Supporting Information

I_2- Catalyzed Synthesis of Substituted Imidazoles from vinyl azides and Benzylamines

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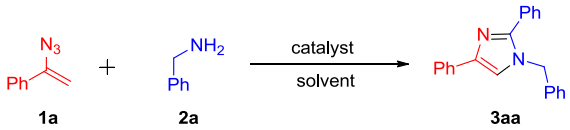
General remark

^{1}H NMR and ^{13}C NMR spectra were recorded on 400MHz and 100MHz in $CDCl_3$. All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All compounds were further characterized by HRMS; copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. Unless otherwise noted, commercially available reagents and solvents were used without further purification.

Table 1. Optimization of reaction condition [a]



1a **2a** **3aa**

entry	catalyst (mol %)	oxidant	solvent	yields(%)[b]
1	I_2(220)		DMF	37
2	KI(10)	TBHP	DMA	34
3	TBAI(10)	TBHP	DMA	26
4	I_2(10)	TBHP	DMF	67
5	I_2(5)	TBHP	DMF	72
6	-	TBHP	DMA	-
7	I_2(5)	TBP	DMF	57
8	I_2(5)	*m*-CPBA	DMF	48
9[c]	I_2(5)	O_2	DMF	26
10	I_2(5)	H_2O_2	DMF	trace
11	I_2(5)	$K_2S_2O_8$	DMF	-
12	I_2(5)	BPO	DMF	43
13	**I_2(5)**	**TBHP**	**DMA**	**76**
14	I_2(5)	TBHP	DMSO	66
15	I_2(5)	TBHP	toluene	60
16	I_2(5)	TBHP	MeCN	64

[a] Reaction conditions: **1a** (0.5 mmol), **2a** (1.5 mmol), solvent (2 mL). [b] Yields of isolated products. [c] The reaction was carried out under O_2 (1 atm). Entry in bold highlights optimized reaction conditions, and the reaction time was monitored by TLC. DMF = *N*,*N*-dimethyl formamide, DMSO = dimethyl sulfoxide, DMA = 2-(dimethylamino)acetaldehyde, TBAI = tetrabutyl ammonium iodide, TBHP = tertbutyl hydroperoxide (5.0-6.0 M in decane), TBP = *di*-tertbutyl peroxide, BPO = benzoyl peroxide.

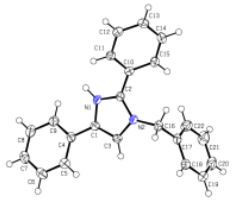
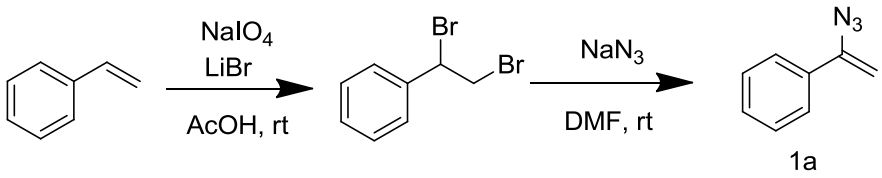


Figure 1. The X-ray structure of **3aa**

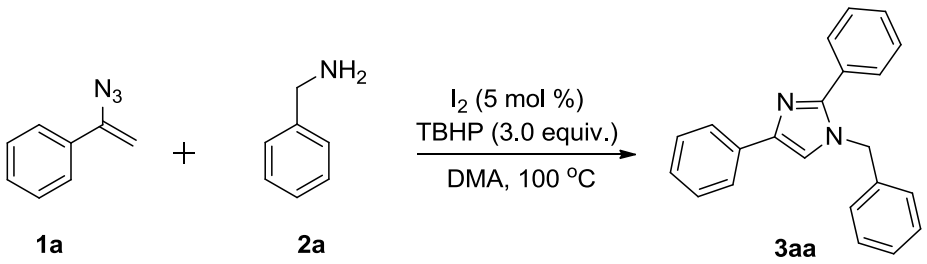
Synthesis of vinyl azides[1] :



The procedure for dibromination of styrene was slightly modified from Sudalai's method. To a solution of styrene (1.00g, 9.6 mmol) and LiBr (1.82g, 21.2 mmol) in acetic acid (10 mL) was added $NaIO_4$ (1.02g, 4.8 mmol) portionwise during 15 minutes. The stirring was continued at room temperature for 5 h. The reaction mixture was diluted with water and extracted with CH_2Cl_2. The organic layers were washed with saturated aq. $NaHCO_3$, $Na_2S_2O_3$, and brine. It was dried over anhydrous $MgSO_4$ and concentrated under reduced pressure to give dibromide (in quantitative yield), which can be used without further purification.

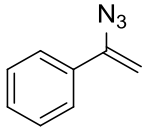
To a solution of dibromide in dry DMF (25 mL) was added NaN_3 (1.87g, 28.8 mmol). The mixture was stirred for 24 h at room temperature, then diluted with water and extracted with diethyl ether. The combined organic layers were washed three times with water, dried with $MgSO_4$. After evaporation of solvents, the crude residue was purified by flash column chromatography (silica gel; hexane : ethyl acetate = 99 : 1) to give vinyl azide 1a (1.27g, 8.8 mmol) in 92% yield.

General procedure for synthesis of substituted imidazoles from vinyl azides and benzylamines :



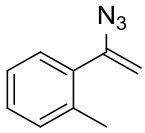
The (1-azidovinyl)benzene (**1a**, 0.5 mmol), phenylmethanamine (**2a**, 1.5 mmol), I_2 (0.025 mmol) and TBHP (1.5 mmol) were mixed in DMA (2 mL) and this mixture was at 100 ^oC for 10 h. The reaction mixture was cooled down to room temperature and then extracted with ethyl acetate (15 ml×3). The combined organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/EtOAc (10:1) to afford the desired imidazoles (**3aa**).

(1-azidovinyl)benzene (1a):



Yellow liquid. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.56-7.54 (m, 2 H), 7.35-7.34 (m, 3 H), 5.43-5.42 (d, *J* = 2.4 Hz, 1 H), 4.95-4.94 (d, *J* = 2.4 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 145.05, 134.29, 129.15, 128.48, 125.59, 98.01.

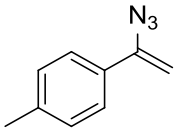
1-(1-azidovinyl)-2-methylbenzene (1b):



Yellow solid, melting point: 133-135 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.30-7.18 (m, 4 H), 5.05 (d, *J* = 0.4 Hz, 1 H), 4.74 (d, *J* = 0.4 Hz, 1 H), 2.39 (s, 3 H); ^{13}C

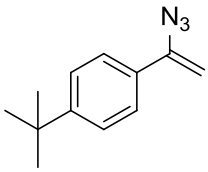
NMR (100 MHz, $CDCl_3$, ppm): δ = 145.44, 136.02, 134.95, 130.43, 129.24, 129.11, 125.90, 102.64, 19.69.

1-(1-azidovinyl)-4-methylbenzene (1c):



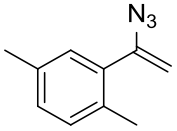
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.44-7.42 (d, *J* = 8 Hz, 2 H), 7.15-7.13 (d, *J* = 8 Hz, 2 H), 5.36 (d, *J* = 2.4 Hz, 1 H), 4.89-4.88 (d, *J* = 2.4 Hz, 1 H), 2.34 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 145.06, 139.17, 131.55, 129.17, 125.50, 97.18, 21.25.

1-(1-azidovinyl)-4-(tert-butyl)benzene (1d):



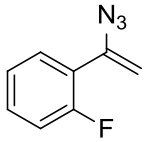
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.54-7.52 (d, *J* = 8 Hz, 2 H), 7.42-7.40 (d, *J* = 8 Hz, 2 H) 5.43 (d, *J* = 2.4 Hz, 1 H), 4.95-4.94 (d, *J* = 2.4 Hz, 1 H), 1.35 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.36, 144.98, 131.51, 125.42, 125.33, 97.29, 34.70, 31.26.

2-(1-azidovinyl)-1,4-dimethylbenzene (1e):



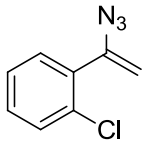
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.12-7.08 (m, 3 H), 5.03-5.02 (d, *J* = 0.8 Hz, 1 H), 4.71 (d, *J* = 0.8 Hz, 1 H), 2.34 (s, 3 H), 2.32 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 145.57, 135.43, 134.74, 132.80, 130.35, 129.84, 129.82, 102.44, 20.87, 19.21.

1-(1-azidovinyl)-2-fluorobenzene (1f):



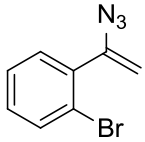
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.50-7.46 (m, 1 H), 7.34-7.29 (m, 1 H), 7.16-7.07 (m, 2 H), 5.42-5.41 (m, 1 H), 5.18-5.17 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.01 (d, *J* = 250 Hz), 139.68 (d, *J* = 3 Hz), 130.56 (d, *J* = 9 Hz), 129.28 (d, *J* = 2 Hz), 124.16 (d, *J* = 4 Hz), 122.38 (d, *J* = 11 Hz), 116.19 (d, *J* = 22 Hz), 103.59 (d, *J* = 9 Hz).

1-(1-azidovinyl)-2-chlorobenzene (1g):



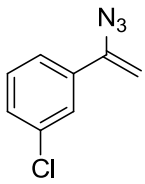
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.44-7.42 (m, 1 H), 7.38-7.25 (m, 3 H), 5.13 (d, *J* = 1.2 Hz, 1 H), 4.90-4.89 (d, *J* = 1.2 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.16, 134.14, 132.72, 130.89, 130.39, 129.99, 126.95, 104.11.

1-(1-azidovinyl)-2-bromobenzene (1h):



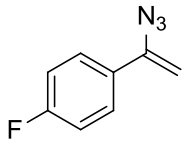
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.63-7.61 (m, 1 H),7.37-7.31 (m, 2 H), 7.27-7.22 (m, 1 H), 5.11 (d, *J* = 1.2 Hz, 1 H), 4.85 (d, *J* = 1.2 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.55, 136.29, 133.15, 131.00, 130.56, 127.54, 122.27, 103.95..

1-(1-azidovinyl)-3-chlorobenzene (1i):



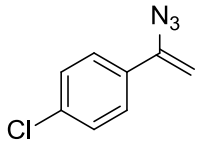
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.54 (m, 1 H), 7.45-7.42 (m, 1 H), 7.32-7.25 (m, 2 H), 5.46-5.45 (d, *J* = 2.4 Hz, 1 H), 4.99-4.98 (d, *J* = 2.4 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.84, 136.03, 134.53, 129.70, 129.12, 125.76, 123.65, 98.81.

1-(1-azidovinyl)-4-fluorobenzene (1j):



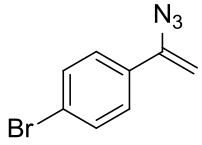
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.54-7.49 (m, 2 H), 7.05-6.99 (m, 2 H), 5.36-5.35 (d, *J* = 2.4 Hz, 1 H), 4.92-4.91 (d, *J* = 2.4 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.28 (d, *J* = 247 Hz), 144.16, 130.46 (d, *J* = 3 Hz), 127.45 (d, *J* = 8 Hz), 115.29 (d, *J* = 22 Hz), 97.57 (d, *J* = 2 Hz).

1-(1-azidovinyl)-4-chlorobenzene (1k):



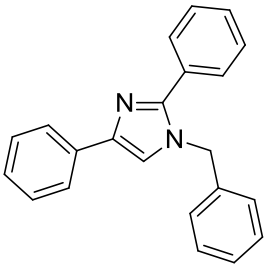
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.48-7.45 (m, 2 H), 7.31-7.23 (m, 2 H), 5.41 (d, *J* = 2.4 Hz, 1 H), 4.95-4.94 (d, *J* = 2.4 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.07, 135.06, 132.73, 128.64, 126.85, 98.14.

1-(1-azidovinyl)-4-bromobenzene (1l):



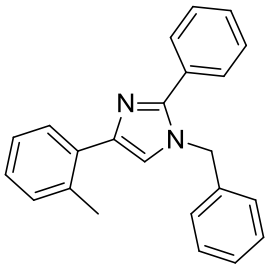
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.46-7.42 (m, 2 H), 7.40-7.36 (m, 2 H), 5.41-5.40 (d, *J* = 2.4 Hz, 1 H), 4.94-4.93 (d, *J* = 2.4 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.12, 133.17, 131.61, 127.12, 123.36, 98.21.

1-benzyl-2,4-diphenyl-1H-imidazole(3aa)[2]:



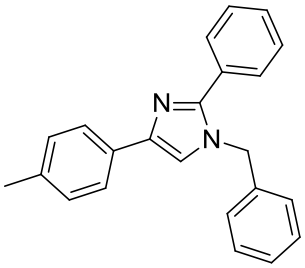
Yellow Solid, mp: 123-124 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.62-7.60 (m, 2 H), 7.44-7.40 (m, 3 H), 7.38-7.29 (m, 5 H), 7.24-7.21 (m, 2 H), 7.14-7.12 (m, 2 H), 5.21 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.79, 141.69, 137.02, 134.22, 130.62, 129.19, 129.17, 128.79, 128.69, 128.14, 126.96, 126.82, 125.08, 116.99, 50.65. HRMS calcd for $C_{22}H_{19}N_2$ $[M+H]^+$ 311.1543; found: 311.1547.

1-benzyl-2-phenyl-4-(o-tolyl)-1H-imidazole (3ba)[3]:



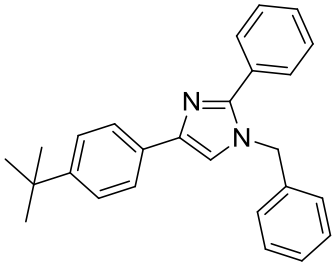
Yellow Solid, mp: 112 – 114 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.97-7.95 (m, 1 H), 7.64-7.60 (m, 2 H), 7.43-7.31 (m, 6 H), 7.23-7.12 (m, 6 H), 5.28 (s, 2 H), 2.50 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.73, 140.86, 137.08, 134.84, 133.44, 130.69, 130.51, 129.02, 129.00, 128.91, 128.60, 128.57, 127.92, 126.78, 126.50, 125.93, 119.62, 50.44, 21.92. HRMS calcd for $C_{23}H_{21}N_2$ $[M+H]^+$ 325.1699; found: 325.1693.

1- benzyl-2-phenyl-4-(p-tolyl)-1H-imidazole (3ca)[2]:



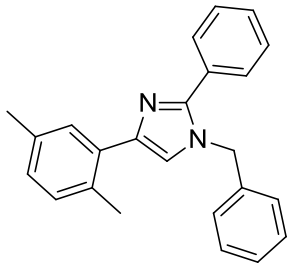
Yellow Solid, mp: 138 - 140^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.73-7.71 (m, 2 H), 7.61-7.59 (m, 2 H), 7.43-7.39 (m, 3 H), 7.37-7.28 (m, 3 H), 7.20-7.16 (m, 3 H), 7.13-7.11 (m, 2 H), 5.19 (s, 2 H), 2.34 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.49, 141.65, 136.97, 136.45, 131.29, 130.56, 129.26, 129.06, 129.02, 128.96, 128.64, 127.97, 126.69, 124.87, 116.44, 50.47, 21.27. HRMS calcd for $C_{23}H_{21}N_2$ $[M+H]^+$ 325.1699; found: 325.1694.

1-benzyl-4-(4-(tert-butyl)phenyl)-2-phenyl-1H-imidazole (3da):



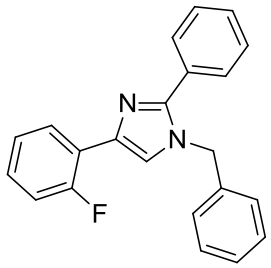
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.77-7.75 (m, 2 H), 7.61-7.59 (m, 2 H), 7.43-7.38 (m, 5 H), 7.36-7.28 (m, 3 H), 7.22 (s, 1 H), 7.12-7.10 (m, 2 H), 5.21 (s, 2 H), 1.33 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 149.78, 148.51, 141.61, 137.04, 131.29, 130.58, 129.06, 129.00, 128.94, 128.63, 127.93, 126.60, 125.45, 124.67, 50.44, 34.56, 31.39. HRMS calcd for $C_{26}H_{27}N_2$ $[M+H]^+$ 367.2169; found: 367.2167.

1-benzyl-4-(2,5-dimethylphenyl)-2-phenyl-1H-imidazole (3ea):



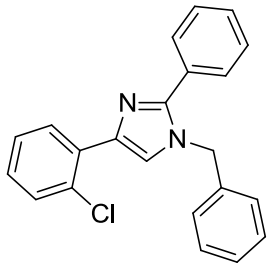
Yellow Solid, mp: 70-72^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82 (s, 1 H), 7.64-7.60 (m, 2 H), 7.44-7.40 (m, 3 H), 7.38-7.24 (m, 3 H), 7.14-7.10 (m, 4 H), 7.00-6.98 (m, 1 H), 5.26 (s, 2 H), 2.44 (s, 3 H), 2.35 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.72, 140.83, 137.12, 125.38, 133.11, 131.62, 130.68, 130.53, 129.05, 129.02, 128.92, 128.61, 127.91, 127.55, 126.49, 119.64, 50.43, 21.51, 20.99. HRMS calcd for $C_{24}H_{23}N_2$ $[M+H]^+$ 339.1856; found: 339.1855.

1-benzyl-4-(2-fluorophenyl)-2-phenyl-1H-imidazole (3fa):



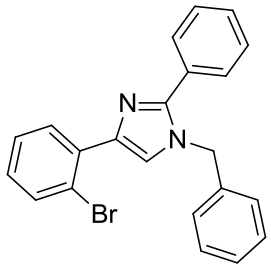
Yellow solid, mp: 68-70 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.32-8.27 (m, 1 H), 7.61-7.59 (m, 2 H), 7.48-7.47 (d, *J* = 4 Hz, 1 H), 7.42-7.40 (m, 3 H), 7.36-7.27 (m, 3 H), 7.22-7.16 (m, 2 H), 7.13-7.05 (m, 3 H), 5.23 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.74 (d, *J* = 246 Hz), 148.10, 136.87, 135.01 (d, *J* = 2 Hz), 130.36, 129.11, 129.05 (d, *J* = 1 Hz), 128.70, 127.98, 127.75, 127.71, 127.66, 127.57, 126.58, 124.32 (d, *J* = 4 Hz), 121.89 (d, *J* = 13 Hz), 121.21 (d, *J* = 14 Hz), 115.40 (d, *J* = 22 Hz), 50.51. HRMS calcd for $C_{22}H_{18}FN_2$ $[M+H]^+$ 329.1449; found: 329.1445.

1-benzyl-4-(2-chlorophenyl)-2-phenyl-1H-imidazole (3ga):



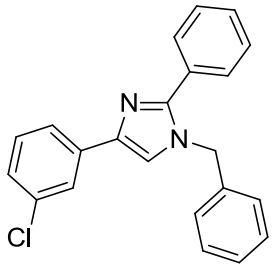
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.32-8.30 (m, 1 H), 7.75 (s, 1 H), 7.61-7.59 (m, 2 H), 7.43-7.38 (m, 4 H), 7.36-7.29 (m, 4 H), 7.19-7.13 (m, 3 H), 5.27 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.75, 137.51, 136.86, 132.39, 130.79, 130.30, 130.14, 129.71, 129.04, 128.66, 127.97, 127.49, 126.90, 126.52, 121.63, 50.56. HRMS calcd for $C_{22}H_{18}ClN_2$ $[M+H]^+$ 345.1153; found: 345.1147, 347.1114.

1-benzyl-4-(2-bromophenyl)-2-phenyl-1H-imidazole (3ha):



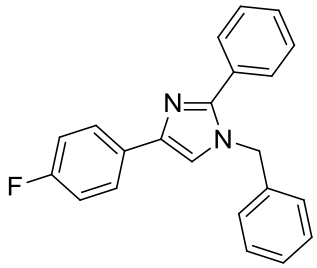
Yellow solid, mp: 106-108 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.21-8.19 (dd, *J* 1= 8 Hz, J2 = 1.6 Hz, 1 H), 7.79 (s, 1 H), 7.62-7.59 (m, 3 H), 7.42-7.40 (m, 3 H), 7.38-7.29 (m, 4 H), 7.16-7.14 (d, *J* = 8 Hz, 2 H), 7.11-7.07 (m, 1 H), 5.27 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.73, 138.78, 136.87, 134.49, 133.52, 130.51, 130.29, 129.04, 129.03, 128.64, 127.96, 127.86, 127.44, 126.53, 121.25, 120.70, 50.57. HRMS calcd for $C_{22}H_{18}BrN_2$ $[M+H]^+$ 389.0648; found: 389.0641, 391.0619.

1-benzyl-4-(3-chlorophenyl)-2-phenyl-1H-imidazole (3ia):



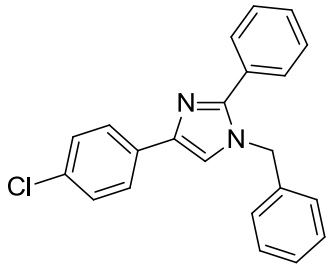
Yellow solid, mp: 96-97 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.84 (s, 1 H), 7.70-7.68 (d, *J* = 8 Hz, 1 H), 7.62-7.60 (m, 2 H), 7.44-7.42 (m, 3 H), 7.38-7.32 (m, 3 H), 7.30-7.26 (m, 2 H), 7.20-7.18 (d, *J* = 8 Hz, 1 H), 7.14-7.13 (m, 2 H), 5.22 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.88, 140.24, 136.65, 135.98, 134.57, 130.25, 129.82, 129.20, 129.10, 129.03, 128.74, 128.44, 128.12, 126.74, 124.98, 122.97, 117.41, 50.59. HRMS calcd for $C_{22}H_{18}ClN_2$ $[M+H]^+$345.1153; found: 345.1146, 347.1114.

1-benzyl-4-(4-fluorophenyl)-2-phenyl-1H-imidazole (3ja)[2]:



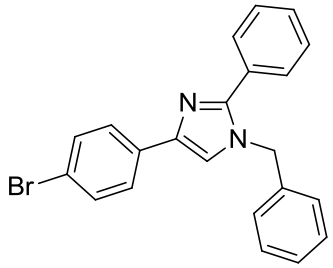
Yellow Solid, mp: 106-107 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.81-7.77 (m, 2 H), 7.62-7.59 (m, 2 H), 7.45-7.41 (m, 3 H), 7.38-7.31 (m, 3 H), 7.19 (s, 1 H), 7.15-7.13 (m, 2 H), 7.07-7.02 (m, 2 H), 5.21 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 162.02 (d, *J* = 243 Hz), 148.70, 140.76, 136.79, 130.38 (d, *J* = 4 Hz), 129.04 (d, *J* = 3 Hz), 128.68, 128.04, 126.71, 126.53 (d, *J* = 8 Hz), 116.42, 115.38 (d, *J* = 21 Hz), 50.54. HRMS calcd for $C_{22}H_{18}FN_2$ $[M+H]^+$ 329.1449; found: 329.1448.

1-benzyl-4-(4-chlorophenyl)-2-phenyl-1H-imidazole (3ka)[2]:



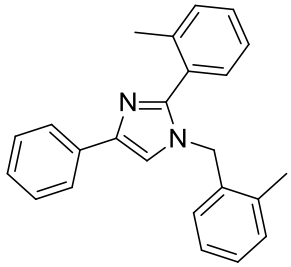
Yellow Solid, mp: 126-128 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.76-7.74 (m, 2 H), 7.61-7.58 (m, 2 H), 7.42-7.41 (m, 3 H), 7.38-7.31 (m, 5 H), 7.22 (s, 1 H), 7.13-7.12 (m, 2 H), 5.20 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.82, 140.49, 136.70, 132.66, 132.31, 130.29, 129.16, 129.08, 129.02, 128.72, 128.68, 128.10, 126.73, 126.19, 116.98, 50.57. HRMS calcd for $C_{22}H_{18}ClN_2$ $[M+H]^+$ 345.1152; found: 345.1146, 347.1113.

1-benzyl-4-(4-bromophenyl)-2-phenyl-1H-imidazole (3la)[2]:



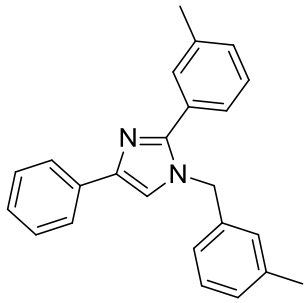
Yellow Solid, mp: 162-164 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.71-7.68 (m, 2 H), 7.61-7.57 (m, 2 H), 7.49-7.45 (m, 2 H), 7.44-7.40 (m, 3 H), 7.38-7.29 (m, 3 H), 7.23 (s, 1 H), 7.14-7.12 (m, 2 H), 5.20 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.84, 140.50, 136.68, 133.11, 131.60, 130.28, 129.16, 129.08, 129.02, 128.71, 128.10, 126.74, 126.52, 120.43, 117.02, 50.58. HRMS calcd for $C_{22}H_{18}BrN_2$ $[M+H]^+$ 389.0648; found: 389.0643, 391.0618.

1-(2-methylbenzyl)-4-phenyl-2-(o-tolyl)-1H-imidazole (3ab):



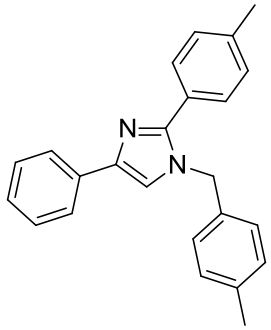
Yellow solid, mp: 104-106 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.83-7.81 (m, 2 H), 7.56-7.27 (m, 5 H), 7.24-7.17 (m, 3 H), 7.15-7.12 (m, 3 H), 6.97-6.96 (d, *J* = 4 Hz, 1 H), 4.90 (s, 2 H), 2.27 (s, 3 H), 2.09 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =148.07, 141.00, 138.72, 135.84, 134.50, 134.30, 130.59, 130.56, 130.43, 130.20, 129.49, 128.54, 128.18, 127.96, 126.68, 126.48, 125.72, 124.83, 115.19, 48.42, 19.93, 18.97. HRMS calcd for $C_{24}H_{23}N_2$ $[M+H]^+$ 339.1856; found: 339.1859.

1-(3-methylbenzyl)-4-phenyl-2-(m-tolyl)-1H-imidazole (3ac):



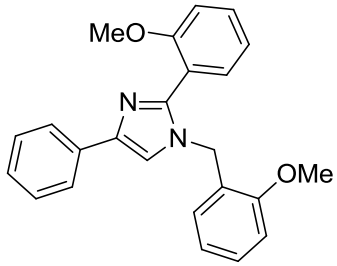
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.49 (s, 1 H), 7.38-7.34 (m, 3 H), 7.31-7.21 (m, 5 H), 7.13-7.11 (d, *J* = 8 Hz, 1 H), 6.95-6.93 (m, 2 H), 5.16 (s, 2 H), 2.37 (s, 3 H), 2.32 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.82, 141.39, 138.81, 138.47, 136.90, 134.17, 130.37, 130.04, 129.78, 128.90, 128.74, 128.55, 128.41, 127.45, 126.77, 125.86, 124.95, 123.88, 116.82, 50.52, 21.46, 21.44. HRMS calcd for $C_{24}H_{23}N_2$ $[M+H]^+$ 339.1856; found: 339.1854.

1-(4-methylbenzyl)-4-phenyl-2-(p-tolyl)-1H-imidazole (3ad)[3]:



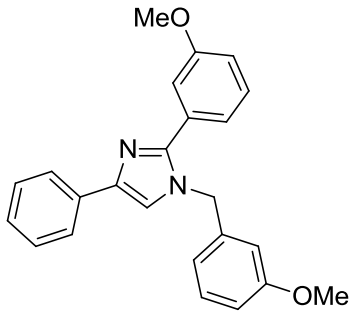
Yellow solid, mp: 94-95 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.83-7.81 (m, 2 H), 7.51-7.49 (m, 2 H), 7.36-7.32 (m, 2 H), 7.23-7.19 (m, 4 H), 7.15-7.13 (m, 2 H), 7.02-7.00 (m, 2 H), 5.13 (s, 2 H), 2.37 (s, 3 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =148.73, 141.34, 138.92, 137.73, 134.24, 133.97, 129.68, 129.33, 128.96, 128.54, 127.68, 126.73, 124.94, 116.68, 50.28, 21.41, 21.16. HRMS calcd for $C_{24}H_{23}N_2$ $[M+H]^+$339.1856; found: 339.1858.

1-(2-methoxybenzyl)-2-(2-methoxyphenyl)-4-phenyl-1H-imidazole (3ae):



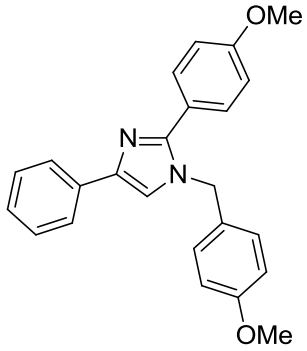
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.51-7.49 (m, 1 H), 7.43-7.38 (m, 1 H), 7.34-7.31 (m, 2 H), 7.24 (s, 1 H), 7.23-7.16 (m, 2 H), 7.05-7.01 (m, 1 H), 6.95-6.81 (m, 4 H), 4.98 (s, 2 H), 3.74 (s, 3 H), 3.70 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =157.65, 156.86, 146.20, 144.11, 134.53, 132.65, 130.84, 129.04, 128.93, 128.40, 126.38, 125.38, 124.82, 120.87, 120.54, 120.28, 116.16, 110.85, 110.22, 55.35, 55.26, 45.57. HRMS calcd for $C_{24}H_{23}N_2O_2$ $[M+H]^+$ 371.1754; found: 371.1755.

1-(3-methoxybenzyl)-2-(3-methoxyphenyl)-4-phenyl-1H-imidazole (3af)[3]:



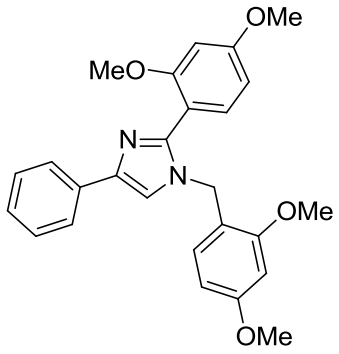
Yellow solid, mp: 120-121 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.38-7.21 (m, 6 H), 7.17-7.15 (m, 2 H), 6.97-6.94 (m, 1 H), 6.85-6.82 (m, 1 H), 6.74-6.72 (d, *J* = 7.6 Hz,1 H), 6.66 (s, 1 H), 5.19 (s, 2 H), 3.76 (s, 3 H), 3.75 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.14, 159.71, 148.45, 141.48, 138.53, 134.05, 131.64, 130.15, 129.68, 128.56, 126.84, 124.96, 121.25, 118.87, 117.01, 115.42, 114.10, 113.19, 112.45, 55.29, 55.28, 50.45. HRMS calcd for $C_{24}H_{23}N_2O_2$ $[M+H]^+$ 371.1754; found: 371.1759.

1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-4-phenyl-1H-imidazole (3ag)[3]:



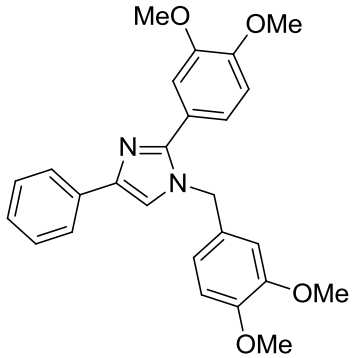
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.53-7.51 (m, 2 H), 7.36-7.32 (m, 2 H), 7.23-7.17 (m 2 H), 7.04-7.02 (m, 2 H), 6.94-6.92 (m, 2 H), 6.85-6.83 (m, 2 H), 5.07 (s, 2 H), 3.79 (s, 3 H), 3.76 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.16, 159.29, 148.43, 141.14, 134.25, 130.45, 128.93, 128.56, 128.14, 126.71, 124.89, 123.05, 116.50, 114.35, 114.06, 55.37, 55.34, 49.98. HRMS calcd for $C_{24}H_{23}N_2O_2$ $[M+H]^+$ 371.1754; found: 371.1755.

1-(2,4-dimethoxybenzyl)-2-(2,4-dimethoxyphenyl)-4-phenyl-1H-imidazole (3ah):



Yellow solid, mp: 105-106 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.80-7.78 (m, 2 H), 7.42-7.40 (d, *J* = 8 Hz, 1 H), 7.31-7.29 (m, 2 H), 7.21-7.15 (m, 2 H), 6.84-6.81 (d, *J* = 8.4 Hz, 1 H), 6.59-6.56 (m, 1 H), 6.52-6.51 (d, *J* = 4 Hz, 1 H),6.41-6.36 (m, 2 H), 4.88 (s, 2 H), 3.84 (s, 3 H), 3.77 (s, 3 H), 3.73 (s, 3 H), 3.71 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 161.99, 160.68, 158.82, 158.03, 145.96, 140.75, 134.63, 133.29, 129.95, 128.35, 126.25, 124.76, 117.87, 115.83, 113.11, 104.80, 104.07, 98.52, 98.35, 55.49, 55.43, 55.39, 55.32, 45.11. HRMS calcd for $C_{26}H_{27}N_2O_4$ $[M+H]^+$ 431.1965; found: 431.1963.

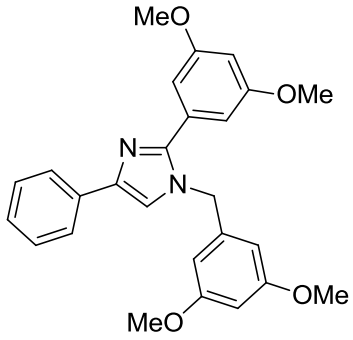
1-(3,4-dimethoxybenzyl)-2-(3,4-dimethoxyphenyl)-4-phenyl-1H-imidazole (3ai):



Yellow solid, mp: 182-184 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.35-7.32 (m, 5 H), 7.32 (s, 1 H), 7.17-7.12 (m, 2 H), 6.87-6.85 (d, *J* = 8 Hz, 1 H), 6.77-6.75 (d, *J* = 8 Hz, 1 H), 6.48-6.40 (m,1 H), 6.39 (s, 1 H), 5.22 (s, 2 H), 3.90 (s, 3 H), 3.85 (s, 3 H), 3.75 (s, 3 H), 3.72 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 149.52, 149.36, 149.19, 148.83, 148.24, 134.92, 130.55, 130.39, 128.82, 128.72, 128.07, 128.01,

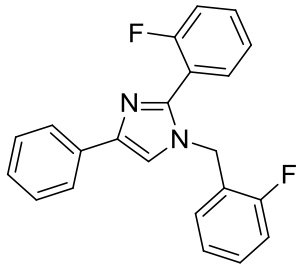
123.75, 121.11, 118.28, 112.03, 111.26, 110.86, 108.98, 55.90, 55.78, 55.72, 48.22. HRMS calcd for $C_{26}H_{27}N_2O_4$ $[M+H]^+$ 431.1965; found: 431.1963.

1-(3,5-dimethoxybenzyl)-2-(3,5-dimethoxyphenyl)-4-phenyl-1H-imidazole (3aj):



Yellow solid, mp: 98-99 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (d, *J* = 8 Hz, 2 H), 7.39-7.35 (m, 2 H), 7.27-7.22 (m, 2 H), 6.76 (d, *J* = 2 Hz, 2 H), 6.51-6.50 (m, 1 H), 6.38-6.37 (d, *J* = 4 Hz,1 H), 6.29-6.28 (d, *J* = 4 Hz, 2 H), 5.15 (s, 2 H), 3.74 (s, 6 H), 3.73 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 161.36, 160.83, 148.36, 141.39, 139.34, 134.02, 132.07, 128.55, 126.85, 124.97, 117.12, 106.95, 104.72, 101.72, 99.52, 55.42, 55.39, 50.58. HRMS calcd for $C_{26}H_{27}N_2O_4$ $[M+H]^+$431.1965; found: 431.1967.

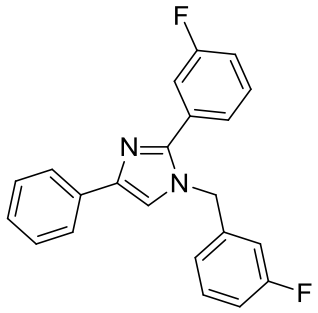
1-(2-fluorobenzyl)-2-(2-fluorophenyl)-4-phenyl-1H-imidazole (3al):



Yellow solid, mp: 72-74 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80(m, 2 H), 7.62-7.58 (m, 1 H), 7.48-7.42 (m, 1 H), 7.37-7.33 (m 2 H), 7.29-7.16 (m, 5 H), 7.07-7.01 (m, 2 H), 6.97-6.93 (m, 1 H), 5.12 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =160.38 (d, *J* = 246 Hz), 160.17 (d, *J* = 247 Hz), 143.42, 142.14, 133.88, 132.69 (d, *J* = 3 Hz), 131.57 (d, *J* = 9 Hz), 130.09 (d, *J* = 8 Hz), 129.51 (d, *J* = 3 Hz), 128.56,

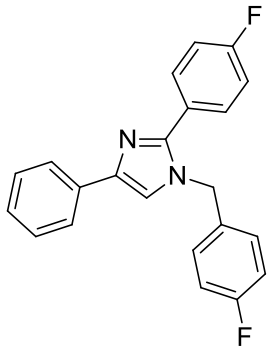
126.91, 124.90, 124.75 (d, *J* = 4 Hz), 124.56 (d, *J* = 4 Hz), 123.58 (d, *J* = 14 Hz), 118.73 (d, *J* = 15 Hz), 116.46, 115.92 (d, *J* = 21 Hz), 115.60 (d, *J* = 21 Hz), 44.41 (m). HRMS calcd for $C_{22}H_{17}F_2N_2$ $[M+H]^+$ 347.1355; found: 347.1358.

1-(3-fluorobenzyl)-2-(3-fluorophenyl)-4-phenyl-1H-imidazole (3am):



Yellow solid, mp: 95-96 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.84-7.82(m, 2 H), 7.41-7.30 (m, 6 H), 7.27-7.24 (m, 2 H), 7.14-7.09 (m 1 H), 7.03-6.99 (m, 1 H), 6.90-6.89 (d, *J* = 7.6 Hz, 1 H), 6.83-6.81 (d, *J* = 8 Hz, 1 H), 5.22 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.21 (d, *J* = 247 Hz), 162.74 (d, *J* = 246 Hz), 147.20, 141.97, 139.09 (d, *J* = 7 Hz), 133.69, 132.27 (d, *J* = 9 Hz), 130.82 (d, *J* = 8 Hz), 130.37 (d, *J* = 8 Hz), 128.65, 127.13, 124.98, 124.47 (d, *J* = 3 Hz), 122.12 (d, *J* = 3 Hz), 117.21, 116.24 (d, *J* = 3 Hz), 116.02 (d, *J* = 4 Hz), 115.19 (d, *J* = 21 Hz), 113.66 (d, *J* = 22 Hz), 50.05. HRMS calcd for $C_{22}H_{17}F_2N_2$ $[M+H]^+$ 347.1355; found: 347.1352.

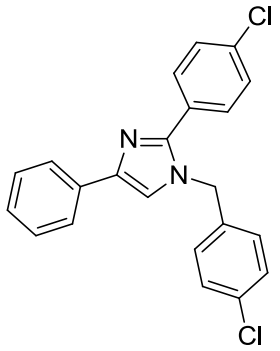
1-(4-fluorobenzyl)-2-(4-fluorophenyl)-4-phenyl-1H-imidazole (3an)[2]:



Yellow Solid, mp: 82-83^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.98-7.96 (m, 2 H), 7.72-7.67 (m, 2 H), 7.54-7.50 (m, 2 H), 7.41-7.38 (m 2 H), 7.29-7.16 (m, 6 H),

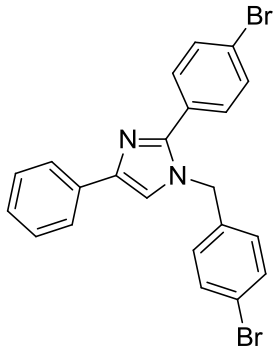
5.29 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.15 (d, *J* = 247 Hz), 162.43 (d, *J* = 246 Hz), 147.49, 141.58, 133.76, 132.33 (d, *J* = 3 Hz), 130.87 (d, *J* = 9 Hz), 128.55, 128.30 (d, *J* = 8 Hz), 126.93, 126.51 (d, *J* = 3 Hz), 124.84, 116.66, 116.49 (d, *J* = 22 Hz), 155.73 (d, *J* = 22 Hz), 49.80. HRMS calcd for $C_{22}H_{17}F_2N_2$ $[M+H]^+$ 347.1355; found: 347.1359.

1-(4-chlorobenzyl)-2-(4-chlorophenyl)-4-phenyl-1H-imidazole (3ao)[2]:



Yellow Solid, mp: 100-101^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.51-7.49 (m, 2 H), 7.39-7.37 (m, 4 H), 7.35-7.30 (m, 2 H), 7.26-7.22 (m, 2 H), 7.03-7.01 (m, 2 H), 5.14 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.38, 141.91, 135.26, 135.08, 134.06, 133.73, 130.18, 129.33, 128.99, 128.76, 128.66, 127.92, 127.11, 124.95, 117.06, 49.95. HRMS calcd for $C_{22}H_{17}Cl_2N_2$ $[M+H]^+$ 379.0764; found: 379.0757, 381.0724, 383.0691.

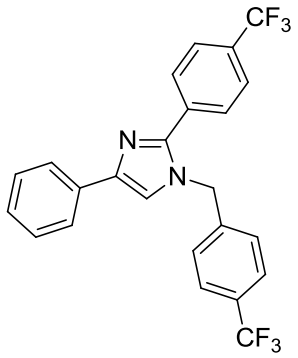
1-(4-bromobenzyl)-2-(4-bromophenyl)-4-phenyl-1H-imidazole (3ap):



Yellow solid, mp: 100-101 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.56-7.54 (m, 2 H), 7.49-7.43 (m, 4 H), 7.39-7.35 (m 2 H), 7.27-7.23 (m, 2 H),

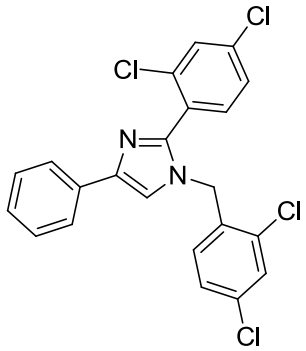
6.98-6.96 (d, *J* = 8 Hz, 2 H), 5.14 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =147.41, 141.98, 135.60, 133.68, 132.29, 131.95, 130.40, 129.16, 128.66, 128.20, 127.13, 124.94, 123.54, 122.14, 117.09, 50.01. HRMS calcd for $C_{22}H_{17}Br_2N_2$ $[M+H]^+$ 466.9753; found: 466.9744, 468.9722, 470.9701.

4-phenyl-1-(4-(trifluoromethyl)benzyl)-2-(4-(trifluoromethyl)phenyl)-1H-imidazole (3aq):



Yellow solid, mp: 107-108 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.72-7.69 (m, 4 H), 7.67-7.63 (m, 2 H), 7.41-7.38 (m, 2 H), 7.30 (s, 1 H), 7.28-7.23 (m, 3 H), 5.31 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.07, 142.46, 140.43, 133.59, 133.46, 131.21, 130.89, 130.76, 130.44, 129.10, 128.71, 127.33, 126.73, 126.23 (q, *J* = 4 Hz,), 125.77 (q, *J* = 4 Hz), 125.24, 125.17, 125.00, 122.53, 122.46, 117.49, 101.65, 50.18. HRMS calcd for $C_{24}H_{17}F_6N_2$ $[M+H]^+$ 447.1291; found: 447.1287.

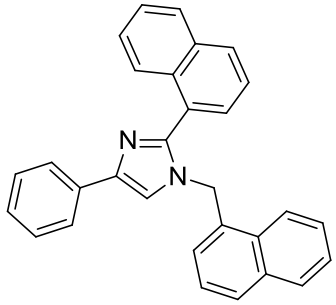
1-(2,4-dichlorobenzyl)-2-(2,4-dichlorophenyl)-4-phenyl-1H-imidazole (3ar):



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.80-7.78 (m, 2 H), 7.51 (d, *J* = 2 Hz, 1 H), 7.40-7.30 (m, 5 H), 7.25-7.22 (m, 2 H), 7.19-7.16 (m, 1 H), 6.85-6.83 (d, *J*

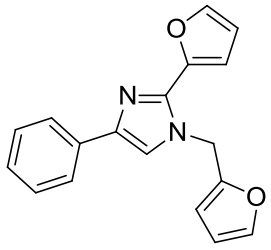
= 8 Hz, 1 H), 5.04 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.81, 142.07, 136.62, 135.50, 134.89, 133.76, 133.56, 133.52, 132.41, 129.91, 129.73, 129.70, 128.64, 128.44, 127.66, 127.57, 127.14, 124.91, 115.93, 47.76. HRMS calcd for $C_{22}H_{15}Cl_4N_2$ $[M+H]^+$446.9984; found: 446.9978, 448.9946, 450.9915, 451.9947, 453.9916.

2-(naphthalen-1-yl)-1-(naphthalen-1-ylmethyl)-4-phenyl-1H-imidazole (3as):



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.98-7.90 (m, 3 H), 7.85-7.78 (m, 4 H), 7.66-7.59 (m, 2 H), 7.56-7.52 (m, 2 H), 7.51-7.40 (m, 3 H), 7.38-7.32 (m, 3 H), 7.25-7.18 (m, 3 H), 5.39 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.07, 141.48, 134.14, 133.85, 133.66, 132.90, 131.95, 130.64, 130.02, 128.95, 128.89, 128.70, 128.55, 128.38, 128.01, 127.06, 126.79, 126.71, 126.36, 126.11, 125.93, 125.83, 125.44, 125.10, 124.90, 122.51, 115.87, 48.60. HRMS calcd for $C_{30}H_{23}N_2$ $[M+H]^+$ 411.1856; found: 411.1859.

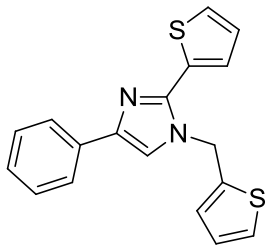
2-(furan-2-yl)-1-(furan-2-ylmethyl)-4-phenyl-1H-imidazole (3at):



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.81-7.79 (m, 2 H), 7.56-7.55 (m, *J* = 4 Hz, 1 H), 7.40-7.34 (m, 3 H), 7.26-7.21 (m, 2 H), 6.94-6.93 (m, 1 H), 6.55-6.54 (m, 1 H), 6.35-6.34 (m, 1 H), 6.30-6.29 (m, 1 H), 5.38 (s, 2 H); ^{13}C NMR (100

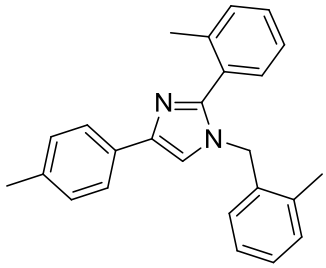
MHz, $CDCl_3$, ppm): δ = 149.32, 145.46, 143.06, 142.78, 141.75, 139.11, 133.73, 128.51, 126.95, 125.01, 116.65, 111.60, 110.66, 110.19, 109.00, 43.92. HRMS calcd for $C_{18}H_{15}N_2O_2$ $[M+H]^+$ 291.1128; found: 291.1126.

4-phenyl-2-(thiophen-2-yl)-1-(thiophen-2-ylmethyl)-1H-imidazole (3au):



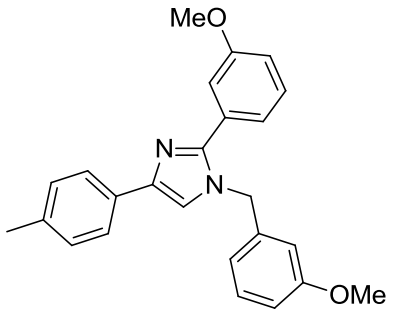
Yellow solid, mp: 92-93 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.42-7.41 (d, *J* = 4 Hz, 1 H), 7.38-7.34 (m, 2 H), 7.31-7.28 (m, 3 H), 7.25-7.22 (m, 2 H), 7.11-7.09 (m, 1 H), 6.99-6.94 (m, 2 H), 5.44 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.05, 141.80, 138.71, 133.70, 131.92, 128.55, 127.55, 127.31, 127.25, 127.08, 127.00, 126.41, 126.06, 125.01, 116.78, 45.89. HRMS calcd for $C_{18}H_{15}N_2S_2$ $[M+H]^+$ 323.0671; found: 323.0675.

1-(2-methylbenzyl)-2-(o-tolyl)-4-(p-tolyl)-1H-imidazole (3cb):



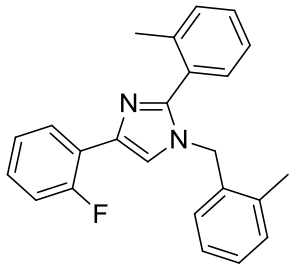
Yellow liquid. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.71-7.69 (m, 2 H), 7.34-7.27 (m, 3 H), 7.24-7.09 (m, 7 H), 6.97-6.95 (d, *J* = 8 Hz, 1 H), 4.90 (s, 2 H), 2.33 (s, 3 H), 2.27 (s, 3 H), 2.09 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.89, 141.08, 138.73, 136.27, 135.82, 134.57, 131.50, 130.56, 130.52, 130.44, 130.28, 129.42, 129.21, 128.13, 127.94, 126.45, 125.68, 124.75, 114.70, 48.37, 21.24, 19.92, 18.96. HRMS calcd for $C_{25}H_{25}N_2$ $[M+H]^+$ 353.2011; found: 353.2019.

1-(3-methoxybenzyl)-2-(3-methoxyphenyl)-4-(p-tolyl)-1H-imidazole (3cf):



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.74-7.2 (m, 2 H), 7.34-7.29 (m, 1 H), 7.27-7.25 (m, 2 H), 7.19-7.15 (m, 4 H), 6.96-6.94 (m, 1 H), 6.85-6.83 (m, 1 H), 6.75-6.73 (d, *J* = 8 Hz, 1 H), 6.67 (s, 1 H), 5.19 (s, 2 H), 3.76 (s, 3 H), 3.75 (s, 3 H), 2.35 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.13, 159.70, 148.28, 141.58, 138.62, 136.46, 131.72, 131.27, 130.13, 129.65, 129.25, 124.88, 121.25, 118.87, 116.58, 115.36, 114.08, 113.18, 112.41, 55.28, 55.27, 50.41, 21.26. HRMS calcd for $C_{25}H_{25}N_2O_2$ $[M+H]^+$ 385.1910; found: 385.1915.

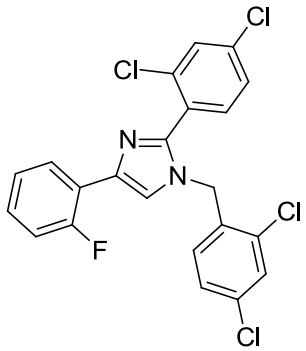
4-(2-fluorophenyl)-1-(2-methylbenzyl)-2-(o-tolyl)-1H-imidazole (3fb):



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.29-7.26 (m, 1 H), 7.51-7.49 (m, 2 H), 7.44-7.43 (d, *J* = 4 Hz, 1 H), 7.24-7.13 (m, 6 H), 7.09-7.01 (m, 3 H), 5.17(s, 2 H), 2.38 (s, 3 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.71 (d, *J* = 246 Hz), 148.18, 139.01, 137.68, 134.79 (d, *J* = 2 Hz), 133.93, 129.66, 129.34, 128.34 (d, *J* = 4 Hz), 127.48 (d, *J* = 9 Hz), 126.59, 124.28 (d, *J* = 3 Hz), 121.00 (d, *J* = 15 Hz), 115.35 (d, *J* = 22 Hz), 50.28, 21.39, 21.13. HRMS calcd for $C_{24}H_{22}FN_2$ $[M+H]^+$ 357.1762; found: 357.1760.

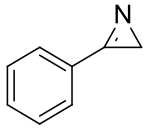
1-(2,4-dichlorobenzyl)-2-(2,4-dichlorophenyl)-4-(2-fluorophenyl)-1H-imidazole

(3fq):



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.22-8.18 (m, 1 H), 7.52-7.51 (d, *J* = 8 Hz, 1 H), 7.46-7.45 (d, *J* = 4 Hz, 1 H), 7.39-7.30 (m, 3 H), 7.23-7.16 (m, 3 H), 7.11-7.06(m, 1 H), 6.84-6.82 (d, *J* = 8 Hz, 1 H), 5.07 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.70 (d, *J* = 245 Hz), 144.32, 136.69, 135.56 (d, *J* = 5 Hz), 134.86, 133.68, 133.44, 132.35, 129.71 (d, *J* = 2 Hz), 129.67, 128.33, 127.95 (d, *J* = 9 Hz), 127.59 (d, *J* = 7 Hz), 124.34, 121.41 (d, *J* = 14 Hz), 120.26 (d, *J* = 14 Hz), 115.45 (d, *J* = 22 Hz), 47.79. HRMS calcd for $C_{22}H_{14}Cl_4FN_2$ $[M+H]^+$ 464.9890; found: 464.9881, 466.9850, 468.9817, 469.9851,471.9824.

3-phenyl-2H-azirine (4)[1]:



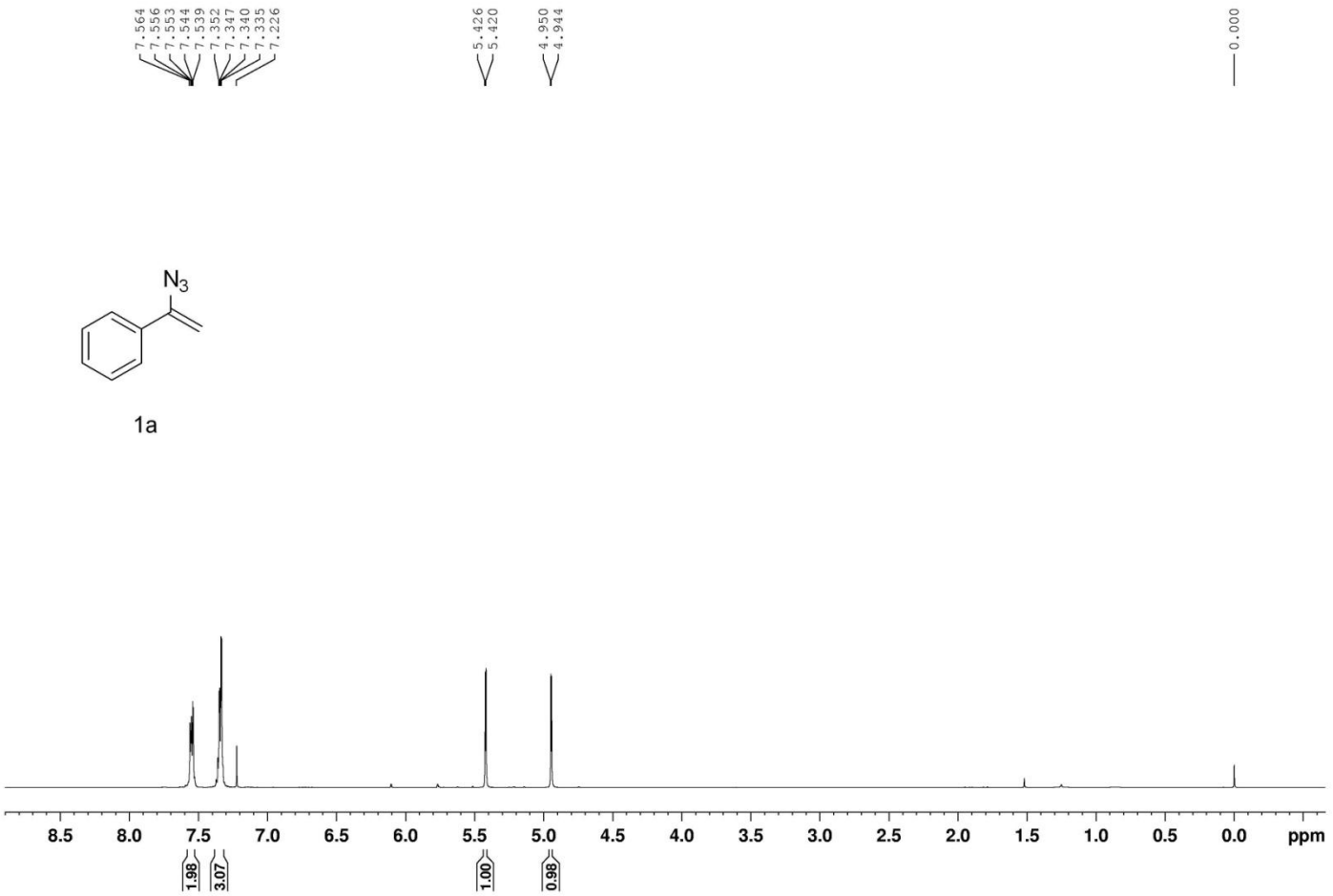
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.92-7.90 (m, 2 H), 7.61-7.53 (m, 3 H), 1.79 (d, *J* = 0.8 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 165.80, 132.94, 129.60, 129.07, 125.50, 19.70. HRMS calcd for C_8H_8N $[M+H]^+$ 118.0651; found: 118.0650.

References

(1) Donthiri, R. R.; Pappula, V.; Reddy, N. N. K.; Bairagi, D.; Adimurthy, S. *J. Org. Chem.* **2014**, *79*, 11277.

(2) Cai, Z.-J.; Wang, S.-Y.; Ji, S.-J. *Org. Lett.* **2012**, *14*, 6068.

(3) Huang, H.; Ji, X.; Wu, W.; Jiang, H. *Adv. Synth. Catal*. **2014**, *355*,170.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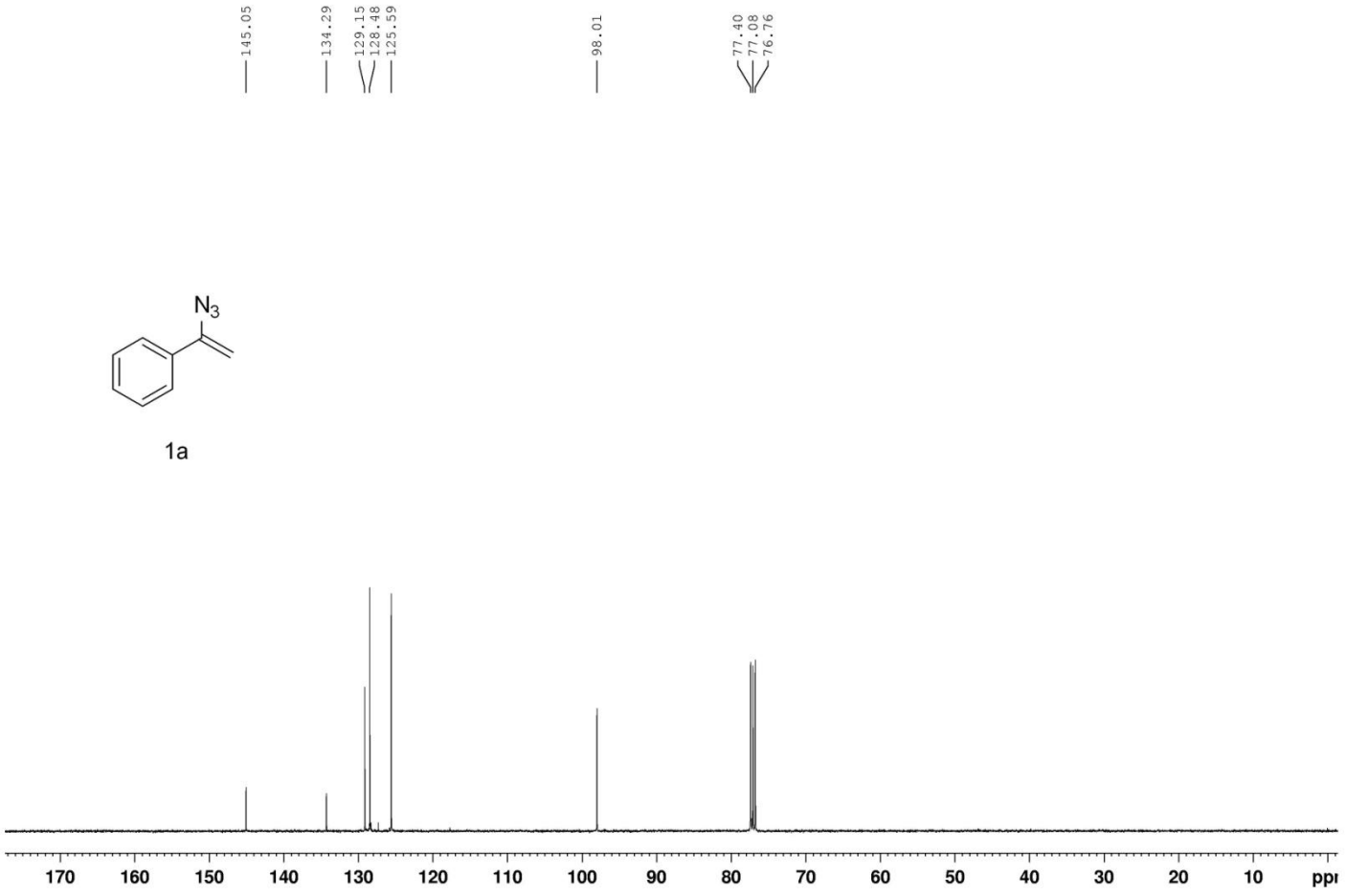
7.544
7.539
7.352
7.347
7.340
7.335
7.226
5.426
5.420
4.950
4.944
0.000
N3
1a
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.98
3.07
1.00
0.98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129.15
128.48
125.59
98.01
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77.08
76.76
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1a
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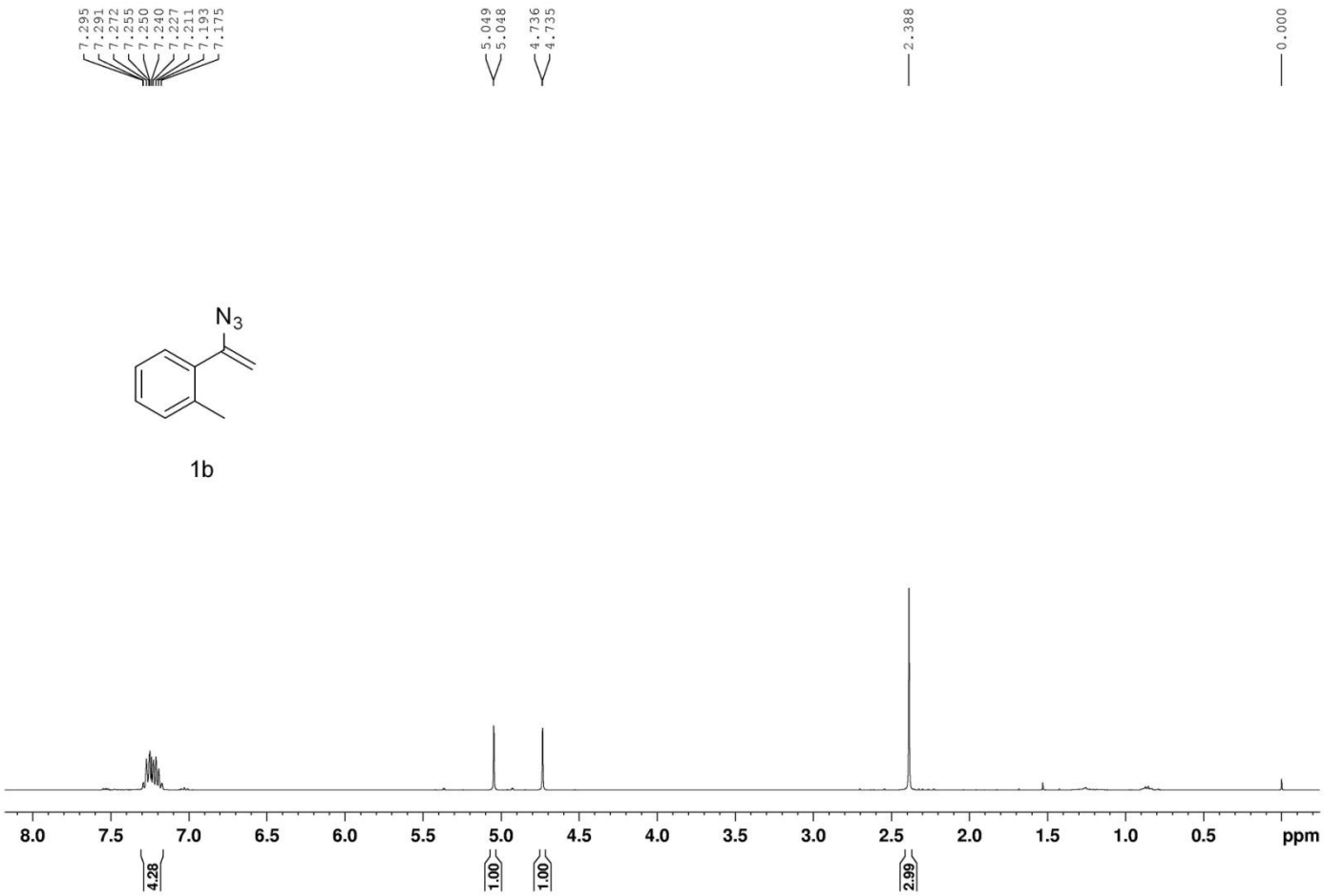
90
80
70
60
50
40
30
20
10
ppm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4.735
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0.000
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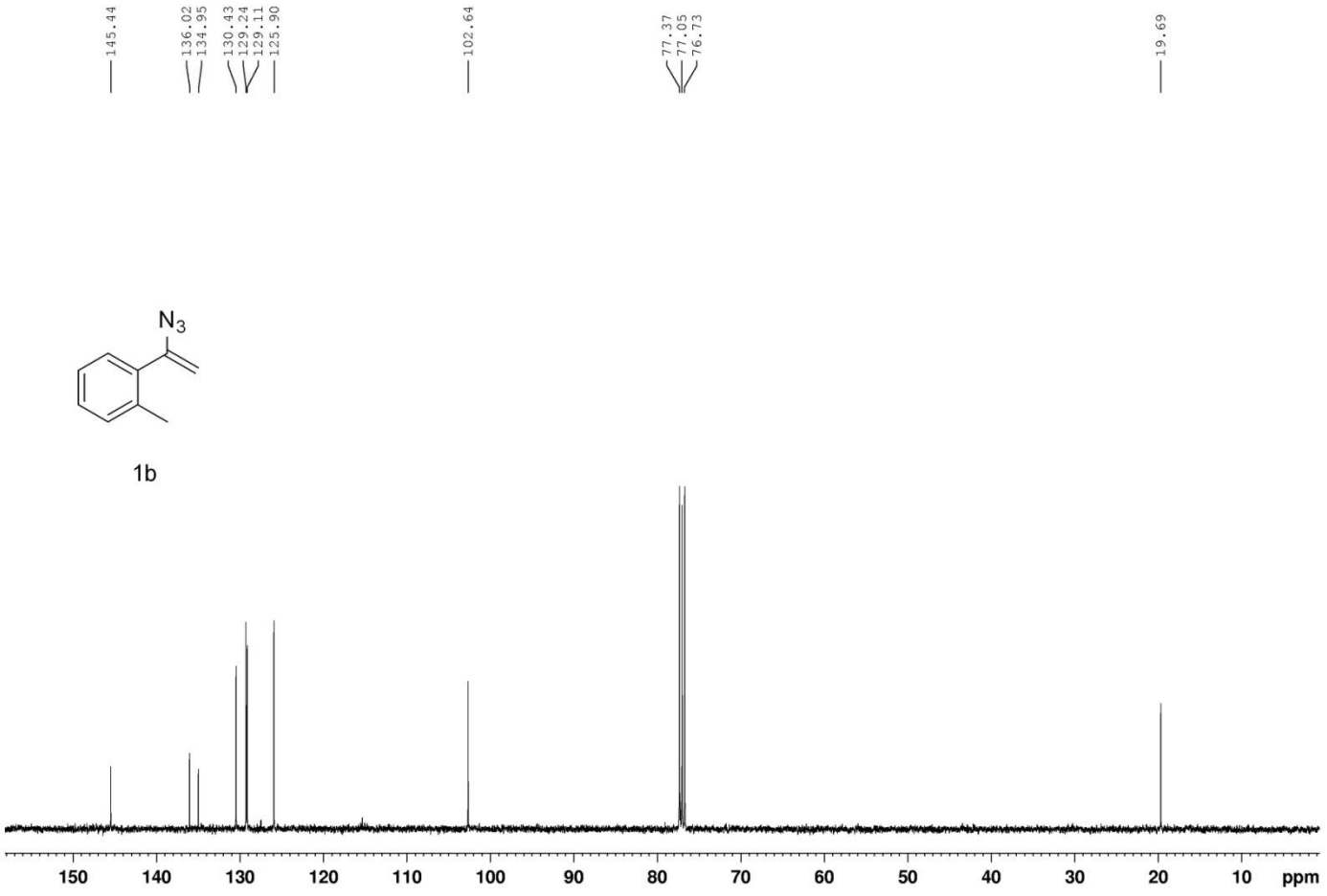
1b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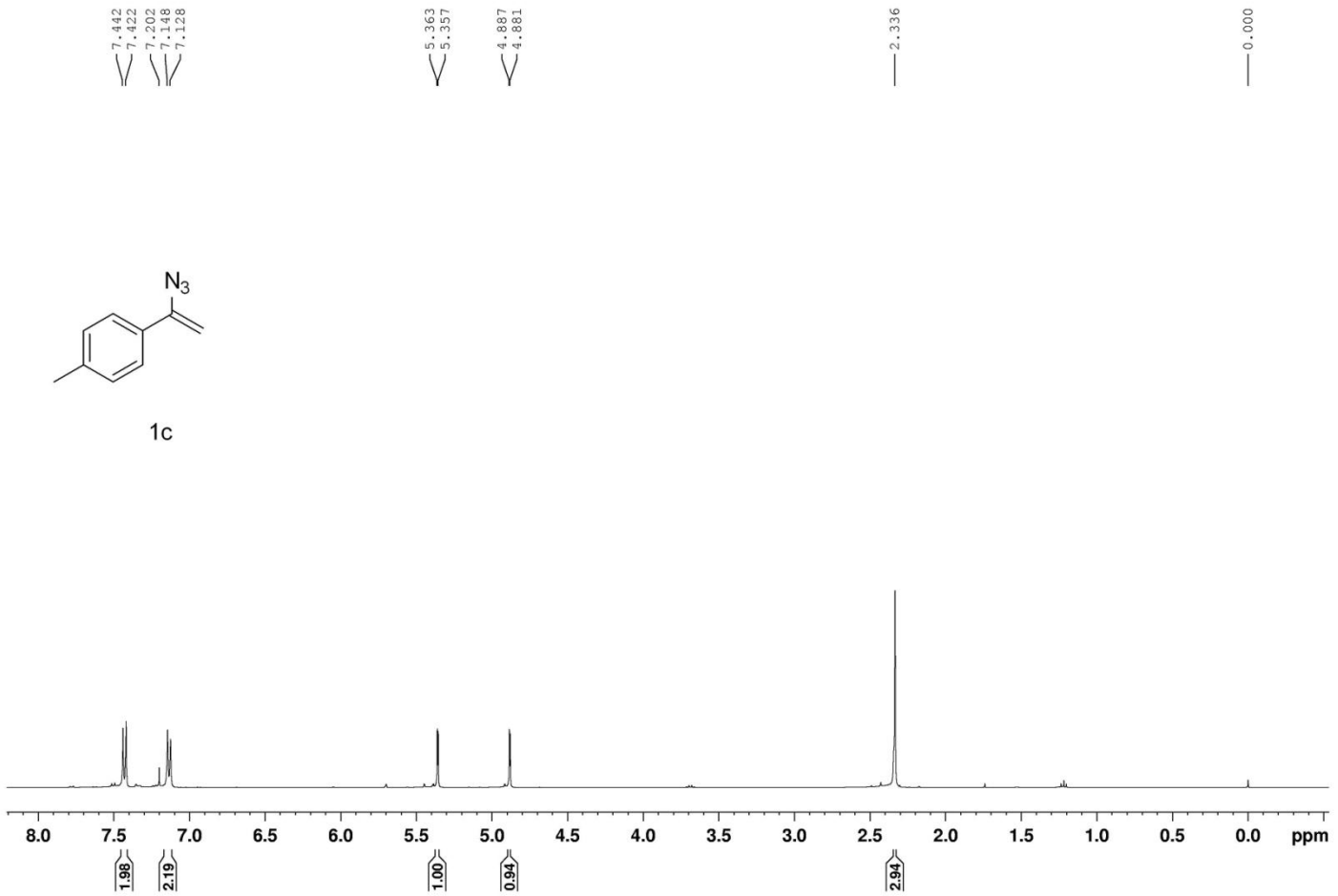
30
20
10
ppm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7.0
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6.0
5.5
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4.5
4.0
3.5
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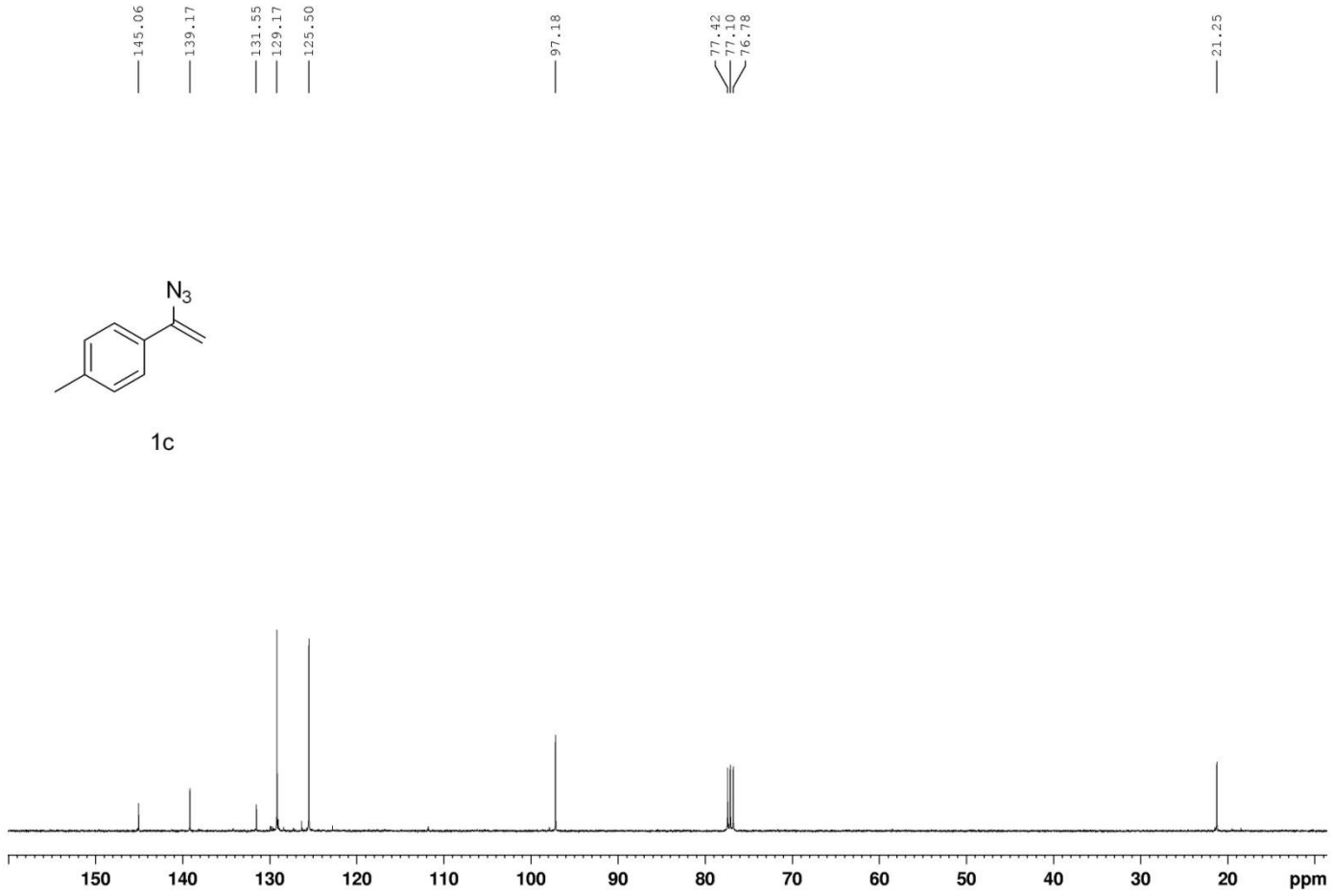
2.94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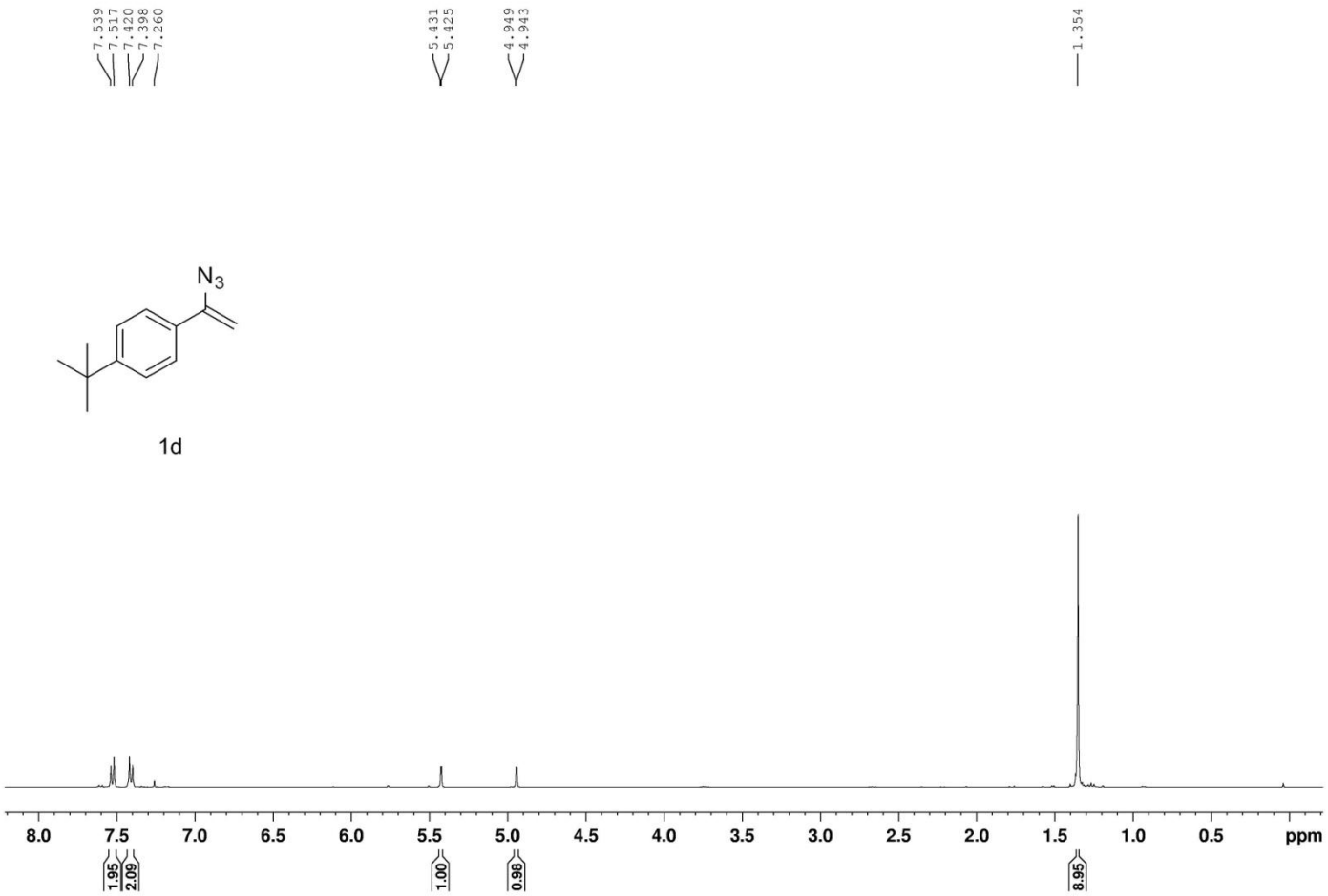
120
110
100
90
80
70
60
50
40
30
20
ppm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4.949
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1d
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
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1.5
1.0
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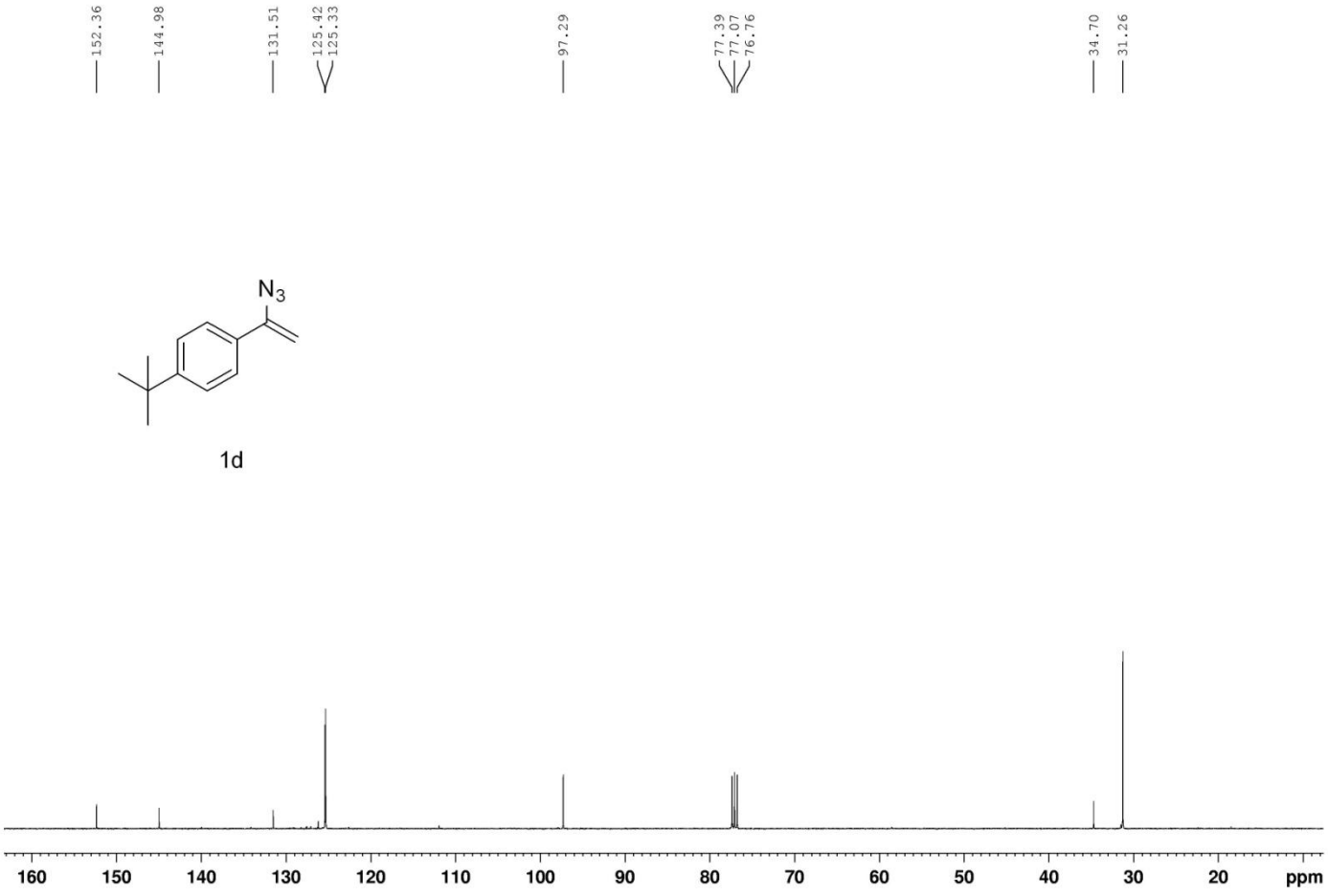
0.98
8.95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97.29
77.39
77.07
76.76
34.70
31.26
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140
130
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100
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70
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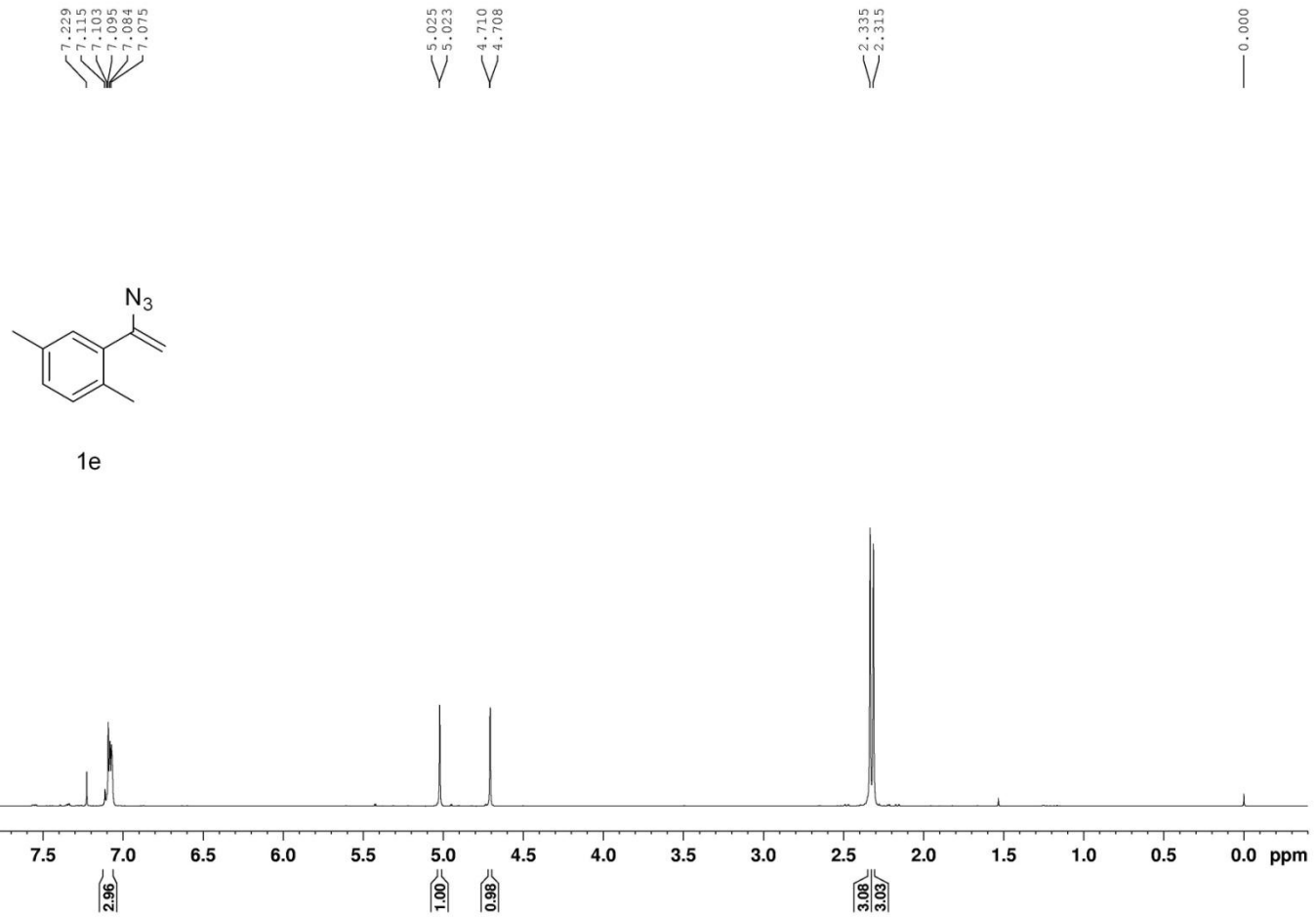
20
ppm

1d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5.023
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4.708
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2.315
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N3
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.00
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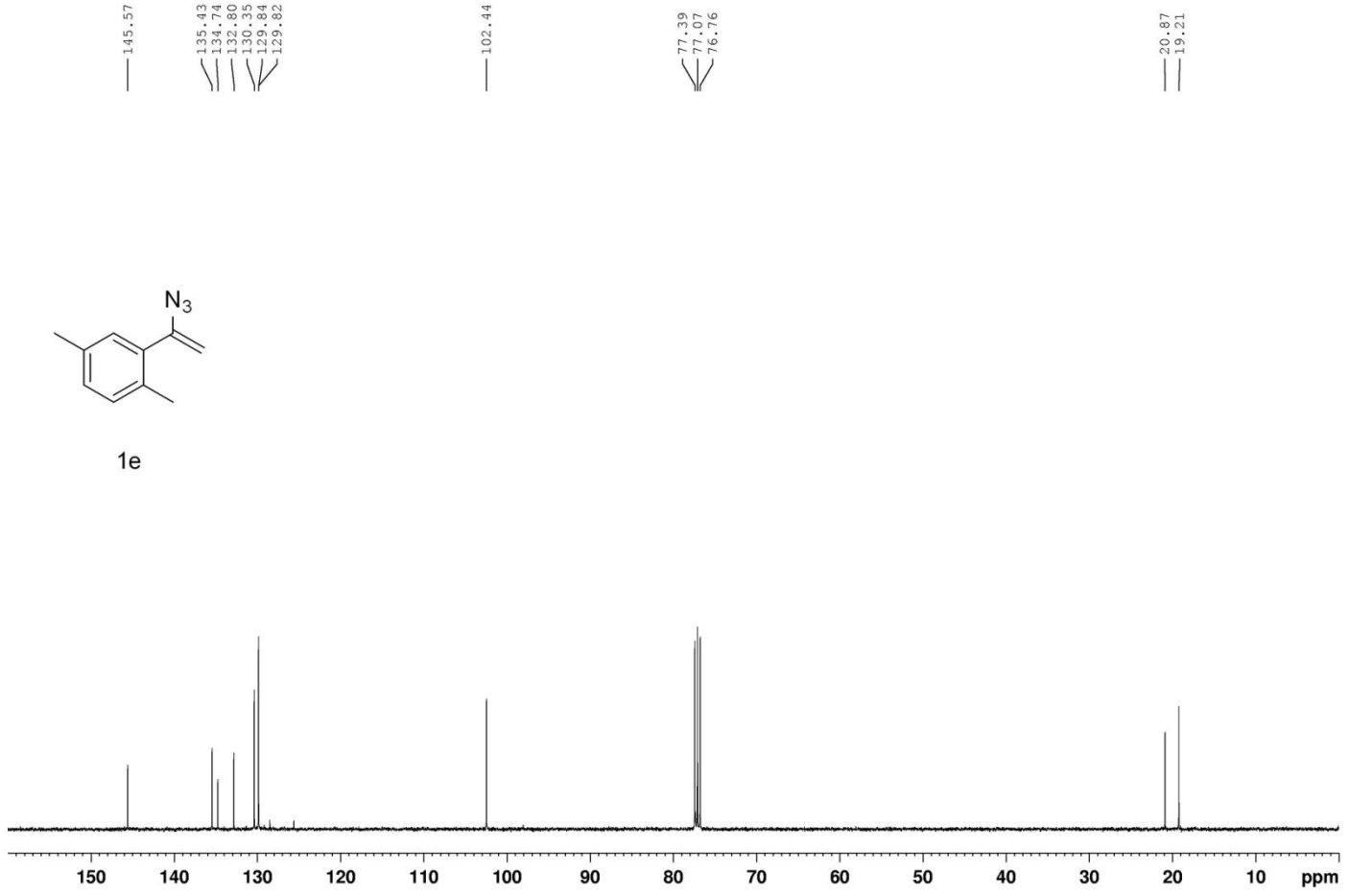
3.08
3.03

1e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102.44
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77.07
76.76
20.87
19.21
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100
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80
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60
50
40
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20
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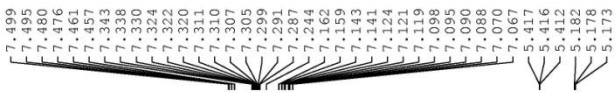
ppm

1e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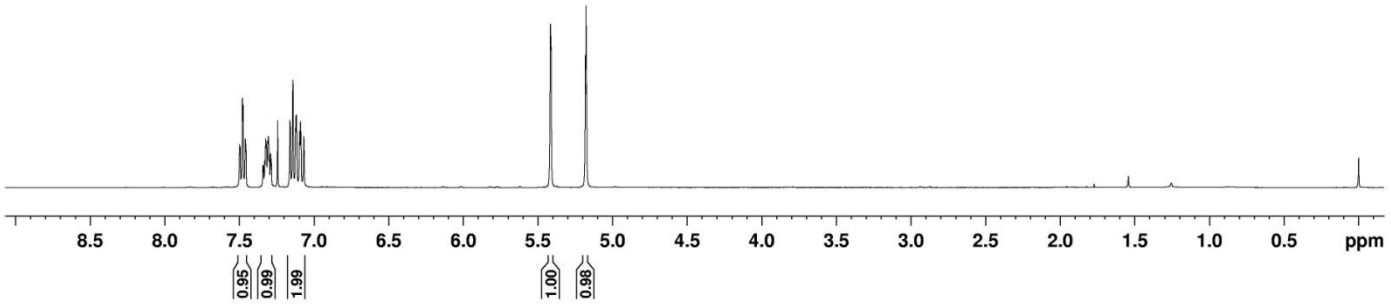
7.324
7.322
7.320
7.311
7.310
7.307
7.305
7.299
7.291
7.287
7.244
7.162
7.159
7.143
7.141
7.124
7.121
7.119
7.098
7.095
7.090
7.088
7.070
7.067
5.417
5.416
5.412
5.182
5.178
5.173

0.000


N3
F

1f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4.0
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2.0
1.5
1.0
0.5
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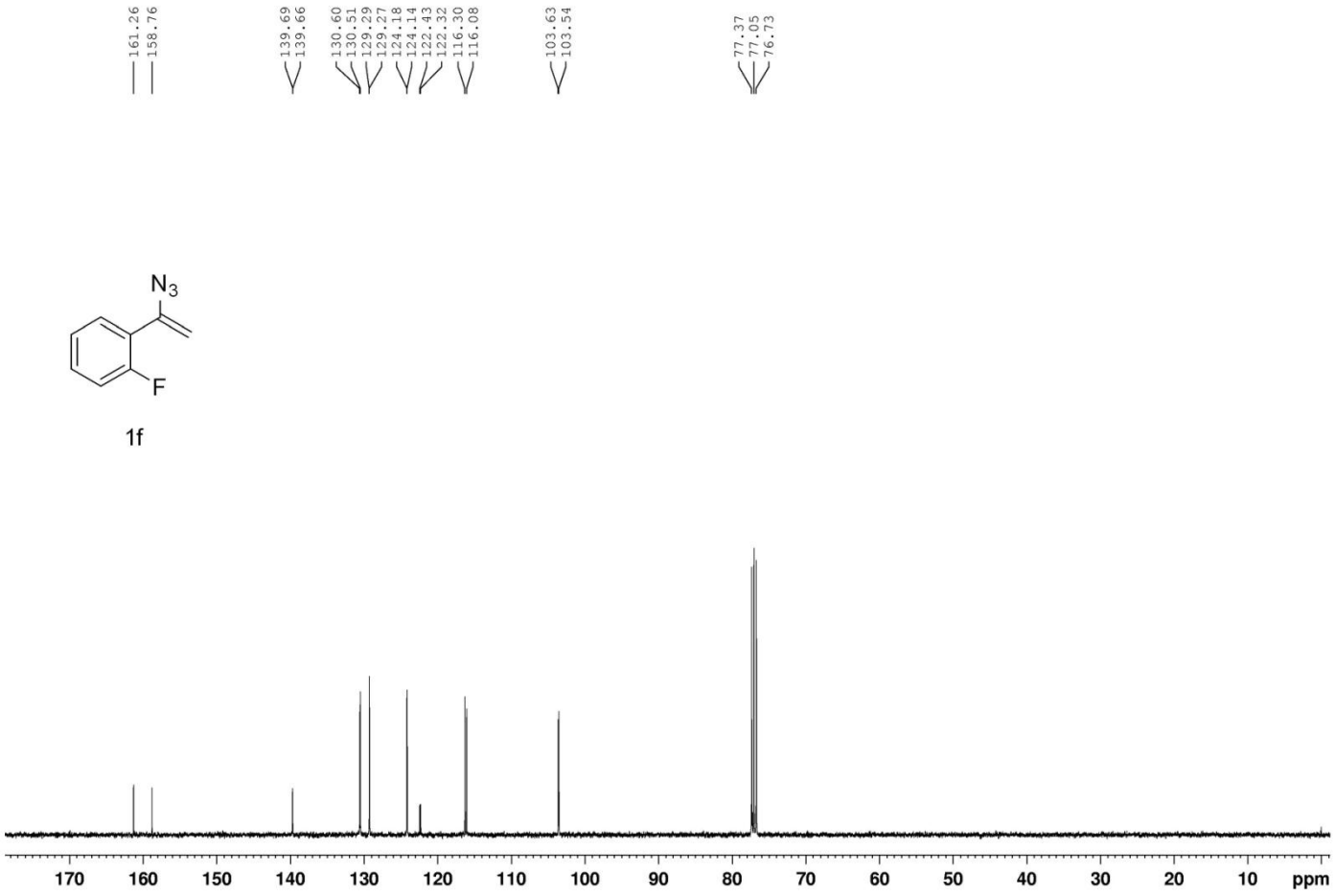
1.00
0.98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139.69
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129.27
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124.14
122.43
122.32
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116.08
103.63
103.54
77.37
77.05
76.73
N3
F
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70
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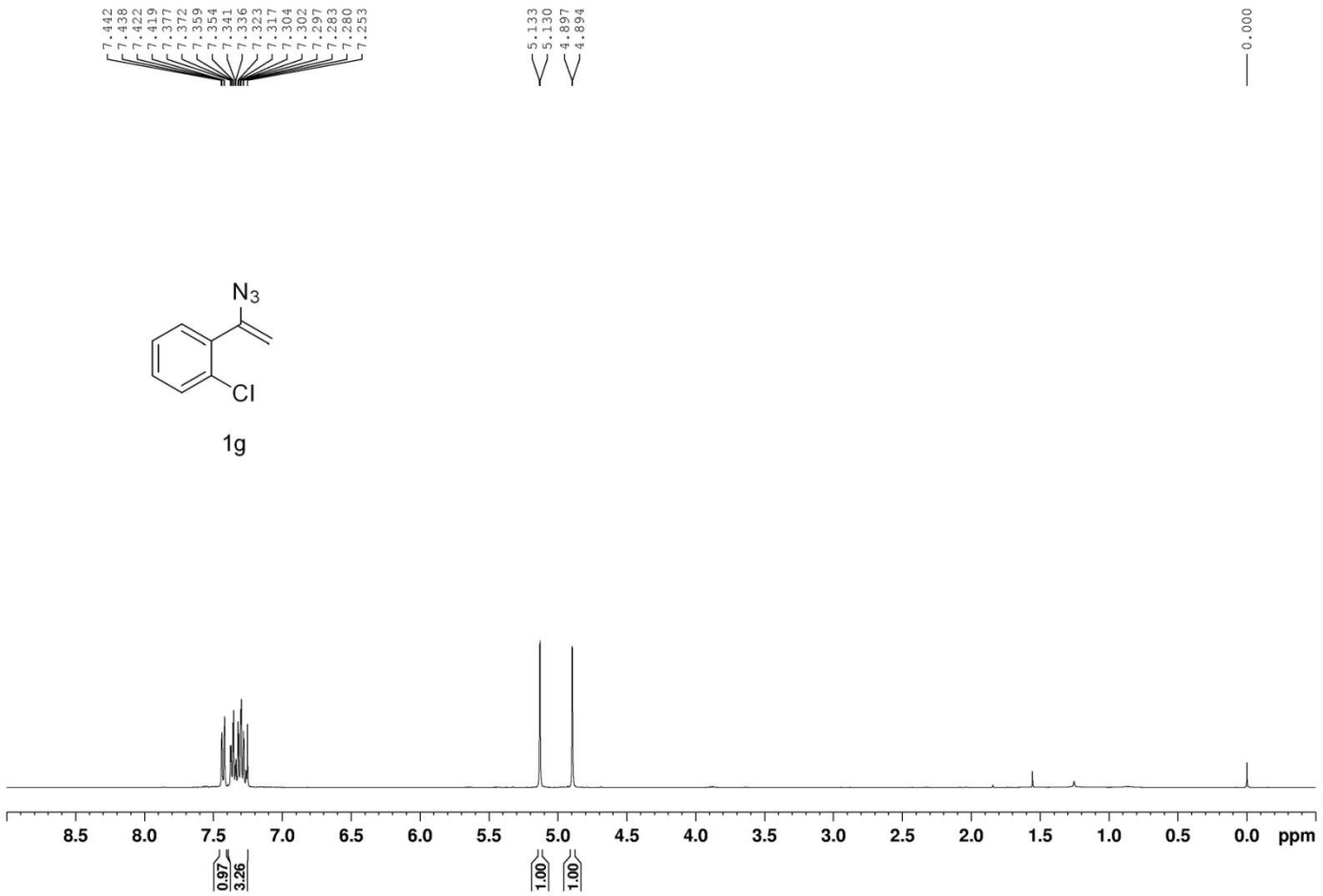
10
ppm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7.372
7.359
7.354
7.341
7.336
7.323
7.317
7.304
7.302
7.297
7.283
7.280
7.253
5.133
5.130
4.897
4.894
0.000
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Cl
1g
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.0
1.5
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ppm
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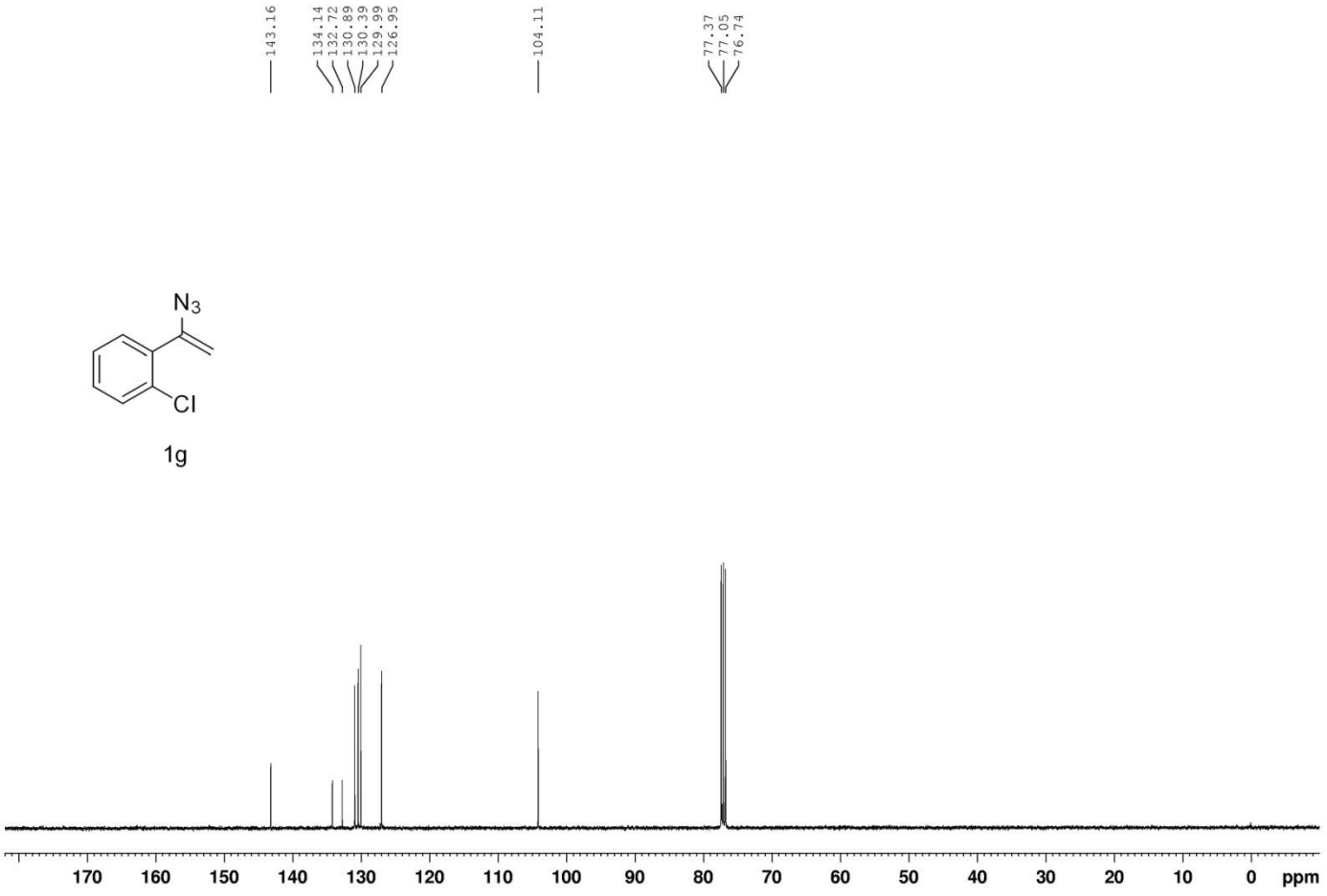
1.00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129.99
126.95
104.11
77.37
77.05
76.74
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Cl
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140
130
120
110
100
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80
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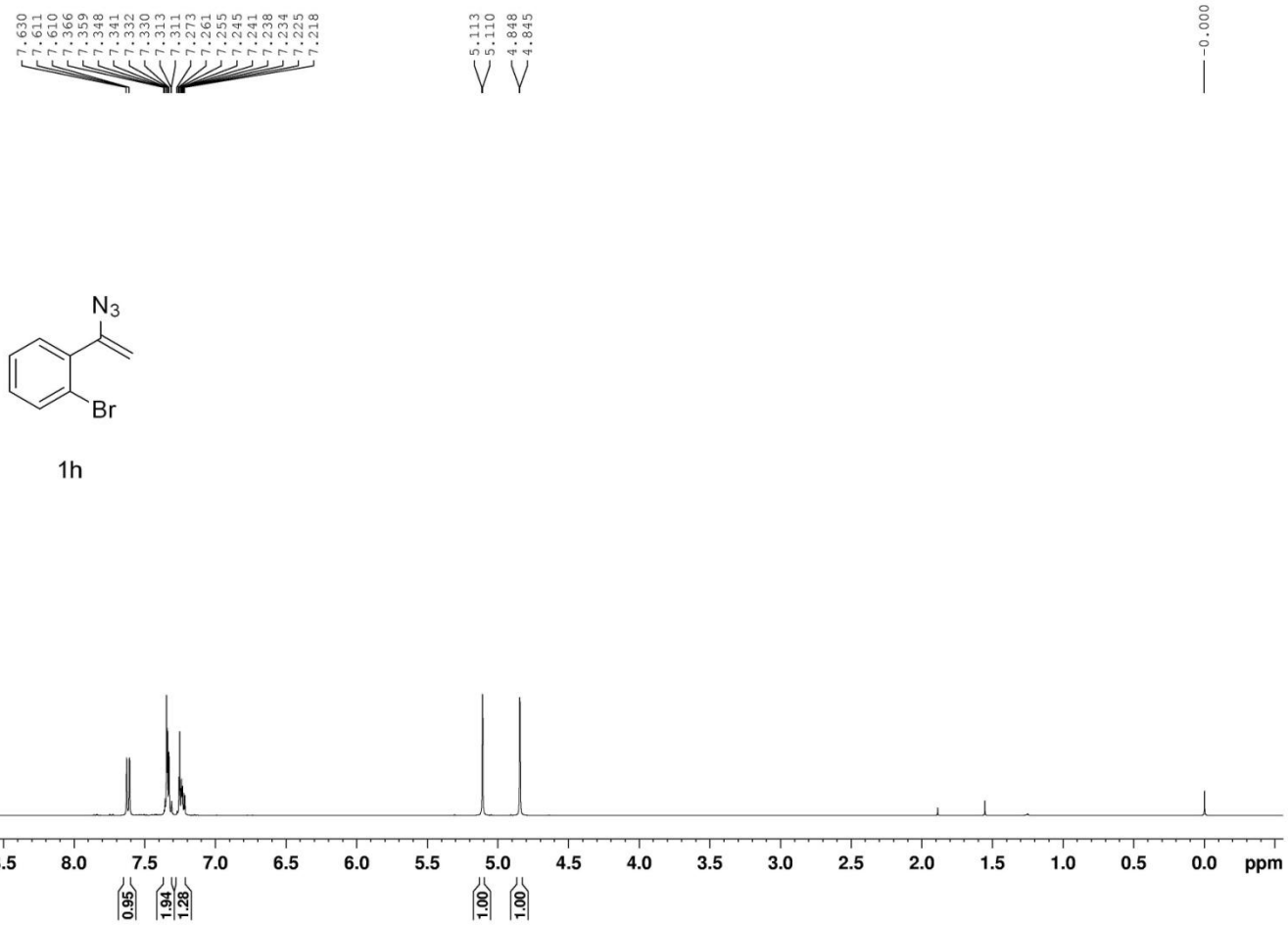
60
50
40
30
20
10
0
ppm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7.332
7.330
7.313
7.311
7.273
7.261
7.255
7.245
7.241
7.238
7.234
7.225
7.218
5.113
5.110
4.848
4.845
0.000
N3
Br
1h
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.5
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0.0
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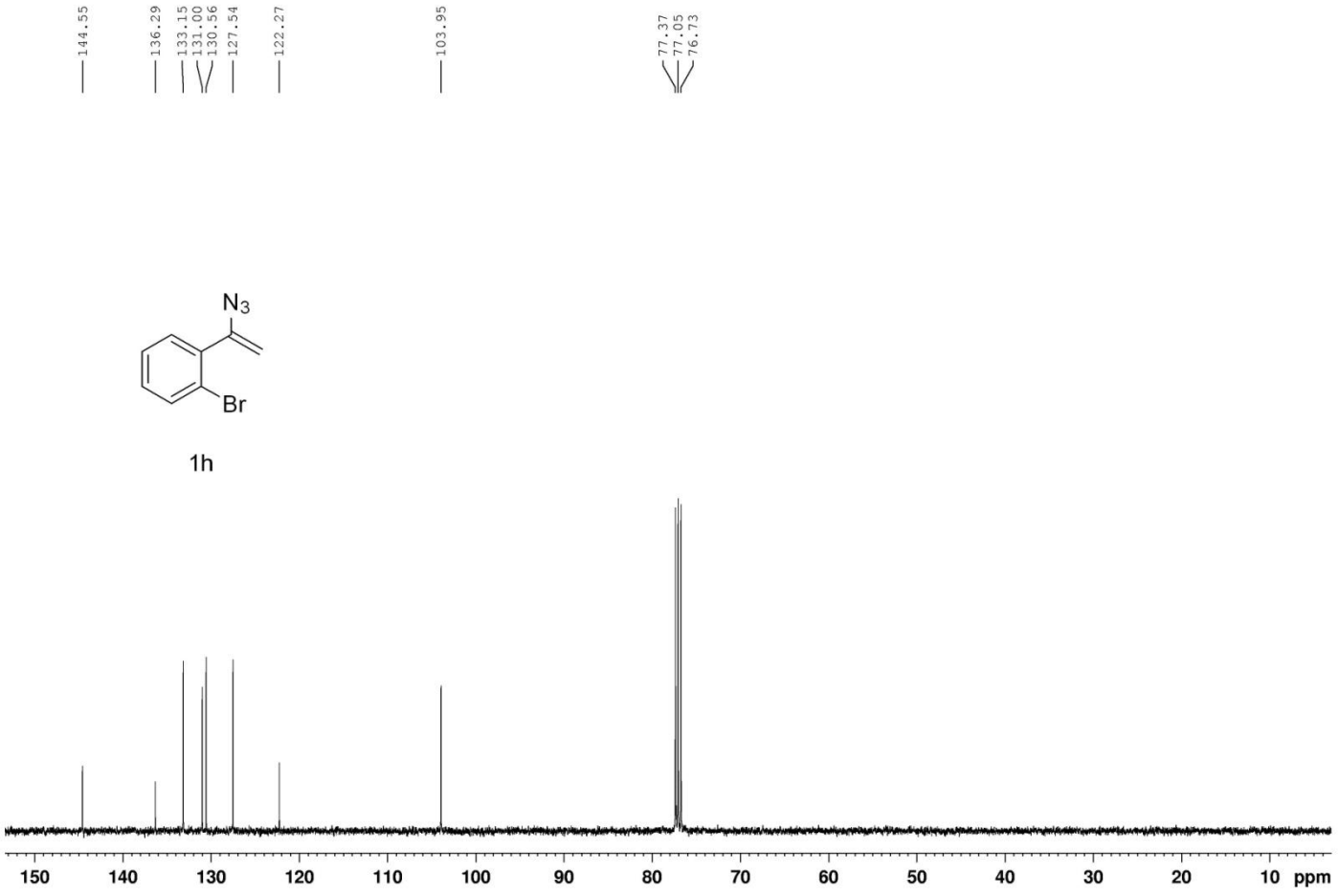
1.00
1.00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122.27
103.95
77.37
77.05
76.73
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140
130
120
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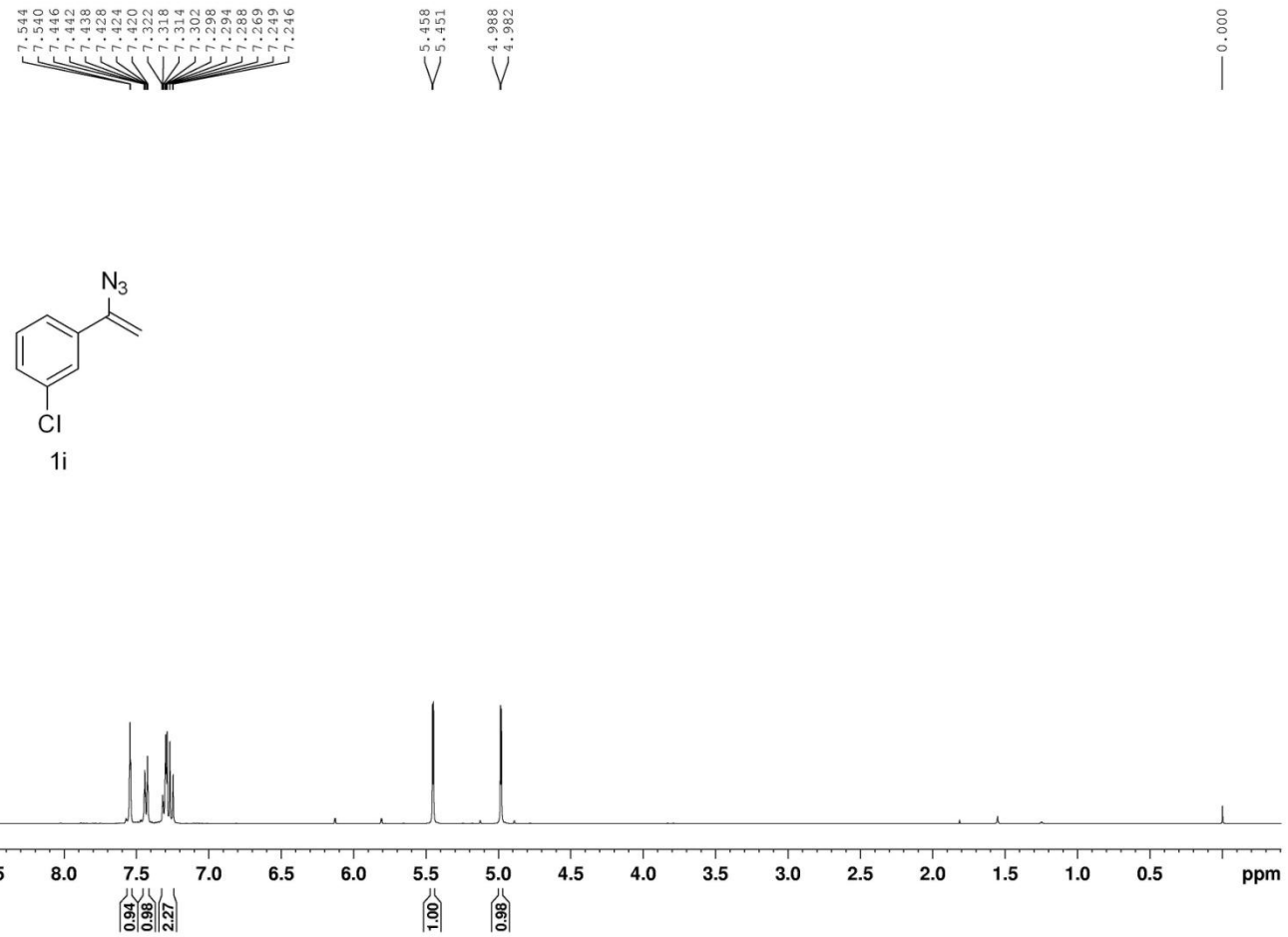
ppm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7.322
7.318
7.314
7.302
7.298
7.294
7.288
7.269
7.249
7.246
5.458
5.451
4.988
4.982
0.000
N3
Cl
1i
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.0
1.5
1.0
0.5
ppm
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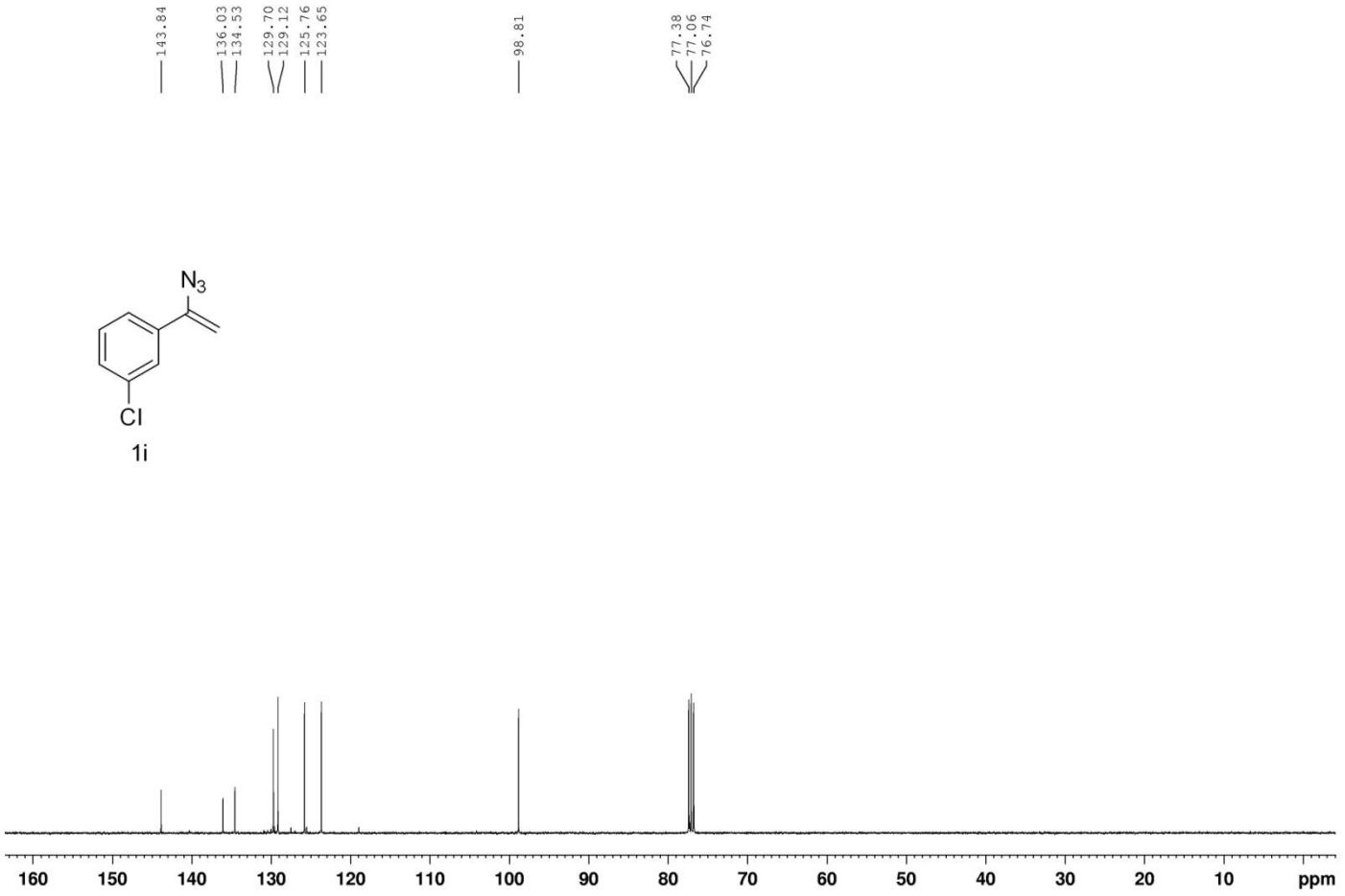
0.98
2.27
1.00
0.98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125.76
123.65
98.81
77.38
77.06
76.74
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Cl
1i
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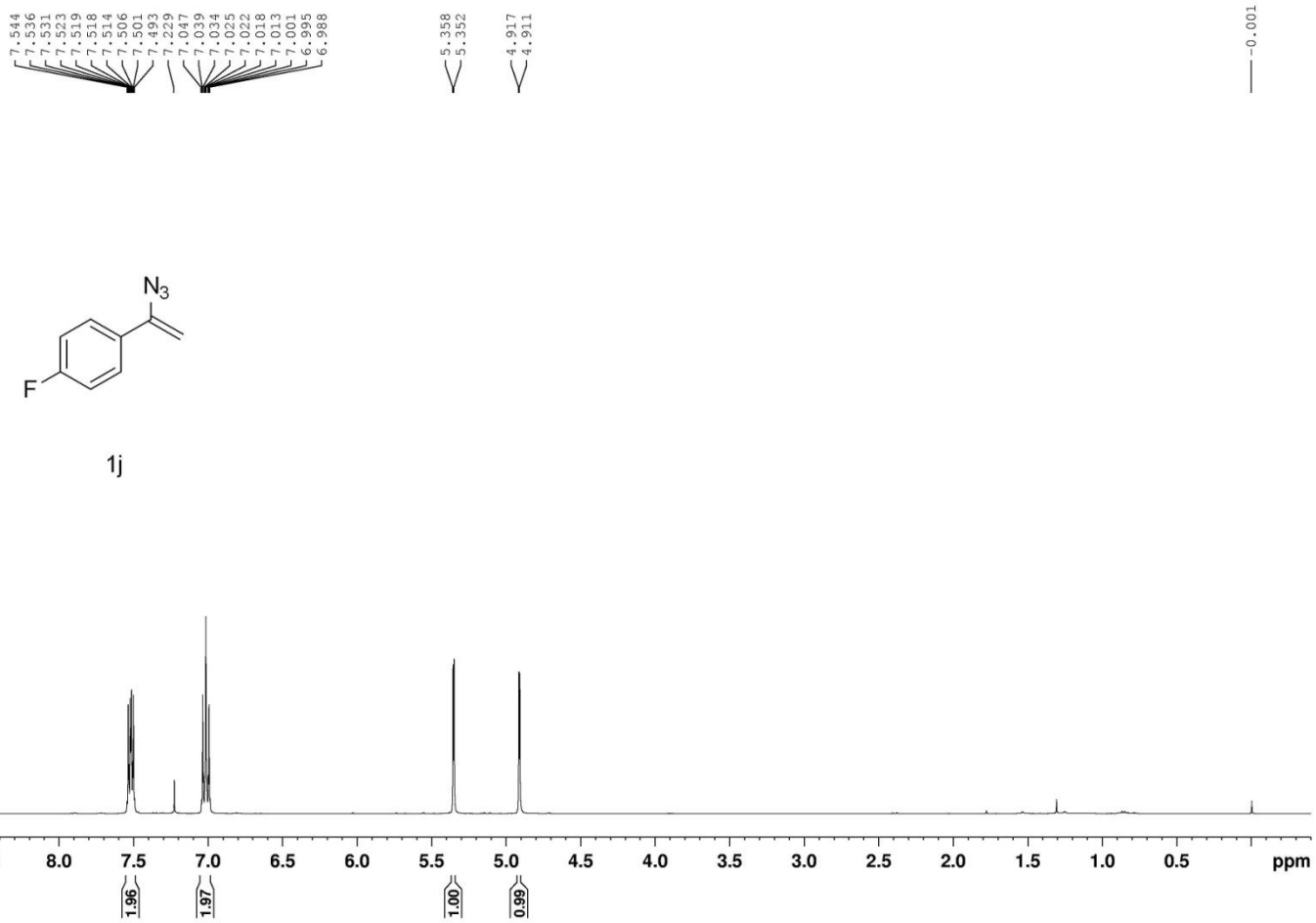
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.514
7.506
7.501
7.493
7.229
7.047
7.039
7.034
7.025
7.022
7.018
7.013
7.001
6.995
6.988
5.358
5.352
4.917
4.911
-0.001
N3
F
1j
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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ppm
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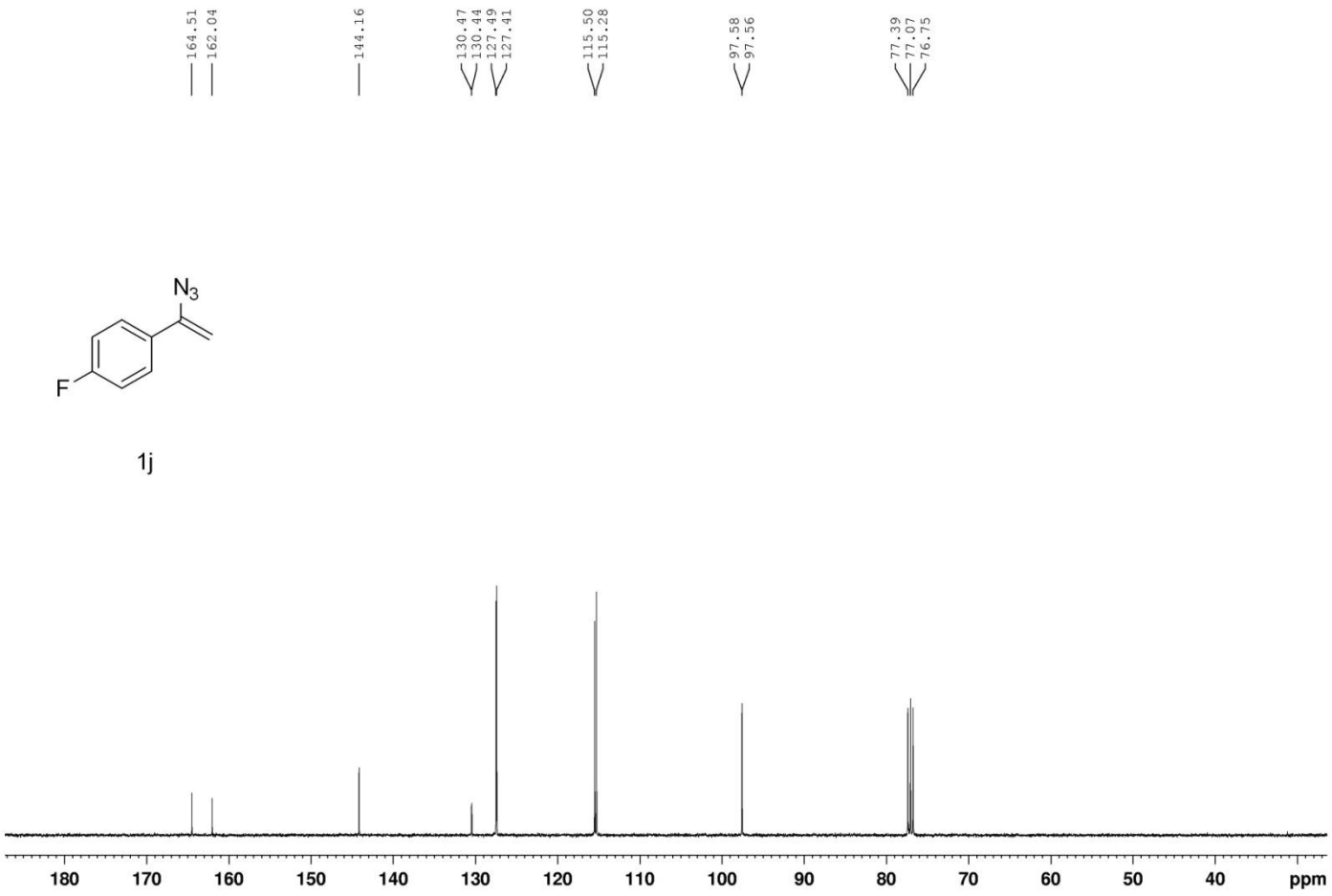
1.97
1.00
0.99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97.58
97.56
77.39
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76.75
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130
120
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100
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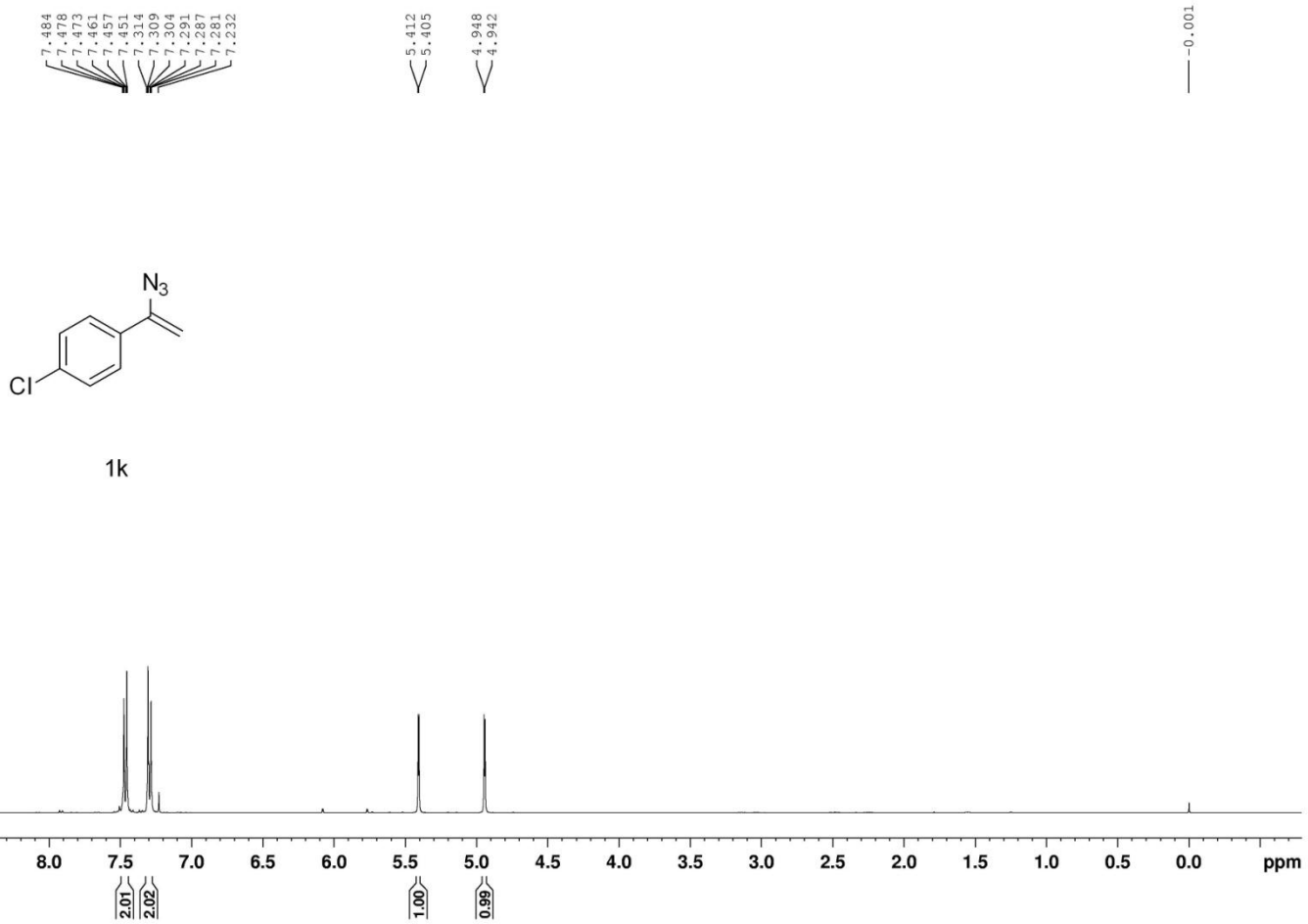
70
60
50
40
ppm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7.309
7.304
7.291
7.287
7.281
7.232
5.412
5.405
4.948
4.942
0.001
N3
Cl
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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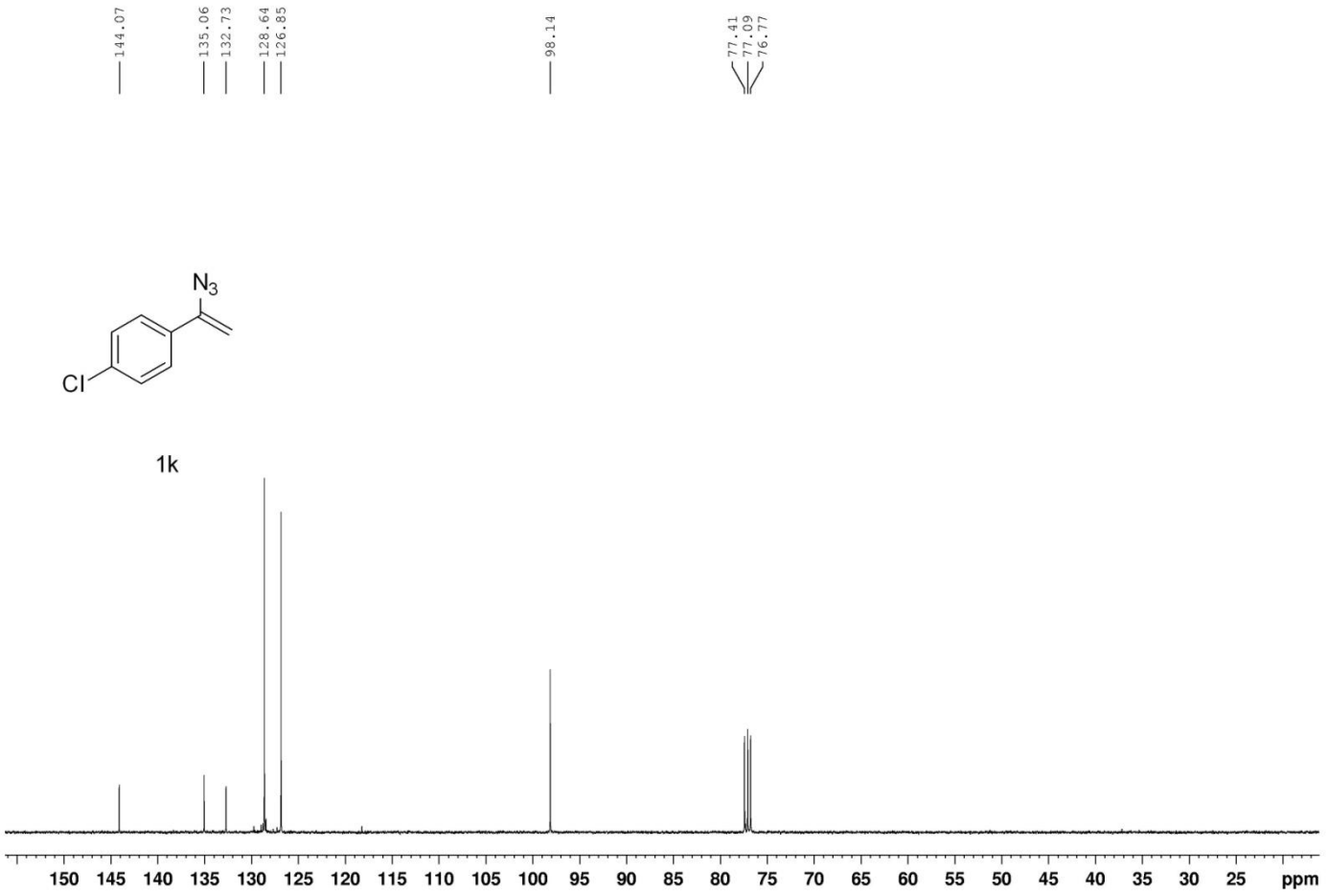
2.0
1.5
1.0
0.5
0.0
ppm
2.01
2.02
1.00
0.99

1k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132.73
128.64
126.85
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77.09
76.77
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Cl
1k
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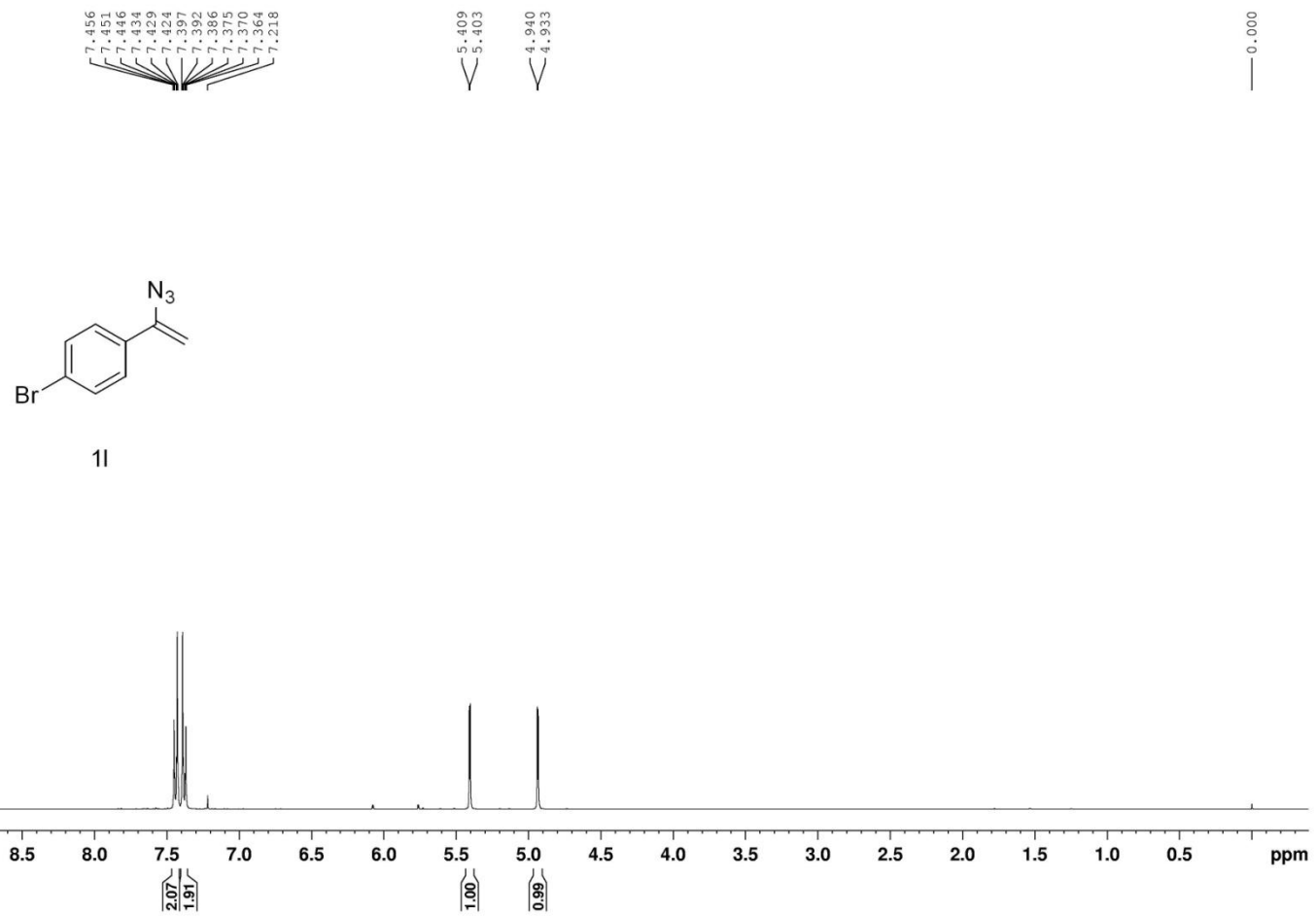
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7.370
7.364
7.218
5.409
5.403
4.940
4.933
0.000
N3
Br
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.07
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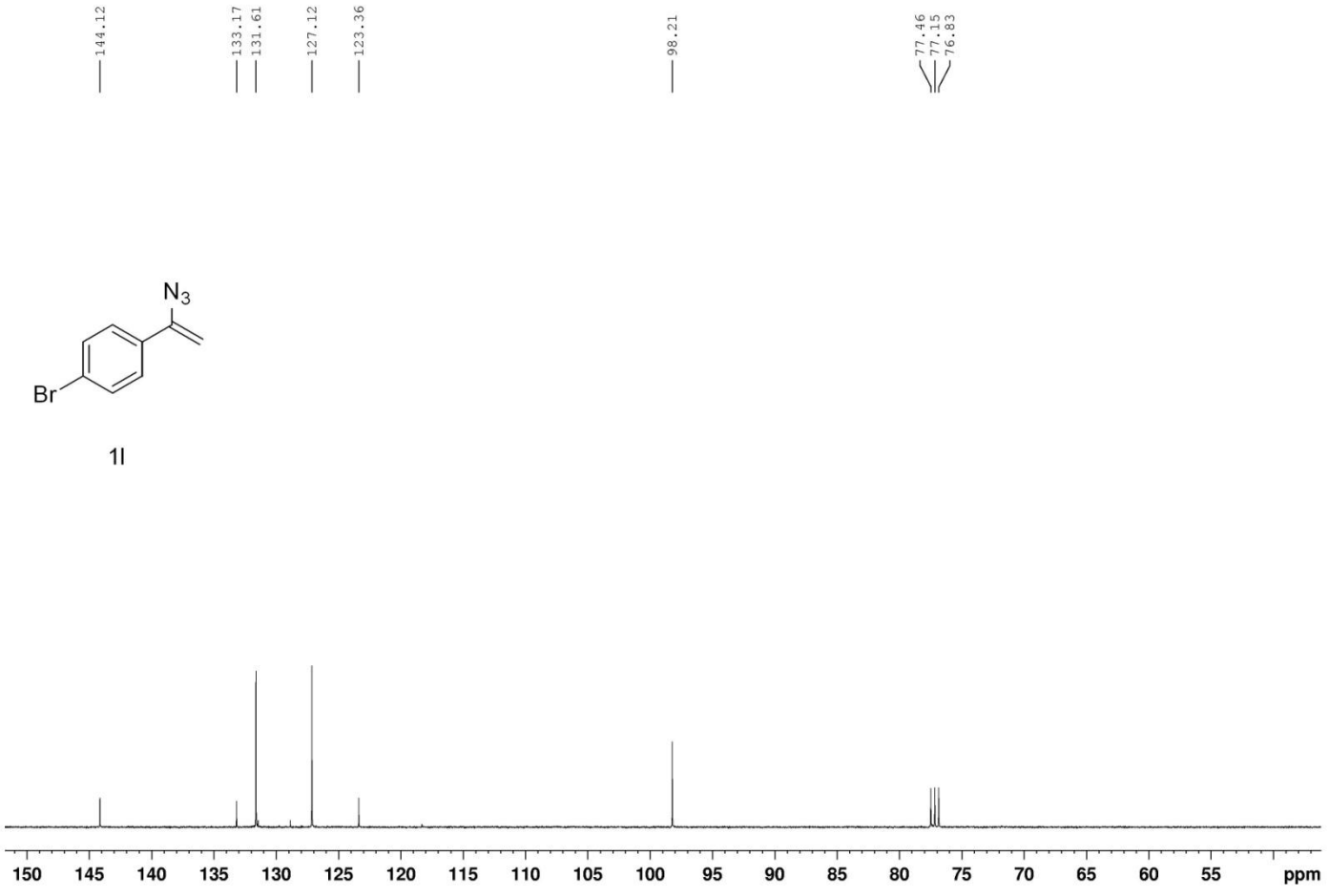
1l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Br
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145
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120
115
110
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80
75
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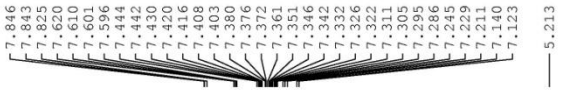
60
55
ppm

1l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7.442
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7.416
7.408
7.403
7.380
7.376
7.372
7.361
7.351
7.346
7.342
7.332
7.326
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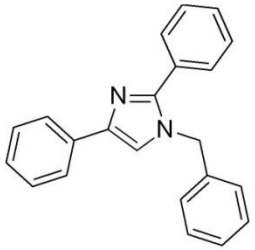
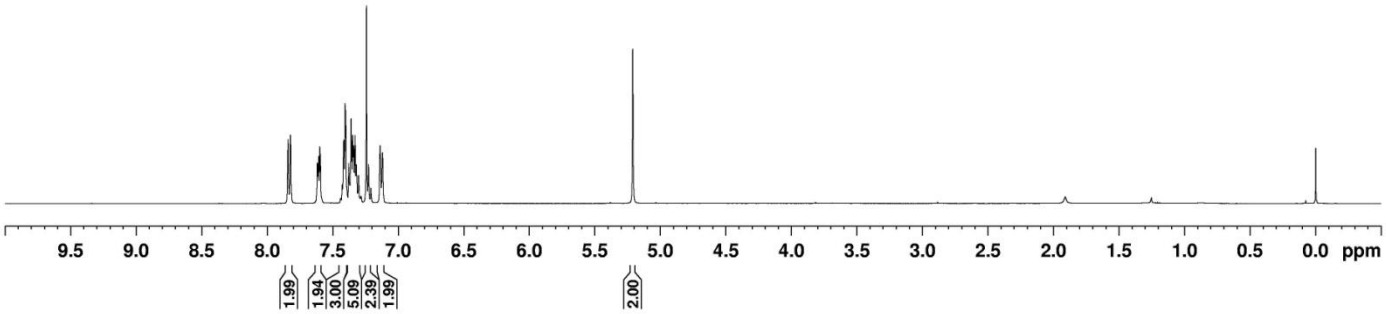

N
N

3aa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5.0
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4.0
3.5
3.0
2.5
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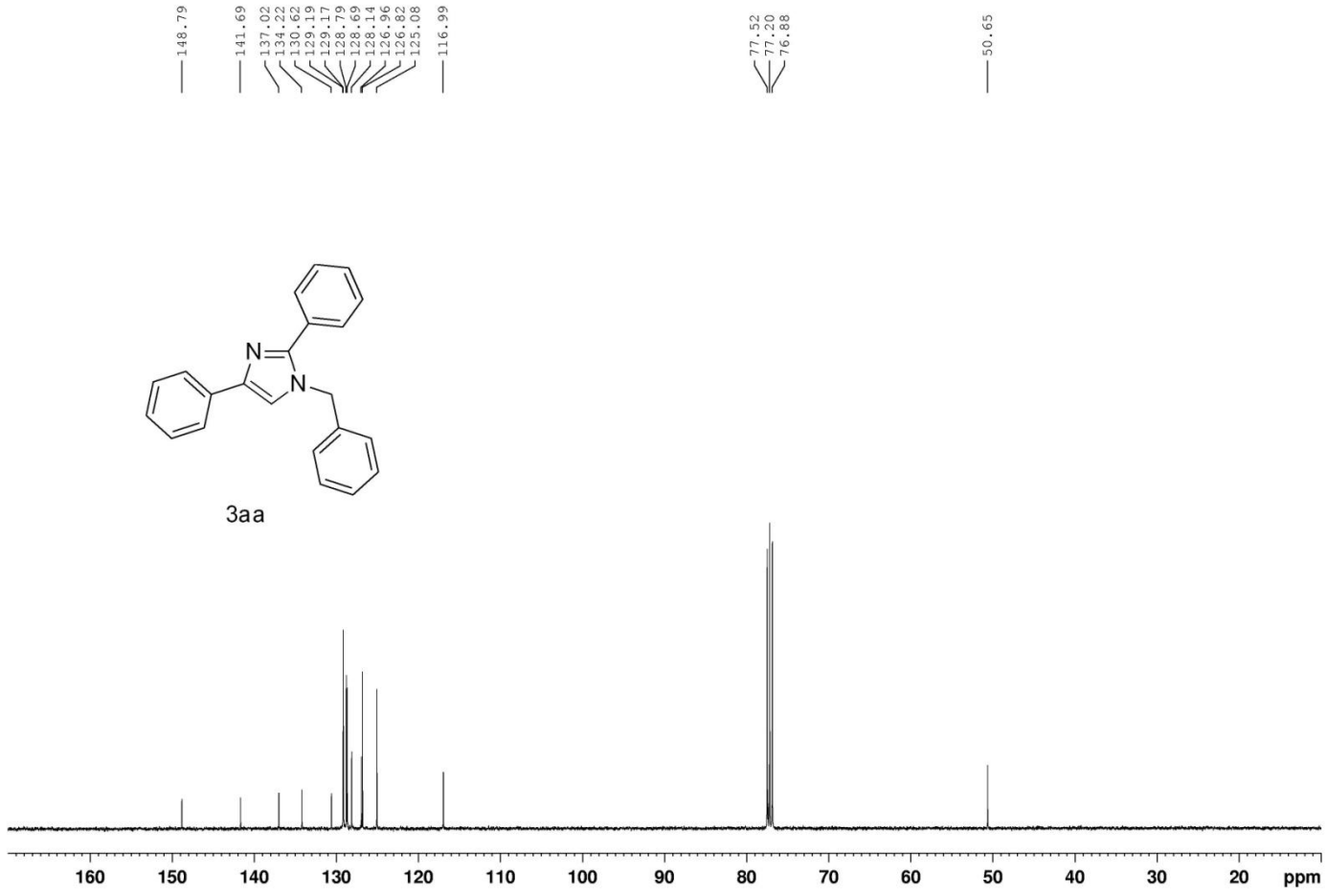
1.99
2.00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128.14
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126.82
125.08
116.99
77.52
77.20
76.88
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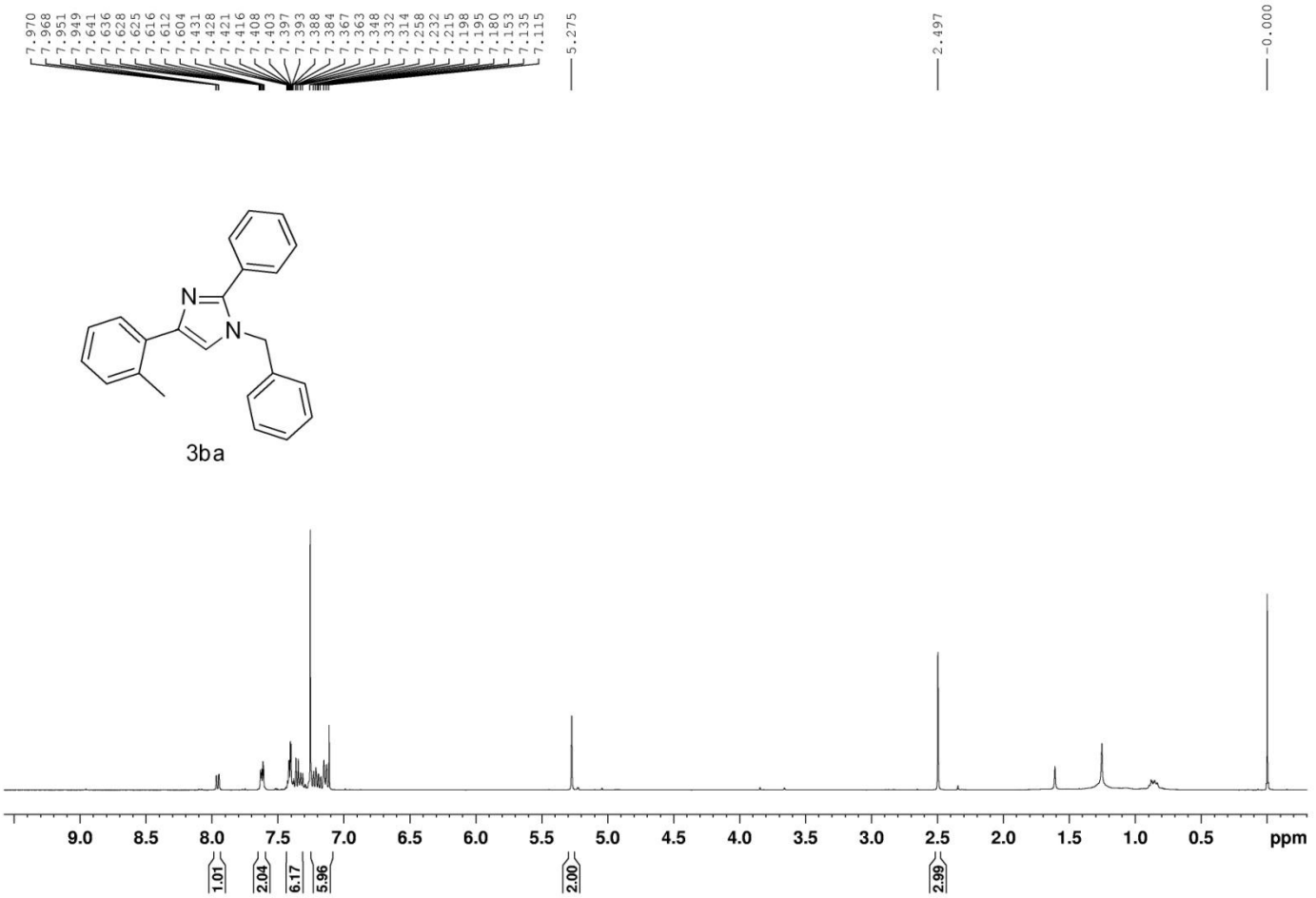
40
30
20
ppm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7.612
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7.431
7.428
7.421
7.416
7.408
7.403
7.397
7.393
7.388
7.384
7.367
7.363
7.348
7.332
7.314
7.258
7.232
7.215
7.198
7.195
7.180
7.153
7.135
7.115
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N
3ba
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8.0
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6.0
5.5
5.0
4.5
4.0
3.5
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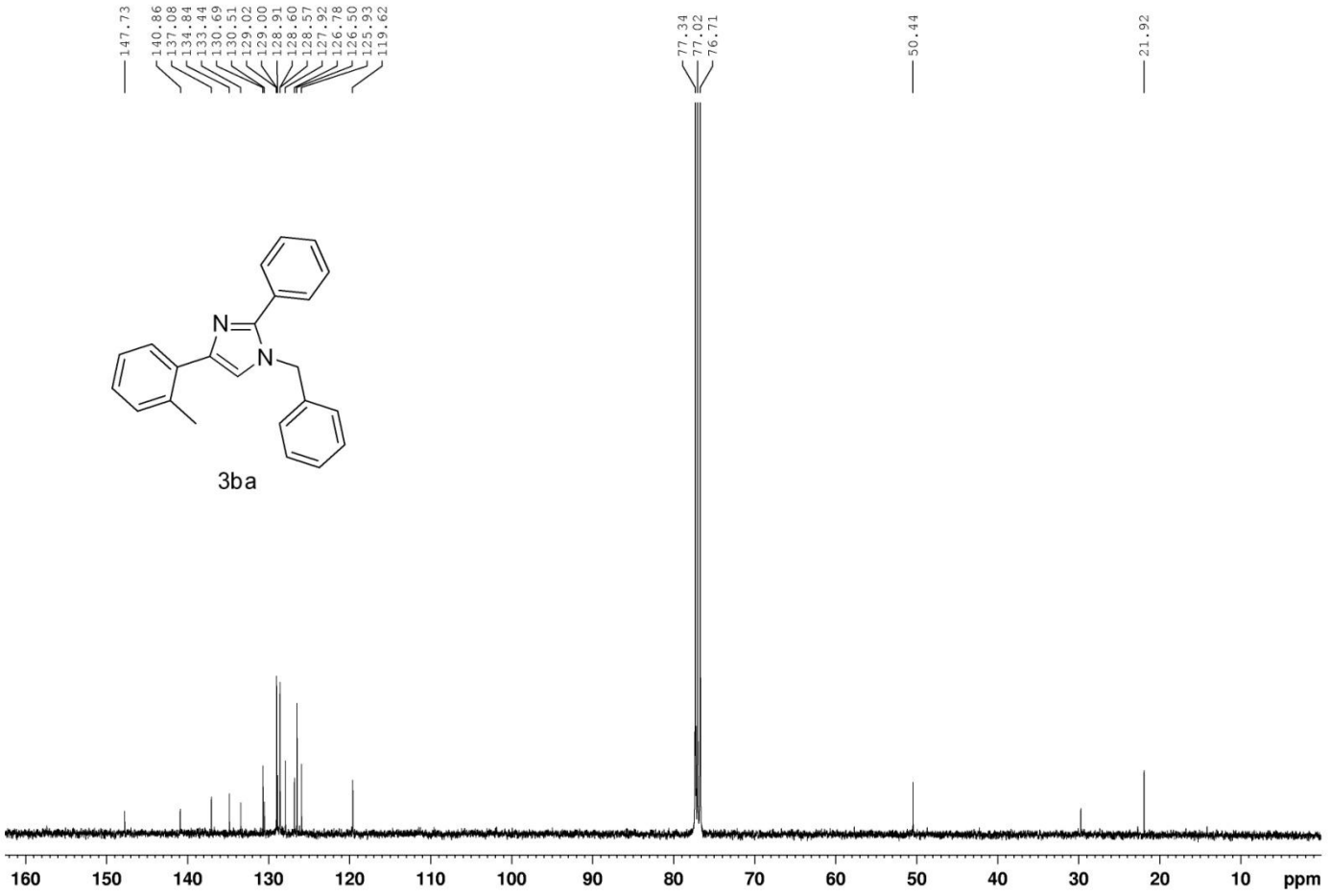
2.99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128.57
127.92
126.78
126.50
125.93
119.62
77.34
77.02
76.71
50.44
21.92
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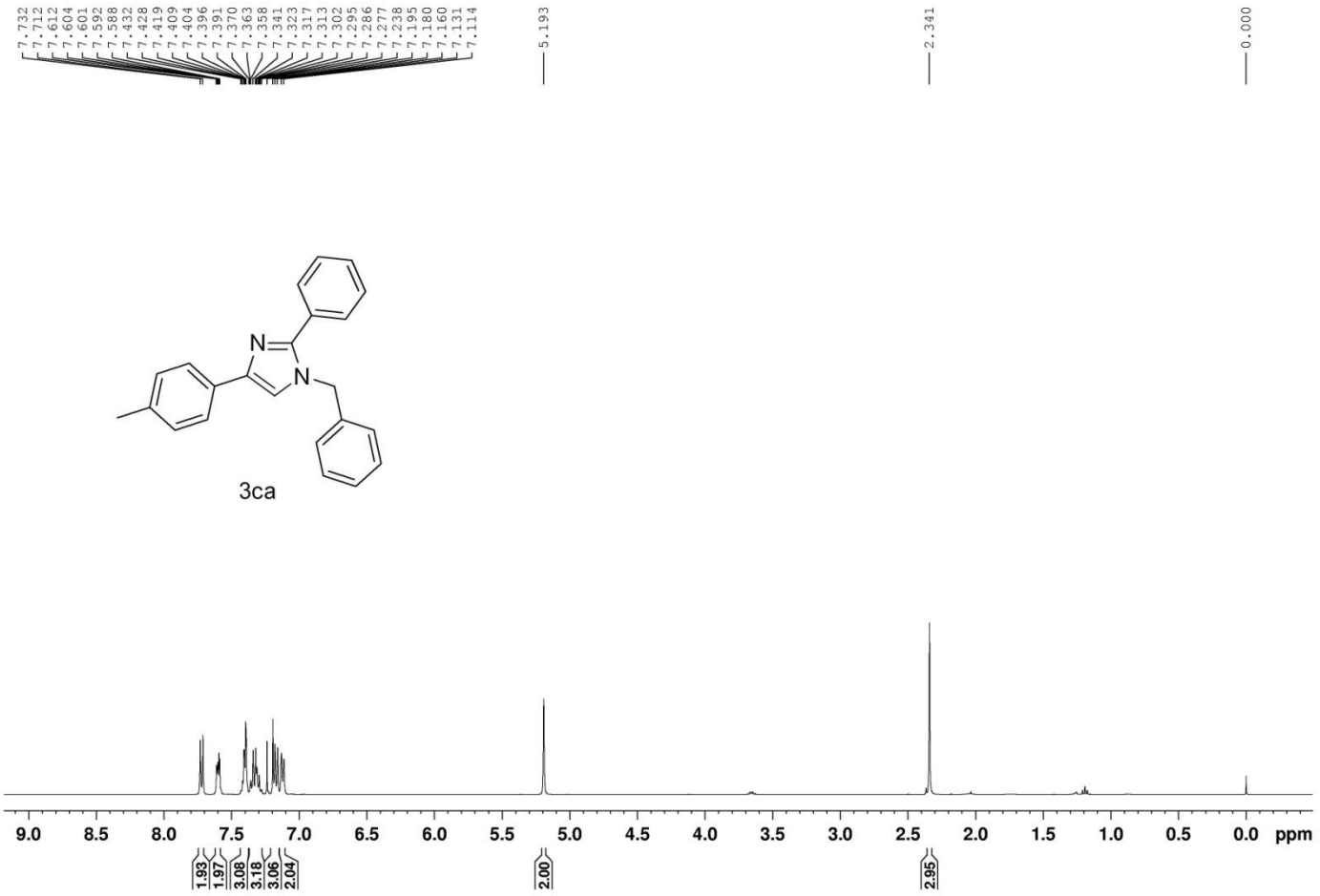
10
ppm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7.391
7.370
7.363
7.358
7.341
7.323
7.317
7.313
7.302
7.295
7.286
7.277
7.238
7.195
7.180
7.160
7.131
7.114
5.193
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8.0
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6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
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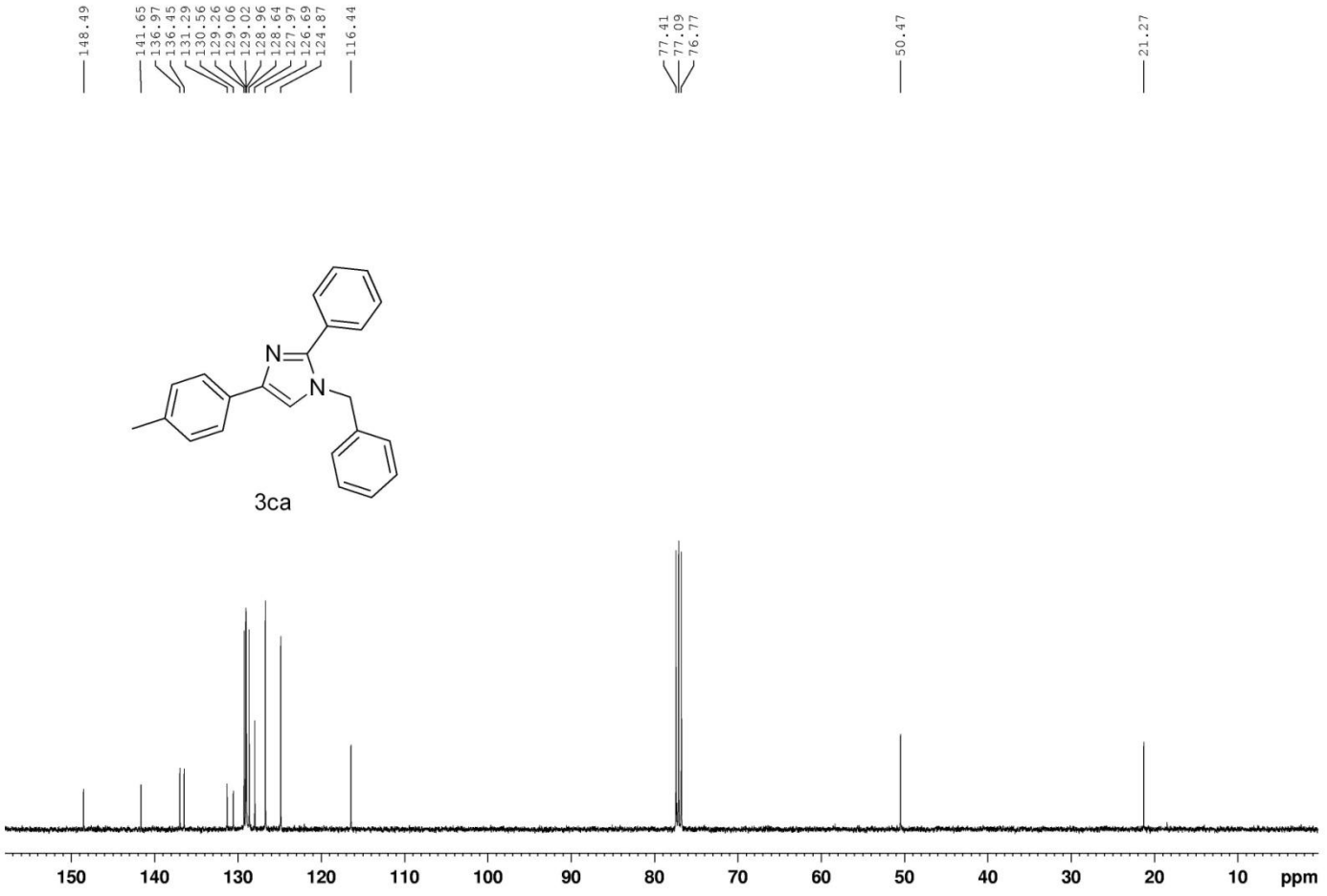
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136.45
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128.96
128.64
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126.69
124.87
116.44
77.41
77.09
76.77
50.47
21.27
N
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3ca
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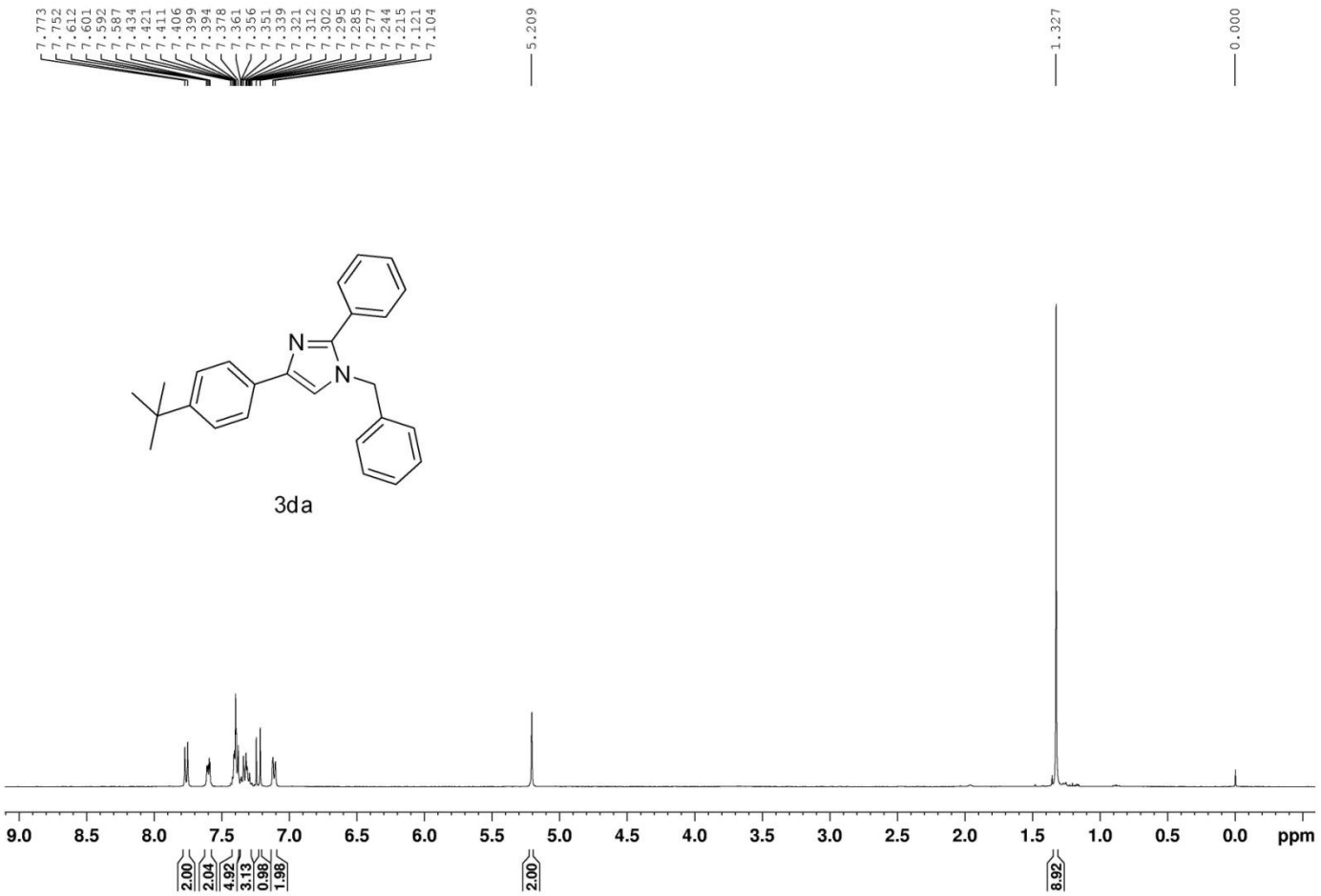
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.421
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7.394
7.378
7.361
7.356
7.351
7.339
7.321
7.312
7.302
7.295
7.285
7.277
7.244
7.215
7.121
7.104
5.209
1.327
0.000
N
N
3da
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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0.0
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3.13
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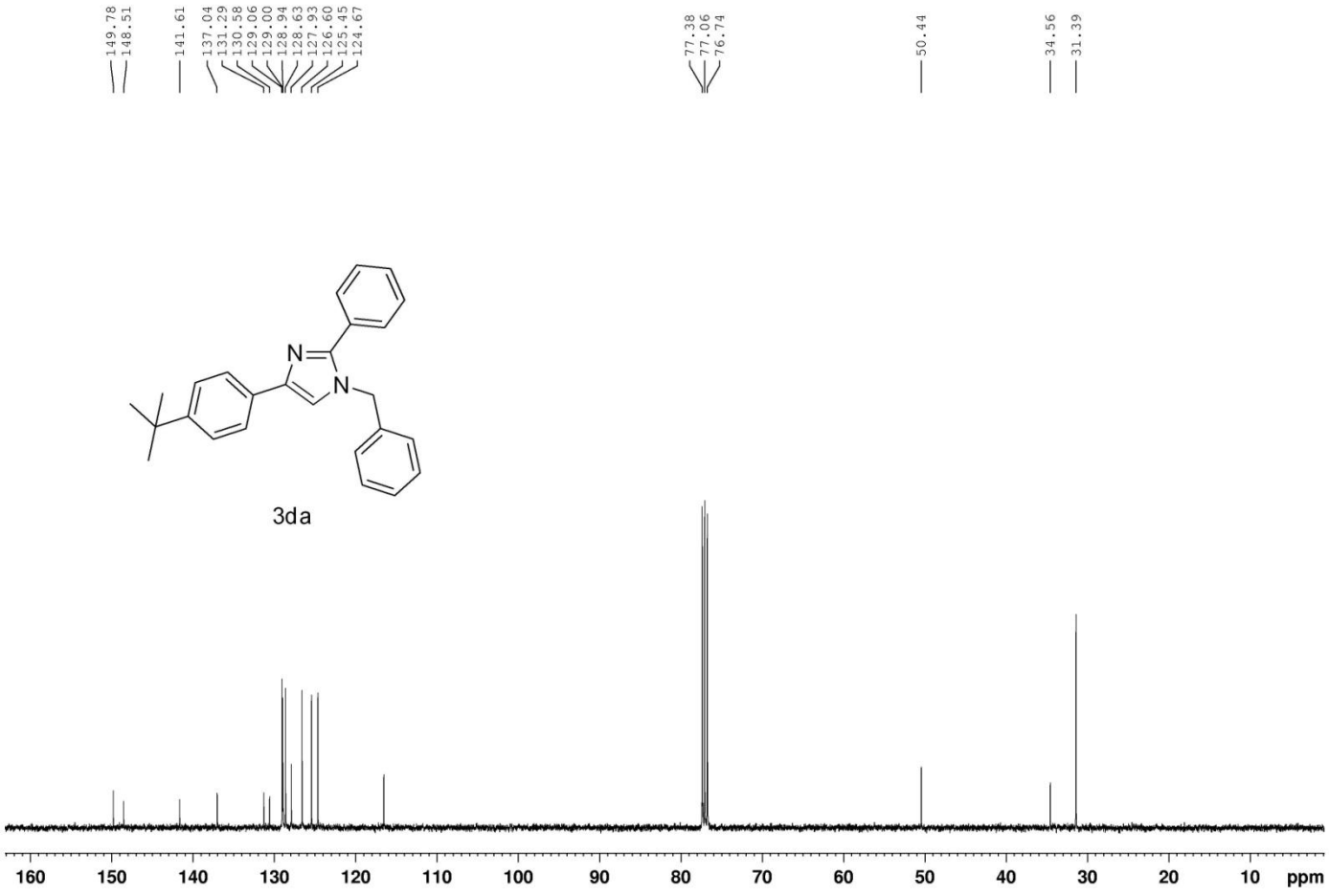
2.00
8.92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130.58
129.06
129.00
128.94
128.63
127.93
126.60
125.45
124.67
77.38
77.06
76.74
50.44
34.56
31.39
N
N
3da
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.823
7.643
7.630
7.622
7.619
7.611
7.606
7.598
7.437
7.424
7.414
7.409
7.401
7.396
7.375
7.371
7.367
7.354
7.350
7.336
7.320
7.309
7.302
7.294
7.284
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7.104
7.096
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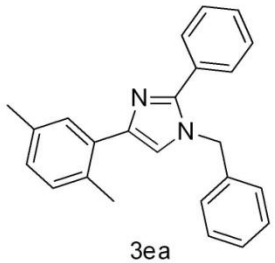
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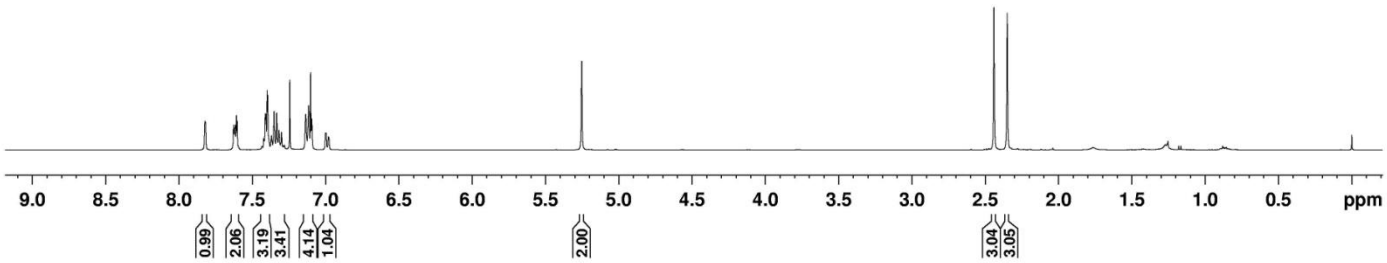
N

3ea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5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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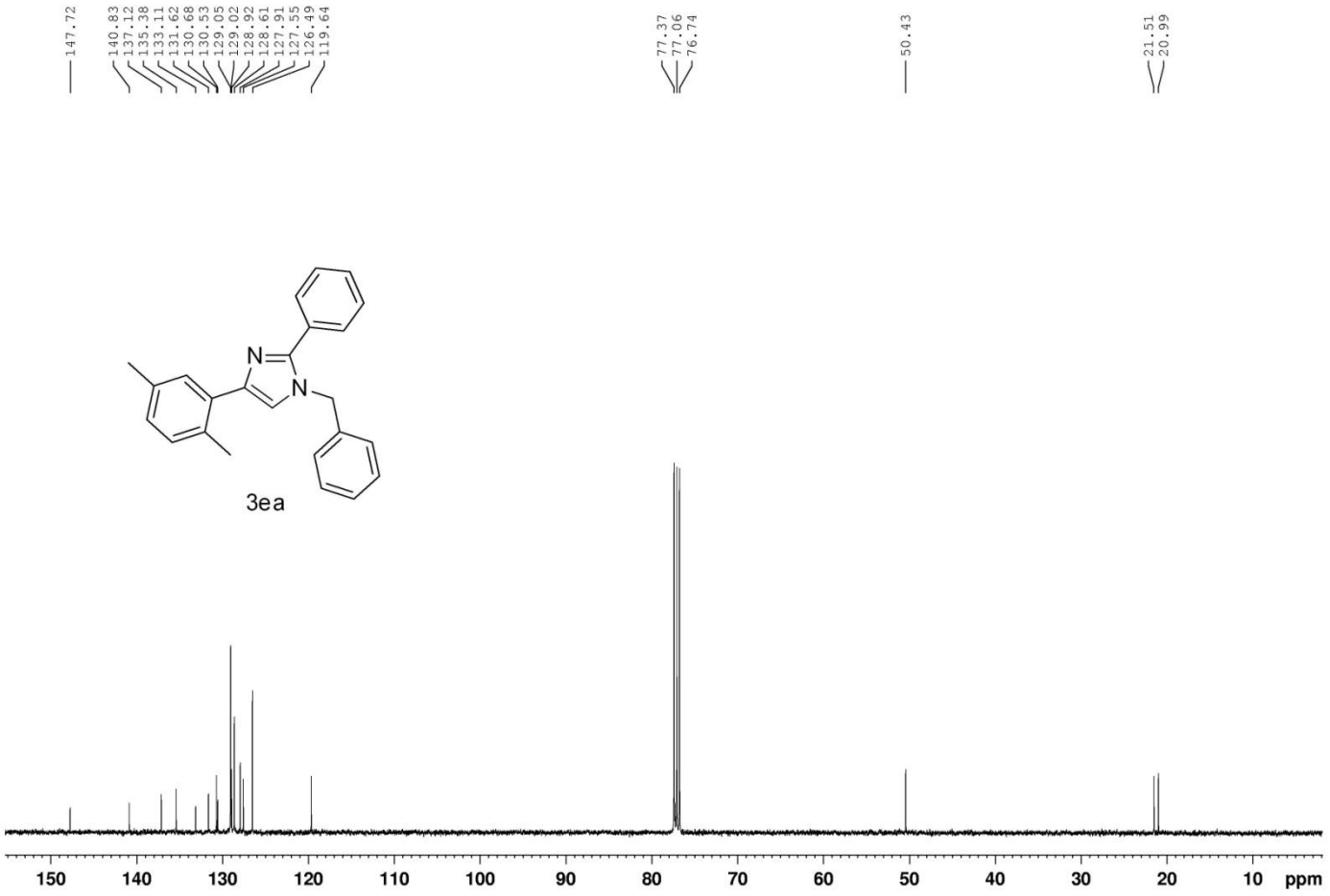
ppm
0.99
2.06
3.19
3.41
4.14
1.04
2.00
3.04
3.05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137.12
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130.53
129.05
129.02
128.92
128.61
127.91
127.55
126.49
119.64
77.37
77.06
76.74
50.43
21.51
20.99
N
N
3ea
150
140
130
120
110
100
90
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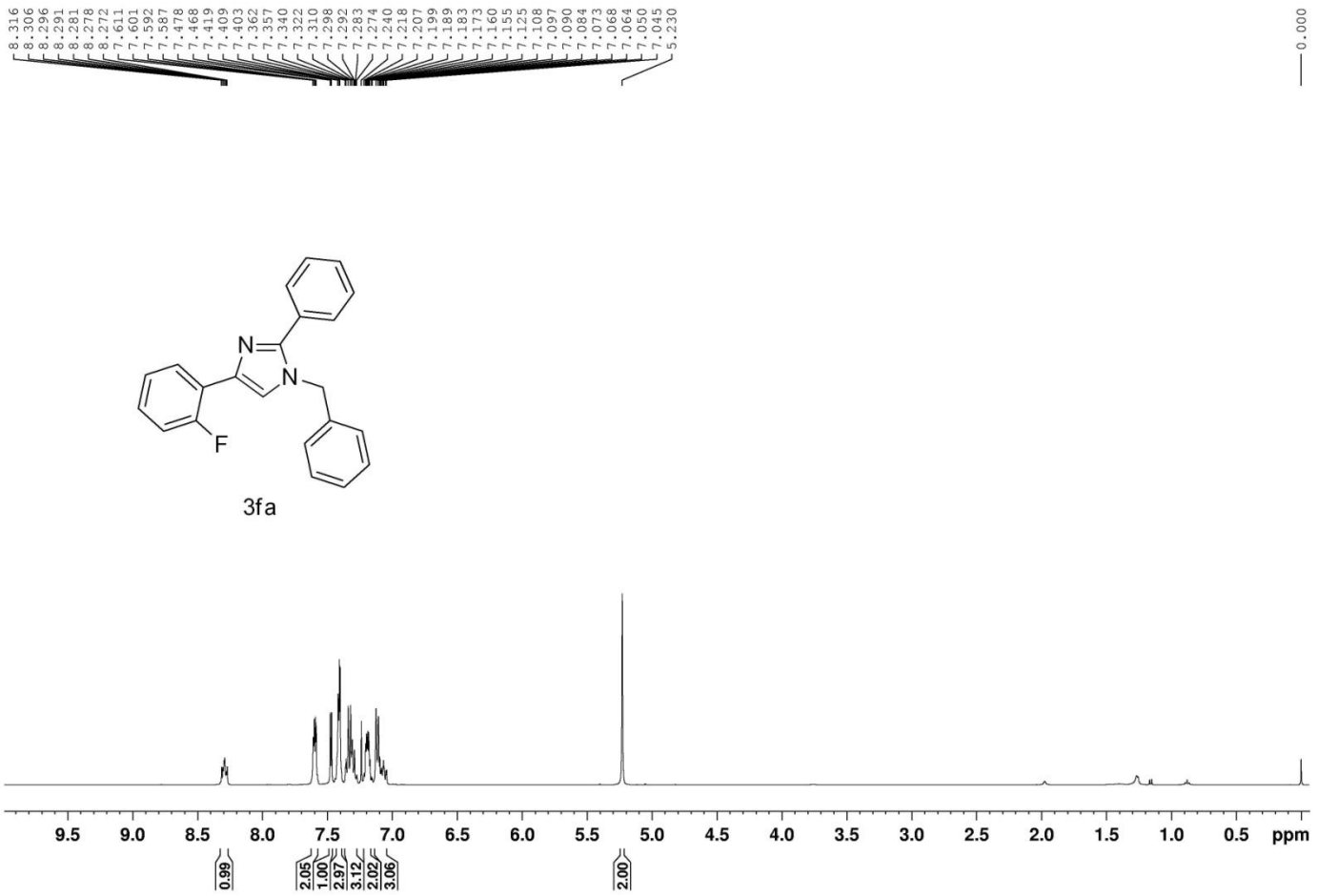
70
60
50
40
30
20
10
ppm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8.278
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7.611
7.601
7.592
7.587
7.478
7.468
7.419
7.409
7.403
7.362
7.357
7.340
7.322
7.310
7.298
7.292
7.283
7.274
7.240
7.218
7.207
7.199
7.189
7.183
7.173
7.160
7.155
7.125
7.108
7.097
7.090
7.084
7.073
7.068
7.064
7.050
7.045
5.230
0.000
N
N
F
3fa
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
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0.5
ppm
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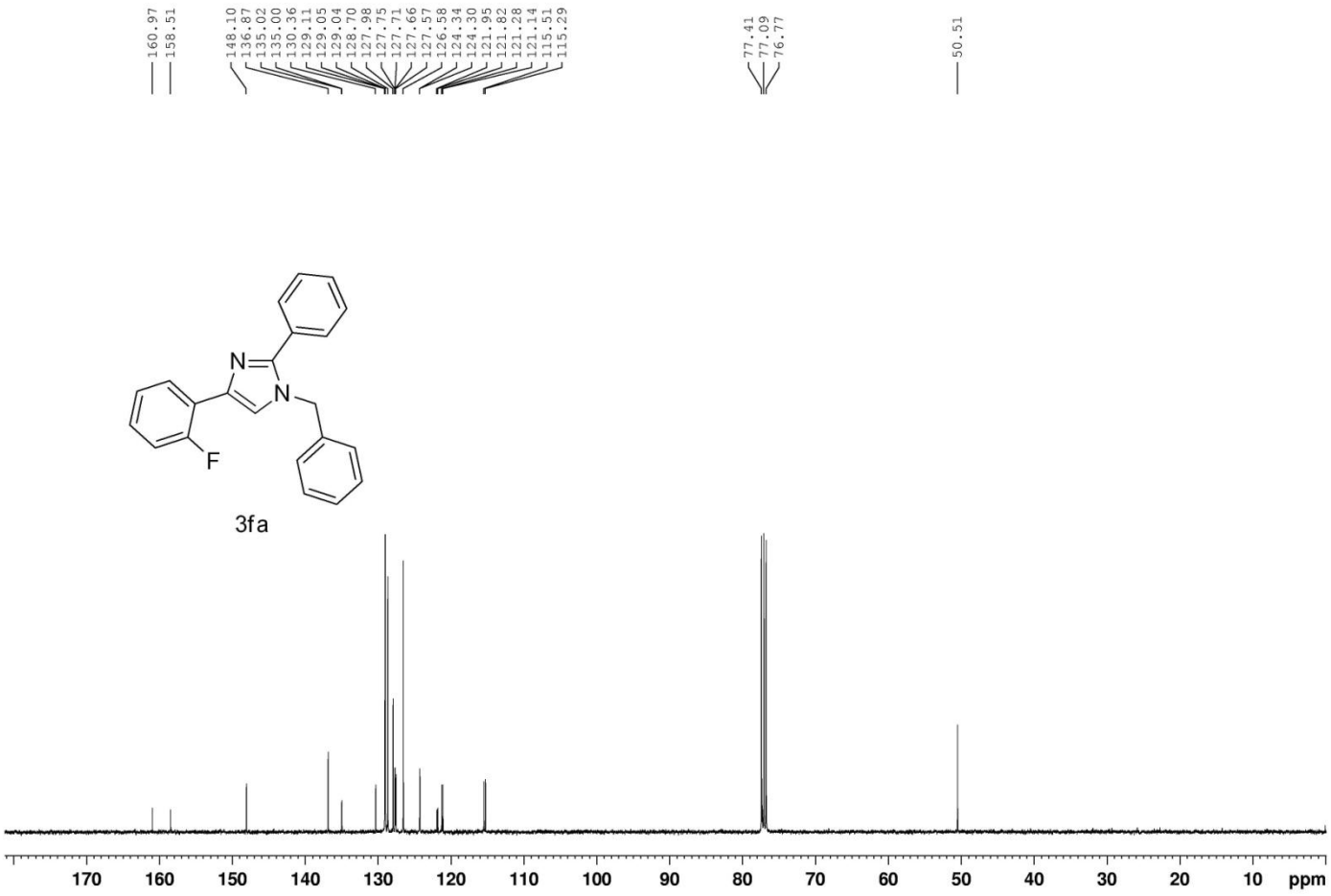
1.00
2.97
3.12
2.02
3.06
2.00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129.11
129.05
129.04
128.70
127.98
127.75
127.71
127.66
127.57
126.58
124.34
124.30
121.95
121.82
121.28
121.14
115.51
115.29
77.41
77.09
76.77
50.51
N
N
F
3fa
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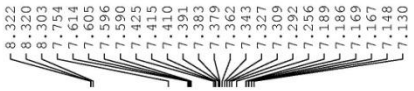
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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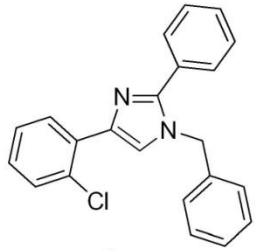
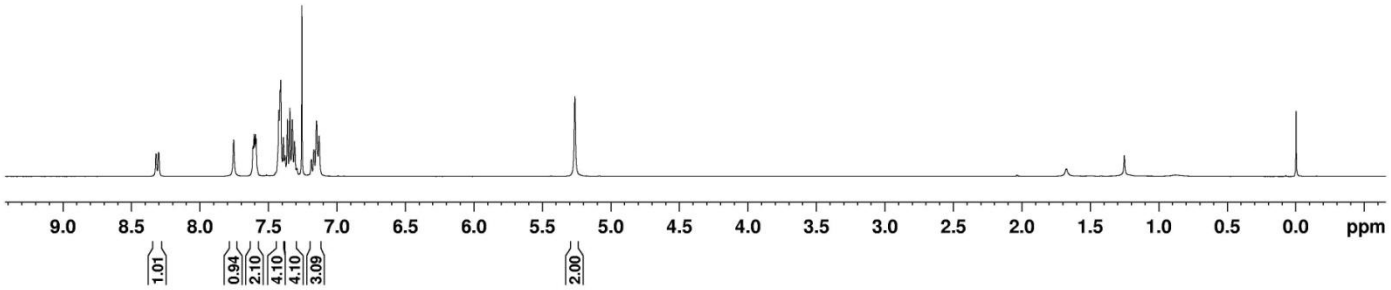
8.320
8.303
7.754
7.614
7.605
7.596
7.590
7.425
7.415
7.410
7.391
7.383
7.379
7.362
7.343
7.327
7.309
7.292
7.256
7.189
7.186
7.169
7.167
7.148
7.130
5.266
0.000


N
N
Cl

3ga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8.0
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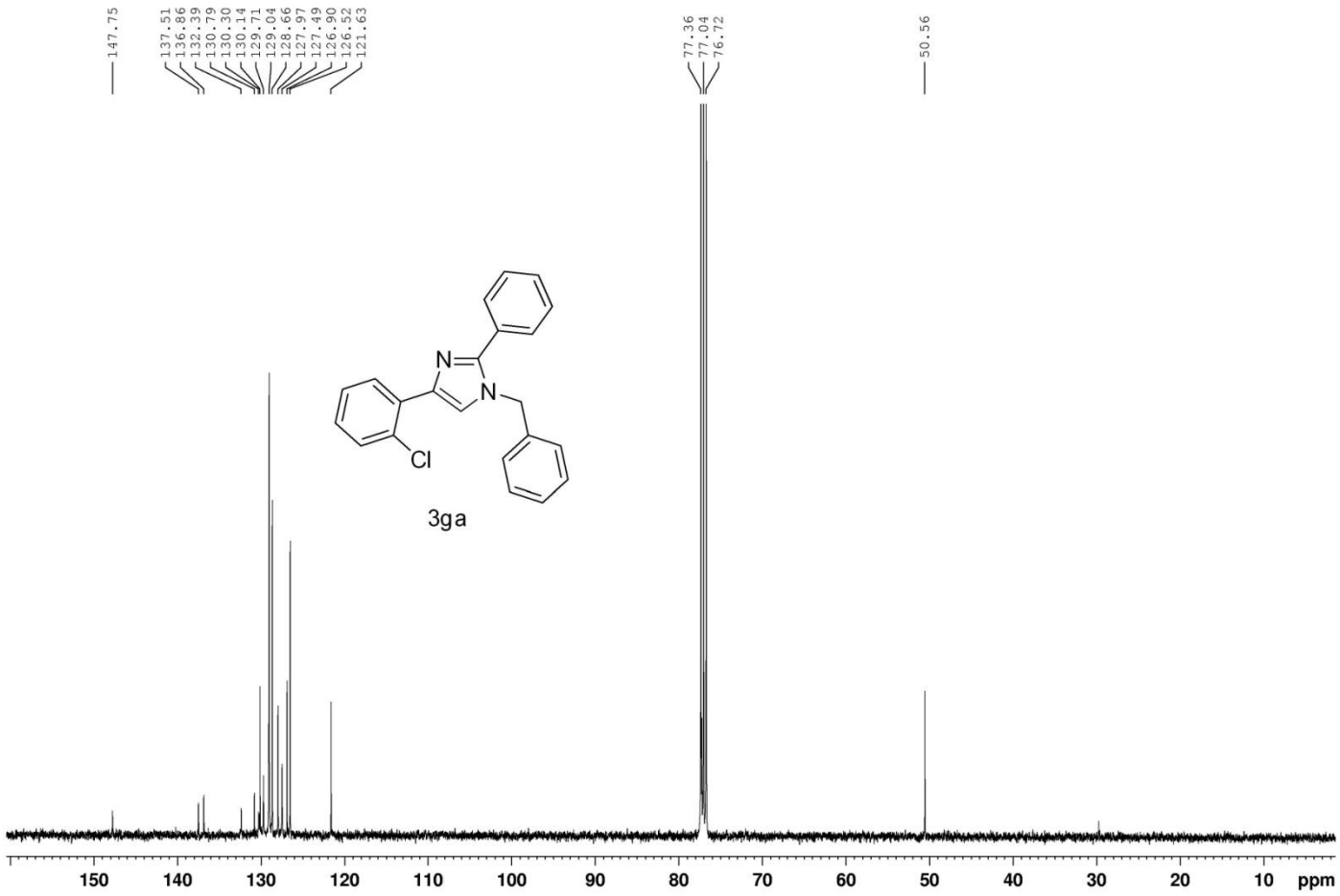
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.01
0.94
2.10
4.10
4.10
3.09
2.00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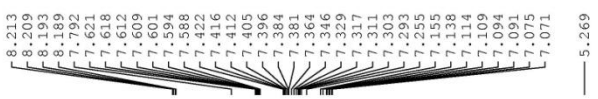
130.30
130.14
129.71
129.04
128.66
127.97
127.49
126.90
126.52
121.63
77.36
77.04
76.72
50.56
N
N
Cl
3ga
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.209
8.193
8.189
7.792
7.621
7.618
7.612
7.609
7.601
7.594
7.588
7.422
7.416
7.412
7.405
7.396
7.384
7.381
7.364
7.346
7.329
7.317
7.311
7.303
7.293
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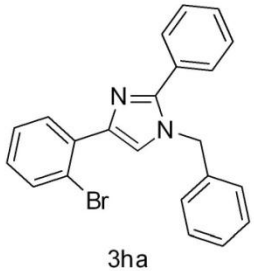
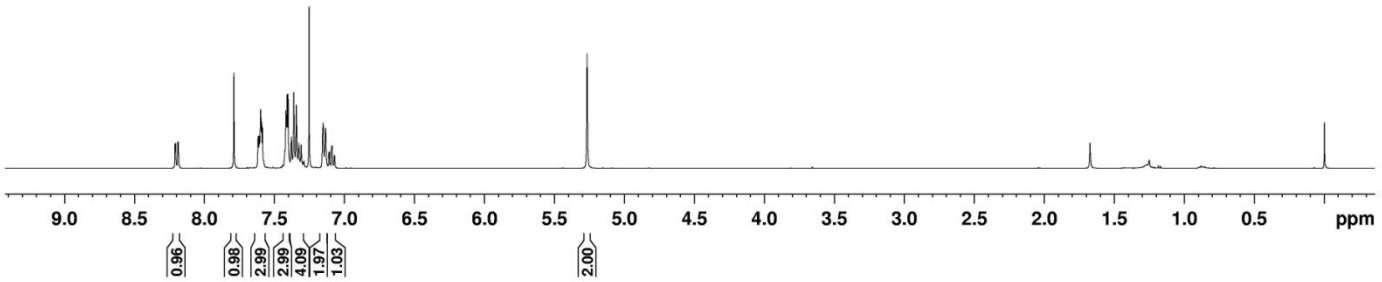
7.155
7.138
7.114
7.109
7.094
7.091
7.075
7.071
5.269
0.000


N
N
Br

3ha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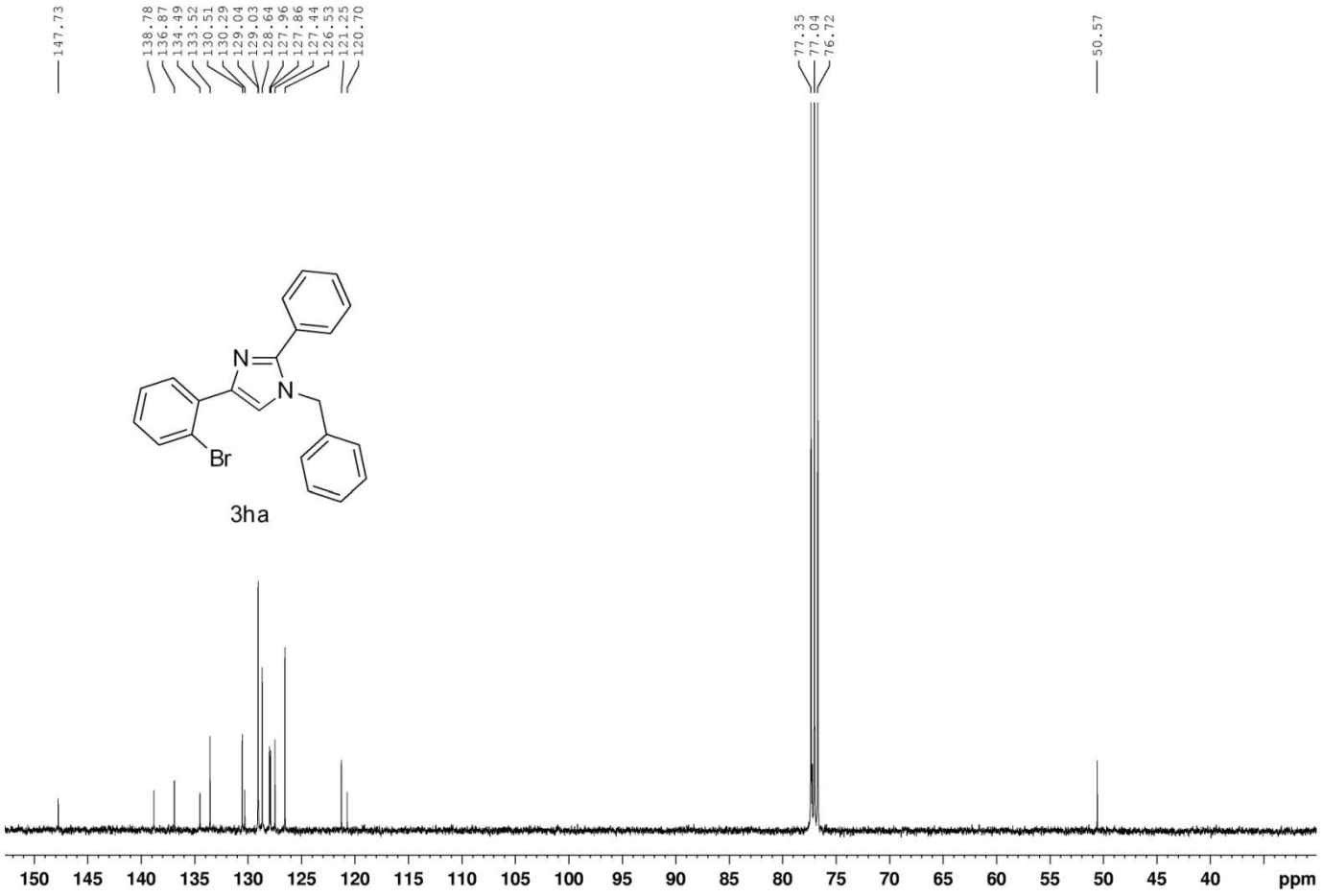
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.96
0.98
2.99
2.99
4.09
1.97
1.03
2.00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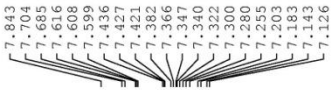
136.87
134.49
133.52
130.51
130.29
129.04
129.03
128.64
127.96
127.86
127.44
126.53
121.25
120.70
77.35
77.04
76.72
50.57
N
N
Br
3ha
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 ppm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7.704
7.685
7.616
7.608
7.599
7.436
7.427
7.421
7.382
7.366
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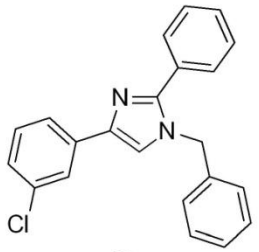
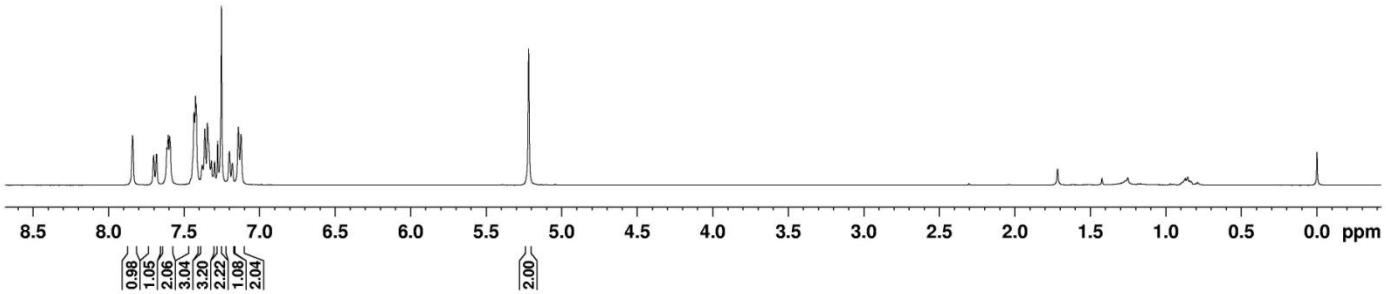
7.340
7.322
7.300
7.280
7.255
7.203
7.183
7.143
7.126

5.221

0.001


N
N
Cl

3ia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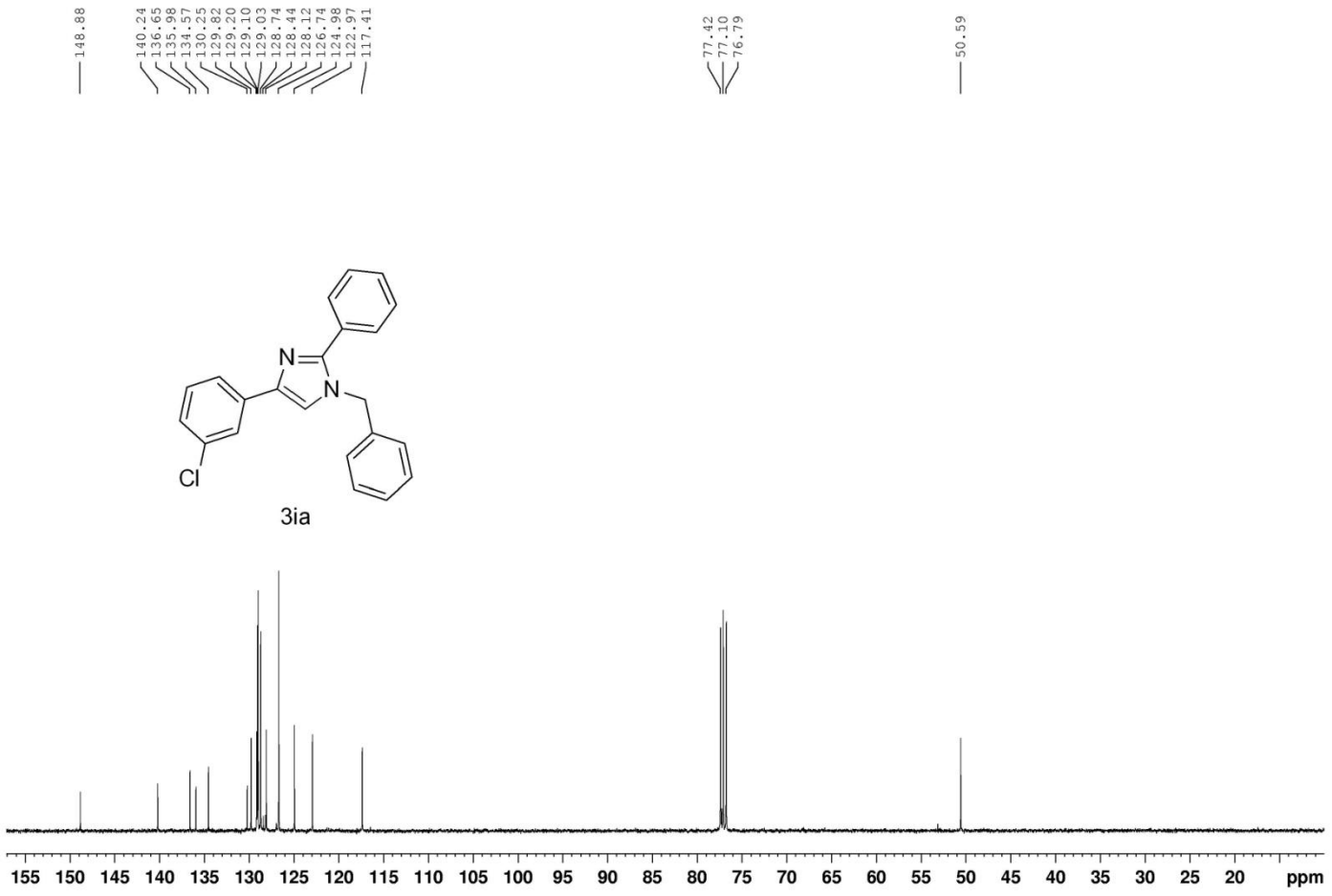
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.98
1.05
2.06
3.04
3.20
2.22
1.08
2.04
2.00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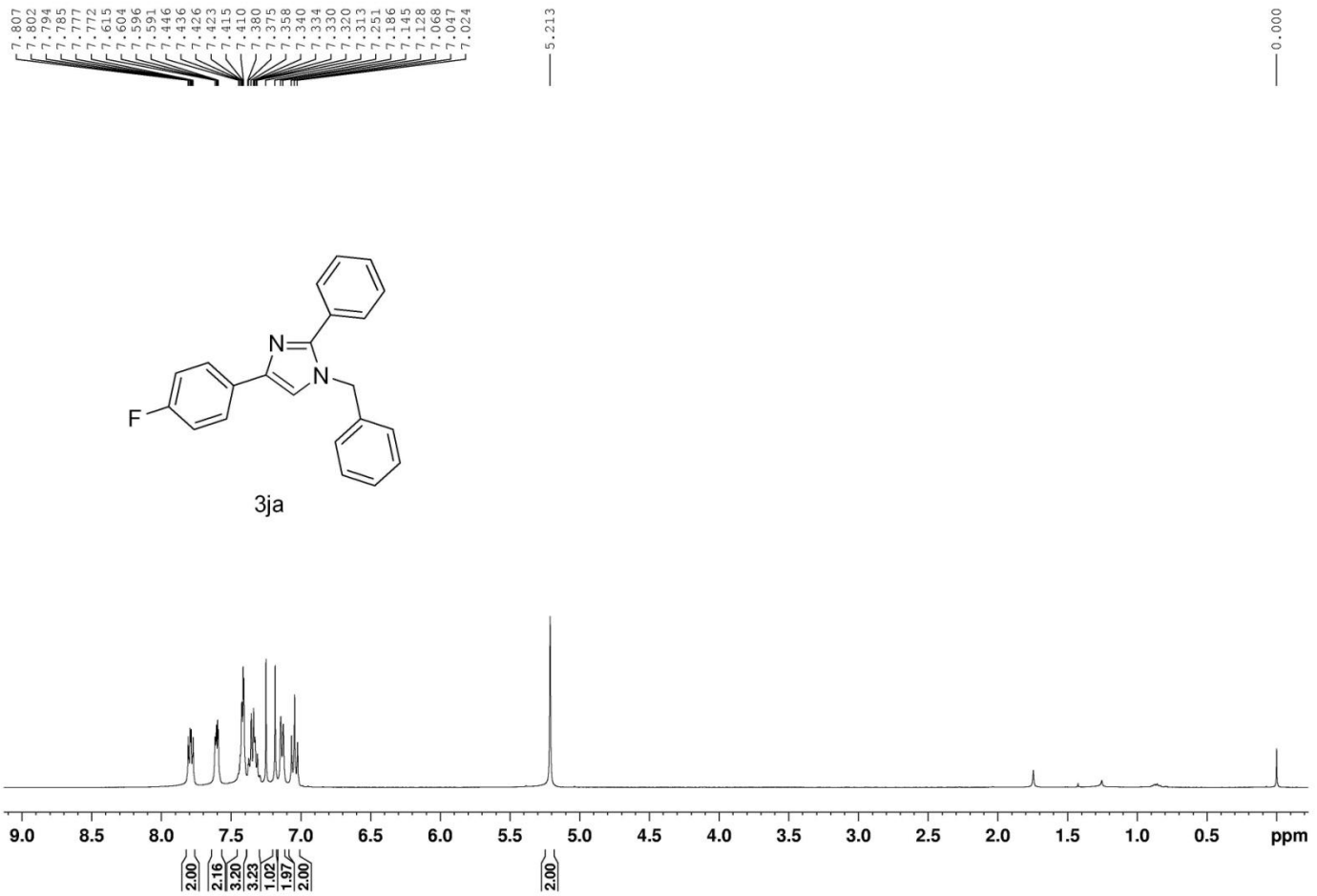
140.24
136.65
135.98
134.57
130.25
129.82
129.20
129.10
129.03
128.74
128.44
128.12
126.74
124.98
122.97
117.41
77.42
77.10
76.79
50.59
N
N
Cl
3ia
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 ppm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7.785
7.777
7.772
7.615
7.604
7.596
7.591
7.446
7.436
7.426
7.423
7.415
7.410
7.380
7.375
7.358
7.340
7.334
7.330
7.320
7.313
7.251
7.186
7.145
7.128
7.068
7.047
7.024
5.213
0.000
N
N
F
3ja
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
ppm
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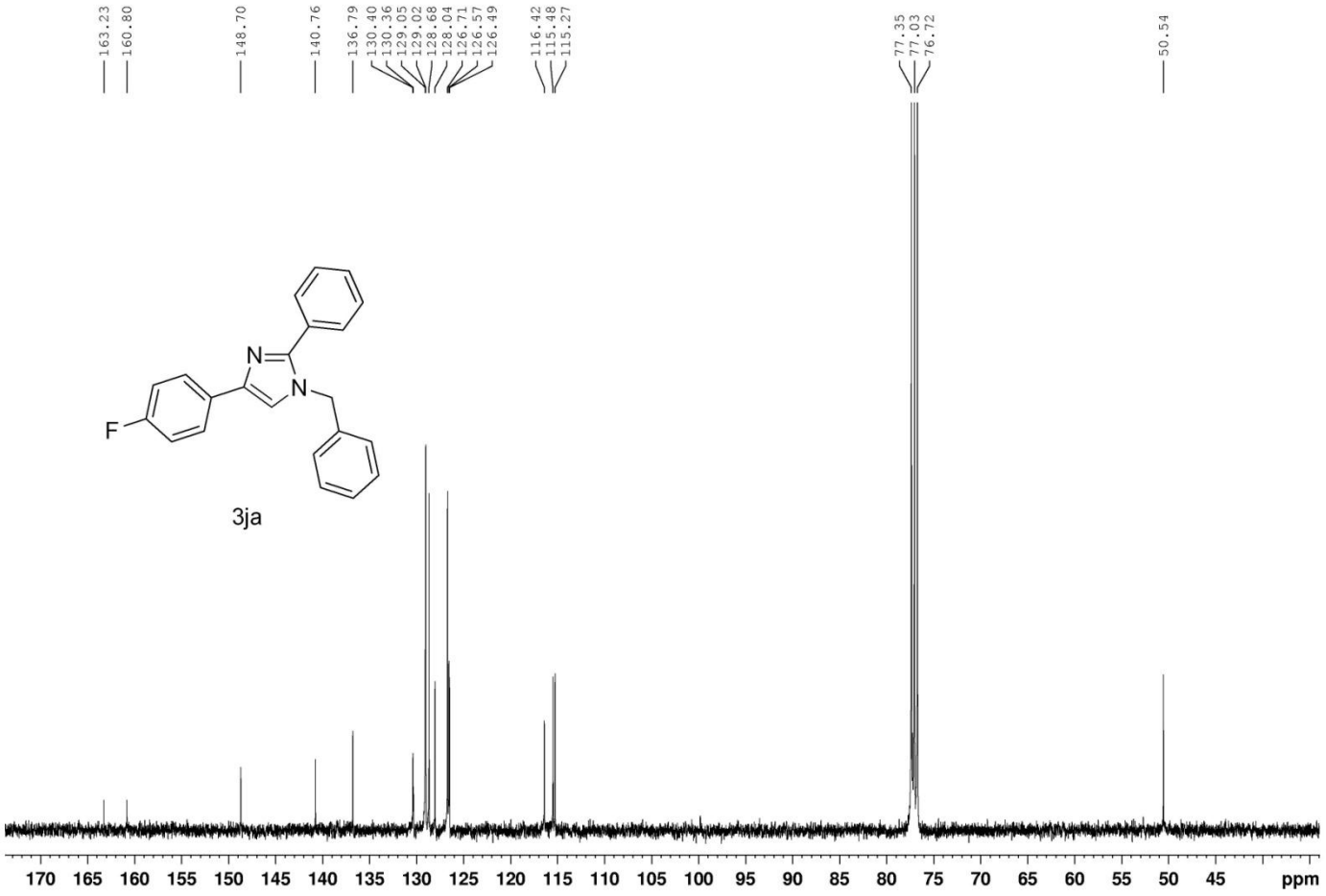
3.20
3.23
1.02
1.97
2.00
2.00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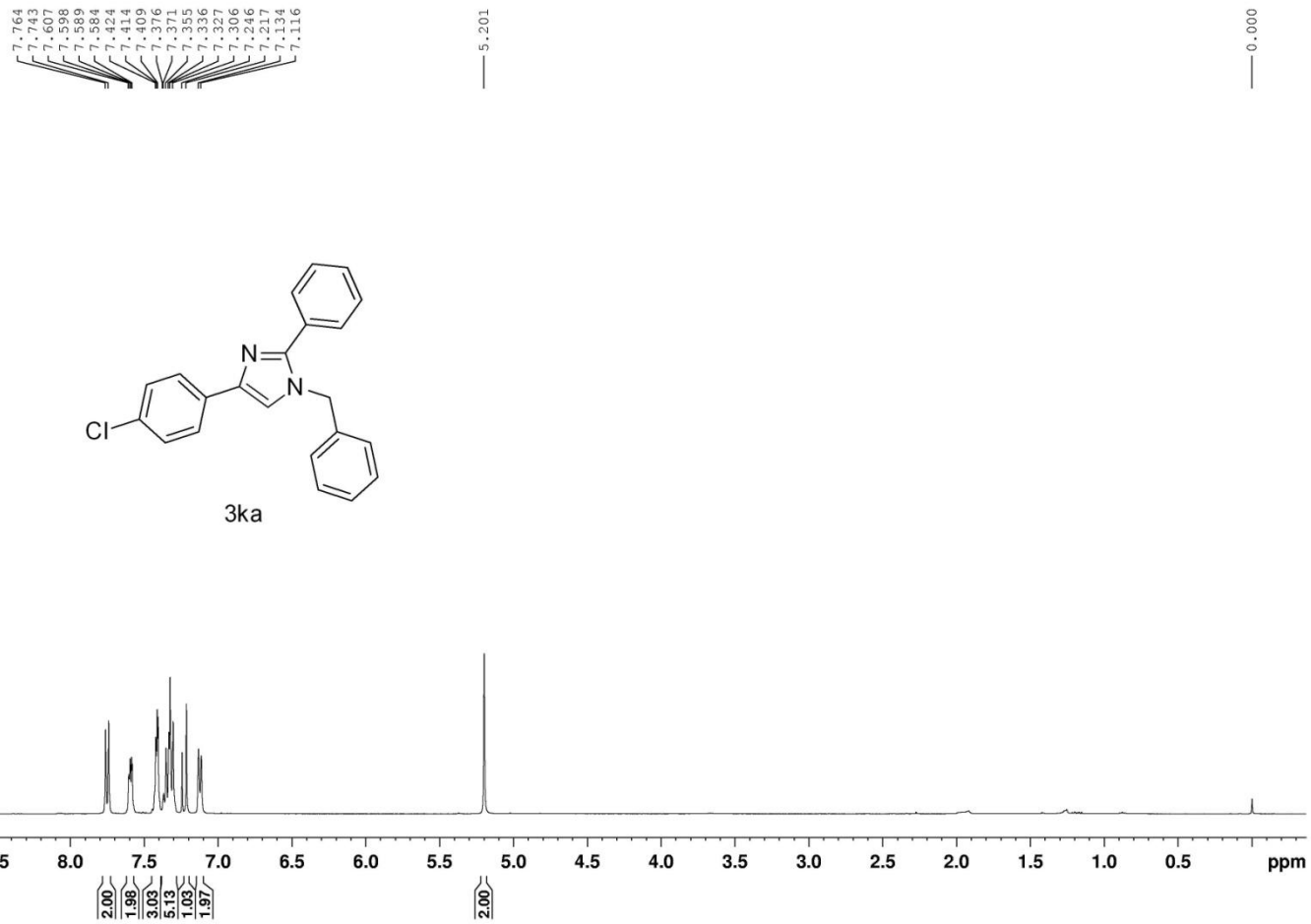
148.70
140.76
136.79
130.40
130.36
129.05
129.02
128.68
128.04
126.71
126.57
126.49
116.42
115.48
115.27
77.35
77.03
76.72
50.54
N
N
F
3ja
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 ppm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7.607
7.598
7.589
7.584
7.424
7.414
7.409
7.376
7.371
7.355
7.336
7.327
7.306
7.246
7.217
7.134
7.116
5.201
0.000
N
N
Cl
3ka
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
ppm
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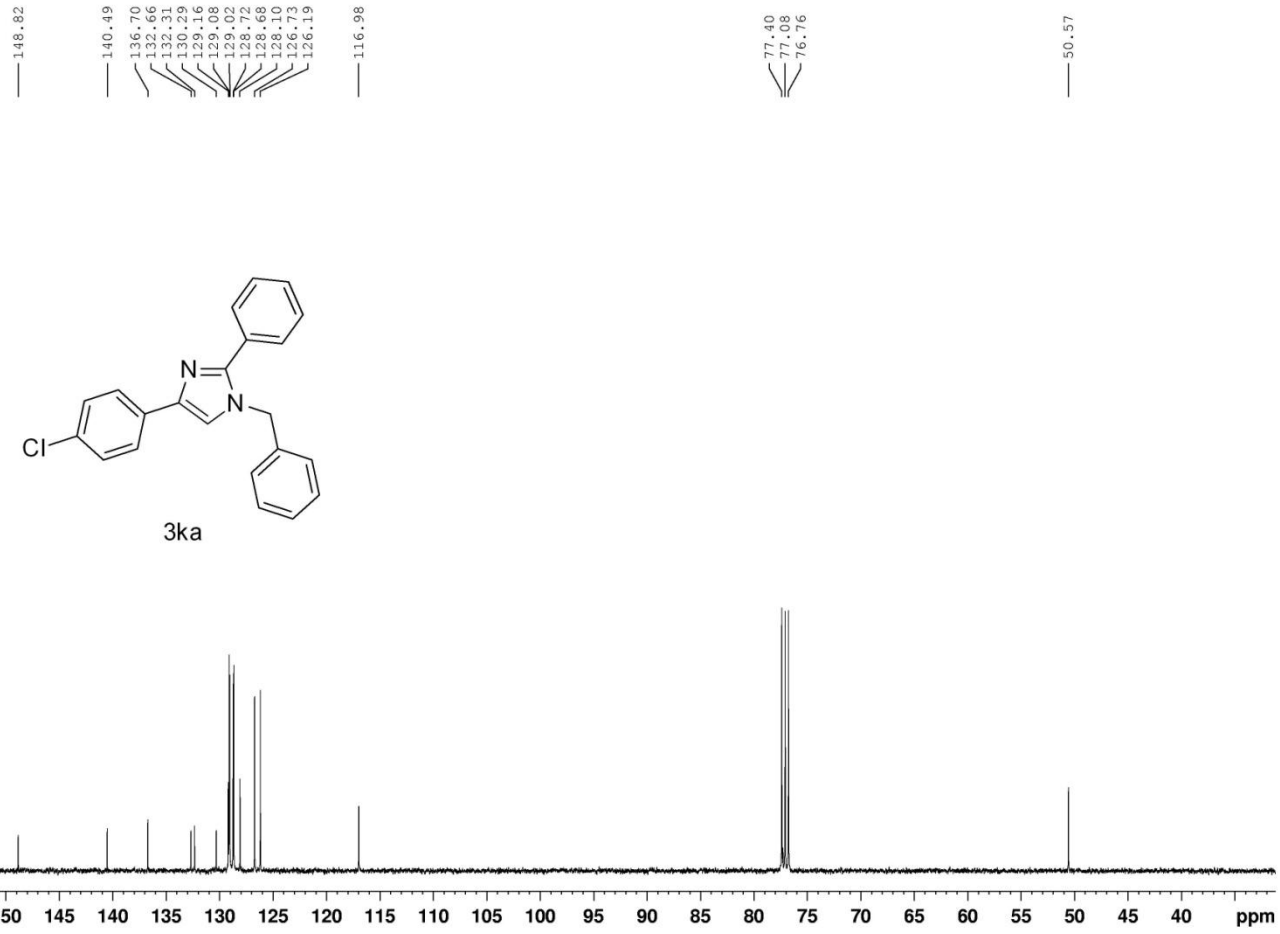
3.03
5.13
1.03
1.97
2.00


148.82
140.49
136.70
132.66
132.31
130.29
129.16
129.08
129.02
128.72
128.68
128.10
126.73
126.19
116.98
77.40
77.08
76.76
50.57
N
N
Cl
3ka
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 ppm


7.713
7.707
7.702
7.690
7.686
7.680
7.607
7.602
7.598
7.589
7.583
7.574
7.485
7.479
7.474
7.462
7.457
7.451
7.435
7.432
7.426
7.424
7.415
7.410
7.400
7.378
7.373
7.368
7.356
7.338
7.330
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7.313
7.303
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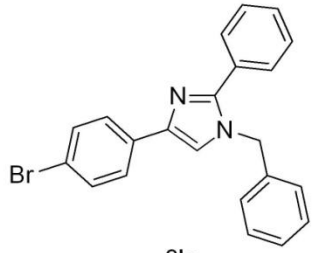
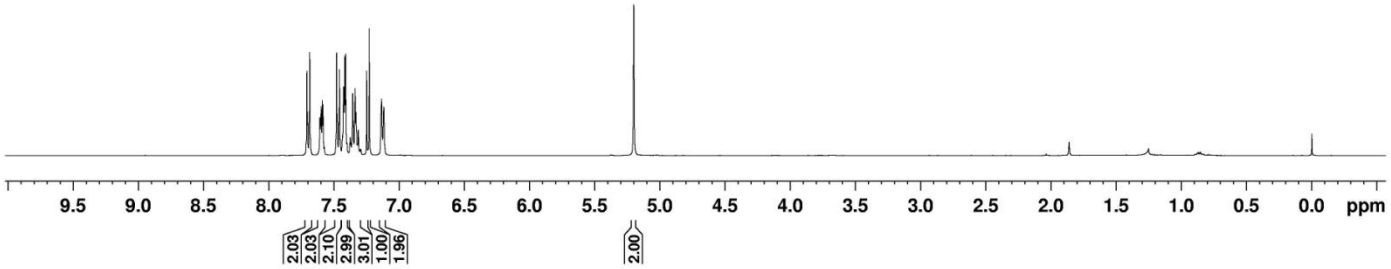
7.134
7.118
5.202

0.000


N
N
Br

3Ia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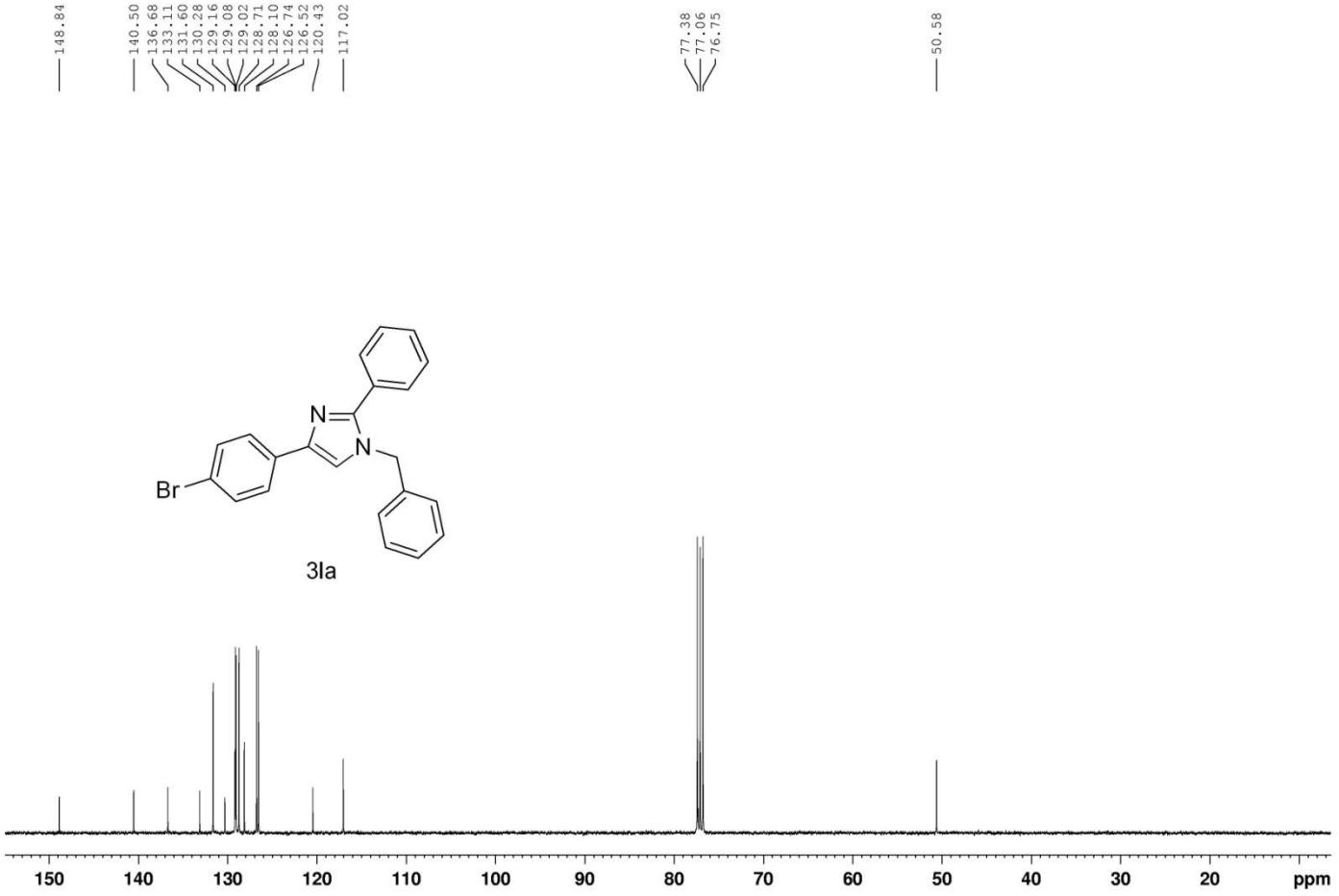
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.03
2.03
2.10
2.99
3.01
1.00
1.96
2.00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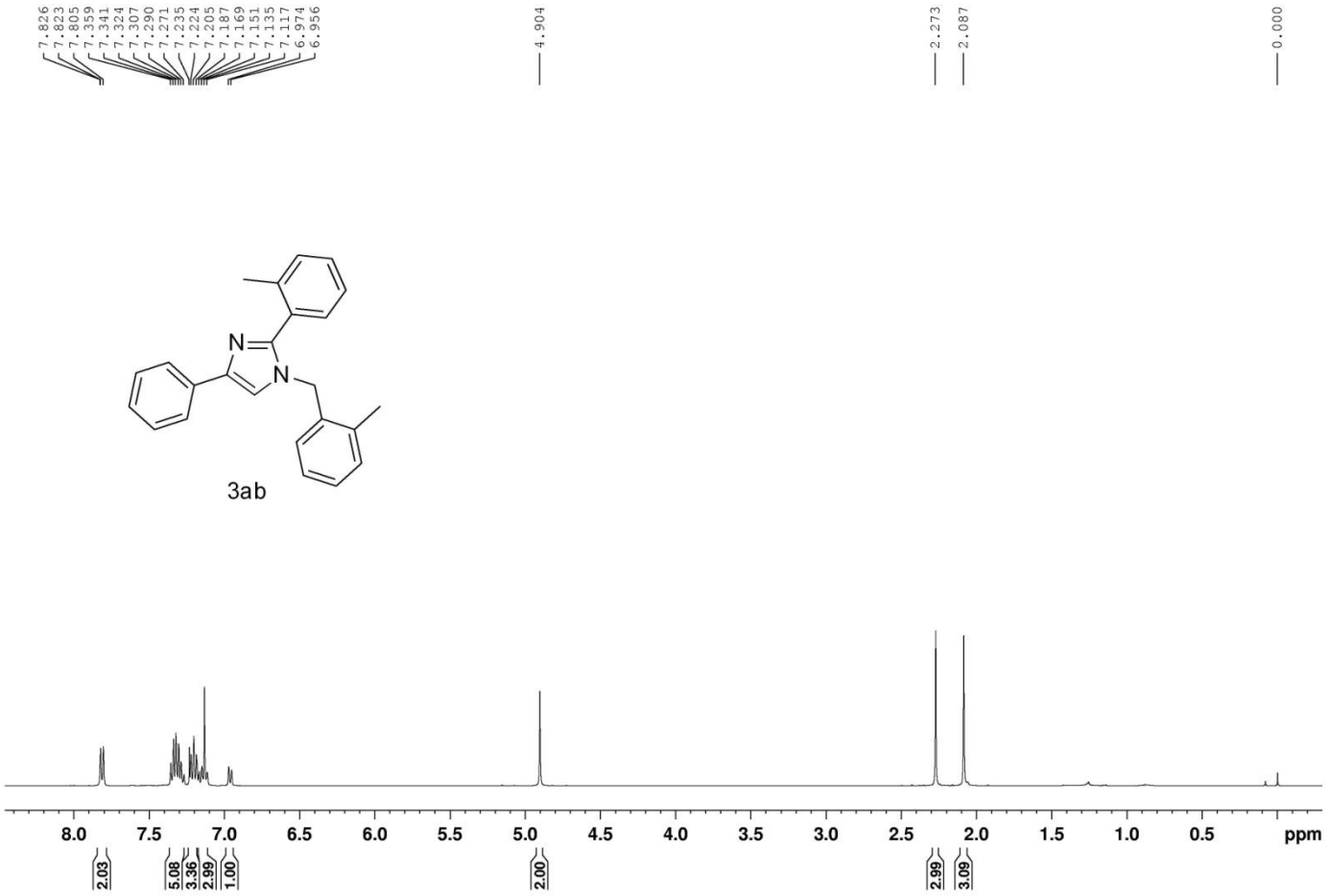
140.50
136.68
133.11
131.60
130.28
129.16
129.08
129.02
128.71
128.10
126.74
126.52
120.43
117.02
77.38
77.06
76.75
50.58
N
N
Br
3la
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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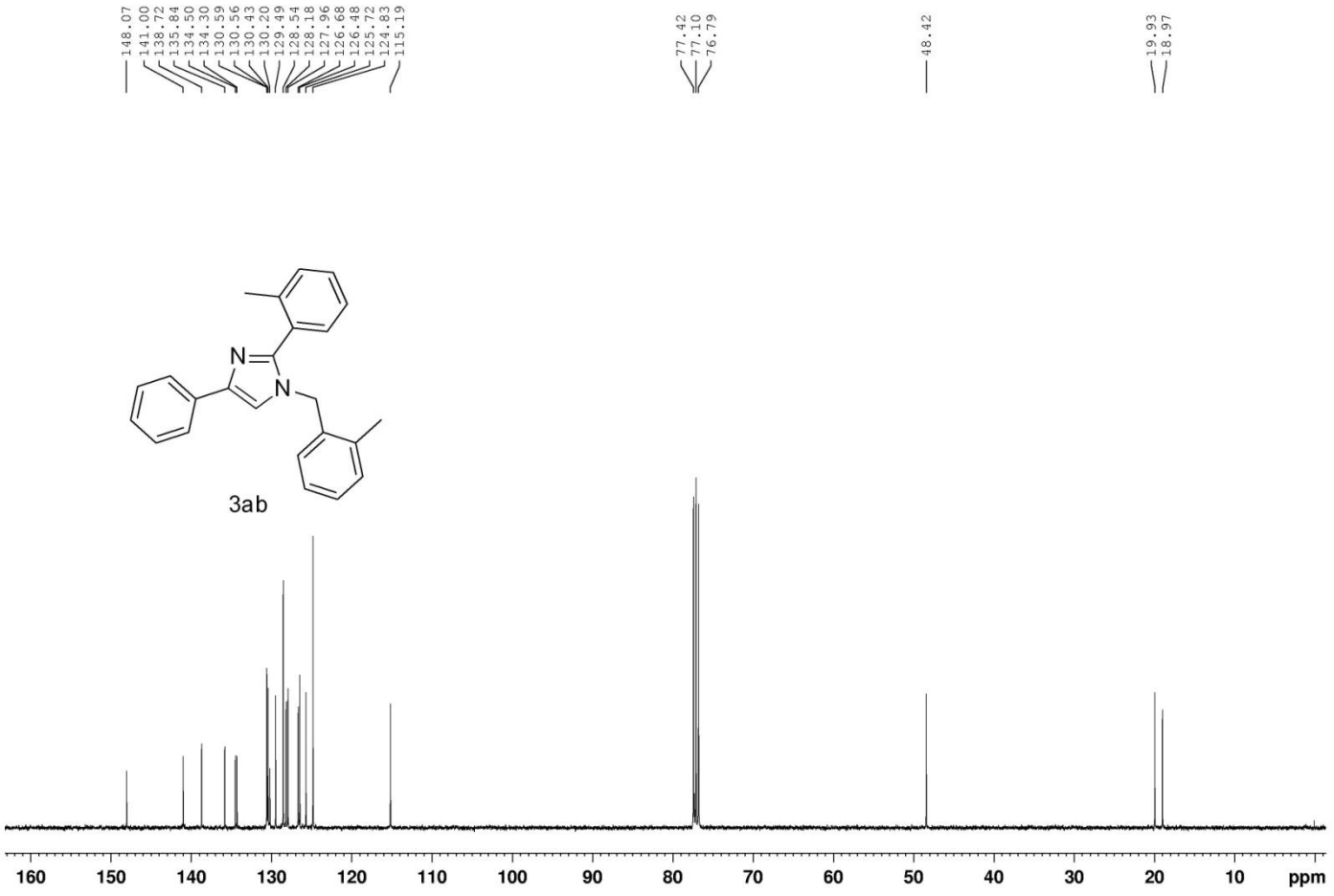
7.290
7.271
7.235
7.224
7.205
7.187
7.169
7.151
7.135
7.117
6.974
6.956
4.904
2.273
2.087
0.000
N
N
3ab
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.03
5.08
3.36
2.99
1.00
2.00
2.99
3.09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18.97
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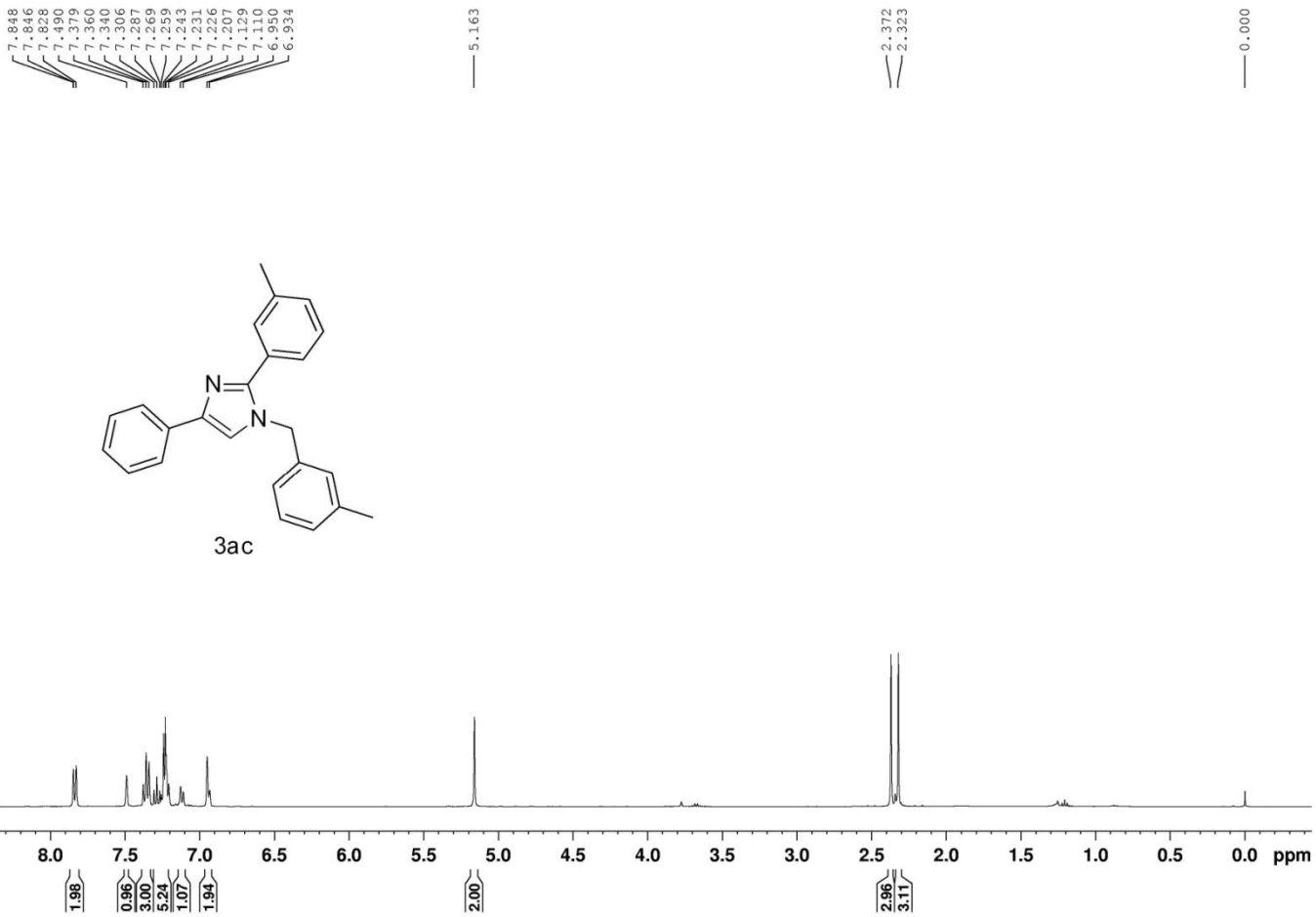
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7.231
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7.207
7.129
7.110
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N
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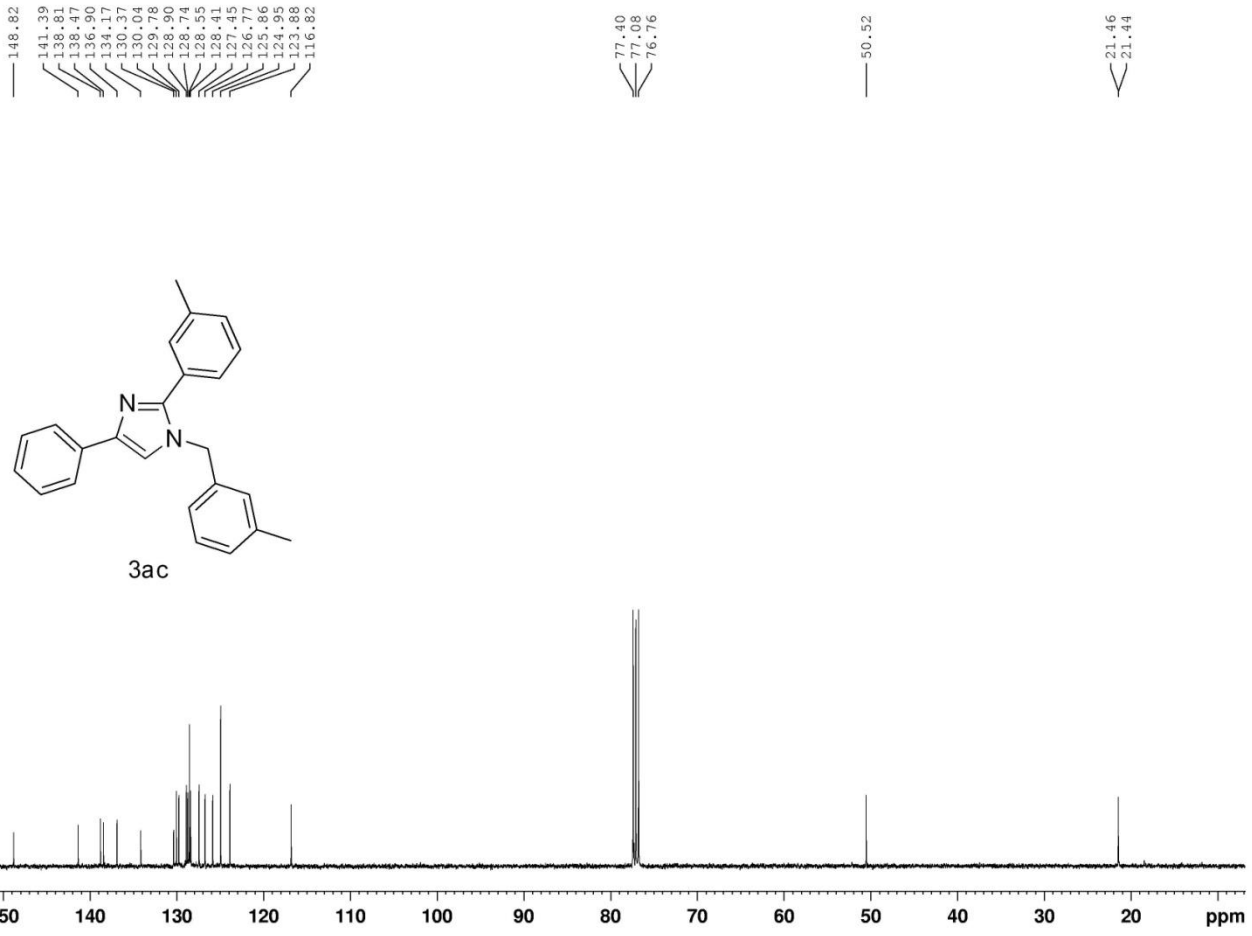
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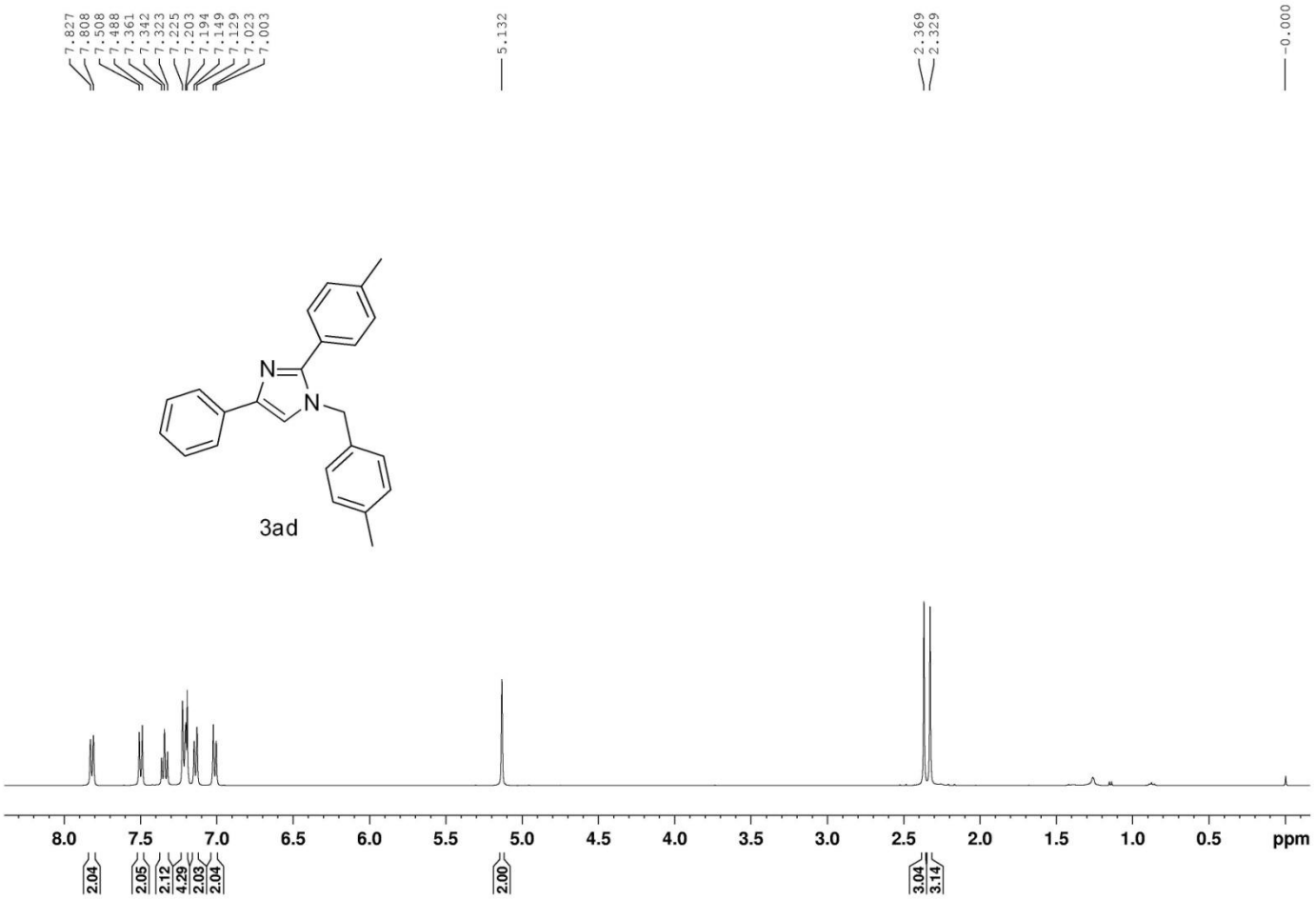
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N
3ad
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6.0
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5.0
4.5
4.0
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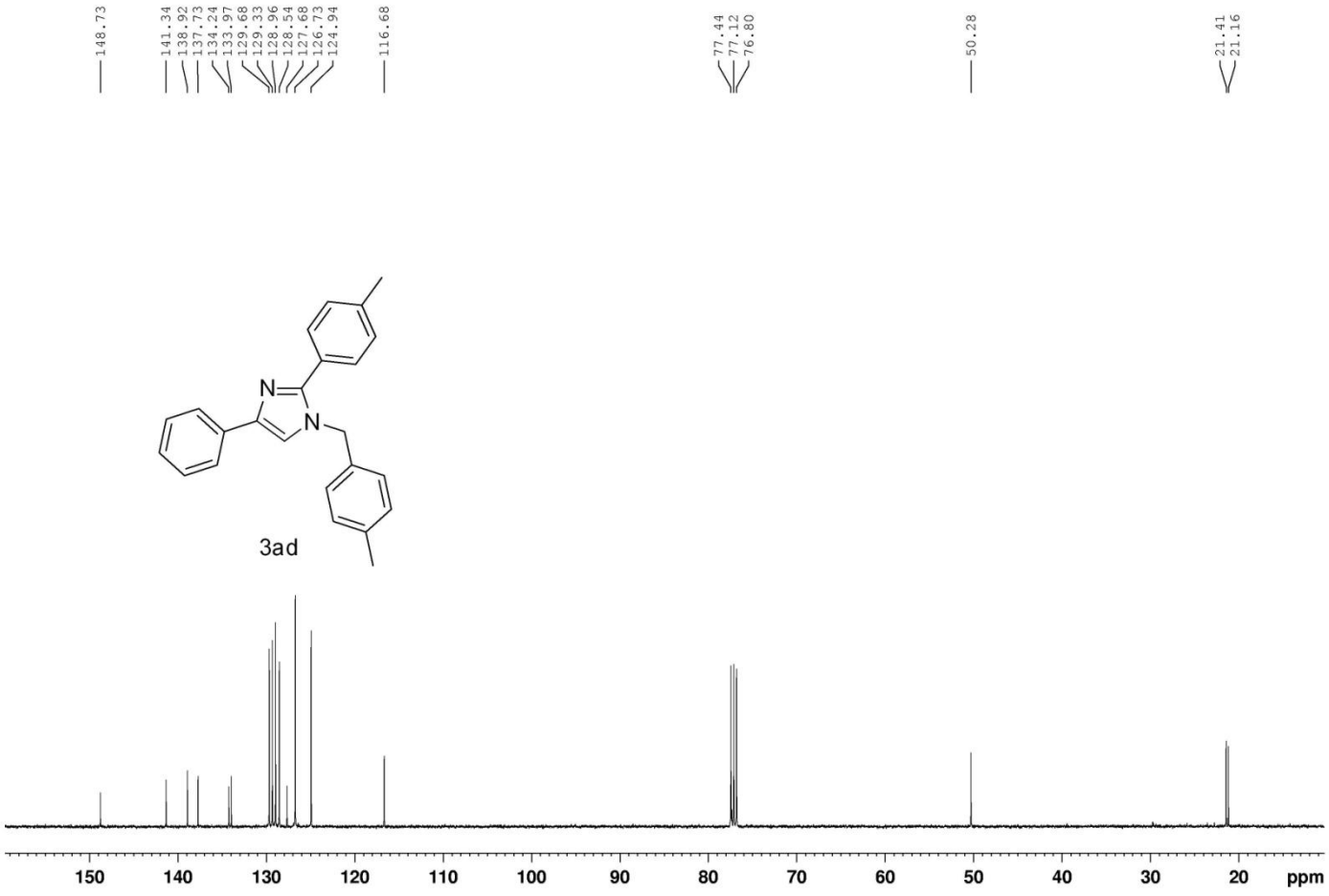
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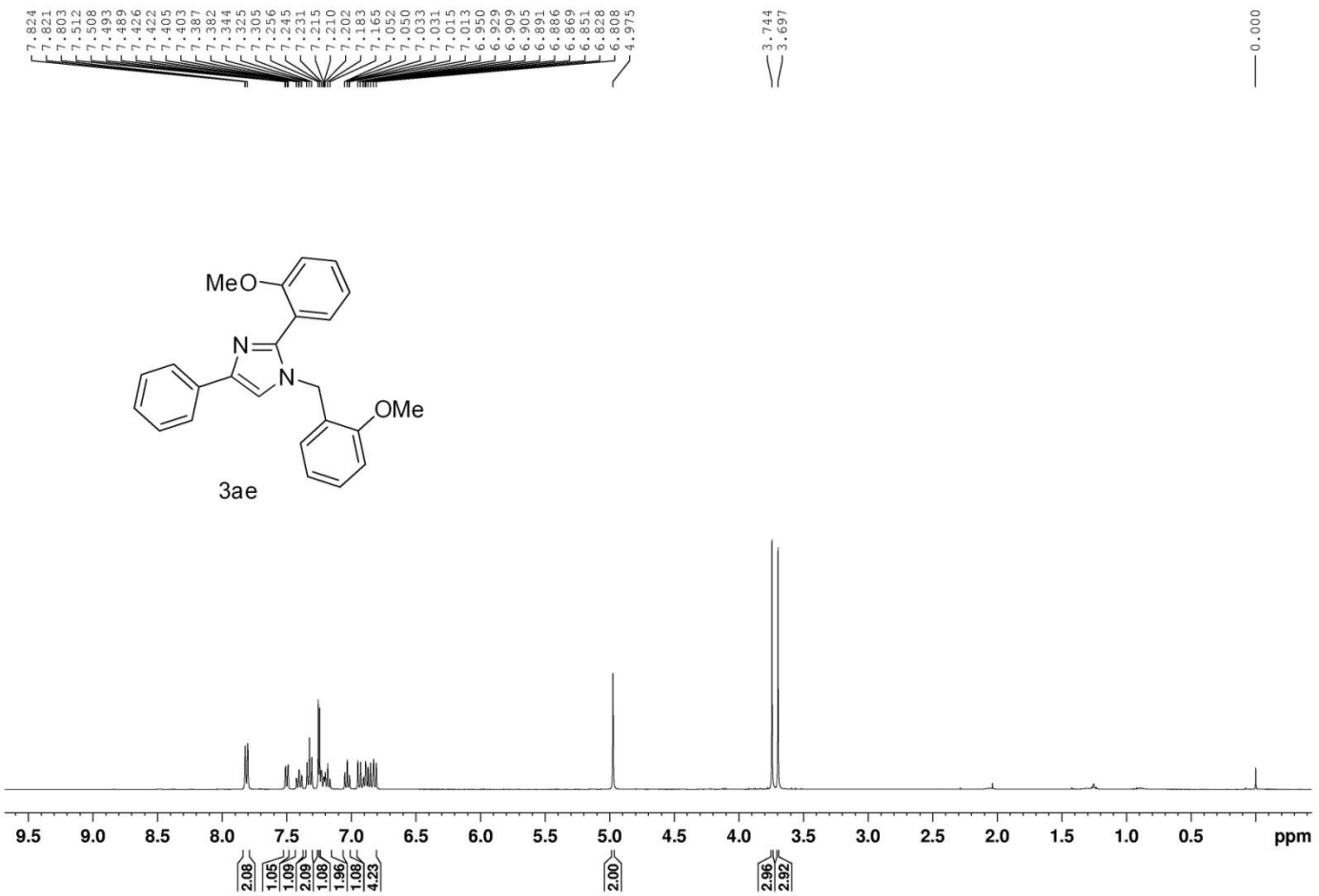
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7.245
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6.909
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3.697
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N
N
OMe
3ae
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1.0
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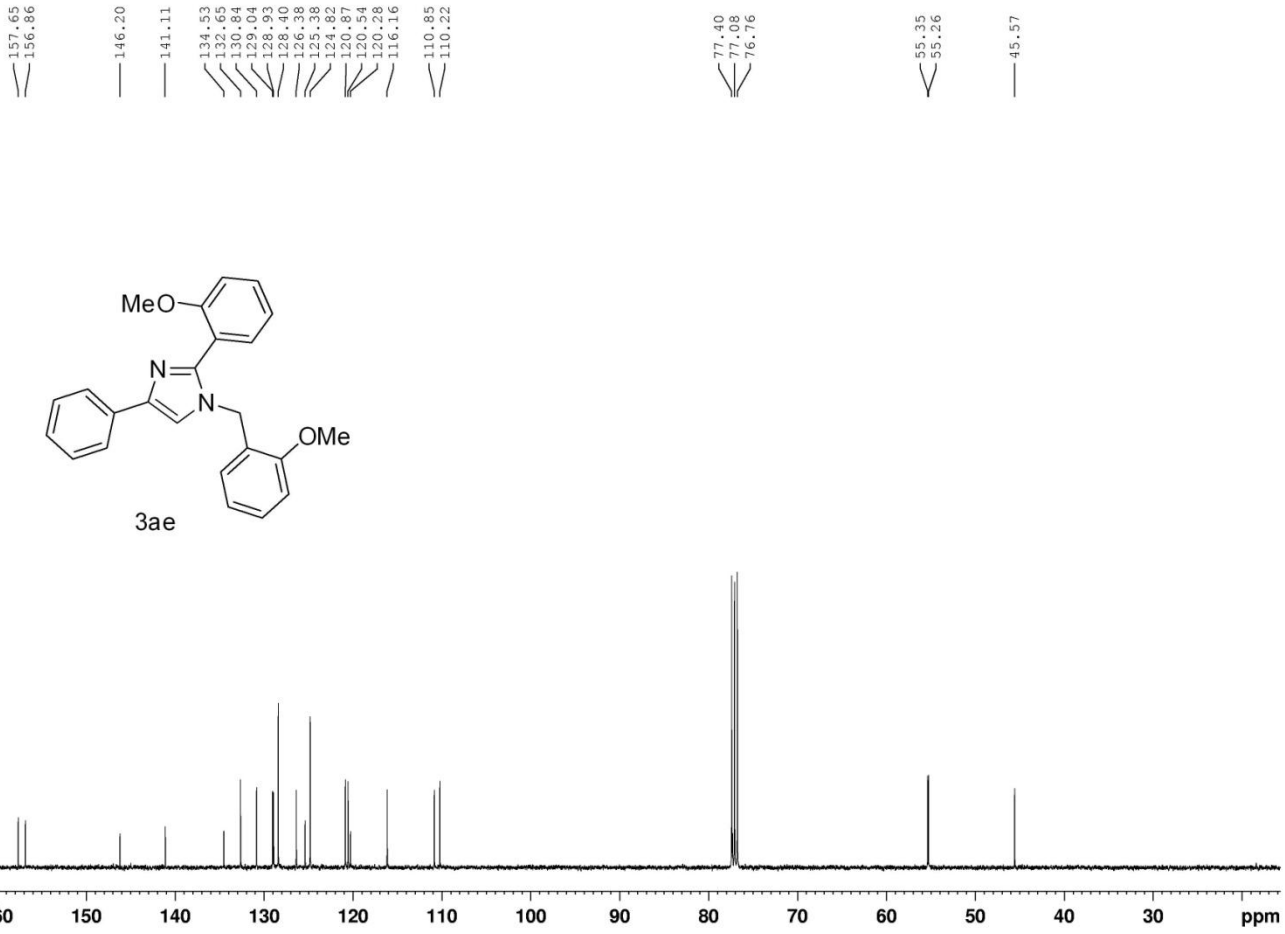
2.92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76.76
55.35
55.26
45.57
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3ae
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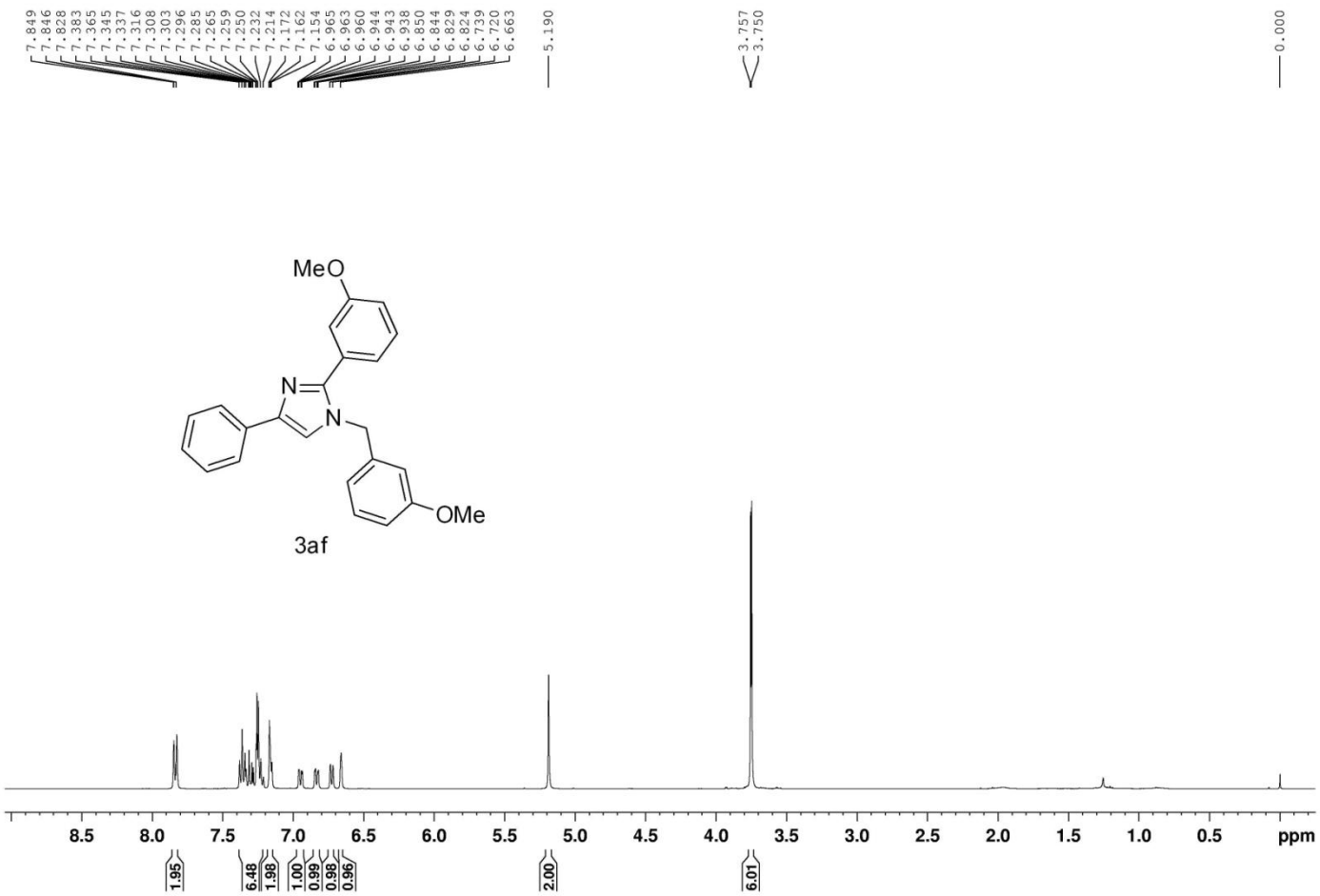
ppm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7.265
7.259
7.250
7.232
7.214
7.172
7.162
7.154
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6.960
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6.943
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N
OMe
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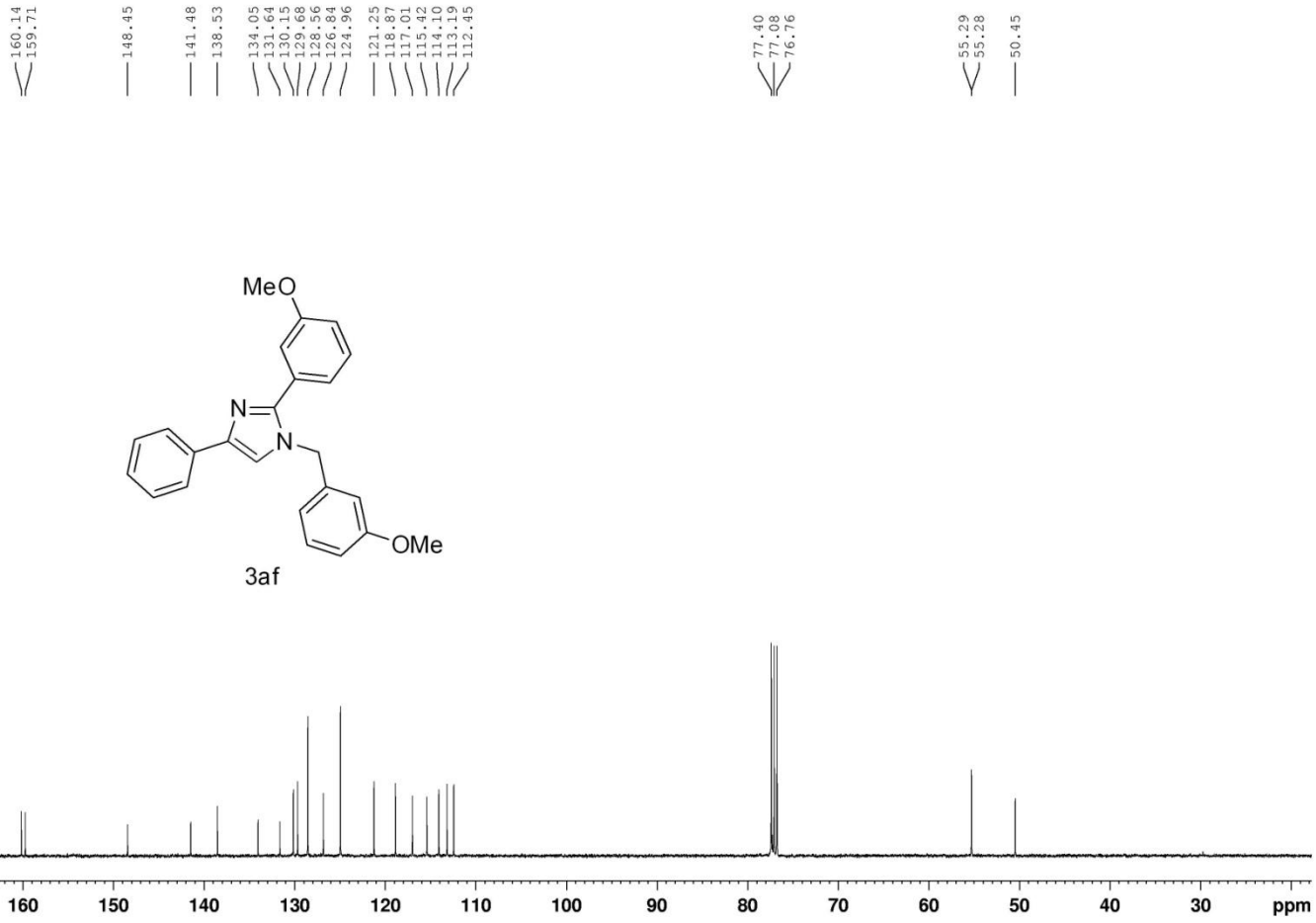
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114.10
113.19
112.45
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77.08
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55.29
55.28
50.45
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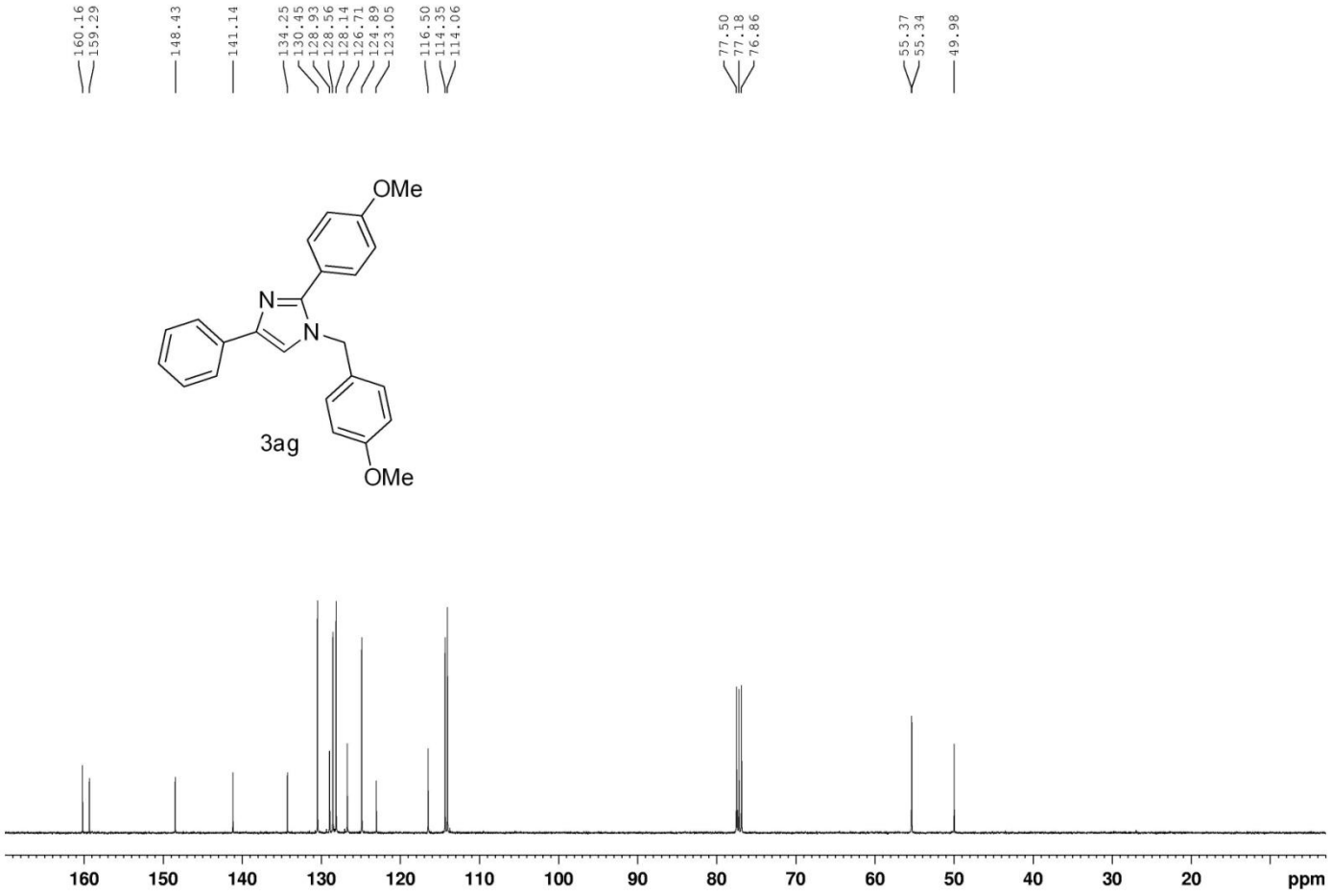
30
ppm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114.06
77.50
77.18
76.86
55.37
55.34
49.98
OMe
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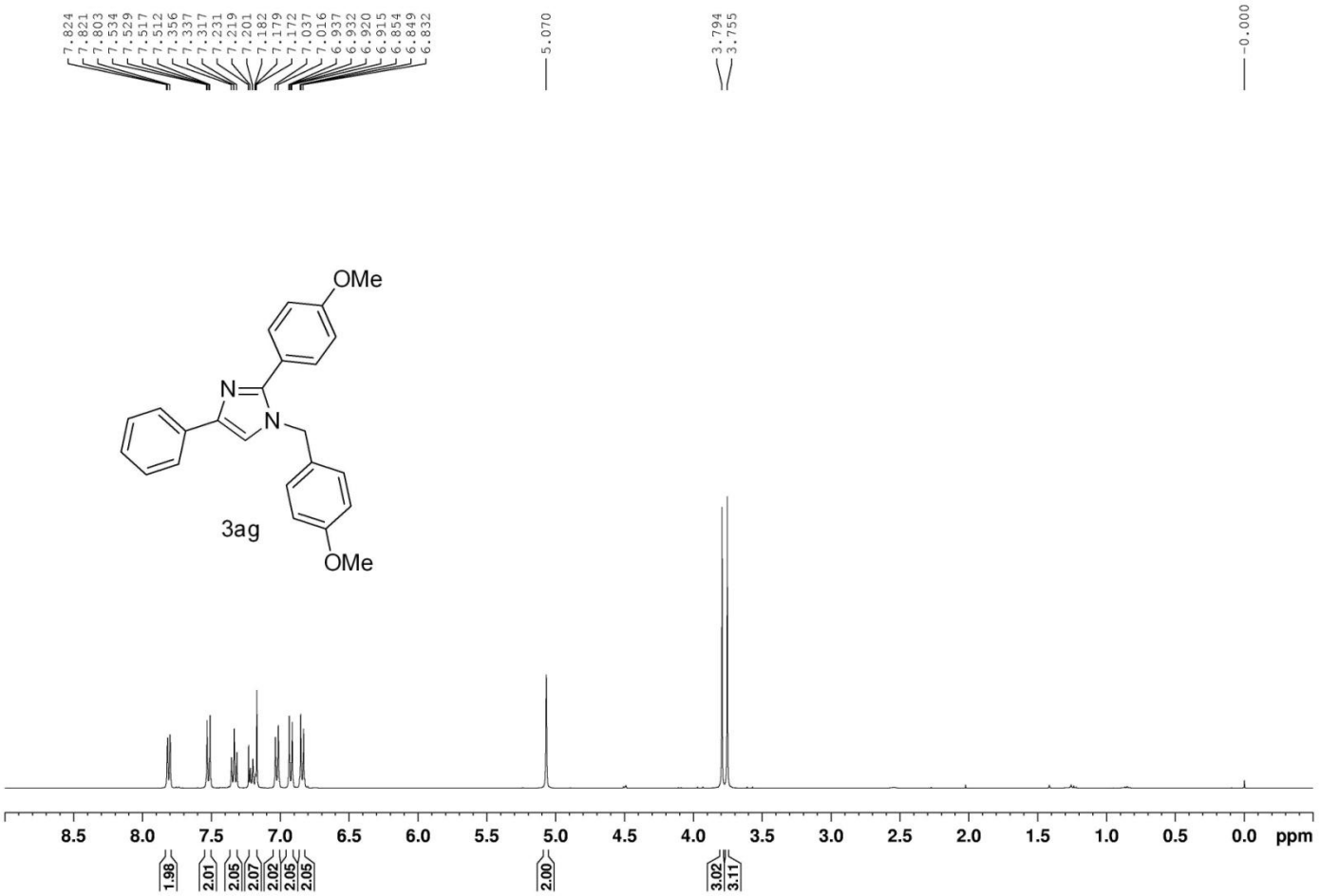
40
30
20
ppm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7.179
7.172
7.037
7.016
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6.932
6.920
6.915
6.854
6.849
6.832
5.070
3.794
3.755
-0.000
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N
N
OMe
3ag
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5.0
4.5
4.0
3.5
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1.0
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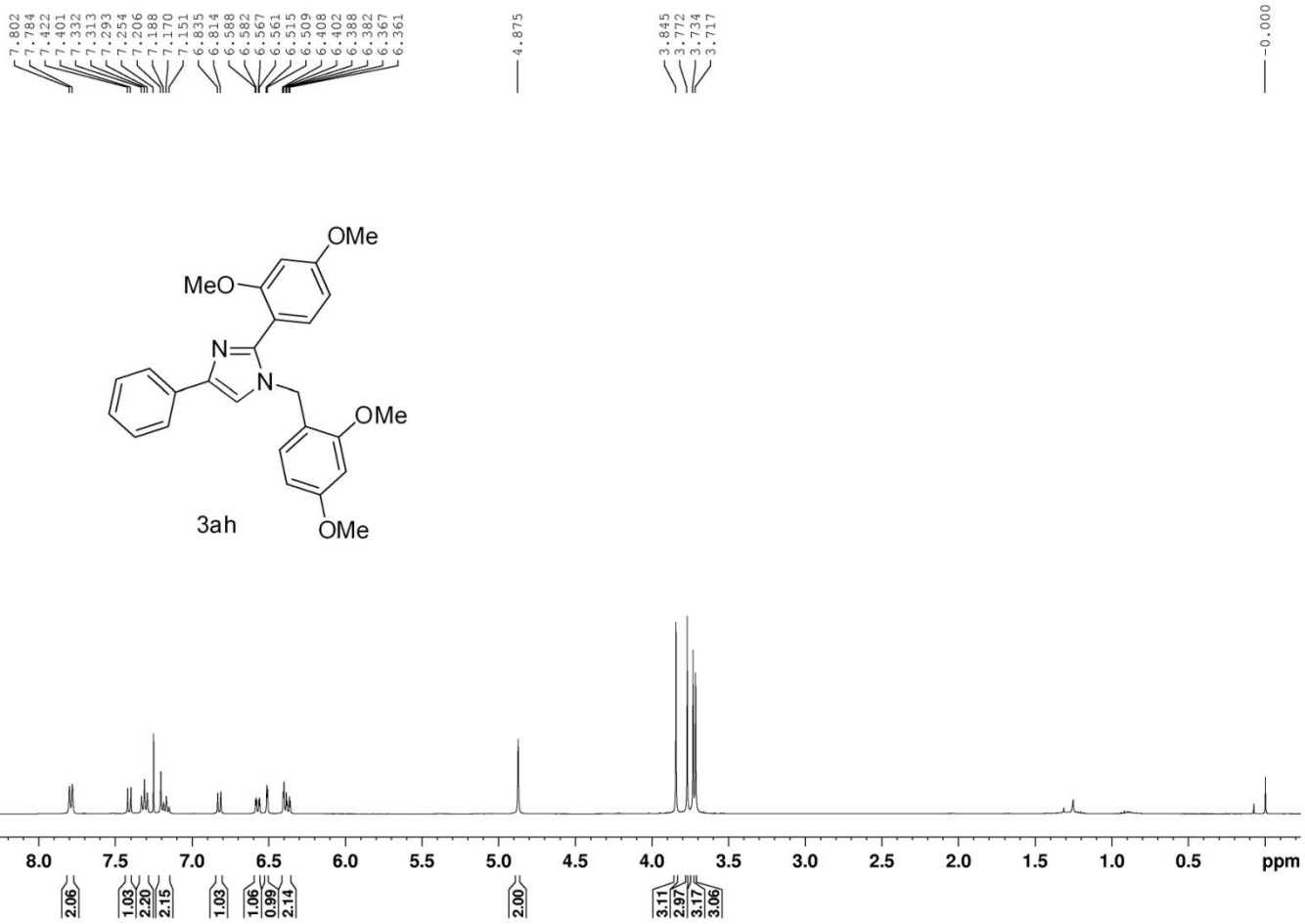
3.11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6.814
6.588
6.582
6.567
6.561
6.515
6.509
6.408
6.402
6.388
6.382
6.367
6.361
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3.734
3.717
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MeO
N
N
OMe
OMe
3ah
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7.5
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
ppm
2.06
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1.03
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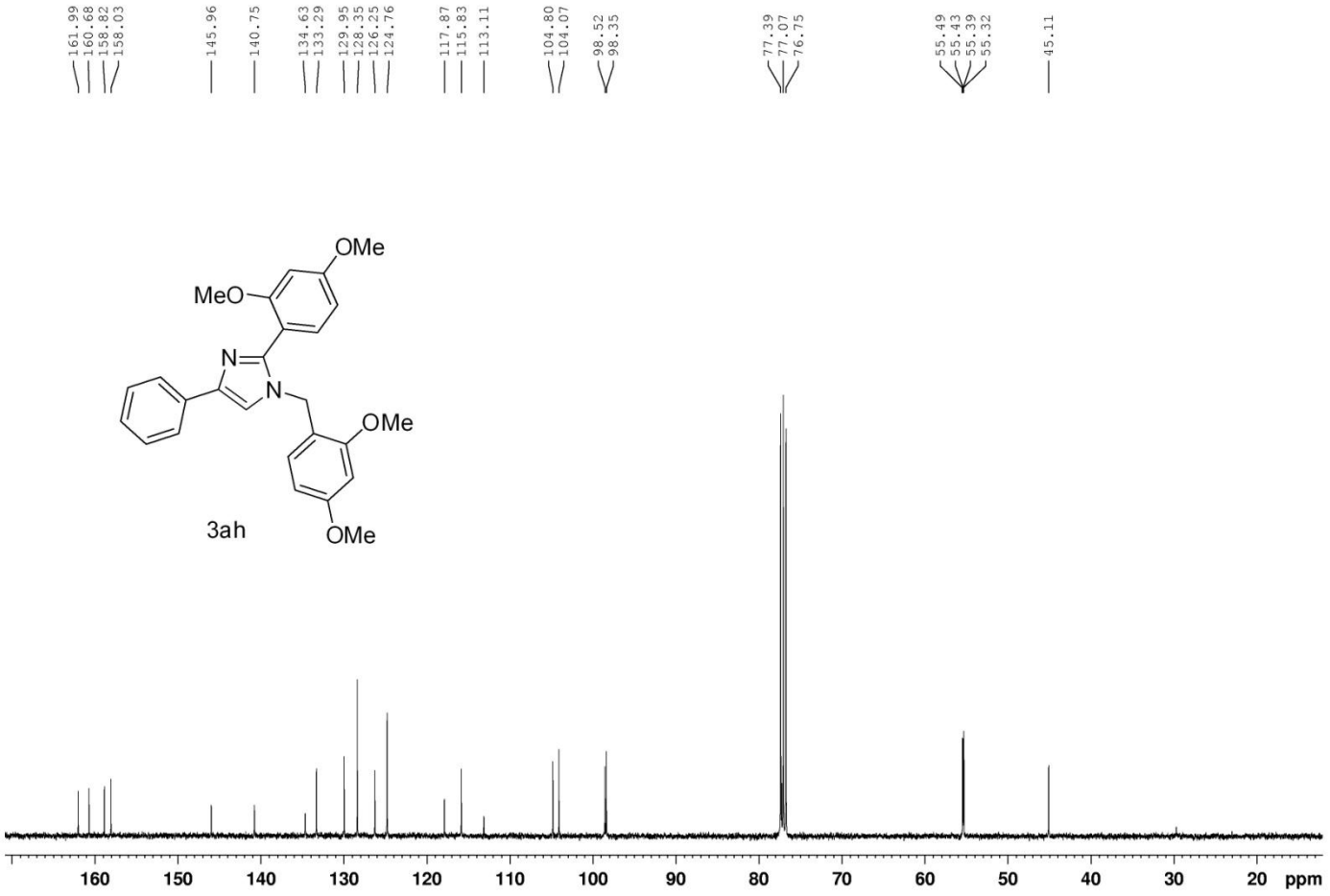
3.17
3.06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113.11
104.80
104.07
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77.39
77.07
76.75
55.49
55.43
55.39
55.32
45.11
OMe
MeO
N
N
OMe
OMe
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80
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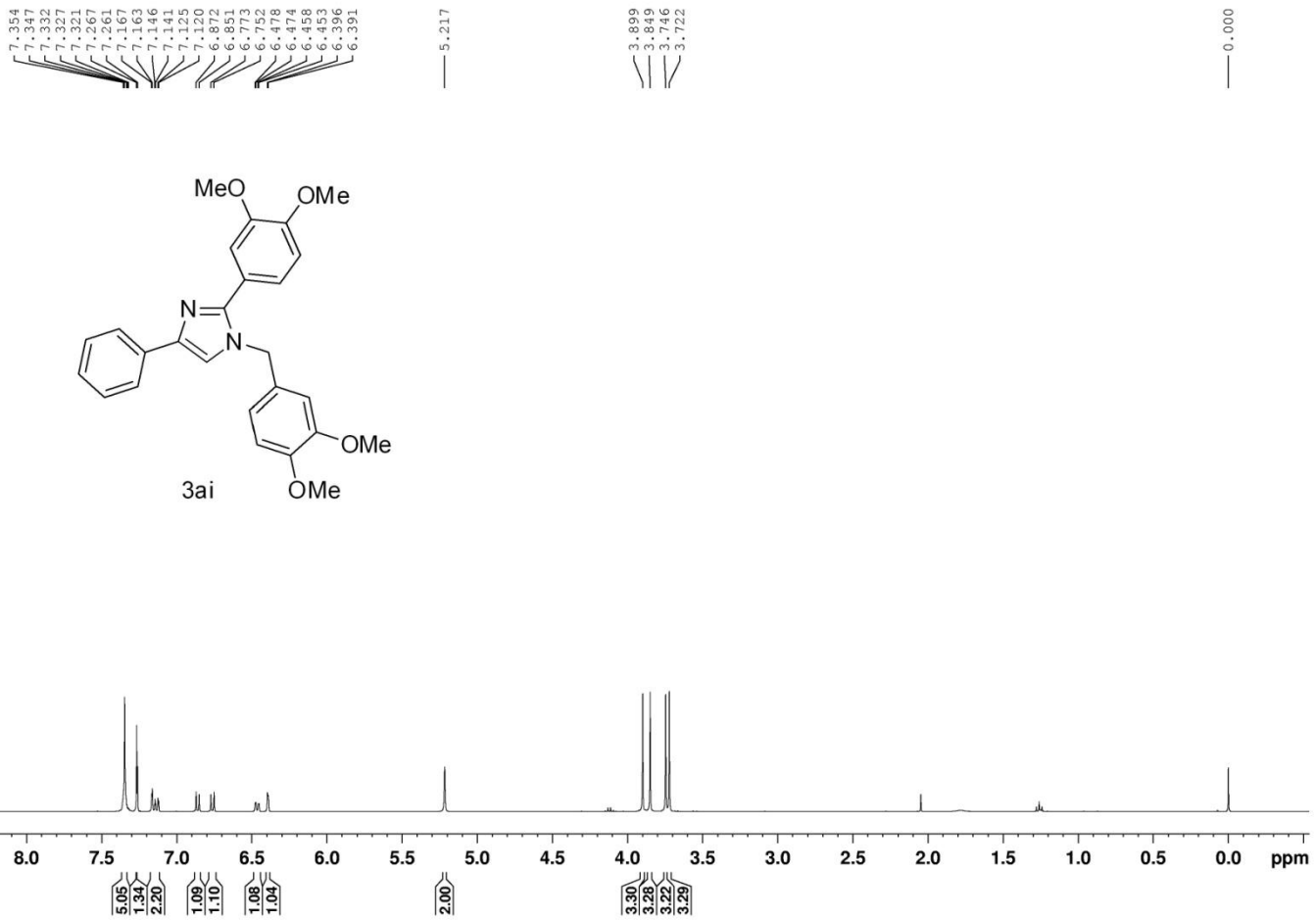
20
ppm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6.391
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OMe
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N
OMe
OMe
3ai
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1.0
0.5
0.0
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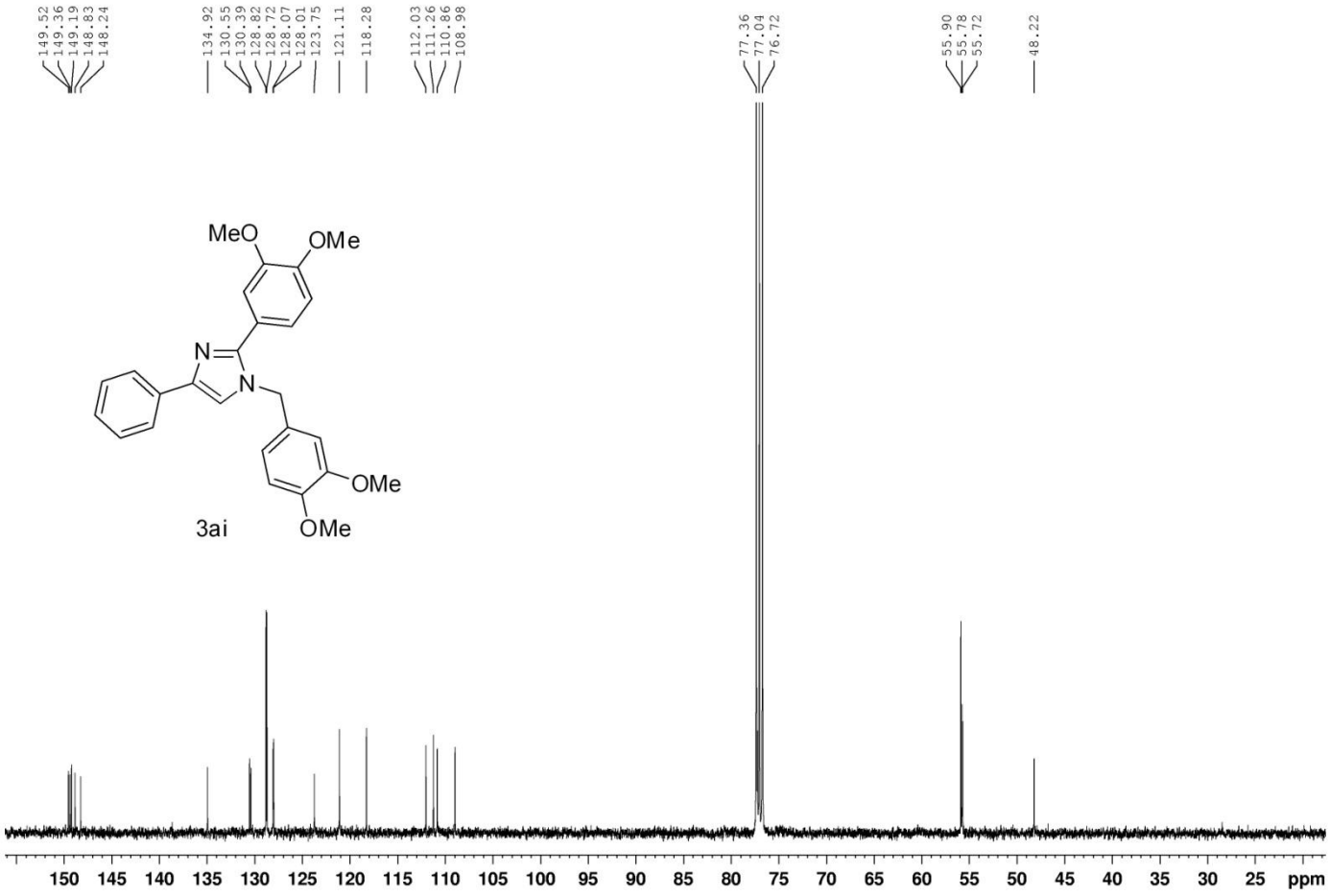
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118.28
112.03
111.26
110.86
108.98
77.36
77.04
76.72
55.90
55.78
55.72
48.22
MeO
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N
N
OMe
OMe
3ai
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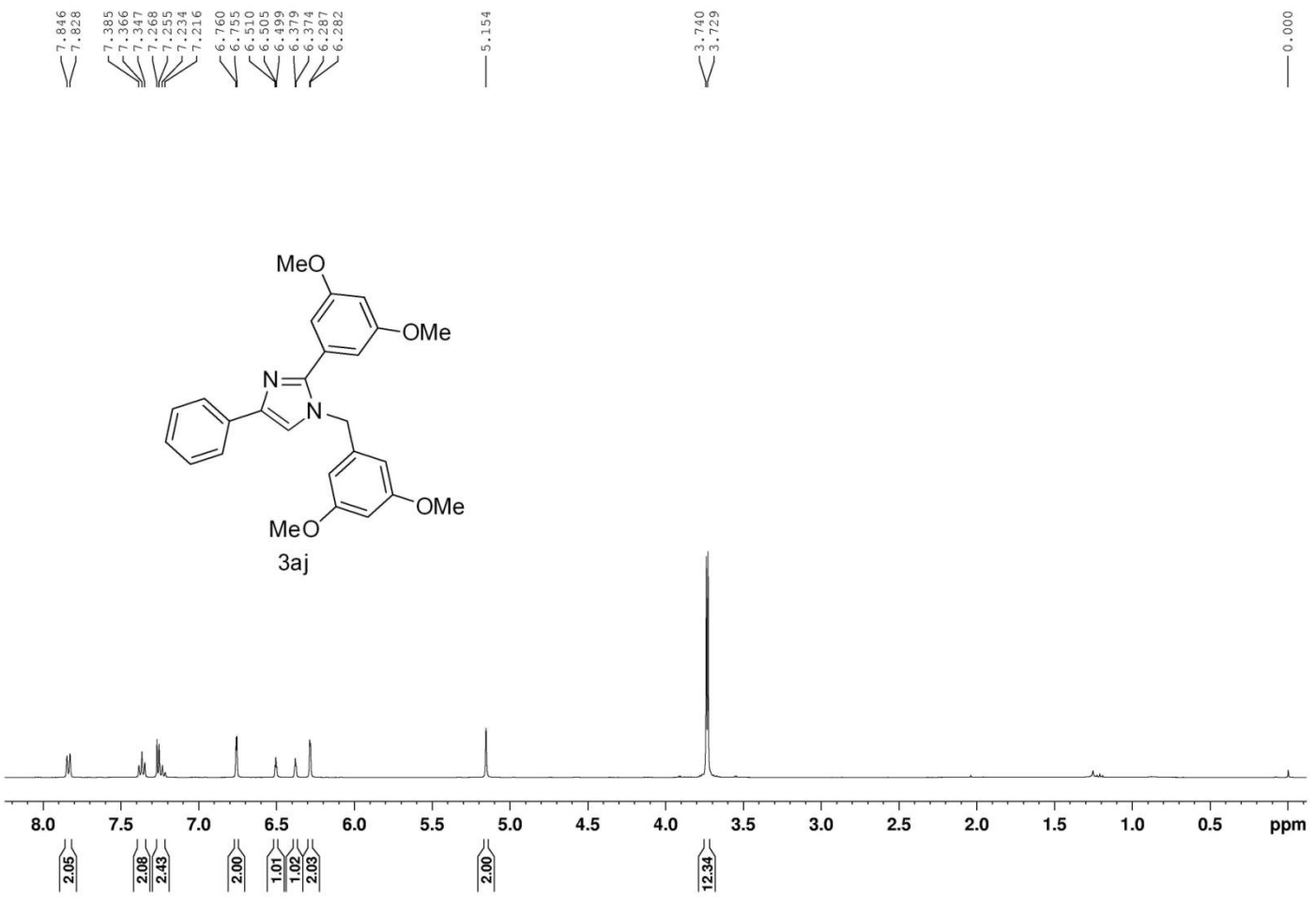
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6.505
6.499
6.379
6.374
6.287
6.282
5.154
3.740
3.729
0.000
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OMe
N
N
OMe
MeO
3aj
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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2.0
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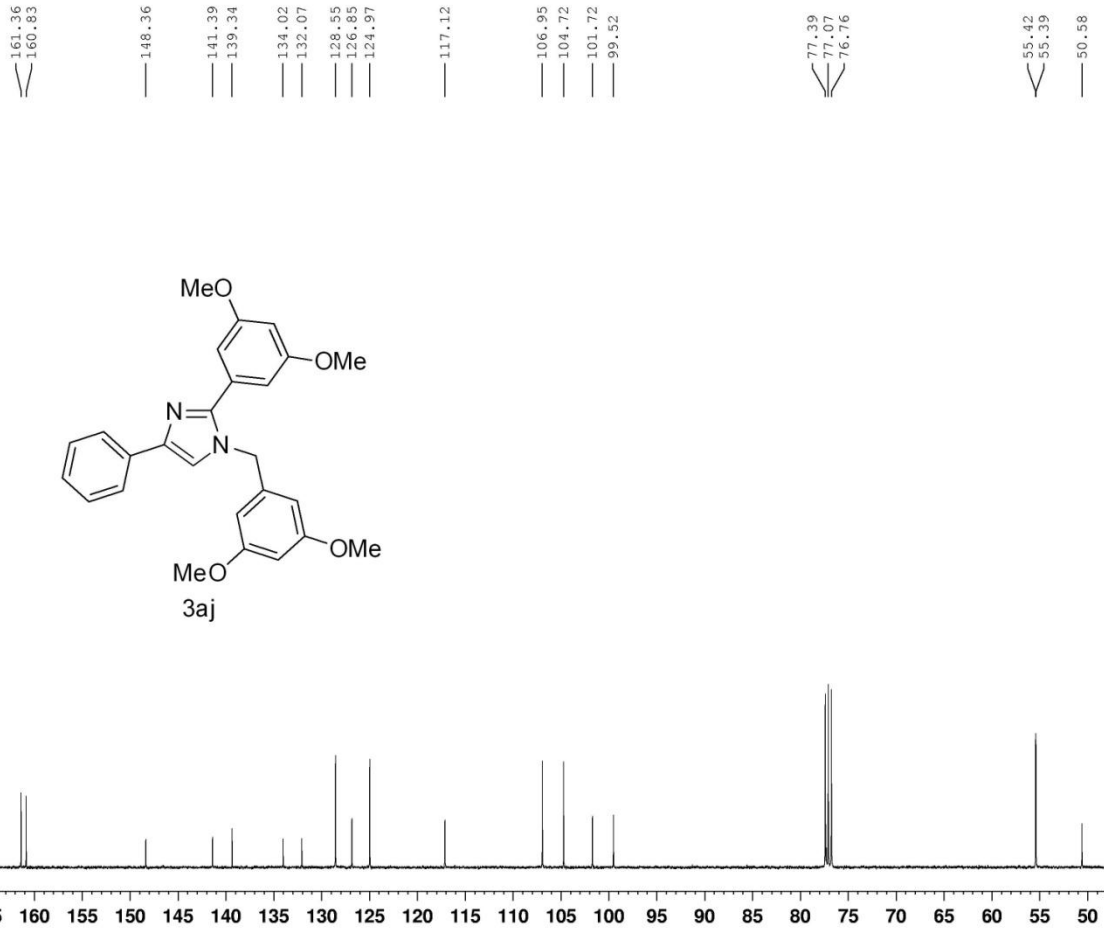
12.34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101.72
99.52
77.39
77.07
76.76
55.42
55.39
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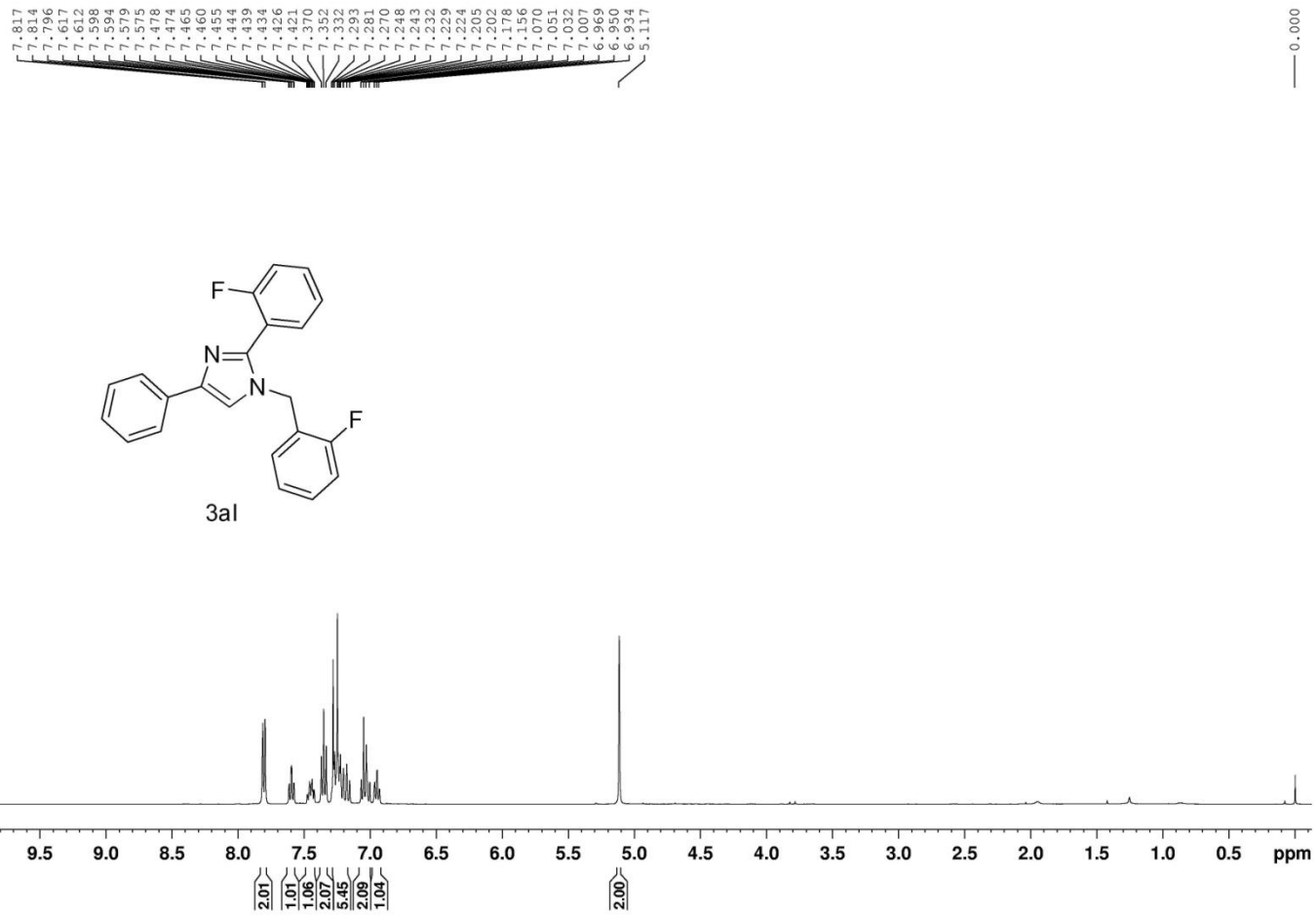
MeO
OMe
N
N
OMe
MeO
3aj
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 ppm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6.934
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N
F
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5.0
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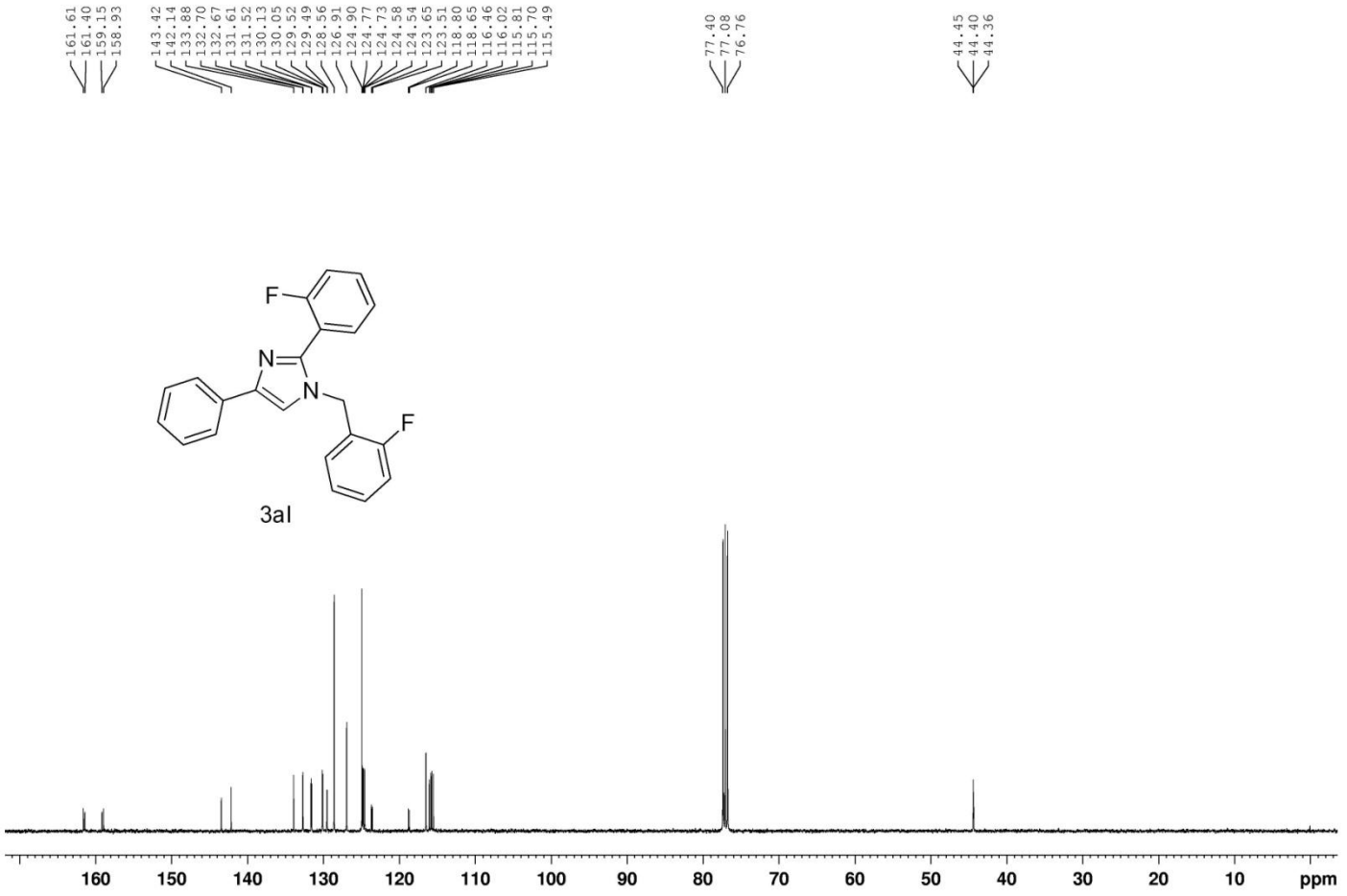
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77.08
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44.36
F
N
N
F
3al
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10
ppm


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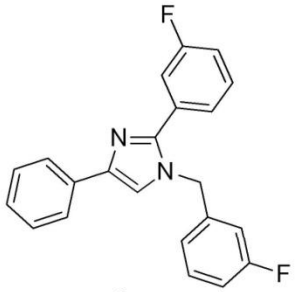
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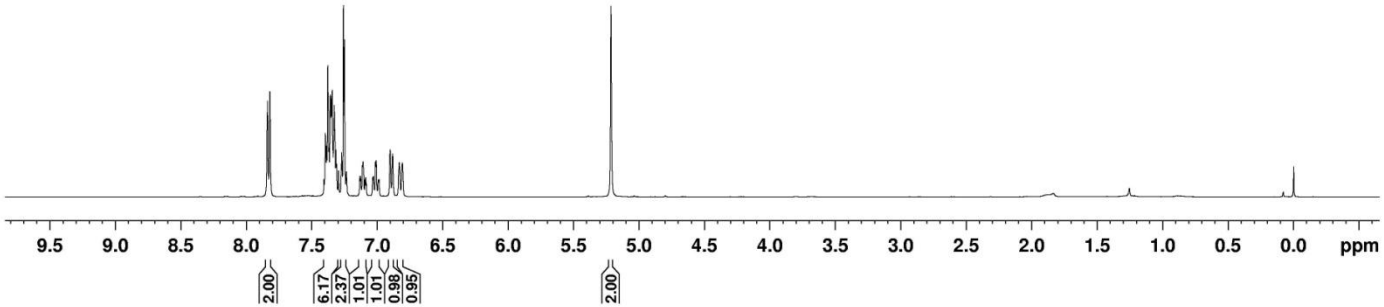
3am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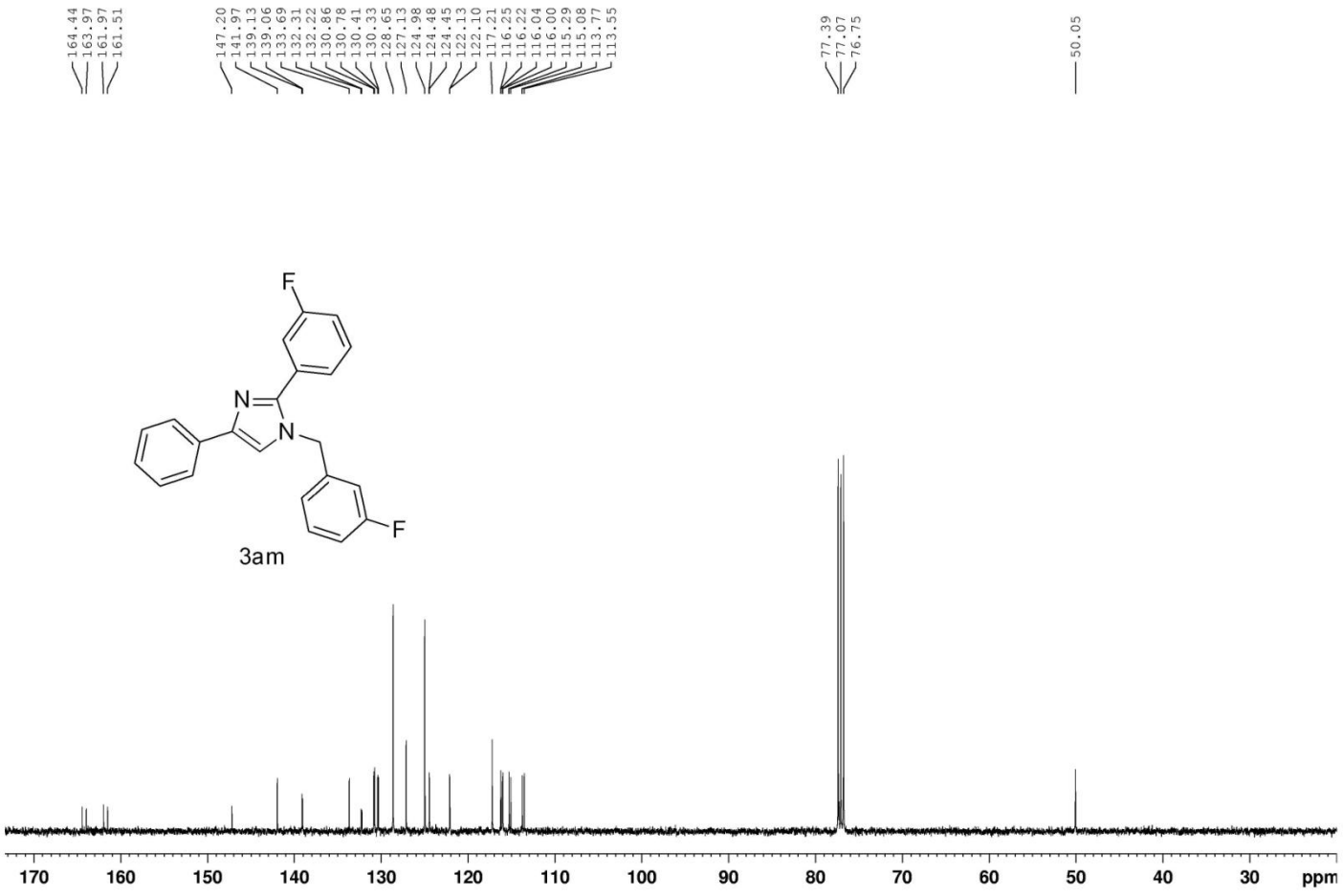
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F
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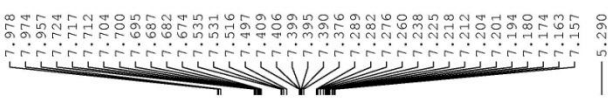
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7.531
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7.395
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7.282
7.276
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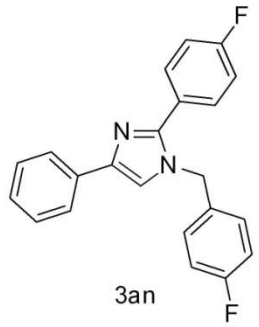
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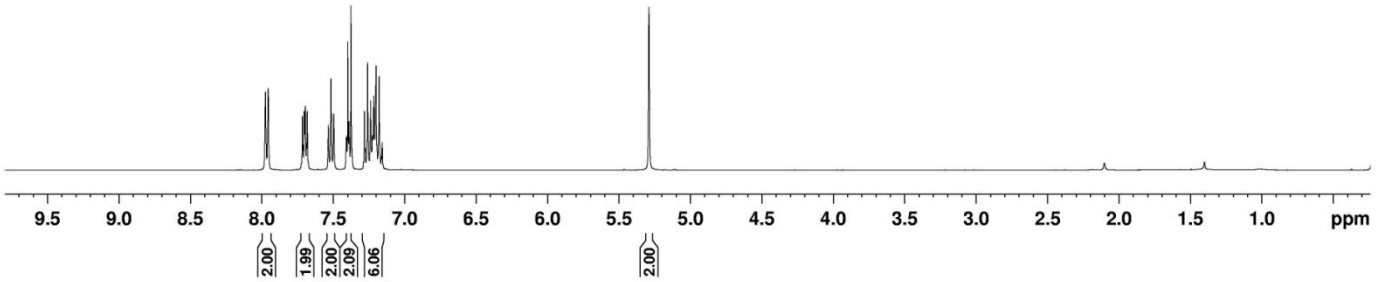
N
N
F

3an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6.0
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4.0
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2.0
1.5
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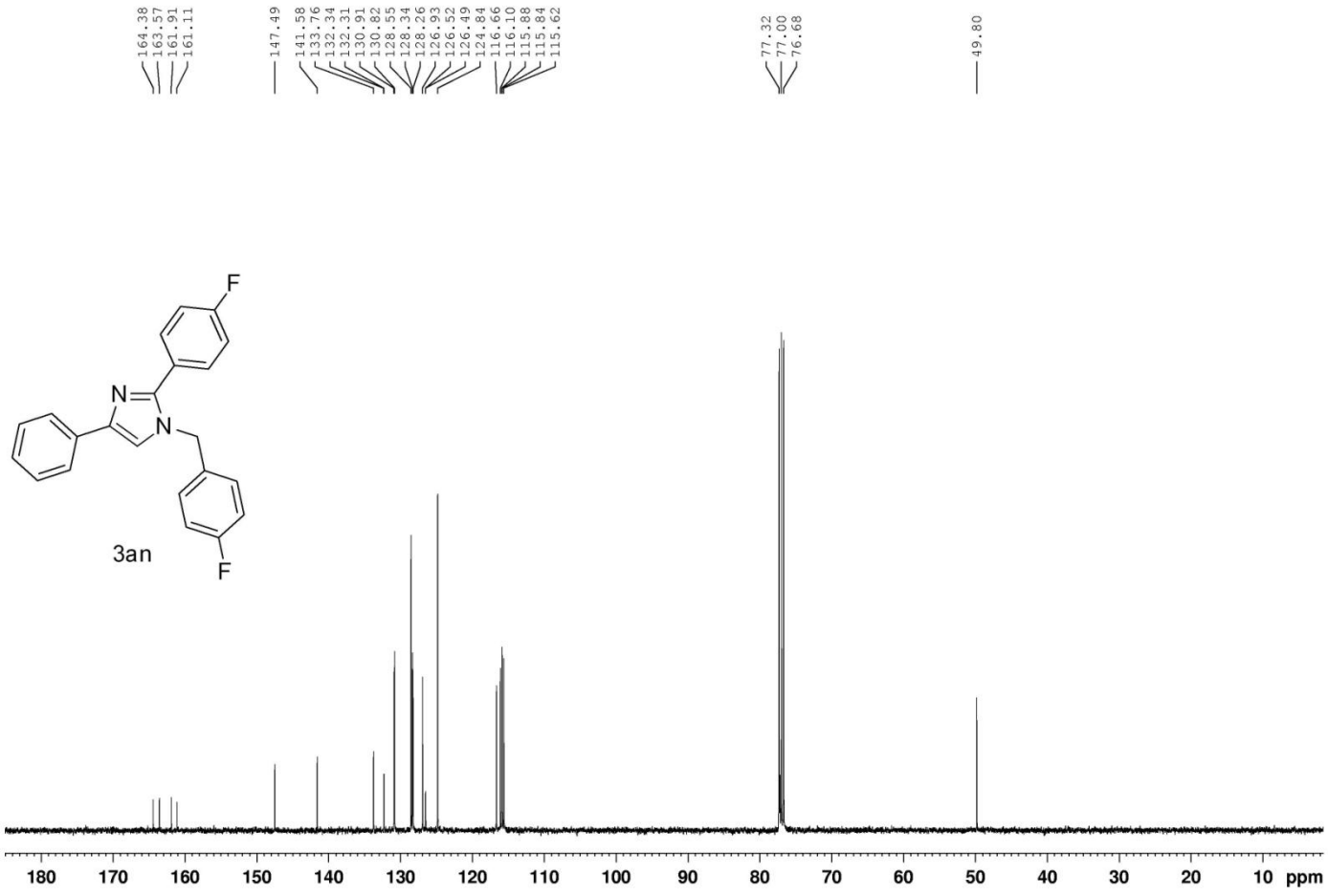
2.09
6.06
2.00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128.34
128.26
126.93
126.52
126.49
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116.66
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115.88
115.84
115.62
77.32
77.00
76.68
49.80
F
N
N
3an
F
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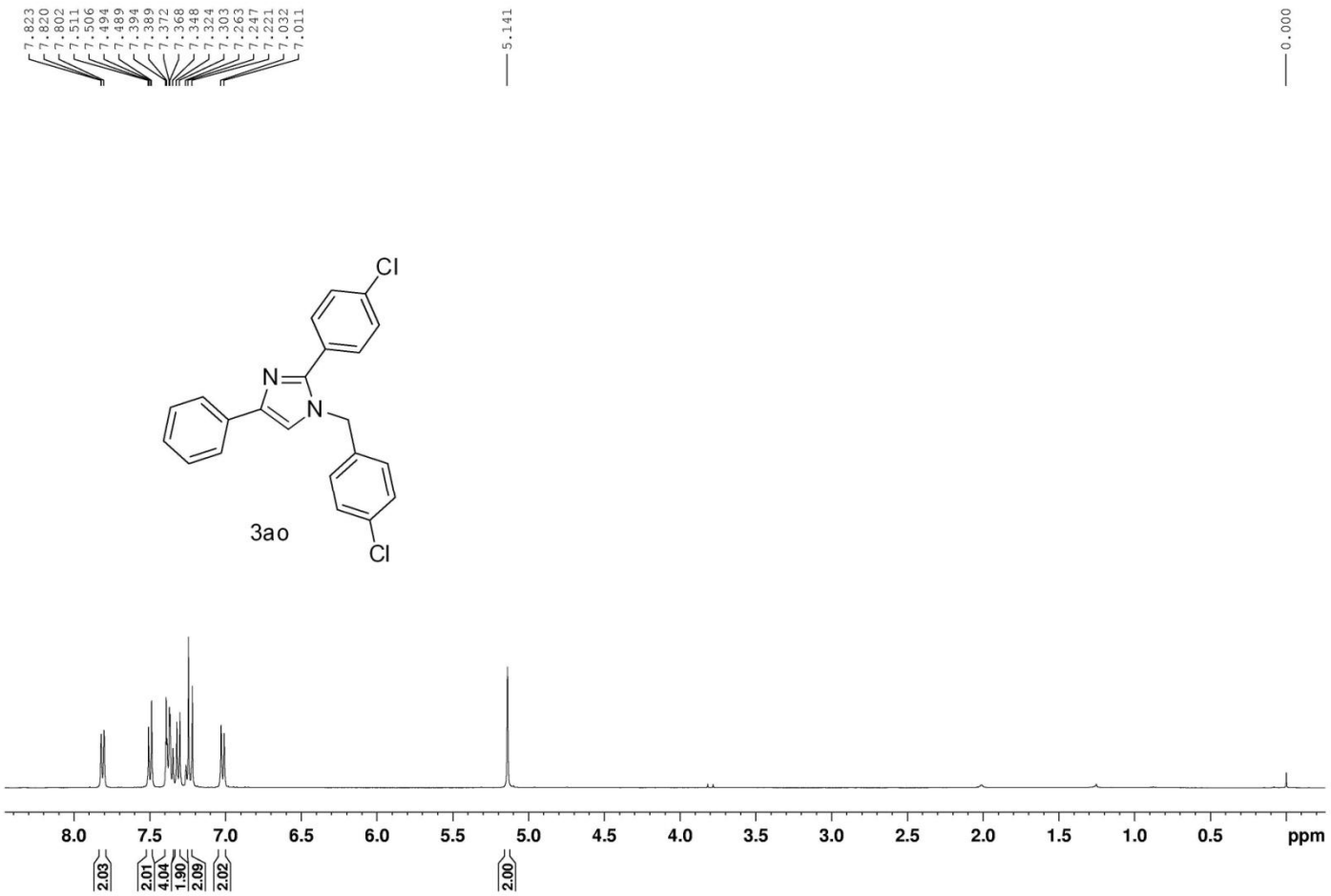
ppm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7.506
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7.394
7.389
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7.368
7.348
7.324
7.303
7.263
7.247
7.221
7.032
7.011
5.141
0.000
Cl
N
N
Cl
3ao
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.0
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ppm
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2.01
4.04
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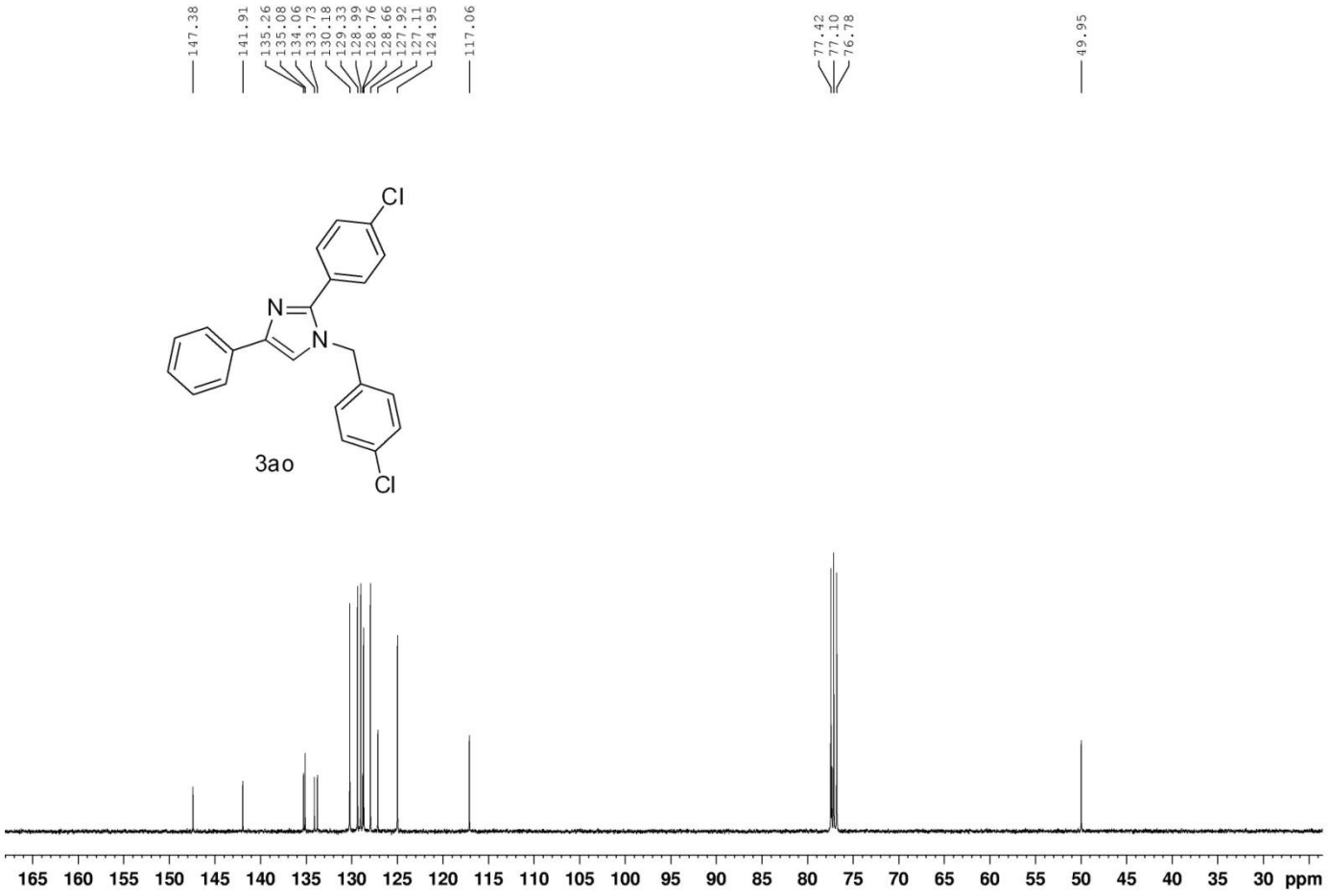
2.02
2.00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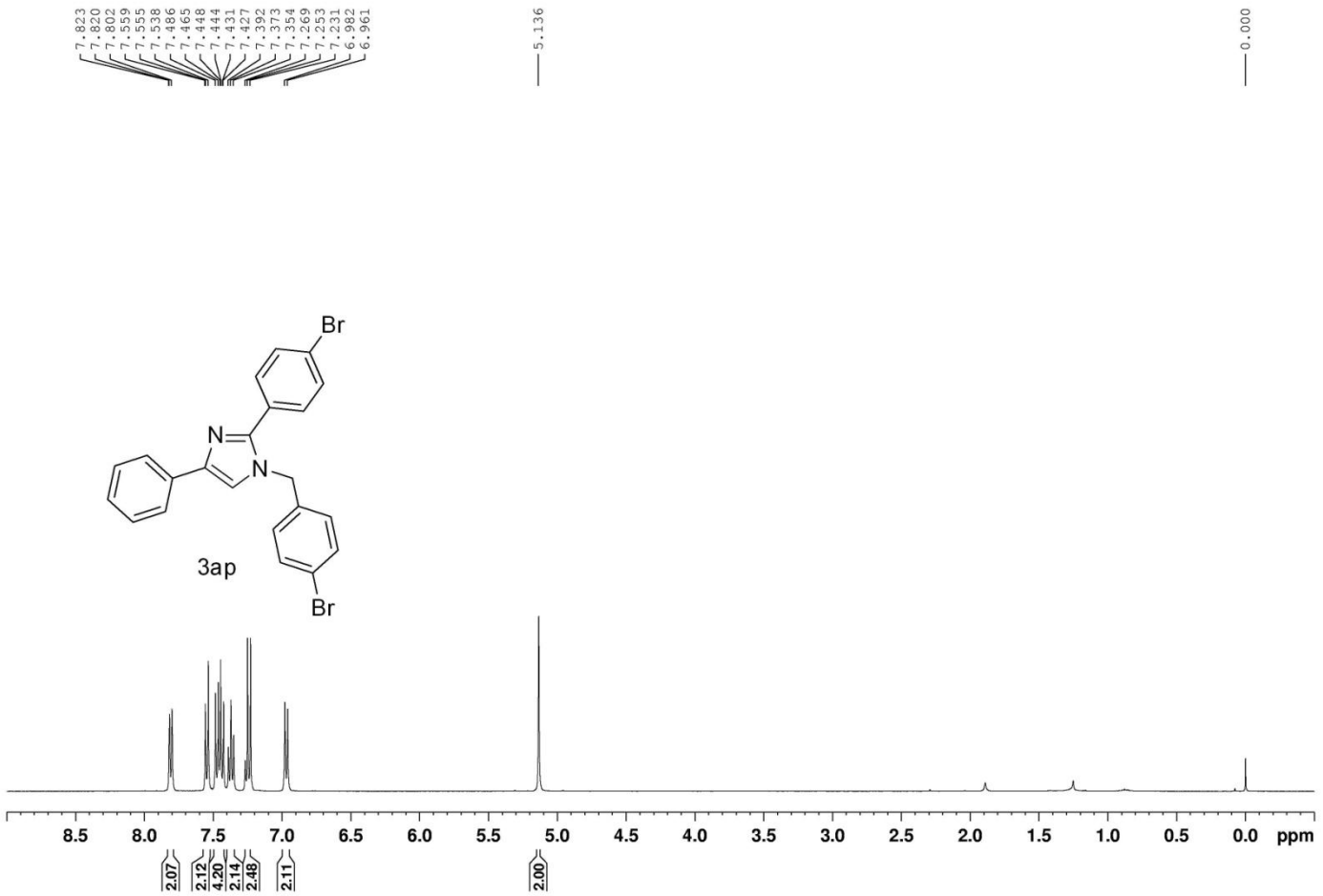
129.33
128.99
128.76
128.66
127.92
127.11
124.95
117.06
77.42
77.10
76.78
49.95
Cl
N
N
Cl
3ao
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 ppm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7.465
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7.431
7.427
7.392
7.373
7.354
7.269
7.253
7.231
6.982
6.961
5.136
0.000
Br
N
N
Br
3ap
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
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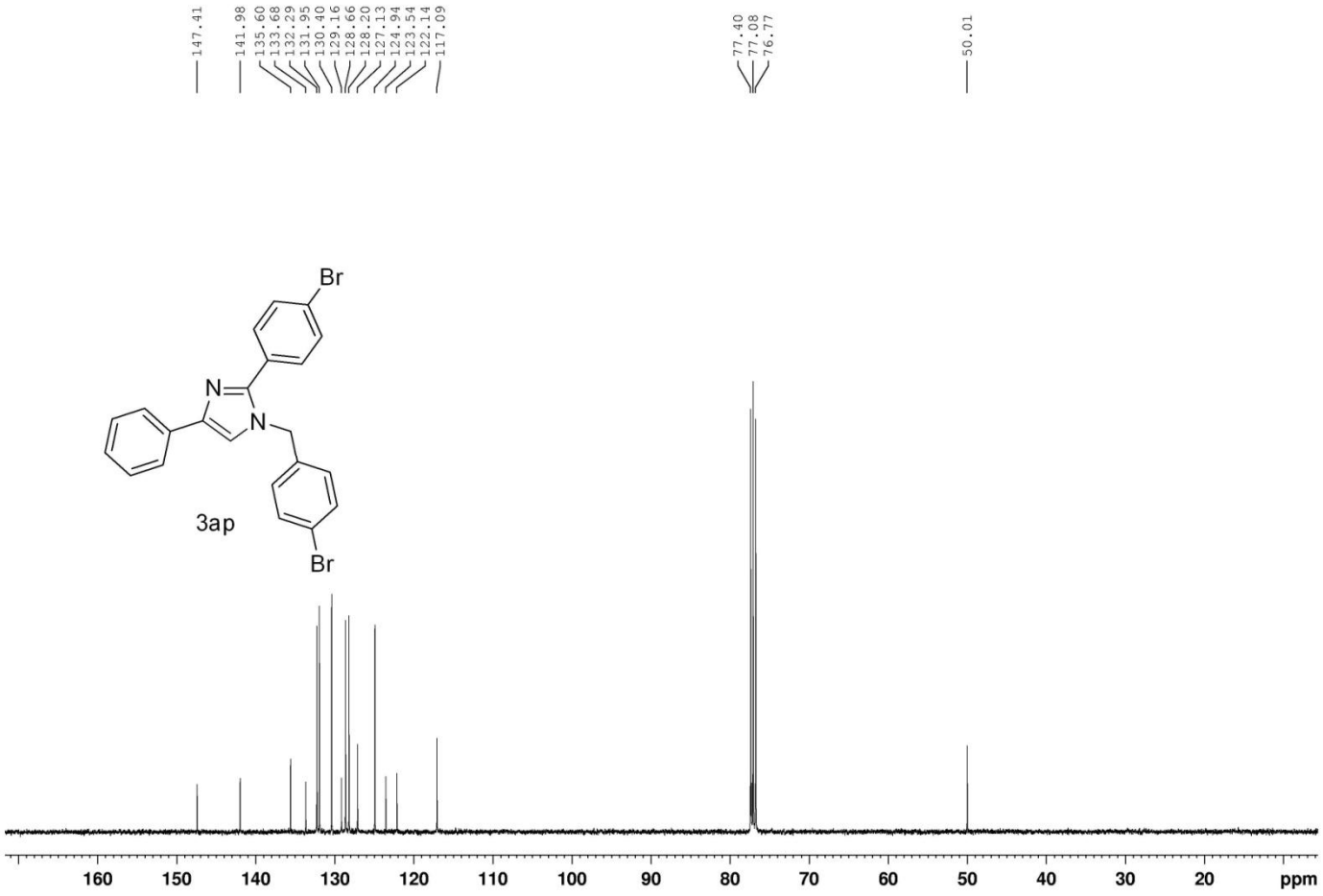
2.00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130.40
129.16
128.66
128.20
127.13
124.94
123.54
122.14
117.09
77.40
77.08
76.77
50.01
Br
N
N
Br
3ap
160
150
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120
110
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90
80
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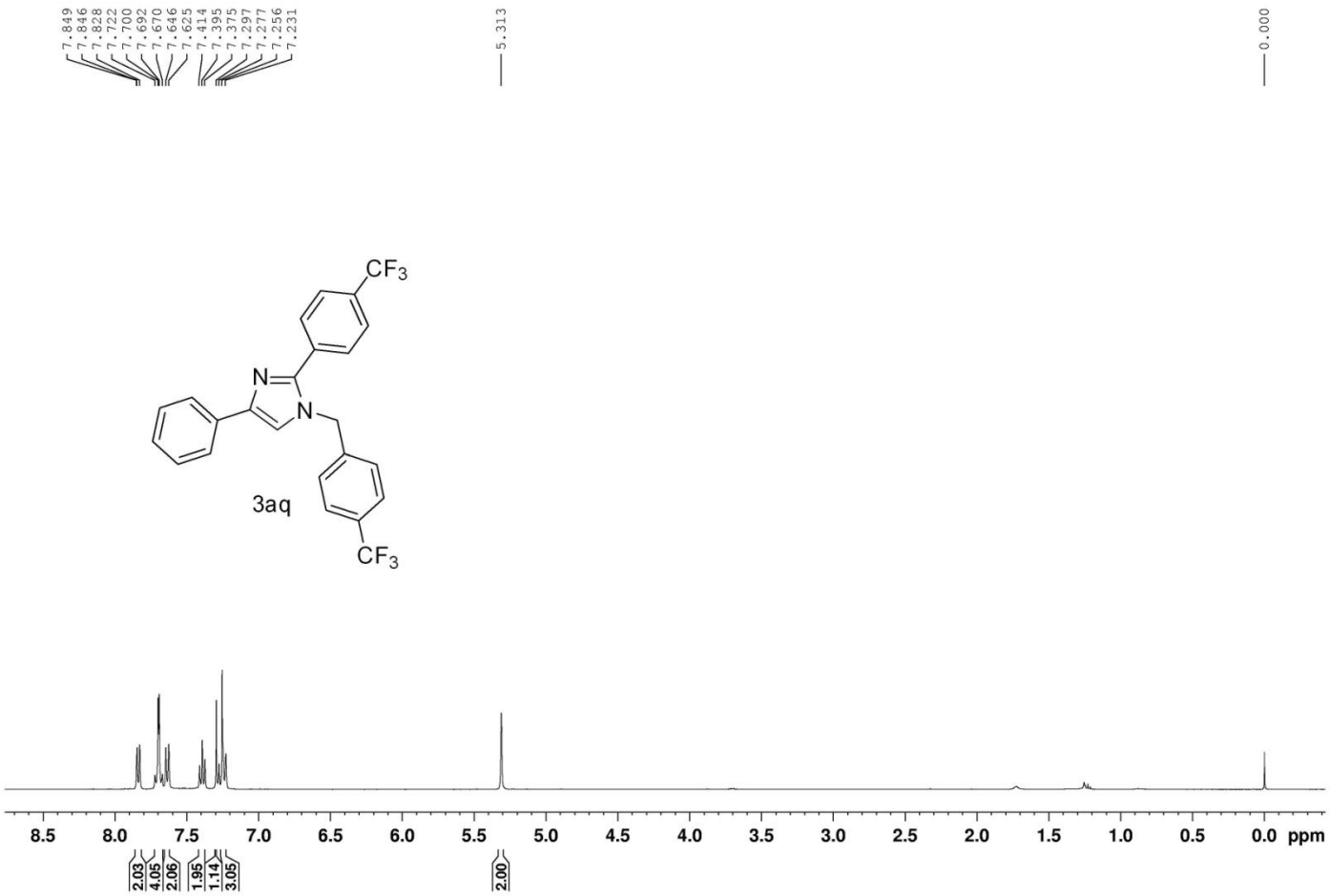
40
30
20
ppm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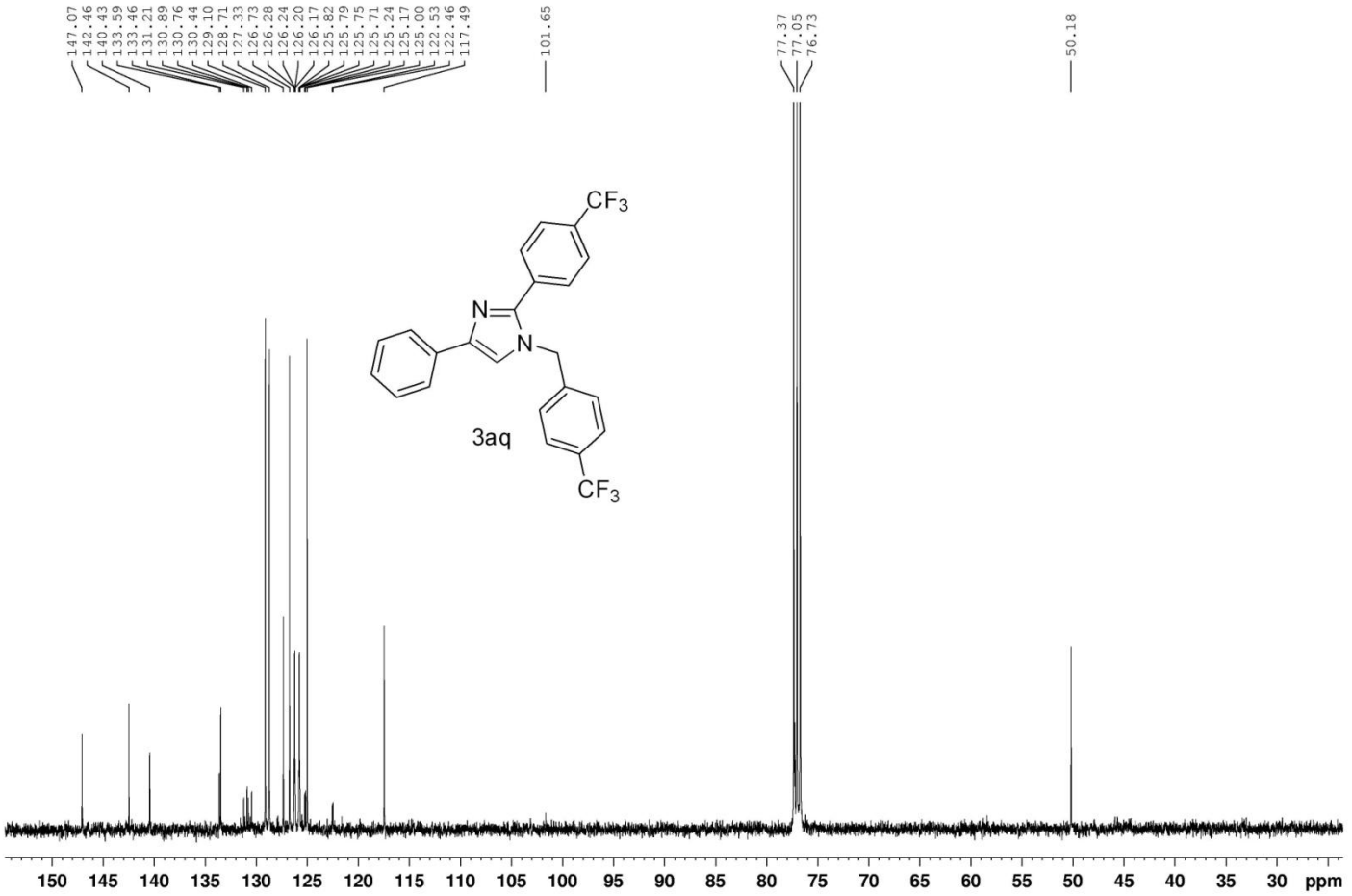
7.625
7.414
7.395
7.375
7.297
7.277
7.256
7.231
5.313
0.000
CF3
N
N
3aq
CF3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
2.03
4.05
2.06
1.95
1.14
3.05
2.00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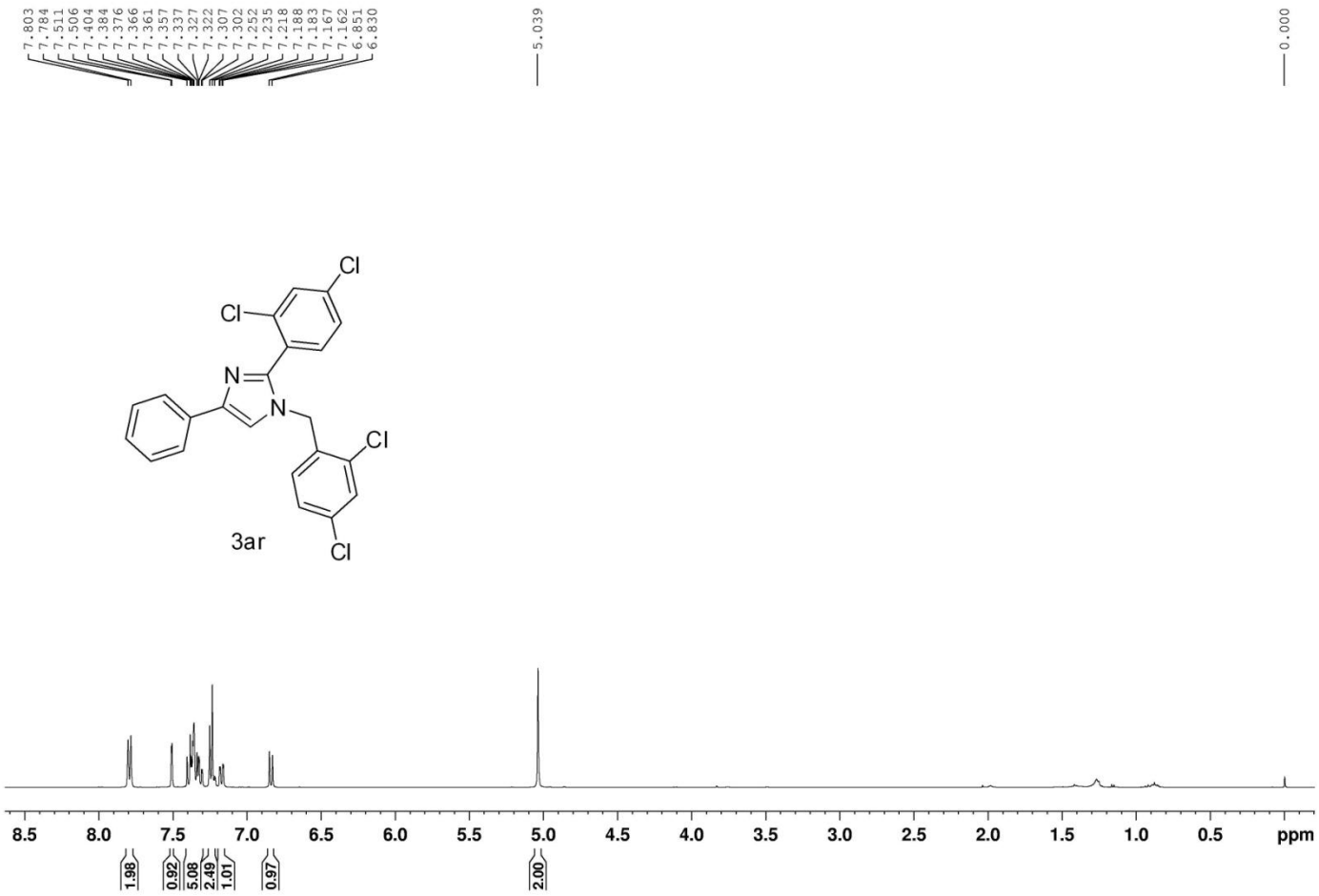
140.43
133.59
133.46
131.21
130.89
130.76
130.44
129.10
128.71
127.33
126.73
126.28
126.24
126.20
126.17
125.82
125.79
125.75
125.71
125.24
125.17
125.00
122.53
122.46
117.49
101.65
77.37
77.05
76.73
50.18
CF3
N
N
3aq
CF3
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 ppm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7.307
7.302
7.252
7.235
7.218
7.188
7.183
7.167
7.162
6.851
6.830
5.039
0.000
Cl
Cl
N
N
Cl
Cl
3ar
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.0
0.5
ppm
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5.08
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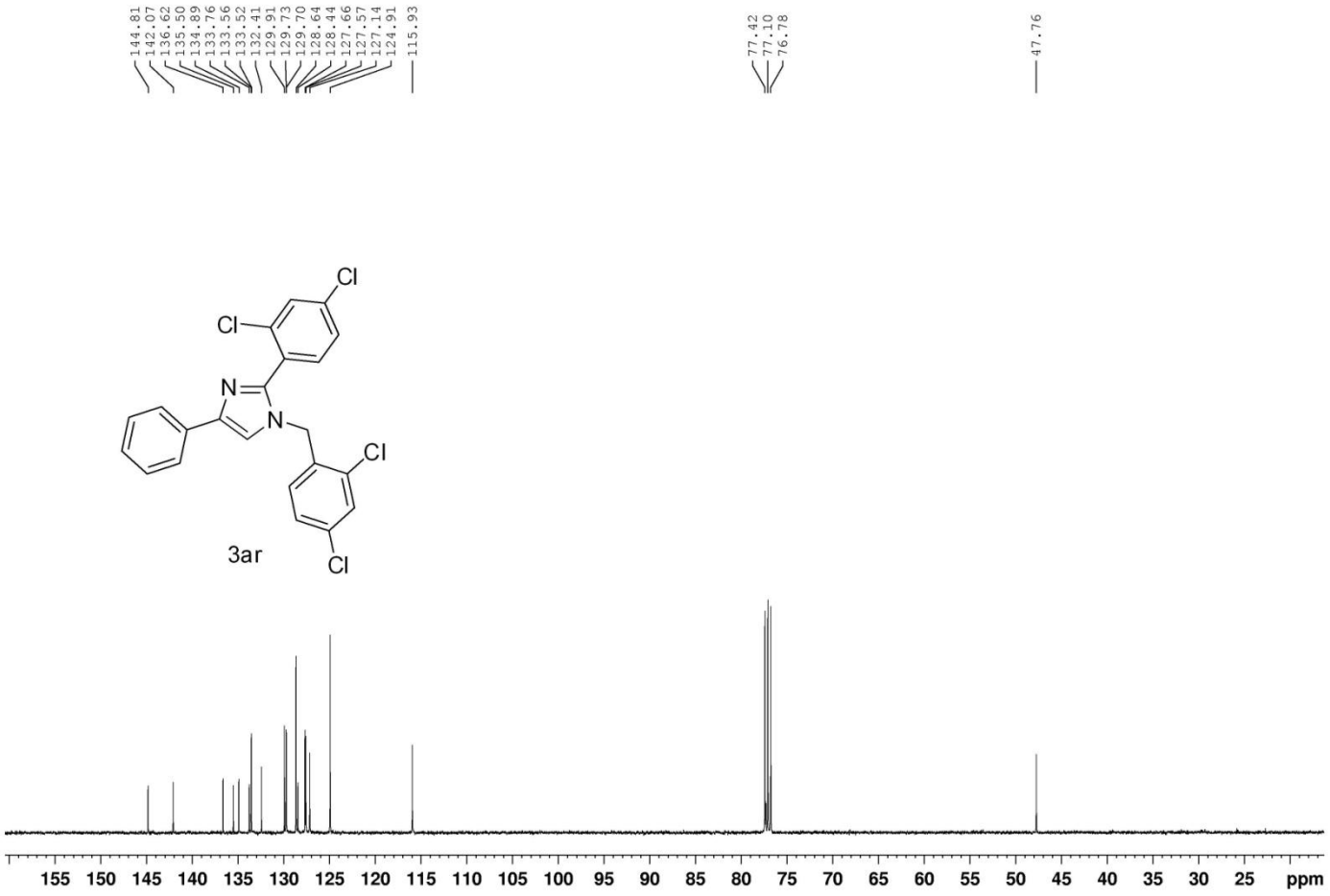
0.97
2.00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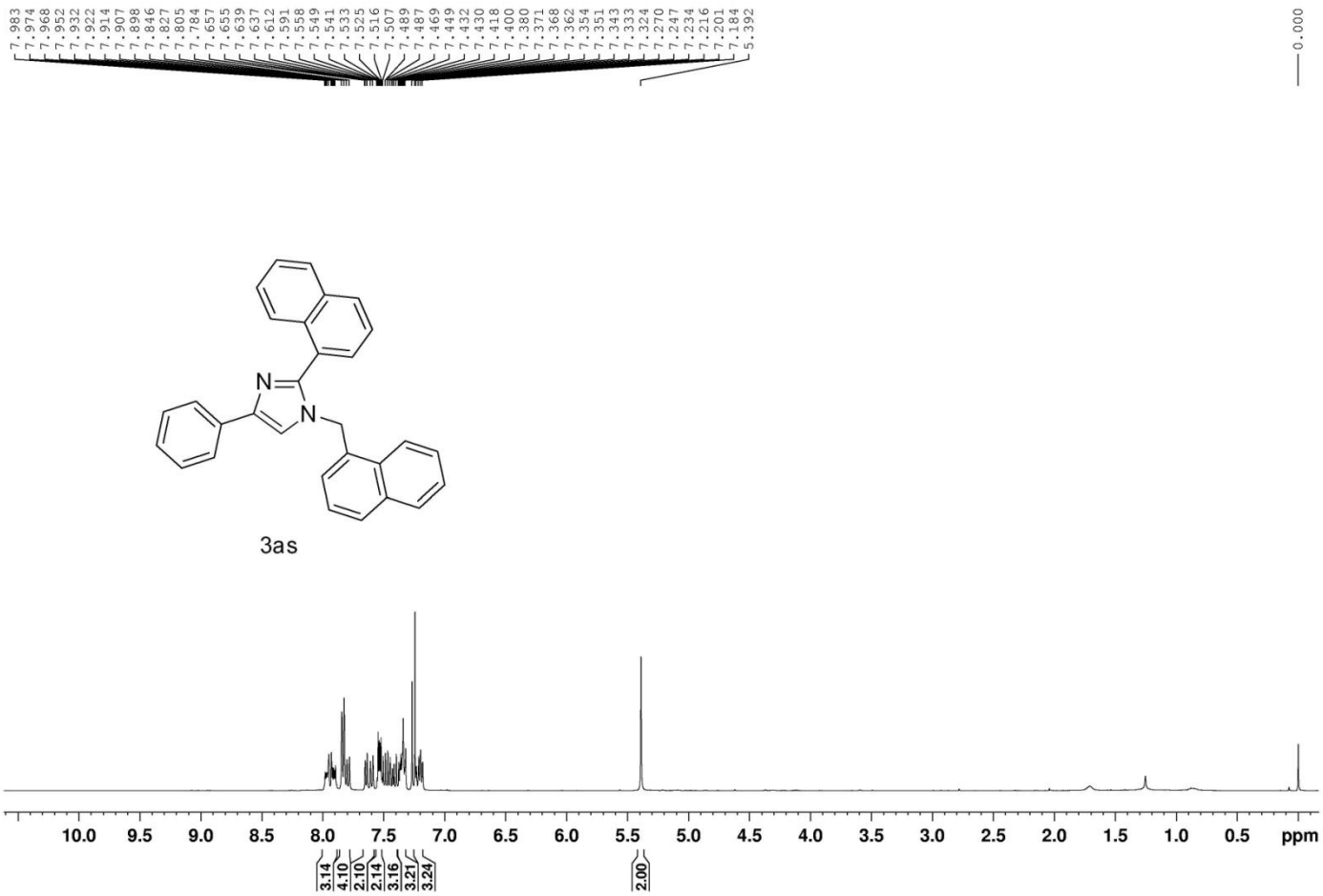
129.73
129.70
128.64
128.44
127.66
127.57
127.14
124.91
115.93
77.42
77.10
76.78
47.76
Cl
Cl
N
N
Cl
Cl
3ar
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 ppm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7.846
7.827
7.805
7.784
7.657
7.655
7.639
7.637
7.612
7.591
7.558
7.549
7.541
7.533
7.525
7.516
7.507
7.489
7.487
7.469
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7.432
7.430
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7.400
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7.371
7.368
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7.354
7.351
7.343
7.333
7.324
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7.247
7.234
7.216
7.201
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N
N
3as
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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
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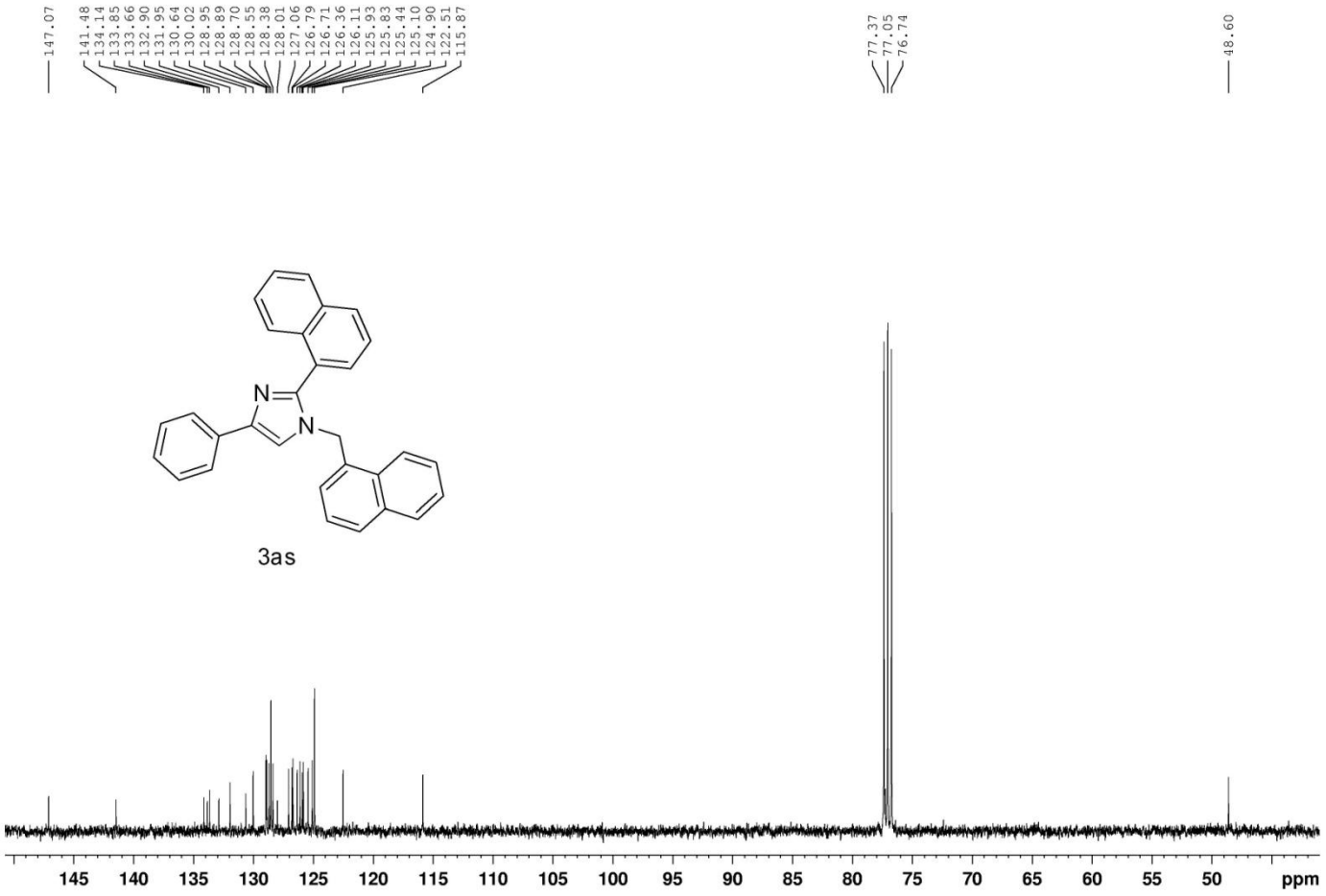
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128.70
128.55
128.38
128.01
127.06
126.79
126.71
126.36
126.11
125.93
125.83
125.44
125.10
124.90
122.51
115.87
77.37
77.05
76.74
48.60
N
N
3as
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115
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80
75
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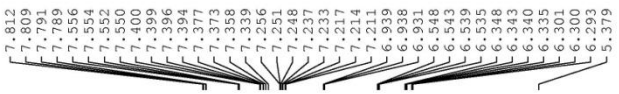
50
ppm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7.377
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7.358
7.339
7.256
7.251
7.248
7.237
7.233
7.217
7.214
7.211
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6.938
6.931
6.548
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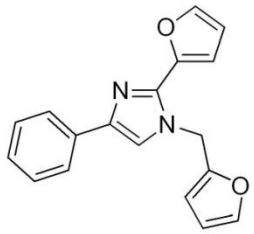
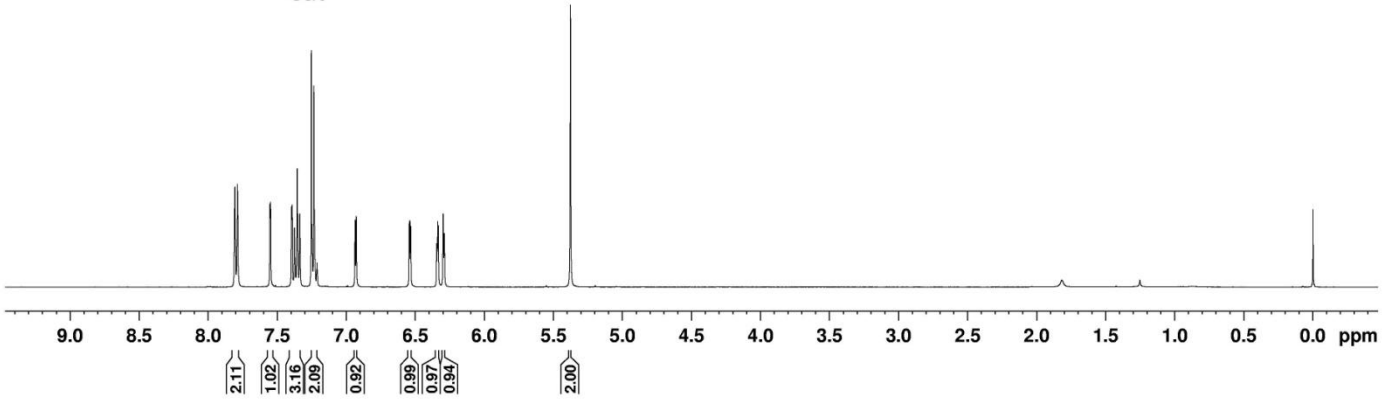

O
N
N
O

3at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5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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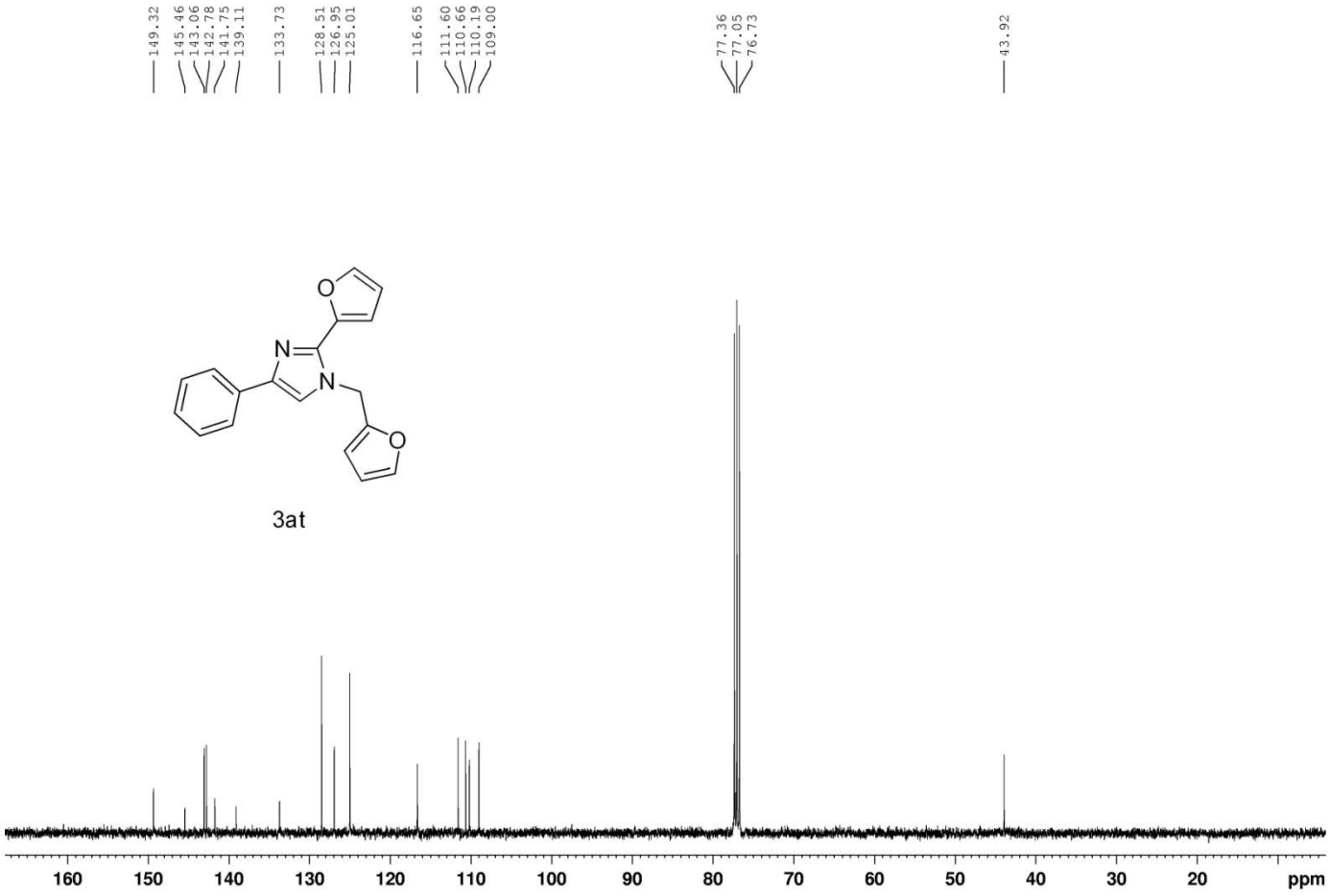
2.00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110.66
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109.00
77.36
77.05
76.73
43.92
O
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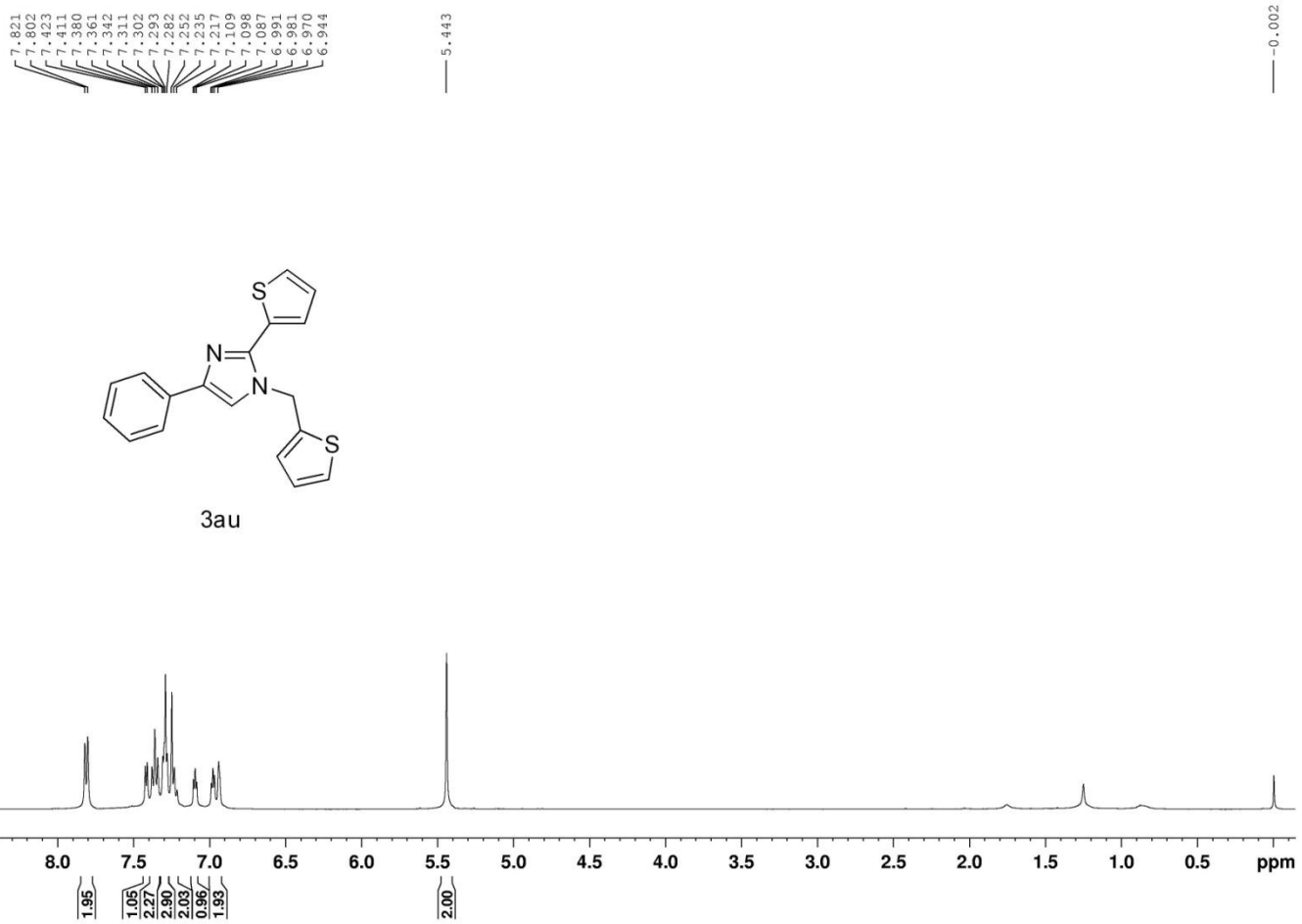
30
20
ppm

3at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7.235
7.217
7.109
7.098
7.087
6.991
6.981
6.970
6.944
5.443
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N
N
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7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
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2.0
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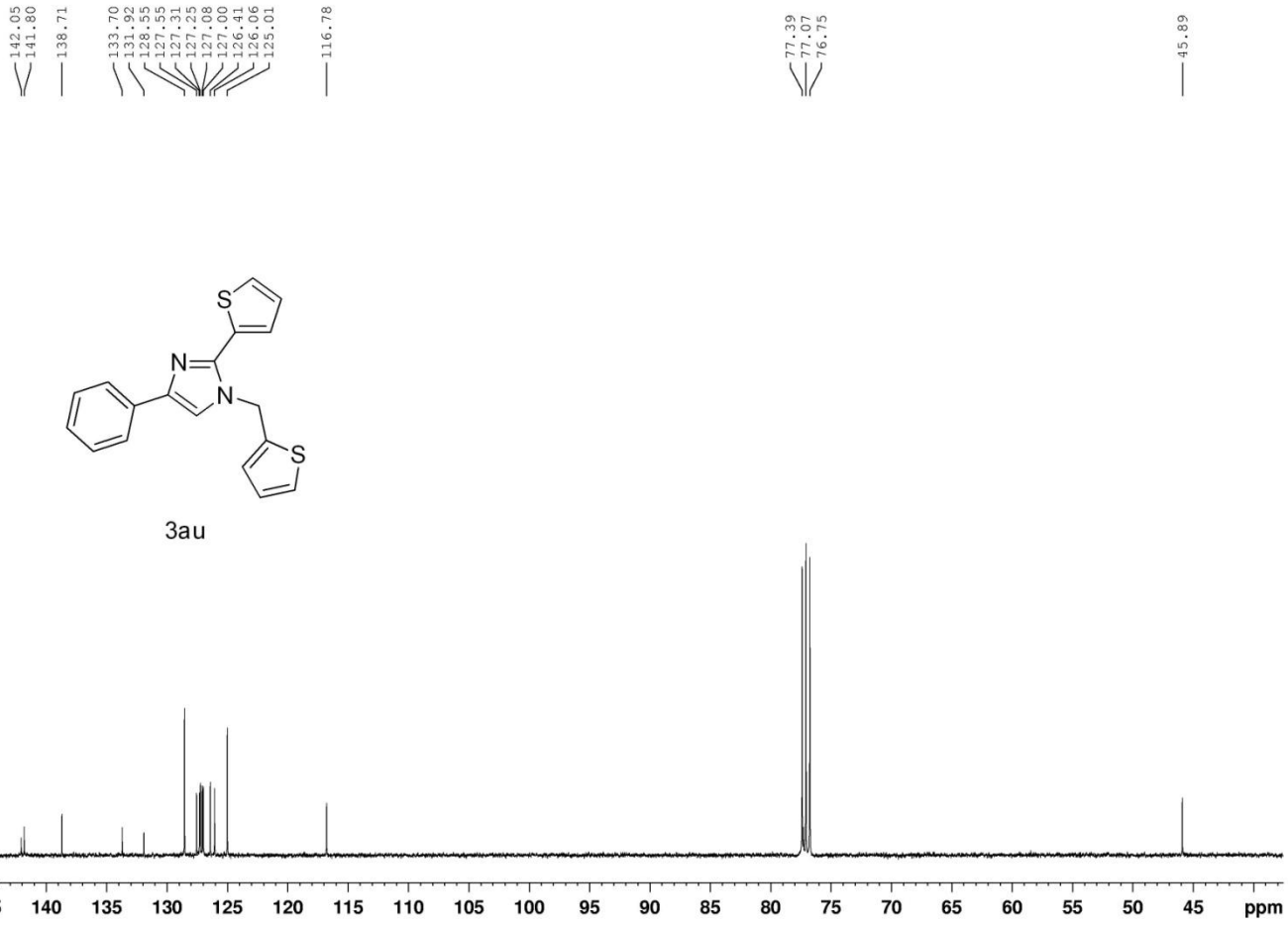
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127.08
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126.41
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76.75
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140
135
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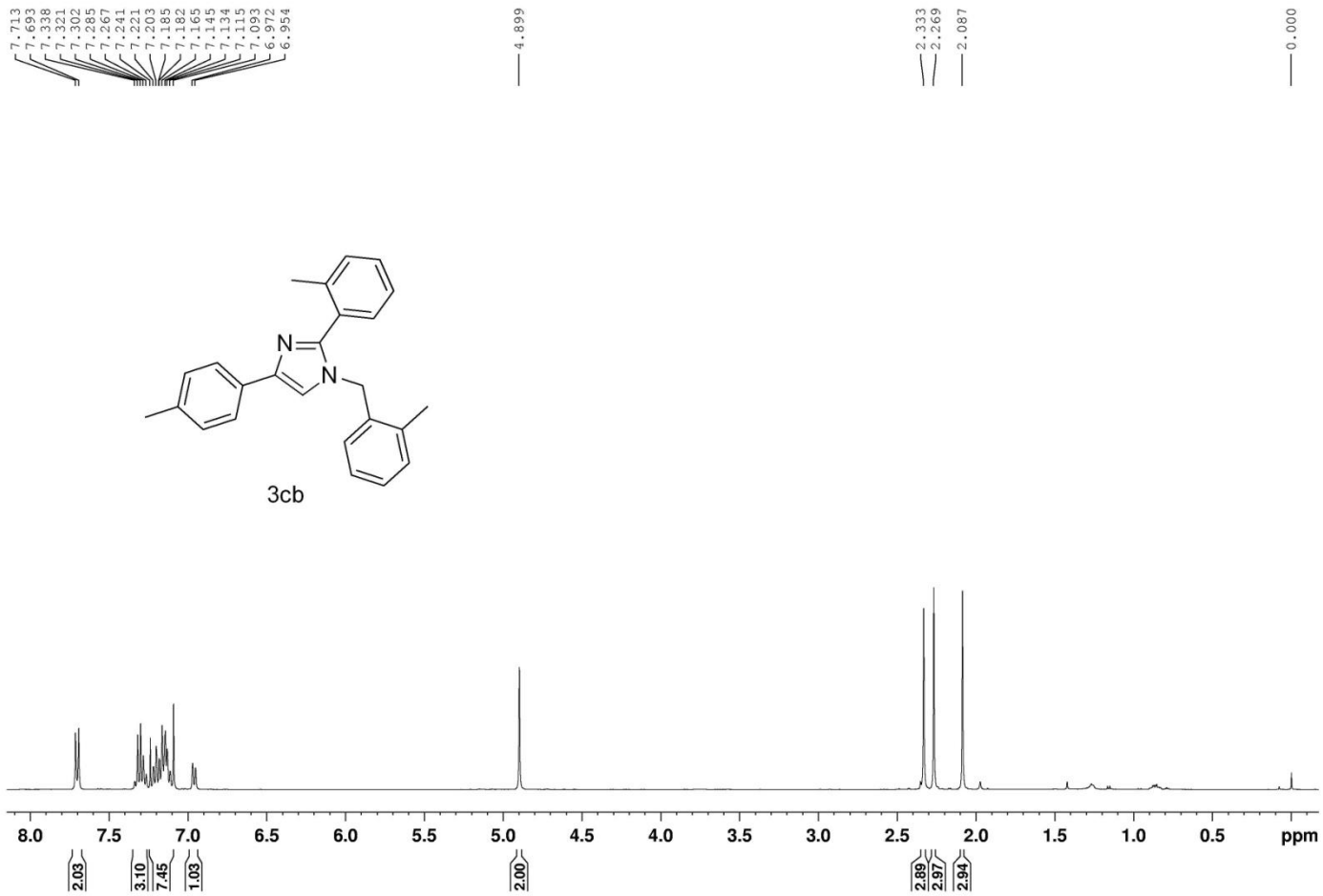
3au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7.145
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7.115
7.093
6.972
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2.269
2.087
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N
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6.0
5.5
5.0
4.5
4.0
3.5
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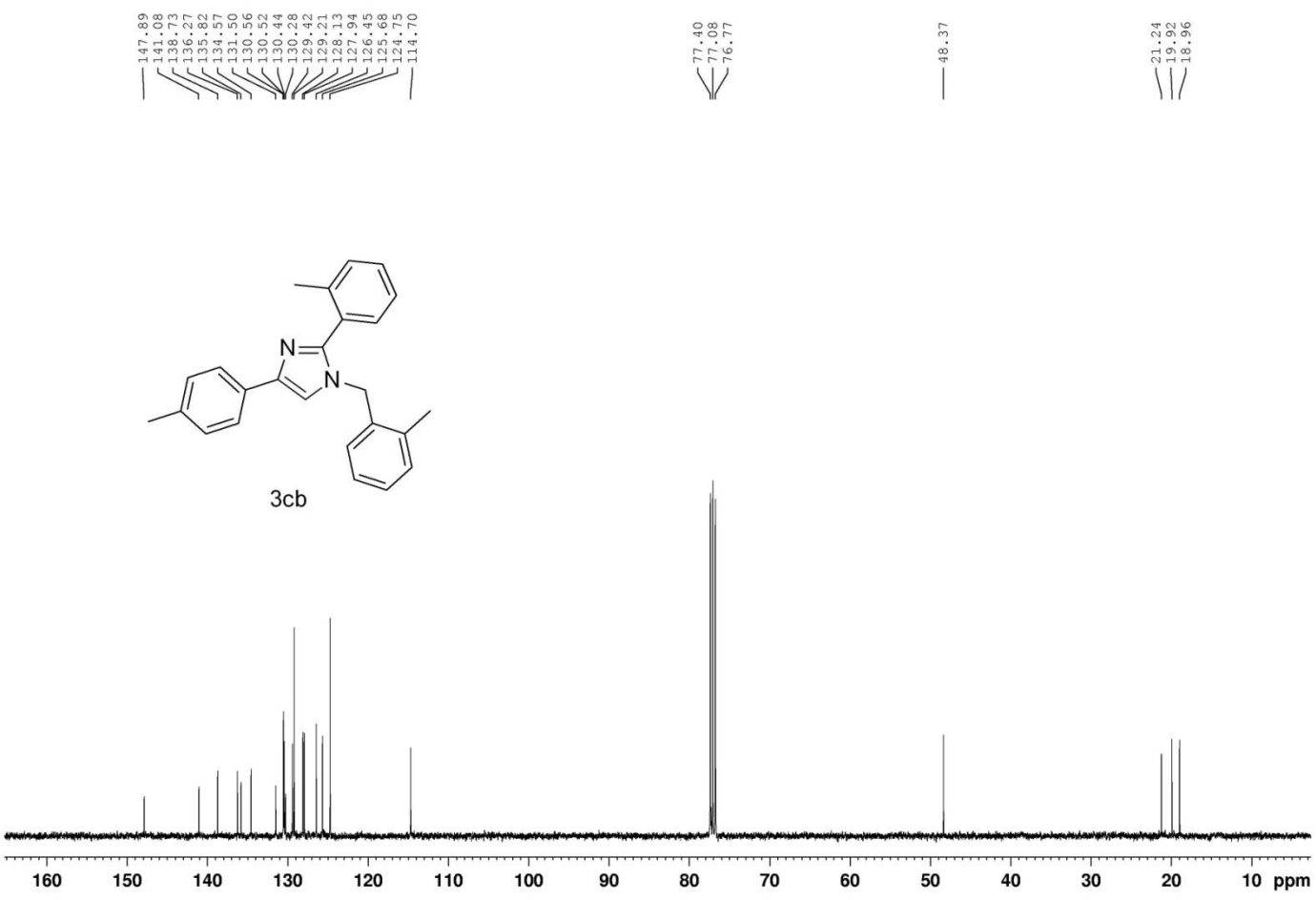
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128.13
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126.45
125.68
124.75
114.70
77.40
77.08
76.77
48.37
21.24
19.92
18.96
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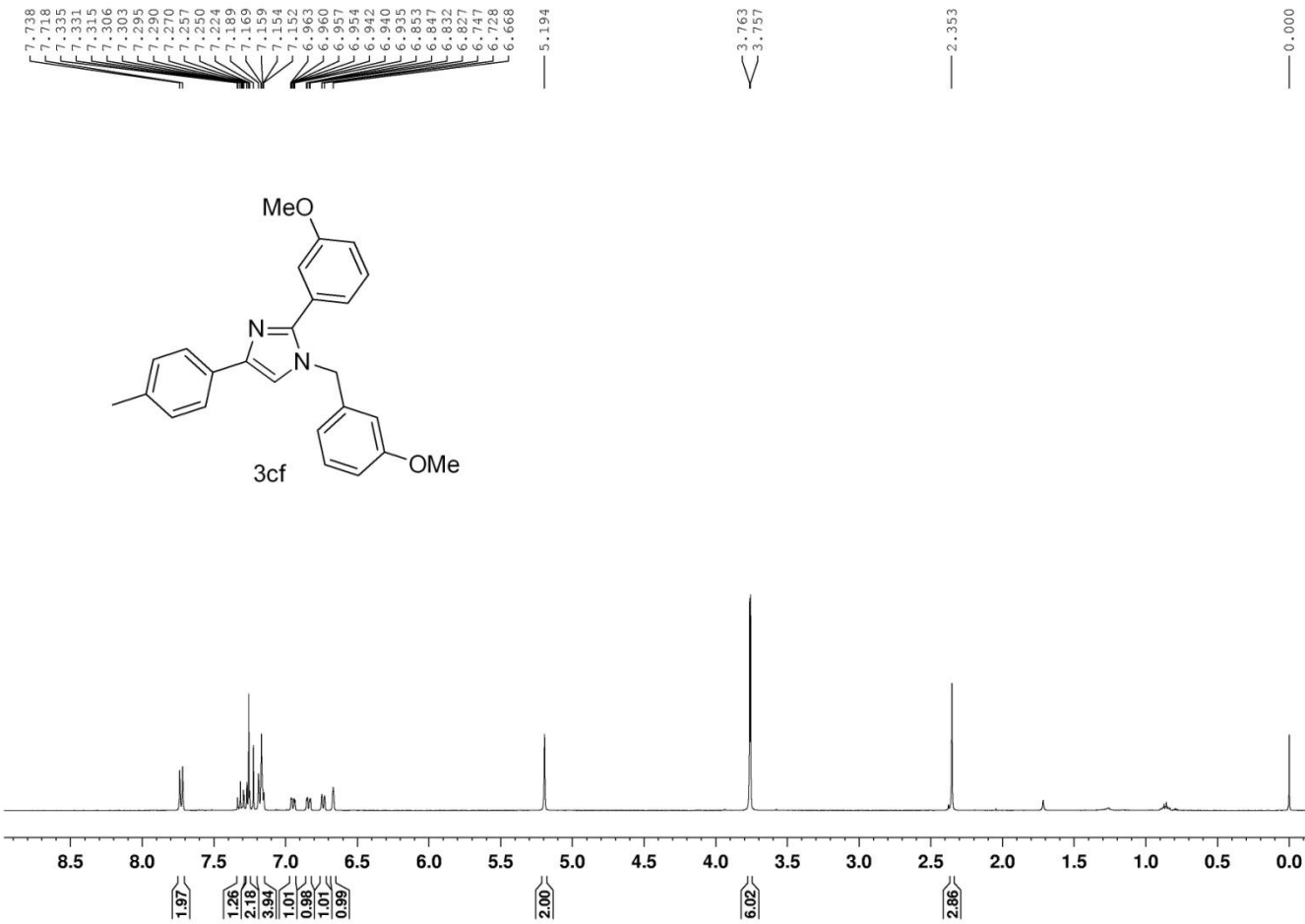
10
ppm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7.169
7.159
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7.152
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6.960
6.957
6.954
6.942
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6.935
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6.847
6.832
6.827
6.747
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6.668
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MeO
N
N
OMe
3cf
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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
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1.01
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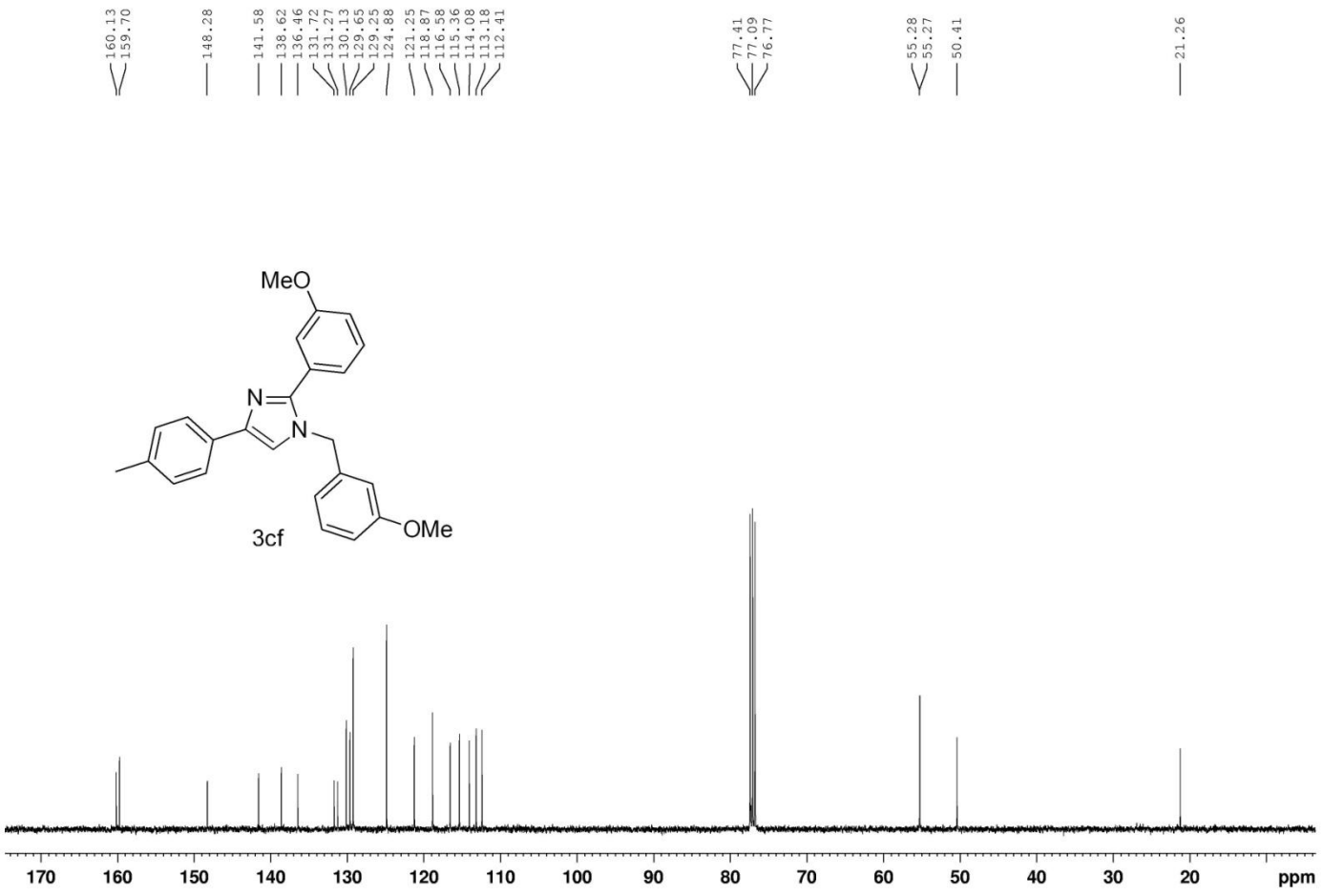
2.86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118.87
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115.36
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112.41
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77.09
76.77
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55.27
50.41
21.26
MeO
N
N
OMe
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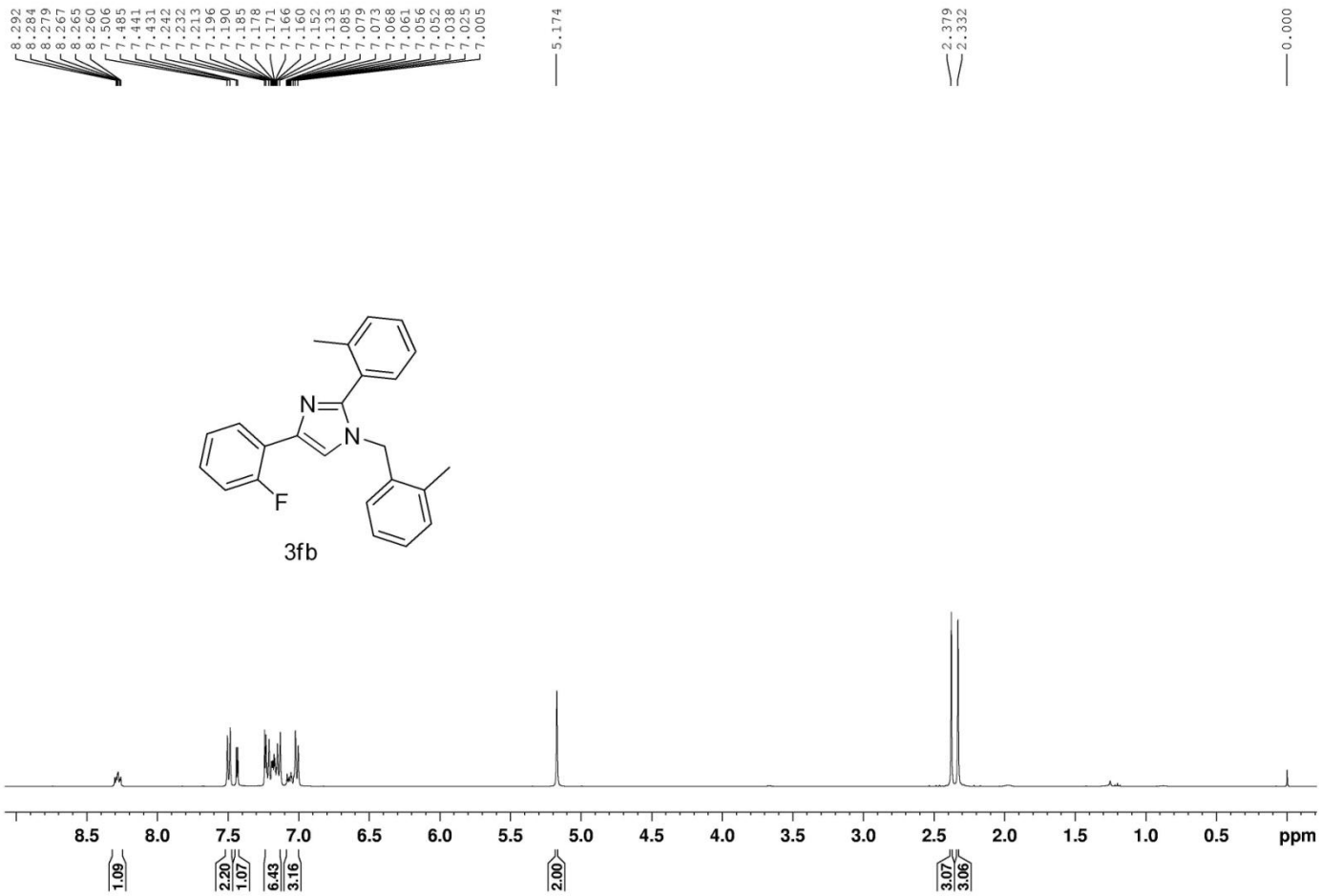
ppm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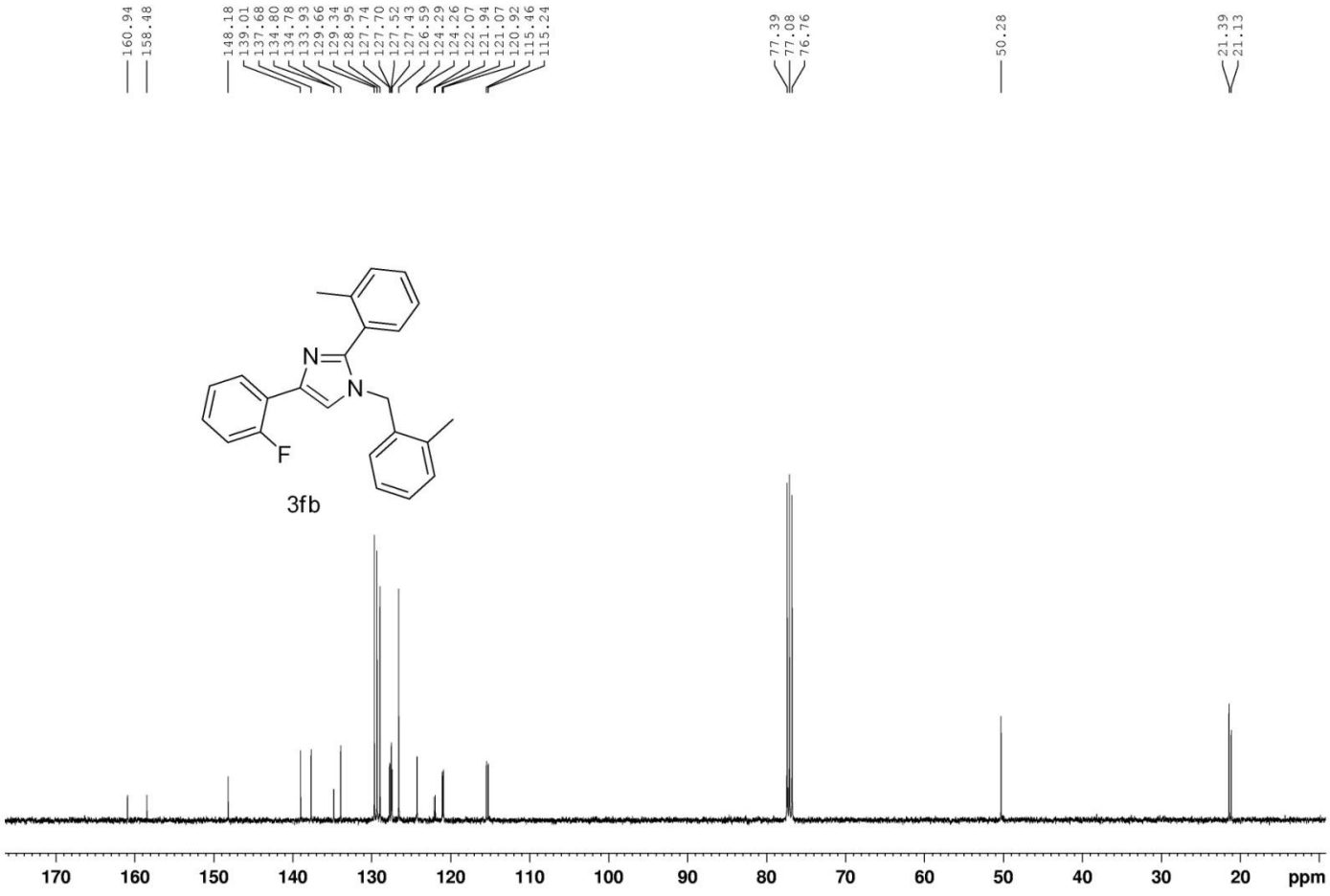
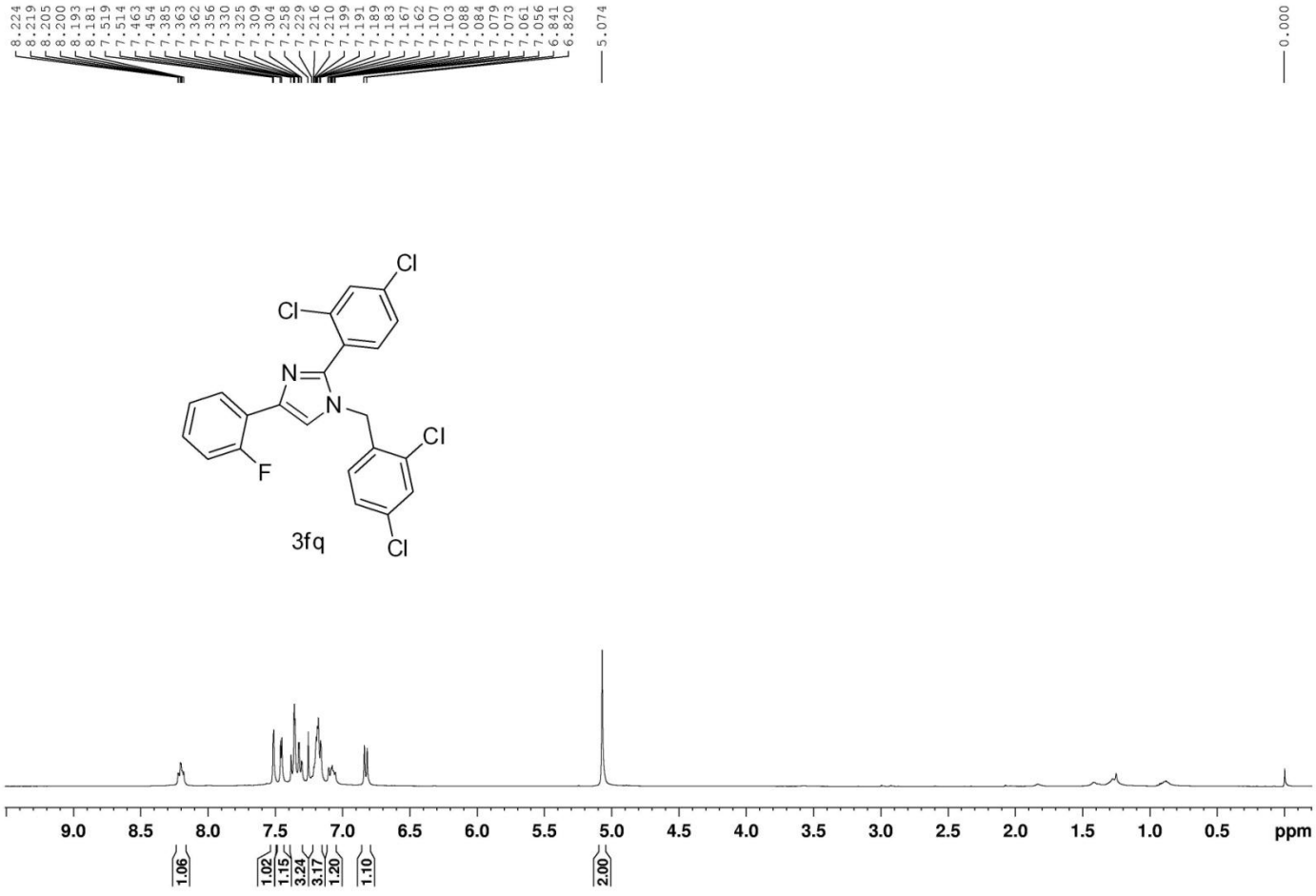
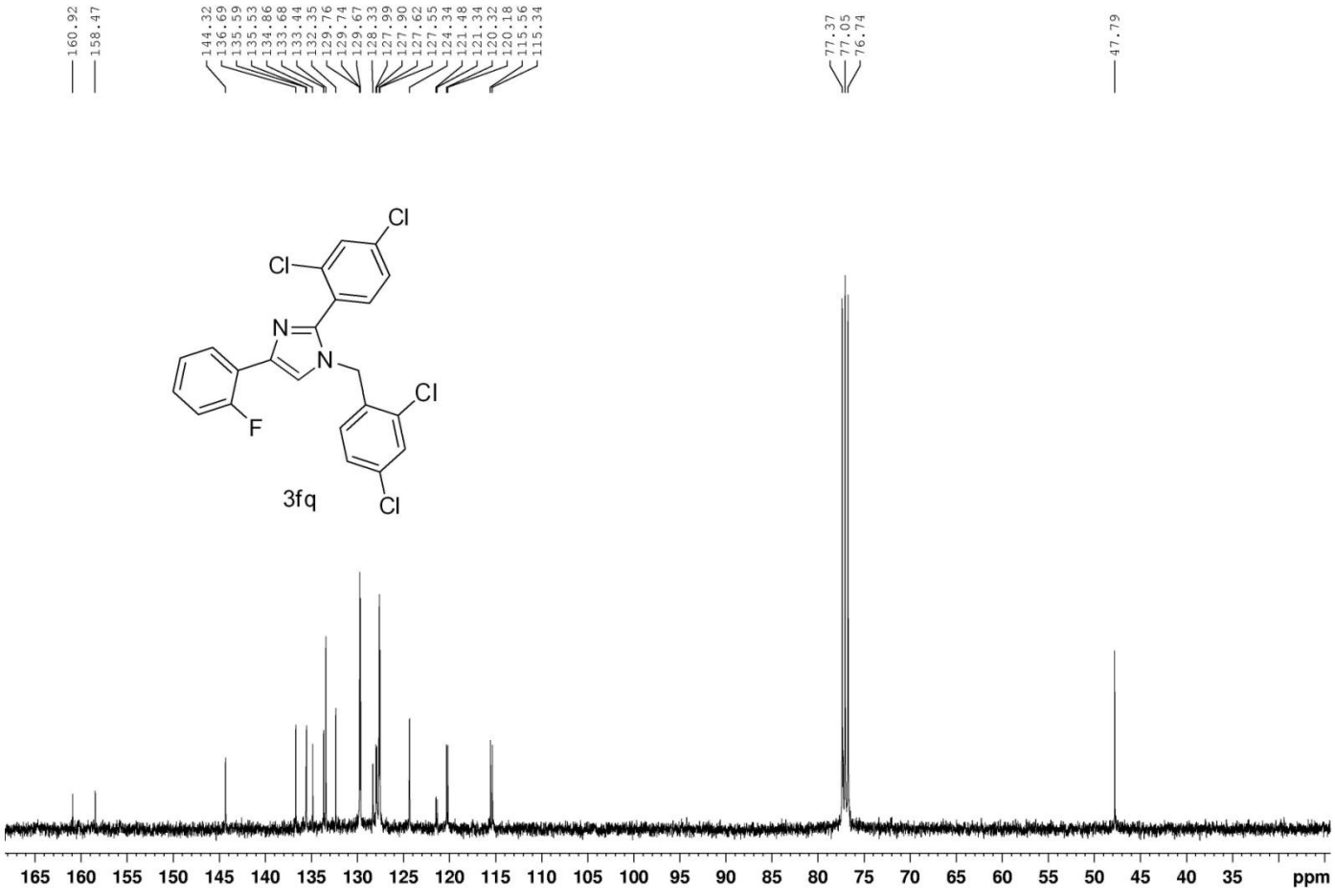
8.279
8.267
8.265
8.260
7.506
7.485
7.441
7.431
7.242
7.232
7.213
7.196
7.190
7.185
7.178
7.171
7.166
7.160
7.152
7.133
7.085
7.079
7.073
7.068
7.061
7.056
7.052
7.038
7.025
7.005
5.174
2.379
2.332
0.000
N
N
F
3fb
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.09
2.20
1.07
6.43
3.16
2.00
3.07
3.06


160.94
158.48
148.18
139.01
137.68
134.80
134.78
133.93
129.66
129.34
128.95
127.74
127.70
127.52
127.43
126.59
124.29
124.26
122.07
121.94
121.07
120.92
115.46
115.24
77.39
77.08
76.76
50.28
21.39
21.13
N
N
F
3fb
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.224
8.219
8.205
8.200
8.193
8.181
7.519
7.514
7.463
7.454
7.385
7.363
7.362
7.356
7.330
7.325
7.309
7.304
7.258
7.229
7.216
7.210
7.199
7.191
7.189
7.183
7.167
7.162
7.107
7.103
7.088
7.084
7.079
7.073
7.061
7.056
6.841
6.820
5.074
0.000
Cl
Cl
N
N
Cl
F
Cl
3fq
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
ppm
1.06
1.02
1.15
3.24
3.17
1.20
1.10
2.00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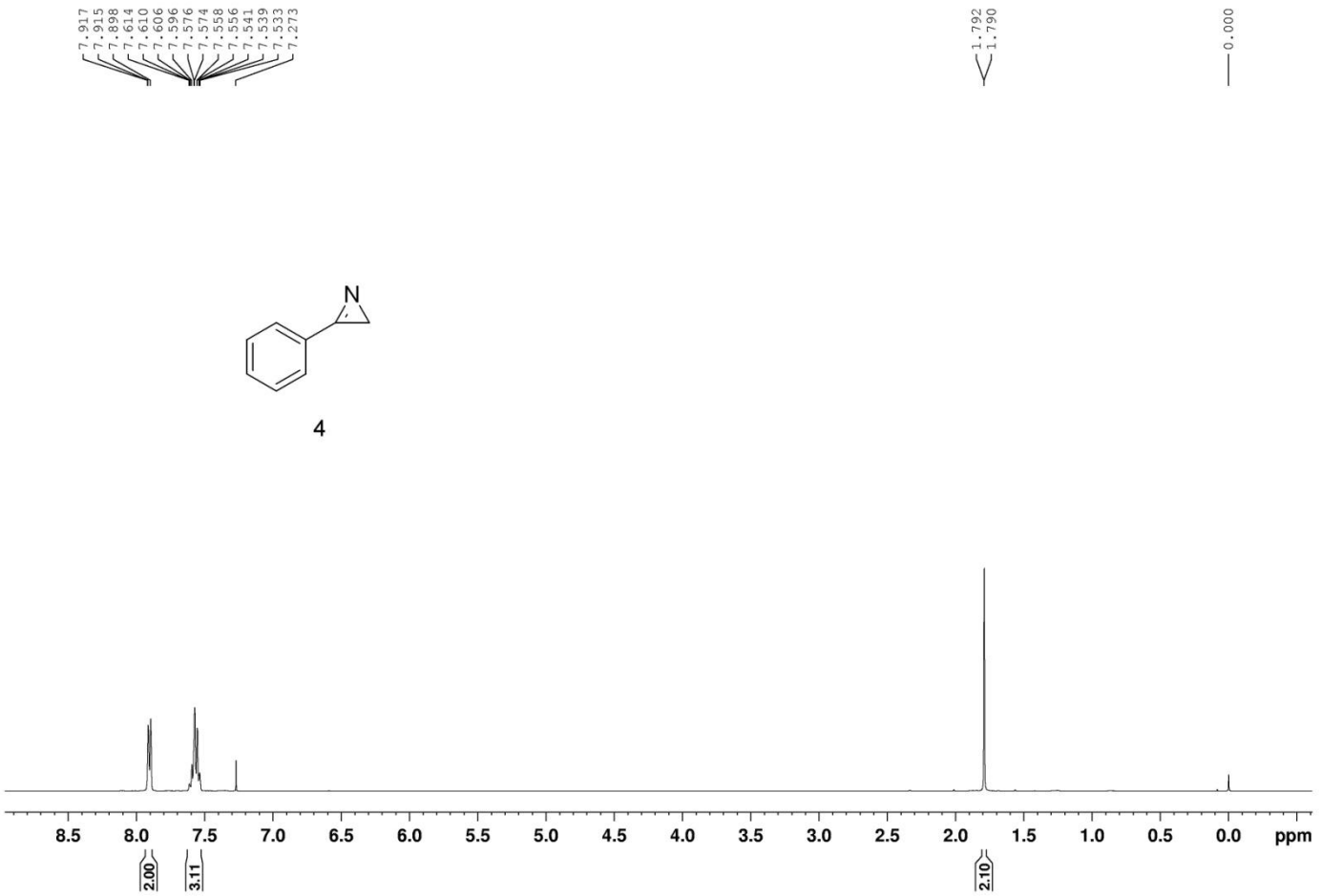
158.47
144.32
136.69
135.59
135.53
134.86
133.68
133.44
132.35
129.76
129.74
129.67
128.33
127.99
127.90
127.62
127.55
124.34
121.48
121.34
120.32
120.18
115.56
115.34
77.37
77.05
76.74
47.79
Cl
Cl
N
N
Cl
F
Cl
3fq
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 ppm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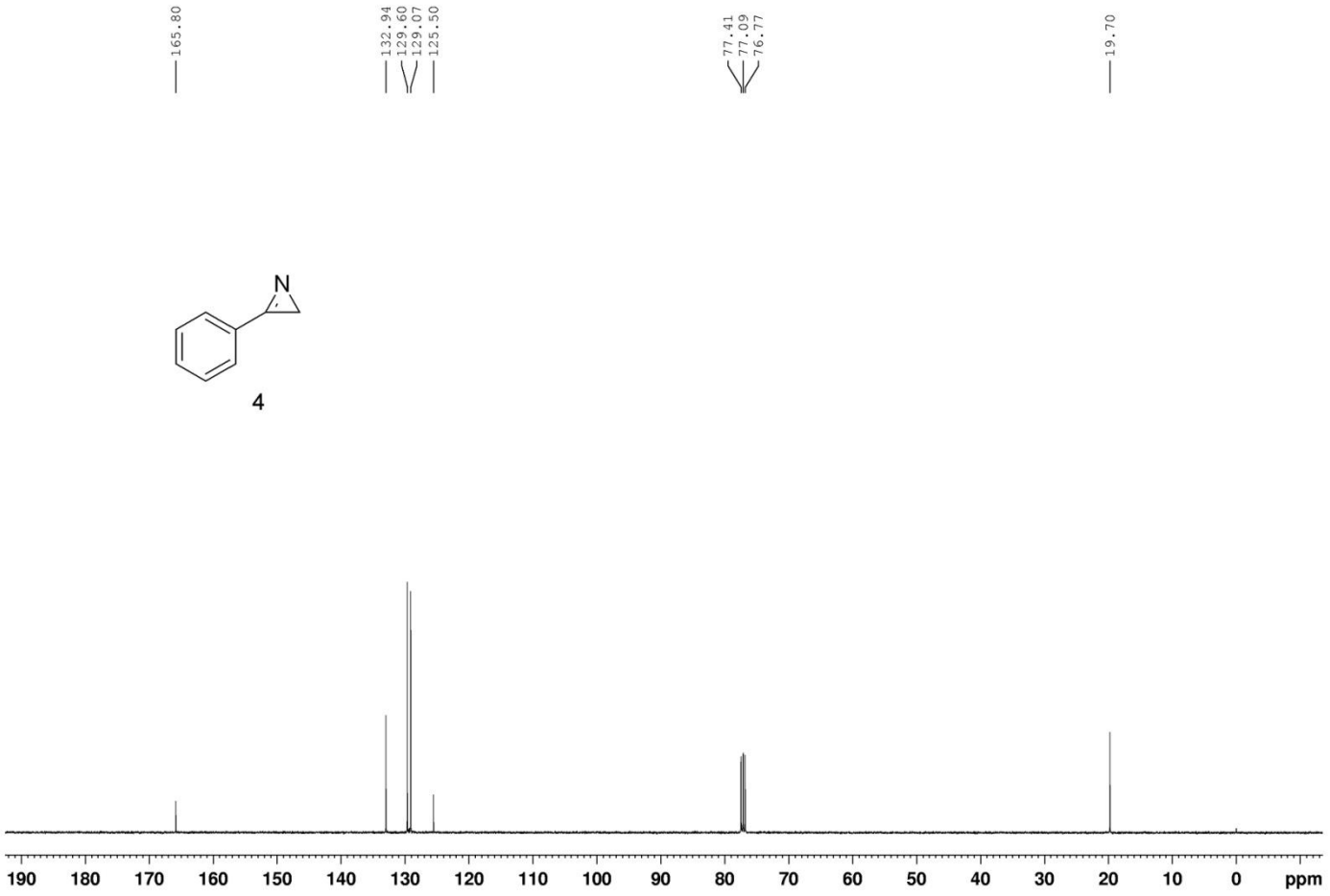
7.915
7.898
7.614
7.610
7.606
7.596
7.576
7.574
7.558
7.556
7.541
7.539
7.533
7.273
1.792
1.790
0.000
N
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
3.11
2.10

4


165.80
132.94
129.60
129.07
125.50
77.41
77.09
76.77
19.70
N
4
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm