Electronic Supplementary Material (ESI) for ChemComm.

Iodine Mediated Oxidative Annulation for One Pot Synthesis of Pyrazines and Quinoxalines Using Multipathway Coupled Domino Strategy†

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Supporting Information

Figure S1. Pharmaceutical and Bioactive natural Pyrazines and Quinoxalines

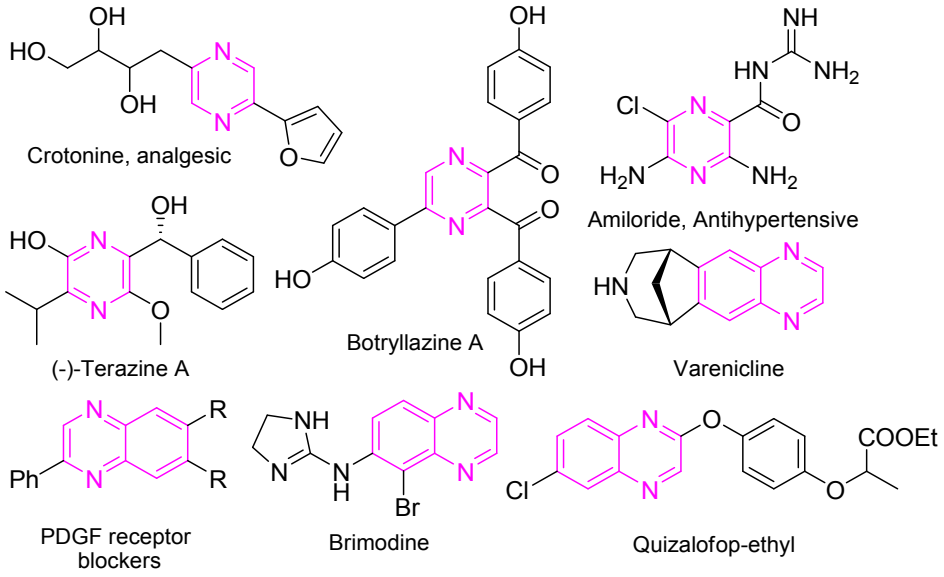


Figure S2. X-ray crystal structure of compound **5k (CCDC -975936)**

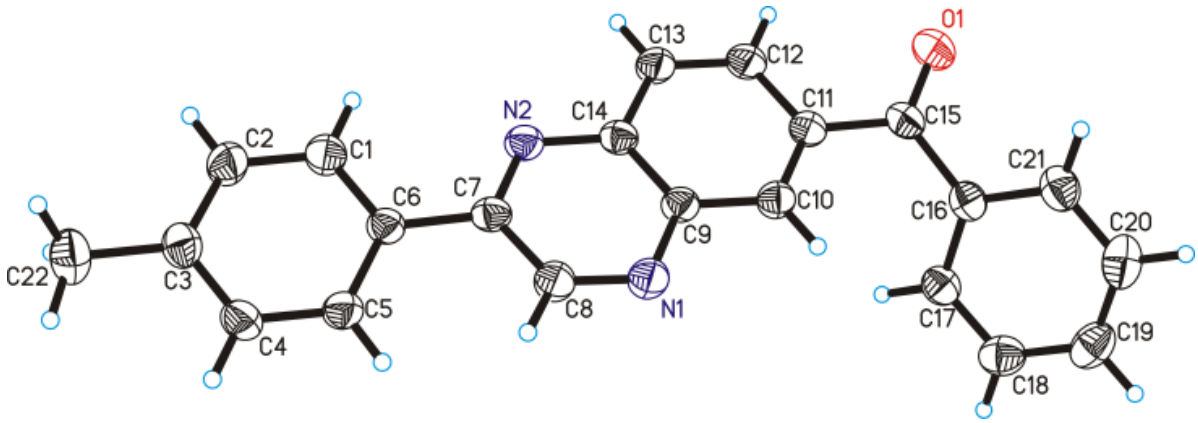
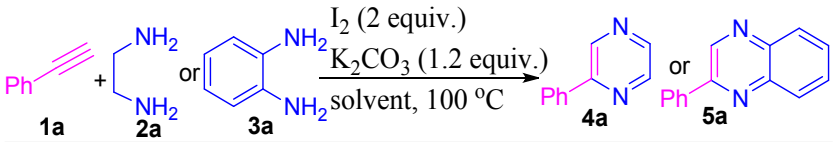


Table S1. Crystal data and structure refinement details for compound **5k**.

Compound	**5k**
Empirical formula	$C_{22}H_{16}N_2O$
Formula weight	324.37
Crystal System	Monoclinic
Space group	P21/c
a (Å)	6.182(4)
b (Å)	28.80(2)
c (Å)	9.743(6)
α (°)	90.00
β (°)	106.28(1)
γ (°)	90.00
V (Å^3)	1664.8(18)
Z	4
D_c (g/cm^3)	1.294
F_{000}	680
μ (mm^{-1})	0.08
θ_{max} (°)	25.38
Total reflections	12951
Unique reflections	3029
Reflections [$I > 2\sigma(I)$]	2154
Parameters	226
R_{int}	0.0533
Goodness-of-fit	1.151
R [$F^2 > 2\sigma(F^2)$]	0.0678
wR (F^2, all data)	0.2328
CCDC No.	975936

Table S2. Details regarding the use of DMSO in stoichiometric amounts for the iodine mediated Pyrazines and Quinoxalines synthesis via MPCD strategy.



entry	solvent	DMSO (equiv.)	temp (°C)	time (h)	yield (%)[b]
1	CCl_4	2	100	12	n.r.
2	DCE	2	100	12	n.r.
3	THF	2	100	12	n.r.
4	dioxane	2	100	12	n.r.
5	THF	3	100	12	n.r.
6	CCl_4	4	100	12	n.r.
7	THF	4	100	12	n.r.
8	dioxane	4	100	12	n.r.

[a] Reaction conditions: **1a** (**1.**0 mmol), **2a**/K_2CO_3 (**1.**0 mmol/1.2 mmol) or **3a** (1.0 mmol) DMSO (2 to 4 mmol) I_2 (2.0 mmol), heated in different solvents at 100 °C for 12 h. [b] Isolated yield. CCl_4 = carbon tetrachloride, DCE = 1,2-dichloroethane, THF = tetrahydrofuran.

1. General Information

All reactions, unless noted, were carried out under an open air atmosphere in flame-dried or oven-dried glassware with magnetic stirring. Analytical thin layer chromatography (TLC) was performed on Dynamic Adsorbents precoated (0.25 mm thickness) silica gel plates with F254 indicator. Visualization was accomplished by UV light (254 nm). Column chromatography was performed with silica gel (60-120 or 100–200 mesh) as the stationary phase. ^{1}H NMR spectra were recorded on a Bruker DRX-400 (400 MHz) spectrometer, and chemical shifts were reported in ppm. The peak information was described as: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = double doublet, bs = broad singlet; coupling constant(s) in Hz. ^{13}C NMR spectra were recorded on a Bruker DRX-400 (75 or 100 MHz) spectrometer with complete proton decoupling. High-resolution mass spectra (HRMS) were performed on QTof and MALDI-ToF/ToF mass spectrometer.

2. General procedure:

2A Pyrazines and Quinoxalines from terminal aryl alkynes: Aryl acetylene **1** (1.0 mmol), I_2 (2.0 mmol), and ethane-1, 2-diamine **2** (1.0 mmol)/K_2CO_3 (1.2 mmol) or benzene-1, 2-diamine **3** (1.0 mmol) were dissolved in DMSO (10 mL) and the mixture was stirred at 100 ^{0}C for 12 h. Upon completion, the mixture was diluted with water and extracted with EtOAc (3×20 mL). The extract was washed with $Na_2S_2O_3$ (5% w/w, aq.), brine and dried over anhydrous sodium sulphate. After removal of the solvent in vacuum, the residue was purified by column chromatography on silica gel to afford the **4** or **5**.

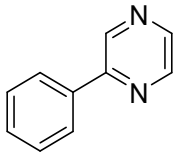
2B Pyrazines and Quinoxalines from terminal aryl alkenes: To a clear solution of IBX (2.0 mmol) in 10 mL of DMSO was added the terminal aryl alkenes **6** (1.0 mmol) followed by iodine (2.0 mmol). The reaction mixture was stirred for 2-3 h, ethane-1, 2-diamine **2** and K_2CO_3 (1.0 mmol/1.2 mmol) or benzene-1, 2-diamine **3** (1.0 mmol) were added, the mixture was heated at 100 ^{0}C for 10 h. Upon completion, the mixture was filtered, diluted with water and extracted with EtOAc (3×20 mL). The extract was washed with $Na_2S_2O_3$ (5% w/w, aq.), brine and dried over anhydrous sodium sulphate. After removal of the solvent in vacuum, the residue was purified by column chromatography on silica gel to afford the **4** or **5**.

2C Pyrazines and Quinoxalines from aromatic ketones: A mixture of aromatic ketone **7** (1.0 mmol), and I_2 (2.0 mmol) in 10 mL of DMSO was stirred at 100 °C for 2-3 h. After disappearance of the reactant, then added ethane-1, 2-diamine **2** and K_2CO_3 (1.0 mmol/1.2 mmol) or benzene-1, 2-diamine **3** (1.0 mmol) and the mixture was heated at 100 ^{0} C for 10 h. Upon completion, the mixture was diluted with water and extracted with EtOAc (3×20 mL). The extract was washed with $Na_2S_2O_3$ (5% w/w, aq.), brine and dried over anhydrous sodium sulphate. After removal of the solvent in vacuum, the residue was purified by column chromatography on silica gel to afford the **4** or **5**.

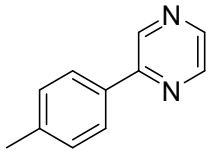
2D Synthesis of 2-iodo-1-phenylethanone (A): phenyl acetylene **1a** (1.0 mmol), and I_2 (2.0 mmol) were dissolved in DMSO (10 mL) and the mixture was stirred at 80 ^{0} C for 1 h. Upon completion, the mixture was diluted with water and extracted with EtOAc (3×20 mL). The extract was washed with $Na_2S_2O_3$ (5% w/w, aq.), brine and dried over anhydrous sodium sulphate. After removal of the solvent in vacuum, the residue was purified by column chromatography on silica gel to afford intermediate **A**.

3. Spectral data

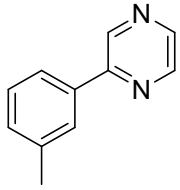
3.1. Spectral data of Pyrazines



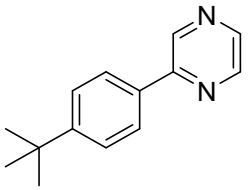
2-Phenylpyrazine (4a):[1] general procedure **2A/2B/2C** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.50 (Hexane/ EtOAc, 8:2); yield 72% (224 mg); light yellow solid; mp 73-74 ˚C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.03 (d, *J* = 1.28 Hz, 1H), 8.64 (dd, *J* = 3.92, 1.59 Hz, 1H), 8.51 (d, *J* = 2.4 Hz, 1H), 8.03−8.01 (m, 2H), 7.52−7.49 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.8, 143.1, 141.9, 141.2, 135.3, 128.9, 128.0, 125.9; IR (KBr) ν: 3019, 1637, 1469, 1080, 756, 668 cm^{-1}; ESIMS m/z $[M+H]^+$: 157.3.



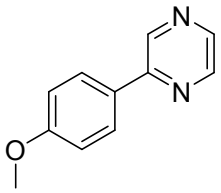
2-(p-Tolyl)-pyrazine (4b):[1] general procedure **2A/2B** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.55 (Hexane/EtOAc, 8:2); yield 75% (254 mg); pale yellow solid; mp 56-57 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.00 (s, 1H), 8.60 (bs, 1H), 8.47 (d, *J* = 2.15 Hz, 1H), 7.91 (d, *J* = 7.97 Hz, 2H), 7.32 (d, *J* = 7.91 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 152.9, 144.1, 142.6, 142.1, 140.2, 133.6, 129.8, 126.9, 21.4; IR (KBr) ν: 3436, 1637, 1467, 1078, 1016, 815, 756 cm^{-1}; ESIMS m/z $[M+H]^+$: 171.3.



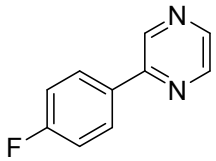
2-(m-Tolyl)-pyrazine (4j):[1] general procedure **2B** has been used; Column chromatography (Hexane/EtOAc) : R_f = 0.55 (Hexane/EtOAc, 8:2); yield 71% (241 mg); light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.02 (s, 1H), 8.62 (bs, 1H), 8.50 (bs, 1H), 7.84 (s, 1H), 7.79 (d, *J* = 7.68 Hz, 1H), 7.40 (t, *J* = 7.59 Hz, 1H), 7.29 (d , *J* = 7.47 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 153.0, 144.1, 142.8, 142.3, 138.8, 136.3, 130.7, 128.9, 127.6, 124.0, 21.5; IR (KBr) ν: 3436, 1637, 1467, 1078, 1016, 815, 756 cm^{-1}; ESIMS m/z $[M+H]^+$: 171.3.



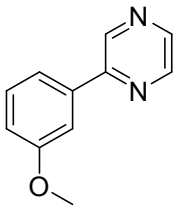
2-(4-(tert-butyl)phenyl)-pyrazine (4k): general procedure **2B** has been used; Column chromatography (Hexane/EtOAc) : R_f = 0.40 (Hexane/EtOAc, 9:1); yield 76% (322 mg); white solid; mp 86-87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.01 (d, *J* = 1.46 Hz, 1H), 8.61 (dd, *J* = 1.58, 2.43 Hz, 1H), 8.47 (d, *J* = 2.53 Hz, 1H), 7.97-7.94 (m, 2H), 7.55-7.52 (m, 2H), 1.37 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 153.4, 153.0, 144.3, 142.7, 142.2, 133.7, 126.8, 126.2, 34.9, 31.4; IR (KBr) ν: 3437, 3021, 1621, 1426, 1215, 1052, 759, 692 cm^{-1}; ESIMS m/z $[M+H]^+$: 213.2.



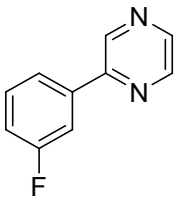
2-(4-Methoxy-phenyl)-pyrazine (4c):[1] general procedure **2A/2B** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/EtOAc, 9:1); yield 76% (283 mg); colorless solid; mp 86-87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.97 (d, *J* = 1.46 Hz, 1H), 8.57 (dd, *J* = 2.50, 1.60 Hz, 1H), 8.43 (d, *J* = 2.53 Hz, 1H), 7.99-7.96 (m, 2H), 7.04-7.01 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.2, 152.6, 144.0, 143.0, 142.3, 137.7, 130.0, 119.2, 115.9, 112.0, 55.4; IR (KBr) ν: 3436, 1637, 1403, 769, 692 cm^{-1}; ESIMS m/z $[M+H]^+$: 187.3.



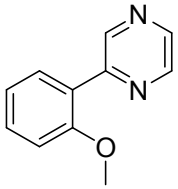
2-(4-Fluorophenyl)-pyrazine (4d):[1] general procedure **2A** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/EtOAc, 8:2); yield 65% (225 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.00 (s, 1H), 8.62 (d, *J* = 1.36 Hz, 1H), 8.50 (d, *J* = 2.27 Hz, 1H), 8.04−8.00 (m, 2H), 7.22-7.18 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 164.0 (d, *J* = 250.3 Hz), 151.8, 144.1, 142.8, 141.8, 132.5, 128.8 (d, *J* = 8.46 Hz), 116.1 (d, *J* = 21.8 Hz); ESIMS m/z $[M+H]^+$: 175.3.



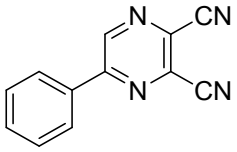
2-(3-Methoxy-phenyl)-pyrazine (4f):[1] general procedure **2A** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/EtOAc, 9:1); yield 68% (252 mg); pale yellow solid; mp 85-86 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.02 (d, *J* = 1.46 Hz, 1H), 8.63 (dd, *J* = 2.33,1.68, Hz, 1H), 8.57(d, *J* = 2.47 Hz, 1H), 7.60-7.56 (m, Hz, 2H), 7.42-7.41(t , *J* = 8.09 Hz, 1H), 7.04-7.04(m, 1H) 3.90(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 157.1, 152.0, 146.5, 142.1, 131.2, 131.0, 125.8, 121.3, 111.4, 55.6; IR (KBr) ν: 3435, 3020, 1638, 1463, 1216, 758; ESIMS m/z $[M+H]^+$: 187.3.



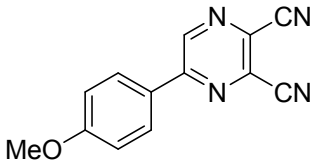
2-(3-Fluoro-phenyl)-pyrazine (4g): general procedure **2A/2C** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/EtOAc, 9:1); yield 63% (219 mg); yellow solid; mp 56-57 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.02 (d, *J* = 1.43 Hz, 1H), 8.65(dd, *J* = 2.36, 1.62 Hz, 1H), 8.54 (d, *J* = 2.47 Hz, 1H), 7.80-7.75 (m, 2H), 7.51-7.45 (m, 1H), 7.20-7.15 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 164.7, 162.2, 151.6, 144.3, 143.6, 142.2, 139.3, 138.7, 138.6, 130.78, 130.70, 122.54, 122.52, 117.0, 116.8, 114.2, 113.9; IR (KBr) ν: 3440, 3021, 1595, 1215, 759, 672 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{10}H_8FN_2$ $[M+H]^+$ 175.0672 found 175.0660.



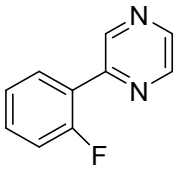
2-(2-Methoxy-phenyl)-pyrazine (4h):[2] general procedure **2A/2B** has been used, Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/EtOAc, 9:1); yield 68% (245 mg); yellow oil, mp 132-133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.15(d, *J* = 1.46 Hz, 1H), 8.65-8.64 (m, 1H), 8.54 (d, *J* = 2.56 Hz, 1H), 7.82 (dd, *J* = 7.63, 1.75 Hz 1H), 7.45-7.41(m, 1H), 7.13-7.09 (m, 1H), 7.04-7.02 (m, 1H), 3.89 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 157.1, 151.9, 146.5, 144.1, 142.1, 131.2, 131.0, 125.8, 121.3, 111.4, 55.6; IR (KBr) ν: 3436, 1637, 1403, 769, 692 cm^{-1}; ESIMS m/z $[M+H]^+$: 187.3.



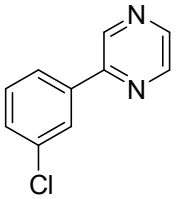
5-phenylpyrazine-2,3-dicarbonitrile (4l):[3] general procedure **2B** has been used; Column chromatography (Hexane/EtOAc); R_f = 0.40 (Hexane/EtOAc, 9:1); yield 65% (267 mg); white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.29 (s, 1H), 8.14-8.12 (m, 2H), 7.64-7.60 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 154.9, 144.1, 133.0, 132.6, 130.8, 130.2, 129.8, 128.0; IR (KBr) ν: 3405, 3021, 1635, 2200, 1406, 1215, 760, 670 cm^{-1}; ESIMS m/z $[M+H]^+$: 207.3.



5-(4-methoxyphenyl-) pyrazine-2,3-dicarbonitrile (4m):[4] general procedure **2B** has been used; Column chromatography (Hexane/EtOAc); R_f = 0.40 (Hexane/EtOAc, 9:1); yield 67% (316 mg); yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.22 (s, 1H), 8.14-8.12 (m, 2H), 7.11-7.09 (m, 2H), 3.94 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 163.8, 154.4, 143.4, 133.3, 130.0, 129.6, 125.0, 115.4, 113.5, 113.2, 55.8; IR (KBr) ν: 3410, 3019, 1635, 1216, 760, 676cm^{-1}; ESIMS m/z $[M+H]^+$: 237.3.

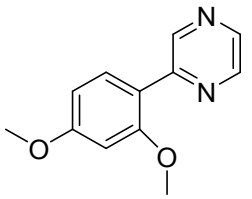


2-(2-fluorophenyl)- pyrazine (4o):[5] general procedure **2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.6 (Hexane/EtOAc, 9:1); yield 69% (240 mg); pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.09 (dd, J = 2.16, 1.68 Hz, 1H), 8.68 (dd, J = 2.38, 1.65 Hz, 1H), 8.53 (d, J = 2.47 Hz, 1H), 7.98-8.02 (m, 1H), 7.42-7.47 (m, 1H), 7.28-7.32 (m, 1H), 7.18-7.23 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.7 (d, J = 251.10 Hz), 149.6, 145.7 (d, J = 12.00 Hz), 144.6, 143.3, 131.7 (d, J = 8.49 Hz), 131.1 (d, J = 2.38 Hz), 125.0 (d, J = 3.10 Hz), 124.6 (d, J = 12.30 Hz), 116.6 (d, J = 22.71 Hz); IR (KBr) ν: 3401, 1623, 1400, 1148, 1074, 762, 669 cm^{-1}; ESIMS m/z $[M+H]^+$:175.2.

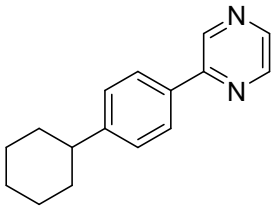


2-(3-chlorophenyl)- pyrazine (4n):[1] general procedure **2C** has been used; Column chromatography (Hexane/ EtOAc); R_f = 0.6 (Hexane/EtOAc, 9:1); yield 66% (396 mg); light

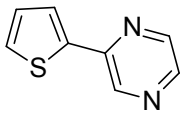
yellow solid; mp 95-96 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.01 (d, *J* = 1.44 Hz, 1H), 8.64 (dd, *J* = 2.44, 1.57 Hz, 1H), 8.54 (d, *J* = 2.49 Hz, 1H), 8.04-8.05 (m, 1H), 7.87-7.90 (m, 1H), 7.44-7.45 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.6, 144.5, 143.7, 142.3, 138.3, 135.5, 130.52, 130.17, 127.3, 125.1; IR (KBr) ν: 3402, 1635, 1463, 1146,1079, 760, 670 cm^{-1}; ESIMS m/z $[M+H]^+$:191.2.



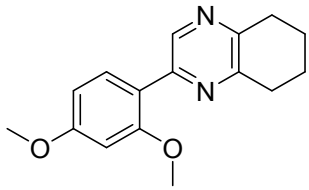
2-(2,4-dimethoxyphenyl)- pyrazine (4p):[6] general procedure **2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.4 (Hexane/EtOAc, 9:1); yield 76 % (328 mg); white solid; mp 75-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.14 (d, *J* = 1.57 Hz, 1H), 8.60 (dd, *J* = 2.54, 1.66 Hz, 1H), 8.39 (d, *J* = 2.57 Hz, 1H), 7.83 (d, *J* = 8.60 Hz, 1H), 6.65 (dd, *J* = 8.60, 2.34 Hz, 1H), 6.57 (d, *J* = 2.32, 1H), 3.89 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 162.5, 158.6, 152.0, 146.3, 144.1, 141.6, 132.3, 118.8, 105.8, 99.0, 55.8, 55.7; IR (KBr) ν: 3404, 1612, 1462, 1126, 1029, 929, 762, 669 cm^{-1}; ESIMS m/z $[M+H]^+$: 217.



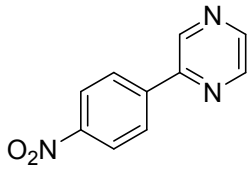
2-(4-cyclohexylphenyl)- pyrazine (4r): general procedure **2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.5 (Hexane/EtOAc, 9:1); yield 75% (357 mg); white solid; mp 176-178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.00 (d, *J* = 1.36 Hz, 1H), 8.61 (dd, *J* = 2.44, 1.60 Hz, 1H), 8.46 (d, *J* = 2.44 Hz, 1H), 7.94 (d, *J* = 8.33, Hz, 2H), 7.35 (d, *J* = 8.13 Hz, 2H), 2.54-2.61 (m, 1H), 1.75-1.90 (m, 5H), 1.37-1.51 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 153.1, 150.4, 144.3, 142.7, 142.2, 134.1, 127.8, 127.1, 44.6, 34.5, 27.0, 26.3; IR (KBr) ν: 3681, 3400, 1634, 1470, 928, 757, 669, 626 cm^{-1}; ESIMS m/z $[M+H]^+$: 239.2.



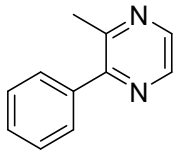
2-(thiophen-2-yl)- pyrazine (4q):[1] general procedure **2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.4 (Hexane/EtOAc, 9:1); yield 76% (246 mg); Slight yellow solid; mp 97-98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.96 (d, *J* = 1.48 Hz, 1H), 8.50 (dd, *J* = 2.52, 1.64 Hz, 1H), 8.40 (d, *J* = 2.58 Hz, 1H), 7.69 (dd, *J* = 3.70, 1.04 Hz, 1H), 7.48 (dd, *J* = 5.04, 1.02, 1H), 7.16 (dd, *J* = 4.99, 3.72 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 148.7, 144.2,142.5, 141.5, 140.8, 129.2, 128.6, 126.0; IR (KBr) ν: 3400, 1631, 1466, 1216, 1069, 928, 759, 670 cm^{-1}; ESIMS m/z $[M+H]^+$: 163.3.



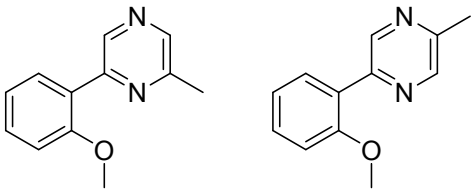
2-(2,4-dimethoxyphenyl)-5,6,7,8-tetrahydroquinoxaline (4u): general procedure **2C** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.4 (Hexane/ EtOAc, 9:1); yield 71 % (383 mg); green oil ; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.80 (s, 1H), 7.73 (d, *J* = 8.56 Hz, 1H), 6.62 (dd, *J* = 8.51, 2.35 Hz, 1H), 6.55 (d, *J* = 2.35 Hz, 1H), 3.85 (s, 3H), 3.851 (s , 3H), 2.97-2.99 (m , 4H), 1.93 –1.94 (m , 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 161.9, 158.4, 152.1, 149.7, 148.6, 142.9, 132.0, 119.5, 105.6, 99.0, 55.78, 55.70, 32.3, 31.8, 23.0; IR (KBr) ν: 3404, 1612, 1452, 1128, 1033, 928, 760, 670 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{16}H_{19}N_2O_2$ $[M+H]^+$ 271.1447 found 271.1445.



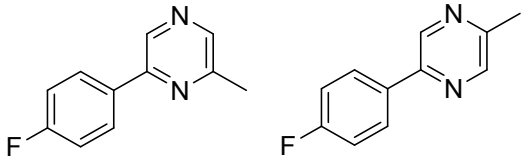
2-(4-nitrophenyl)- pyrazine (4s): general procedure **2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.5 (Hexane/EtOAc, 9:1); yield 56 % (224 mg); light yellow solid; mp 178-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.12, (d, *J* = 1.16 Hz, 1H), 8.71 (s, 1H), 8.63 (d, *J* = 2.36 Hz, 1H), 8.37 (d, *J* = 8.85 Hz, 2H), 8.22 (d, *J* = 8.90 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 150.5, 148.9, 144.7, 144.6, 142.7, 142.4, 128.0, 124.4; IR (KBr) ν: 3403, 2402, 1632, 1401, 1022, 761, 669 cm^{-1}; ESIMS m/z $[M+H]^+$: 202.2.



2-methyl-3-phenylpyrazine (4t):[7] general procedure **2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.6 (Hexane/EtOAc, 9:1); yield 70% (190 mg); white solid; mp 36-37 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.48 (dd, *J* = 2.49, 0.59 Hz, 1H), 8.44 (d, *J* = 2.47, 1H), 7.56-7.59 (m, 2H), 7.42-7.51 (m, 3H), 2.64 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 154.2, 152.0, 142.3, 141.7, 138.8, 129.1, 128.9, 128.6, 23.3; IR (KBr) ν: 3402, 1634, 1399, 927, 760, 669 cm^{-1}; ESIMS m/z $[M+H]^+$:171.2.

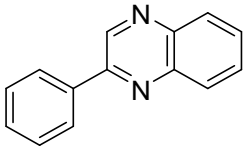


2-(2-methoxyphenyl)-6-methylpyrazine and 2-(2-methoxyphenyl)-5-methylpyrazine (4i): general procedure **2A** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/ EtOAc, 9:1); yield 81% (324 mg); colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.00 (d, J = 1.49 Hz, 1H), 8.91 (s, 1H), 7.80-7.77 (m, 2H), 7.42-7.38 (m, 2H), 7.11-7.07(m, 2H); 7.02-7.00 (m, 2H); 3.87 (s, 3H); 2.61(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.25, 160.23, 153.2, 152.1, 151.5, 149.6, 143.8, 142.7, 141.0, 139.1, 138.1, 137.9, 130.0, 119.3, 118.9, 115.6, 115.5, 112.3, 111.9, 55.4, 21.7, 21.2; IR (KBr) ν: 3436, 3019, 2401, 1680, 1470, 1216, 1039, 759 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{12}H_{13}N_2O$ $[M+H]^+$ 201.1028 found 201.1024.

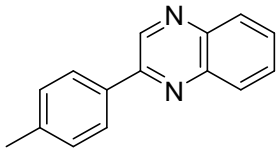


2-(4-fluorophenyl)-6-methylpyrazine and 2-(4-fluorophenyl)-5-methylpyrazine (4e): general procedure **2A** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/ EtOAc, 9:1); yield 77% (290 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.88 (d, J = 1.35 Hz, 1H), 8.80 (s, 1H), 8.51 (d, J = 0.98 Hz, 1H), 8.41 (s, 1H), 7.79-7.7 (m, 4H), 7.49-7.43 (m, 2H) 7.17-7.12 (m, 2H), 2.63 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 162.1, 153.4, 152.6, 150.3, 148.5, 143.9, 143.2, 140.8, 138.8, 130.5, 130.4, 122.4, 121.1, 116.6, 116.4, 116.2, 114.0, 113.8, 113.7, 113.5, 21.6, 21.2; IR (KBr) ν: 3432, 3019, 2400, 1633, 1404, 1215, 757 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{11}H_{10}FN_2$ $[M+H]^+$ 189.0828 found 189.0835.

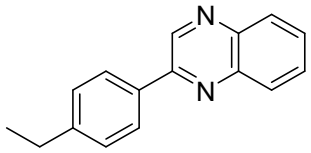
3.2. Spectral data of Quinoxalines



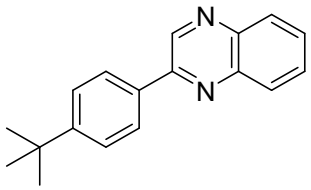
2-Phenylquinoxaline (5a):[1] general procedure **2A/2B/2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.50 (Hexane/EtOAc, 8:2); yield 76% (314 mg); light yellow solid; mp 80-81 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.33 (s, 1H), 8.21−8.11 (m, 4H), 7.80−7.73 (m, 2H), 7.59−7.51 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.9, 143.3, 142.3, 141.6, 136.8, 130.3, 129.6, 129.5, 129.1, 127.5; IR (KBr) ν: 3437, 3019, 1634, 1409, 1050, 759 cm^{-1}; ESIMS m/z $[M+H]^+$: 207.3.



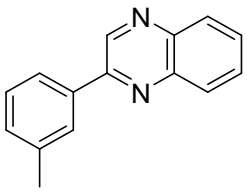
2-(p-Tolyl)-quinoxaline (5b):[1] general procedure **2A/2B** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.55 (Hexane/EtOAc, 8:2); yield 78 % (343 mg); light yellow solid; mp 89-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.29 (s, 1H), 8.13−8.08 (m, 4H), 7.75 (m, 2H), 7.35 (d, *J* = 7.9 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.8, 143.3, 142.3, 141.4, 140.5, 134.0, 130.1, 129.9, 129.5, 129.2, 129.1, 127.4, 21.4; IR (KBr) ν: 3435, 3019, 1636, 1421, 1215, 1048, 928, 757, 669 cm^{-1}; ESIMS m/z $[M+H]^+$: 221.3.



2-(4-ethylphenyl)-quinoxaline (5e):[3] general procedure **2A/2B** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.55 (Hexane/EtOAc, 8:2); yield 77 % (360 mg); pale yellow solid; mp 77-78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.31 (s, 1H), 8.15−8.09 (m, 4H), 7.77-7.72 (m, 2H), 7.40 (d, *J* = 8.20 Hz, 2H), 2.75 (q, *J* = 15.01, 7.47 Hz, 2H) 1.30 (t, *J* = 7.52 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.9, 146.8, 143.3, 142.3, 141.4, 134.2, 130.2, 129.5, 129.3, 129.0, 128.7, 127.5, 28.7, 15.4; IR (KBr) ν: 3434, 3019, 2400, 1637, 1422, 1216, 757 cm^{-1}; ESIMS m/z $[M+H]^+$: 235.3.

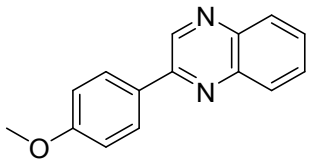


2-(4-tert-Butyl-phenyl)-quinoxaline (5d):[8] general procedure **2A/2C** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.40 (Hexane/EtOAc, 9:1); yield 79% (414 mg); colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.31 (s, 1H), 8.16-8.10 (m, 4H), 7.79-7.71 (m,2H), 7.60 -7.58(m,2H),1.39 (s, 9H)); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 153.6, 151.9, 143.4, 142.4, 141.5, 134.1, 130.2, 129.6, 129.2, 127.4, 126.2, 34.9, 31.3; IR (KBr) ν: 3437, 3021, 1621, 1426, 1215, 1052, 759 cm^{-1}; ESIMS m/z $[M+H]^+$: 263.2.

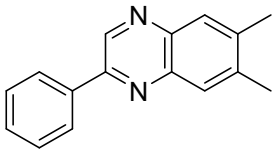


2-m-tolylquinoxalin (5f):[3] general procedure **2A** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.55 (Hexane/EtOAc, 8:2); yield 74% (329 mg); colorless solid; mp 83-84 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.31 (s, 1H), 8.17-8.11 (m, 2H), 8.02 (s, 1H), 7.98-7.96

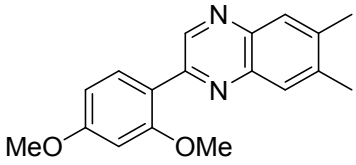
(m, 1H), 7.81-7.33 (m, 2H) 7.46 (T, J = 7.63 Hz, 1H) 7.35-7.33 (m, 1H) 2.50 (S, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 152.1, 143.5, 142.3, 141.5, 138.9, 136.7, 131.0, 130.2, 129.6, 129.4, 129.1, 129.0, 128.2, 124.7, 21.5; IR (KBr) ν: 3436, 1637, 1403, 1215, 758 cm^{-1}; ESIMS m/z $[M+H]^+$: 221.3.



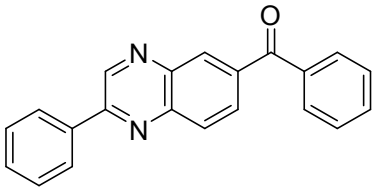
2-(4-Methoxyphenyl)-quinoxaline (5c):[1] general procedure **2A/2B/2C** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/ EtOAc, 8:2); yield 80% (378 mg); colorless solid; mp 104-105 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.16 (s, 1H), 8.05−8.03 (m, 2H), 7.99-7.96 (m, 2H), 7.64-7.57 (m, 2H), 6.95-6.93(m, 2H), 3.76 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 161.4, 151.4, 143.0, 142.3, 141.2, 130.1, 129.4, 129.3, 129.07, 129.03, 128.9, 114.5, 55.4; IR (KBr) ν: 3440, 3020, 1613, 1423, 1216, 759 cm^{-1}; ESIMS m/z $[M+H]^+$: 237.3.



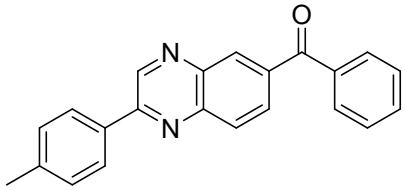
6,7-dimethyl-2-phenylquinoxaline (5m):[9] general procedure **2B** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.55 (Hexane/ EtOAc, 8:2); yield 79% (354 mg); Yellow solid; Mp 120-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.22 (s, 1H), 8.17-8.15 (m, 2H), 7.90 (s, 1H),7.85 (s, 1H), 7.57-7.47 (m, 3H) 2.51 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.0, 142.5, 141.3, 140.8, 140.7, 140.2, 137.2, 129.9, 129.1, 128.8, 128.2, 127.5, 20.49, 20.46; IR (KBr) ν: 3416, 3020, 1622, 1393, 1215, , 759 cm^{-1}; ESIMS m/z $[M+H]^+$: 235.3.



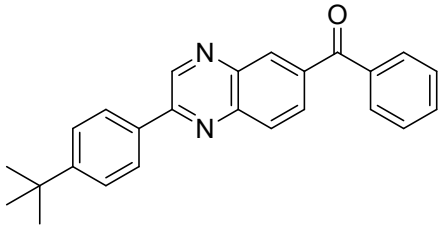
2-(2,4-dimethoxyphenyl)-6,7-dimethylquinoxaline (5n): general procedure **2C** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.4 (Hexane/ EtOAc, 8:2); yield 88 % (517 mg); white solid ; ^{1}H NMR (400 MHz, $CDCl_3$) δ =9.23 (s, 1H), 7.89-7.86 (m, 2H), 7.82 (s, 1H), 6.68 (dd, J = 2.38, 8.60 Hz, 1H), 6.59 (d, J = 2.32 Hz, 1H), 3.887 (s, 3H), 3.886 (s, 3H), 2.49 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 162.5,158.8,151.2,146.5, 141.8, 140.2, 139.9, 139.5, 132.7, 128.6, 128.2, 120.0, 106.0, 99.6, 55.8, 55.7, 20.5, 20.4; IR (KBr) ν: 3407, 2924, 2852, 1608, 1282, 1209, 1030, 871, 831 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{18}H_{19}N_2O_2$ $[M + H]^+$ 295.1447 found 295.1445.



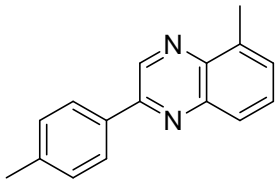
Phenyl(2-phenylquinoxalin-6-yl)methanone (5j):[3] general procedure **2A** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/ EtOAc, 9:1); yield 69% (427 mg); colorless solid; mp 131-132 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ = 9.42 (s,1H), 8.50 (s, 1H), 8.27-8.24 (m, 4H), 7.91-7.89 (m, 2H), 7.65-7.52 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 195.8, 153.5, 144.5, 144.3, 140.7, 138.0, 137.2, 136.4, 133.0, 132.4, 130.9, 130.4, 130.3, 130.2, 129.4, 128.6, 127.6; IR (KBr) ν: 3406, 2958, 1651, 1319, 1309, 840, 695 cm^{-1}; ESIMS m/z $[M+H]^+$: 311.3.



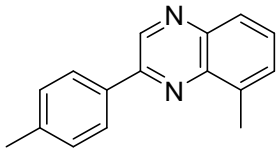
Phenyl (2-p-tolylquinoxalin-6-yl)methanone (5k): general procedure **2A** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/ EtOAc, 9:1); yield 76% (492 mg); light yellow solid; mp 156-157 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ = 9.38 (s, 1H), 8.47 (s, 1H), 8.24 (s, 2H), 8.15 (d, J = 8.02 Hz, 2H), 7.90 (d, J = 7.36 Hz, 2H), 7.64 (t, J = 7.35 Hz, 1H), 7.53 (t, J = 7.49 Hz, 2H), 7.39 (d, J = 7.98 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 195.6, 153.2, 144.3, 144.2, 141.2, 140.4, 137.6, 137.1, 133.4, 132.8, 132.3, 130.1, 130.0, 129.9, 128.5, 127.6, 21.5; IR (KBr) ν: 3436, 3019, 1656, 1421, 1215, 1048, 757 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{22}H_{17}N_2O$ $[M+H]^+$ 325.1341 found 325.1352.



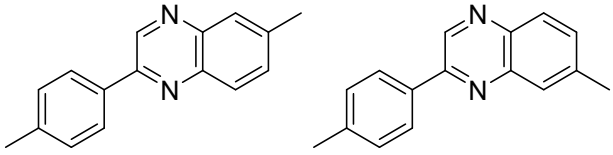
2-(4-tert-Butyl-phenyl)-quinoxalin-6-yl]-phenyl-methanone (5l): general procedure **2A** has been used; Column chromatography (Hexane/EtOAc): R_f = 0.40 (Hexane/ EtOAc, 9:1); yield 73% (534 mg); colorless solid; mp 179-180 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ = 9.39 (s, 1H), 8.485-8.483 (m, 1H), 8.254-8.252 (m, 2H), 8.20-8.17 (m, 2H), 7.91-7.89 (m, 2H), 7.64-7.51 (m, 4H), 7.55-7.51(m, 2H), 1.4 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 195.7, 154.4, 153.4, 144.5, 144.3, 140.5, 137.7, 137.3, 133.5, 132.9, 132.4, 130.27, 130.24, 130.1, 128.6, 127.6, 126.4, 35.0, 31.3; IR (KBr) ν: 3435, 3019, 1654, 1404, 1215, 757 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{25}H_{23}N_2O$ $[M+H]^+$ 367.1810 found 367.1807.



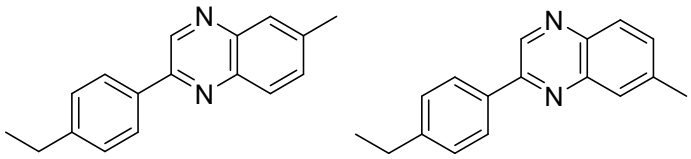
5-Methyl-2-p-tolylquinoxaline (5i): general procedure **2A/2B** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.40 (Hexane/EtOAc, 9:1); yield 40% (187 mg); light yellow solid; mp 95-96 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ = 9.30 (s, 1H), 8.16 (d, *J* = 7.86 Hz, 2H), 7.92 (t, *J* = 5.16 Hz, 1H), 7.60 (d, *J* = 5.04 Hz, 2H), 7.36 (d, *J* = 7.66 Hz, 2H), 2.87 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 150.2, 142.5, 141.4, 141.3, 140.3, 137.8, 134.3, 130.1, 129.8, 129.0, 127.3, 126.8, 21.4, 17.1; IR (KBr) ν: 3437, 3020, 1631, 1414, 1215, 1050, 758 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{16}H_{15}N_2$ $[M+H]^+$ 235.1235 found 235.1234.



8-Methyl-2-p-tolylquinoxaline (5i): general procedure **2A/2B** has been used; Column chromatography (Hexane/ EtOAc): R_f = 0.45 (Hexane/EtOAc, 9:1); yield 36% (168 mg); light yellow solid; mp 94-95 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ = 9.31 (s, 1H), 8.10 (d, *J* = 7.97 Hz, 2H), 7.83 (d, *J* = 8.37 Hz, 1H), 7.65 (t, *J* = 7.37 Hz, 1H), 7.56 (d, *J* = 6.89 Hz, 1H), 7.37(d, *J* = 7.88 Hz, 2H), 2.82 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.4, 142.5, 141.9, 140.6, 140.3, 137.3, 134.1, 129.98, 129.91, 129.4, 127.48, 127.43, 21.4, 17.3; IR (KBr) ν: 3437, 3022, 1632, 1414, 1216, 1050, 759 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{16}H_{15}N_2$ $[M+H]^+$ 235.1235 found 235.1234.



6-Methyl-2-p-tolylquinoxaline and 7-Methyl-2-p-tolylquinoxaline (5g):[11] general procedure **2A** has been used; Column chromatography (hexane/EtOAc): R_f = 0.60 (Hexane/ EtOAc, 9:1); yield 78% (368 mg); Brown solid; mp 102-103 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ = 9.24 (d, *J* = 9.82 Hz, 1H), 8.09-8.06 (m, 2H), 8.02-7.96 (m, 1H), 7.88 (d, *J* = 17.86 Hz, 1H), 7.60-7.53 (m, 1H), 7.31 (d, *J* = 7.94 Hz, 2H), 2.59 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.6, 151.0, 143.1, 142.3, 141.4, 140.7, 140.6, 140.2, 140.1, 139.9, 139.7, 134.1, 132.4, 131.5, 129.8, 129.0, 128.5, 128.3, 127.9, 127.3, 127.2, 21.8, 21.7, 21.3; IR (KBr) ν: 3437, 3021, 1634, 1414, 1215, 1050, 759 cm^{-1}; ESIMS m/z $[M+H]^+$: 235.3.



2-(4-ethylphenyl)-6-methylquinoxaline and 2-(4-ethylphenyl)-7-methylquinoxaline (5h): general procedure **2A** has been used; Column chromatography (hexane/EtOAc): R_f = 0.40 (Hexane/ EtOAc, 9:1); yield 85% (421 mg); light yellow solid; mp 95-96 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.24 (d, *J* = 9.81 Hz, 1H), 8.11-8.09 (m, 2H), 8.03-7.97 (m, 1H), 7.89 (d, *J* = 17.86 Hz, 1H), 7.60-7.53 (m, 1H), 7.38 (d, *J* = 7.94 Hz, 2H), 2.74 (q, *J* = 15.08 Hz, 2H), 2.60 (s, 3H), 1.29 (t, *J* = 7.62 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 151.8, 151.1, 146.6, 146.5, 143.2, 142.4, 141.5, 140.7, 140.6, 139.9, 139.8, 134.4, 132.4, 131.6, 129.0, 128.6, 128.5, 128.4, 127.9, 127.5, 127.4, 28.7, 21.84, 21.80, 15.4; IR (KBr) ν: 3437, 3021, 1621, 1426, 1215, 1052, 759 cm^{-1}; HRMS (ESI-TOF) Calcd for $C_{17}H_{17}N_2$ $[M+H]^+$ 249.1392 found 249.1390.

4. References

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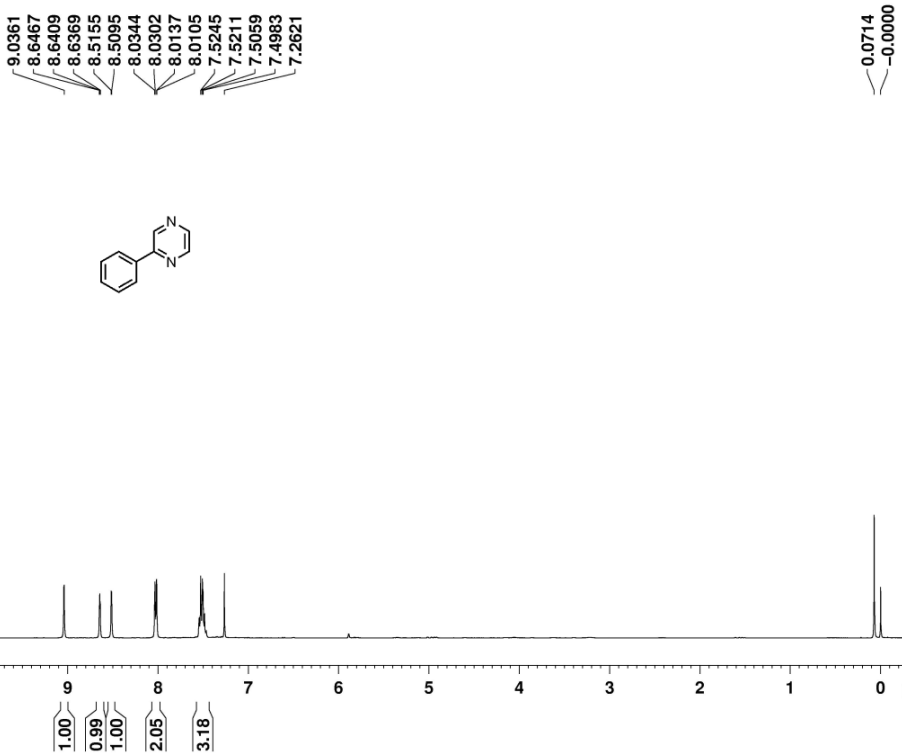
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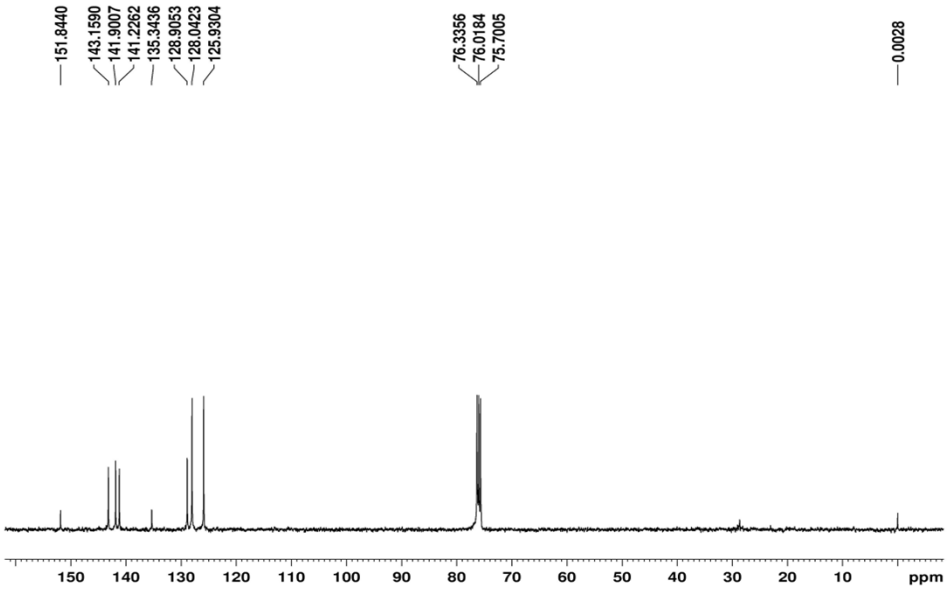
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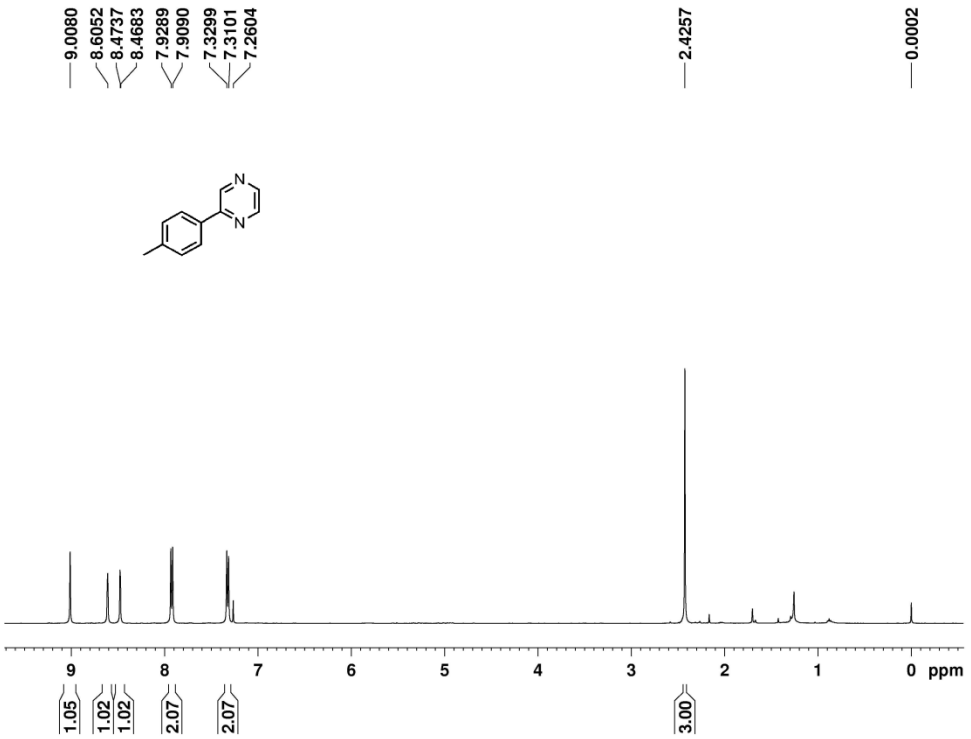
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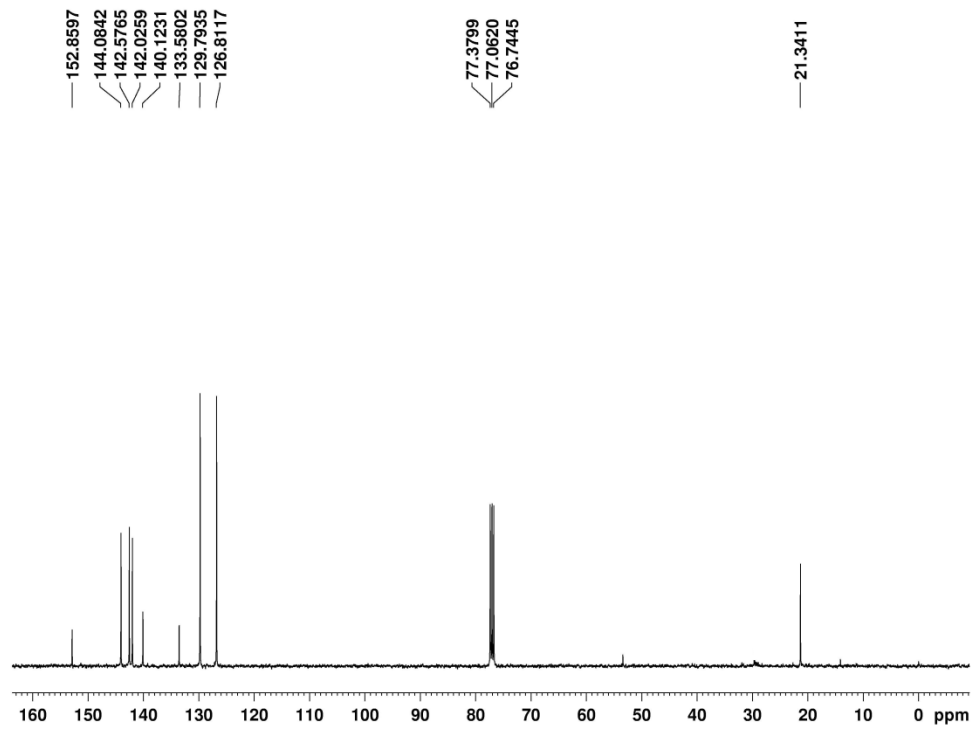
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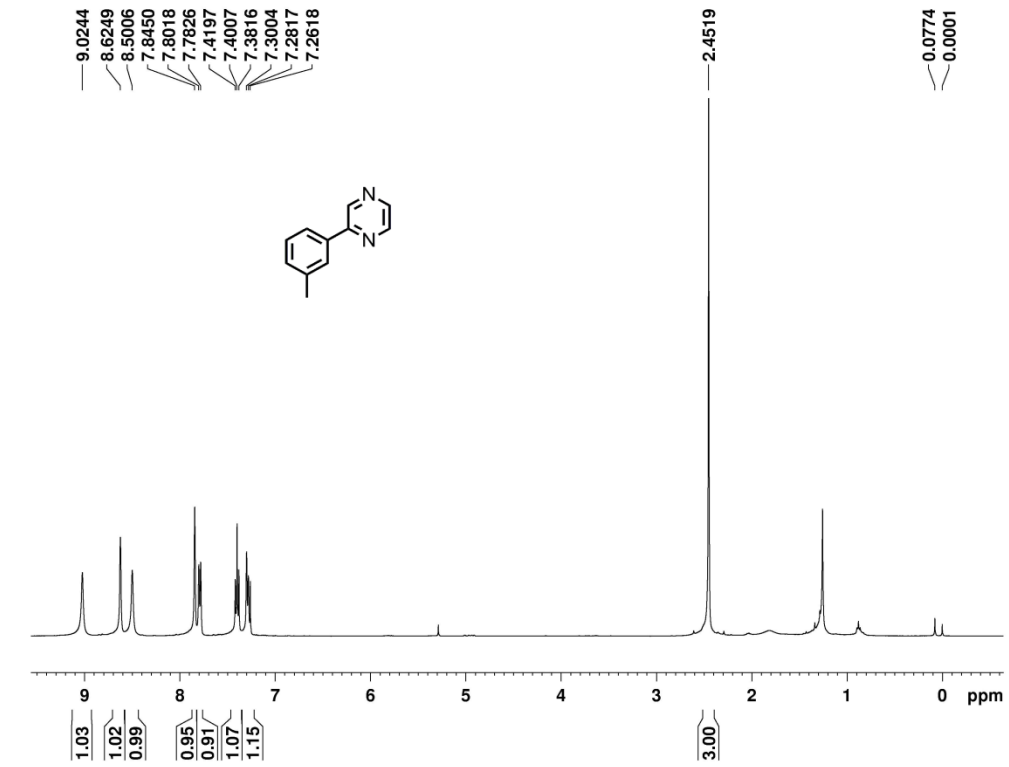
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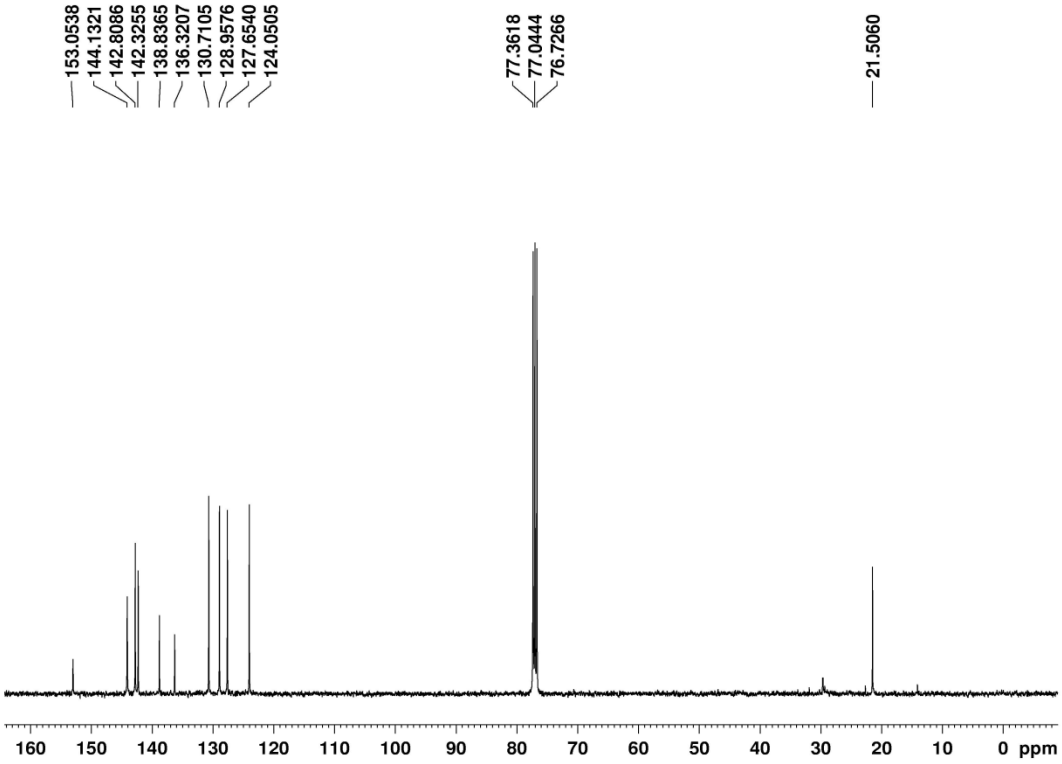
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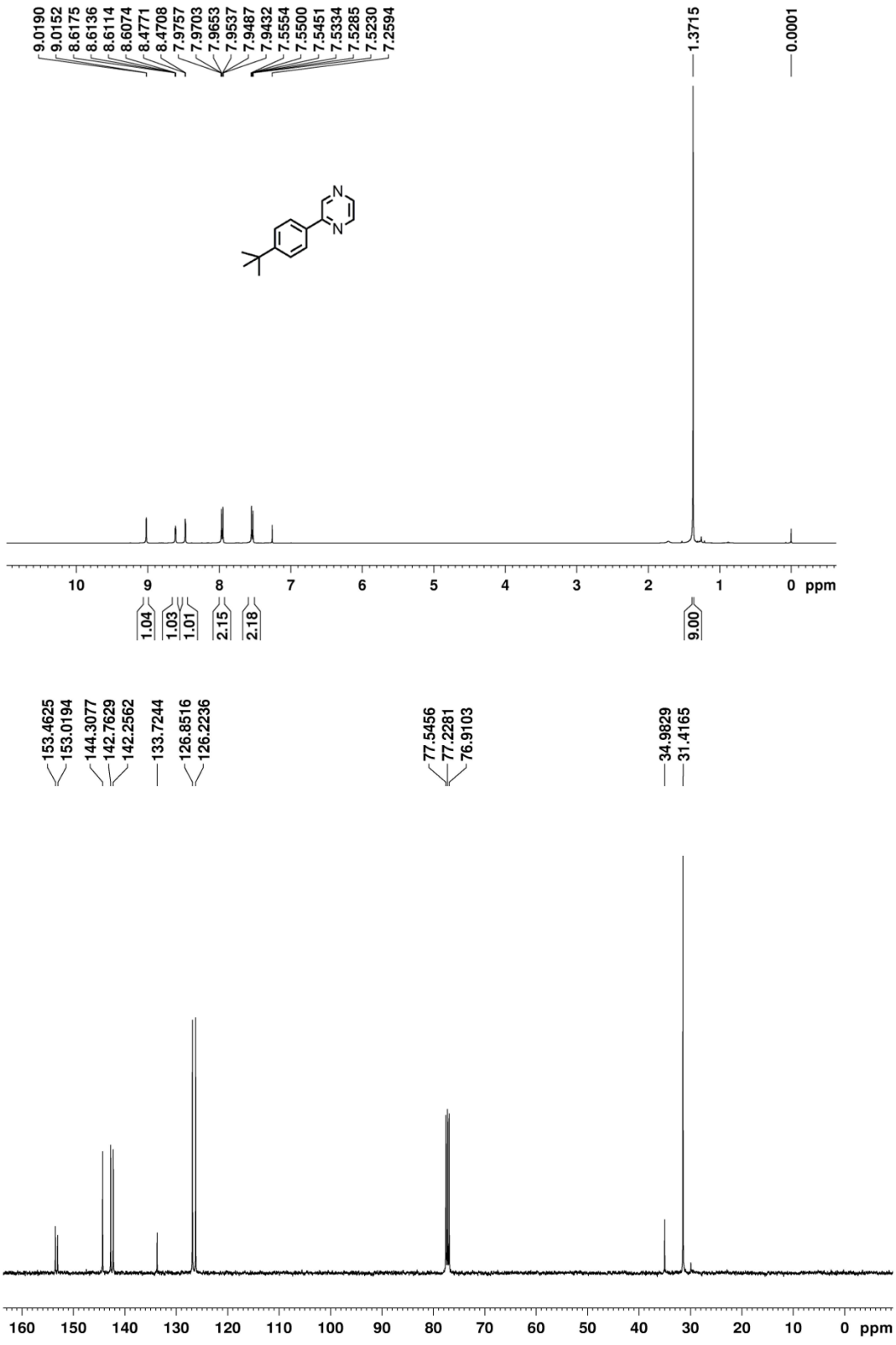
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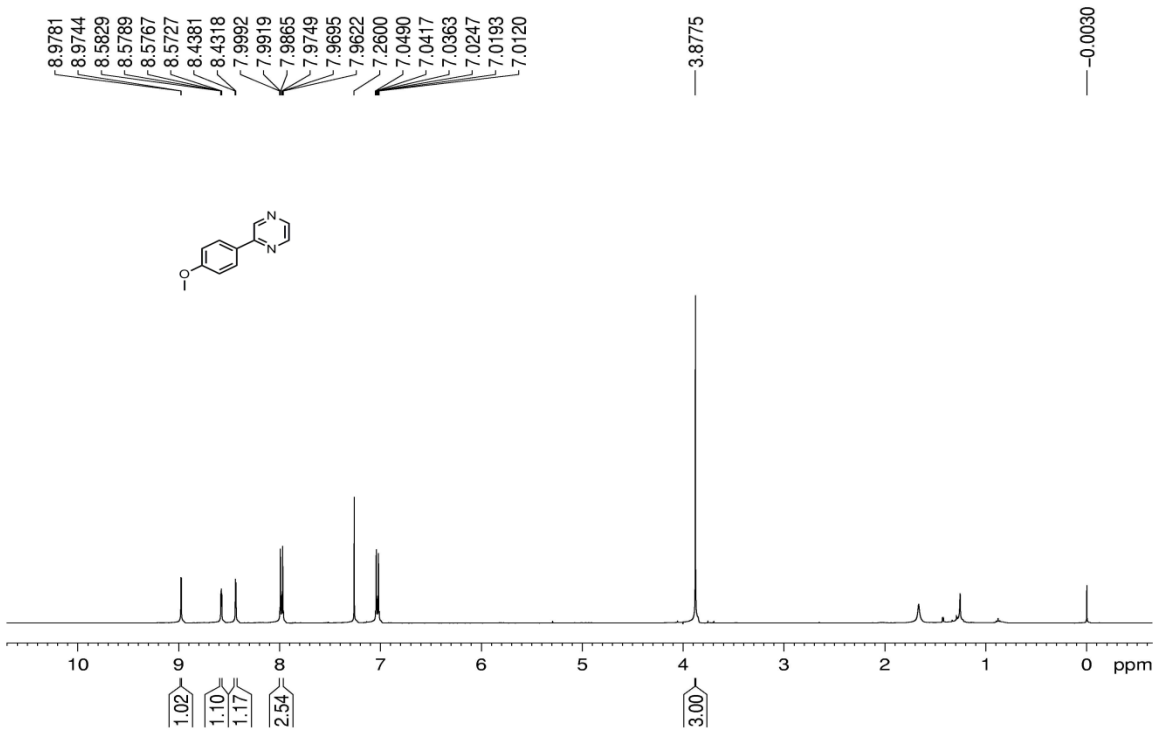
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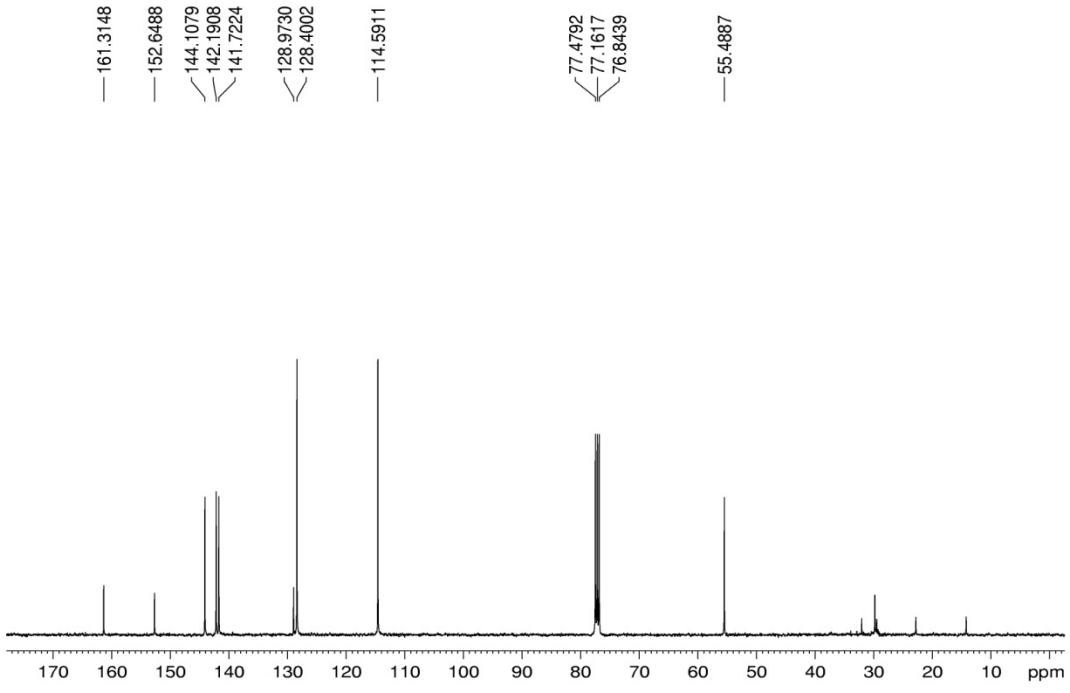
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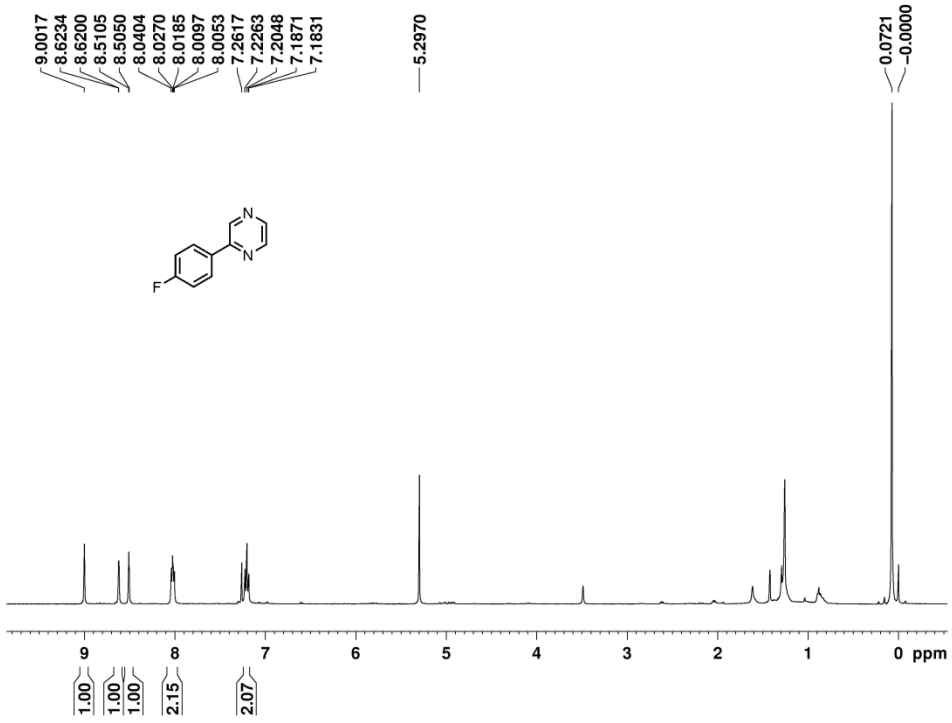
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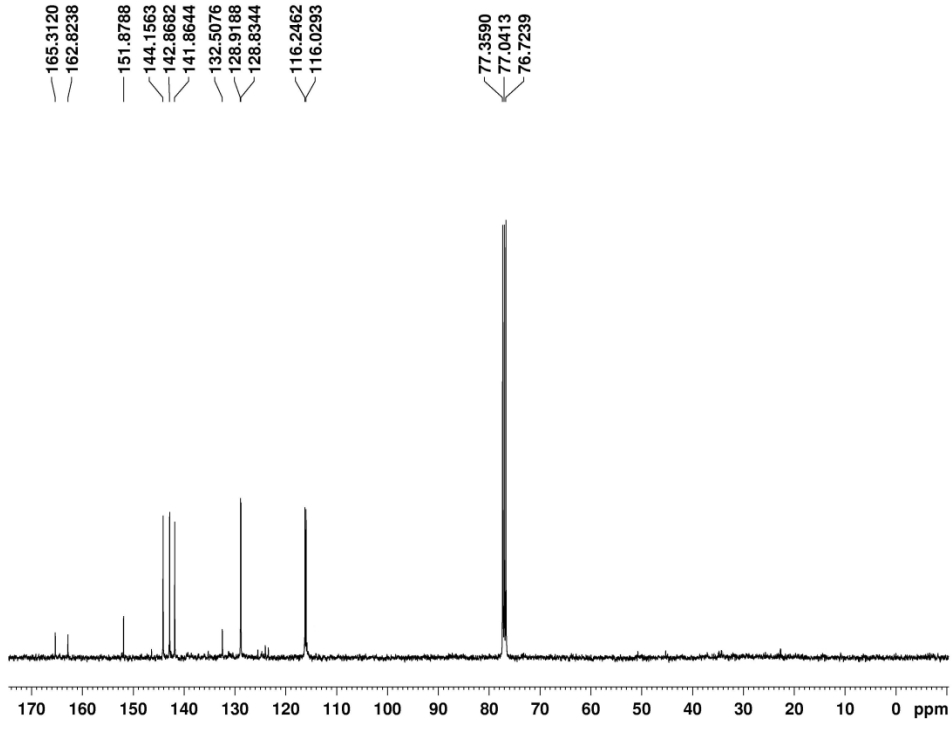
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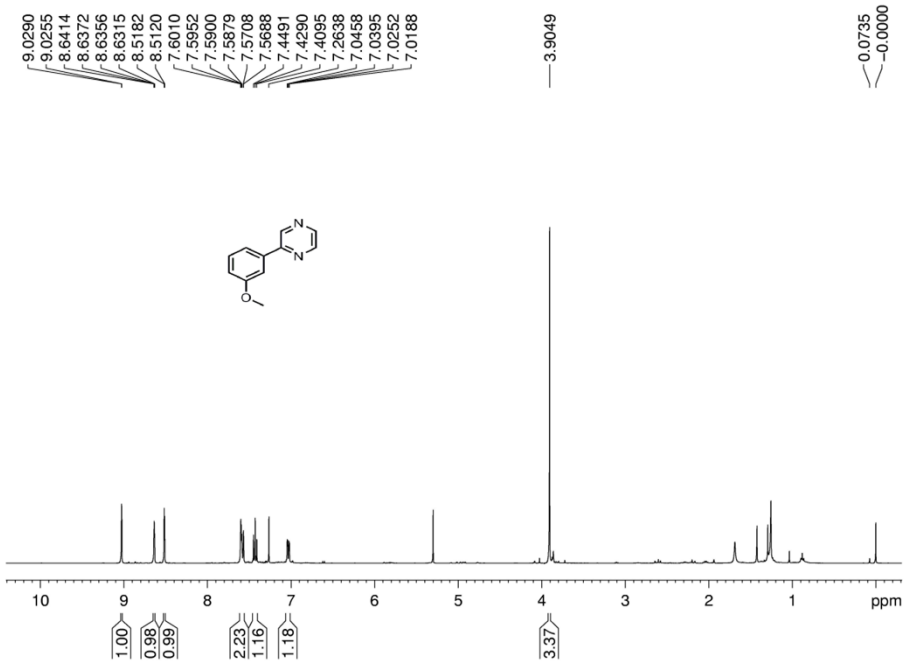
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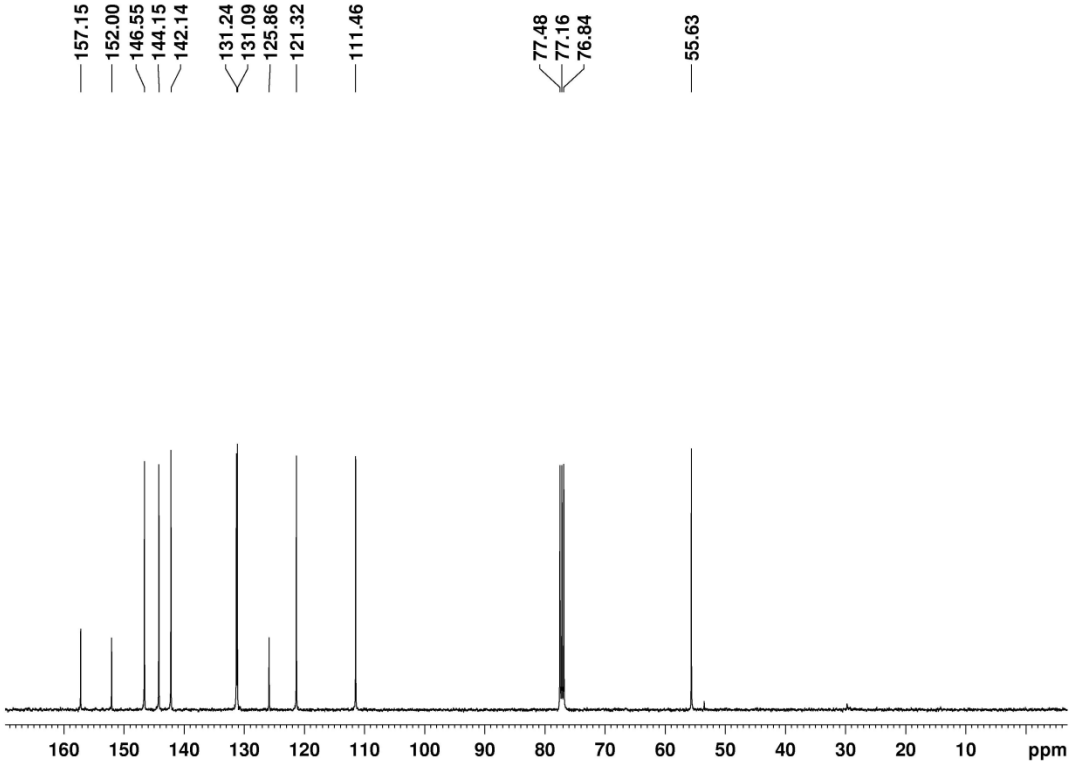
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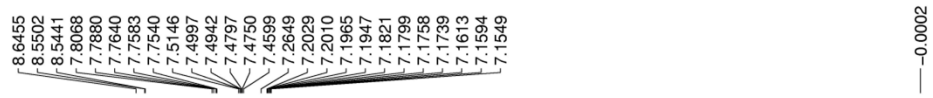
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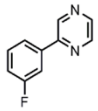
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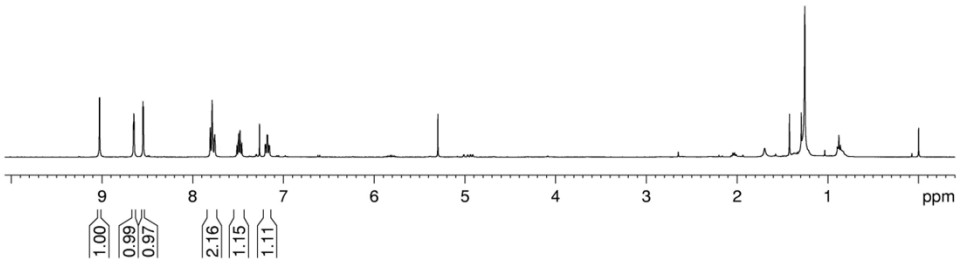
9
8
7
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5
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ppm
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0.99
0.97
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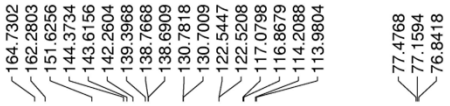
1.15
1.11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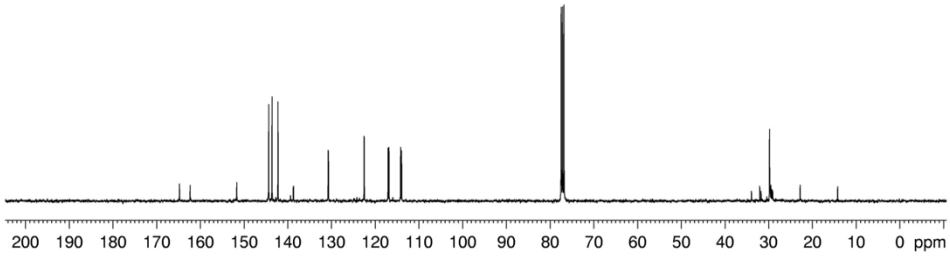
151.6256
144.3734
143.6156
142.2604
139.3968
138.7668
138.6909
130.7818
130.7009
122.5447
122.5208
117.0798
116.8679
114.2088
113.9804
77.4768
77.1594
76.8418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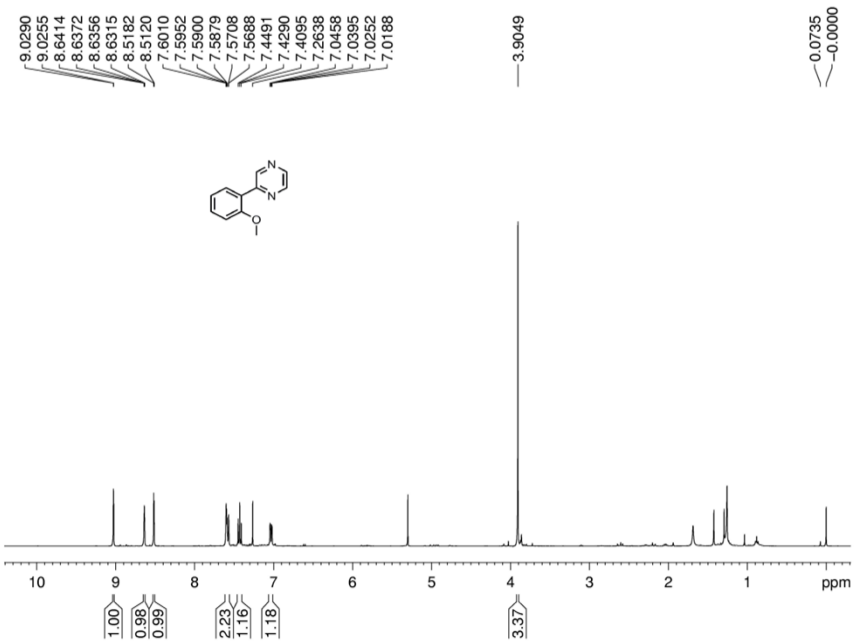
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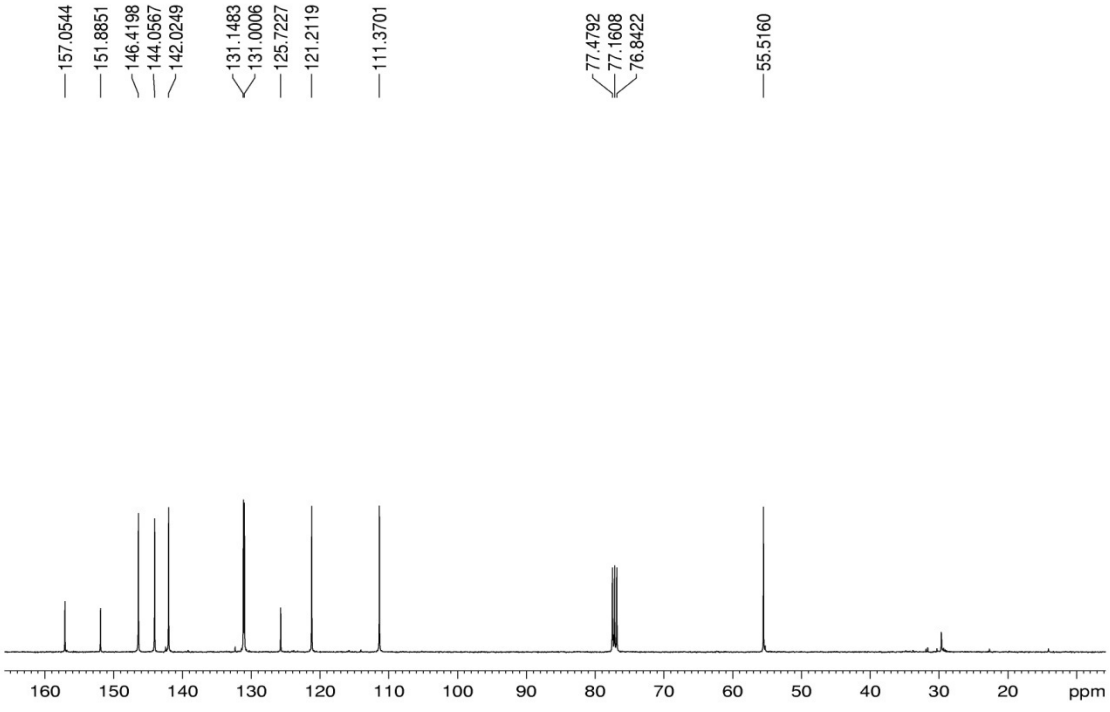
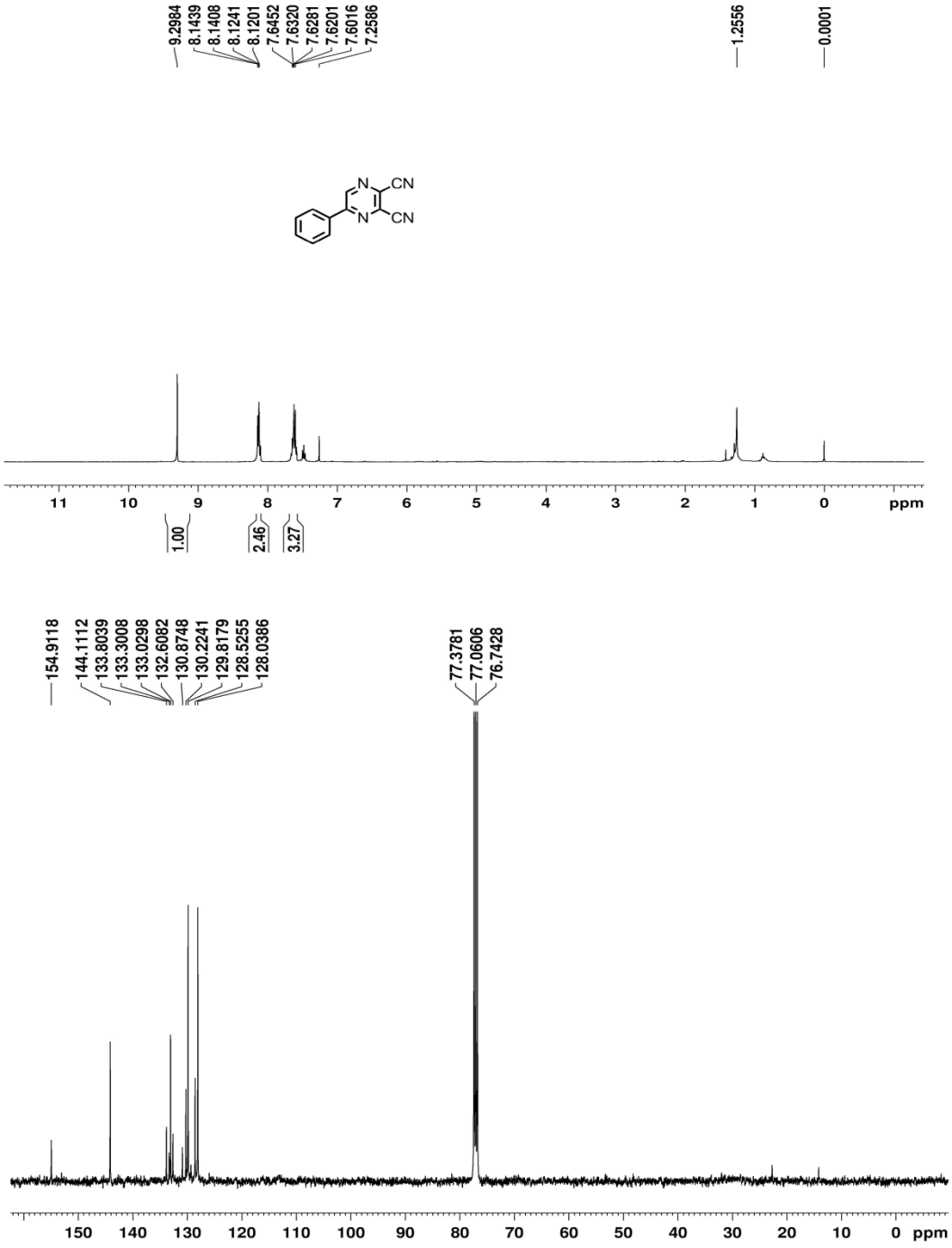
9.0255
8.6414
8.6372
8.6356
8.6315
8.5182
8.5120
7.6010
7.5952
7.5900
7.5879
7.5708
7.5688
7.4491
7.4290
7.4095
7.2638
7.0458
7.0395
7.0252
7.0188
3.9049
0.0735
-0.0000
N
N
O
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.98
0.99
2.23
1.16
1.18
3.37


157.0544
151.8851
146.4198
144.0567
142.0249
131.1483
131.0006
125.7227
121.2119
111.3701
77.4792
77.1608
76.8422
55.5160
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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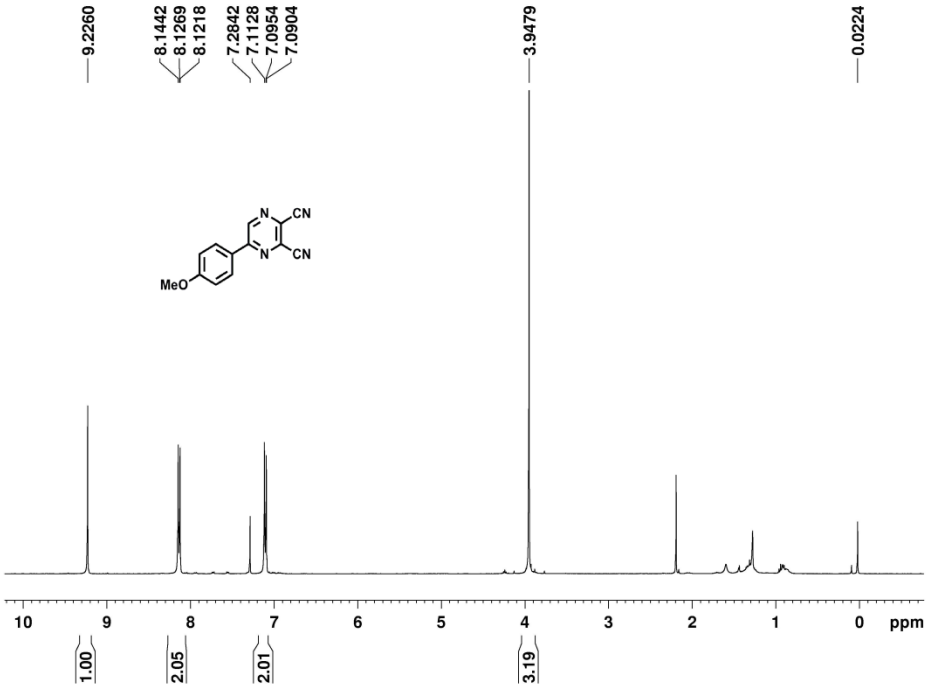
8.1439
8.1408
8.1241
8.1201
7.6452
7.6320
7.6281
7.6201
7.6016
7.2586
1.2556
0.0001
CN
CN
N
N
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.46
3.27
154.9118
144.1112
133.8039
133.3008
133.0298
132.6082
130.8748
130.2241
129.8179
128.5255
128.0386
77.3781
77.0606
76.7428
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


9.2260
8.1442
8.1269
8.1218
7.2842
7.1128
7.0954
7.0904
3.9479
0.0224
N
CN
CN
N
MeO
10
9
8
7
6
5
4
3
2
1
0
ppm
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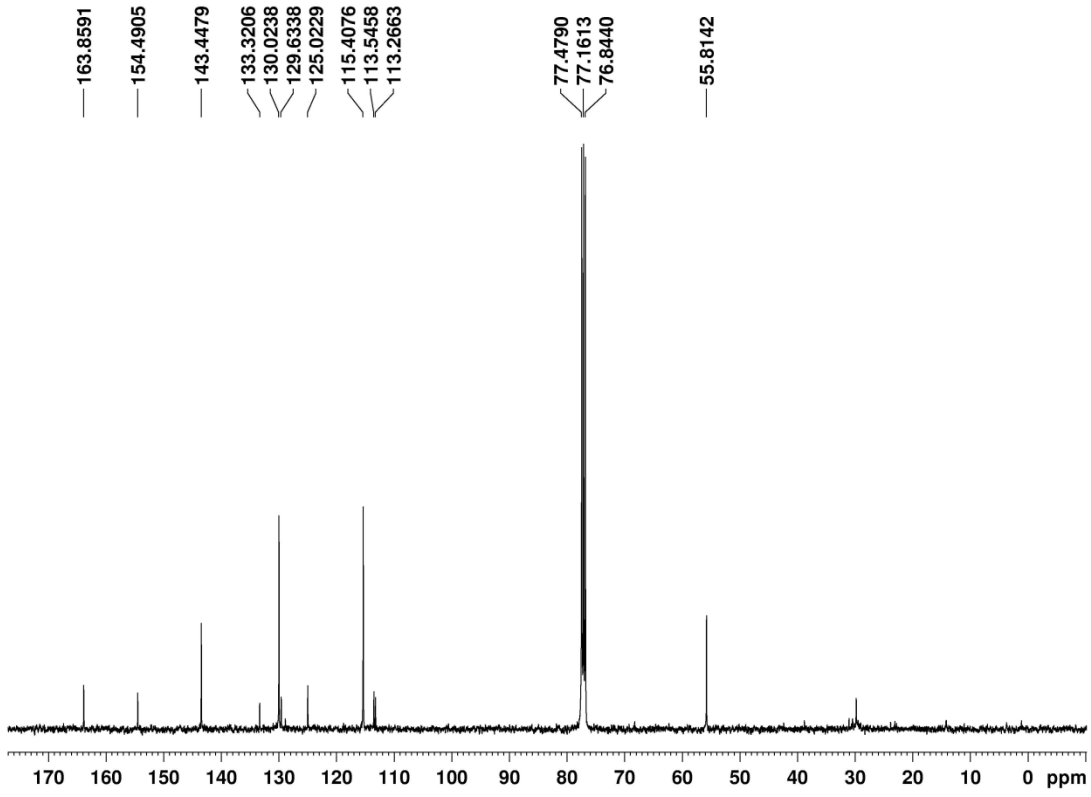
2.05
2.01
3.19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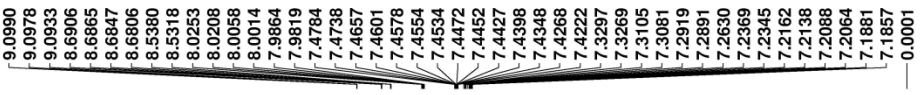
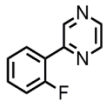
154.4905
143.4479
133.3206
130.0238
129.6338
125.0229
115.4076
113.5458
113.2663
77.4790
77.1613
76.8440
55.8142
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


9.0990
9.0978
9.0933
8.6906
8.6865
8.6847
8.6806
8.5380
8.5318
8.0253
8.0208
8.0058
8.0014
7.9864
7.9819
7.4784
7.4738
7.4657
7.4601
7.4578
7.4554
7.4534
7.4472
7.4452
7.4427
7.4398
7.4348
7.4268
7.4222
7.3297
7.3269
7.3105
7.3081
7.2919
7.2891
7.2630
7.2369
7.2345
7.2162
7.2138
7.2088
7.2064
7.1881
7.1857
0.0001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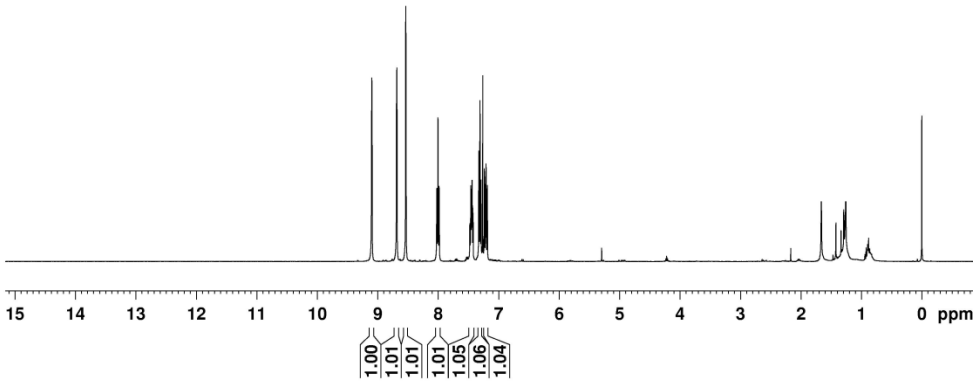
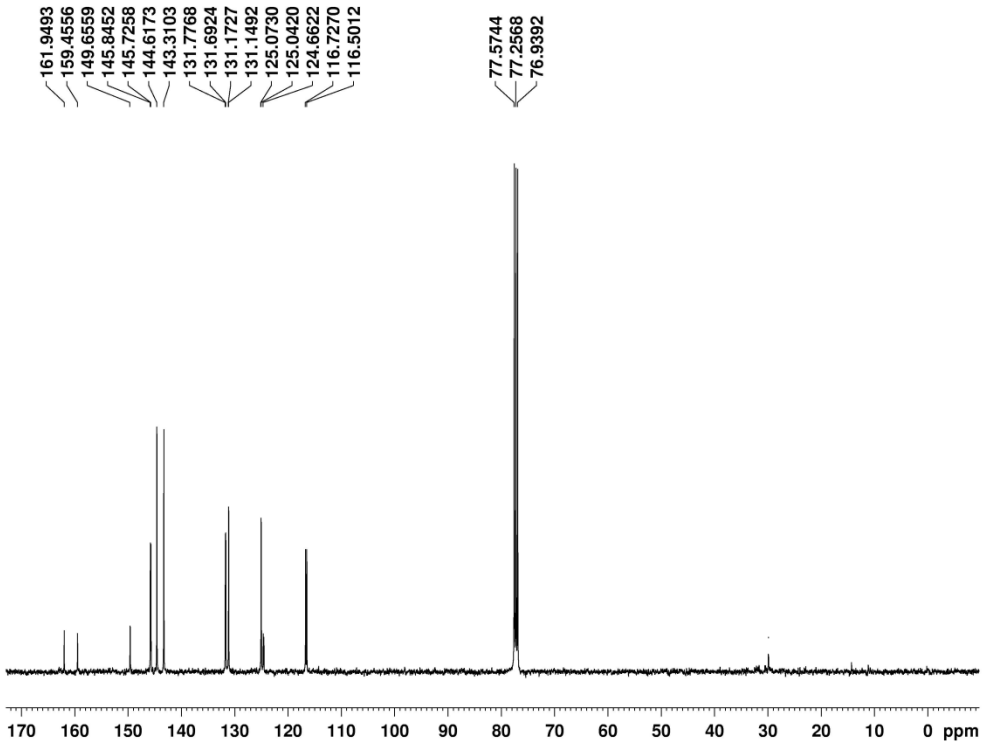
N
F


15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.01
1.01
1.01
1.05
1.06
1.04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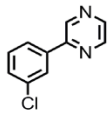
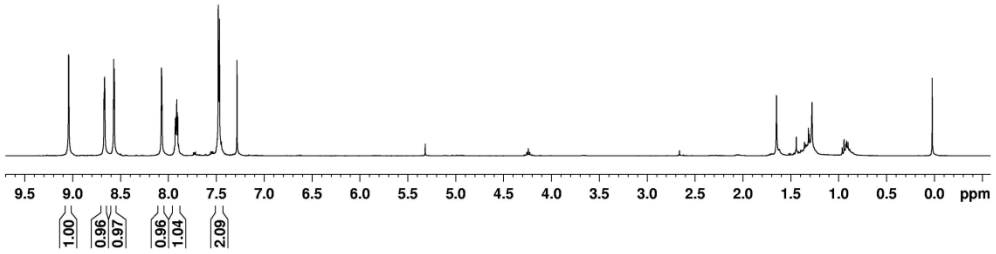
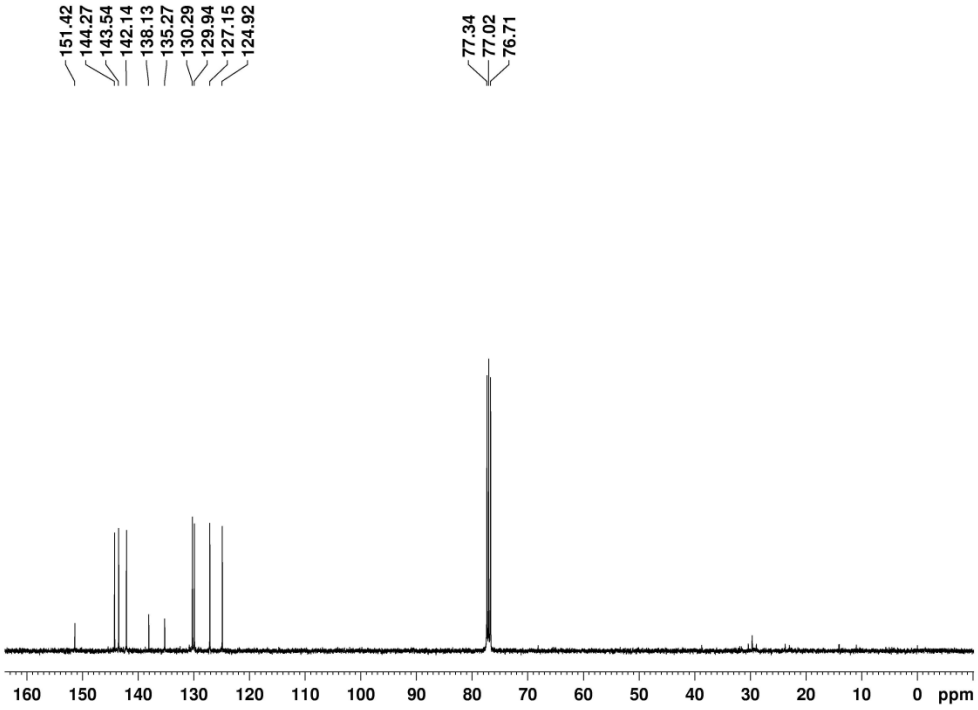
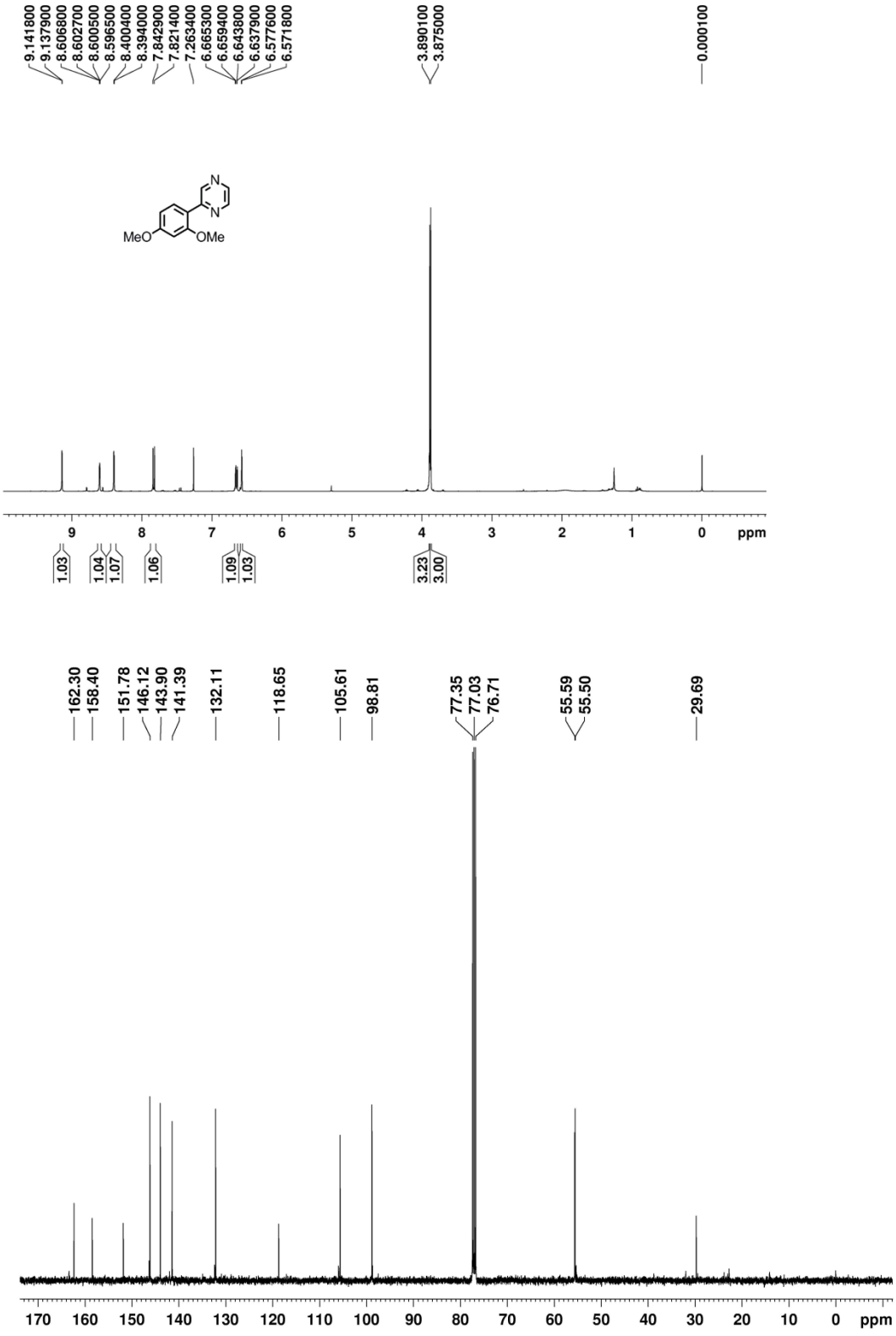
159.4556
149.6559
145.8452
145.7258
144.6173
143.3103
131.7768
131.6924
131.1727
131.1492
125.0730
125.0420
124.6622
116.7270
116.5012
77.5744
77.2568
76.9392
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.66
8.57
8.57
8.08
8.07
8.07
8.07
8.07
7.93
7.93
7.92
7.92
7.92
7.91
7.90
7.48
7.47
7.47
7.47
7.28
0.02


N
N
Cl


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.96
0.97
0.96
1.04
2.09


151.42
144.27
143.54
142.14
138.13
135.27
130.29
129.94
127.15
124.92
77.34
77.02
76.71
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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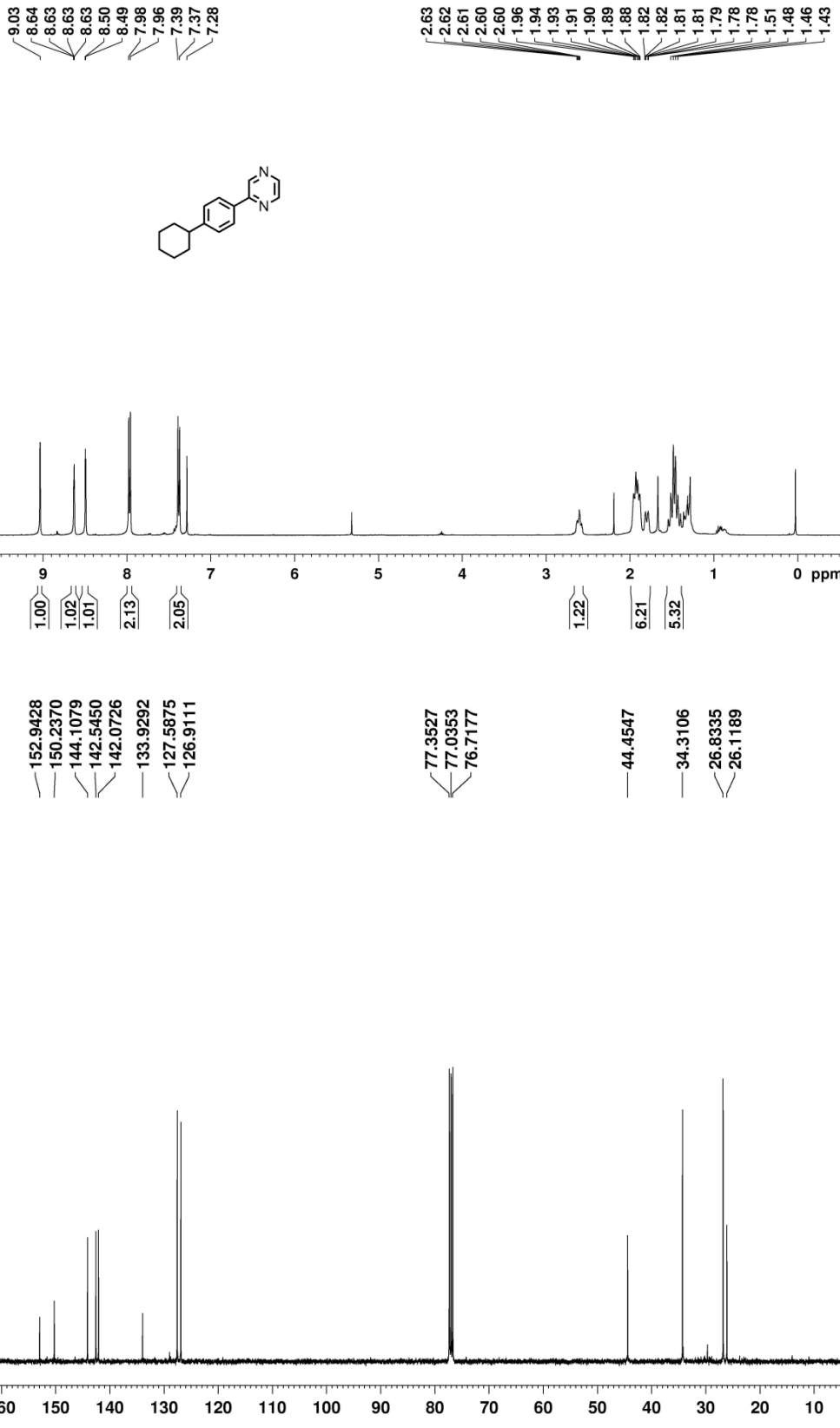
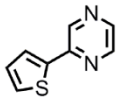
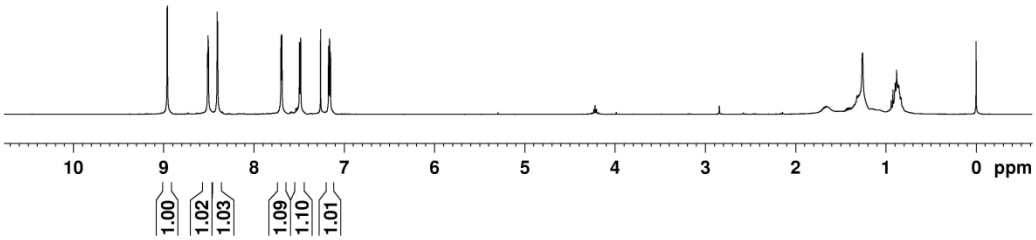
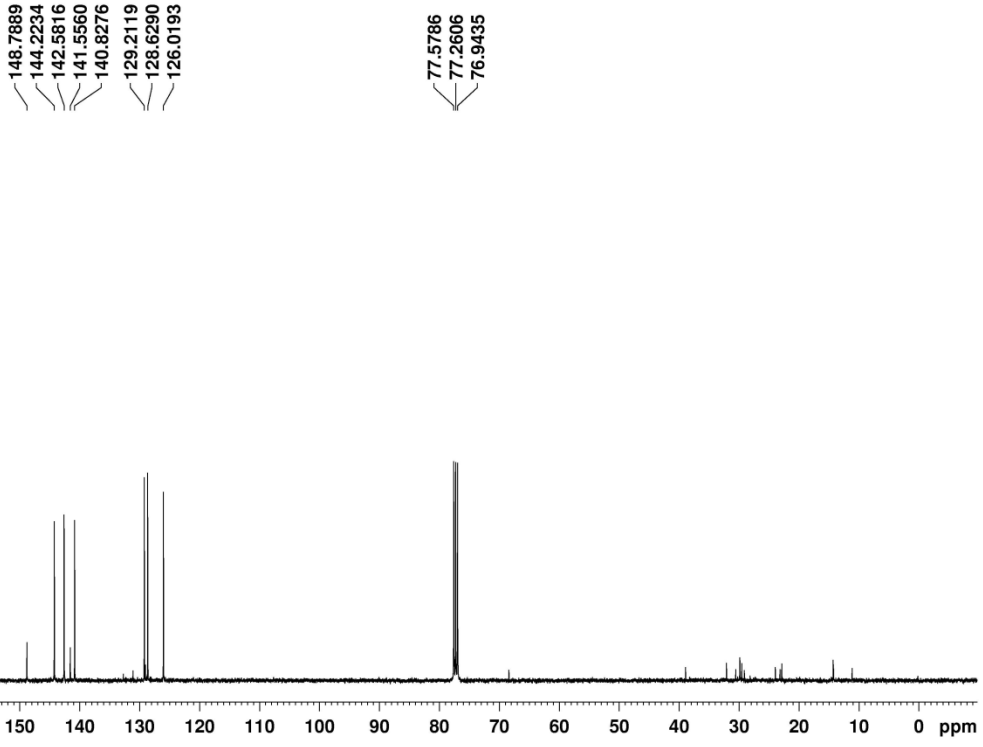
9.137900
8.606800
8.602700
8.600500
8.596500
8.400400
8.394000
7.842900
7.821400
7.263400
6.665300
6.659400
6.643800
6.637900
6.577600
6.571800
3.890100
3.875000
0.000100
MeO
OMe
N
N
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.04
1.07
1.06
1.09
1.03
3.23
3.00
162.30
158.40
151.78
146.12
143.90
141.39
132.11
118.65
105.61
98.81
77.35
77.03
76.71
55.59
55.50
29.69
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

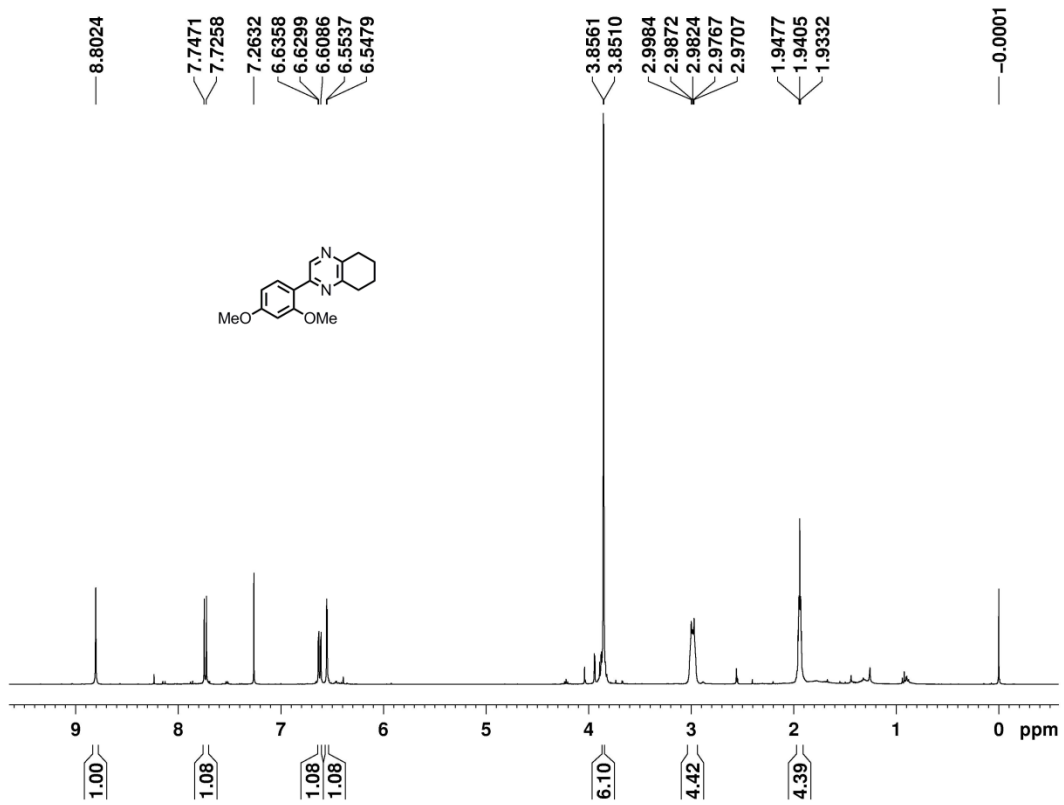

9.03
8.64
8.63
8.63
8.63
8.50
8.49
7.98
7.96
7.39
7.37
7.28
2.63
2.62
2.61
2.60
2.60
1.96
1.94
1.93
1.91
1.90
1.89
1.88
1.82
1.82
1.81
1.81
1.79
1.78
1.78
1.51
1.48
1.46
1.43
N
N
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.02
1.01
2.13
2.05
1.22
6.21
5.32
152.9428
150.2370
144.1079
142.5450
142.0726
133.9292
127.5875
126.9111
77.3527
77.0353
76.7177
44.4547
34.3106
26.8335
26.1189
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

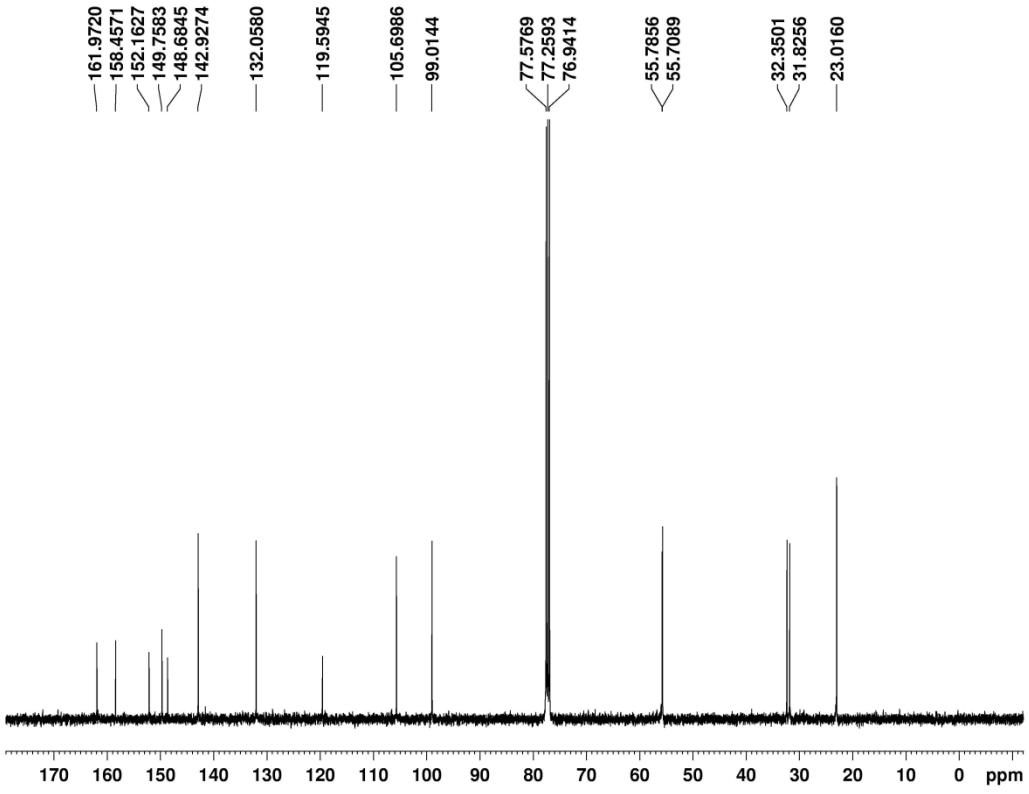

8.9624
8.9587
8.5140
8.5099
8.5077
8.5038
8.4078
8.4014
7.7009
7.6983
7.6916
7.6890
7.4968
7.4942
7.4842
7.4816
7.2623
7.1740
7.1647
7.1615
7.1521
0.0001


N
N
S


10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.02
1.03
1.09
1.10
1.01


148.7889
144.2234
142.5816
141.5560
140.8276
129.2119
128.6290
126.0193
77.5786
77.2606
76.9435
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.8024
7.7471
7.7258
7.2632
6.6358
6.6299
6.6086
6.5537
6.5479
3.8561
3.8510
2.9984
2.9872
2.9824
2.9767
2.9707
1.9477
1.9405
1.9332
-0.0001
N
N
MeO
OMe
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.08
1.08
1.08
6.10
4.42
4.39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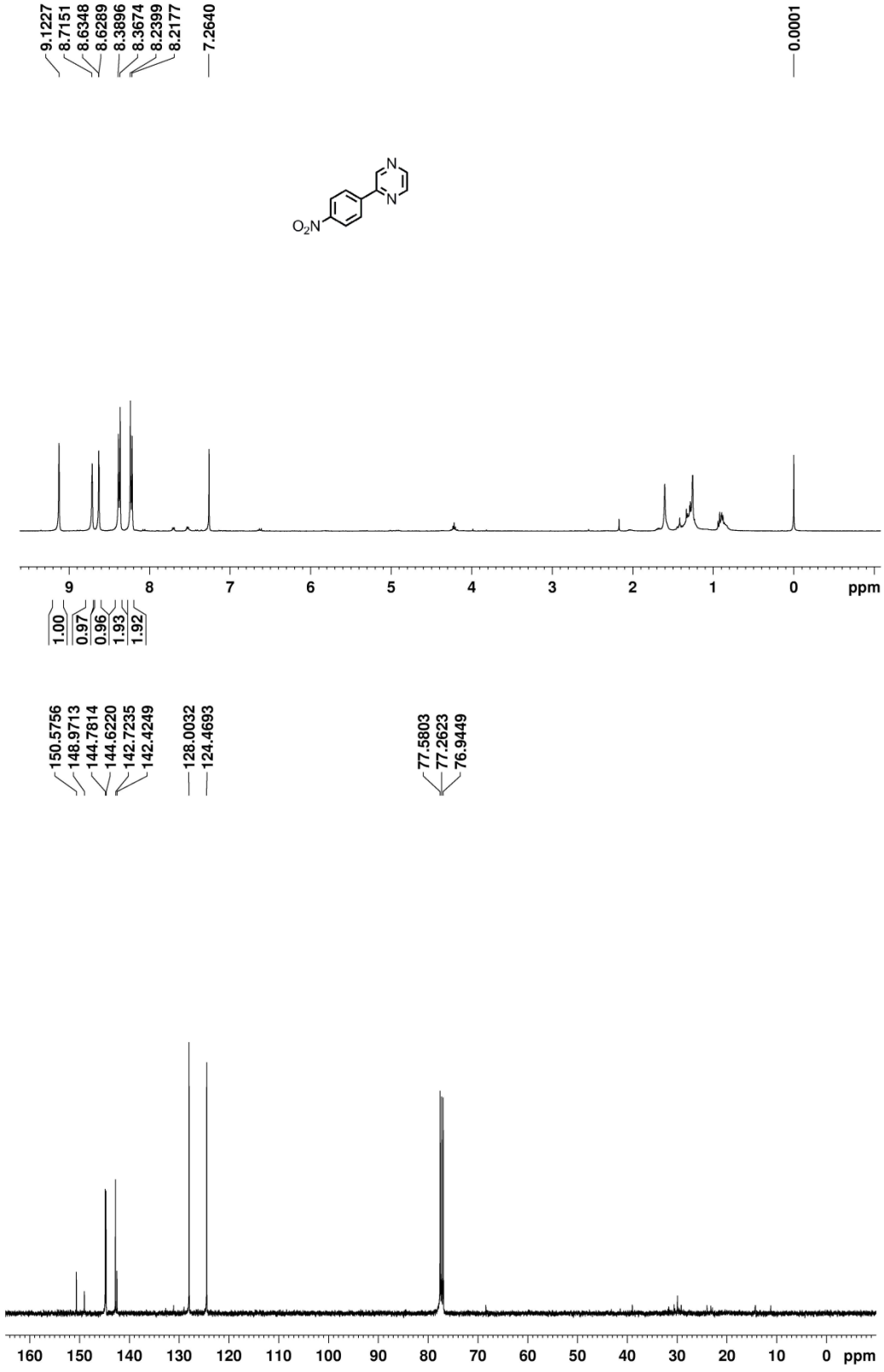
152.1627
149.7583
148.6845
142.9274
132.0580
119.5945
105.6986
99.0144
77.5769
77.2593
76.9414
55.7856
55.7089
32.3501
31.8256
23.0160
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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8.6348
8.6289
8.3896
8.3674
8.2399
8.2177
7.2640
0.0001
O2N
N
N
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.97
0.96
1.93
1.92
150.5756
148.9713
144.7814
144.6220
142.7235
142.4249
128.0032
124.4693
77.5803
77.2623
76.9449
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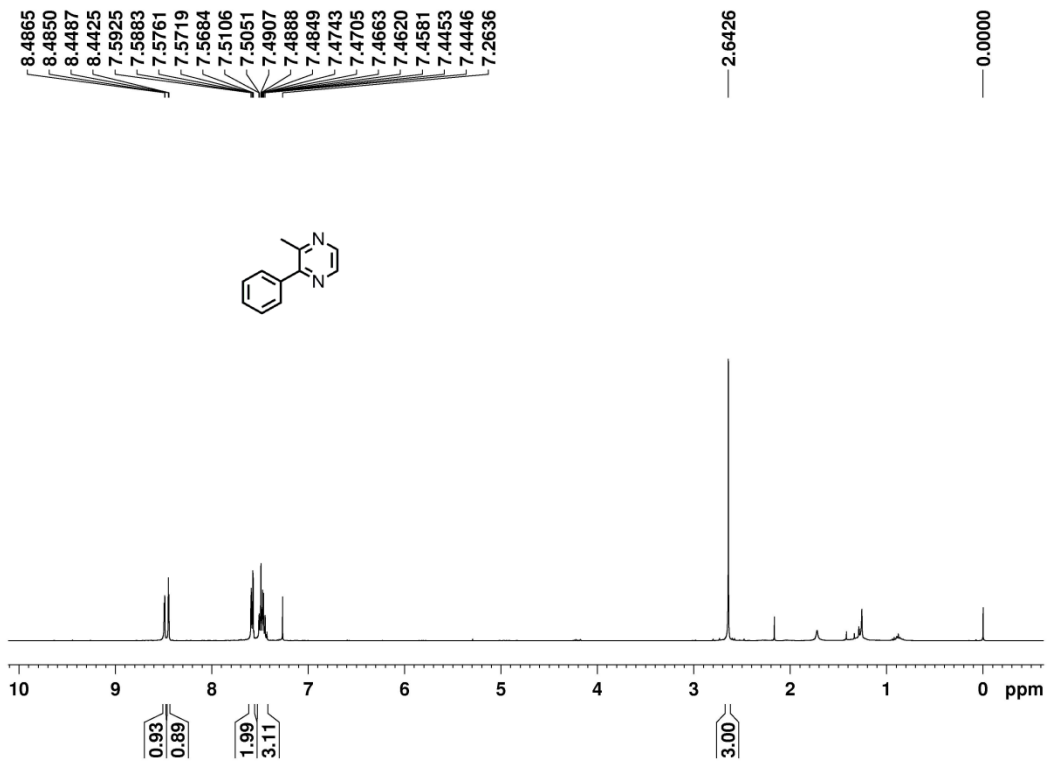
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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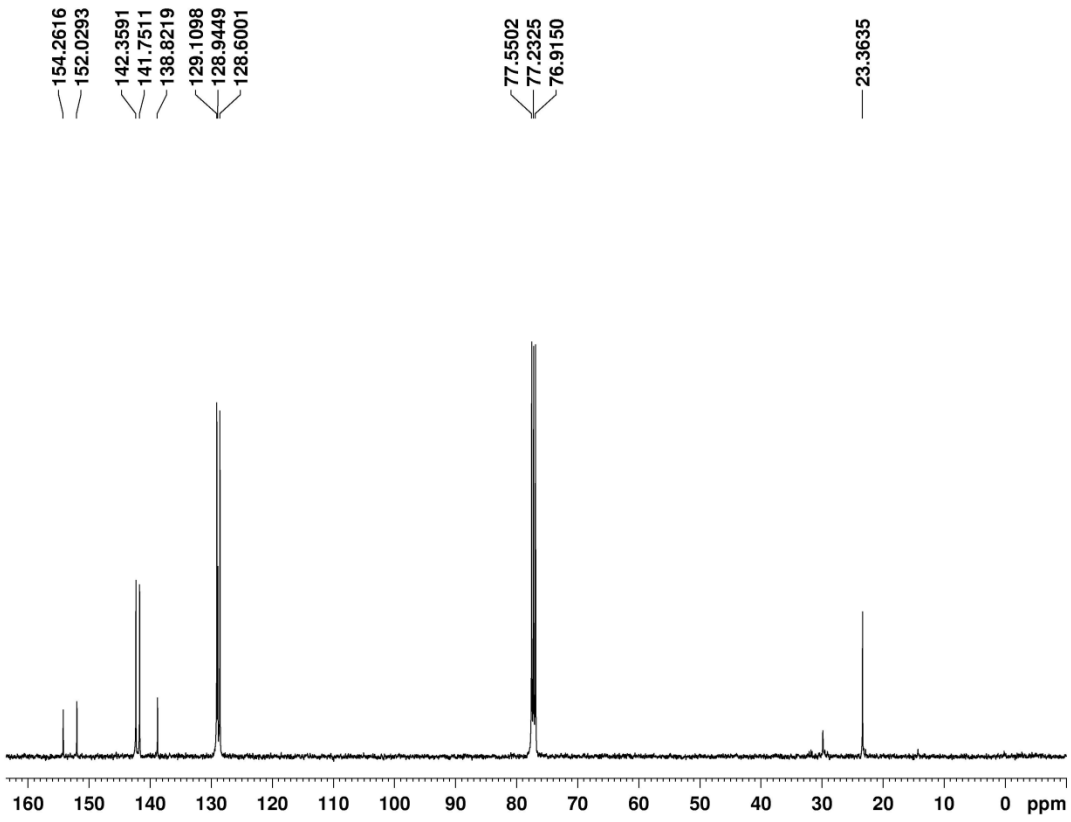
8.4850
8.4487
8.4425
7.5925
7.5883
7.5761
7.5719
7.5684
7.5106
7.5051
7.4907
7.4888
7.4849
7.4743
7.4705
7.4663
7.4620
7.4581
7.4453
7.4446
7.2636
2.6426
0.0000
N
N
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
0.89
1.99
3.11
3.00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142.3591
141.7511
138.8219
129.1098
128.9449
128.6001
77.5502
77.2325
76.9150
23.3635
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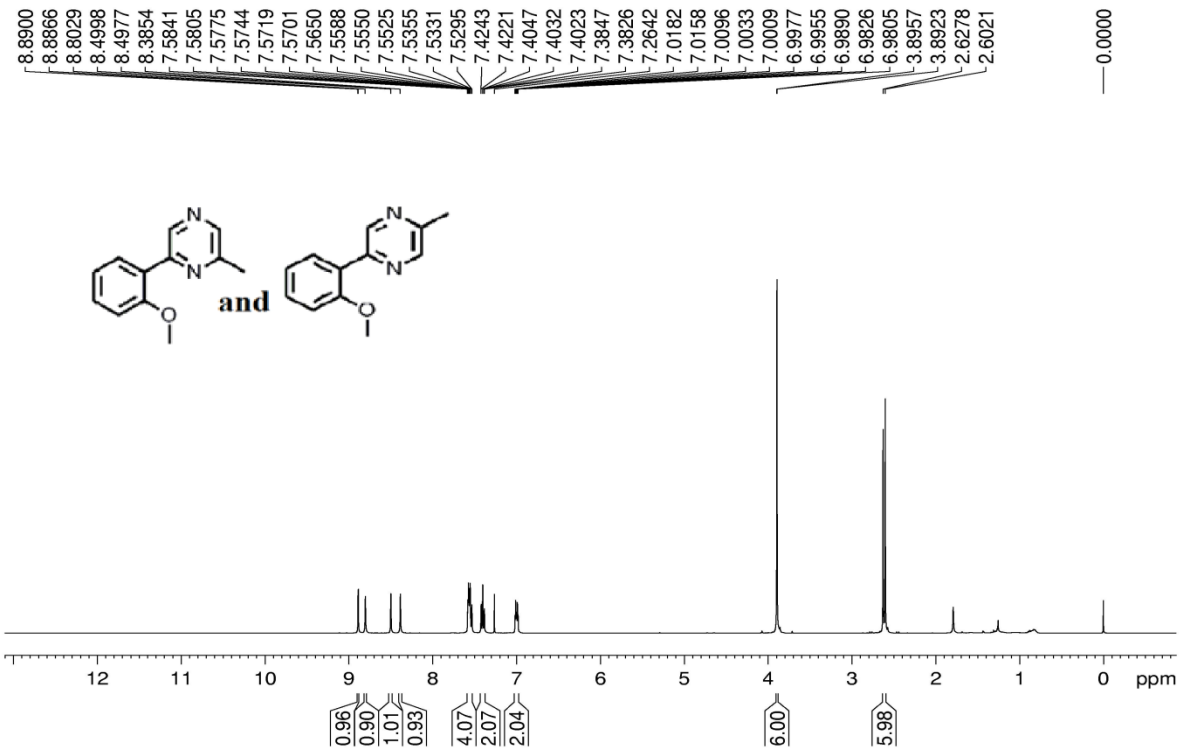
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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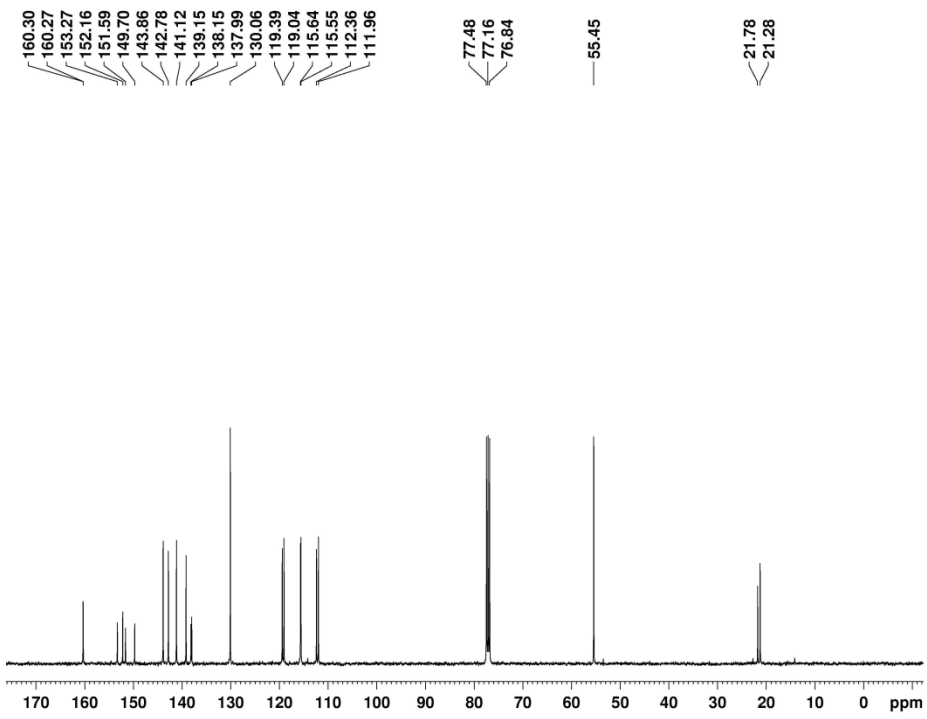
8.4998
8.4977
8.3854
7.5841
7.5805
7.5775
7.5744
7.5719
7.5701
7.5650
7.5588
7.5550
7.5525
7.5355
7.5331
7.5295
7.4243
7.4221
7.4047
7.4032
7.4023
7.3847
7.3826
7.2642
7.0182
7.0158
7.0096
7.0033
7.0009
6.9977
6.9955
6.9890
6.9826
6.9805
3.8957
3.8923
2.6278
2.6021
0.0000
and
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
0.90
1.01
0.93
4.07
2.07
2.04
6.00
5.98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153.27
152.16
151.59
149.70
143.86
142.78
141.12
139.15
138.15
137.99
130.06
119.39
119.04
115.64
115.55
112.36
111.96
77.48
77.16
76.84
55.45
21.78
21.28
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.8904
8.8869
8.8077
8.5164
8.5143
8.4170
7.7907
7.7871
7.7847
7.7805
7.7762
7.7696
7.7684
7.7489
7.7387
7.7233
7.7172
7.7131
7.4922
7.4884
7.4768
7.4718
7.4681
7.4568
7.4534
7.4489
7.4371
7.4336
7.2639
7.1754
7.1713
7.1688
7.1665
7.1642
7.1572
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7.1456
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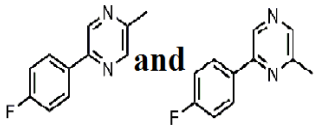
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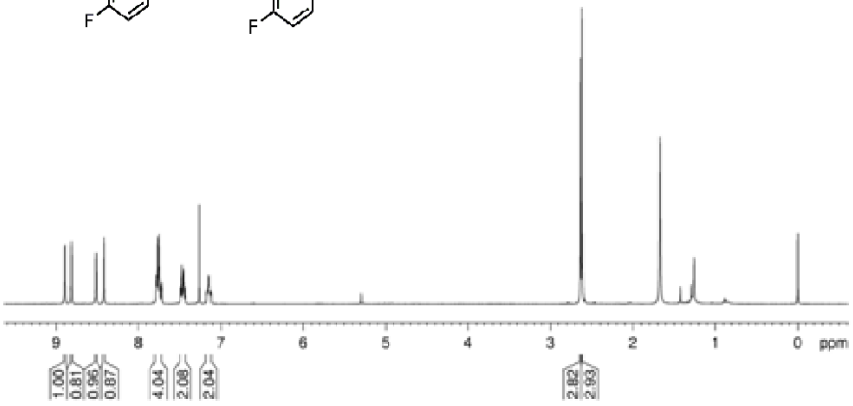
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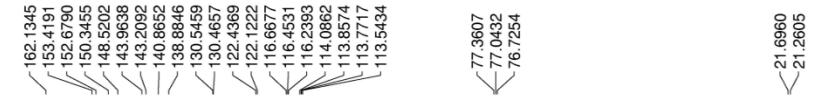
2.93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122.1222
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116.4531
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113.8574
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77.0432
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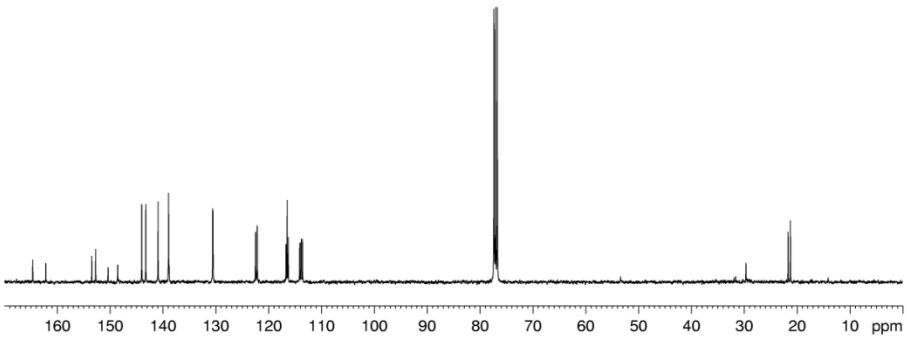
21.2605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10
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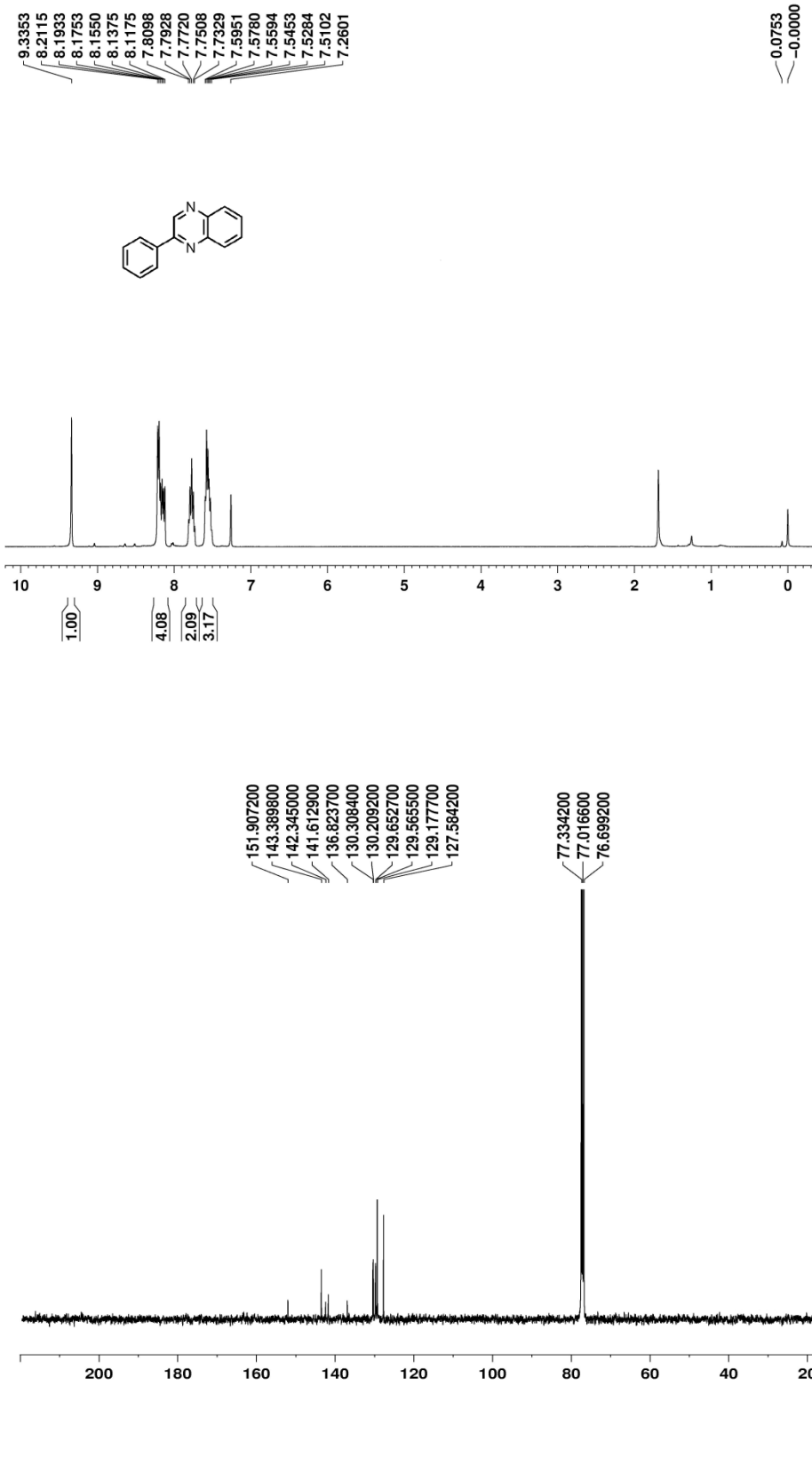
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7.5453
7.5284
7.5102
7.2601
0.0753
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N
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8
7
6
5
4
3
2
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0
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4.08
2.09
3.17
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129.177700
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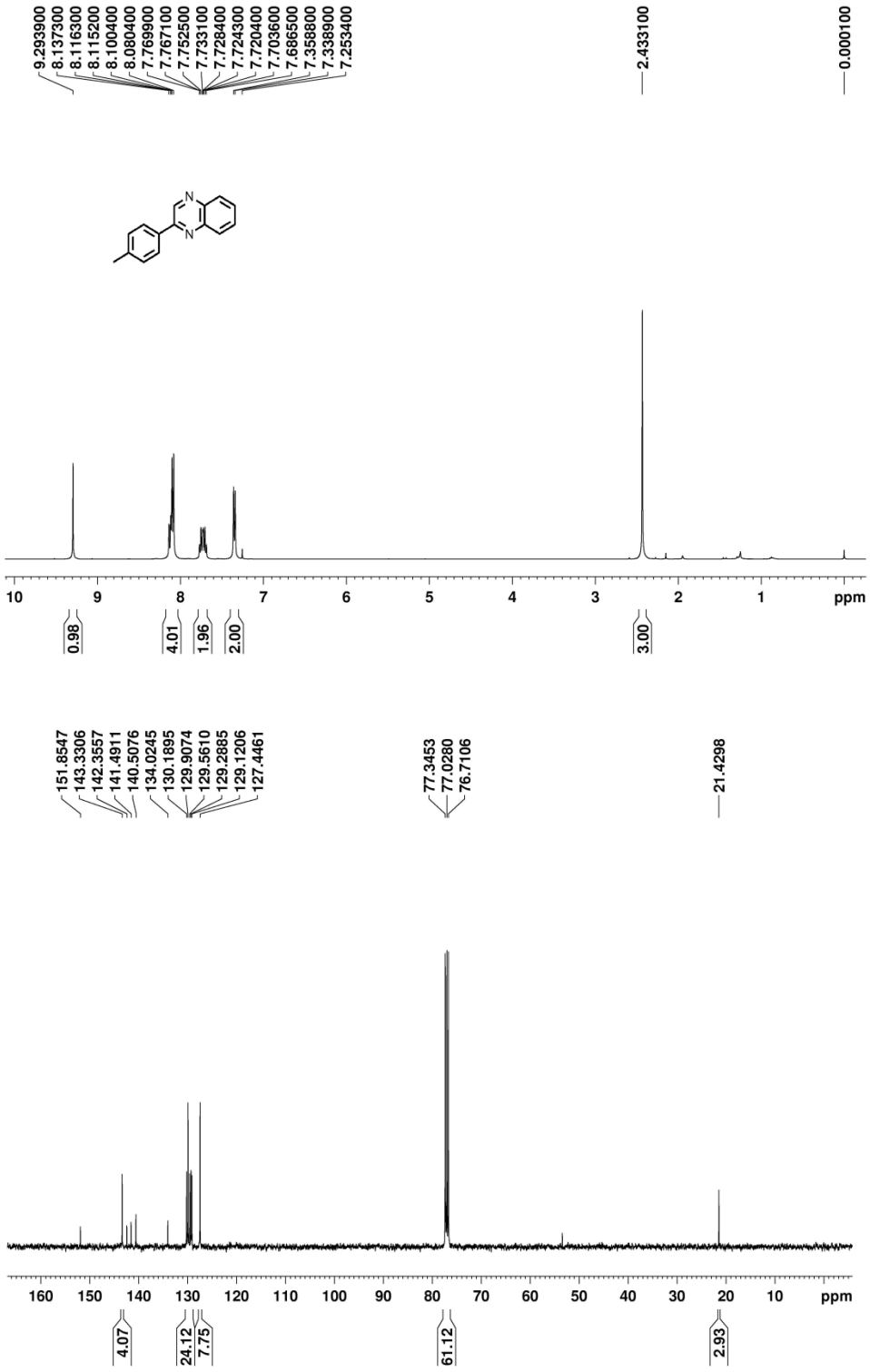
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7.728400
7.724300
7.720400
7.703600
7.686500
7.358800
7.338900
7.253400
2.433100
0.000100
N
N
10
9
8
7
6
5
4
3
2
1
ppm
0.98
4.01
1.96
2.00
3.00
151.8547
143.3306
142.3557
141.4911
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130.1895
129.9074
129.5610
129.2885
129.1206
127.4461
77.3453
77.0280
76.7106
21.4298
160
150
140
130
120
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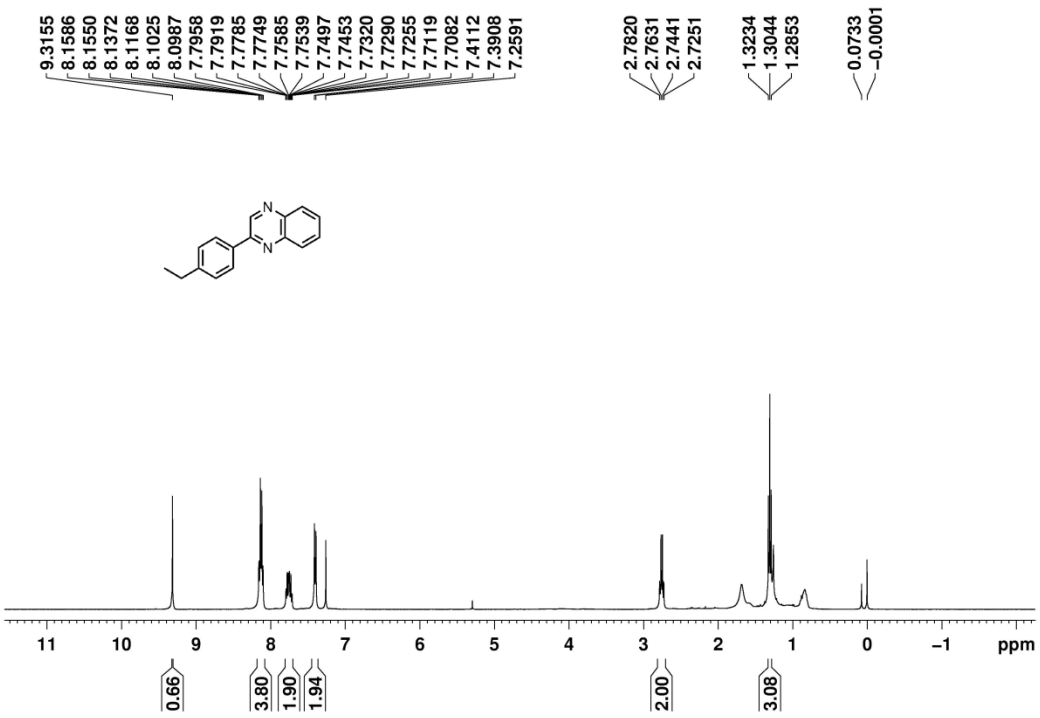
2.93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7.7749
7.7585
7.7539
7.7497
7.7453
7.7320
7.7290
7.7255
7.7119
7.7082
7.4112
7.3908
7.2591
2.7820
2.7631
2.7441
2.7251
1.3234
1.3044
1.2853
0.0733
-0.0001
N
N
11
10
9
8
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−1
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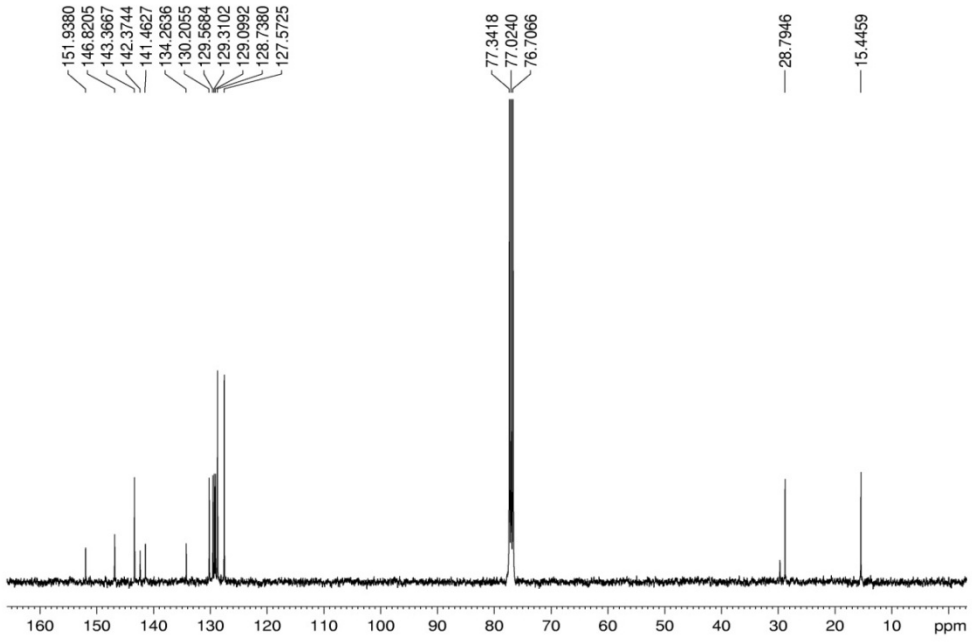
3.08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128.7380
127.5725
77.3418
77.0240
76.7066
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150
140
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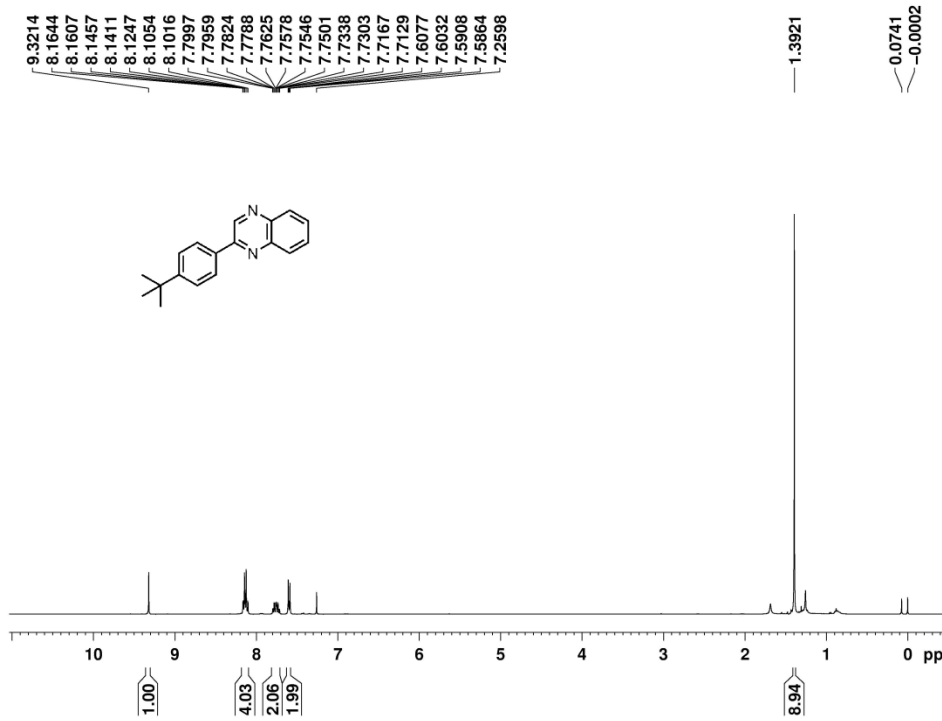
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7.7788
7.7625
7.7578
7.7546
7.7501
7.7338
7.7303
7.7167
7.7129
7.6077
7.6032
7.5908
7.5864
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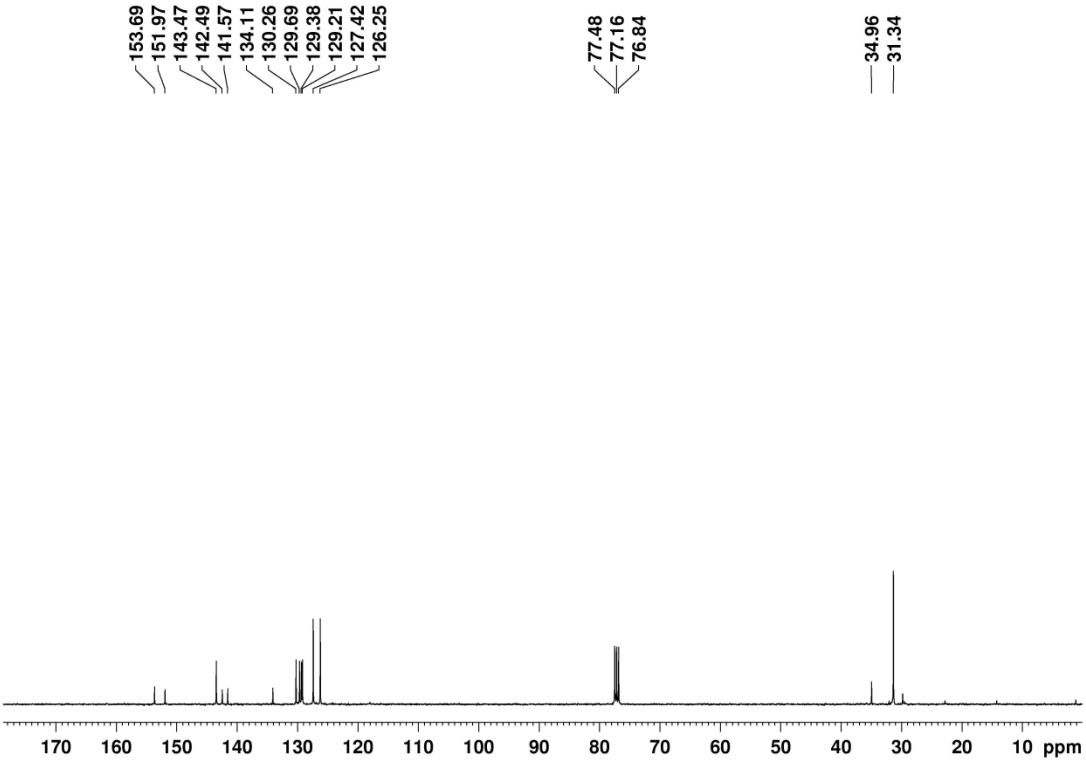
2.06
1.99
8.94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31.34
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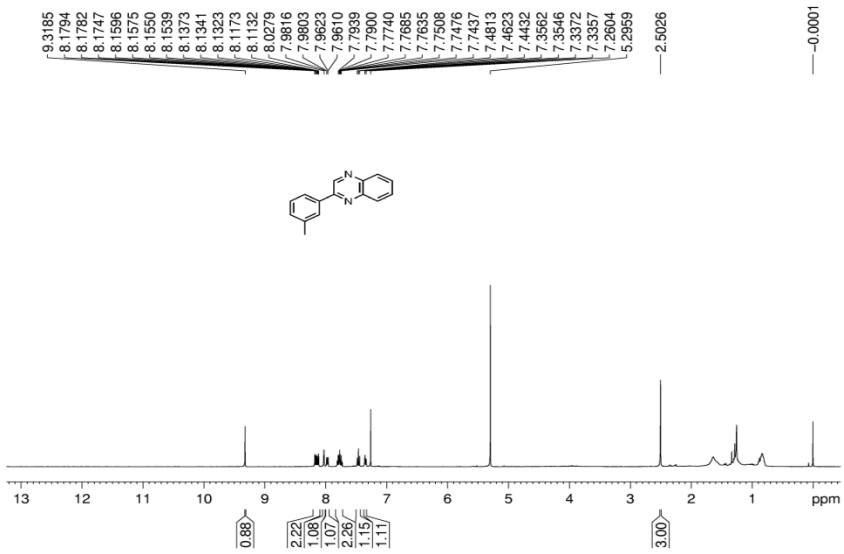
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8.1550
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8.1132
8.0279
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7.9623
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7.7939
7.7900
7.7740
7.7685
7.7635
7.7508
7.7476
7.7437
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7
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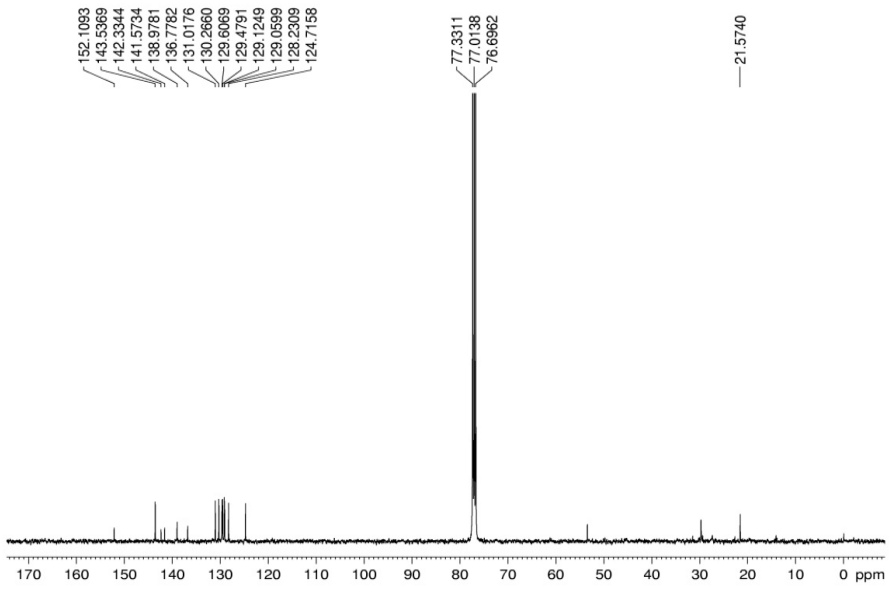
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129.0599
128.2309
124.7158
77.3311
77.0138
76.6962
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150
140
130
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110
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70
60
50
40
30
20
10
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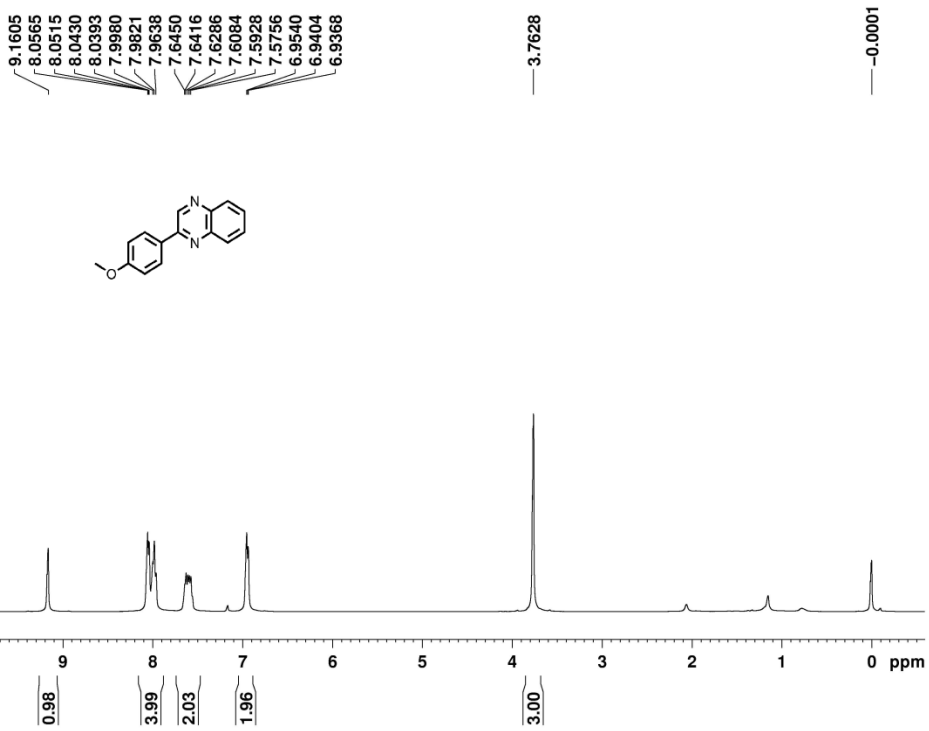
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7.6286
7.6084
7.5928
7.5756
6.9540
6.9404
6.9368
3.7628
-0.0001
N
N
O
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7
6
5
4
3
2
1
0 ppm
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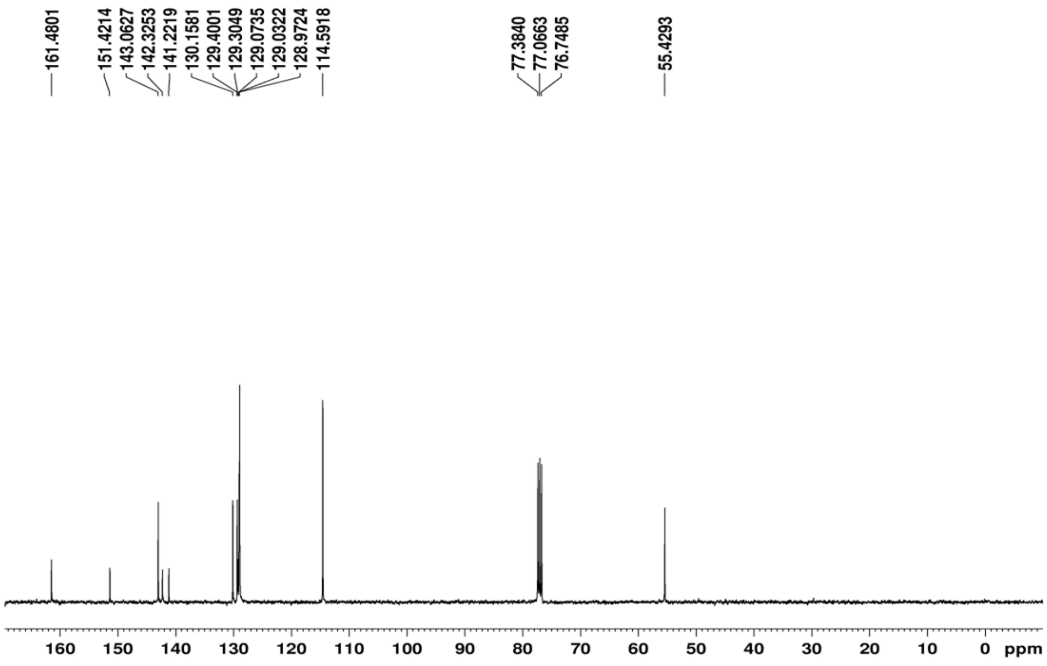
2.03
1.96
3.00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129.0322
128.9724
114.5918
77.3840
77.0663
76.7485
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150
140
130
120
110
100
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60
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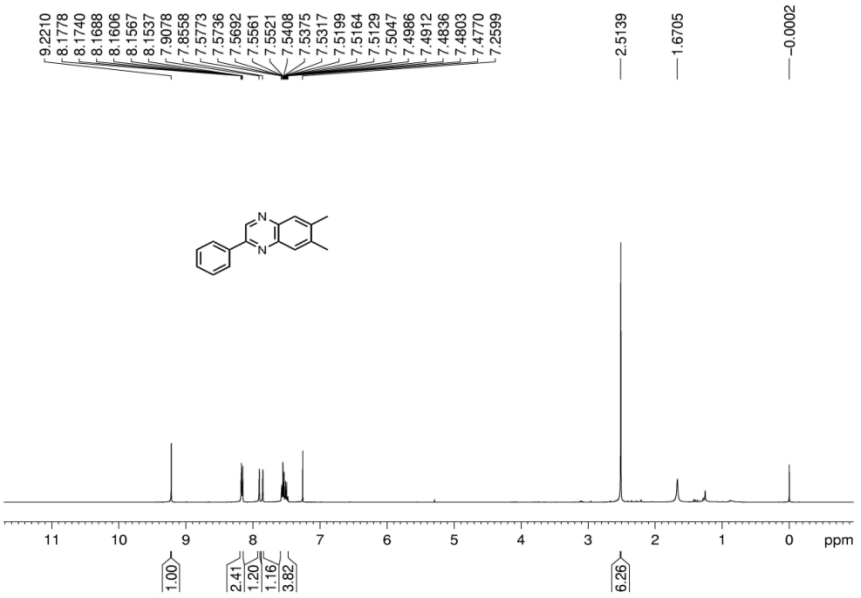
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7.5692
7.5561
7.5521
7.5408
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7.5317
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7.4986
7.4912
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7.4803
7.4770
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0.0002
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N
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10
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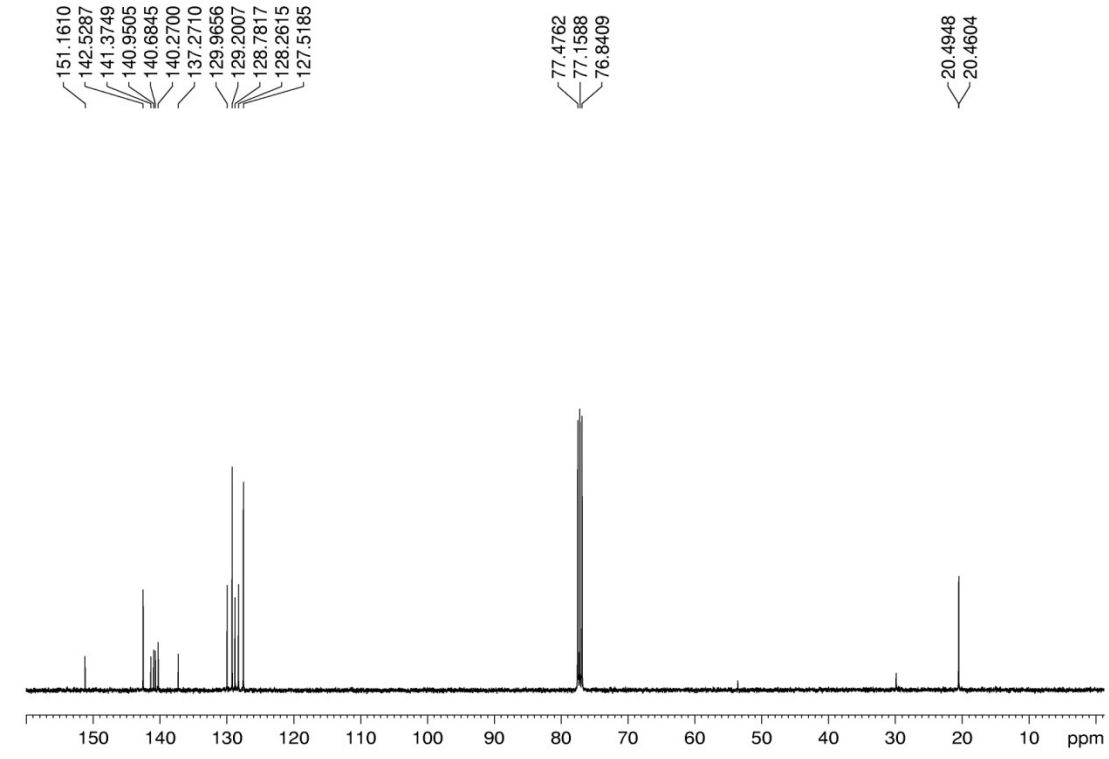
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77.1588
76.8409
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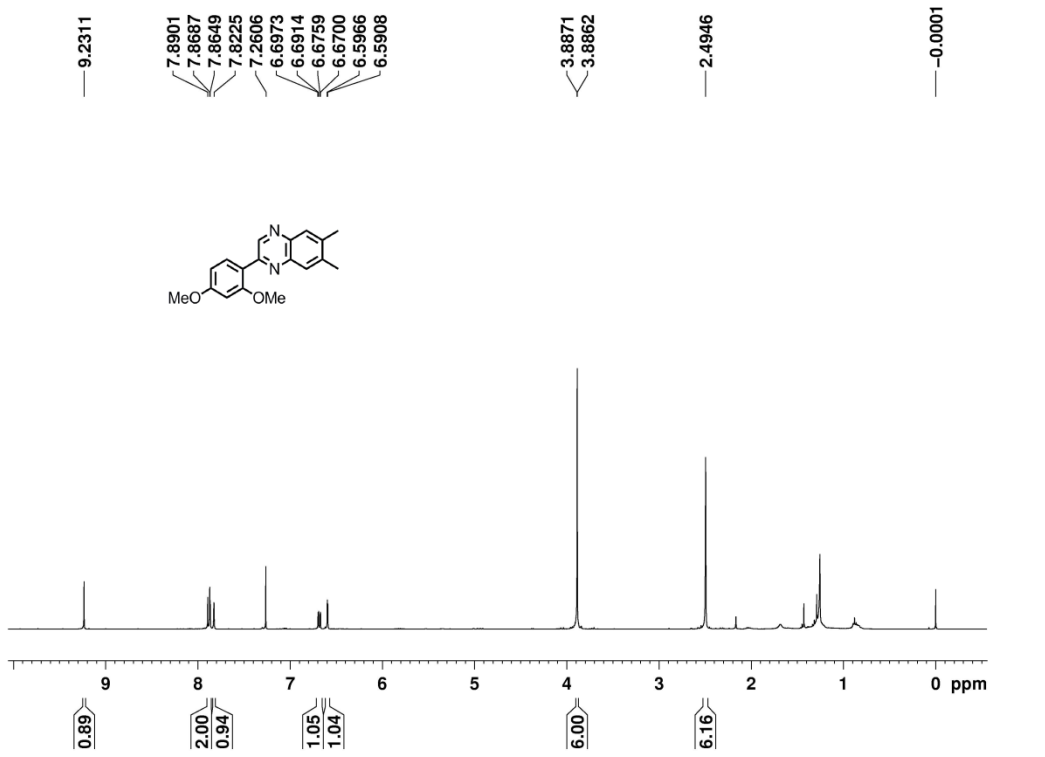
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6.6759
6.6700
6.5966
6.5908
3.8871
3.8862
2.4946
0.0001
MeO
OMe
9
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3
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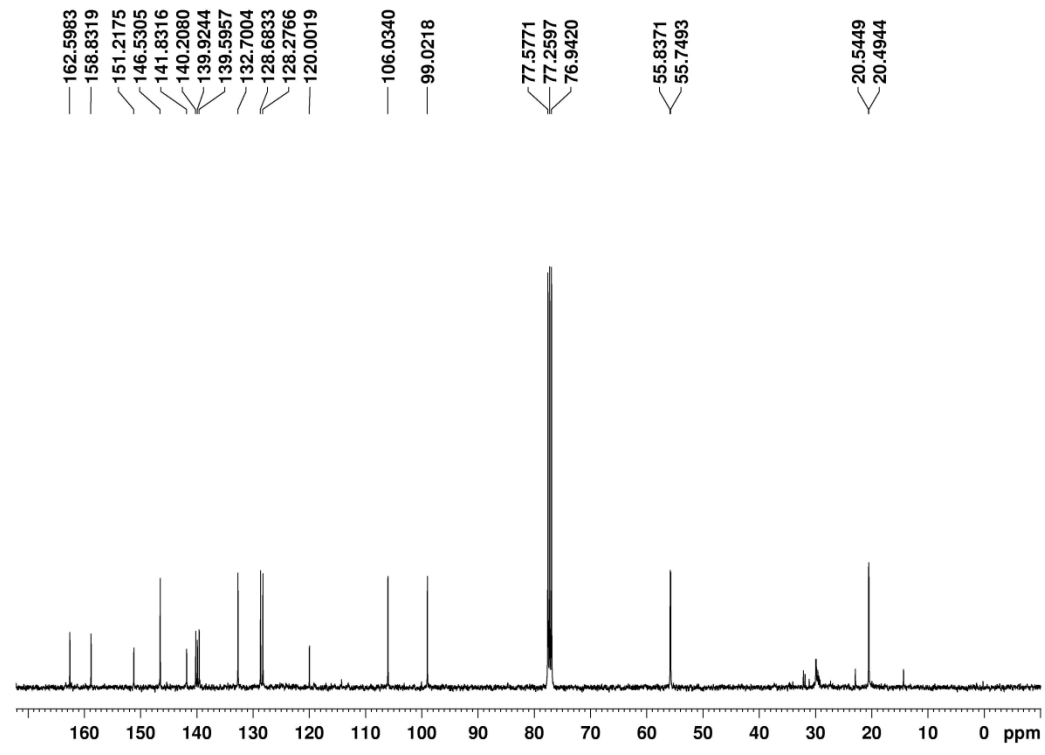
6.16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120.0019
106.0340
99.0218
77.5771
77.2597
76.9420
55.8371
55.7493
20.5449
20.4944
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


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8.5012
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8.2731
8.2658
8.2496
8.2462
7.9185
7.9056
7.9010
7.8974
7.6577
7.6421
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7.5922
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7.5452
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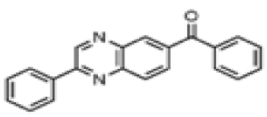
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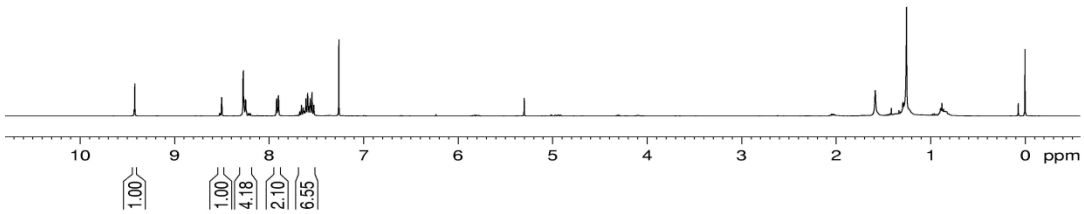
N
O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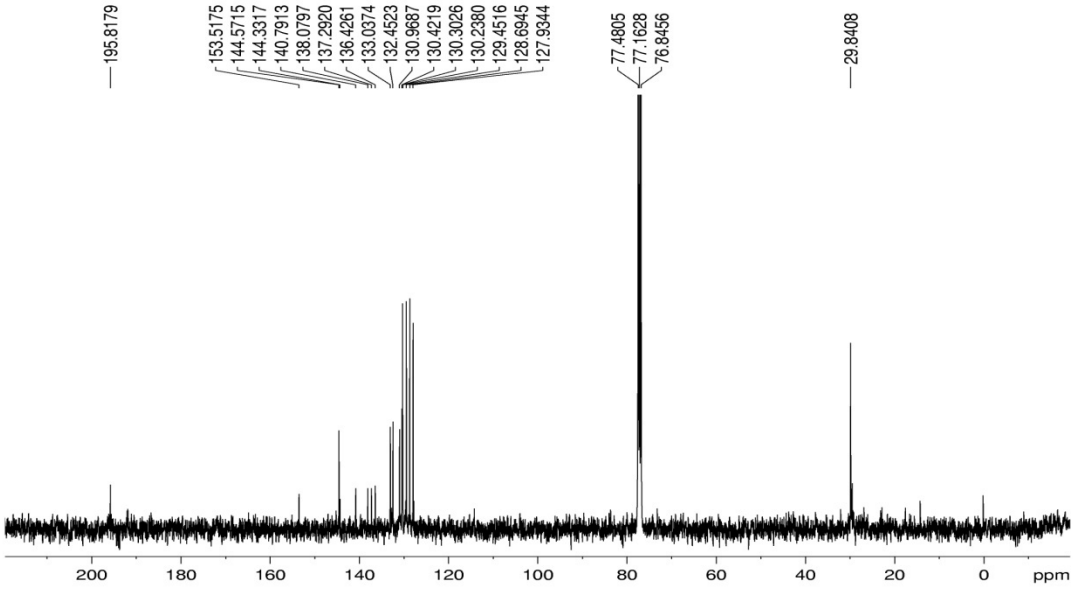
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.00
4.18
2.10
6.55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130.4219
130.3026
130.2380
129.4516
128.6945
127.9344
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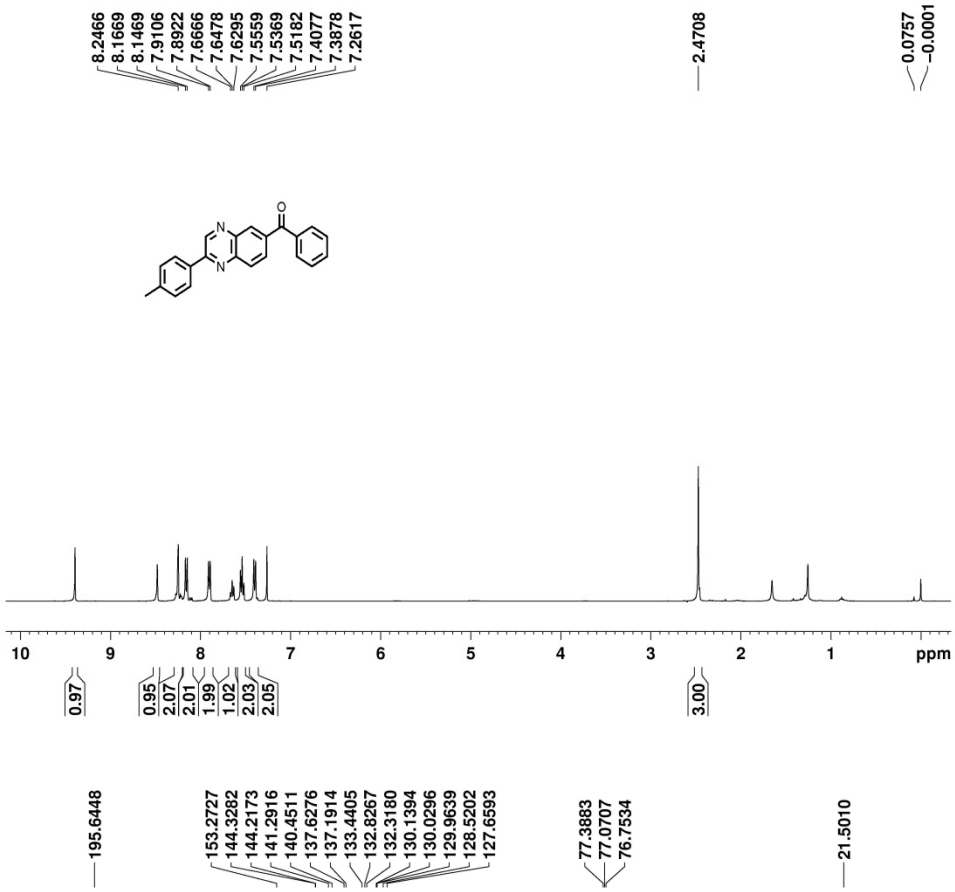
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7.5182
7.4077
7.3878
7.2617
2.4708
0.0757
-0.0001
O
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N
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9
8
7
6
5
4
3
2
1
ppm
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0.95
2.07
2.01
1.99
1.02
2.03
2.05
3.00
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144.2173
141.2916
140.4511
137.6276
137.1914
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132.8267
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77.3883
77.0707
76.7534
21.5010
210
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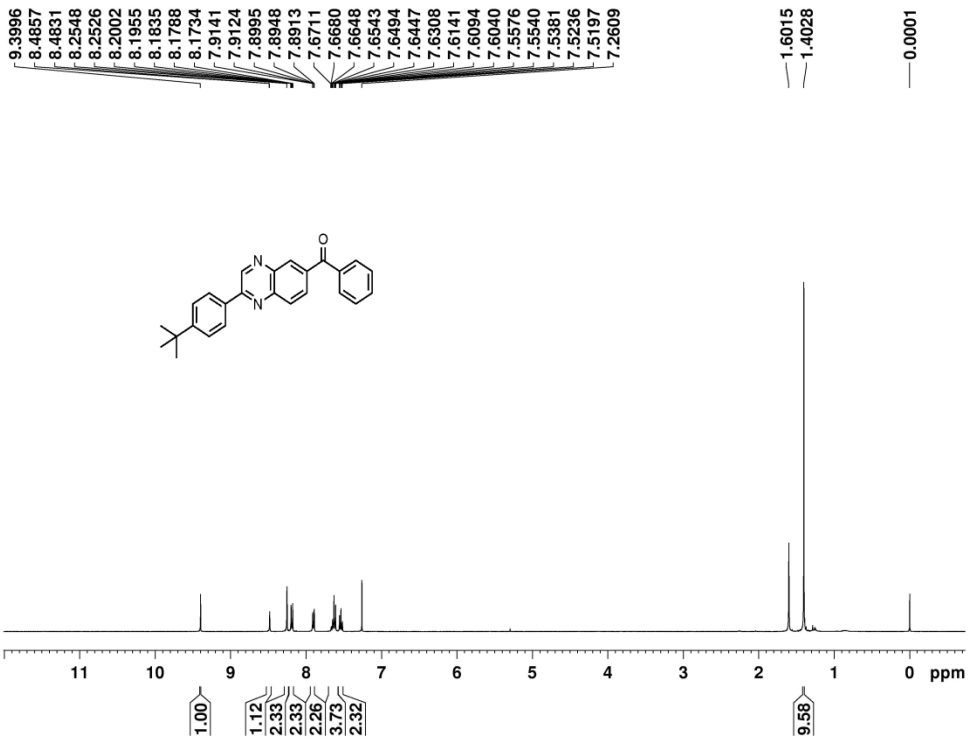
ppm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7.6094
7.6040
7.5576
7.5540
7.5381
7.5236
7.5197
7.2609
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1.4028
0.0001
O
N
N
11
10
9
8
7
6
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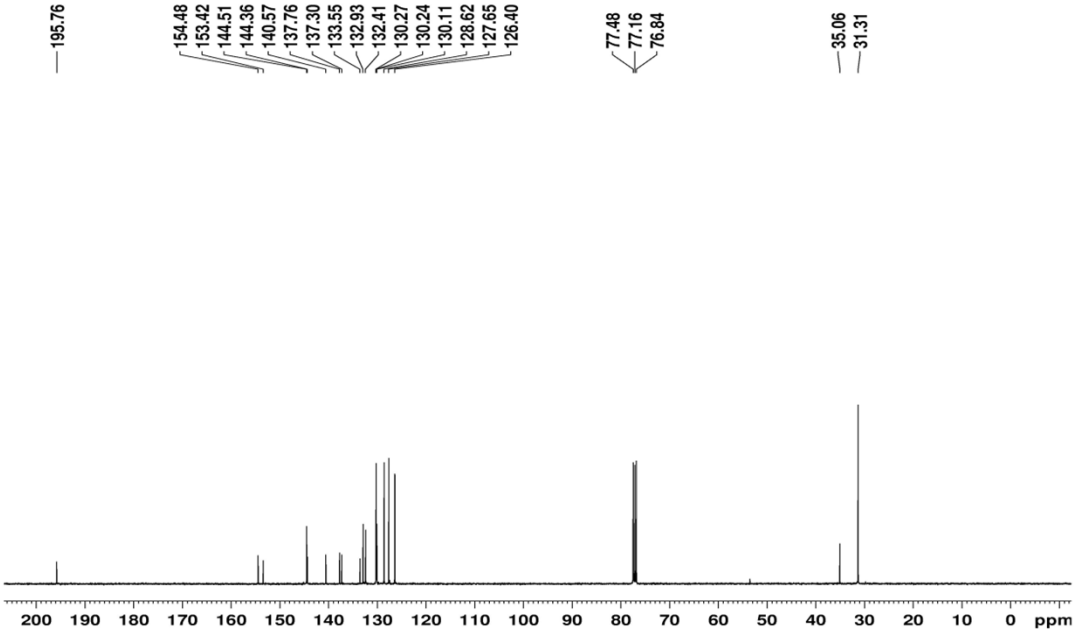
2.32
9.58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140.57
137.76
137.30
133.55
132.93
132.41
130.27
130.24
130.11
128.62
127.65
126.40
77.48
77.16
76.84
35.06
31.31
200
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140
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120
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100
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80
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60
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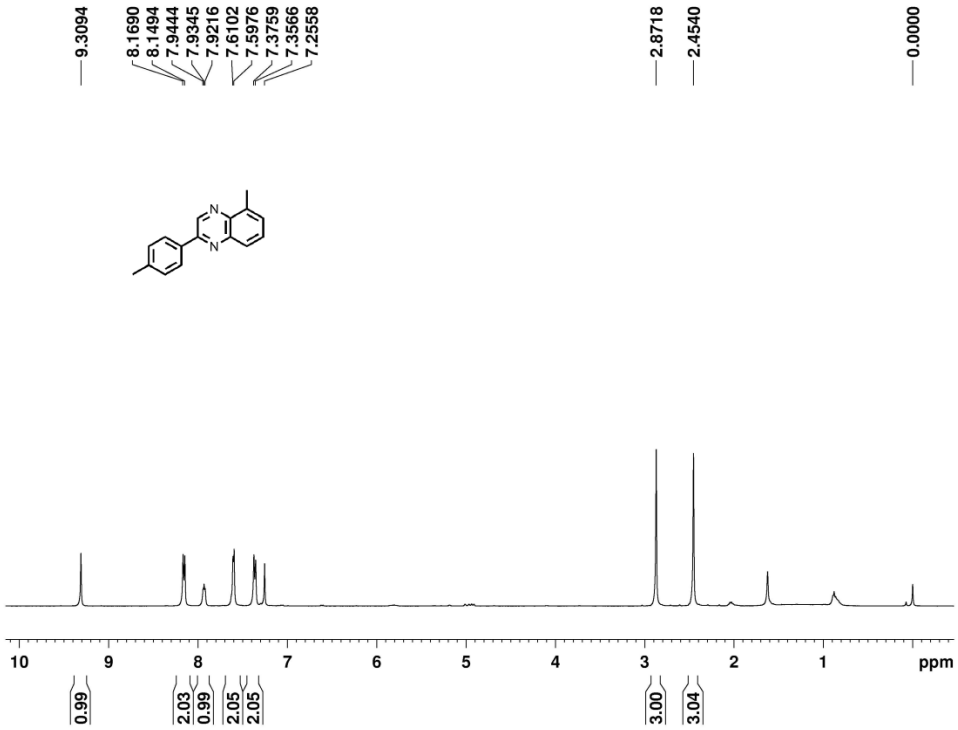
ppm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7.2558
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2.4540
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N
N
10
9
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ppm
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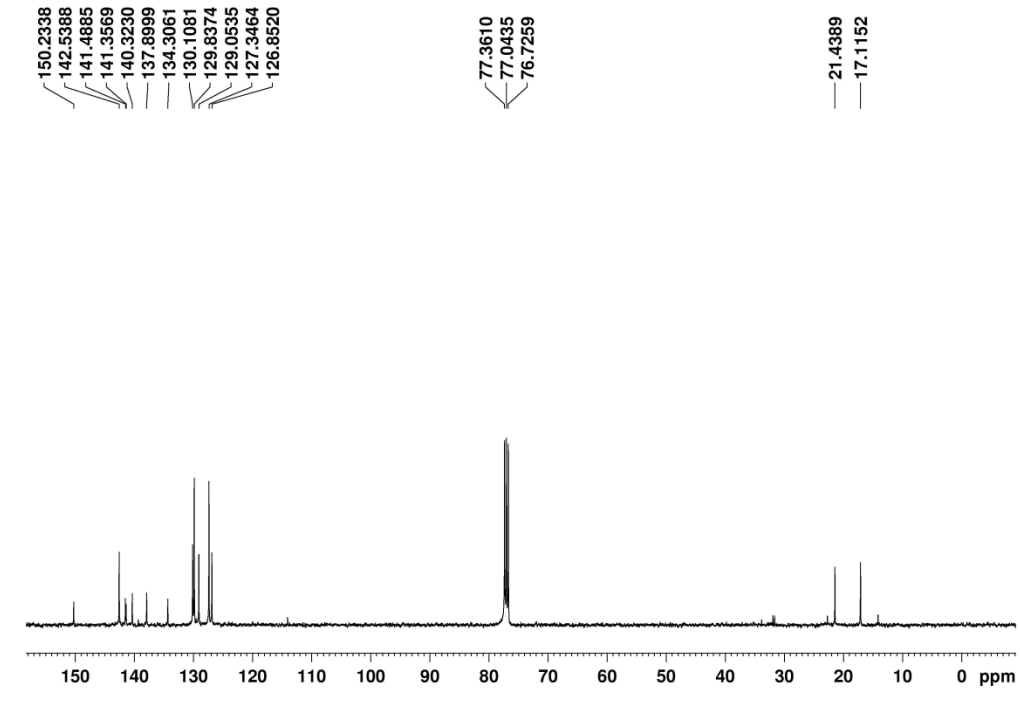
3.04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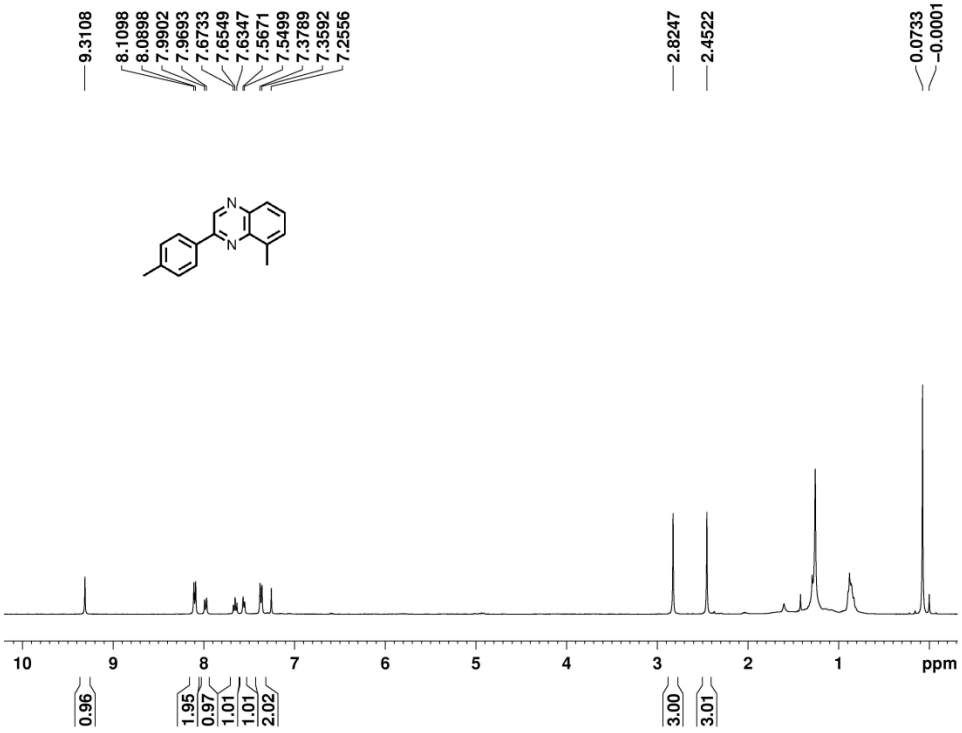
129.8374
129.0535
127.3464
126.8520
77.3610
77.0435
76.7259
21.4389
17.1152
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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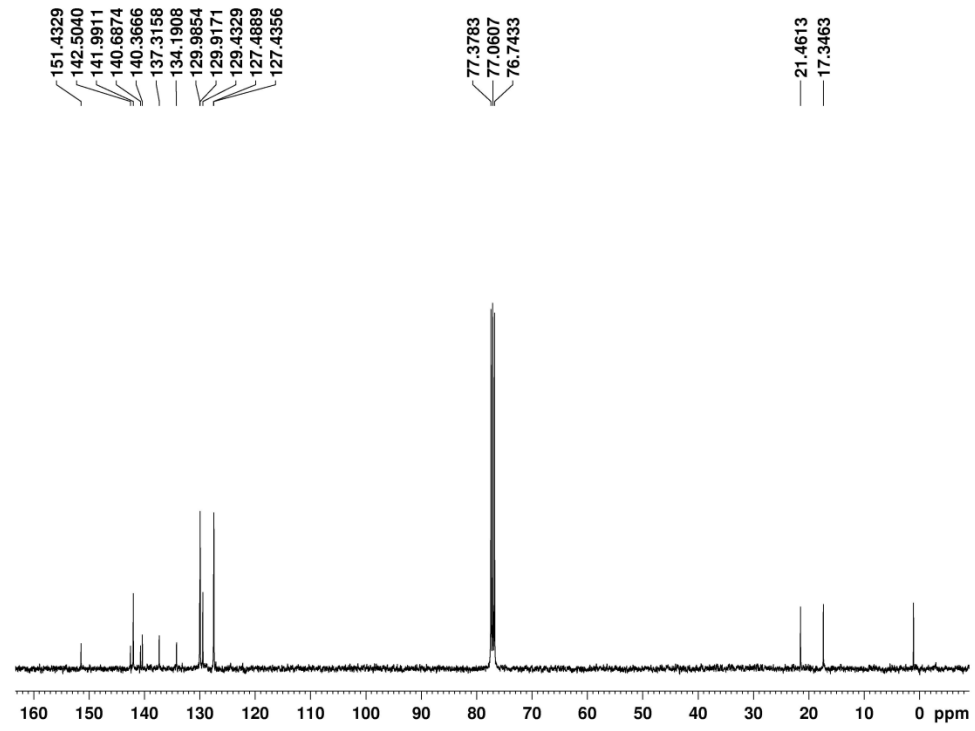
8.1098
8.0898
7.9902
7.9693
7.6733
7.6549
7.6347
7.5671
7.5499
7.3789
7.3592
7.2556
2.8247
2.4522
0.0733
-0.0001
N
N
10
9
8
7
6
5
4
3
2
1
ppm
0.96
1.95
0.97
1.01
1.01
2.02
3.00
3.01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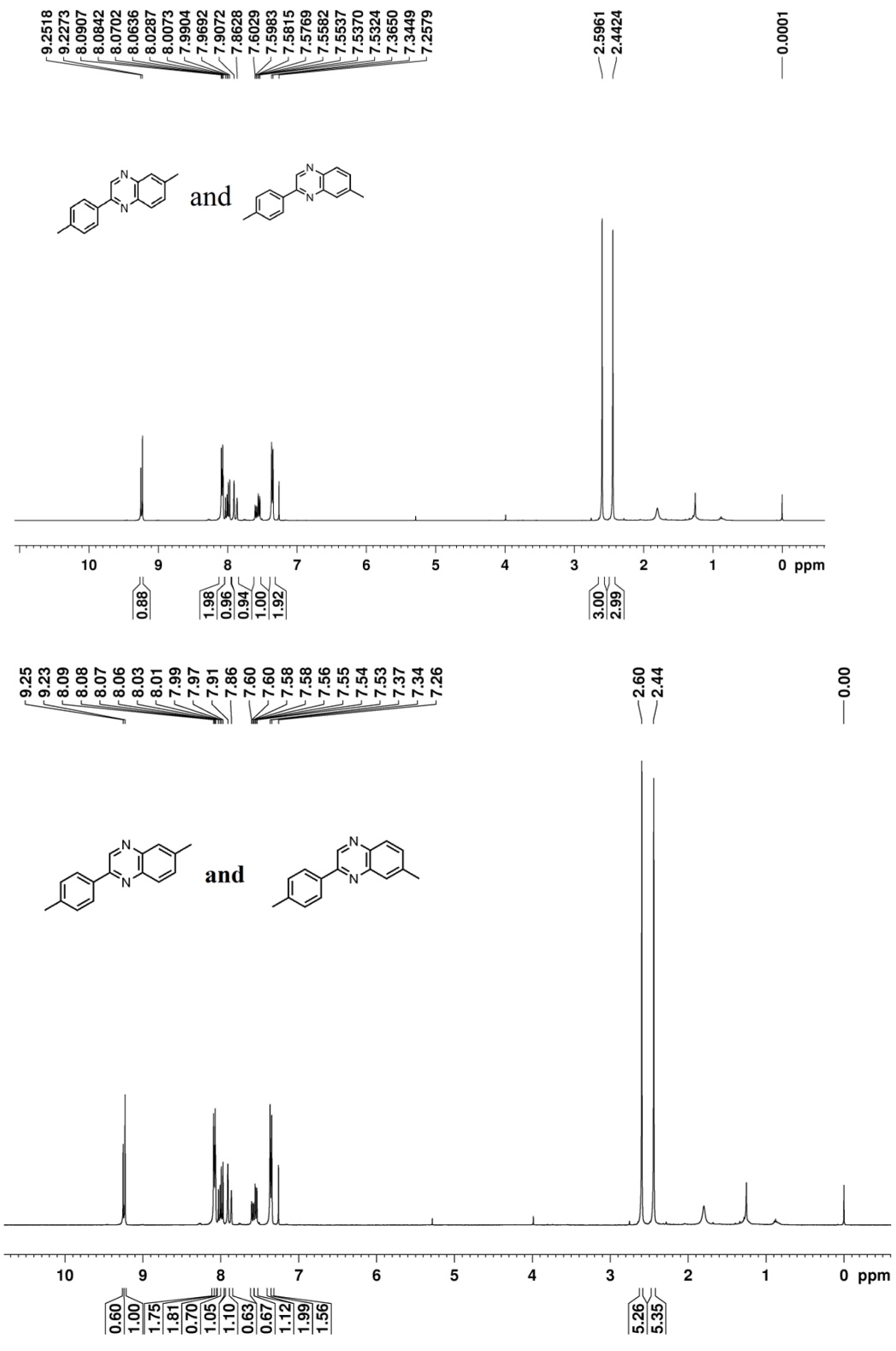
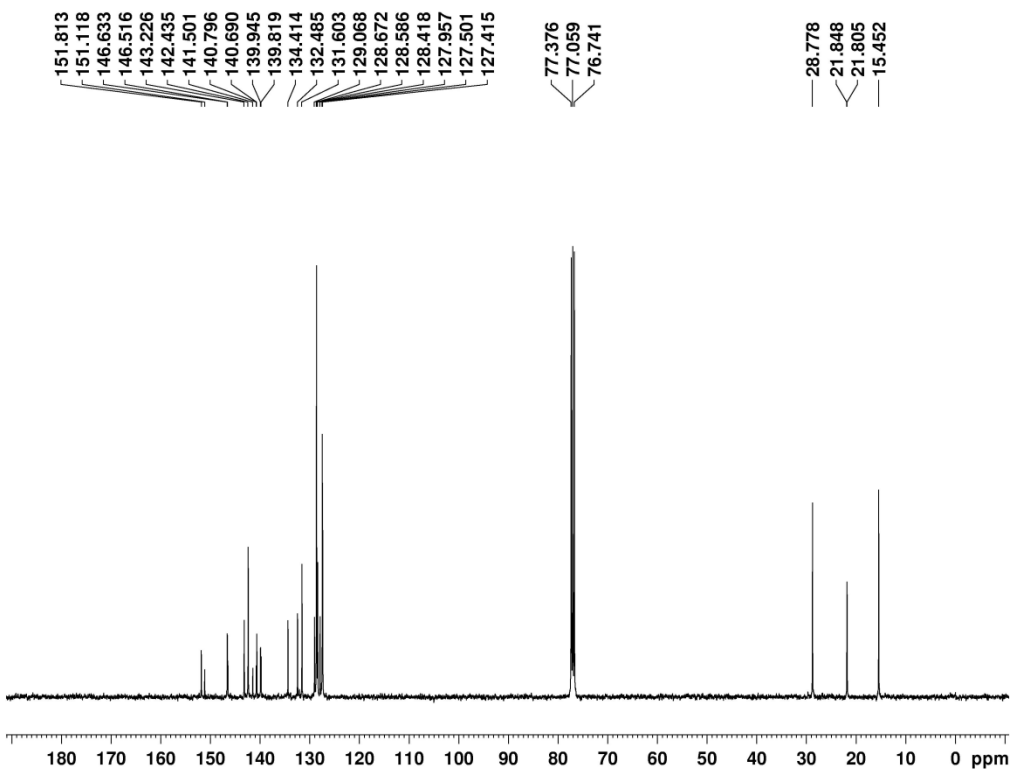
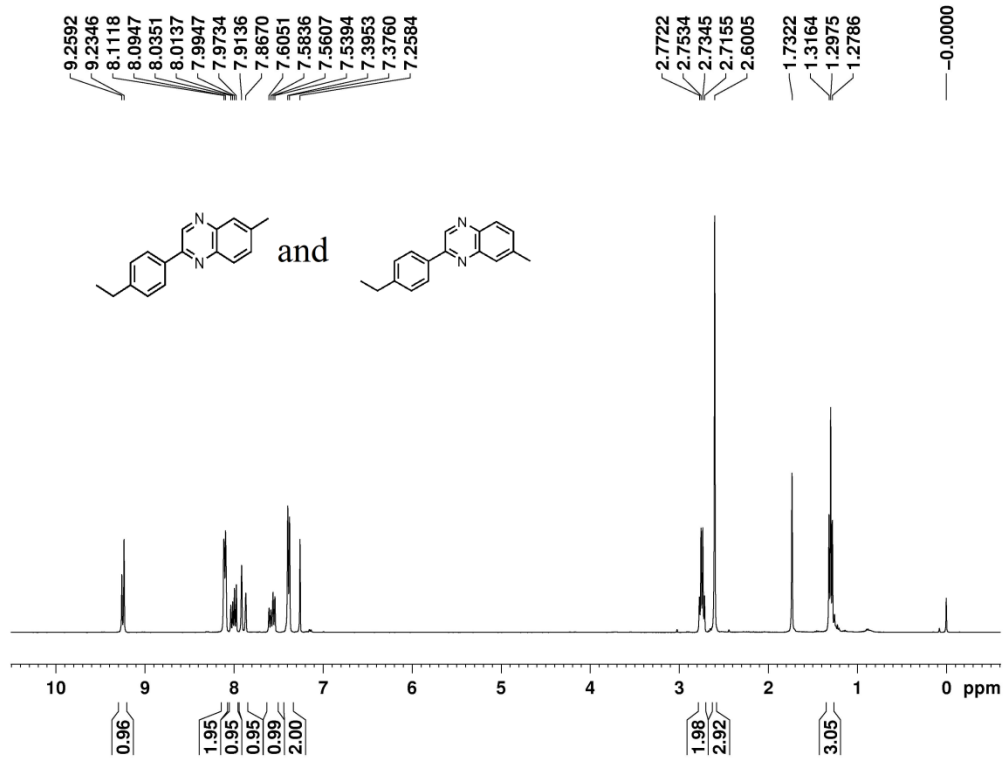
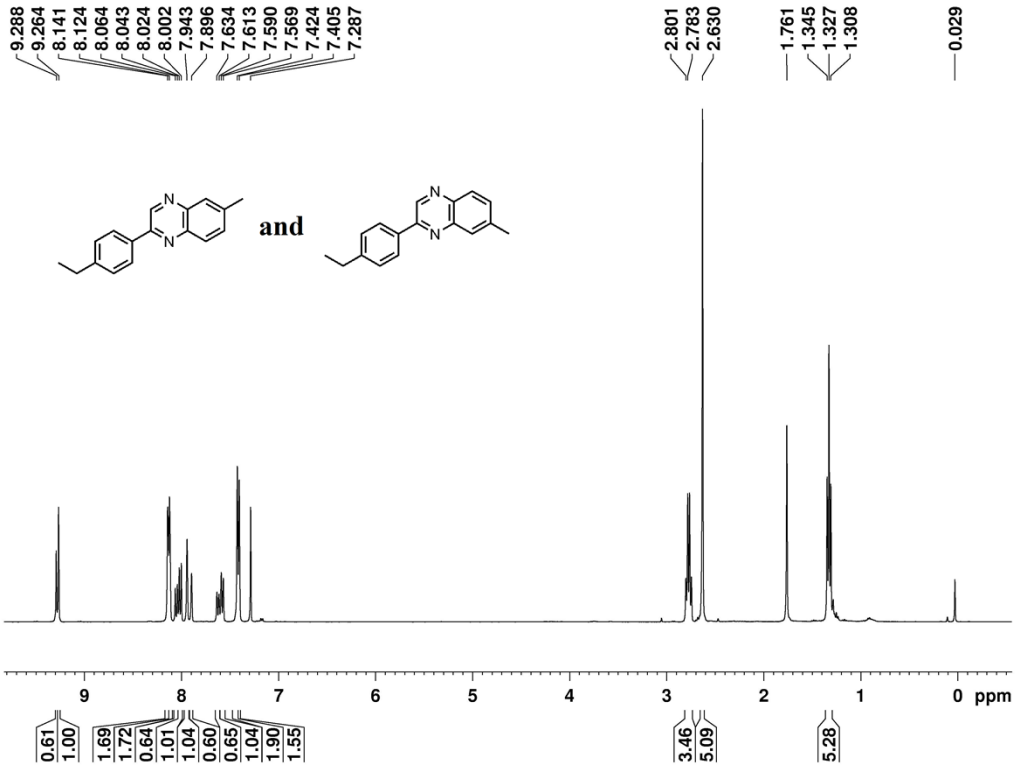
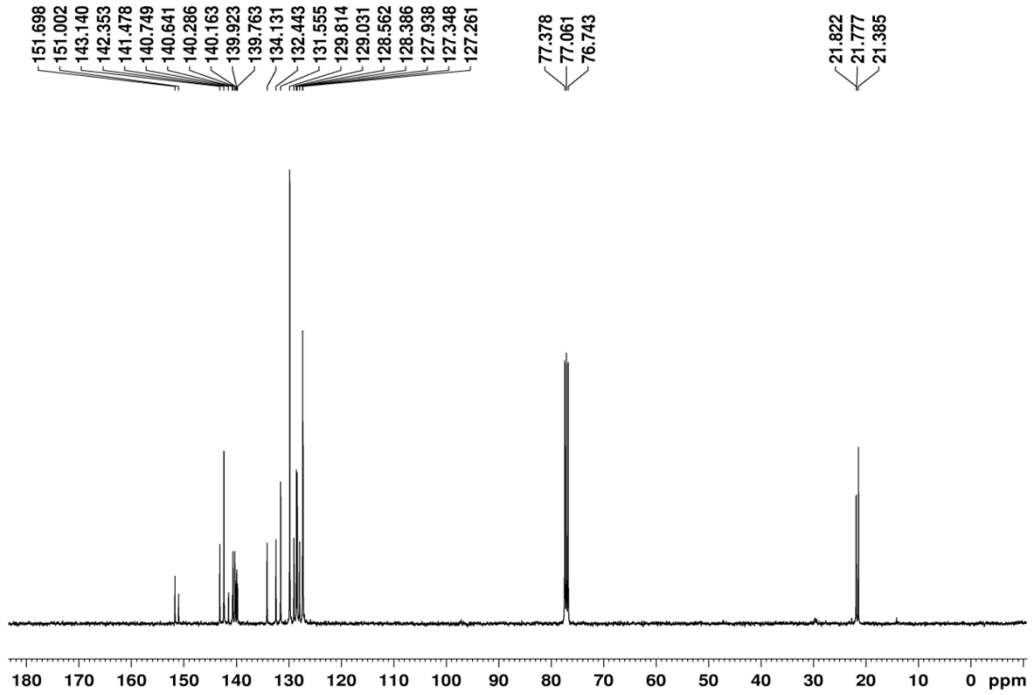
142.5040
141.9911
140.6874
140.3666
137.3158
134.1908
129.9854
129.9171
129.4329
127.4889
127.4356
77.3783
77.0607
76.7433
21.4613
17.3463
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

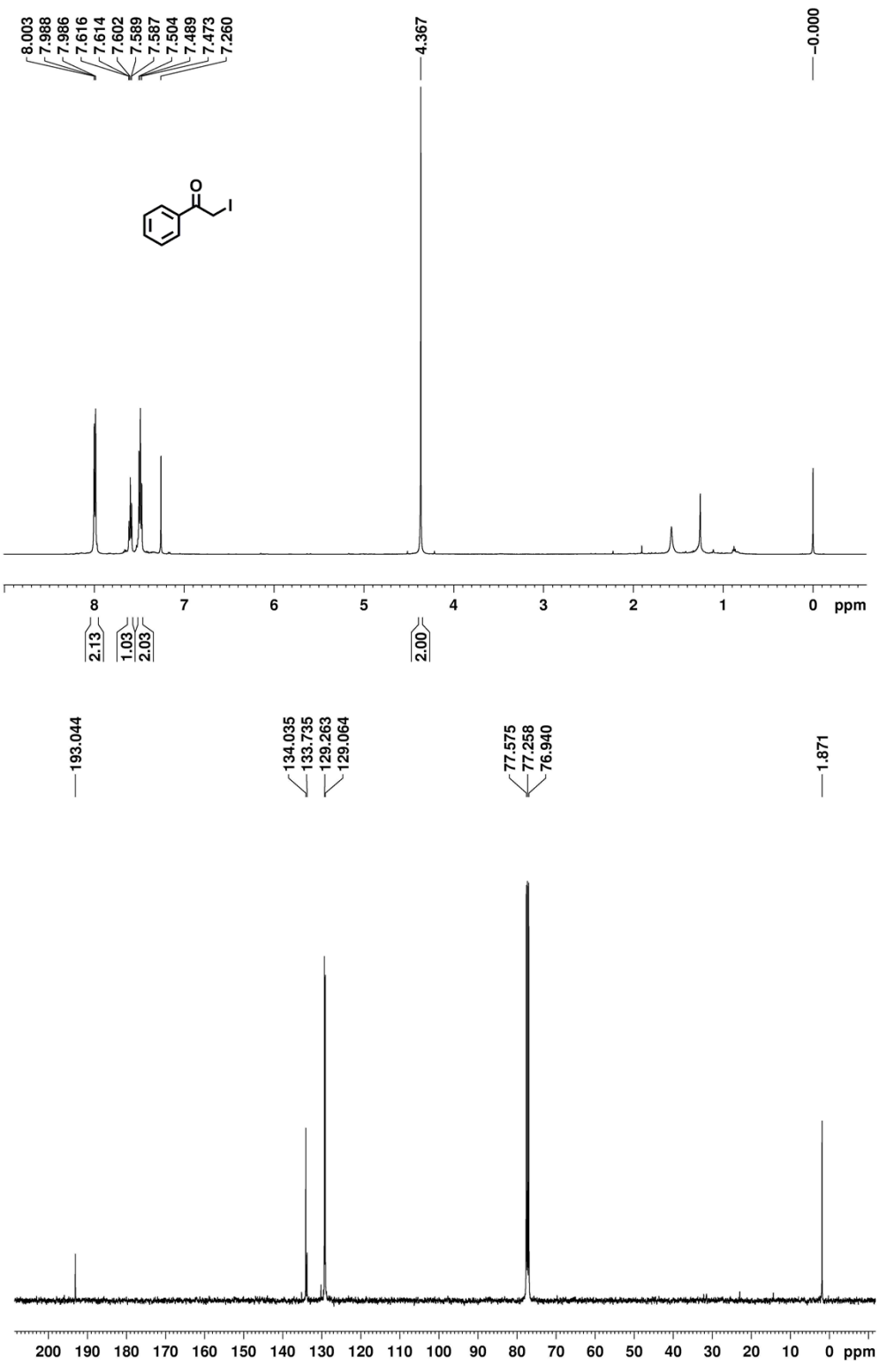

9.2518
9.2273
8.0907
8.0842
8.0702
8.0636
8.0287
8.0073
7.9904
7.9692
7.9072
7.8628
7.6029
7.5983
7.5815
7.5769
7.5582
7.5537
7.5370
7.5324
7.3650
7.3449
7.2579
2.5961
2.4424
0.0001
and
10
9
8
7
6
5
4
3
2
1
0 ppm
0.88
1.98
0.96
0.94
1.00
1.92
3.00
2.99
9.25
9.23
8.09
8.08
8.07
8.06
8.03
8.01
7.99
7.97
7.91
7.86
7.60
7.60
7.58
7.58
7.56
7.55
7.54
7.53
7.37
7.34
7.26
2.60
2.44
0.00
and
10
9
8
7
6
5
4
3
2
1
0 ppm
0.60
1.00
1.75
1.81
0.70
1.05
1.10
0.63
0.67
1.12
1.99
1.56
5.26
5.35


151.813
151.118
146.633
146.516
143.226
142.435
141.501
140.796
140.690
139.945
139.819
134.414
132.485
131.603
129.068
128.672
128.586
128.418
127.957
127.501
127.415
77.376
77.059
76.741
28.778
21.848
21.805
15.452
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


9.2592
9.2346
8.1118
8.0947
8.0351
8.0137
7.9947
7.9734
7.9136
7.8670
7.6051
7.5836
7.5607
7.5394
7.3953
7.3760
7.2584
2.7722
2.7534
2.7345
2.7155
2.6005
1.7322
1.3164
1.2975
1.2786
-0.0000
and
10 9 8 7 6 5 4 3 2 1 0 ppm
0.96
1.95
0.95
0.95
0.99
2.00
1.98
2.92
3.05


9.288
9.264
8.141
8.124
8.064
8.043
8.024
8.002
7.943
7.896
7.634
7.613
7.590
7.569
7.424
7.405
7.287
2.801
2.783
2.630
1.761
1.345
1.327
1.308
0.029
and
9
8
7
6
5
4
3
2
1
0 ppm
0.61
1.00
1.69
1.72
0.64
1.01
1.04
0.60
0.65
1.04
1.90
1.55
3.46
5.09
5.28


151.698
151.002
143.140
142.353
141.478
140.749
140.641
140.286
140.163
139.923
139.763
134.131
132.443
131.555
129.814
129.031
128.562
128.386
127.938
127.348
127.261
77.378
77.061
76.743
21.822
21.777
21.385
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.003
7.988
7.986
7.616
7.614
7.602
7.589
7.587
7.504
7.489
7.473
7.260
4.367
0.000
O
I
8
7
6
5
4
3
2
1
0 ppm
2.13
1.03
2.03
2.00
193.044
134.035
133.735
129.263
129.064
77.575
77.258
76.940
1.871
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm