hz, 2H), 2.20 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.7, 148.3, 146.4, 139.7, 134.0, 129.3, 129.1, 128.5, 128.4, 127.5, 127.3, 118.8, 114.0, 79.7, 72.8, 57.0, 41.3; HRMS (ESI-TOF) calcd for $C_{23}H_{19}NO$ $[M+Na]^+$ 348.1364, found 348.1268.

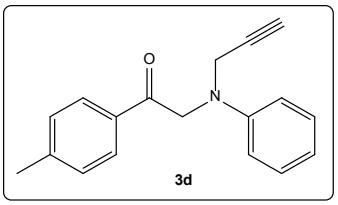


1-(4-Methoxyphenyl)-2-(phenyl(prop-2-yn-1-yl)amino)ethan-1-one (3c)[2]: White solid



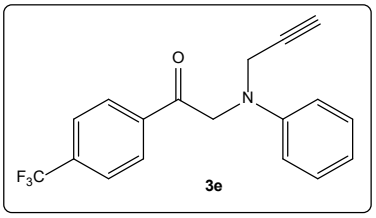
(purified by column chromatography, hexane/EtOAc 10:1), 70% yield, m.p. = 118–119 °C (lit.,[2] 117–118 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92–7.87 (m, 2H), 7.16–7.10 (m, 2H), 6.88–6.84 (m, 2H), 6.73–6.66 (m, 3H), 4.70 (s, 2H), 4.09 (d, *J* = 2.5 Hz, 2H), 3.77 (s, 3H), 2.18 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.5, 163.9, 148.3, 130.2, 129.3, 128.4, 118.6, 114.0, 113.9, 79.9, 72.7, 56.6, 55.6, 41.3.

2-(Phenyl(prop-2-yn-1-yl)amino)-1-(*p*-tolyl)ethan-1-one (3d)[2]: White solid, 76% yield



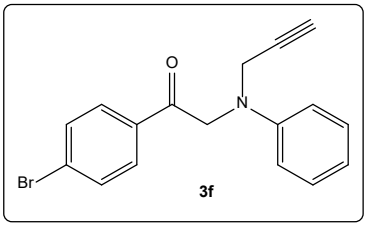
(purified by column chromatography, hexane/EtOAc 20:1), m.p.: 72–73 °C (lit.,[2] 73–75 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90–7.78 (m, 2H), 7.24–7.19 (m, 2H), 7.18–7.12 (m, 2H), 6.76–6.67 (m, 3H), 4.75 (s, 2H), 4.11 (d, *J* = 2.5 Hz, 2H), 2.35 (s, 3H), 2.19 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.6, 147.2, 143.5, 131.8, 128.5, 128.2, 127.0, 117.6, 112.8, 78.7, 71.6, 55.8, 40.2, 20.7.

2-(Phenyl(prop-2-yn-1-yl)amino)-1-(4-(trifluoromethyl)phenyl)ethan-1-one (3e): Reddish-



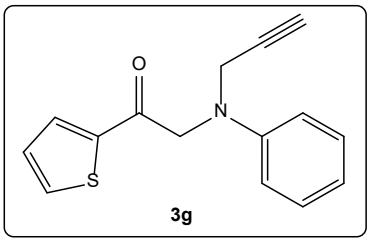
brown solid (purified by column chromatography, hexane/EtOAc 10:1), 40% yield, m.p.: 92–93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13–8.08 (m, 2H), 7.78–7.73 (m, 2H), 7.27–7.21 (m, 2H), 6.88–6.75 (m, 3H), 4.85 (s, 2H), 4.18 (d, *J* = 2.4 Hz, 2H), 2.28 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.5, 148.1, 138.0, 134.9 (q, $^2J_{C–F}$ = *32.6 Hz*), 129.4, 128.3, 125.9 (q, $^3J_{C–F}$ = *3.7 Hz*), 124.9 (q, $^1J_{C–F}$ = 273.0 Hz), 122.2, 119.2, 114.2, 79.4, 73.1, 57.3, 41.3; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{14}F_3NO$ $[M+Na]^+$ 340.0925, found 340.0835.

1-(4-Bromophenyl)-2-(phenyl(prop-2-yn-1-yl)amino)ethan-1-one (3f)[2]: White solid (purified

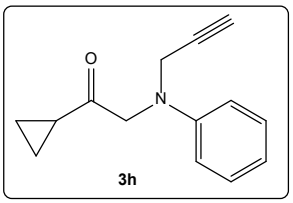


by column chromatography, hexane/EtOAc 20:1), 55% yield, m.p.: 108–109 °C (lit.,[2] 108–109 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86–7.74 (m, 2H), 7.61–7.51 (m, 2H), 7.19–7.13 (m, 2H), 6.82–6.61 (m, 3H), 4.72 (s, 2H), 4.10 (d, *J* = 2.5 Hz, 2H), 2.20 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.3, 148.1, 134.0, 132.2, 129.5, 129.3, 128.9, 119.0, 114.1, 79.5, 72.9, 56.9, 41.3.

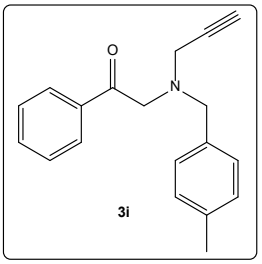
2-(Phenyl(prop-2-yn-1-yl)amino)-1-(thiophen-2-yl)ethan-1-one (3g): Greenish solid (purified by column chromatography, hexane/EtOAc 10:1), 75% yield, m.p.: 89–90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.59 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.20–7.14 (m, 2H), 7.08 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.79–6.72 (m, 3H), 4.60 (s, 2H), 4.12 (d, *J* = 2.4 Hz, 2H), 2.20 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 148.1, 141.1, 134.2, 132.3, 129.3, 128.2, 119.2, 114.3, 79.4, 73.0, 58.0, 41.4; HRMS (ESI-TOF) m/z: calcd for $C_{15}H_{13}NOS$ $[M+H]^+$ 256.0791, found 256.0850.



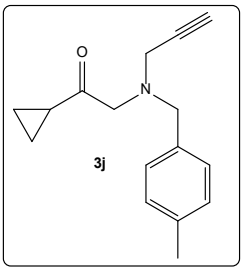
1-Cyclopropyl-2-(phenyl(prop-2-yn-1-yl)amino)ethan-1-one (3h)[2]: Pale yellow oil (purified by column chromatography, hexane/EtOAc 20:1), 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21–7.15 (m, 2H), 6.75 (tt, *J* = 7.3, 1.0 Hz, 1H), 6.72–6.67 (m, 2H), 4.15 (s, 2H), 4.07 (d, *J* = 2.5 Hz, 2H), 2.19 (t, *J* = 2.4 Hz, 1H), 2.09 (m, 1H), 1.04–0.99 (m, 2H), 0.86–0.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.4, 147.9, 129.3, 118.7, 113.7, 79.4, 72.7, 61.3, 41.4, 29.7, 17.7, 11.6.



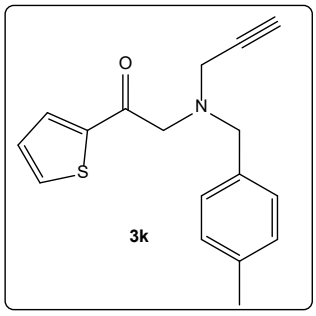
2-((4-Methylbenzyl)(prop-2-yn-1-yl)amino)-1-phenylethan-1-one (3i): Brownish yellow oil (purified by column chromatography, hexane/EtOAc 20:1), 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88–7.82 (m, 2H), 7.45–7.40 (m, 1H), 7.34–7.28 (m, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 2H), 3.89 (s, 2H), 3.62 (s, 2H), 3.40 (d, *J* = 2.5 Hz, 2H), 2.21 (s, 3H), 2.19 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 137.1, 136.1, 134.8, 133.2, 129.3, 129.1, 128.5, 128.3, 78.4, 74.0, 59.1, 57.8, 42.3, 21.2.



1-Cyclopropyl-2-((4-methylbenzyl)(prop-2-yn-1-yl)amino)ethan-1-one (3j): Brownish yellow oil (purified by column chromatography, hexane/EtOAc 20:1), 88% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.1 Hz, 2H), 7.06 (d, *J* = 7.5 Hz, 2H), 3.58 (s, 2H), 3.42 (s, 2H), 3.35 (d, *J* = 2.4 Hz, 2H), 2.27 (s, 3H), 2.24–2.12 (m, 2H), 1.00–0.94 (m, 2H), 0.84–0.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.1, 137.1, 134.8, 129.2, 129.1, 78.3, 73.6, 63.3, 57.6, 42.4, 21.2, 18.2, 11.2; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{19}NO$ $[M+Na]^+$ 264.1359; found: 264.1321.

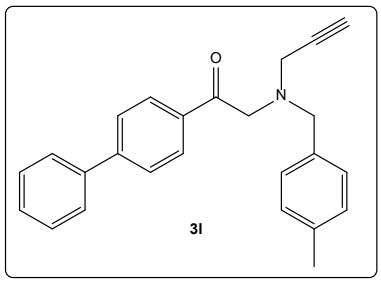


2-((4-methylbenzyl)(prop-2-yn-1-yl)amino)-1-(thiophen-2-yl)ethan-1-one (3k): Maroon oil



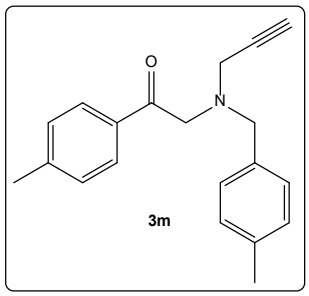
(purified by column chromatography, hexane/EtOAc 20:1), 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.55 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.22–7.17 (m, 2H), 7.08–7.00 (m, 3H), 3.79 (s, 2H), 3.66 (s, 2H), 3.40 (d, *J* = 2.4 Hz, 2H), 2.25 (s, 3H), 2.22 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.6, 142.1, 137.2, 134.5, 133.8, 132.7, 129.4, 129.1, 127.9, 78.2, 73.9, 60.2, 57.8, 42.4, 21.2; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{17}NOS$ $[M+Na]^+$ 306.0923; found: 306.0852.

1-([1,1'-Biphenyl]-4-yl)-2-((4-methylbenzyl)(prop-2-yn-1-yl)amino)ethan-1-one (3l): Orange solid



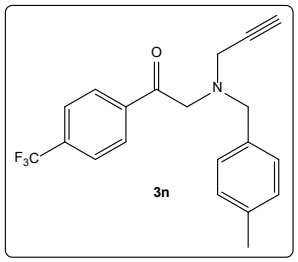
(purified by column chromatography, hexane/EtOAc 20:1), 57% yield, m.p.: 117–118 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97–7.90 (m, 2H), 7.56–7.48 (m, 4H), 7.37–7.32 (m, 2H), 7.30–7.25 (m, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 3.91 (s, 2H), 3.65 (s, 2H), 3.42 (d, *J* = 2.4 Hz, 2H), 2.22 (s, 3H), 2.20 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 145.9, 139.9, 137.1, 134.8, 129.3, 129.2, 129.0, 128.9, 128.3, 127.3, 127.2, 78.5, 74.0, 59.2, 57.8, 42.4, 21.2; HRMS (ESI-TOF) m/z: calcd for $C_{25}H_{23}NO$ $[M+Na]^+$ 376.1672; found: 376.1567.

2-((4-Methylbenzyl)(prop-2-yn-1-yl)amino)-1-(*p*-tolyl)ethan-1-one (3m): Brownish-yellow oil



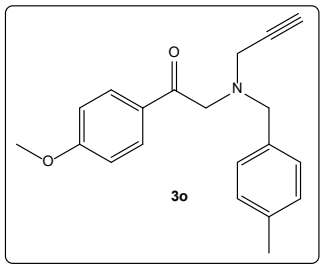
(purified by column chromatography, hexane/EtOAc 20:1), 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78–7.72 (m, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 7.8 Hz, 2H), 6.99 (d, *J* = 7.9 Hz, 2H), 3.85 (s, 2H), 3.61 (s, 2H), 3.38 (d, *J* = 2.5 Hz, 2H), 2.25 (s, 3H), 2.19 (s, 3H), 2.17 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 144.0, 137.0, 134.8, 133.6, 129.3, 129.2, 129.1, 128.4, 78.5, 74.0, 59.0, 57.7, 42.3, 21.7, 21.2.

2-((4-Methylbenzyl)(prop-2-yn-1-yl)amino)-1-(4-(trifluoromethyl)phenyl)ethan-1-one (3n):

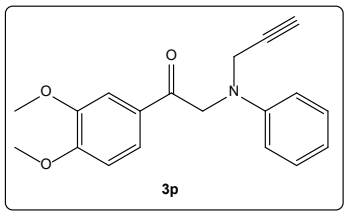


Brown oil (purified by column chromatography, hexane/EtOAc 10:1), 55% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98–7.93 (m, 2H), 7.62–7.56 (m, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.03–6.99 (m, 2H), 3.88 (s, 2H), 3.61 (s, 2H), 3.39 (d, *J* = 2.5 Hz, 2H), 2.23–2.21 (m, 4H).

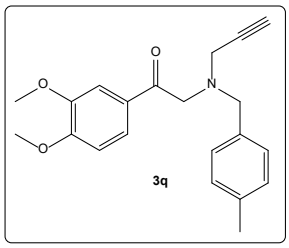
1-(4-Methoxyphenyl)-2-((4-methylbenzyl)(prop-2-yn-1-yl)amino)ethan-1-one (3o): Maroon Oil (purified by column chromatography, hexane/EtOAc 10:1), 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93–7.87 (m, 2H), 7.20–7.16 (m, 2H), 7.03 (d, *J* = 7.5 Hz, 2H), 6.85–6.80 (m, 2H), 3.86 (s, 2H), 3.77 (s, 3H), 3.63 (s, 2H), 3.41 (d, *J* = 2.4 Hz, 2H), 2.24 (s, 3H), 2.21 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.8, 163.6, 137.1, 134.8, 130.6, 129.3, 129.1, 113.6, 78.5, 73.8, 59.0, 57.7, 55.5, 42.3, 21.2; HRMS (ESI-TOF) m/z: calcd for $C_{20}H_{21}NO_2$ $[M+Na]^+$ 330.1465; found 330.1385.



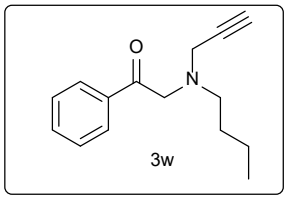
1-(3,4-Dimethoxyphenyl)-2-(phenyl(prop-2-yn-1-yl)amino)ethan-1-one (3p): Yellowish-orange solid (purified by column chromatography, hexane/EtOAc 10:1), 50% yield; m.p.: 144–145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.49 (d, *J* = 2.0 Hz, 1H), 7.20–7.13 (m, 2H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.80–6.63 (m, 3H), 4.75 (s, 2H), 4.12 (d, *J* = 2.4 Hz, 2H), 3.89 (s, 3H), 3.85 (s, 3H), 2.20 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.6, 153.8, 149.3, 148.3, 129.2, 128.5, 122.4, 118.7, 113.9, 110.2, 110.1, 79.8, 72.7, 56.5, 56.2, 56.1, 41.3; HRMS (ESI-TOF) m/z: calcd for $C_{19}H_{19}NO_3$ $[M+Na]^+$ 332.1257; found: 332.1234.



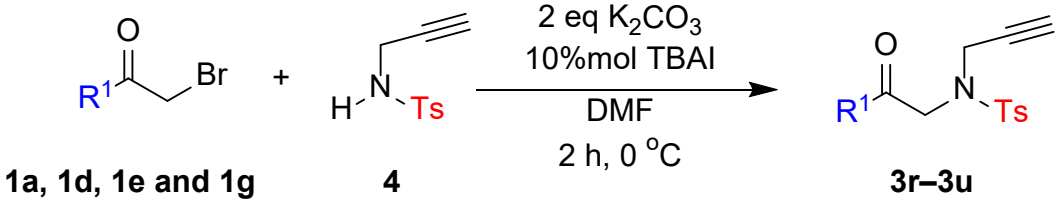
1-(3,4-Dimethoxyphenyl)-2-((4-methylbenzyl)(prop-2-yn-1-yl)amino)ethan-1-one (3q): Reddish brown oil (purified by column chromatography, hexane/EtOAc 10:1), 60% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.47 (d, *J* = 2.0 Hz, 1H), 7.18–7.14 (m, 2H), 7.04–6.99 (m, 2H), 6.75 (d, *J* = 8.4 Hz, 1H), 3.85 (s, 2H), 3.83 (s, 3H), 3.81 (s, 3H), 3.62 (s, 2H), 3.39 (d, *J* = 2.4 Hz, 2H), 2.23–2.20 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.8, 153.4, 148.9, 137.0, 134.8, 129.24, 129.22, 129.1, 123.0, 110.5, 110.0, 78.5, 73.8, 59.0, 57.7, 56.03, 55.96, 42.3, 21.1; HRMS (ESI-TOF) m/z: calcd for $C_{19}H_{19}NO_3$ $[M+Na]^+$ 332.1257; found: 332.1234.



2-(butyl(prop-2-yn-1-yl)amino)-1-phenylethan-1-one (3w): Reddish brown oil (purified by column chromatography, hexane/EtOAc 20:1), 65% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.90 (m, 2H), 7.49 – 7.44 (m, 1H), 7.39 – 7.34 (m, 2H), 3.90 (s, 2H), 3.50 (d, J = 2.5 Hz, 2H), 2.56 – 2.48 (m, 2H), 2.16 (t, J = 2.5 Hz, 1H), 1.45 – 1.37 (m, 2H), 1.24 (ddd, J = 9.8, 7.4, 6.1 Hz, 2H), 0.82 (t, J = 7.4 Hz, 3H).



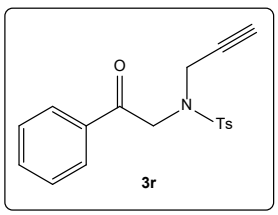
4. General Procedure for the Synthesis of *N*–Tosylated Compounds (3r-3u)



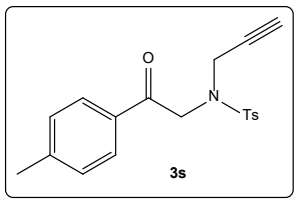
Scheme S3. Preparation of *N*-sulfonyl (tosyl) protected β-ketopropargyl amines **3r–3u**

N-tosylated compounds **3r–3u** were synthesized using a standard *N*-alkylation protocol, adapted from procedures reported in similar studies.[3] Accordingly, in a round-bottom flask, a mixture of the corresponding α-bromo ketone (**1a, 1d, 1e** and **1g**) (1.0 equiv), *N*-propargyl-4-methylbenzenesulfonamide (**4**) (1.1 equiv), potassium carbonate (K_2CO_3) (2.0 equiv), and tetrabutylammonium iodide (TBAI) (10 mol%) in dimethylformamide (DMF) was prepared. The reaction mixture was heated to 60 °C for 2 hours, with progress monitored by TLC. After completion, the work-up and purification were performed as described above for **3a–3q**. The desired products **3r–3u** were afforded after purification by column chromatography in excellent yields (77% to 97%).[4]

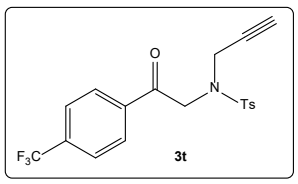
4-methyl-*N*-(2-oxo-2-phenylethyl)-*N*-(prop-2-yn-1-yl)benzenesulfonamide (3r)[4]: white solid (purified by column chromatography, hexane/EtOAc 10:1), 97% yield; m.p.: 73–74 ºC (lit.,[4] 80–82 ºC); ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.88–7.85 (m, 2H), 7.70–7.67 (m, 2H), 7.54–7.50 (m, 1H), 7.42–7.37 (m, 2H), 7.25–7.21 (m, 2H), 4.73 (s, 2H), 4.21 (d, J = 2.5 Hz, 2H), 2.35 (s, 3H), 2.04 (t, J = 2.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.3, 143.9, 136.1, 134.8, 133.9, 129.7, 128.9, 128.0, 127.7, 76.6, 74.5, 51.5, 37.4, 21.6.



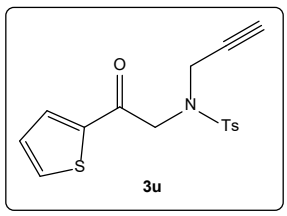
4-methyl-*N*-(2-oxo-2-(*p*-tolyl)ethyl)-*N*-(prop-2-yn-1-yl)benzenesulfonamide (3s)[4]: white solid (purified by column chromatography, hexane/EtOAc 10:1), 95% yield; m.p.: 84–85 °C (lit.,[4] 84–86 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.3 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 8.3 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 4.67 (s, 2H), 4.17 (d, *J* = 2.7 Hz, 2H), 2.28 (s, 3H), 2.26 (s, 3H), 2.02 (t, *J* = 2.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8, 144.9, 143.9, 136.1, 132.3, 129.7, 129.5, 128.1, 127.6, 76.6, 74.7, 51.4, 37.4, 21.7, 21.6.



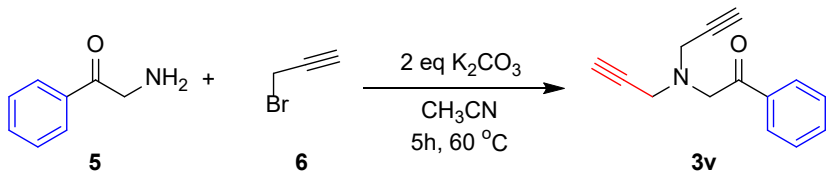
4-methyl-*N*-(2-oxo-2-(4-(trifluoromethyl)phenyl)ethyl)-*N*-(prop-2-yn-1-yl)benzenesulfonamide (3t)[4]: Light yellow solid (purified by column chromatography, hexane/EtOAc 10:1), 80% yield; m.p.: 86–87 °C (lit.,[4] 68–70 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 2H), 7.67–7.61 (m, 4H), 7.22 (d, *J* = 8.0 Hz, 2H), 4.70 (s, 2H), 4.16 (d, *J* = 2.5 Hz, 2H), 2.33 (s, 3H), 2.04 (t, *J* = 2.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8, 144.1, 137.5, 135.7, 134.9 (q, $^2J_{C-F}$ = *32.8 Hz*), 129.8, 128.5, 127.6, 125.9 (q, $^3J_{C-F}$ = *3.7 Hz*), 124.8 (q, $^1J_{C-F}$ = 273 Hz) 76.2, 74.8, 52.0, 37.5, 21.5.



4-methyl-*N*-(2-oxo-2-(thiophen-2-yl)ethyl)-*N*-(prop-2-yn-1-yl)benzenesulfonamide (3u)[5]: White solid (purified by column chromatography, hexane/EtOAc 10:1), 77% yield; m.p.: 130–132 °C (lit.,[5] not reported); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 3.9, 1.1 Hz, 1H), 7.71–7.66 (m, 2H), 7.62 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.27–7.22 (m, 2H), 7.08 (dd, *J* = 5.0, 3.8 Hz, 1H), 4.61 (s, 2H), 4.18 (d, *J* = 2.5 Hz, 2H), 2.36 (s, 3H), 2.05 (t, *J* = 2.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.5, 144.0, 141.0, 135.8, 134.6, 132.8, 129.7, 128.4, 127.7, 76.4, 74.6, 51.7, 37.6, 21.6.



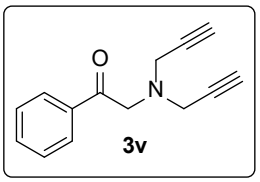
5. Synthesis of *N,N*–Dipropargyl-2-aminoacetophenone (3v)



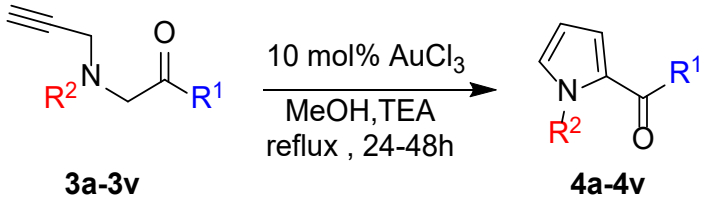
Scheme S4. Synthesis of N,N-dipropargyl substituted *β*–aminoacetophenone **3v**.

In a round-bottom flask, a mixture of 2-aminoacetophenone (**5**) (1.0 equiv), propargyl bromide (**6**) (2.0 equiv) and potassium carbonate (K_2CO_3) (2.0 equiv) in CH_3CN was heated at 60 °C for 5 hours. The reaction progress was monitored by TLC. Upon completion, the work-up and purification were performed as described above. The final product **3v** was isolated in 70% yield.

2-(di(prop-2-yn-1-yl)amino)-1-phenylethan-1-one (3v): Brown oil (purified by column chromatography, hexane/EtOAc 20:1), 70% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98–7.90 (m, 2H), 7.53–7.47 (m, 1H), 7.43–7.36 (m, 2H), 4.03 (s, 2H), 3.54 (d, J = 2.5 Hz, 4H), 2.22 (t, J = 2.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.1, 135.7, 133.4, 128.6, 128.1, 78.4, 74.0, 58.0, 42.9.



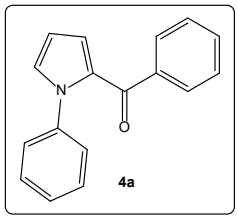
6. General Procedure for the Synthesis of Pyrrole Derivatives (4a–4v)



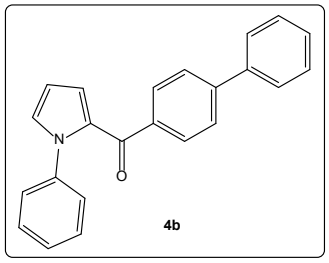
Scheme S5. Gold(III)-catalyzed synthesis of polysubstituted pyrrole derivatives **4a–4v**.

To a vial were sequentially added gold(III) chloride ($AuCl_3$) (0.1 mmol, 0.10 equiv), corresponding *N*-propargyl-β-aminoketone derivative (**3a–3v**) (1 mmol, 1.0 equiv), methanol (2 mL), and finally triethylamine (TEA) (2 mmol, 2.0 equiv). The vial was sealed, and the reaction mixture was heated at reflux temperature of solvent for 24-48 hours (the heating plate temperature was conducted as 80 °C). The progress of the reaction was monitored by thin-layer chromatography (TLC). Upon completion, the mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The resulting residue was dissolved in ethyl acetate, washed with water, dried over anhydrous magnesium sulfate ($MgSO_4$), filtered, and concentrated in vacuo. The crude product was purified by column chromatography on silica gel using a mixture of hexane and ethyl acetate as the eluent to afford the desired pyrrole products (**4a-4v**) (20-90% yield).

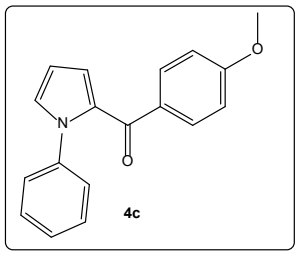
Phenyl(1-phenyl-1H-pyrrol-2-yl)methanone (4a)[6]: Compound 4a was purified by column chromatography on silica gel (hexane/EtOAc = 20:1) to give a brown solid (21 mg, 43% isolated yield, 70% NMR yield) after 24 h; m.p. 65–66 °C (lit. ref.[6] reports an oil) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82–7.74 (m, 2H), 7.45–7.39 (m, 2H), 7.36–7.27 (m, 4H), 7.27–7.18 (m, 3H), 6.99 (dd, *J* = 2.6, 1.6 Hz, 1H), 6.77 (dd, *J* = 3.9, 1.7 Hz, 1H), 6.22 (dd, *J* = 4.0, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.8, 139.6, 138.0, 130.9, 130.02, 130.01, 128.5, 127.8, 127.1, 126.4, 124.5, 122.3, 108.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{13}NO$ $[M+Na]^+$ 270.0889; found: 270.0853.



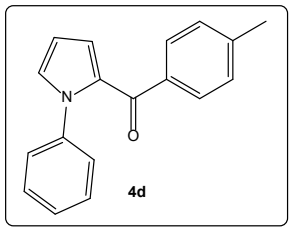
[1,1'-Biphenyl]-4-yl(1-phenyl-1H-pyrrol-2-yl)methanone (4b): Compound 4b purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a yellowish solid (19 mg, 29% isolated yield, 40% NMR yield) after 48 h; m.p.: 109–110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93–7.87 (m, 2H), 7.62–7.55 (m, 4H), 7.42–7.25 (m, 8H), 7.05 (dd, *J* = 2.6, 1.7 Hz, 1H), 6.87 (dd, *J* = 3.9, 1.7 Hz, 1H), 6.28 (dd, *J* = 4.0, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.4, 144.8, 140.6, 140.2, 137.8, 131.2, 131.0, 130.2, 129.0, 128.9, 128.1, 127.5, 127.3, 126.9, 125.5, 123.2, 109.5; HRMS (ESI-TOF) m/z: calcd for $C_{23}H_{17}NO$ $[M+Na]^+$ 346.1202; found: 346.1146.



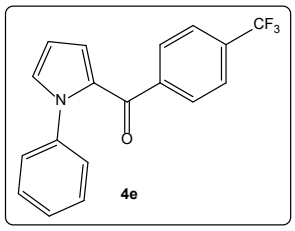
(4-Methoxyphenyl)(1-phenyl-1H-pyrrol-2-yl)methanone (4c): Compound 4c purified by column chromatography on silica gel (hexane/EtOAc, 10:1) to give a maroon solid(21 mg, 38% isolated yield; 55% NMR yield) after 48 h; m.p.: 110–111 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86–7.79 (m, 2H), 7.35–7.20 (m, 5H), 7.01 (dd, *J* = 2.6, 1.6 Hz, 1H), 6.88–6.84 (m, 2H), 6.78 (dd, *J* = 3.9, 1.7 Hz, 1H), 6.24 (dd, *J* = 3.9, 2.6 Hz, 1H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.8, 161.8, 139.6, 130.8, 130.6, 130.2, 129.4, 127.9, 126.3, 124.3, 121.3, 112.4, 108.2, 54.4; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{15}NO_2$ $[M+Na]^+$ 300.0995; found: 300.0976.



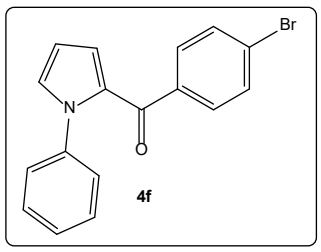
(1-Phenyl-1H-pyrrol-2-yl)(*p*-tolyl)methanone (4d): Compound 4d purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a white solid(22 mg, 42% isolated yield; 65% NMR yield) after 24 h; m.p.: 111–112 °C ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77–7.71 (m, 2H), 7.36–7.22 (m, 5H), 7.20–7.16 (m, 2H), 7.03 (dd, *J* = 2.6, 1.7 Hz, 1H), 6.80 (dd, *J* = 3.9, 1.7 Hz, 1H), 6.26 (dd, *J* = 3.9, 2.6 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.7, 142.6, 140.7, 136.3, 131.2, 130.7, 129.8, 128.9, 128.8, 127.4, 125.5, 122.9, 109.3, 21.6; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{15}NO$ $[M+Na]^+$ 284.1046; found: 284.1010.



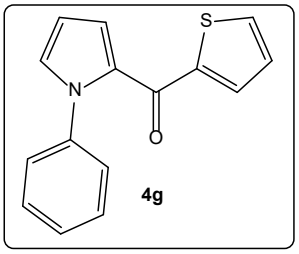
(1-Phenyl-1H-pyrrol-2-yl)(4-(trifluoromethyl)phenyl)methanone (4e): Compound 4e purified by column chromatography on silica gel (hexane/EtOAc, 10:1) to give a brownish-yellow oil (11 mg, 17% isolated yield; 30% NMR yield) after 24 h ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91–7.87 (m, 2H), 7.66–7.63 (m, 2H), 7.40–7.30 (m, 3H), 7.28–7.23 (m, 2H), 7.08 (dd, *J* = 2.6, 1.6 Hz, 1H), 6.80 (dd, *J* = 4.0, 1.7 Hz, 1H), 6.29 (dd, *J* = 4.0, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.3, 141.17, 141.16, 139.4, 132.5 (q, $^{2}J_{C–F}$ = 33.0 Hz), 130.9, 129.6, 128.6, 127.9, 126.7 (×2), 124.6 (q, $^{1}J_{C–F}$ = 273 Hz), 124.2 (q, $^{3}J_{C–F}$ = 3.7 Hz), 122.9, 108.7; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{12}F_3NO$ $[M+Na]^+$ 338.0763; found: 338.0688.



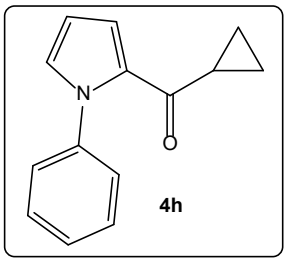
(4-Bromophenyl)(1-phenyl-1H-pyrrol-2-yl)methanone (4f): Compound 4f purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a yellow solid(22 mg, 34% isolated yield; 45% NMR yield) after 24 h; m.p.: 123–124 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69–7.65 (m, 2H), 7.53–7.49 (m, 2H), 7.37–7.27 (m, 3H), 7.24–7.20 (m, 2H), 7.04 (dd, *J* = 2.7, 1.6 Hz, 1H), 6.78 (dd, *J* = 4.0, 1.6 Hz, 1H), 6.26 (dd, *J* = 4.0, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.6, 140.5, 137.8, 131.5, 131.4, 131.1, 130.7, 129.0, 127.6, 126.8, 125.6, 123.4, 109.6; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{12}{}^{79}BrNO$ $[M(^{79}Br)+Na]^+$ 347.9994; found: 347.9912.



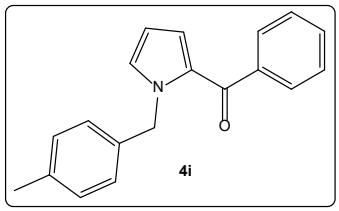
(1-Phenyl-1H-pyrrol-2-yl)(thiophen-2-yl)methanone (4g): Compound 4g purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a reddish-brown solid(22 mg, 44% isolated yield; 65% NMR yield) after 24 h, m.p.: 66–67°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.51 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.33–7.18 (m, 5H), 7.06–7.01 (m, 2H), 7.00 (dd, *J* = 2.7, 1.6 Hz, 1H), 6.25 (dd, *J* = 4.0, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.2, 143.5, 139.4, 131.7, 131.6, 129.9, 129.7, 127.9, 126.6, 126.4, 124.5, 120.6, 108.4; HRMS (ESI-TOF) m/z: calcd for $C_{15}H_{11}NOS$ $[M+Na]^+$ 276.0454; found: 276.0413.



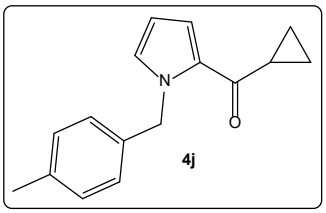
Cyclopropyl(1-phenyl-1H-pyrrol-2-yl)methanone (4h): Compound 4h purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a orange oil (16 mg, 38% isolated yield; 60% NMR yield) after 48 h, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.22 (m, 3H), 7.21–7.16 (m, 3H), 6.90 (dd, *J* = 2.7, 1.7 Hz, 1H), 6.26 (dd, *J* = 4.0, 2.6 Hz, 1H), 2.44–2.34 (m, 1H), 1.02–0.96 (m, 2H), 0.81–0.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.5, 141.1, 132.2, 130.8, 128.6, 127.6, 126.1, 119.6, 109.3, 29.7, 17.9, 10.2; HRMS (ESI-TOF) m/z: calcd for $C_{14}H_{13}NO$ $[M+Na]^+$ 234.0889; found: 234.0850.



(1-(4-Methylbenzyl)-1H-pyrrol-2-yl)(phenyl)methanone (4i): Compound 4i purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a maroon oil (17 mg, 30% isolated yield; 48% NMR yield) after 48 h; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74–7.67 (m, 2H), 7.46–7.41 (m, 1H), 7.38–7.33 (m, 2H), 7.06–7.00 (m, 4H), 6.93 (dd, *J* = 2.6, 1.7 Hz, 1H), 6.69 (dd, *J* = 4.1, 1.7 Hz, 1H), 6.12 (dd, *J* = 4.0, 2.5 Hz, 1H), 5.55 (s, 2H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.2, 140.0, 137.2, 135.2, 131.4, 130.8, 130.1, 129.34, 129.28, 128.0, 127.3, 123.5, 108.6, 52.2, 21.1; HRMS (ESI-TOF) m/z: calcd for $C_{19}H_{17}NO$ $[M+Na]^+$ 298.1202; found: 298.1148.

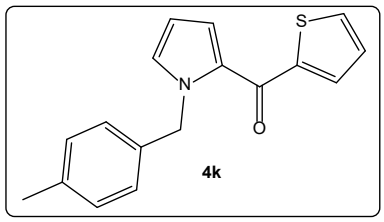


Cyclopropyl(1-(4-methylbenzyl)-1H-pyrrol-2-yl)methanone (4j): Compound 4j purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a pinkish-orange oil(9 mg, 19% isolated yield; 30% NMR yield) after 48 h; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (dd, *J* = 4.1, 1.7 Hz, 1H), 7.04–7.00 (m, 2H), 6.96–6.92 (m, 2H), 6.81 (dd, *J* = 2.6, 1.7 Hz, 1H), 6.13

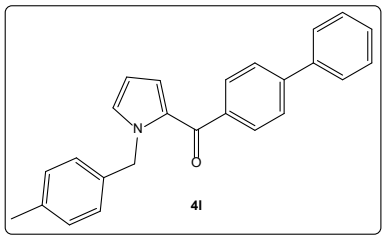


(dd, J = 4.1, 2.6 Hz, 1H), 5.47 (s, 2H), 2.44–2.35 (m, 1H), 2.23 (s, 3H), 1.04–0.98 (m, 2H), 0.81–0.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 137.0, 135.3, 130.0, 129.2, 129.1, 127.2, 119.5, 108.5, 52.3, 21.1, 17.9, 10.0; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{17}NO$ $[M+Na]^+$ 262.1202; found: 262.1153.

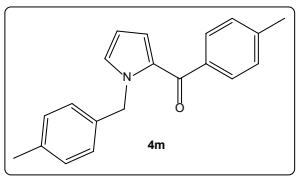
(1-(4-Methylbenzyl)-1H-pyrrol-2-yl)(thiophen-2-yl)methanone (4k): Compound 4k purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a bright orange oil(18 mg, 32% isolated yield; 46% NMR yield) after 48 h ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, J = 3.7, 1.2 Hz, 1H), 7.52 (dd, J = 4.9, 1.2 Hz, 1H), 7.06–6.98 (m, 6H), 6.91 (dd, J = 2.6, 1.7 Hz, 1H), 6.15 (dd, J = 4.0, 2.6 Hz, 1H), 5.49 (s, 2H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 143.8, 136.2, 134.1, 131.4, 131.0, 129.6, 128.9, 128.3, 126.5, 126.2, 120.5, 107.7, 51.0, 20.1; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{15}NOS$ $[M+Na]^+$ 304.0767; found: 304.0729.



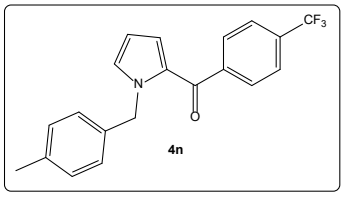
[1,1'-Biphenyl]-4-yl(1-(4-methylbenzyl)-1H-pyrrol-2-yl)methanone (4l): Compound 4l purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a colorless oil(18 mg, 15% isolated yield; 30% NMR yield) after 48 h ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82–7.77 (m, 2H), 7.59–7.55 (m, 4H), 7.42–7.37 (m, 2H), 7.34–7.29 (m, 1H), 7.10–6.99 (m, 4H), 6.94 (dd, J = 2.5, 1.7 Hz, 1H), 6.75 (dd, J = 4.0, 1.7 Hz, 1H), 6.15 (dd, J = 4.0, 2.5 Hz, 1H), 5.57 (s, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.7, 144.2, 140.3, 138.7, 137.2, 135.2, 130.7, 130.2, 129.9, 129.4, 128.9, 127.9, 127.33, 127.28, 126.7, 123.3, 108.6, 52.2, 21.1; HRMS (ESI-TOF) m/z: calcd for $C_{25}H_{21}NO$ $[M+Na]^+$ 374.1515; found: 374.1500.



(1-(4-Methylbenzyl)-1H-pyrrol-2-yl)(*p*-tolyl)methanone (4m): Compound 4m purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a colorless oil(16 mg, 28% isolated yield; 45% NMR yield) after 48 h; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.58 (m, 2H), 7.18 – 7.14 (m, 2H), 7.08 – 6.97 (m, 4H), 6.91 (dd, J = 2.5, 1.7 Hz, 1H), 6.68 (dd, J = 4.0, 1.7 Hz, 1H), 6.11 (dd, J = 4.0, 2.5 Hz, 1H), 2.34 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.0, 142.0, 137.2, 137.2, 135.3, 130.4, 130.3, 129.5, 129.4, 128.7, 127.3, 123.1, 108.4, 52.1, 21.6, 21.1; HRMS (ESI-TOF) m/z: calcd for $C_{20}H_{19}NO$ $[M+Na]^+$ 312.1359; found: 312.1288.

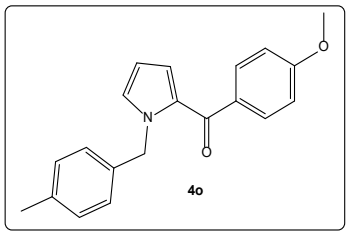


(1-(4-Methylbenzyl)-1H-pyrrol-2-yl)(4-(trifluoromethyl)phenyl)methanone (4n): Compound 4n purified by column chromatography on silica gel (hexane/EtOAc, 10:1) to give a yellowish-



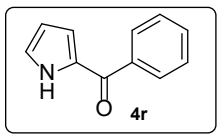
orange oil(7 mg, 10% isolated yield; 20% NMR yield) after 48 h ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.07–7.01 (m, 4H), 6.97 (dd, *J* = 2.5, 1.7 Hz, 1H), 6.66 (dd, *J* = 4.1, 1.7 Hz, 1H), 6.14 (dd, *J* = 4.1, 2.5 Hz, 1H), 5.55 (s, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.6, 143.1, 137.4, 134.9, 133.0 (q, $^2J_{C–F}$ = 33.0 Hz), 131.6, 129.6, 129.40, 129.38, 127.3, 125.0 (q, *J* = 3.7 Hz), 124.1 122.5 (q, $^1J_{C–F}$ = 273.0 Hz), 109.0, 52.4, 21.1; HRMS (ESI-TOF) m/z: calcd for $C_{20}H_{16}F_3NO$ $[M+H]^+$ 344.1257; found: 344.1293.

(4-Methoxyphenyl)(1-(4-methylbenzyl)-1H-pyrrol-2-yl)methanone (4o): Compound 4o purified by column chromatography on silica gel (hexane/EtOAc, 10:1) to give an orange oil(17



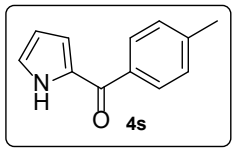
mg, 28% isolated yield; 43% NMR yield) after 48 h; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76–7.71 (m, 2H), 7.05–6.99 (m, 4H), 6.90 (dd, *J* = 2.6, 1.7 Hz, 1H), 6.87–6.84 (m, 2H), 6.67 (dd, *J* = 4.0, 1.7 Hz, 1H), 6.12 (dd, *J* = 4.0, 2.5 Hz, 1H), 5.52 (s, 2H), 3.79 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.2, 162.5, 137.1, 135.3, 132.5, 131.6, 130.3, 130.2, 129.3, 127.3, 122.5, 113.3, 108.3, 55.4, 52.0, 21.1; HRMS (ESI-TOF) m/z: calcd for $C_{20}H_{19}NO_2$ $[M+Na]^+$ 328.1308; found: 328.1271.

Phenyl(1H-pyrrol-2-yl)methanone (4r)[7]: Purified by column chromatography on silica gel



(hexane/EtOAc, 10:1) to afford 4r as white solid; reaction time 24 h; yield (90 %); m.p.: 77–78 ºC (lit.,[7] 78–80 ºC);; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.85–7.79 (m, 2H), 7.47–7.42 (m, 1H), 7.40–7.34 (m, 2H), 7.07 (td, *J* = 2.7, 1.4 Hz, 1H), 6.79 (ddd, *J* = 3.8, 2.4, 1.4 Hz, 1H), 6.22 (dt, *J* = 3.8, 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.2, 138.6, 131.9, 131.2, 129.1, 128.4, 126.1, 120.1, 111.0.

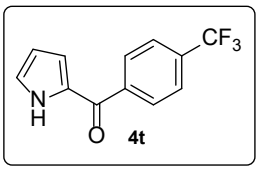
(1H-pyrrol-2-yl)(*p*-tolyl)methanone (4s)[8]: Purified by column chromatography on silica gel



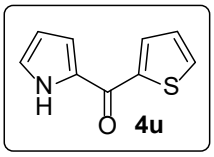
(hexane/EtOAc, 10:1) to afford 4s as white solid; reaction time 24 h; yield (87 %); m.p.: 118–119 °C (lit.,[8] 119–121 ºC); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.90 (s, 1H), 7.78–7.73 (m, 2H), 7.23–7.19 (m, 2H), 7.07 (td, *J* = 2.7, 1.3 Hz, 1H),

6.82 (ddd, J = 3.8, 2.5, 1.3 Hz, 1H), 6.26 (dt, J = 3.9, 2.5 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.6, 142.5, 135.6, 131.2, 129.2, 129.0, 125.2, 119.2, 110.9, 21.6.

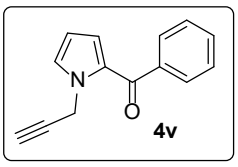
(1H-pyrrol-2-yl)(4-(trifluoromethyl)phenyl)methanone (4t)[9]: Purified by column chromatography on silica gel (hexane/EtOAc, 10:1) to afford 4t as off-white solid; reaction time 24 h; yield (75 %); m.p.: 103–104 °C (lit.,[9] not reported); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 7.89 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 8.1 Hz, 2H), 7.14–7.08 (m, 1H), 6.80–6.73 (m, 1H), 6.29–6.22 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.7, 141.6, 133.3 ($^2J_{C–F}$ = 32.6 Hz), 130.8, 129.3, 126.8, 125.4 ($^3J_{C–F}$ = 3.7 Hz), 125.2 ($^1J_{C–F}$ = 273.0 Hz), 120.7, 111.4.



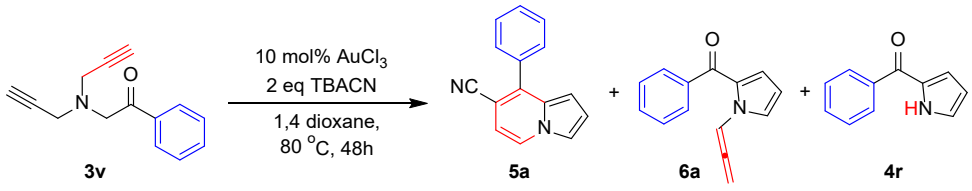
(1H-pyrrol-2-yl)(thiophen-2-yl)methanone (4u)[10]: Purified by column chromatography on silica gel (hexane/EtOAc, 10:1) to afford 4u as brown solid; reaction time 24 h; yield (85 %); m.p.: 69–70 °C (lit.,[10] not reported); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.29 (s, 1H), 7.84 (dd, J = 3.8, 1.2 Hz, 1H), 7.55 (dd, J = 4.9, 1.2 Hz, 1H), 7.10–7.06 (m, 3H), 6.29–6.25 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 142.8, 132.4, 132.3, 130.7, 127.9, 125.7, 117.9, 111.1.



Phenyl(1-(prop-2-yn-1-yl)-1H-pyrrol-2-yl)methanone (4v)[11]: Compound 4v purified by column chromatography on silica gel (hexane/EtOAc, 20:1) to give a reddish-brown oil(11 mg, 26% isolated yield; 40% NMR yield) after 48 h ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76–7.72 (m, 2H), 7.49–7.45 (m, 1H), 7.41–7.36 (m, 2H), 7.26–7.21 (m, 1H), 6.71 (dd, J = 4.1, 1.7 Hz, 1H), 6.16 (dd, J = 4.0, 2.6 Hz, 1H), 5.24 (d, J = 2.6 Hz, 2H), 2.39 (t, J = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.2, 139.6, 131.6, 129.8, 129.2, 128.1, 123.7, 108.8, 78.3, 74.1, 38.7.



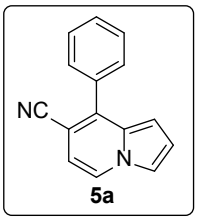
7. Experimental Procedure for the Gold-Catalyzed Reaction of Substrate 3v



Scheme S6. Gold(III)-catalyzed reaction of **3v** in the presence of TBACN.

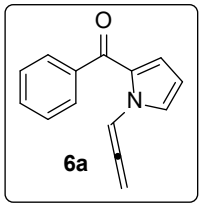
To a solution of the *N*,*N*-dipropargylamino ketone **3v** (1.0 mmol, 1.0 equiv) in 1,4-dioxane (2 mL) were added tetrabutylammonium cyanide (TBACN) (2.0 mmol, 2.0 equiv) and gold(III) chloride ($AuCl_3$) (0.1 mmol, 0.10 equiv). The reaction mixture was heated at 80 °C for 48 hours, and the progress was monitored by thin-layer chromatography (TLC). Upon completion, the mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The resulting residue was diluted with ethyl acetate and washed sequentially with water and brine. The organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$), filtered, and concentrated in vacuo. The crude material was purified by column chromatography to isolate the indolizine derivative **5a** (20% yield), corresponding allene derivative **6a** (35% yield) and the depropargylated pyrrole product **4r** (25% yield).

8-phenylindolizine-7-carbonitrile (5a)[11]: Purified by column chromatography on silica gel



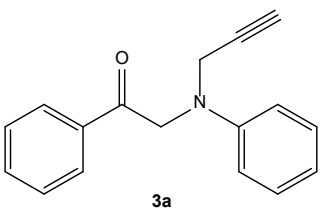
(hexane/EtOAc, 20:1) to afford 5a as yellow solid; reaction time 48 h; yield (20 %); m.p.: 140–142 °C (lit.,[11] 147-148 ºC); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 1.0, 7.2 Hz, 1H), 7.65–7.62 (m, 2H), 7.55–7.50 (m, 4H), 6.92 (dd, *J* = 2.6, 4.2 Hz, 1H), 6.69 (d, *J* = 7.2 Hz, 1H), 6.59 (dt, *J* = 1.2, 4.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 134.9, 131.3, 129.5, 129.1, 128.7, 124.2, 118.9, 116.7, 115.9, 111.1, 105.6, 98.1.

Phenyl(1-(propa-1,2-dien-1-yl)-1*H*-pyrrol-2-yl)methanone (6a)[12]: Purified by column

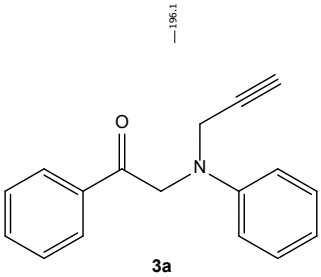


chromatography on silica gel (hexane/EtOAc, 20:1) to afford 6a as yellow oil; reaction time 48 h; yield (35 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (t, *J* = 6.6 Hz, 1H), 7.75–7.71 (m, 2H), 7.50–7.45 (m, 1H), 7.41–7.36 (m, 2H), 7.20 (dd, *J* = 2.8, 1.6 Hz, 1H), 6.71 (dd, *J* = 4.0, 1.6 Hz, 1H), 6.18 (dd, *J* = 4.0, 2.8 Hz, 1H), 5.45 (d, *J* = 6.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1, 186.4, 139.7, 131.7, 129.2, 128.1, 127.7, 124.2, 110.0, 99.4, 87.0.

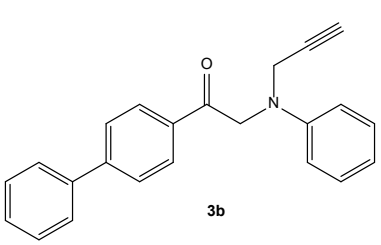
8. NMR spectra for the substrates and products



3a

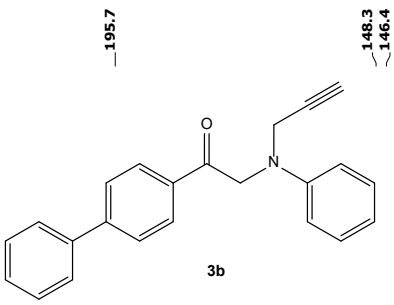


3a


O
N

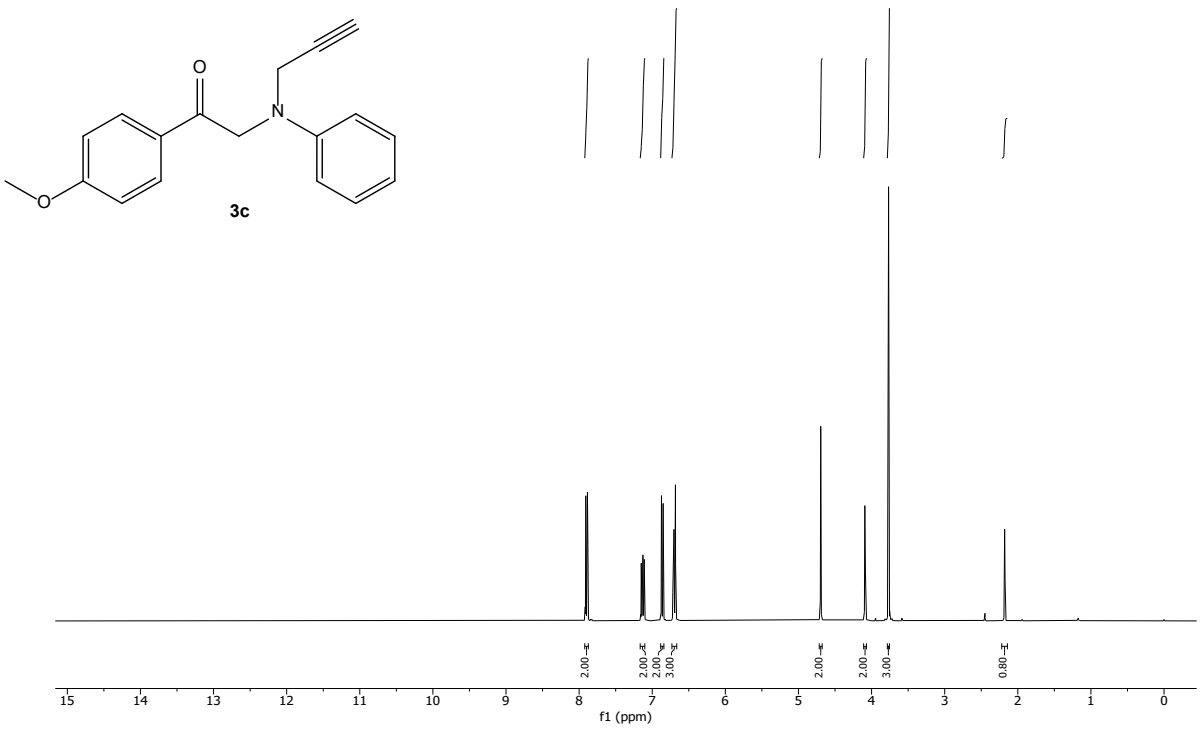
3b

2.06
2.16
2.56
2.44
1.06
2.07
3.00
2.00
2.00
0.84
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

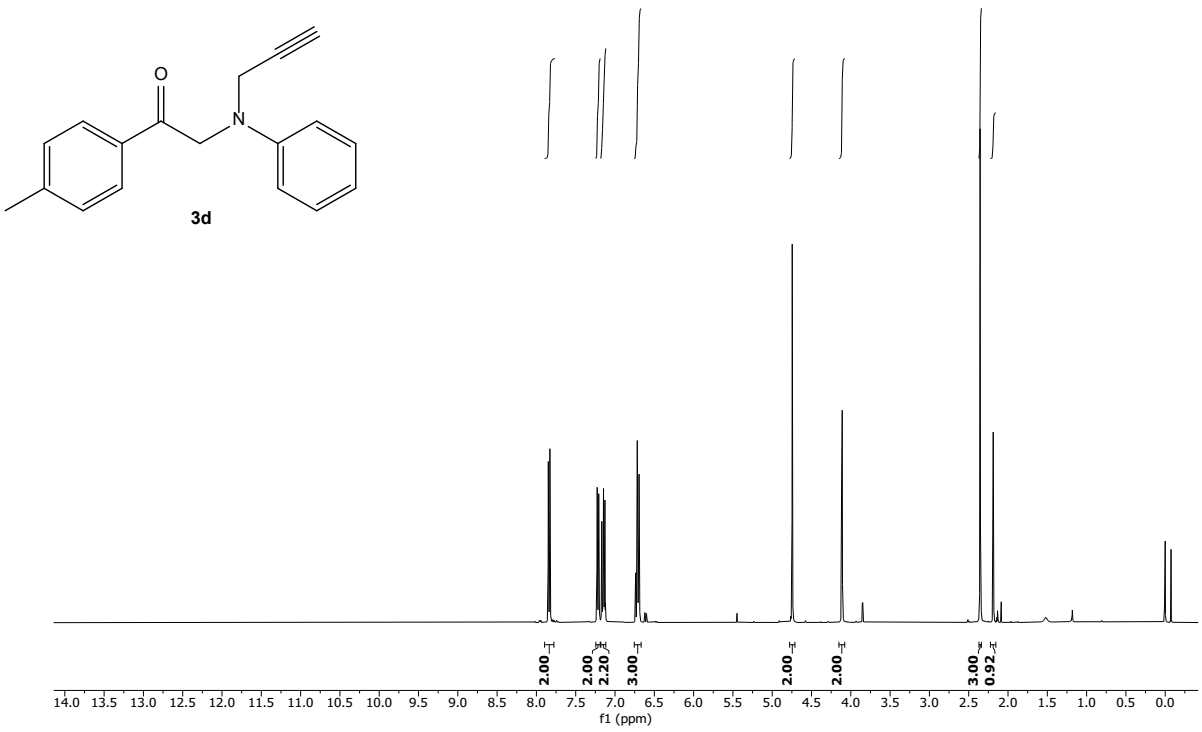

O
N

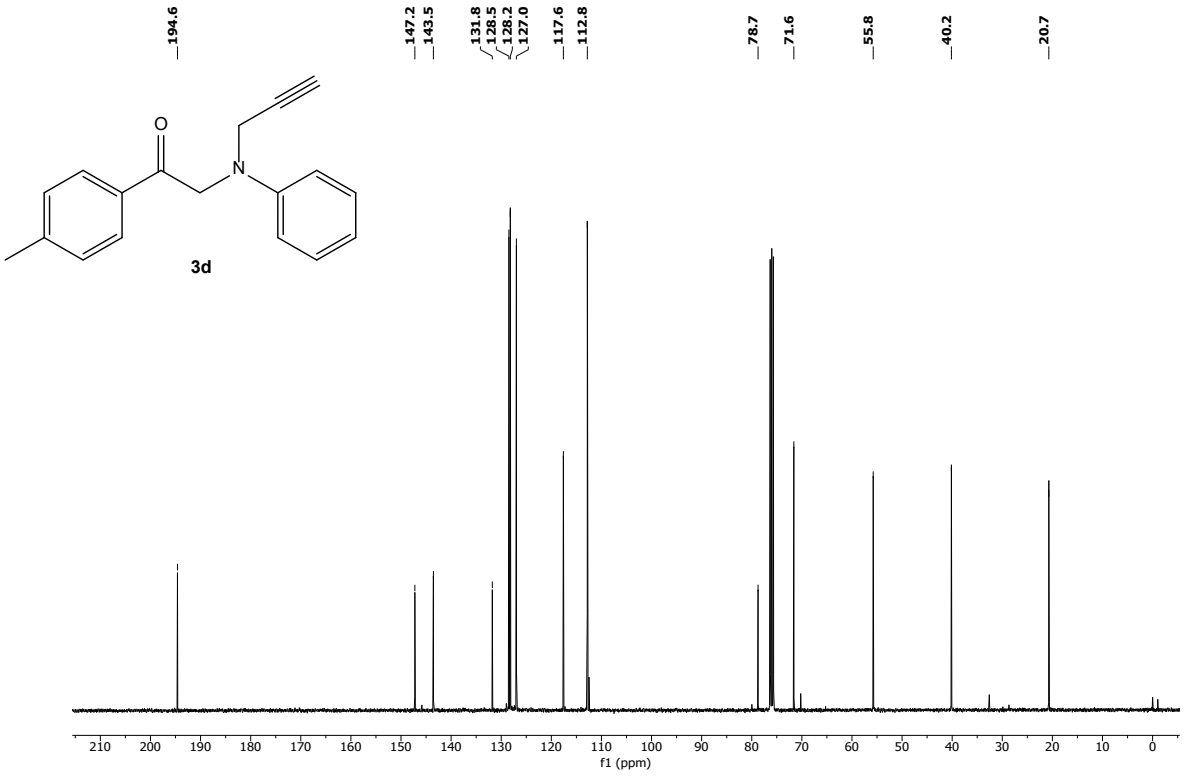
3b

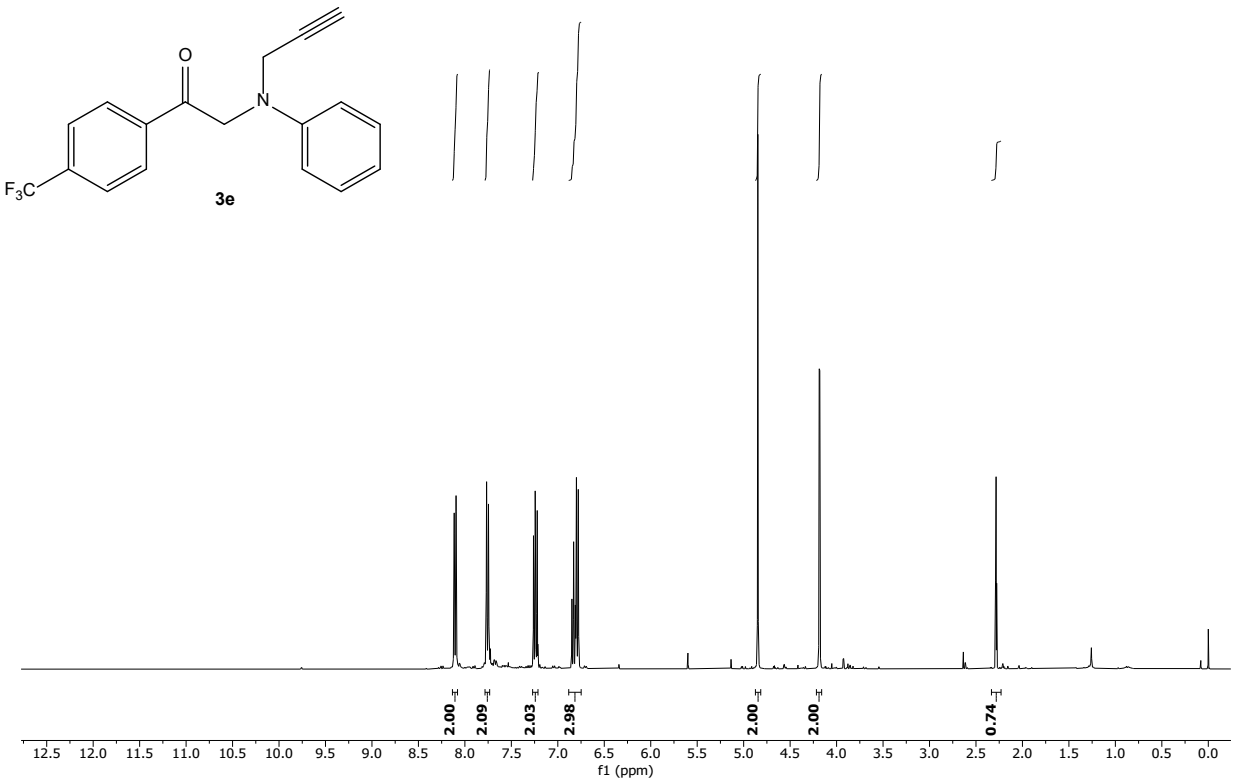
195.7
148.3
146.4
139.7
134.0
129.3
129.1
128.5
128.4
127.5
127.3
118.8
114.0
79.7
72.8
57.0
41.3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

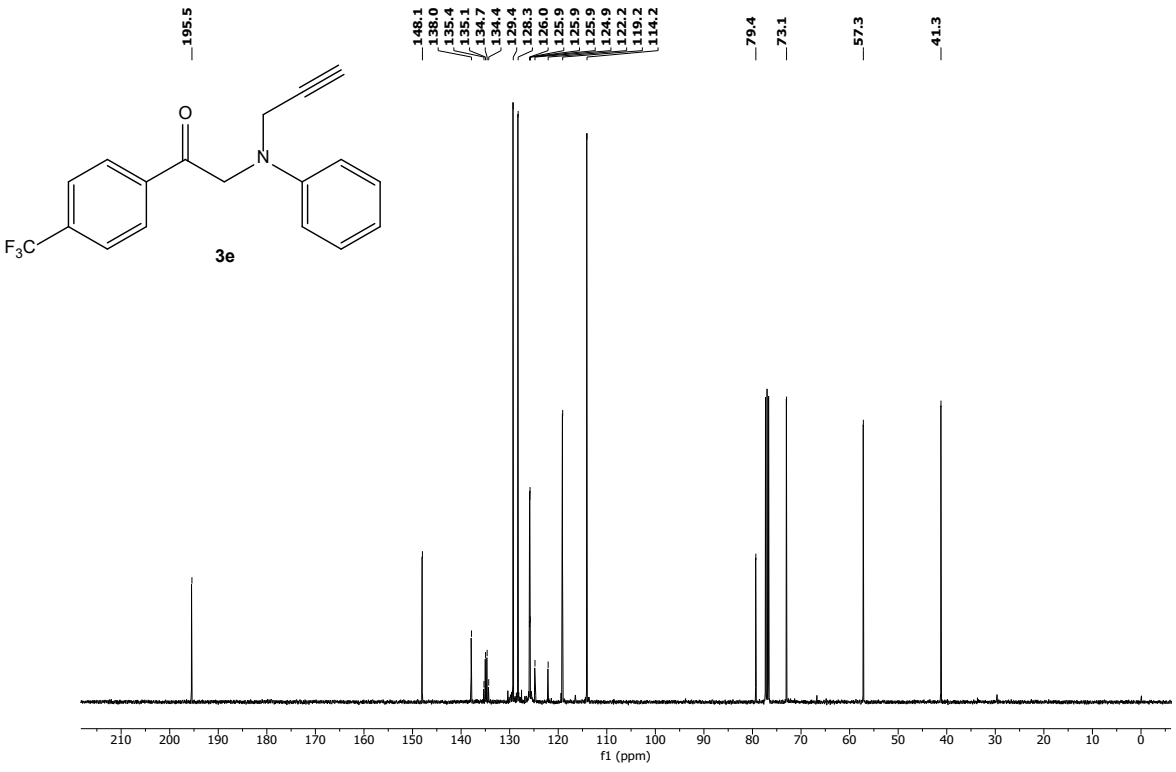

O
N
O
3c
2.00
2.00
2.00
3.00
2.00
2.00
3.00
0.80
f1 (ppm)


194.5
163.9
148.3
130.2
129.3
128.4
118.6
114.0
113.9
79.9
72.7
56.6
55.6
41.3
O
N
O
3c
f1 (ppm)


O
N
3d
2.00
2.00
2.20
3.00
2.00
2.00
3.00
0.92
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


194.6
147.2
143.5
131.8
128.5
128.2
127.0
117.6
112.8
78.7
71.6
55.8
40.2
20.7
O
N
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
F3C
3e
2.00
2.09
2.03
2.98
2.00
2.00
0.74
f1 (ppm)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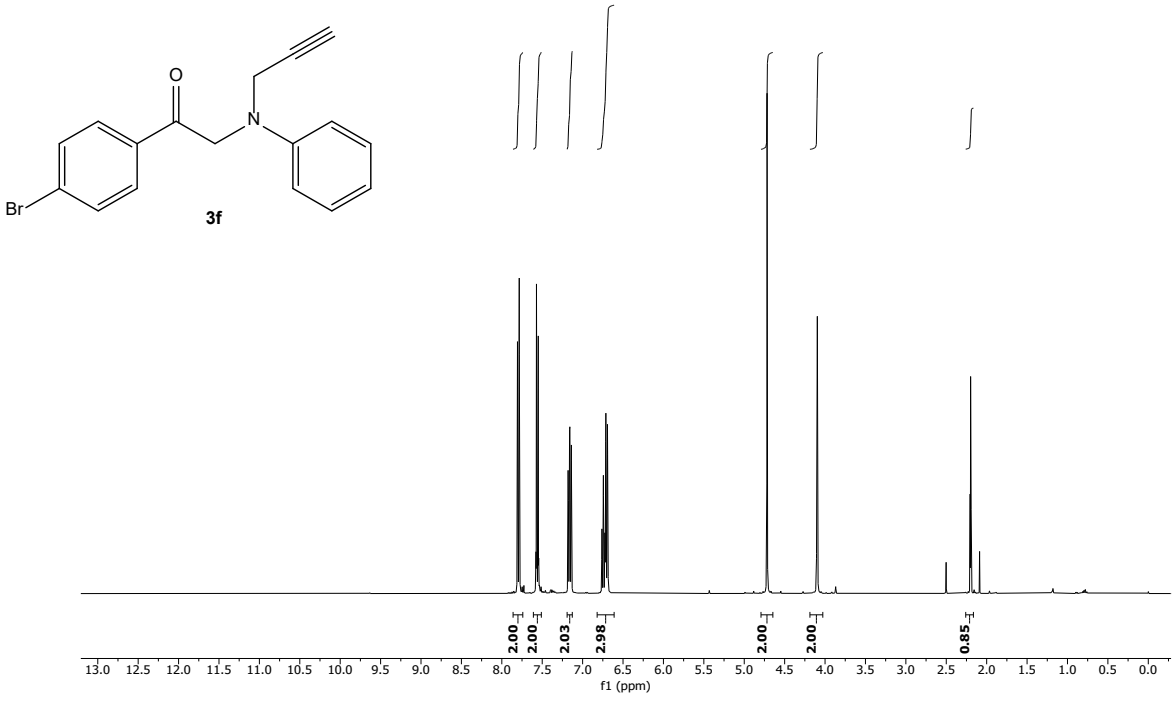
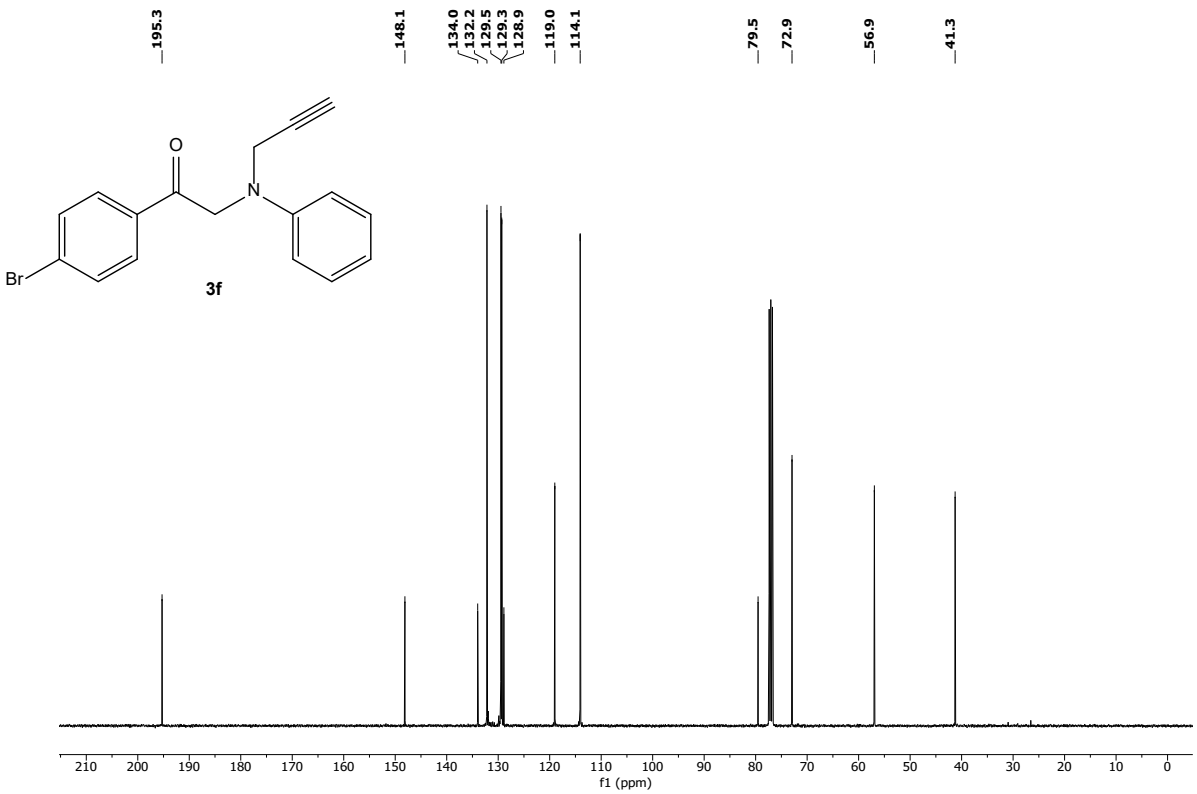
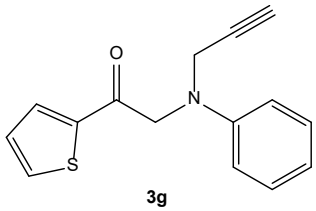
148.1
138.0
135.4
135.1
134.7
134.4
129.4
128.3
126.0
125.9
125.9
125.9
124.9
122.2
119.2
114.2
79.4
73.1
57.3
41.3
O
N
F3C
3e
f1 (ppm)


O
N
Br
3f
2.00
2.00
2.03
2.98
2.00
2.00
0.85
f1 (ppm)


195.3
148.1
134.0
132.2
129.5
129.3
128.9
119.0
114.1
79.5
72.9
56.9
41.3
O
N
Br
3f
f1 (ppm)


O
N
S

3g

1.00
0.95
2.10
1.00
3.00
2.04
2.04
0.90
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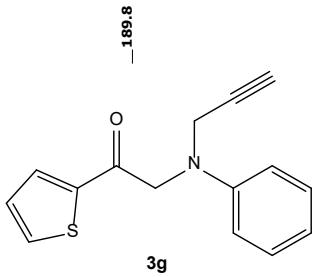
f1 (ppm)


O
N
S

3g

189.8
148.1
141.1
134.2
132.3
129.3
128.2
119.2
114.3
79.4
73.0
58.0
41.4
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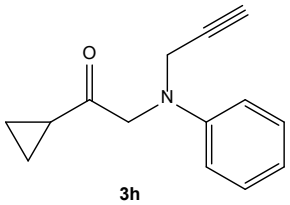
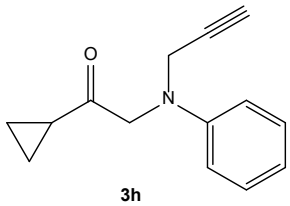
f1 (ppm)


O
N

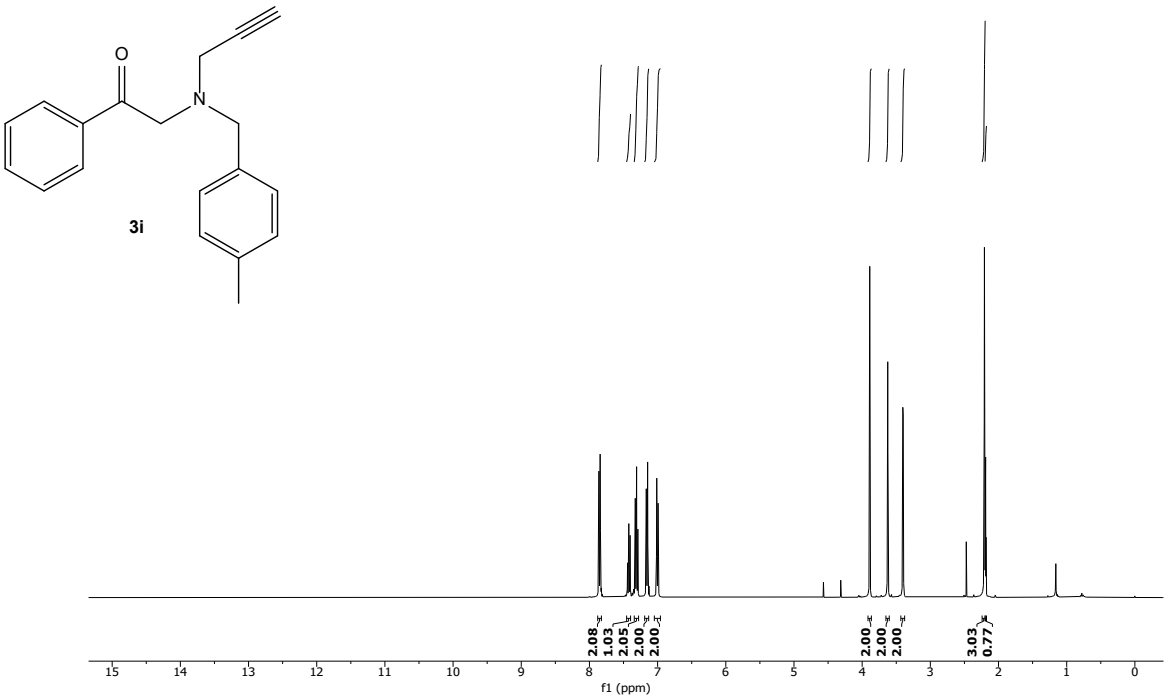
3h

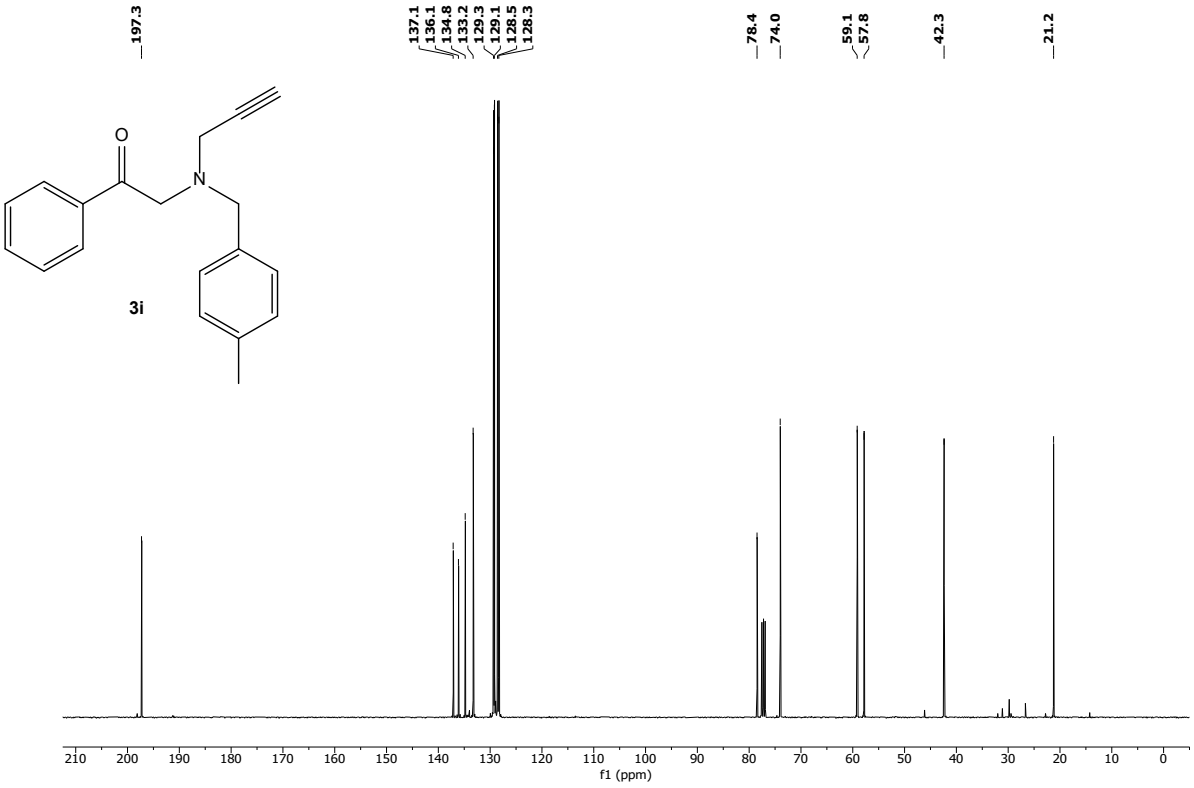
2.09
1.00
2.00
2.02
2.00
1.00
1.02
2.13
2.10
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

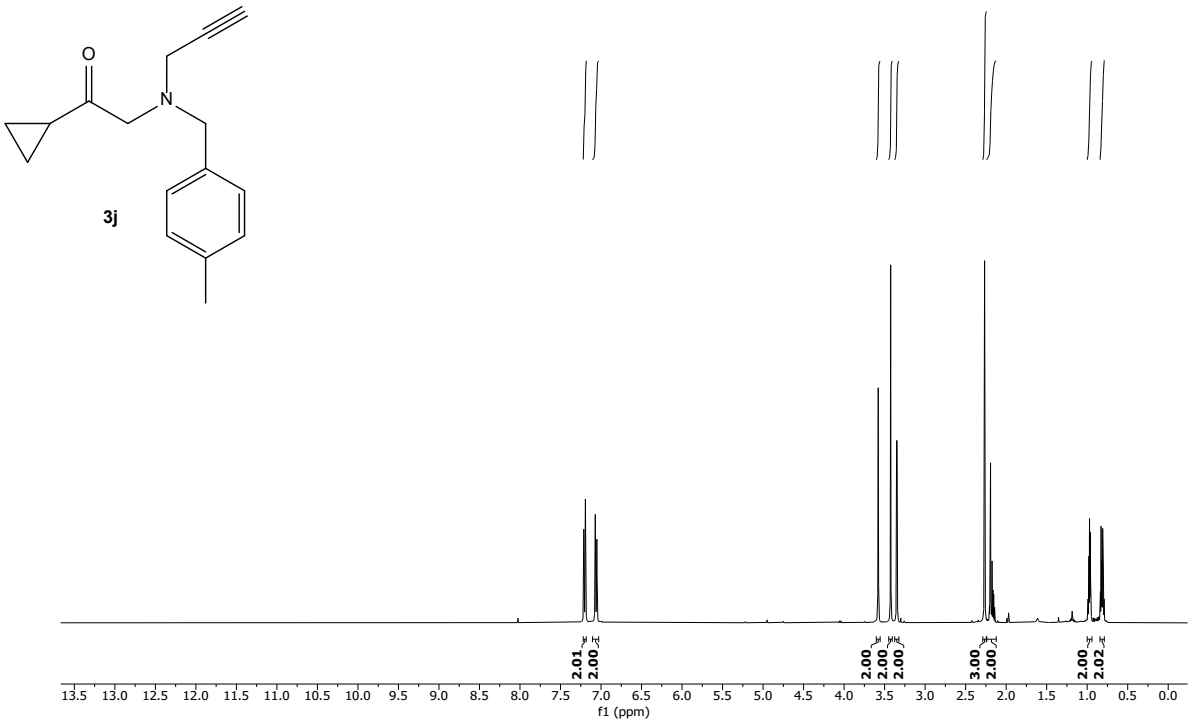

O
N

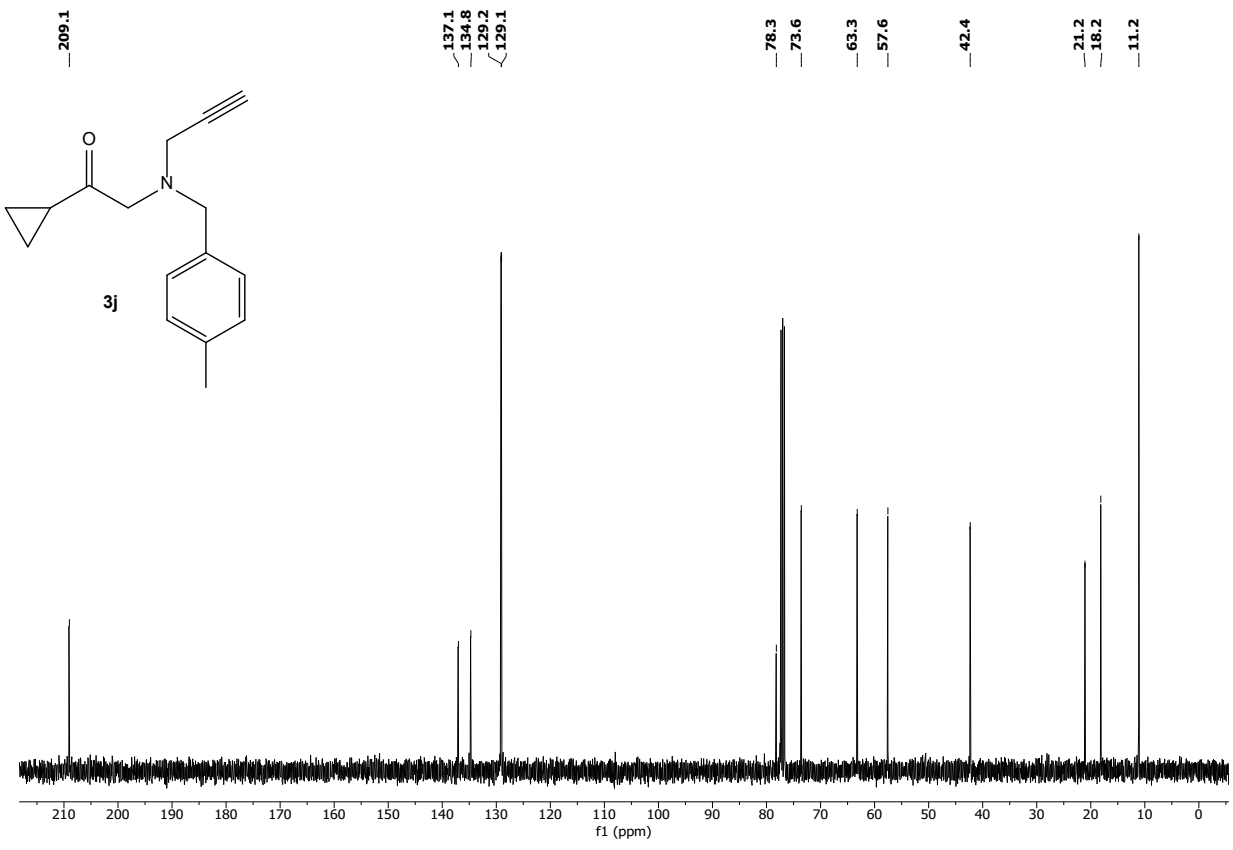
3h

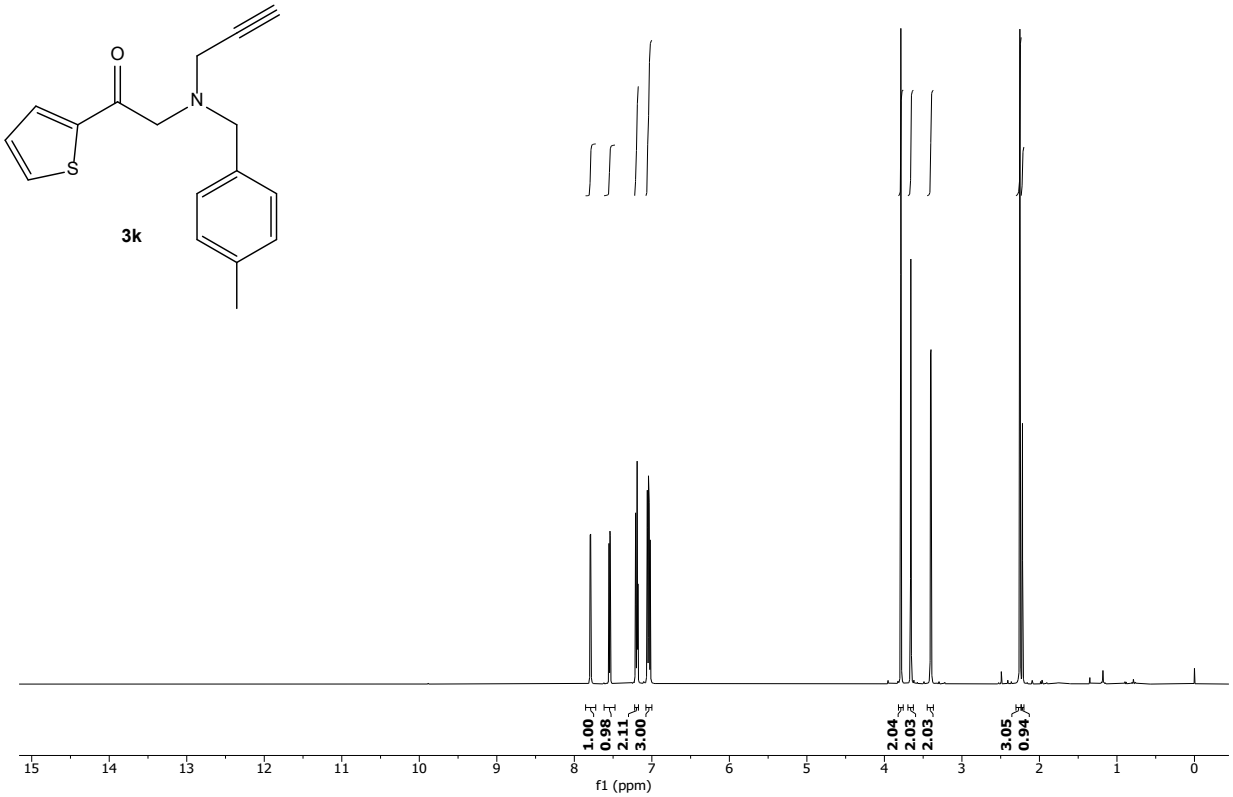
209.4
147.9
129.3
118.7
113.7
79.4
72.7
61.3
41.4
29.7
17.7
11.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

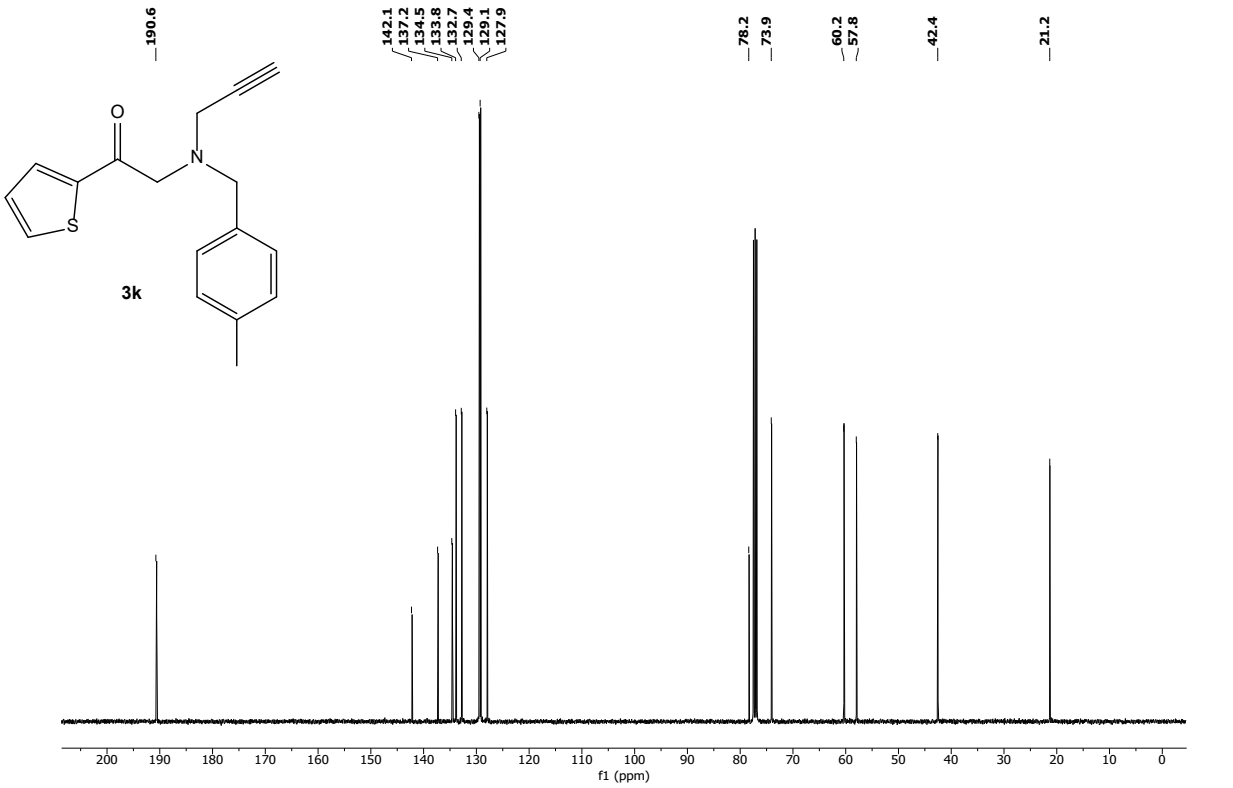

O
N
3i
2.08
1.03
2.05
2.00
2.00
2.00
2.00
2.00
3.03
0.77
f1 (ppm)

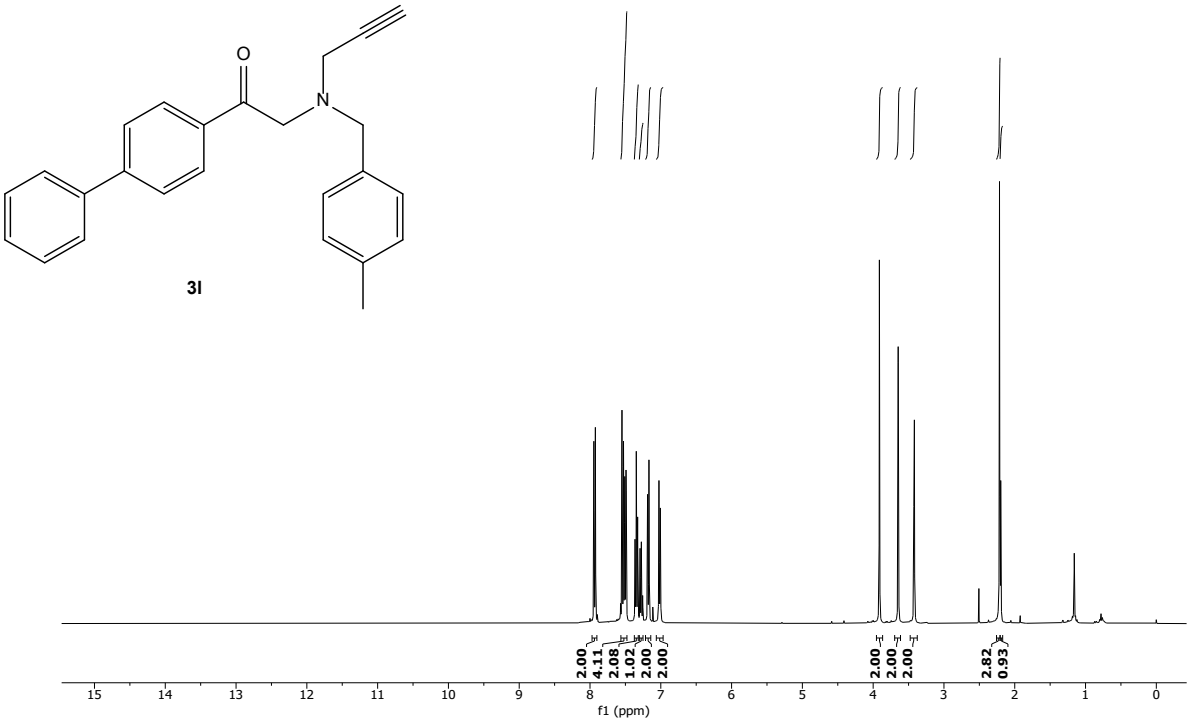

197.3
137.1
136.1
134.8
133.2
129.3
129.1
128.5
128.3
78.4
74.0
59.1
57.8
42.3
21.2
O
N
3i
f1 (ppm)

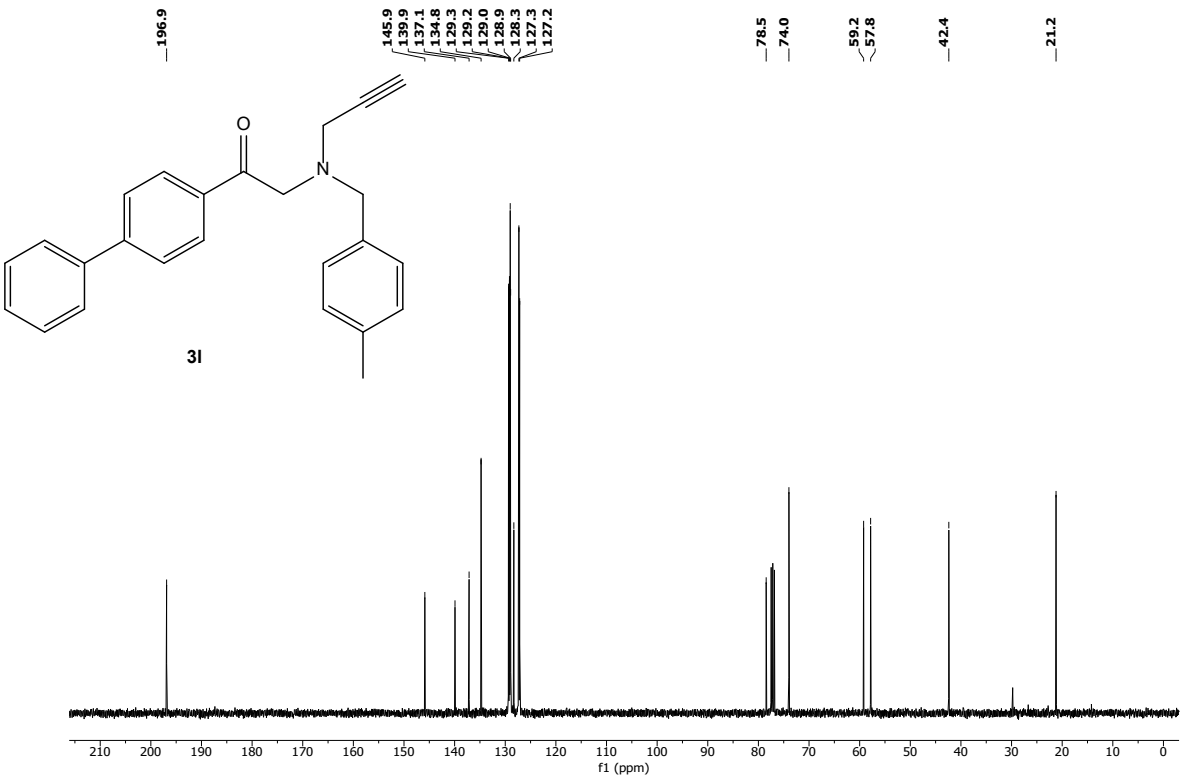

O
N
3j
2.01
2.00
2.00
2.00
2.00
3.00
2.00
2.00
2.02
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

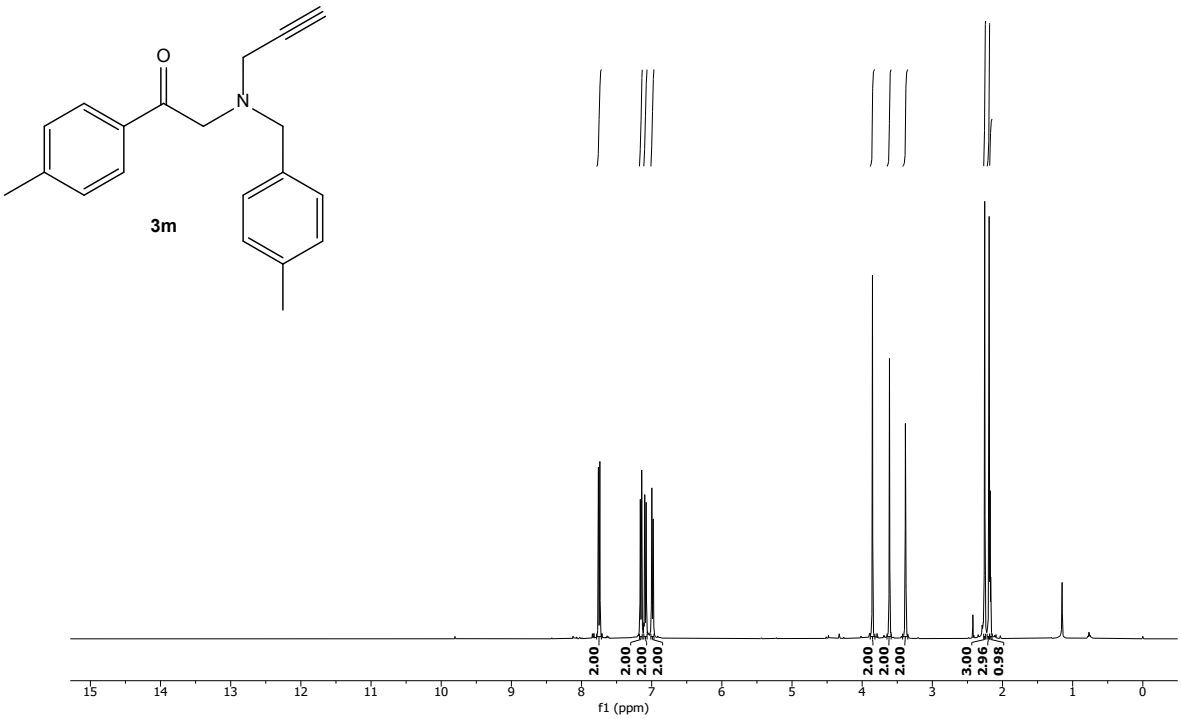

209.1
137.1
134.8
129.2
129.1
78.3
73.6
63.3
57.6
42.4
21.2
18.2
11.2
O
N
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

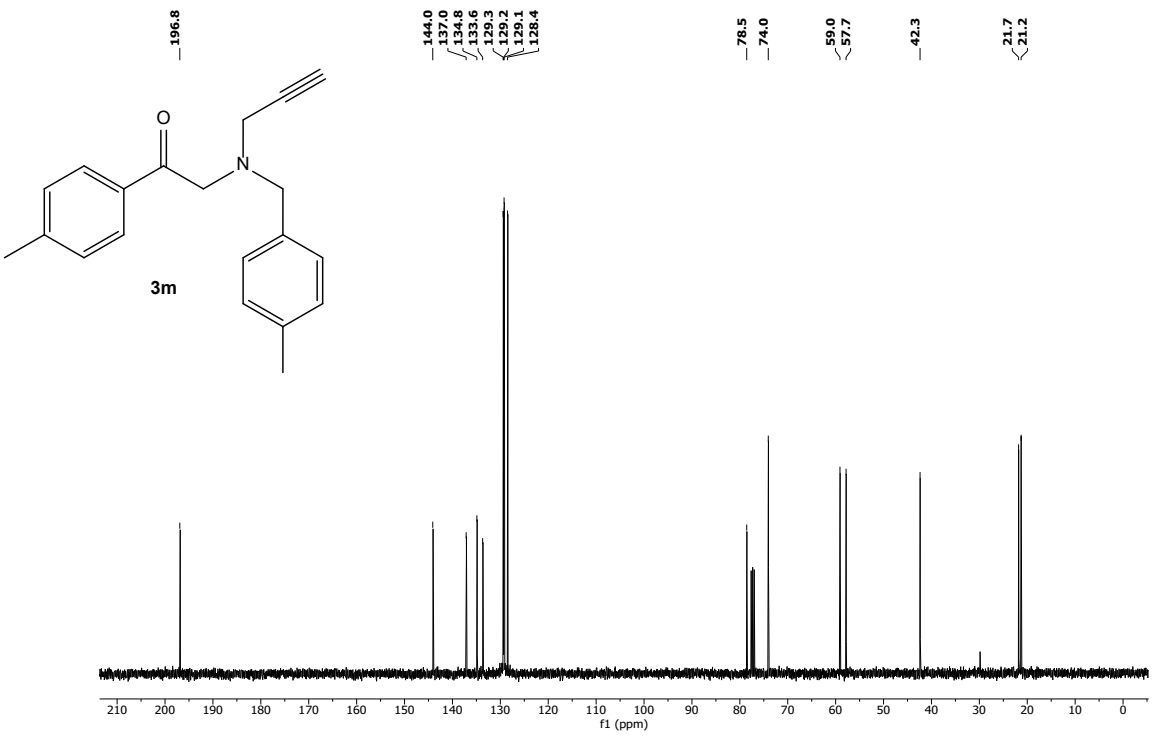

O
N
S
3k
1.00
0.98
2.11
3.00
2.04
2.03
2.03
3.05
0.94
f1 (ppm)


190.6
142.1
137.2
134.5
133.8
132.7
129.4
129.1
127.9
78.2
73.9
60.2
57.8
42.4
21.2
O
N
S
3k
f1 (ppm)


O
N
3l
2.00
4.11
2.08
1.02
2.00
2.00
2.00
2.00
2.00
2.82
0.93
f1 (ppm)


196.9
145.9
139.9
137.1
134.8
129.3
129.2
129.0
128.9
128.3
127.3
127.2
78.5
74.0
59.2
57.8
42.4
21.2
O
N
3l
f1 (ppm)


O
N
3m
2.00
2.00
2.00
2.00
2.00
2.00
3.00
2.96
0.98
f1 (ppm)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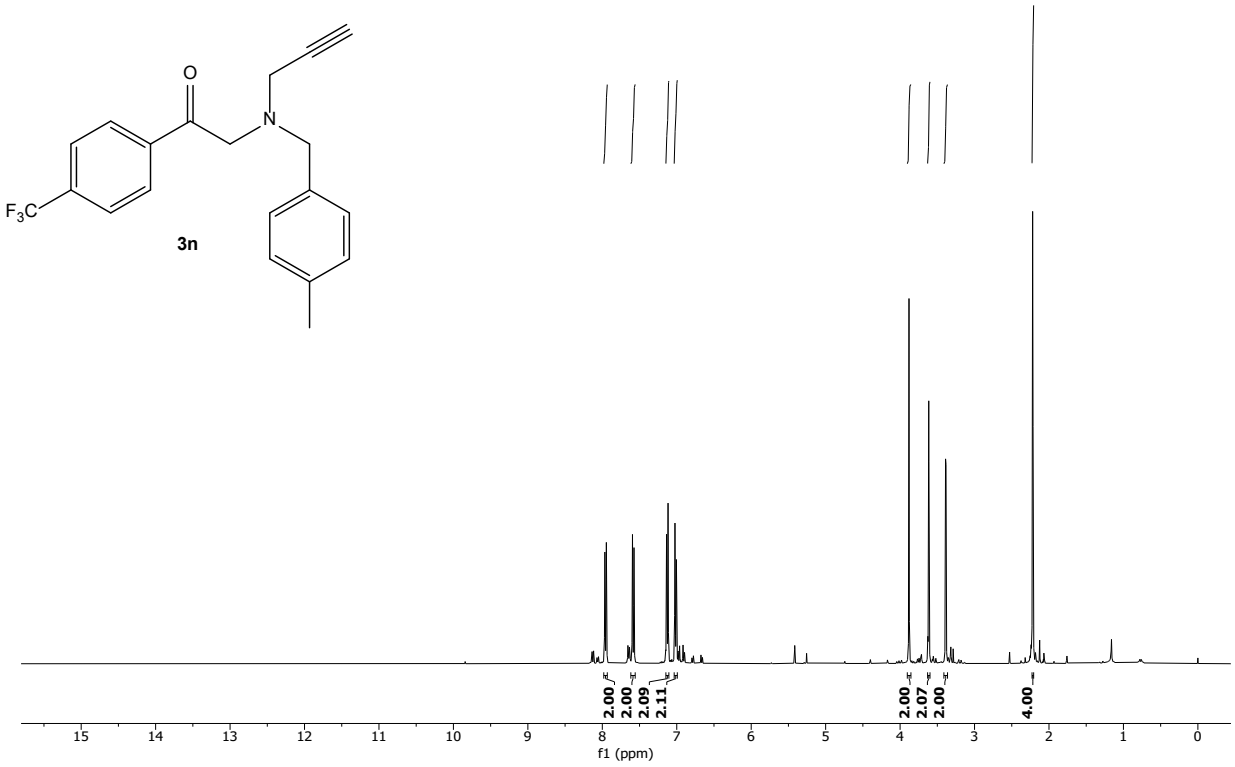
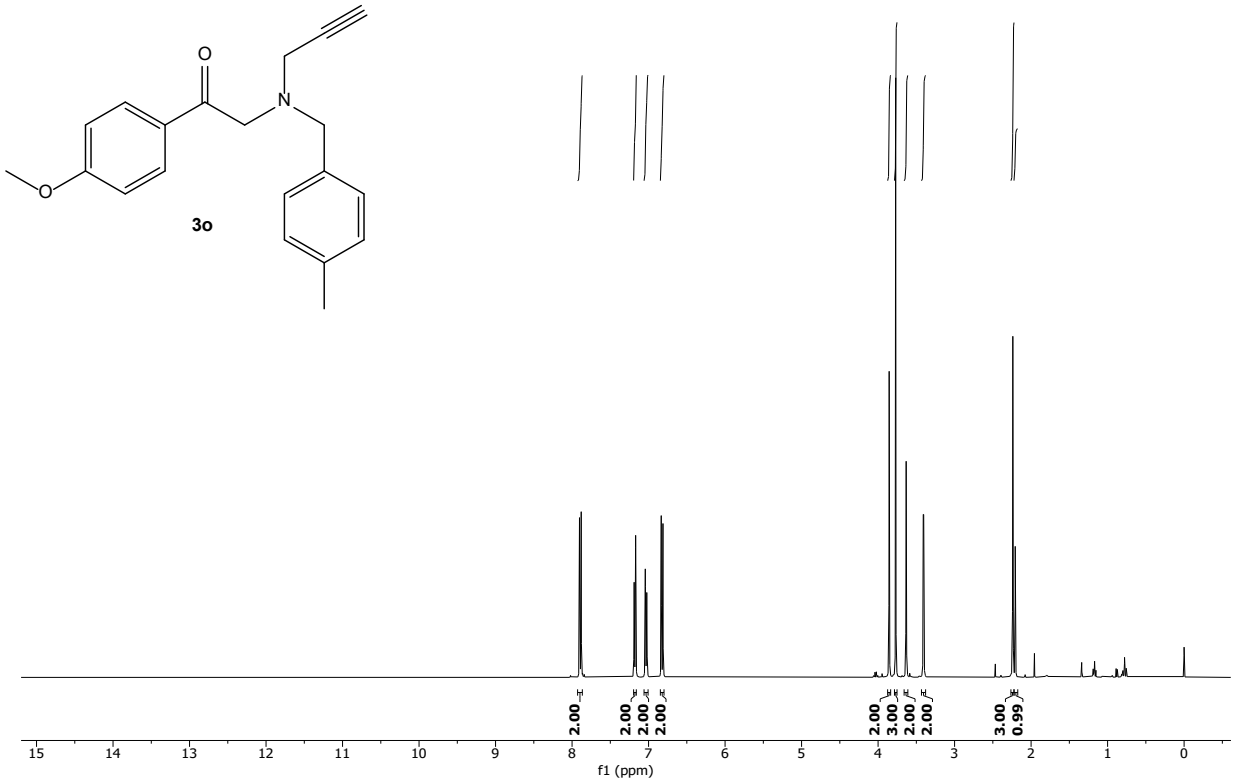
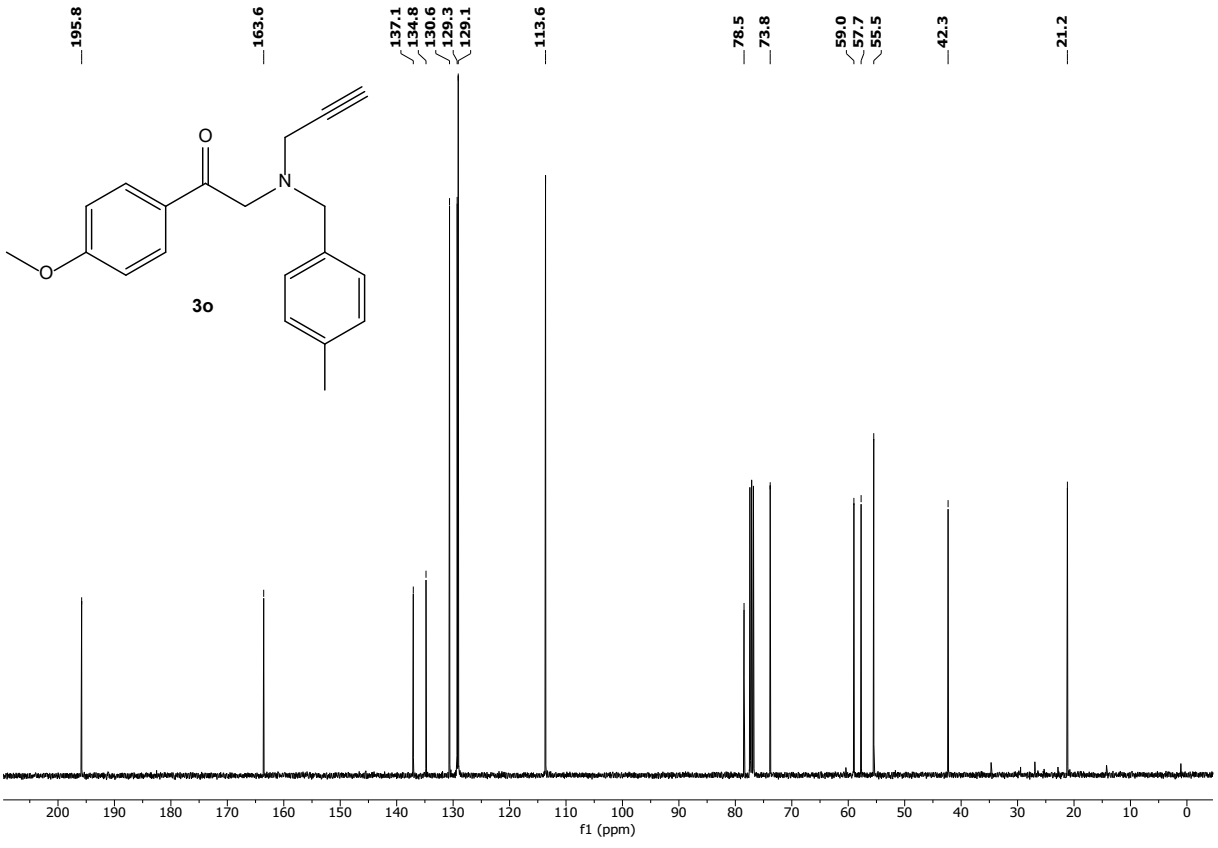
144.0
137.0
134.8
133.6
129.3
129.2
129.1
128.4
78.5
74.0
59.0
57.7
42.3
21.7
21.2
O
N
3m
f1 (ppm)


O
N
F3C
3n
2.00
2.00
2.09
2.11
2.00
2.07
2.00
4.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


O
N
O
3o
2.00
2.00
2.00
2.00
2.00
3.00
2.00
2.00
3.00
0.99
f1 (ppm)


195.8
163.6
137.1
134.8
130.6
129.3
129.1
113.6
78.5
73.8
59.0
57.7
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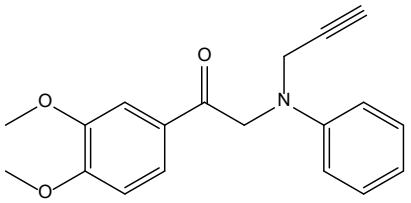
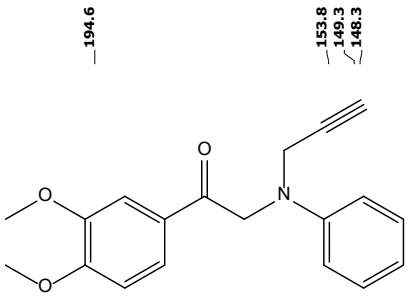
42.3
21.2
O
N
O
3o
f1 (ppm)


O
O
O
N

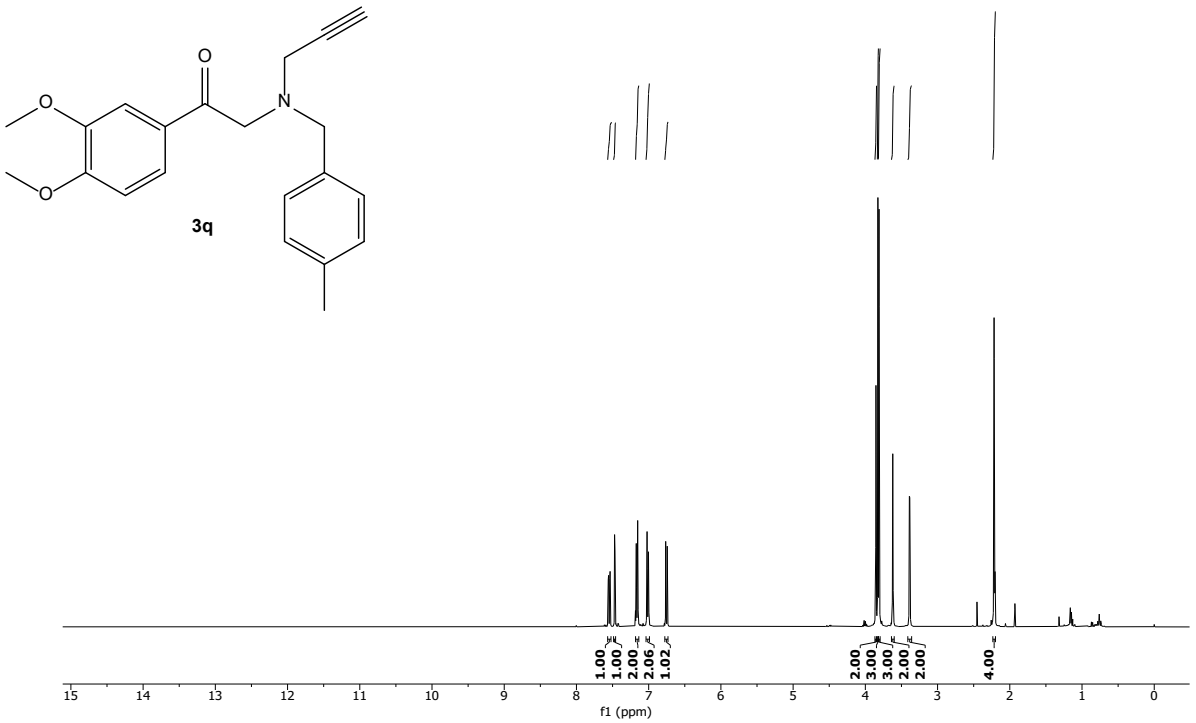
3p

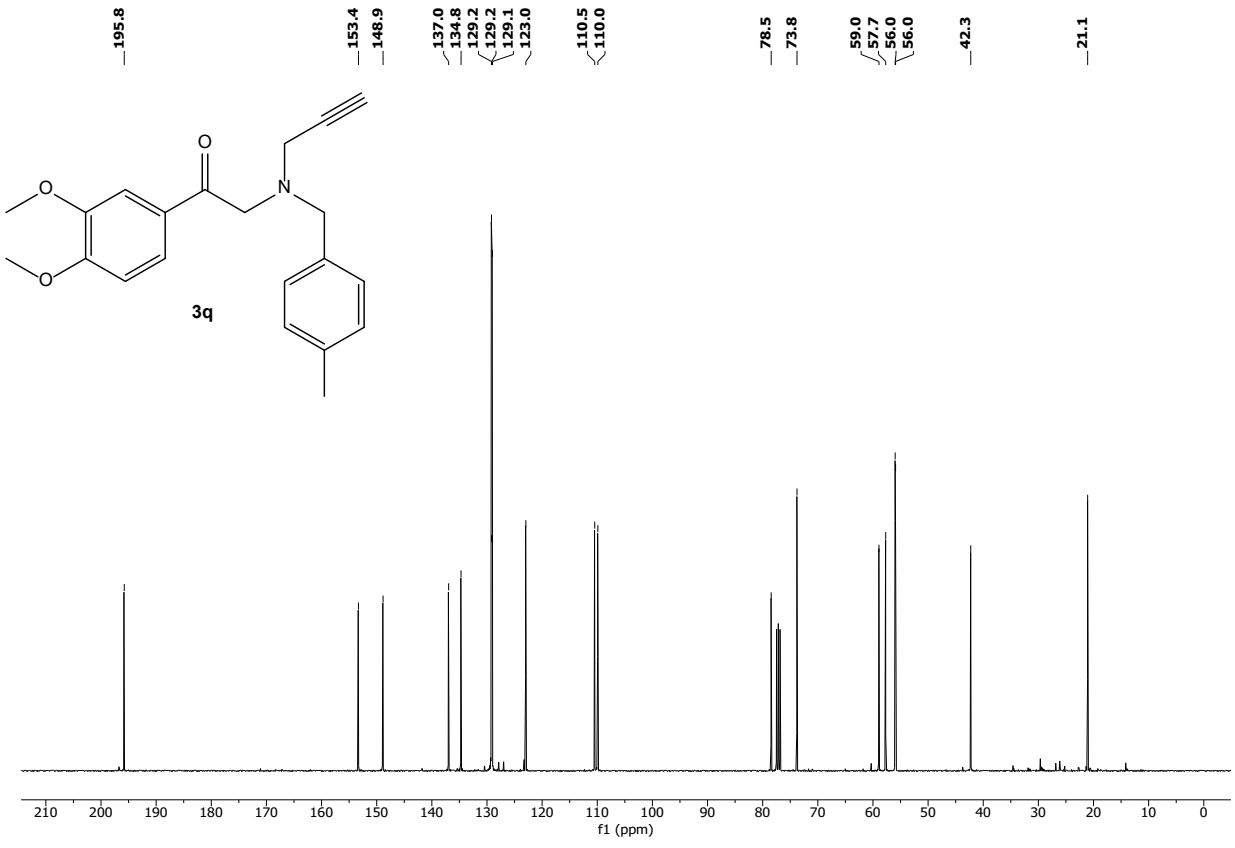
1.00
1.00
2.11
1.00
3.00
2.00
2.00
3.00
3.00
0.87
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

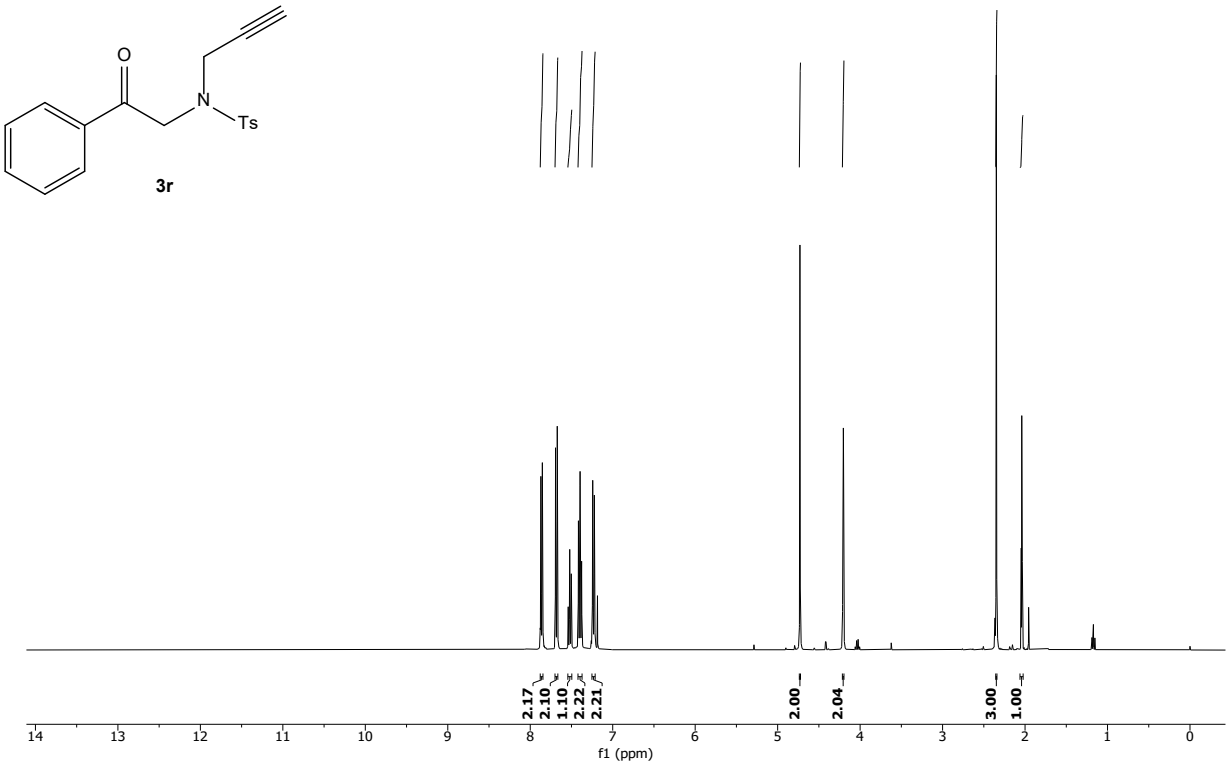

O
O
O
N

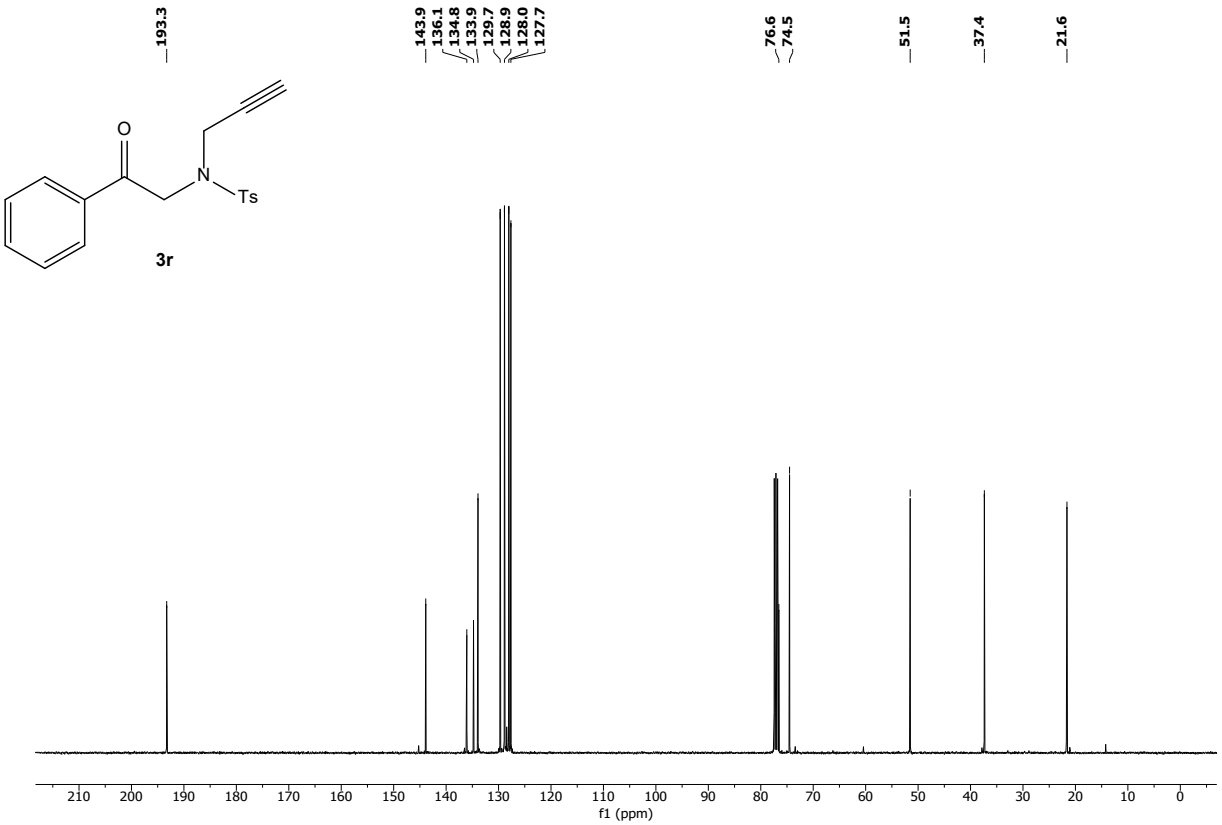
3p

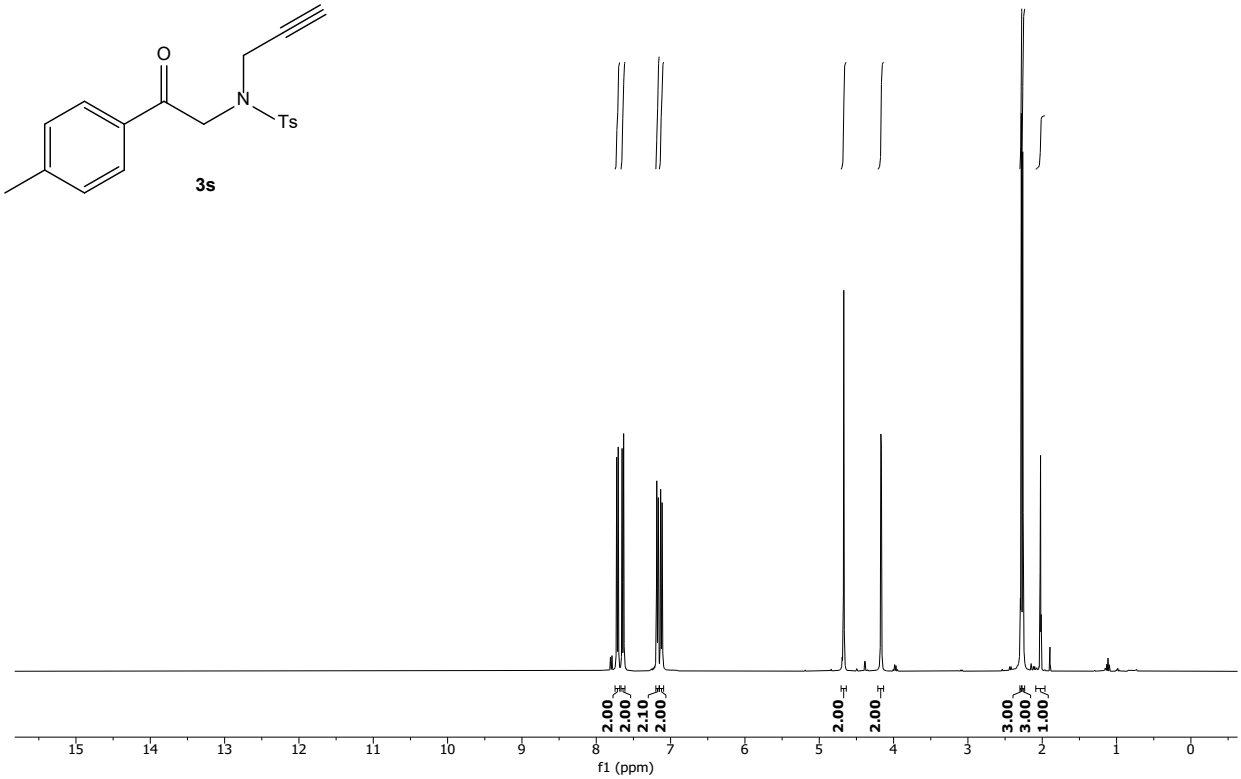
194.6
153.8
149.3
148.3
129.2
128.5
122.4
118.7
113.9
110.2
110.1
79.8
72.7
56.5
56.1
56.0
41.3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

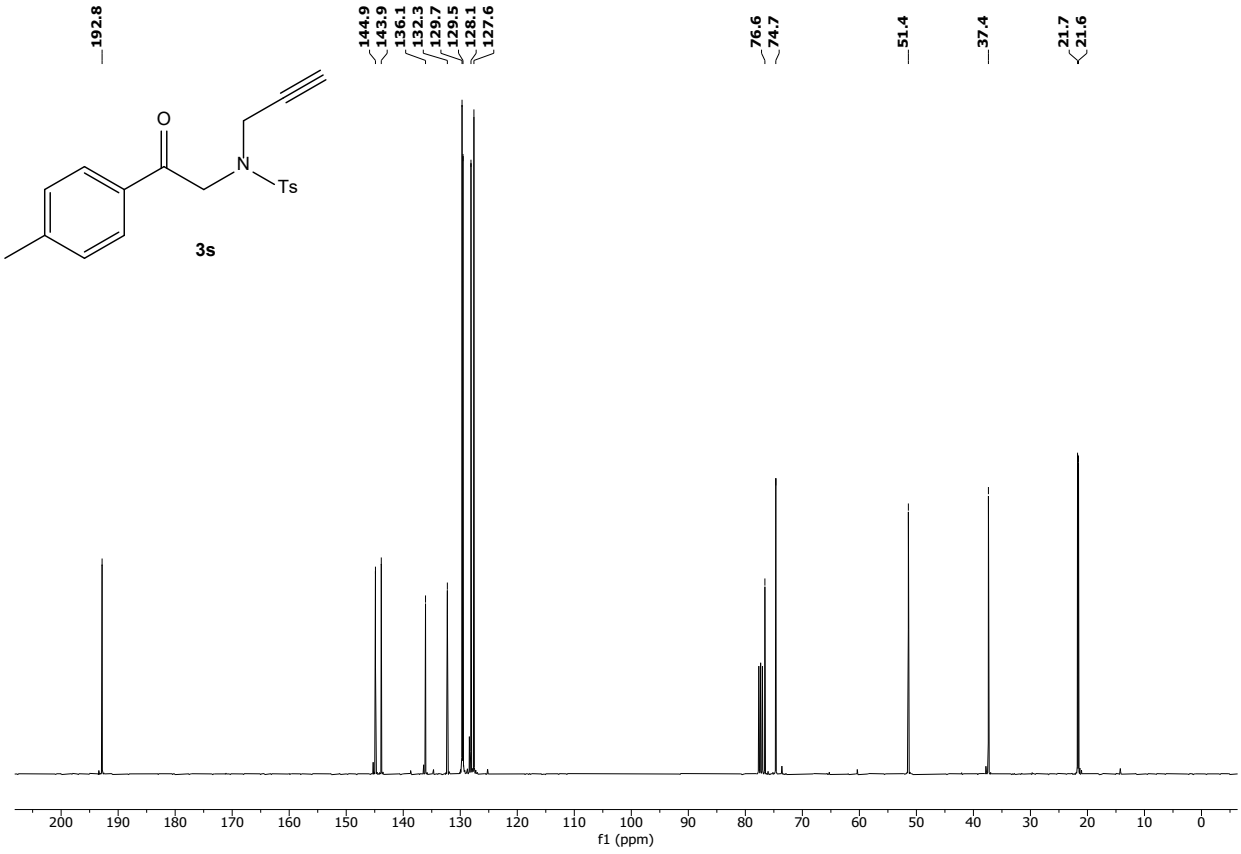

O
O
O
N
3q
1.00
1.00
2.00
2.06
1.02
2.00
3.00
3.00
2.00
2.00
4.00
f1 (ppm)

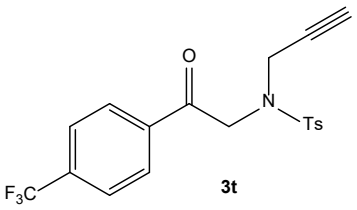

195.8
153.4
148.9
137.0
134.8
129.2
129.2
129.1
123.0
110.5
110.0
78.5
73.8
59.0
57.7
56.0
56.0
42.3
21.1
O
O
O
N
3q
f1 (ppm)


O
N
Ts
3r
2.17
2.10
1.10
2.22
2.21
2.00
2.04
3.00
1.00
f1 (ppm)

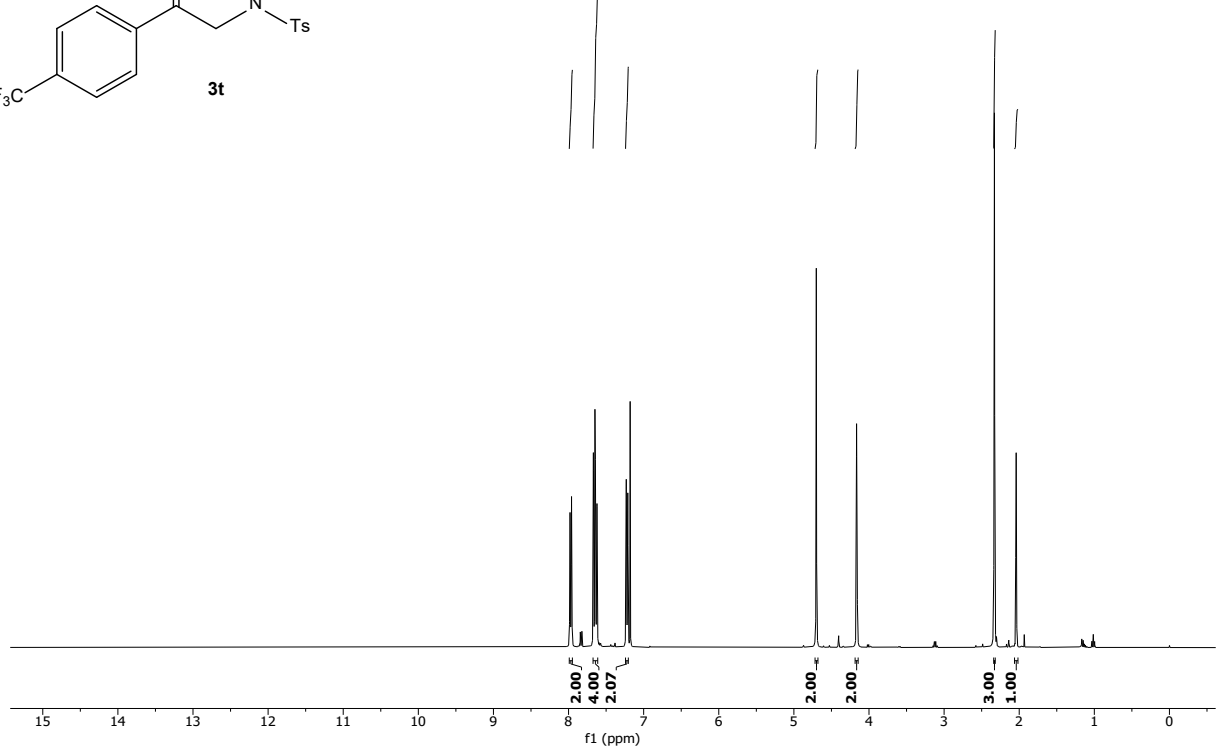

193.3
143.9
136.1
134.8
133.9
129.7
128.9
128.0
127.7
76.6
74.5
51.5
37.4
21.6
O
N
Ts
3r
f1 (ppm)

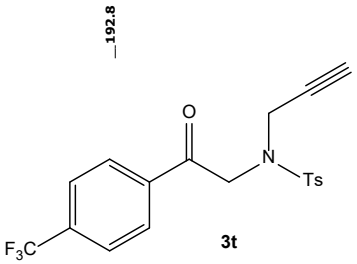

O
N
Ts
3s
2.00
2.00
2.10
2.00
2.00
2.00
3.00
3.00
1.00
f1 (ppm)


192.8
144.9
143.9
136.1
132.3
129.7
129.5
128.1
127.6
76.6
74.7
51.4
37.4
21.7
21.6
O
N
Ts
3s
f1 (ppm)


O
N
Ts
F3C

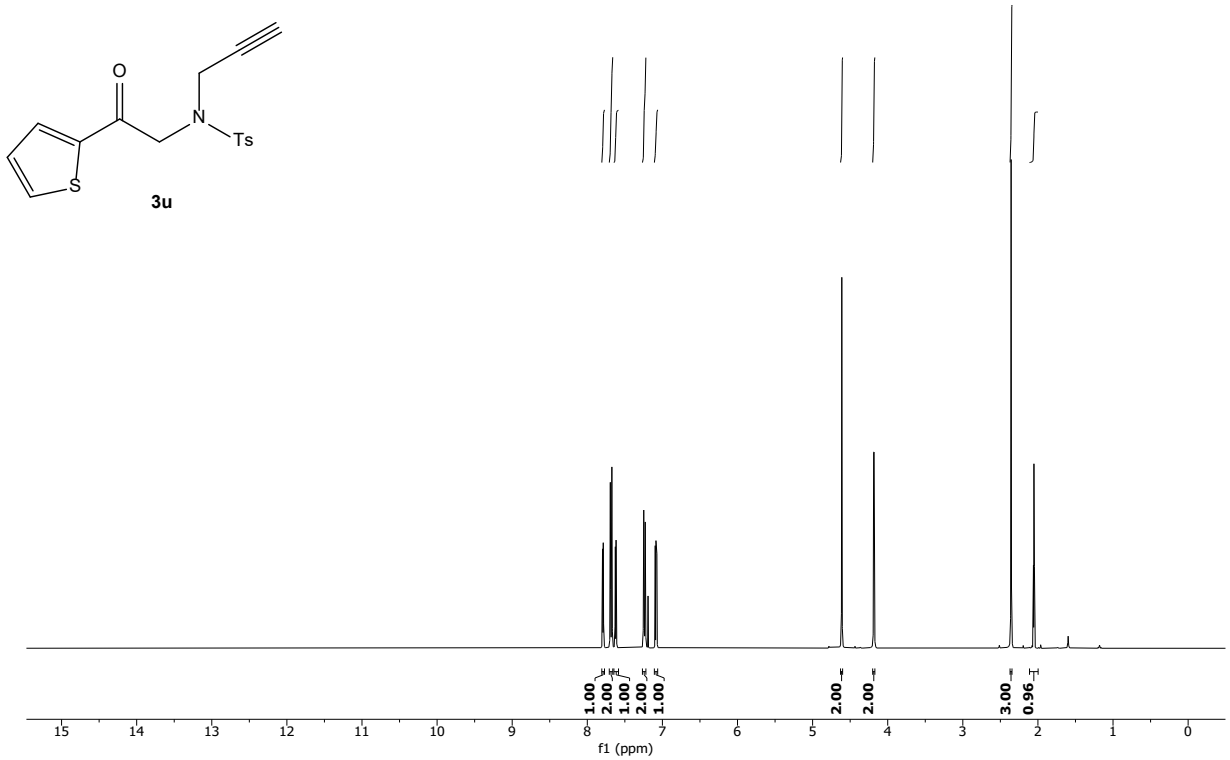
3t

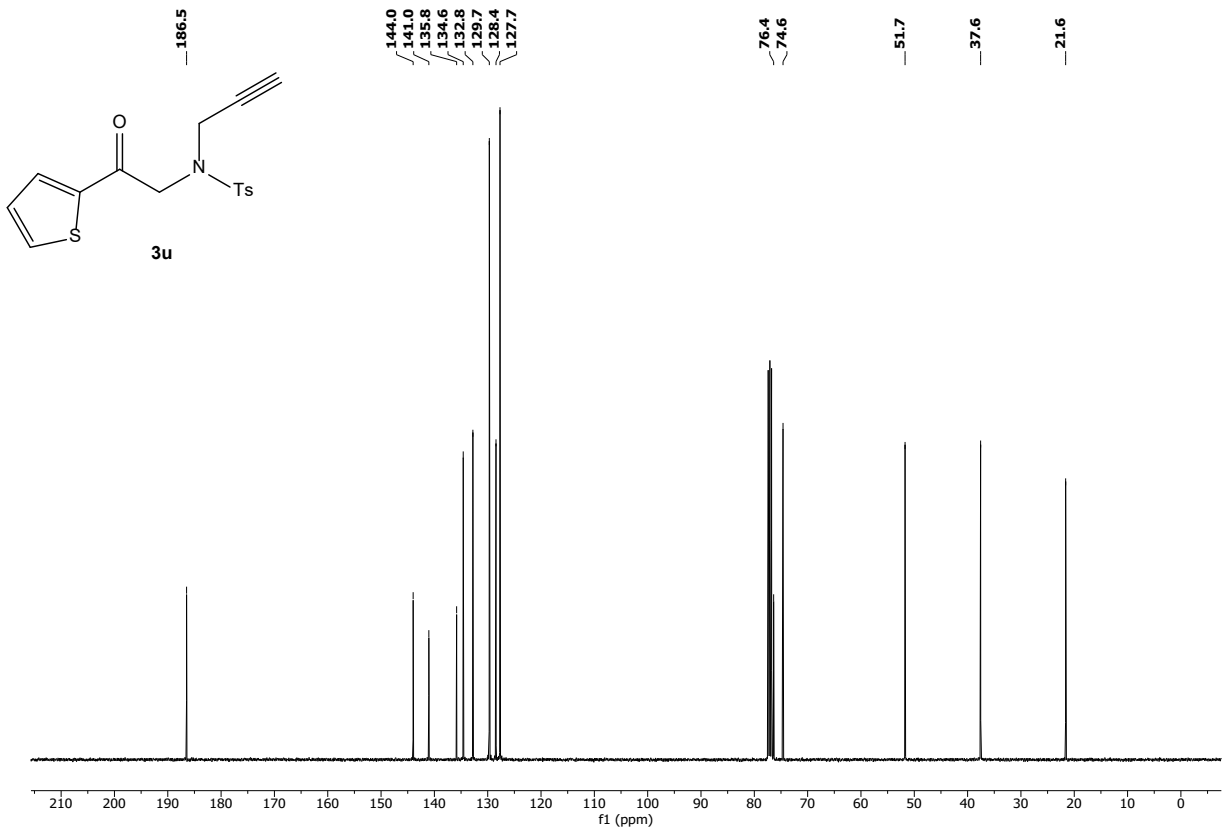

2.00
4.00
2.07
2.00
2.00
3.00
1.00
f1 (ppm)

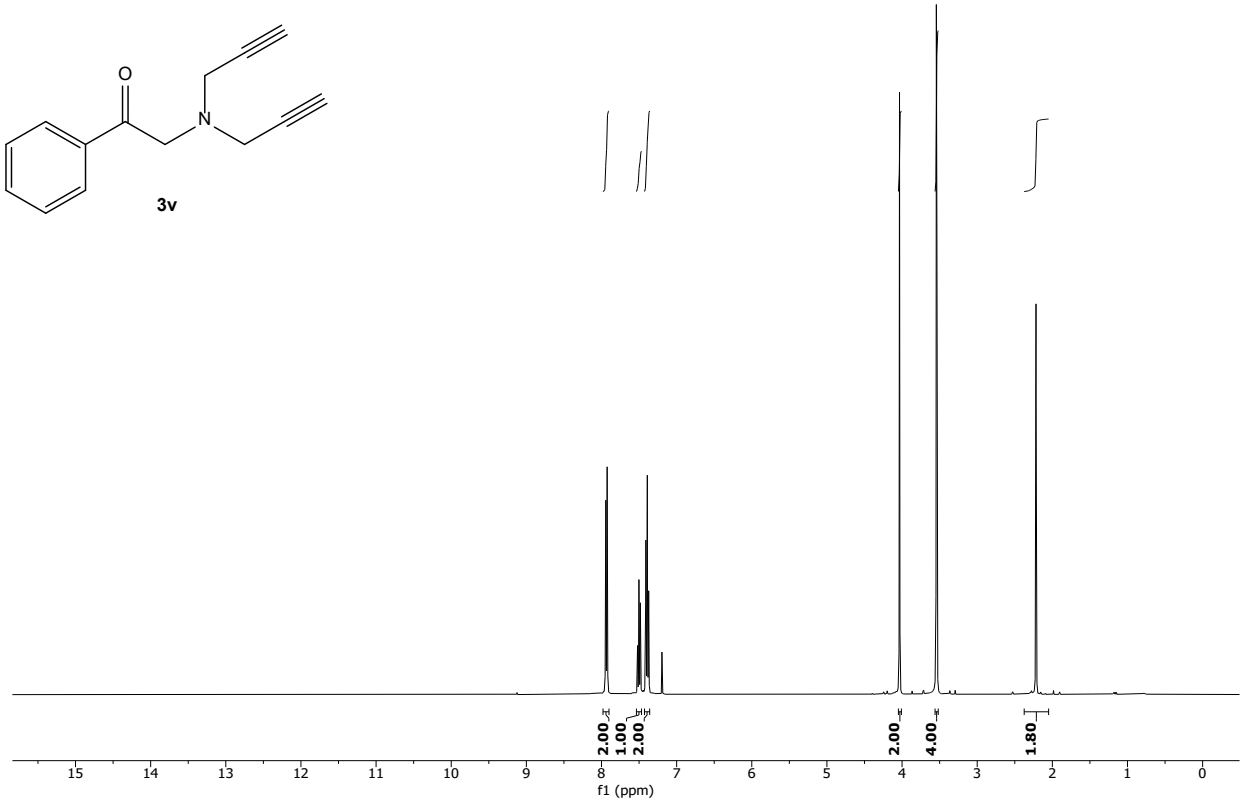

O
N
Ts
F3C

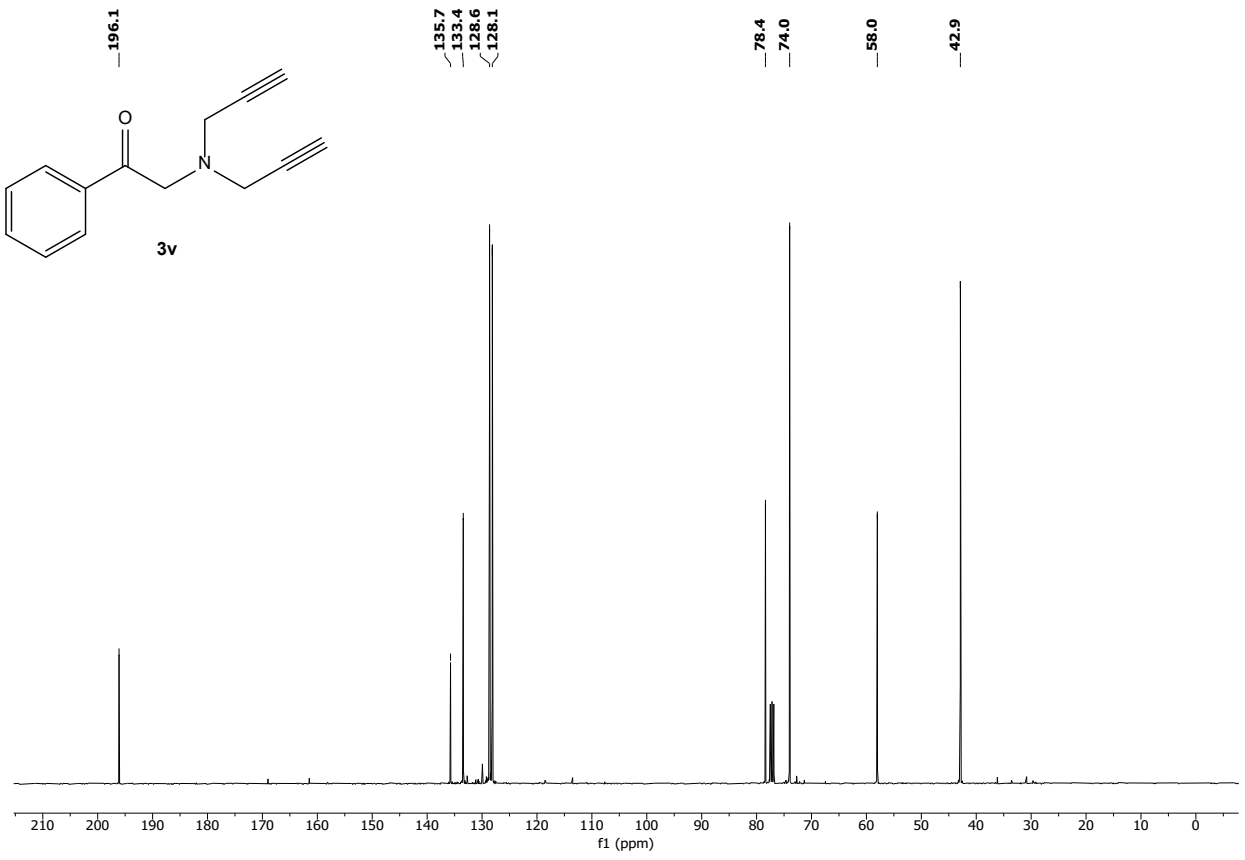
3t

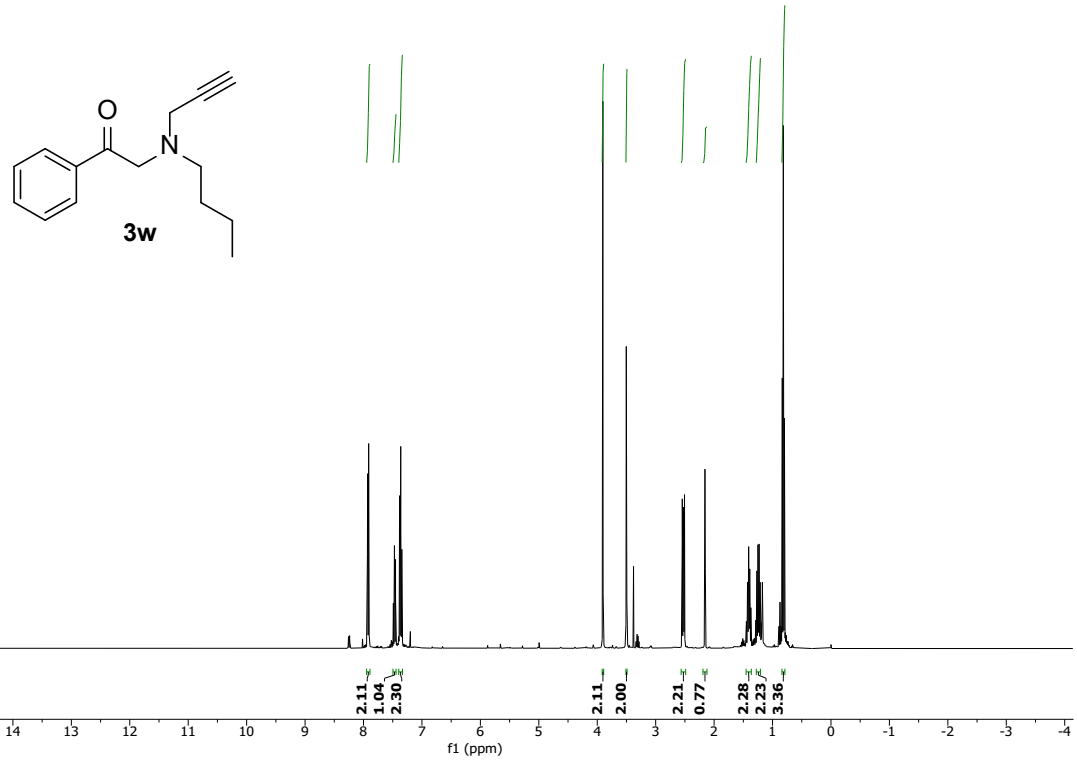
192.8
144.1
137.5
135.7
135.4
135.1
134.8
134.4
129.8
128.5
127.6
125.9
125.9
125.8
125.8
124.8
122.1
76.2
74.8
52.0
37.5
21.5
f1 (ppm)

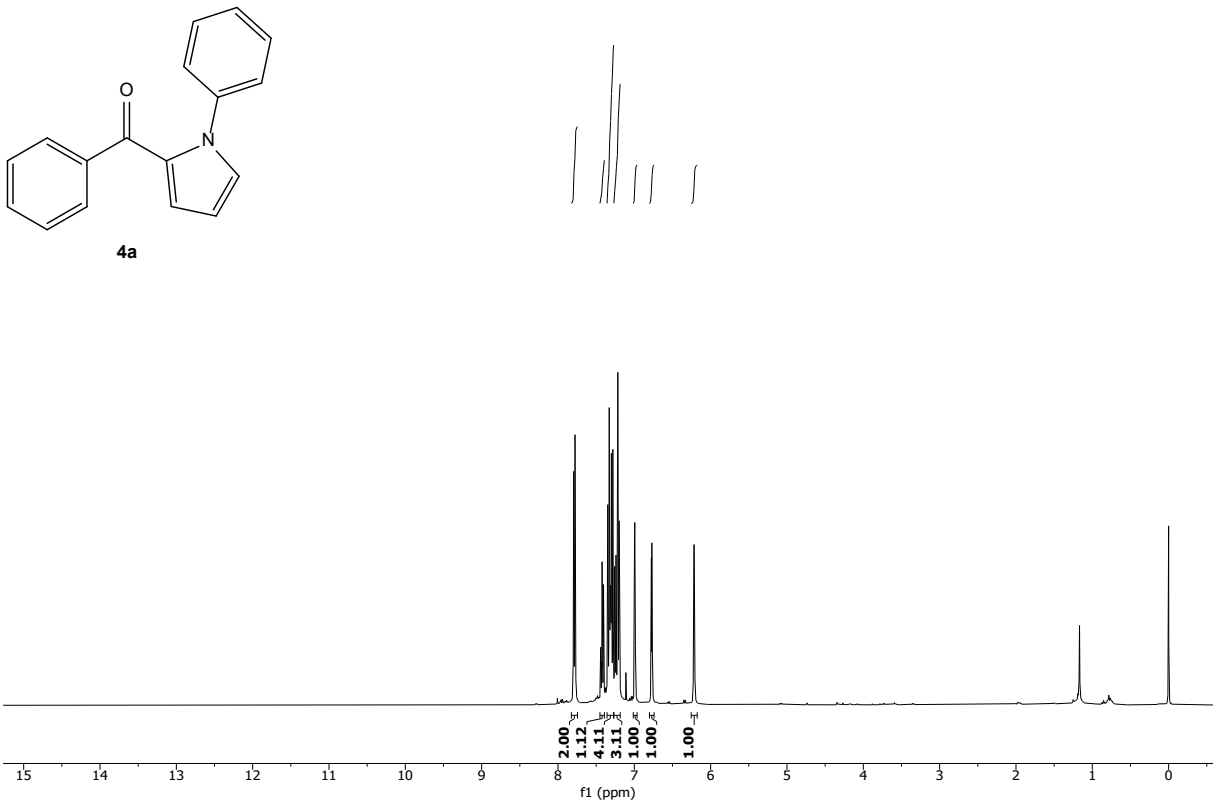

O
N
Ts
S
3u
1.00
2.00
1.00
2.00
1.00
2.00
2.00
3.00
0.96
f1 (ppm)

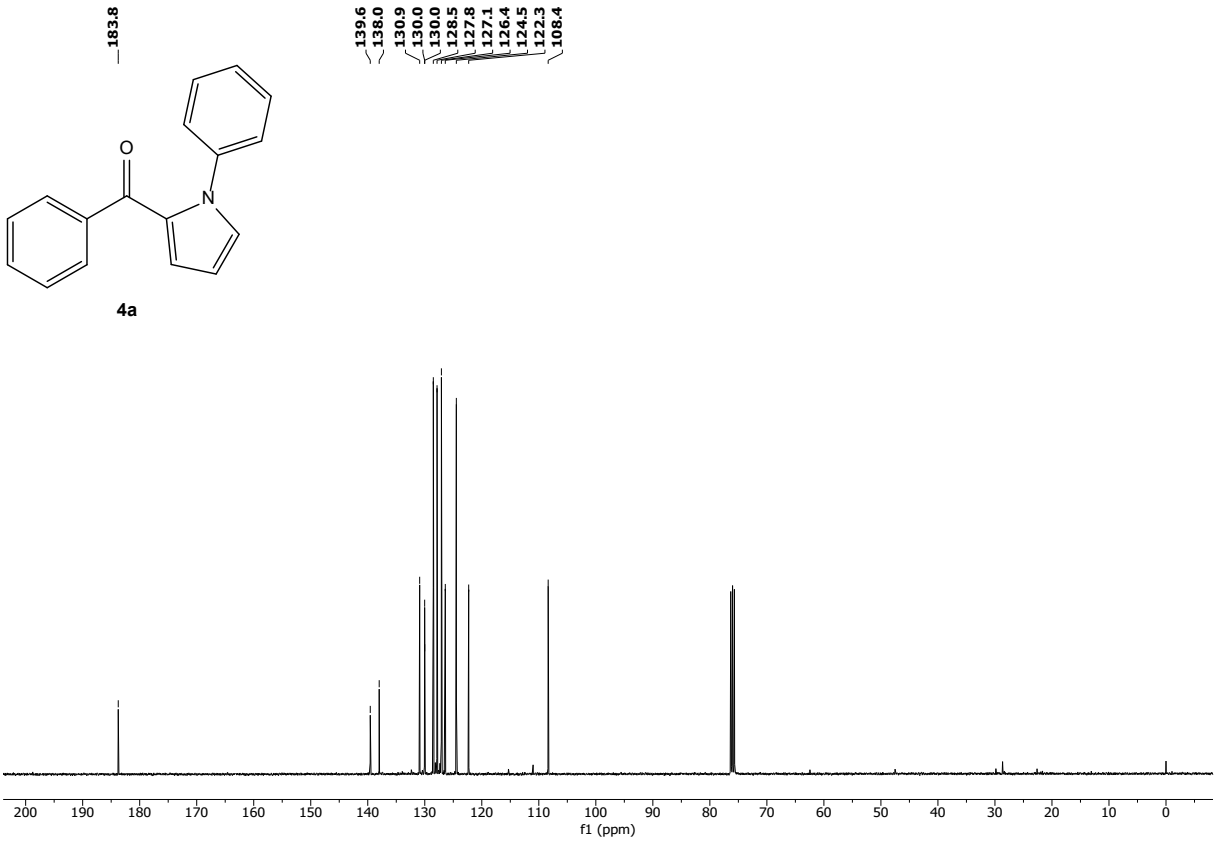

186.5
144.0
141.0
135.8
134.6
132.8
129.7
128.4
127.7
76.4
74.6
51.7
37.6
21.6
O
N
Ts
S
3u
f1 (ppm)

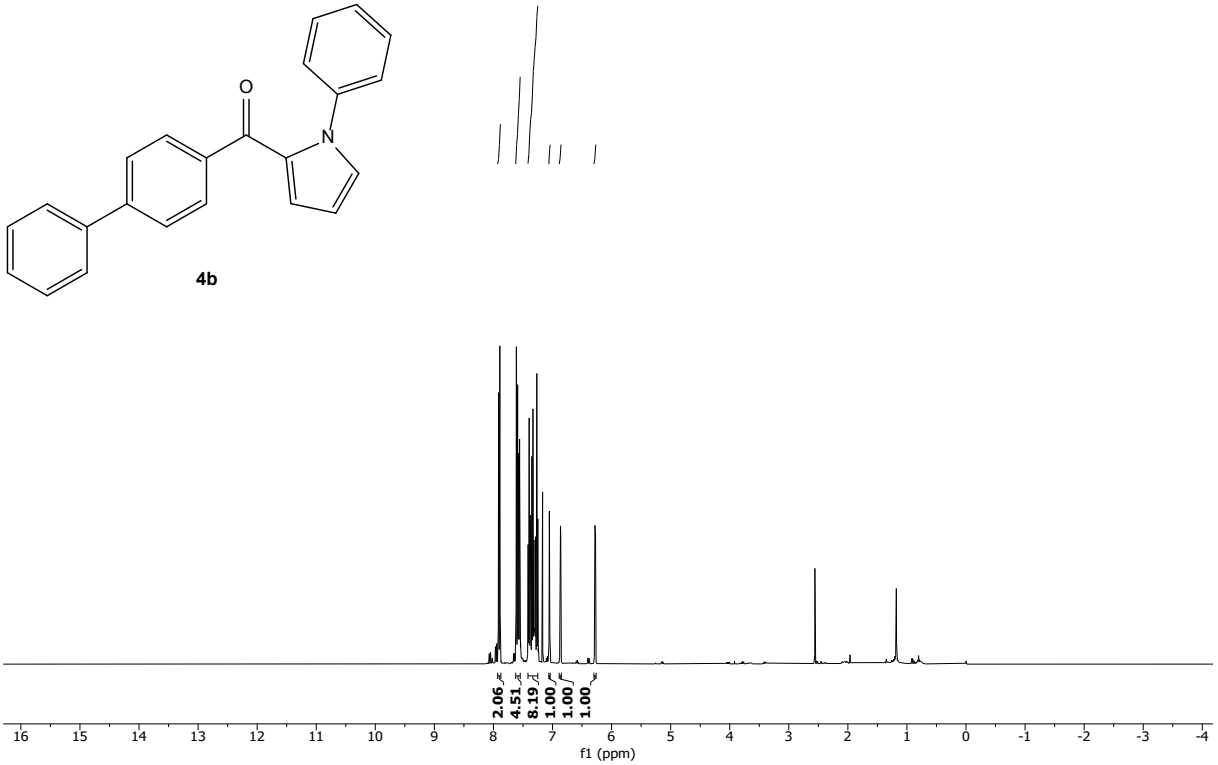

O
N
3v
2.00
1.00
2.00
2.00
4.00
1.80
f1 (ppm)

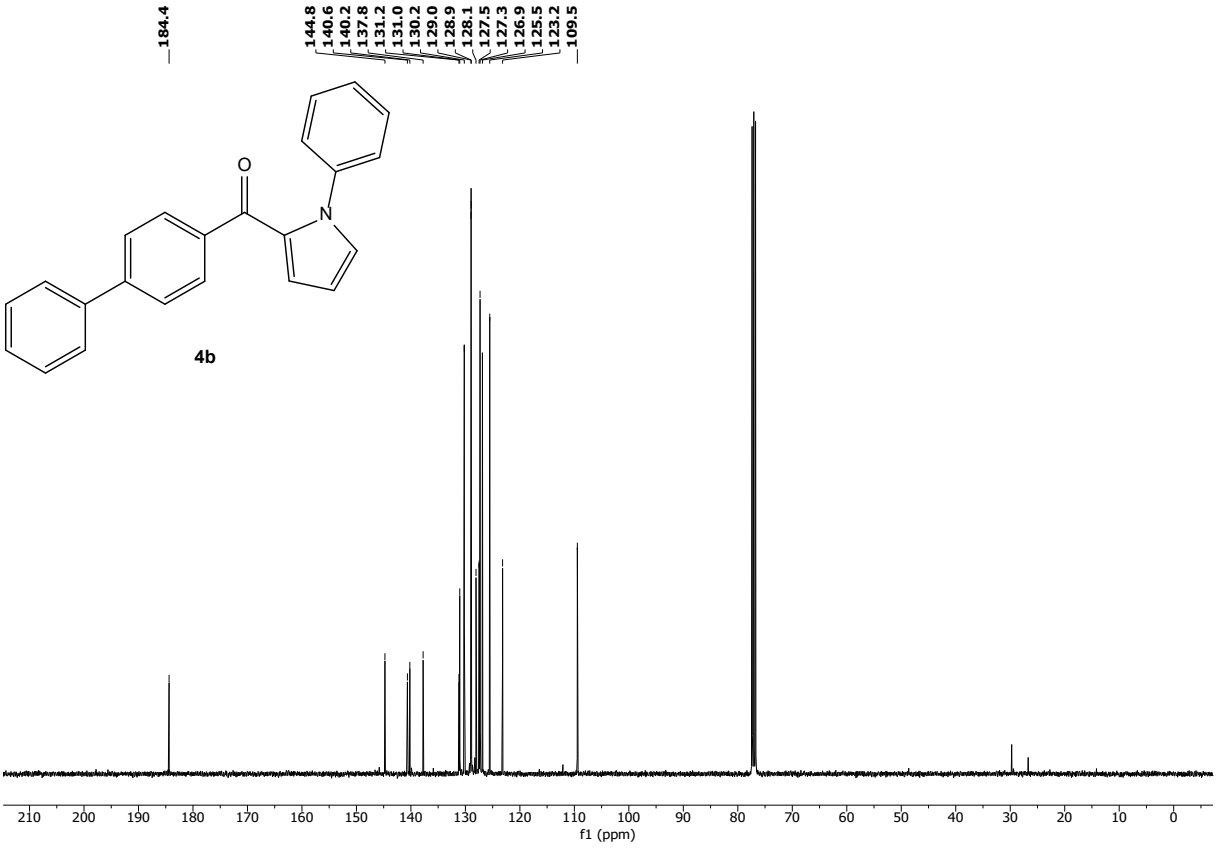

196.1
135.7
133.4
128.6
128.1
78.4
74.0
58.0
42.9
O
N
3v
f1 (ppm)

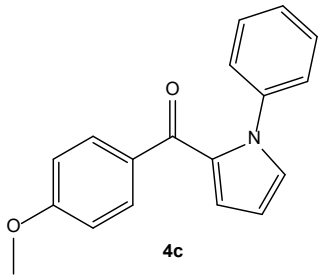

O
N
3w
2.11
1.04
2.30
2.11
2.00
2.21
0.77
2.28
2.23
3.36
f1 (ppm)


O
N
4a
2.00
1.12
4.11
3.11
1.00
1.00
1.00
f1 (ppm)


183.8
139.6
138.0
130.9
130.0
130.0
128.5
127.8
127.1
126.4
124.5
122.3
108.4
O
N
4a
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
4b
2.06
4.51
8.19
1.00
1.00
1.00
f1 (ppm)

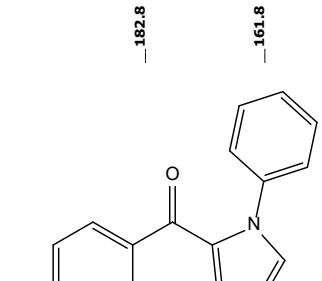

184.4
144.8
140.6
140.2
137.8
131.2
131.0
130.2
129.0
128.9
128.1
127.5
127.3
126.9
125.5
123.2
109.5
O
N
4b
f1 (ppm)


O
N
O

4c

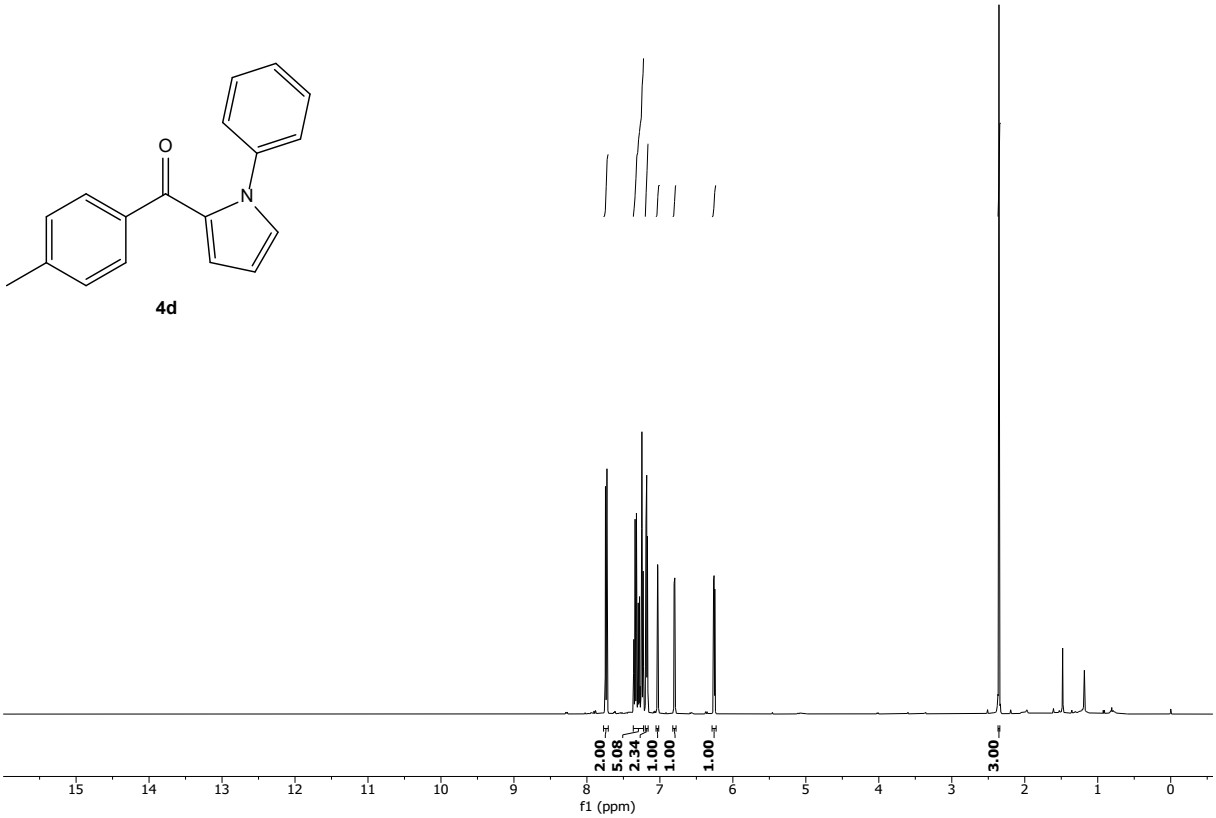
2.00
5.03
1.00
2.00
1.00
1.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

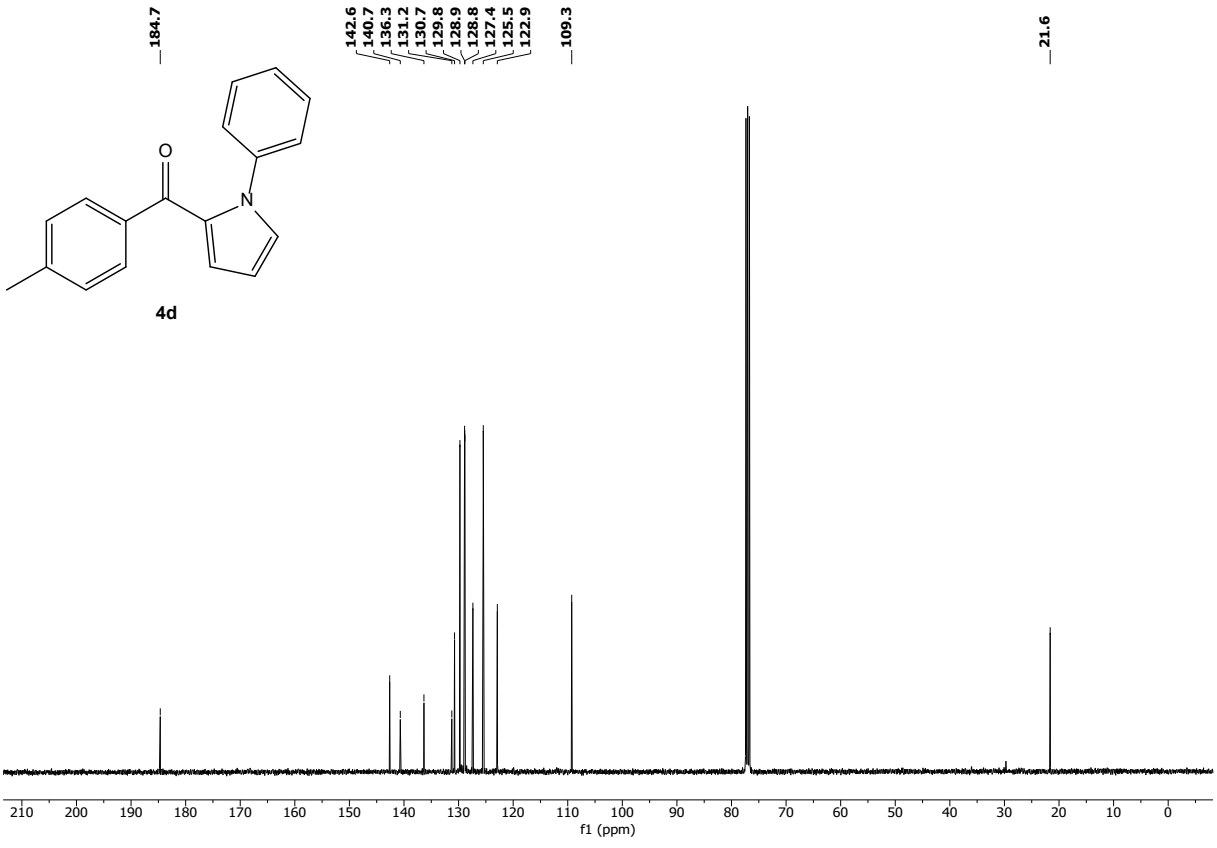
Z

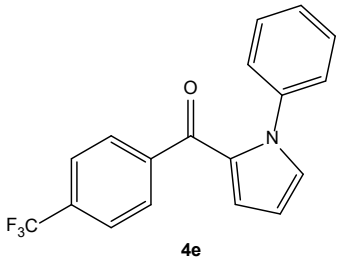

O
N
O

4c

182.8
161.8
139.6
130.8
130.6
130.2
129.4
127.9
126.3
124.3
121.3
112.4
108.2
54.4
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

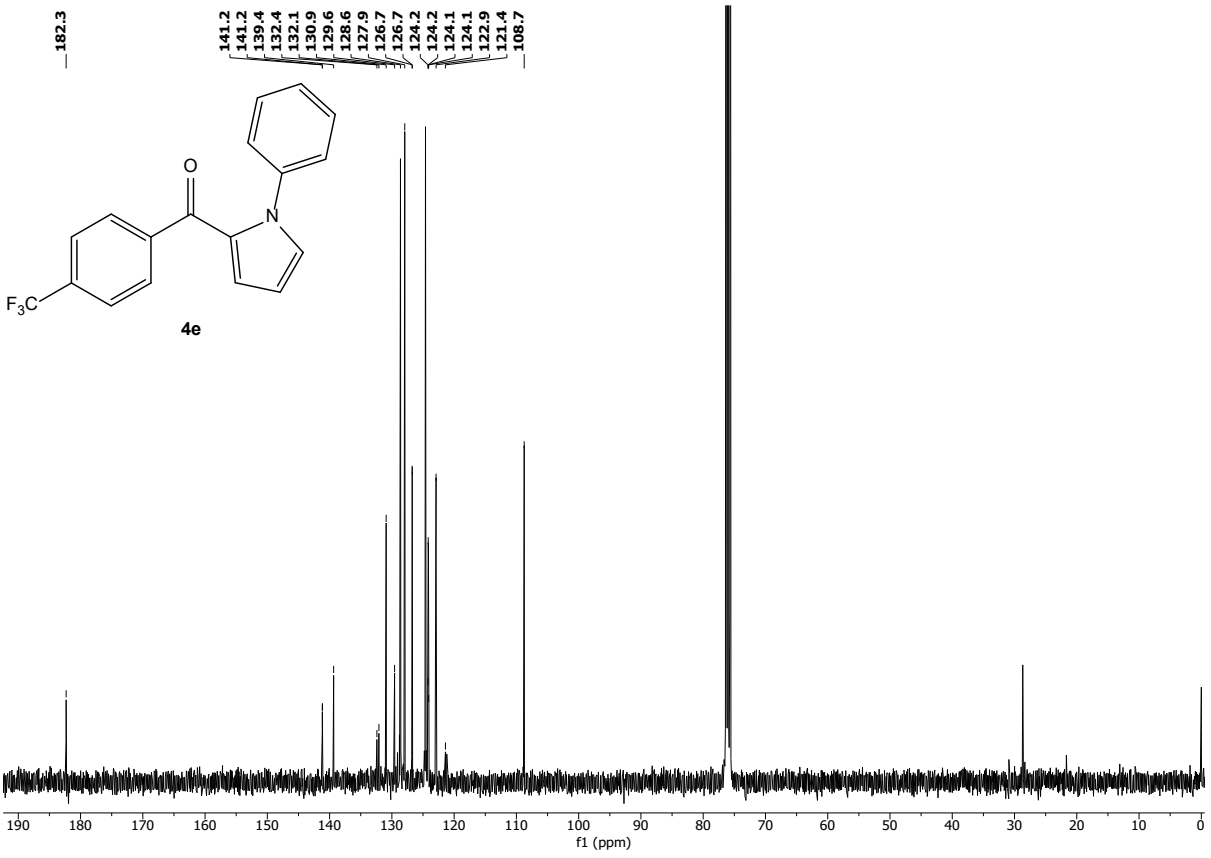

O
N
4d
2.00
5.08
2.34
1.00
1.00
1.00
3.00
f1 (ppm)


184.7
142.6
140.7
136.3
131.2
130.7
129.8
128.9
128.8
127.4
125.5
122.9
109.3
21.6
O
N
4d
f1 (ppm)

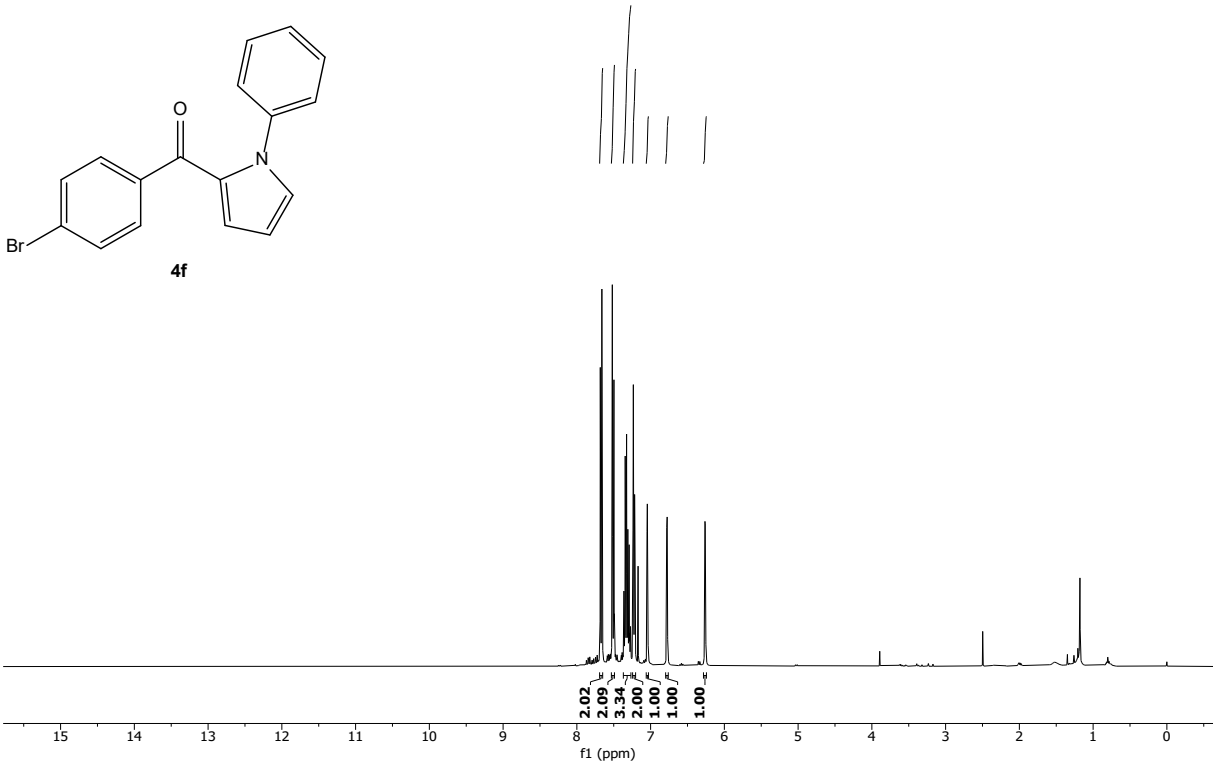

O
N
F3C

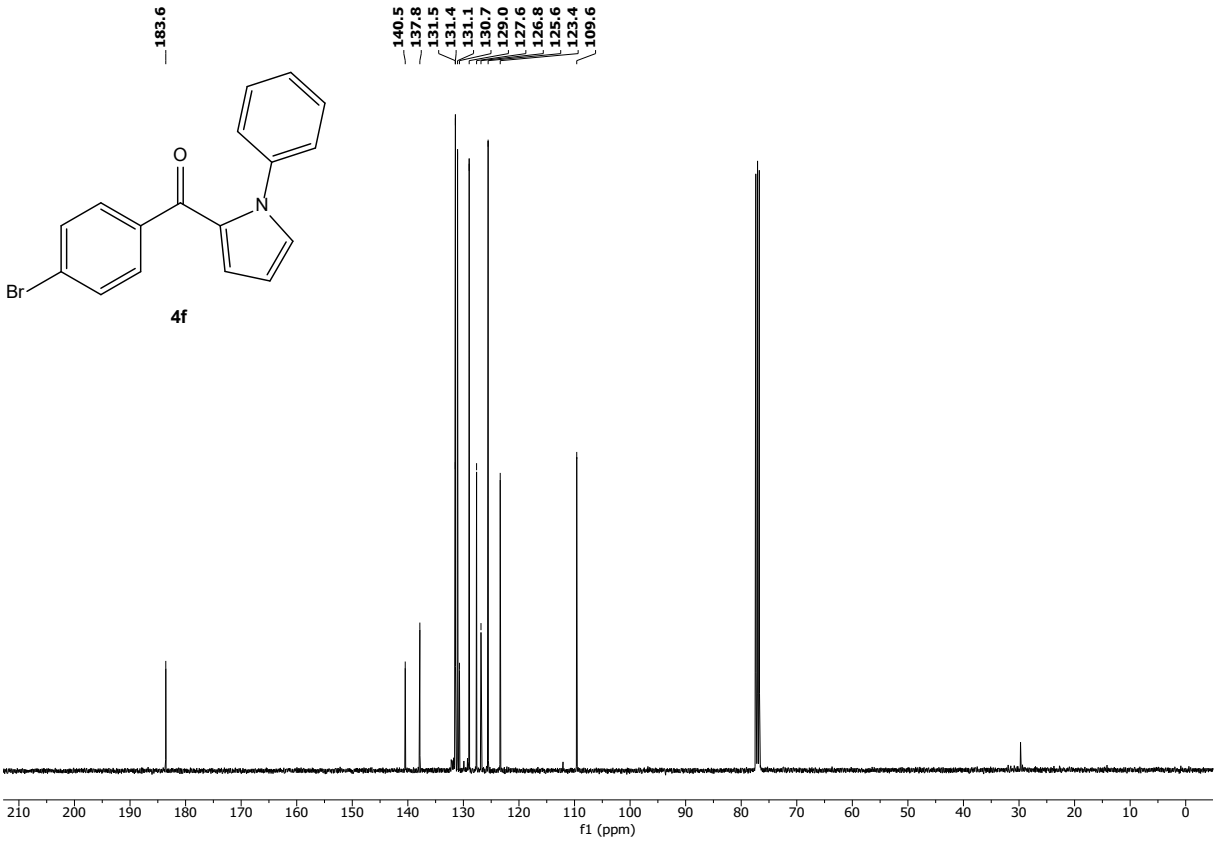
4e

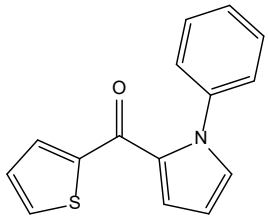
2.00
2.29
3.20
2.00
1.00
1.00
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


182.3
141.2
141.2
139.4
132.4
132.1
130.9
129.6
128.6
127.9
126.7
126.7
124.2
124.2
124.1
124.1
122.9
121.4
108.7
O
N
F3C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

4e

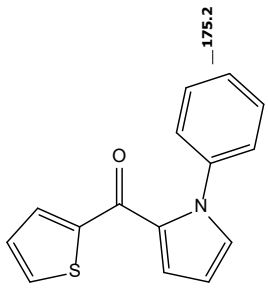

O
N
Br
4f
2.02
2.09
3.34
2.00
1.00
1.00
1.00
f1 (ppm)


183.6
140.5
137.8
131.5
131.4
131.1
130.7
129.0
127.6
126.8
125.6
123.4
109.6
O
N
Br
4f
f1 (ppm)


O
N
S

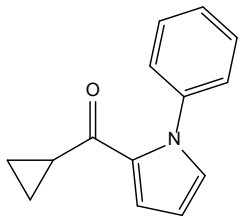
4g

1.00
1.00
5.07
2.00
1.00
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


O
N
S

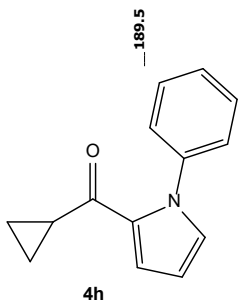
4g

175.2
143.5
139.4
131.7
131.6
129.9
129.7
127.9
126.6
126.4
124.5
120.6
108.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N

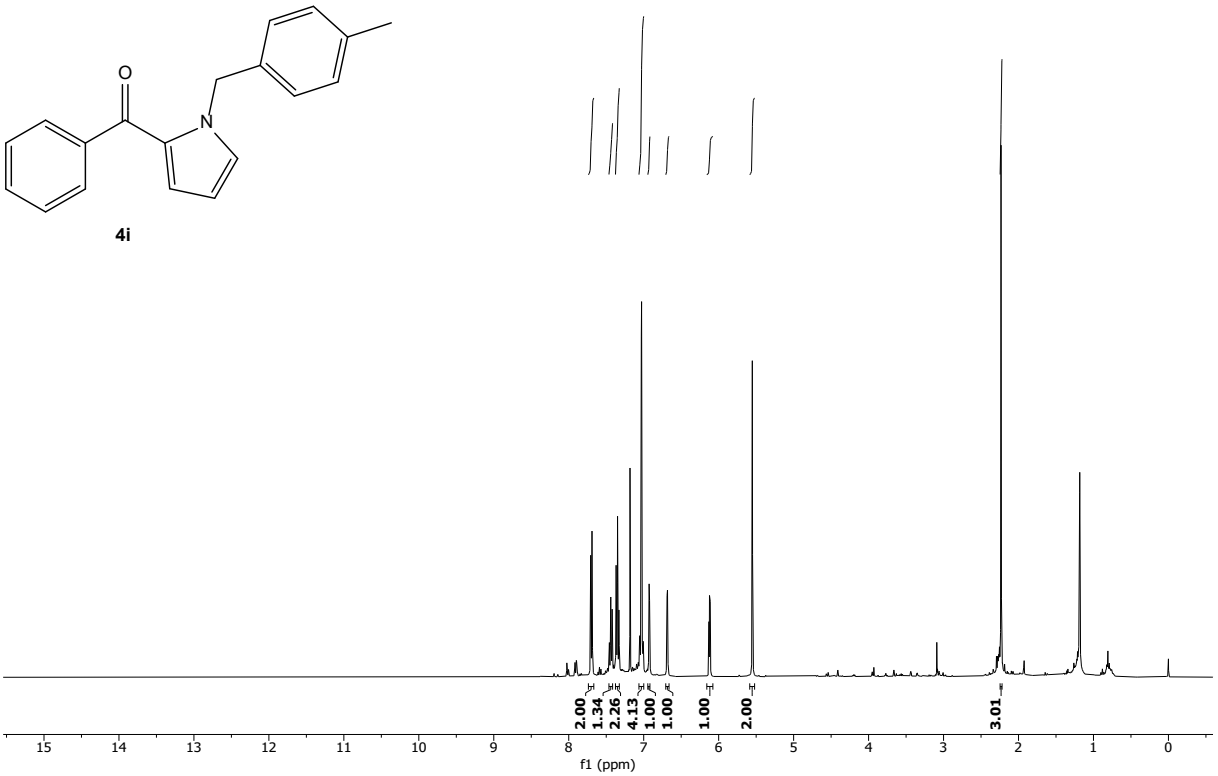
4h

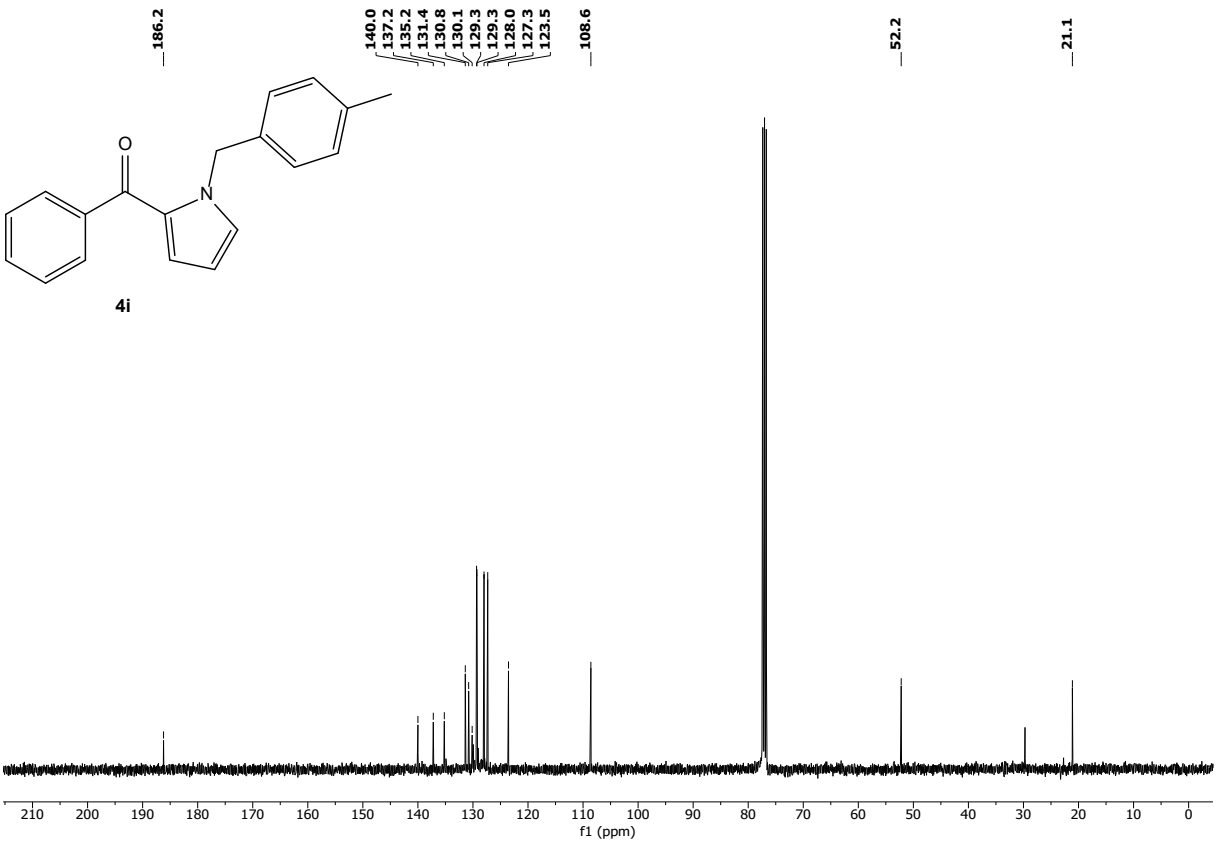
2.68
3.03
1.00
0.85
1.00
2.00
2.35
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

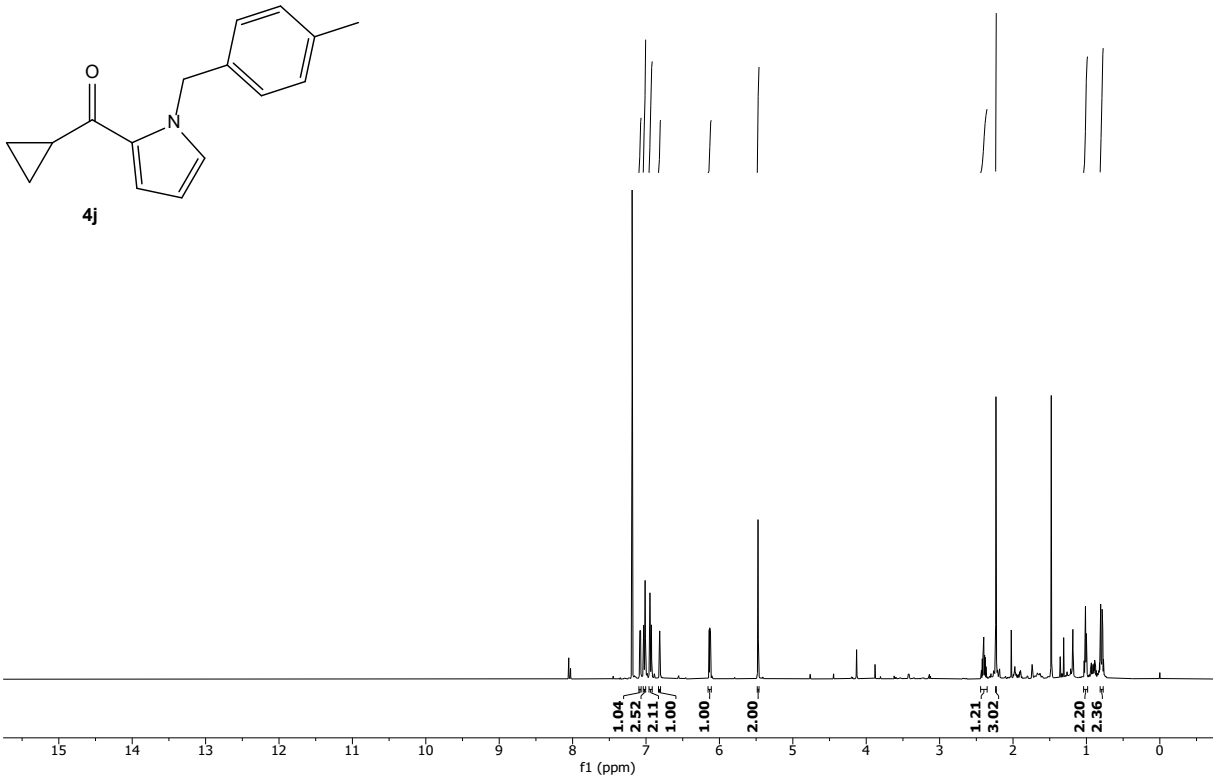

O
N

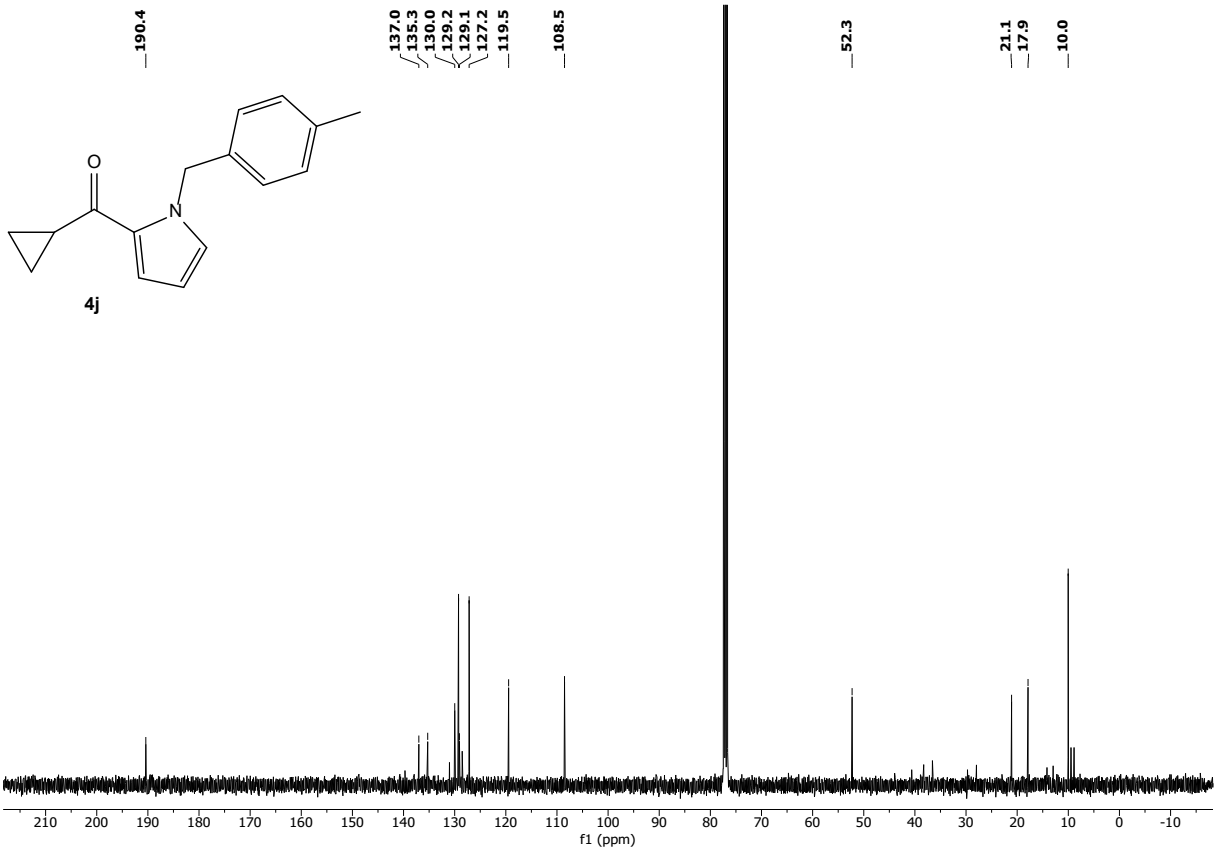
4h

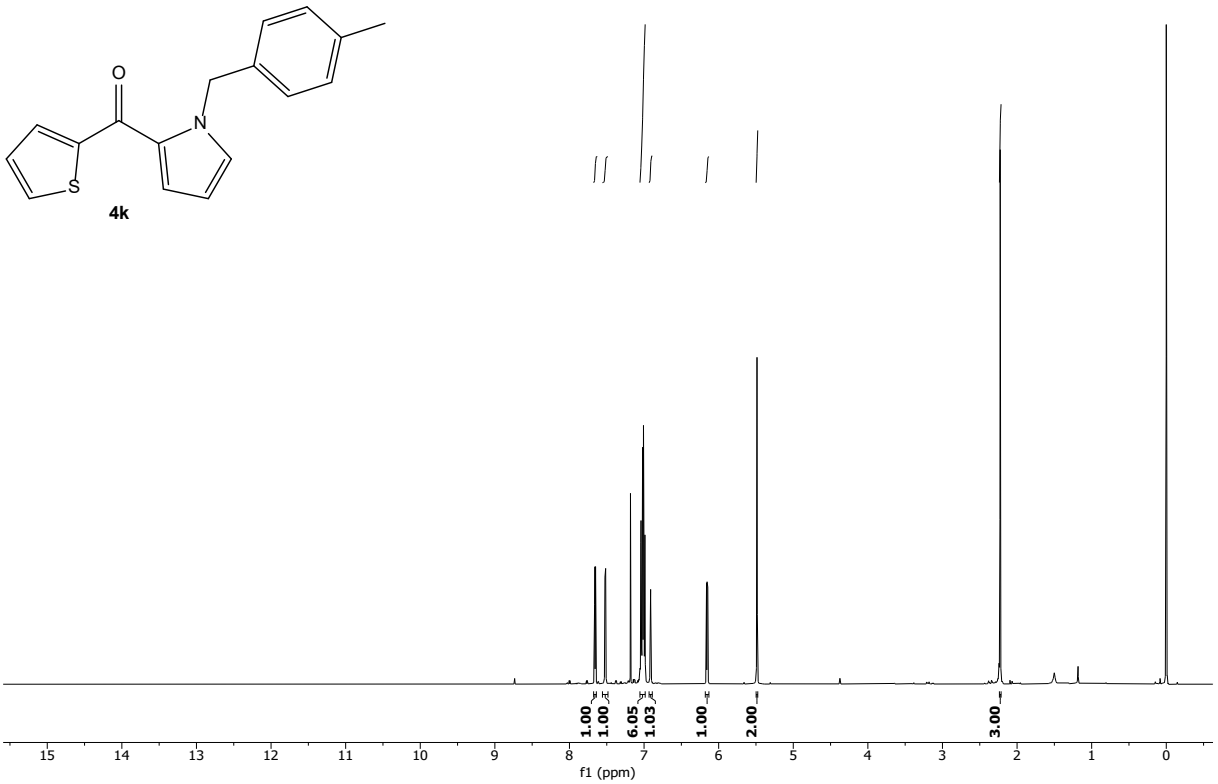
189.5
141.1
132.2
130.8
128.6
127.6
126.1
119.6
109.3
29.7
17.9
10.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

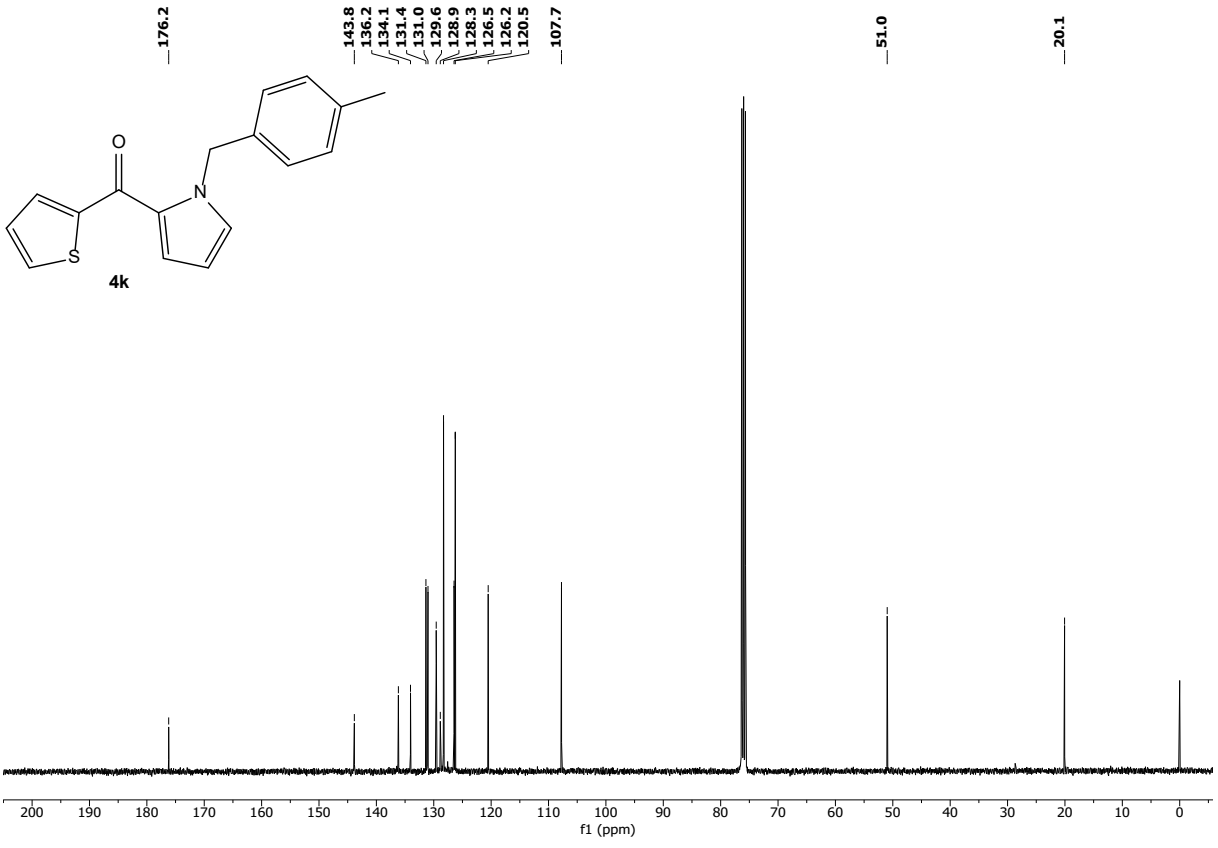

O
N
4i
2.00
1.34
2.26
4.13
1.00
1.00
1.00
2.00
3.01
f1 (ppm)

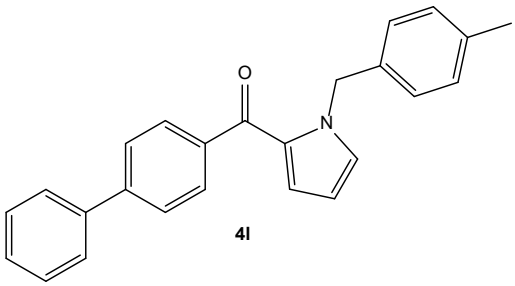

186.2
140.0
137.2
135.2
131.4
130.8
130.1
129.3
129.3
128.0
127.3
123.5
108.6
52.2
21.1
O
N
4i
f1 (ppm)


O
N
4j
1.04
2.52
2.11
1.00
1.00
2.00
1.21
3.02
2.20
2.36
f1 (ppm)


190.4
137.0
135.3
130.0
129.2
129.1
127.2
119.5
108.5
52.3
21.1
17.9
10.0
O
N
4j
f1 (ppm)

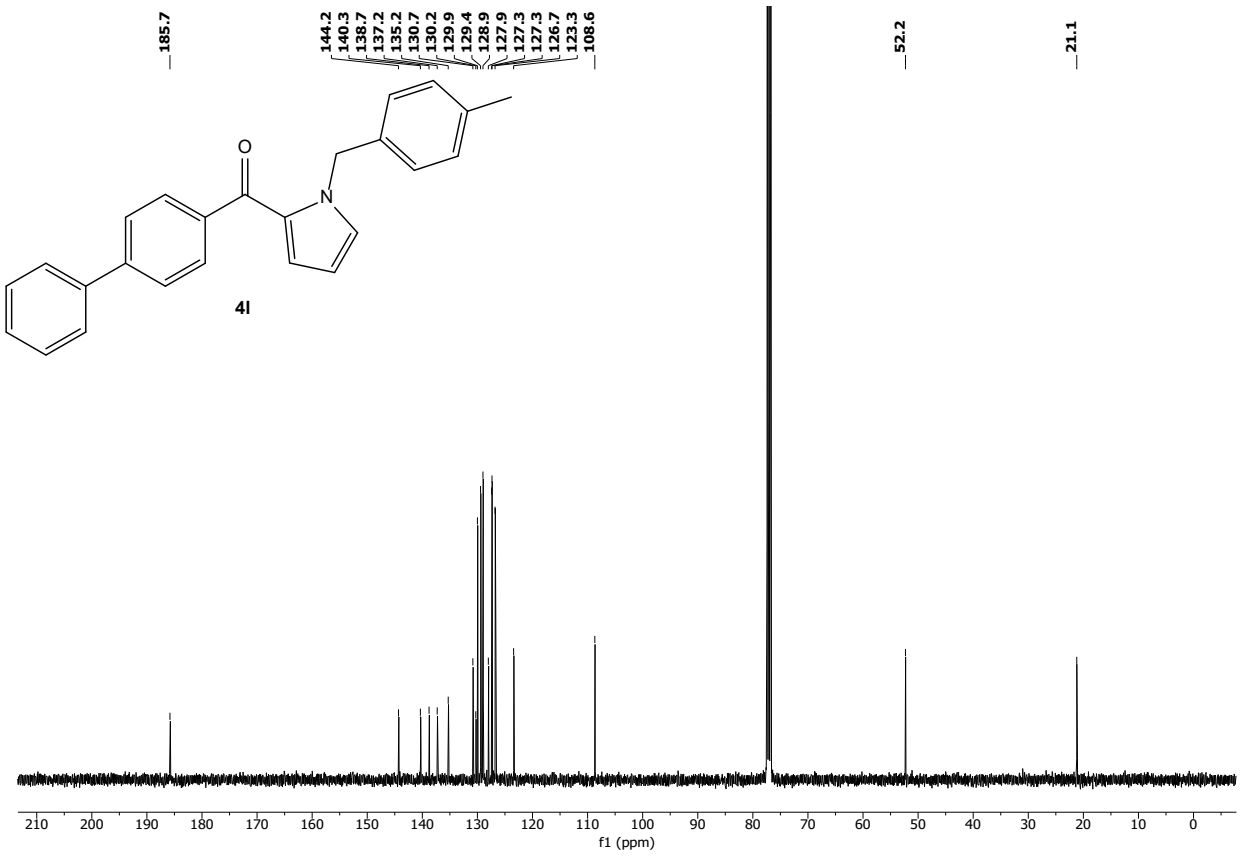

O
N
S
4k
1.00
1.00
6.05
1.03
1.00
2.00
3.00
f1 (ppm)

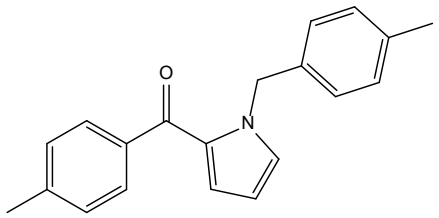

176.2
143.8
136.2
134.1
131.4
131.0
129.6
128.9
128.3
126.5
126.2
120.5
107.7
51.0
20.1
O
N
S
4k
f1 (ppm)


O
N

4l

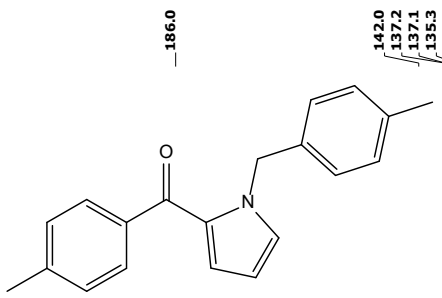
2.00
4.01
2.16
1.04
3.96
1.00
1.00
1.00
2.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


185.7
144.2
140.3
138.7
137.2
135.2
130.7
130.2
129.9
129.4
128.9
127.9
127.3
127.3
126.7
123.3
108.6
52.2
21.1
O
N
4l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N

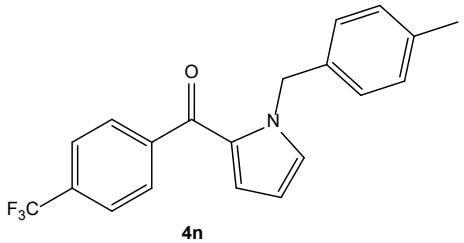
4m

2.00
2.00
4.00
1.00
1.00
1.00
2.00
3.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


O
N

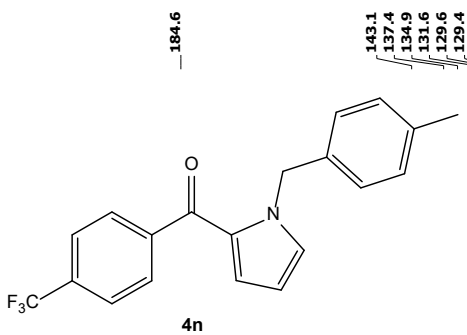
4m

186.0
142.0
137.2
137.1
135.3
130.5
130.3
129.5
129.3
128.7
127.3
123.1
108.4
52.1
21.5
21.1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
F3C

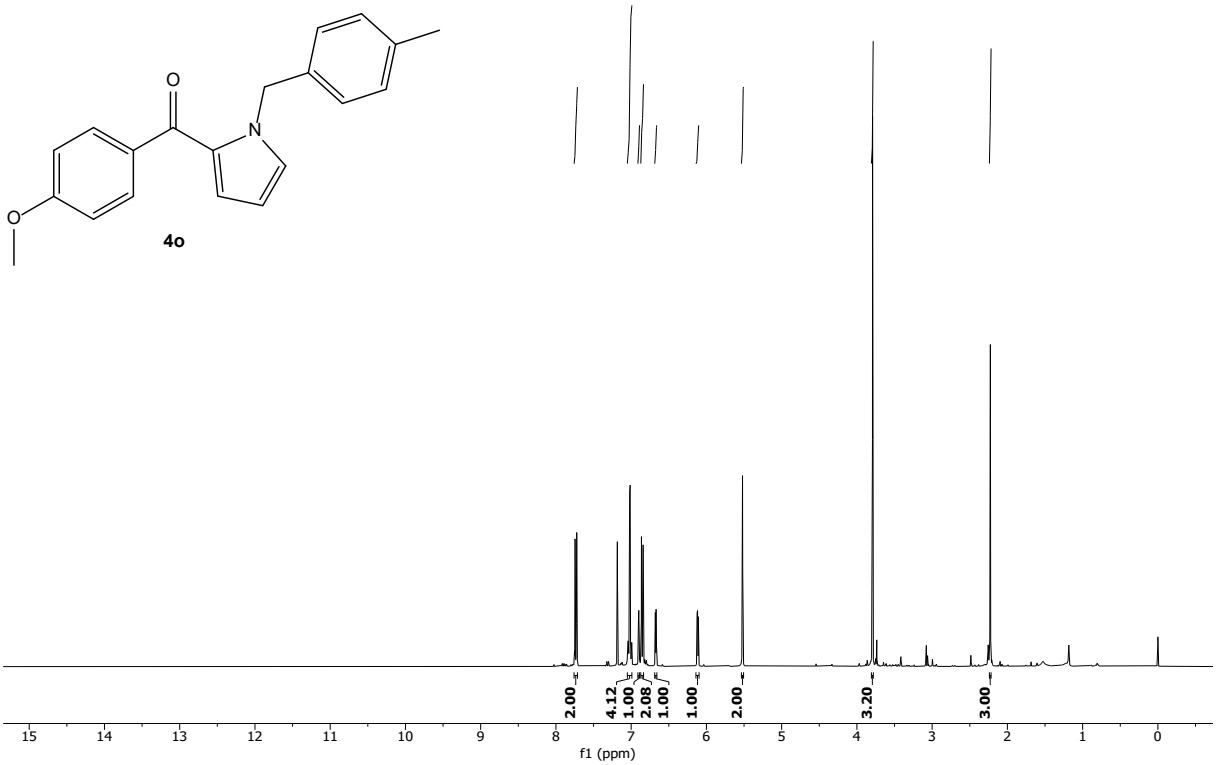
4n

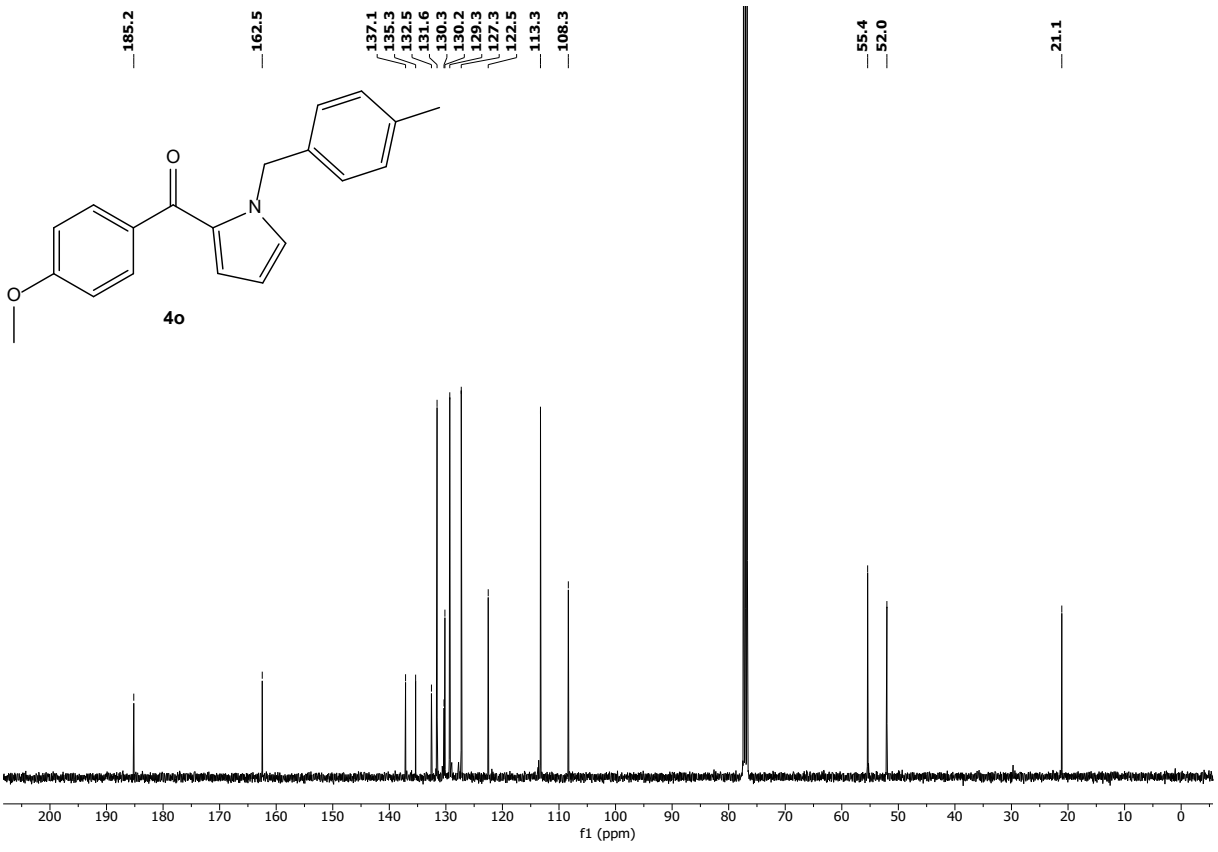
2.00
2.17
4.29
1.00
1.06
1.00
2.00
3.04
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

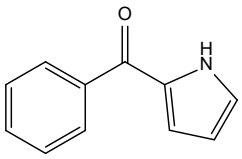

O
N
F3C

4n

184.6
143.1
137.4
134.9
131.6
129.6
129.4
129.4
127.3
125.1
125.0
124.1
109.0
52.4
21.1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

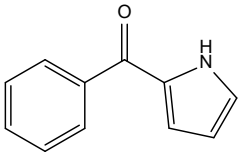

O
N
O
4o
2.00
4.12
1.00
2.08
1.00
1.00
2.00
3.20
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


185.2
162.5
137.1
135.3
132.5
131.6
130.3
130.2
129.3
127.3
122.5
113.3
108.3
55.4
52.0
21.1
O
N
O
4o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
H
N

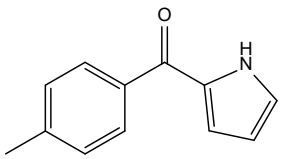
4r

1.00
2.00
1.00
2.00
1.00
1.00
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


O
H
N

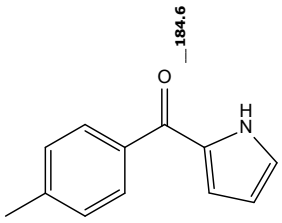
4r

185.2
138.6
131.9
131.2
129.1
128.4
126.1
120.1
111.0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
H
N

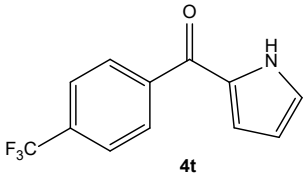
4s

1.00
2.00
2.04
1.00
1.00
1.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

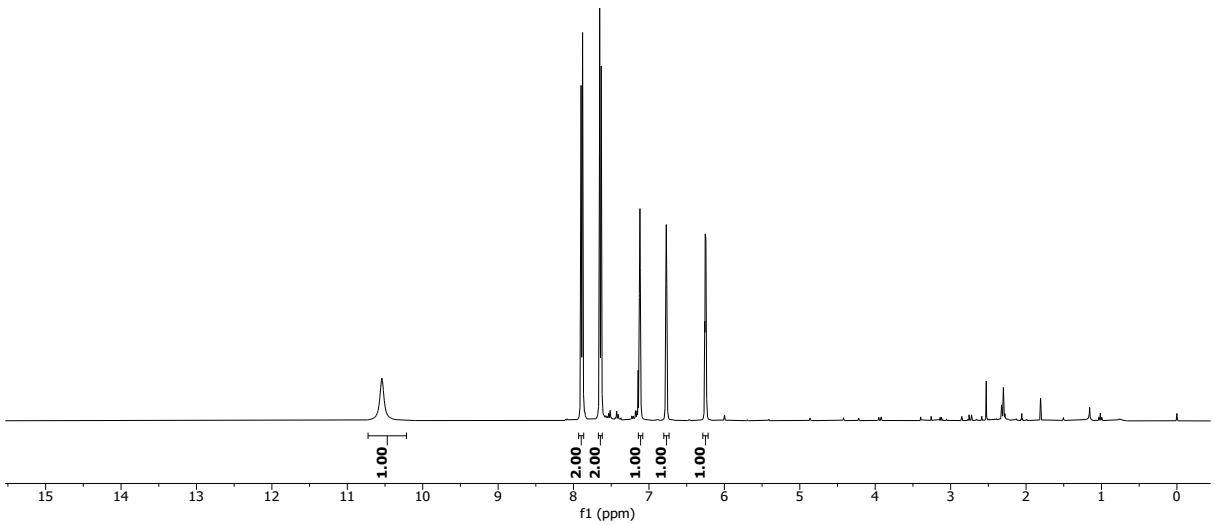

O
H
N

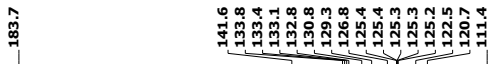
4s

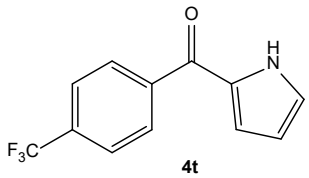
184.6
142.5
135.6
131.2
129.2
129.0
125.2
119.2
111.0
21.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
H
N
F3C

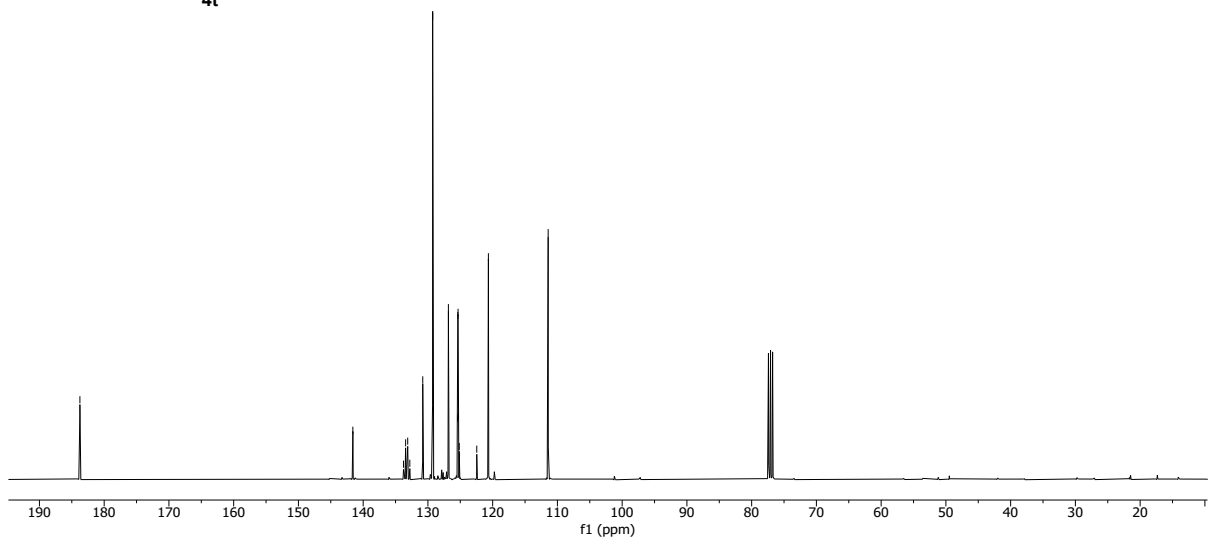
4t

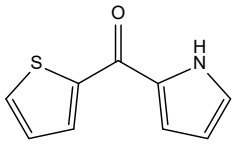

1.00
2.00
2.00
1.00
1.00
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


183.7
141.6
133.8
133.4
133.1
132.8
130.8
129.3
126.8
125.4
125.4
125.3
125.3
125.2
122.5
120.7
111.4


O
H
N
F3C

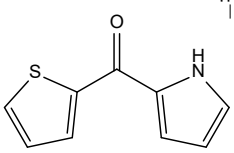
4t


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


O
S
H
N

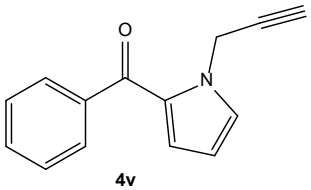
4u

1.00
1.00
1.00
3.00
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


O
S
H
N

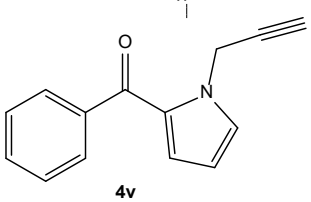
4u

175.9
142.8
132.4
132.3
130.7
127.9
125.7
117.9
111.1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N

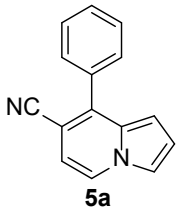
4v

2.00
1.00
2.00
1.00
1.00
1.00
2.00
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


O
N

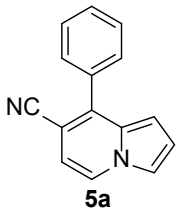
4v

186.2
139.6
131.6
129.8
129.2
128.1
123.7
108.8
78.3
74.1
38.7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


NC
N

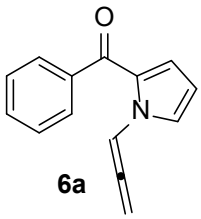
5a

1.02
2.00
4.00
1.00
1.00
1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
f1 (ppm)


NC
N

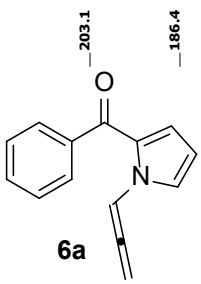
5a

140.4
134.9
131.3
129.5
129.1
128.7
124.2
118.9
116.7
115.9
111.1
105.6
98.1
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
N

6a

1.00
2.21
1.42
2.22
1.00
1.00
1.00
2.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


O
N

6a

203.1
186.4
139.7
131.7
129.7
129.2
128.1
127.7
124.2
110.0
99.4
87.0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

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