Direct Arylations On Water: Synthesis of 2,5-Disubstituted Oxazoles Balsoxin and Texaline

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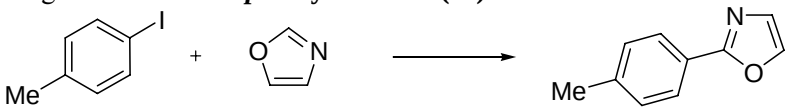
Part A: Experimental Procedures

General

NMR spectra were obtained from a Brüker AC250 (250MHz) instrument and calibrated to residual solvent peaks: ^{1}H - $CDCl_3$, 7.26 ppm and ^{13}C – $CDCl_3$, 77.0 ppm. The ^{1}H-NMR data is presented as follows: chemical shift (in ppm on the δ scale), integration, multiplicity (s= singlet, d= doublet, t= triplet, q= quartet, m= multiplet), coupling constant (J in Hz) and structural assignment. The ^{13}C-NMR data is reported as ppm on the δ scale, followed by the structural assignment. High resolution mass spectrometry was performed by the EPSRC National Mass Spectrometry Service Centre, Swansea, using Finnigan MAT 95XP and Finnigan MAT 900XLT instruments ES analysis. The data is presented as the ionisation method, followed by the calculated and measured masses. TLC was preformed on Merck 60 F254 silica plates and visualised by UV light and/or $KMnO_4$ stain. Compound purification was carried out by wet flash column chromatography using Merck Kieselgel 60 (particle size 35-70). Eluent constitution is quoted as ratios or percentages. All solvents were dried before use unless otherwise stated. Anhydrous solvents were obtained from a solvent purification system supplied by www.glasscontoursolventsystems.com or a PureSolv solvent purification system supplied by Innovative Technologies Inc. All other chemicals were purchased from a chemical supplier and used as received.

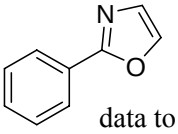
General procedure for Negishi reactions: **2-*p*-Tolyl-oxazole (6c)**



4c **5** **6c**

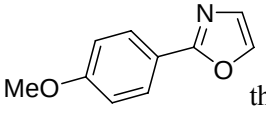
Oxazole (0.30 g, 4.41 mmol, 1.4 equiv) was dissolved in THF (20 mL) under N_2 atmosphere at -78 ˚C, treated with n-BuLi (1.6 M in hexane, 3.35 ml, 5.35 mmol, 1.2 equiv based on oxazole) maintaining an internal temperature below -60 ˚C. After stirring for 10 min, solid $ZnCl_2$ (1.20 g, 9.45mmol, 3.0 equiv) is added portion wise to avoid clumping, the cooling bath is removed, contents warmed to room temperature. Once at ambient temperature, the catalyst $Pd(PPh_3)_4$ (0.079g, 0.22 mmol, 5 mol%) and the *p*-methyl iodobenzene (**4c**, 0.686 g, 3.15 mmol, 1.0 equiv) were added and the contents heated to 60 ˚C and stirred for four hours. The solvent was removed under reduced pressure and the contents were partitioned between NH_4Cl and EtOAc. Extraction and washing with NH_4Cl (followed by filtration of $MgSO_4$) as well as column chromatography in 100% DCM afforded product **6c** as a colorless oil (0.376 g, 75 % yield). **^{1}H NMR** (250 MHz, $CDCl_3$) δ 7.82-7.78 (2H, d, *J*= 6.5 Hz), 7.53 (1H, s), 7.12-7.06 (3H, m) 2.24 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 162.1 (quat), 140.5 (quat), 138.2 (CH), 129.4 (CH), 128.2 (CH), 126.2 (CH), 124.8 (quat), 21.4 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{10}H_9NO$ 159.0679, found 159.0676.

2-Phenyl-oxazole (6a)



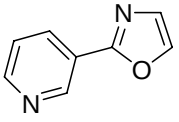
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a colorless oil (0.458 g, 83 % yield), with identical spectral data to that previously reported.[1]

2-(4-Methoxy-pheny)-oxazole (6b)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave **6b** as a colorless oil (0.474 g, 86 % yield) with identical spectral data to that previously reported.[2]

3-Oxazol-2-yl-pyridine (6d)



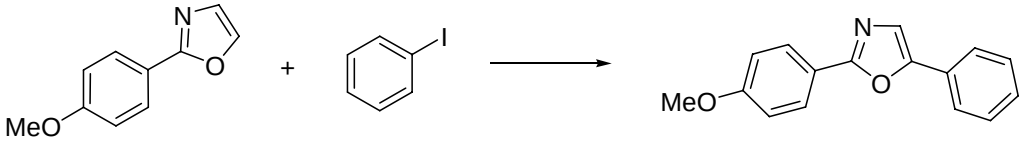
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a colorless oil (0.359g, 78 % yield), **^{1}H NMR** (250 MHz,

[1] Hiemstra, H.; Houwing, H.; Possel, O.; Van Leusen, A. *Can. J. Chem.*, **1979**, 57, 3168.
[2] Reeder, M.; Gleaves, H.; Hoover, S.; Imbordino, R.; Pangborn, J. *J. Org. Proc. Res. Dev.* **2003**, 7, 696.

$CDCl_3$) δ 9.40 (1 H, d, *J*= 1.5 Hz), 8.83 (1 H, dd, *J*= 4.9 Hz, 1.6 Hz), 8.46 (1 H, dt, *J*= 10.1 Hz, 2.0 Hz), 7.94 (1 H, d, *J*= 0.8 Hz), 7.50 (1 H, m), 7.41 (1 H, d, *J*= 0.8 Hz); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 159.4 (quat), 150.9 (CH), 147.5 (CH), 139.3 (CH), 133.8 (CH), 128.7 (CH), 123.8 (quat), 123.7 (CH); **HRMS** (EI) *m/z* calcd for $C_8H_6N_2O$ 146.0475, found 146.0472.

Direct Arylations. Compounds **8a**, **b** and **c**, **13a**, **b** and **c**, **14a**, **b** and **c**, **15a** and **c**, **17a** have been previously reported in the literature. [3,4]

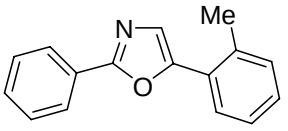
Representative procedure: **2-(4-Methoxy-phenyl)-5-phenyl-oxazole (8b)**



6b **8b**

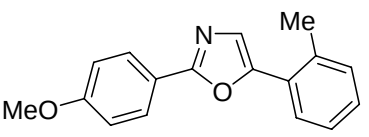
Ag_2CO_3 (317 mg, 1.15 mmol, 2 equiv), PPh_3 (15.2 mg, 0.058mmol, 10 mol %), $Pd(dppf)Cl_2$ DCM (0.024 g, 5 % mol) were put into a carousel tube and mixed well. The aryl iodide (0.078 ml, 0.692 mmol, 1.2 equiv) followed by *p*-methoxyphenyl-2-oxazole (0.101 g, 0.577 mmol, 1 equiv) were added via pipette. Lastly 4-7 ml of distilled water was added via washbottle and the tube was heated to 60˚C and stirred 24 hrs. The dark mixture/melt was filtered through celite using DCM and acetone to wash several times. TLC analysis showed a bright blue spot (UV 254 nm) with R_f= 0.20 (DCM, 100%). Purification by chromatography (SiO_2, CH_2Cl_2 100%) gave the pure product (120 mg, 83%) with identical spectral data to that previously reported.

2-Phenyl-5-*p*-tolyl-oxazole (9a)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (113 mg, 83 % yield, mp. 62-63 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.04-8.00 (2H, m), 7.54-7.51 (2H, m), 7.40-7.37 (3H, m), 7.31 (1H, s), 7.18-7.15 (2H, m), 2.30 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 160.7 (quat), 150.7 (quat), 134.8 (quat), 131.2 (CH), 130.3 (CH), 128.8 (CH), 127.4 (quat), 127.2 (quat), 126.7 (CH), 126.2 (CH), 21.9 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{16}H_{13}NO$ 235.0992, found 235.0993.

2-(4-Methoxy-phenyl)-5-*o*-tolyl-oxazole (9b)

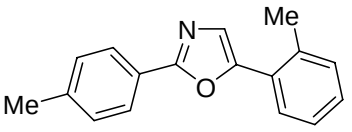


Prepared according to the general procedure. Purification by flash chromatography (silica, DCM/acetone 99:1) gave the coupled product as a

[3] Pulici, M.; Quartieri, F.; Felder, E. *J. Comb. Chem.*, **2005**, *7*, 463.
[4] Keni, M.; Tepe, J. *J. Org. Chem.*, **2005**, *70*, 4211.

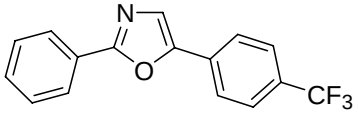
white solid (150 mg, 98 % yield, mp. 71-73 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.22-8.18 (2H, m), 7.92 (1H, m), 7.45 (1H, s), 7.46-7.41 (3H, m), 7.17-7.13 (2H, m), 4.02 (3H, s), 2.68 (3H, s)**; ^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.2 (quat), 160.7 (quat), 150.0 (quat), 134.5 (quat), 131.0 (CH), 128.0 (CH), 127.8 (CH), 127.3 (quat), 126.4 (CH), 126.0 (CH), 125.9 (CH), 120.1 (quat), 114.1 (CH), 55.2 (CH_3), 21.8 (CH_3)**; HRMS** (EI) *m/z* calcd for $C_{17}H_{15}NO_2$ 265.1097, found 265.1094.

5-*o*-Tolyl-2-*p*-tolyl-oxazole (9c)



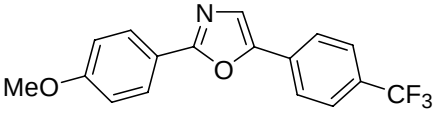
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (129 mg, 90 % yield, mp. 87-89 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.24-8.21 (2H, m), 7.99 (1H, m), 7.54-7.48 (6H, m); 2.74 (3H, s), 2.62 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.0 (quat), 150.3 (quat), 140.5 (quat), 134.7 (quat), 131.1 (CH), 129.4 (CH), 128.2 (CH), 127.3 (quat), 126.7 (CH), 126.2 (CH), 126.1 (CH), 126.0 (CH), 124.7 (quat), 21.8 (CH_3), 21.4 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{17}H_{15}NO$ 249.1148, found 249.1146.

2-Phenyl-5-(4-trifluoromethyl-phenyl)-oxazole (10a)



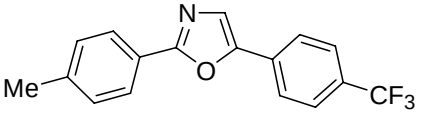
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (134 mg, 80 % yield, mp. 97-99 ˚C). **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.13-8.09 (2H, m), 7.79 (2H, d, *J*= 8.2 Hz), 7.67 (2H, d, *J*= 8.2 Hz), 7.52-7.47 (4H, m); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.9 (quat), 149.7 (quat), 131.2 (quat), 130.7 (quat), 128.8 (CH), 127.0 (quat), 126.4 (CH), 125.2 (CH), 124.1 (CH)-(not all peaks assigned); **HRMS** (EI) *m/z* calcd for $C_{16}H_{10}F_3NO$ 289.0709, found 289.0708.

2-(4-Methoxy-phenyl)-5-(4-trifluoromethyl-phenyl)-oxazole (10b)



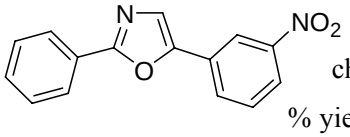
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (178 mg, 97 % yield, mp. 132-133 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.07-8.03 (2H, m), 7.79 (2H, d, *J*= 8.2 Hz), 7.68 (2H, d, *J*= 8.7 Hz), 7.50 (1H, s), 7.02-6.98 (2H, m), 3.88 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 162.1 (quat), 161.7 (quat), 149.3 (quat), 131.4 (quat), 128.2 (CH), 125.1 (CH), 124.0 (CH), 119.8 (quat), 114.3 (CH), 55.4 (CH_3)-(not all peaks assigned); **HRMS** (EI) *m/z* calcd for $C_{17}H_{12}F_3NO_2$ 319.0815, found 319.0812.

2-*p*-Tolyl-5-(4-trifluoromethyl-phenyl)-oxazole (10c)



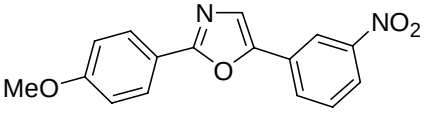
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (144 mg, 82 % yield, mp. 98-100 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.02-7.99 (2H, m), 7.80 (2H, d, *J*= 7.5 Hz), 7.67 (2H, d, *J*= 7.5 Hz), 7.53 (1H, s), 7.32-7.28 (2H, m), 2.35 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 162.2 (quat), 149.5 (quat), 141.1 (quat), 131.3 (quat), 129.6 (CH), 126.4 (CH), 125.1 (CH), 124.3 (quat), 124.1 (CH), 21.6 (CH_3)- (not all peaks assigned); **HRMS** (EI) *m/z* calcd for $C_{17}H_{12}F_3NO$ 303.0866, found 303.0867.

5-(3-Nitro-phenyl)-2-phenyl-oxazole (11a)



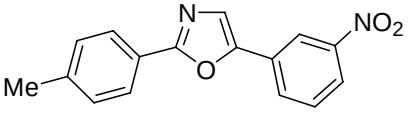
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave **11a** as a pale yellow solid (129 mg, 84 % yield, mp. 145-147 ˚C). **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.53 (1H, t, *J*= 1.9Hz), 8.19-8.10 (3H, m), 8.00 (1H, m), 7.63 (1H, m), 7.59 (1H, s), 7.52-7.49 (3H, m); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 162.1 (quat), 148.9 (quat), 148.8 (quat), 130.9 (CH), 130.0 (CH), 129.6 (quat), 129.5 (CH), 128.9 (CH), 126.8 (quat), 126.5 (CH), 125.5 (CH), 122.7 (CH), 118.8 (CH); **HRMS** (EI) *m/z* calcd for $C_{15}H_{10}N_2O_3$ 266.0686, found 266.0687.

2-(4-Methoxy-phenyl)-5-(3-nitro-phenyl)-oxazole (11b)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a yellow solid (145 mg, 85 % yield, mp. 196-198 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.53 (1H, t, *J*= 1.8 Hz), 8.17 (1H, m), 8.09-8.06 (2H, m), 8.00 (1H, m), 7.62 (1H, t, *J*= 7.5 Hz), 7.56 (1H, s), 7.04-7.00 (2H, m), 3.89 (3H, s)**; ^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.8 (quat), 148.8 (quat), 148.4 (quat), 130.0 (CH), 129.8 (quat), 129.4 (CH), 128.3 (CH), 128.2 (quat), 125.3 (CH), 122.5 (CH), 119.6 (quat), 118.7 (CH), 114.4 (CH), 55.5 (CH_3)**; HRMS** (EI) *m/z* calcd for $C_{16}H_{12}N_2O_4$ 296.0792, found 296.0790.

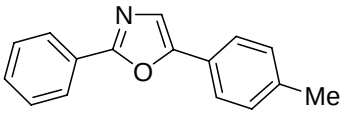
5-(3-Nitro-phenyl)-2-*p*-tolyl-oxazole (11c)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a pale yellow solid (129 mg, 80 % yield, 157-159 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.55 (1H, t, *J*= 2.0 Hz), 8.15 (1H, m), 8.02-7.97 (3H, m), 7.61 (1H, t, *J*= 8.3 Hz), 7.56 (1H, s), 7.32-7.26 (2H, m), 2.43 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 162.4 (quat), 148.7 (quat), 148.5 (quat), 141.3 (quat),

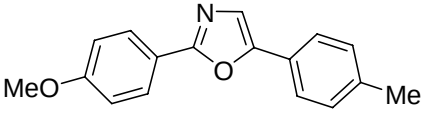
130.0 (CH), 129.7 (quat), 129.6 (CH), 129.4 (CH), 126.5 (CH), 125.4 (CH), 124.1 (quat), 122.6 (CH), 118.7 (CH), 21.5 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{16}H_{12}N_2O_3$ 280.0842, found 280.0843.

2-Phenyl-5-*p*-tolyl-oxazole (12a)



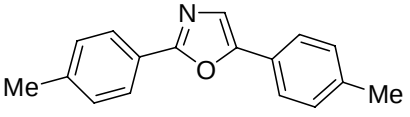
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (102 mg, 75 % yield, mp. 74-75 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.04-8.00 (2H, m), 7.55-7.51 (2H, m), 7.40-7.37 (3H, m), 7.31 (1H, s), 7.18-7.15 (2H, m), 2.30 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.8 (quat), 151.5 (quat), 138.5 (quat), 130.2 (CH), 129.6 (CH), 128.8 (CH), 127.5 (quat), 126.2 (CH), 125.3 (quat), 124.1 (CH), 122.8 (CH), 21.3 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{16}H_{13}NO$ 235.0992, found 235.0994.

2-(4-Methoxy-phenyl)-5-*p*-tolyl-oxazole (12b)



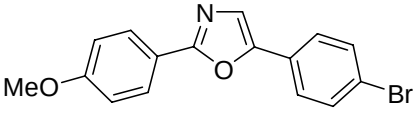
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (149 mg, 97 % yield, mp. 102-104 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 7.98-7.94 (2H, m,), 7.53-7.50 (2H, m, 7.27 (1H, s), 7.18-7.14 (2H, m), 6.93-6.89 (2H, m), 3.79 (3H, s), 2.31 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.3 (quat), 160.9 (quat), 150.9 (quat), 138.2 (quat), 129.5 (CH), 127.9 (CH), 125.4 (quat), 124.0 (CH), 122.5 (CH), 120.3 (quat), 114.2 (CH), 55.4 (CH_3), 21.3 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{17}H_{15}NO_2$ 265.1097, found 265.1096.

2,5-Di-*p*-tolyl-oxazole (12c)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (140 mg, 97 % yield, mp. 106-107 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.19 (2H, d, *J*= 8.3Hz), 7.80 (2H, d, *J*= 7.8Hz), 7.57 (1H, s), 7.45-7.41 (4H, m), 2.60 (3H, s), 2.58 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.0 (quat), 151.1 (quat), 140.4 (quat), 138.3 (quat), 129.5 (CH), 129.4 (CH), 126.1 (CH), 125.3 (quat), 124.8 (quat), 124.0 (CH), 122.6 (CH), 21.4 (CH_3), 21.3 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{17}H_{15}NO$ 249.1148, found 249.1147.

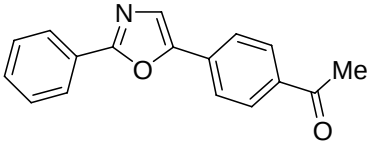
5-(4-Bromo-phenyl)-2-(4-methoxy-phenyl)-oxazole (15b)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white

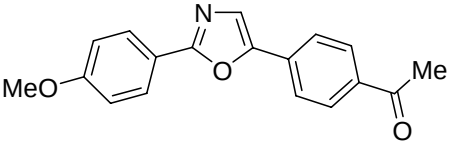
solid (158 mg, 83 % yield, mp. 137-139 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.03-7.99 (2H, m), 7.53 (4H, s), 7.38 (1H, s), 6.99-6.96 (2H, m), 3.85 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.4 (quat), 149.6 (quat), 132.0 (CH), 127.9 (CH), 127.0 (quat), 125.4 (CH), 123.7 (CH and quat), 121.9 (quat), 119.9 (quat), 114.2 (CH); **HRMS** (EI) *m/z* calcd for $C_{16}H_{12}BrNO_2$ (Br^{79}) 329.0046, found 329.0060, calcd for $C_{16}H_{12}BrNO_2$ (Br^{81}) 331.0026, found 331.0009.

1-[4-(2-Phenyl-oxazol-5-5-yl)-phenyl]-ethanone (16a)



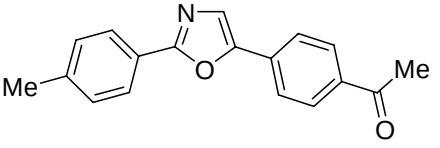
Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (131 mg, 86 % yield, mp. 105-106 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.11-8.07 (2H, m), 8.01-7.98 (2H, m), 7.77-7.73 (2H, m), 7.53 (1H, s), 7.48-7.45 (3H, m), 2.59 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 196.9 (quat), 161.9 (quat), 150.1 (quat), 136.3 (quat), 131.9 (quat), 130.62 (CH), 129.0 (CH), 128.8 (CH), 127.0 (quat), 126.4 (CH), 125.5 (CH), 123.9 (CH), 26.5 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{17}H_{13}NO_2$ 263.0941, found 263.0950.

1-{4-[2-(4-Methoxy-phenyl)oxazol-5-yl]-pheny}-ethanone (16b)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a off white solid (151 mg, 89 % yield, mp. 148-150 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.04-7.80 (4H, m), 7.76-7.72 (2H, m), 7.51 (1H, s), 6.99-6.96 (2H, m), 3.86 (3H, s), 2.60 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 197.1 (quat), 162.1 (quat), 161.6 (quat), 149.6 (quat), 136.2 (quat), 132.1 (quat), 129.0 (CH), 128.1 (CH), 125.4 (CH), 123.7 (CH), 119.8 (quat), 114.3 (CH), 55.4 (CH_3), 26.5 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{18}H_{15}NO_3$ 293.1046, found 293.1044.

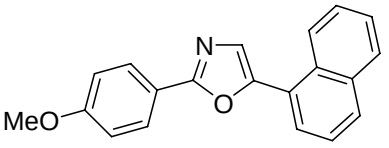
1-[4-(2-*p*-Tolyl-oxazol-5-yl)-phenyl]-ethanone (16c)



Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (149 mg, 93 % yield, mp. 132-134 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 7.87-7.82 (4H, m), 7.62-7.59 (2H, d, *J*= 8.5 Hz), 7.38 (1H, s), 7.13 (2H, d, *J*= 8.0 Hz), 2.45 (3H, s), 2.26 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 197.0 (quat), 162.2 (quat), 149.8 (quat), 141.1 (quat), 136.2 (quat), 132.1 (quat), 129.5 (CH), 129.0 (CH), 126.4 (CH), 125.5 (CH), 124.3 (quat), 123.8 (CH), 26.5 (CH_3), 21.5 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{18}H_{15}NO_2$ 277.1097, found 277.1095.

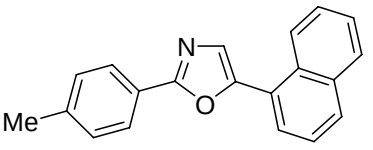
2-(4-Methoxy-phenyl)-5-naphthalen-1-yl-oxazole (17b)

Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (132 mg, 76 % yield, 72-74 ˚C); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.37 (1H, m), 8.12-8.08 (2H, m), 7.92-7.81 (3H, m), 7.59-7.51 (4H, m), 7.04-7.00 (2H, m), 3.89 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.6 (quat), 161.4 (quat), 149.9 (quat), 133.9 (quat), 130.1 (quat), 129.3 (CH), 128.7 (CH), 128.0 (CH), 127.0 (CH), 126.5 (CH), 126.2 (2x CH), 125.5 (quat), 125.3 (CH), 124.9 (CH), 120.2 (quat), 114.3 (CH), 55.3 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{20}H_{15}NO_2$ 301.1097, found 301.1092.



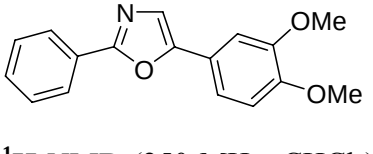
5-Naphthalen-1-yl-2-*p*-tolyl-oxazole (17c)

Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (133 mg, 81 % yield, mp. 114-116 ˚C). **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.38 (1H, m), 8.09-8.05 (2H, m), 7.94-7.82 (3H, m), 7.63-7.52 (4H, m), 7.34-7.30 (2H, m); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.7 (quat), 150.1 (quat), 140.6 (quat), 133.9 (quat), 130.1 (quat), 129.5 (CH), 129.4 (CH), 128.7 (CH), 127.0 (CH), 126.7 (CH), 126.3 (CH), 126.2 (CH), 125.4 (quat), 125.3 (CH), 124.9 (CH), 124.8 (quat), 21.5 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{20}H_{15}NO$ 285.1148, found 285.1144.



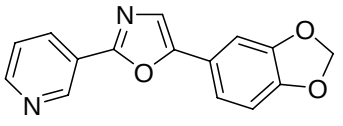
Balsoxin (18)

Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (136 mg, 84 % yield) with identical spectral data to that previously reported: **^{1}H NMR** (250 MHz, $CHCl_3$) δ 8.11-8.07 (2H, m), 7.50-7.44 (3H, m), 7.33 (1H, s), 7.30 (1H, dd, *J*= 2.00Hz, 8.4Hz), 7.19 (1H, d, *J*= 2.0Hz), 6.93 (1H, d, *J*= 8.4Hz), 3.90 (3H, CH_3), 3.85 (3H, CH_3); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 160.5 (quat), 151.2 (quat), 149.4 (quat), 149.3 (quat), 130.1 (CH), 128.7 (CH), 127.5 (quat), 126.1 (CH), 122.2 (CH), 121.0 (quat), 117.2 (CH), 111.4 (CH), 107.4 (CH), 56.0 (CH_3), 55.9 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{17}H_{15}NO_3$ 281.1046, found 281.1046.



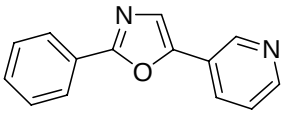
Texaline (19)

Prepared according to the general procedure. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as a white solid (114 mg, 74 % yield) with identical spectral data and melting point to that previously reported.



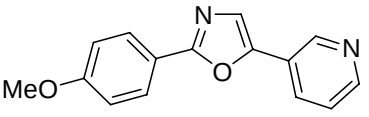
^{1}H NMR (250 MHz, $CDCl_3$) δ 9.29 (1H, d, *J*= 1.5Hz), 8.66 (1H, dd, *J*= 1.7, 4.9Hz), 8.30 (1H, m), 7.38 (1H, dd, *J*= 4.9, 8.0Hz), 7.31 (1H, s), 7.21 (1H, dd, *J*= 1.8, 8.0Hz), 7.14 (1H, d, *J*= 1.7Hz), 6.90 (1H, d, *J*= 8.3Hz), 6.00 (2H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 158.12 (quat), 151.83 (quat), 150.75, 148.23 (quat), 148.14 (quat), 147.40 (CH), 133.12 (CH), 123.63 (quat), 123.49 (CH), 122.47 (CH), 121.68 (quat), 118.53 (CH), 108.85 (CH), 104.82 (CH), 101.42 (CH_2); **HRMS** (EI) *m/z* calcd for $C_{15}H_{10}N_2O_3$ 266.0685, found 266.0684.

3-(2-Phenyl-oxazol-5-yl)-pyridine



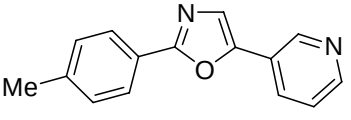
Prepared according to the general procedure. Purification by flash chromatography (silica, EtOAc 100%) gave the coupled product as a white solid (42 mg, 36 % yield); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.99 (1H, dd, *J*= 0.77, 2.3 Hz), 8.57 (1H, dd, *J*= 1.6, 4.8 Hz), 8.12-8.08 (2H, m), 7.98 (1H, ddd, *J*= 1.7, 2.2, 8.0 Hz), 7.52-7.47 (4H, m), 7.35 (1H, ddd, *J*= 0.8, 4.9, 8.0 Hz); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 161.9 (quat), 149.3 (CH), 148.4 (quat), 145.6 (CH), 131.1 (CH), 130.6 (CH), 128.8 (CH), 127.0 (quat), 126.4 (CH), 124.7 (CH), 124.3 (quat), 123.6 (CH); **HRMS** (EI) *m/z* calcd for $C_{14}H_{10}N_2O$ 222.0793, found 222.0791.

3-[2-(4-Methoxy-phenyl)-oxazol-5-yl]-pyridine



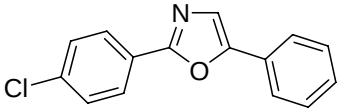
Prepared according to the general procedure. Purification by flash chromatography (silica, 1:1 hexane/ethyl acetate) gave the coupled product as a white solid (44 mg, 30 % yield); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.98 (1H, s), 8.57-8.55 (2H, m), 8.08-8.03 (2H, m), 7.96 (1H, m), 7.49 (1H, s) 7.39-7.34 (1H, m), 7.02-6.98 (2H, m), 3.88 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 162.1 (quat.), 161.6 (CH), 149.0 (quat.), 147.8 (quat.), 145.4 (CH), 131.0 (CH), 128.1 (CH), 124.6 (CH), 123.6 (quat.), 119.8 (quat.), 114.3 (CH), 55.4 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{15}H_{12}N_2O_2$ 252.0895, found 252.0895.

3-(2-*p*-Tolyl-oxazol-5-yl)-pyridine



Prepared according to the general procedure. Purification by flash chromatography (silica, 1:1 hexane/ethyl acetate) gave the coupled product as a white solid (45 mg, 33 % yield); **^{1}H NMR** (250 MHz, $CDCl_3$) δ 8.98 (1H, s), 8.57 (1H, s), 8.01-7.95 (3H, m), 7.51 (1H, s), 7.37-7.26 (2H, m), 2.42 (3H, s); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 162.2 (quat.), 149.1 (CH), 148.1 (quat.), 145.5 (CH), 141.1 (quat.), 131.1 (CH), 129.6 (CH), 126.4 (CH), 124.6 (CH), 124.4 (quat.), 123.6 (quat.), 21,5 (CH_3); **HRMS** (EI) *m/z* calcd for $C_{15}H_{12}N_2O$ 236.0950, found 236.0950.

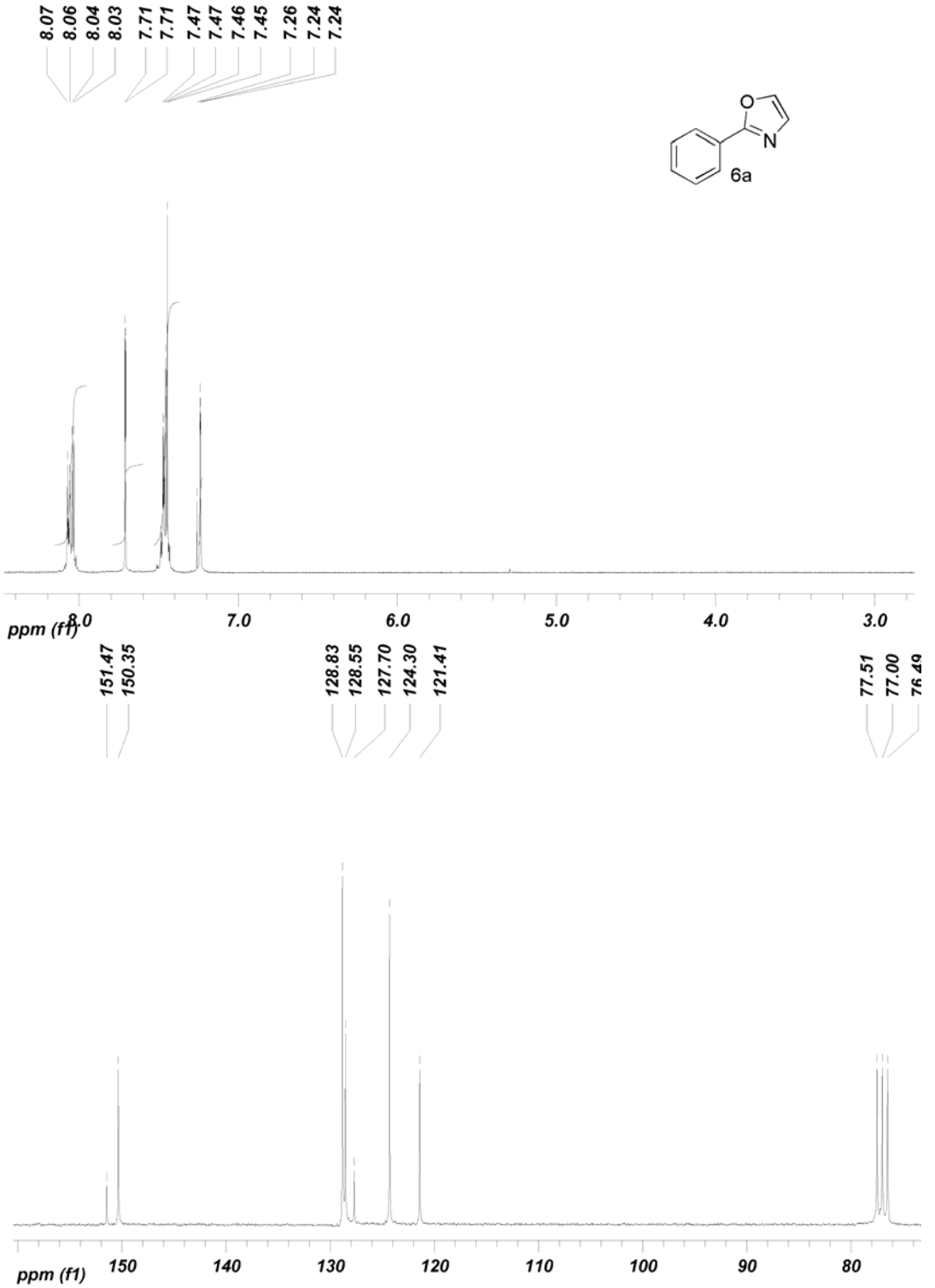
2-(4-Chloro-phenyl)-5-phenyloxazole

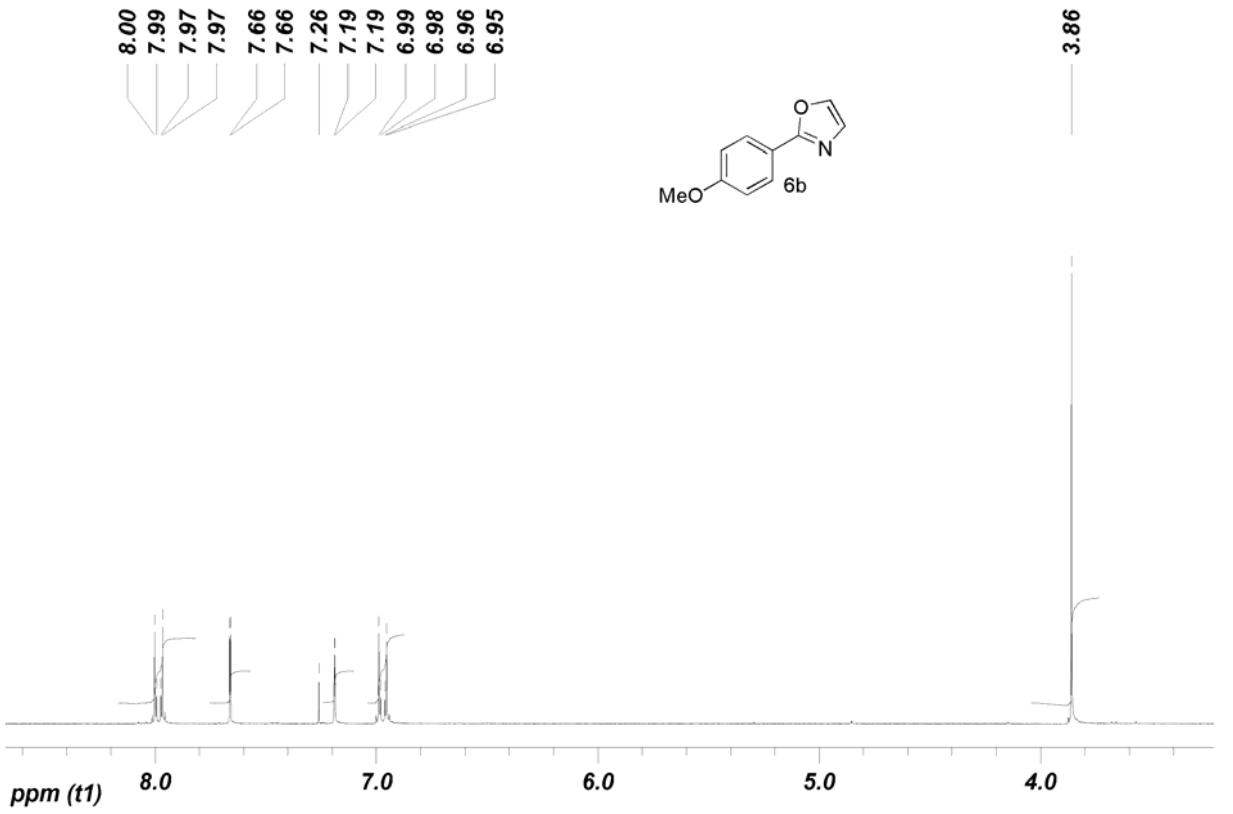


Prepared according to the general procedure for the direct arylation on the 5-position. Purification by flash chromatography (silica, DCM 100%) gave the coupled product as an off white solid (105 mg, 71 % yield) with identical spectral data to that previously reported.[5] **^{1}H NMR** (250 MHz, $CDCl_3$) 8.04-8.01 (2H, m), 7.72-7.69 (2H, m), 7.48-7.41 (6H, m); **^{13}C NMR** (63 MHz, $CDCl_3$) δ 160.1 (quat), 151.5 (quat), 136.3 (quat), 129.1 (CH), 129.0 (CH), 128.6 (CH), 127.8 (quat), 127.5 (CH), 125.9 (quat), 124.2 (CH), 123.5 (CH).

[5] Clark, A. D. *Tetrahedron* **1999**, *55*, 3637-3648.

^{1}H and ^{13}C NMR

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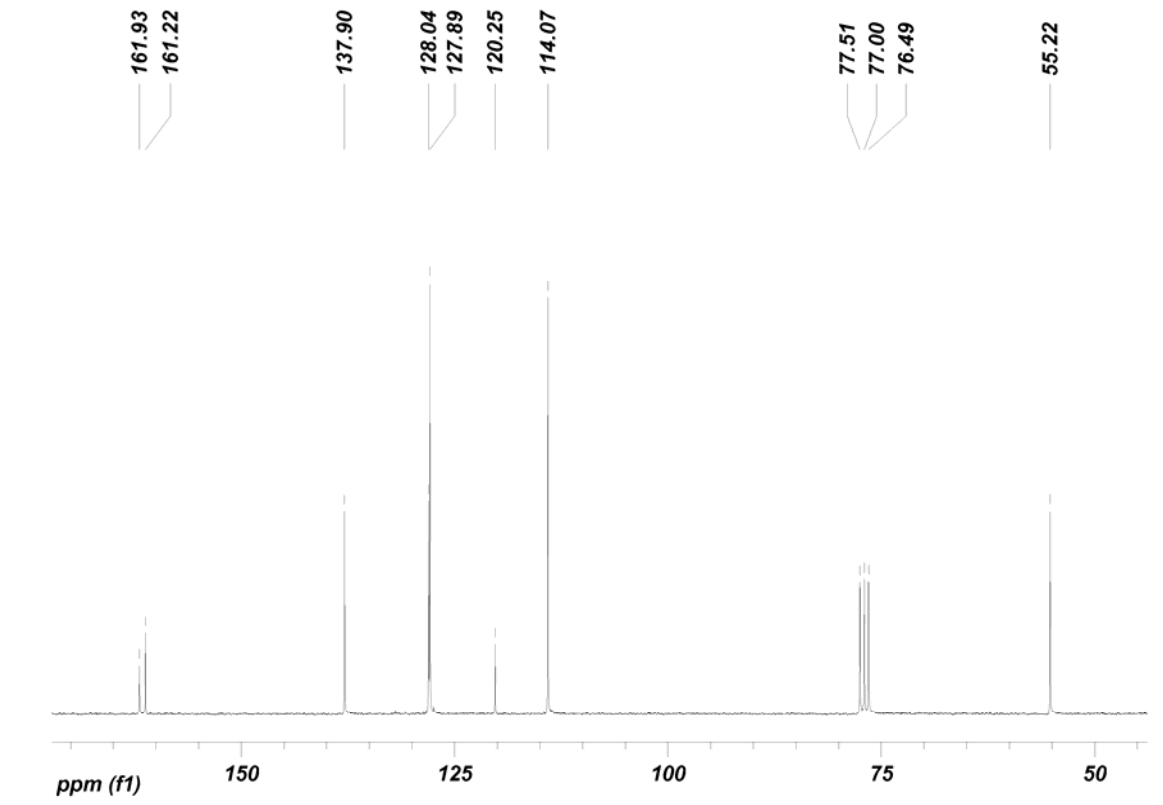
4.0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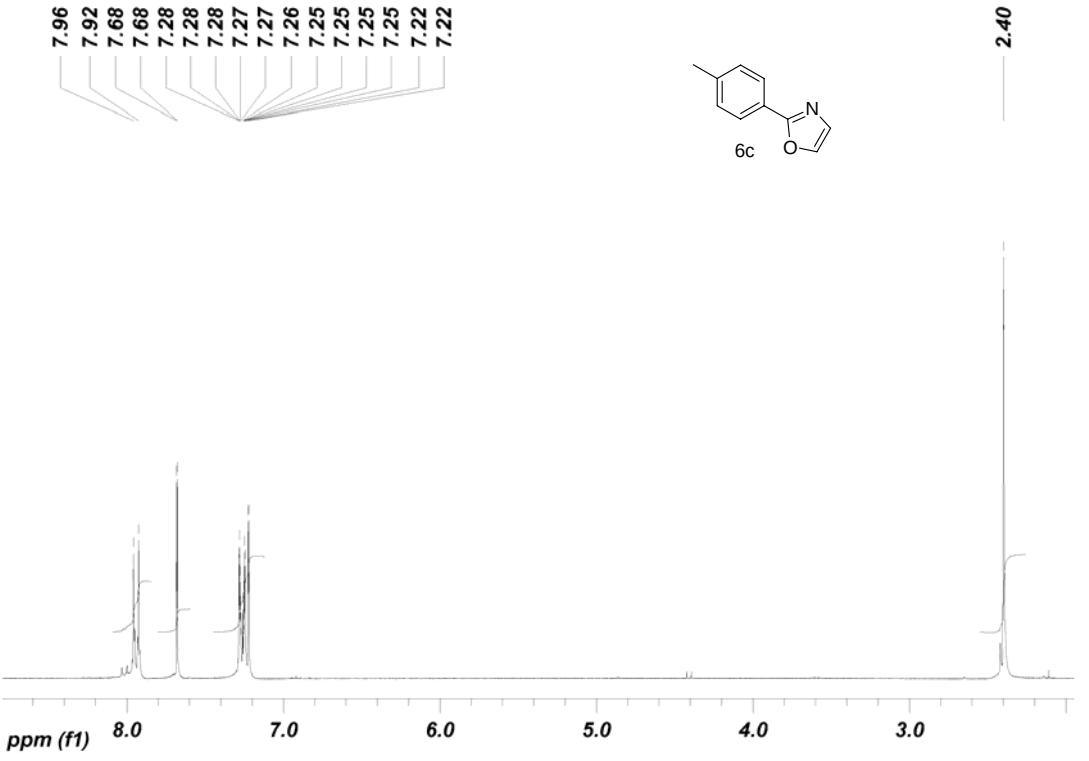
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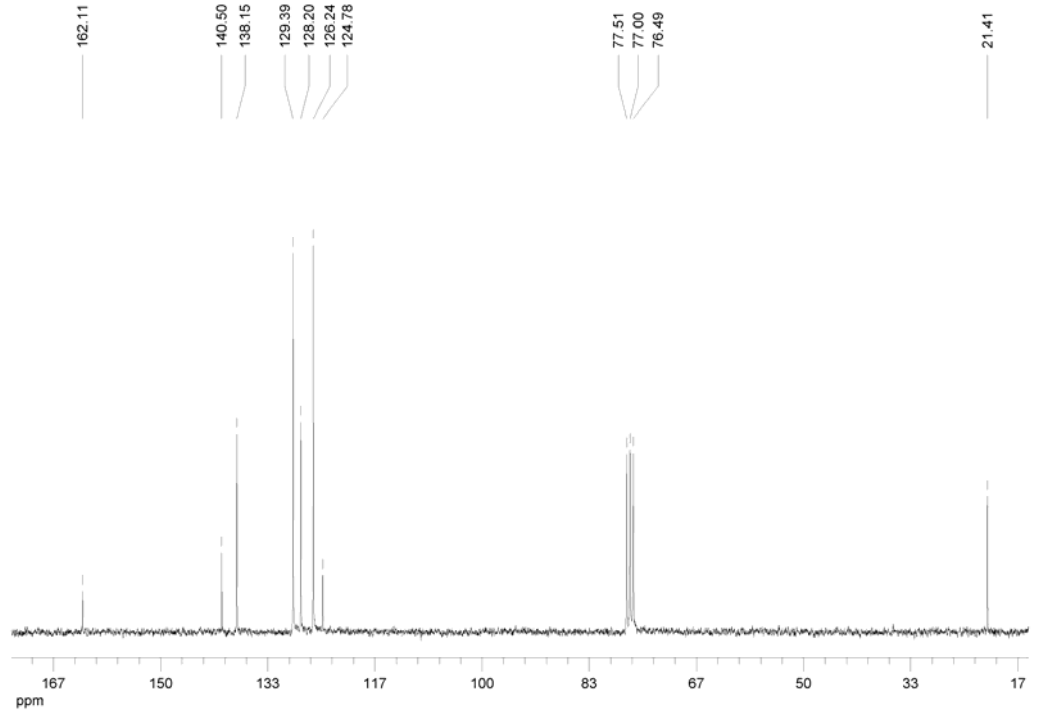
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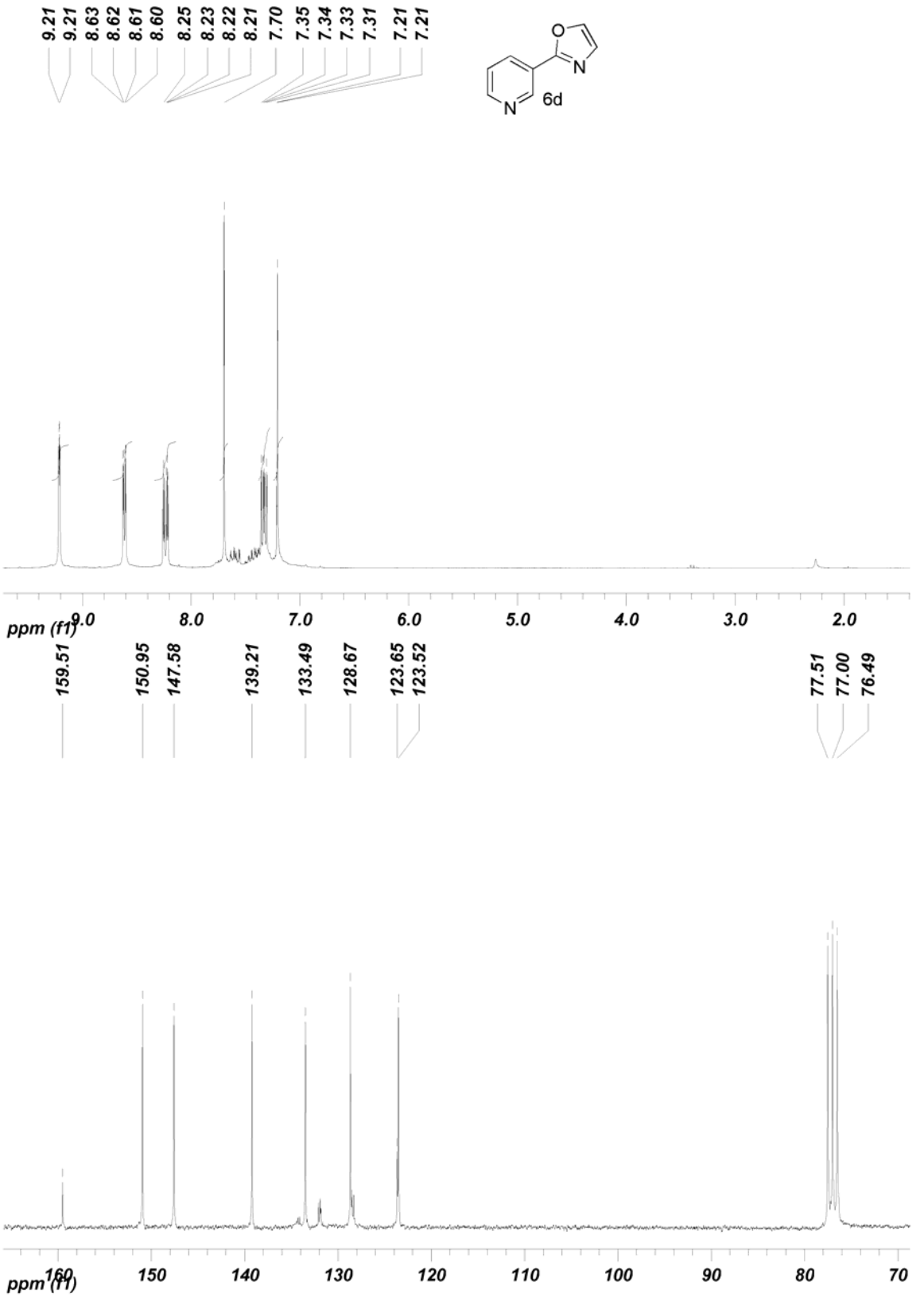
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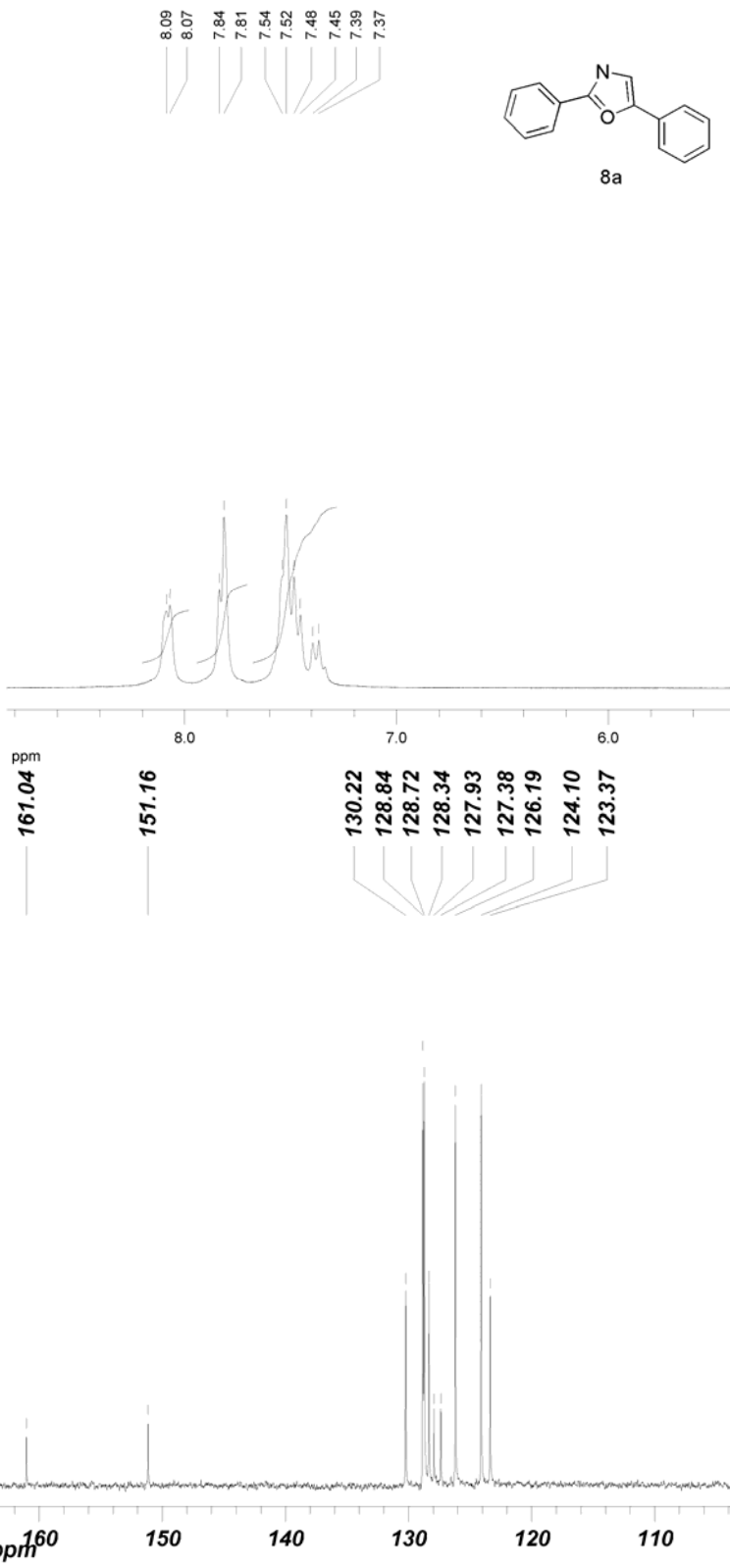
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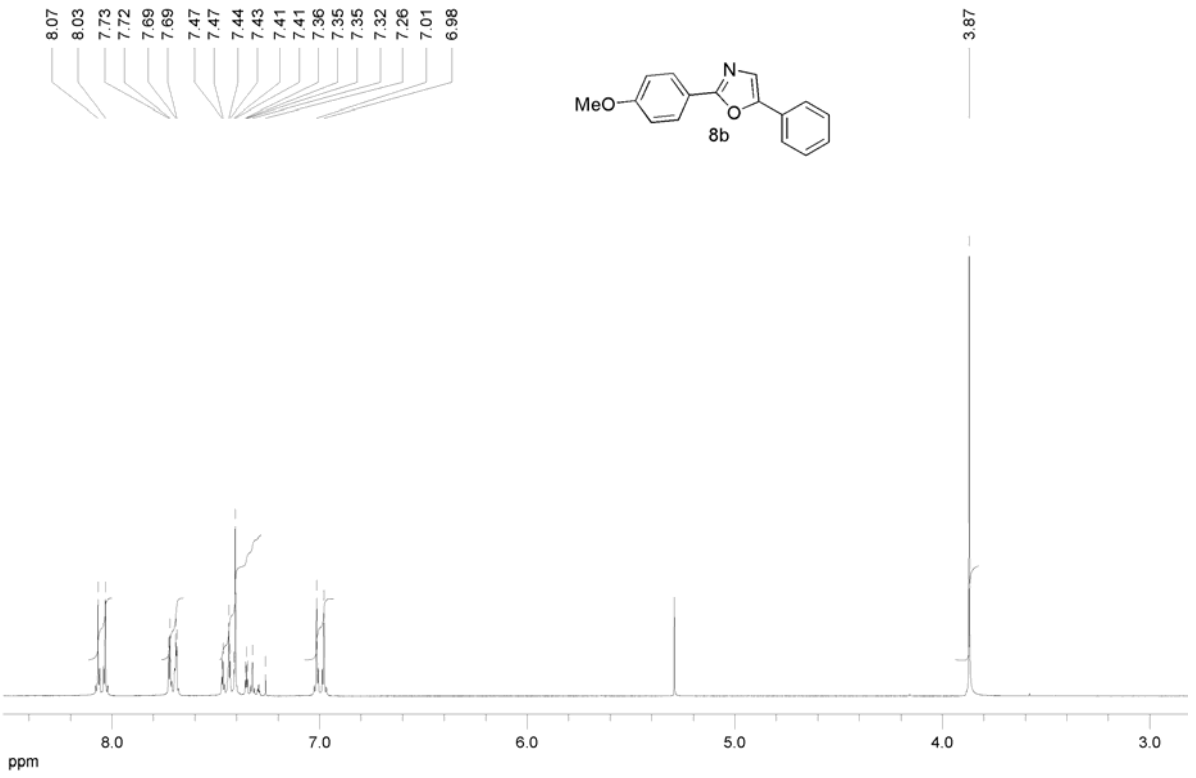
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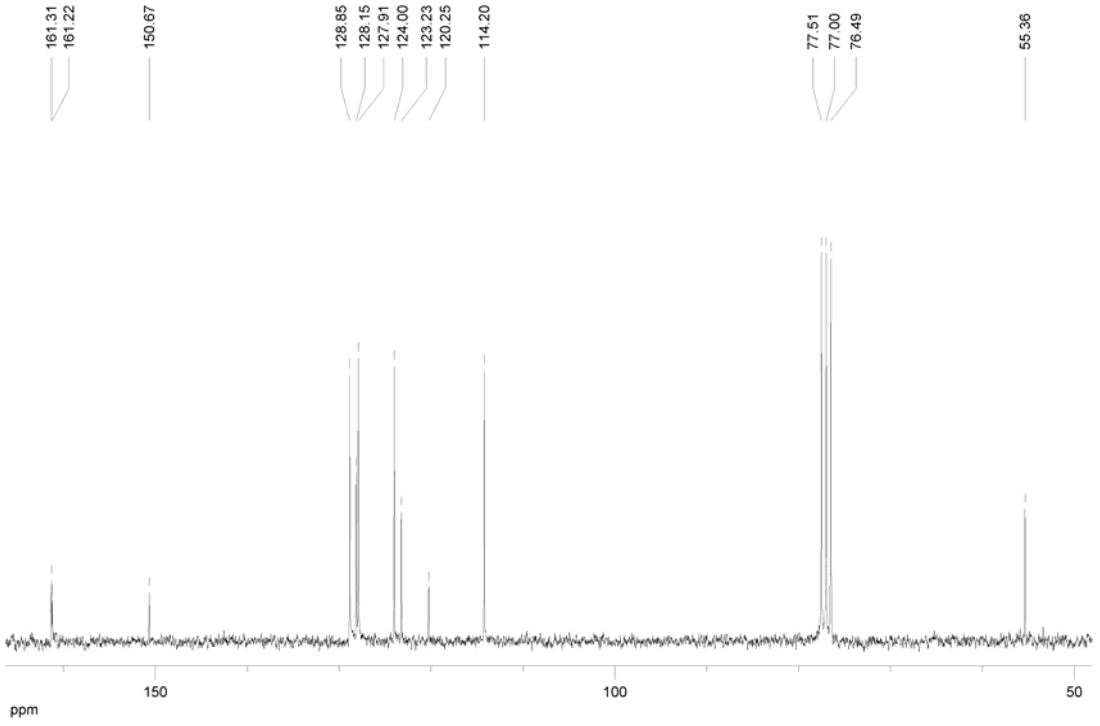
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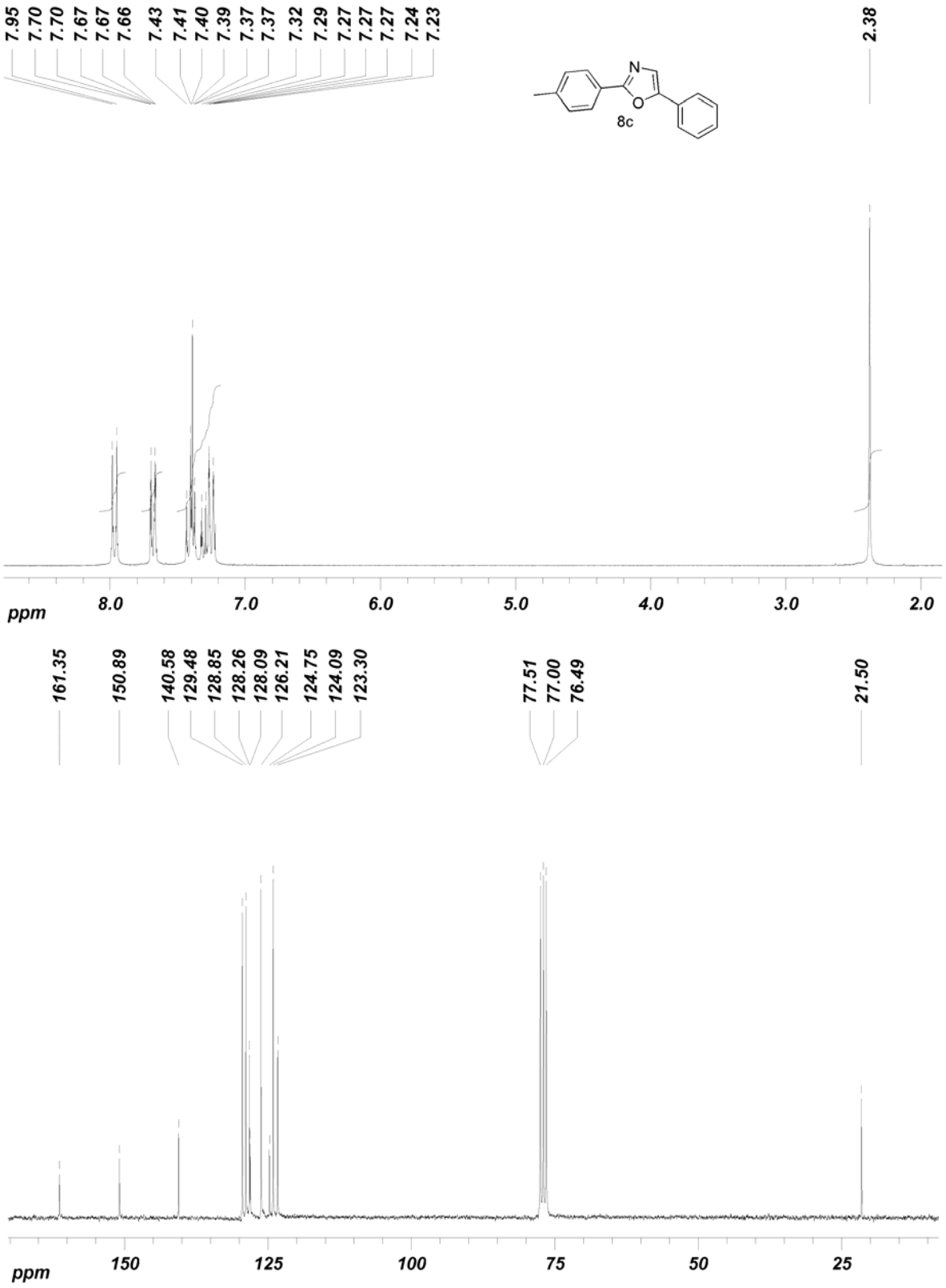
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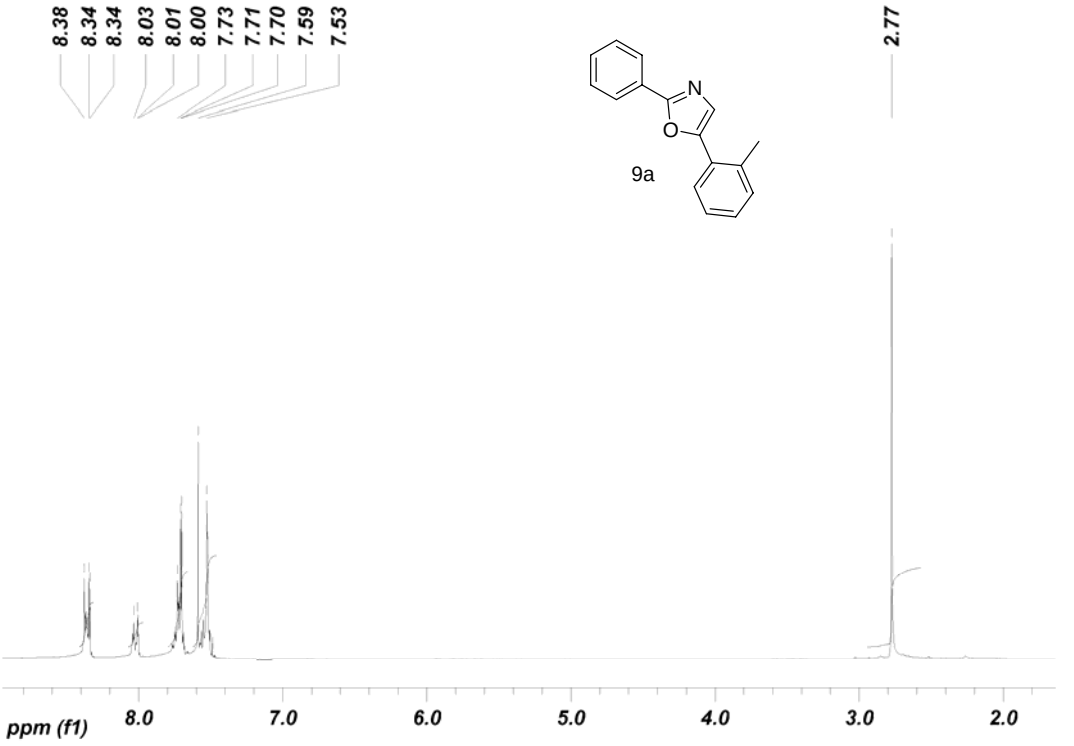
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8.00
7.73
7.71
7.70
7.59
7.53
2.77
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O
9a
ppm (f1)
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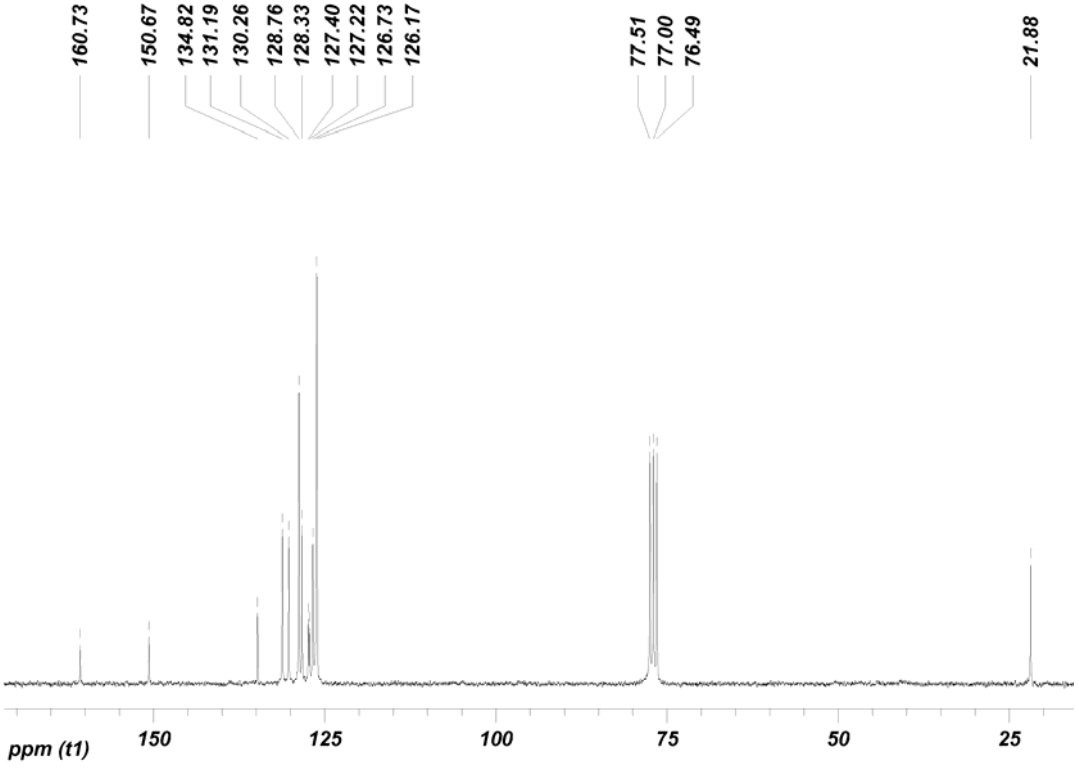
7.0
6.0
5.0
4.0
3.0
2.0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150.67
134.82
131.19
130.26
128.76
128.33
127.40
127.22
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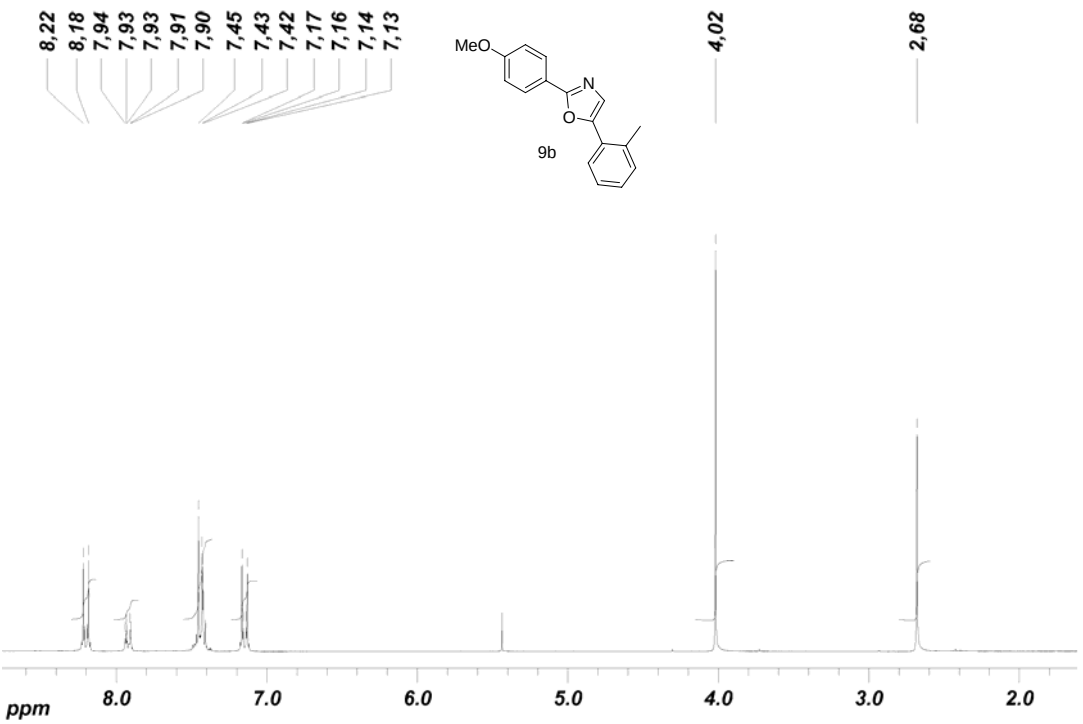
126.17
77.51
77.00
76.49
21.88
ppm (t1)
150
125
100
75
50
25


8,22
8,18
7,94
7,93
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7,91
7,90
7,45
7,43
7,42
7,17
7,16
7,14
7,13
MeO
N
O
9b
4,02
2,68
ppm
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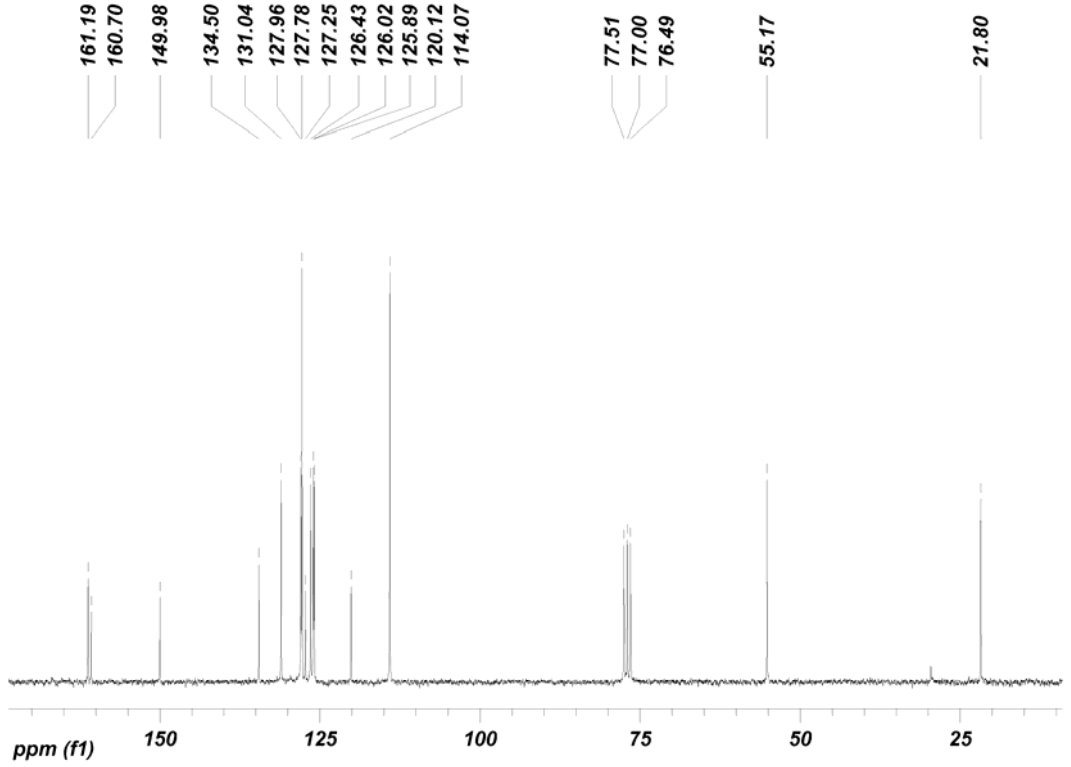
7.0
6.0
5.0
4.0
3.0
2.0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160.70
149.98
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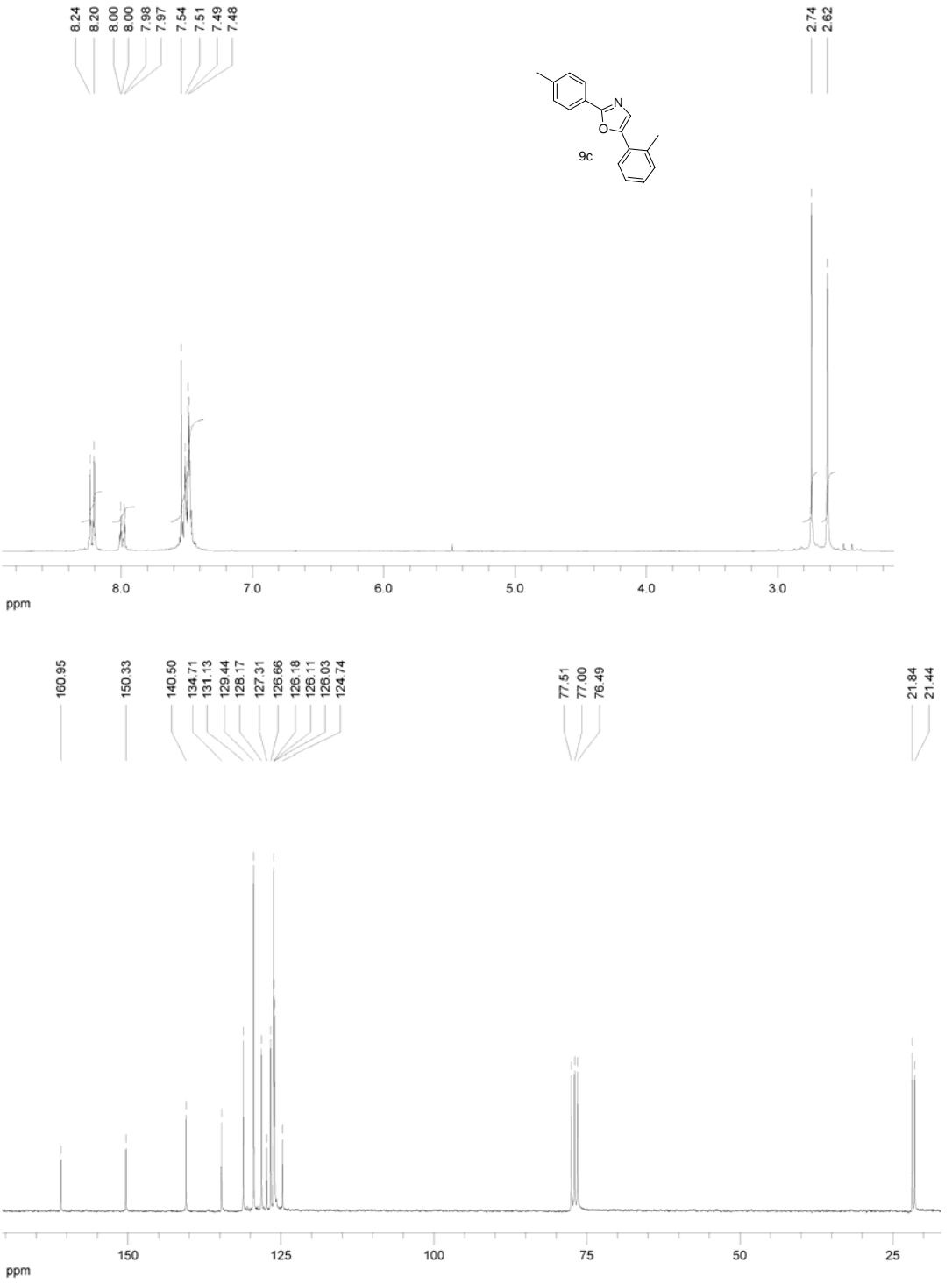
131.04
127.96
127.78
127.25
126.43
126.02
125.89
120.12
114.07
77.51
77.00
76.49
55.17
21.80
ppm (f1)
150
125
100
75
50
25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8.20
8.00
8.00
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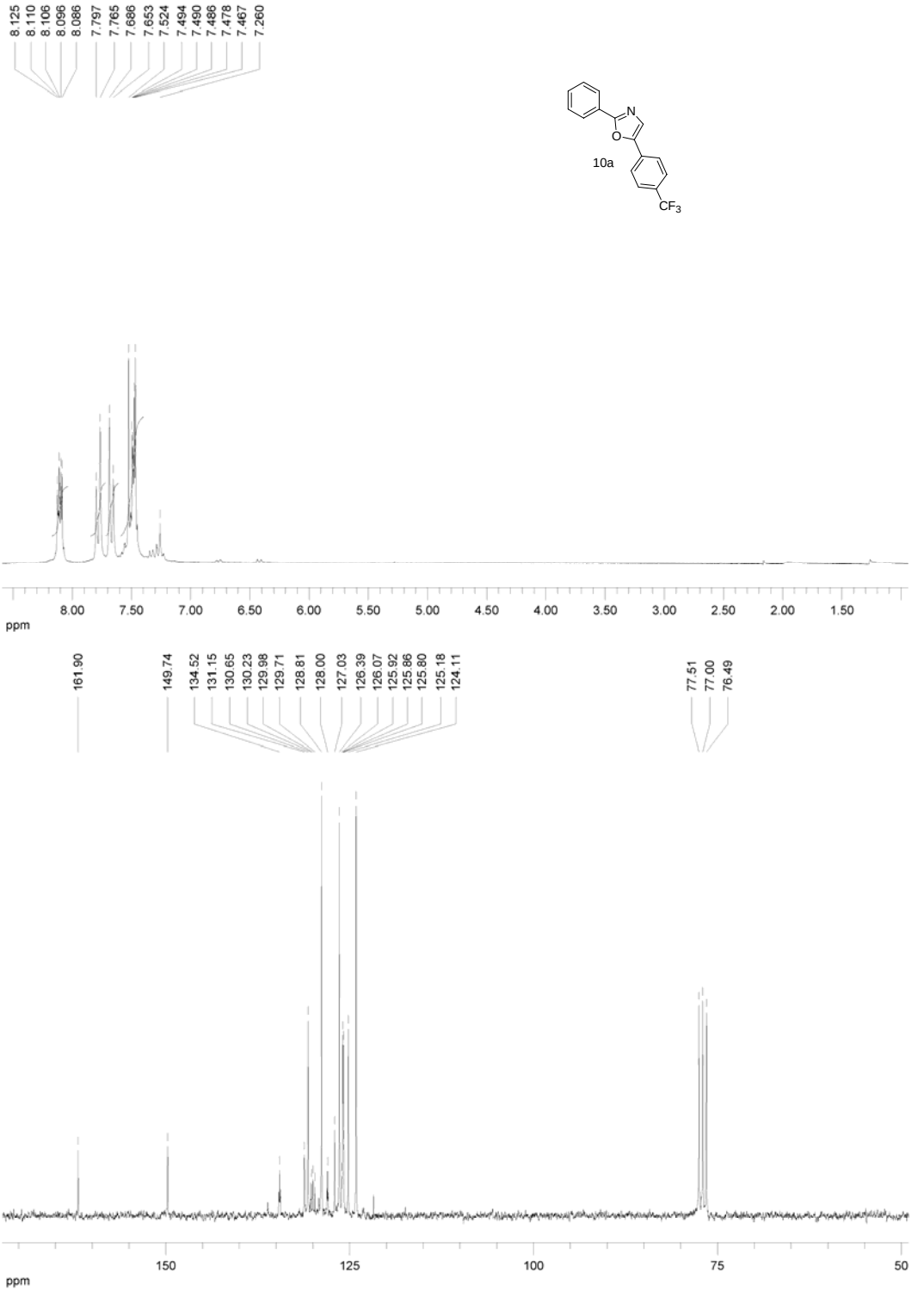
7.97
7.54
7.51
7.49
7.48
2.74
2.62
N
O
9c
8.0
7.0
6.0
5.0
4.0
3.0
ppm
160.95
150.33
140.50
134.71
131.13
129.44
128.17
127.31
126.66
126.18
126.11
126.03
124.74
77.51
77.00
76.49
21.84
21.44
150
125
100
75
50
25
ppm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8.110
8.106
8.096
8.086
7.797
7.765
7.686
7.653
7.524
7.494
7.490
7.486
7.478
7.467
7.260
N
O
10a
CF3
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
ppm
161.90
149.74
134.52
131.15
130.65
130.23
129.98
129.71
128.81
128.00
127.03
126.39
126.07
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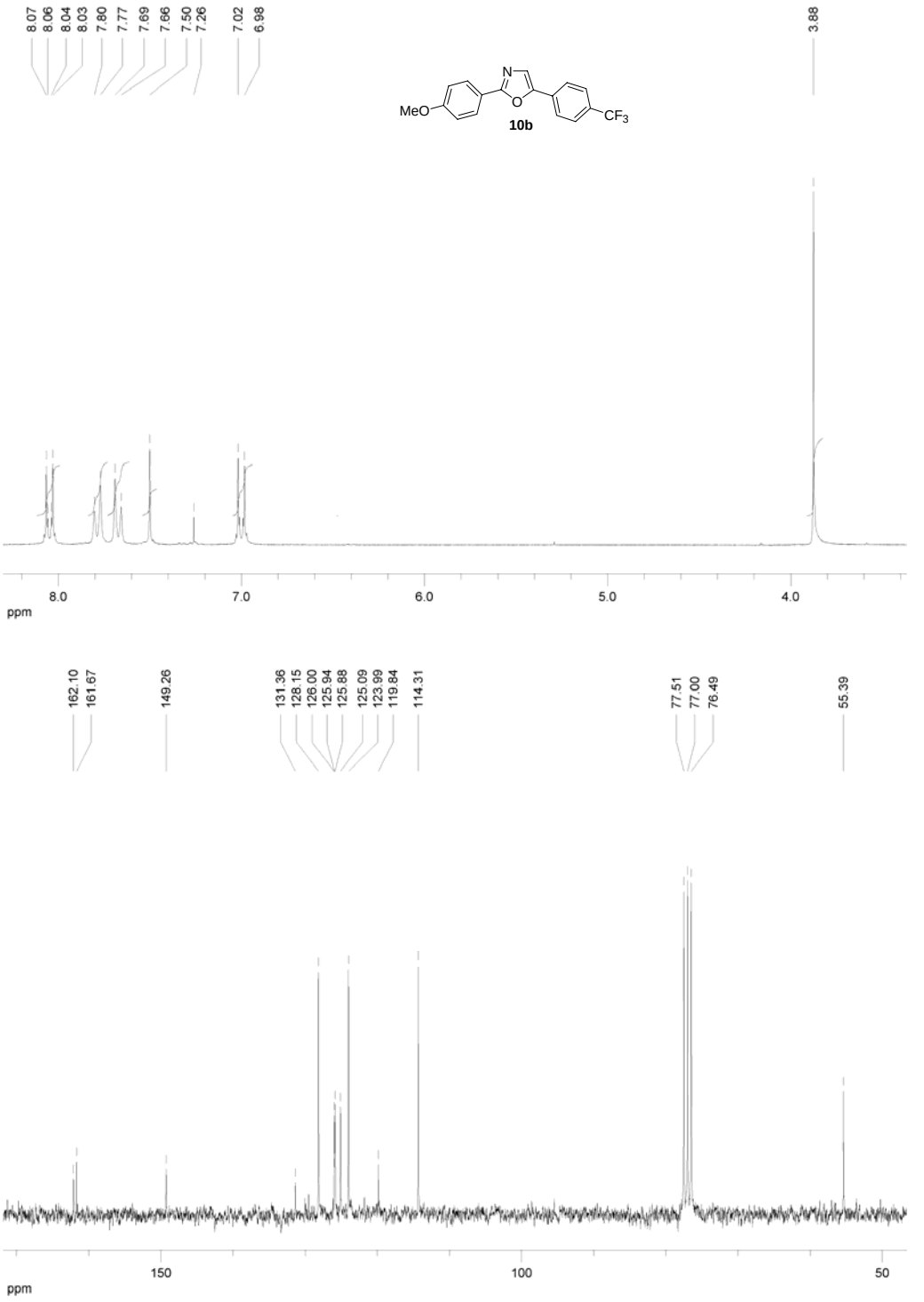
125.80
125.18
124.11
77.51
77.00
76.49
150
125
100
75
50
ppm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8.06
8.04
8.03
7.80
7.77
7.69
7.66
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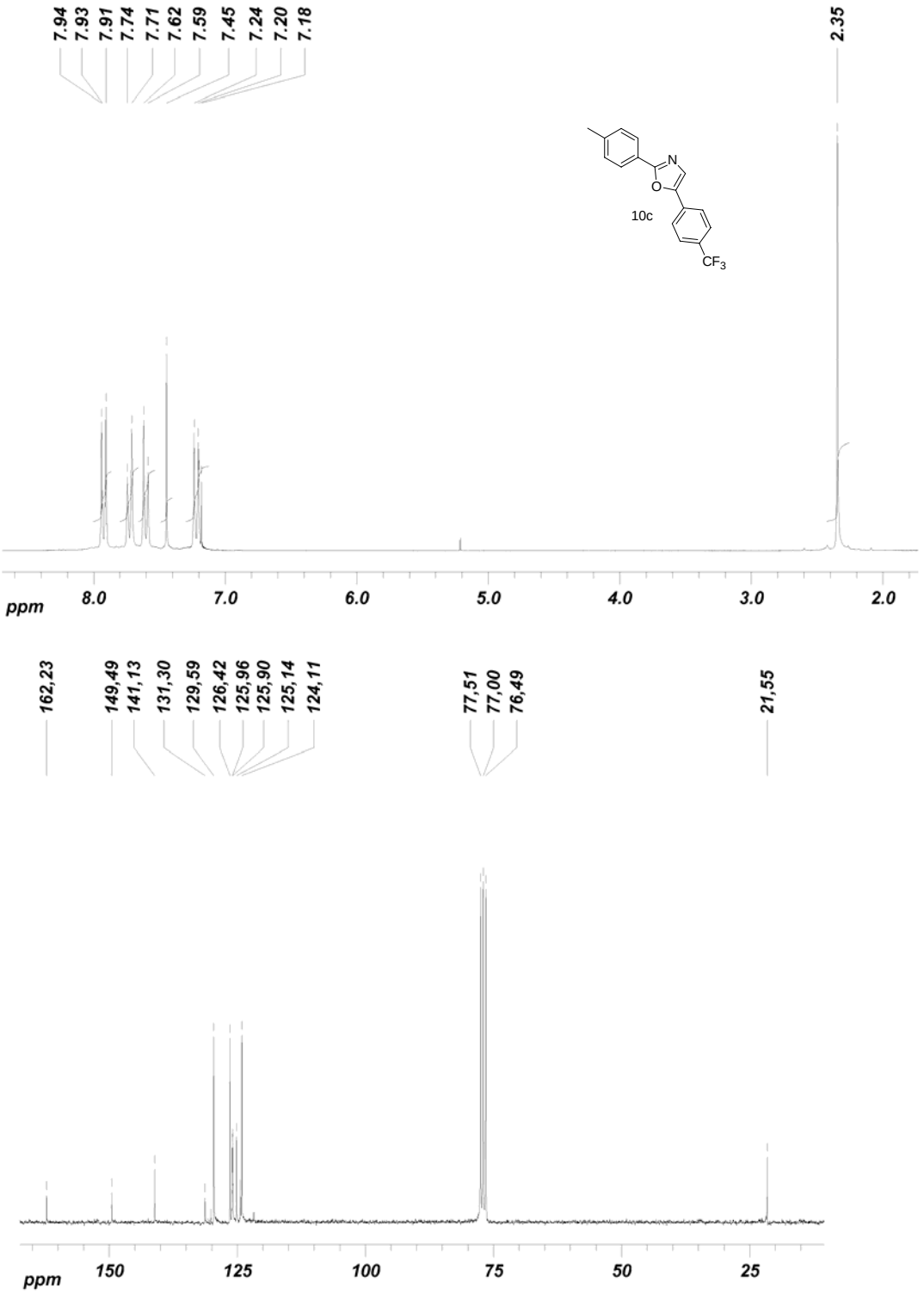
7.26
7.02
6.98
3.88
MeO
N
O
CF3
10b
8.0
7.0
6.0
5.0
4.0
ppm
162.10
161.67
149.26
131.36
128.15
126.00
125.94
125.88
125.09
123.99
119.84
114.31
77.51
77.00
76.49
55.39
150
100
50
ppm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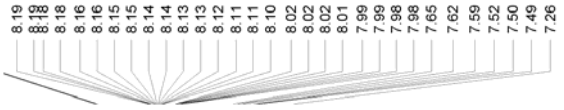
7.93
7.91
7.74
7.71
7.62
7.59
7.45
7.24
7.20
7.18
2.35
N
O
10c
CF3
ppm
8.0
7.0
6.0
5.0
4.0
3.0
2.0
162,23
149,49
141,13
131,30
129,59
126,42
125,96
125,90
125,14
124,11
77,51
77,00
76,49
21,55
ppm
150
125
100
75
50
25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8.18
8.18
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8.15
8.14
8.14
8.13
8.13
8.12
8.11
8.11
8.10
8.02
8.02
8.02
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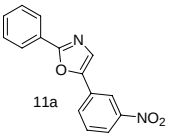
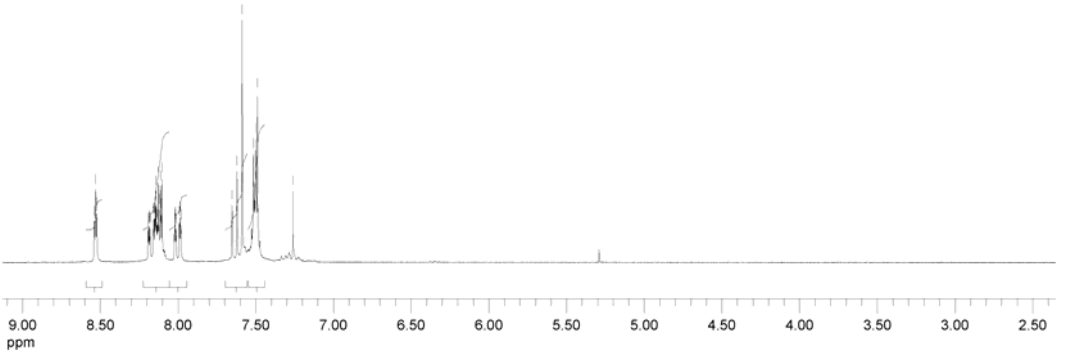
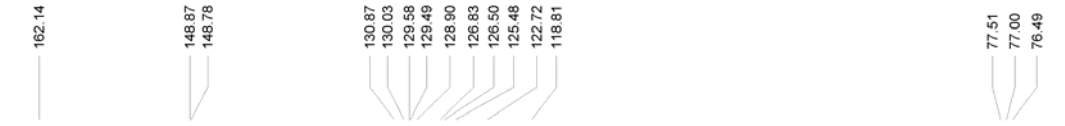
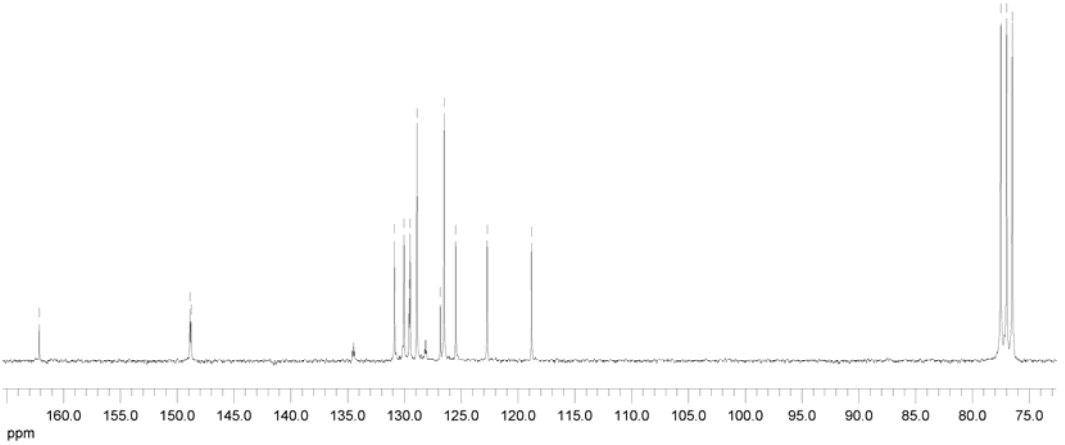
7.62
7.59
7.52
7.50
7.49
7.26


N
O
NO2

11a


9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
ppm


162.14
148.87
148.78
130.87
130.03
129.58
129.49
128.90
126.83
126.50
125.48
122.72
118.81
77.51
77.00
76.49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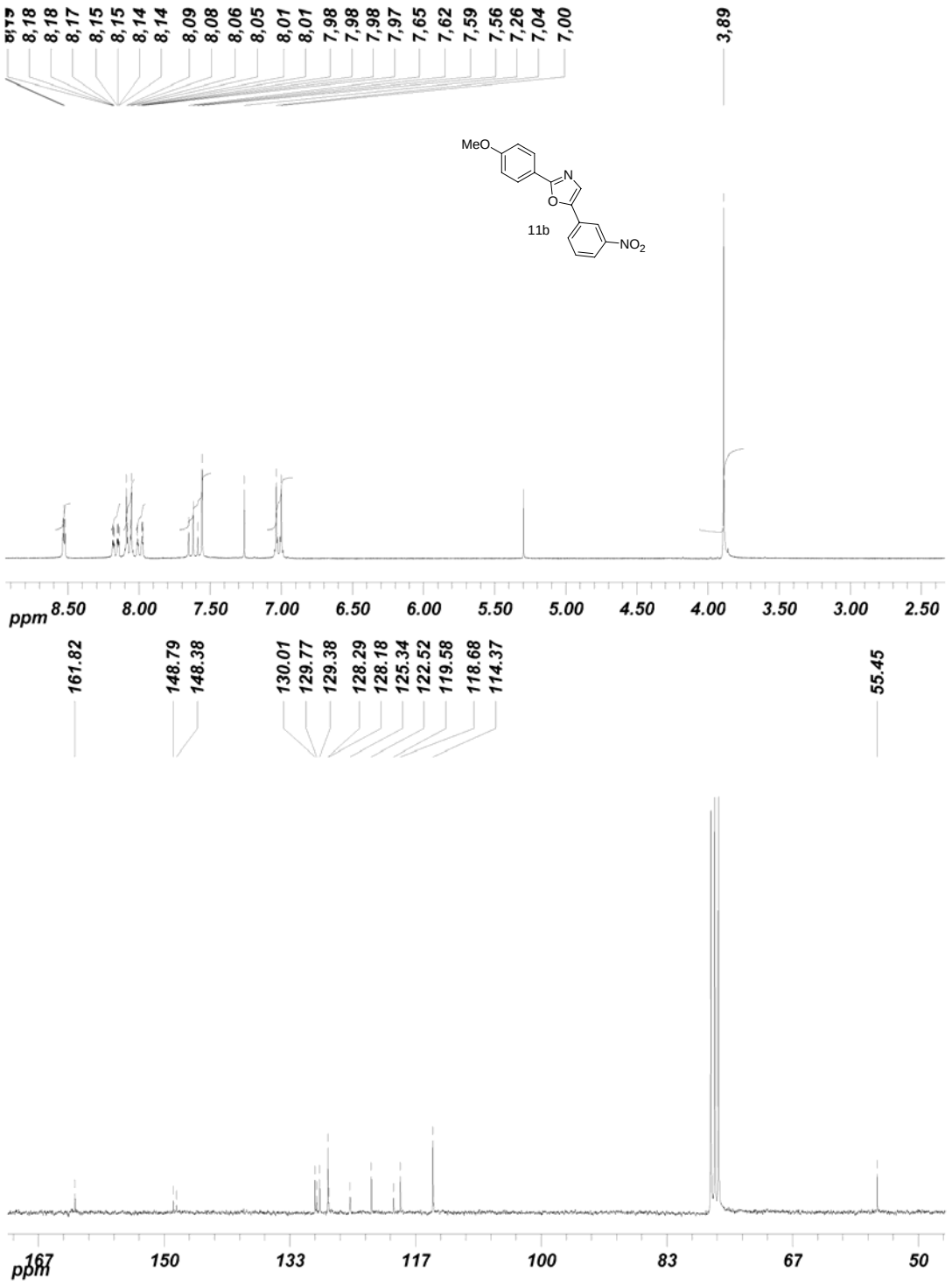
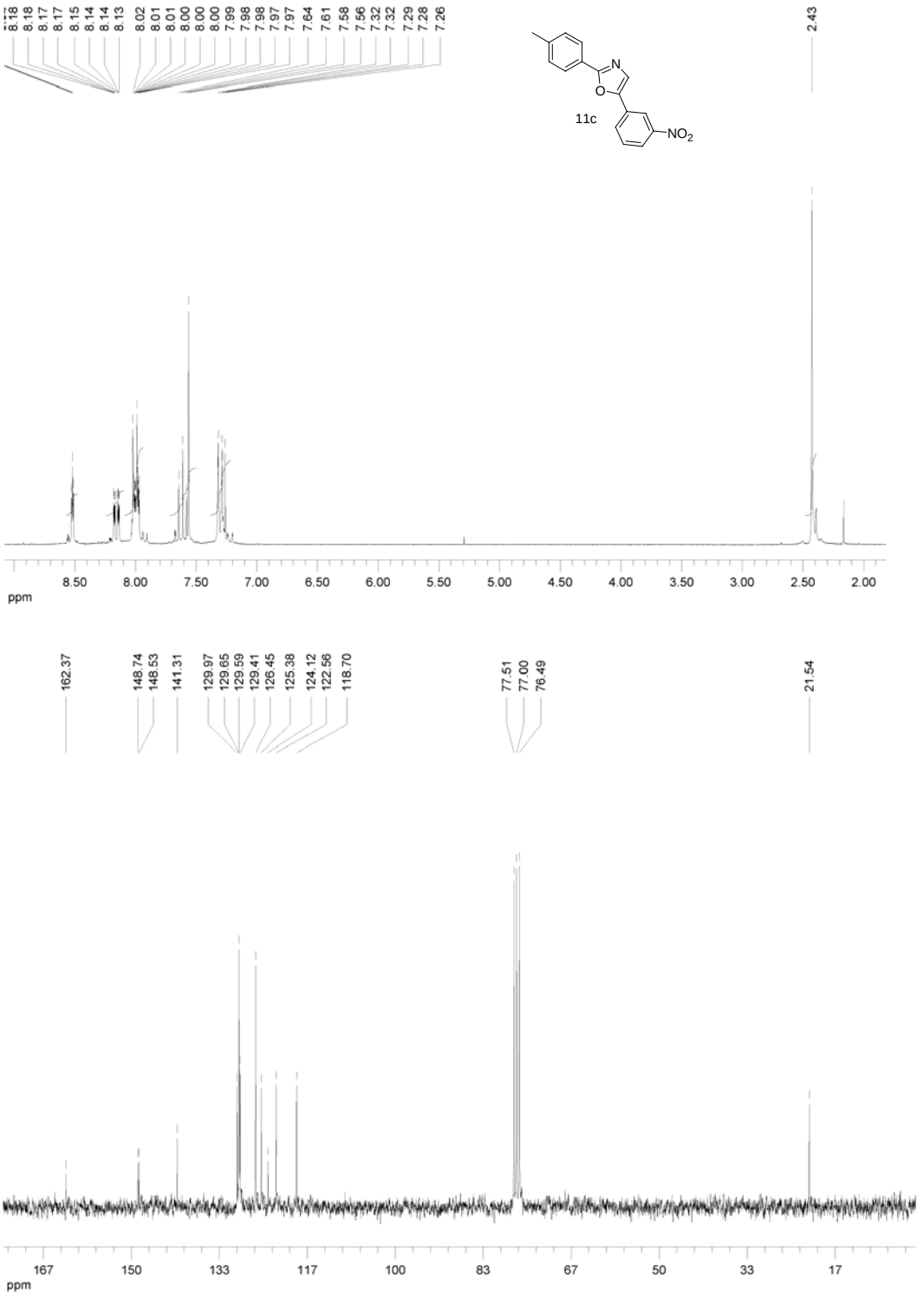
155.0
150.0
145.0
140.0
135.0
130.0
125.0
120.0
115.0
110.0
105.0
100.0
95.0
90.0
85.0
80.0
75.0
ppm


8,18
8,18
8,17
8,15
8,15
8,14
8,14
8,09
8,08
8,06
8,05
8,01
8,01
7,98
7,98
7,98
7,97
7,65
7,62
7,59
7,56
7,26
7,04
7,00
3,89
MeO
N
O
11b
NO2
ppm 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50
161.82
148.79
148.38
130.01
129.77
129.38
128.29
128.18
125.34
122.52
119.58
118.68
114.37
55.45
ppm 167 150 133 117 100 83 67 50


8.18
8.18
8.17
8.17
8.15
8.14
8.14
8.13
8.02
8.01
8.01
8.00
8.00
8.00
7.99
7.98
7.98
7.97
7.97
7.64
7.61
7.58
7.56
7.32
7.32
7.29
7.28
7.26
2.43
N
O
11c
NO2
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
ppm
162.37
148.74
148.53
141.31
129.97
129.65
129.59
129.41
126.45
125.38
124.12
122.56
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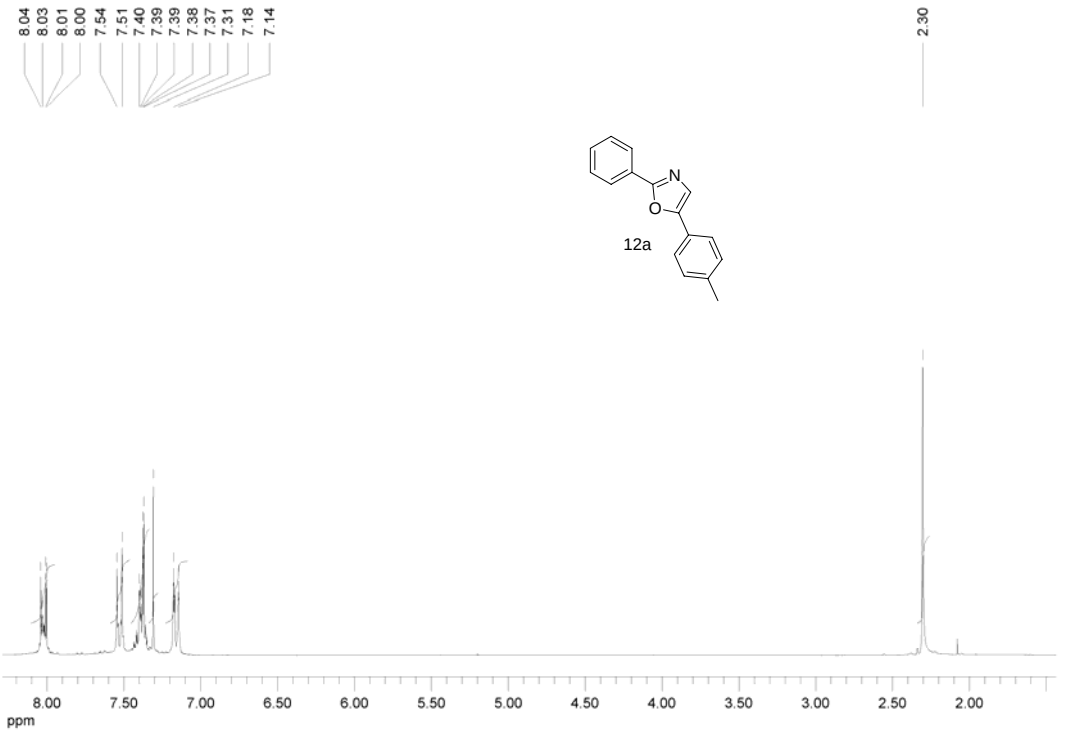
77.00
76.49
21.54
167
150
133
117
100
83
67
50
33
17
ppm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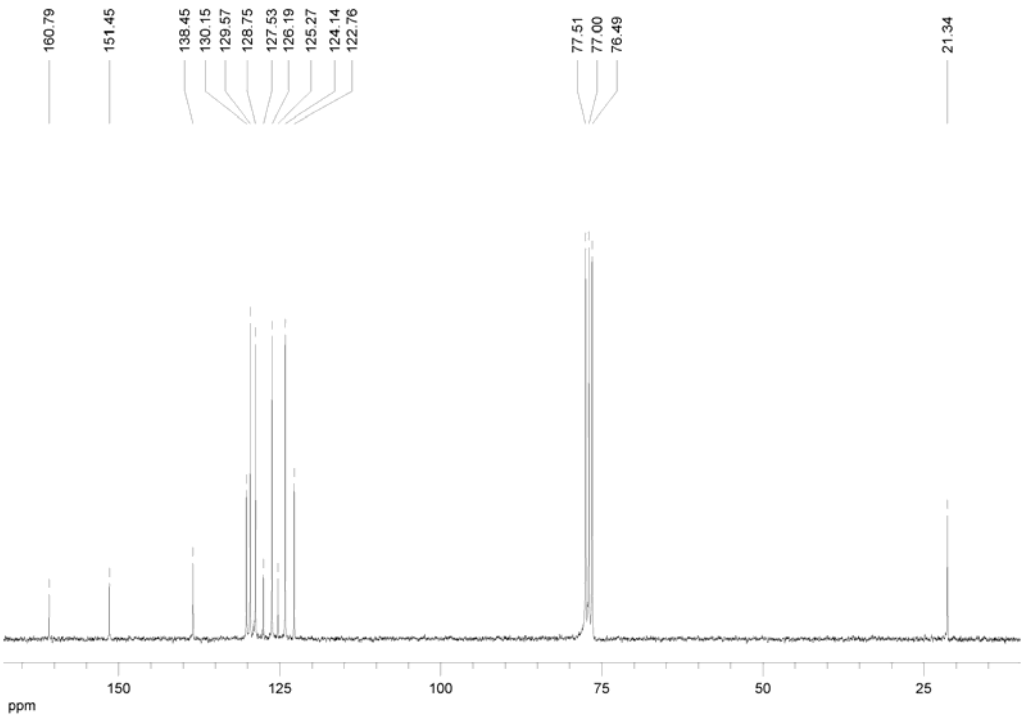
8.03
8.01
8.00
7.54
7.51
7.40
7.39
7.39
7.38
7.37
7.31
7.18
7.14
2.30
N
O
12a
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
ppm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138.45
130.15
129.57
128.75
127.53
126.19
125.27
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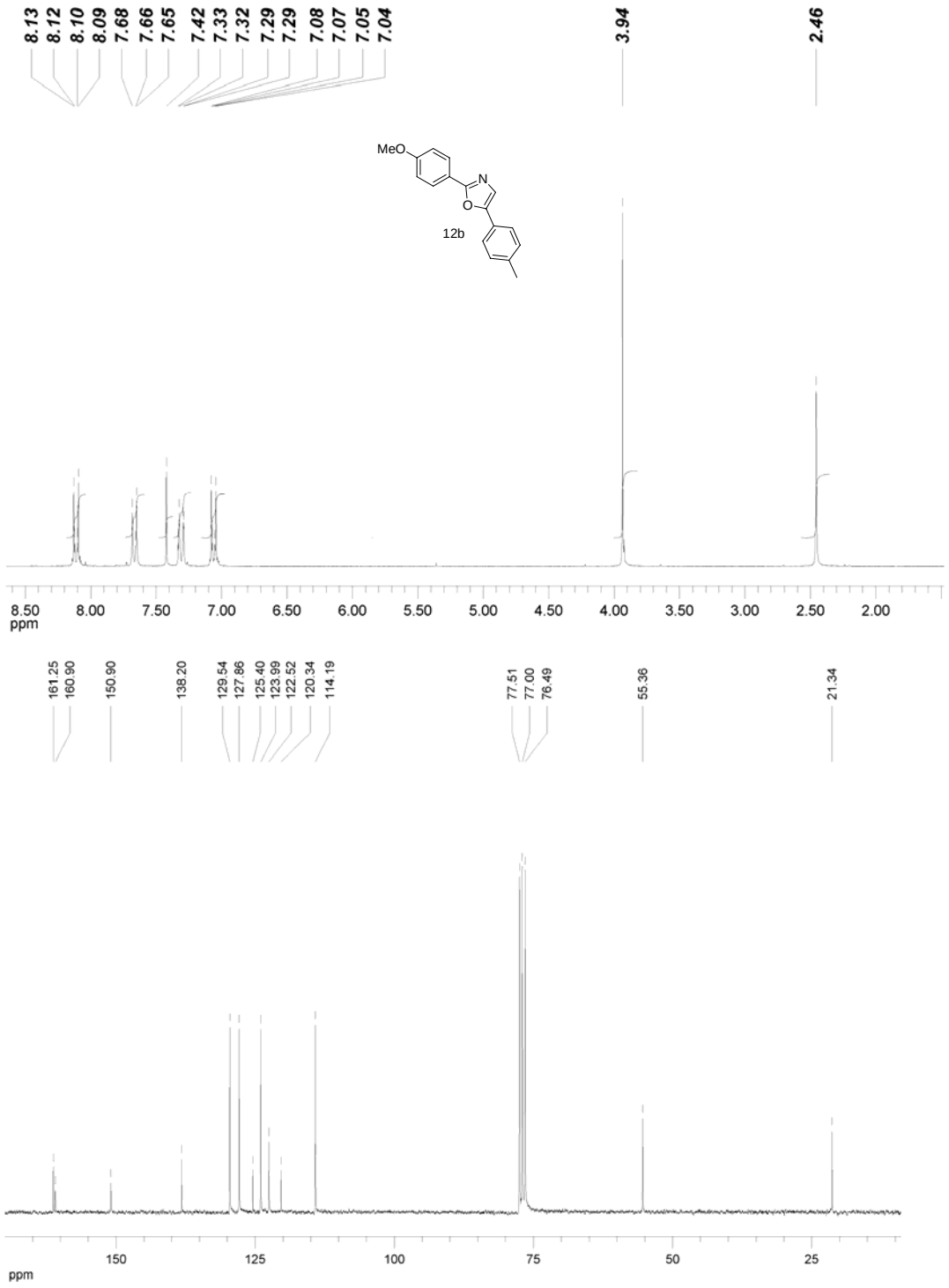
122.76
77.51
77.00
76.49
21.34
150
125
100
75
50
25
ppm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8.09
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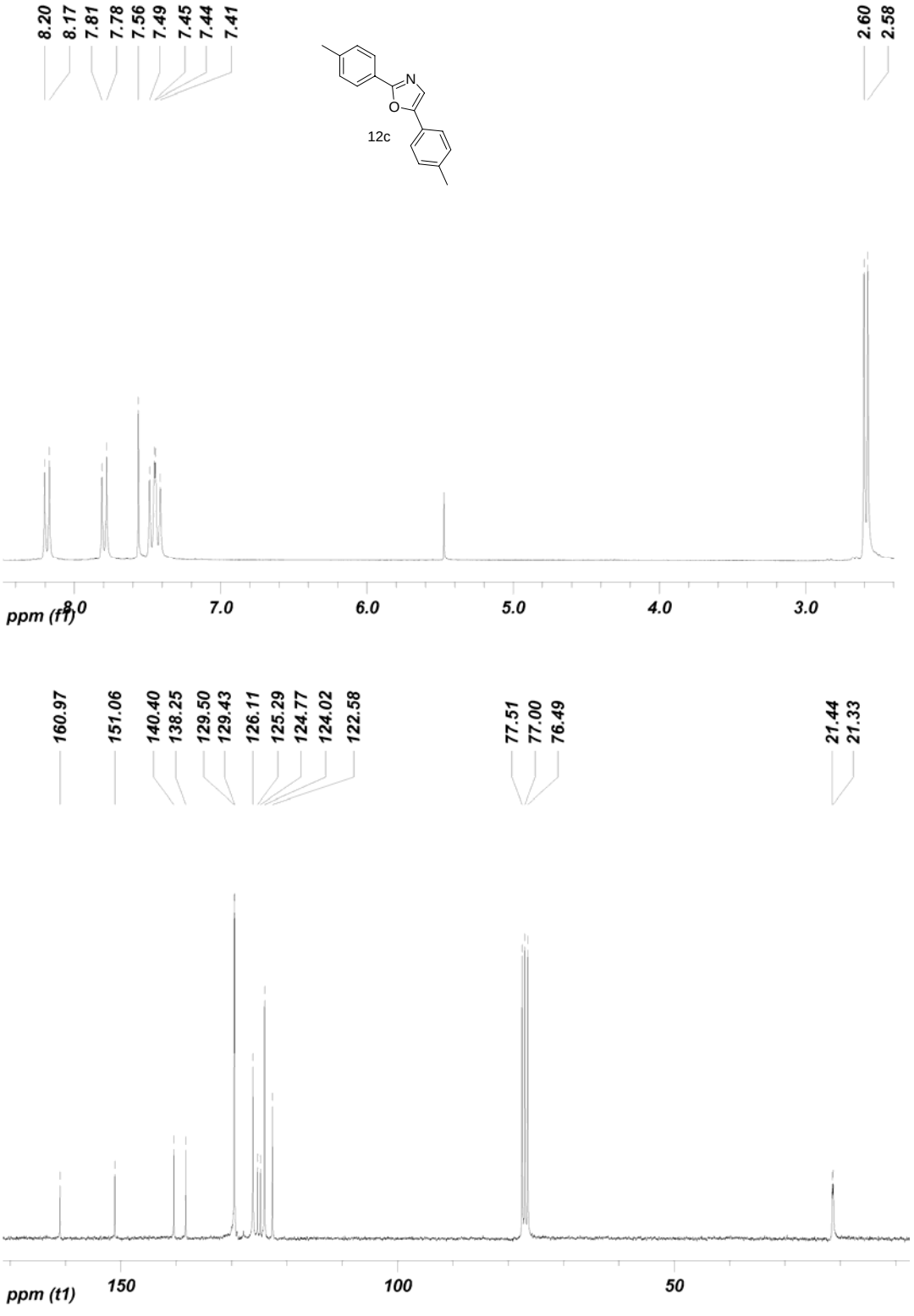
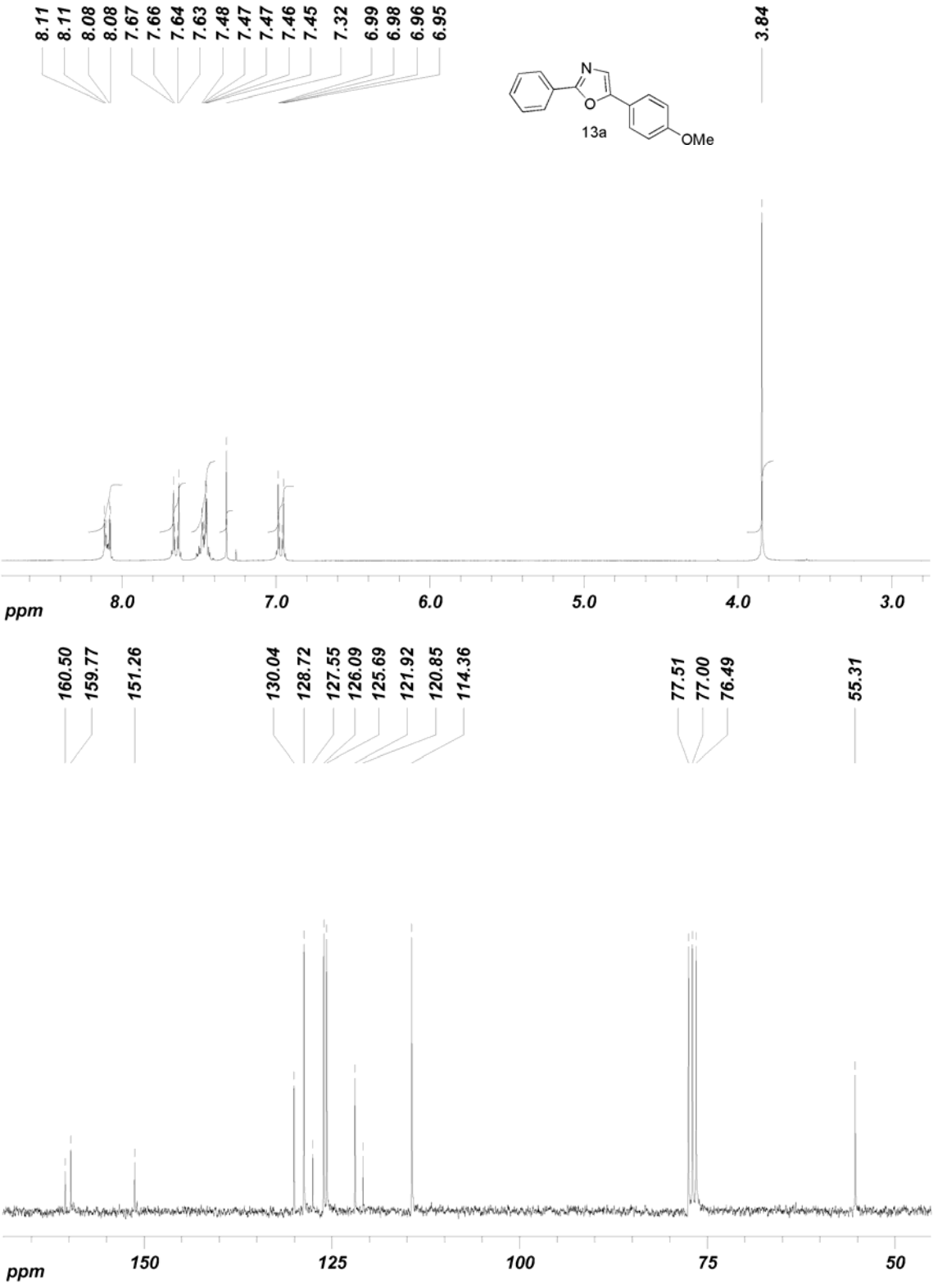
7.66
7.65
7.42
7.33
7.32
7.29
7.29
7.08
7.07
7.05
7.04
3.94
2.46
MeO
N
O
12b
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
ppm
161.25
160.90
150.90
138.20
129.54
127.86
125.40
123.99
122.52
120.34
114.19
77.51
77.00
76.49
55.36
21.34
150
125
100
75
50
25
ppm


8.20
8.17
7.81
7.78
7.56
7.49
7.45
7.44
7.41
2.60
2.58
12c
ppm (f1)
8.0
7.0
6.0
5.0
4.0
3.0
160.97
151.06
140.40
138.25
129.50
129.43
126.11
125.29
124.77
124.02
122.58
77.51
77.00
76.49
21.44
21.33
ppm (t1)
150
100
50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8.11
8.08
8.08
7.67
7.66
7.64
7.63
7.48
7.47
7.47
7.46
7.45
7.32
6.99
6.98
6.96
6.95
3.84
N
O
13a
OMe
ppm
8.0
7.0
6.0
5.0
4.0
3.0
160.50
159.77
151.26
130.04
128.72
127.55
126.09
125.69
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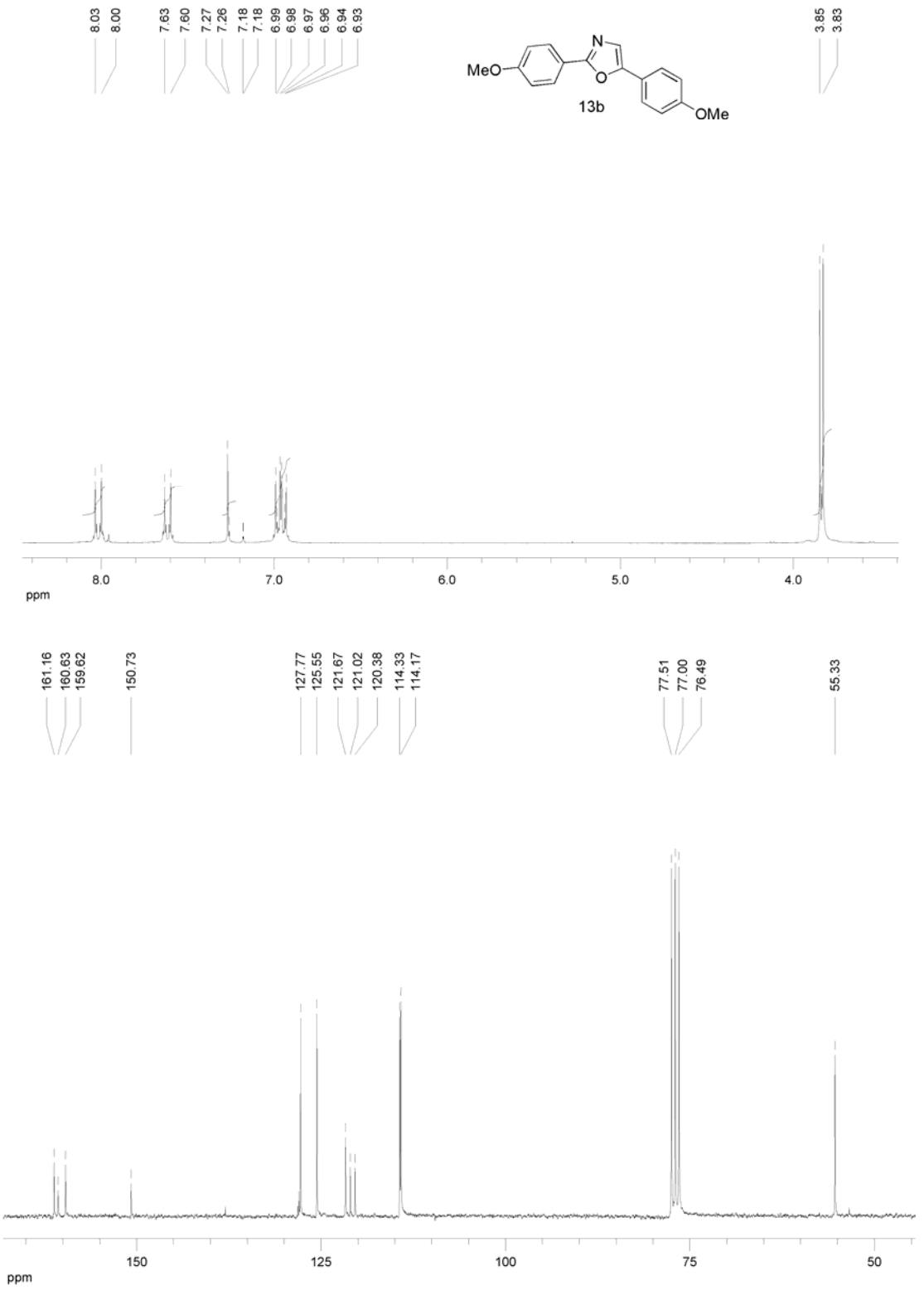
120.85
114.36
77.51
77.00
76.49
55.31
ppm
150
125
100
75
50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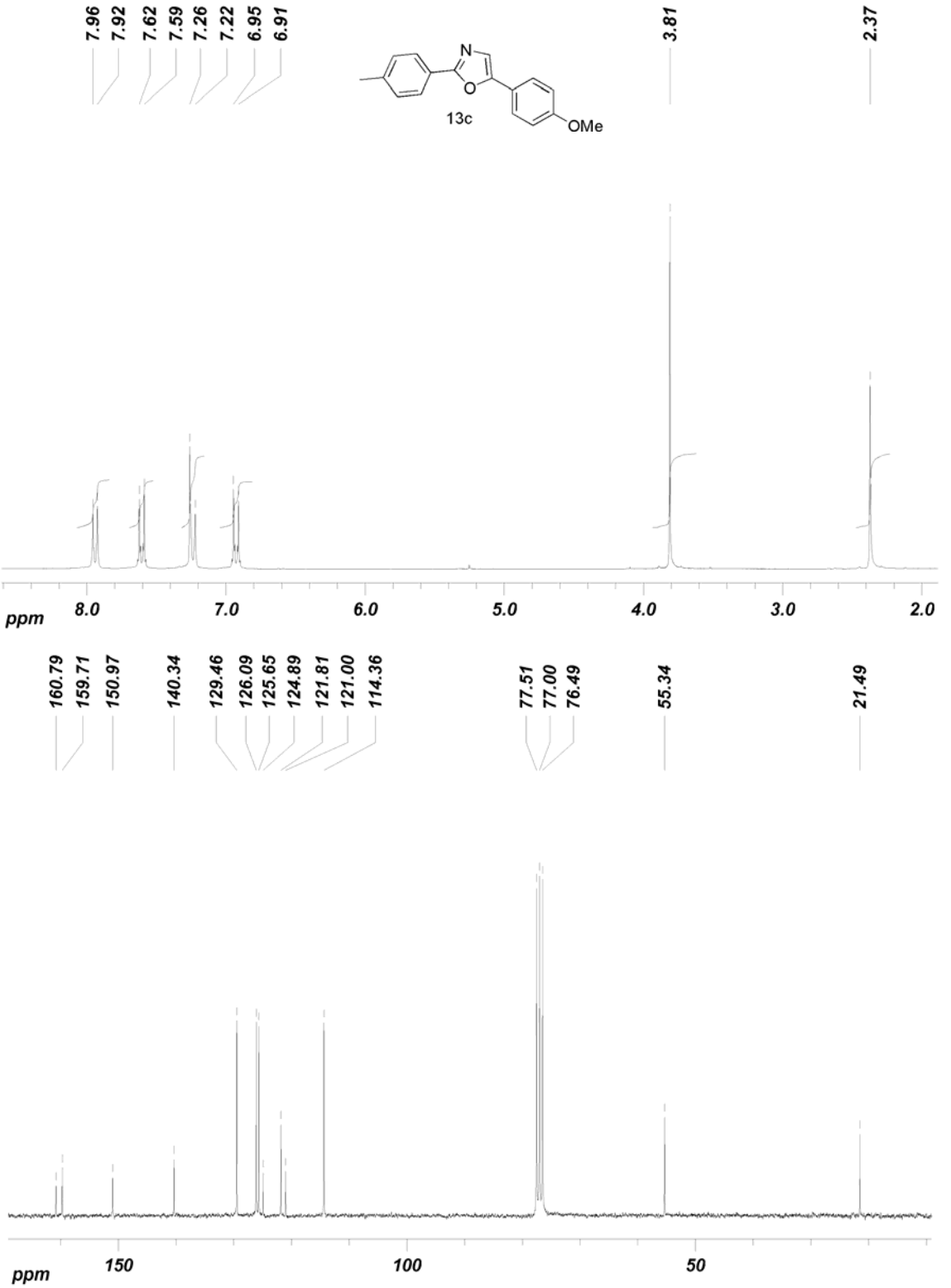
8.00
7.63
7.60
7.27
7.26
7.18
7.18
6.99
6.98
6.97
6.96
6.94
6.93
3.85
3.83
MeO
N
O
OMe
13b
8.0
7.0
6.0
5.0
4.0
ppm
161.16
160.63
159.62
150.73
127.77
125.55
121.67
121.02
120.38
114.33
114.17
77.51
77.00
76.49
55.33
150
125
100
75
50
ppm


7.96
7.92
7.62
7.59
7.26
7.22
6.95
6.91
3.81
2.37
N
O
13c
OMe
ppm
8.0
7.0
6.0
5.0
4.0
3.0
2.0
160.79
159.71
150.97
140.34
129.46
126.09
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124.89
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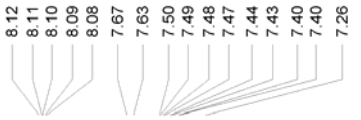
121.00
114.36
77.51
77.00
76.49
55.34
21.49
ppm
150
100
50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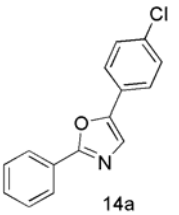
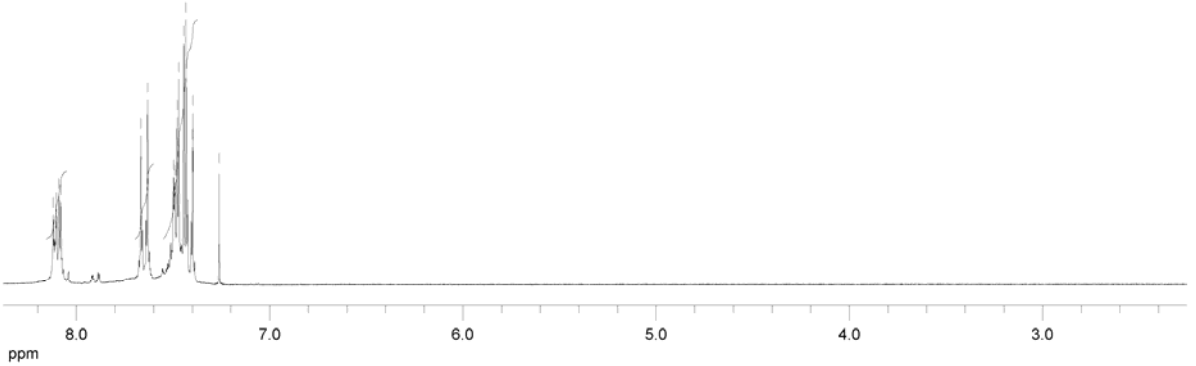
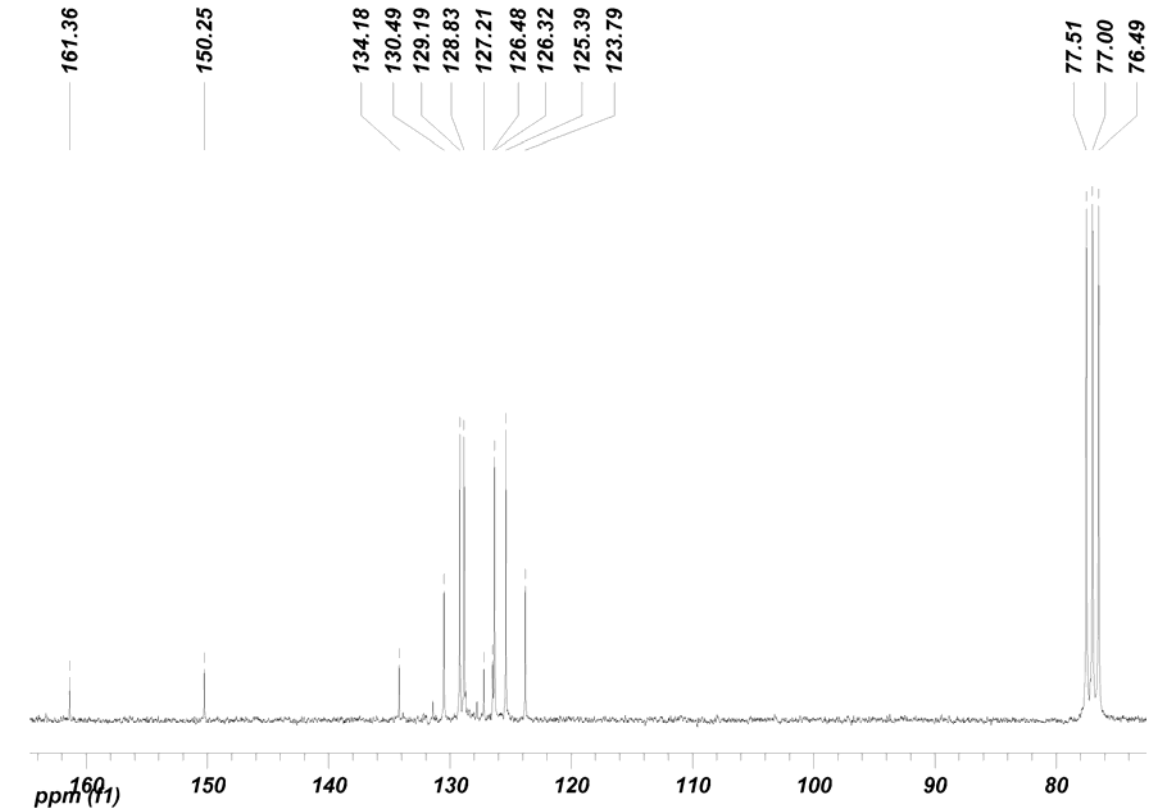
8.11
8.10
8.09
8.08
7.67
7.63
7.50
7.49
7.48
7.47
7.44
7.43
7.40
7.40
7.26


Cl
O
N

14a


8.0
7.0
6.0
5.0
4.0
3.0
ppm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150.25
134.18
130.49
129.19
128.83
127.21
126.48
126.32
125.39
123.79
77.51
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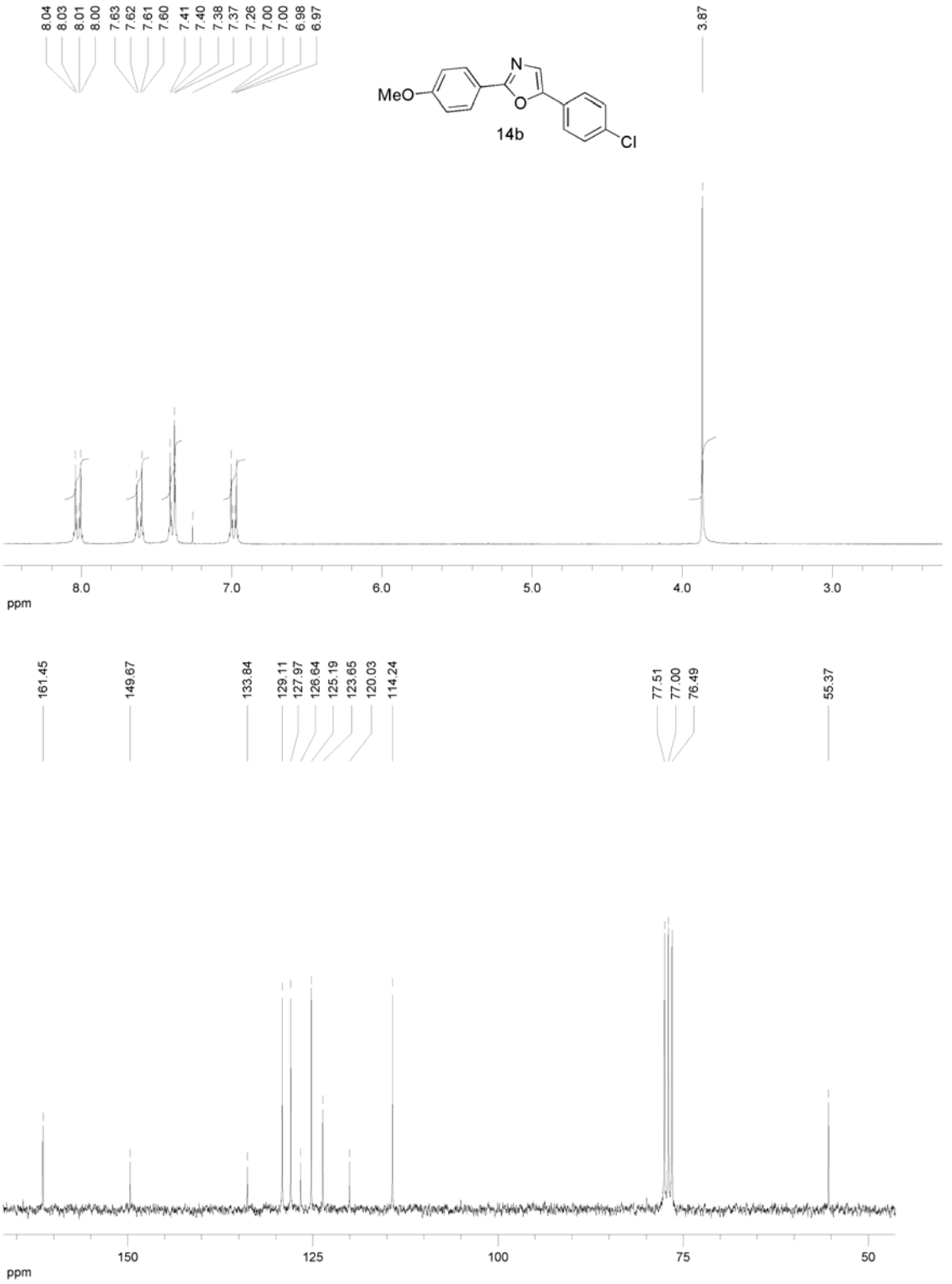
150
140
130
120
110
100
90
80
ppm (f1)


8.04
8.03
8.01
8.00
7.63
7.62
7.61
7.60
7.41
7.40
7.38
7.37
7.26
7.00
7.00
6.98
6.97
3.87
MeO
N
O
Cl
14b
8.0
7.0
6.0
5.0
4.0
3.0
ppm
161.45
149.67
133.84
129.11
127.97
126.64
125.19
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120.03
114.24
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55.37
150
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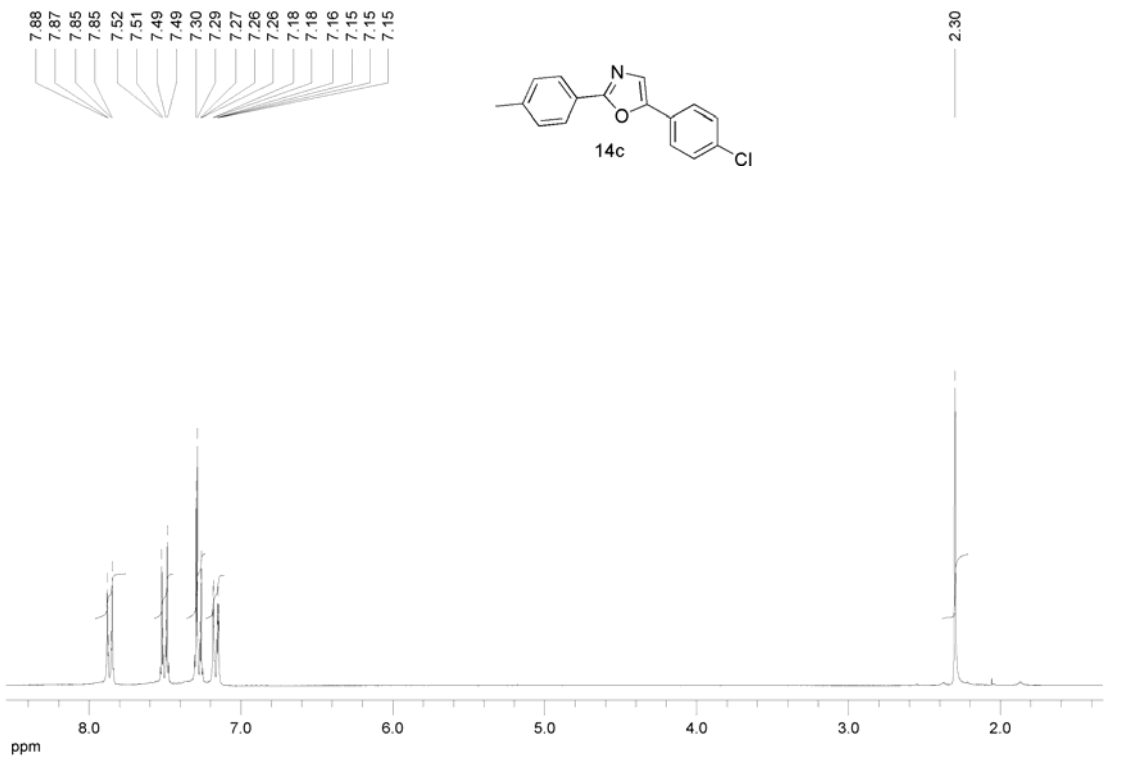
100
75
50
ppm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7.85
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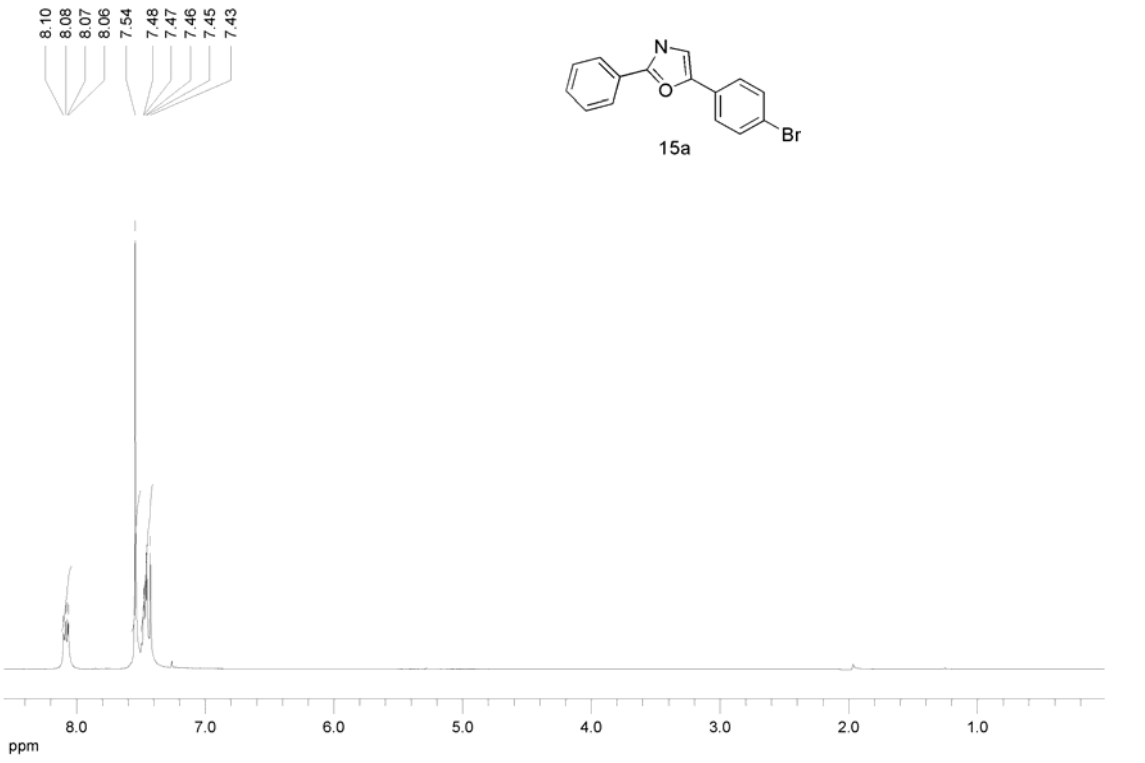
7.51
7.49
7.49
7.30
7.29
7.27
7.26
7.26
7.18
7.18
7.16
7.15
7.15
7.15
2.30
N
O
Cl
14c
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm
161.52
149.84
140.74
133.92
129.47
129.07
126.54
126.22
125.23
124.51
123.67
77.51
77.00
76.49
21.47
150
125
100
75
50
25
ppm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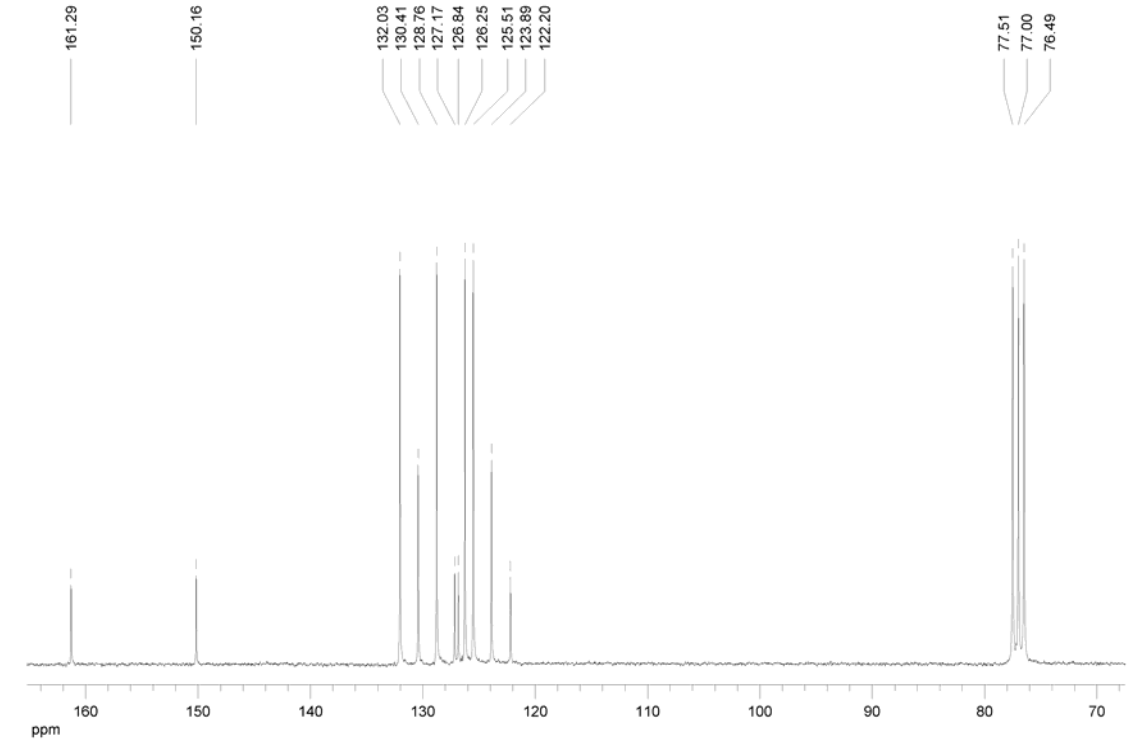
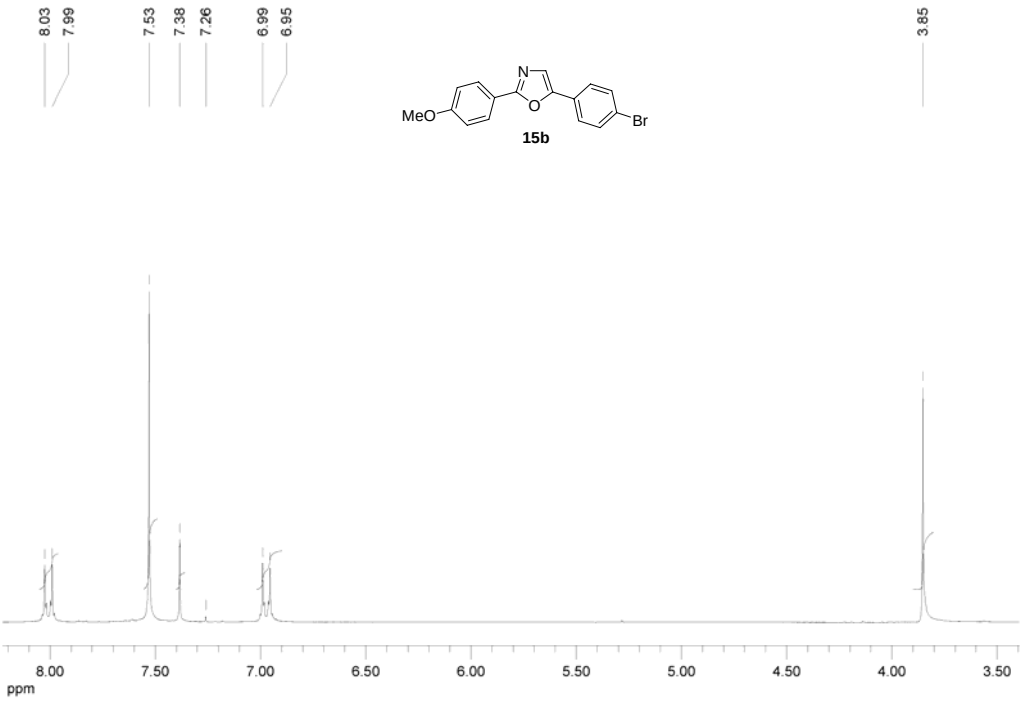
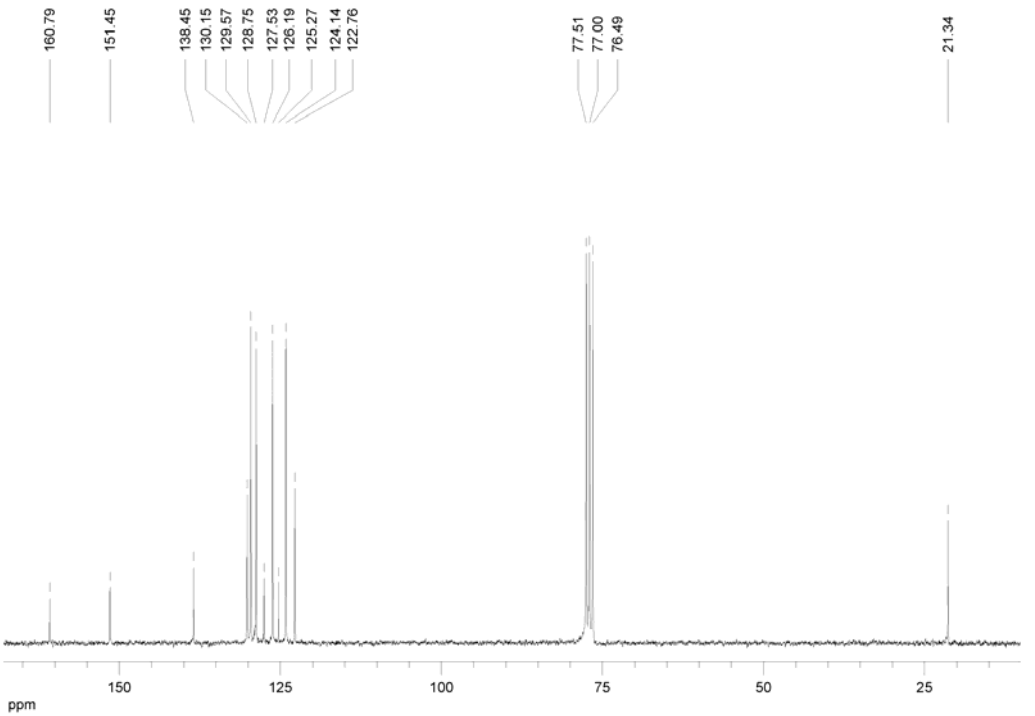
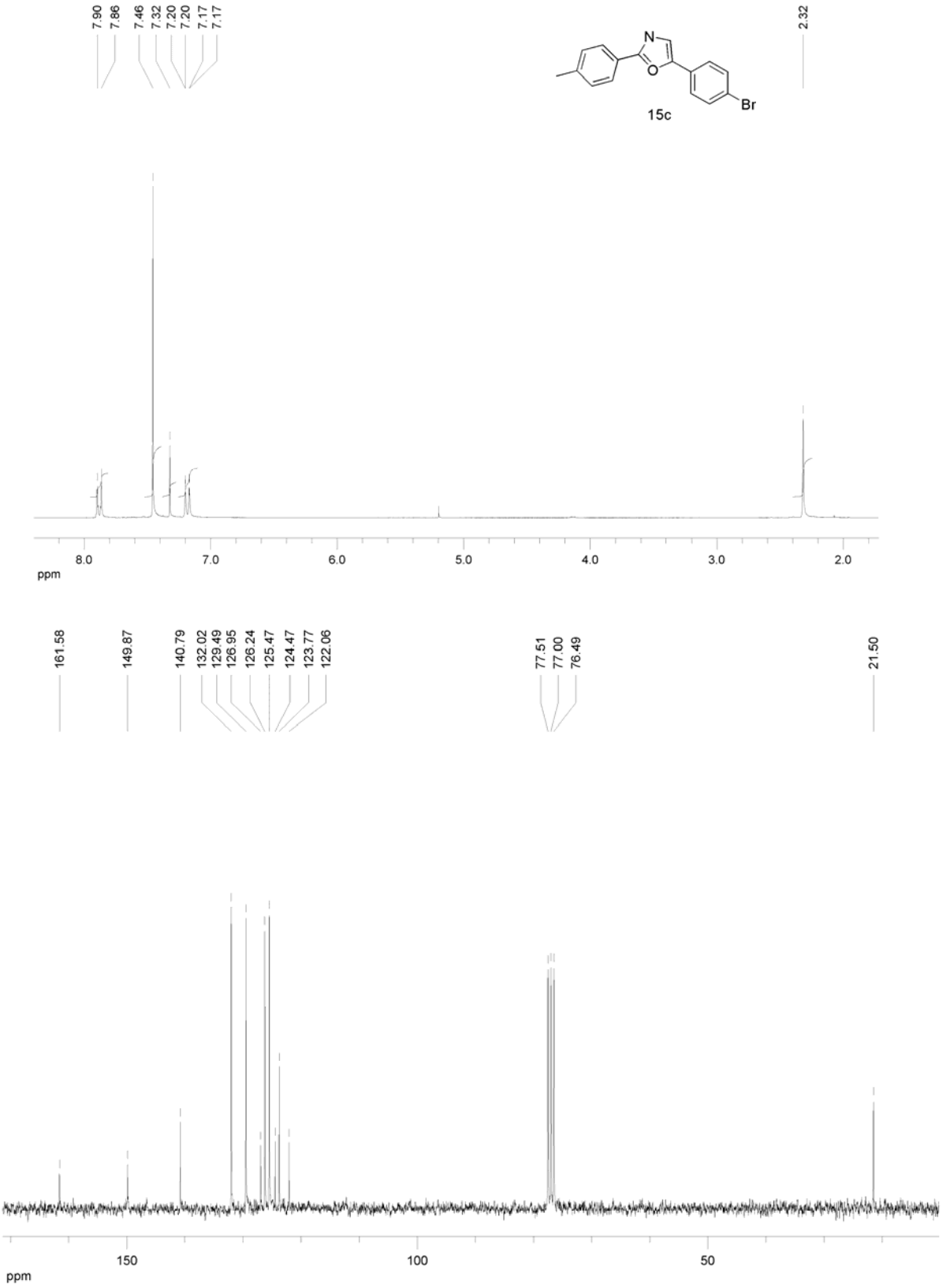
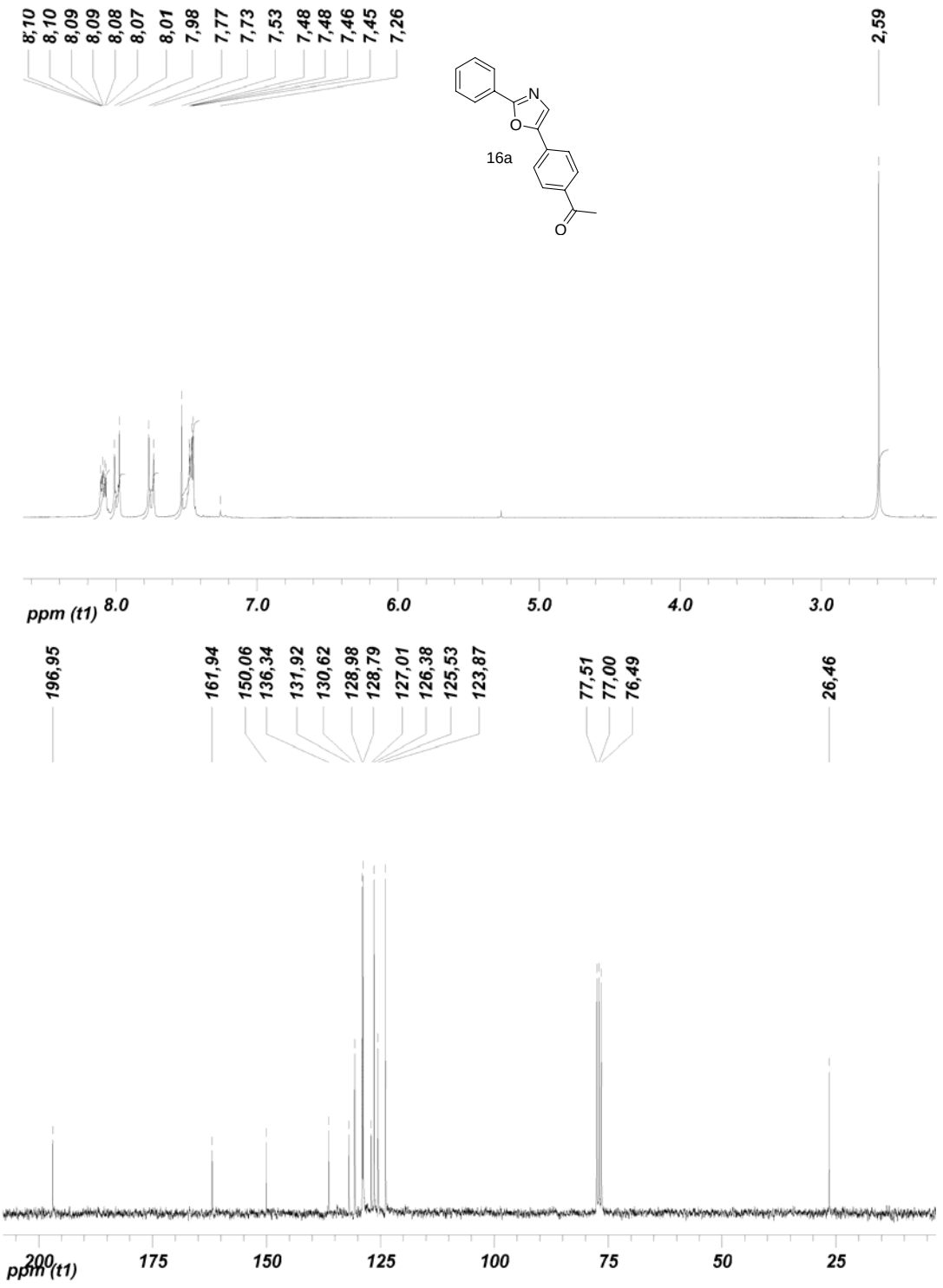
8.07
8.06
7.54
7.48
7.47
7.46
7.45
7.43
N
O
Br
15a
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm

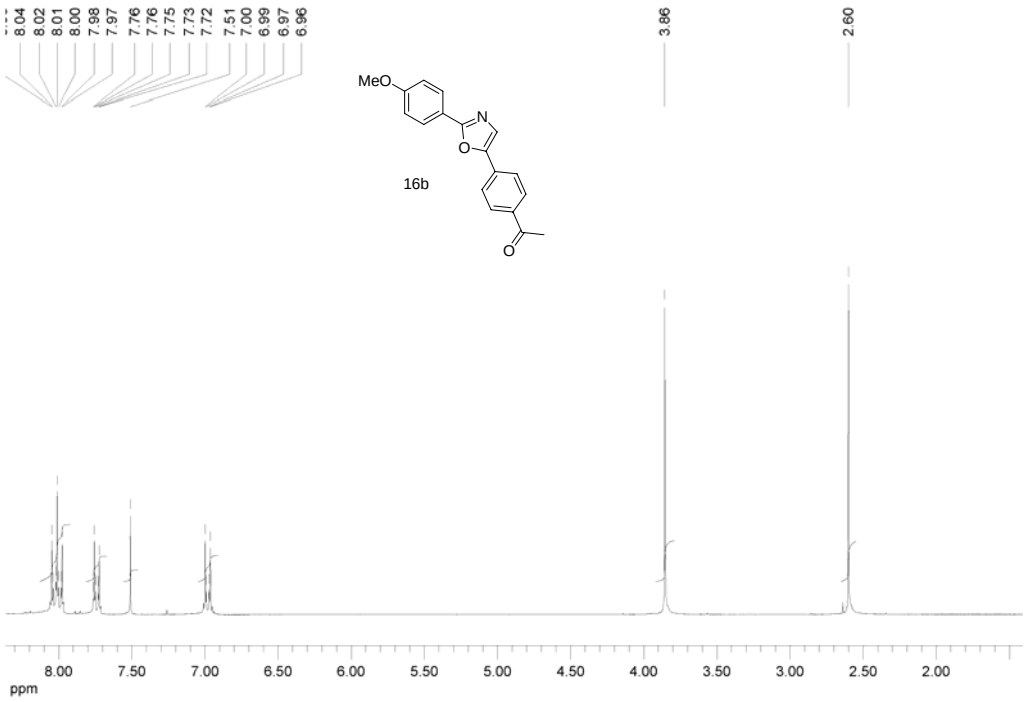

161.29
150.16
132.03
130.41
128.76
127.17
126.84
126.25
125.51
123.89
122.20
77.51
77.00
76.49
160
150
140
130
120
110
100
90
80
70
ppm

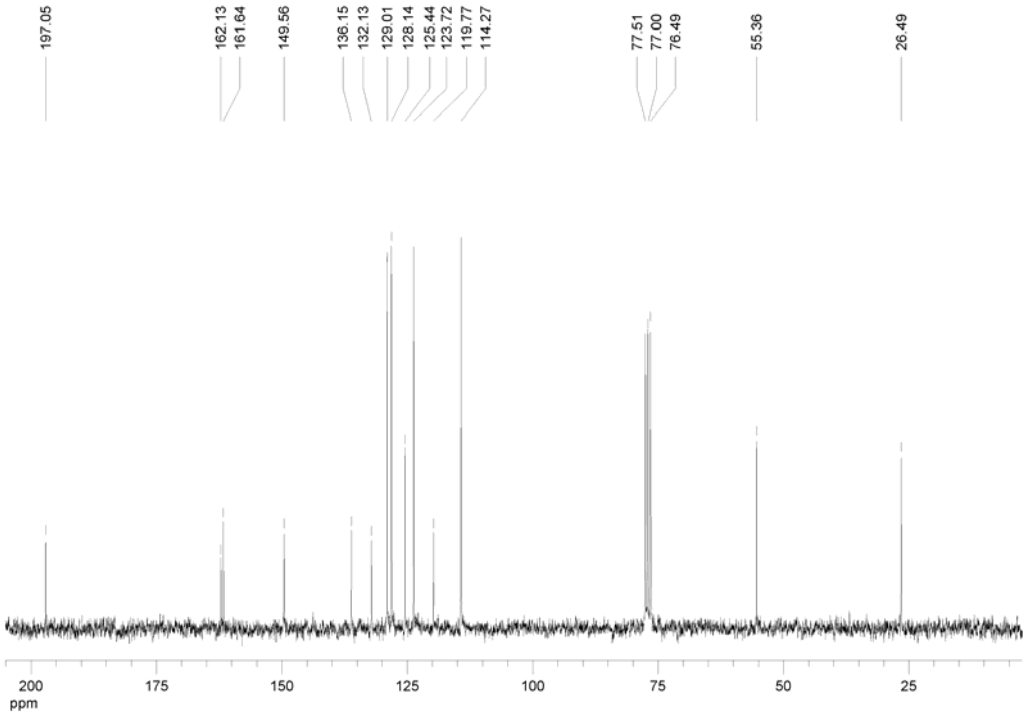

8.03
7.99
7.53
7.38
7.26
6.99
6.95
3.85
N
O
MeO
Br
15b
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
ppm


160.79
151.45
138.45
130.15
129.57
128.75
127.53
126.19
125.27
124.14
122.76
77.51
77.00
76.49
21.34
150
125
100
75
50
25
ppm


7.90
7.86
7.46
7.32
7.20
7.20
7.17
7.17
2.32
N
O
Br
15c
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm
161.58
149.87
140.79
132.02
129.49
126.95
126.24
125.47
124.47
123.77
122.06
77.51
77.00
76.49
21.50
150
100
50
ppm


8,10
8,10
8,09
8,09
8,08
8,07
8,01
7,98
7,77
7,73
7,53
7,48
7,48
7,46
7,45
7,26
2,59
N
O
O
16a
ppm (t1)
8.0
7.0
6.0
5.0
4.0
3.0
196,95
161,94
150,06
136,34
131,92
130,62
128,98
128,79
127,01
126,38
125,53
123,87
77,51
77,00
76,49
26,46
200
175
150
125
100
75
50
25
ppm (t1)


8.04
8.02
8.01
8.00
7.98
7.97
7.76
7.76
7.75
7.73
7.72
7.51
7.00
6.99
6.97
6.96
3.86
2.60
MeO
N
O
16b
O
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
ppm


197.05
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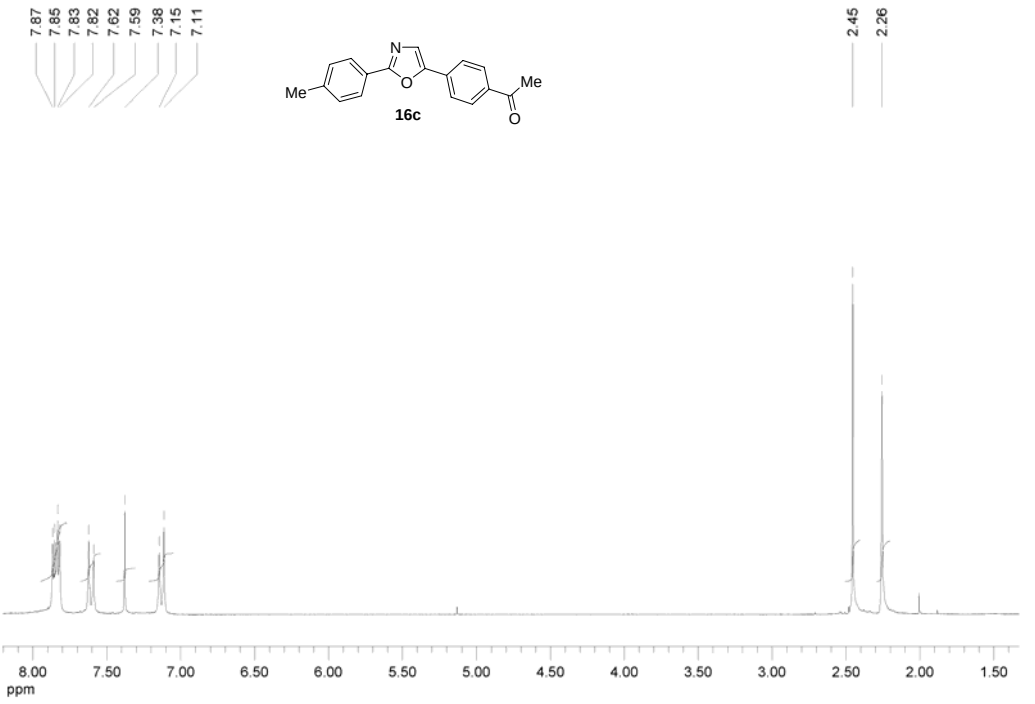
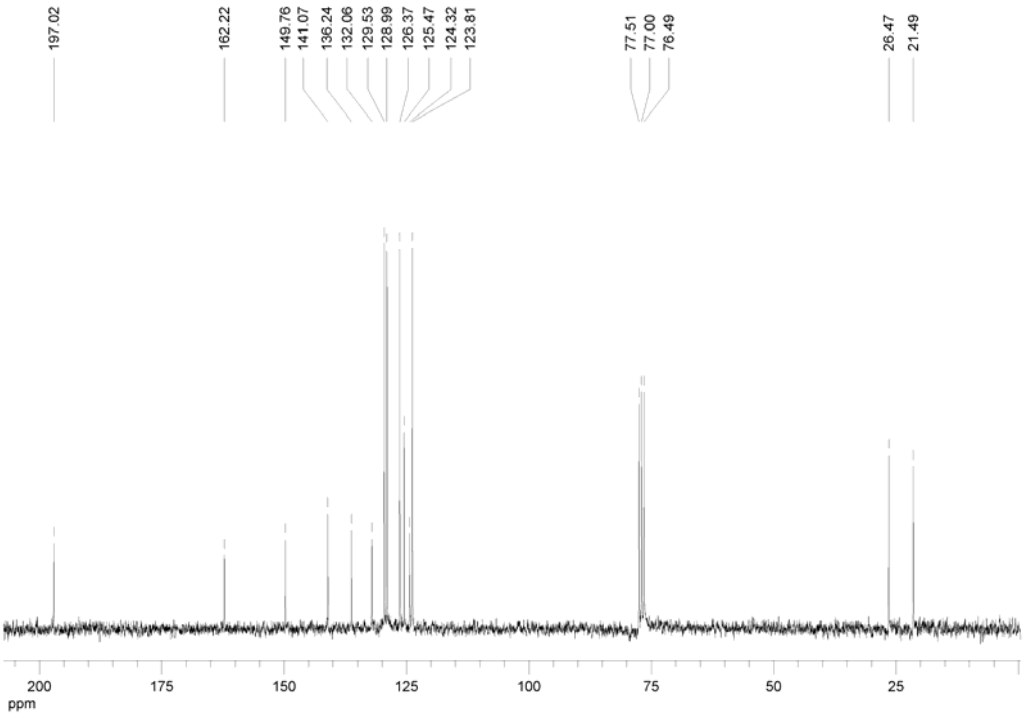
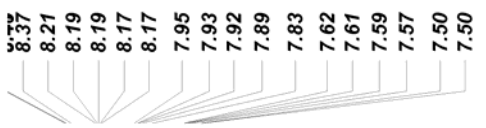
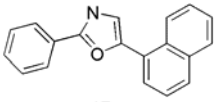
161.64
149.56
136.15
132.13
129.01
128.14
125.44
123.72
119.77
114.27
77.51
77.00
76.49
55.36
26.49
200
175
150
125
100
75
50
25
ppm

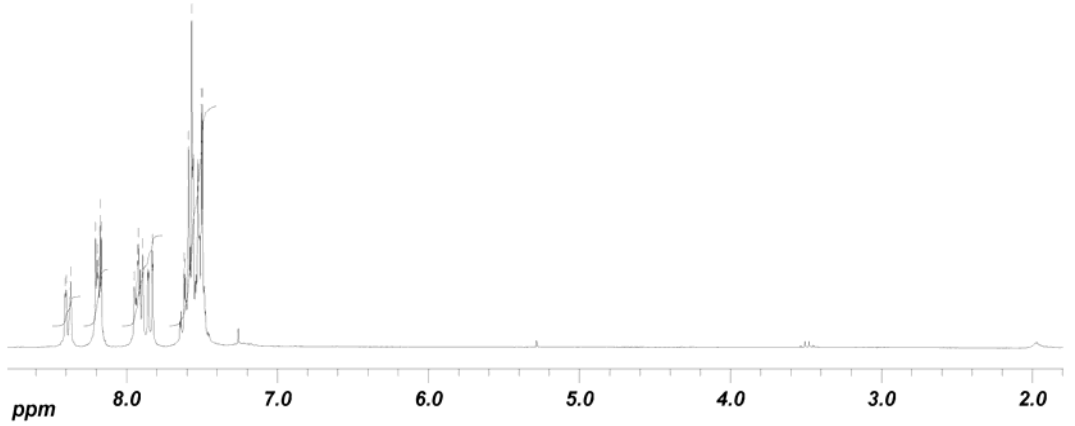

7.87
7.85
7.83
7.82
7.62
7.59
7.38
7.15
7.11
N
O
Me
Me
O
16c
2.45
2.26
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
ppm


197.02
162.22
149.76
141.07
136.24
132.06
129.53
128.99
126.37
125.47
124.32
123.81
77.51
77.00
76.49
26.47
21.49
200
175
150
125
100
75
50
25
ppm


8.37
8.21
8.19
8.19
8.17
8.17
7.95
7.93
7.92
7.89
7.83
7.62
7.61
7.59
7.57
7.50
7.50


N
O

17a


ppm
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6.0
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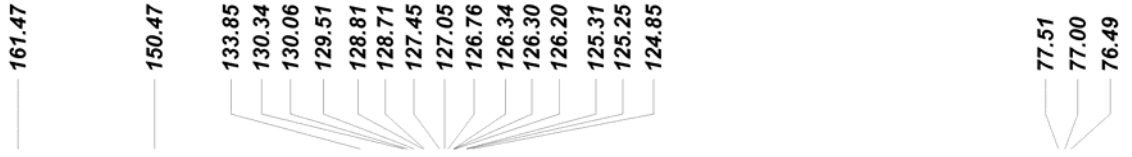
4.0
3.0
2.0


161.47
150.47
133.85
130.34
130.06
129.51
128.81
128.71
127.45
127.05
126.76
126.34
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126.20
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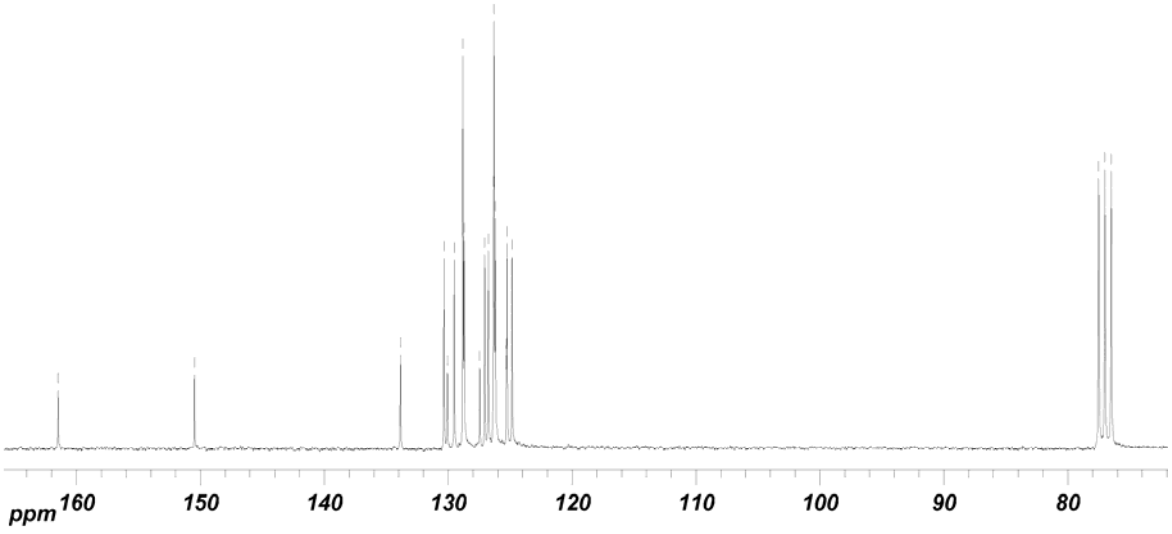
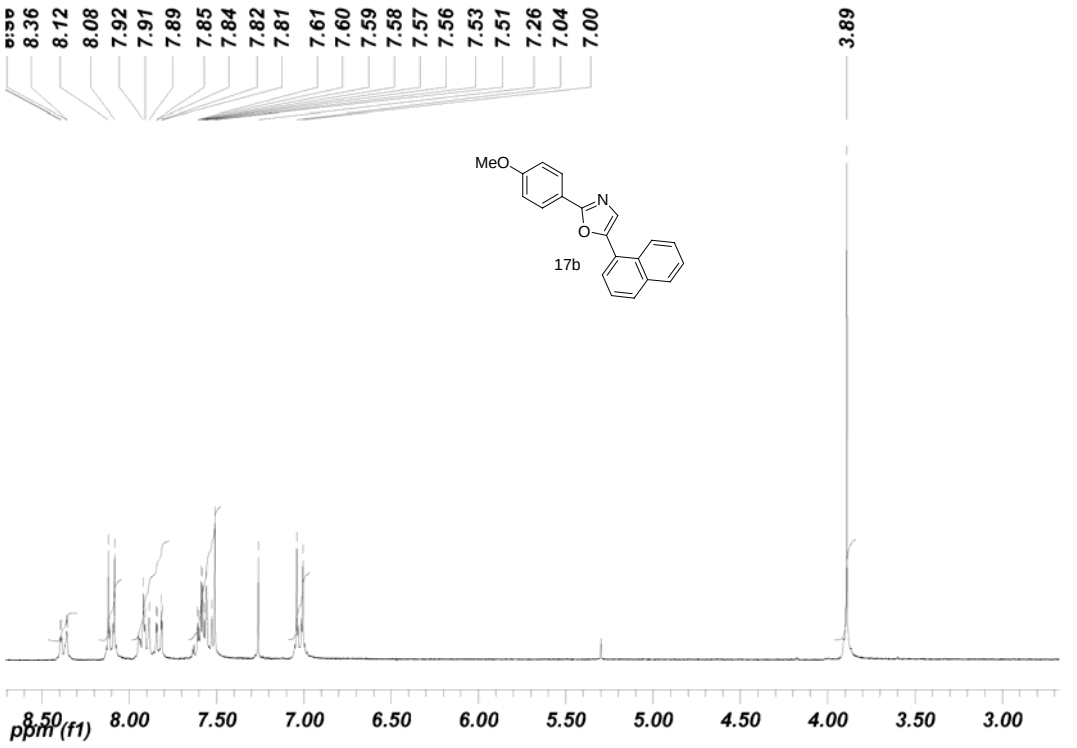
125.25
124.85
77.51
77.00
76.49


ppm
160
150
140
130
120
110
100
90
80


8.36
8.12
8.08
7.92
7.91
7.89
7.85
7.84
7.82
7.81
7.61
7.60
7.59
7.58
7.57
7.56
7.53
7.51
7.26
7.04
7.00
3.89
MeO
N
O
17b
8.50
8.00
7.50
7.00
6.50
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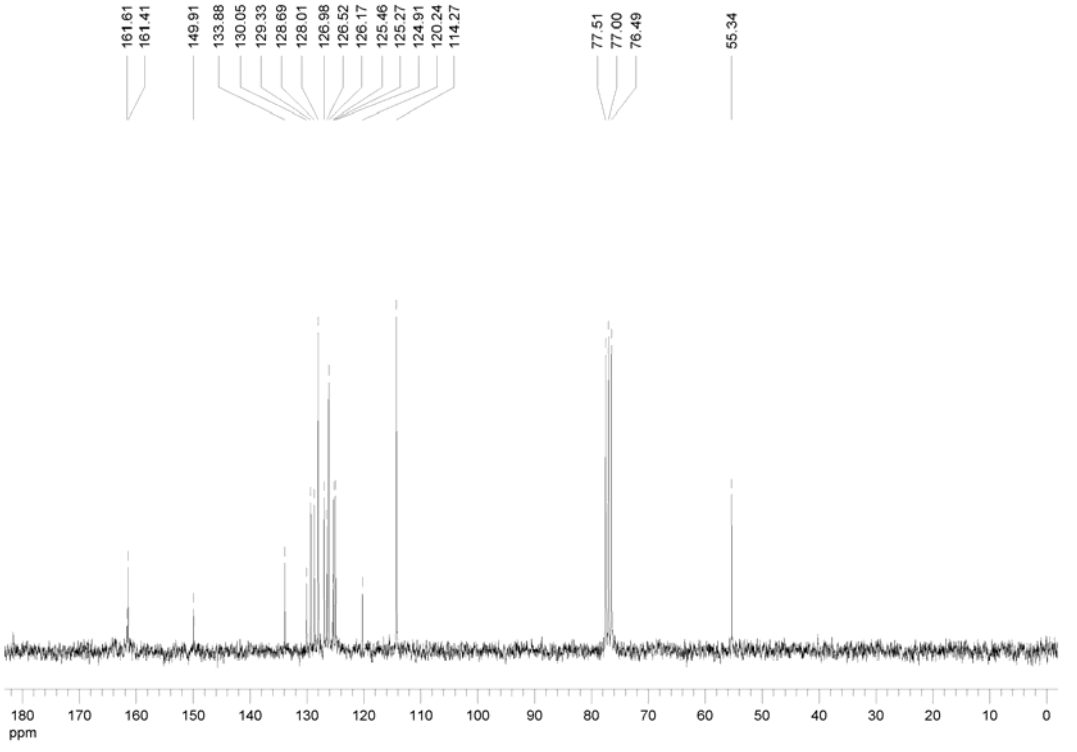
5.00
4.50
4.00
3.50
3.00
ppm (f1)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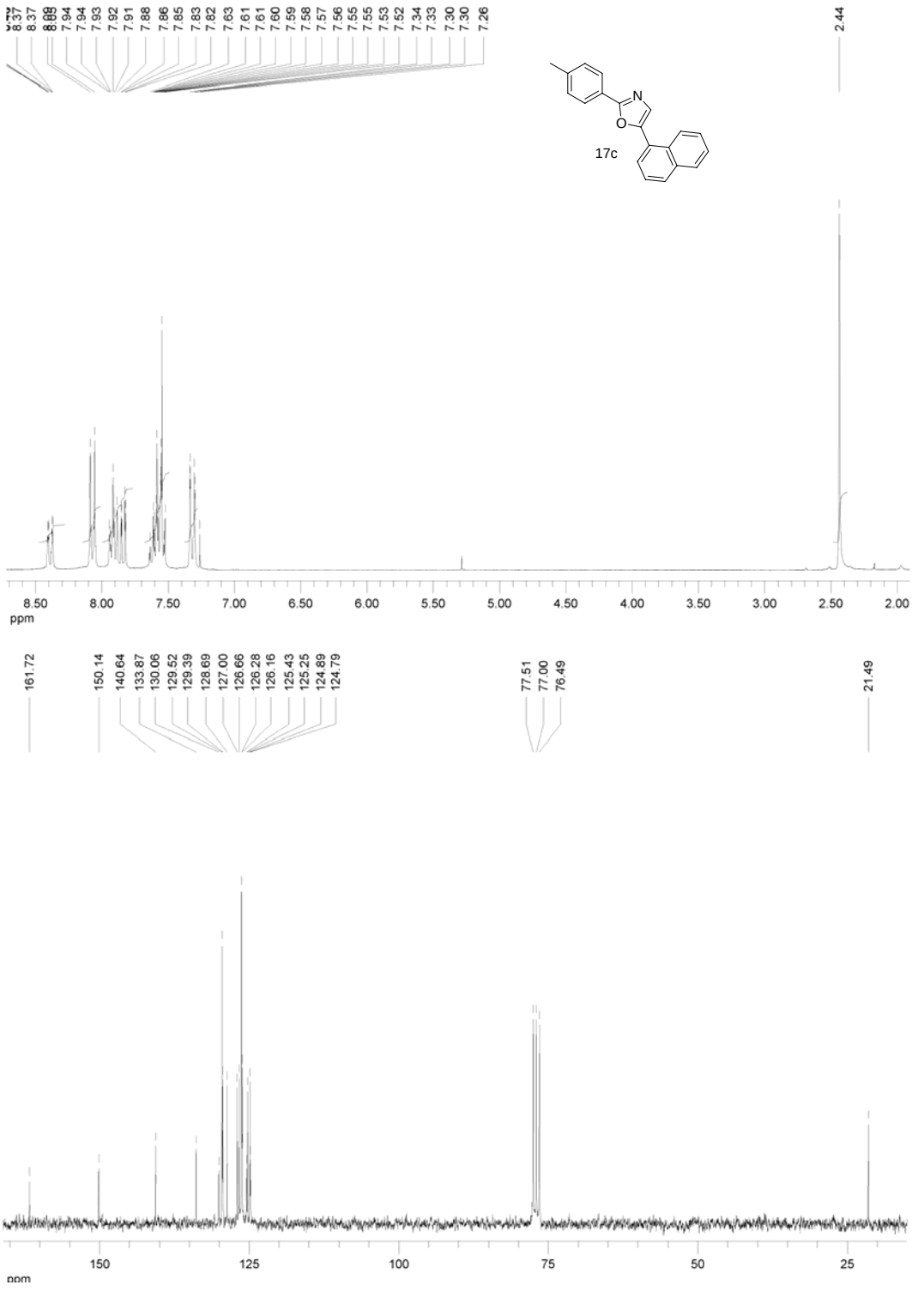
161.41
149.91
133.88
130.05
129.33
128.69
128.01
126.98
126.52
126.17
125.46
125.27
124.91
120.24
114.27
77.51
77.00
76.49
55.34
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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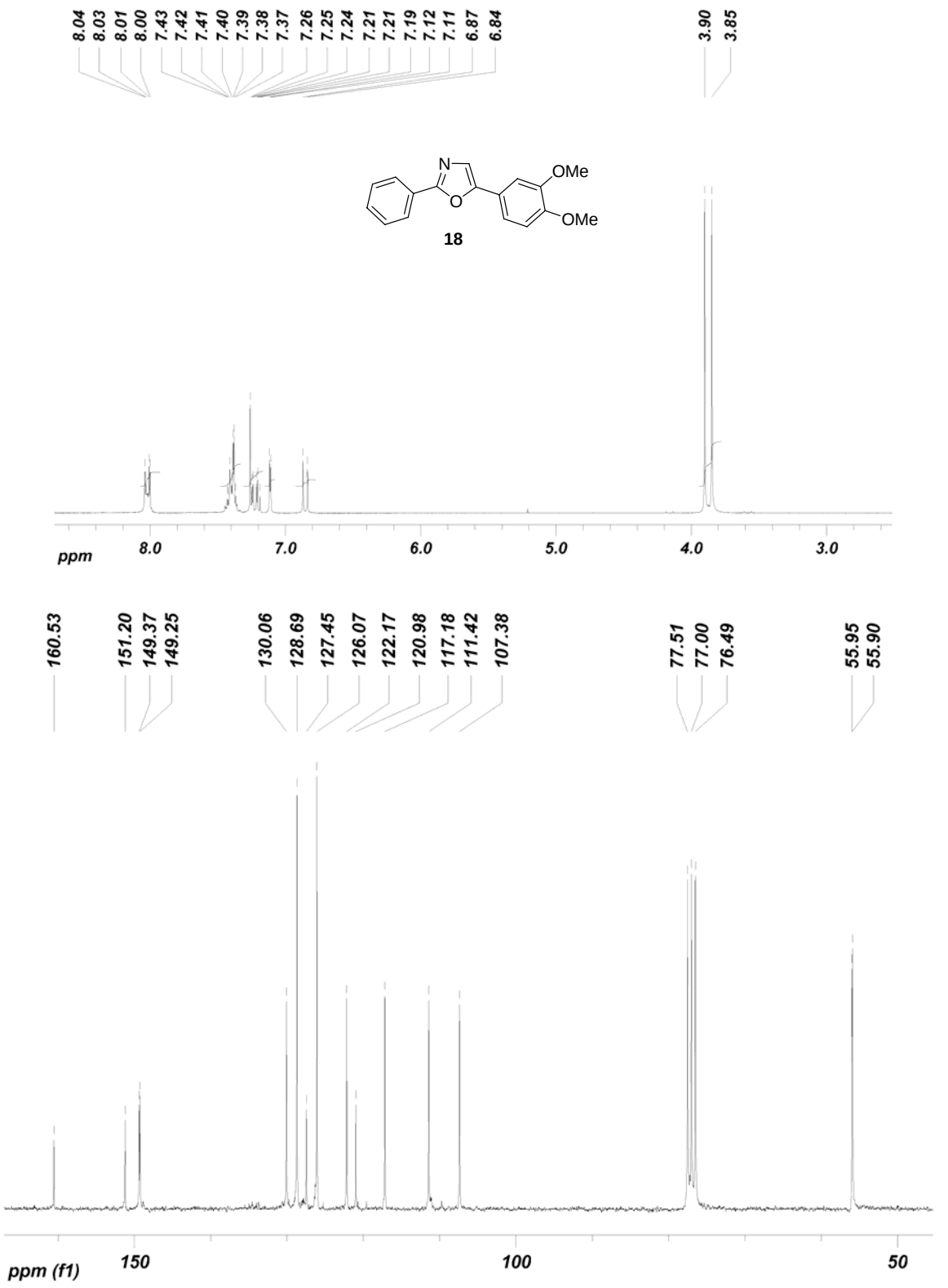
8.37
7.94
7.94
7.93
7.92
7.91
7.88
7.86
7.85
7.83
7.82
7.63
7.61
7.61
7.60
7.59
7.58
7.57
7.56
7.55
7.55
7.53
7.52
7.34
7.33
7.30
7.30
7.26
2.44
N
O
17c
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
ppm
161.72
150.14
140.64
133.87
130.06
129.52
129.39
128.69
127.00
126.66
126.28
126.16
125.43
125.25
124.89
124.79
77.51
77.00
76.49
21.49
150
125
100
75
50
25
ppm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8.03
8.01
8.00
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.26
7.25
7.24
7.21
7.21
7.19
7.12
7.11
6.87
6.84
3.90
3.85
N
O
OMe
OMe
18
ppm
8.0
7.0
6.0
5.0
4.0
3.0
160.53
151.20
149.37
149.25
130.06
128.69
127.45
126.07
122.17
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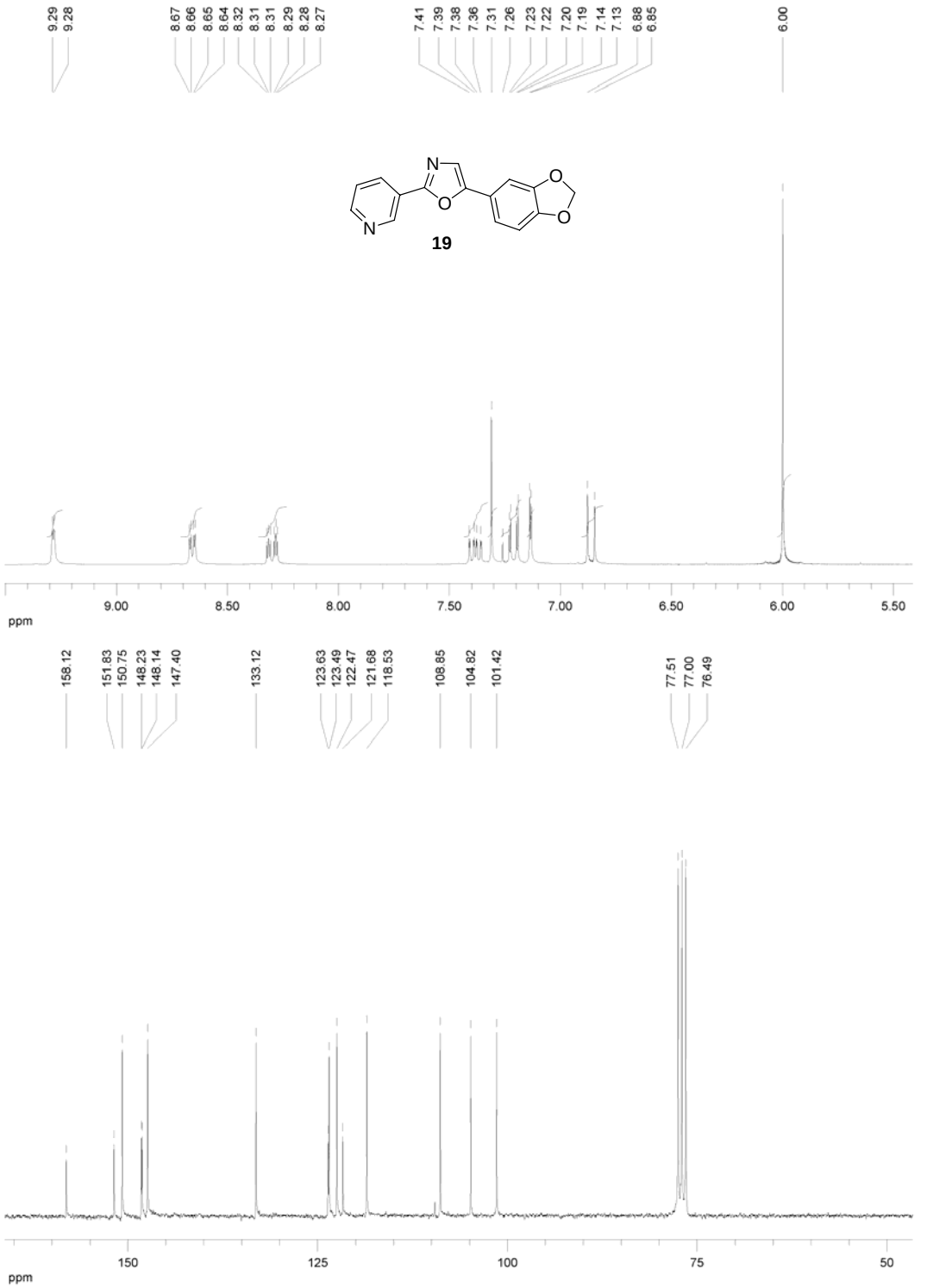
107.38
77.51
77.00
76.49
55.95
55.90
ppm (f1)
150
100
50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8.66
8.65
8.64
8.32
8.31
8.31
8.29
8.28
8.27
7.41
7.39
7.38
7.36
7.31
7.26
7.23
7.22
7.20
7.19
7.14
7.13
6.88
6.85
6.00
N
O
N
O
O
19
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
ppm
158.12
151.83
150.75
148.23
148.14
147.40
133.12
123.63
123.49
122.47
121.68
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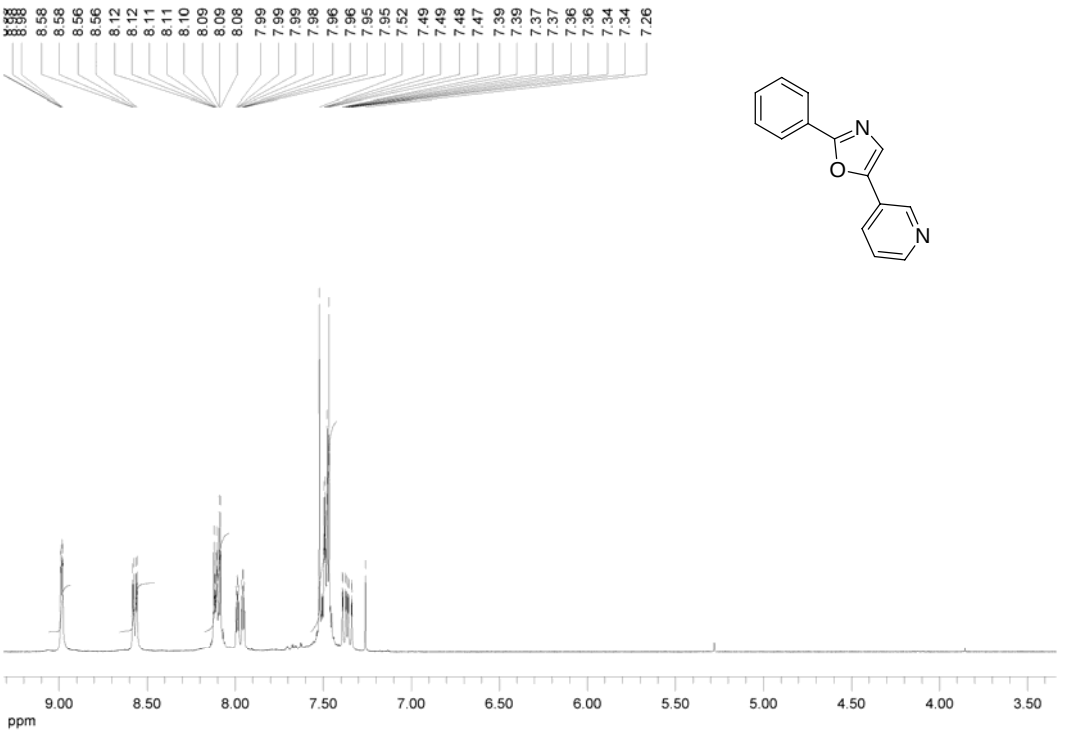
108.85
104.82
101.42
77.51
77.00
76.49
150
125
100
75
50
ppm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8.58
8.56
8.56
8.56
8.12
8.11
8.11
8.10
8.09
8.09
8.08
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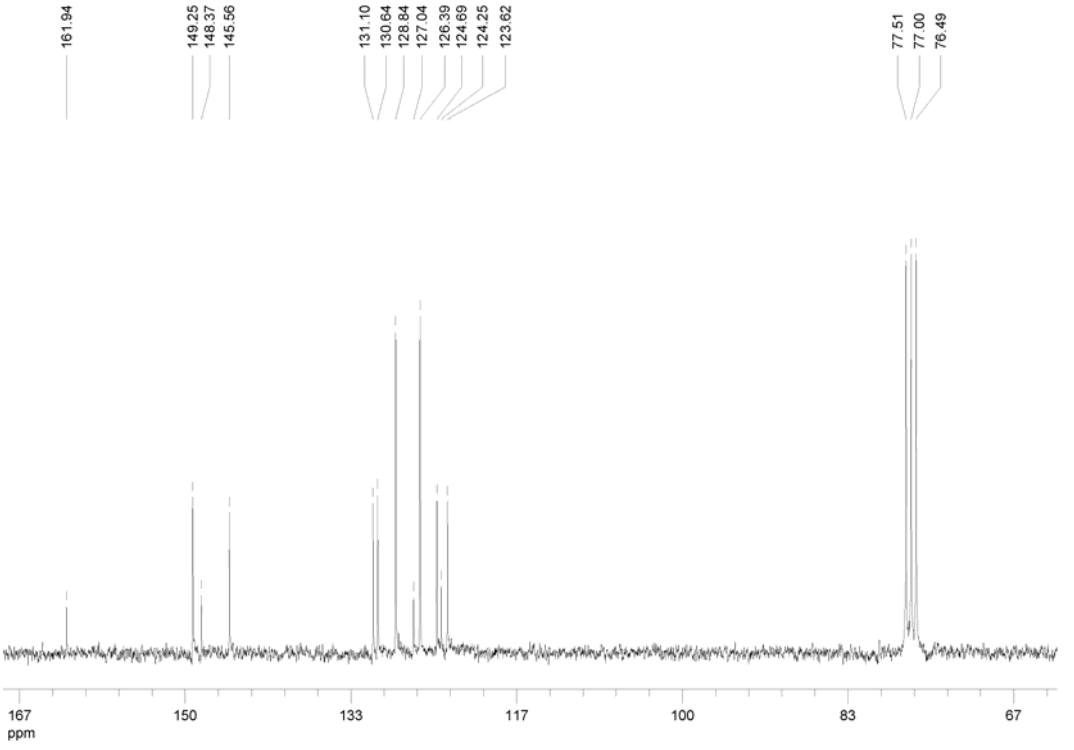
7.99
7.99
7.98
7.96
7.96
7.95
7.95
7.52
7.49
7.49
7.48
7.47
7.39
7.39
7.37
7.37
7.36
7.36
7.34
7.34
7.26
N
O
N
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
ppm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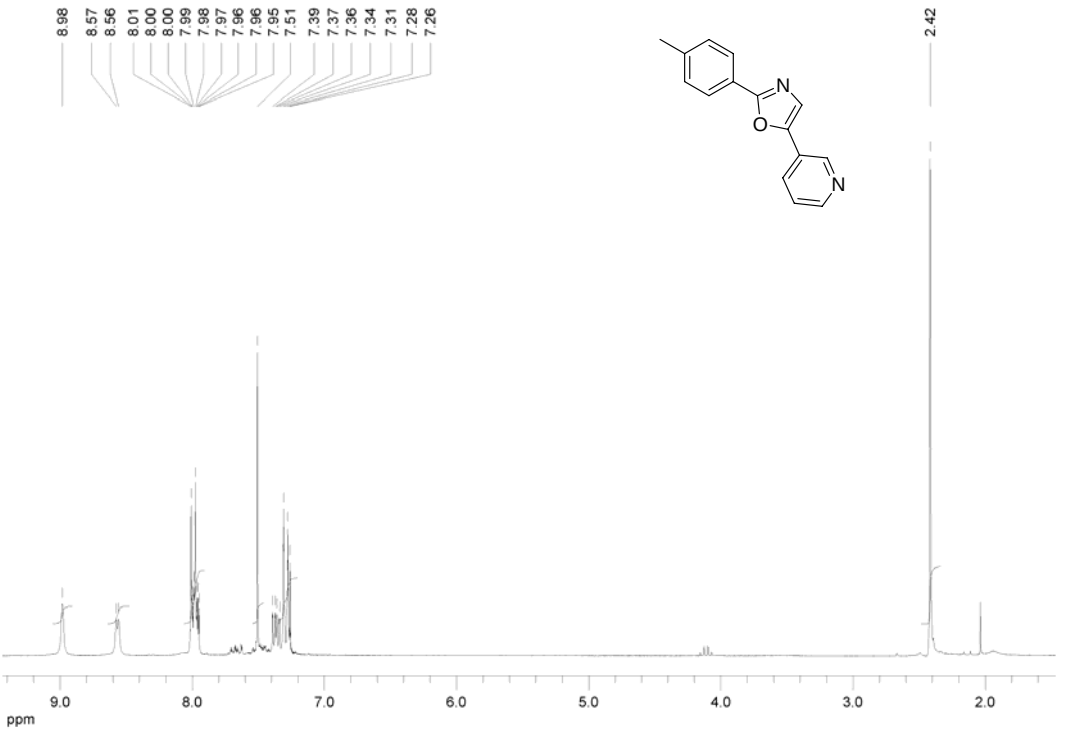
149.25
148.37
145.56
131.10
130.64
128.84
127.04
126.39
124.69
124.25
123.62
77.51
77.00
76.49
167
150
133
117
100
83
67
ppm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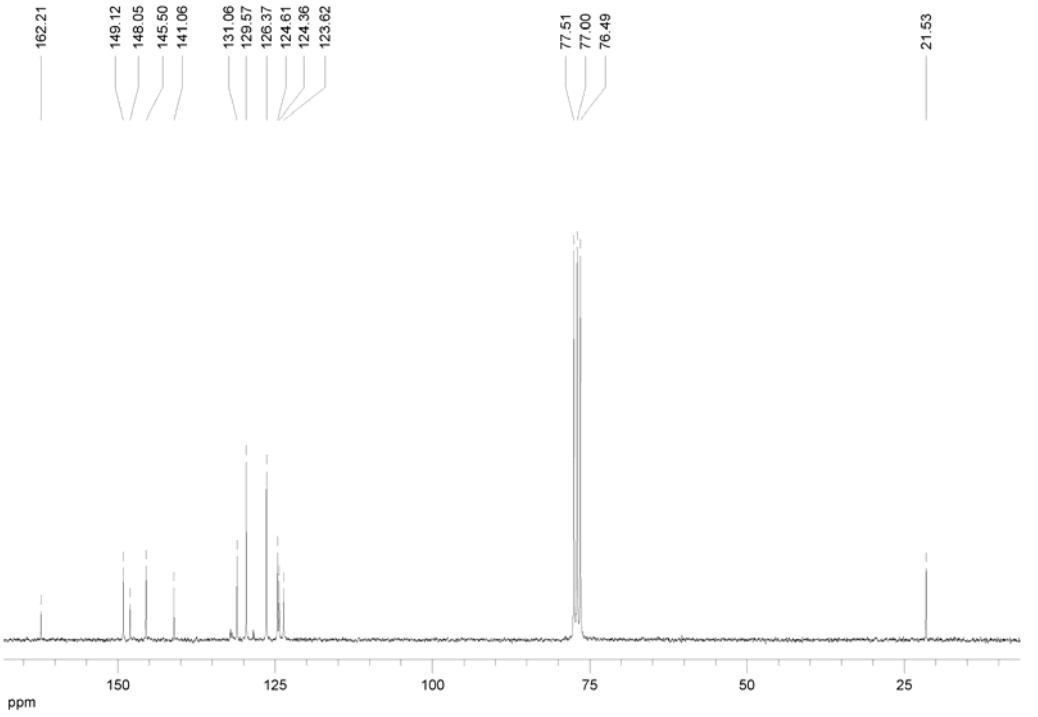
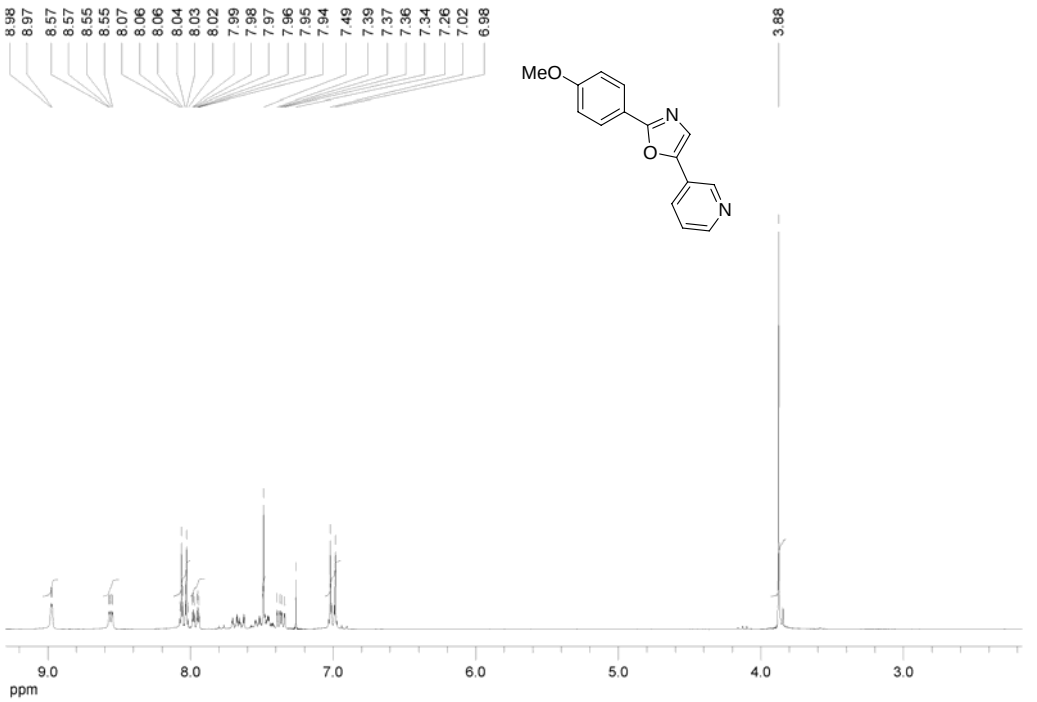
8.57
8.56
8.01
8.00
8.00
7.99
7.98
7.97
7.96
7.96
7.95
7.51
7.39
7.37
7.36
7.34
7.31
7.28
7.26
2.42
N
O
N
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm


162.21
149.12
148.05
145.50
141.06
131.06
129.57
126.37
124.61
124.36
123.62
77.51
77.00
76.49
21.53
150
125
100
75
50
25
ppm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8.57
8.55
8.55
8.07
8.06
8.06
8.04
8.03
8.02
7.99
7.98
7.97
7.96
7.95
7.94
7.49
7.39
7.37
7.36
7.34
7.26
7.02
6.98
3.88
MeO
N
O
N
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8.0
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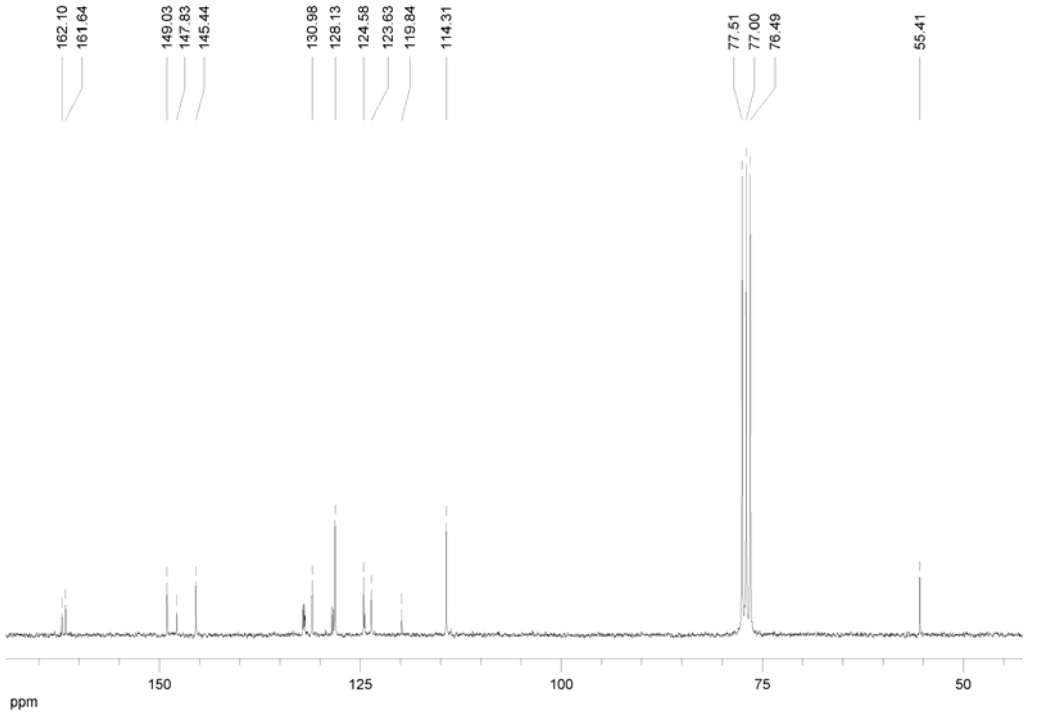
6.0
5.0
4.0
3.0
ppm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119.84
114.31
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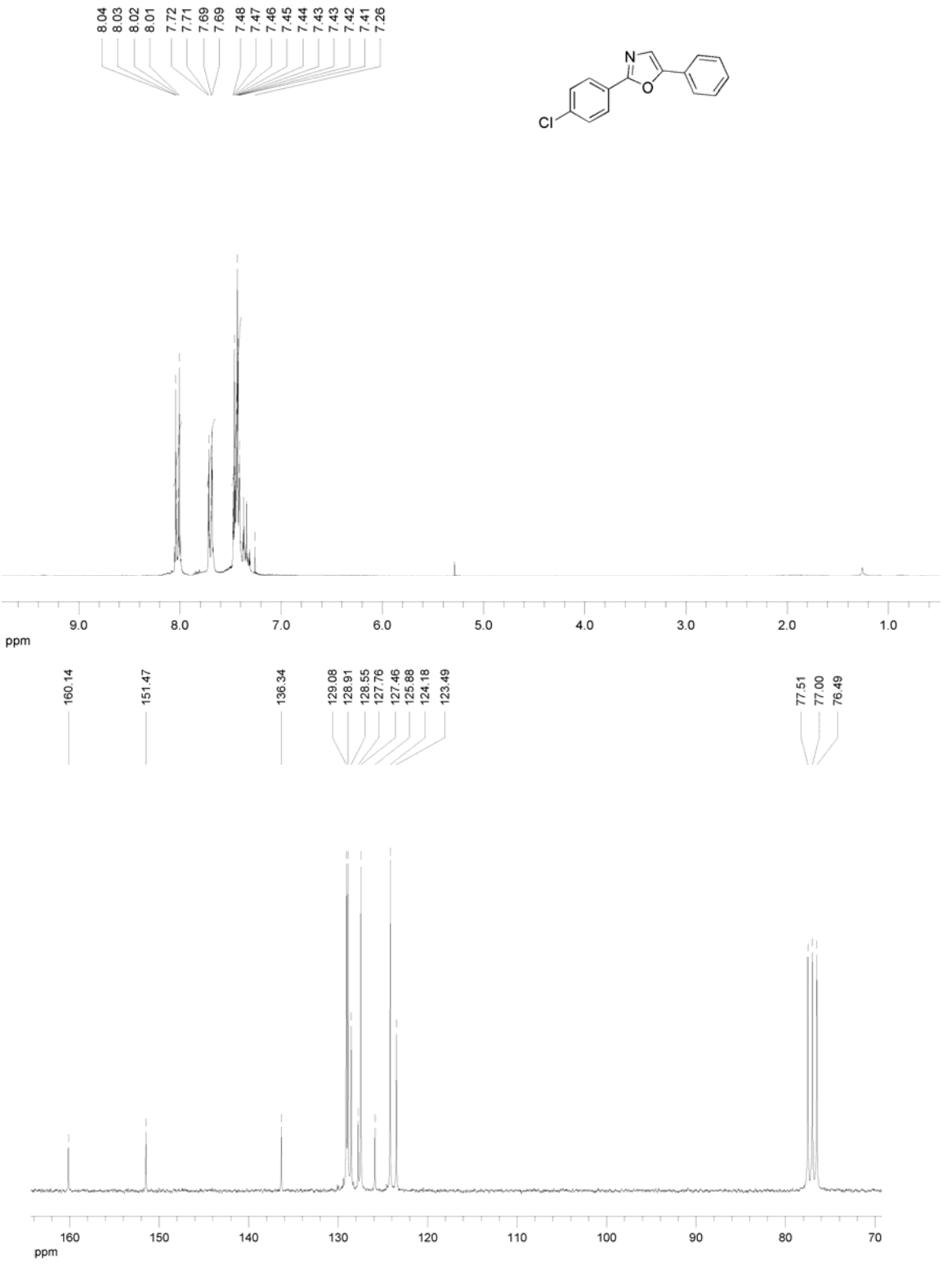
77.00
76.49
55.41
150
125
100
75
50
ppm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8.03
8.02
8.01
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7.69
7.69
7.48
7.47
7.46
7.45
7.44
7.43
7.43
7.42
7.41
7.26
N
O
Cl
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
160.14
151.47
136.34
129.08
128.91
128.55
127.76
127.46
125.88
124.18
123.49
77.51
77.00
76.49
160
150
140
130
120
110
100
90
80
70
ppm

X-Ray structure of 3-[2-*p*-Tolyl-oxazol-5-yl]-pyridine

(ORTEP thermal ellipsoids 50% probability)