

Electronic Supplementary Information

Pd NPs confined novel covalent organic polymer for catalytic application

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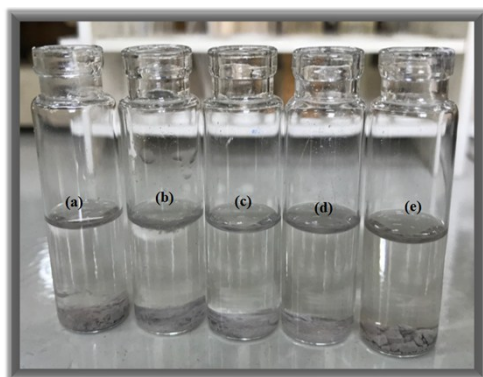


Figure S1. Solubility of **1** in various solvents viz. (a) DMSO, (b) H₂O, (c) CH₃CN, (d) 1,4-dioxane and (e) CH₃OH.

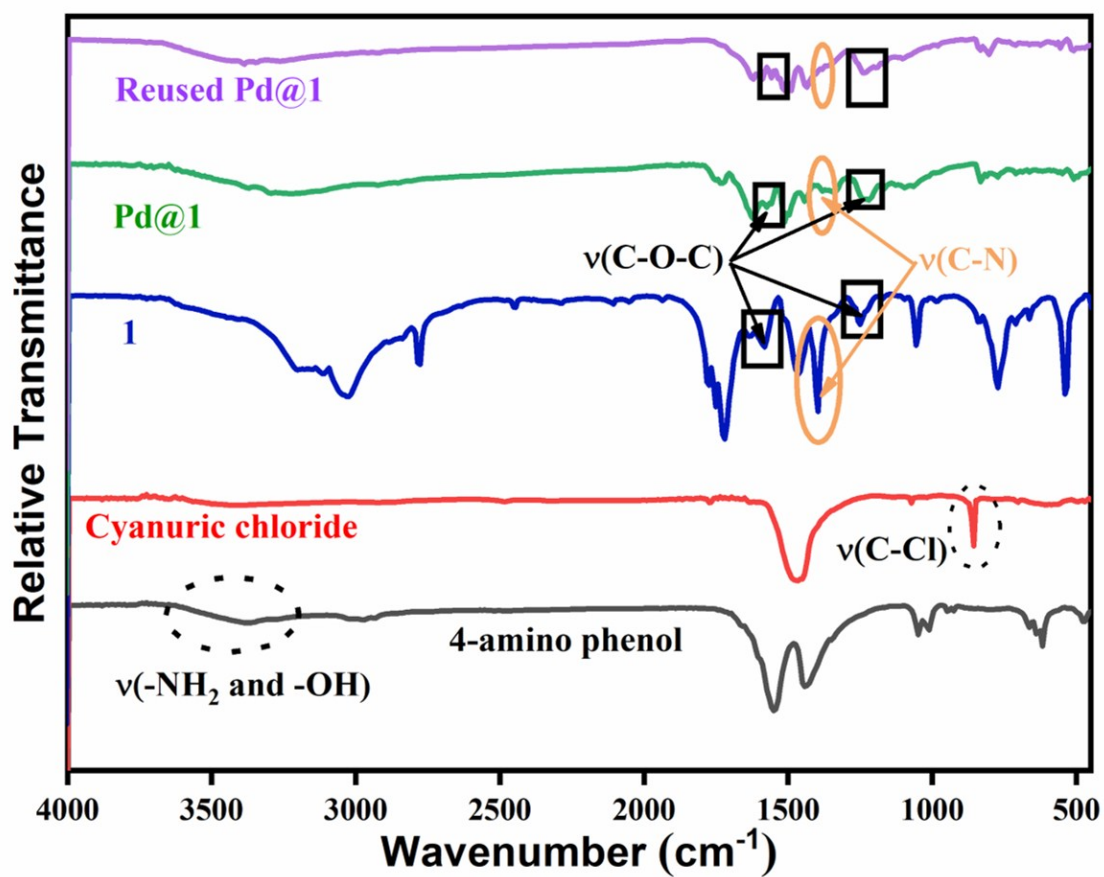


Figure S2. FT-IR Spectra of *p*-amino phenol, cyanuric chloride, **1**, Pd@**1** and reused Pd@**1**.

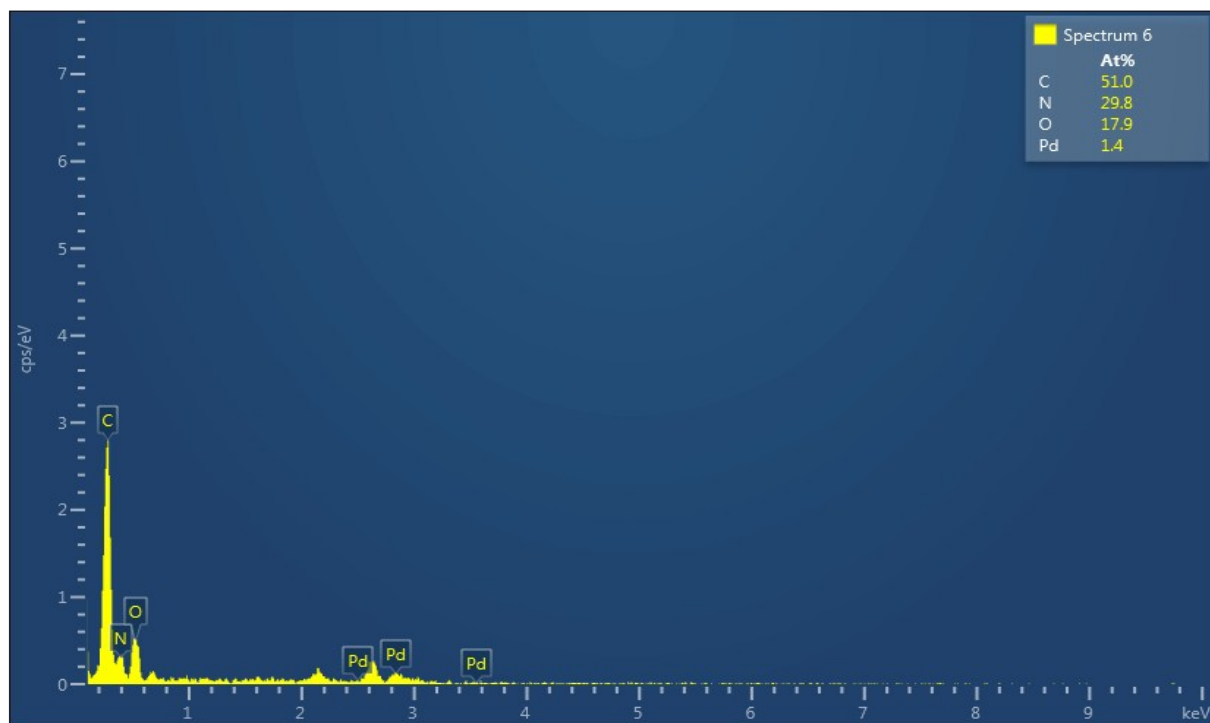


Figure S3. EDX spectra of Pd@1.

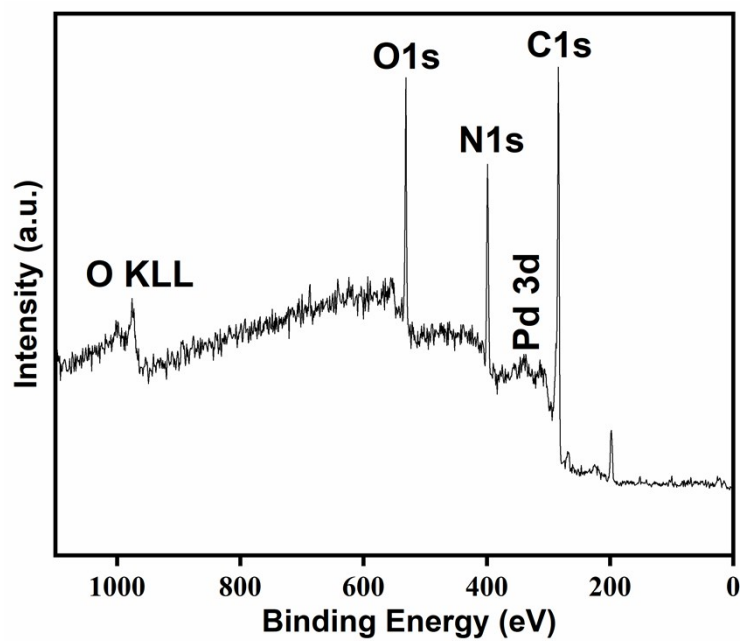


Figure S4. XPS Complete survey scan spectrum of Pd@1.

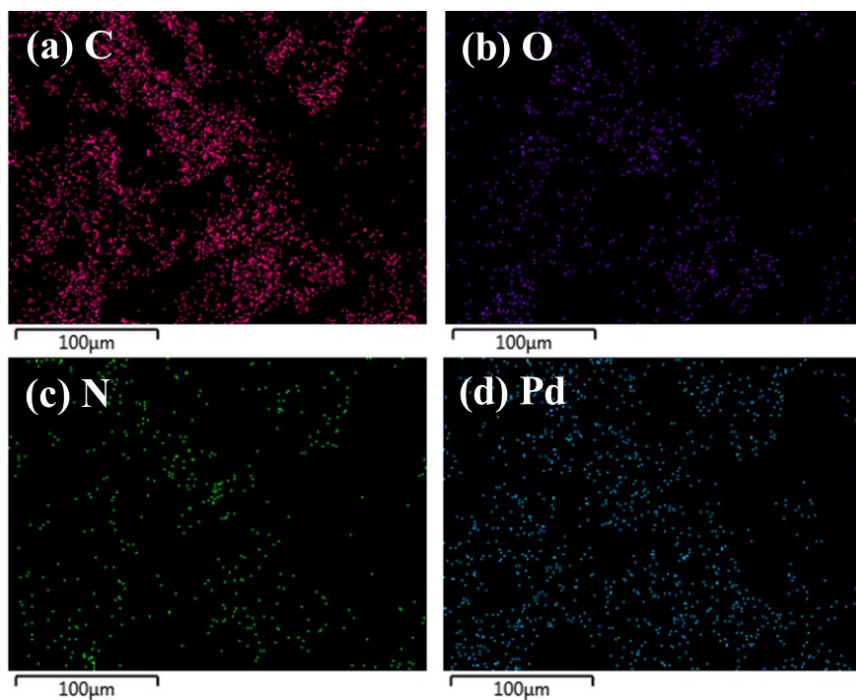


Figure S5. Elemental mapping of Pd@1.

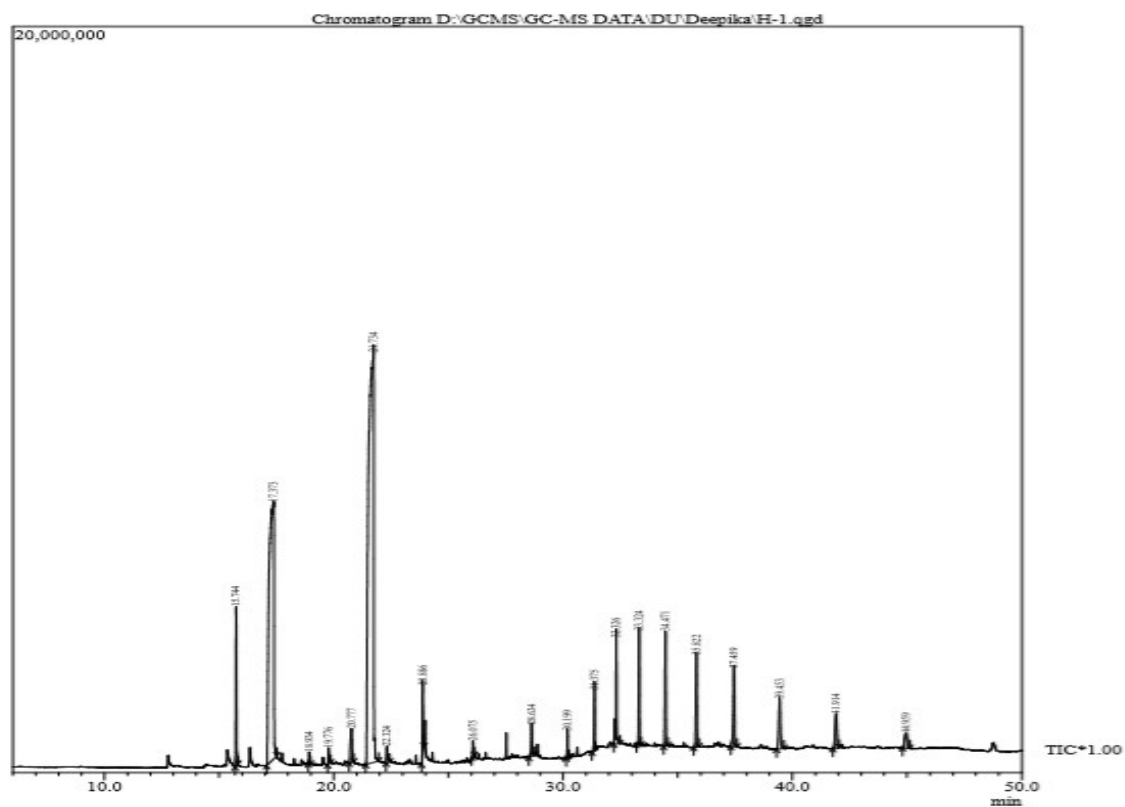


Figure S6. Gas Chromatograph of hot filtration test.

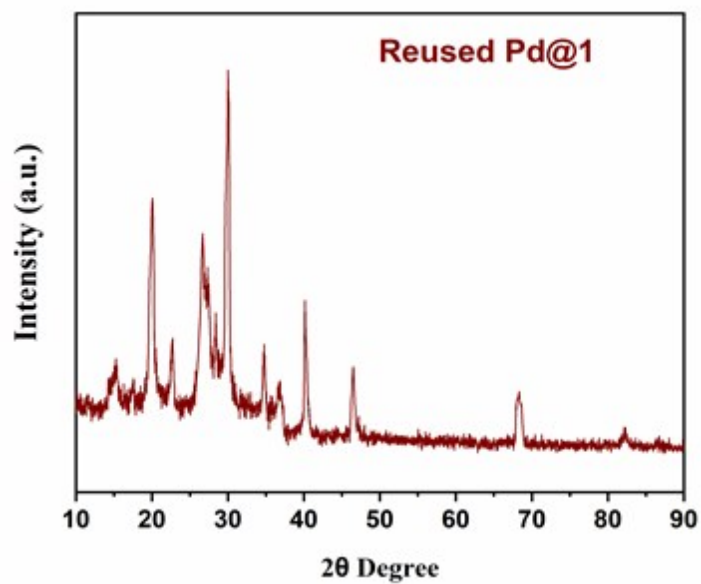


Figure S7. Powder XRD pattern for reused Pd@1.

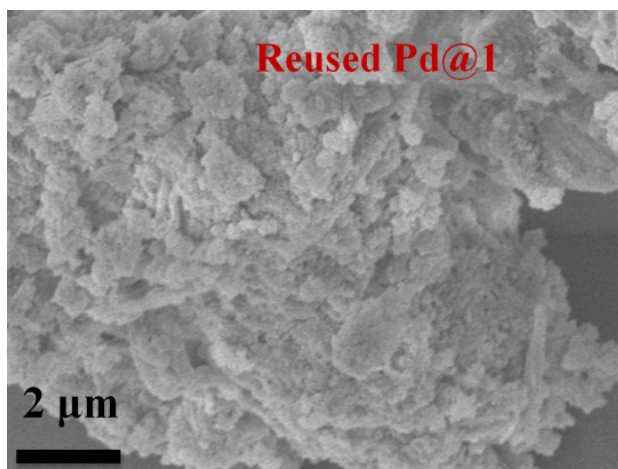


Figure S8. FE-SEM image of reused Pd@1.

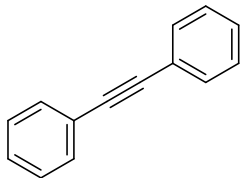
Table S1. Reusability of Pd@1.^a

Number of Cycle	1	2	3	4	5	6	7	8
Yield (%)	96	96	95	94	94	92	92	90

^aReaction conditions: aryl halide (1.2 mmol), alkyne (1 mmol), CuI (5 mg), catalyst (10 mg), base (1.5 mmol) solvent (3 mL).

¹H and ¹³C NMR chemical shift for 3a-3x

3a. 1,2-diphenylethyne

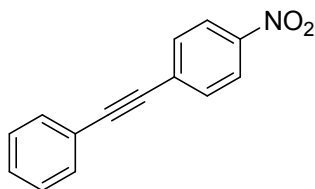


¹H-NMR (400 MHz, CDCl₃) δ 7.54 (d, *J* = 7.8 Hz, 5H), 7.37 (d, *J* = 6.9 Hz, 5H).

¹³C-NMR (101 MHz, CDCl₃) δ 133.77, 132.88, 130.49, 129.54, 123.05.

HRMS-ESI: calculated: 178.0783 [C₁₄H₁₀], Observed: 179.0846 [C₁₄H₁₀ +H].

3b. 1-nitro-4-(phenylethynyl)benzene

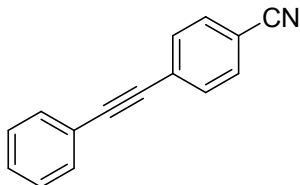


¹H-NMR (400 MHz, CDCl₃) δ 8.22 (d, *J* = 8.7 Hz, 2H), 7.66 (d, *J* = 8.7 Hz, 2H), 7.52-7.57 (m, 2H), 7.39 (dd, *J* = 4.8, 1.1 Hz, 3H)

¹³C-NMR (101 MHz, CDCl₃) δ 147.94, 139.72, 132.81, 125.80, 124.61, 123.07, 95.62, 88.53

HRMS-ESI: 223.0633 [C₁₄H₉NO₂], Observed: 224.0123 [C₁₄H₉NO₂ +H].

3c. 4-(phenylethynyl)benzonitrile

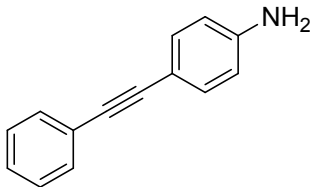


¹H-NMR (400 MHz, CDCl₃) δ 7.84 (d, *J* = 8.7 Hz, 2H), 7.59-7.62 (dd, 2H), 7.53 (d, *J* = 7.8 Hz, 2H), 7.35 (d, *J* = 7.3 Hz, 3H).

¹³C-NMR (101 MHz, CDCl₃) δ 139.44, 134.09, 133.45, 132.99, 132.74, 130.07, 129.39, 122.71, 119.37, 112.83, 100.77.

HRMS-ESI: calculated: 203.0745 [C₁₅H₉N], Observed: 204.0818 [C₁₅H₉N +H].

3d. 4-(phenylethynyl)aniline

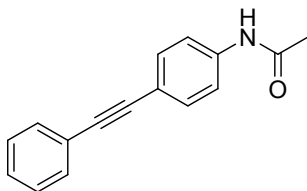


¹H-NMR (400 MHz, CDCl₃) δ 7.40 (d, *J* = 9.4 Hz, 2H), 7.10 (t, *J* = 8.2 Hz, 2H), 6.76 (d, *J* = 7.7 Hz, 2H), 6.60-6.64 (t, *J* = 8.4 Hz, 2H), 6.12 (s, 2H)

¹³C-NMR (101 MHz, CDCl₃) δ 145.31, 136.90, 133.84, 129.59, 120.69, 117.05, 110.47, 95.75, 89.83

HRMS-ESI: calculated: 193.0889 [C₁₄H₁₁N], Observed: 194.0961 [C₁₄H₁₁N +H].

3e. N-(4-(phenylethynyl)phenyl)acetamide

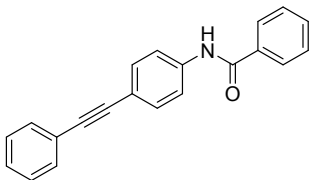


¹H-NMR (400 MHz, CDCl₃) δ 9.84 (s, 1H), 7.84 (d, *J* = 7.3 Hz, 2H), 7.52-7.57 (m, 4H), 7.45-7.50 (m, 3H), 2.04 (s, 3H)

¹³C-NMR (101 MHz, CDCl₃) δ 164.38, 136.91, 133.84, 129.59, 124.81, 120.69, 117.05, 110.47, 95.75, 89.83

HRMS-ESI: calculated: 235.0997 [C₁₆H₁₃NO], Observed: 236.1078 [C₁₆H₁₃NO +H].

3f. N-(4-(phenylethynyl)phenyl)benzamide

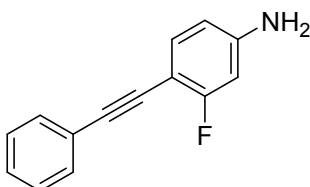


¹H-NMR (400 MHz, DMSO-D₆) δ 10.36 (s, 1H), 7.94 (d, *J* = 7.4 Hz, 2H), 7.78 (d, *J* = 8.8 Hz, 2H), 7.44-7.55 (m, 4H), 7.34-7.38 (m, 6H)

^{13}C -NMR (101 MHz, $\text{DMSO}-d_6$) δ 166.22, 139.16, 135.29, 132.22, 131.95, 129.45, 129.16, 128.91, 128.23, 122.77, 122.32, 115.68, 83.99, 81.17

HRMS-ESI: calculated: 296.9771 [$\text{C}_{21}\text{H}_{15}\text{NO}$], Observed: 297.9844 [$\text{C}_{21}\text{H}_{15}\text{NO} + \text{H}$].

3g. 3-fluoro-4-(phenylethynyl)aniline

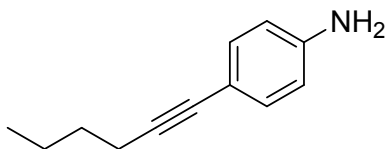


^1H -NMR (400 MHz, CDCl_3) δ 7.48-7.50 (m, 1H), 7.29-7.35 (m, 2H), 7.16 (dd, J = 8.1, 2.9 Hz, 2H), 6.82-6.86 (m, 1H), 6.69 (dd, J = 8.8, 5.1 Hz, 2H), 3.91 (s, 2H)

^{13}C -NMR (101 MHz, CDCl_3) 156.61, 154.23, 140.67, 132.23, 128.91, 128.42, 119.41, 119.16, 115.97, 115.23, 108.75, 83.54

HRMS-ESI: calculated: 211.0194 [$\text{C}_{14}\text{H}_{10}\text{FN}$], Observed: 212.0121 [$\text{C}_{14}\text{H}_{10}\text{FN} + \text{H}$].

3h. 4-(hex-1-yn-1-yl)aniline

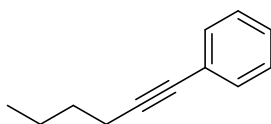


^1H -NMR (400 MHz, CDCl_3) δ 7.40 (d, J = 9.3 Hz, 2H), 6.51 (d, J = 9.3 Hz, 2H), 6.10 (s, 2H), 2.41 (t, J = 7.2, 2H), 1.42 (m, 2H), 1.24-1.29 (m, 2H), 0.90 (t, J = 7.5 Hz, 3H)

^{13}C -NMR (101 MHz, CDCl_3) δ 144.26, 132.47, 127.71, 119.51, 115.44, 109.43, 29.47, 22.71

HRMS-ESI: calculated: 173.1265 [$\text{C}_{12}\text{H}_{15}\text{N}$], Observed: 174.1277 [$\text{C}_{12}\text{H}_{15}\text{N} + \text{H}$].

3i. hex-1-yn-1-ylbenzene

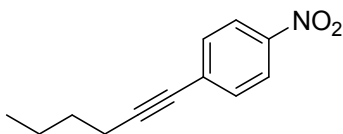


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.53 (d, J = 8.2 Hz, 2H), 7.44-7.41 (d, 3H), 2.41 (t, J = 7.1 Hz, 2H), 1.65 (m, 2H), (m, 3H), 1.49 (m, 2H), .93 (t, J = 6.9 Hz, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 145.06, 132.06, 131.03, 122.77, 97.14, 79.34, 30.24, 20.71, 18.87, 12.57

HRMS-ESI: calculated: 158.1096 [$\text{C}_{12}\text{H}_{14}$], Observed: 159.0311 [$\text{C}_{12}\text{H}_{14} + \text{H}$].

3j. 4-(hex-1-yn-1-yl)-4-nitrobenzene

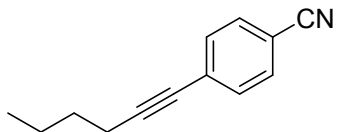


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.13 (d, J = 8.2 Hz, 2H), 7.49 (d, J = 8.7 Hz, 2H), 2.44 (t, J = 7.1 Hz, 2H), 1.56-1.63 (m, 2H), 1.42-1.50 (m, 2H), 0.94 (t, J = 7.3 Hz, 3H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 147.56, 139.79, 133.51, 124.44, 103.75, 97.62, 31.72, 23.13, 20.16, 14.90

HRMS-ESI: calculated: 203.0938 [$\text{C}_{12}\text{H}_{13}\text{NO}_2$], Observed: 204.1017 [$\text{C}_{12}\text{H}_{13}\text{NO}_2 + \text{H}$].

3k. 4-(hex-1-yn-1-yl)benzonitrile

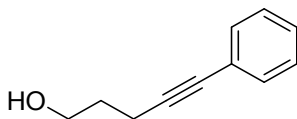


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.12 (d, J = 8.3 Hz, 2H), 7.90 (d, J = 5.5 Hz, 2H), 2.43 (t, J = 7.1 Hz, 2H), 1.55-1.62 (m, 2H), 1.43-1.51 (m, 2H), 0.93 (t, J = 7.5 Hz, 3H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 138.59, 133.07, 132.16, 131.98, 118.30, 111.77, 100.41, 40.85, 30.55, 29.76, 21.70

HRMS-ESI: calculated: 204.1197 [$\text{C}_{13}\text{H}_{13}\text{N}$], Observed: 205.1169 [$\text{C}_{13}\text{H}_{13}\text{N} + \text{H}$].

3l. 5-phenylpent-4-yn-1-ol

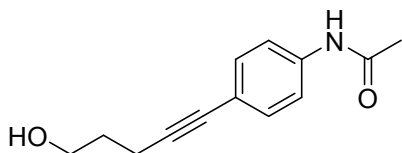


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.60 (d, $J = 8.7$ Hz, 2H), 7.40 (dd, $J = 14.2, 8.7$ Hz, 3H), 4.478 (s, 1H), 3.423-3.403 (t, $J = 7.3$ Hz, 2H), 2.455-2.419 (t, $J = 7.1$ Hz, 2H), 1.632-1.560 (q, $J = 7.3$ Hz, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 133.51, 126.12, 103.75, 85.11, 61.99, 31.88, 14.94

HRMS-ESI: calculated: 146.0723 [$\text{C}_{11}\text{H}_{12}\text{O}$], Observed: 147.0723 [$\text{C}_{11}\text{H}_{12} + \text{H}$].

3m. N-(4-(5-hydroxypent-1-yn-1-yl)phenyl)acetamide

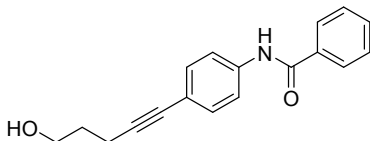


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 9.69 (s, 1H), 7.73 (t, $J = 1.9$ Hz, 1H), 7.35 (d, $J = 9.8$ Hz, 1H), 7.04-7.13 (m, 2H), 4.40 (s, 1H), 4.05 (q, $J = 7.1$ Hz, 2H), 3.64 (t, $J = 6.3$ Hz, 2H), 2.08 (s, 2H), 1.19 (t, $J = 7.1$ Hz, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 169.69, 139.63, 130.21, 123.01, 118.57, 98.67, 85.13, 65.70, 31.05, 24.31, 15.89

HRMS-ESI: calculated: 217.1103 [$\text{C}_{13}\text{H}_{15}\text{NO}_2$], Observed: 218.1782 [$\text{C}_{13}\text{H}_{15}\text{NO}_2 + \text{H}$].

3n. N-(4-(5-hydroxypent-1-yn-1-yl)phenyl)benzamide

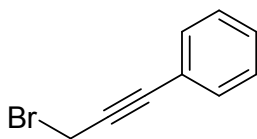


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.05 (s, 1H), 7.91 (d, $J = 8.0$ Hz, 2H), 7.46-7.55 (m, 6H), 7.33 (t, $J = 7.1$ Hz, 1H), 3.60 (t, $J = 6.3$ Hz, 2H), 3.23 (s, 1H), 2.19 (d, $J = 7.0, 2.7$ Hz, 2H), 1.62-1.69 (m, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 165.66, 136.17, 134.90, 132.70, 129.34, 128.01, 127.20, 125.25, 103.38, 88.01, 82.68, 66.85, 24.27, 18.20

HRMS-ESI: calculated: 279.1259 [$\text{C}_{18}\text{H}_{17}\text{NO}_2$], Observed: 280.1395 [$\text{C}_{18}\text{H}_{17}\text{NO}_2 + \text{H}$].

3o. 4-(3-bromoprop-1-yn-1-yl)benzene

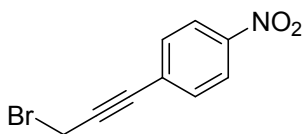


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.35 (d, $J = 7.3$ Hz, 2H), 7.00 (t, $J = 7.6$ Hz, 1H), 6.78 (t, $J = 7.8$ Hz, 2H), 4.08 (s, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 137.61, 131.92, 130.07, 127.62, 94.44, 88.92, 41.16

HRMS-ESI: calculated: 193.9731 [$\text{C}_9\text{H}_7\text{Br}$], Observed: 194.8495 [$\text{C}_9\text{H}_7\text{Br}+\text{H}$].

3p. 4-(3-bromoprop-1-yn-1-yl)-4-nitrobenzene

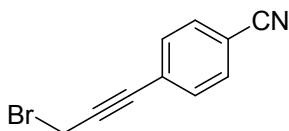


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.88-7.94 (m, 4H), 4.27 (s, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 147.94, 139.32, 125.65, 120.74, 111.15, 102.93, 29.62

HRMS-ESI: calculated: 238.9582 [$\text{C}_9\text{H}_6\text{BrNO}_2$], Observed: 239.8180 [$\text{C}_9\text{H}_6\text{BrNO}_2+\text{H}$].

3q. 4-(3-bromoprop-1-yn-1-yl)benzonitrile

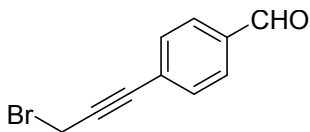


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.72 (d, $J = 7.8$ Hz, 2H), 7.53 (d, $J = 7.3$ Hz, 2H), 4.34 (s, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 132.59, 129.30, 128.54, 121.87, 106.28, 81.64, 74.10, 29.68

HRMS-ESI: calculated: 218.9684 [$\text{C}_{10}\text{H}_6\text{BrN}$], Observed: 219.8721 [$\text{C}_{10}\text{H}_6\text{BrN}+\text{H}$].

3r. 4-(3-bromoprop-1-yn-1-yl)benzaldehyde

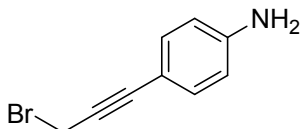


^1H -NMR (400 MHz, CDCl_3) δ 9.92 (s, 1H), 7.70 (d, J = 8.5 Hz, 2H), 7.63 (d, J = 8.5 Hz, 2H), 4.04 (s, 2H)

^{13}C -NMR (101 MHz, CDCl_3) δ 191.19, 135.11, 132.50, 131.05, 129.62, 90.27, 86.58, 14.28

HRMS-ESI: calculated: 221.9680 [$\text{C}_{10}\text{H}_7\text{BrO}$], Observed: 222.8180 [$\text{C}_{10}\text{H}_7\text{BrO}+\text{H}$].

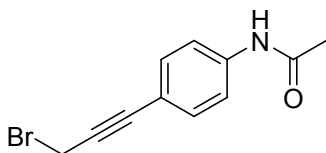
3s. 4-(3-bromoprop-1-yn-1-yl)aniline



^1H -NMR (400 MHz, CDCl_3) δ 7.24 (d, J = 8.8 Hz, 2H), 6.54 (d, J = 8.8 Hz, 2H), 6.05 (s, 2H), 3.78 (s, 2H)

^{13}C -NMR (101 MHz, CDCl_3) δ 133.45, 130.18, 129.40, 122.71, 82.52, 74.88, 30.54 HRMS-ESI: calculated: 208.9789 [$\text{C}_9\text{H}_6\text{BrN}$], Observed: 209.9735 [$\text{C}_9\text{H}_6\text{BrN}+\text{H}$].

3t. N-(4-(3-bromoprop-1-yn-1-yl)phenyl)acetamide

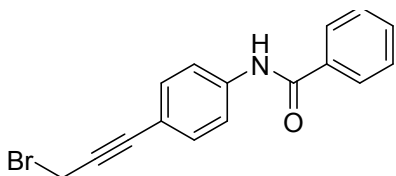


^1H -NMR (400 MHz, CDCl_3) δ 8.92 (s, 1H), 7.79 (t, J = 1.9 Hz, 1H), 7.36 (d, J = 8.1 Hz, 1H), 7.16 (d, J = 6.9 Hz, 1H), 7.09 (t, J = 8.1 Hz, 1H), 4.09 (s, 2H), 2.13 (s, 3H)

^{13}C -NMR (101 MHz, CDCl_3) δ 169.85, 139.54, 130.29, 127.26, 123.29, 122.50, 118.82, 90.26, 85.19, 24.45, 14.13

HRMS-ESI: calculated: 250.9946 [$\text{C}_{11}\text{H}_{10}\text{BrNO}$], Observed: 251.8180 [$\text{C}_{11}\text{H}_{10}\text{BrNO}+\text{H}$].

3u. N-(4-(3-bromoprop-1-yn-1-yl)phenyl)benzamide

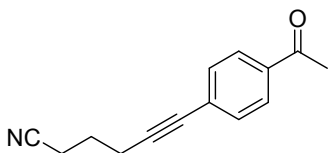


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.16 (s, 1H), 7.91 (d, J = 8.0 Hz, 2H), 7.46-7.55 (m, 6H), 7.33 (t, J = 7.1 Hz, 1H), 4.080 (s, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 165.65, 135.88, 134.79, 132.31, 129.05, 128.60, 127.21, 125.44, 121.98, 91.12, 85.63, 15.75

HRMS-ESI: calculated: 313.0102 [$\text{C}_{16}\text{H}_{12}\text{BrNO}$], Observed: 314.0239 [$\text{C}_{16}\text{H}_{12}\text{BrNO}+\text{H}$].

3v. 6-(4-acetylphenyl)hex-5-ynenitrile

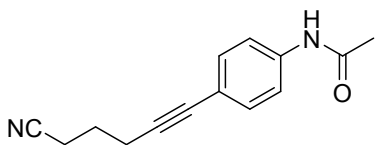


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.88 (d, J = 7.0 Hz, 2H), 7.69 (d, J = 7.0 Hz, 2H), 2.88 (s, 3H), 2.24-2.28 (q, 2H), 1.99 (t, J = 2.7 Hz, 2H), 1.74-1.78 (m, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 196.68, 151.88, 130.85, 127.27, 118.98, 113.63, 81.87, 70.49, 26.12, 24.30, 17.51, 16.00

HRMS-ESI: calculated: 211.0997 [$\text{C}_{14}\text{H}_{13}\text{NO}$], Observed: 212.0187 [$\text{C}_{14}\text{H}_{13}\text{NO}+\text{H}$].

3w. N-(4-(5-cyanopent-1-yn-1-yl)phenyl)acetamide

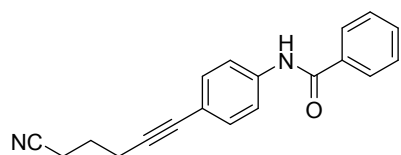


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 9.84 (s, 1H), 7.76 (t, J = 1.8 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.16 (d, J = 6.9 Hz, 1H), 7.10 (t, J = 8.0 Hz, 1H), 2.40-2.49 (m, 4H), 2.17-2.11 (s, 3H), 1.81-1.91 (m, 2H)

$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 169.47, 139.22, 130.29, 127.19, 123.06, 118.40, 110.32, 100.94, 75.55, 29.77, 24.47, 18.54, 16.51

HRMS-ESI: calculated: 226.1106 [$\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}$], Observed: 227.1251 [$\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}+\text{H}$].

3x. N-(4-(5-cyanopent-1-yn-1-yl)phenyl)benzamide

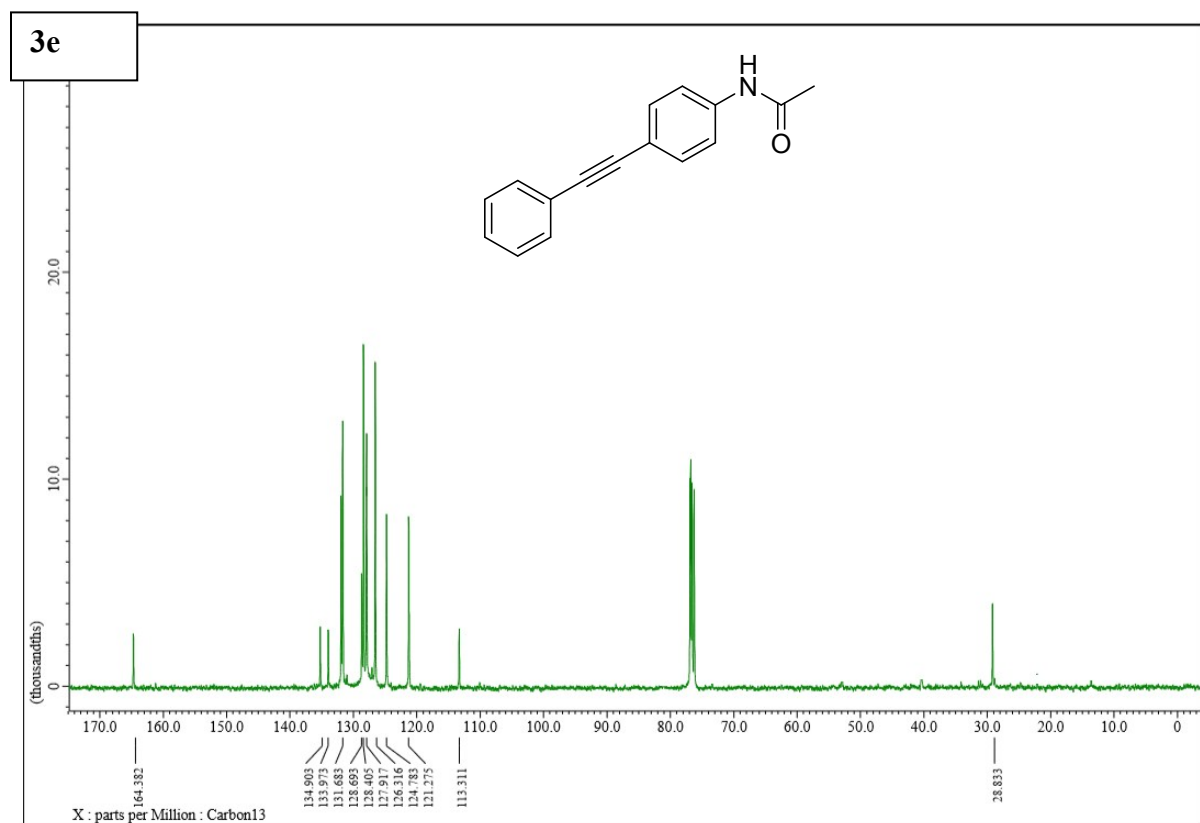
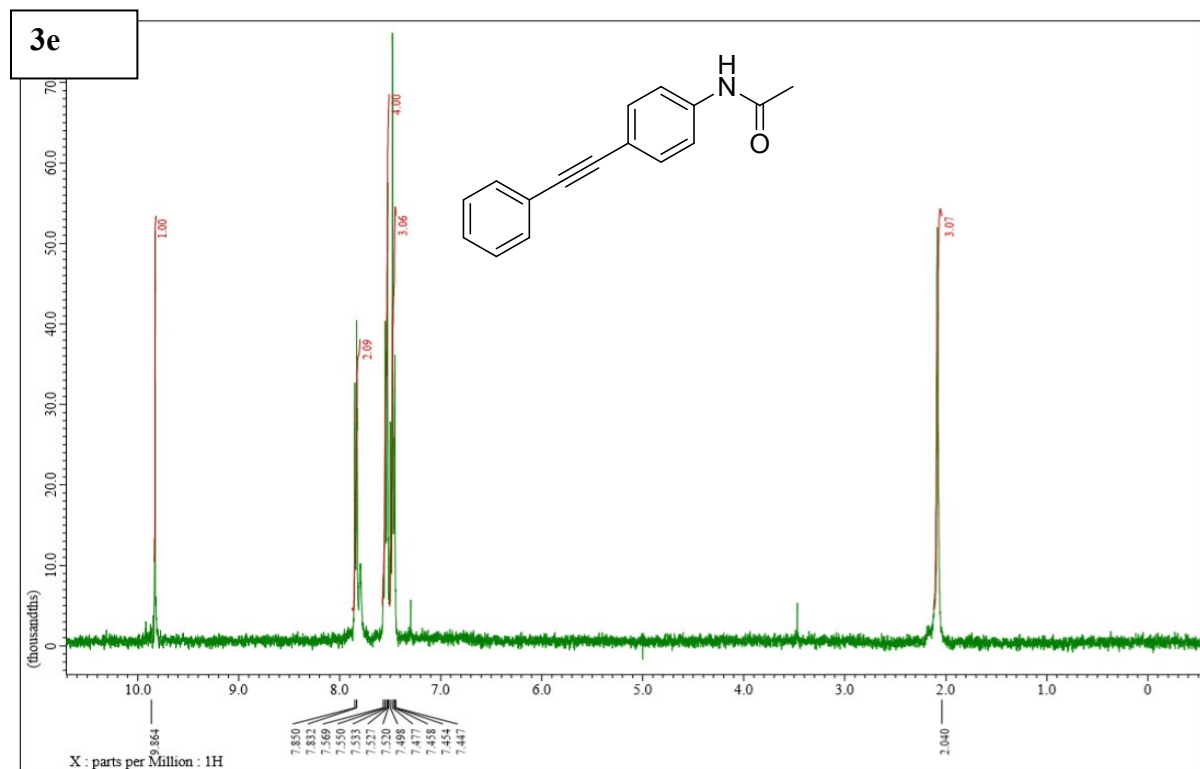


$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.27 (s, 1H), 7.89 (d, $J = 7.3$ Hz, 2H), 7.78 (d, $J = 7.3$ Hz, 2H) 7.51-7.55 (m, 2H), 7.44-7.48 (m, 2H), 7.29-7.33 (t, $J = 7.3$ Hz, 1H), 2.37-2.45 (m, 2H), 1.78-1.85 (m, 4H)

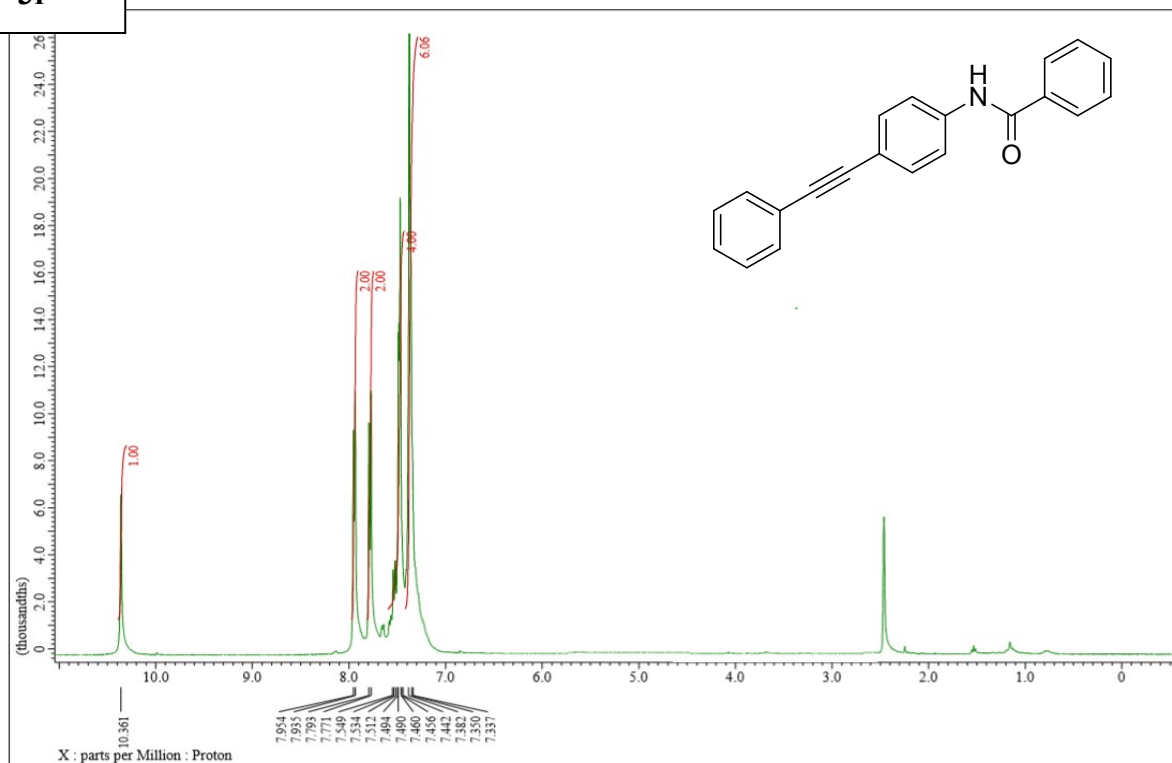
$^{13}\text{C-NMR}$ (101 MHz, CDCl_3) δ 165.33, 135.87, 134.55, 132.38, 129.04, 128.58, 127.20, 125.25, 119.02, 114.12, 102.99, 75.37, 29.79, 24.27, 18.20

HRMS-ESI: calculated: 288.1263 [$\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}$], Observed: 289.1310 [$\text{C}_{19}\text{H}_{16}\text{N}_2\text{O} + \text{H}$].

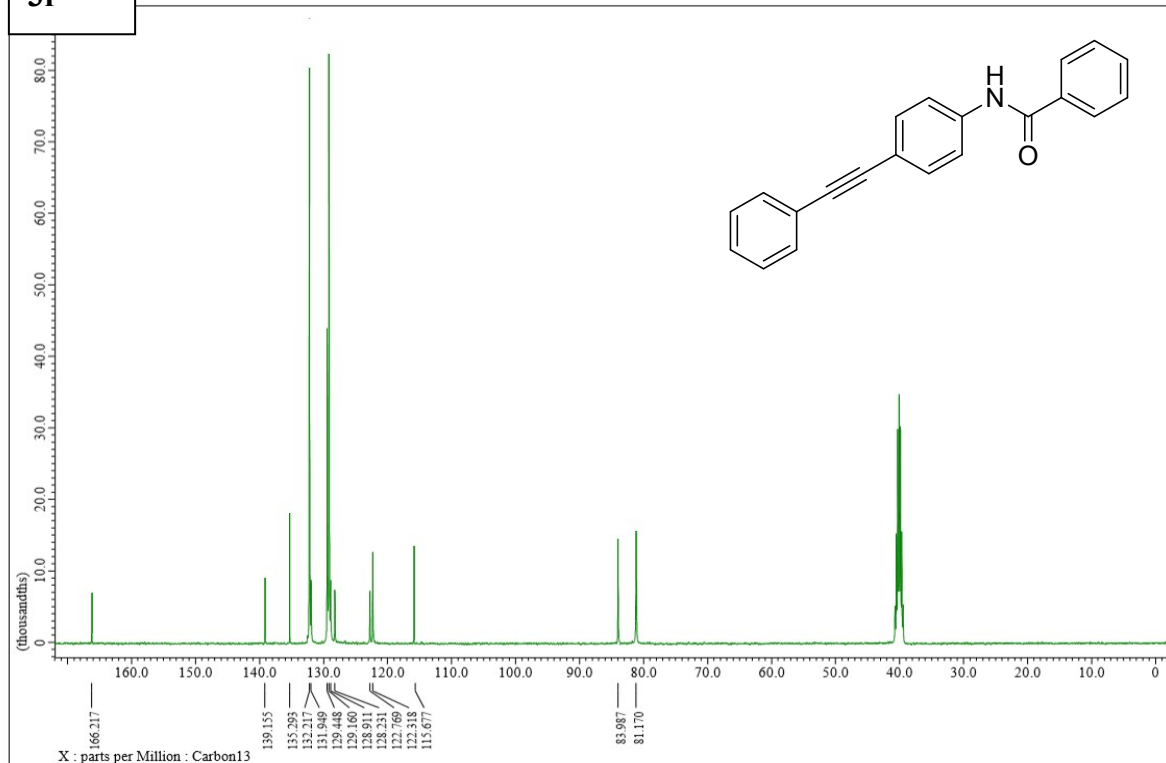
¹H and ¹³C Spectra



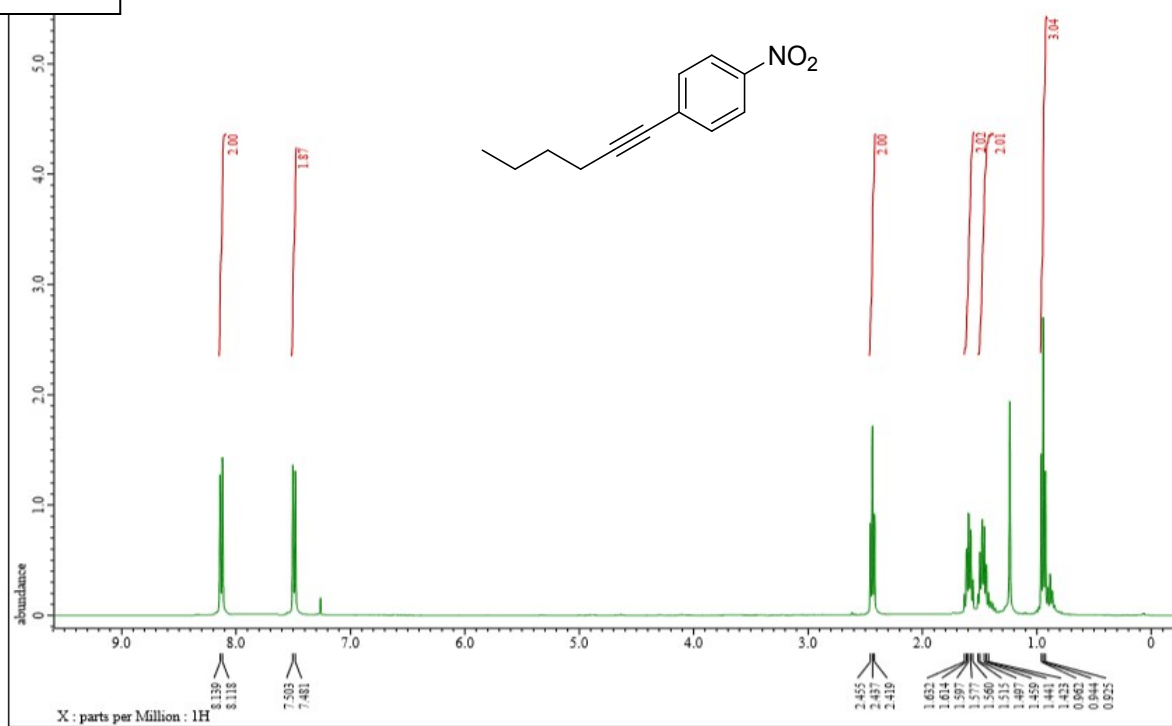
3f



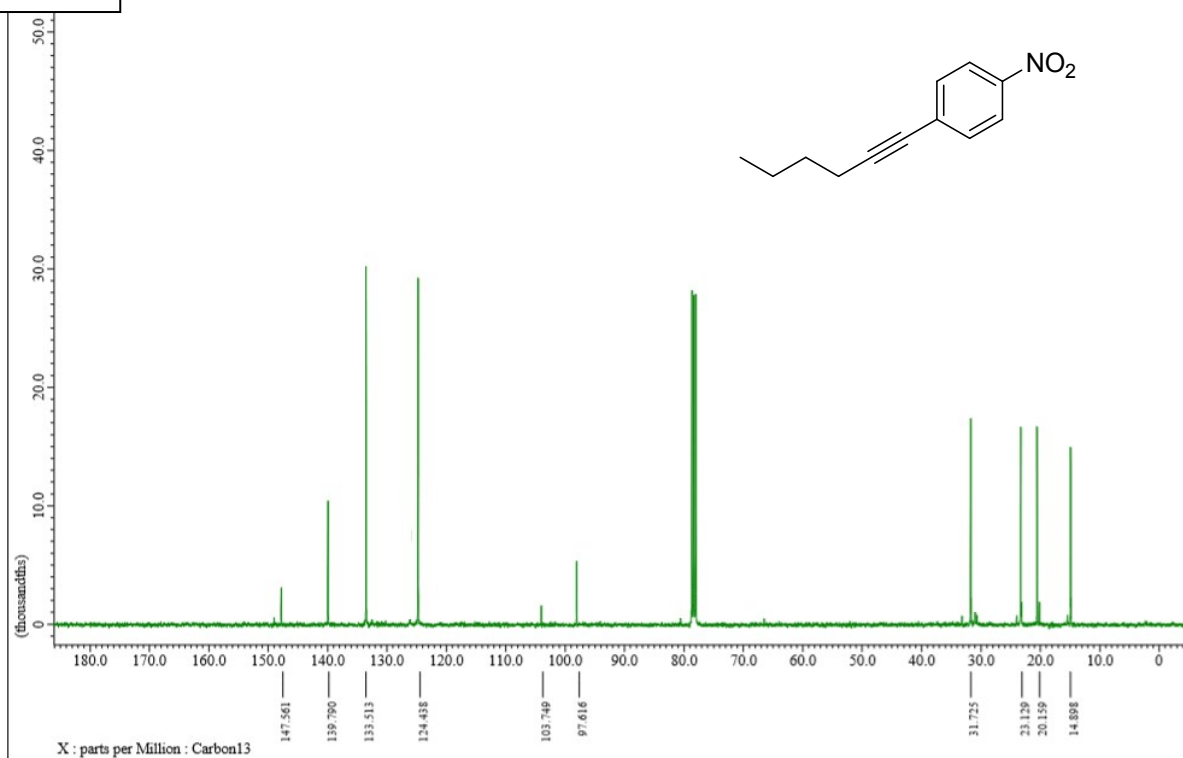
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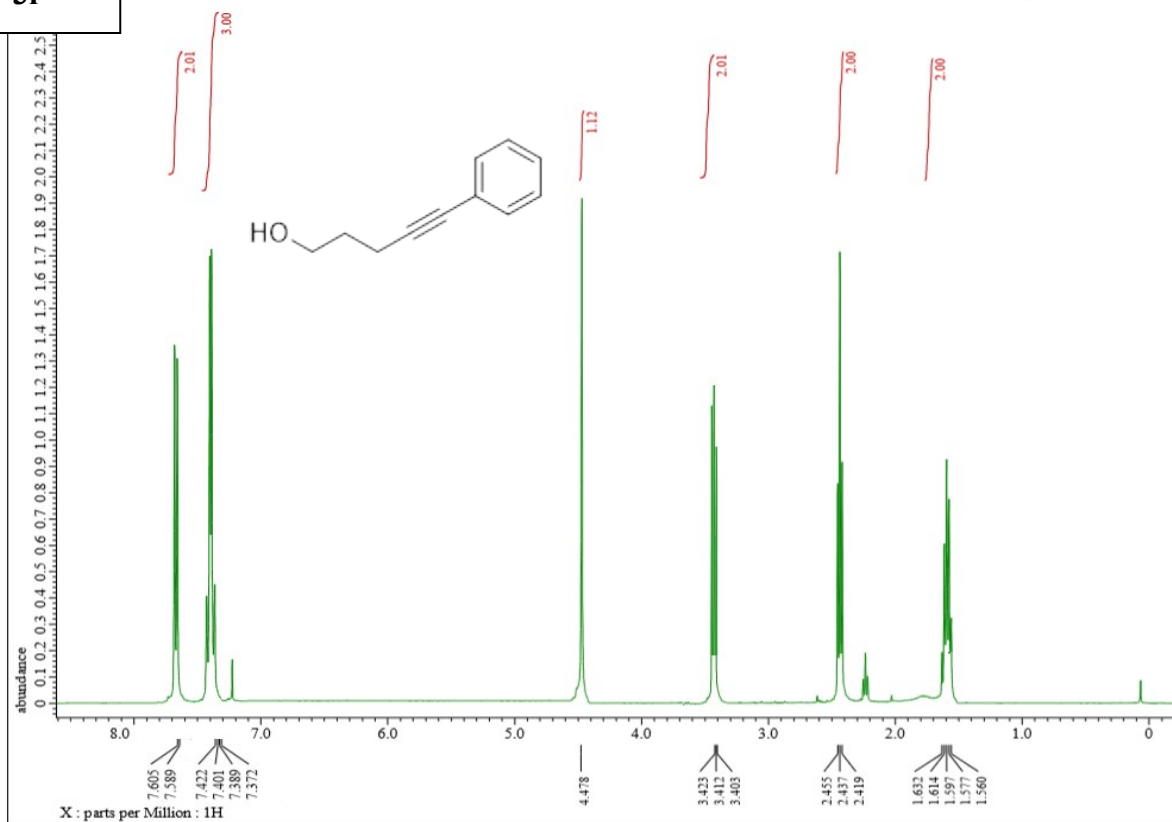
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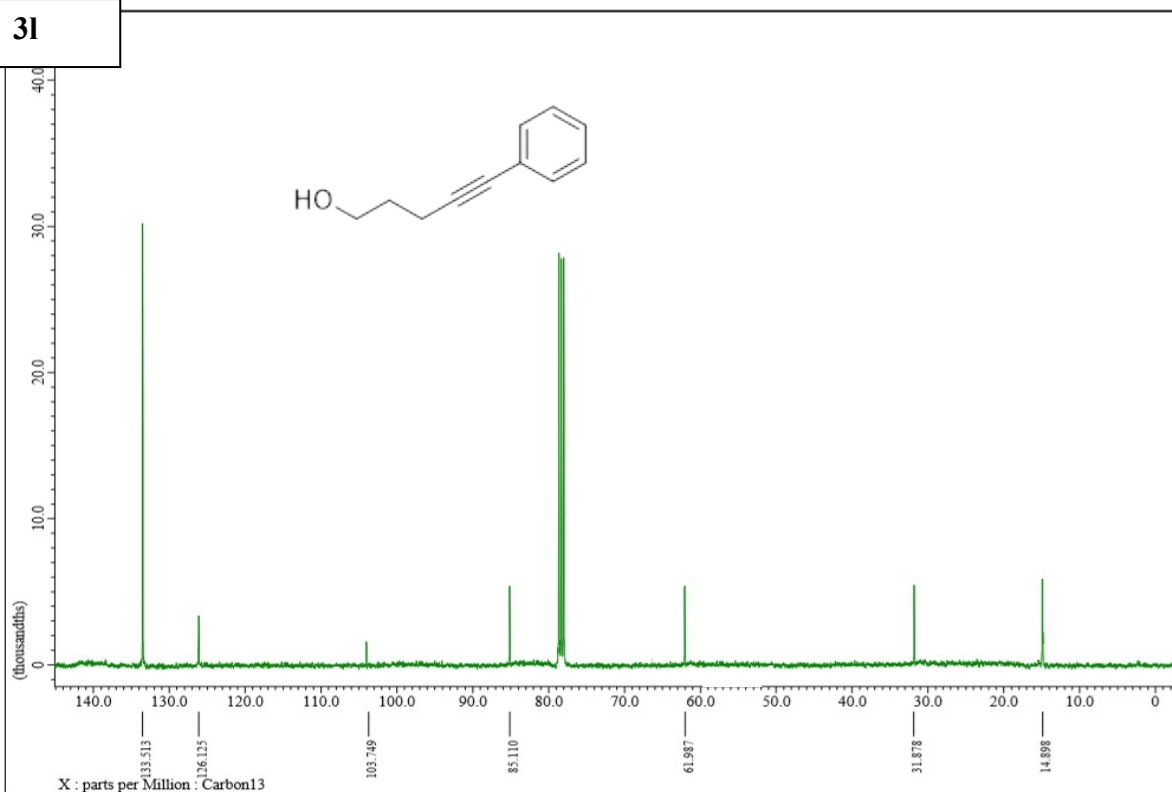
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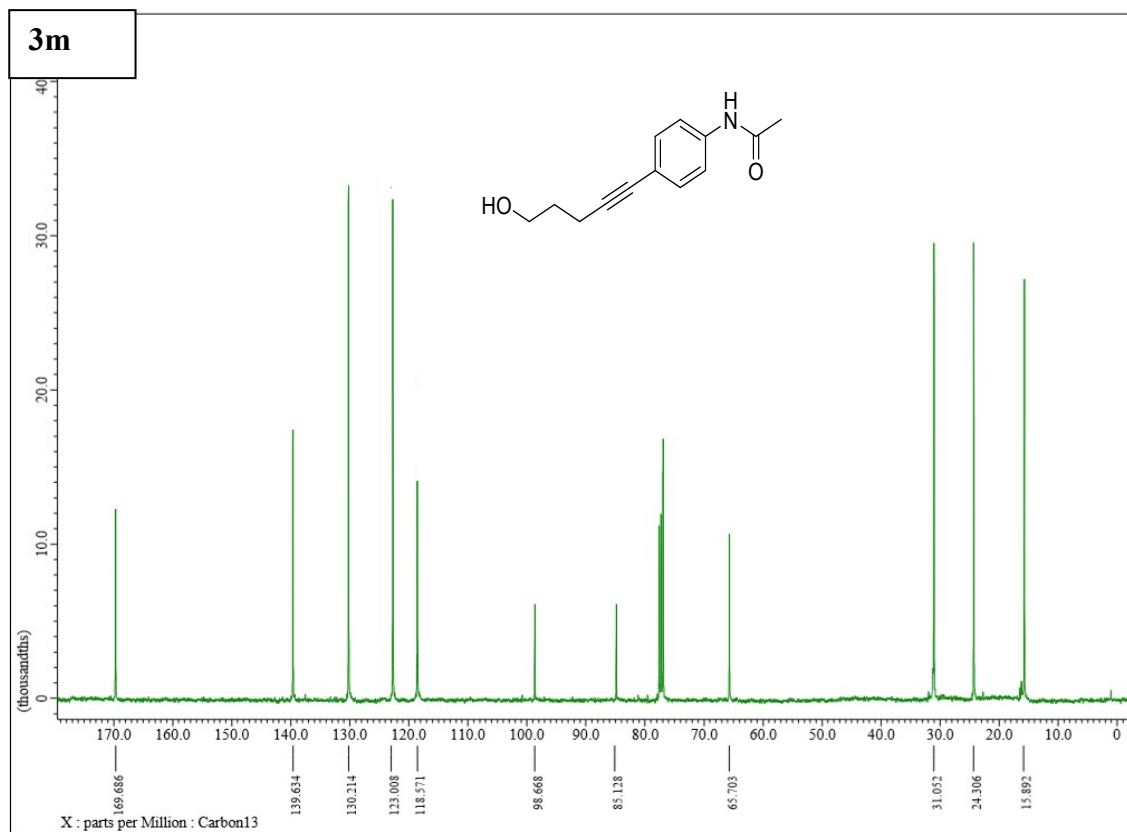
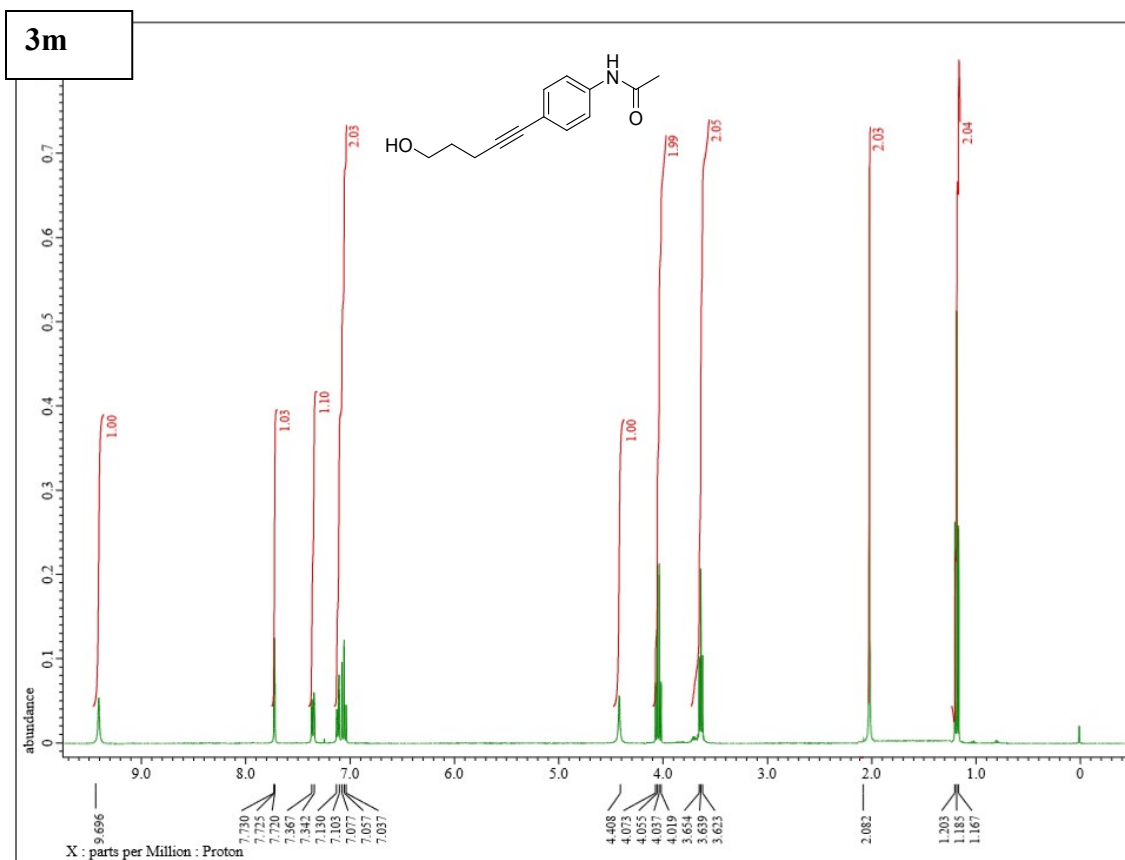


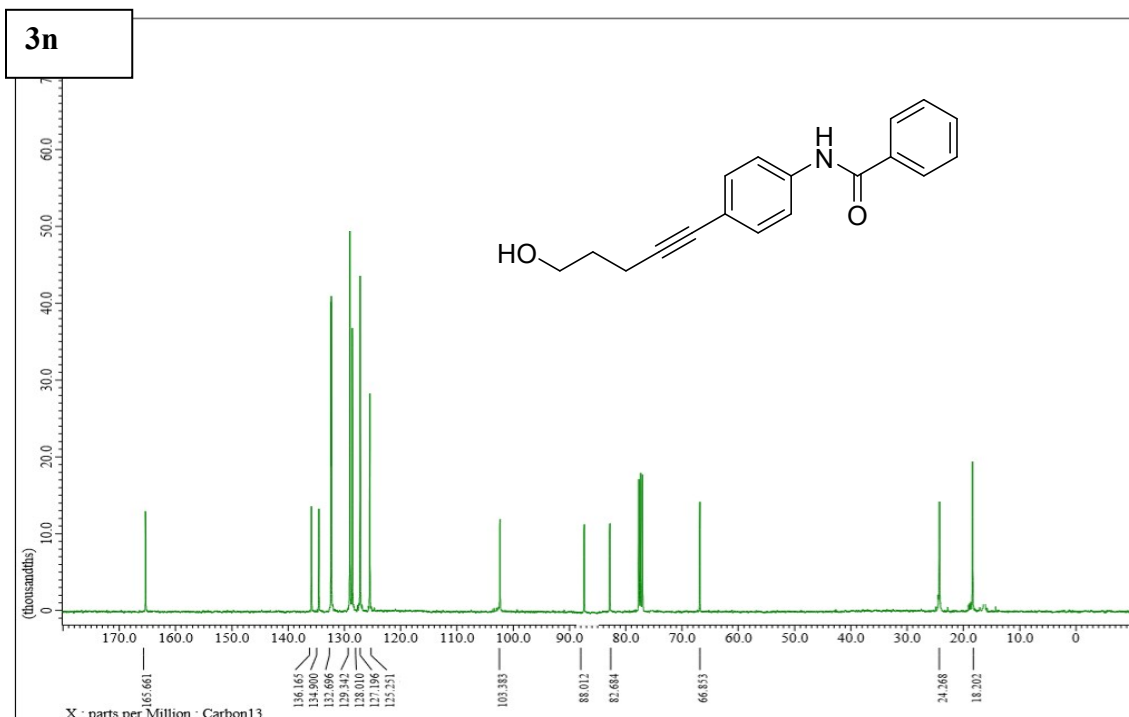
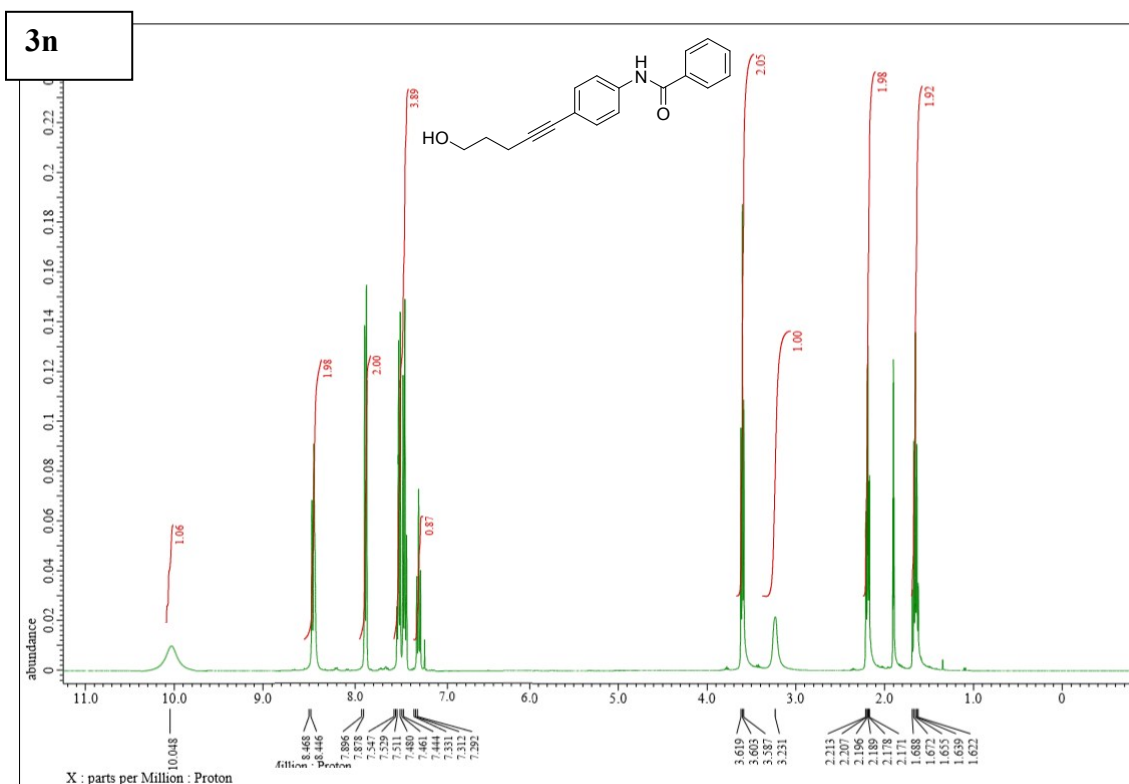
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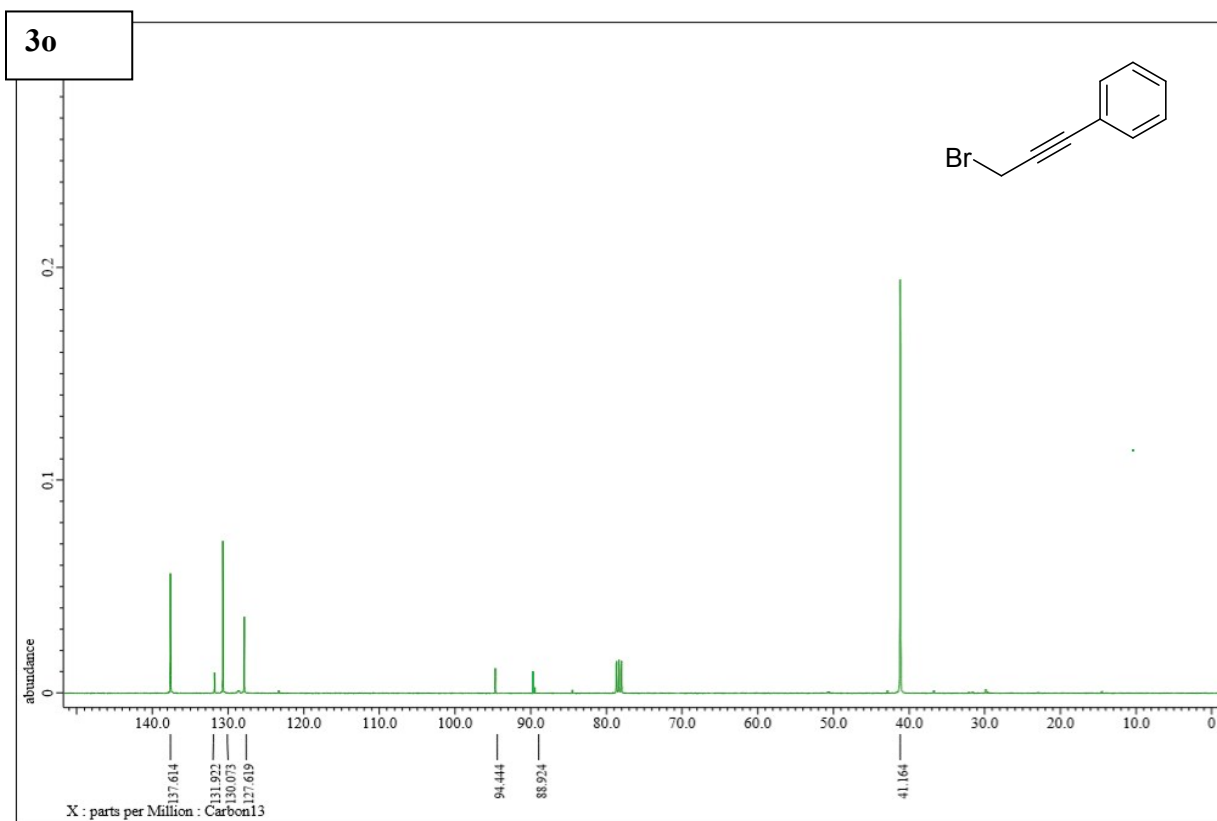
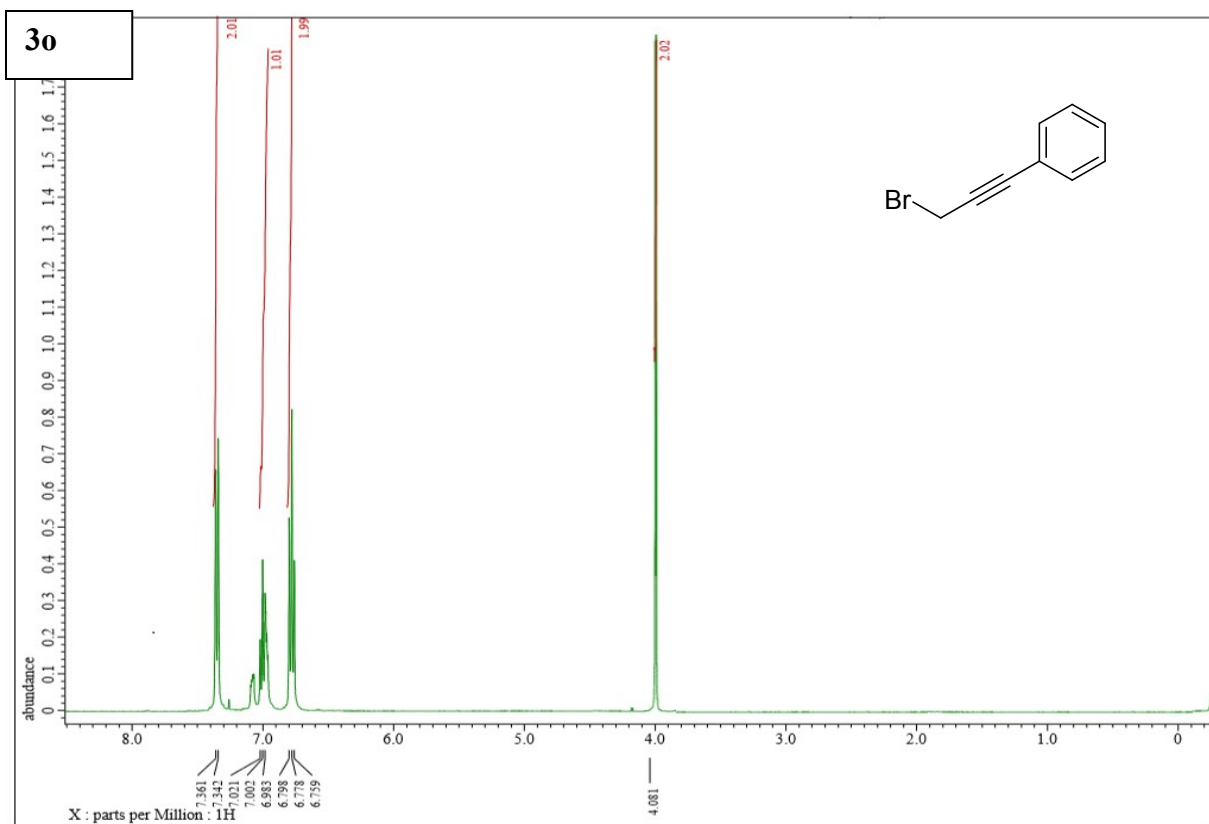


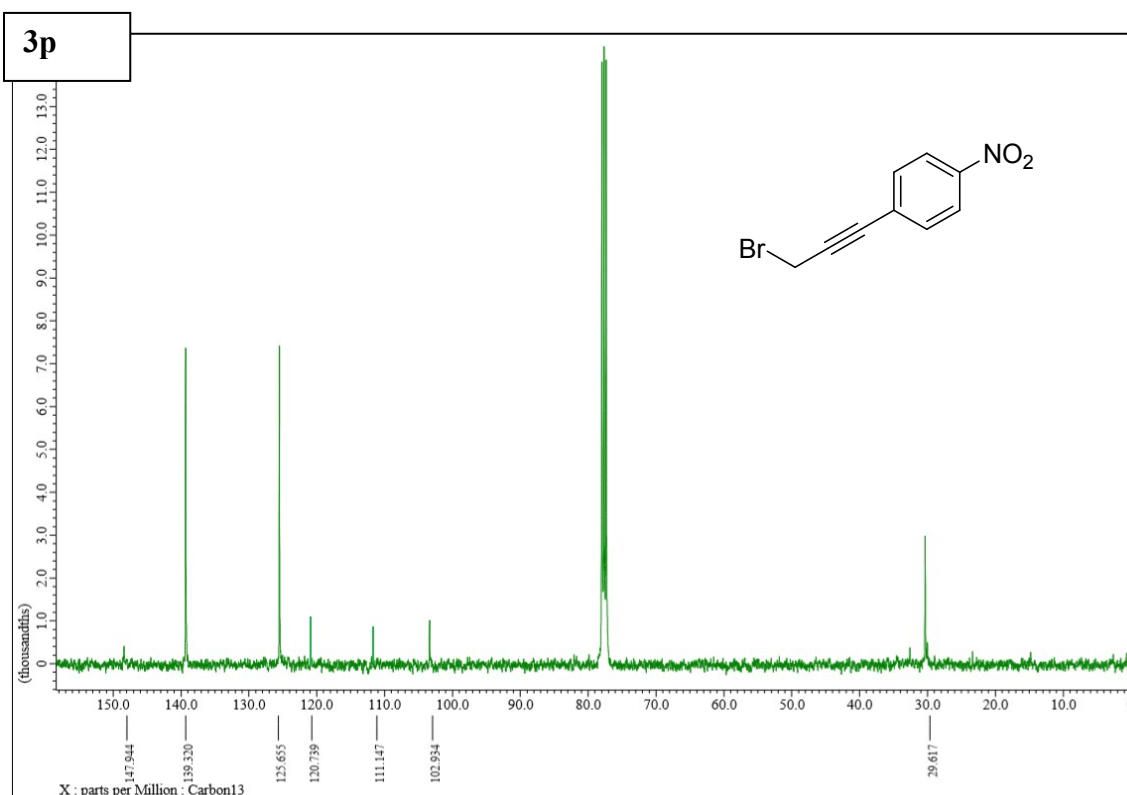
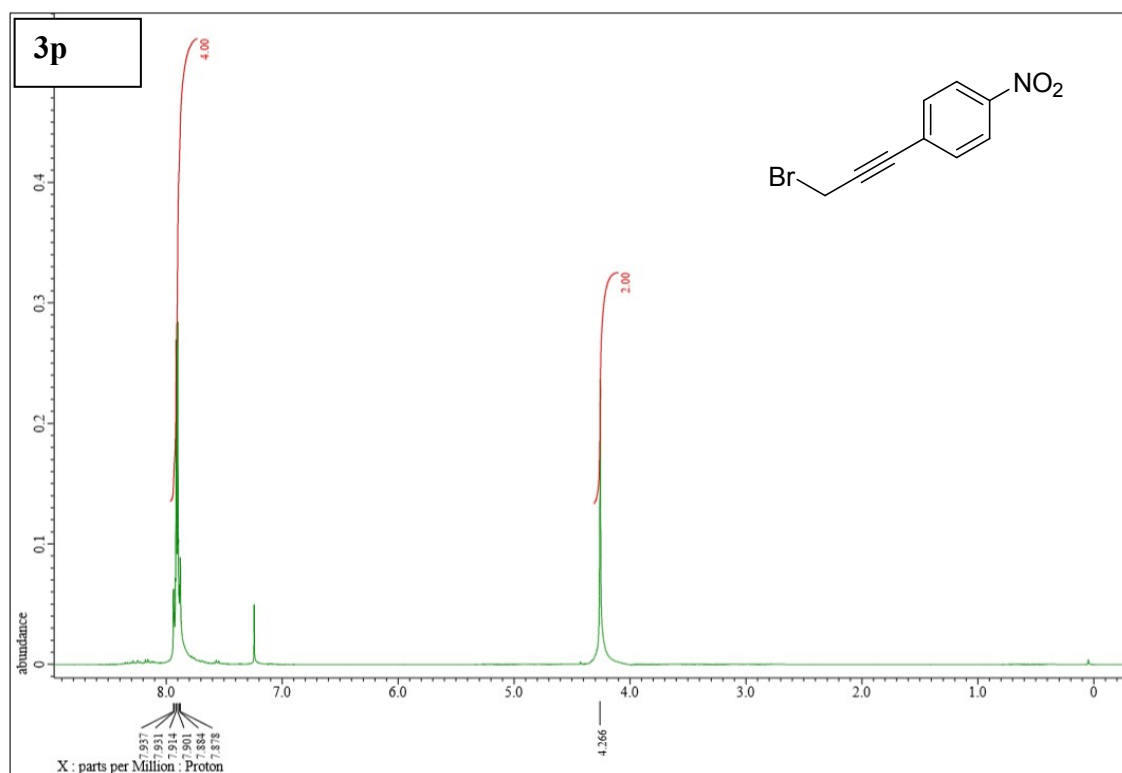
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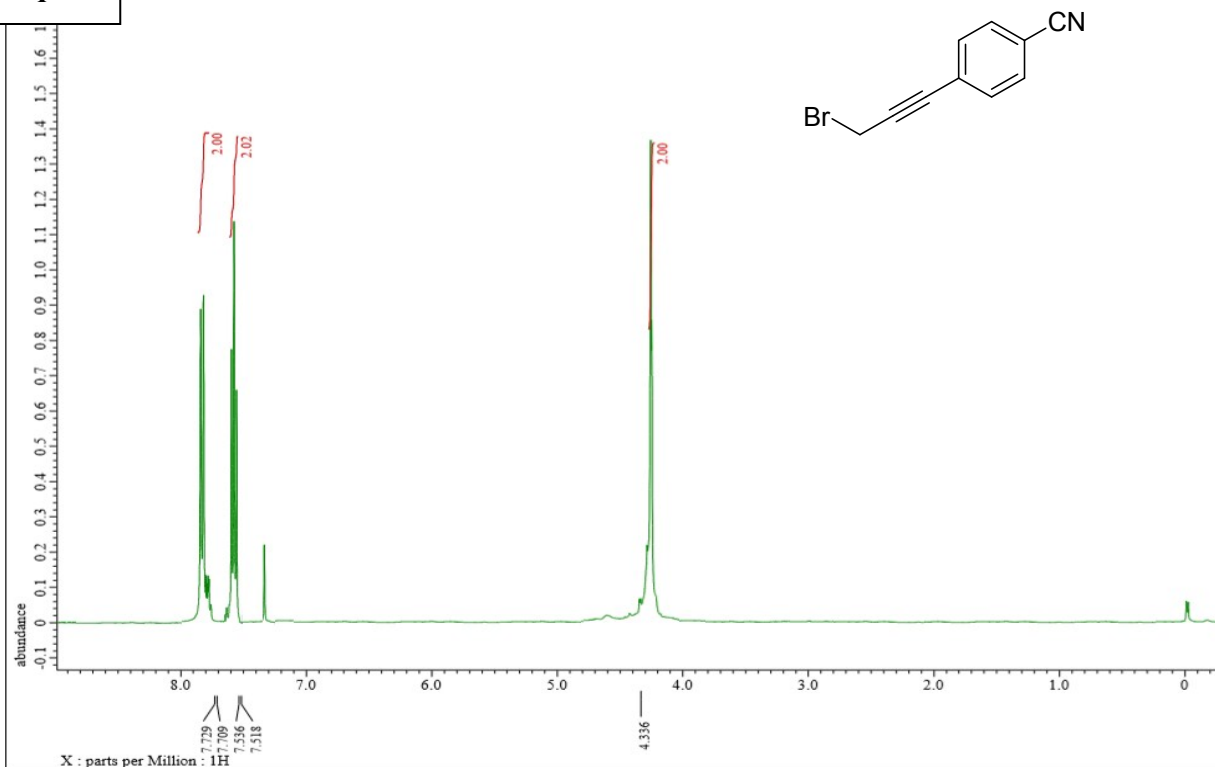




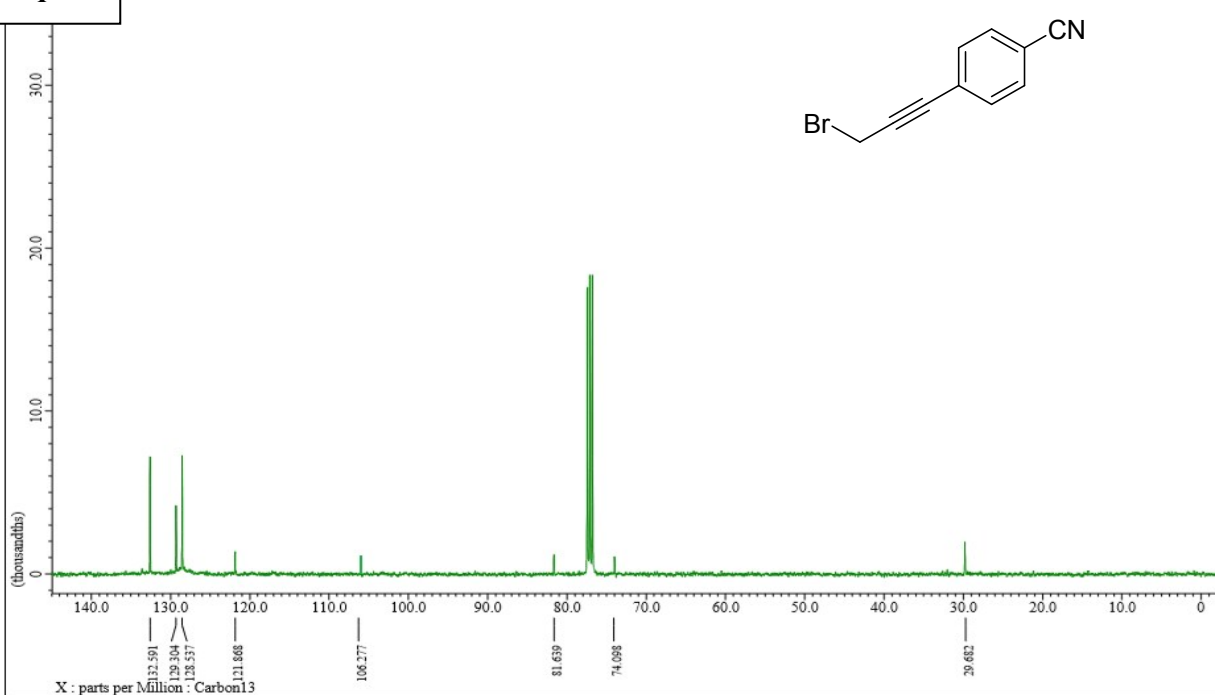


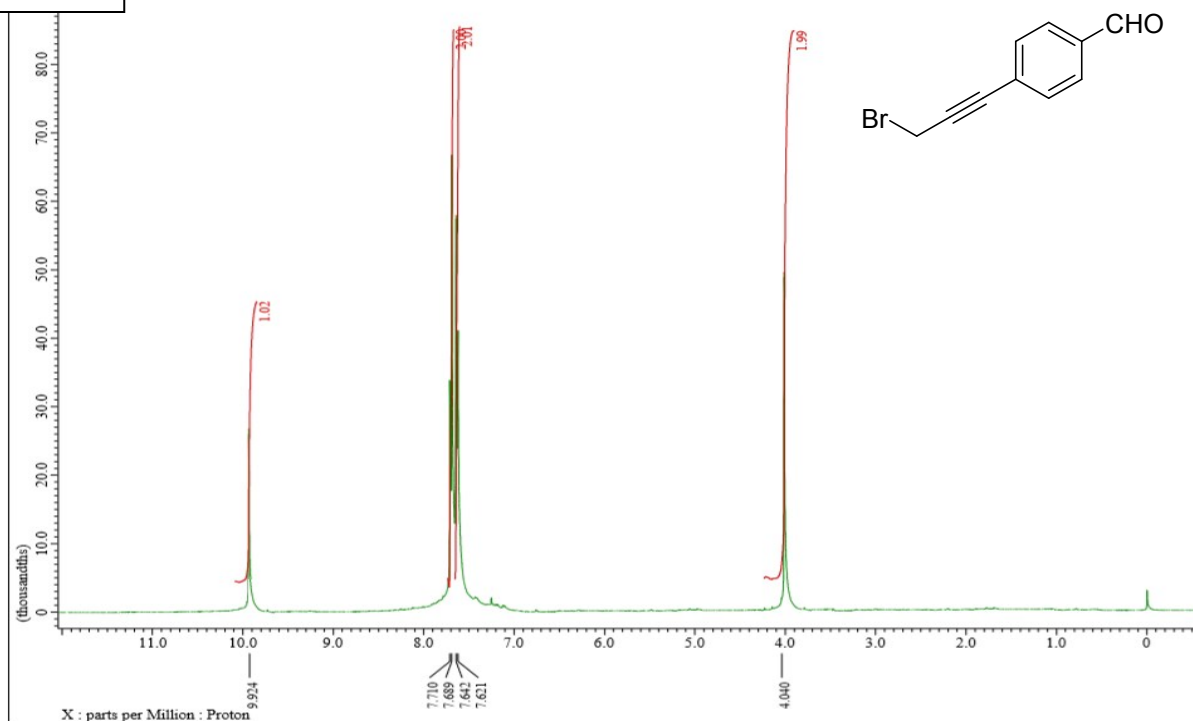
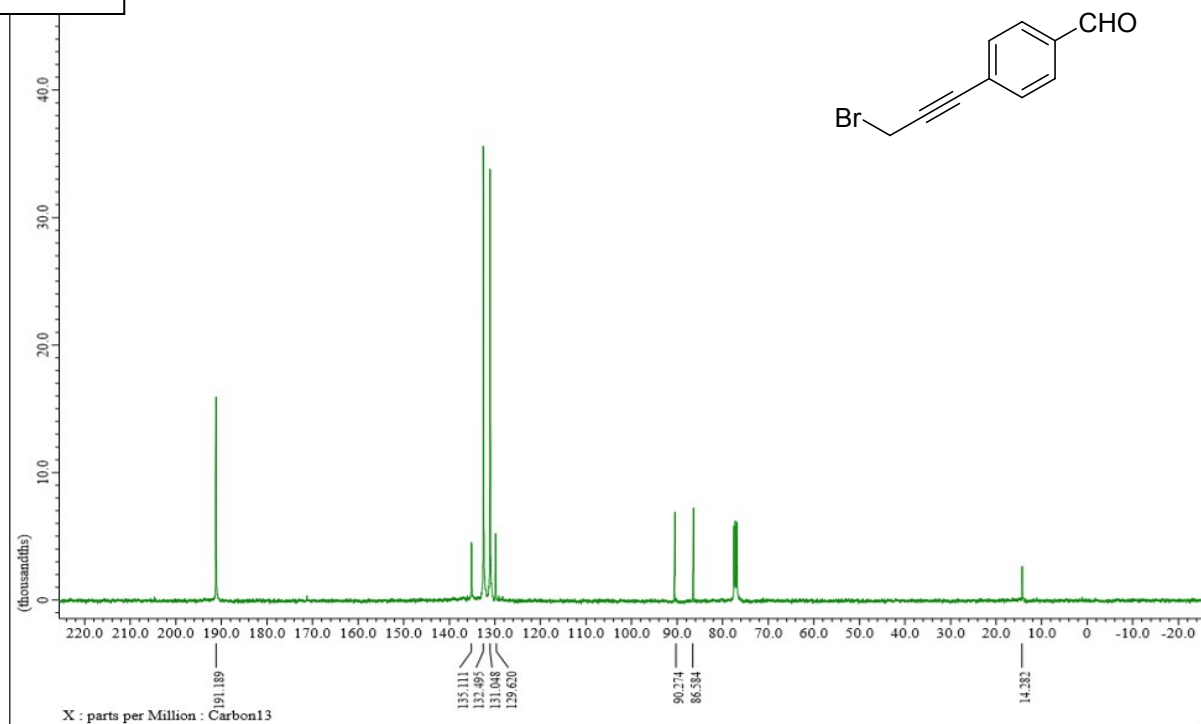


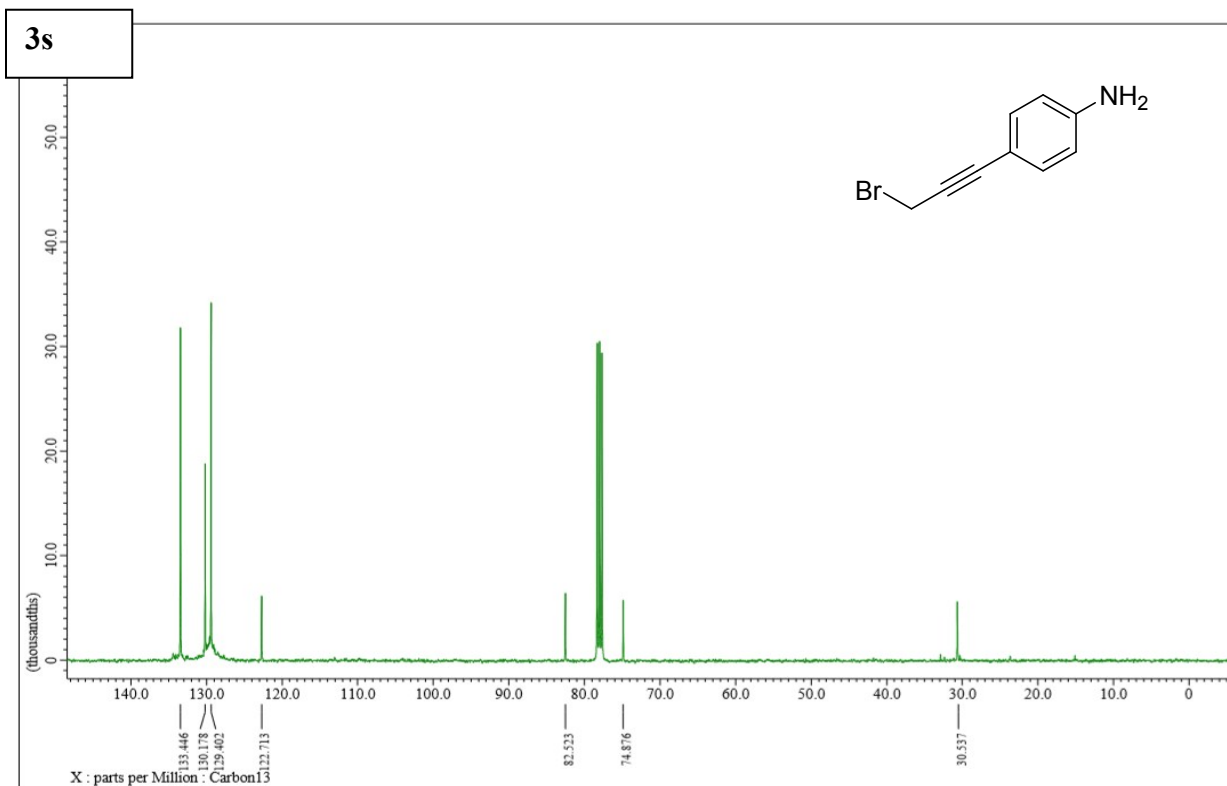
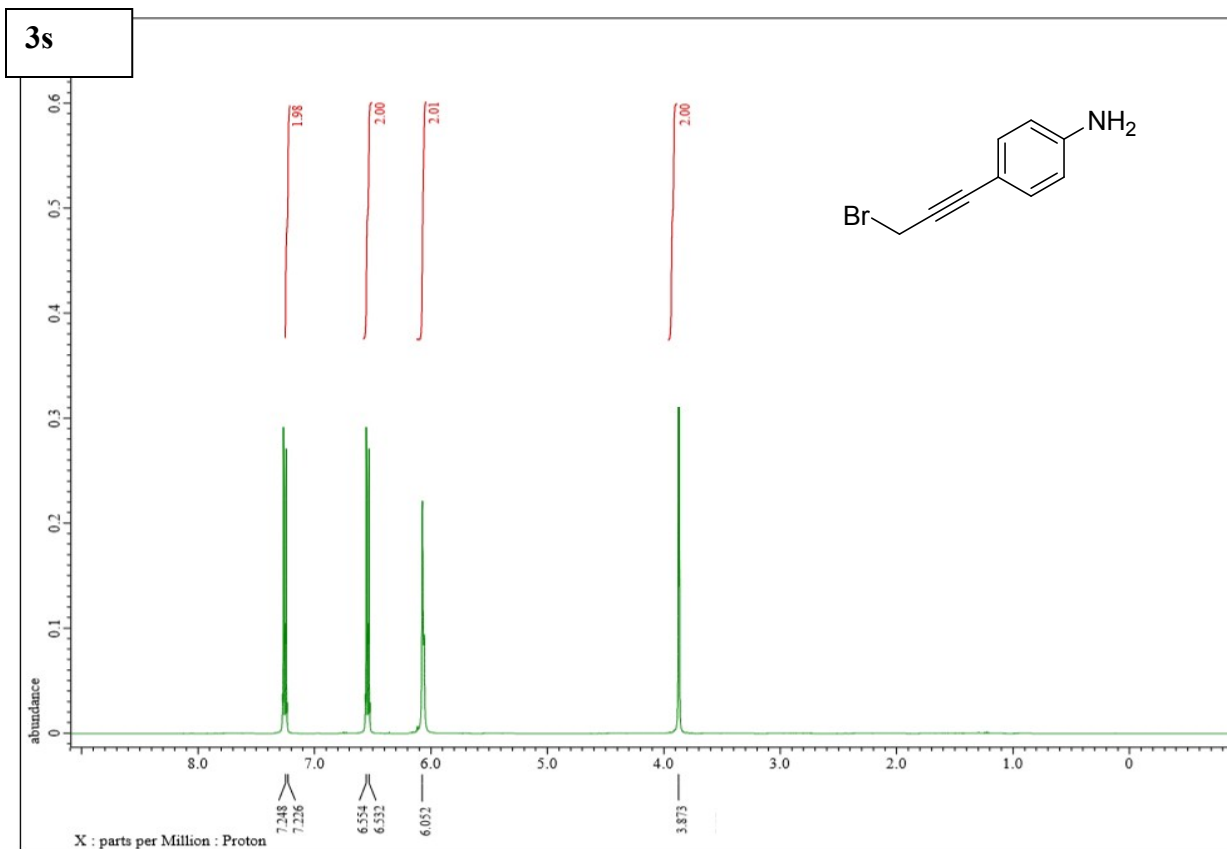
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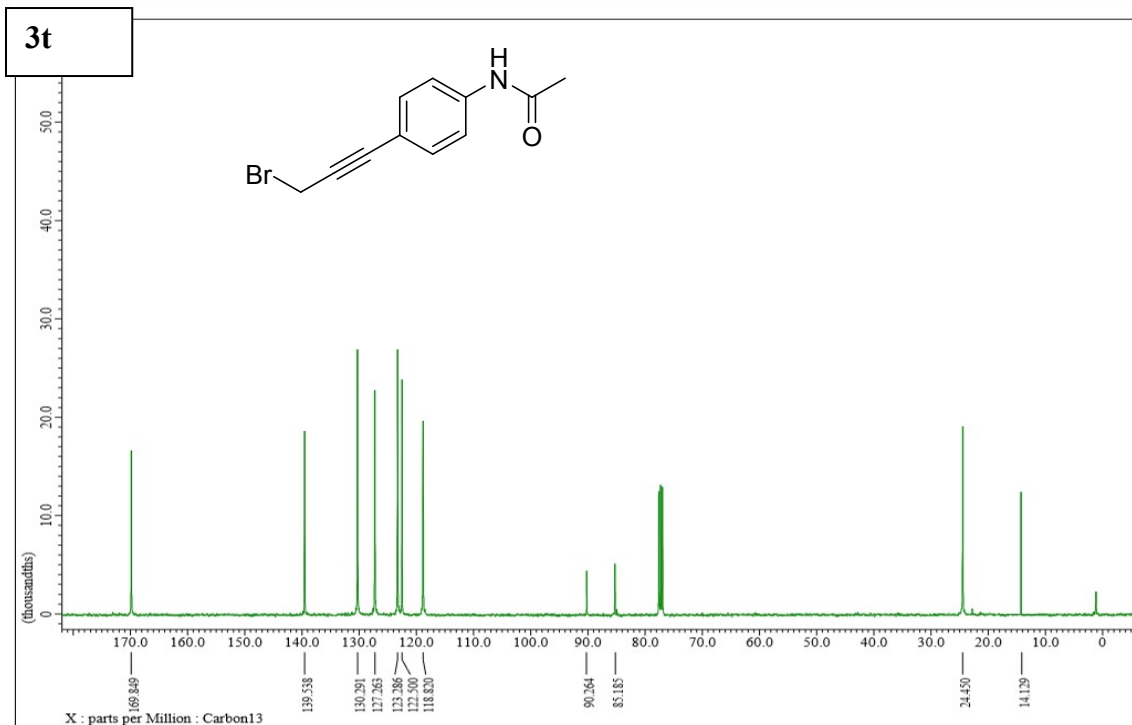
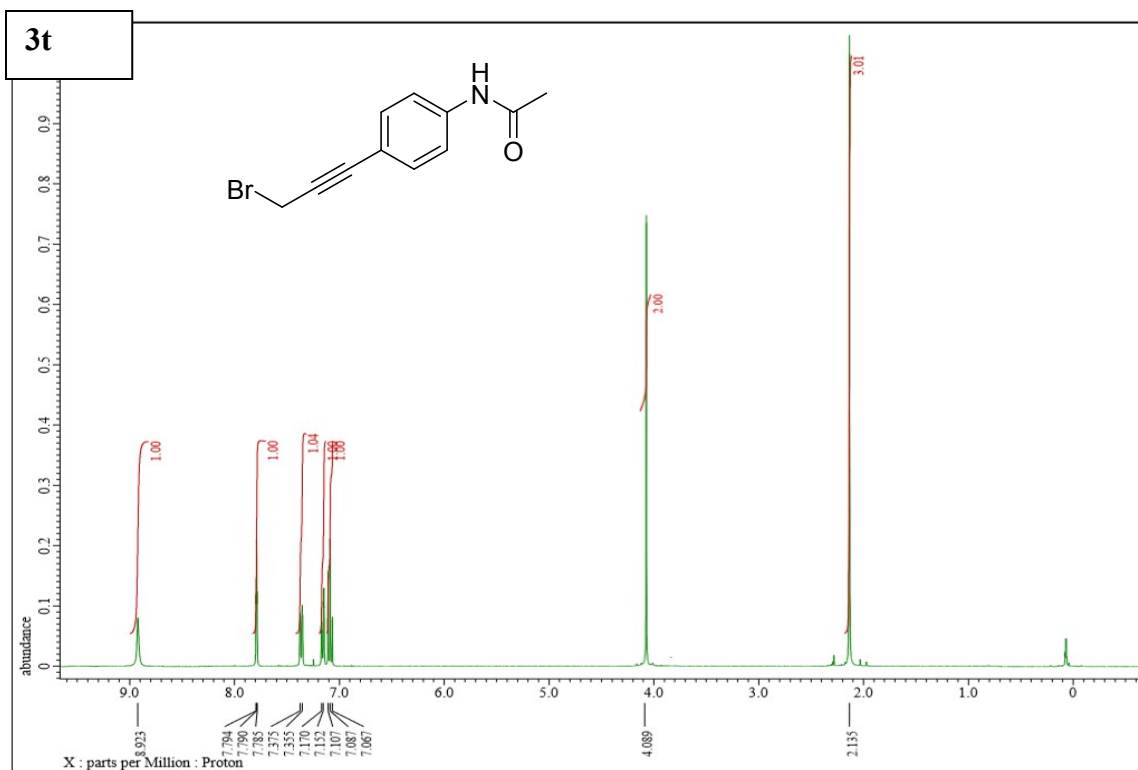


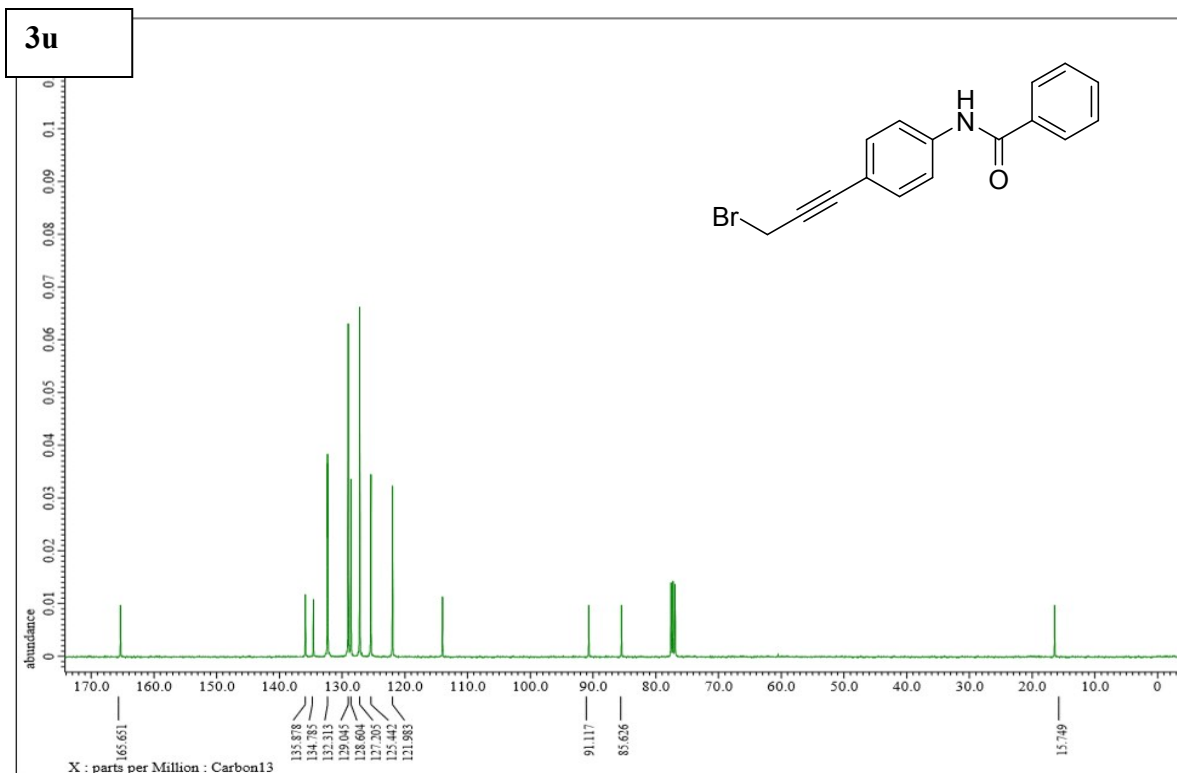
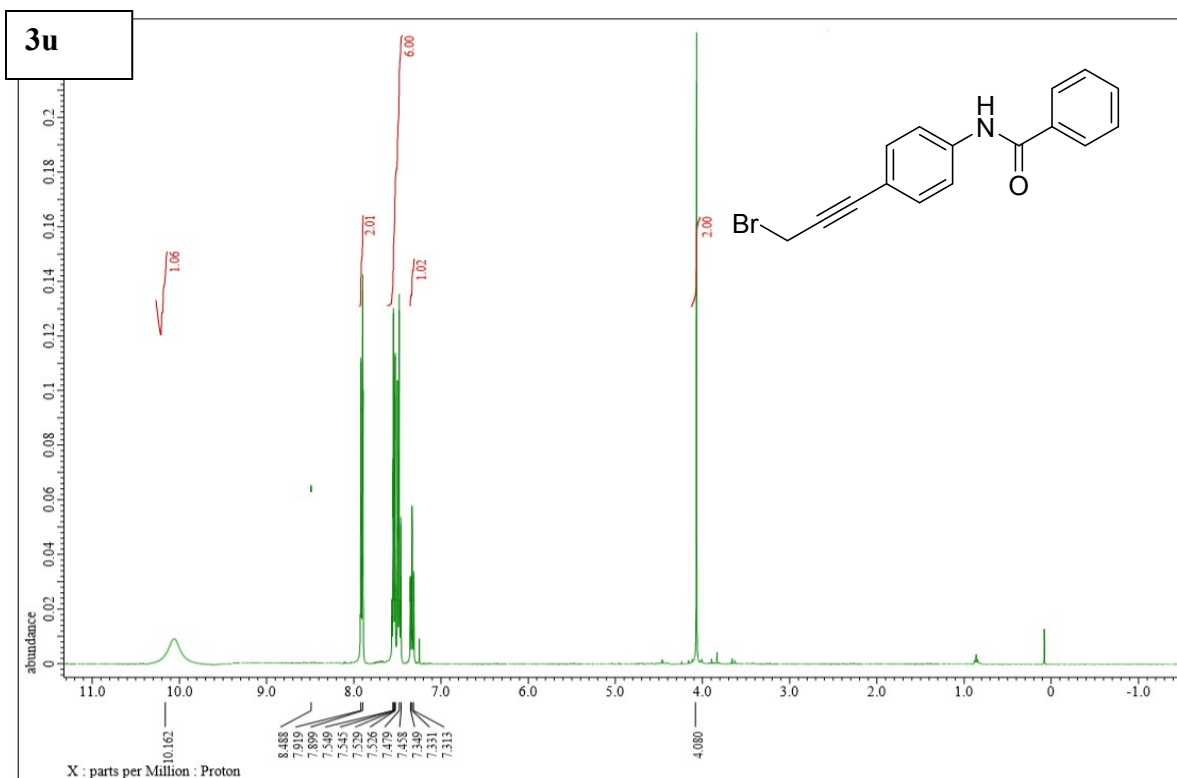
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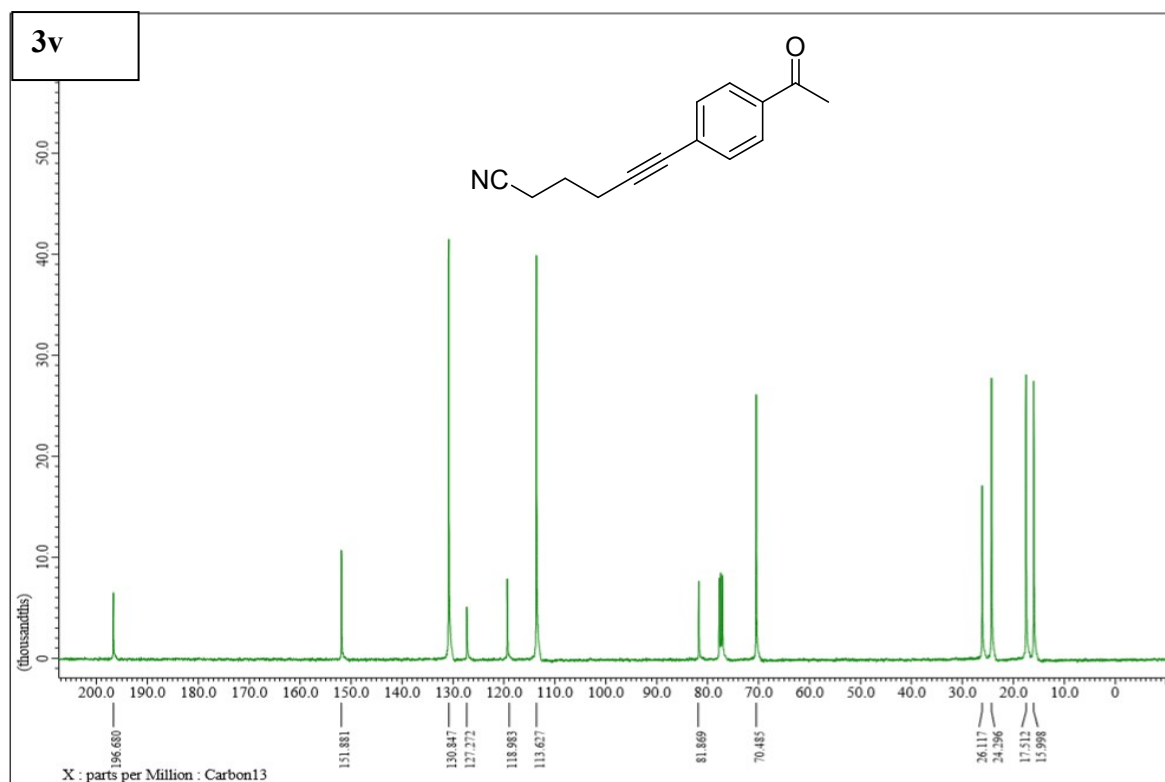
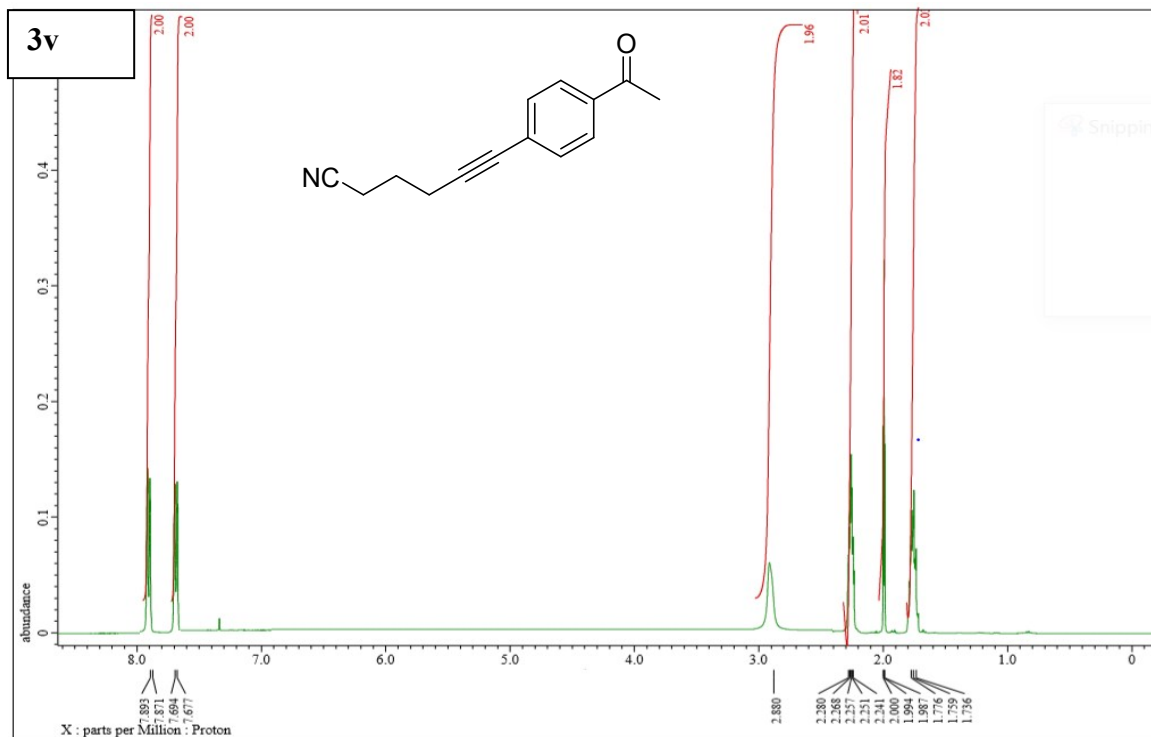


3r**3r**

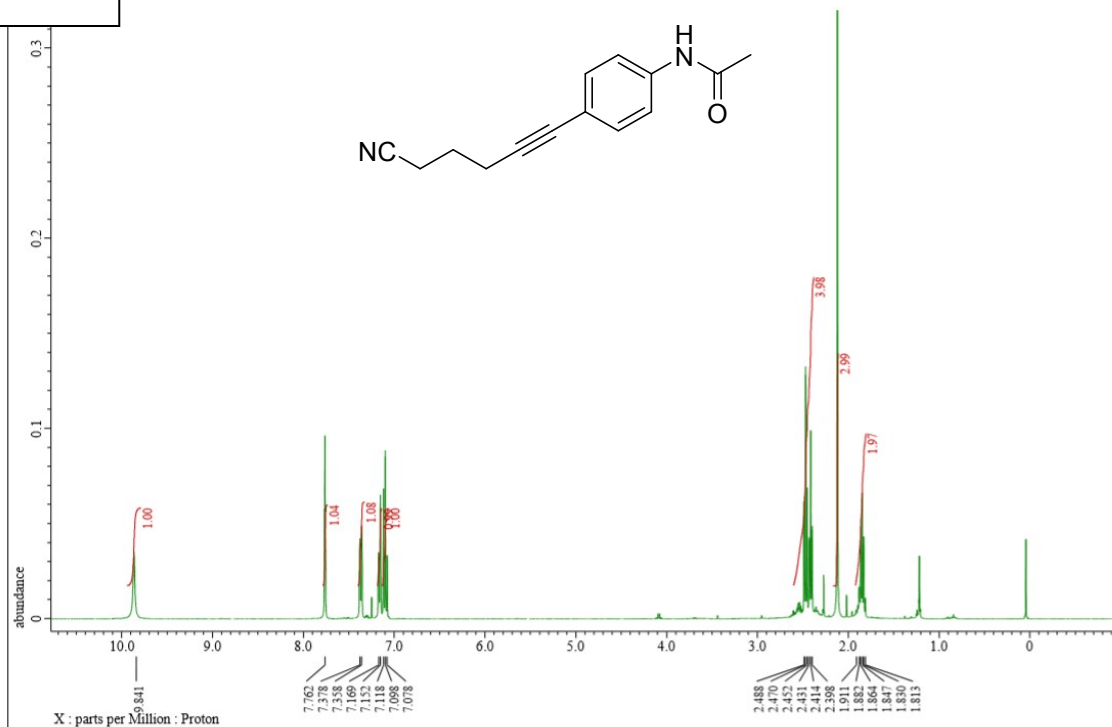








3w



3w

