

Supplementary Information

Dendrimer-encapsulated Pd (0) nanoparticles immobilized on nanosilica as a highly active and recyclable catalyst for the copper-, and phosphine free Sonogashira–Hagihara coupling reactions in water

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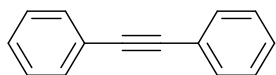
(1) Chemistry Department, College of Sciences, Shiraz University, Shiraz, Iran

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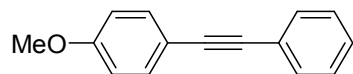
(3) Students Research Committee, School of Pharmacy, Shahid Beheshti University of Medical Sciences, Tehran, Iran

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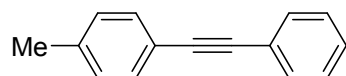
E-mail: sardarian@susc.ac.ir



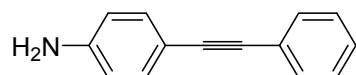
$^1\text{H-NMR}$ (250 MHz, CDCl_3) δ : 7.23-7.28 (m, 6H), 7.43-7.47 (m, 4H) ppm; $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ : 89.5, 123.3, 128.3, 129.2, 131.6 ppm; MS (m/e)= 178 [M^+]; Elemental Analysis: Calcd. C: 94.33, H: 5.67, Found. C: 94.14, H: 5.62.



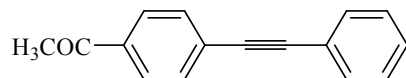
$^1\text{H-NMR}$ (250 MHz, CDCl_3) δ : 3.76 (s, 3H, CH_3), 6.79 (d, 2H, $J=8.2$ Hz, Ar-H), 7.21-7.25 (m, 3H, Ar-H), 7.37-7.44 (m, 4H, Ar-H) ppm; $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ : 55.2, 88.0, 89.4, 114.0, 115.3, 123.6, 127.9, 128.3, 131.4, 133.0, 159.6 ppm; MS (m/e)= 208 [M^+]; Elemental Analysis: Calcd. C: 86.50, H: 5.82, Found. C: 86.36, H: 5.78.



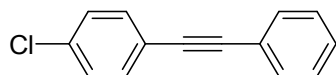
$^1\text{H-NMR}$ (CDCl_3 , 250 MHz) δ : 2.22 (s, 3H, CH_3), 7.14 (d, 2H, $J=8.4$ Hz, Ar-H), 7.19-7.42 (m, 7H, Ar-H) ppm; $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ : 21.5, 88.7, 89.6, 120.2, 123.5, 128.1, 128.3, 129.1, 131.5, 131.7, 138.4 ppm; MS (m/e)= 192 [M^+]; Elemental Analysis: Calcd. C: 93.70, H: 6.30, Found. C: 93.51, H: 6.27.



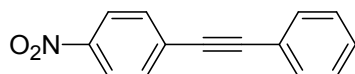
$^1\text{H-NMR}$ (CDCl_3 , 250 MHz) δ : 3.62 (s, 2H, NH_2), 6.52 (s, 2H, Ar-H), 7.22-7.40 (m, 7H, Ar-H) ppm; $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ : 87.3, 90.2, 112.5, 114.7, 123.9, 127.7, 128.3, 131.3, 132.9, 146.7 ppm.



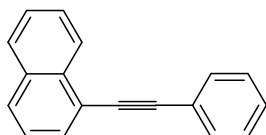
$^1\text{H-NMR}$ (250 MHz, CDCl_3) δ : 2.51 (s, 3H, CH_3), 7.16-7.33 (m, 3H, Ar-H), 7.45-7.54 (m, 4H, Ar-H), 7.86 (d, 2H, $J=7.5$ Hz, Ar-H) ppm; $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ : 27.0, 88.9, 92.9, 123.0, 128.2, 128.3, 128.8, 129.5, 132.0, 132.2, 136.5, 197.6 ppm.



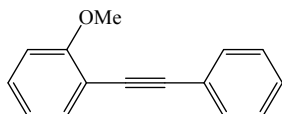
^1H NMR (250 MHz, CDCl_3) δ : 7.13-7.43 (m, 9H, Ar-H) ppm; ^{13}C NMR (62.9 MHz, CDCl_3) δ : 88.2, 90.3, 121.8, 122.9, 128.4, 128.5, 128.7, 131.6, 132.8, 134.2 ppm.



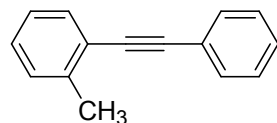
^1H -NMR (250 MHz, CDCl_3) δ : 7.37-7.41 (m, 3H, Ar-H), 7.54-7.57 (m, 2H, Ar-H), 7.68 (d, 2H, J = 12.5 Hz, Ar-H), 8.22 (d, 2H, J = 7.5 Hz, Ar-H) ppm; ^{13}C -NMR (62.9 MHz, CDCl_3) δ : 87.5, 94.7, 122.0, 123.6, 128.5, 129.2, 130.2, 131.8, 132.2, 146.9 ppm; MS (m/e)= 224 [M^+]; Elemental Analysis: Calcd. C: 75.32, H: 4.07, N: 6.27, Found. C: 75.24, H: 4.14, N: 6.20.



^1H -NMR (250 MHz, CDCl_3) δ : 7.26-7.74 (m, 11H, Ar-H), 8.36 (d, 1H, J = 8.2 Hz, Ar-H); ^{13}C -NMR (62.9 MHz, CDCl_3) δ : 87.5, 94.3, 120.9, 123.4, 125.3, 125.6, 126.2, 126.4, 126.8, 128.3, 128.42, 128.47, 128.8, 130.4, 131.7, 133.2, 133.3, 141.1 ppm; MS (m/e)= 228 [M^+]; Elemental Analysis: Calcd. C: 94.69, H: 5.31, Found. C: 94.53, H: 5.39.

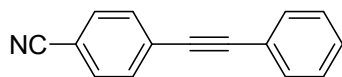


^1H NMR (250 MHz, CDCl_3) δ : 3.82 (s, 3H, CH_3), 6.87 (d, 2H, J = 7.25 Hz, Ar-H), 7.31-7.33 (m, 3H, Ar-H), 7.45-7.53 (m, 4H, Ar-H) ppm; ^{13}C NMR (CDCl_3 , 62.9 MHz): δ : 55.8, 85.6, 93.3, 110.6, 112.4, 120.4, 123.5, 128.0, 128.1, 129.7, 131.6, 133.5, 159.8 ppm.

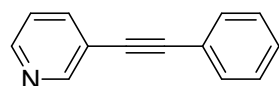


^1H NMR (250 MHz, CDCl_3) δ : 2.44 (s, 3H, CH_3), 7.14-7.46 (m, 9H, Ar-H) ppm; ^{13}C NMR (CDCl_3 , 62.9 MHz) δ : 20.7, 86.01, 94.2, 123.0, 125.5, 128.1, 128.30, 128.35, 129.4, 131.5,

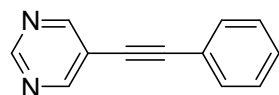
131.8, 140.1 ppm; MS (m/e)= 192 [M⁺]; Elemental Analysis: Calcd. C: 93.70, H: 6.30, Found. C: 93.91, H: 6.18.



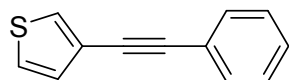
¹H-NMR (250 MHz, CDCl₃) δ: 7.28-7.31 (m, 3H, Ar-H), 7.44-7.53 (m, 6H, Ar-H) ppm; ¹³C-NMR (62.9 MHz, CDCl₃) δ: 87.7, 93.7, 111.4, 118.5, 122.2, 128.2, 128.5, 129.1, 131.7, 132.03, 132.06 ppm; MS (m/e)= 203 [M⁺]; Elemental Analysis: Calcd. C: 88.64, H: 4.47, N: 6.89, Found. C: 88.53, H: 4.34, N: 6.72.



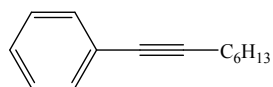
¹H-NMR (250 MHz, CDCl₃) δ: 7.26-7.29 (m, 4H, Ar-H), 7.44-7.47 (m, 2H, Ar-H), 7.70 (m, 1H, Ar-H), 8.45 (m, 1H, Ar-H), 8.68 (s, 1H, Ar-H) ppm; ¹³C-NMR (62.9 MHz, CDCl₃) δ: 85.9, 92.7, 120.5, 122.4, 123.0, 128.4, 128.8, 131.6, 138.4, 148.4, 152.1 ppm; MS (m/e)= 179 [M⁺]; Elemental Analysis: Calcd. C: 87.12, H: 5.07, N: 7.81, Found. C: 87.23, H: 4.92, N: 7.79.



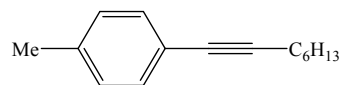
¹H-NMR (250 MHz, CDCl₃) δ: 7.29-7.48 (m, 5H, Ar-H), 8.77 (s, 2H, Ar-H), 9.06 (s, 1H, Ar-H) ppm; ¹³C-NMR (62.9 MHz, CDCl₃) δ: 82.3, 96.3, 119.9, 121.7, 128.5, 128.7, 129.1, 129.3, 131.7, 139.3, 156.6, 158.5 ppm; MS (m/e)= 180 [M⁺]; Elemental Analysis: Calcd. C: 79.98, H: 4.48, N: 15.54, Found. C: 79.90, H: 4.59, N: 15.51.



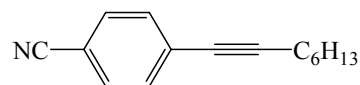
¹H-NMR (250 MHz, CDCl₃) δ: 7.31-7.42 (m, 5H, Ar-H), 7.59-7.64 (m, 3H, Ar-H) ppm; ¹³C-NMR (62.9 MHz, CDCl₃) δ: 84.7, 89.1, 123.3, 125.5, 127.2, 128.5, 128.7, 129.3, 129.9, 131.7, 132.6 ppm; MS (m/e)= 184 [M⁺]; Elemental Analysis: Calcd. C: 78.22, H: 4.39, Found. C: 78.09, H: 4.48.



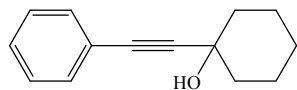
$^1\text{H-NMR}$ (250 MHz, CDCl_3) δ : 0.83 (t, 3H, $J = 7.0$ Hz, CH_3), 1.20-1.55 (m, 8H, CH_2), 2.31 (t, 2H, $J = 7.0$ Hz, CH_2), 7.15-7.21 (m, 3H, Ar-H), 7.28-7.33 (m, 2H, Ar-H) ppm;; $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ : 14.0, 19.3, 22.5, 28.5, 28.7, 31.3, 80.5, 90.4, 124.0, 127.4, 128.1, 131.5 ppm.



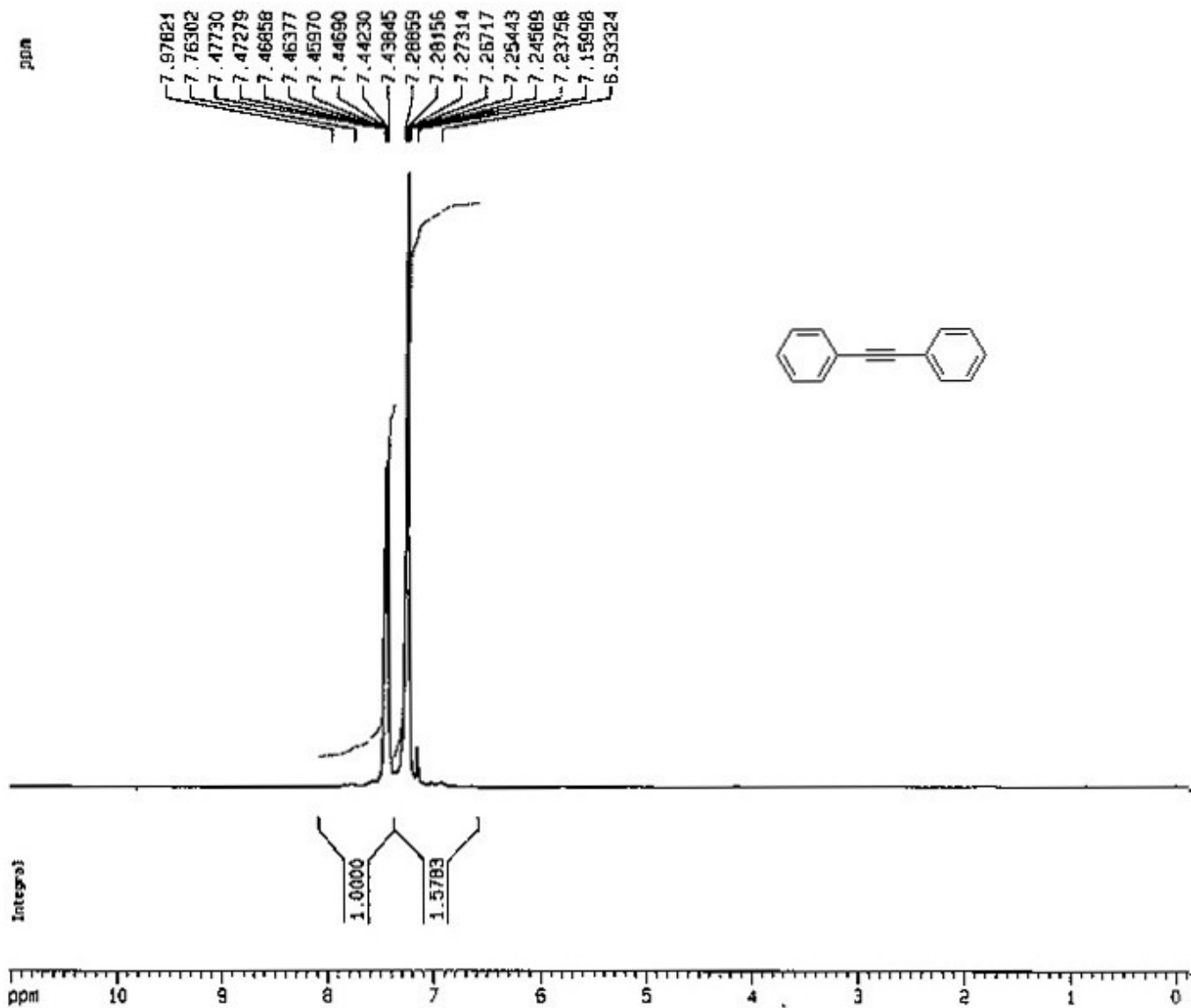
$^1\text{H-NMR}$ (250 MHz, CDCl_3) δ : 0.93 (t, 3H, $J = 7.0$ Hz, $-\text{CH}_2\text{CH}_3$), 1.31-1.65 (m, 8H, $-\text{CH}_2$), 2.35 (s, 3H, CH_3), 2.41 (t, 2H, $J = 7.0$ Hz, CH_2), 7.10 (d, 2H, $J = 8.5$ Hz, Ar-H), 7.31 (d, 2H, $J = 8.0$ Hz, Ar-H) ppm; $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ : 14.0, 19.4, 21.3, 22.5, 28.6, 28.7, 31.3, 80.5, 89.5, 121.0, 128.8, 131.3, 137.3 ppm.

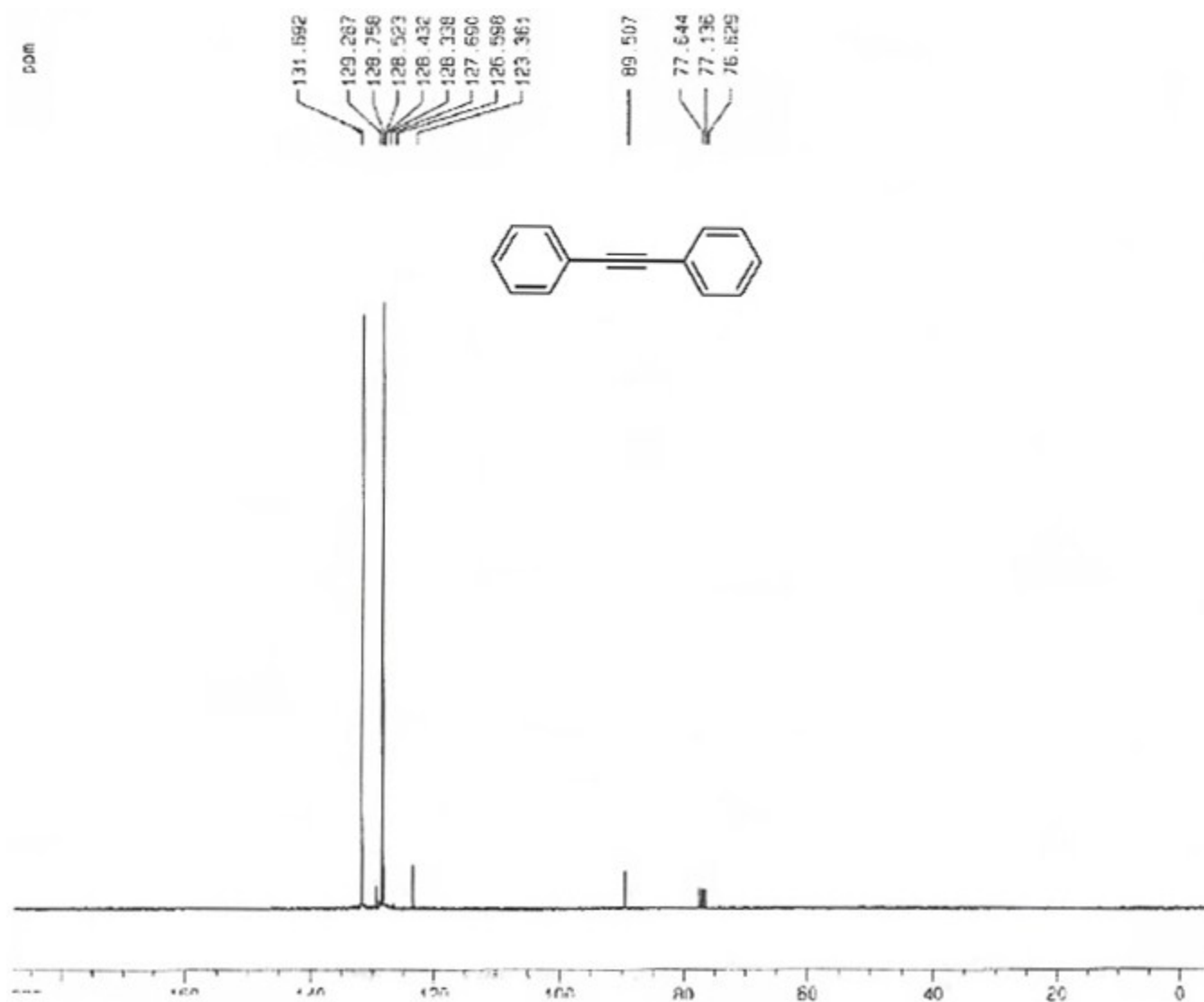


$^1\text{H-NMR}$ (250 MHz, CDCl_3) δ : 0.89 (t, 3H, $J = 7.0$ Hz, $-\text{CH}_2\text{CH}_3$), 1.24-1.63 (m, 8H, $-\text{CH}_2$), 2.41 (t, 2H, $J = 7.0$ Hz, CH_2), 7.42 (d, 2H, $J = 8.75$ Hz, Ar-H), 7.56 (d, 2H, $J = 8.75$ Hz, Ar-H) ppm.



$^1\text{H-NMR}$ (250 MHz, CDCl_3) δ : 1.27-1.29 (s, 1H, OH), 1.55-1.77 (m, 7H, $-\text{CH}_2$), 1.98-2.04 (m, 2H, $-\text{CH}_2$), 2.27 (s, 1H, CH_2), 7.26-7.31 (m, 3H, Ar-H), 7.40-7.45 (m, 2H, Ar-H) ppm.

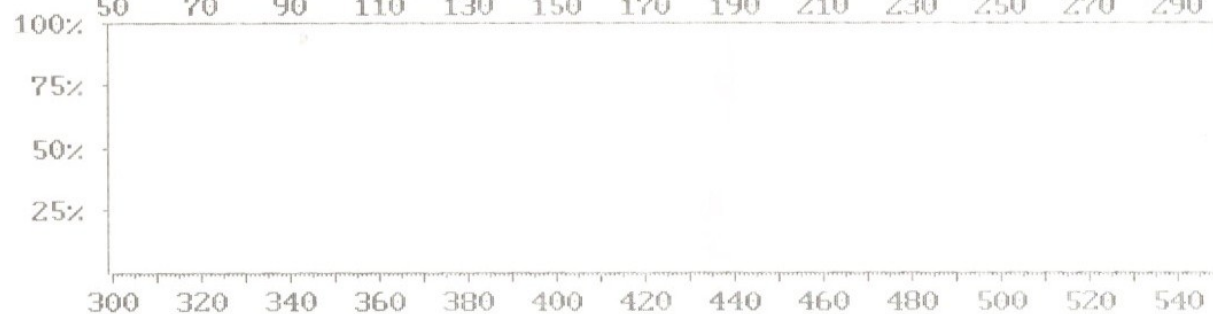
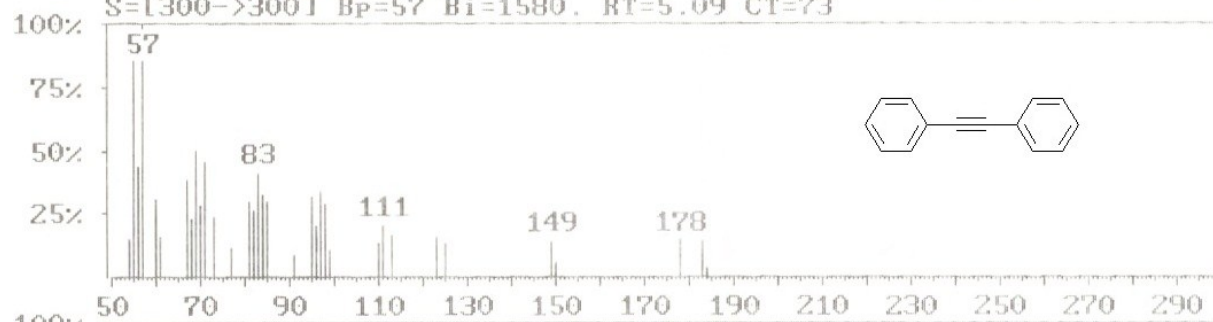




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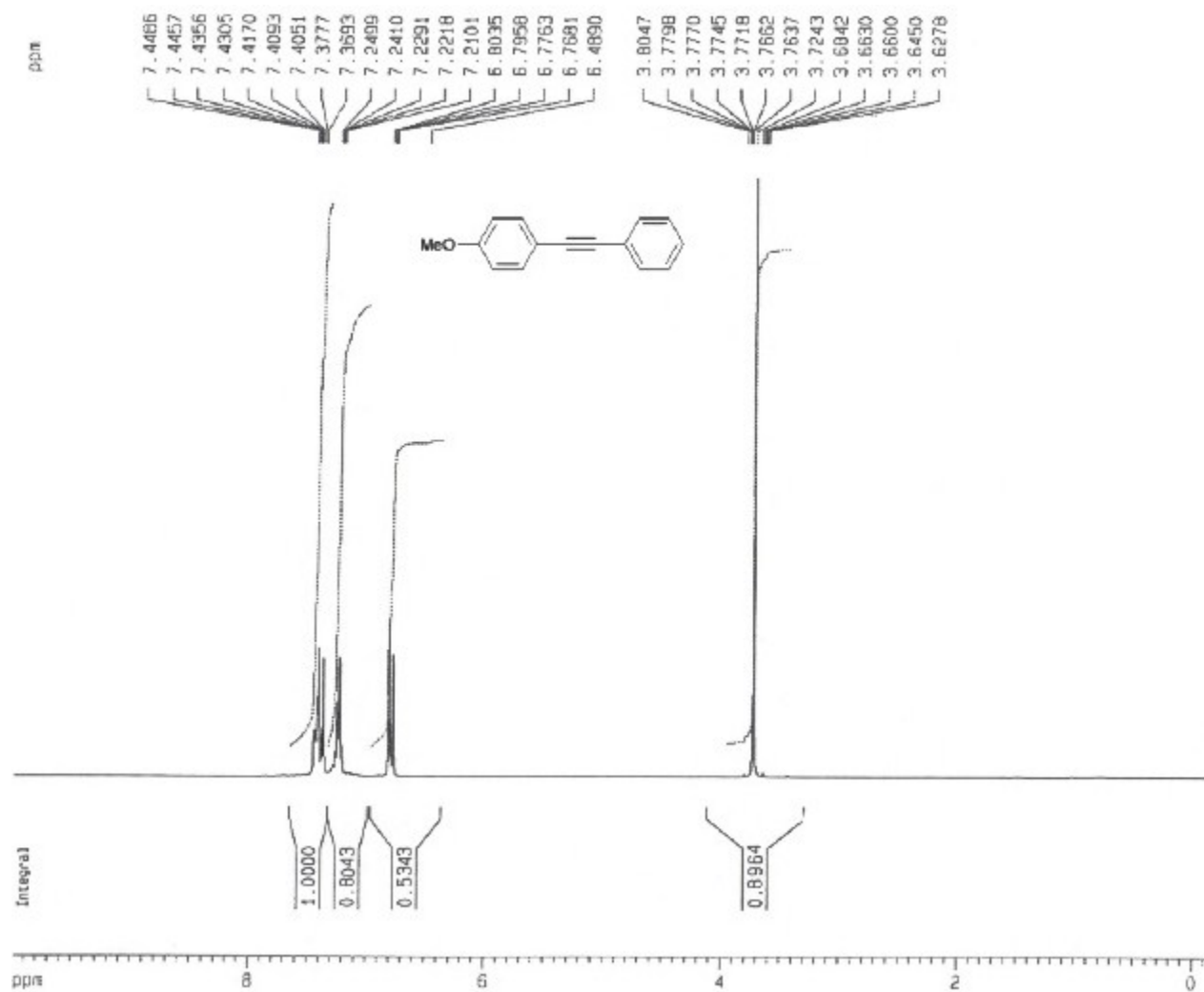
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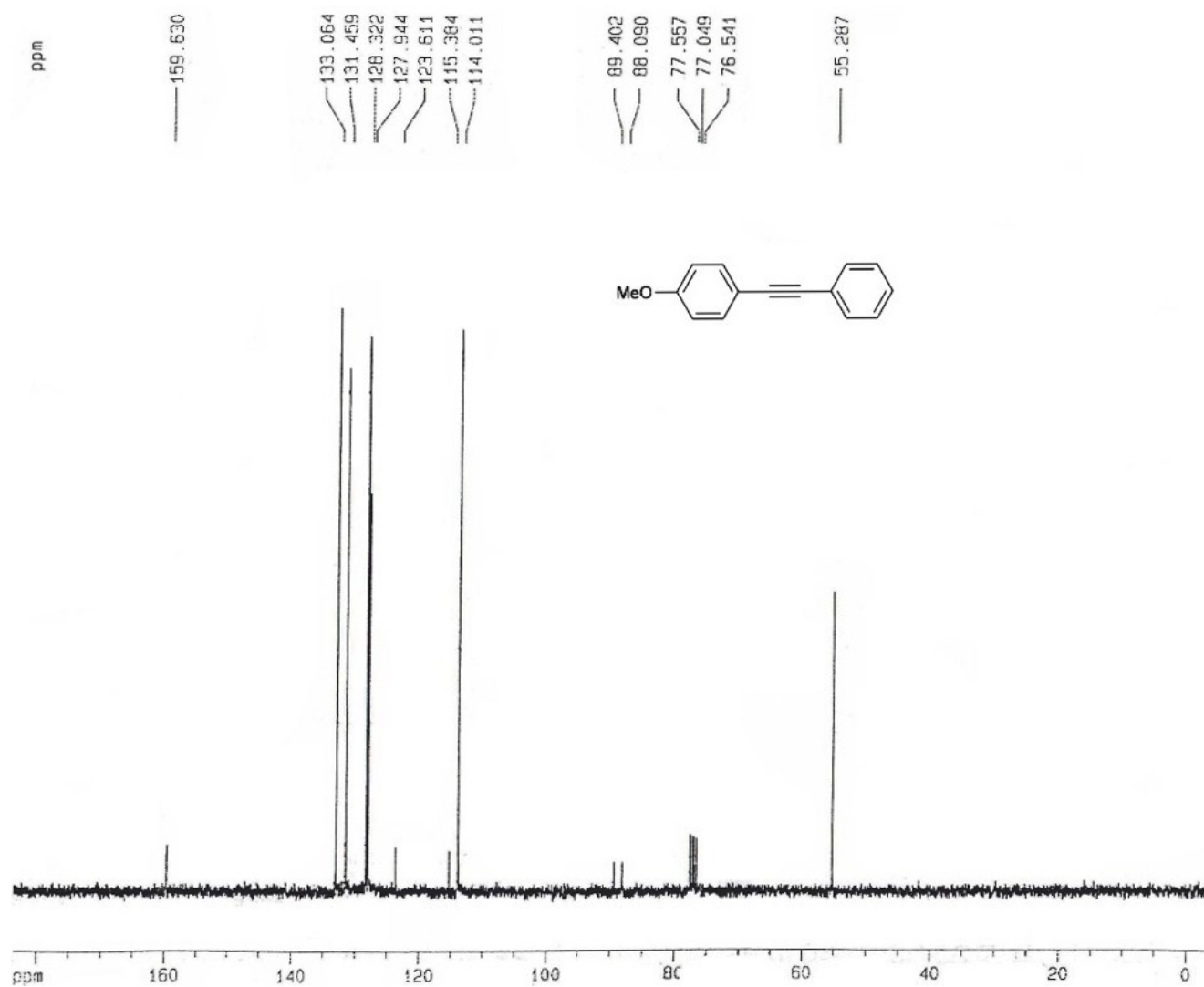
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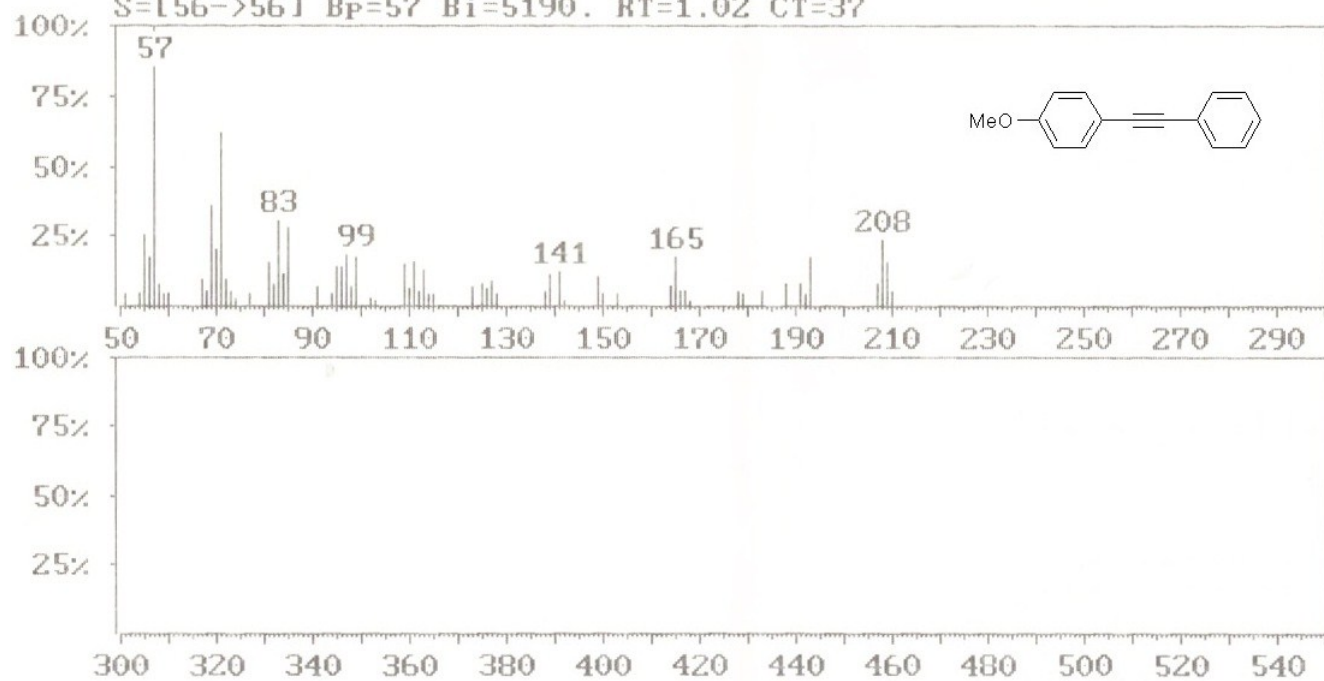




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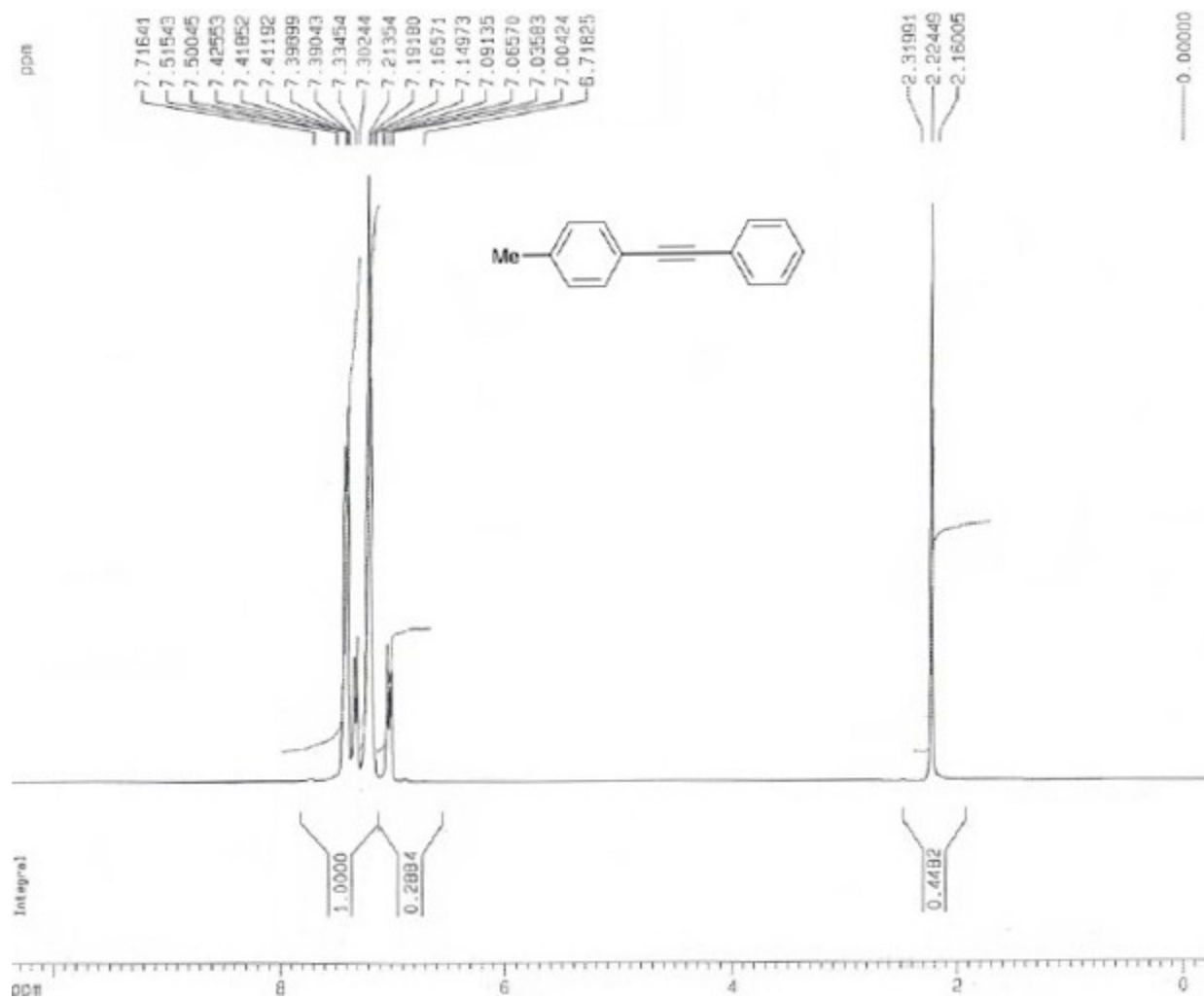
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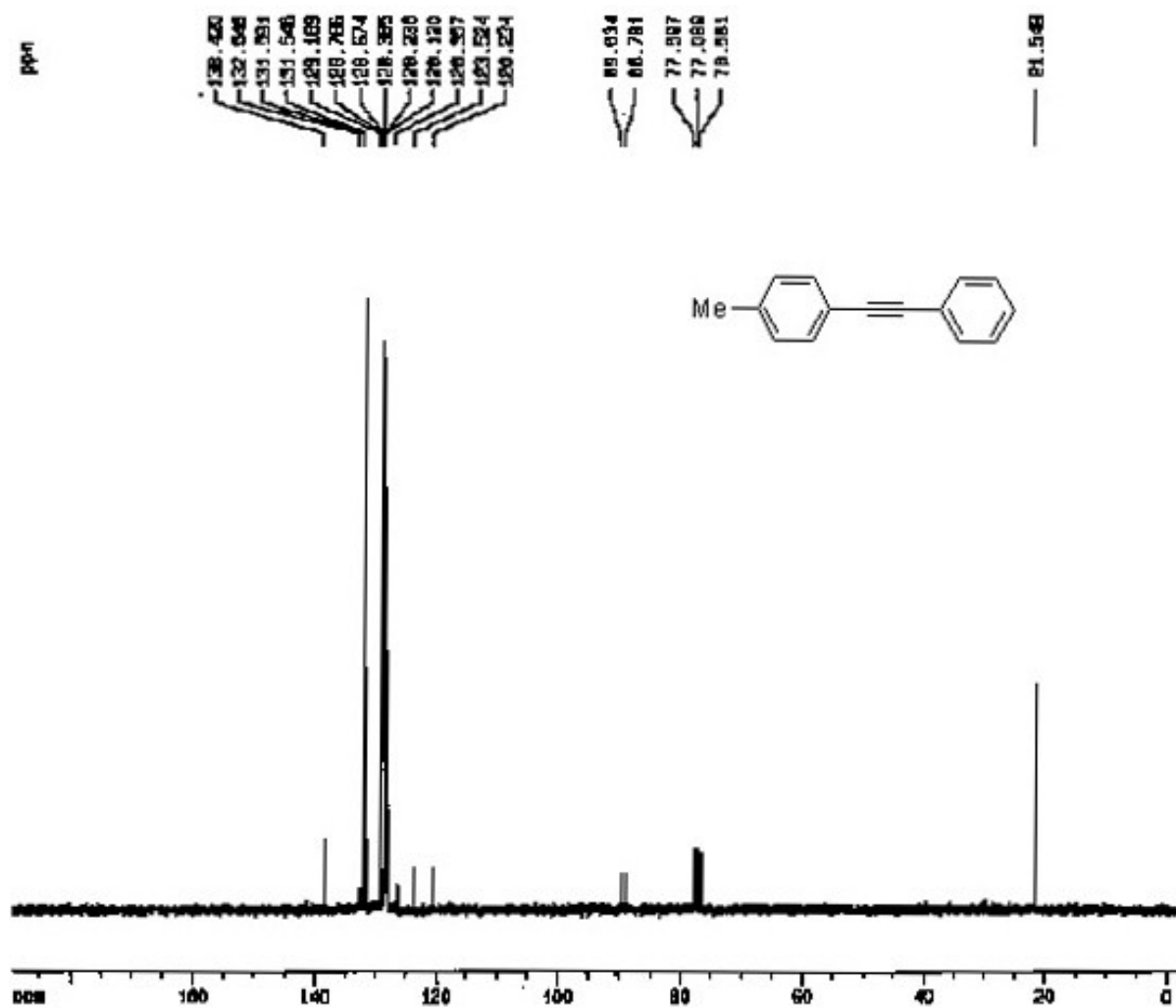
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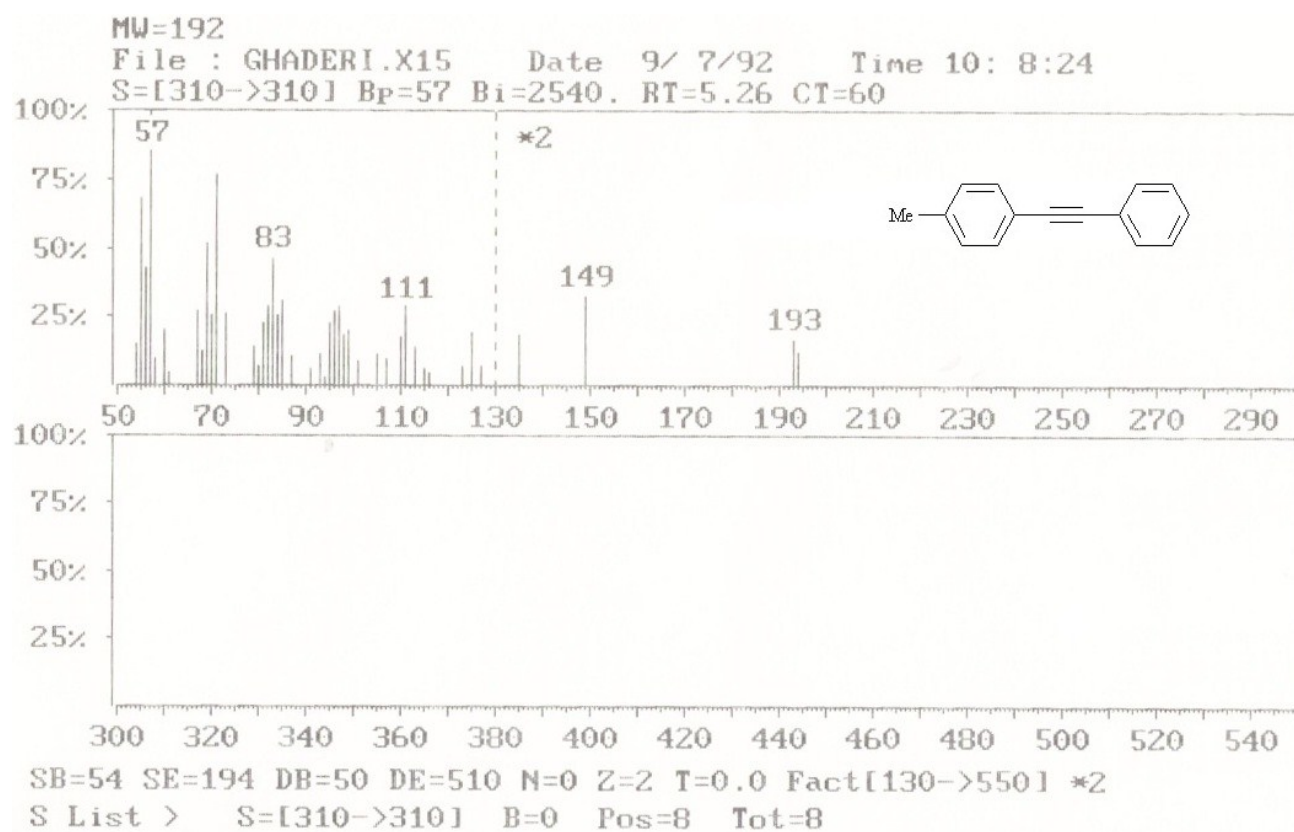


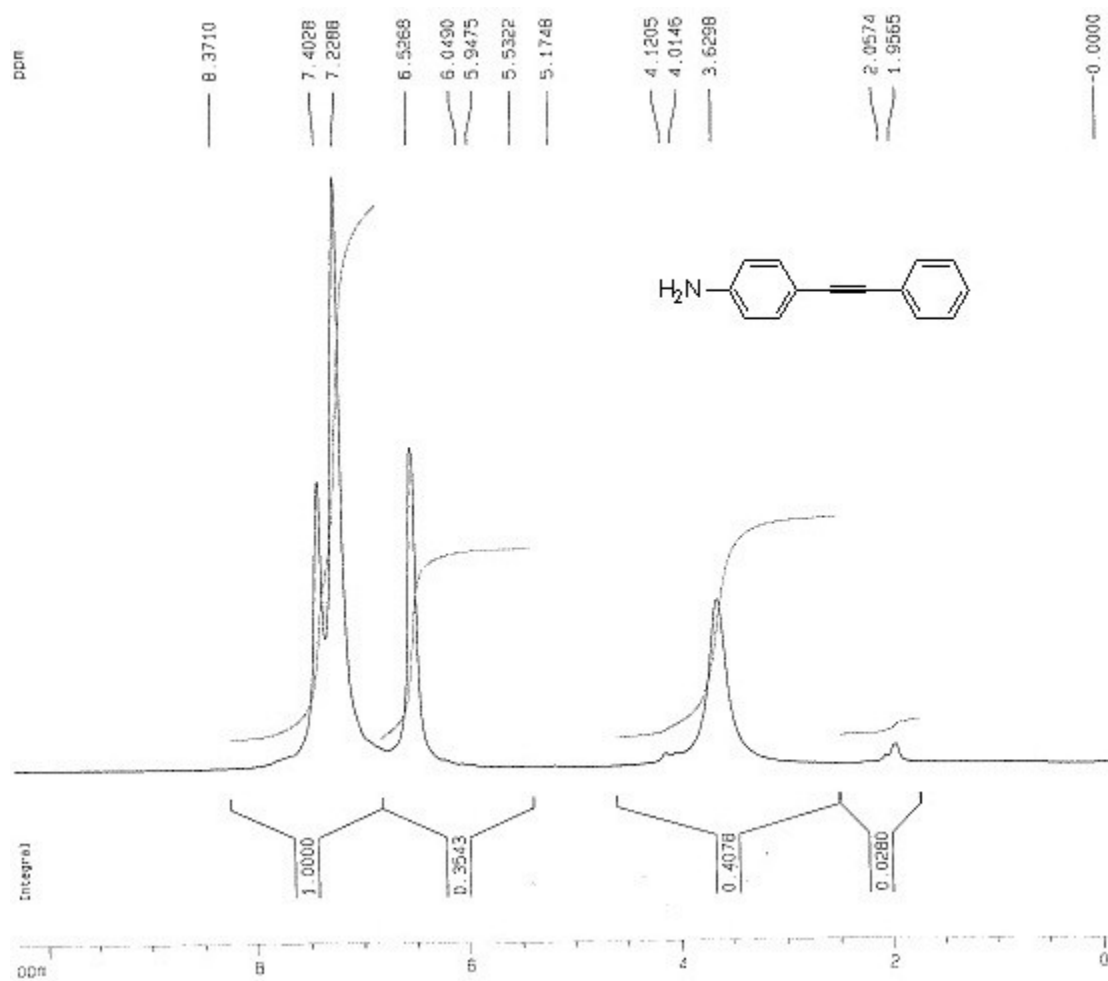
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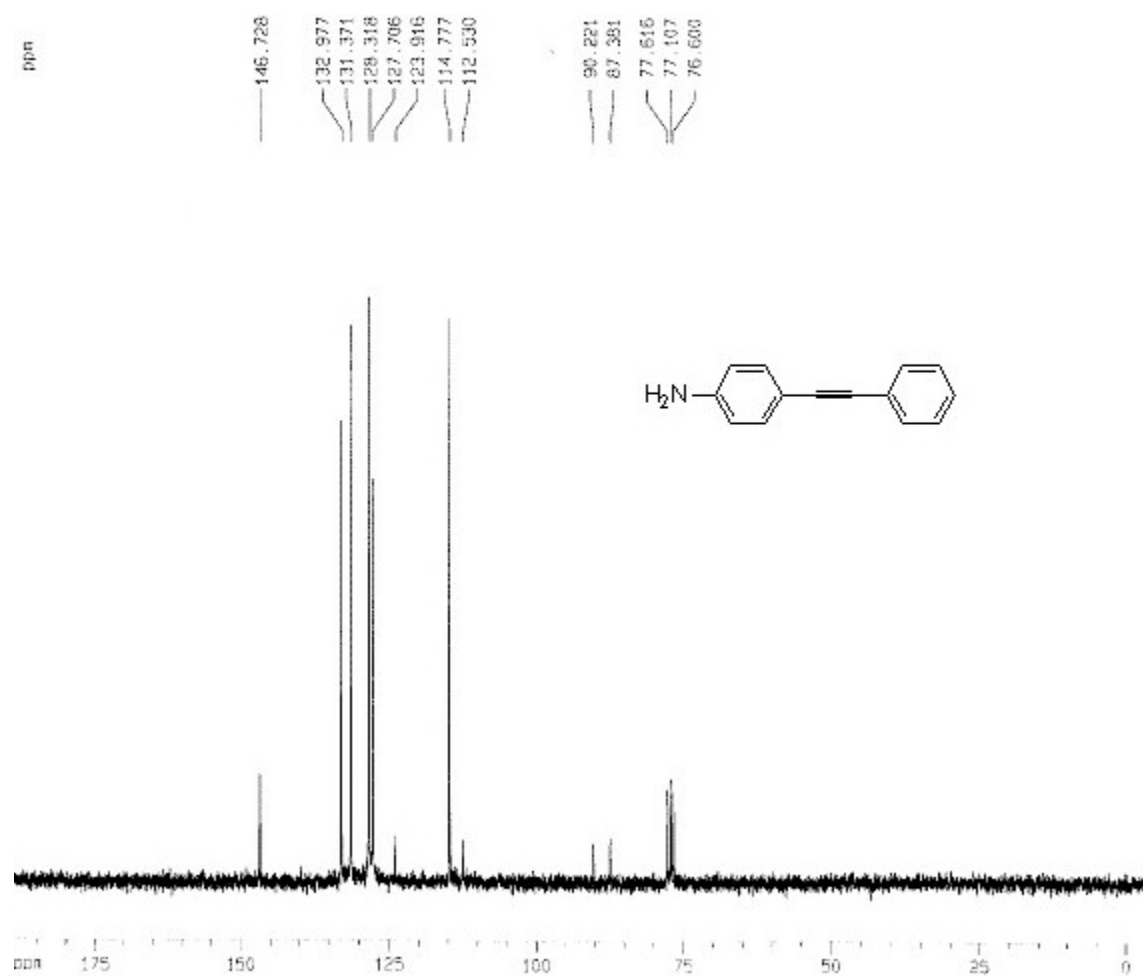
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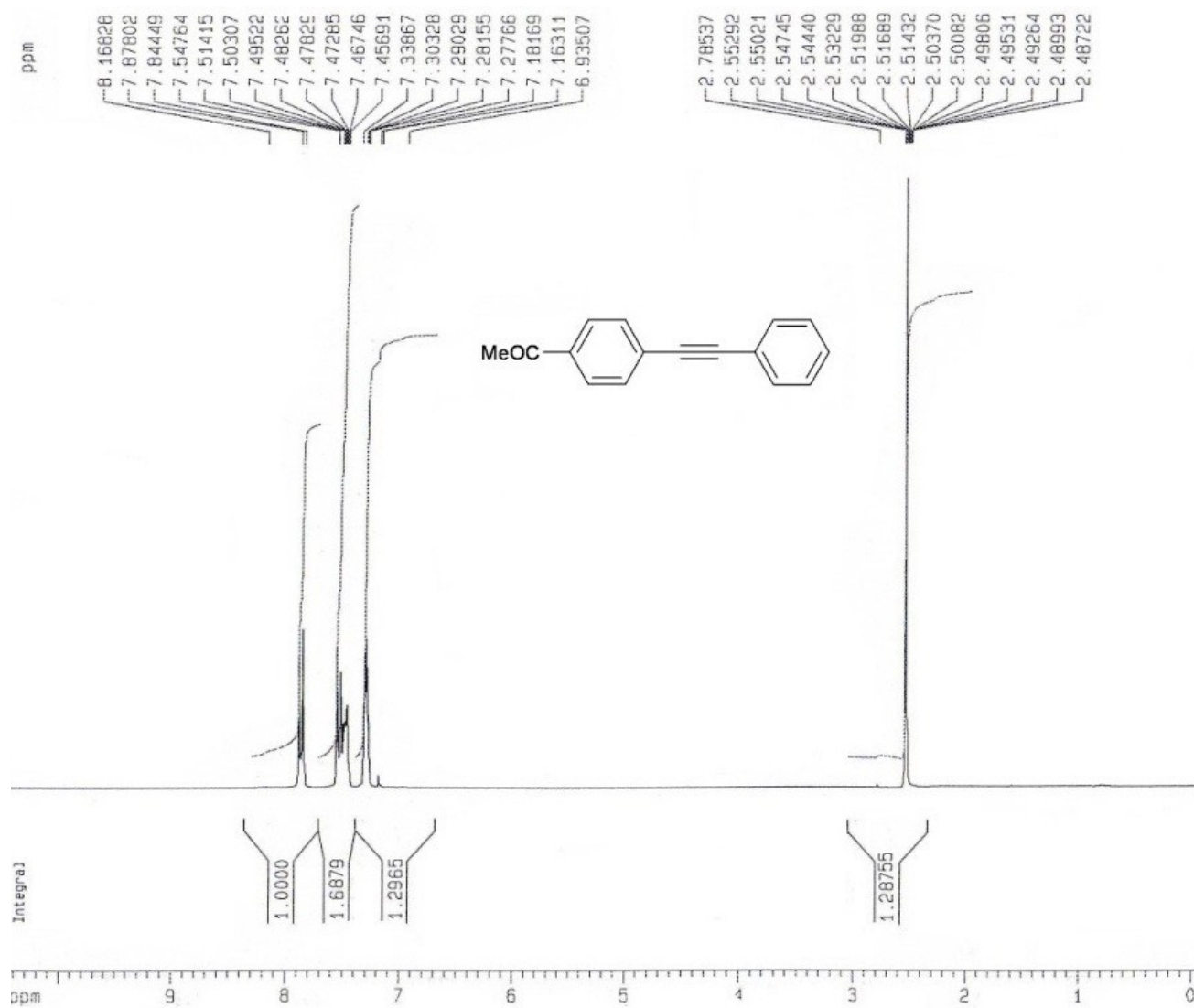


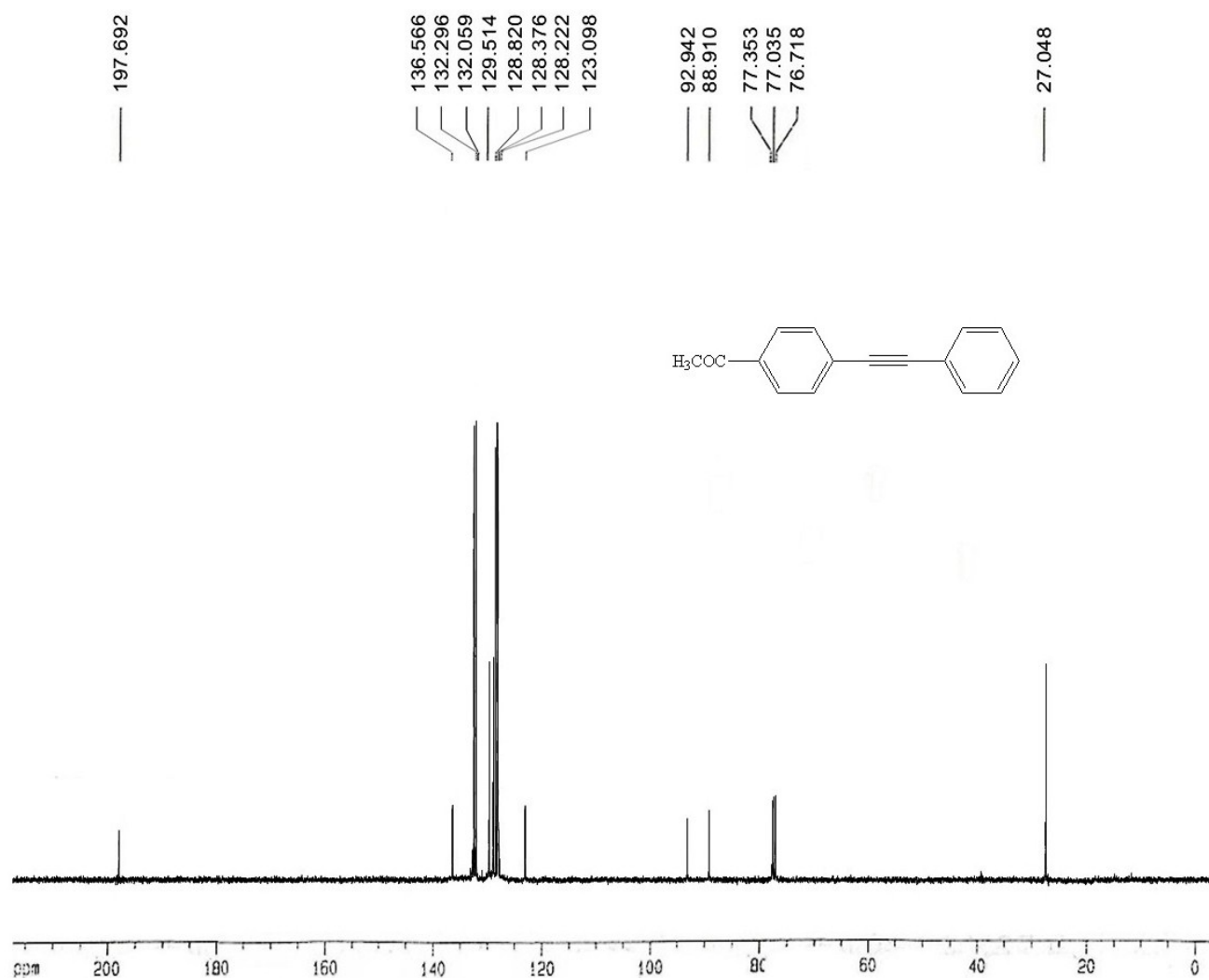


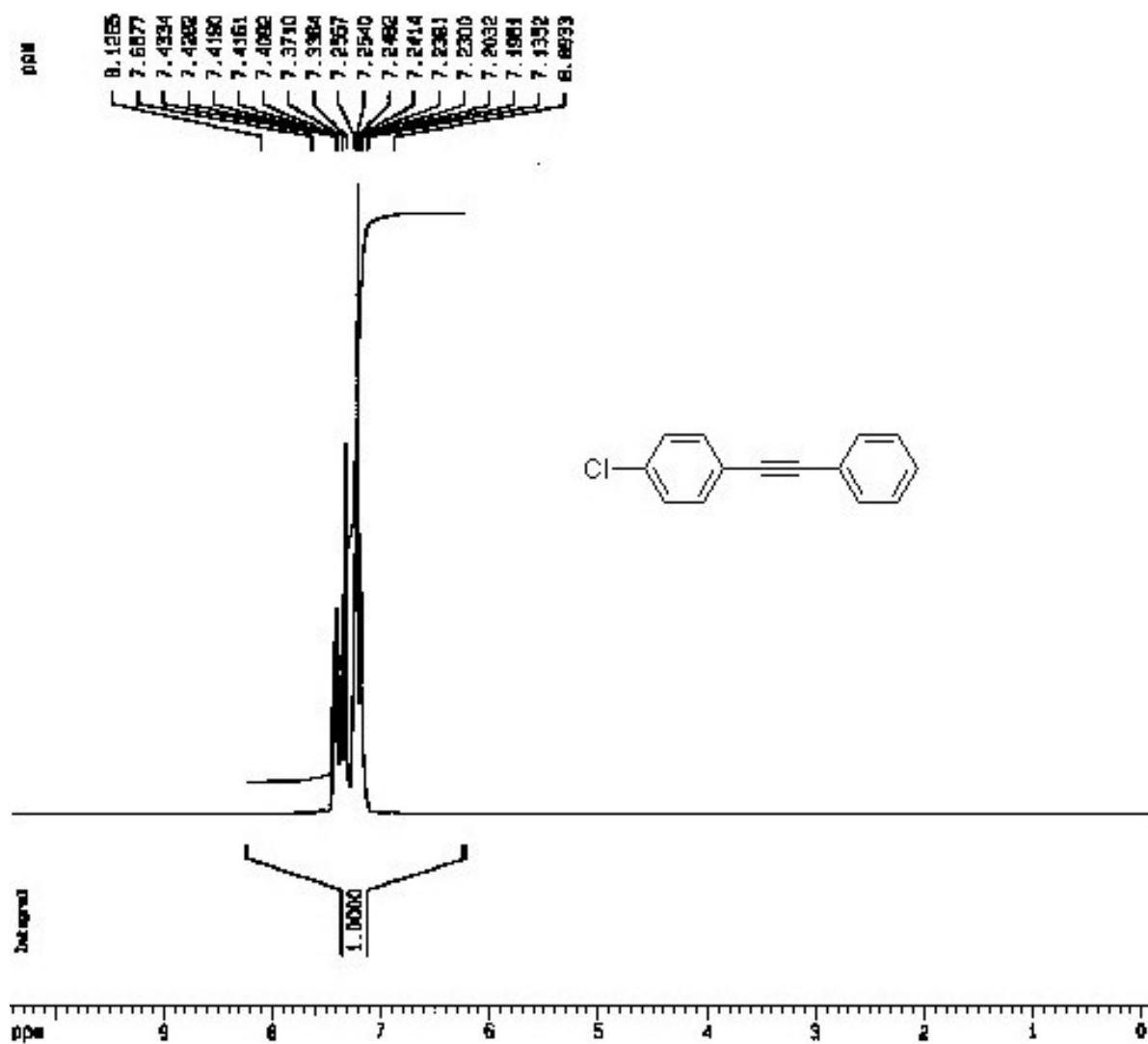


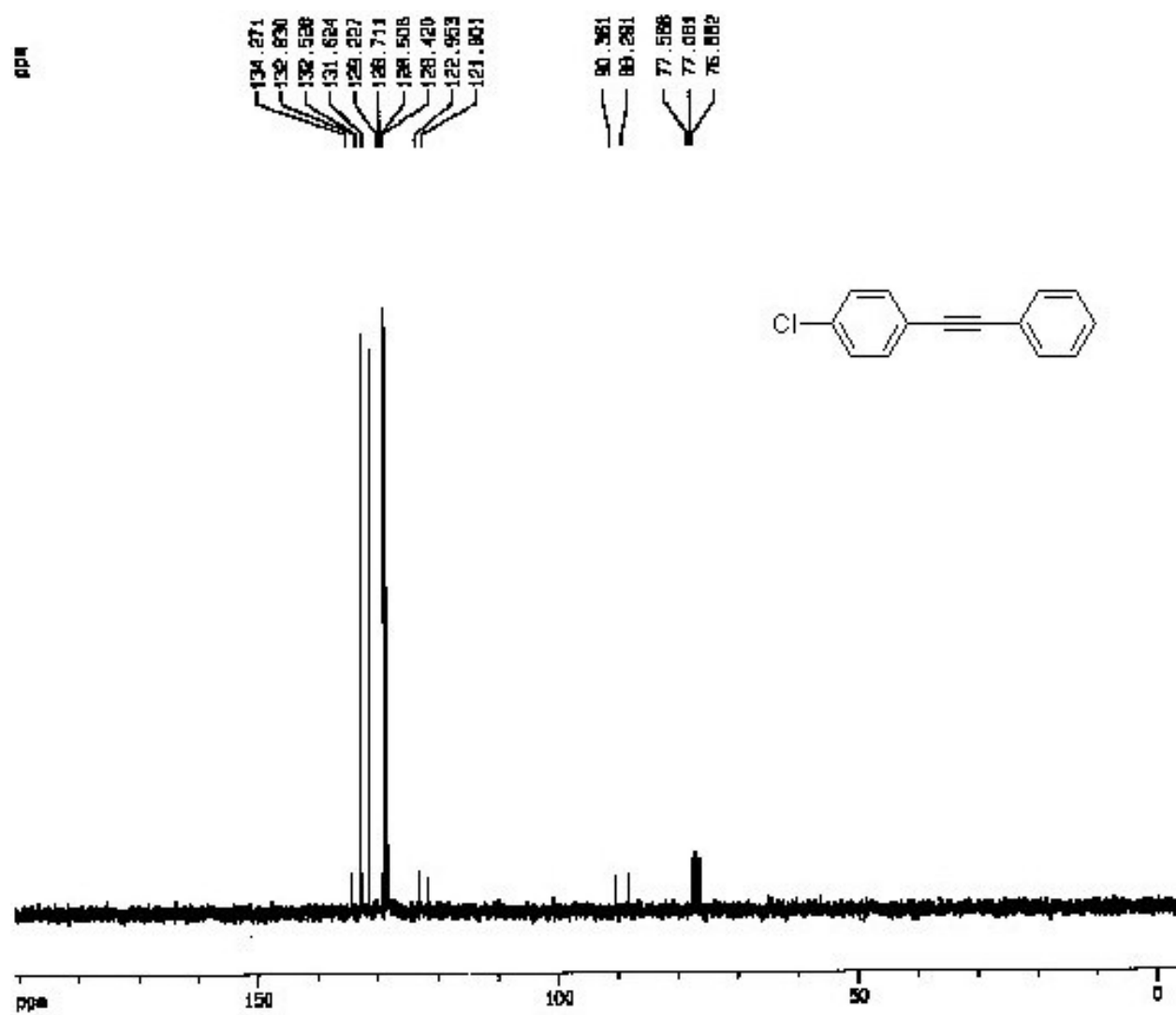


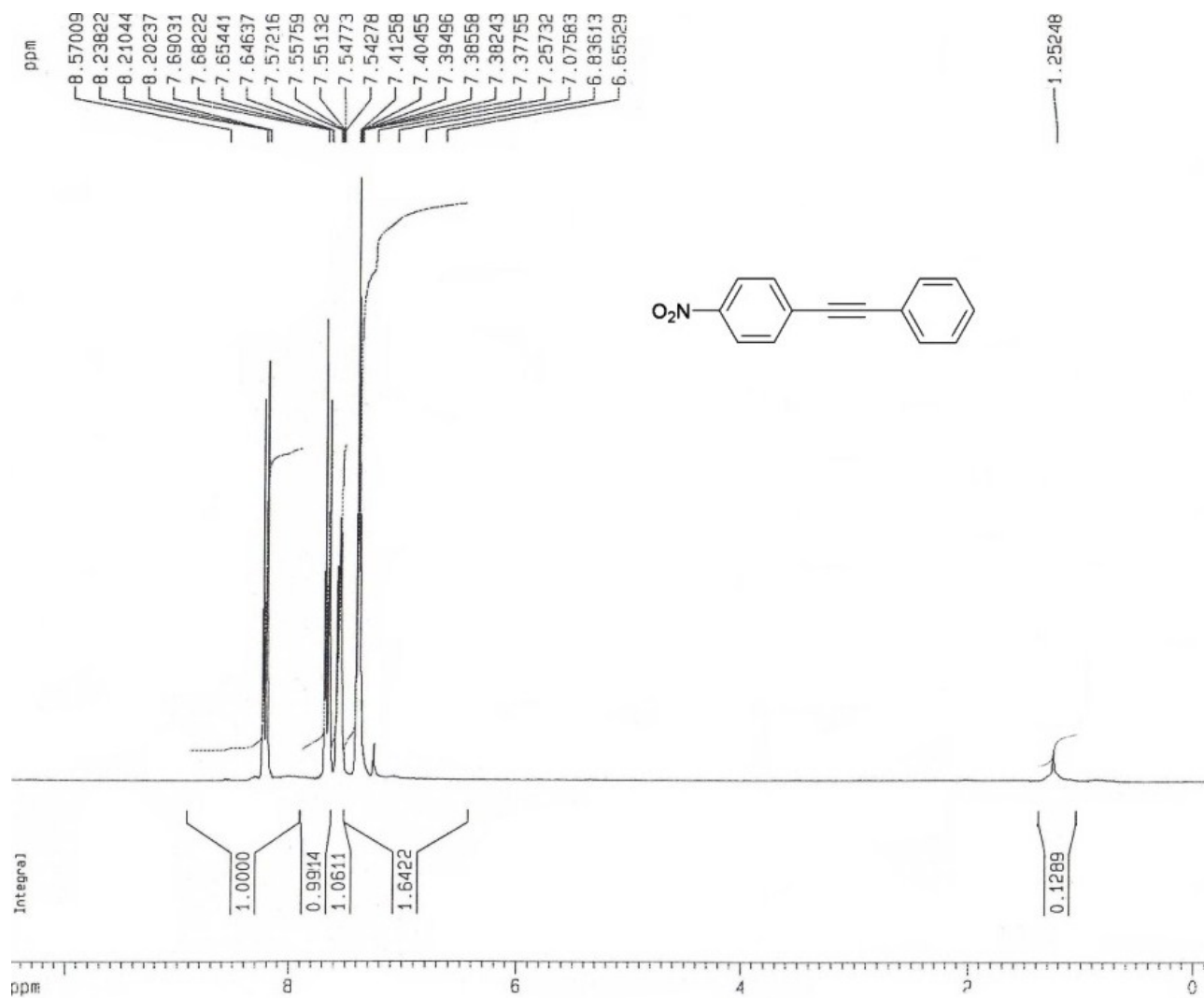


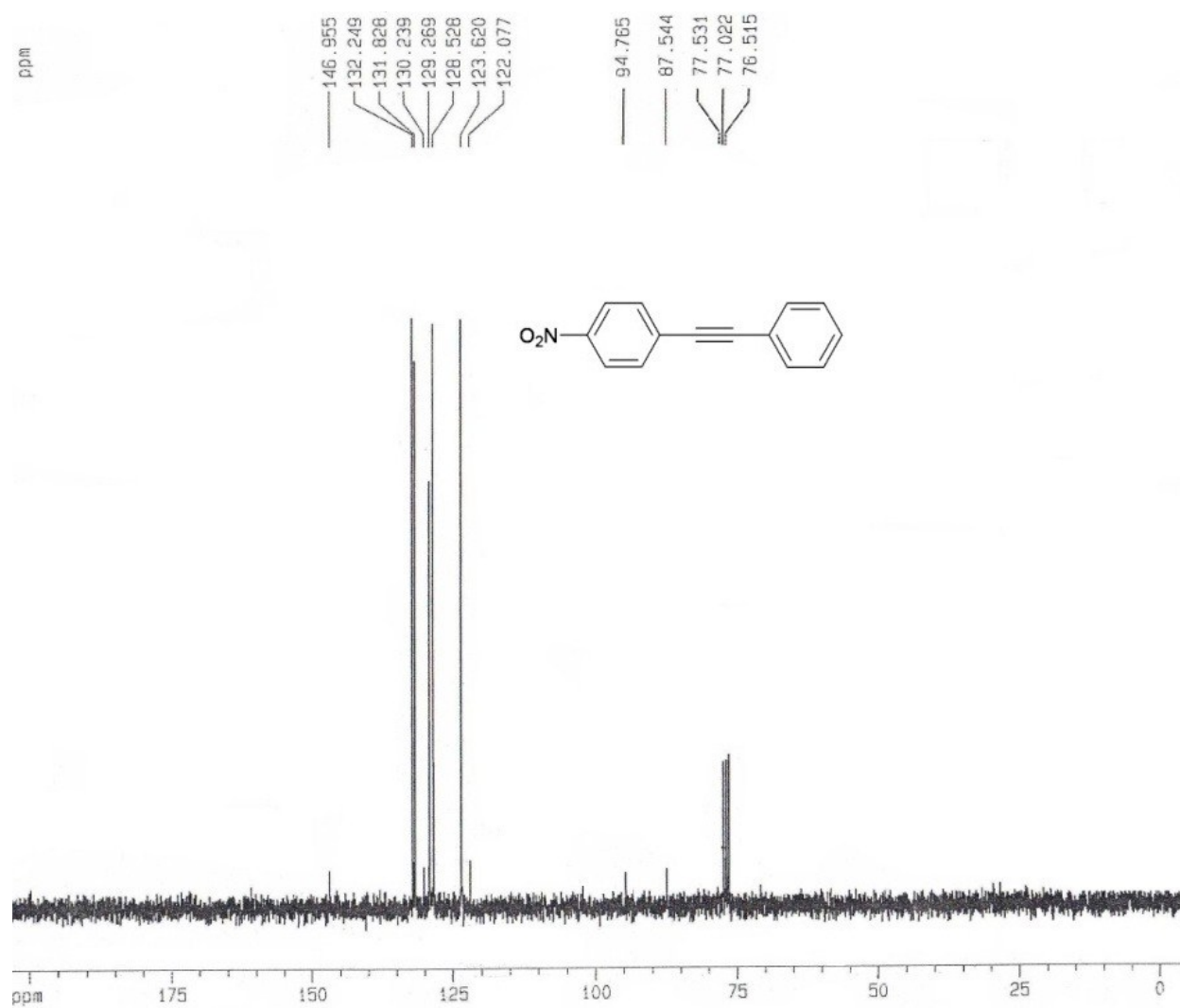


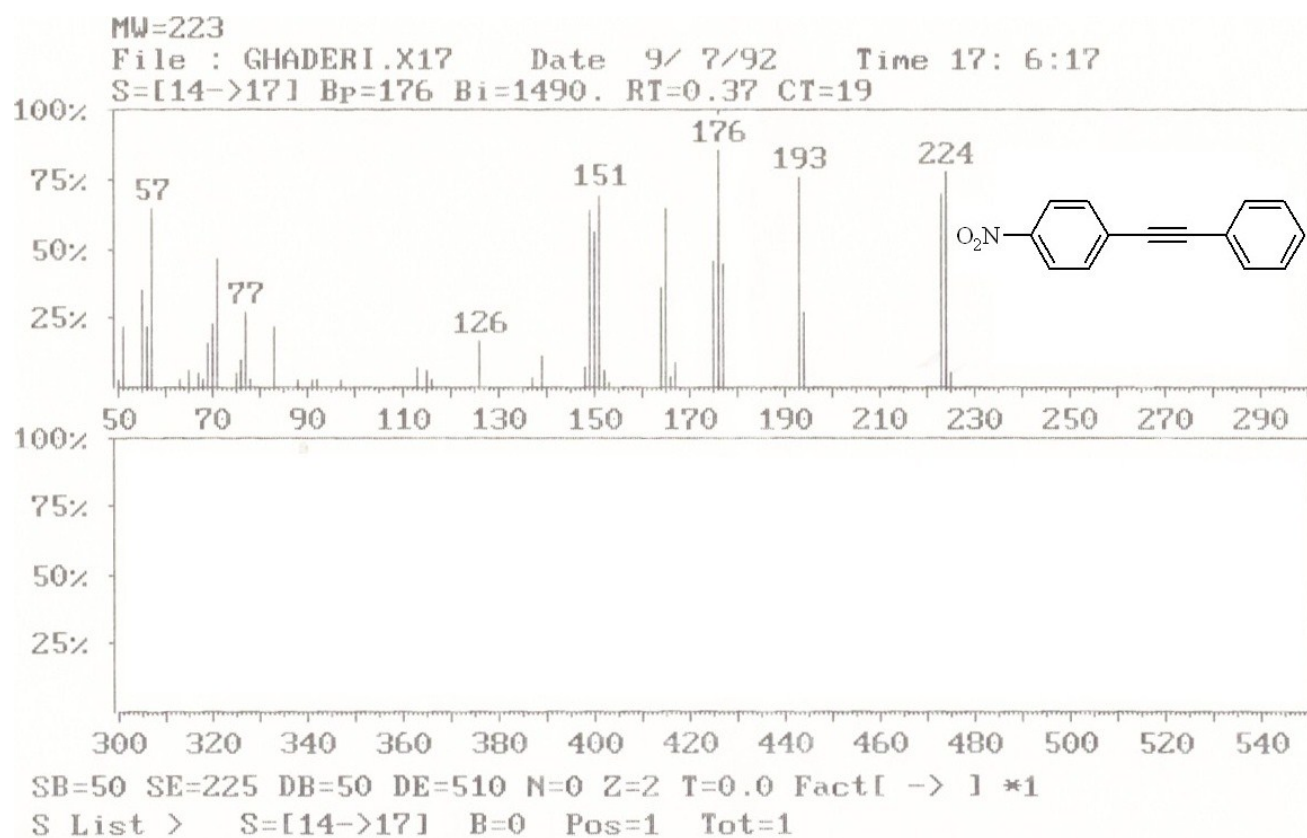


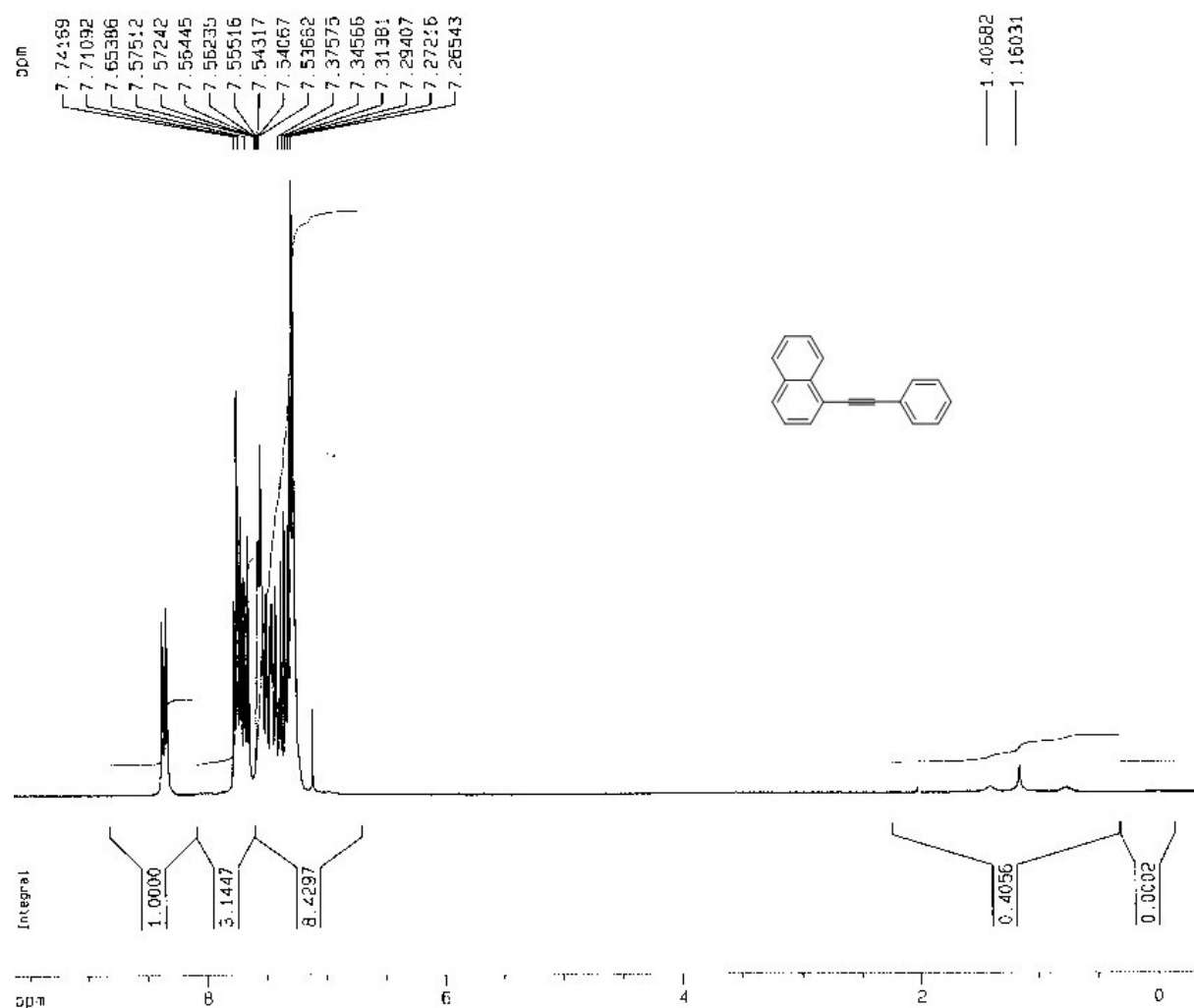


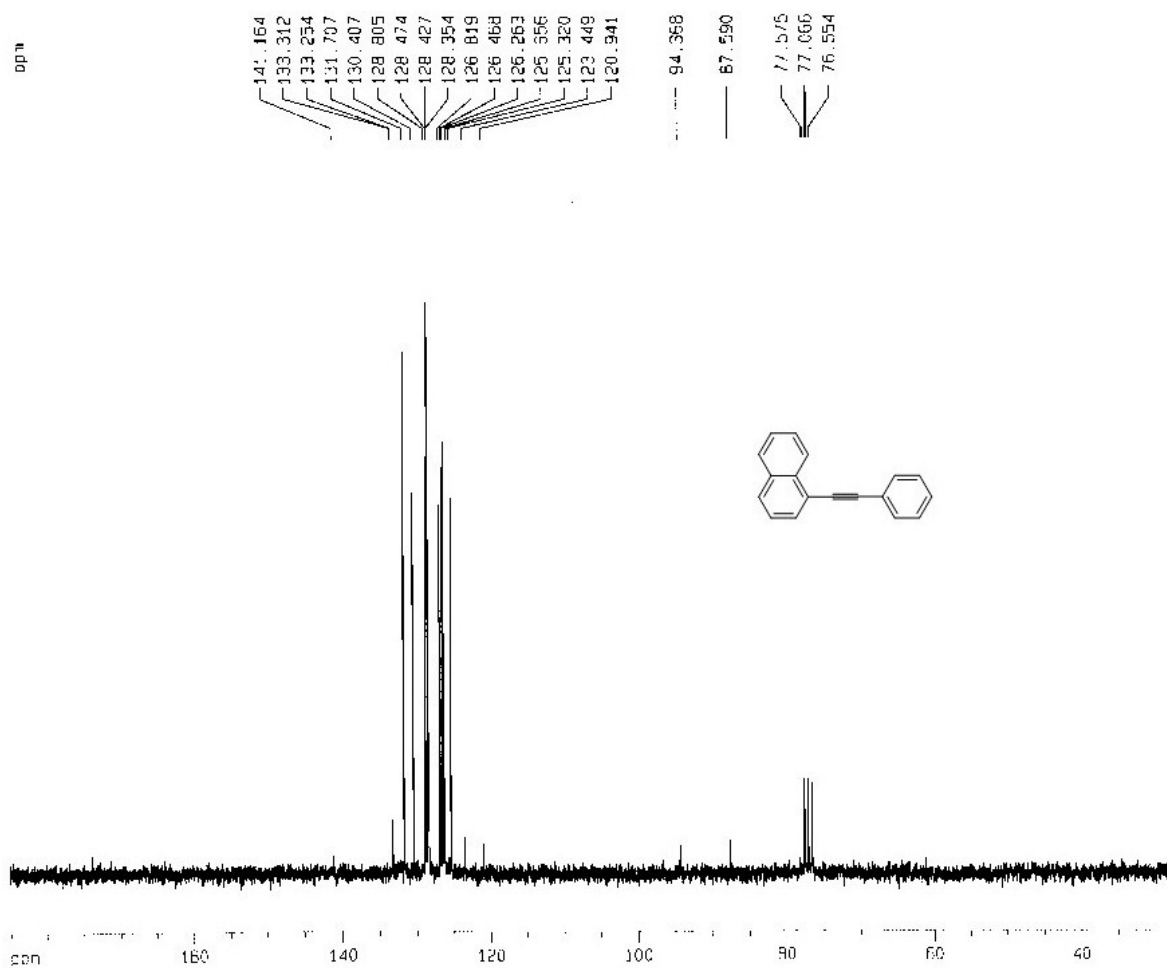


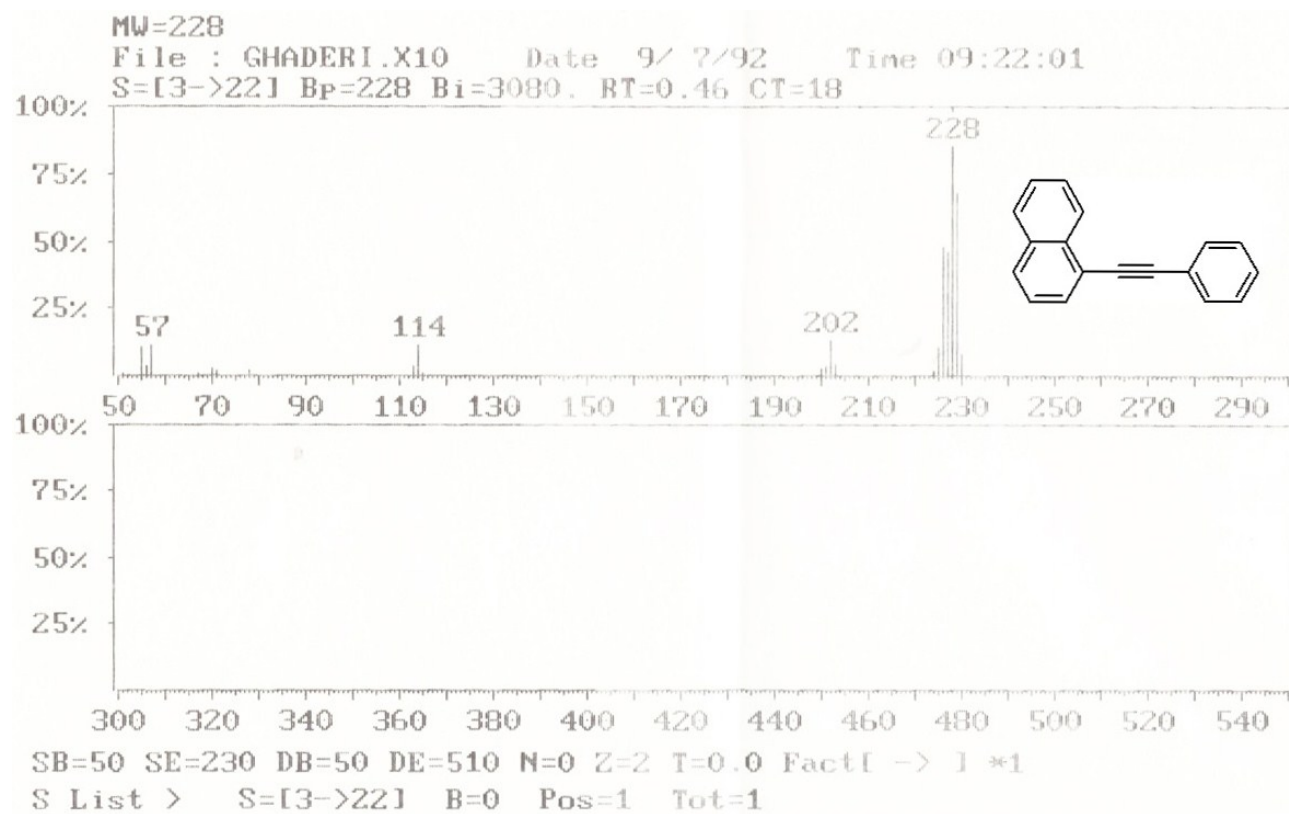


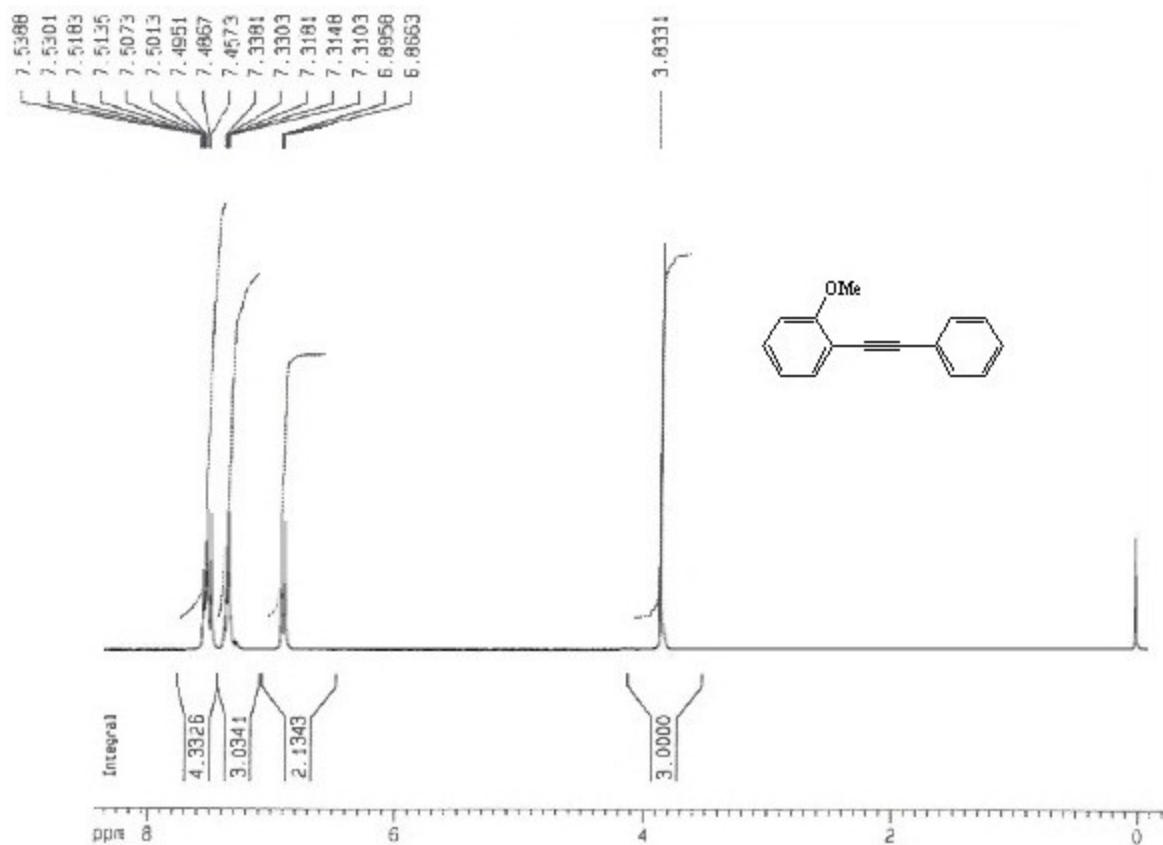


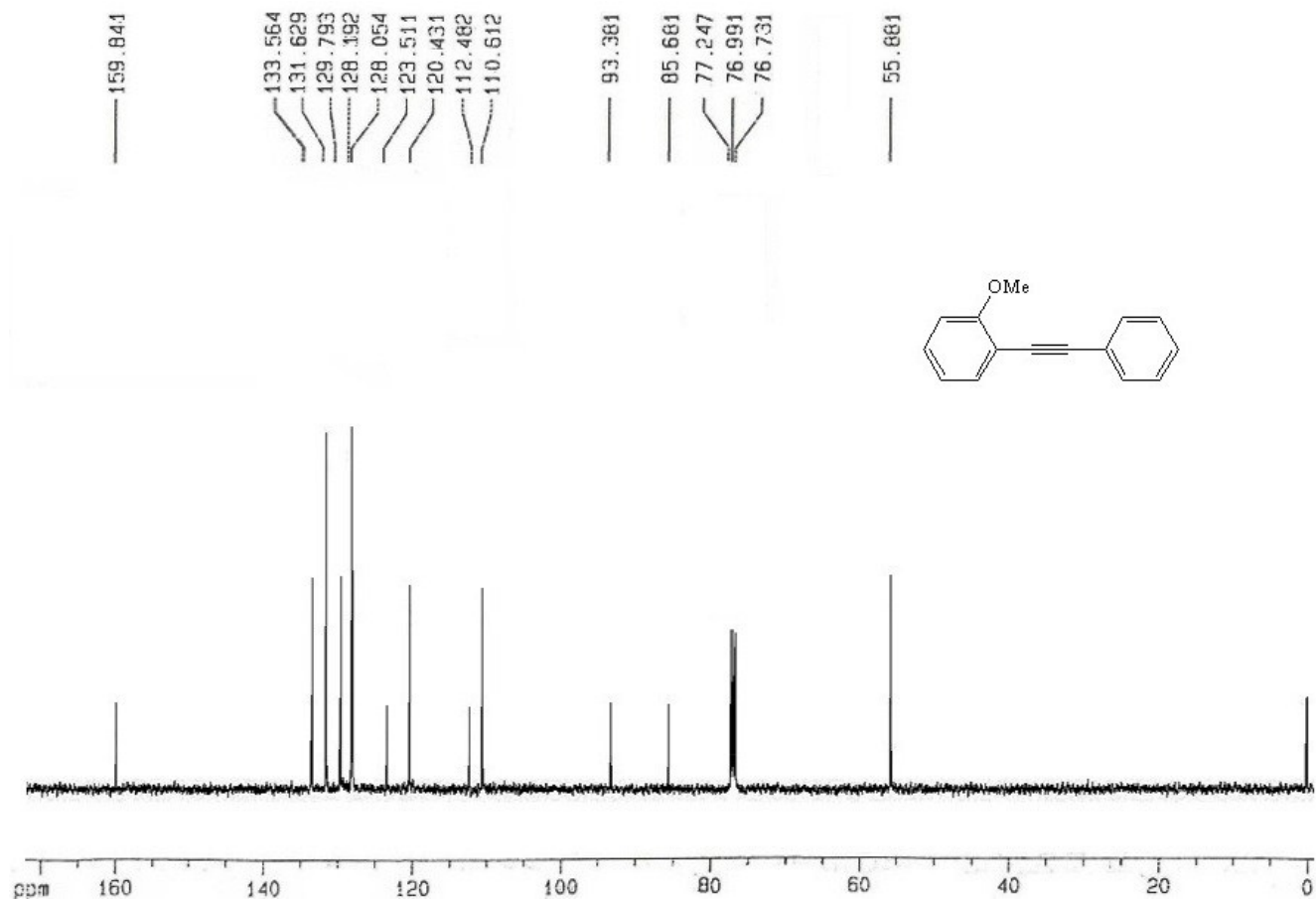


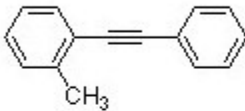


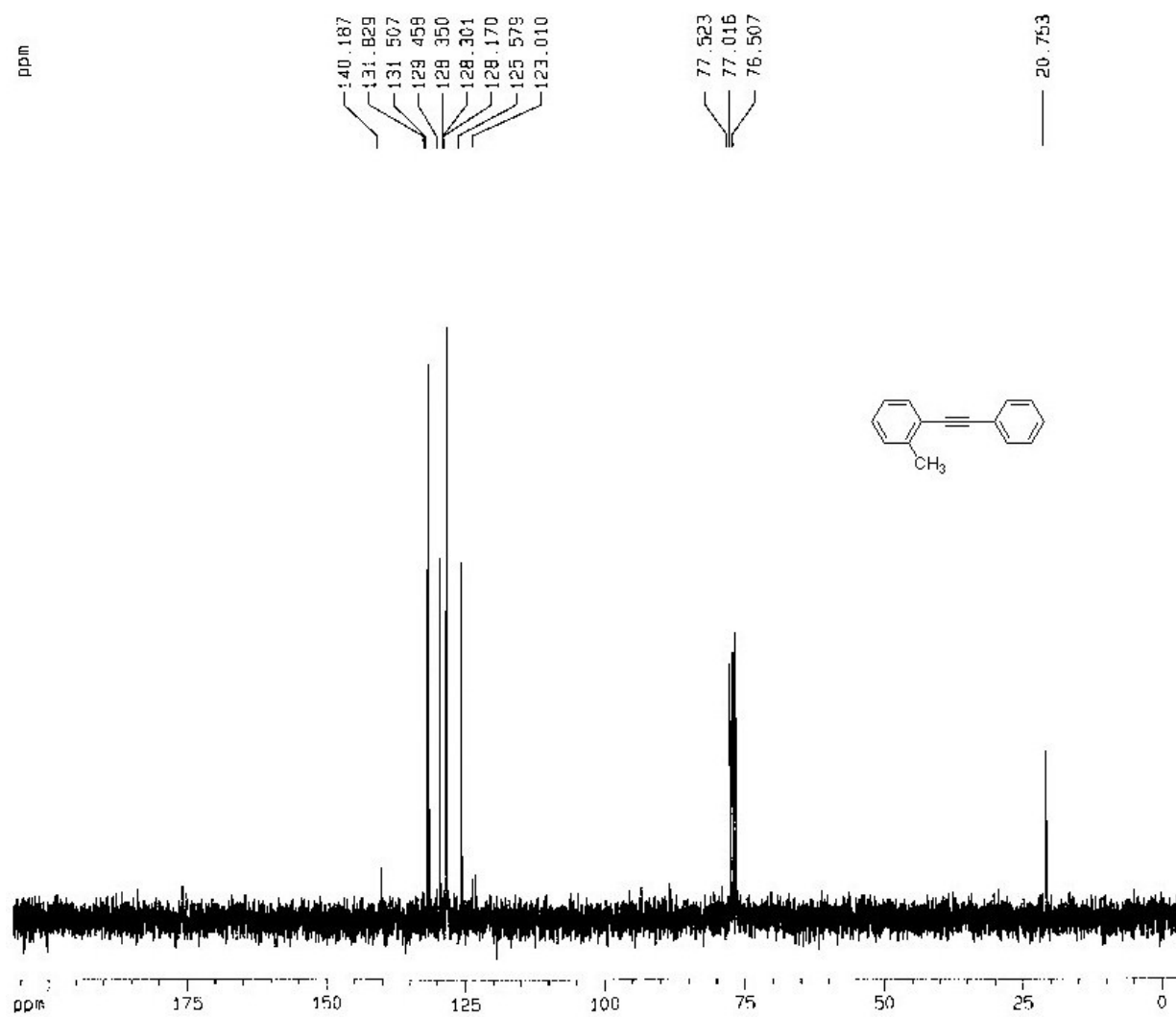








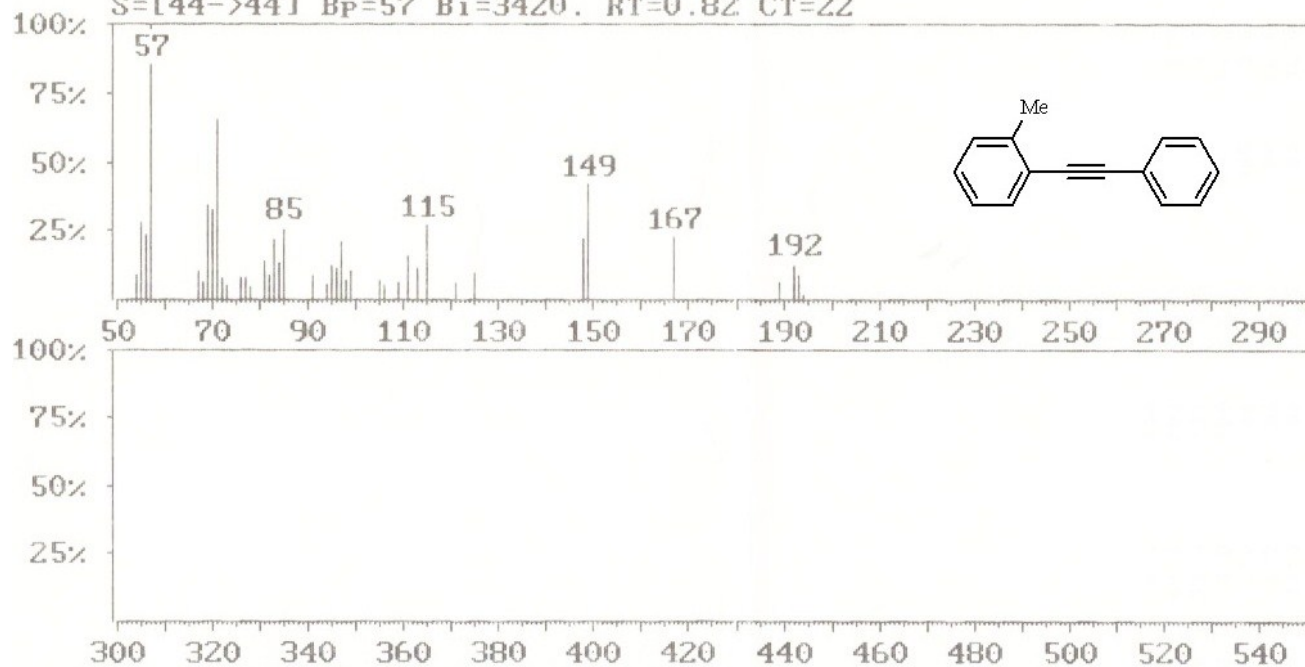




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