Electronic Supplementary Material (ESI) for ChemComm.
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SUPPORTING INFORMATION

Direct synthesis of nitroaryl acetylenes from acetylenes and nitroarenes *via* oxidative nucleophilic substitution of hydrogen.

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1. General information

^{1}H and ^{13}C NMR spectra were recorded on a Bruker 500 MHz (500 MHz for ^{1}H and 125 MHz ^{13}C spectra), a Varian-NMR-vnmrs600 (600 MHz for ^{1}H and 150 MHz ^{13}C spectra) instruments. Chemical shifts δ are expressed in ppm referred to TMS (internal standards), and coupling constants in Hertz. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q) and multiplet (m). Electrospray mass spectra (ESI) were obtained on SYNAPT G2-S HDMS. Infrared spectra are recorded on a Perkin-Elmer Model 1600 FT-IR spectrophotometer.

Materials and Methods: THF was dried using sodium/benzophenone under an argon atmosphere and distilled prior to use. Silica gel (Merck 60, 230-400 mesh) was used for column chromatography. Hexane or hexane/ethyl acetate mixtures were used for elution. TLC analyses were performed on Merck Kieselgel 60 F_{254} Alufolien with hexane/ethyl acetate mixtures. 1-Octyl 2,4-dinitrofenyl sulfide was obtained according to literature method.[1] Other chemicals were obtained from commercial sources and used directly.

2. General procedures for synthesis of the acetylenes.

2.1. Synthesis of the dinitrophenylacetylenes from *m*-dinitrobenzene.

To a solution of acetylene (3.0 mmol) and HMPA (0.59 mL, 0.60 g, 3.3 mmol) in dry THF (10 mL) at – 70 °C under argon, 2.5 M BuLi in hexane (1.2 mL, 3.0 mmol) was added in portions in 3 min. After the addition was completed, the mixture was stirred at – 70 °C for 30 min. A solution of the *m*-dinitrobenzene (0,25 g, 1.5 mmol) in THF (2.0 mL) was added (colour changed to blue immediately) and the resultant mixture was stirred for 10 min at – 70 °C. A solution of 0.68 g (3.0 mmol) of DDQ in THF (2.0 mL) was added and the mixture was stirred at – 70 °C for 20 min. The cooling bath was removed, the mixture was stirred for 1h at RT, then concentrated and the residue was subject to column chromatography (SiO_2, hexane/AcOEt).

2.2. Synthesis of the nitroarylacetylenes from other nitrobenzenes, 1-nitronaphtalene and nitropyridines

To a mixture of acetylene (3.0 mmol) in dry THF (7 mL) and HMPA (5 mL) at – 70 °C under argon, 2.5 M BuLi in hexane (1.2 mL, 3.0 mmol) was added in portions in 4 min. After the

[1] R. W. Bost, P. K. Starnes, E. L. Wood, *J. Am. Chem. Soc.*, 1951, **73**, 1968

addition was completed, the mixture was stirred at – 70 °C for 30 min. A solution of the nitroarene (1.5 mmol) in THF (2.0 mL) was added (colour changed to brown or dark-green immediately) and the resultant mixture was stirred for 1h at – 70 °C. A solution of 0.68 g (3.0 mmol) of DDQ in THF (2.0 mL) was added and the mixture was stirred at – 70 °C for 20 min. The cooling bath was removed, the mixture was stirred for 1h at RT, then concentrated and the residue was subject to column chromatography (SiO_2, hexane/AcOEt)

1,3-Dinitro-4-(phenylethynyl)benzene (1a). Yellow solid (0.224 g, 56%), mp. 111 – 113 °C (lit. mp. 109 – 110 °C)[2]. IR (KBr): 3119, 2213, 1606, 1592, 1535, 1519, 1336, 1065, 1011, 834, 765, 738, 690 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.94 (d, *J* = 2.2 Hz, 1H), 8.43 (dd, *J* = 8.6 Hz, 2.2 Hz, 1H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.61 – 7.65 (m, 2H), 7.40 – 7.48 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.4, 146.3, 135.5, 132.4, 130.4, 128.7, 126.9, 124.9, 121.3, 120.5, 103.6, 83.9.

1,3-Dinitro-2-(phenylethynyl)benzene (1a'). Orange solid (0.064 g, 16%), mp. 100 – 103 °C (lit. mp. 105 °C)[3]. ^1H NMR (500 MHz, $CDCl_3$): δ 8.18 (d, *J* = 8.0 Hz, 2H), 7.56 – 7.64 (m, 3H), 7.36 – 7.46 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.6, 132.5, 130.4, 128.6, 128.1, 128.0, 121.3, 113.6, 106.0, 78.6.

4-(4-Methoxy-phenylethynyl)-1,3-dinitrobenzene (1c). Yellow–brown solid (0.202 g, 45%), mp. 170 – 173 °C (lit. mp 175 - 177 °C).[2] IR (KBr): 3096, 2937, 2204, 1596, 1513, 1337, 1254, 1138, 1026, 835 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.94 (d, *J* = 2.2 Hz, 1H), 8.41 (dd, *J* = 8.6 Hz, 2.2 Hz, 1H), 7.85 (d, *J* = 8.6 Hz, 1H), 7.57 – 7.59 and 6.92 – 6.94 (4H, AA'XX'), 3,86 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.4, 145.8, 135.2, 134.4, 128.0, 126.8, 125.4, 120.6, 114.4, 113.3, 104.7, 83.7, 55.4. HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{15}H_{10}N_2O_5Na$, 321.0487; found: 321.0485.

2-(4-Methoxy-phenylethynyl)-1,3-dinitrobenzene (1c'). Yellow–brown solid (0.112 g, 25%), mp. 176 – 179 °C. IR (KBr): 3086, 2940, 2209, 1600, 1531, 1511, 1343, 1252, 1170 1028, 828, 740 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.58 (m, 3H), 6.91 – 6.92 (AA'XX', 2H), 3.85 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.4, 151.4, 134.4, 128.0, 127.3, 114.3, 114.1, 113.3, 107.1, 78.2, 55.4. HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{15}H_{10}N_2O_5Na$, 321.0487; found: 321.0487.

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[2] B. Prueger, G. E. Hofmeister, C. B. Jacobsen, D. G. Alberg, M. Nielsen, K. A. Jorgensen, *Chem. Eur. J.*, 2010, **16**, 3783

[3] S. D. Carter, T. W. Wallace, *J. Chem. Res.*, 1985, **5**, 1601

1-Methoxy-2,4-dinitro-5-(phenylethynyl)benzene (2a). Orange solid (0.048 g, 10%), mp. 126 – 129 °C. IR (KBr): 2942, 2211, 1611, 1584, 1523, 1335, 1301, 1250, 1042, 982, 831, 765, 693 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.76 (s, 1H), 7.63 – 7.66 (m, 2H), 7.40 – 7.46 (m, 3H), 7.33 (s, 1H), 4.11 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.7, 132.4, 132.0, 130.3, 128.7, 128.5, 125.2, 123.7, 121.4, 118.3, 102.1, 84.3, 57.5. HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{15}H_{10}N_2O_5Na$, 321.0487; found: 321.0479.

1-Methoxy-2,4-dinitro-3-(phenylethynyl)benzene (2a'). Yellow solid (0.200 g, 45%), mp. 145 – 148 °C. IR (KBr): 2952, 2204, 1610, 1578, 1541, 1518, 1343, 1305, 1268, 1065, 762, 688, 658 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (d, *J* = 9.3 Hz, 1H), 7.56 – 7.60 (m, 2H), 7.35 – 7.45 (m, 3H), 7.08 (d, *J* = 9.3 Hz, 1H), 4.03 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.1, 132.5, 130.3, 128.5, 127.9, 121.1, 114.4, 111.3, 104.7, 78.3, 57.3. HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{15}H_{10}N_2O_5Na$, 321.0487; found: 321.0480.

2,4-Dinitro-1-octylsulfanyl-5-(phenylethynyl)benzene (3a). Orange–brown oil (0.065 g, 11%). ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.04 (s, 1H), 7.64 – 7.66 (m, 2H), 7.60 (s, 1H), 7.41 – 7.46 (m, 3H), 3.07 (t, *J* = 7.5 Hz, 2H), 1.80 – 1.85 (m, 2H), 1.52 – 1.58 (m, 2H), 1.24 – 1.36 (m, 8H), 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.6, 144.1, 142.8, 132.4, 131.3, 130.3, 128.6, 128.5, 123.3, 121.4, 102.2, 84.3, 33.9, 32.7, 31.7, 29.1, 29.0, 27.3, 22.6, 14.0. EI (*m / z*): 412 (6, $M^{+\cdot}$), 411 (18), 299 (14), 187 (18), 181 (17), 169 (15), 131 (25).

2,4-Dinitro-1-octylsulfanyl-3-(phenylethynyl)benzene (3a'). Orange solid (0.483 g, 78%), mp. 54 – 56 °C. IR (KBr): 2957, 2925, 2852, 2218, 1584, 1558, 1539, 1515, 1335, 931, 825, 758, 688 cm^{-1}.^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.4 Hz, 1H), 7.57 – 7.59 (m, 2H), 7.37 – 7.45 (m, 4H), 3.04 (t, *J* = 7.5 Hz, 2H), 1.66 – 1.74 (m, 2H), 1.40 – 1.48 (m, 2H), 1.22 – 1.36 (m, 8H), 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 152.4, 146.0, 138.7, 132.4, 130.3, 128.5, 126.7, 125.8, 121.1, 113.4, 104.8, 78.4, 33.4, 31.7, 29.0, 28.9, 28.7, 28.4, 22.6, 14.0. HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{22}H_{24}N_2O_4SNa$, 435.1354; found: 435.1354

2-Nitro-1-phenylethynyl-4-trifluoromethylbenzene (4a).[4] Yellow–orange solid (0.198 g, 45%), mp. 55 – 57 °C. IR (KBr): 2214, 1627, 1534, 1321, 1184, 1124, 1082, 900, 840, 763, 689 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.36 (s, 1H), 7.82 – 7.87 (m, 2H), 7.61 – 7.64 (m, 2H), 7.38 – 7.46 (m, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.4, 135.3, 132.3, 130.5 (q, *J* = 35 Hz), 129.9, 129.2 (q, *J* = 3.5 Hz), 128.6, 122.7 (q, *J* = 272 Hz), 122.4, 122.2 (q, *J* = 3.5

[4] R. Zhou, W. Wang, Z.-J.Jiang, H.-Y. Fu, X.-L. Zheng, C.-C. Zhang, H. Chen, R.-X. Li, *Catalysis Science and Technology,* 2014, **4**, 746

Hz), 121.7, 100.4, 83.8. ^{19}F NMR (500 MHz, $CDCl_3$): δ -63.0 (s), HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{15}H_8NO_2F_3Na$, 314.0405; found: 314.0403.

1-Nitro-2-phenylethynyl-3-trifluoromethylbenzene (4a'). Yellow–orange oil. (0.026g, 6%), ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.1 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.60 – 7.63 (m, 2H), 7.54 – 7.58 (m, 1H), 7.38 – 7.46 (m, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.6, 134.0 (q, *J* = 31 Hz), 133.3, 132.2, 130.0 (q, *J* = 6.3 Hz), 128.6 (q, *J* = 9.1 Hz), 128.0, 127.3, 122.6 (q, *J* = 273 Hz), 121.7, 117.1, 104.2, 79.8. ^{19}F NMR (500 MHz, $CDCl_3$): δ -62.5 (s), HRMS–EI (*m / z*): $M^{+\cdot}$ calcd for $C_{15}H_8NO_2F_3$, 291.0507; found: 291.0508.

1-Nitro-2-(phenylethynyl)naphthalene (5a). Light–brown solid (0.171 g, 42%), mp. 100 – 102 °C. IR (KBr): 2210, 1598, 1526, 1375, 1337, 864, 817, 757, 688 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.54 – 7.67 (m, 5H), 7.36 – 7.40 (m, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 150.0, 133.1, 132.0, 130.5, 129.3, 129.1, 128.6, 128.2, 128.0, 127.9, 124.3, 122.0, 121.8, 114.3, 97.2, 83.3. HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{18}H_{11}NO_2Na$, 296.0687; found: 296.0687.

3-Nitro-4-(phenylethynyl)pyridine (6a). Light–brown solid (0.242 g, 78%), mp. 114 – 116 °C. IR (KBr): 3054, 2218, 1603, 1589, 1535, 1348, 836, 762 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.31 (s, 1H), 8.78 (d, *J* = 5.1 Hz, 1H), 7.62 – 7.65 (m, 2H), 7.59 (d, *J* = 5.1 Hz, 1H), 7.40 – 7.46 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.0, 146.1, 144.8, 132.5, 130.3, 128.6, 127.4, 126.9, 121.2, 102.9, 82.9. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{13}H_9N_2O_2$, 225.0664; found: 225.0658.

3-Nitro-4-(4-tolylethynyl)pyridine (6b). Light–yellow solid (0.255 g, 72%), mp. 90 – 91 °C. IR (KBr): 3054, 2917, 2213, 1593, 1534, 1508, 1345, 1224, 815 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.30 (s, 1H), 8.76 (d, *J* = 5.1 Hz, 1H), 7.56 (d, *J* = 5.1 Hz, 1H), 7.52 – 7.54 and 7.21 – 7.23 (4H, AA'XX'), 2.40 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.9, 146.1, 141.0, 132.5, 129.4, 127.3, 127.1, 118.2, 103.5, 82.6, 21.7. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{14}H_{11}N_2O_2$, 239.0821; found: 239.0822.

4-(4-Methoxy-phenylethynyl)-3-nitropyridine (6c). Brown solid (0.277 g, 73%), mp. 153 – 155 °C. IR (KBr): 2219, 2196, 1596, 1346, 1255, 828 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.29 (s, 1H), 8.74 (d, *J* = 5.1 Hz, 1H), 7.57 – 7.59 and 6.92 – 6.94 (4H, AA'XX'), 7.54 (d, *J* = 5.1 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.4, 152.8, 146.2, 134.4, 127.3, 127.1, 114.4, 113.3, 103.9, 82.5, 55.4. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{14}H_{11}N_2O_3$, 255.0770; found: 255.0768.

6-Methoxy-3-nitro-2-(phenylethynyl)pyridine (7a). Light–brown solid (0.295 g, 77%), mp. 116 – 117 °C. IR (KBr): 3090, 2217, 1582, 1324, 1065, 1011, 835, 758 cm^{-1}. ^{1}H NMR

(500 MHz, $CDCl_3$): δ 8.32 (d, *J* = 9.1 Hz, 1H), 7.68 – 7.72 (m, 2H), 7.38 – 7.44 (m, 3H), 6.78 (d, *J* = 9.1 Hz, 1H), 4.08 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 141.7, 136.6, 135.5, 132.6, 129.9, 128.5, 121.6, 111.1, 97.5, 86.0, 54.9. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{14}H_{11}N_2O_3$, 255.0770; found: 255.0767.

6-Methoxy-3-nitro-2-(4-tolylethynyl)pyridine (7b). Yellow solid (0.284 g, 71%), mp. 122 – 124 °C. IR (KBr): 3100, 2205, 1583, 1320, 1062, 1013, 812, 774 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.31 (d, *J* = 9.1 Hz, 1H), 7.58 – 7.60 and 7.20 – 7.22 (4H, AA'XX'), 6.75 (d, *J* = 9.1 Hz, 1H), 4.08 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 141.6, 140.5, 136.8, 135.5, 132.6, 129.3, 118.6, 110.8, 98.2, 85.7, 54.9, 21.7. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{15}H_{13}N_2O_3$, 269.0926; found: 269.0924.

2-(4-Methoxy-phenylethynyl)-6-methoxy-3-nitropyridine (7c). Yellow–green solid (0.310 g, 73%), mp. 117– 119 °C. IR (KBr): 3076, 2955, 2199, 1742, 1581, 1511, 1325, 1252, 1154, 1063, 1013, 822, 773 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.31 (d, *J* = 9.1 Hz, 1H), 7.64 – 7.65 and 6.91 – 6.93 (4H, AA'XX'), 6.74 (d, *J* = 9.1 Hz, 1H), 4.08 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 161.1, 141.4, 137.0, 135.5, 134.4, 114.2, 113.7, 110.6, 98.5, 85.5, 55.4, 54.9. HRMS–ESI (*m / z*): $[M+Na]^+$ calcd for $C_{15}H_{12}N_2O_4Na$, 307.0695; found: 307.0689.

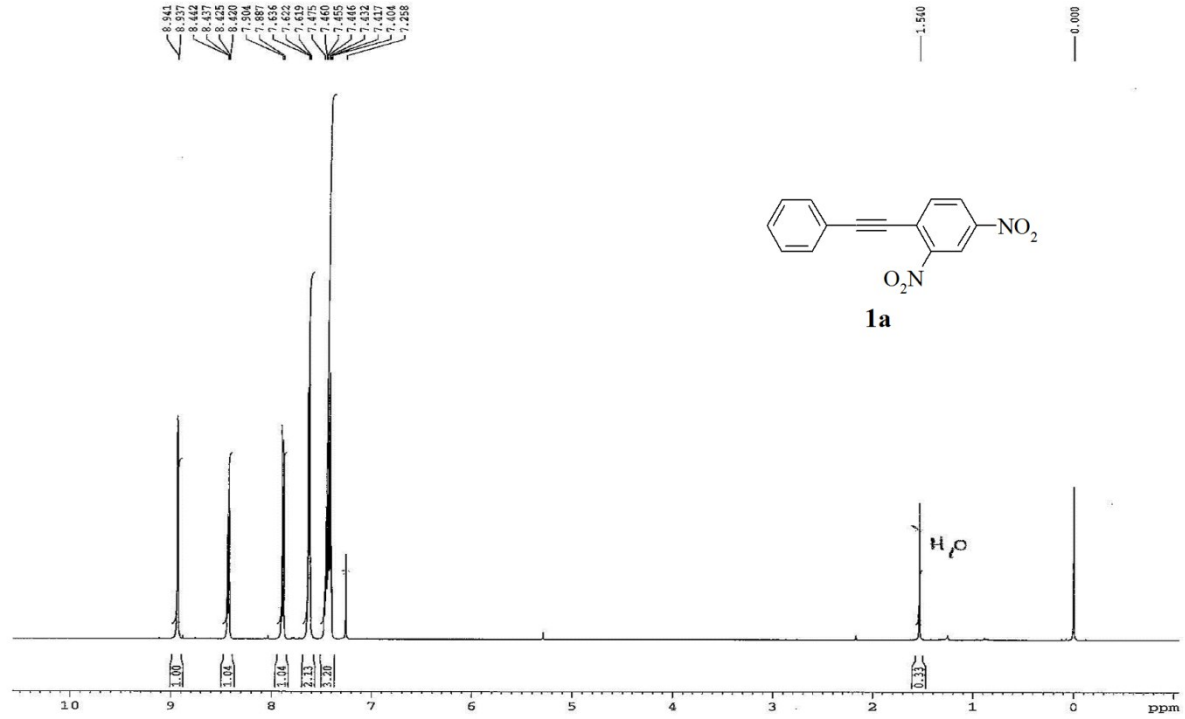
2-(4-Fluoro-phenylethynyl)-6-methoxy-3-nitropyridine (7d). Light–brown solid (0.340 g, 83%), mp. 101 – 102 °C. IR (KBr): 3093, 2211, 1580, 1323, 1064, 1016, 835, 775 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.32 (d, *J* = 9.1 Hz, 1H), 7.67 – 7.70 (m, 2H), 7.07 – 7.12 (m, 2H), 6.78 (d, *J* = 9.1 Hz, 1H), 4.08 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 163.5 (d, *J* = 250 Hz), 136.5, 135.5, 134.7 (d, *J* = 8.7 Hz), 117.8 (d, *J* = 3.7 Hz), 116.0, 115.9 111.2, 96.4, 85.8, 54.9. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{14}H_{10}N_2O_3F$, 273.0675; found: 273.0665.

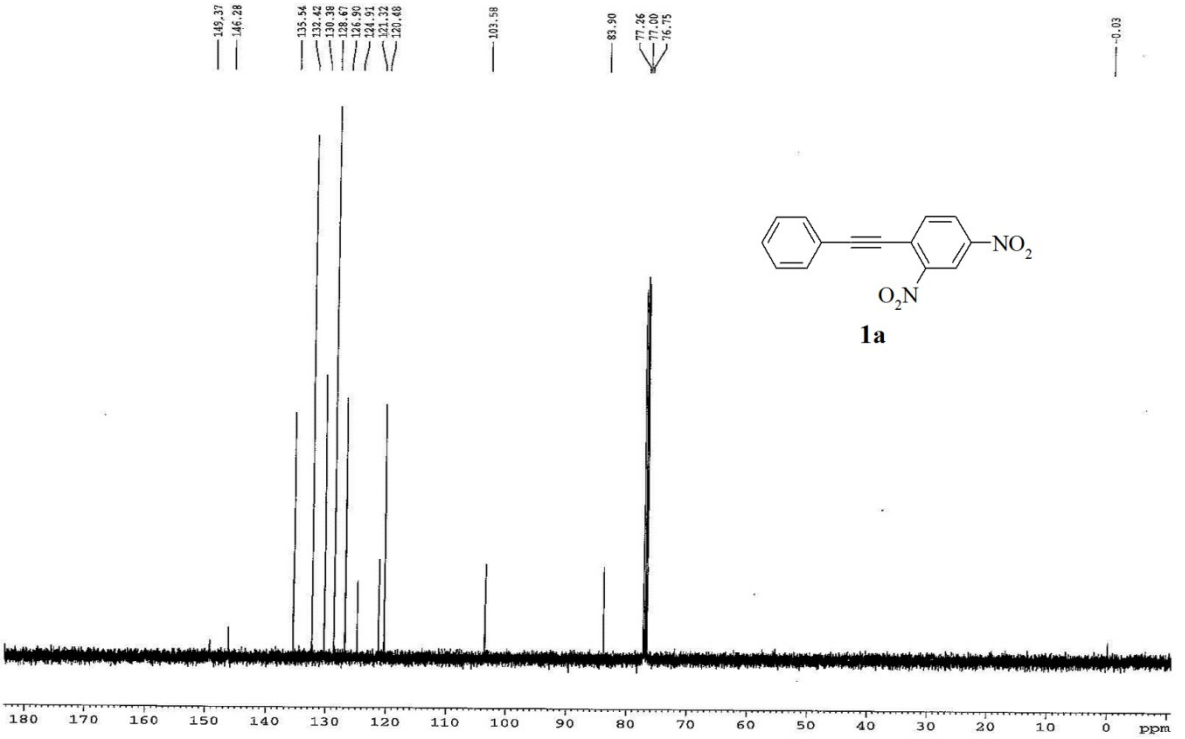
6-Methoxy-3-nitro-2-(trimethylsilanylethynyl)pyridine (7e). Light–brown solid (0.255 g, 68%), mp. 92– 94 °C. IR (KBr): 2956, 2898, 2656, 2113, 1590, 1520, 1473, 1417, 1322, 1246, 1070, 1019, 954, 849, 774, 671 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.25 (d, *J* = 9.1 Hz, 1H), 6.76 (d, *J* = 9.1 Hz, 1H), 4.05 (s, 3H), 0.32 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.3, 142.4, 135.9, 135.3, 111.5, 105.0, 99.7, 54.9, -0.56. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{11}H_{15}N_2O_3Si$, 251.0852; found: 251.0855.

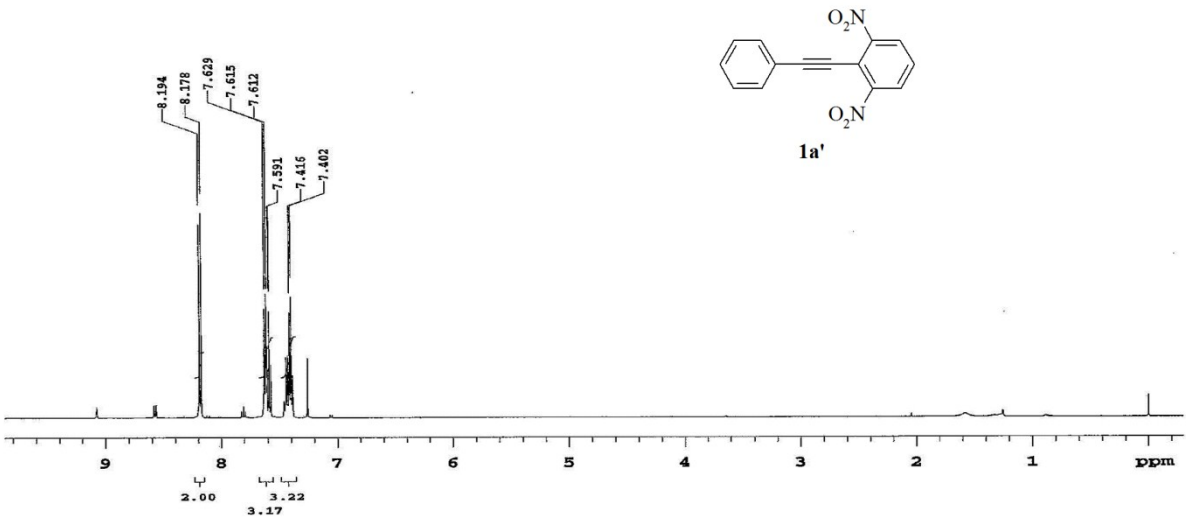
2-(Hex-1-ynyl)-6-methoxy-3-nitropyridine (7f). Yellow oil (0.132 g, 40%), IR (film): 2957, 2230, 1586, 1319, 1085, 1027, 1009, 835, 778 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.24 (d, *J* = 9.0 Hz, 1H), 6.72 (d, *J* = 9.0 Hz, 1H), 4.04 (s, 3H), 2.55 (t, *J* = 7.1 Hz, 2H), 1.65 – 1.71 (m, 2H), 1.49 – 1.57 (m, 2H), 0.97 (t, *J* = 7.1 Hz, 3H),. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2,

141.9, 136.9, 135.4, 110.6, 100.8, 77.5, 54.8, 30.1, 22.0, 19.7, 13.6. HRMS–ESI (*m / z*): $[M+H]^+$ calcd for $C_{12}H_{15}N_2O_3$, 235.1083; found: 235.1073.

3. Copies of ^{1}H and ^{13}C NMR spectra of the compounds 1-7



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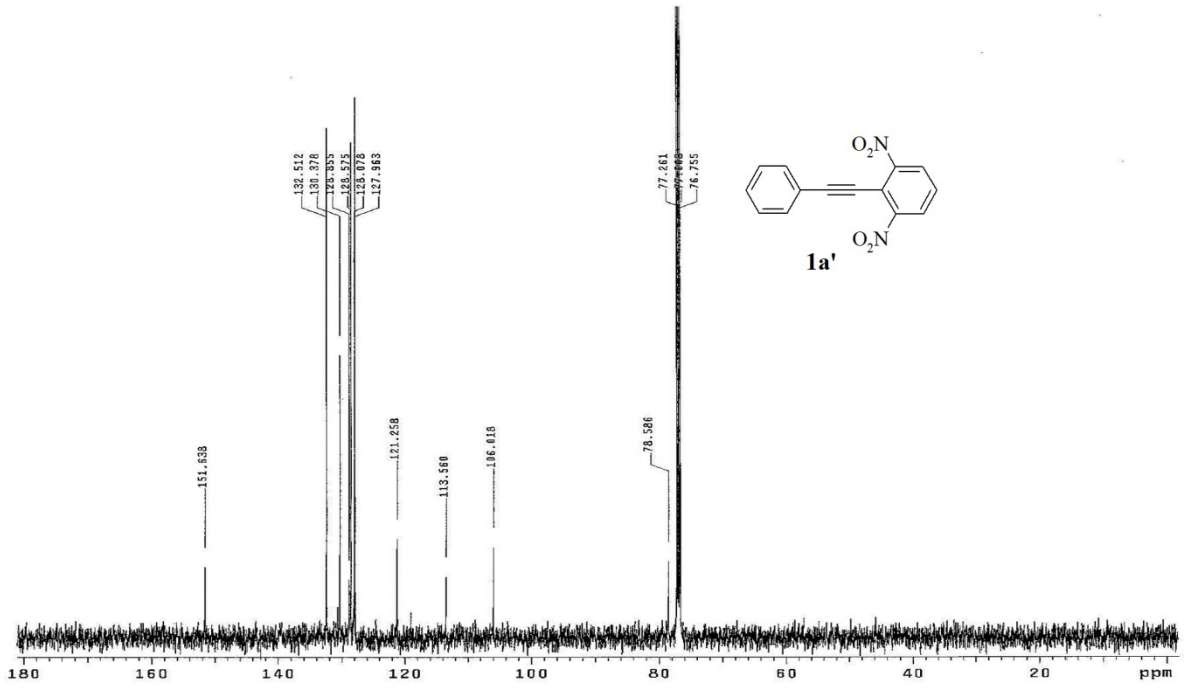
3.17

O2N
O2N

1a'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40
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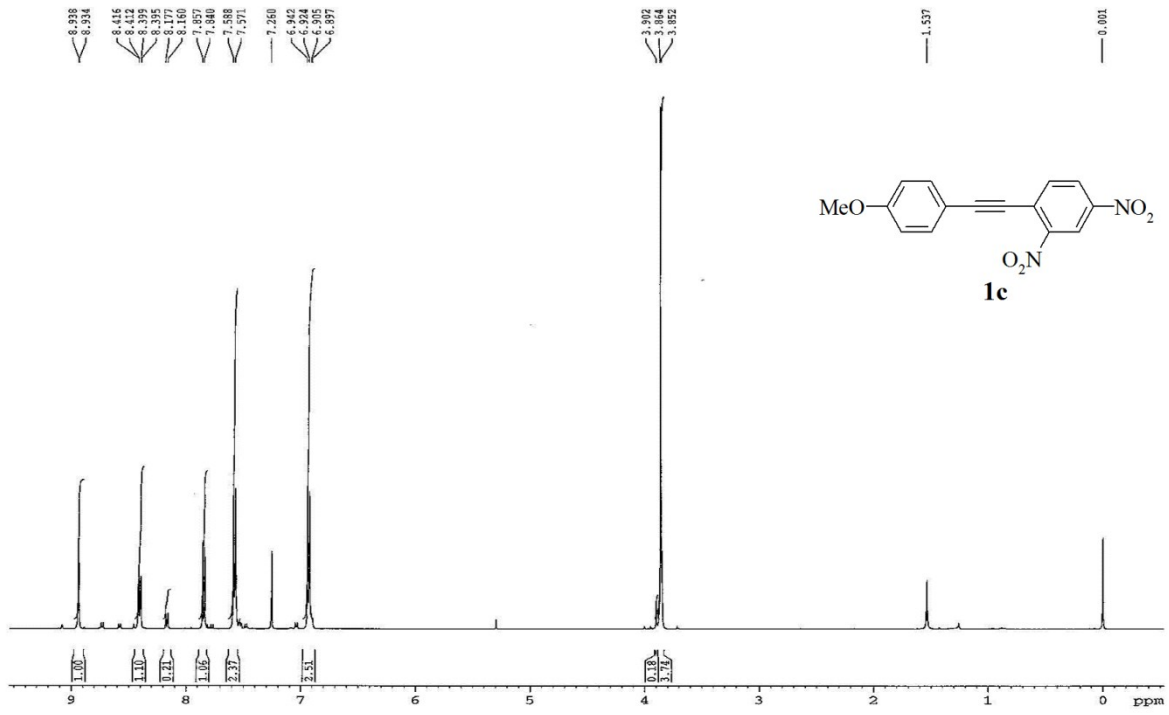
ppm

O2N
O2N

1a'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7.840
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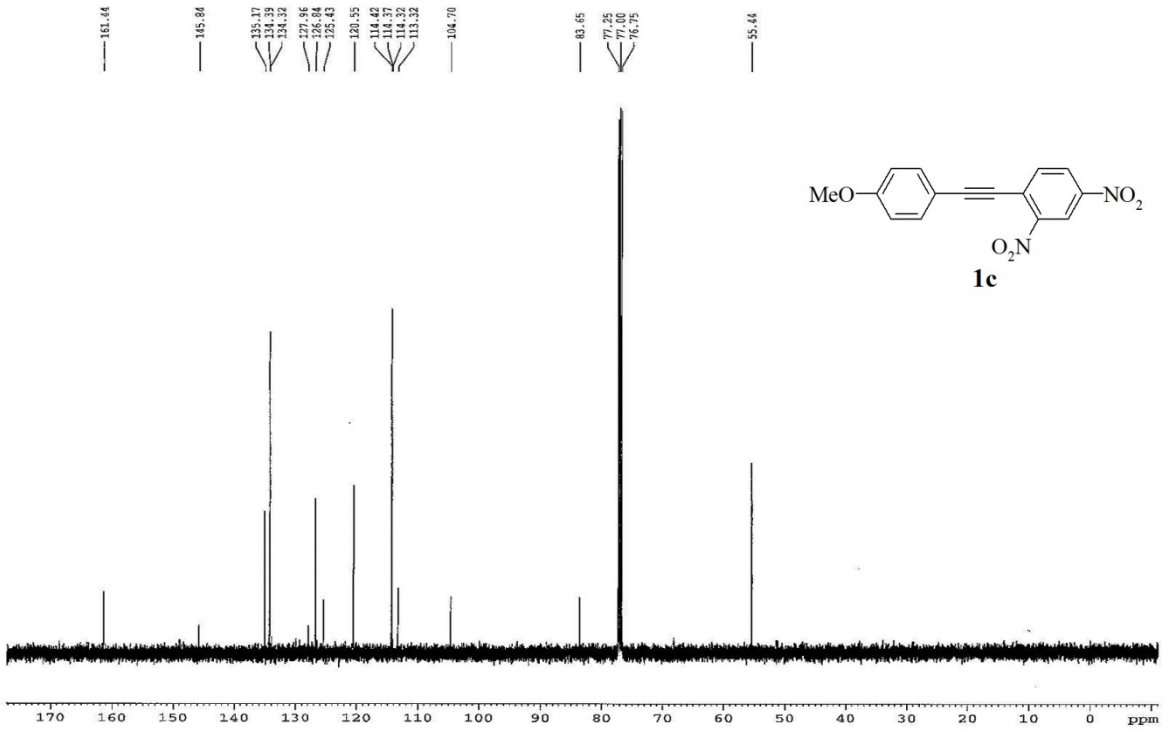
7.260
6.942
6.924
6.905
6.897
3.902
3.864
3.852
1.537
0.001
MeO
NO2
O2N
1c
1.00
1.10
0.21
1.06
2.37
2.51
0.18
3.74
9
8
7
6
5
4
3
2
1
0
ppm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135.17
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127.96
126.84
125.43
120.55
114.42
114.37
114.32
113.32
104.70
83.65
77.25
77.00
76.75
55.44
MeO
NO2
O2N
1c
170
160
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140
130
120
110
100
90
80
70
60
50
40
30
20
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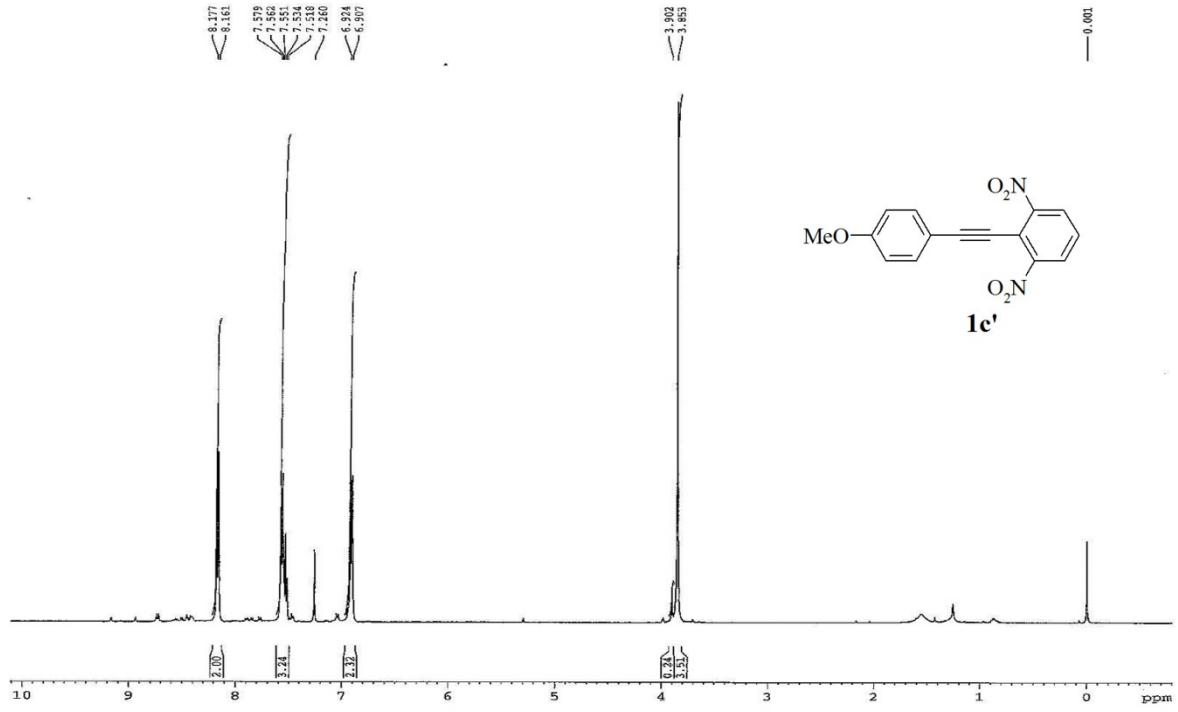
0
ppm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8.161
7.579
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7.518
7.260
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3.902
3.853
0.001
MeO
O_2N
O_2N
1c'
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6.74
3.53
10
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6
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3
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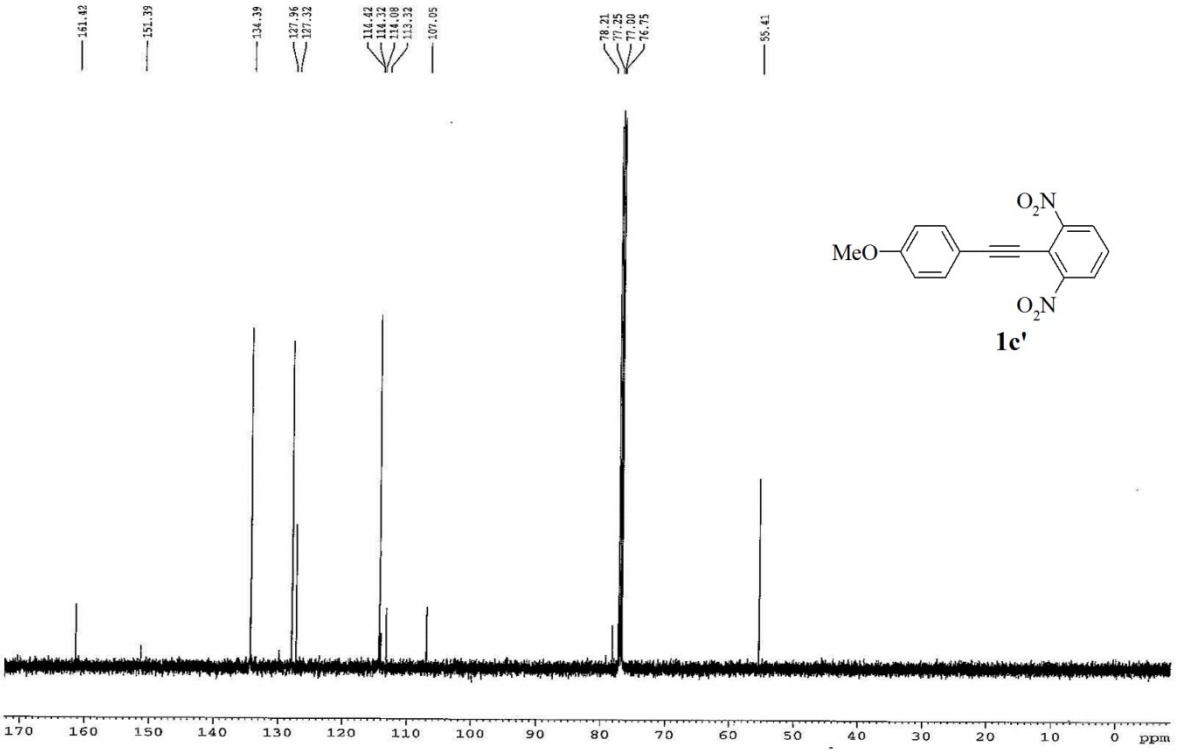
ppm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114.08
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107.05
78.21
77.25
77.00
76.75
55.41
MeO
O_2N
O_2N
1c'
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140
130
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100
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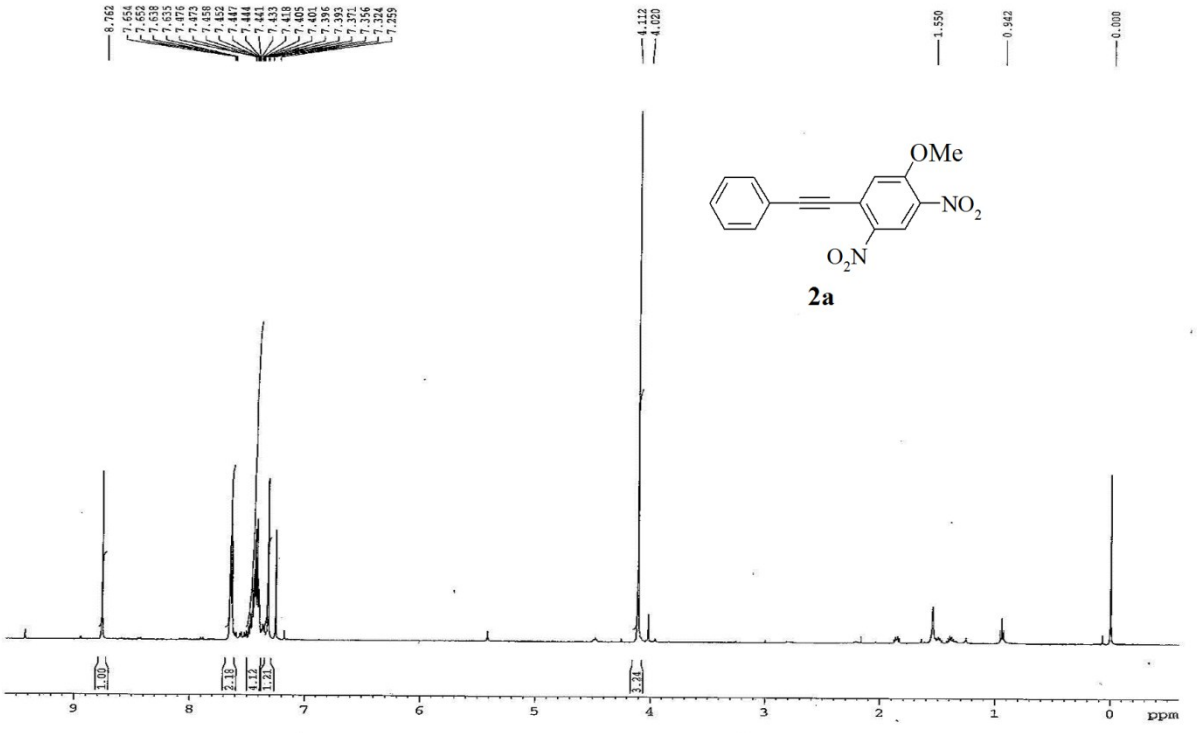
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7.458
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7.444
7.441
7.433
7.418
7.405
7.401
7.396
7.393
7.371
7.356
7.324
7.259
4.112
4.020
1.550
0.842
0.000
OMe
NO2
O2N
2a
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1.12
1.21
3.24
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8
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6
5
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0
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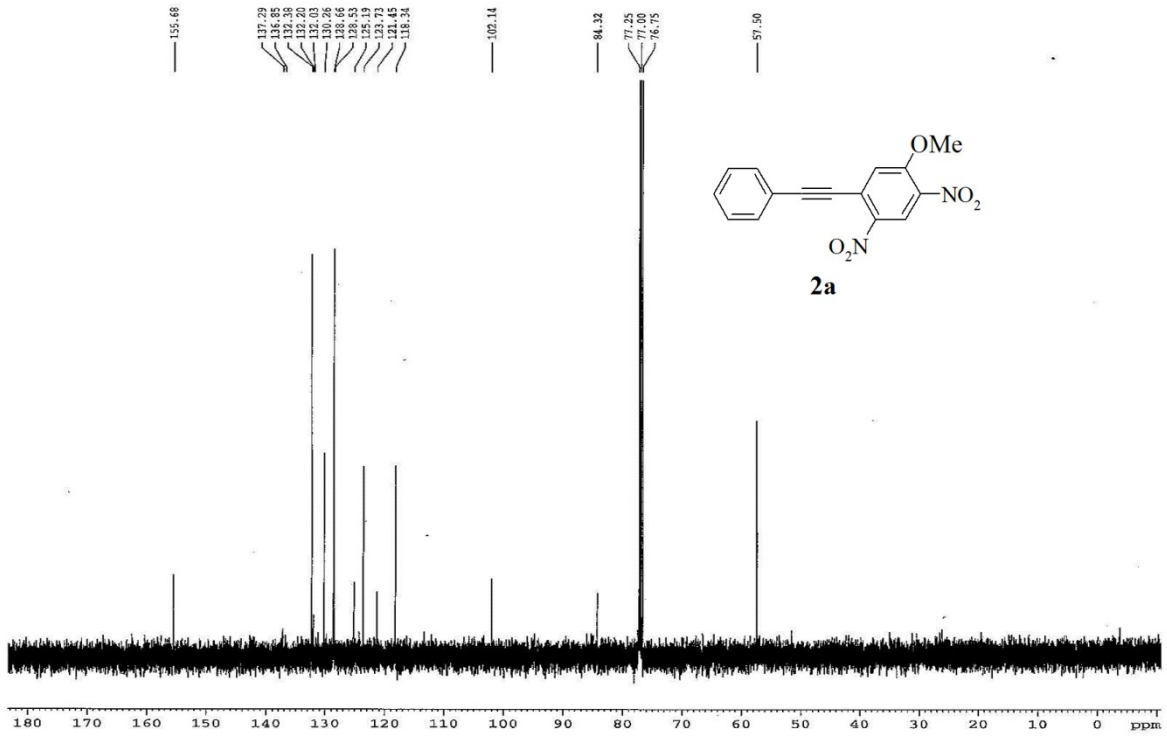
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137.29
136.85
132.38
132.03
131.03
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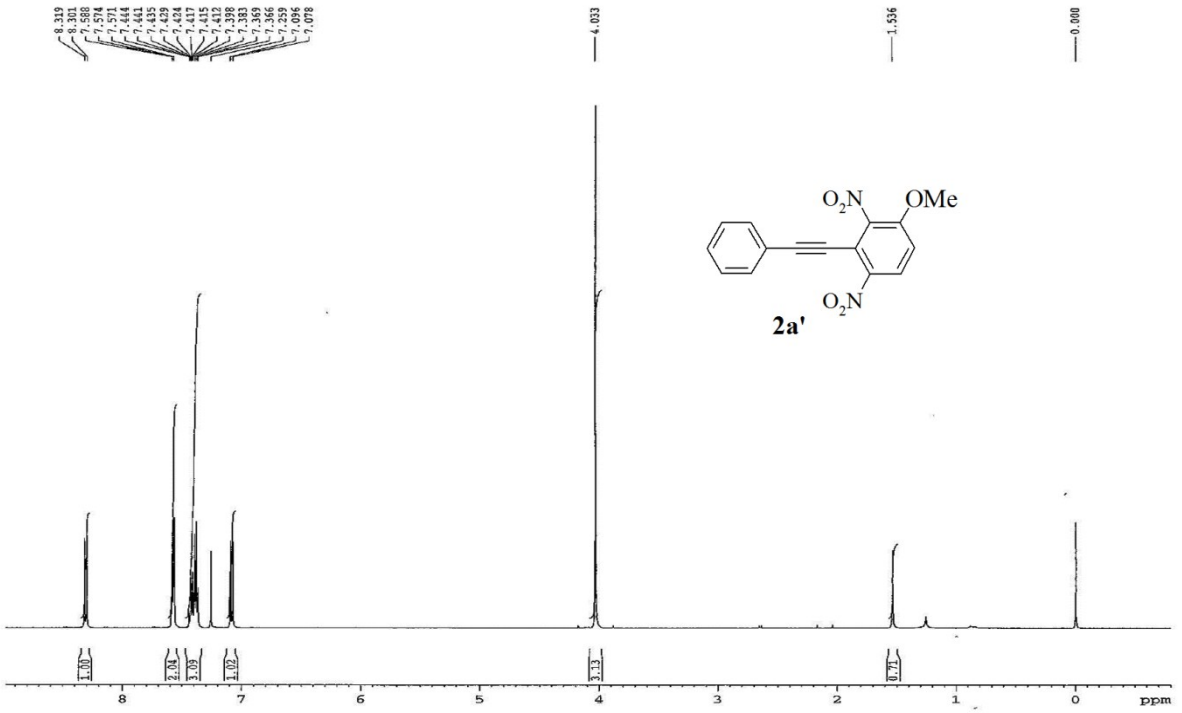
128.66
128.53
125.19
123.73
121.45
118.34
102.14
84.32
77.25
77.00
76.75
57.50
OMe
NO2
O2N
2a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.301
7.588
7.574
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7.444
7.441
7.435
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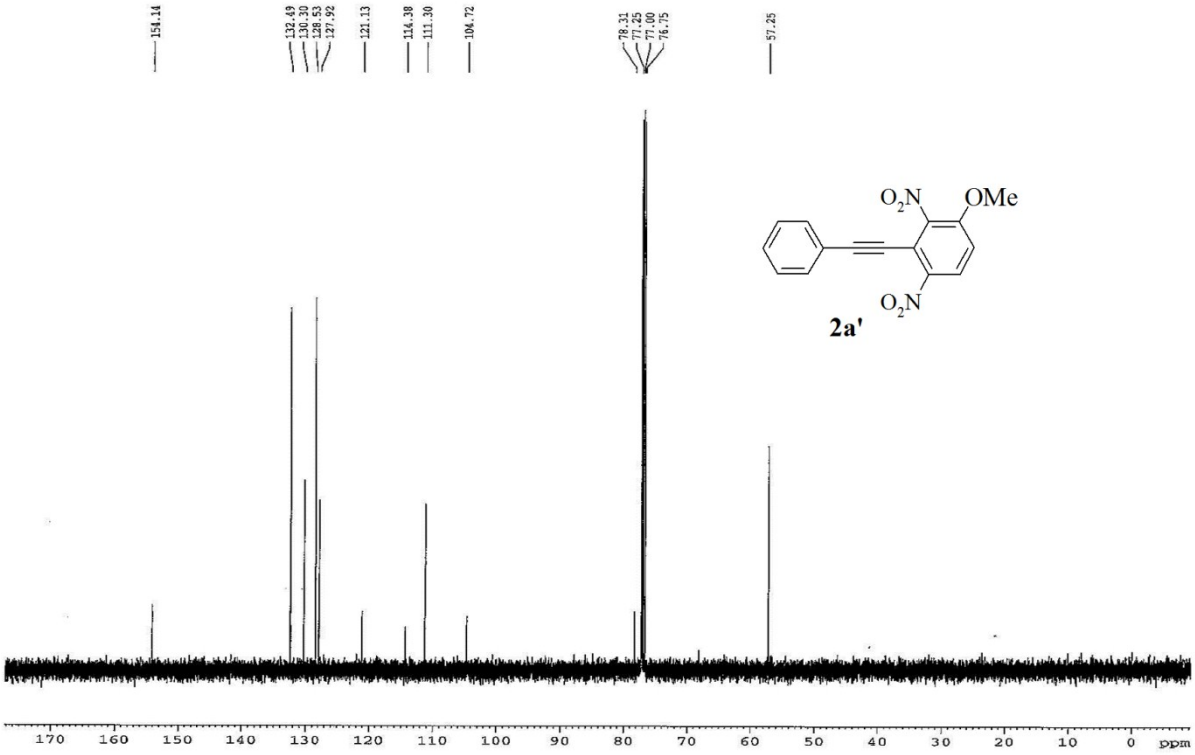
7.424
7.417
7.415
7.412
7.398
7.383
7.369
7.366
7.259
7.096
7.078
4.033
1.536
0.000
O2N
OMe
O2N
2a'
1.00
2.04
3.09
1.02
3.13
6.71
8
7
6
5
4
3
2
1
0
ppm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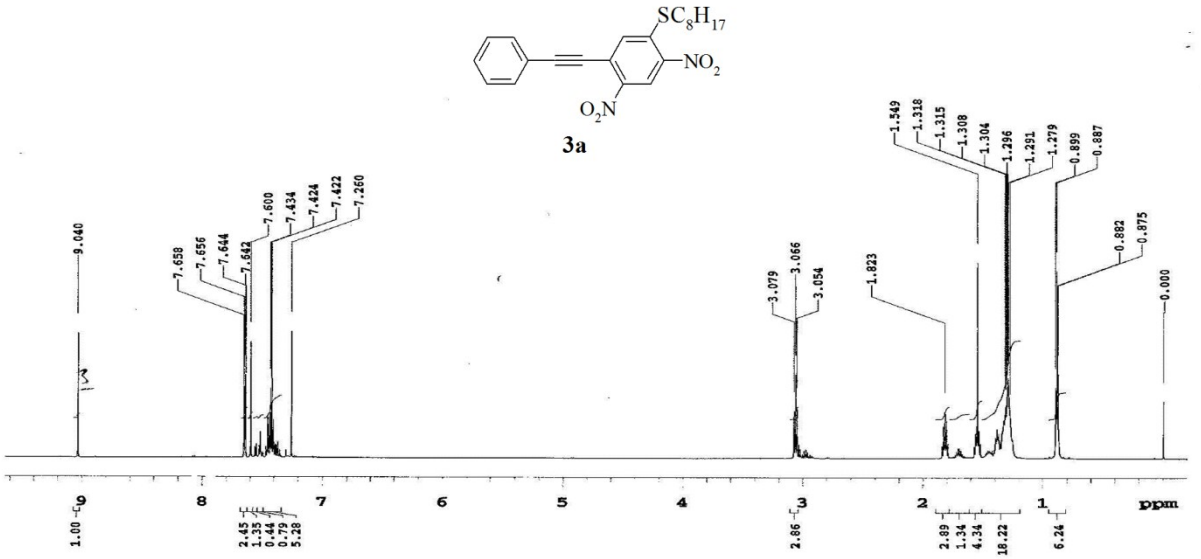
129.53
127.92
121.13
114.38
111.30
104.72
78.31
77.25
77.00
76.75
57.25
O2N
OMe
O2N
2a'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


SC8H17
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O2N
3a
9.040
7.658
7.656
7.644
7.642
7.600
7.434
7.424
7.422
7.260
3.079
3.066
3.054
1.823
1.549
1.318
1.315
1.308
1.304
1.296
1.291
1.279
0.899
0.887
0.882
0.875
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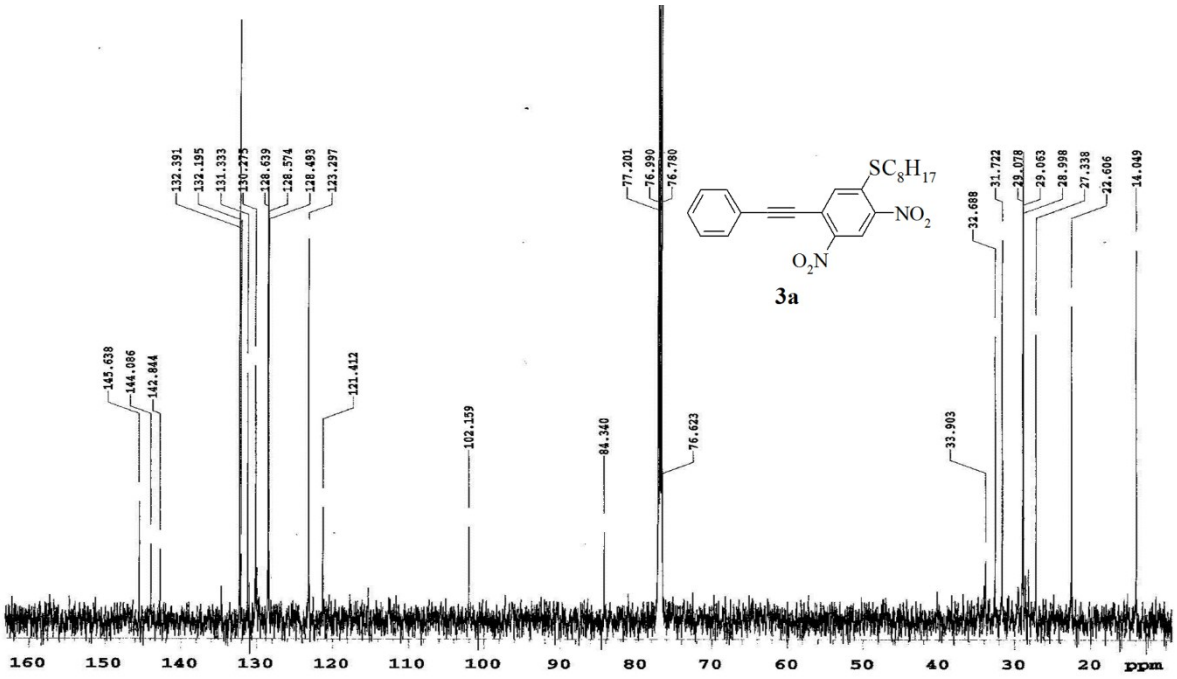
ppm


SC8H17
NO2
O2N
3a
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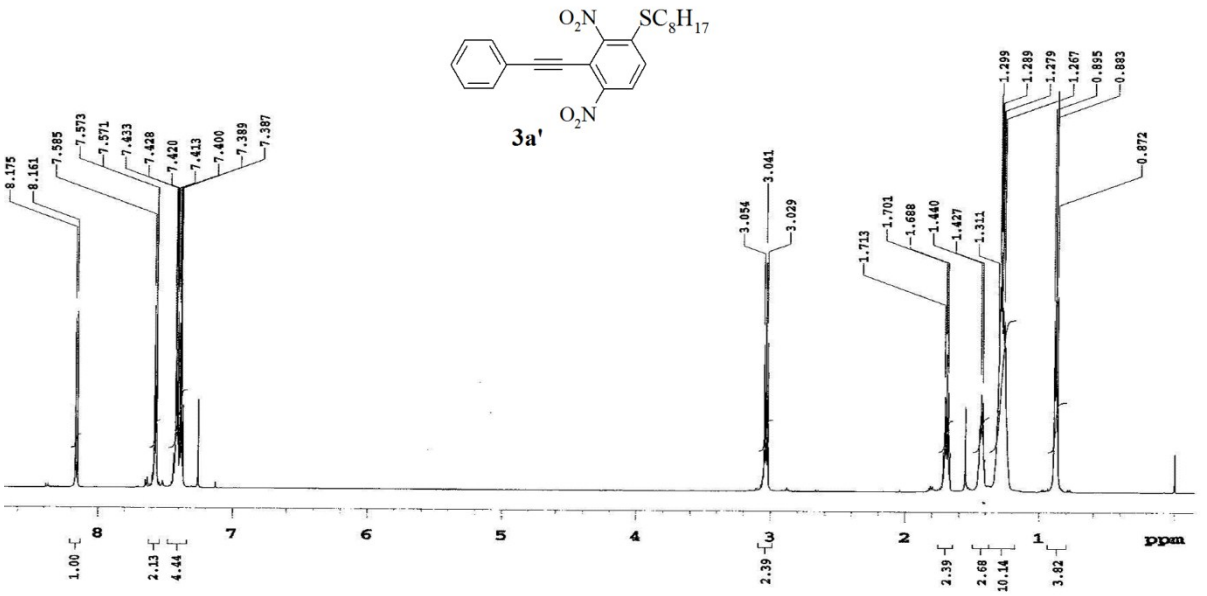
144.086
142.844
132.391
132.195
131.333
130.275
128.639
128.574
128.493
123.297
121.412
102.159
84.340
77.201
76.990
76.780
76.623
33.903
32.688
31.722
29.078
29.063
28.998
27.338
22.606
14.049
ppm


3a'
8.175
8.161
7.585
7.573
7.571
7.433
7.428
7.420
7.413
7.400
7.389
7.387
3.054
3.041
3.029
1.713
1.701
1.688
1.440
1.427
1.311
1.299
1.289
1.279
1.267
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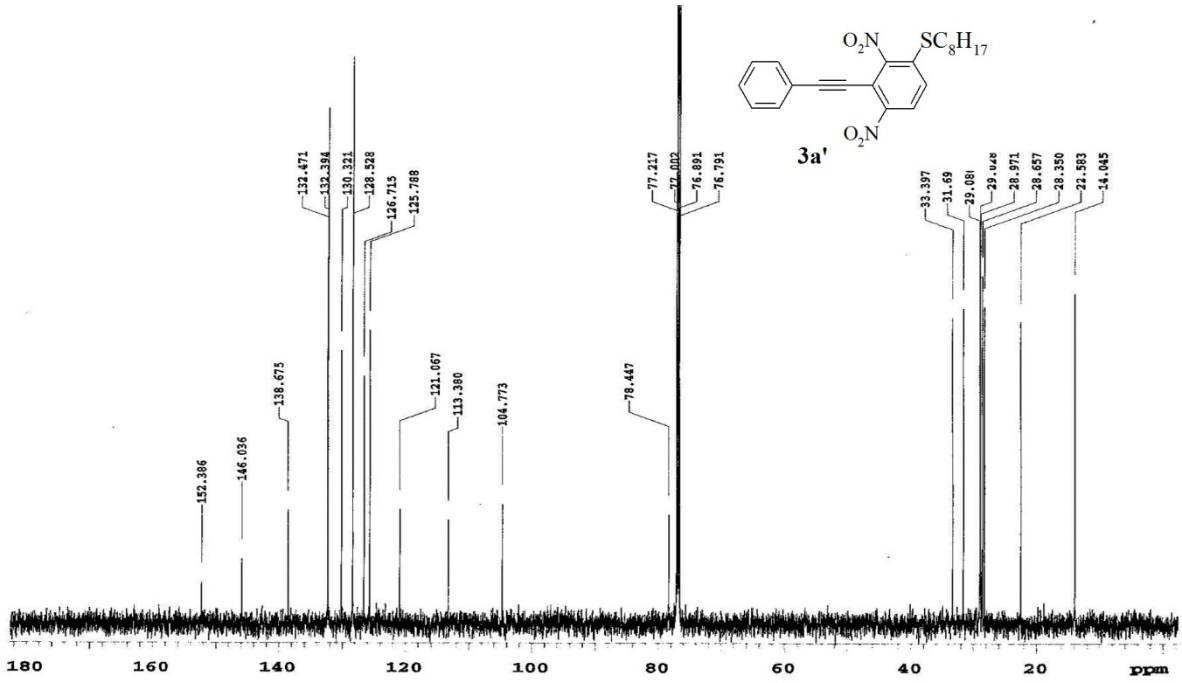
0.883
0.872
ppm


3a'
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146.036
138.675
132.471
132.384
130.321
128.528
126.715
125.788
121.067
113.380
104.773
78.447
77.217
77.002
76.891
76.791
33.397
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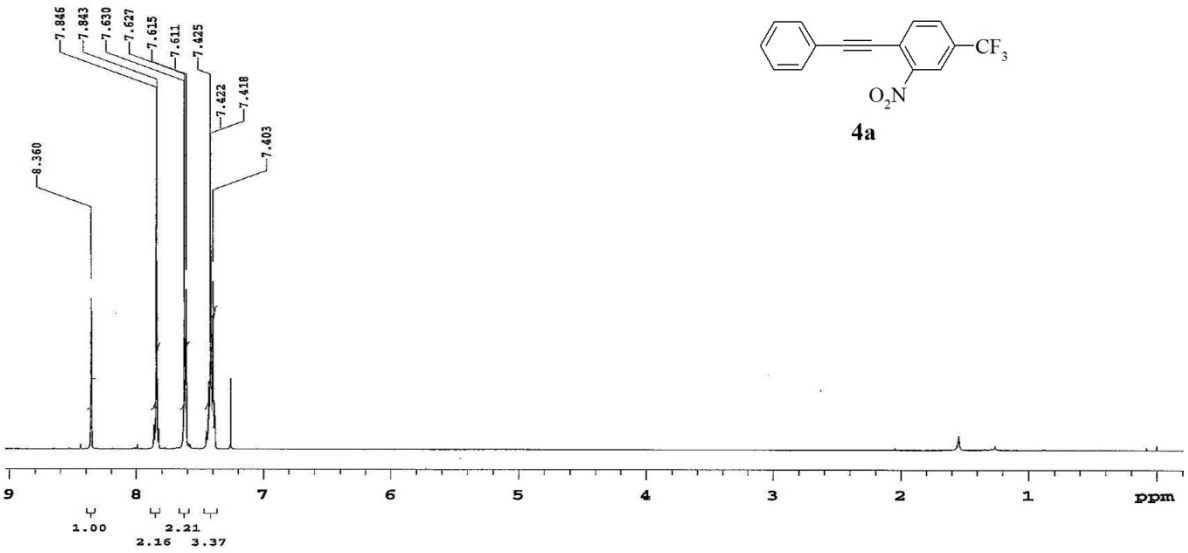
29.081
28.971
28.657
28.350
22.583
14.045
ppm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7.630
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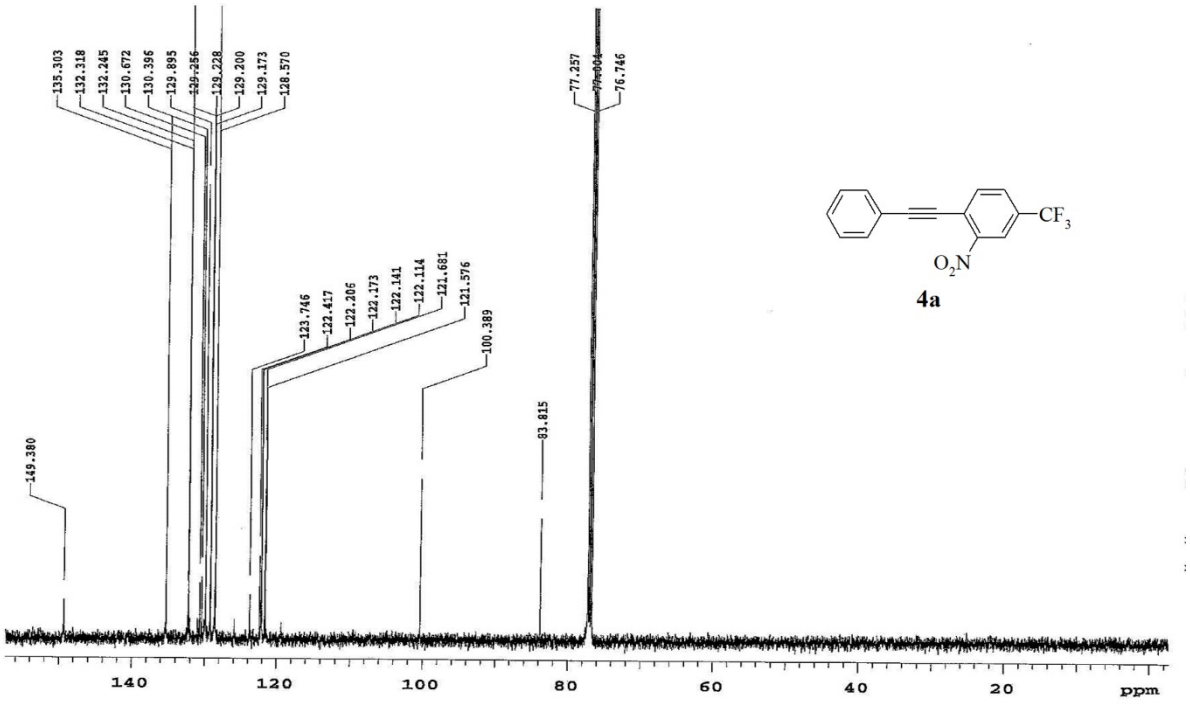
7.425
7.422
7.418
7.403
8.360
9
8
7
6
5
4
3
2
1
ppm
1.00
2.21
2.16
3.37
CF3
O2N

4a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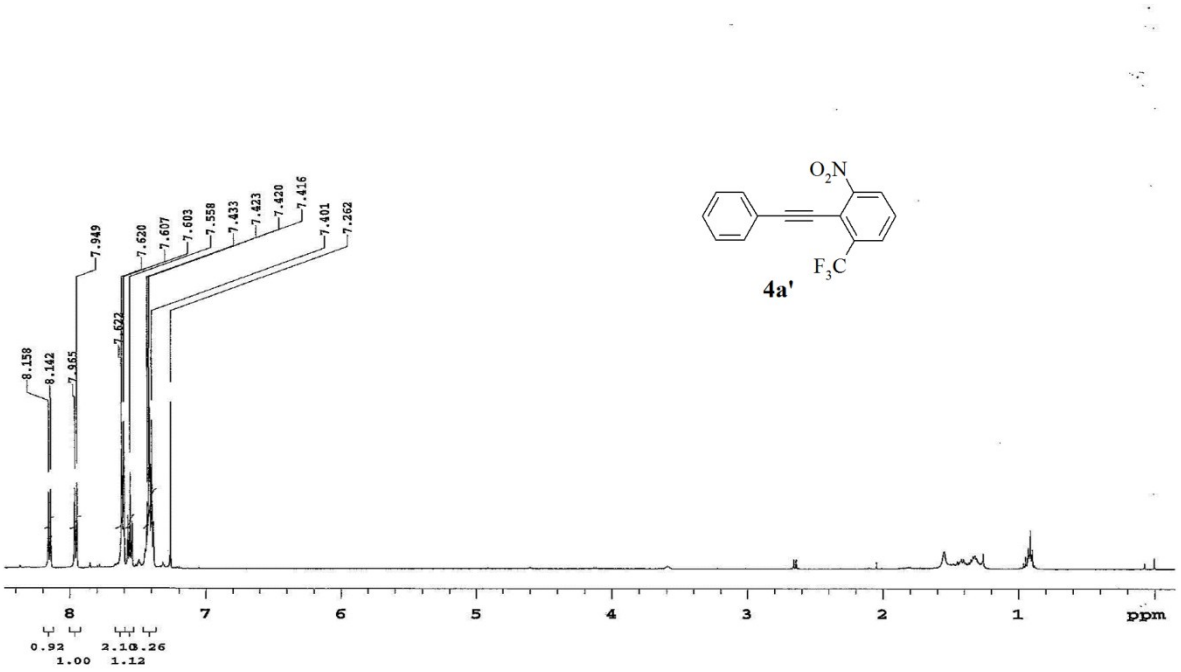
132.318
132.245
130.672
130.396
129.895
129.256
129.228
129.200
129.173
128.570
123.746
122.417
122.206
122.173
122.141
122.114
121.681
121.576
100.389
83.815
77.257
77.004
76.746
149.380
140
120
100
80
60
40
20
ppm
CF3
O2N

4a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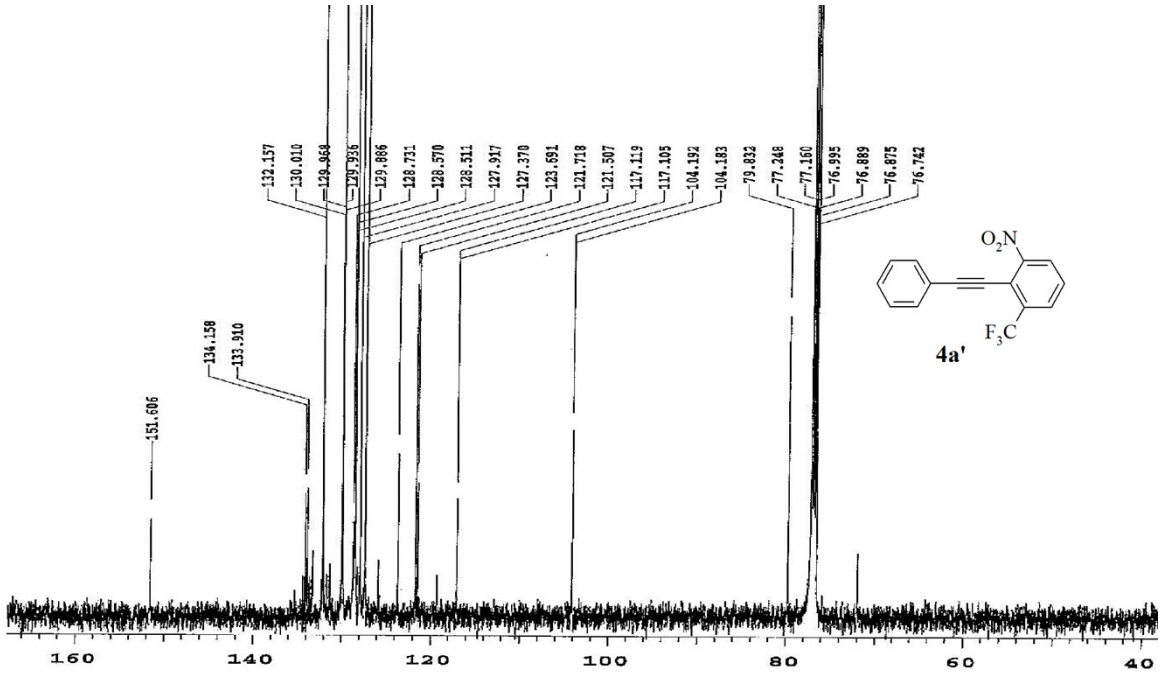
8.142
7.949
7.865
7.622
7.620
7.607
7.603
7.558
7.433
7.423
7.420
7.416
7.401
7.262
8
7
6
5
4
3
2
1
ppm
0.92
1.00
2.10
1.12
0.26
O2N
F3C
4a'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129.963
129.936
129.886
128.731
128.570
128.511
127.917
127.370
123.691
121.718
121.507
117.119
117.105
104.192
104.183
79.832
77.248
77.160
76.995
76.889
76.875
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134.158
133.910
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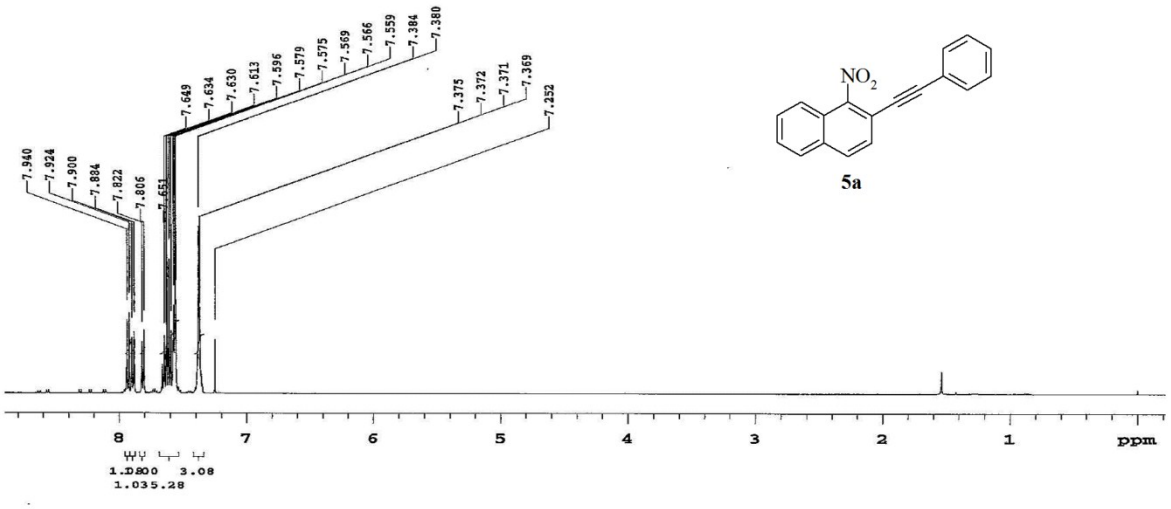
160
140
120
100
80
60
40
O2N
F3C
4a'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7.924
7.900
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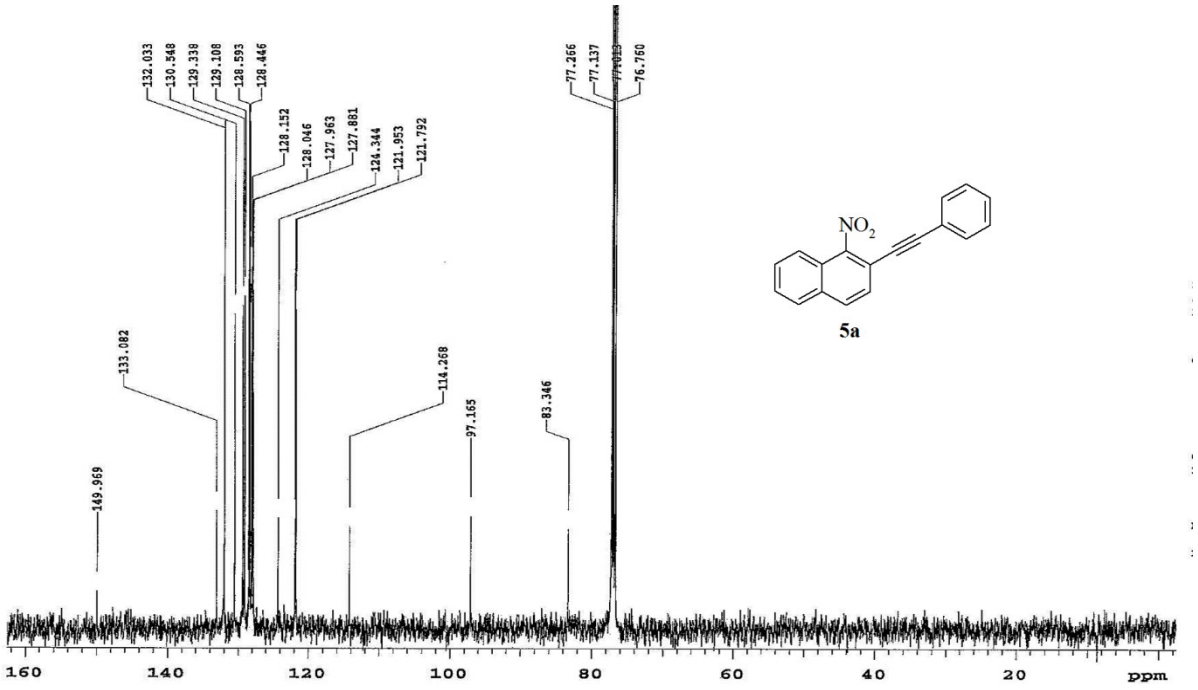
7.822
7.806
7.651
7.649
7.634
7.630
7.613
7.596
7.579
7.575
7.569
7.566
7.559
7.384
7.380
7.375
7.372
7.371
7.369
7.252
8
7
6
5
4
3
2
1
ppm
1.035.28
3.08

NO2

5a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130.548
129.338
129.108
128.593
128.446
128.152
128.046
127.963
127.881
124.344
121.953
121.792
77.266
77.137
76.760
133.082
114.268
97.165
83.346
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120
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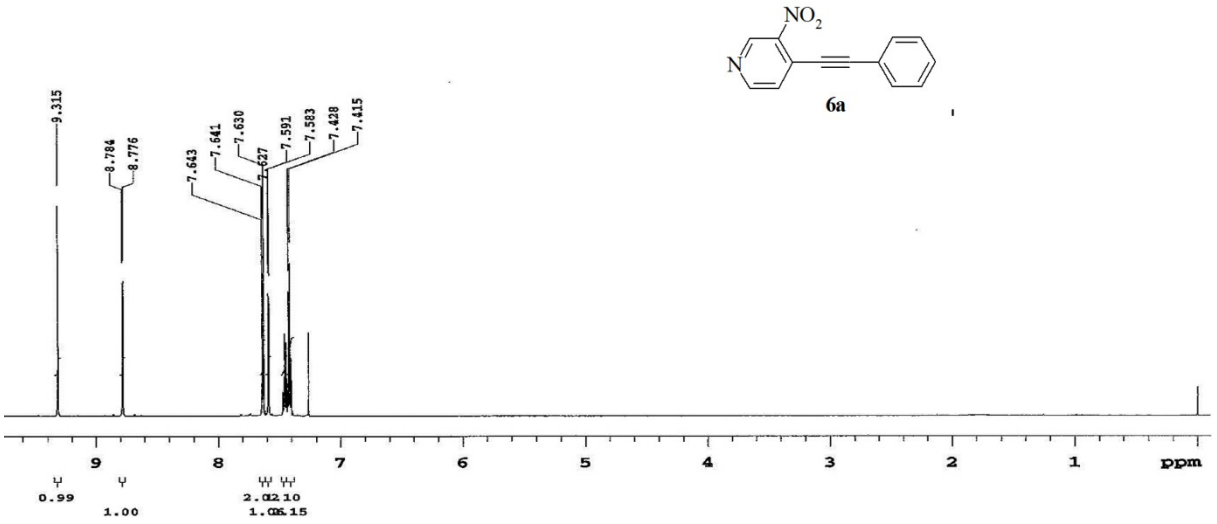
80
60
40
20
ppm

NO2

5a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8.776
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7.641
7.630
7.627
7.591
7.583
7.428
7.415
9
8
7
6
5
4
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2
1
ppm
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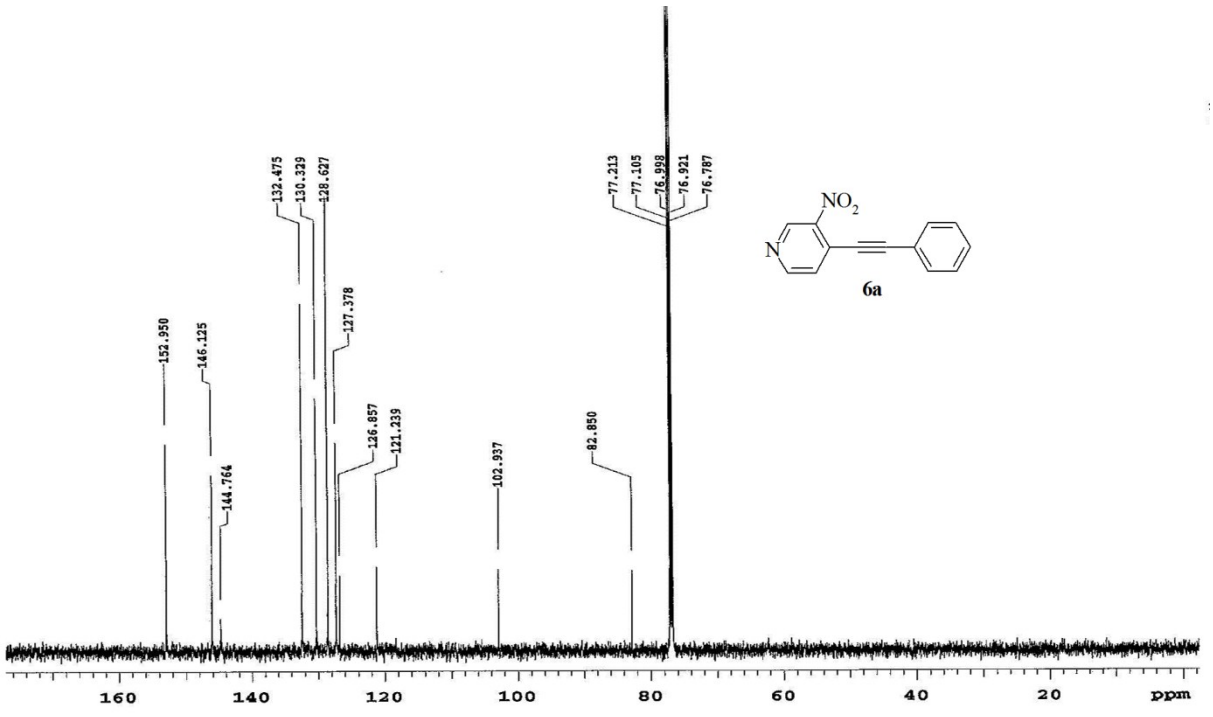
2.10
1.00
5.15

NO2
N

6a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127.378
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121.239
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82.850
77.213
77.105
76.998
76.921
76.787
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146.125
144.764
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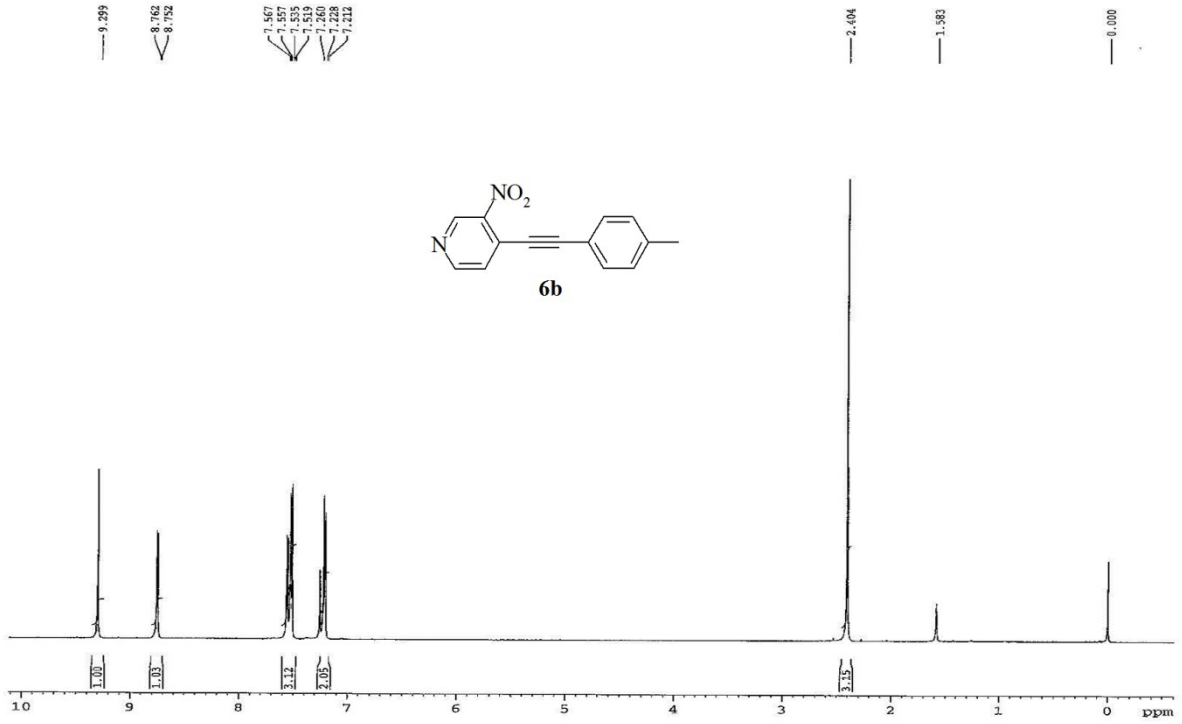
80
60
40
20
ppm

NO2
N

6a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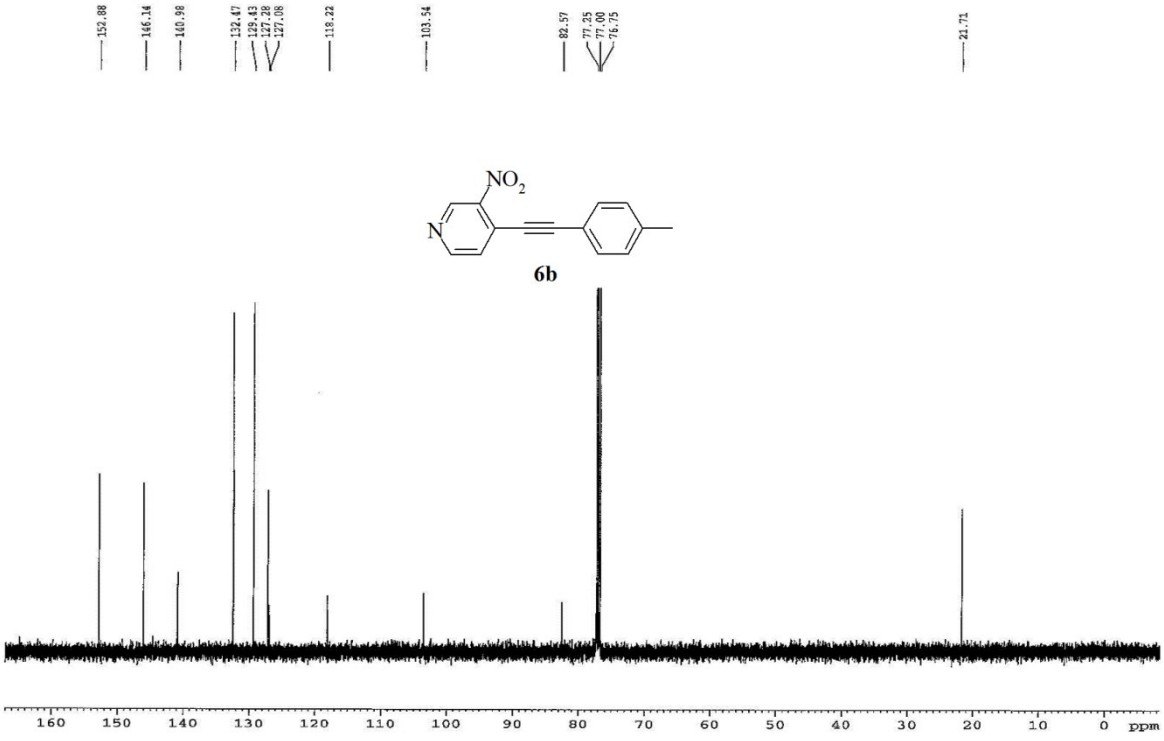
7.535
7.519
7.260
7.228
7.212
2.404
1.583
0.000
NO2
N
6b
1.00
1.03
3.12
2.05
3.15
10
9
8
7
6
5
4
3
2
1
0
ppm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132.47
129.43
127.28
127.08
118.22
103.54
82.57
77.25
77.00
76.75
21.71
NO2
N
6b
160
150
140
130
120
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100
90
80
70
60
50
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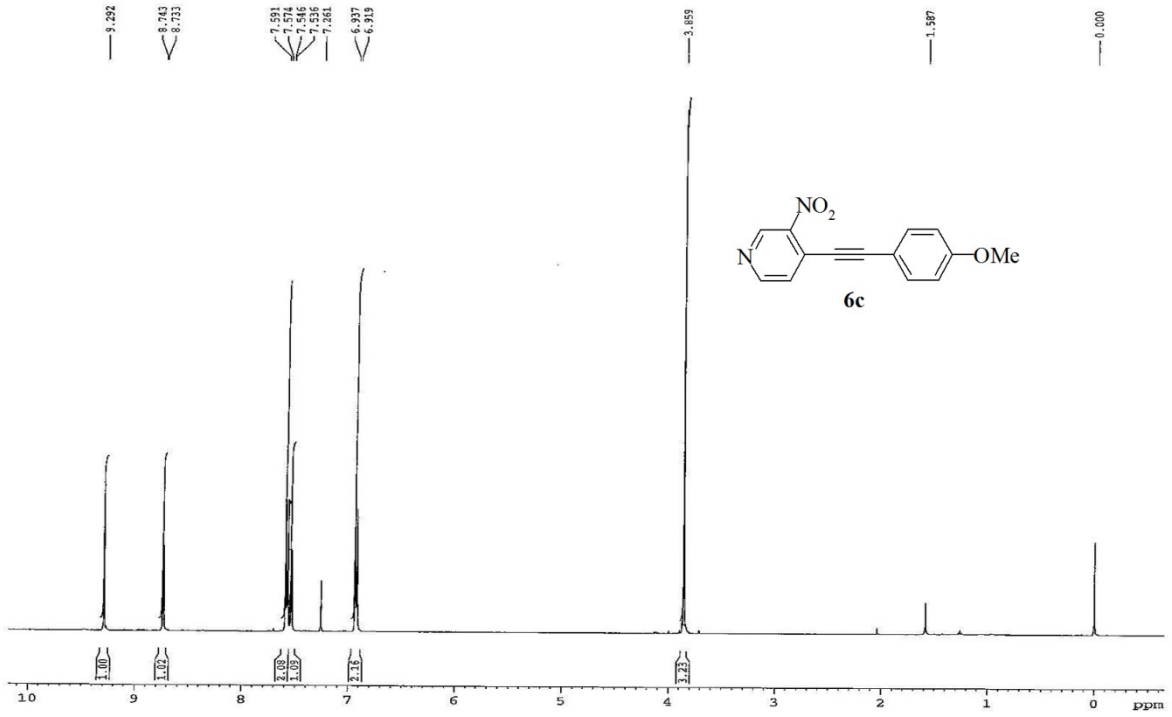
30
20
10
0
ppm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7.566
7.546
7.261
6.937
6.919
3.859
1.587
0.000
NO2
N
OMe
6c
1.00
1.02
2.08
1.08
2.16
3.23
10
9
8
7
6
5
4
3
2
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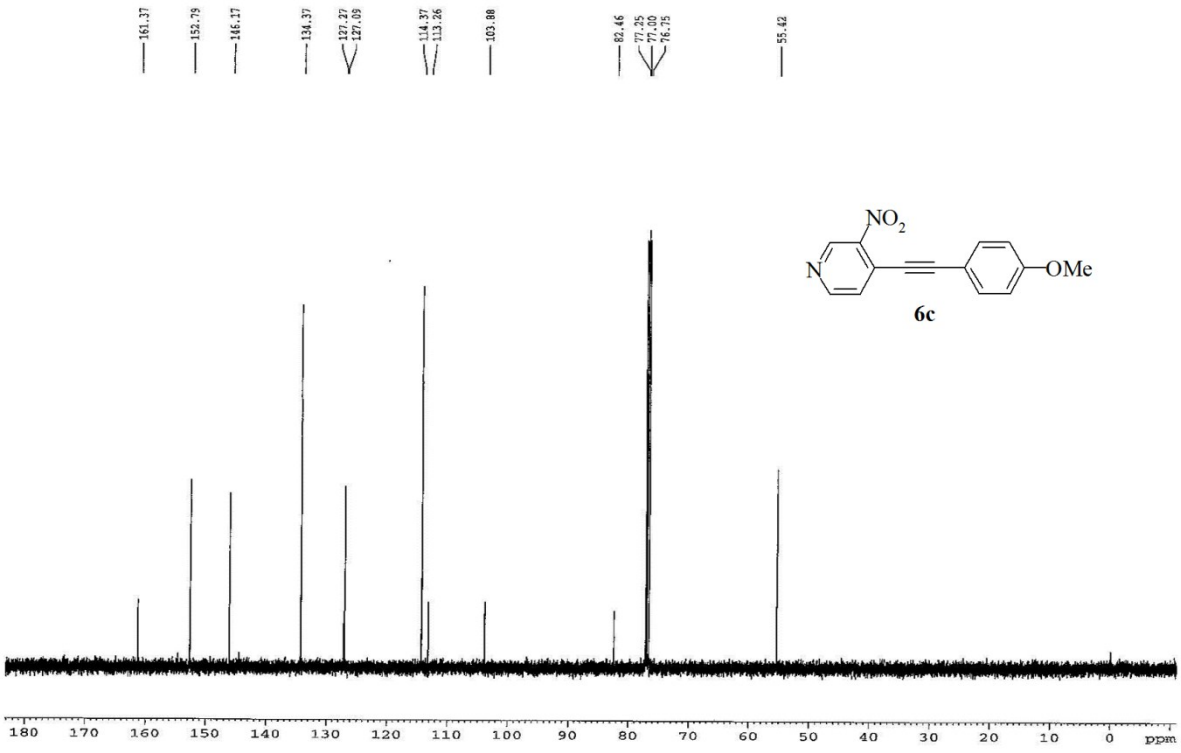
0
ppm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127.27
127.09
114.37
113.26
103.88
82.46
77.25
77.00
76.75
55.42
NO2
N
OMe
6c
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170
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140
130
120
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100
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80
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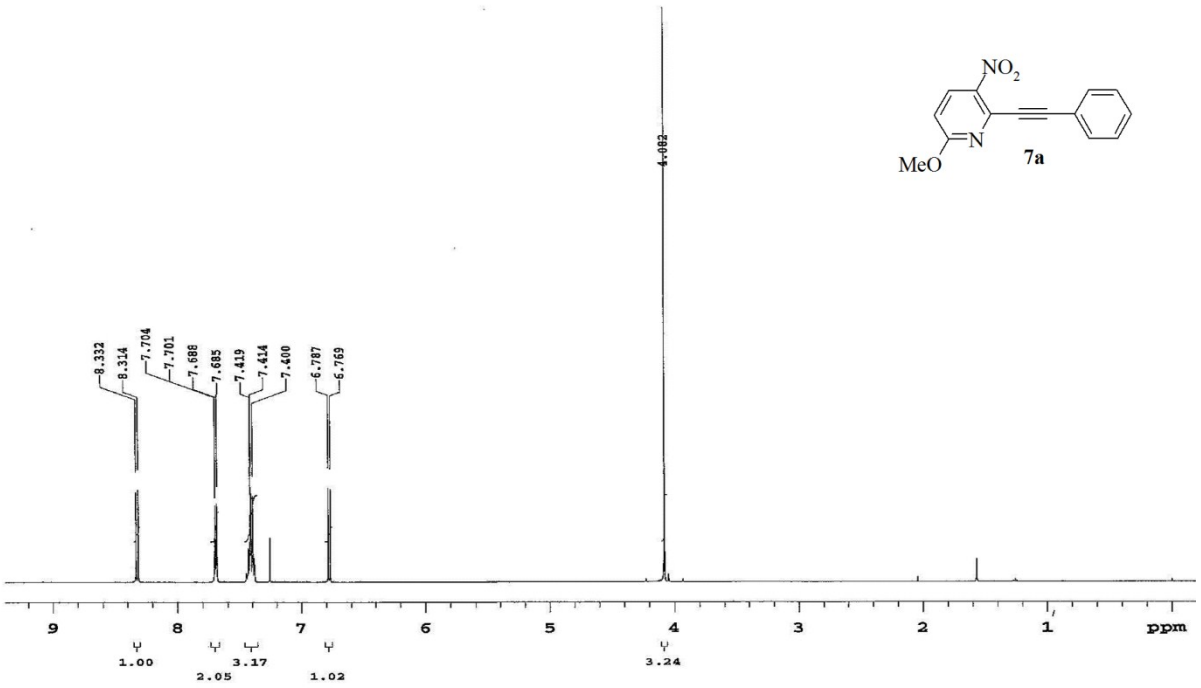
60
50
40
30
20
10
0
ppm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7.414
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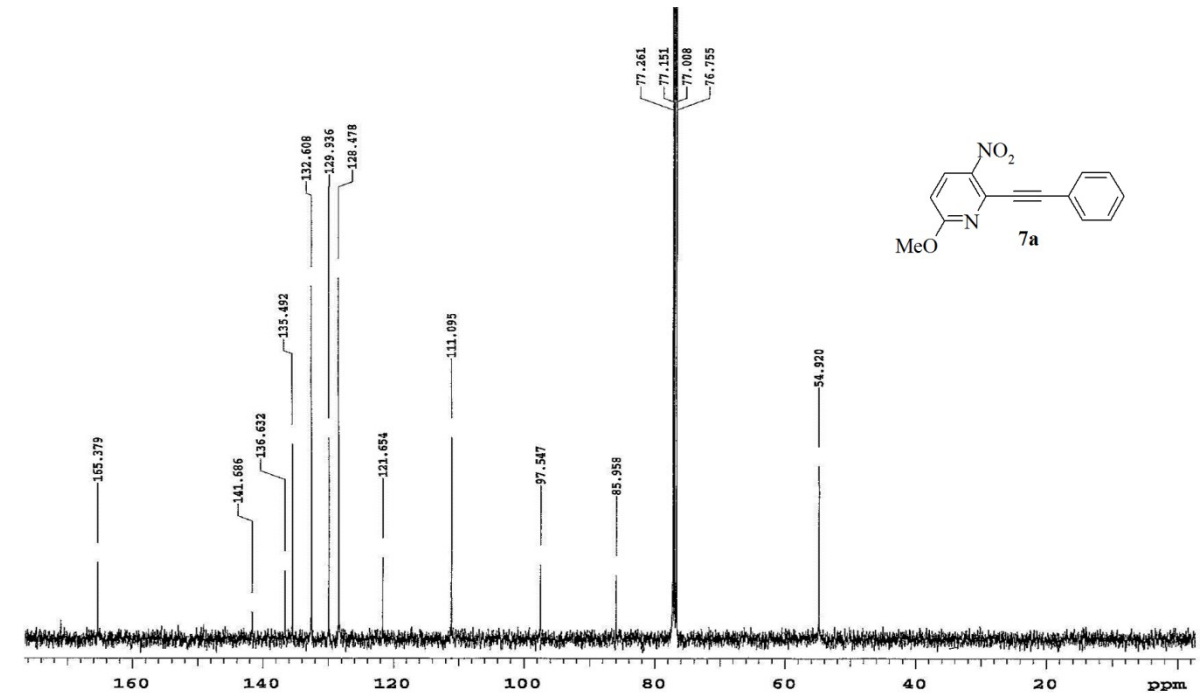
9
8
7
6
5
4
3
2
1
ppm
1.00
2.05
3.17
1.02
3.24
NO2
N
MeO
7a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77.008
76.755
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129.936
128.478
135.492
111.095
54.920
136.632
141.686
165.379
121.654
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85.958
160
140
120
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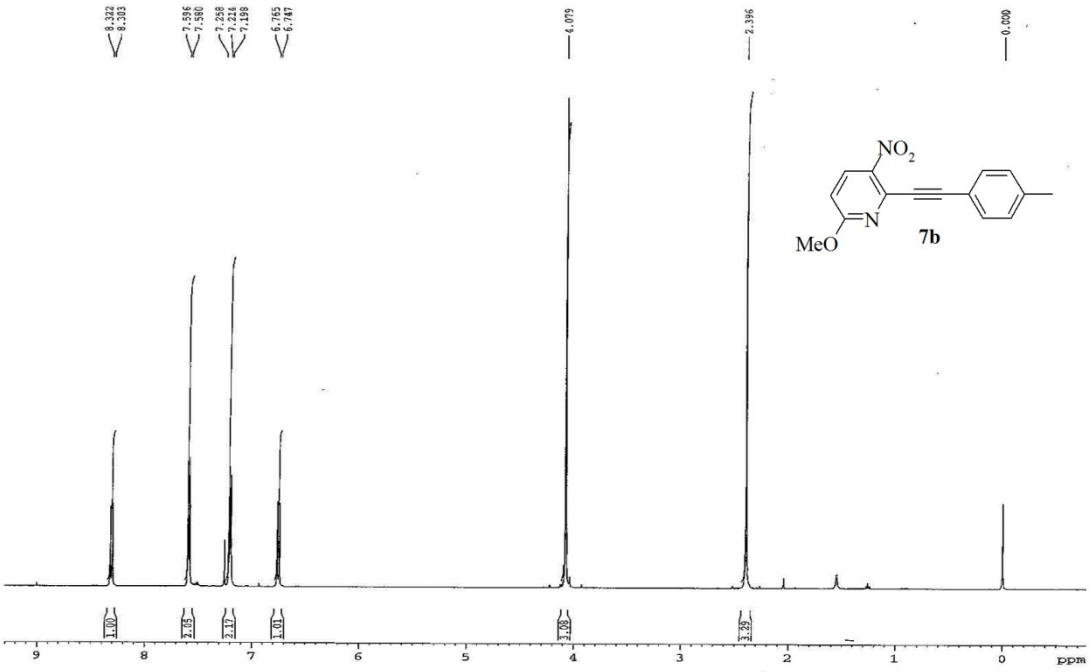
80
60
40
20
ppm
NO2
N
MeO
7a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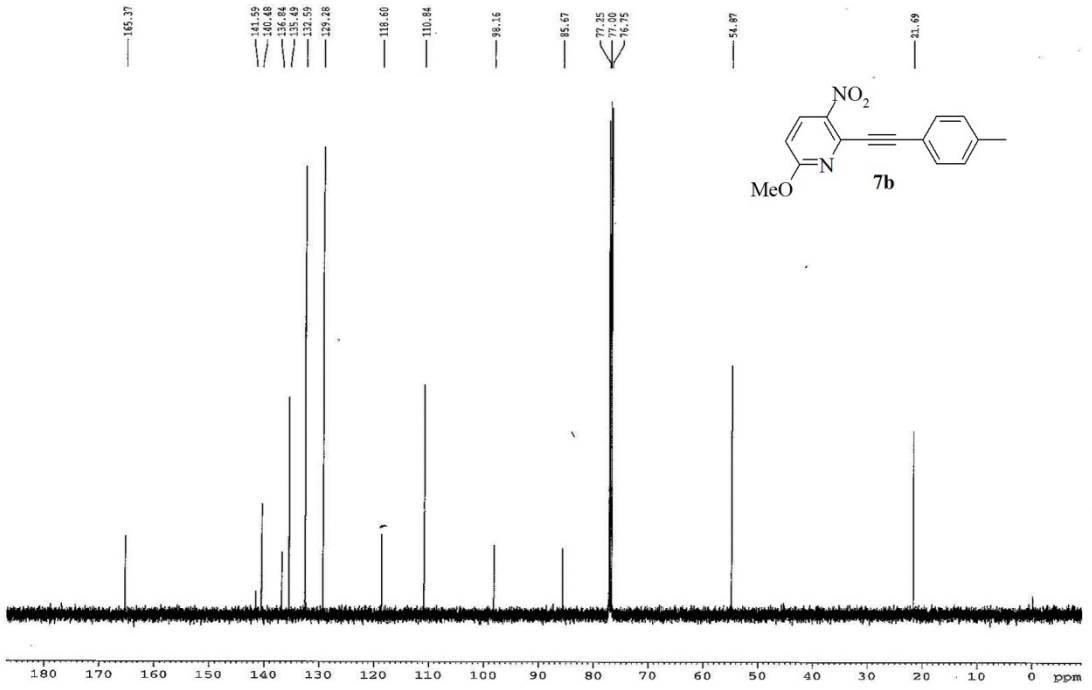
8.303
7.586
7.580
7.238
7.224
7.198
6.765
6.747
4.079
2.396
0.000
NO2
N
MeO
7b
1.00
2.08
2.17
1.01
3.00
3.29
9
8
7
6
5
4
3
2
1
0
ppm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135.49
132.59
129.28
118.60
110.84
98.16
85.67
77.25
77.00
76.75
54.87
21.69
NO2
N
MeO
7b
180
170
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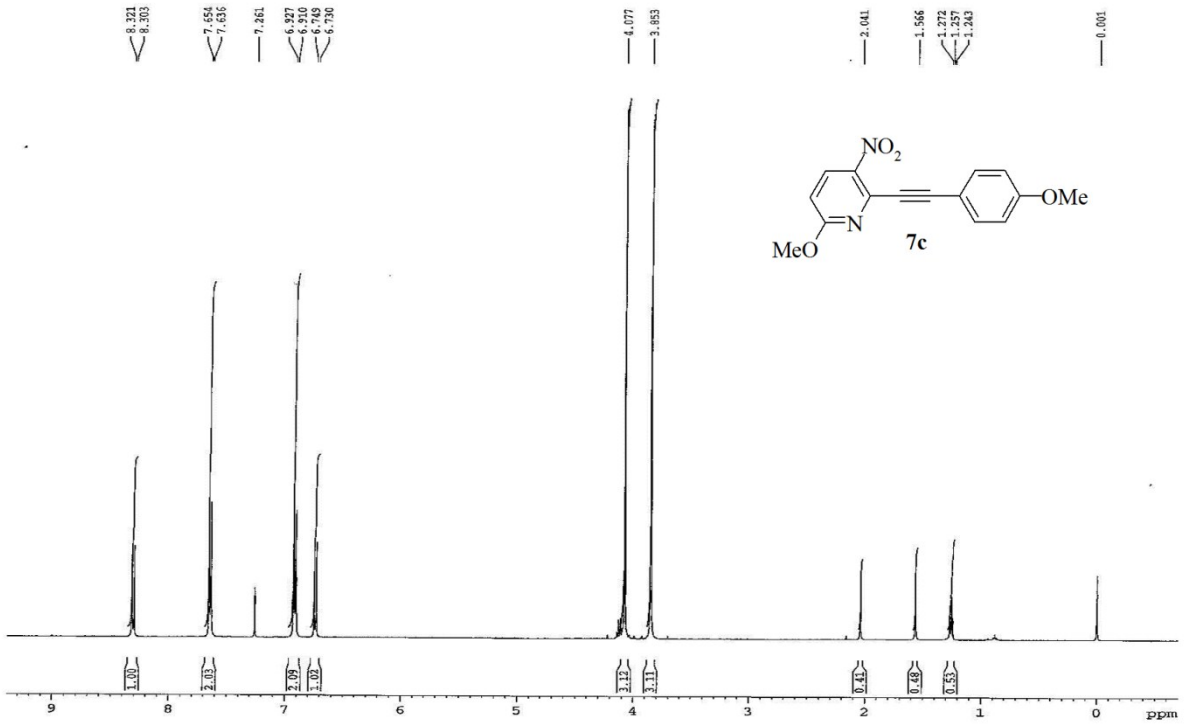
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.303
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7.261
6.927
6.910
6.749
6.730
4.077
3.853
2.041
1.566
1.272
1.257
1.243
0.001
NO2
OMe
N
MeO
7c
1.00
2.03
2.09
1.02
3.12
3.11
0.41
0.48
0.53
9
8
7
6
5
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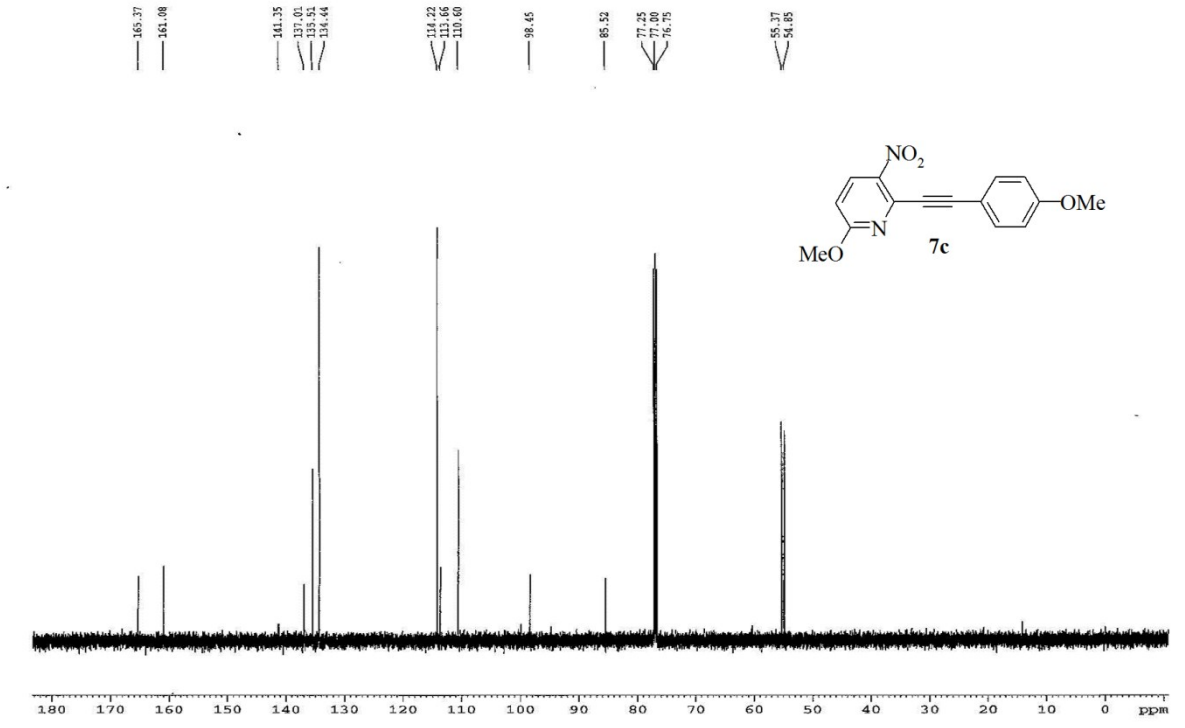
3
2
1
0
ppm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134.44
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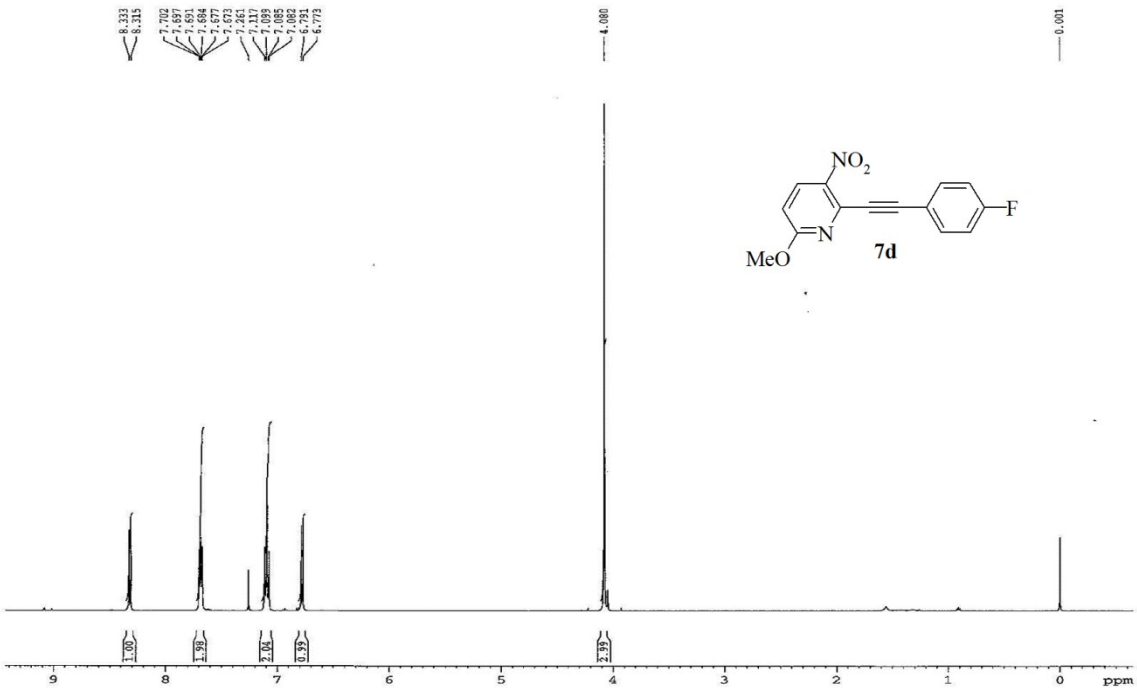
113.66
110.60
98.45
85.52
77.25
77.00
76.75
55.37
54.85
NO2
OMe
N
MeO
7c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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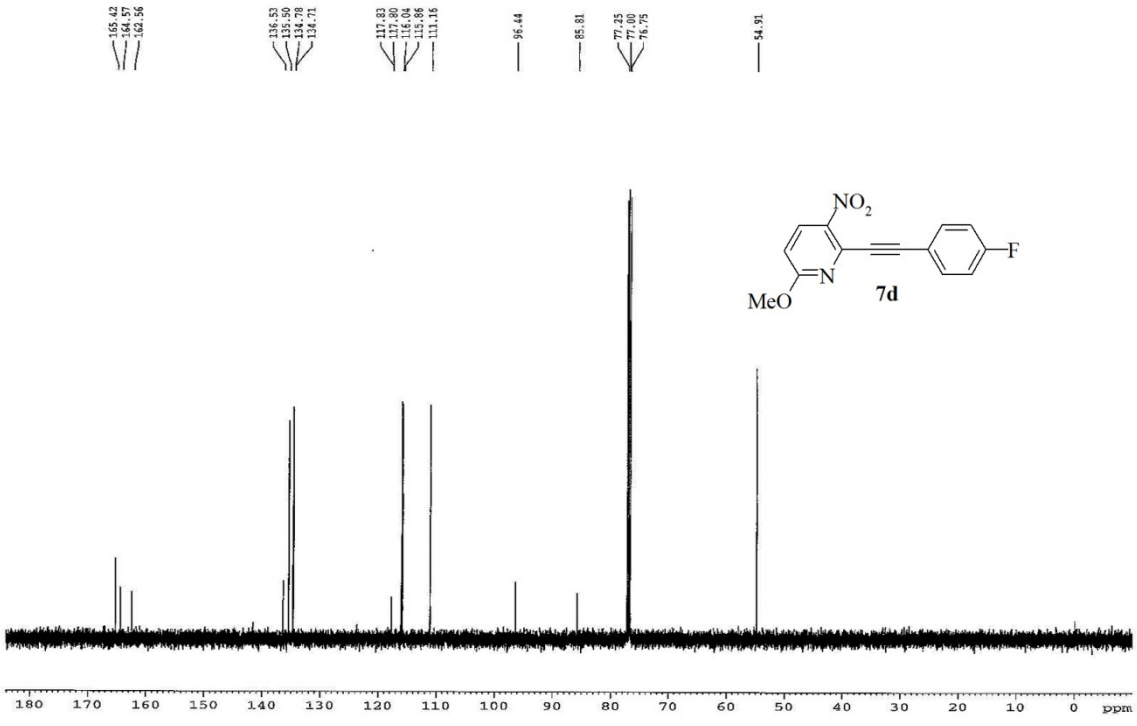
8.315
7.702
7.697
7.691
7.684
7.677
7.673
7.261
7.117
7.099
7.085
7.082
6.791
6.773
4.080
0.001
NO2
F
N
MeO
7d
1.00
1.98
2.04
0.99
2.98
9
8
7
6
5
4
3
2
1
0
ppm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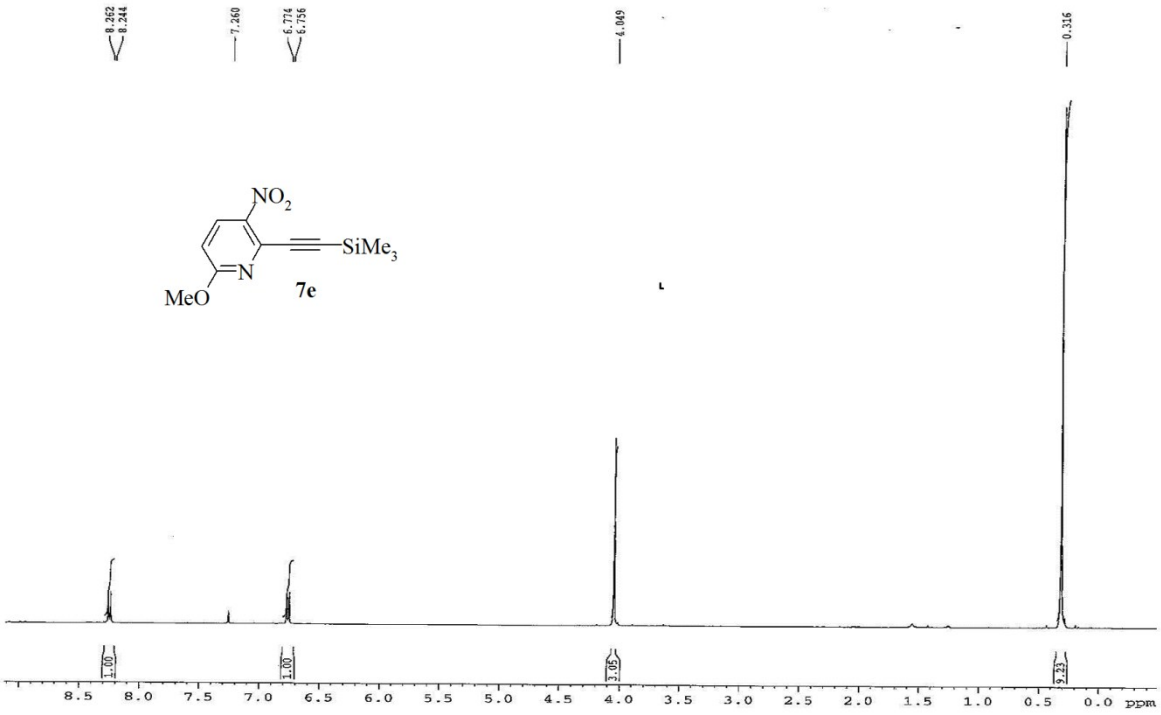
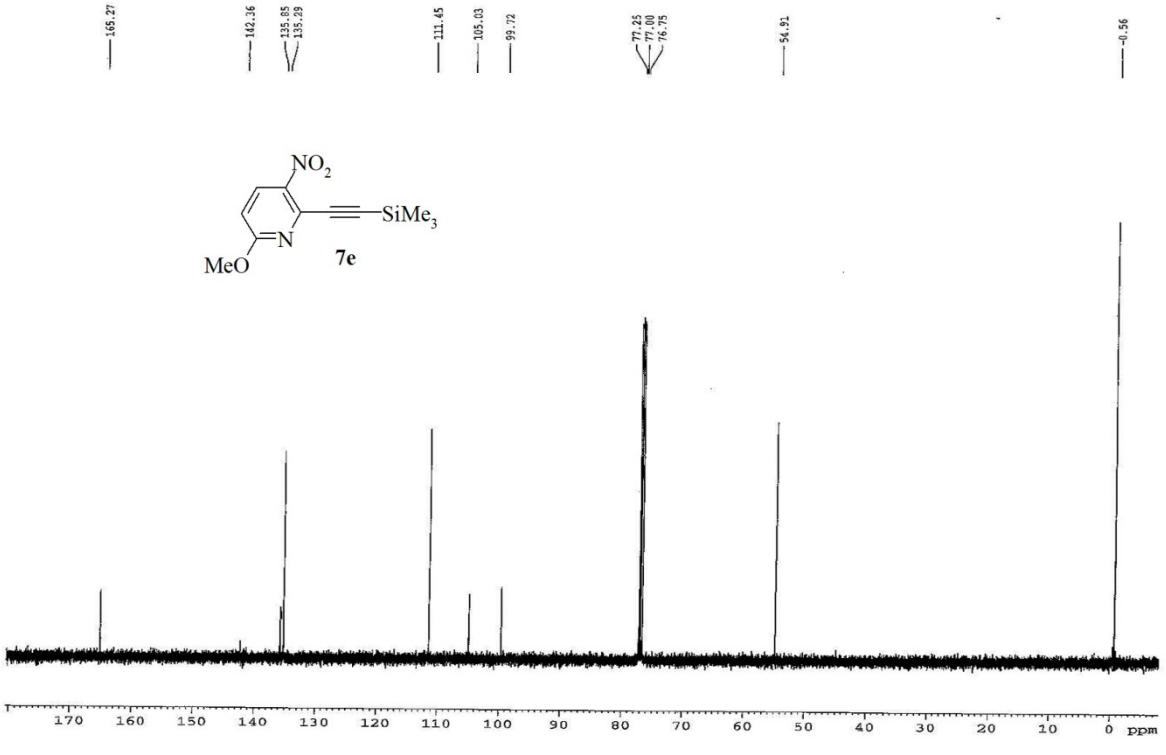
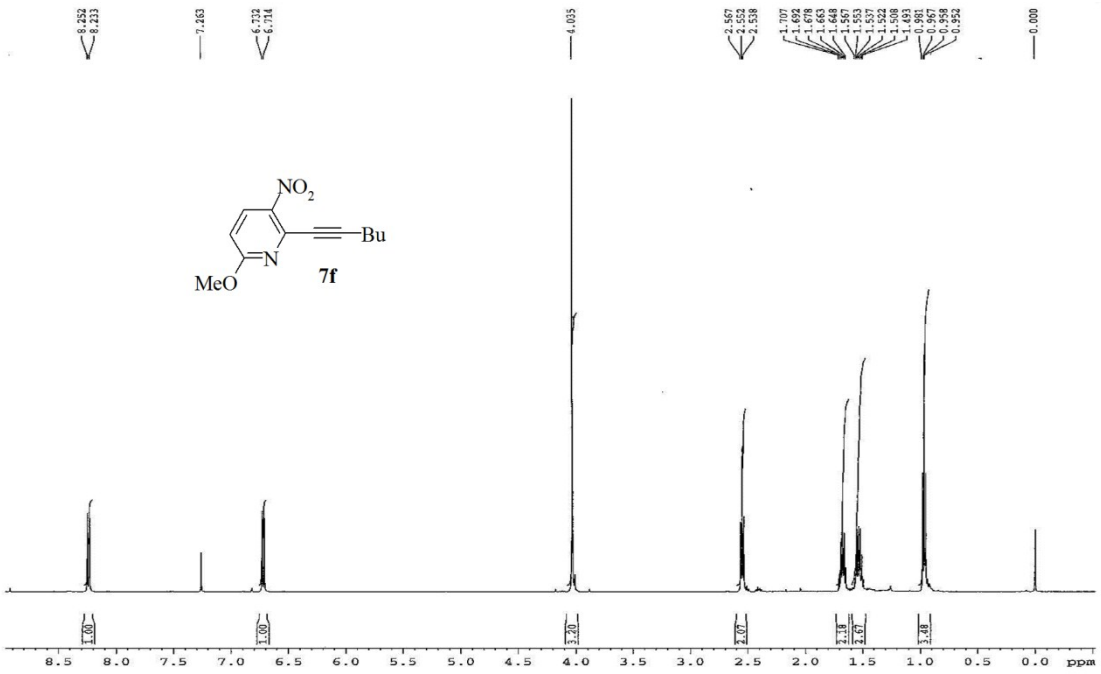
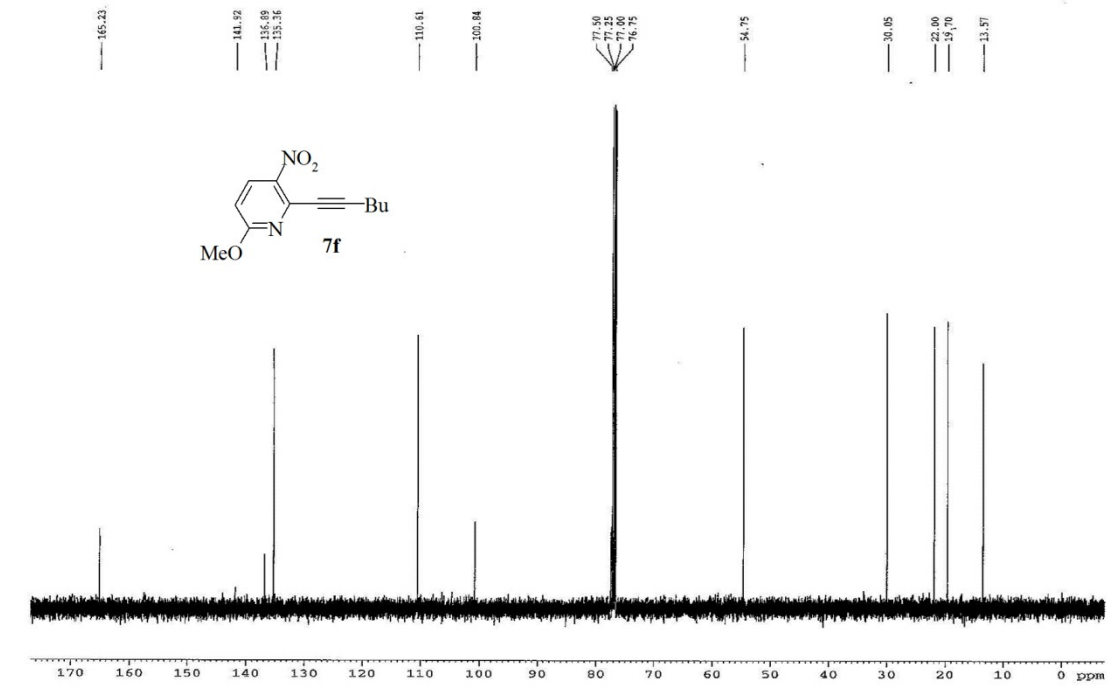
164.57
162.56
136.53
135.50
134.78
134.71
117.83
117.80
116.04
115.86
111.16
96.44
85.81
77.25
77.00
76.75
54.91
NO2
F
N
MeO
7d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.262
8.244
7.260
6.774
6.756
4.049
0.316
NO2
SiMe3
N
MeO
7e
1.00
1.00
3.05
9.29
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 ppm


165.27
142.36
135.85
135.39
111.45
105.03
99.72
77.25
77.00
76.75
54.91
-0.56
NO2
SiMe3
N
MeO
7e
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.252
8.233
7.263
6.732
6.714
4.035
2.567
2.552
2.538
1.707
1.692
1.678
1.663
1.648
1.567
1.553
1.537
1.522
1.508
1.493
0.981
0.967
0.958
0.952
0.000
NO2
Bu
N
MeO
7f
1.00
1.00
3.20
2.07
2.18
2.67
3.48
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
ppm


165.23
141.92
136.89
135.36
110.61
100.84
77.50
77.25
77.00
76.75
54.75
30.05
22.00
19.70
13.57
NO2
Bu
N
MeO
7f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm