Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Facile synthesis of fully substituted 1*H*-imidazoles from oxime esters via dual photoredox/copper catalyzed multicomponent reactions

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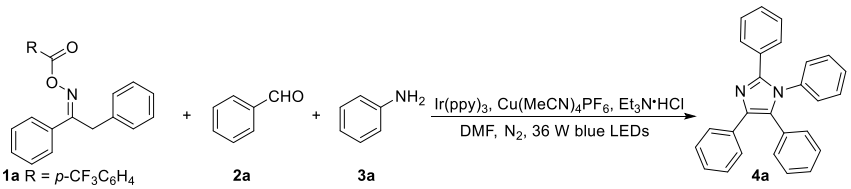
Supporting Information

Table of Contents

1.General information. All commercially available reagents were used without further purification. Column chromatography was performed on silica gel (200-300 mesh). ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a 400 MHz NMR spectrometer. ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectra were recorded on a 500 MHz NMR spectrometer. Chemical shifts (δ) were reported in ppm, and coupling constants (J) were given in Hertz (Hz). Data were reported as s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet. High-resolution mass spectra (HRMS) were recorded on an AB SCIEX Triple TOF 5600+ mass spectrometer. Melting points were uncorrected. Substrate**s 1a–1o** were prepared according to the literature procedure.[1]

2. Optimization of reaction conditions

Table S1. Optimization of Reaction Conditions[a]



1a R = *p*-$CF_3C_6H_4$ **2a** **3a** **4a**

Entry	PC	[Cu]	Additive	Solvent	Yield [%]
1	$Ir(dF(CF_3)ppy_2)dtbbpyPF_6$	CuCN	Et_3N HCl	DMF	0
2	$Ir(ppy_2dtbbpy)PF_6$	CuCN	Et_3N HCl	DMF	0
3	$Ir(dF(CF_3)ppy_2(5,5\text{-}dF(CF_3)bpy_2))PF_6$	CuCN	Et_3N HCl	DMF	0
4	$Ir(dF(CF_3)ppy_2bpy)PF_6$	CuCN	Et_3N HCl	DMF	0
5	$Ir(ppy)_3$	CuCN	Et_3N HCl	DMF	51
6	4CzIPN	CuCN	Et_3N HCl	DMF	0
7	4DPAIPN	CuCN	Et_3N HCl	DMF	0
8	Acr-$Mes^+ClO_4^-$	CuCN	Et_3N HCl	DMF	0
9	Eosin Y	CuCN	Et_3N HCl	DMF	0
10	Rhodamine B	CuCN	Et_3N HCl	DMF	0
11	Rose begal	CuCN	Et_3N HCl	DMF	0
12	Methylene blue	CuCN	Et_3N HCl	DMF	0
13	$Ir(ppy)_3$	CuBr	Et_3N HCl	DMF	81
14	$Ir(ppy)_3$	CuCl	Et_3N HCl	DMF	79
15	$Ir(ppy)_3$	CuI	Et_3N HCl	DMF	77
16	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	DMF	90
17	$Ir(ppy)_3$	CuSCN	Et_3N HCl	DMF	41
18	$Ir(ppy)_3$	CuTc	Et_3N HCl	DMF	48

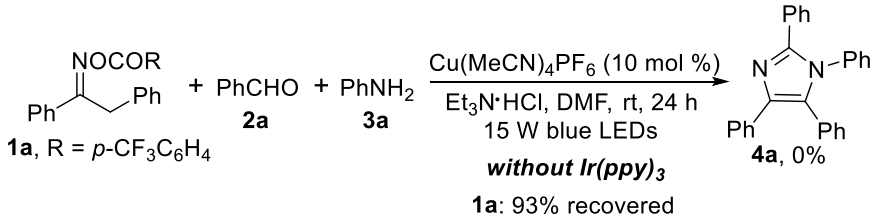
19	$Ir(ppy)_3$	Cu(OAc)	Et_3N HCl	DMF	82
20	$Ir(ppy)_3$	Cu(OTf)	Et_3N HCl	DMF	73
21	$Ir(ppy)_3$	$Cu(OAc)_2$	Et_3N HCl	DMF	48
22	$Ir(ppy)_3$	$Cu(OTf)_2$	Et_3N HCl	DMF	46
23	$Ir(ppy)_3$	$Cu(acac)_2$	Et_3N HCl	DMF	49
24	$Ir(ppy)_3$	$Cu(NO_3)_2$	Et_3N HCl	DMF	37
25	$Ir(ppy)_3$	$CuCl_2$	Et_3N HCl	DMF	53
26	$Ir(ppy)_3$	$CuBr_2$	Et_3N HCl	DMF	52
27	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N	DMF	60
28	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Cs_2CO_3	DMF	0
29	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Na_2CO_3	DMF	53
30	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	K_2CO_3	DMF	70
31	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Na_2HPO_4	DMF	57
32	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	K_2HPO_4	DMF	40
33	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	$NaHCO_3$	DMF	74
34	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	NaH_2PO_4	DMF	35
35	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	TFA	DMF	0
36	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	TMG	DMF	30
37	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	DMA	60
38	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	DMSO	73
39	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	MeCN	71
40	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	Dioxane	0
41	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	DCE	53
42	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	MeOH	0
43	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	NMP	36
44	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	EA	59
45	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	THF	3
46	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	toluene	36
47	-	$Cu(MeCN)_4PF_6$	Et_3N HCl	DMF	0
48	$Ir(ppy)_3$	-	Et_3N HCl	DMF	0
49	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	-	DMF	50
50[c]	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	DMF	0
51[d]	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	DMF	77
52[e]	$Ir(ppy)_3$	$Cu(MeCN)_4PF_6$	Et_3N HCl	DMF	19

[a]All reactions were carried out with **1a** (76.6 mg, 0.20 mmol), **2a** (42.4 mg, 0.40 mmol, 2.0 equiv), **3a** (37.2 mg, 0.40 mmol, 2.0 equiv), photocatalyst (0.0020 mmol), copper catalyst (0.020 mmol), additive (0.40 mmol, 2 equiv) in solvent (2.0 mL) at room temperature under N_2 for 24 h under irradiation with a 15 W blue LED lamp unless otherwise stated. [b]Isolated yield based on **1a**. [c]The reaction was conducted in the dark.[d] In the air atmosphere. [e]18 W CFL lamp was used. $Cu(acac)_2$ = cupric acetylacetonate. CuTC = copper(I) thiophene-2-carboxylate. NEt_3 = triethylamine, TMG = tetramethylguanidine, DCE = dichloroethane, DMF = *N*,*N*-dimethylformamide.

3.General procedure for the synthesis of fully substituted 1*H*-imidazoles (Scheme 2 and Scheme 3). To a reaction tube equipped with a magnetic stir bar were added oxime ester **1** (0.20 mmol), aldehyde **2** (0.40 mmol), amine **3**(0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N·HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. After that, the mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 40:1 ~ 10:1) to give products **4**.

4. Mechanistic studies

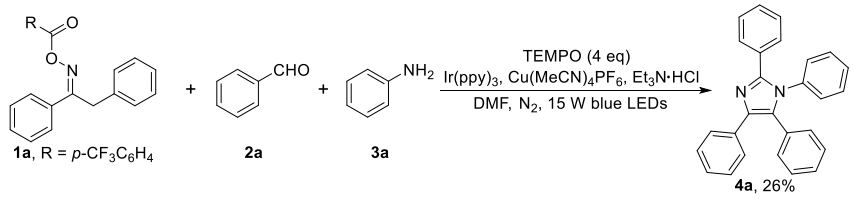
4.1 The experiment in the absence of $Ir(ppy)_3$



To a reaction tube equipped with a magnetic stir bar were added oxime ester **1a** (76.6 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N·HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **3a** was not observed. After that, the mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with H_2O, brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1) to afford the recovered oxime ester **1a** (71.5 mg, 93% recovered). Such results are not contradictory with previous reports about copper-mediated/catalyzed N-O bond

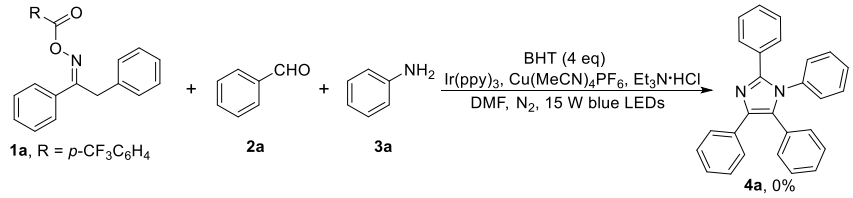
cleavage reactions of oxime esters, which need to be conducted under heating conditions.

4.2 The experiment of the addition of radical scavenger TEMPO



To a reaction tube equipped with a magnetic stir bar were added oxime ester **1a** (76.6 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N·HCl$ (55.2 mg, 0.40 mmol), TEMPO (125.0 mg, 0.80 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. Afterwards, the mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1) to give product **4a** (19.3 mg, 26%).

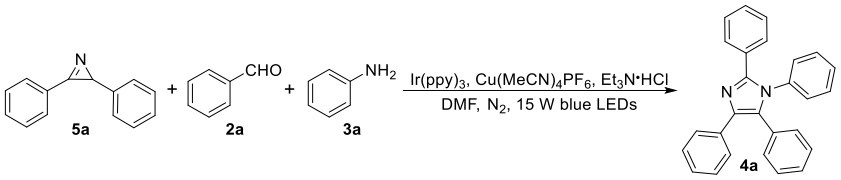
4.3 The experiment of the addition of radical scavenger BHT



To a reaction tube equipped with a magnetic stir bar were added oxime ester **1a** (76.6 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N·HCl$ (55.2 mg, 0.40 mmol), BHT (176.3 mg, 0.80 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **4a** was not observed.

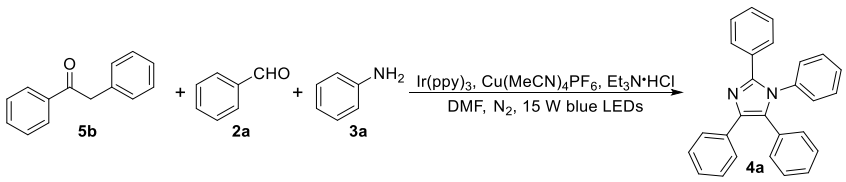
4.4 The possible reaction between compounds 5a-d, aldehyde 2a, and amine 3a

4.4.1 The possible reaction between 2,3-diphenyl-2*H*-azirine (5a), aldehyde 2a, and amine 3a



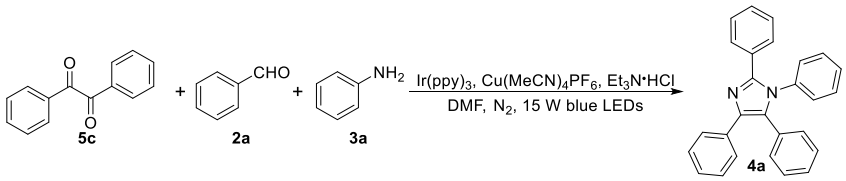
To a reaction tube equipped with a magnetic stir bar were added azirine **5a** (38.6 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N \cdot HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **4a** was not observed.

4.4.2 The possible reaction between 1,2-diphenylethan-1-one (5b), aldehyde 2a, and amine 3a



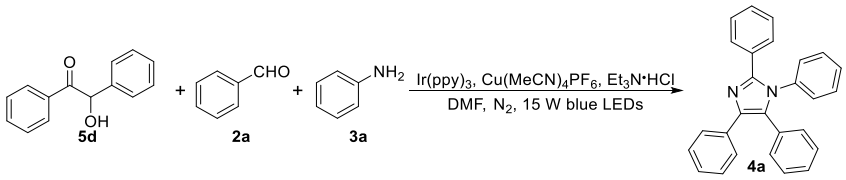
To a reaction tube equipped with a magnetic stir bar were added azirine **5b** (39.2 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N \cdot HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **4a** was not observed.

4.4.3 The possible reaction between benzil (5c), aldehyde 2a, and amine 3a (Scheme 2d)



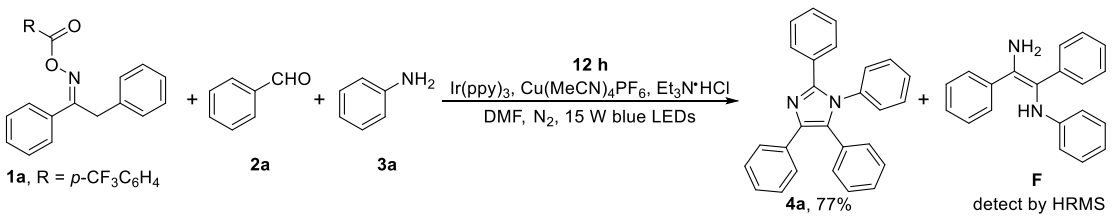
To a reaction tube equipped with a magnetic stir bar were added azirine **5c** (42.0 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N·HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **4a** was not observed.

4.4.4 The possible reaction between 2-hydroxy-1,2-diphenylethan-1-one (5d) aldehyde 2a, and amine 3a

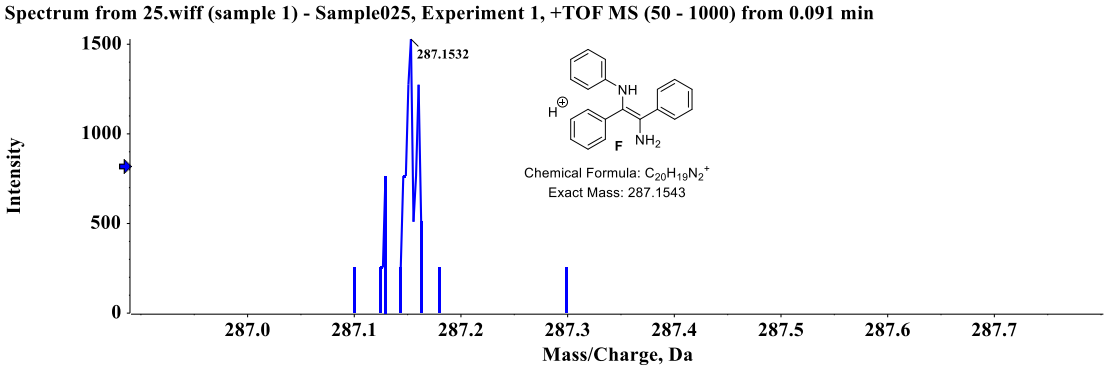


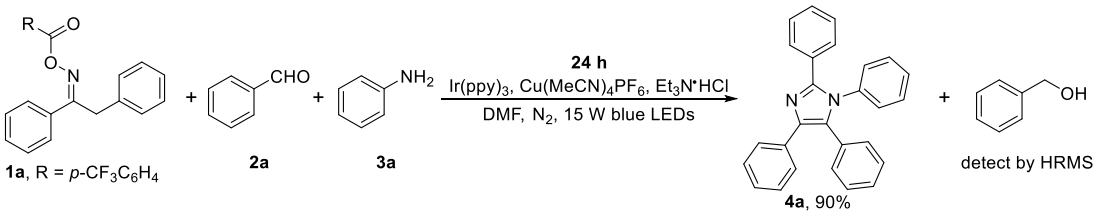
To a reaction tube equipped with a magnetic stir bar were added azirine **5d** (42.4 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N·HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **4a** was not observed.

4.5 Intermediates trapping experiments



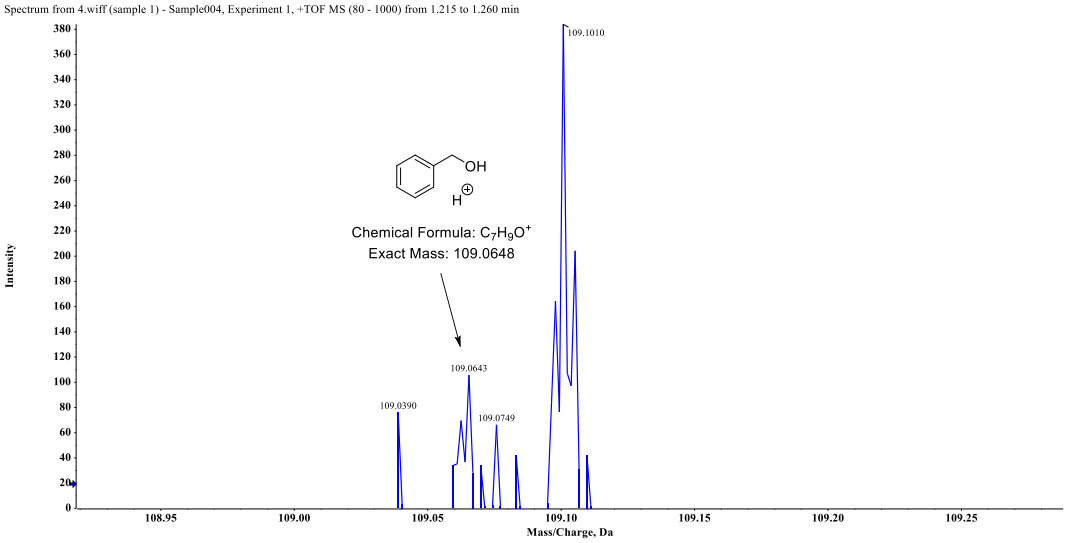
To a reaction tube equipped with a magnetic stir bar were added oxime ester **1a** (76.6 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N \cdot HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 12 h. After that, a trace amount of the crude reaction mixture was subjected to the HRMS analysis, which indicated that the intermediates **F** could be formed. Afterwards, the mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1) to give product **4a** (57.1 mg, 77%).





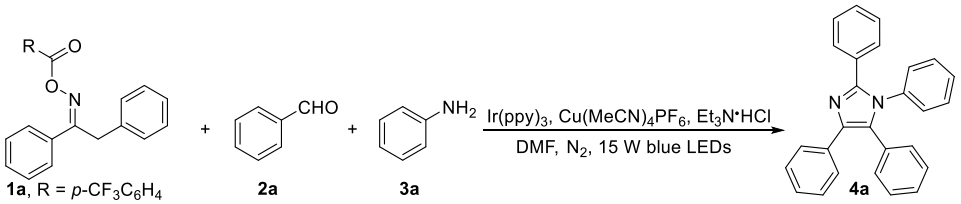
To a reaction tube equipped with a magnetic stir bar were added oxime ester **1a** (76.6 mg, 0.20 mmol), aldehyde **2a** (42.4 mg, 0.40 mmol), amine **3a** (37.3 mg, 0.40 mmol), $Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), $Cu(MeCN)_4PF_6$ (7.5 mg, 0.020 mmol), $Et_3N \cdot HCl$ (55.2 mg, 0.40 mmol), and DMF (2.0 mL). The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at 25 ^oC under nitrogen atmosphere for 24 h. After that, a trace amount of the crude reaction mixture was subjected to the HRMS analysis, which indicated that benzyl alcohol could be formed. Afterwards, the

mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1) to give product **4a** (67.1 mg, 90%).



4.6 Fluorescence quenching experiments

The luminescence quenching experiment was taken using a FluoroMax-4 Spectrophotometer. The experiments were carried out with the 3 x 10^{-5} mol/L of $Ir(ppy)_3$ in DMF at 25 ^{o}C under nitrogen atmosphere. The concentrations of quencher (**1a**, **2a**, **3a**, Et_3N·HCl) in DMF were 1 mmol/L, 2 mmol/L, 3 mmol/L, 4 mmol/L. The excitation wavelength was 384 nm and the emission intensity was collected at 523 nm. The ratio of I_0/I was plotted as a function of the quencher concentration (I_0 = emission intensity of the photocatalyst in isolation at the specified wavelength; I = observed emission intensity of the photocatalyst with added quencher).



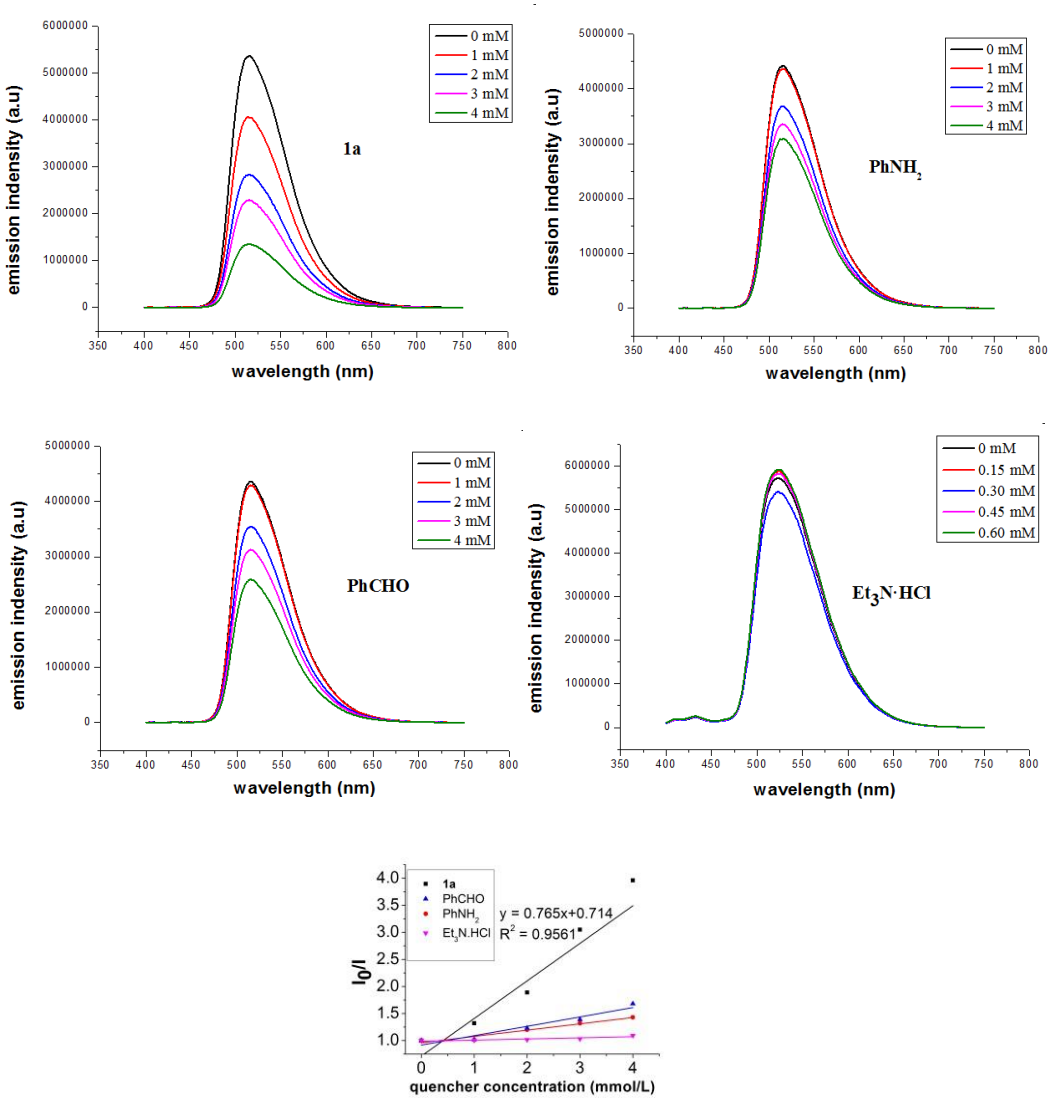
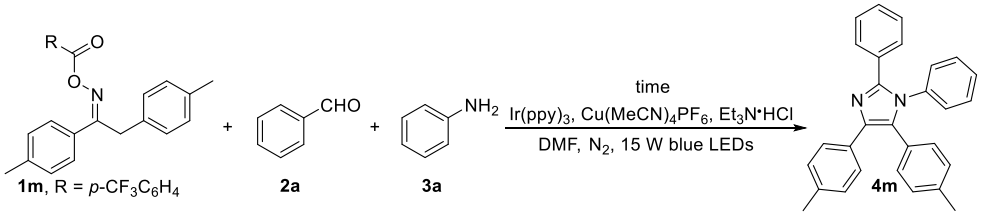


Figure S3. Emission quenching experiments with oxime ester **1a**, PhCHO **2a**, $PhNH_2$ **3a**, or $Et_3N \cdot HCl$ as quenchers.

4.7 Light on/off experiments



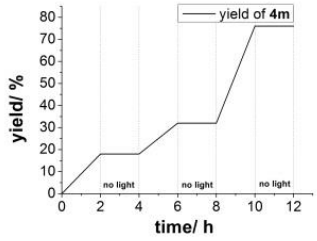


Figure S4 Light on-off experiments

The yield of **4m** was determined by ^{1}H NMR using 1,2-dibromoethane as an internal standard. The results revealed that a radical chain process was not the major reaction pathway.

4.8 Reductive potential of substrate

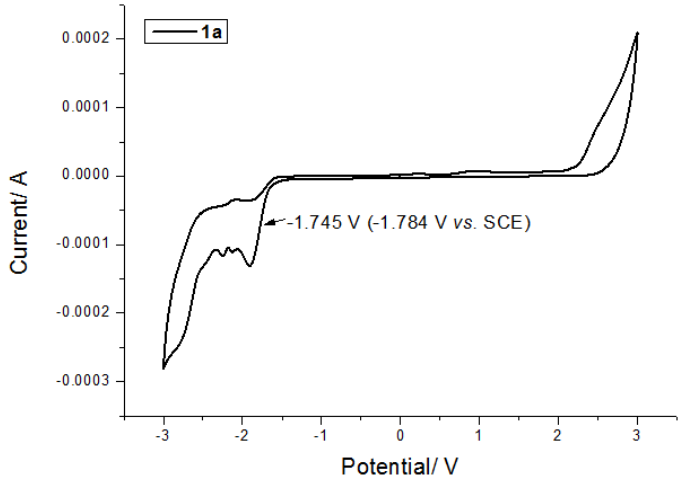
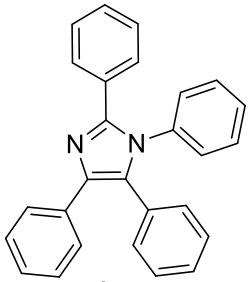


Figure S3. Cyclic voltammogram of 1a

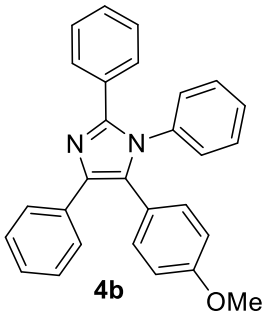
$E_{1/2}^{Red}$ (**1a**) = -1.78 V *vs.* SCE

5.Characterization data



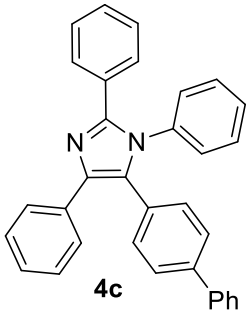
4a

White solid (0.20 mmol scale, 67.1 mg, 90%; 3.0 mmol scale, 0.98 g, 88%); mp 178-179 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.6 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.30 – 7.16 (m, 12H), 7.12 (d, J = 6.1 Hz, 2H), 7.03 (d, J = 7.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 138.2, 137.0, 134.4, 131.1, 130.8, 130.6, 130.4, 129.0, 128.9, 128.4, 128.3, 128.2, 128.12, 128.05, 127.9, 127.6, 127.4, 126.6; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{21}N_2$ 373.1699, found 373.1676.



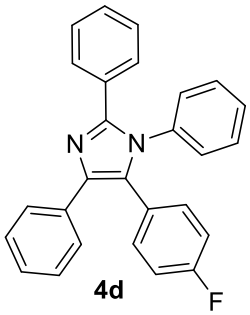
4b

White solid (44.3 mg, 55%); mp 179-180 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.60 (m, 2H), 7.45 – 7.39 (m, 2H), 7.29 – 7.17 (m, 9H), 7.07 – 7.00 (m, 4H), 6.78 – 6.72 (m, 2H), 3.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 146.7, 138.0, 137.1, 134.5, 132.3, 130.7, 130.5, 129.0, 128.9, 128.4, 128.2, 128.14, 128.11, 128.0, 127.3, 126.4, 122.7, 113.8, 55.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2O$ 403.1805, found 403.1823.



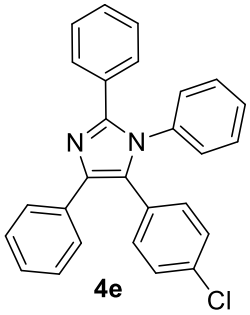
4c

White solid (65.5 mg, 73%); mp 177-178 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.63 (m, 2H), 7.59 – 7.53 (m, 2H), 7.52 – 7.42 (m, 4H), 7.41 – 7.36 (m, 2H), 7.32 – 7.29 (m, 1H), 7.27 – 7.18 (m, 9H), 7.18 – 7.15 (m, 2H), 7.08 – 7.01 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.0, 140.2, 140.1, 138.5, 137.0, 134.4, 131.3, 131.1, 130.43, 130.40, 129.1, 128.9, 128.7, 128.4, 128.3, 128.23, 128.21, 128.15, 128.0, 127.5, 126.81, 126.78, 126.6; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{33}H_{25}N_2$ 449.2012, found 449.2009.



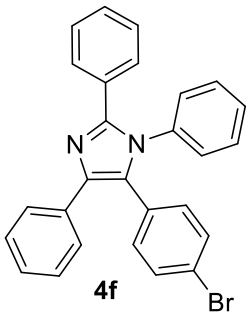
4d

White solid (51.5 mg, 66%); mp 165-166 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.55 (m, 2H), 7.44 – 7.40 (m, 2H), 7.30 – 7.19 (m, 9H), 7.11 – 7.07 (m, 2H), 7.04 – 7.00 (m, 2H), 6.94 – 6.89 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.4 (d, J = 248.4 Hz), 147.0, 138.4, 136.9, 134.2, 132.9 (d, J = 8.1 Hz), 130.3, 129.7, 129.2, 129.0, 128.9, 128.4, 128.3, 128.2, 128.1, 127.4, 126.7, 126.6 (d, J = 3.6 Hz), 115.5 (d, J = 21.6 Hz); HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}FN_2$ 391.1605, found 391.1614.



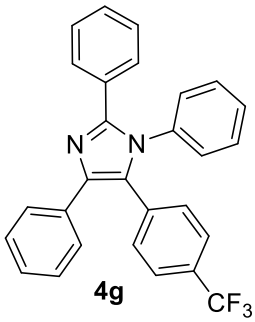
4e

White solid (66.7 mg, 82%); mp 170-171 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 2H), 7.43 – 7.39 (m, 2H), 7.32 – 7.22 (m, 9H), 7.20 – 7.18 (m, 2H), 7.06 – 7.01 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.3, 138.7, 136.8, 134.0, 132.3, 129.9, 129.4, 129.3, 129.0, 128.7, 128.6, 128.5, 128.40, 128.36, 128.3, 128.1, 127.5, 126.9, 126.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$ 407.1310, found 407.1323.

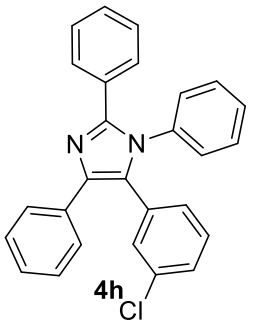


4f

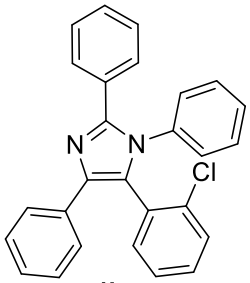
White solid (70.4 mg, 78%); mp 174-175 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.55 (m, 2H), 7.43 – 7.38 (m, 2H), 7.35 – 7.32 (m, 2H), 7.31 – 7.19 (m, 9H), 7.04 – 7.01 (m, 2H), 6.99 – 6.95 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.3, 138.7, 136.8, 134.1, 132.5, 131.6, 130.2, 129.5, 129.4, 129.3, 128.9, 128.5, 128.4, 128.34, 128.25, 128.1, 127.5, 126.9, 122.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}BrN_2$ 451.0804, found 451.0832.



White solid (60.8 mg, 69%); mp 163-164 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.1 Hz, 2H), 7.49 (d, J = 8.3 Hz, 2H), 7.46 – 7.39 (m, 2H), 7.29 – 7.22 (m, 9H), 7.18 – 7.10 (m, 2H), 7.08 – 7.00 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 138.0 (q, J = 1.4 Hz), 136.78, 136.75, 132.0, 131.0, 130.2, 130.1, 129.1, 128.9, 128.55, 128.55 (q, J = 33.9 Hz), 128.5, 128.42, 128.38, 128.3, 128.2, 127.2, 125.1 (q, J = 3.8 Hz), 124.4 (q, J = 270.1 Hz); HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{20}F_3N_2$ 441.1573, found 441.1578.

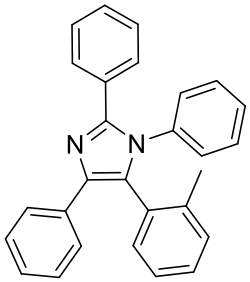


White solid (51.3 mg, 63%); mp 169-170 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 – 7.70 (m, 1H), 7.44 – 7.41 (m, 2H), 7.37 (dt, J = 7.2, 1.6 Hz, 1H), 7.28 – 7.22 (m, 9H), 7.16 – 7.10 (m, 4H), 7.05 – 7.01 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.0, 136.8, 136.3, 134.1, 131.4, 131.0, 130.2, 130.1, 129.3, 129.1, 128.9, 128.44, 128.38, 128.34, 128.32, 128.2, 128.1, 127.3, 126.5, 125.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$ 407.1310, found 407.1322.



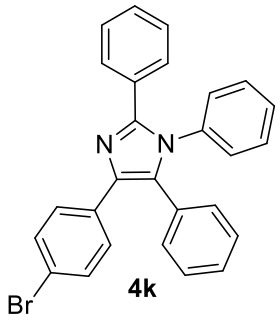
4i

White solid (55.3 mg, 68%); mp 166-167 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.51 (m, 1H), 7.44 – 7.37 (m, 2H), 7.37 – 7.26 (m, 4H), 7.27 – 7.17 (m, 5H), 7.13 – 7.05 (m, 5H), 6.92 – 6.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.7, 137.0, 136.9, 133.9, 133.7, 132.8, 132.1, 130.1, 129.9, 129.8, 129.6, 129.2, 129.1, 128.9, 128.4, 128.3, 128.02, 127.98, 127.9, 127.3, 126.5; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$ 407.1310, found 407.1315.



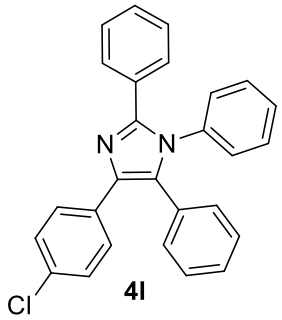
4j

White solid (49.5 mg, 64%); mp 164-165 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.35 (m, 3H), 7.33 – 7.28 (m, 3H), 7.26 – 7.17 (m, 4H), 7.17 – 7.13 (m, 2H), 7.12 – 7.03 (m, 5H), 6.90 – 6.83 (m, 2H), 2.12 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.4, 139.5, 137.3, 137.1, 134.2, 131.3, 131.1, 130.5, 130.2, 130.1, 129.9, 129.1, 129.0, 128.4, 128.2, 128.1, 128.0, 127.9, 127.4, 127.0, 125.4, 20.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2$ 387.1856, found 387.1863.



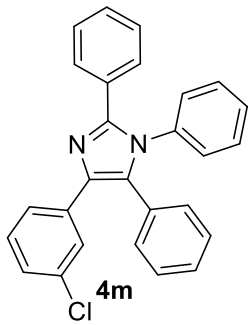
4k

White solid (69.1 mg, 77%); mp 167-168 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.43 (m, 2H), 7.41 (dd, J = 7.8, 1.9 Hz, 2H), 7.39 – 7.32 (m, 2H), 7.30 – 7.20 (m, 9H), 7.15 – 7.08 (m, 2H), 7.07 – 6.99 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1, 137.2, 136.9, 133.4, 131.2, 131.1, 131.0, 130.33, 130.30, 129.1, 128.87, 128.86, 128.5, 128.4, 128.3, 128.2, 128.1, 120.5; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}BrN_2$ 451.0804, found 451.0823.



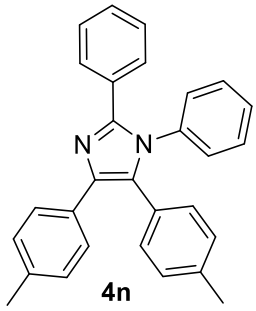
4l

White solid (65.9 mg, 81%); mp 170-171 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 2H), 7.43 – 7.40 (m, 2H), 7.31 – 7.21 (m, 9H), 7.21 – 7.18 (m, 2H), 7.06 – 7.01 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.2, 138.7, 136.8, 134.0, 132.3, 129.4, 129.3, 129.1, 129.04, 128.95, 128.7, 128.5, 128.41, 128.35, 128.3, 128.1, 127.6, 127.5, 126.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$ 407.1310, found 407.1316.



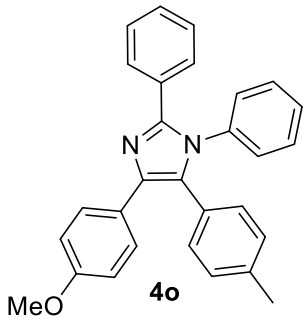
4m

White solid (53.7 mg, 66%); mp 166-167 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.55 (m, 2H), 7.42 (dd, J = 7.8, 1.9 Hz, 2H), 7.33 – 7.18 (m, 10H), 7.17 – 7.09 (m, 2H), 7.07 – 6.97 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 138.8, 136.7, 134.1, 133.9, 132.4, 130.9, 130.2, 129.6, 129.3, 129.21, 129.18, 128.9, 128.5, 128.4, 128.3, 128.2, 128.11, 128.09, 127.5, 126.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$ 407.1310, found 407.1326.



4n

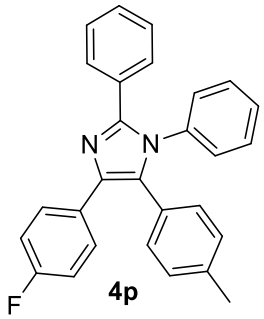
White solid (65.7 mg, 82%); mp 168-169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.4 Hz, 2H), 7.43 – 7.37 (m, 2H), 7.26 – 7.17 (m, 6H), 7.07 – 6.95 (m, 8H), 2.29 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 138.1, 137.5, 137.1, 136.0, 131.6, 130.8, 130.5, 130.4, 129.0, 128.91, 128.85, 128.8, 128.4, 128.03, 127.95, 127.6, 127.2, 21.2, 21.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{29}H_{25}N_2$ 401.2012, found 401.2008.



4o

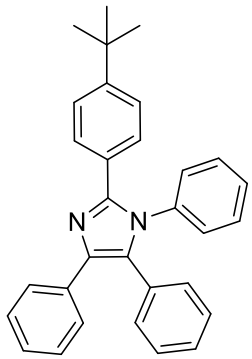
White solid (54.1 mg, 65%); mp 177-178 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.51 (m, 2H), 7.41 (dd, J = 7.6, 2.0 Hz, 2H), 7.29 – 7.19 (m, 6H), 7.05 – 6.97 (m, 6H), 6.83 – 6.78 (m, 2H), 3.78 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.4, 146.6, 137.9, 137.6, 137.2, 130.9, 130.6, 130.0, 129.03, 128.97, 128.9, 128.5, 128.4,

128.1, 128.0, 127.6, 127.2, 113.5, 55.1, 21.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{29}H_{25}N_2O$ 417.1961, found 417.1969.



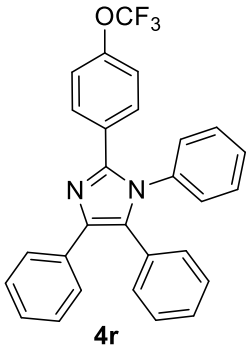
4p

White solid (51.0 mg, 63%); mp 166-167 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.53 (m, 2H), 7.43 – 7.38 (m, 2H), 7.29 – 7.21 (m, 6H), 7.05 – 7.01 (m, 4H), 7.00 – 6.97 (m, 2H), 6.96 – 6.91 (m, 2H), 2.30 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.8 (d, J = 245.7 Hz), 146.8, 137.9, 137.2, 137.1, 130.8, 130.7, 130.6, 130.4, 129.2, 129.0, 128.94 (d, J = 7.7 Hz), 128.88, 128.4, 128.2 (d, J = 3.7 Hz), 128.1, 127.3, 116.0 (d, J = 21.4 Hz), 21.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{22}FN_2$ 405.1762, found 405.1777.



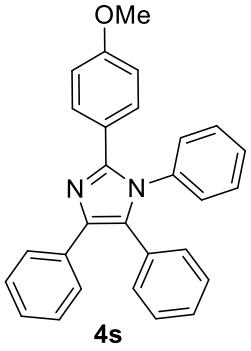
4q

White solid (60.9 mg, 71%); mp 171-172 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 7.62 – 7.58 (m, 2H), 7.35 (d, J = 8.5 Hz, 2H), 7.29 – 7.17 (m, 11H), 7.13 – 7.10 (m, 2H), 7.07 – 7.03 (m, 2H), 1.27 (s, 9H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 151.2, 146.9, 138.0, 137.1, 134.4, 131.0, 130.6, 130.6, 129.0, 128.4, 128.24, 128.15, 128.1, 127.8, 127.5, 127.3, 126.5, 125.0, 34.5, 31.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{31}H_{29}N_2$ 429.2325, found 429.2332.



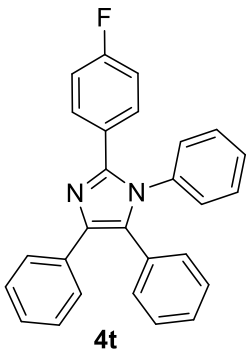
4r

White solid (58.4 mg, 64%); mp 162-163 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 7.1 Hz, 2H), 7.46 (d, J = 8.8 Hz, 2H), 7.35 – 7.15 (m, 9H), 7.14 – 7.10 (m, 2H), 7.08 (d, J = 8.5 Hz, 2H), 7.04 (dd, J = 7.7, 1.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0 (q, J = 2.0 Hz), 145.5, 138.4, 136.8, 134.2, 131.2, 131.0, 130.3, 130.2, 129.24, 129.15, 128.5, 128.4, 128.3, 128.2, 128.1, 127.3, 126.7, 120.4, 120.3 (q, J = 256.0 Hz); HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{20}F_3N_2O$ 457.1522, found 457.1534.



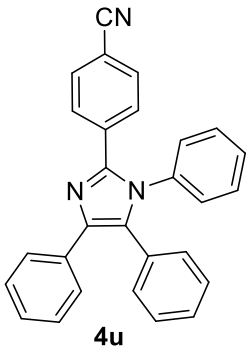
4s

White solid (63.6 mg, 79%); mp 176-177 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 – 7.58 (m, 2H), 7.37 – 7.33 (m, 2H), 7.26 – 7.14 (m, 9H), 7.13 – 7.09 (m, 2H), 7.04 – 7.00 (m, 2H), 6.77 – 6.73 (m, 2H), 3.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 146.8, 137.9, 137.1, 134.4, 131.0, 130.6, 130.4, 130.2, 129.0, 128.4, 128.2, 128.1, 128.0, 127.8, 127.3, 126.4, 123.0, 113.4, 55.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2O$ 403.1805, found 403.1821.



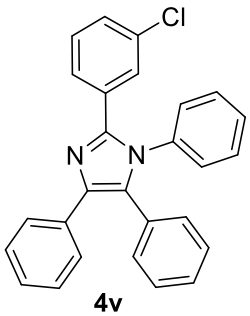
4t

White solid (52.3 mg, 67%); mp 164-165 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.55 (m, 2H), 7.44 – 7.36 (m, 2H), 7.30 – 7.16 (m, 9H), 7.14 – 7.10 (m, 2H), 7.06 – 6.99 (m, 2H), 6.96 – 6.89 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6 (d, J = 248.7 Hz), 146.0, 138.2, 136.9, 134.2, 131.1, 130.83, 130.79 (d, J = 8.2 Hz), 130.5, 129.1, 128.37, 128.36, 128.35 (d, J = 3.4 Hz), 128.3, 128.2 128.0, 127.3, 126.7, 115.2 (d, J = 21.7 Hz); HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}FN_2$ 391.1605, found 391.1611.



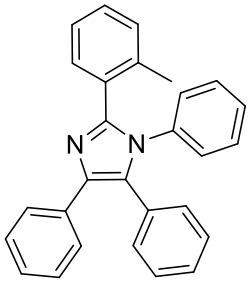
4u

White solid (50.0 mg, 63%); mp 167-168 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 – 7.56 (m, 2H), 7.54 (d, J = 8.2 Hz, 2H), 7.51 (d, J = 7.8 Hz, 2H), 7.35 – 7.19 (m, 9H), 7.15 – 7.10 (m, 2H), 7.06 (d, J = 7.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.6, 139.1, 136.6, 134.6, 133.9, 132.1, 131.8, 131.0, 129.9, 129.4, 128.9, 128.4, 128.3, 128.2, 127.3, 126.9, 118.6, 111.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{20}N_3$ 398.1652, found 398.1653.



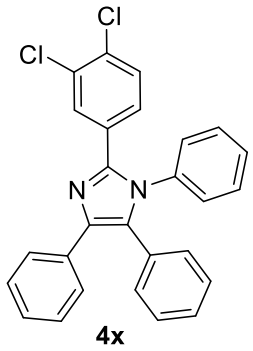
4v

White solid (49.6 mg, 61%); mp 173-174 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 7.5 Hz, 2H), 7.55 (s, 1H), 7.31 – 7.16 (m, 11H), 7.15 – 7.09 (m, 3H), 7.07 – 7.01 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 138.5, 136.7, 134.2, 134.1, 132.2, 131.3, 131.0, 130.3, 129.2, 129.0, 128.5, 128.43, 128.35, 128.30, 128.27, 128.2, 128.1, 127.3, 126.7; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$ 407.1310, found 407.1318.



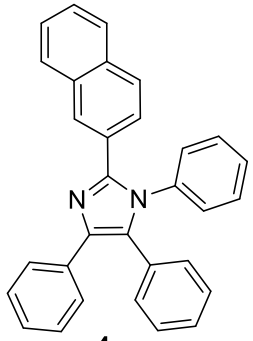
4w

White solid (45.6 mg, 59%); mp 175-176 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.58 (m, 2H), 7.26 – 7.21 (m, 6H), 7.19 – 7.14 (m, 4H), 7.16 – 7.07 (m, 4H), 7.08 – 7.03 (m, 1H), 6.91 – 6.84 (m, 2H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 138.1, 137.6, 136.4, 134.5, 131.1, 130.9, 130.7, 130.5, 130.0, 129.2, 128.9, 128.5, 128.4, 128.1, 127.8, 127.7, 127.6, 127.4, 126.5, 125.2, 20.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2$ 387.1856, found 387.1863.



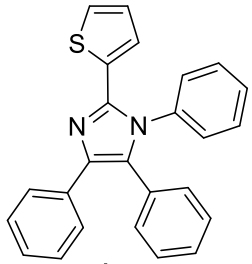
4x

White solid (44.1 mg, 50%); mp 176-177 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, J = 2.1 Hz, 1H), 7.61 – 7.56 (m, 2H), 7.32 – 7.18 (m, 10H), 7.13 – 7.09 (m, 3H), 7.06 – 7.02 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$ δ 144.3, 138.6, 136.5, 134.0, 132.4, 132.3, 131.5, 131.0, 130.5, 130.4, 130.1, 129.9, 129.3, 128.7, 128.4, 128.22, 128.17, 128.1, 127.5, 127.3, 126.8; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{19}Cl_2N_2$ 441.0920, found 441.0936.



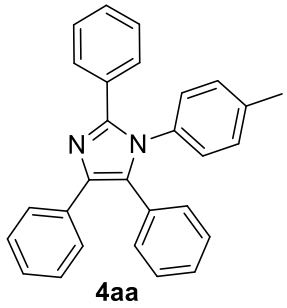
4y

White solid (52.4 mg, 62%); mp 180-181 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.79 – 7.72 (m, 1H), 7.71 – 7.60 (m, 4H), 7.53 (dd, J = 8.6, 1.7 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.32 – 7.18 (m, 9H), 7.19 – 7.12 (m, 2H), 7.08 (d, J = 7.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 138.5, 137.1, 134.4, 132.9, 132.8, 131.1, 131.0, 130.5, 129.1, 128.49, 128.46, 128.4, 128.33, 128.30, 128.2, 128.0, 127.8, 127.6, 127.51, 127.45, 126.6, 126.5, 126.2, 126.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{31}H_{23}N_2$ 423.1856, found 423.1865.



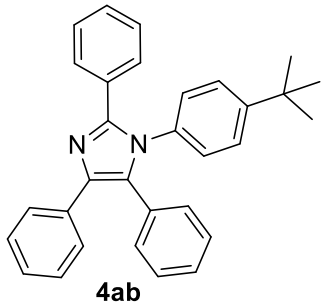
4z

White solid (55.3 mg, 73%); mp 167-168 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.58 (dd, J = 7.2, 1.6 Hz, 2H), 7.38 – 7.33 (m, 3H), 7.26 – 7.21 (m, 3H), 7.21 – 7.17 (m, 6H), 7.15 – 7.12 (m, 2H), 6.83 (dd, J = 5.1, 3.7 Hz, 1H), 6.67 (dd, J = 3.7, 1.1 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.1, 138.2, 136.6, 134.1, 133.1, 131.0, 130.2, 129.3, 129.1, 128.9, 128.3, 128.1, 128.0, 127.3, 127.1, 126.6, 126.3, 126.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{25}H_{19}N_2S$ 379.1263, found 379.1271.



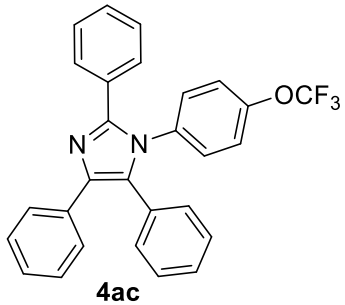
4aa

White solid (68.0 mg, 88%); mp 160-161 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 2H), 7.47 – 7.42 (m, 2H), 7.27 – 7.20 (m, 8H), 7.20 – 7.16 (m, 1H), 7.15 – 7.11 (m, 2H), 7.03 (d, J = 8.2 Hz, 2H), 6.93 – 6.89 (m, 2H), 2.30 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.9, 138.13, 138.09, 134.5, 134.4, 131.1, 130.9, 130.7, 130.6, 129.6, 128.9, 128.3, 128.12, 128.08, 128.06, 128.0, 127.8, 127.4, 126.5, 21.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2$ 387.1856, found 387.1868.



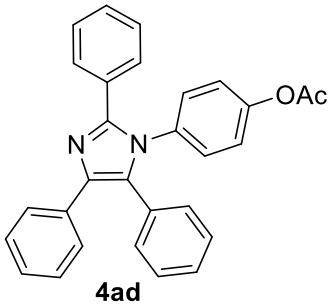
4ab

White solid (73.7 mg, 86%); mp 161-162 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 2H), 7.45 – 7.40 (m, 2H), 7.27 – 7.17 (m, 11H), 7. 27 – 7.16 (m, 2H), 6.97 – 6.92 (m, 2H), 1.27 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.4, 147.0, 138.2, 134.5, 134.3, 131.1, 130.9, 130.7, 130.6, 128.9, 128.2, 128.1, 128.0, 127.82, 127.79, 127.4, 126.5, 125.9, 34.6, 31.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{31}H_{29}N_2$ 429.2325, found 429.2334.



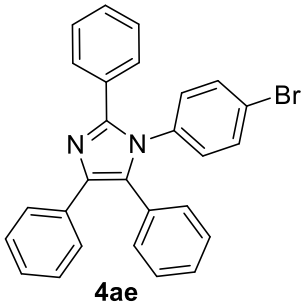
4ac

White solid (56.6 mg, 62%); mp 162-163 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.54 (m, 2H), 7.40 (dd, J = 7.7, 2.0 Hz, 2H), 7.31 – 7.16 (m, 9H), 7.15 – 7.06 (m, 4H), 7.06 – 7.02 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6 (q, J = 2.0 Hz), 147.0, 138.5, 135.5, 134.1, 131.0, 130.6, 130.2, 130.1, 129.8, 129.0, 128.52, 128.50, 128.22, 128.17, 127.4, 126.8, 121.2, 120.2 (q, J = 256.9 Hz); HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{20}F_3N_2O$ 457.1522, found 457.1555.



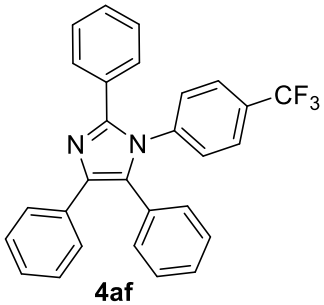
4ad

White solid (57.7 mg, 67%); mp 179-180 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 2H), 7.44 – 7.41 (m, 2H), 7.27 – 7.21 (m, 8H), 7.20 – 7.16 (m, 1H), 7.14 – 7.11 (m, 2H), 7.04 – 6.98 (m, 4H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 150.1, 147.0, 138.3, 134.3, 134.2, 131.0, 130.7, 130.3, 130.2, 129.2, 128.9, 128.4, 128.3, 128.14, 128.11, 128.0, 127.4, 126.6, 122.1, 21.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{29}H_{23}N_2O_2$ 431.1754, found 431.1756.



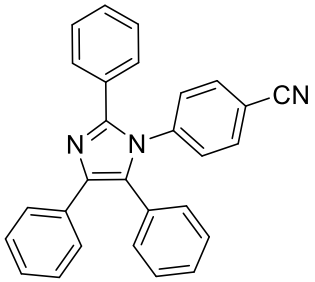
4ae

White solid (72.1 mg, 80%); mp 177-178 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 – 7.55 (m, 2H), 7.43 – 7.39 (m, 2H), 7.38 – 7.34 (m, 2H), 7.30 – 7.21 (m, 8H), 7.21 – 7.16 (m, 1H), 7.14 – 7.09 (m, 2H), 6.91 – 6.86 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.9, 138.5, 136.1, 134.1, 132.3, 131.1, 130.5, 130.3, 130.1, 129.8, 129.0, 128.52, 128.47, 128.23, 128.18, 128.15, 127.3, 126.7, 122.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}BrN_2$ 451.0804, found 451.0819.



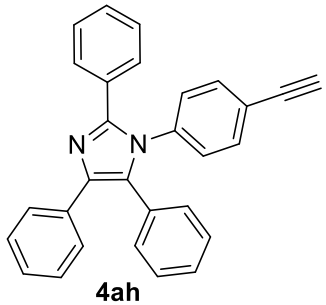
4af

White solid (47.6 mg, 54%); mp 173-174 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, J = 6.8 Hz, 2H), 7.49 (d, J = 8.2 Hz, 2H), 7.39 – 7.35 (m, 2H), 7.28 – 7.16 (m, 9H), 7.14 – 7.08 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.9, 140.1, 138.7, 134.0, 131.0, 130.4, 130.1, 129.9 (q, J = 31.6 Hz), 129.0, 128.7, 128.60, 128.58, 128.30, 128.28, 128.2, 127.4, 126.8, 126.2 (q, J = 3.9 Hz), 123.5(q, J = 273.2 Hz) ; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{20}F_3N_2$ 441.1573, found 441.1566.



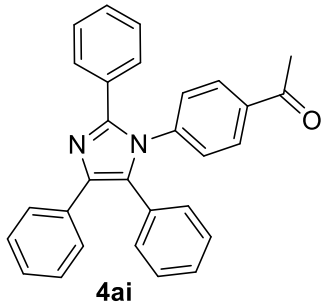
4ag

White solid (40.4 mg, 51%); mp 170-171 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 2H), 7.55 – 7.51 (m, 2H), 7.38 – 7.35 (m, 2H), 7.34 – 7.23 (m, 8H), 7.23 – 7.18 (m, 1H), 7.12 – 7.09 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.9, 140.9, 138.9, 133.8, 132.9, 131.0, 130.2, 129.9, 129.8, 129.1, 128.8, 128.7, 128.5, 128.4, 128.2, 127.4, 126.9, 117.8, 112.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{20}N_3$ 398.1652, found 398.1677.



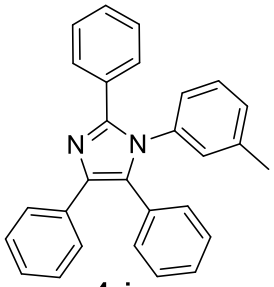
4ah

White solid (45.2 mg, 57%); mp 168-169 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 7.5 Hz, 2H), 7.41 (d, J = 7.0 Hz, 2H), 7.36 (d, J = 8.1 Hz, 2H), 7.30 – 7.16 (m, 9H), 7.11 (d, J = 7.1 Hz, 2H), 6.97 (d, J = 8.0 Hz, 2H), 3.11 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 138.5, 137.3, 134.2, 132.8, 131.0, 130.6, 130.3, 130.2, 129.0, 128.5, 128.4, 128.3, 128.20, 128.15, 128.1, 127.4, 126.7, 122.0, 82.4, 78.7; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{29}H_{21}N_2$ 397.1699, found 397.1703.



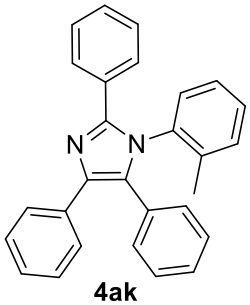
4ai

White solid (54.7 mg, 66%); mp 171-172 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 8.5 Hz, 2H), 7.62 – 7.55 (m, 2H), 7.43 – 7.37 (m, 2H), 7.31 – 7.18 (m, 9H), 7.14 – 7.08 (m, 4H), 2.56 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.9, 146.9, 141.1, 138.7, 136.3, 134.1, 131.0, 130.5, 130.24, 130.15, 129.1, 129.0, 128.6, 128.5, 128.3, 128.24, 128.17, 127.4, 126.8, 26.6; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{29}H_{23}N_2O$ 415.1805, found 415.1835.



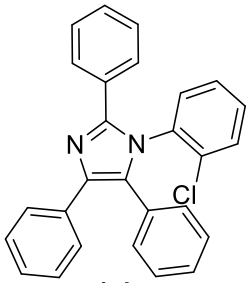
4aj

White solid (45.6 mg, 59%); mp 166-167 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (dd, J = 7.4, 1.8 Hz, 2H), 7.44 (dd, J = 7.7, 2.0 Hz, 2H), 7.26 – 7.16 (m, 9H), 7.15 – 7.10 (m, 3H), 7.07 (d, J = 7.6 Hz, 1H), 6.86 – 6.82 (m, 2H), 2.20 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.8, 139.0, 138.1, 137.0, 134.5, 131.1, 130.9, 130.7, 130.6, 129.0, 128.91, 128.85, 128.7, 128.23, 128.15, 128.1, 128.0, 127.9, 127.4, 126.5, 125.5, 21.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2$ 387.1856, found 387.1847.



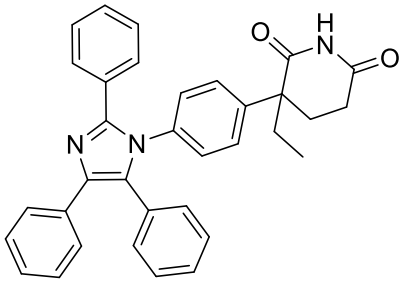
4ak

White solid (40.9 mg, 53%); mp 164-165 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 – 7.61 (m, 2H), 7.47 – 7.43 (m, 2H), 7.27 – 7.17 (m, 10H), 7.16 – 7.13 (m, 2H), 7.13 – 7.10 (m, 3H), 1.88 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.7, 138.3, 136.2, 136.0, 134.4, 131.0, 130.74, 130.67, 130.6, 130.5, 129.3, 129.0, 128.3, 128.2, 128.12, 128.09, 127.9, 127.3, 126.62, 126.56, 17.6; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2$ 387.1856, found 387.1834.



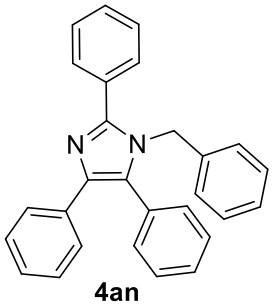
4al

White solid (49.6 mg, 61%); mp 162-163 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 7.6 Hz, 2H), 7.50 – 7.44 (m, 2H), 7.37 – 7.29 (m, 2H), 7.28 – 7.15 (m, 13H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1, 138.3, 135.1, 134.2, 133.3, 130.9, 130.84, 130.80, 130.5, 130.32, 130.25, 130.2, 128.5, 128.34, 128.31, 128.24, 128.16, 128.1, 127.4, 127.2, 126.6; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}ClN_2$ 407.1310, found 407.1301.



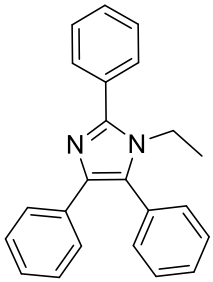
4am

White solid (52.2 mg, 51%); mp 177-178 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.63 – 7.55 (m, 2H), 7.41 – 7.36 (m, 2H), 7.28 – 7.13 (m, 11H), 7.12 – 7.06 (m, 2H), 7.05 – 7.00 (m, 2H), 2.65 – 2.50 (m, 1H), 2.30 – 2.13 (m, 3H), 2.02 – 1.85 (m, 2H), 0.81 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 172.1, 146.8, 139.0, 138.3, 136.5, 134.1, 131.0, 130.6, 130.3, 130.2, 128.94, 128.87, 128.4, 128.3, 128.11, 128.09, 128.06, 127.3, 126.9, 126.6, 50.8, 32.7, 29.0, 27.4, 8.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{34}H_{30}N_3O_2$ 512.2333, found 512.2340.



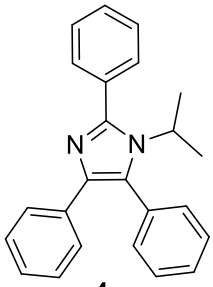
4an

White solid (53.3 mg, 69%); mp 167-168 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.62 (m, 2H), 7.61 – 7.54 (m, 2H), 7.43 – 7.37 (m, 3H), 7.37 – 7.27 (m, 3H), 7.25 – 7.17 (m, 7H), 7.17 – 7.11 (m, 1H), 6.84 – 6.78 (m, 2H), 5.11 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 138.0, 137.5, 134.4, 131.1, 131.0, 130.9, 130.0, 129.1, 128.9, 128.8, 128.59, 128.57, 128.5, 128.1, 127.3, 126.8, 126.3, 126.0, 48.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}N_2$ 387.1856, found 387.1885.



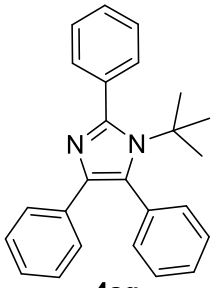
4ao

White solid (40.2 mg, 62%); mp 172-173 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 – 7.69 (m, 2H), 7.55 – 7.52 (m, 2H), 7.52 – 7.47 (m, 5H), 7.47 – 7.43 (m, 3H), 7.22 – 7.18 (m, 2H), 7.15 – 7.11 (m, 1H), 3.95 (q, J = 7.2 Hz, 2H), 1.02 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 137.7, 134.5, 131.5, 131.3, 131.0, 129.3, 129.1, 129.0, 128.8, 128.61, 128.57, 128.0, 126.7, 126.1, 39.6, 16.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{23}H_{21}N_2$ 325.1699, found 325.1686.



4ap

White solid (33.8 mg, 50%); mp 175-176 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 – 7.63 (m, 2H), 7.51 – 7.48 (m, 6H), 7.48 – 7.44 (m, 4H), 7.18 – 7.14 (m, 2H), 7.12 – 7.08 (m, 1H), 4.47 (hept, J = 7.0 Hz, 1H), 1.25 (d, J = 7.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.5, 137.8, 134.5, 132.4, 132.3, 132.1, 130.0, 128.9, 128.8, 128.7, 128.3, 127.9, 126.6, 126.0, 49.3, 23.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{24}H_{23}N_2$ 339.1856, found 339.1867.



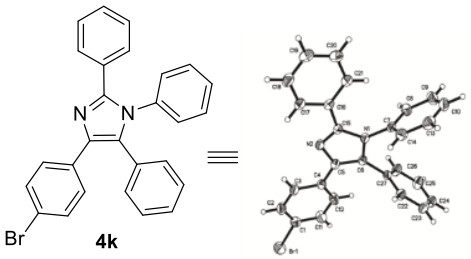
4aq

White solid (22.6 mg, 32%); mp 177-178 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.53 (m, 2H), 7.49 – 7.46 (m, 2H), 7.45 – 7.43 (m, 3H), 7.42 – 7.40 (m, 3H), 7.29 – 7.25 (m, 2H), 7.12 – 7.03 (m, 3H), 1.31 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 137.9, 136.8, 135.0, 134.7, 132.4, 130.2, 129.8, 128.6, 128.5, 128.4, 128.0, 127.7, 127.2, 125.9, 59.8, 33.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{25}H_{25}N_2$ 353.2012, found 353.2010.

6. X-ray structure of product 4k

X-ray structure of 4k with thermal ellipsoids shown at the 30% probability level

(CCDC 2165867)



Crystal data and structure refinement for product 4k

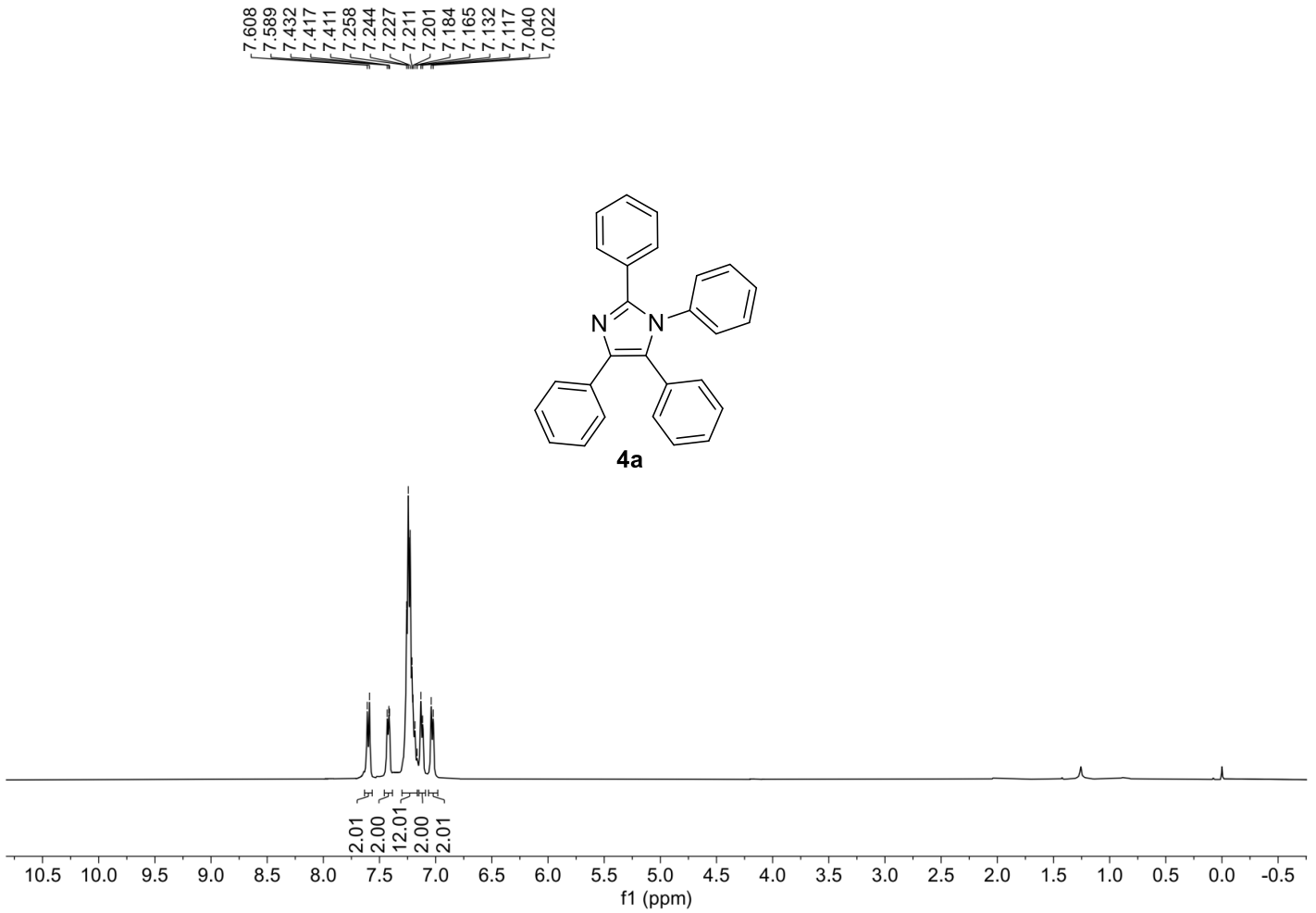
Identification code	**4k**	
Empirical formula	C27 H19 Br N2	
Formula weight	451.35	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.7856(7) Å	α = 94.494(2) °.
	b = 10.4391(7) Å	β = 95.410(2) °.
	c = 11.5402(7) Å	γ = 114.329(2) °.
Volume	1060.43(12) Å^3	
Z	2	
Density (calculated)	1.414 Mg/m^3	
Absorption coefficient	1.954 mm^{-1}	
F(000)	460	
Crystal size	0.300 x 0.220 x 0.200 mm^3	
Theta range for data collection	2.159 to 27.517 °.	
Index ranges	-12<=h<=12, -13<=k<=13, -14<=l<=14	
Reflections collected	16521	
Independent reflections	4840 [R(int) = 0.0307]	
Completeness to theta = 25.242 °	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5116	
Refinement method	Full-matrix least-squares on F^2	

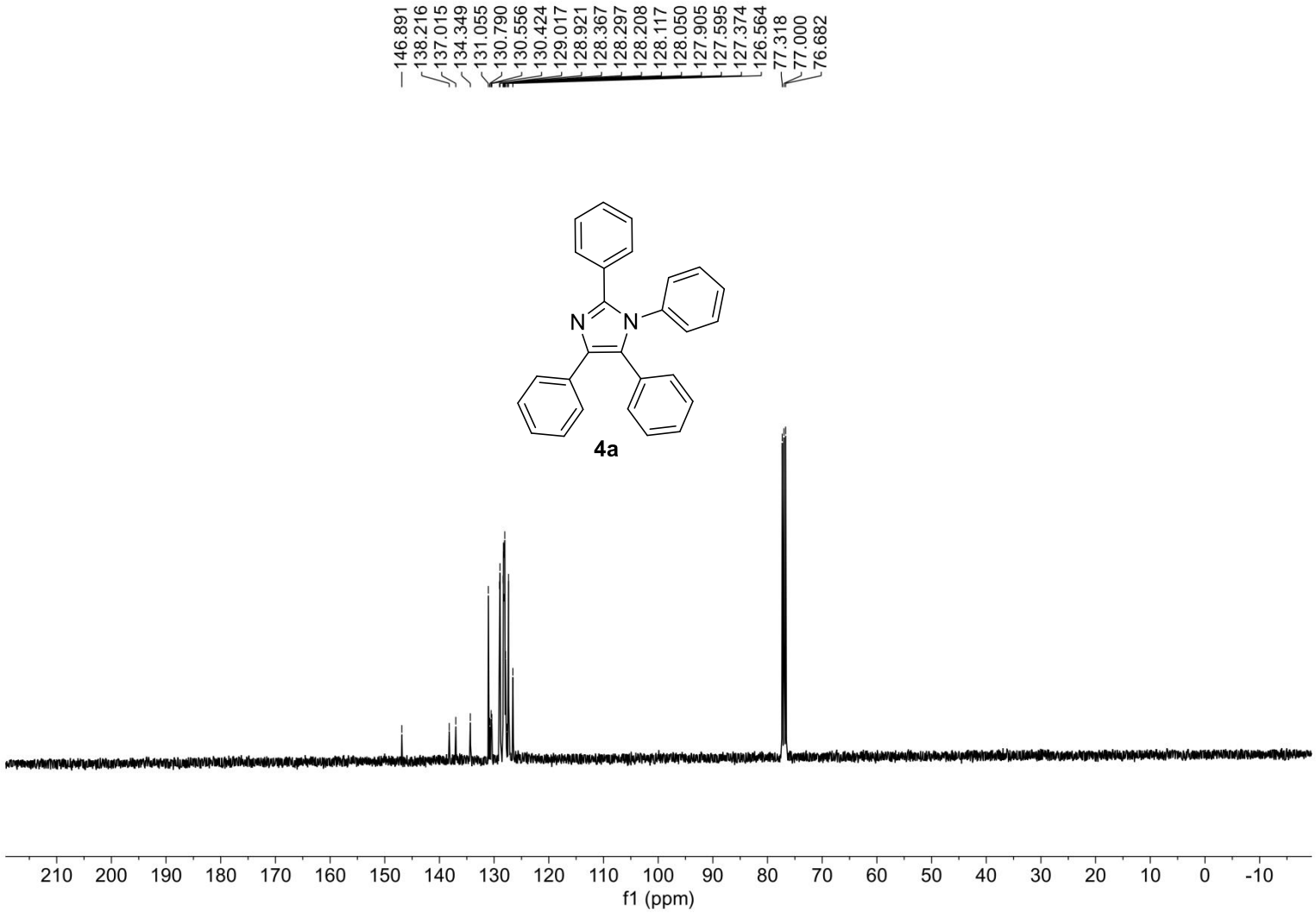
Data / restraints / parameters	4840 / 0 / 271
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.0957
R indices (all data)	R1 = 0.0611, wR2 = 0.1055
Extinction coefficient	n/a
Largest diff. peak and hole	0.589 and -0.451 e.$Å^{-3}$

7. References

(1) J. Ke, Y. Tang, H. Yi, Y. Li, Y. Cheng, C. Liu and A. Lei, Copper-Catalyzed Radical/Radical C_{sp3}-H/P-H Cross-Coupling: α-Phosphorylation of Aryl Ketone O-Acetyloximes. *Angew. Chem., Int. Ed.*, 2015, **54**, 6604-6607.

8. NMR spectra

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137.015
134.349
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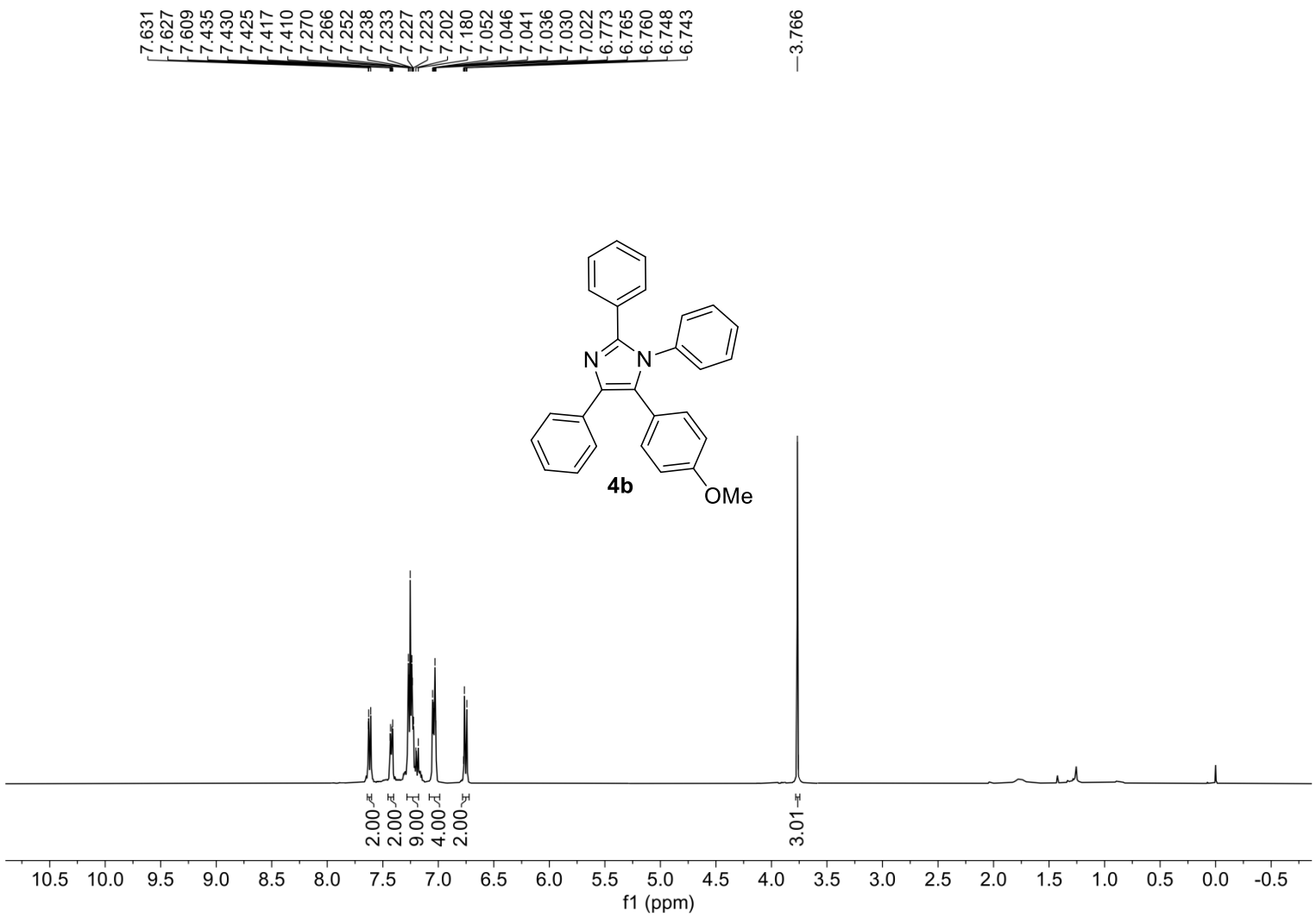
130.790
130.556
130.424
129.017
128.921
128.367
128.297
128.208
128.117
128.050
127.905
127.595
127.374
126.564
77.318
77.000
76.682
N
N
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.627
7.609
7.435
7.430
7.425
7.417
7.410
7.270
7.266
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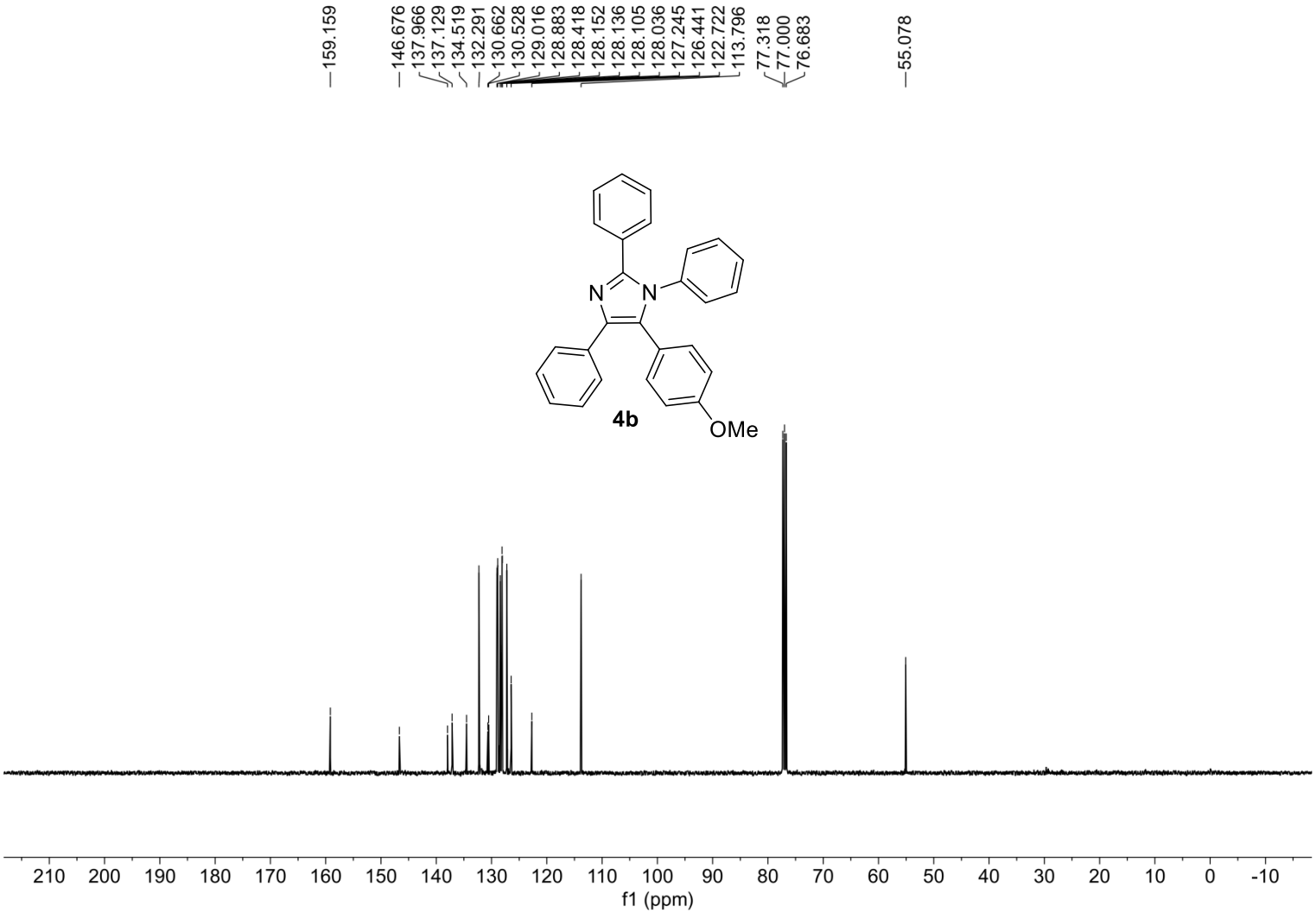
7.238
7.233
7.227
7.223
7.202
7.180
7.052
7.046
7.041
7.036
7.030
7.022
6.773
6.765
6.760
6.748
6.743
3.766
N
N
4b
OMe
2.00
2.00
9.00
4.00
2.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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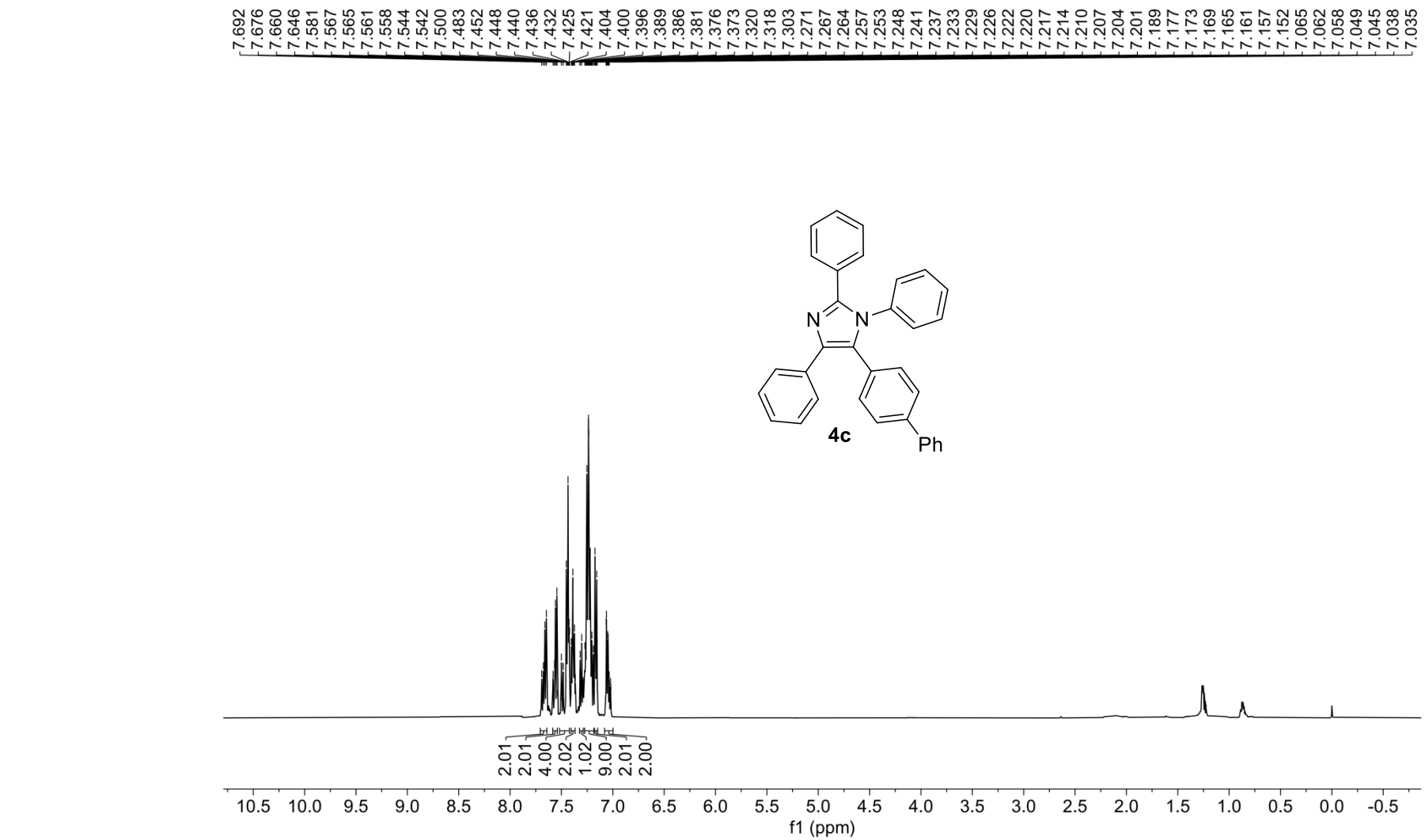
146.676
137.966
137.129
134.519
132.291
130.662
130.528
129.016
128.883
128.418
128.152
128.136
128.105
128.036
127.245
126.441
122.722
113.796
77.318
77.000
76.683
55.078
N
N
OMe
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.646
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7.567
7.565
7.561
7.558
7.544
7.542
7.500
7.483
7.452
7.448
7.440
7.436
7.432
7.425
7.421
7.404
7.400
7.396
7.389
7.386
7.381
7.376
7.373
7.320
7.318
7.303
7.271
7.267
7.264
7.257
7.253
7.248
7.241
7.237
7.233
7.229
7.226
7.222
7.220
7.217
7.214
7.210
7.207
7.204
7.201
7.189
7.177
7.173
7.169
7.165
7.161
7.157
7.152
7.065
7.062
7.058
7.049
7.045
7.038
7.035
N
N
4c
Ph
2.01
2.01
4.00
2.02
1.02
9.00
2.01
2.00
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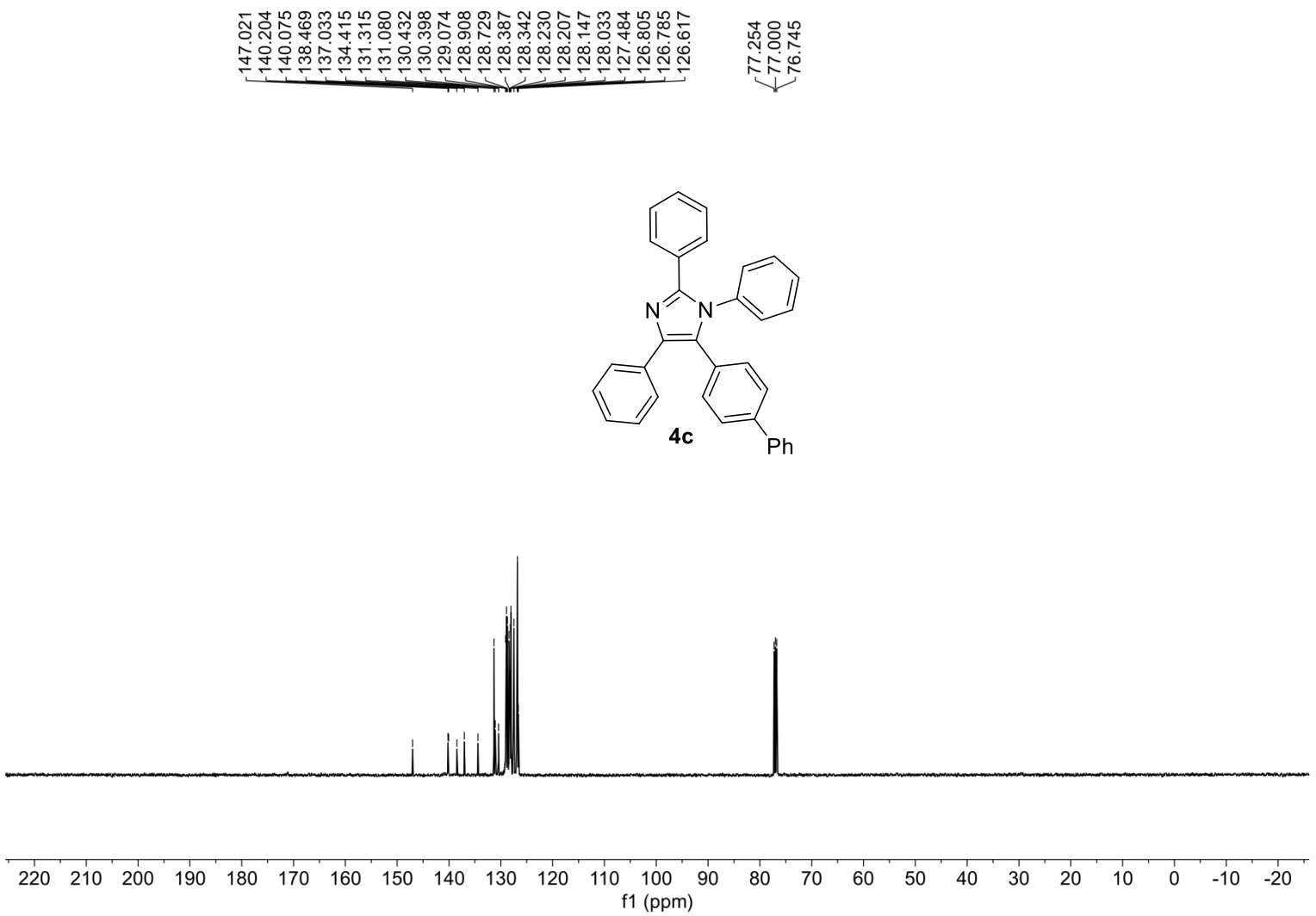
f1 (ppm)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134.415
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131.080
130.432
130.398
129.074
128.908
128.729
128.387
128.342
128.230
128.207
128.147
128.033
127.484
126.805
126.785
126.617
77.254
77.000
76.745
N
N
Ph
4c
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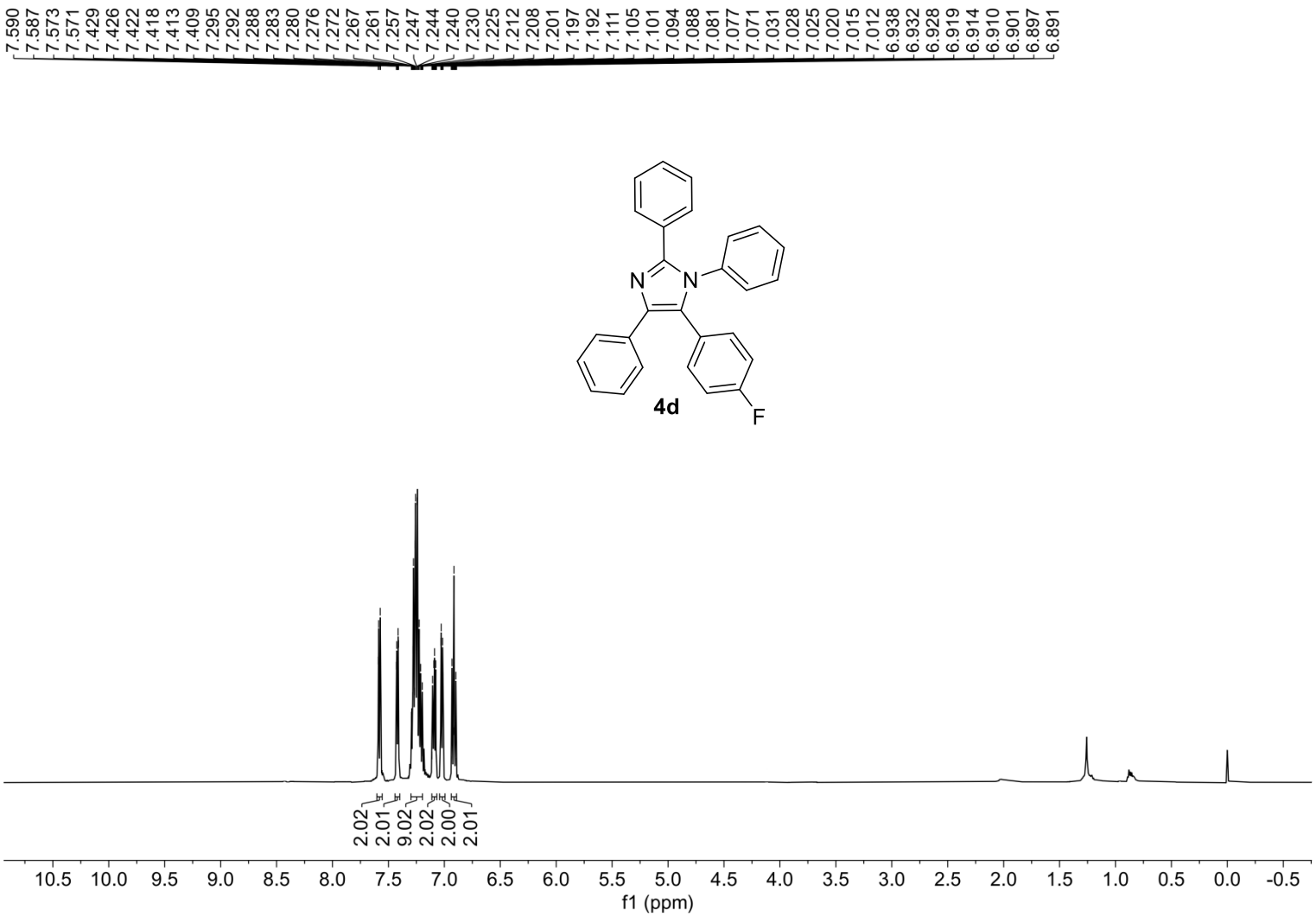
f1 (ppm)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7.587
7.573
7.571
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7.426
7.422
7.418
7.413
7.409
7.295
7.292
7.288
7.283
7.280
7.276
7.272
7.267
7.261
7.257
7.247
7.244
7.240
7.230
7.225
7.212
7.208
7.201
7.197
7.192
7.111
7.105
7.101
7.094
7.088
7.081
7.077
7.071
7.031
7.028
7.025
7.020
7.015
7.012
6.938
6.932
6.928
6.919
6.914
6.910
6.901
6.897
6.891
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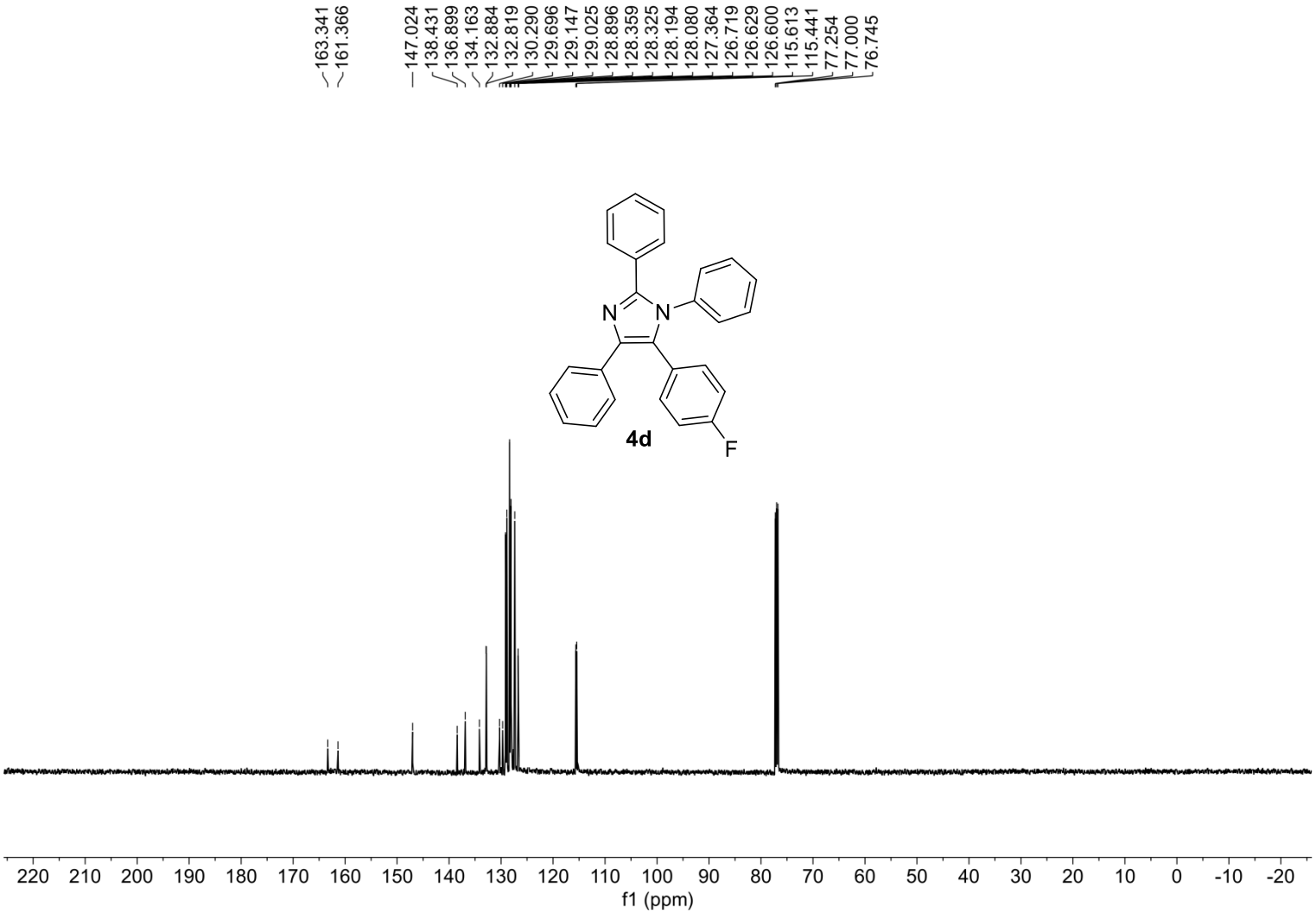
N
F
4d
2.02
2.01
9.02
2.02
2.00
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.163
132.884
132.819
130.290
129.696
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129.025
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128.359
128.325
128.194
128.080
127.364
126.719
126.629
126.600
115.613
115.441
77.254
77.000
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N
N
F
4d
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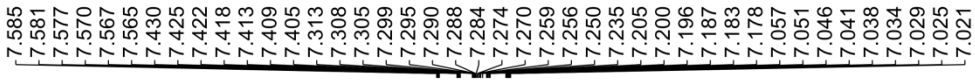
f1 (ppm)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7.581
7.577
7.570
7.567
7.565
7.430
7.425
7.422
7.418
7.413
7.409
7.405
7.313
7.308
7.305
7.299
7.295
7.290
7.288
7.284
7.274
7.270
7.259
7.256
7.250
7.235
7.205
7.200
7.196
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7.038
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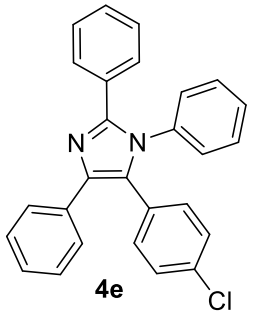
7.025
7.021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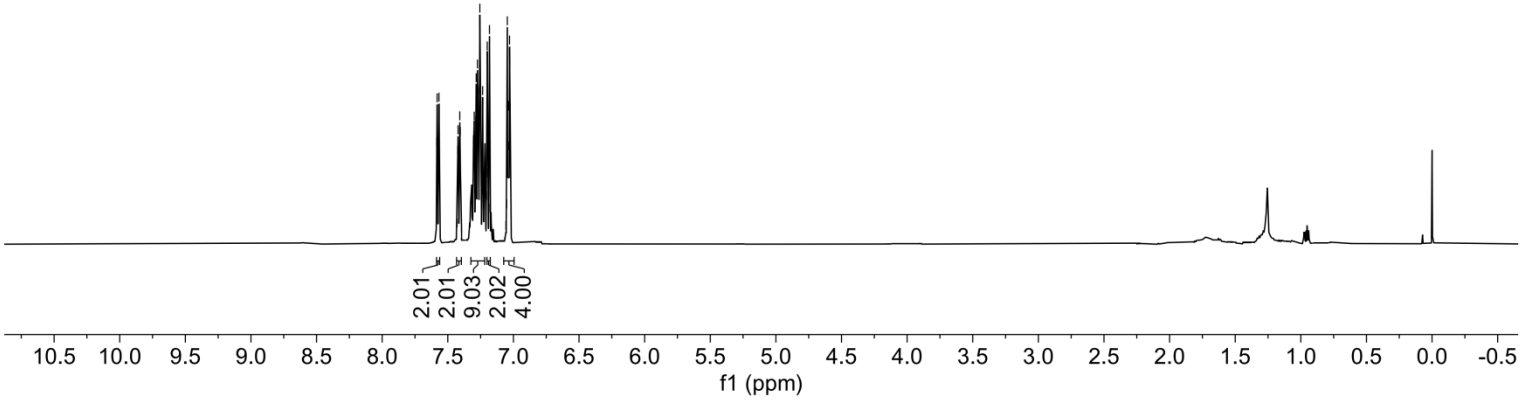
Cl

4e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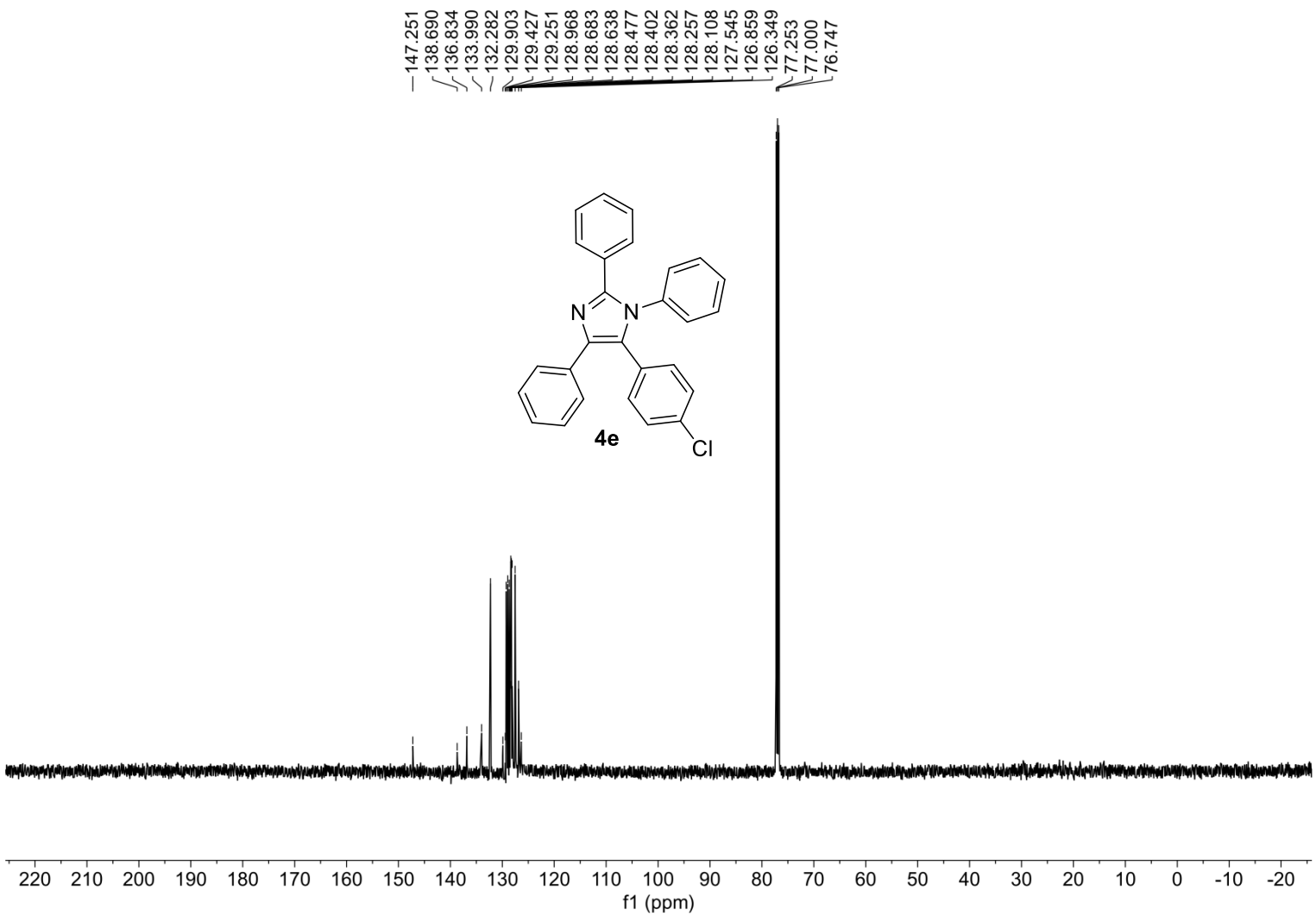
2.01
9.03
2.02
4.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.402
128.362
128.257
128.108
127.545
126.859
126.349
77.253
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Cl
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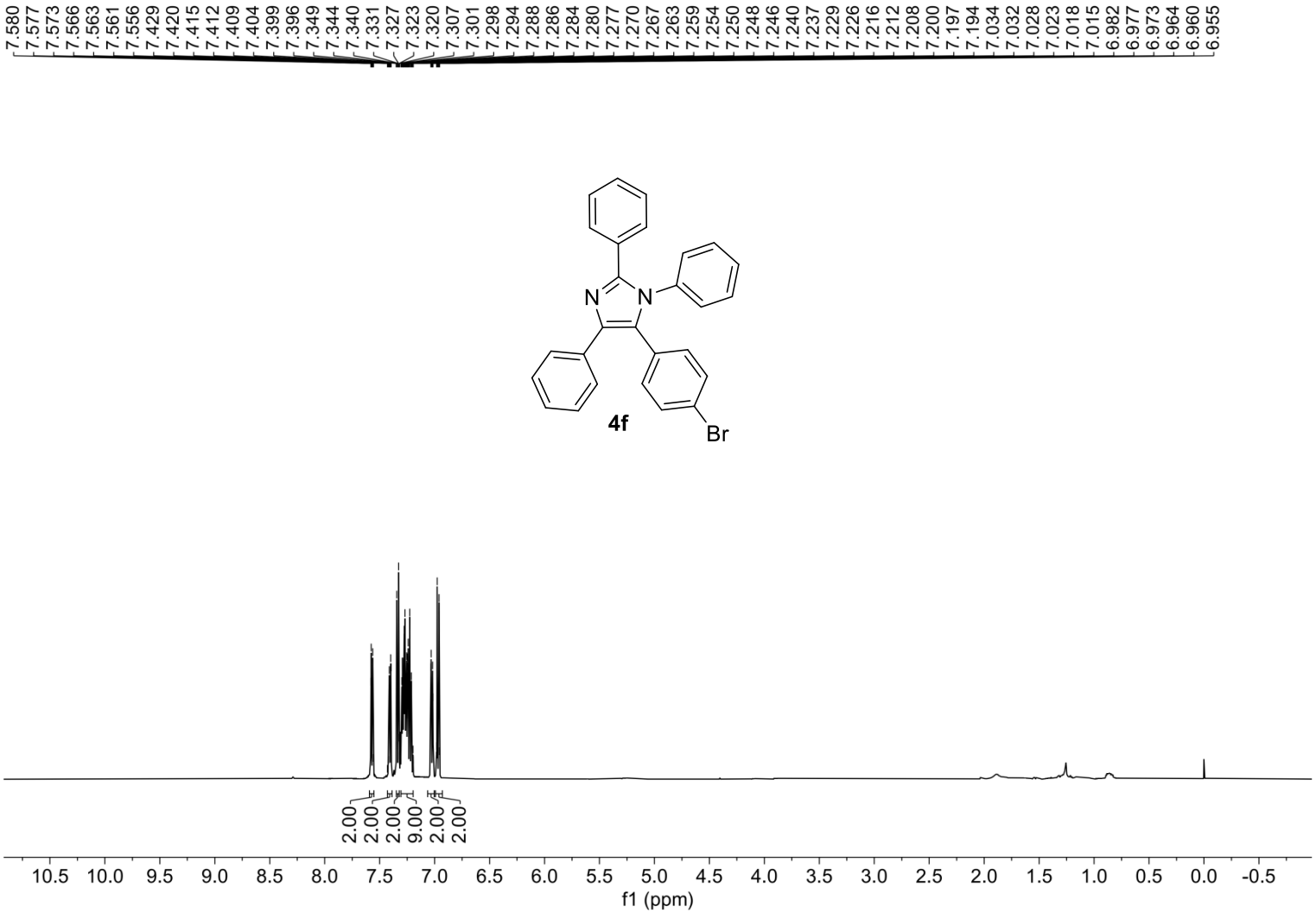
f1 (ppm)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7.404
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7.340
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7.327
7.323
7.320
7.307
7.301
7.298
7.294
7.288
7.286
7.284
7.280
7.277
7.270
7.267
7.263
7.259
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7.015
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6.960
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4f
Br
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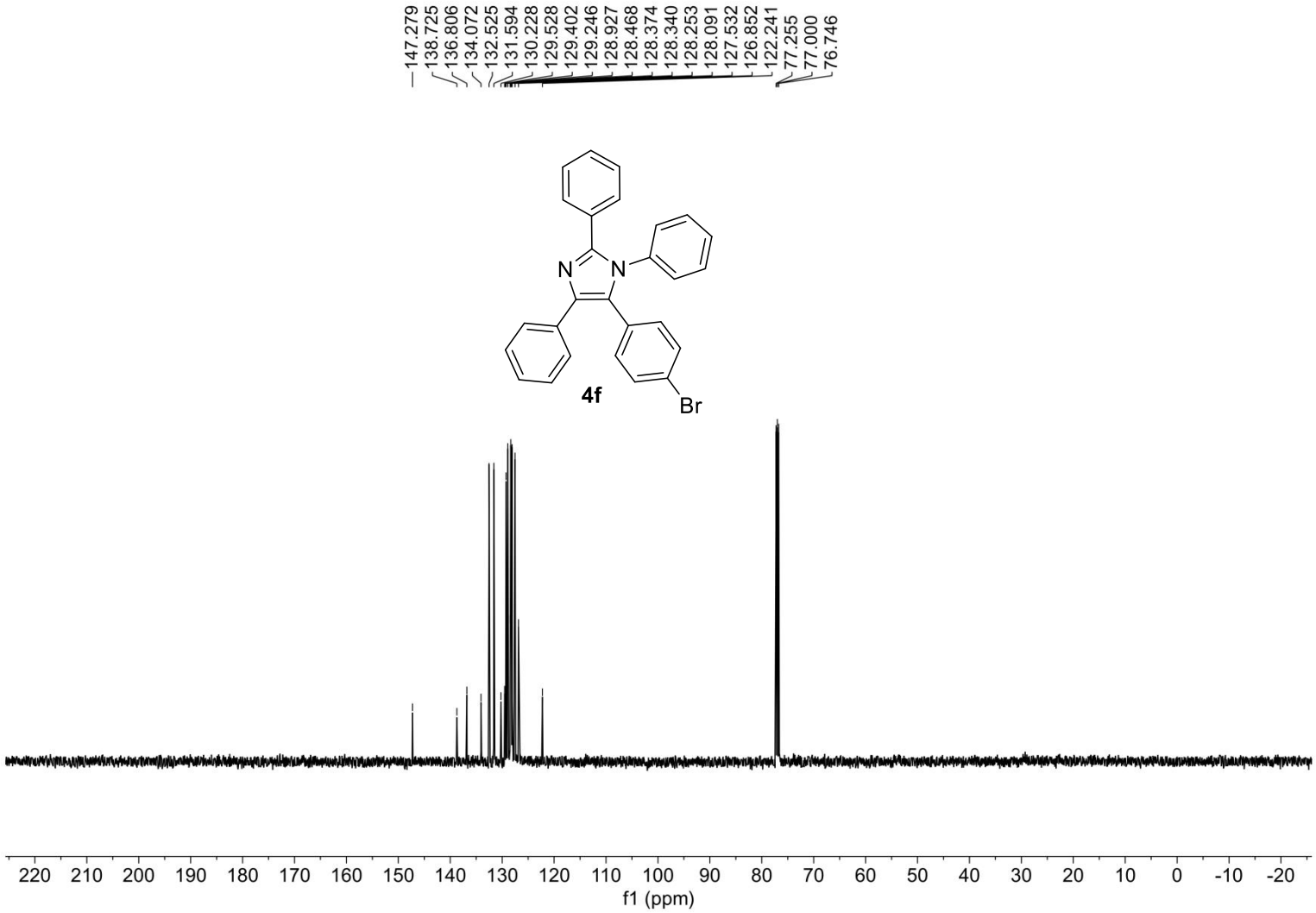
2.00
2.00
9.00
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.852
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Br
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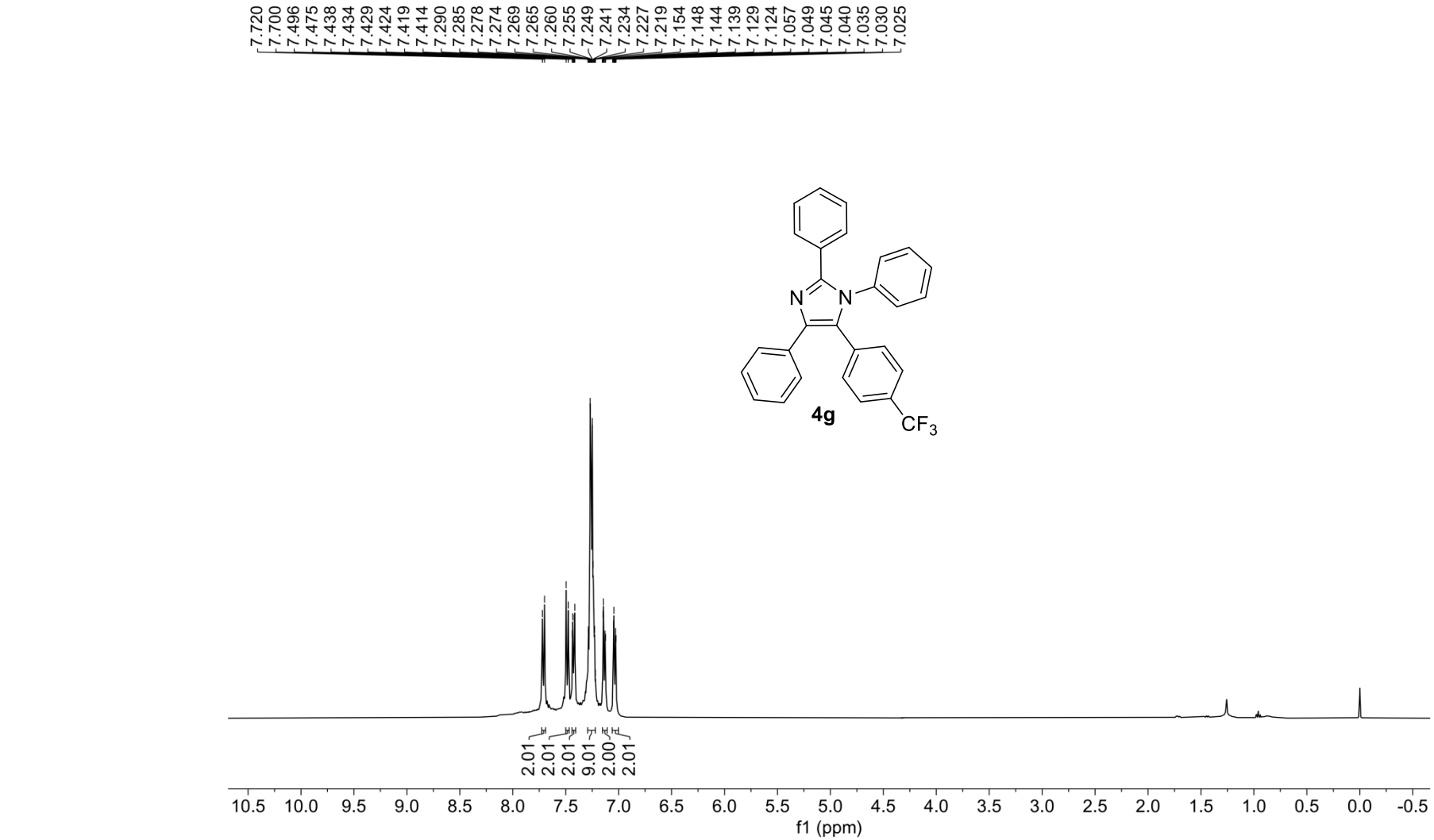
f1 (ppm)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7.045
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7.035
7.030
7.025
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2.01
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2.00
2.01
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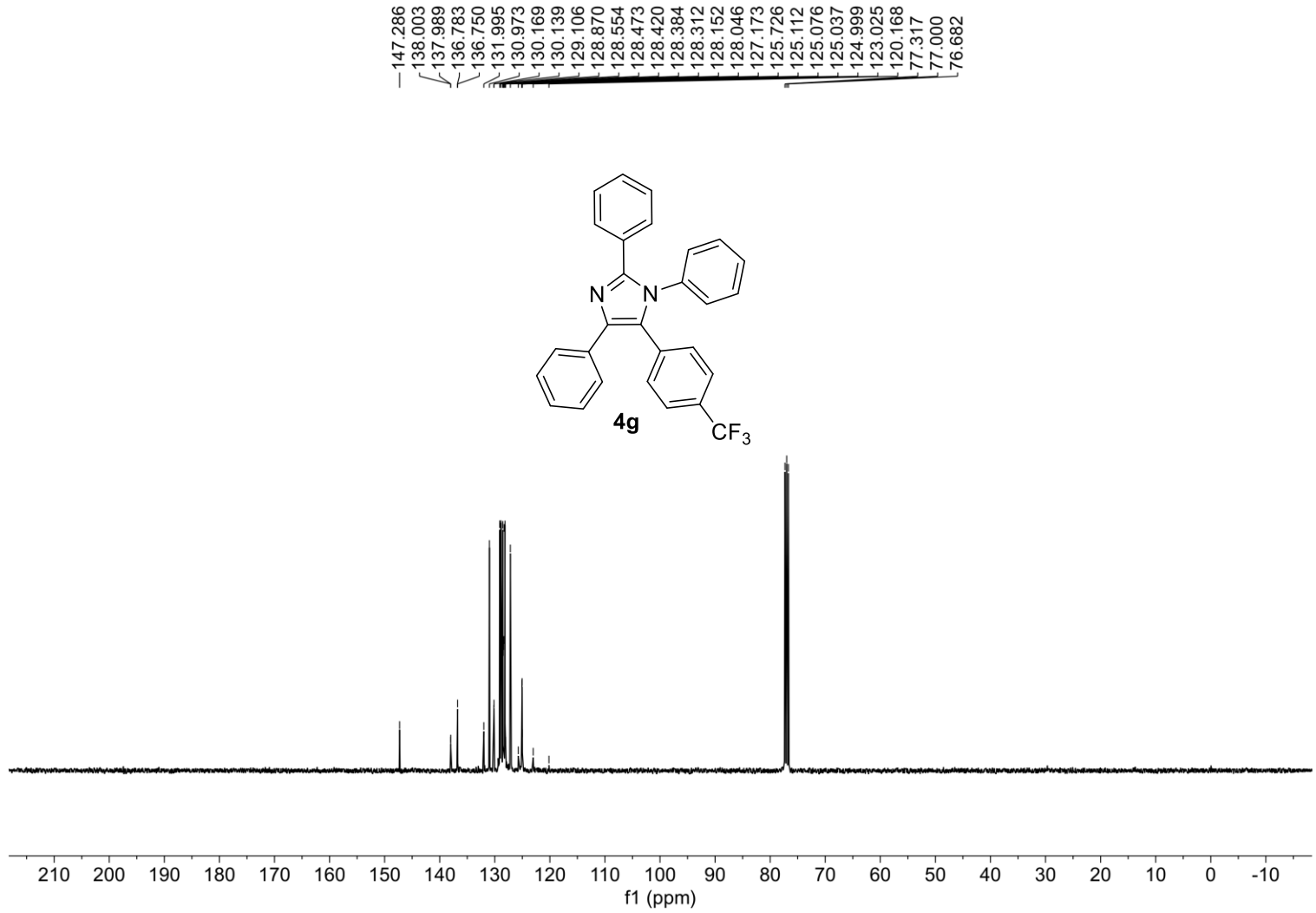
f1 (ppm)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130.169
130.139
129.106
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128.554
128.473
128.420
128.384
128.312
128.152
128.046
127.173
125.726
125.112
125.076
125.037
124.999
123.025
120.168
77.317
77.000
76.682
N
N
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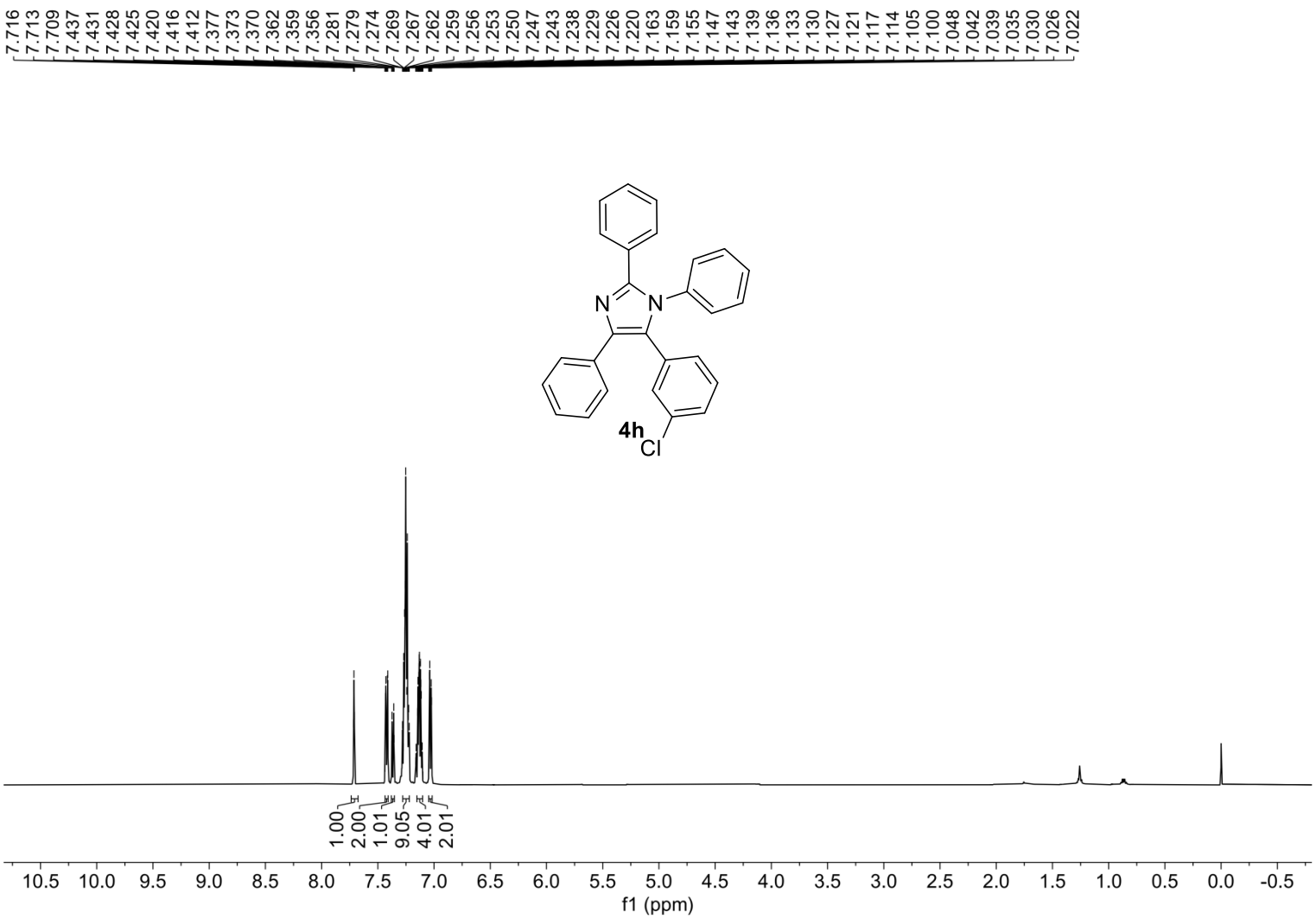
f1 (ppm)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7.420
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7.370
7.362
7.359
7.356
7.281
7.279
7.274
7.269
7.267
7.262
7.259
7.256
7.253
7.250
7.247
7.243
7.238
7.229
7.226
7.220
7.163
7.159
7.155
7.147
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7.139
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7.130
7.127
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4h
Cl
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2.00
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4.01
2.01
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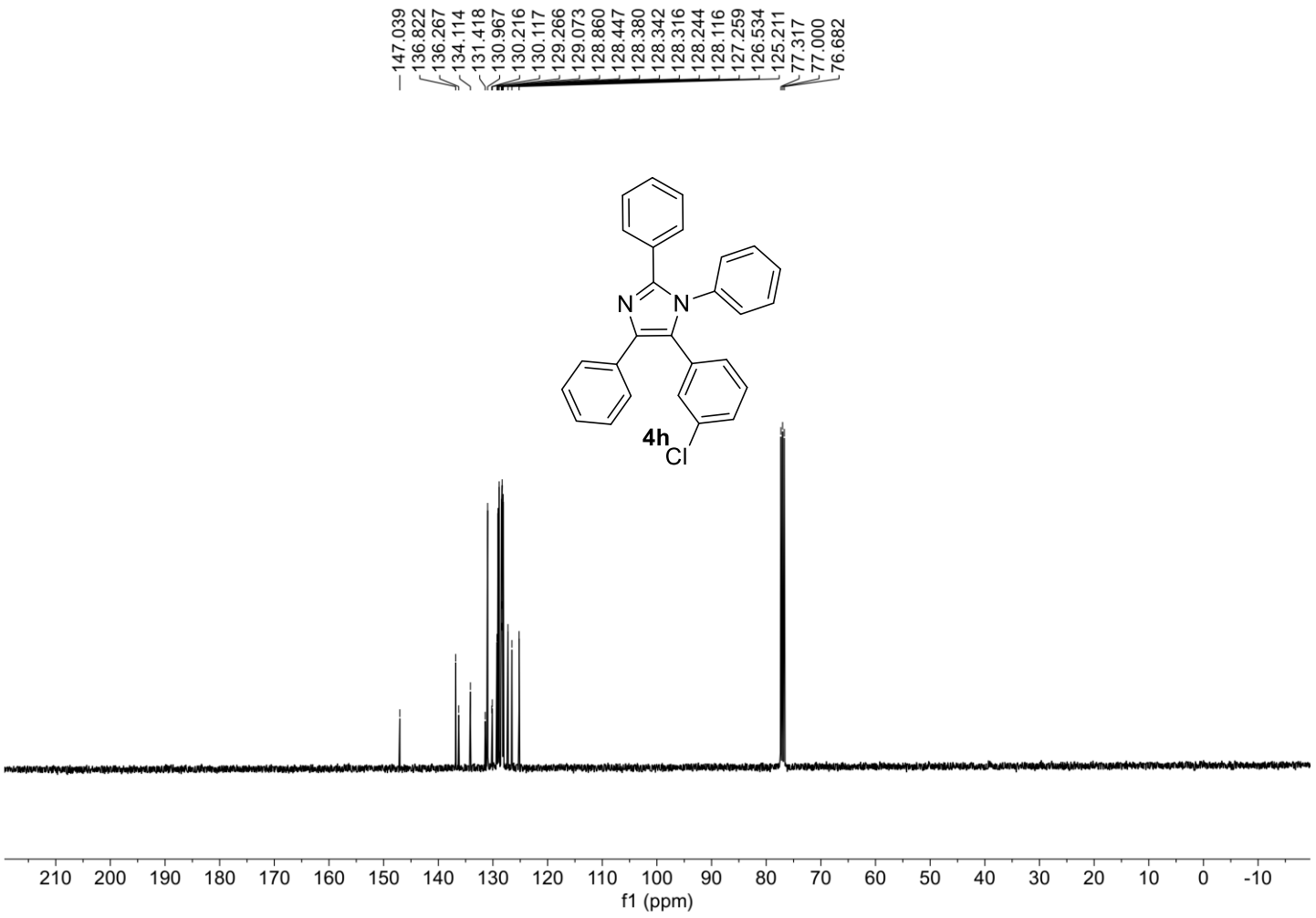
f1 (ppm)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125.211
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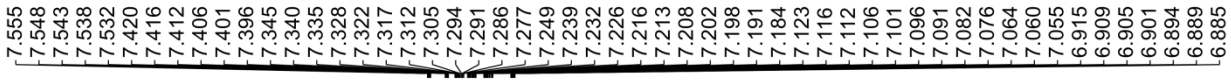
77.000
76.682
N
N
4h
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.294
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7.277
7.249
7.239
7.232
7.226
7.216
7.213
7.208
7.202
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7.191
7.184
7.123
7.116
7.112
7.106
7.101
7.096
7.091
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7.060
7.055
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6.909
6.905
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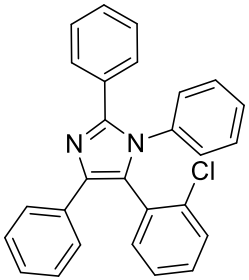
6.889
6.885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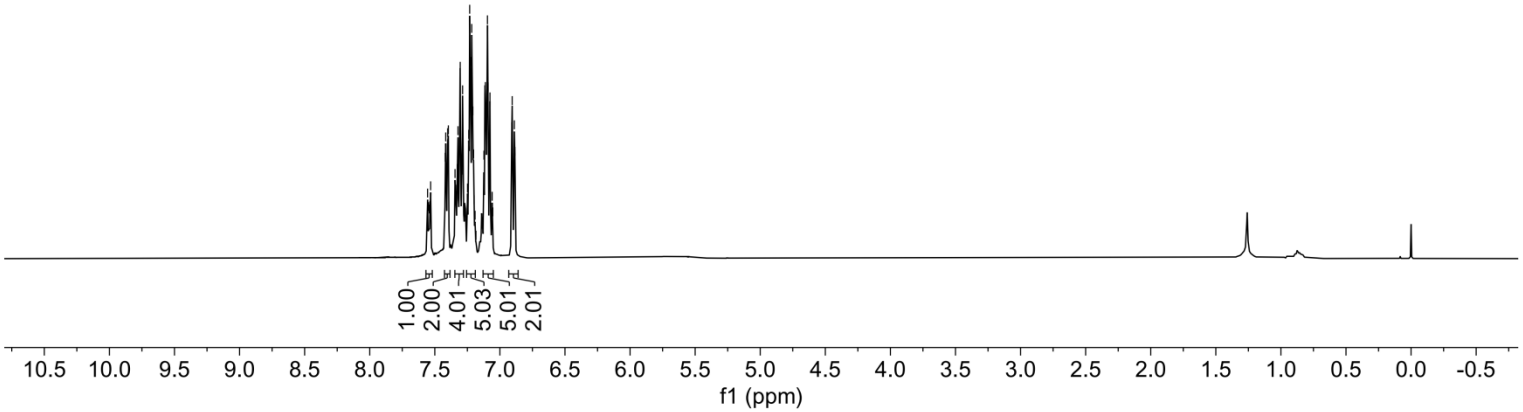
N
Cl

4i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4.01
5.03
5.01
2.01
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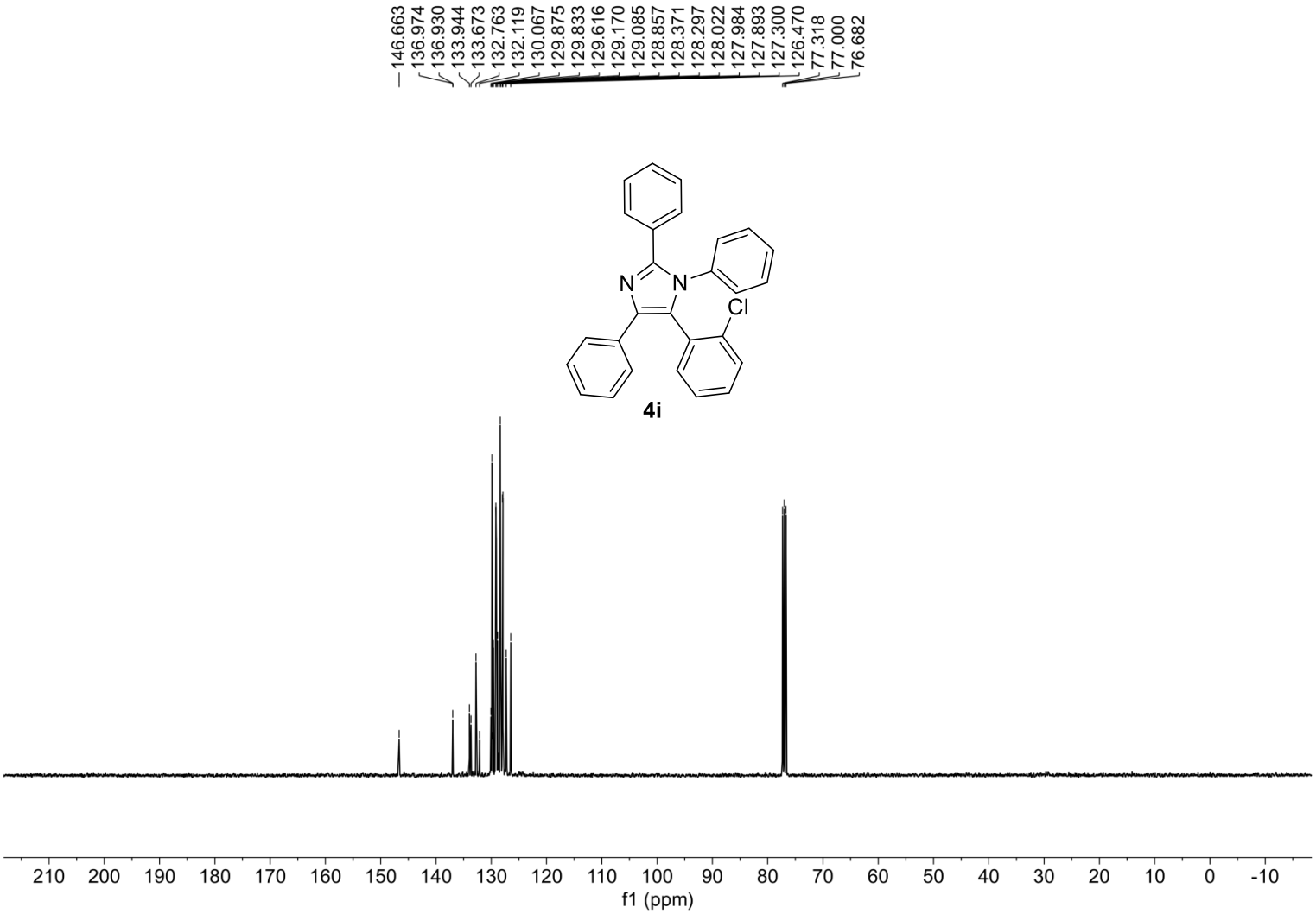
f1 (ppm)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129.085
128.857
128.371
128.297
128.022
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127.893
127.300
126.470
77.318
77.000
76.682
N
N
Cl
4i
210
200
190
180
170
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140
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100
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80
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60
50
40
30
20
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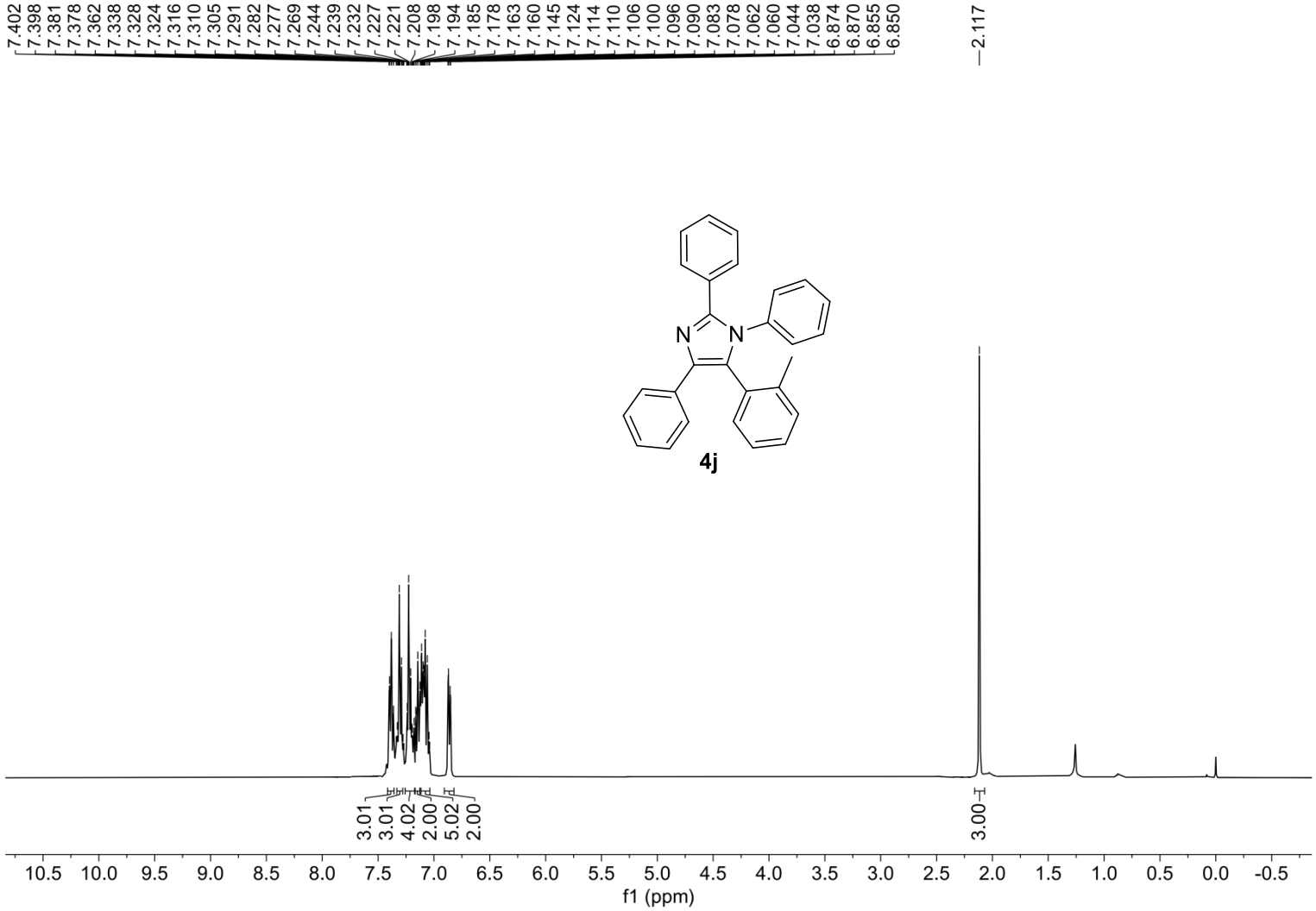
0
-10
f1 (ppm)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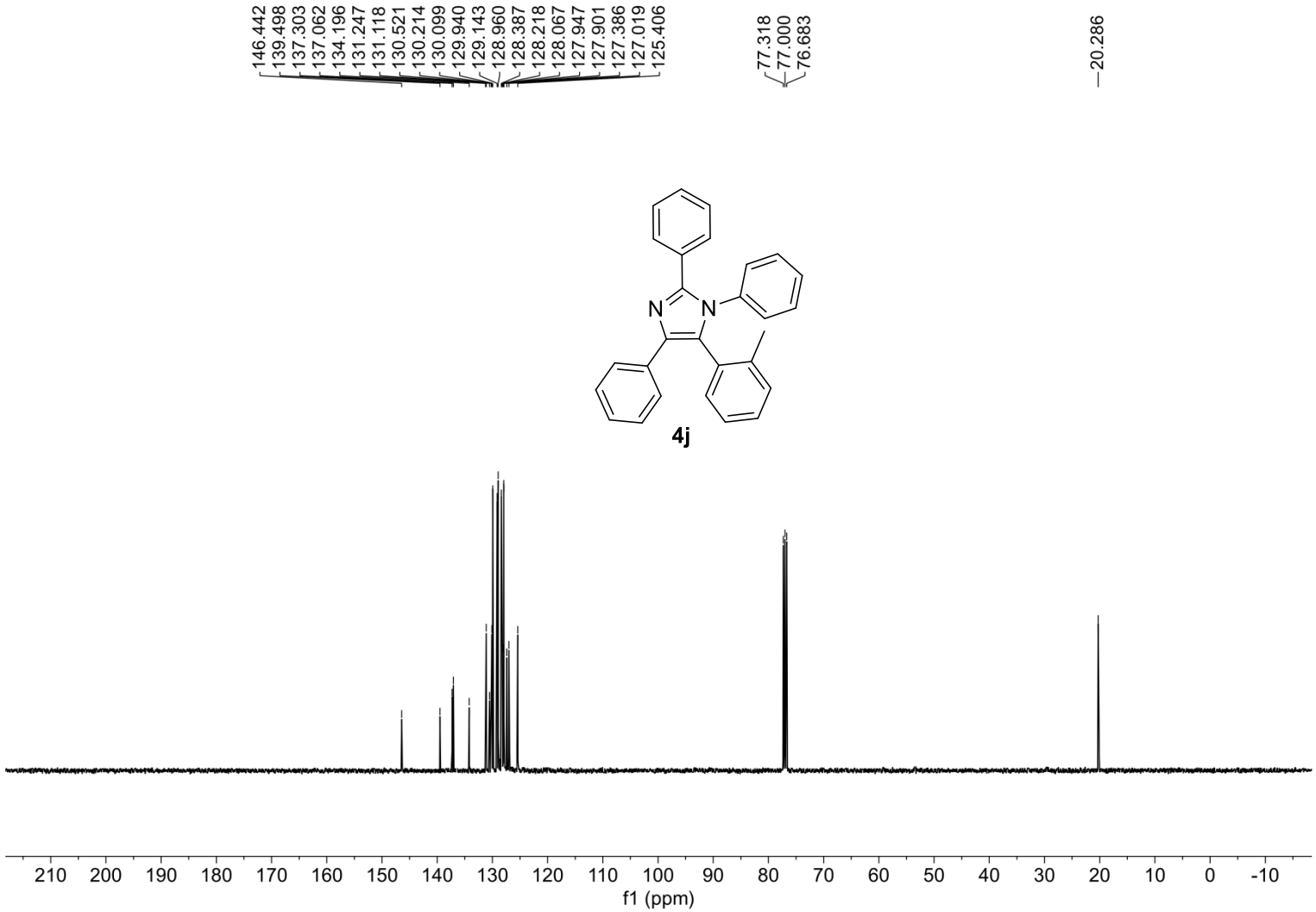
7.305
7.291
7.282
7.277
7.269
7.244
7.239
7.232
7.227
7.221
7.208
7.198
7.194
7.185
7.178
7.163
7.160
7.145
7.124
7.114
7.110
7.106
7.100
7.096
7.090
7.083
7.078
7.062
7.060
7.044
7.038
6.874
6.870
6.855
6.850
2.117
N
N
4j
3.01
3.01
4.02
2.00
5.02
2.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.387
128.218
128.067
127.947
127.901
127.386
127.019
125.406
77.318
77.000
76.683
20.286
N
N
4j
210
200
190
180
170
160
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140
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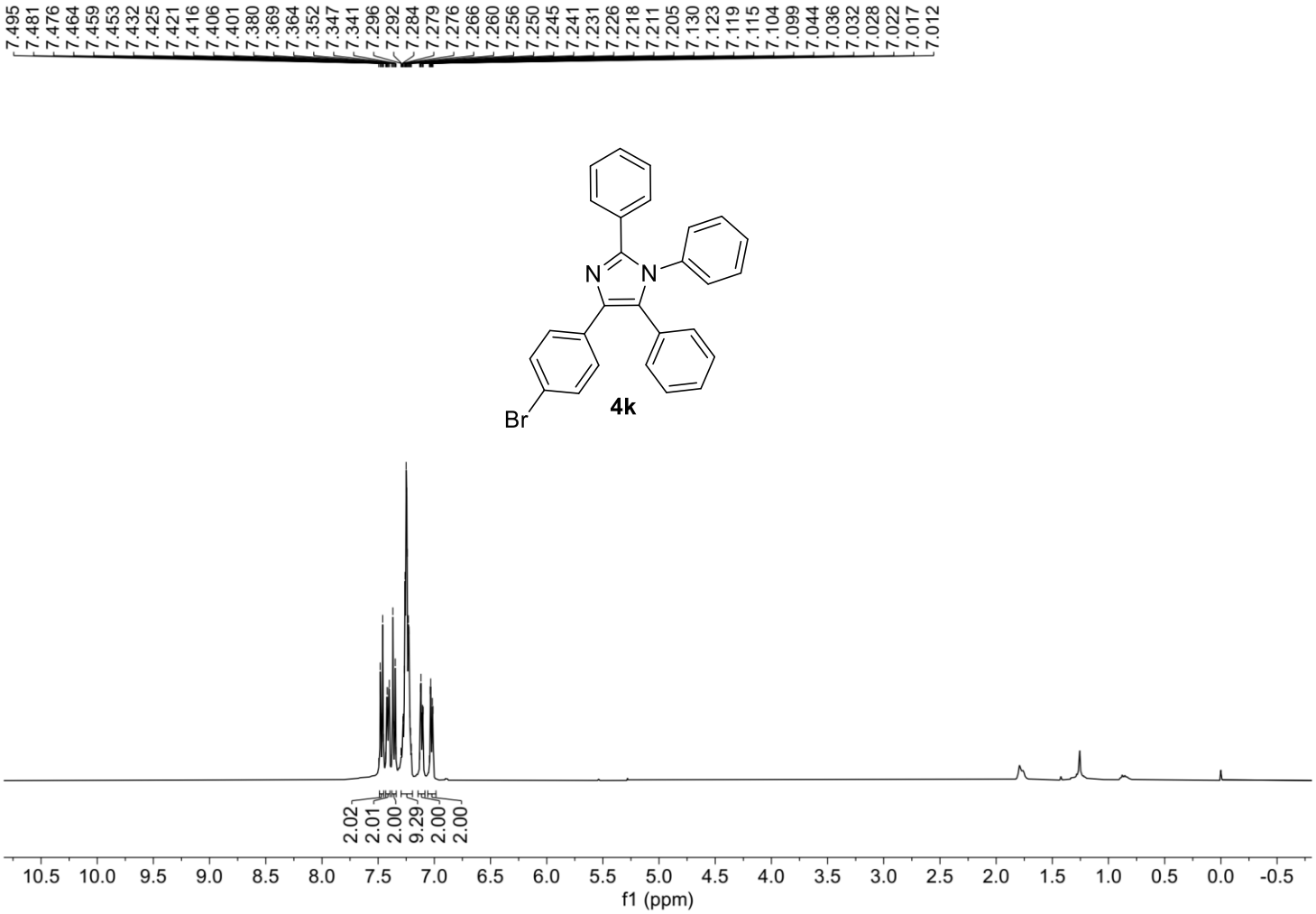
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.425
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7.416
7.406
7.401
7.380
7.369
7.364
7.352
7.347
7.341
7.296
7.292
7.284
7.279
7.276
7.266
7.260
7.256
7.250
7.245
7.241
7.231
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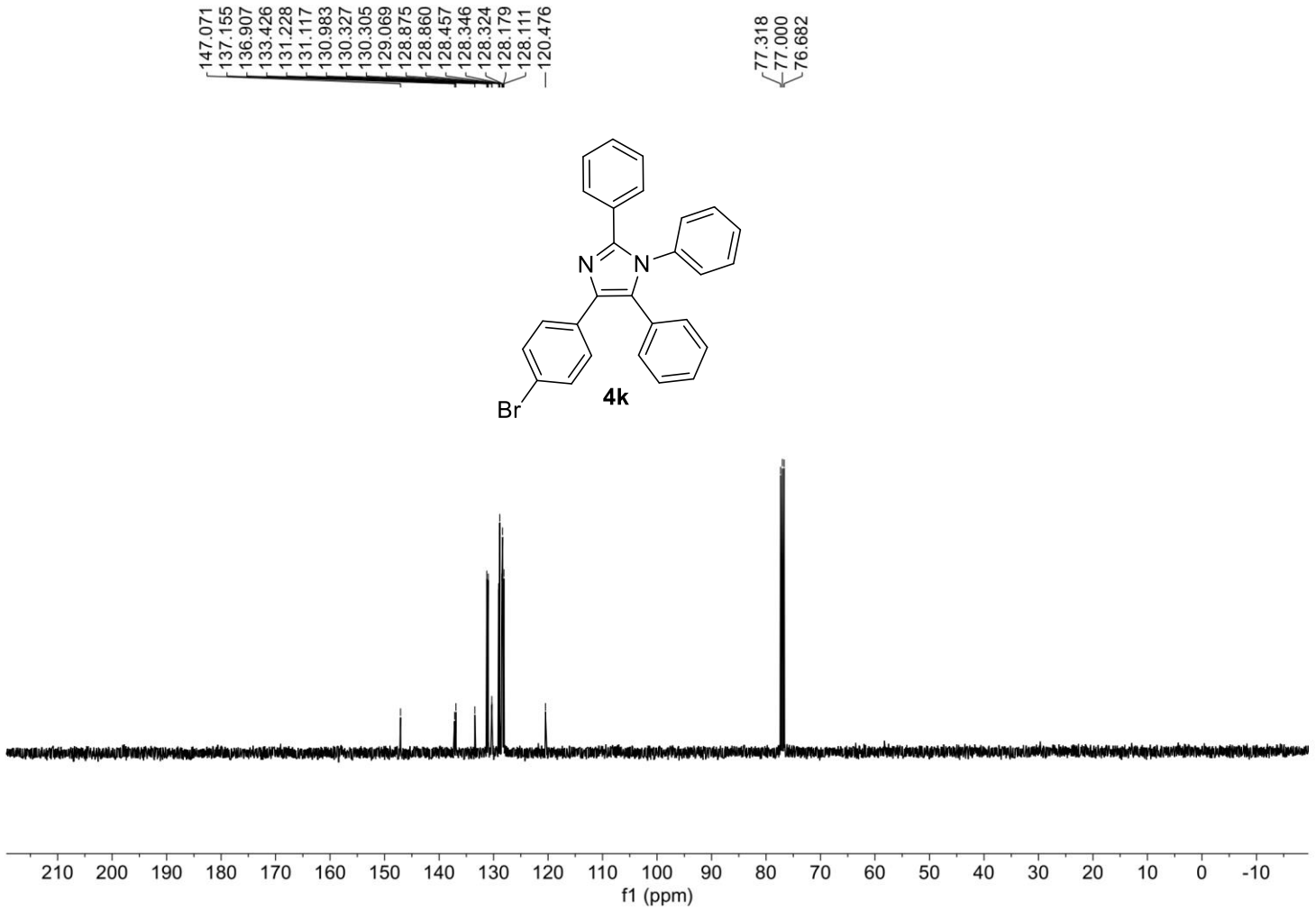
7.218
7.211
7.205
7.130
7.123
7.119
7.115
7.104
7.099
7.044
7.036
7.032
7.028
7.022
7.017
7.012
N
N
Br
4k
2.02
2.01
2.00
9.29
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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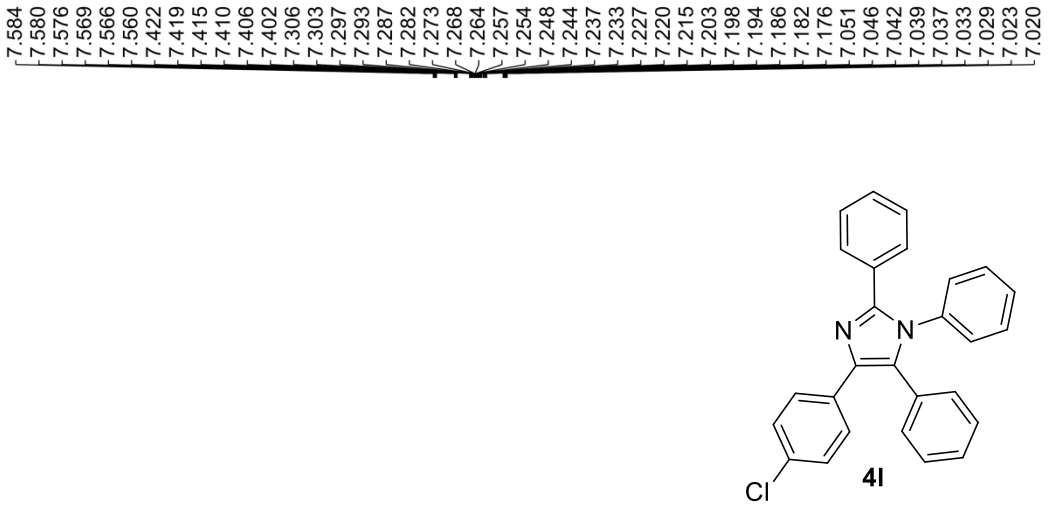
130.305
129.069
128.875
128.860
128.457
128.346
128.324
128.179
128.111
120.476
77.318
77.000
76.682
N
N
Br
4k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.415
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7.406
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7.306
7.303
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7.293
7.287
7.282
7.273
7.268
7.264
7.257
7.254
7.248
7.244
7.237
7.233
7.227
7.220
7.215
7.203
7.198
7.194
7.186
7.182
7.176
7.051
7.046
7.042
7.039
7.037
7.033
7.029
7.023
7.020
N
N
Cl
4l
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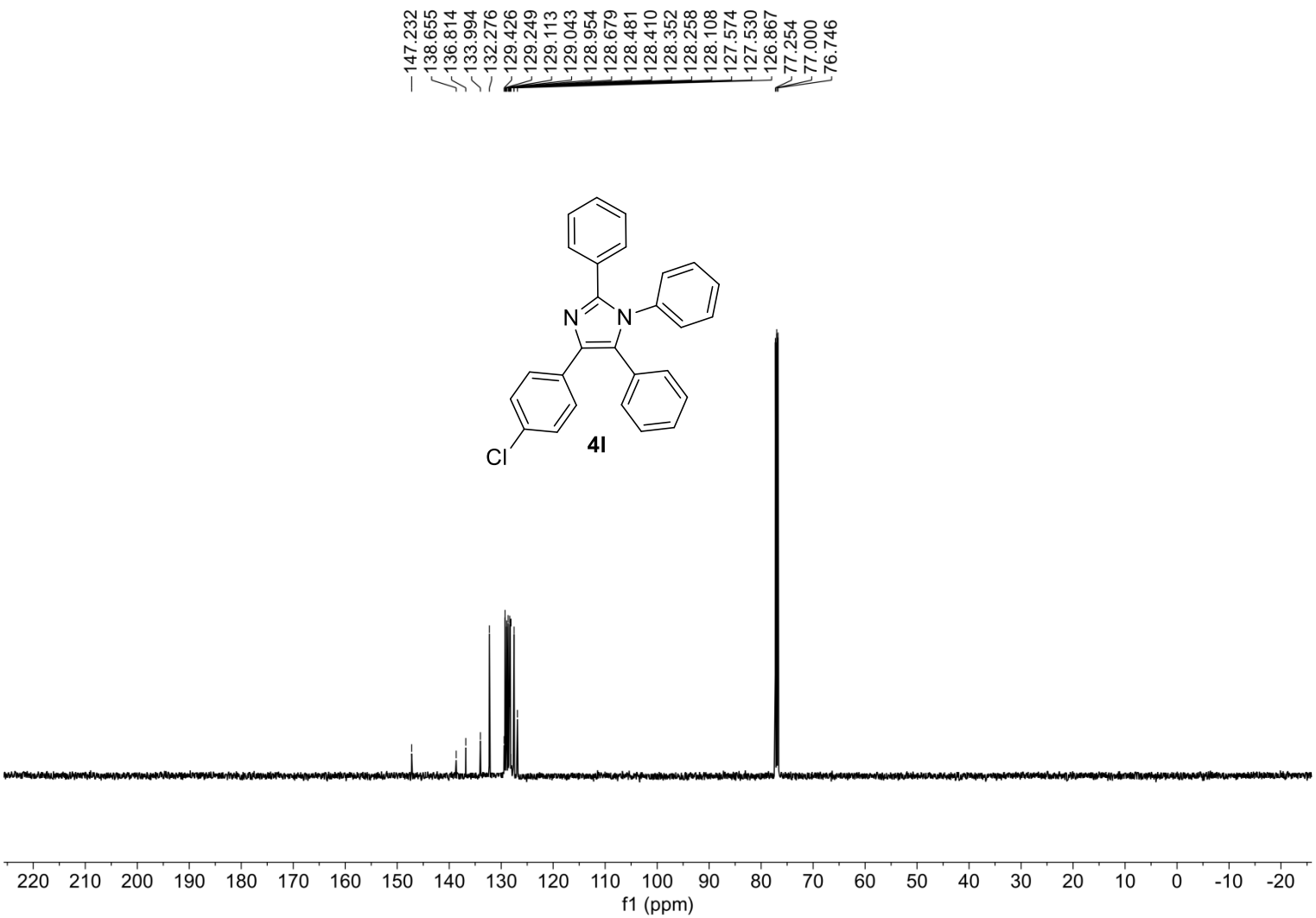
2.00
9.00
2.01
4.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.249
129.113
129.043
128.954
128.679
128.481
128.410
128.352
128.258
128.108
127.574
127.530
126.867
77.254
77.000
76.746
N
N
Cl
4l
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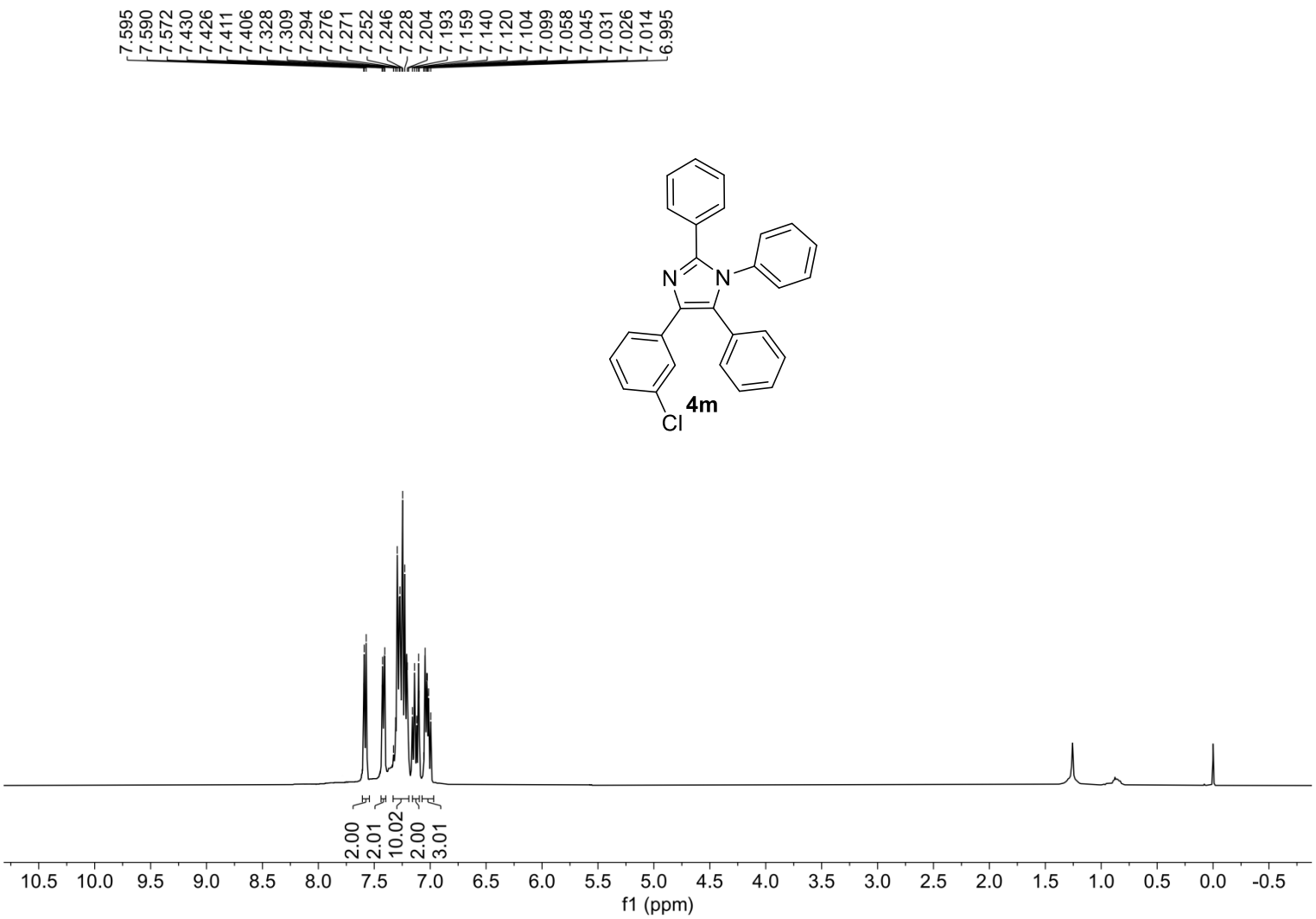
f1 (ppm)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7.411
7.406
7.328
7.309
7.294
7.276
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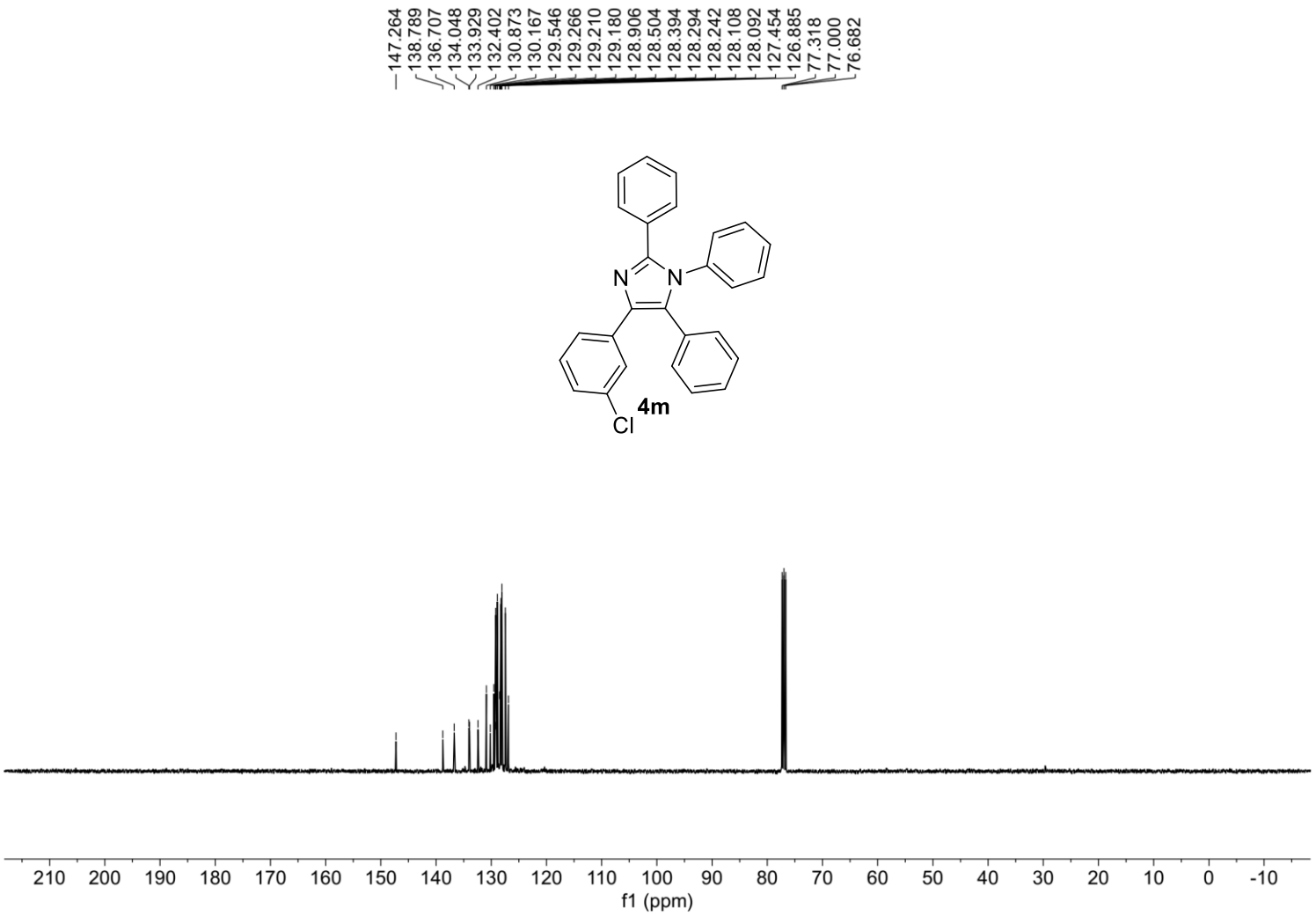
7.252
7.246
7.228
7.204
7.193
7.159
7.140
7.120
7.104
7.099
7.058
7.045
7.031
7.026
7.014
6.995
N
N
Cl
4m
2.00
2.01
10.02
2.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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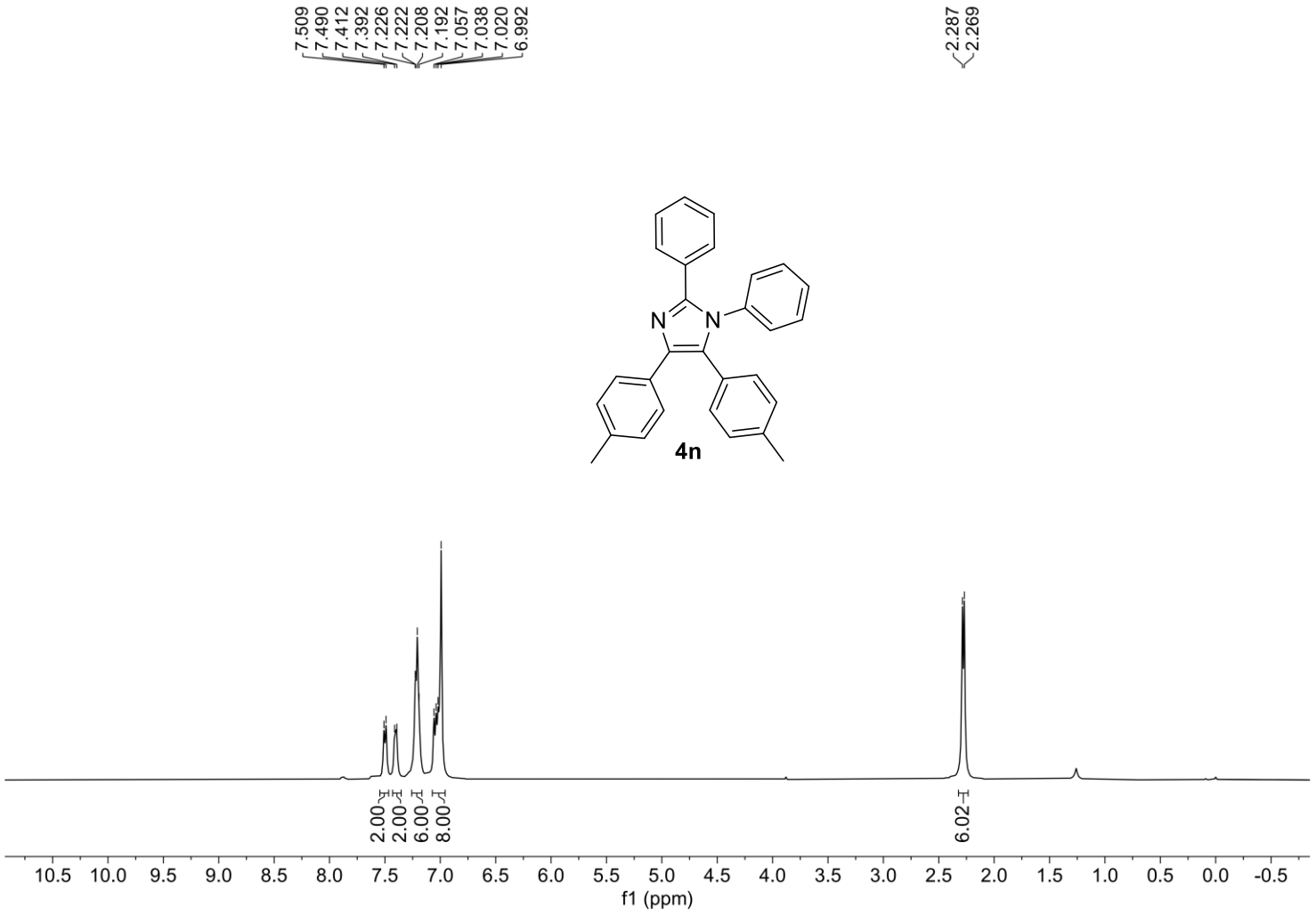
128.504
128.394
128.294
128.242
128.108
128.092
127.454
126.885
77.318
77.000
76.682
N
N
Cl
4m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.412
7.392
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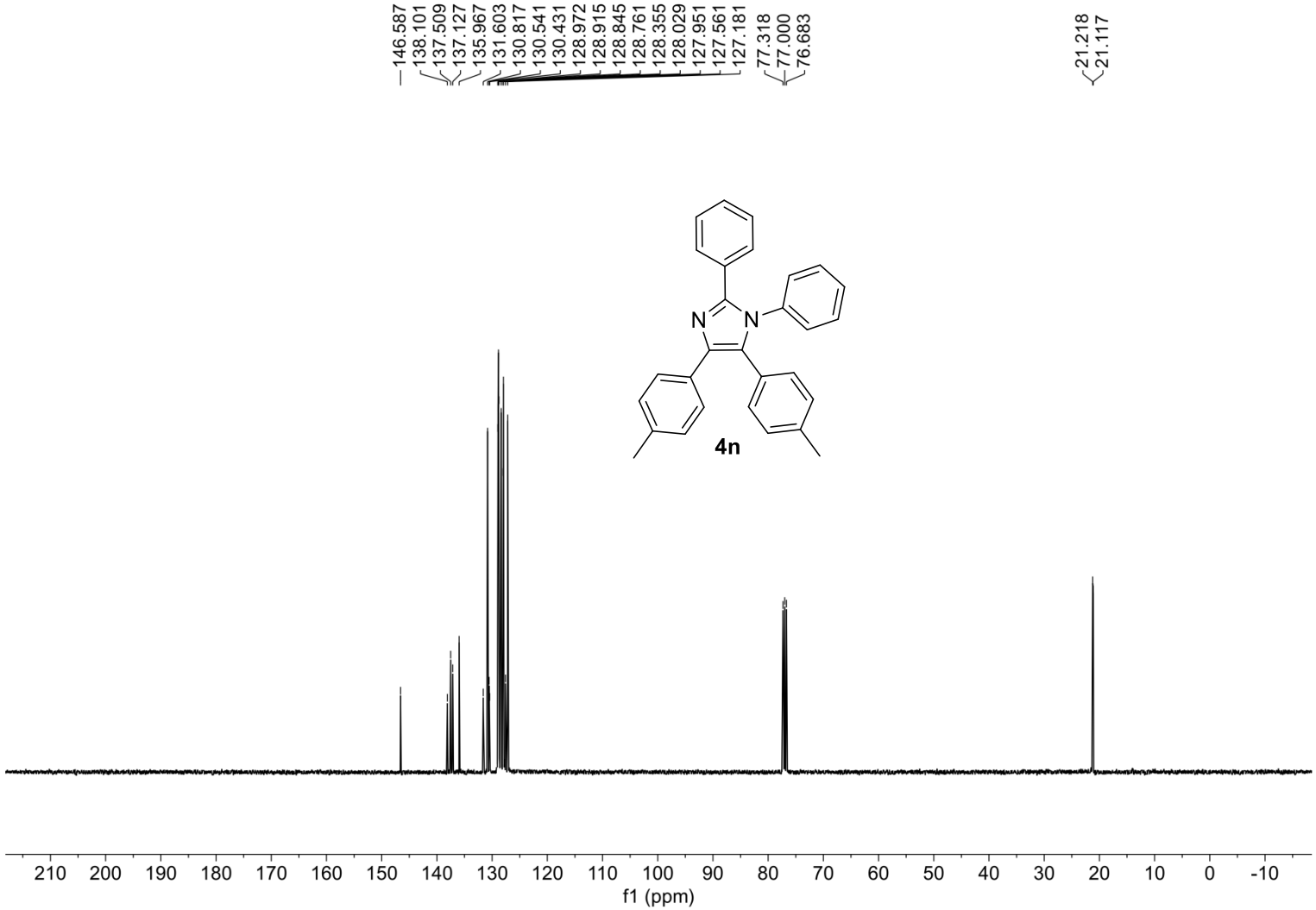
7.222
7.208
7.192
7.057
7.038
7.020
6.992
2.287
2.269
N
N
4n
2.00
2.00
6.00
8.00
6.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.845
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128.029
127.951
127.561
127.181
77.318
77.000
76.683
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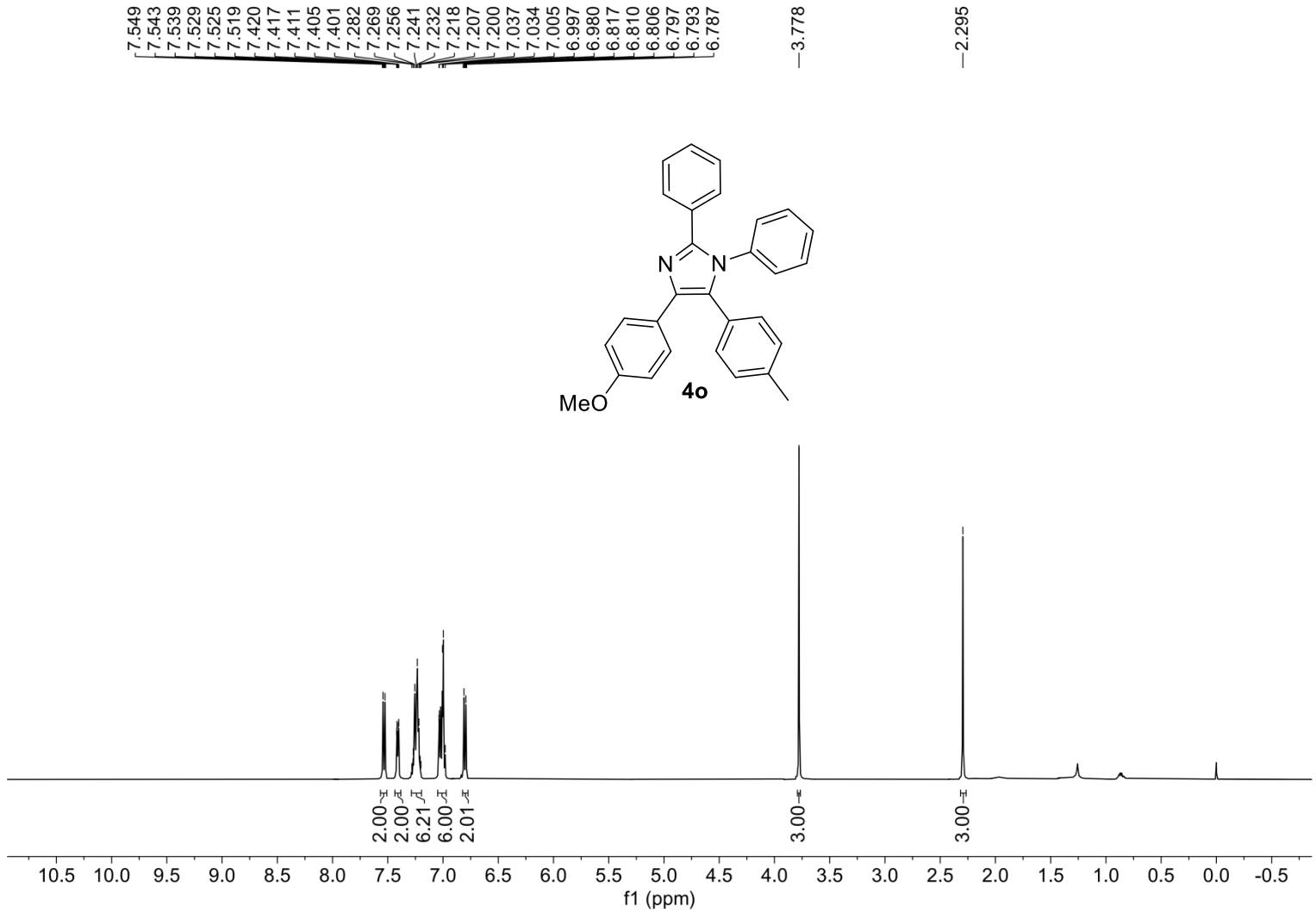
21.117
N
N
4n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.282
7.269
7.256
7.241
7.232
7.218
7.207
7.200
7.037
7.034
7.005
6.997
6.980
6.817
6.810
6.806
6.797
6.793
6.787
3.778
2.295
N
N
MeO
4o
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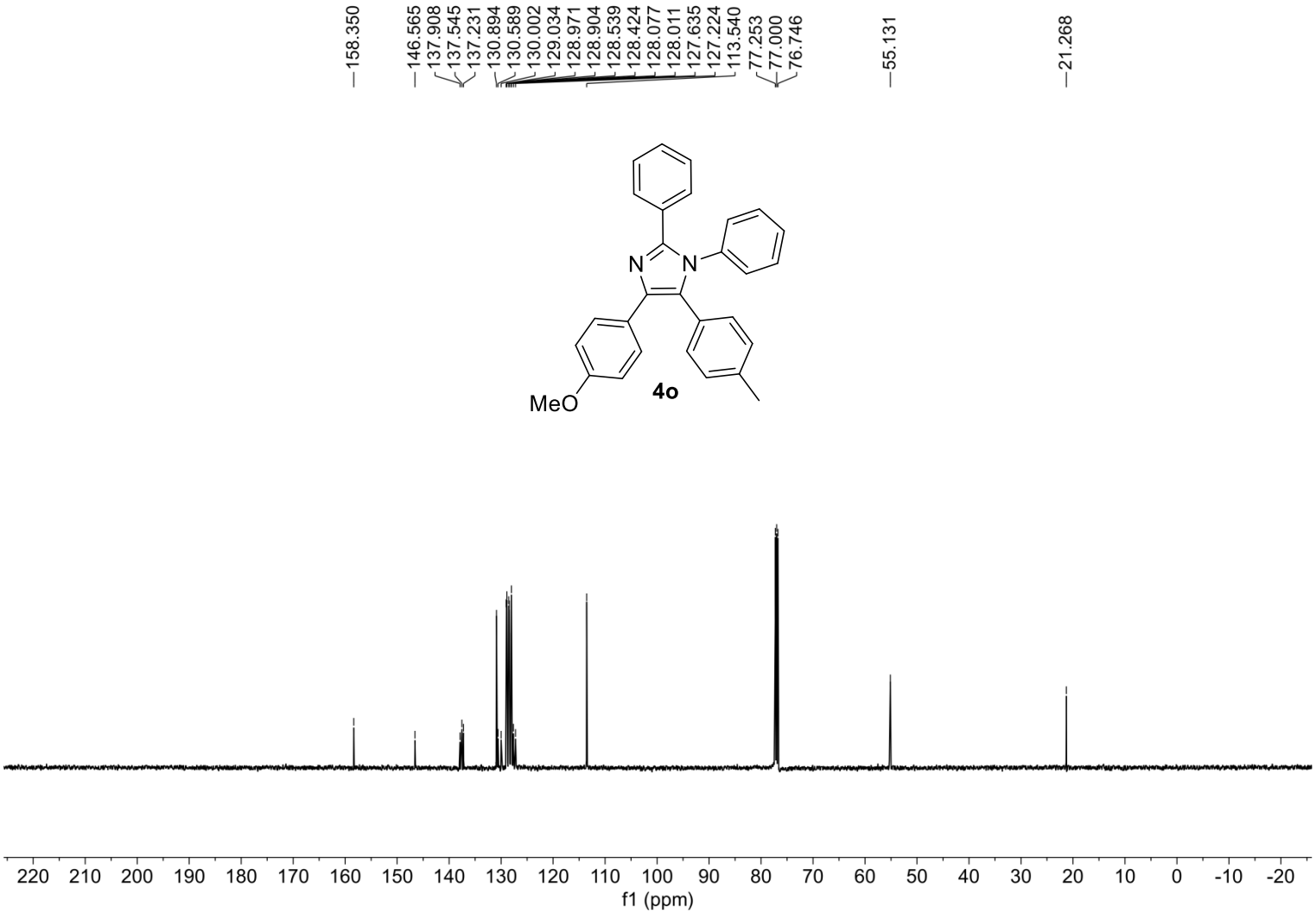
2.00
6.21
6.00
2.01
3.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.077
128.011
127.635
127.224
113.540
77.253
77.000
76.746
55.131
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N
MeO
4o
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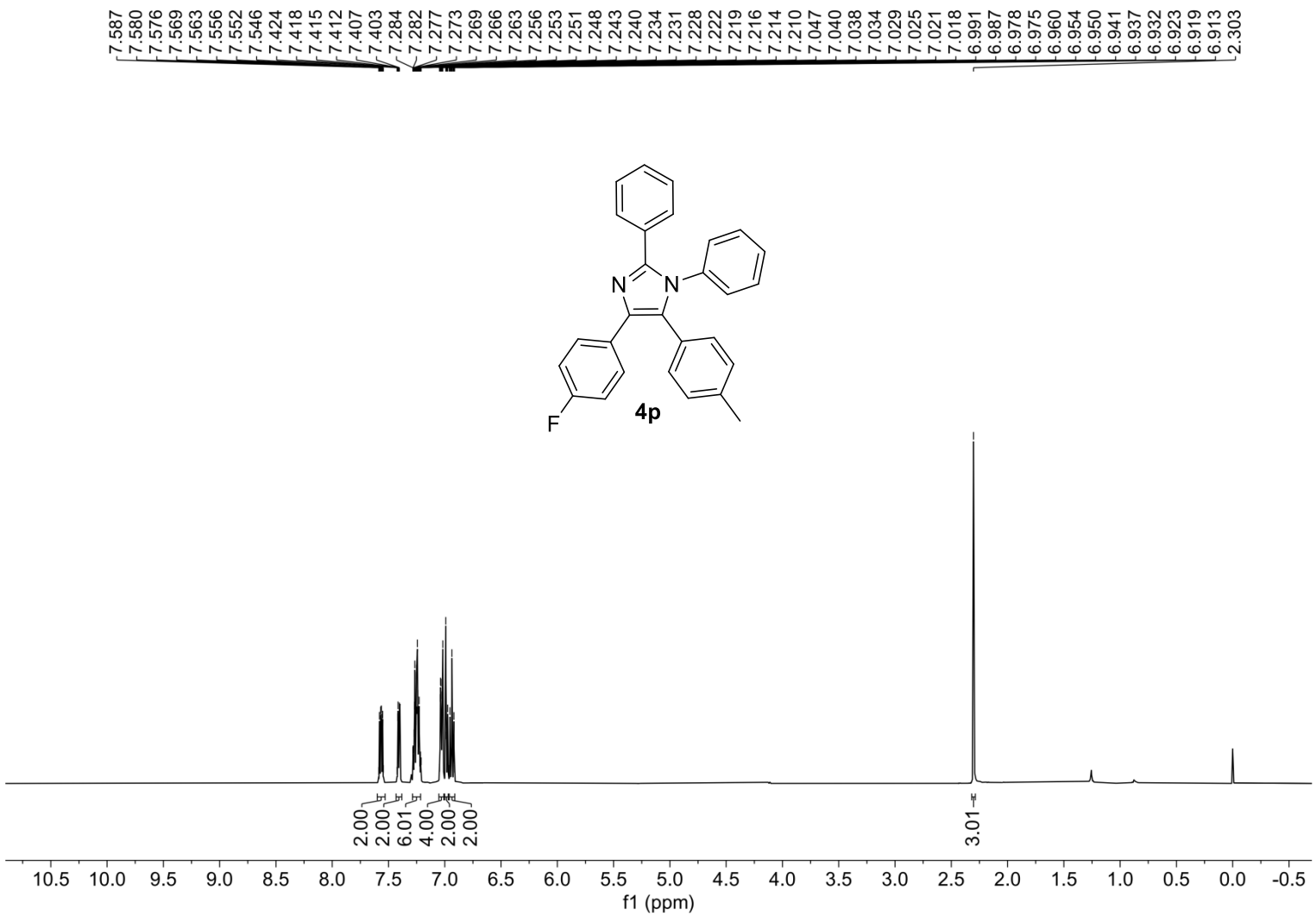
f1 (ppm)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7.282
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7.273
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7.263
7.256
7.253
7.251
7.248
7.243
7.240
7.234
7.231
7.228
7.222
7.219
7.216
7.214
7.210
7.047
7.040
7.038
7.034
7.029
7.025
7.021
7.018
6.991
6.987
6.978
6.975
6.960
6.954
6.950
6.941
6.937
6.932
6.923
6.919
6.913
2.303
N
N
F
4p
2.00
2.00
6.01
4.00
2.00
2.00
3.01
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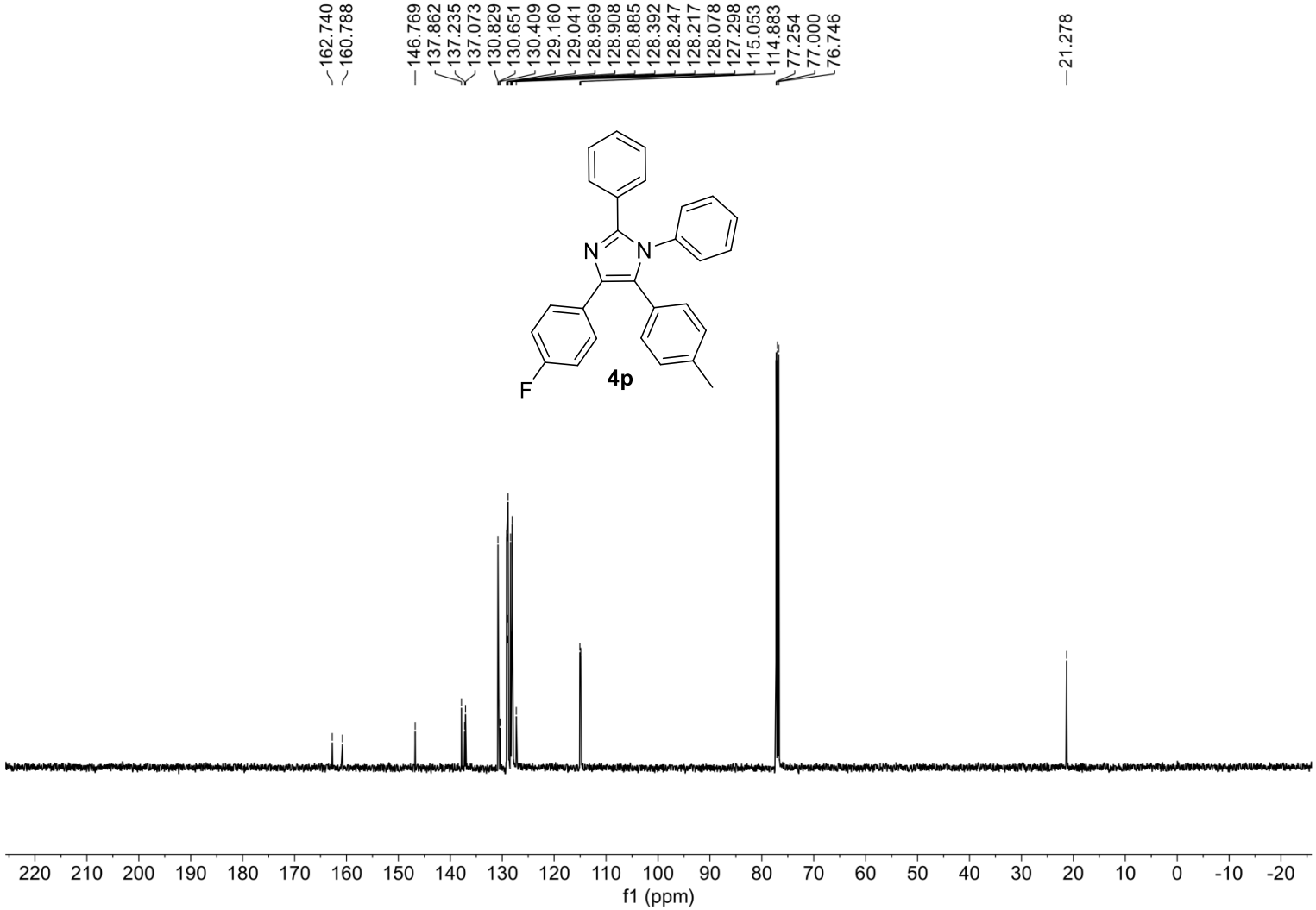
f1 (ppm)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128.908
128.885
128.392
128.247
128.217
128.078
127.298
115.053
114.883
77.254
77.000
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N
F
4p
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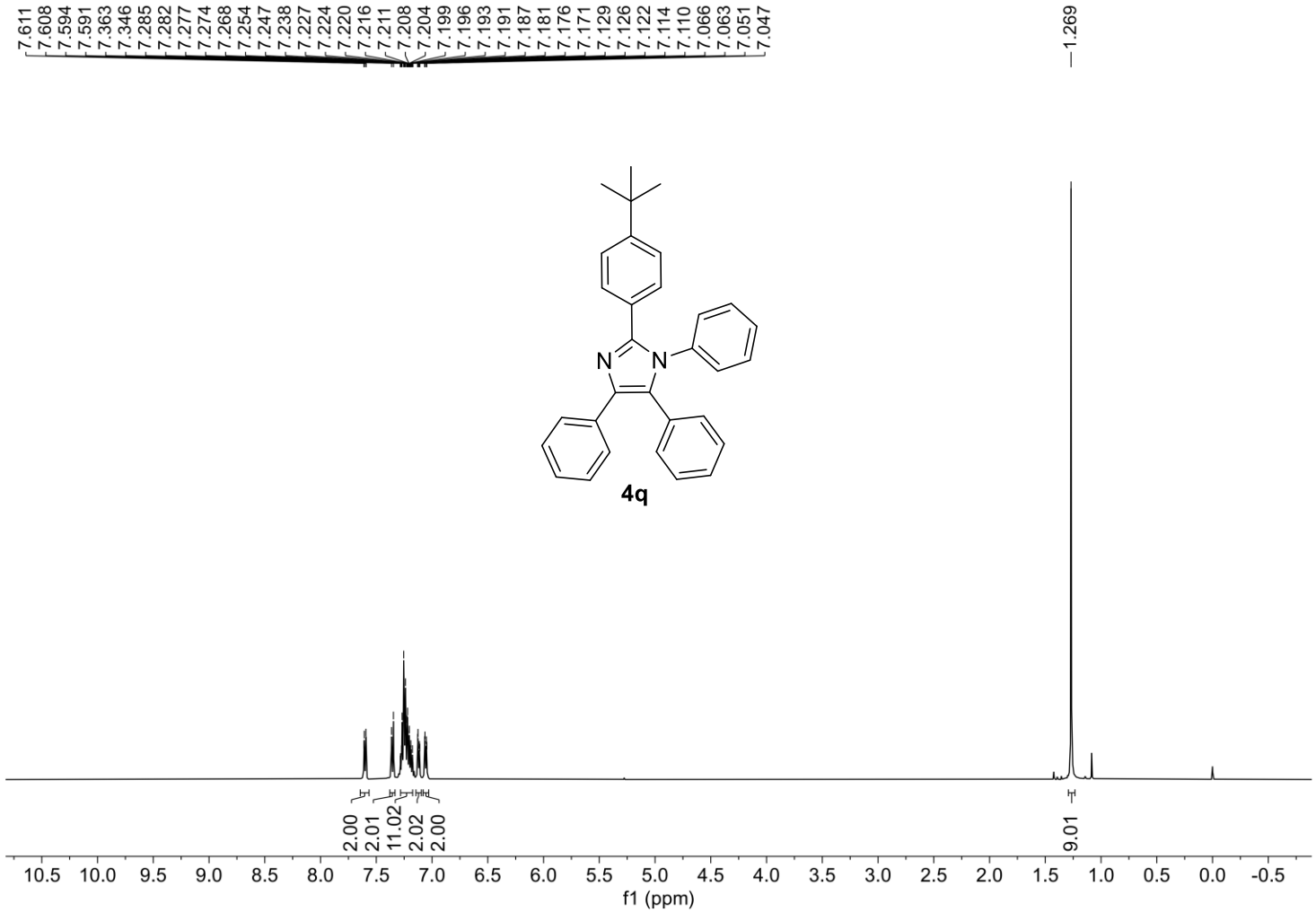
f1 (ppm)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7.216
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7.193
7.191
7.187
7.181
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7.171
7.129
7.126
7.122
7.114
7.110
7.066
7.063
7.051
7.047
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2.01
11.02
2.02
2.00
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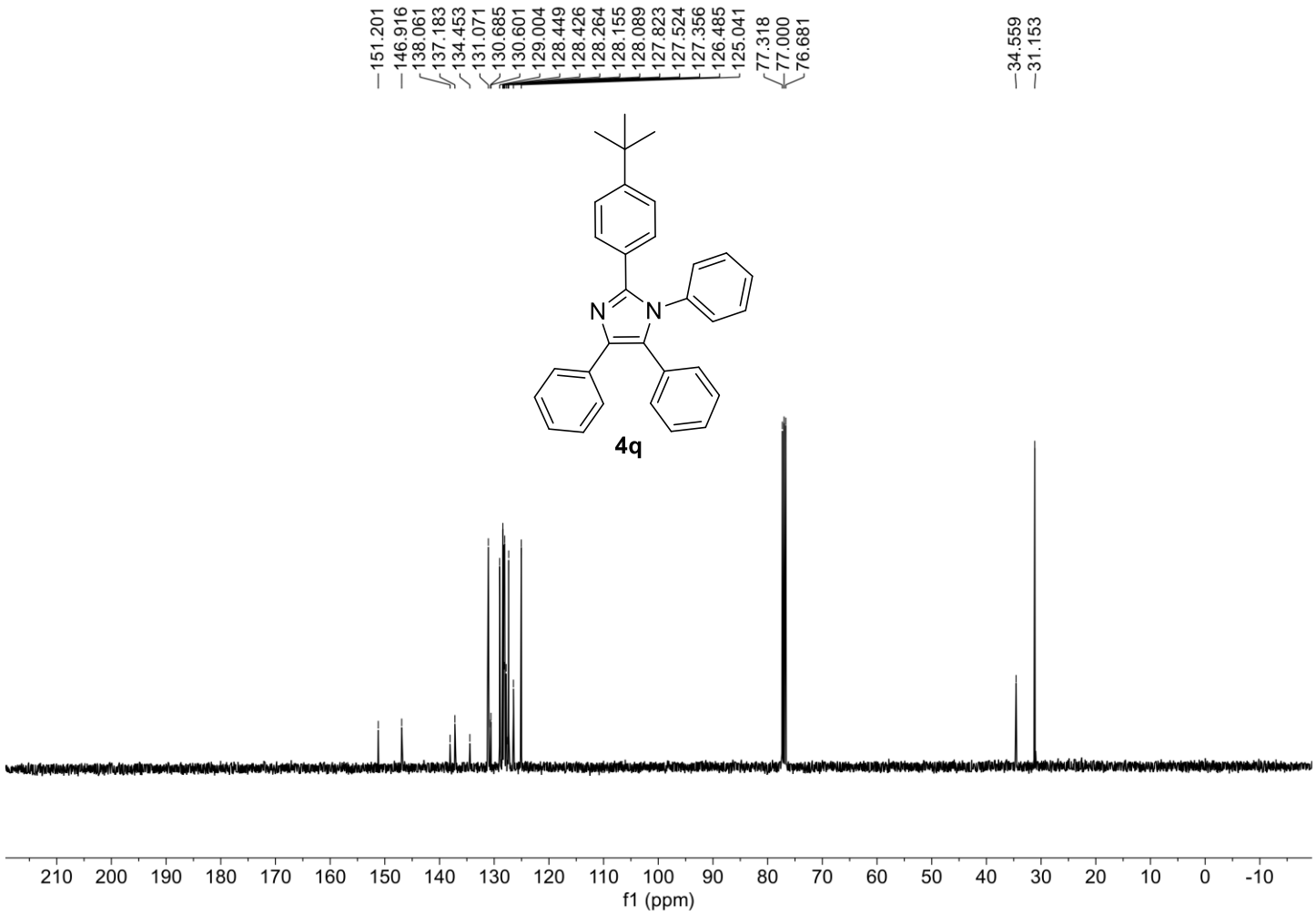
f1 (ppm)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126.485
125.041
77.318
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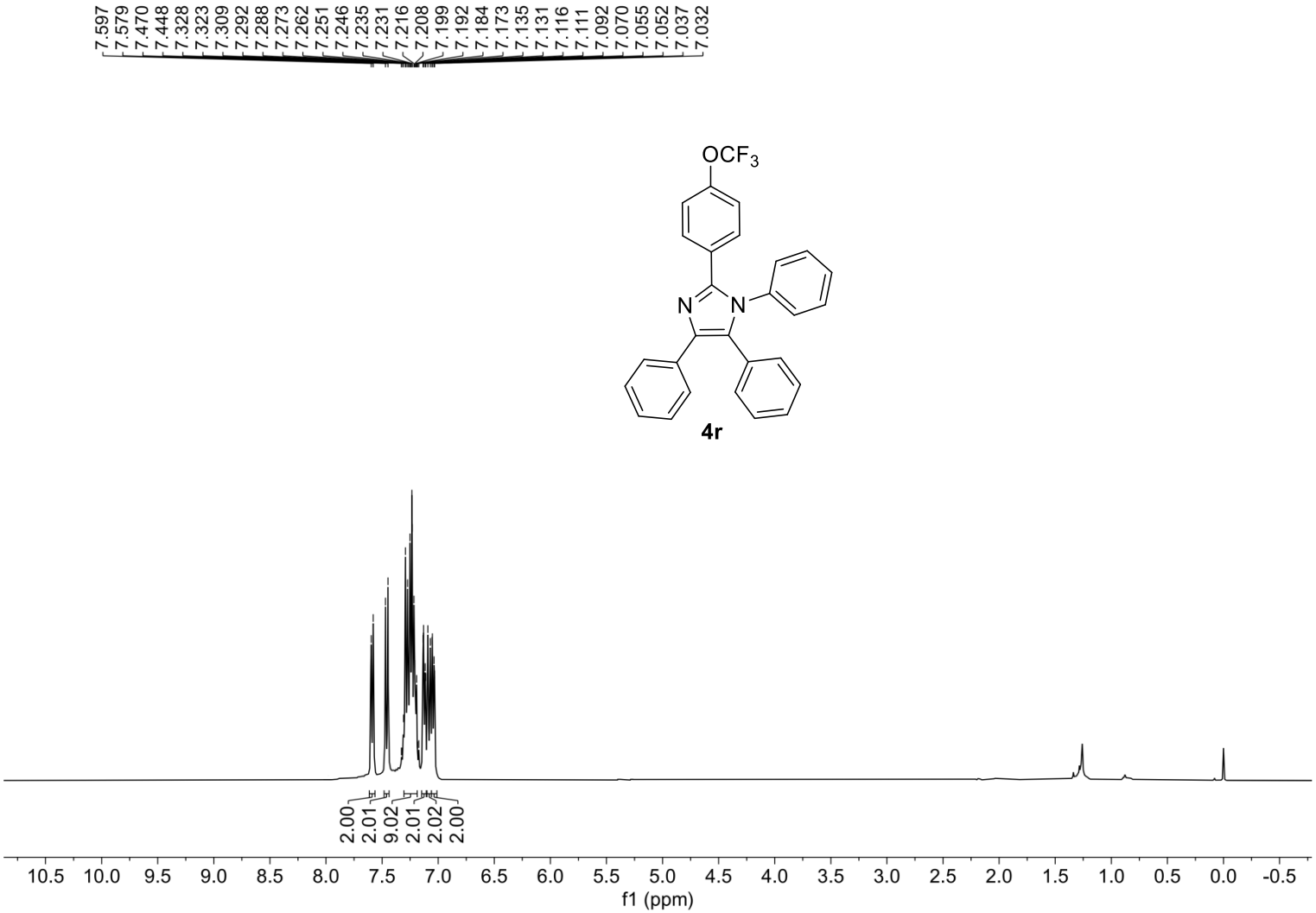
31.153
N
N
4q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.235
7.231
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7.208
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7.192
7.184
7.173
7.135
7.131
7.116
7.111
7.092
7.070
7.055
7.052
7.037
7.032
OCF3
N
N
4r
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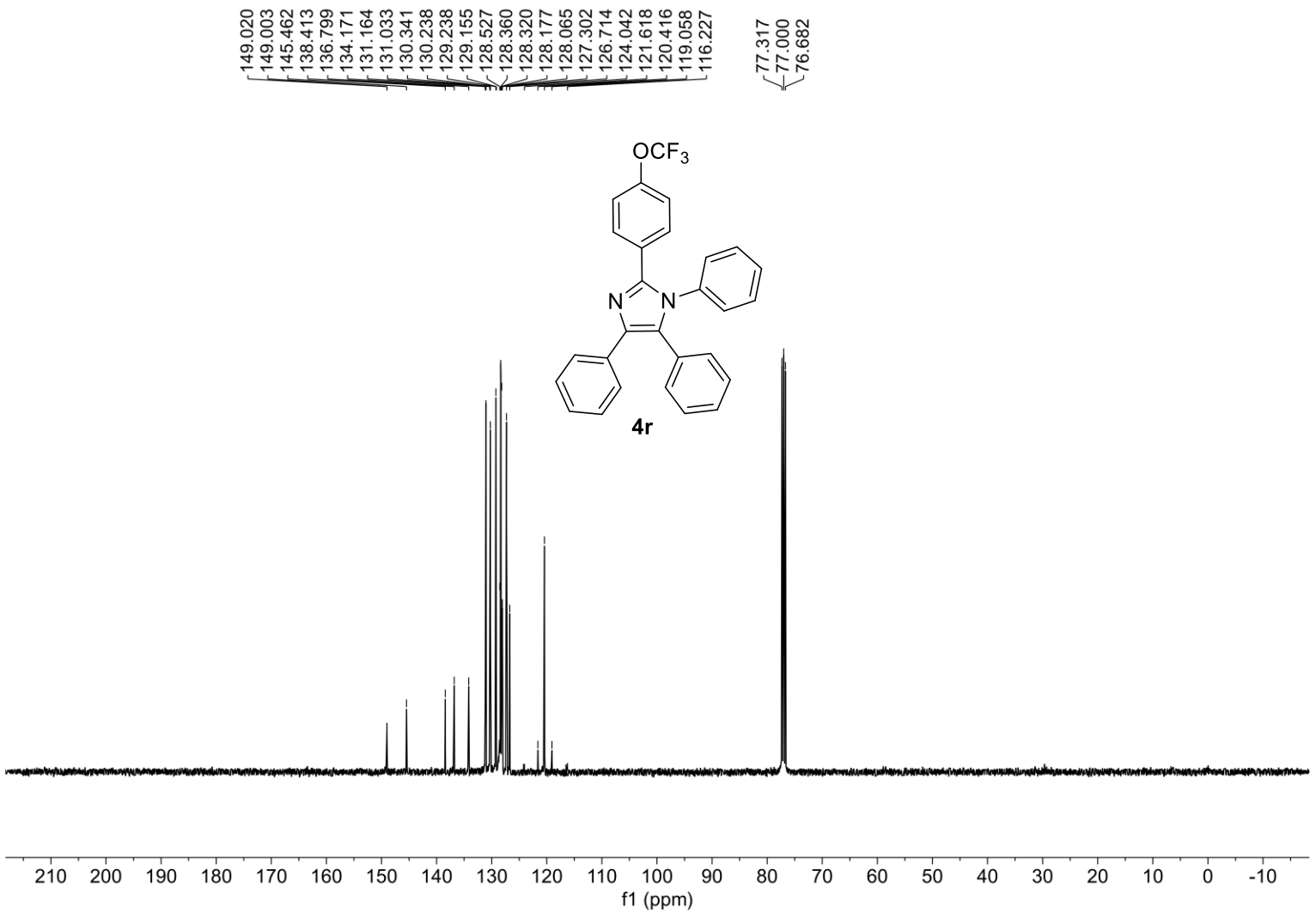
2.01
9.02
2.01
2.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.065
127.302
126.714
124.042
121.618
120.416
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116.227
77.317
77.000
76.682
OCF3
N
N
4r
210
200
190
180
170
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30
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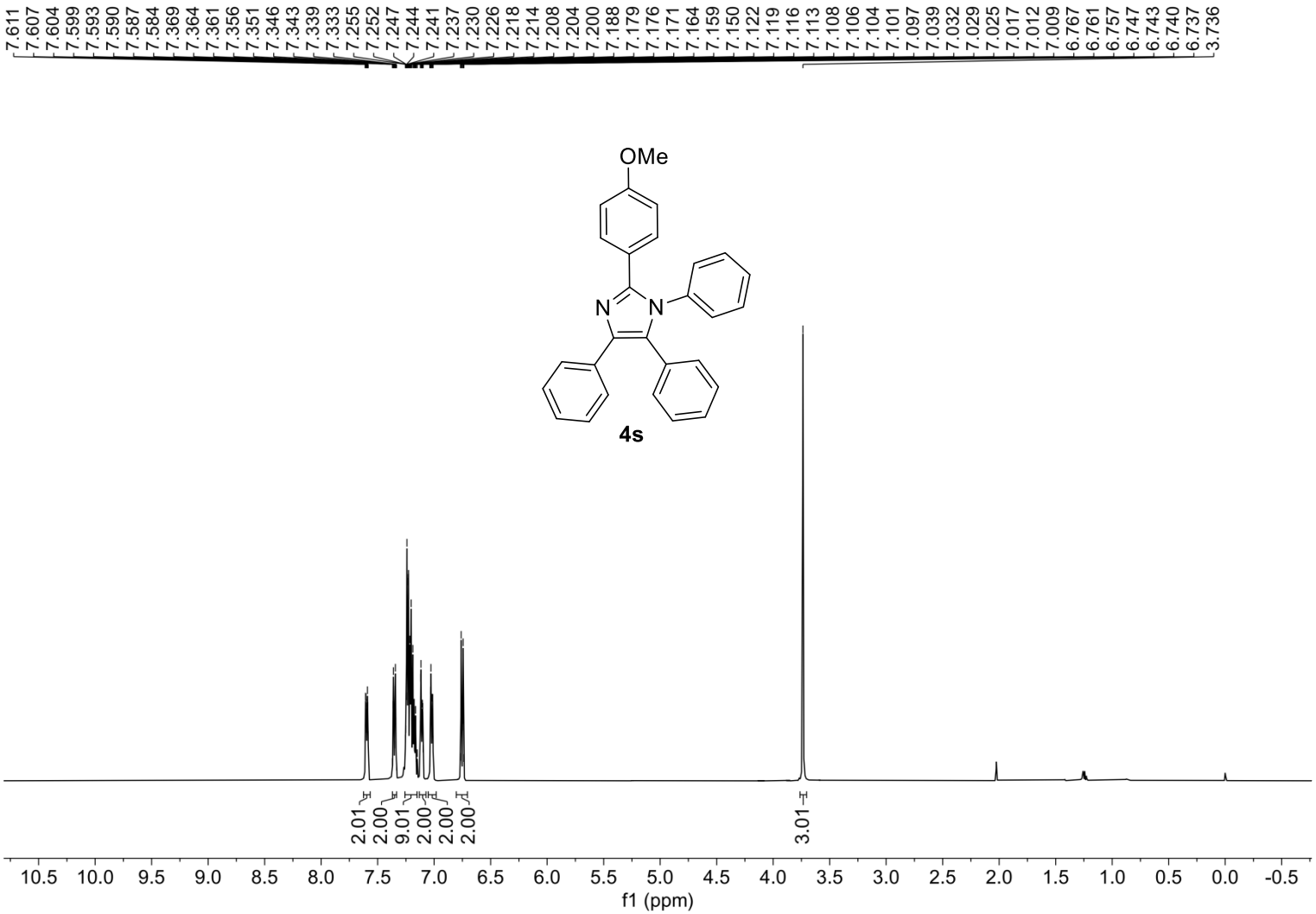
0
-10
f1 (ppm)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7.214
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7.150
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7.113
7.108
7.106
7.104
7.101
7.097
7.039
7.032
7.029
7.025
7.017
7.012
7.009
6.767
6.761
6.757
6.747
6.743
6.740
6.737
3.736
OMe
N
N
4s
2.01
2.00
9.01
2.00
2.00
2.00
3.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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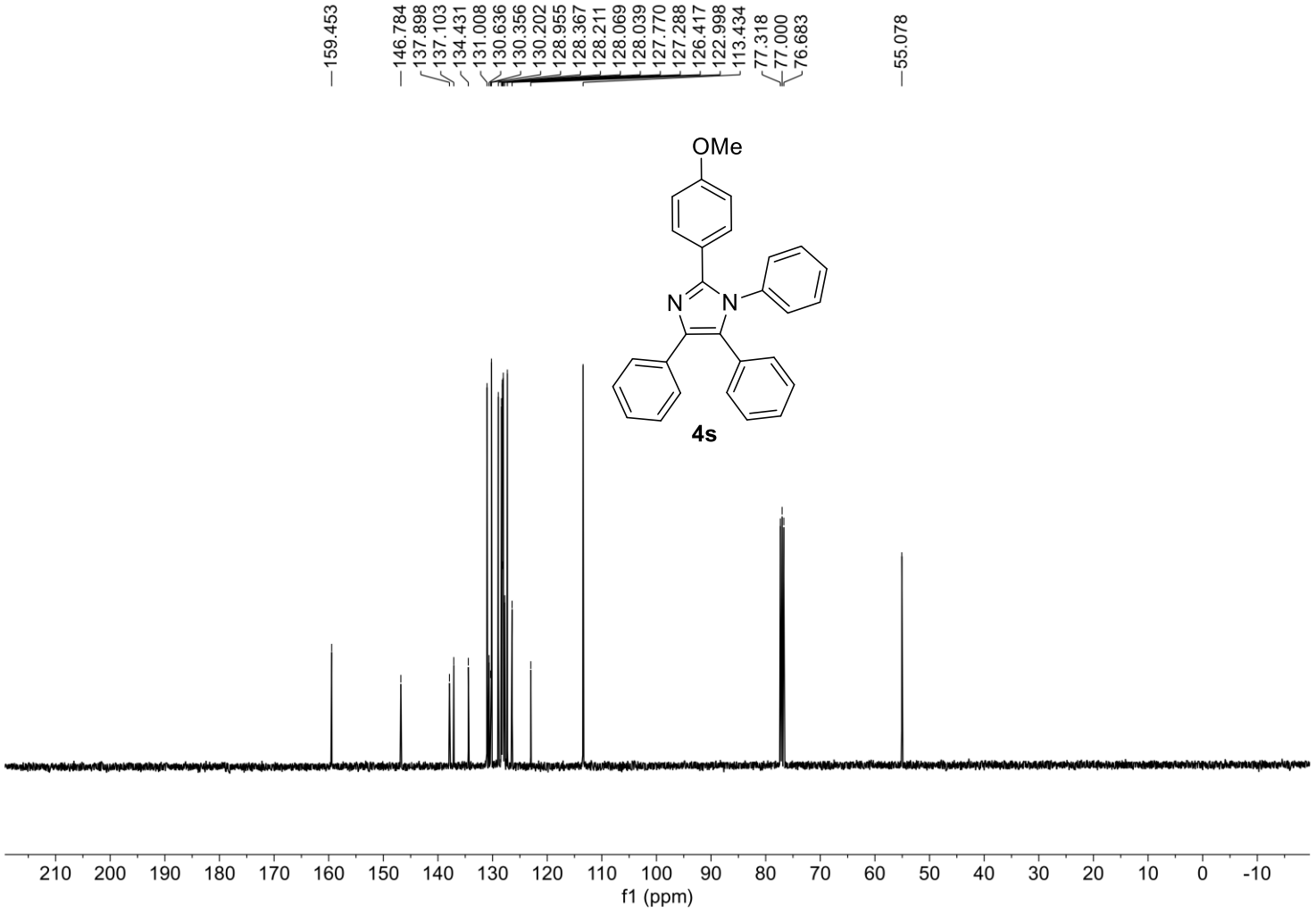
-0.5
f1 (ppm)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130.356
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128.069
128.039
127.770
127.288
126.417
122.998
113.434
77.318
77.000
76.683
55.078
OMe
N
N
4s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.597
7.593
7.575
7.419
7.414
7.405
7.398
7.389
7.384
7.292
7.277
7.271
7.267
7.259
7.250
7.233
7.229
7.214
7.207
7.199
7.190
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7.112
7.107
7.036
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7.018
7.013
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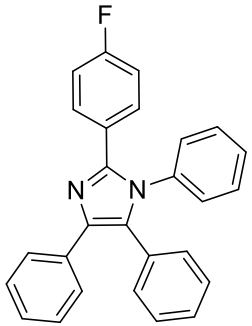
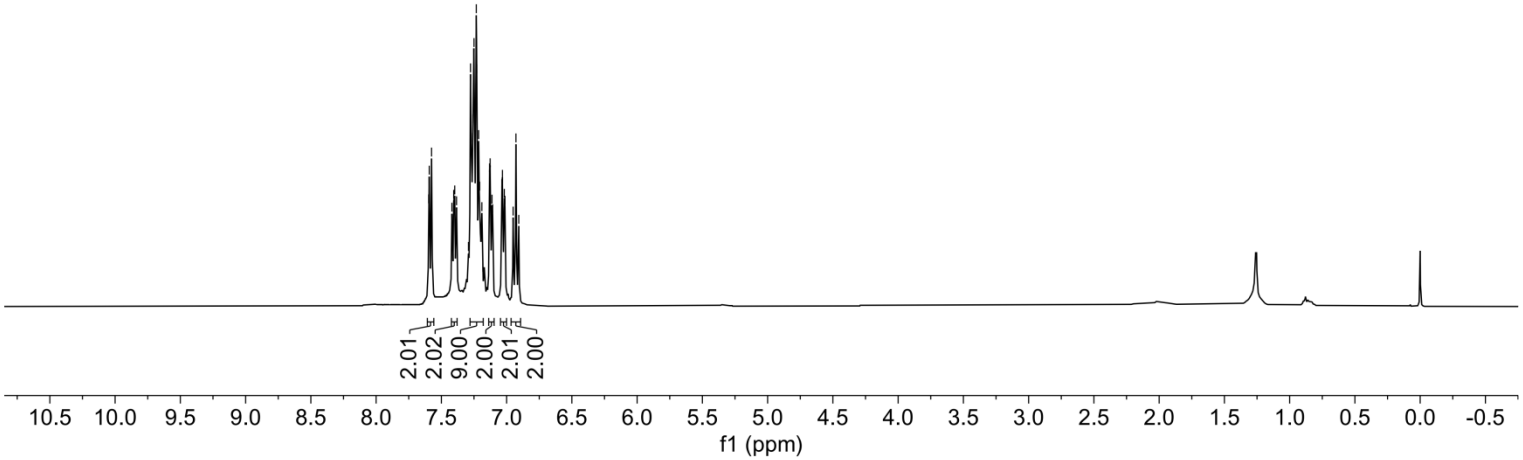
6.929
6.907


F
N
N

4t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2.02
9.00
2.00
2.01
2.00
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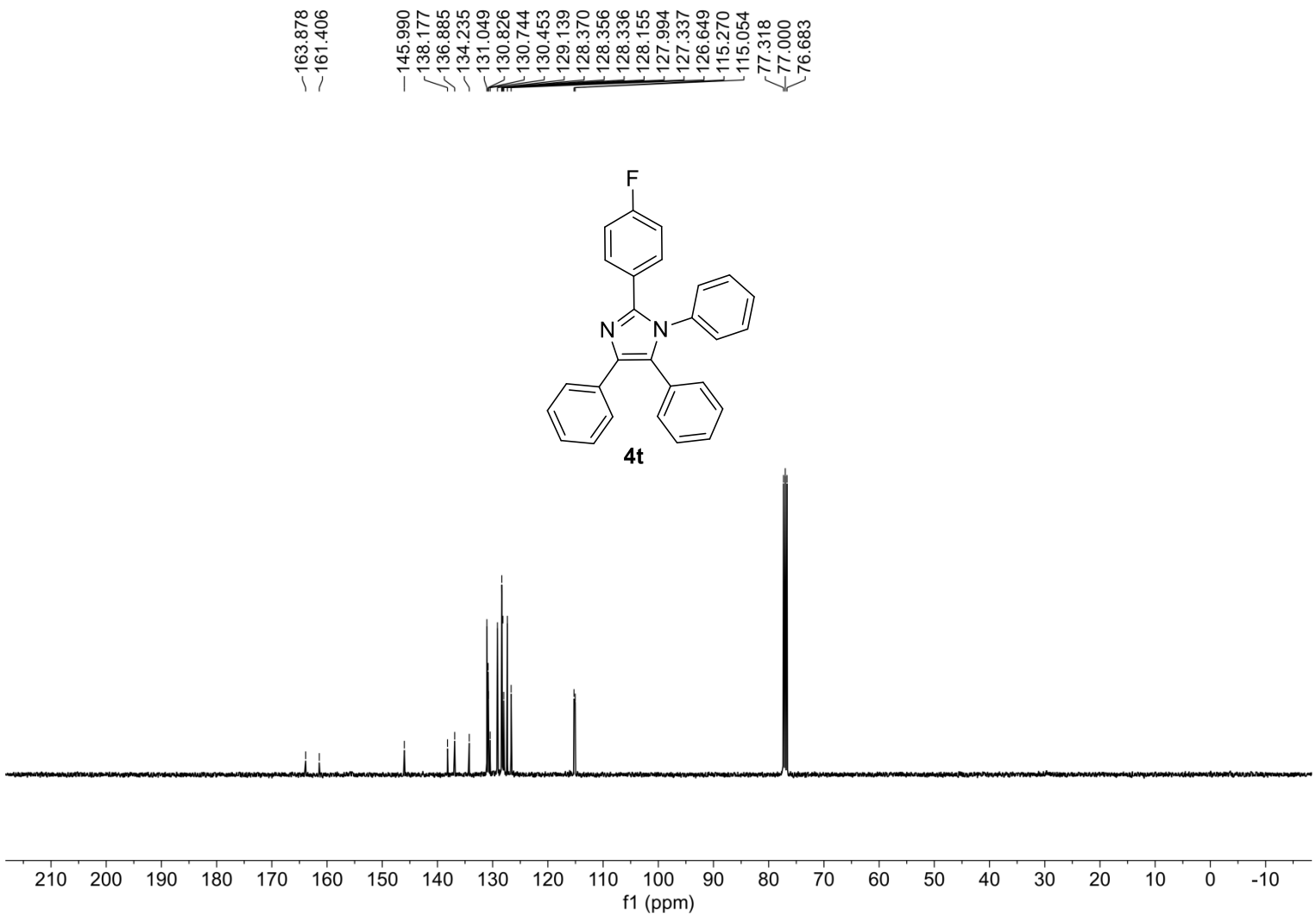
f1 (ppm)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130.826
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130.453
129.139
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128.356
128.336
128.155
127.994
127.337
126.649
115.270
115.054
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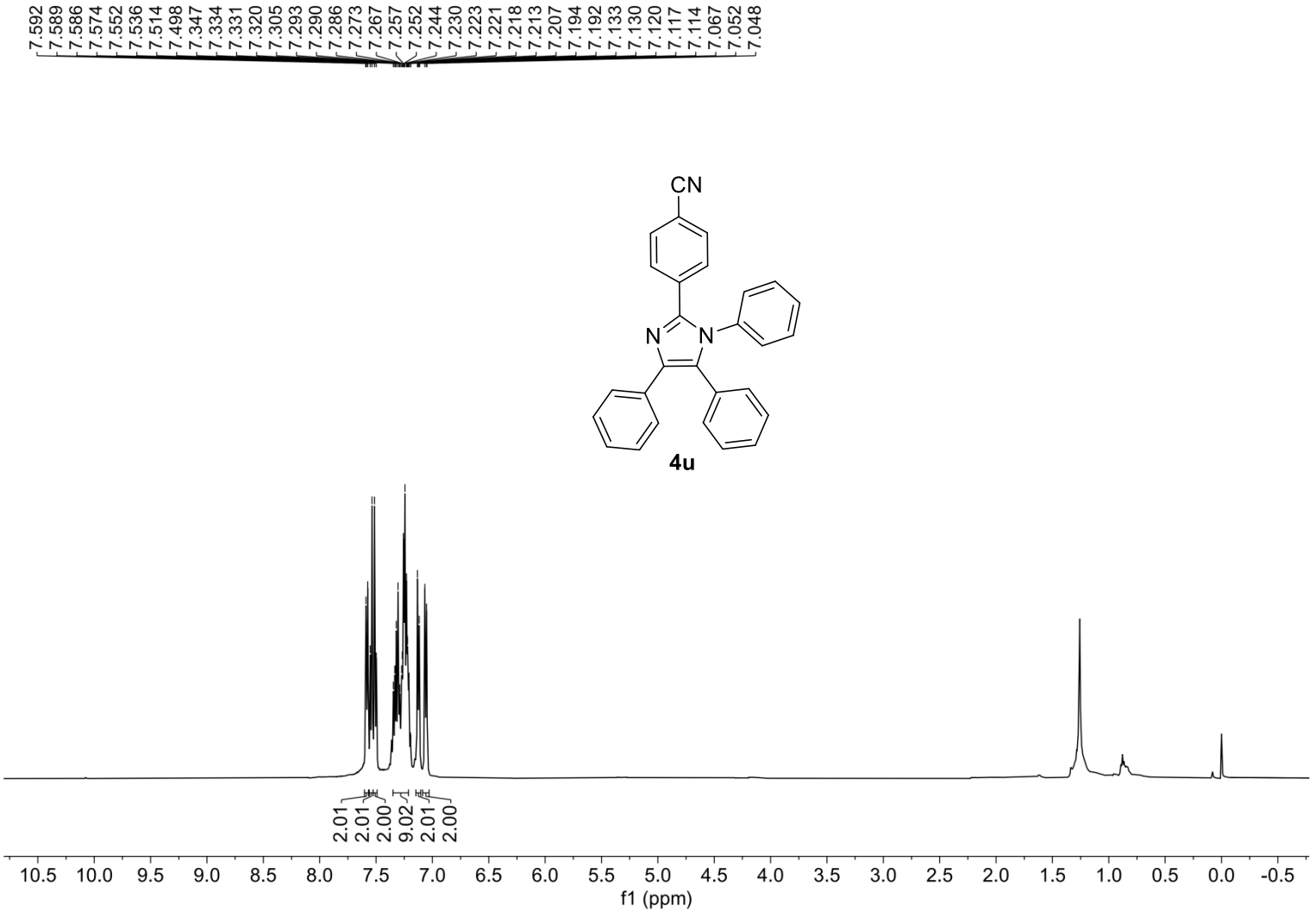
77.000
76.683
F
N
N
4t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.514
7.498
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7.334
7.331
7.320
7.305
7.293
7.290
7.286
7.273
7.267
7.257
7.252
7.244
7.230
7.223
7.221
7.218
7.213
7.207
7.194
7.192
7.133
7.130
7.120
7.117
7.114
7.067
7.052
7.048
CN
N
N
4u
2.01
2.01
2.00
9.02
2.01
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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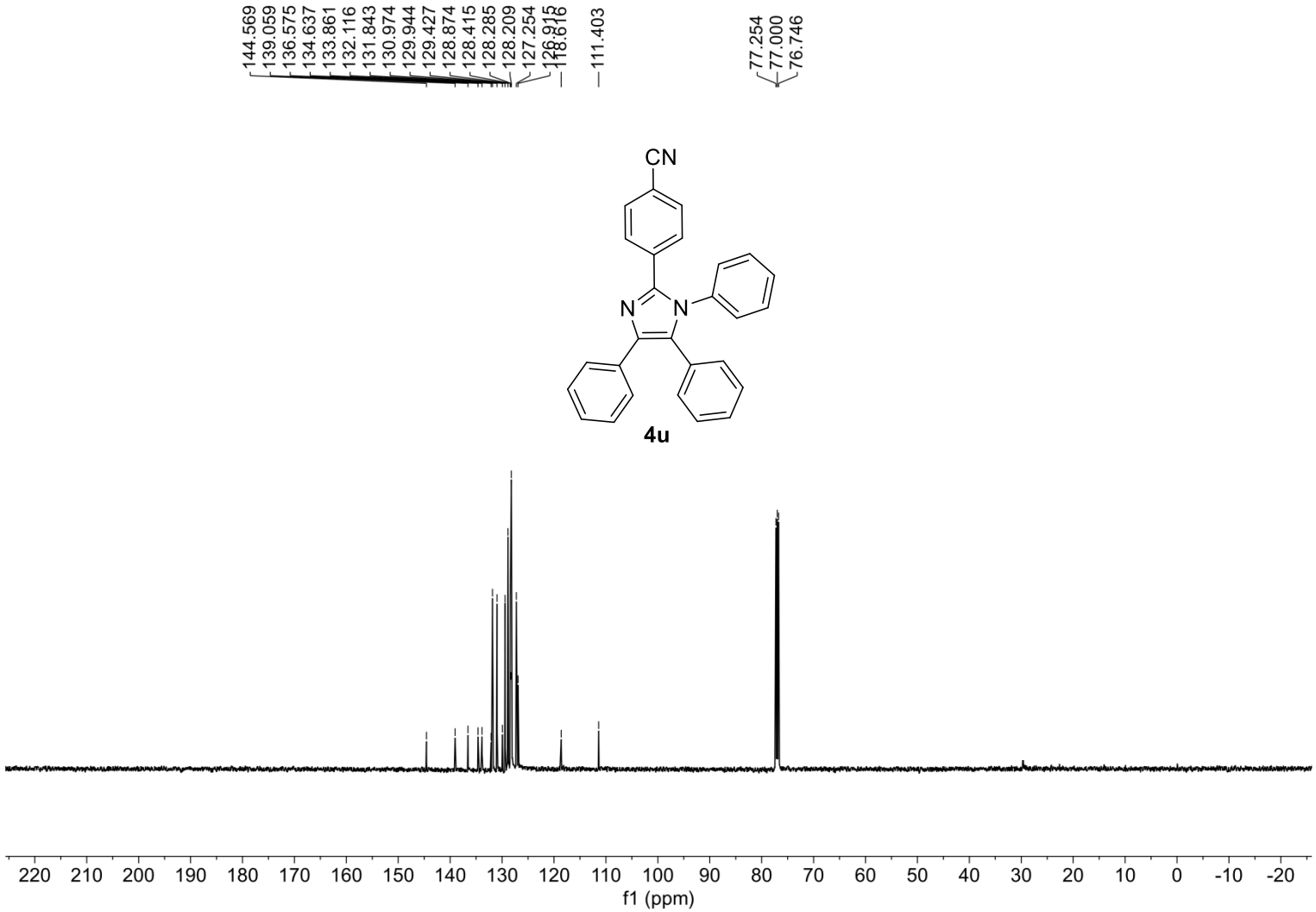
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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130.974
129.944
129.427
128.874
128.415
128.285
128.209
127.254
126.915
118.616
111.403
77.254
77.000
76.746
CN
N
N
4u
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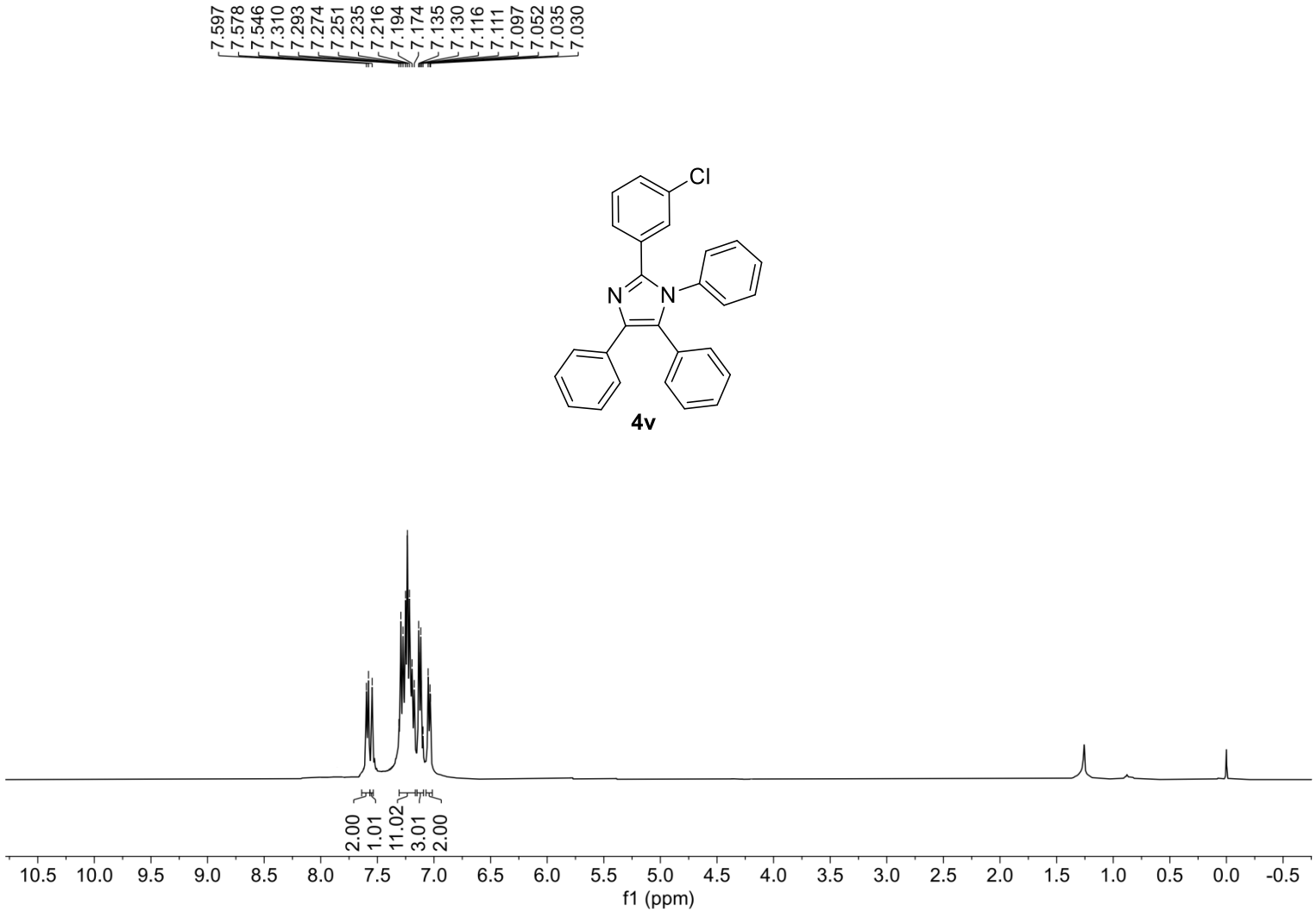
f1 (ppm)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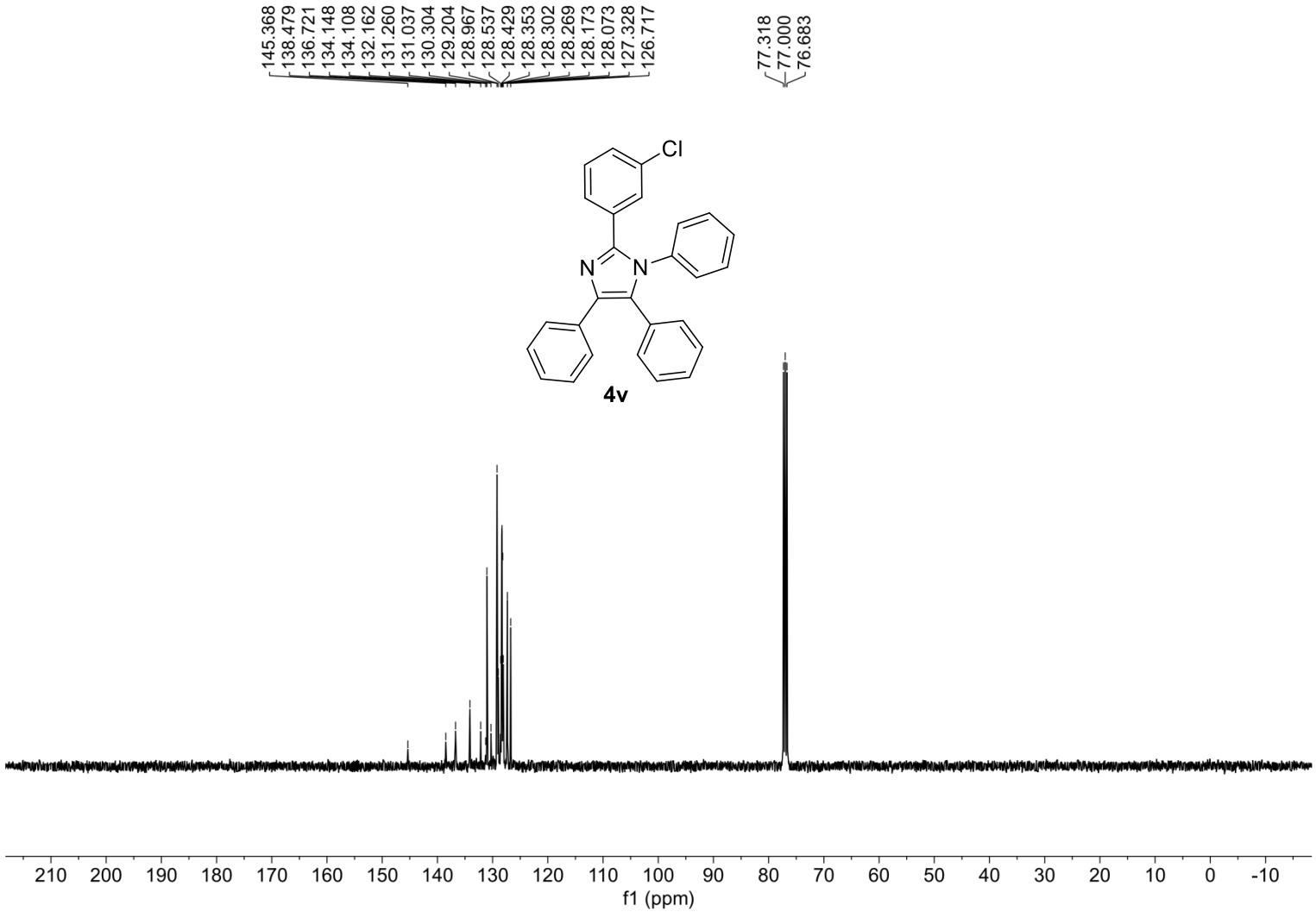
7.274
7.251
7.235
7.216
7.194
7.174
7.135
7.130
7.116
7.111
7.097
7.052
7.035
7.030
Cl
N
N
4v
2.00
1.01
11.02
3.01
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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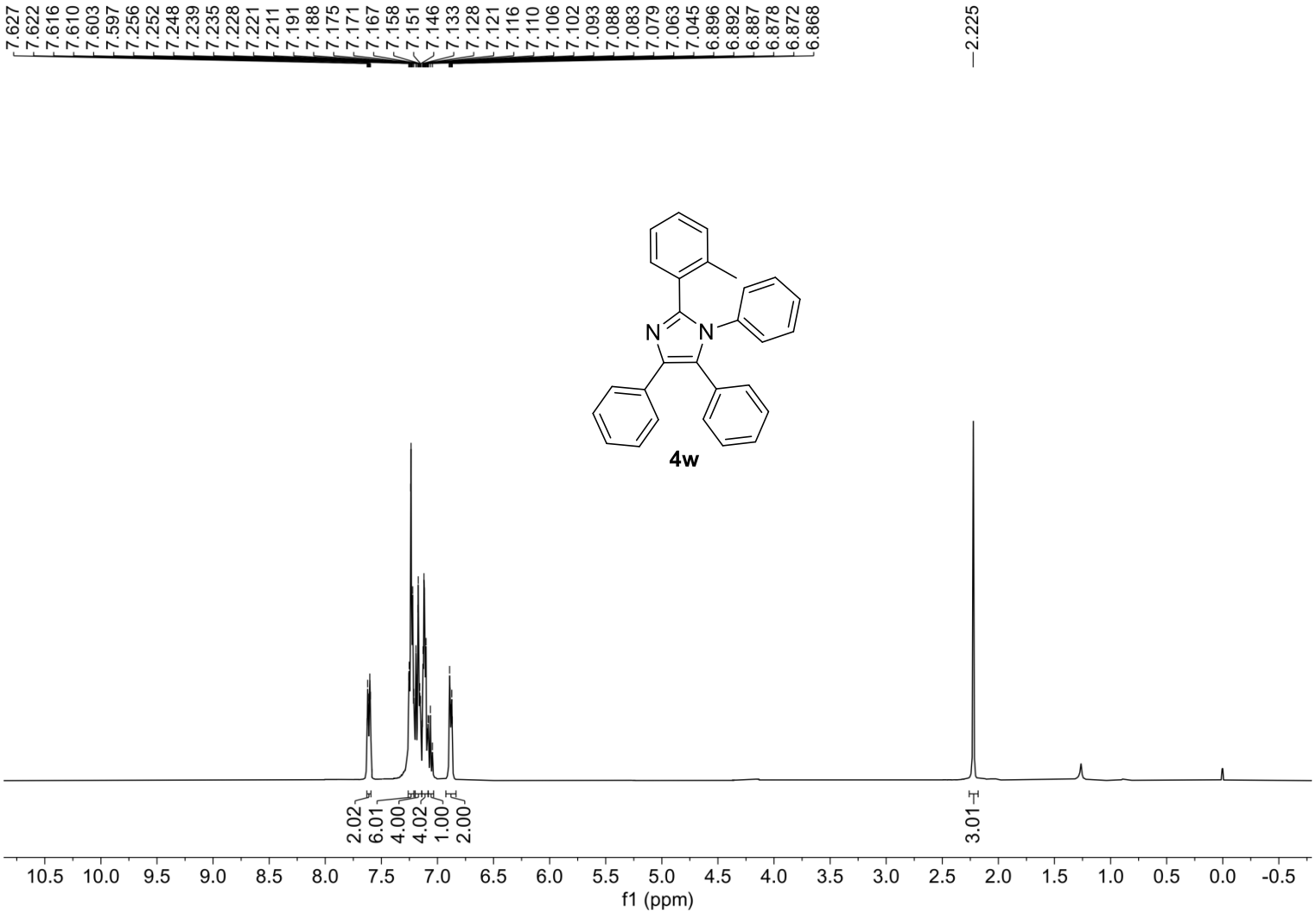
136.721
134.148
134.108
132.162
131.260
131.037
130.304
129.204
128.967
128.537
128.429
128.353
128.302
128.269
128.173
128.073
127.328
126.717
77.318
77.000
76.683
Cl
N
N
4v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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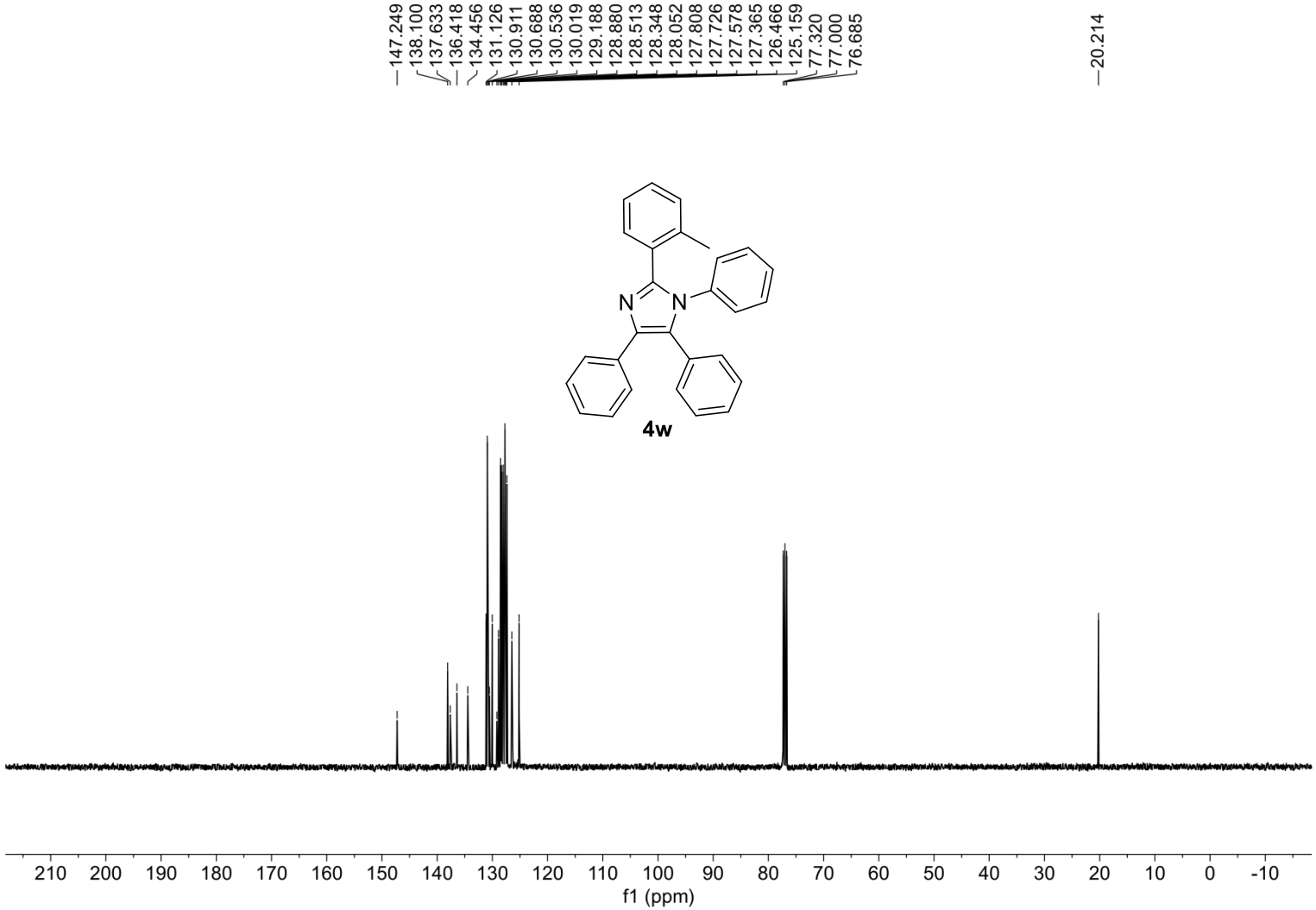
7.616
7.610
7.603
7.597
7.256
7.252
7.248
7.239
7.235
7.228
7.221
7.211
7.191
7.188
7.175
7.171
7.167
7.158
7.151
7.146
7.133
7.128
7.121
7.116
7.110
7.106
7.102
7.093
7.088
7.083
7.079
7.063
7.045
6.896
6.892
6.887
6.878
6.872
6.868
2.225
N
N
4w
2.02
6.01
4.00
4.02
1.00
2.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.348
128.052
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127.726
127.578
127.365
126.466
125.159
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77.000
76.685
20.214
N
N
4w
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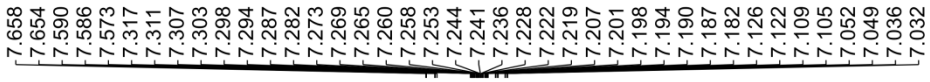
f1 (ppm)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7.303
7.298
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7.282
7.273
7.269
7.265
7.260
7.258
7.253
7.244
7.241
7.236
7.228
7.222
7.219
7.207
7.201
7.198
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7.122
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7.105
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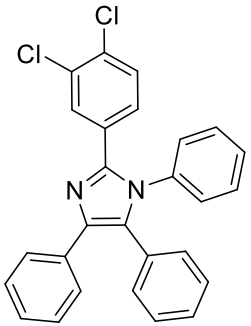
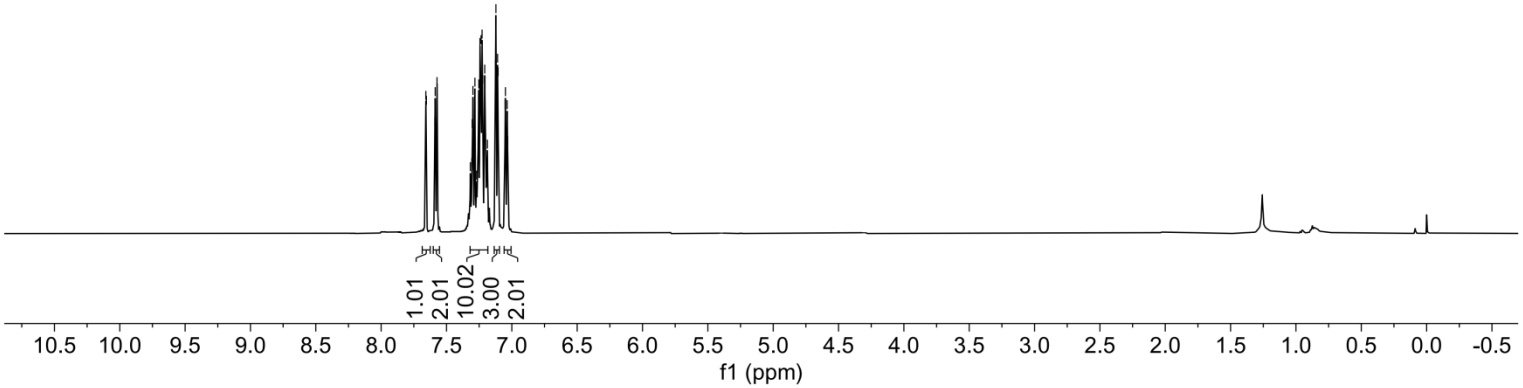
7.032


Cl
Cl
N
N

4x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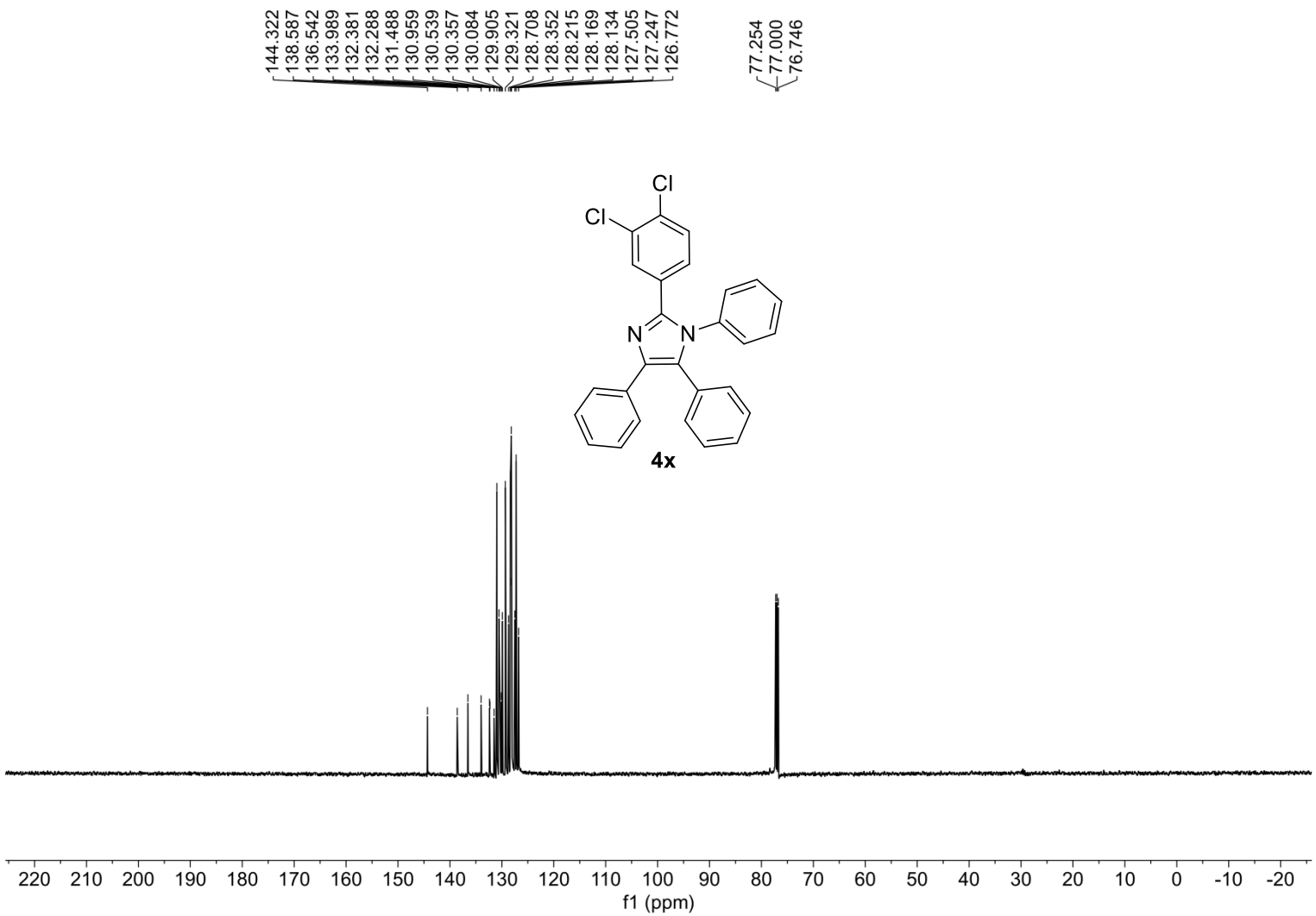
2.01
10.02
3.00
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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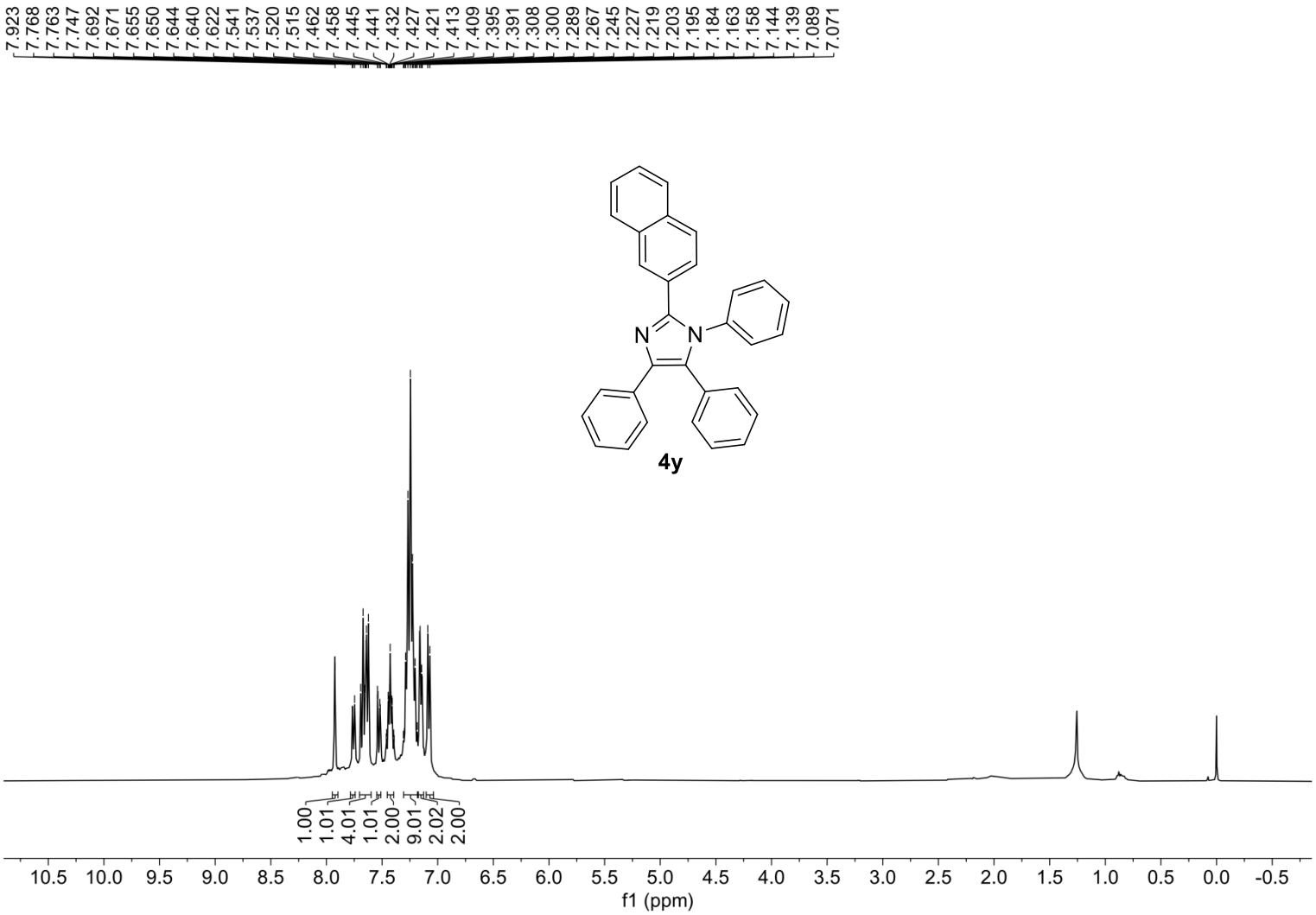
130.357
130.084
129.905
129.321
128.708
128.352
128.215
128.169
128.134
127.505
127.247
126.772
77.254
77.000
76.746
Cl
Cl
N
N
4x
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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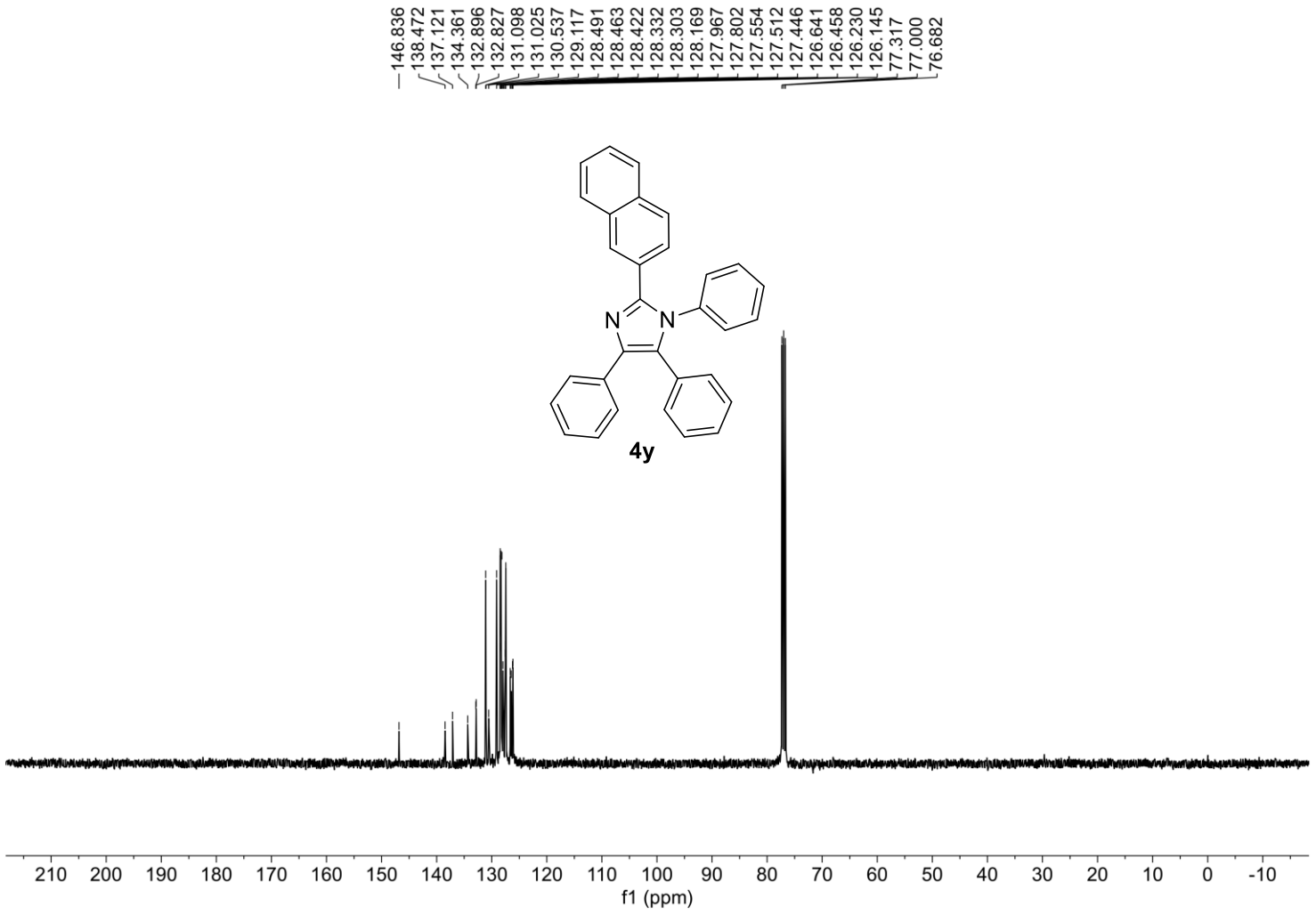
7.537
7.520
7.515
7.462
7.458
7.445
7.441
7.432
7.427
7.421
7.413
7.409
7.395
7.391
7.308
7.300
7.289
7.267
7.245
7.227
7.219
7.203
7.195
7.184
7.163
7.158
7.144
7.139
7.089
7.071
N
N
4y
1.00
1.01
4.01
1.01
2.00
9.01
2.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.169
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127.802
127.554
127.512
127.446
126.641
126.458
126.230
126.145
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77.000
76.682
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N
4y
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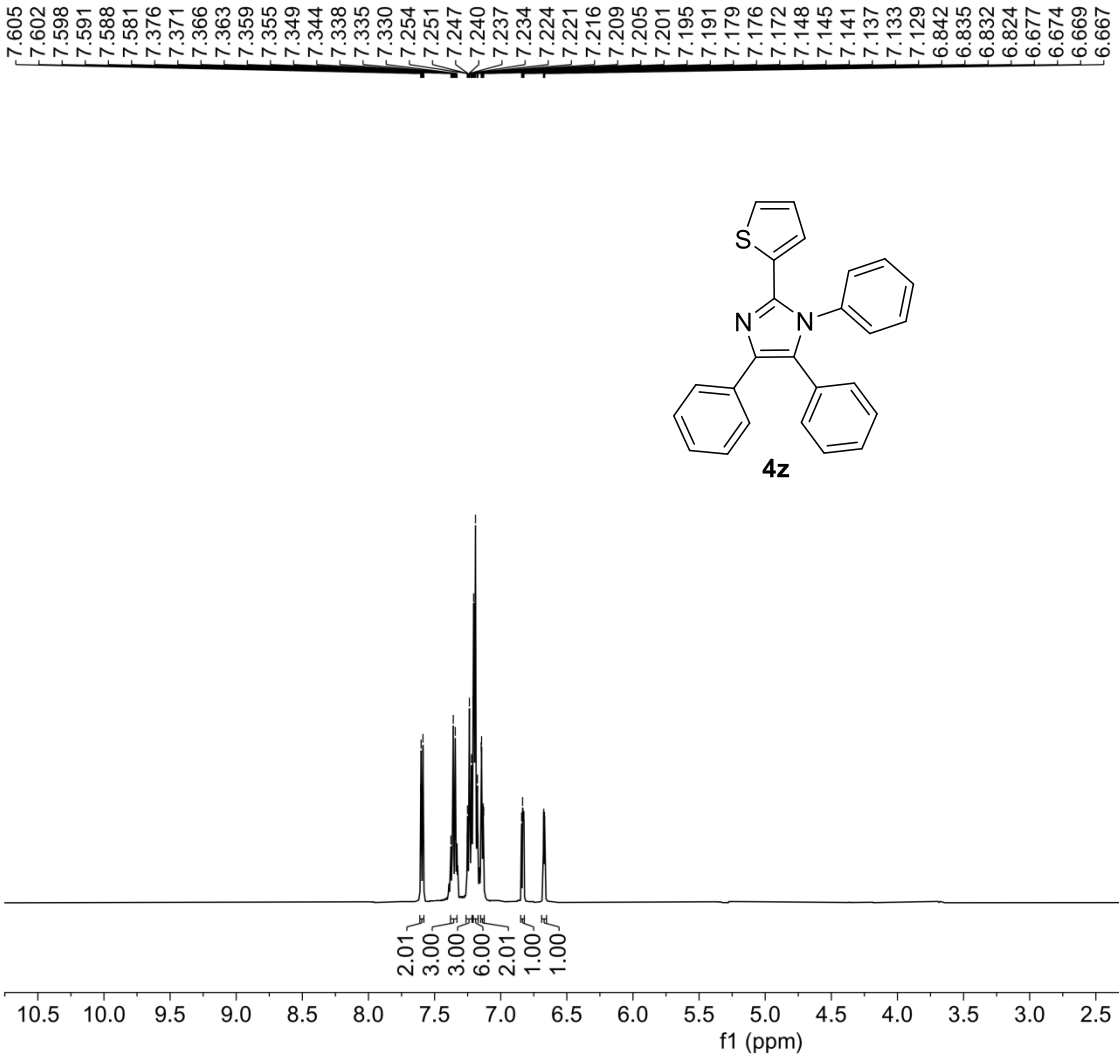
f1 (ppm)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7.344
7.338
7.335
7.330
7.254
7.251
7.247
7.240
7.237
7.234
7.224
7.221
7.216
7.209
7.205
7.201
7.195
7.191
7.179
7.176
7.172
7.148
7.145
7.141
7.137
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6.669
6.667
S
N
N
4z
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3.00
3.00
6.00
2.01
1.00
1.00
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5.0
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2.5
2.0
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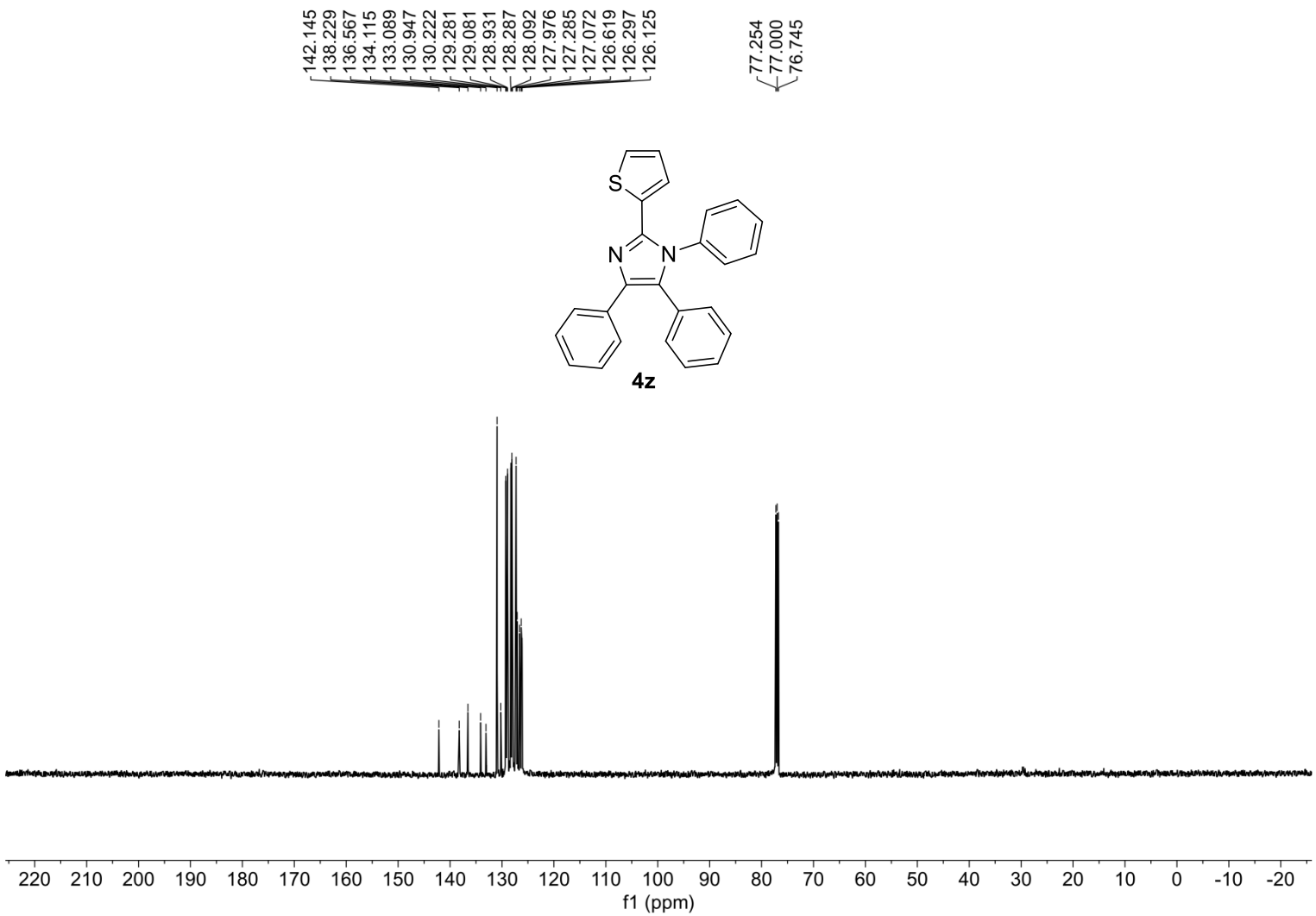
0.5
0.0
-0.5
f1 (ppm)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128.287
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127.285
127.072
126.619
126.297
126.125
77.254
77.000
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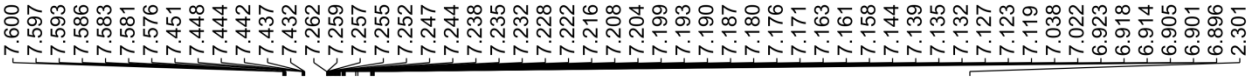
S
N
N
4z
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.444
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7.437
7.432
7.262
7.259
7.257
7.255
7.252
7.247
7.244
7.238
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7.232
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7.222
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7.208
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7.199
7.193
7.190
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7.176
7.171
7.163
7.161
7.158
7.144
7.139
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7.132
7.127
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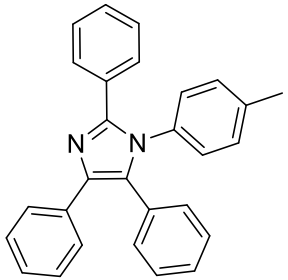
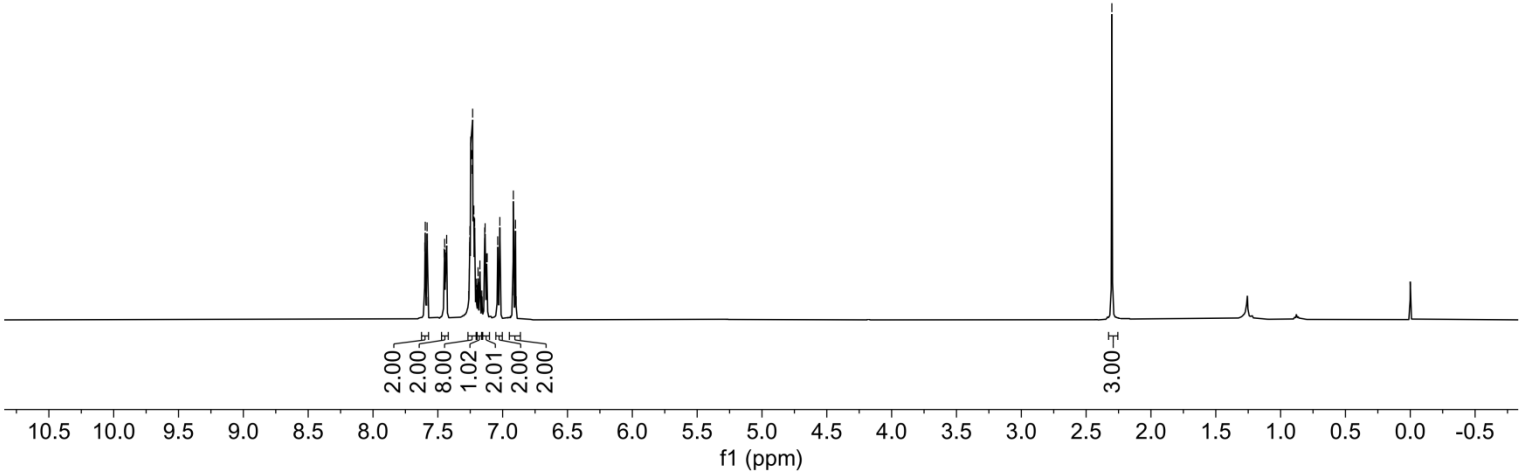

N
N

4aa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2.00
2.00
3.00
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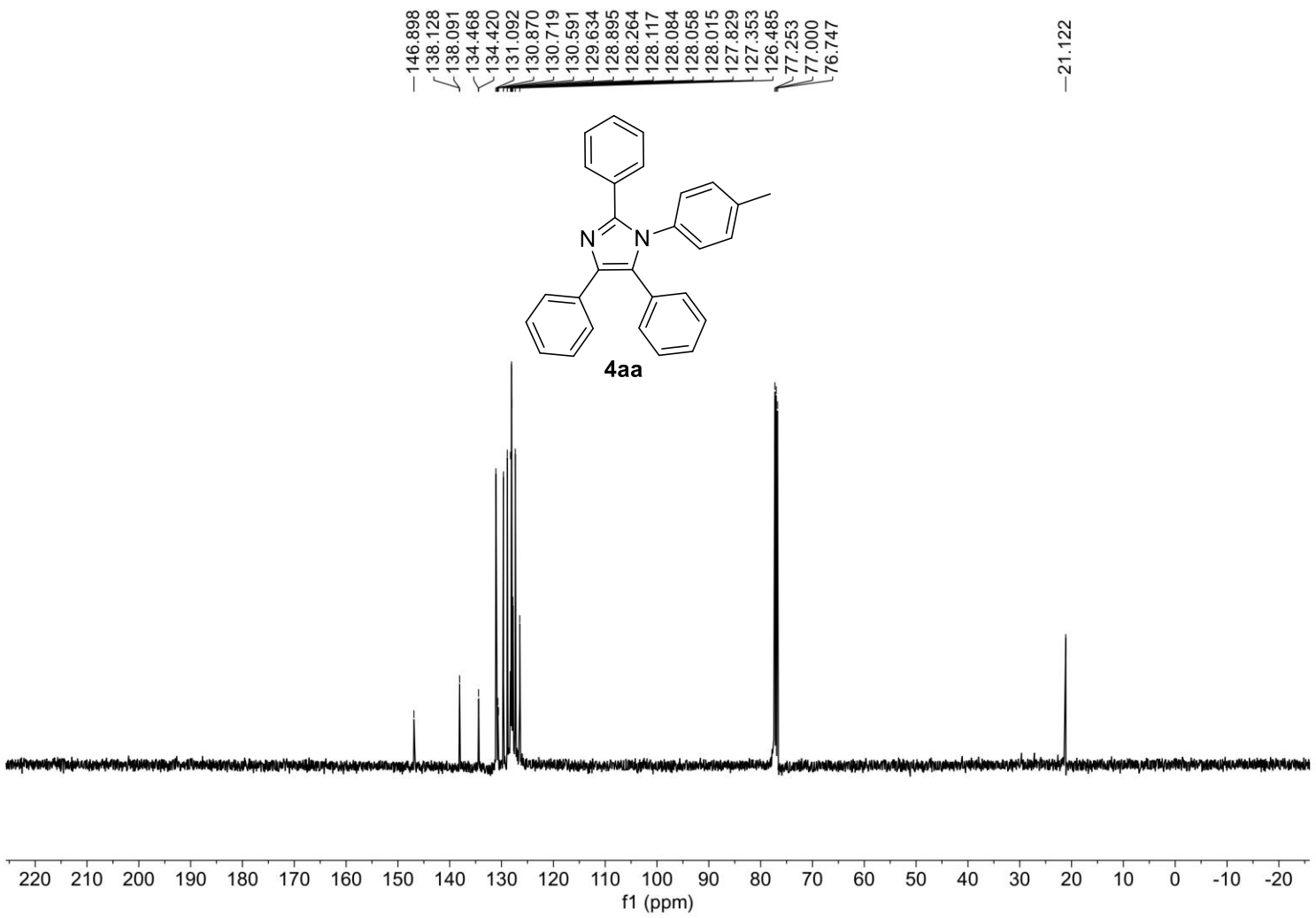
f1 (ppm)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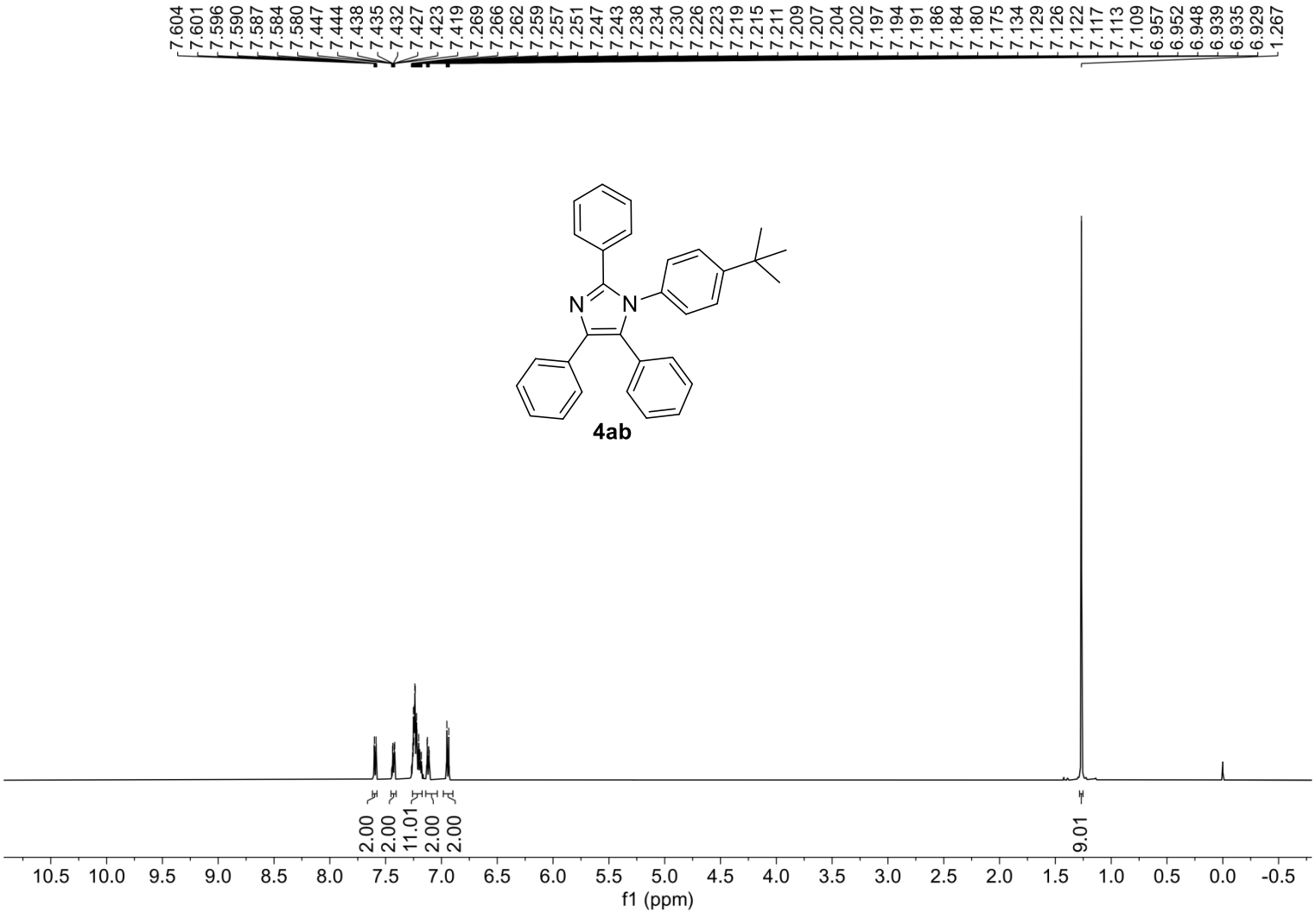
128.117
128.084
128.058
128.015
127.829
127.353
126.485
77.253
77.000
76.747
21.122
N
N
4aa
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.427
7.423
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7.266
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7.251
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7.243
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6.935
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2.00
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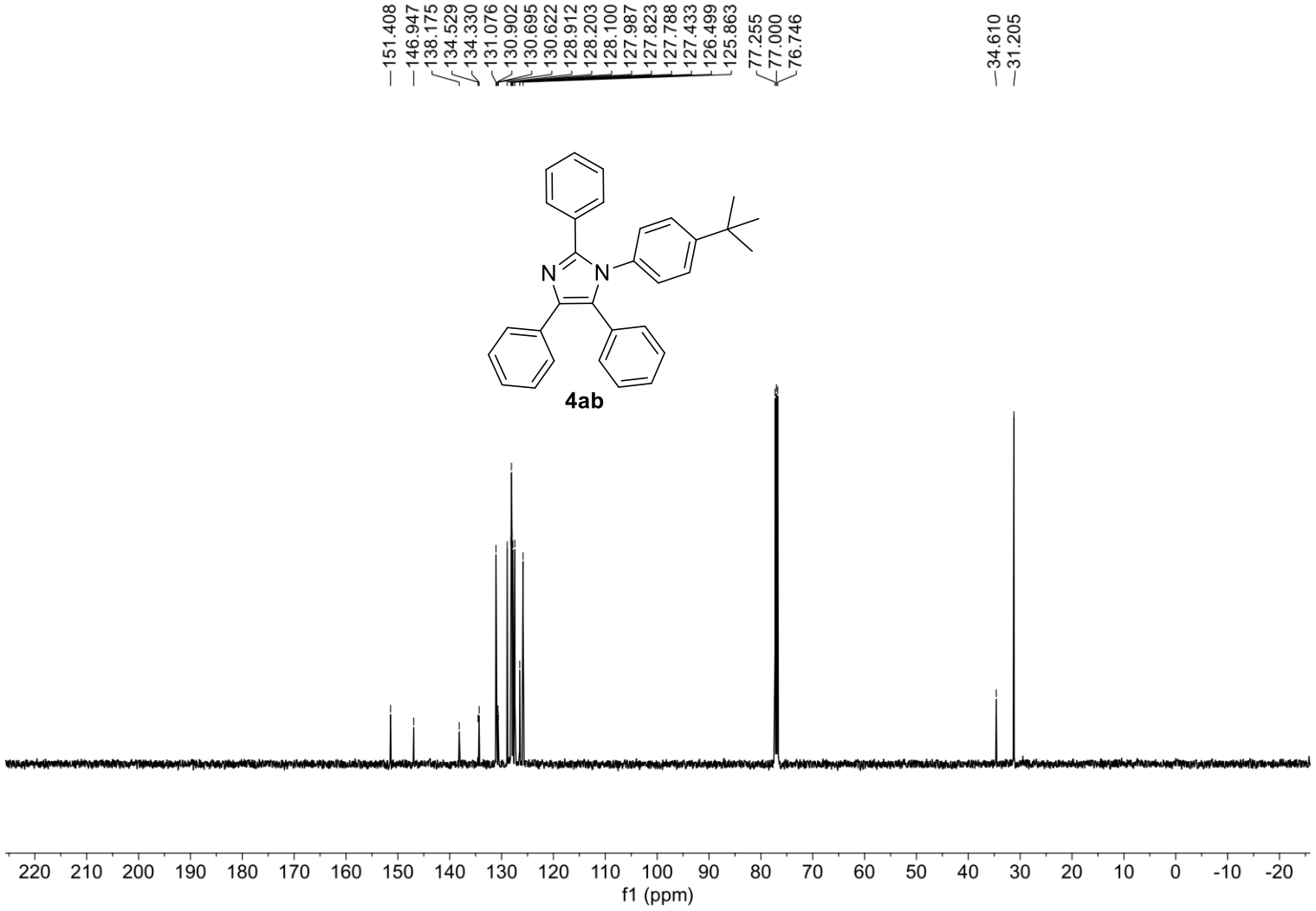
f1 (ppm)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127.433
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77.000
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N
N
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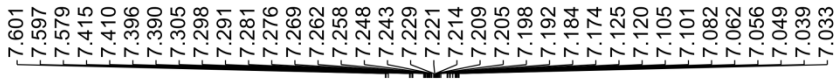
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7.269
7.262
7.258
7.248
7.243
7.229
7.221
7.214
7.209
7.205
7.198
7.192
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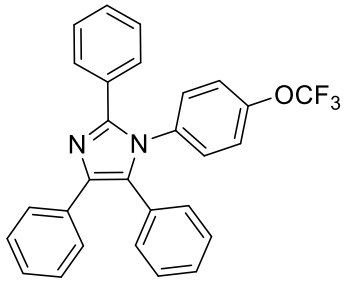
7.120
7.105
7.101
7.082
7.062
7.056
7.049
7.039
7.033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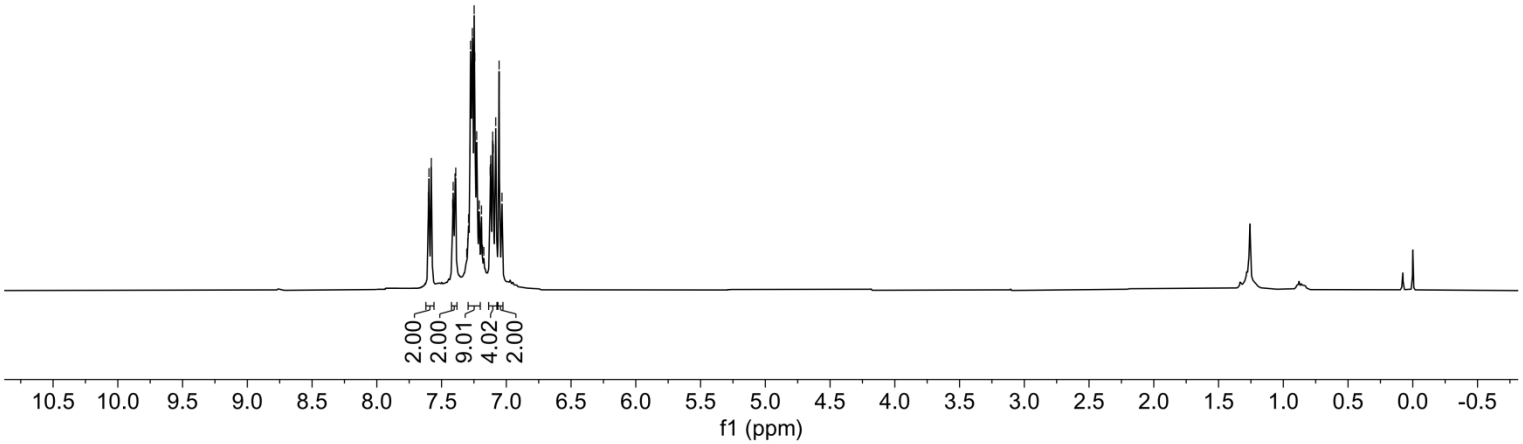
4ac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4.02
2.00
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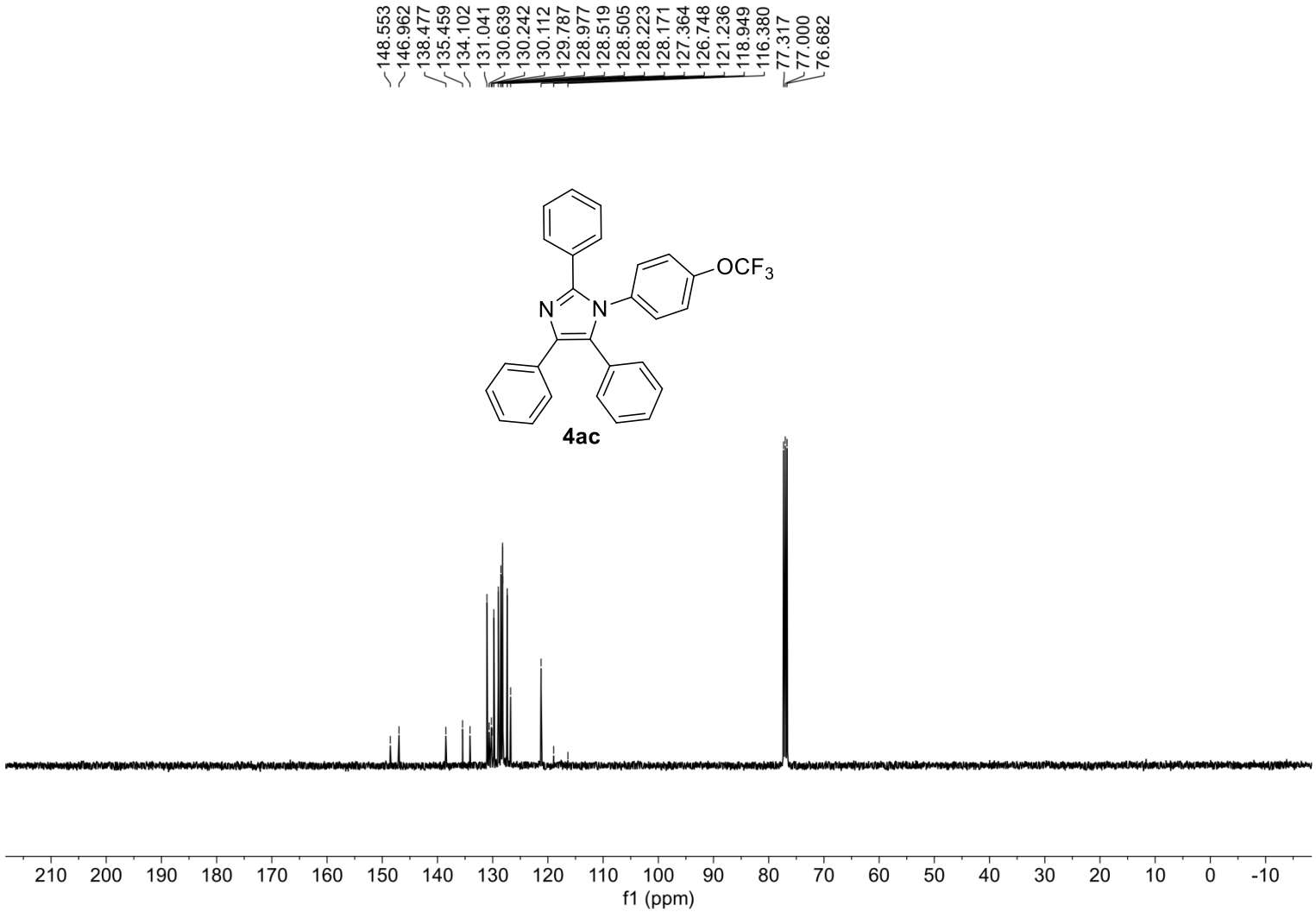
f1 (ppm)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128.505
128.223
128.171
127.364
126.748
121.236
118.949
116.380
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OCF3
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N
4ac
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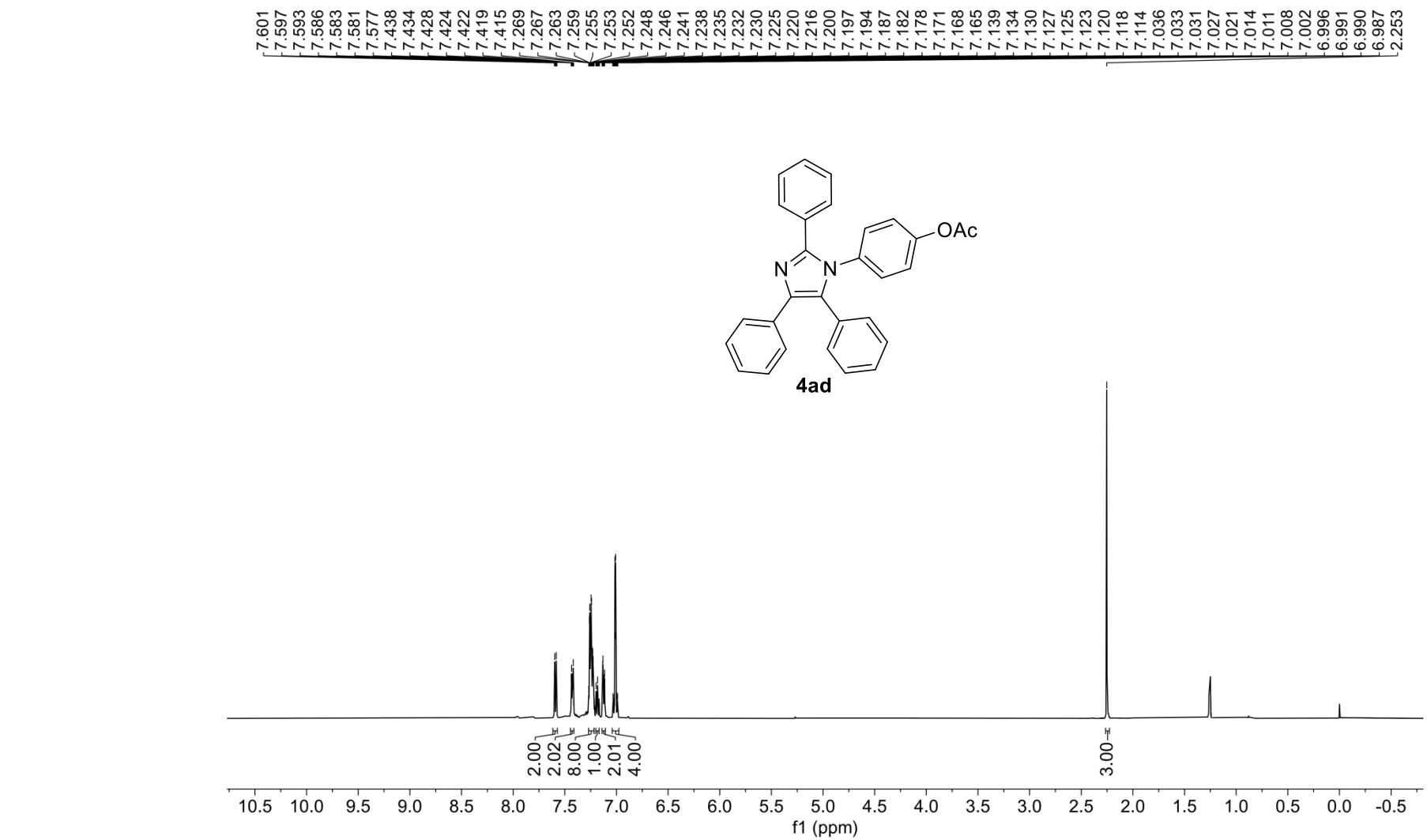
f1 (ppm)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7.438
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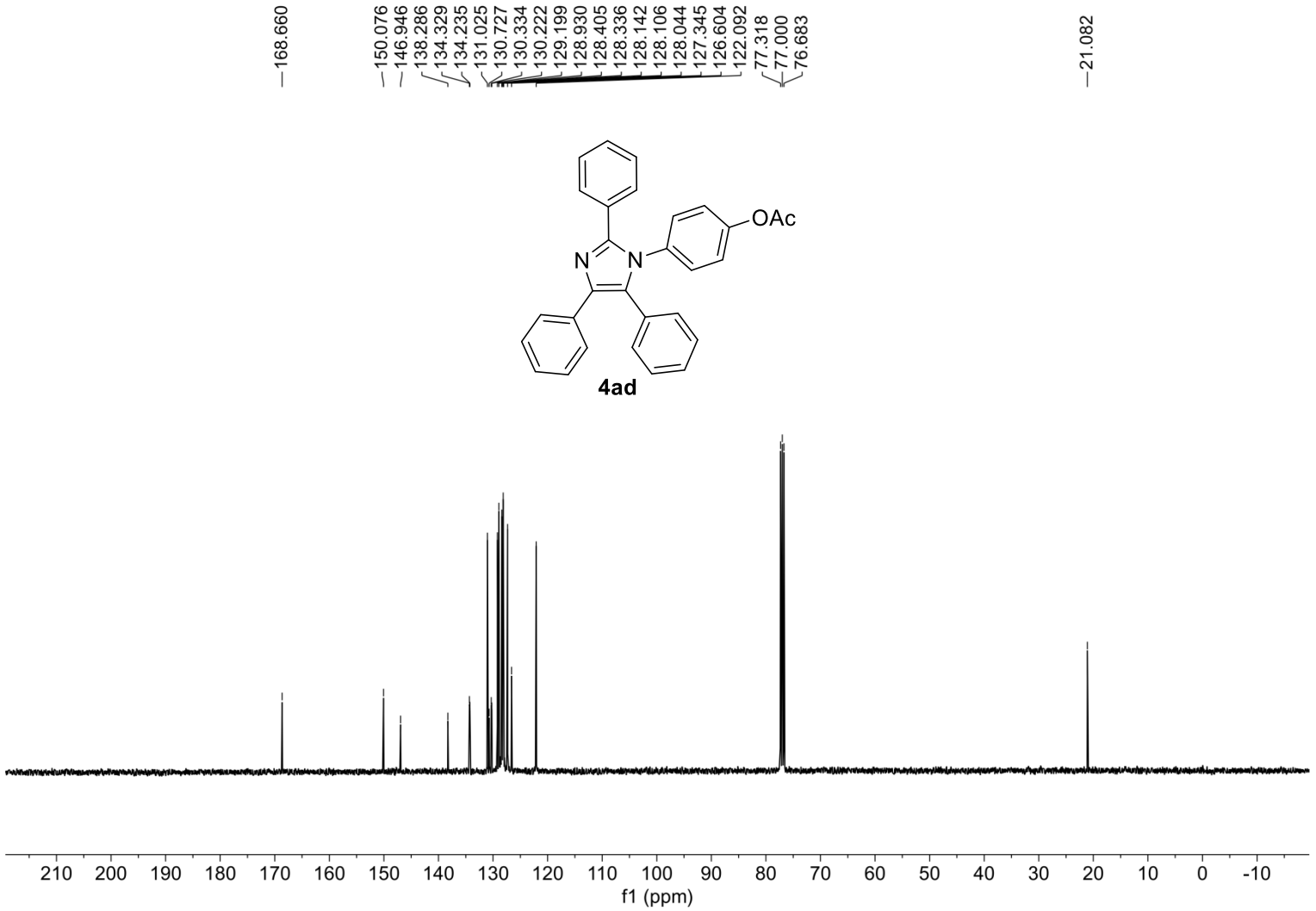
7.428
7.424
7.422
7.419
7.415
7.269
7.267
7.263
7.259
7.255
7.253
7.252
7.248
7.246
7.241
7.238
7.235
7.232
7.230
7.225
7.220
7.216
7.200
7.197
7.194
7.187
7.182
7.178
7.171
7.168
7.165
7.139
7.134
7.130
7.127
7.125
7.123
7.120
7.118
7.114
7.036
7.033
7.031
7.027
7.021
7.014
7.011
7.008
7.002
6.996
6.991
6.990
6.987
2.253
OAc
N
N
4ad
2.00
2.02
8.00
1.00
2.01
4.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.336
128.142
128.106
128.044
127.345
126.604
122.092
77.318
77.000
76.683
21.082
OAc
N
N
4ad
210
200
190
180
170
160
150
140
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120
110
100
90
80
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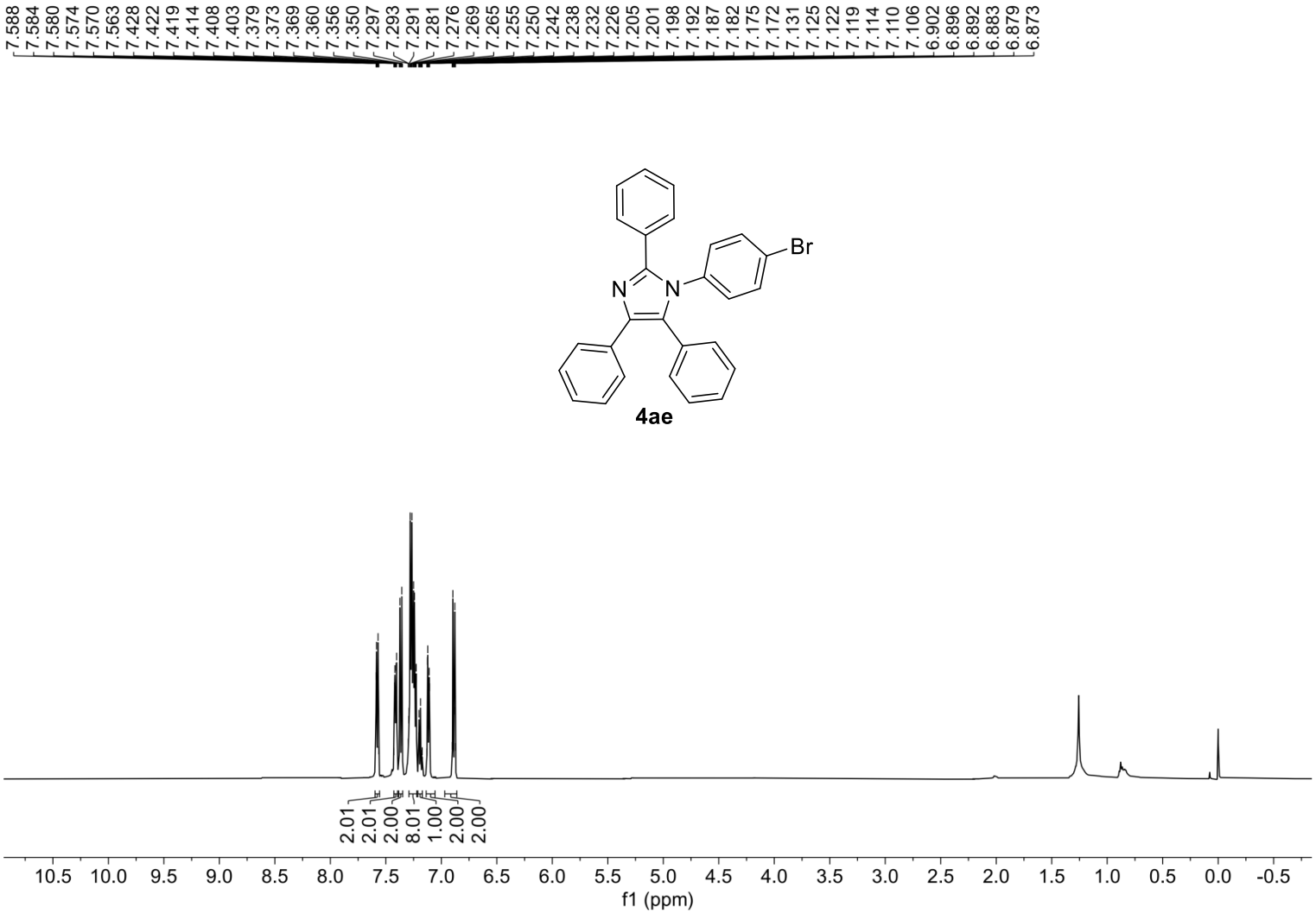
60
50
40
30
20
10
0
-10
f1 (ppm)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7.422
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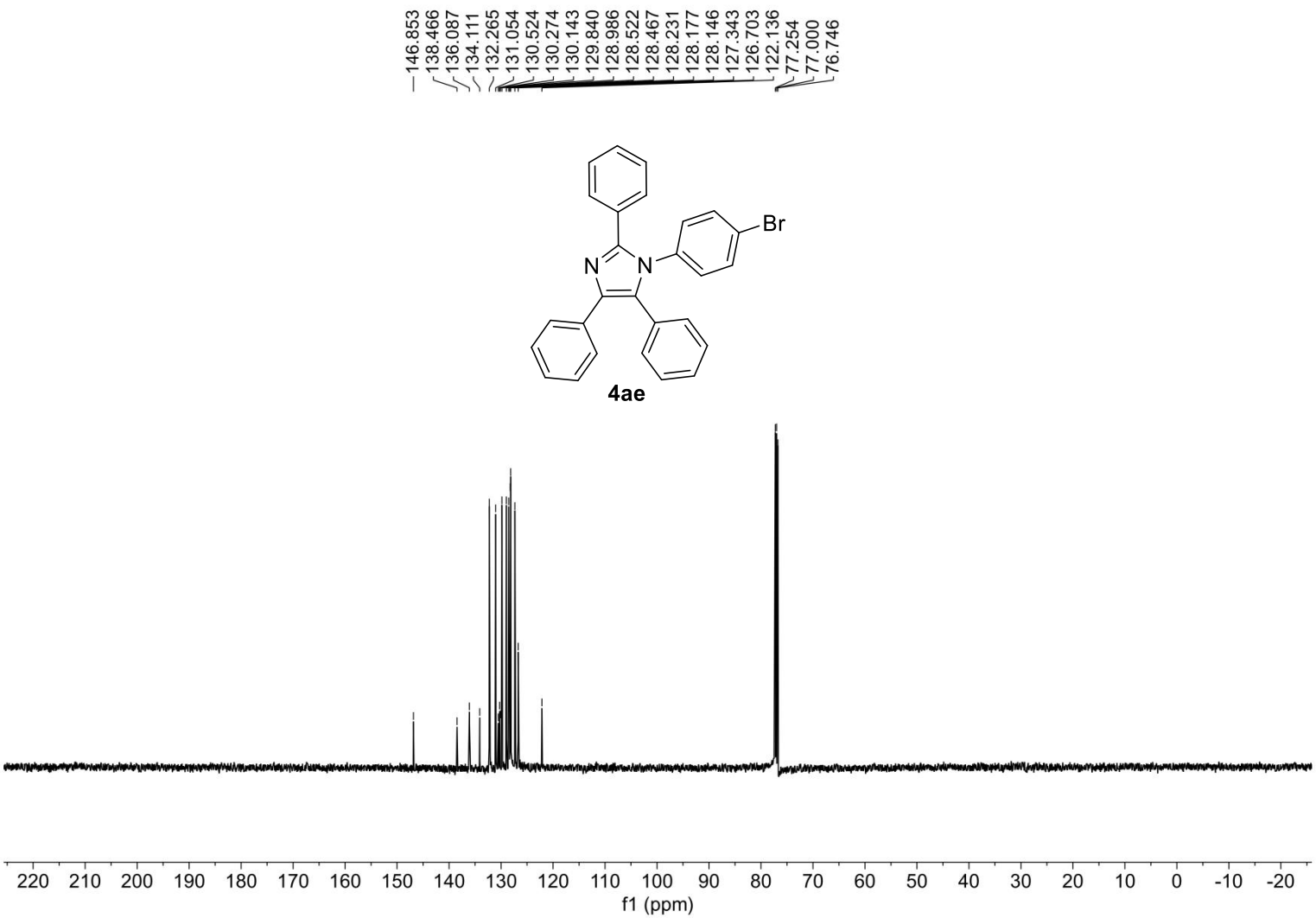
7.408
7.403
7.379
7.373
7.369
7.360
7.356
7.350
7.297
7.293
7.291
7.281
7.276
7.269
7.265
7.255
7.250
7.242
7.238
7.232
7.226
7.205
7.201
7.198
7.192
7.187
7.182
7.175
7.172
7.131
7.125
7.122
7.119
7.114
7.110
7.106
6.902
6.896
6.892
6.883
6.879
6.873
Br
N
N
4ae
2.01
2.01
2.00
8.01
1.00
2.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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132.265
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130.274
130.143
129.840
128.986
128.522
128.467
128.231
128.177
128.146
127.343
126.703
122.136
77.254
77.000
76.746
Br
N
N
4ae
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.595
7.581
7.494
7.477
7.386
7.383
7.371
7.367
7.279
7.269
7.262
7.248
7.236
7.233
7.221
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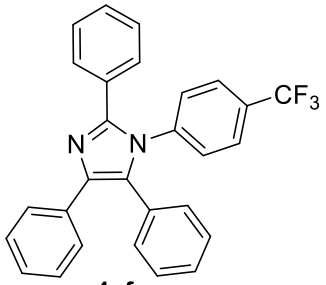
7.197
7.187
7.182
7.176
7.168
7.119
7.111
7.102
7.097
7.094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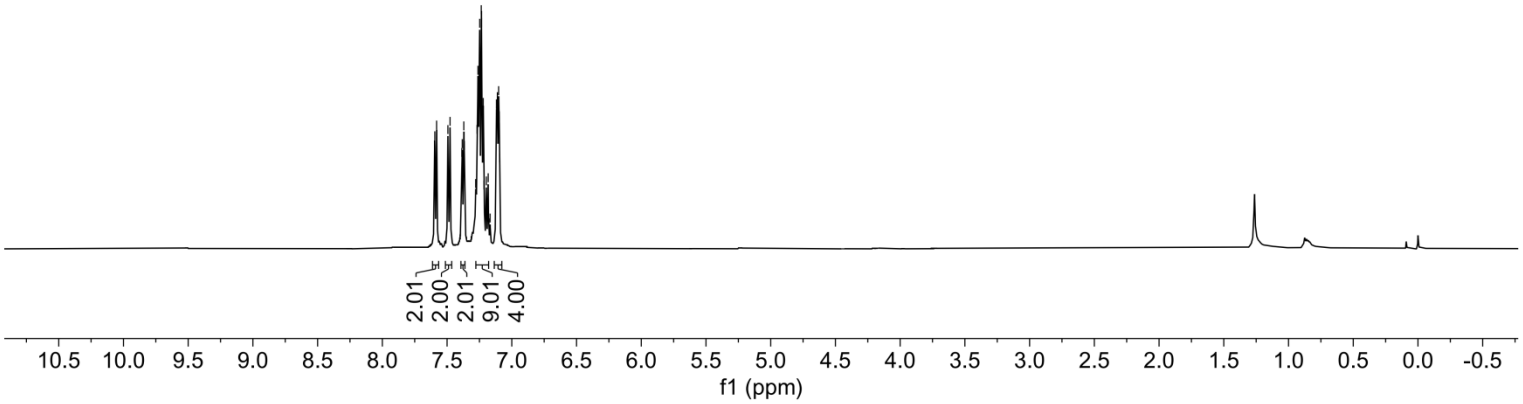
N

4af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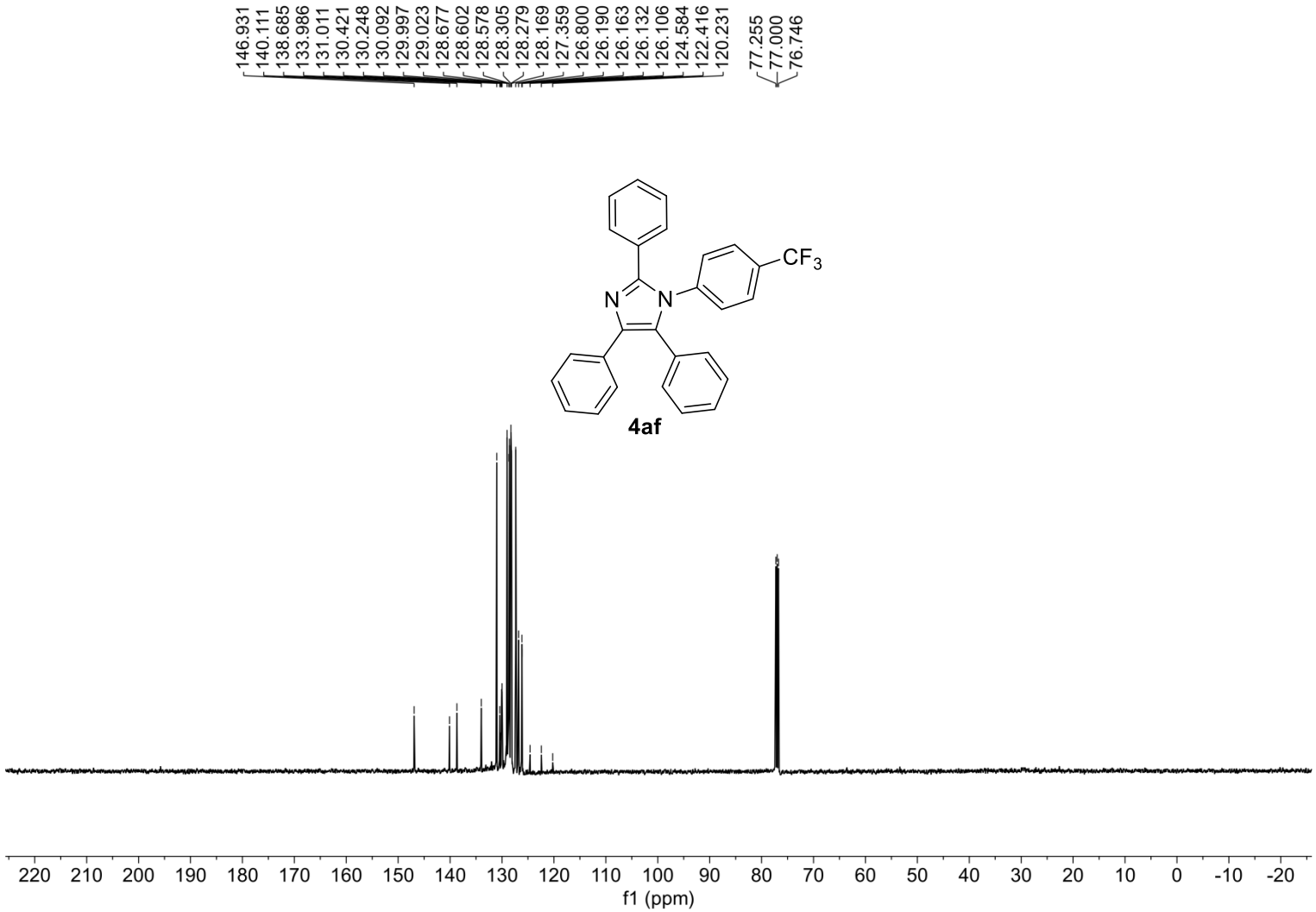
2.00
2.01
9.01
4.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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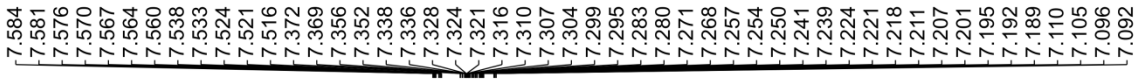
128.305
128.279
128.169
127.359
126.800
126.190
126.163
126.132
126.106
124.584
122.416
120.231
77.255
77.000
76.746
CF3
N
N
4af
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.538
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7.524
7.521
7.516
7.372
7.369
7.356
7.352
7.338
7.336
7.328
7.324
7.321
7.316
7.310
7.307
7.304
7.299
7.295
7.283
7.280
7.271
7.268
7.257
7.254
7.250
7.241
7.239
7.224
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7.189
7.110
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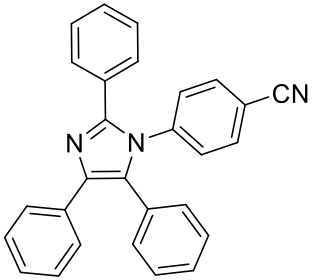
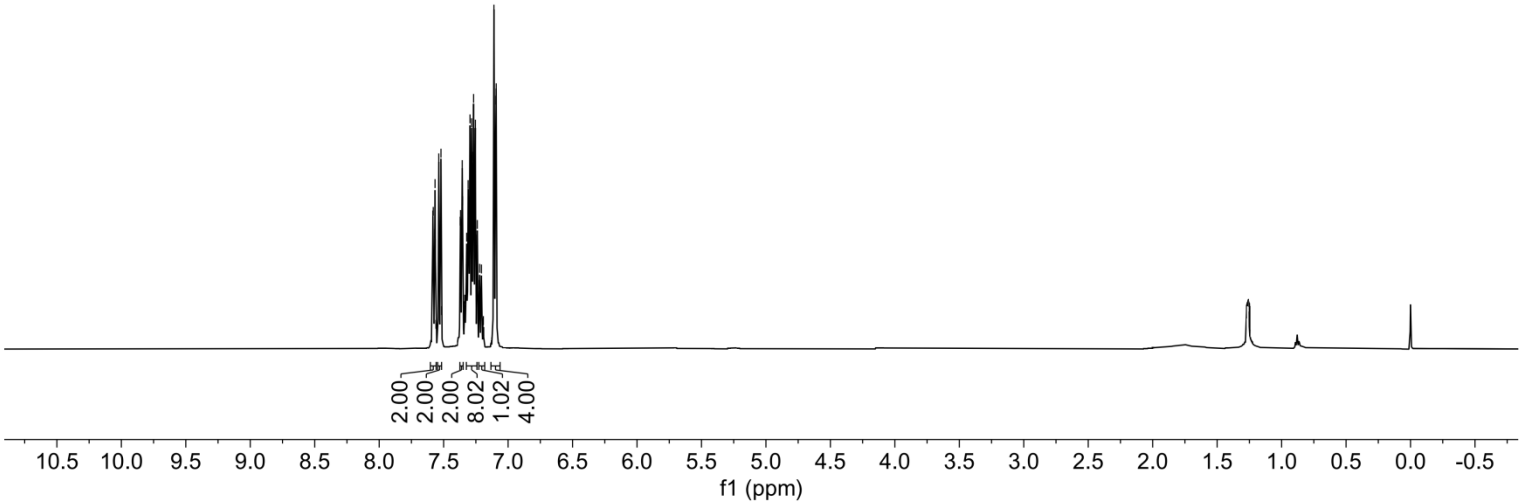
7.096
7.092


CN
N
N

4ag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2.00
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1.02
4.00
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10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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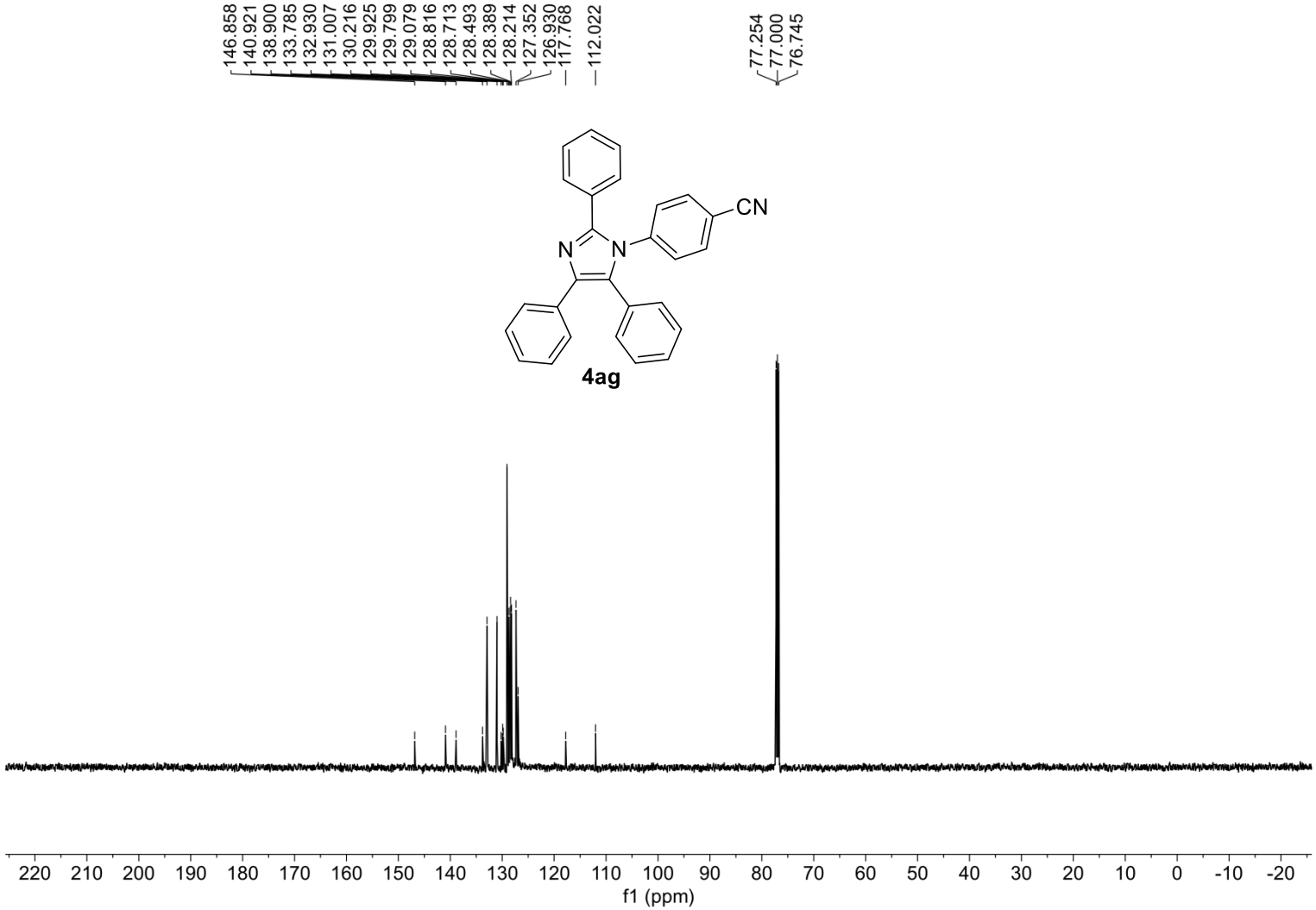
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.352
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112.022
77.254
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CN
N
N
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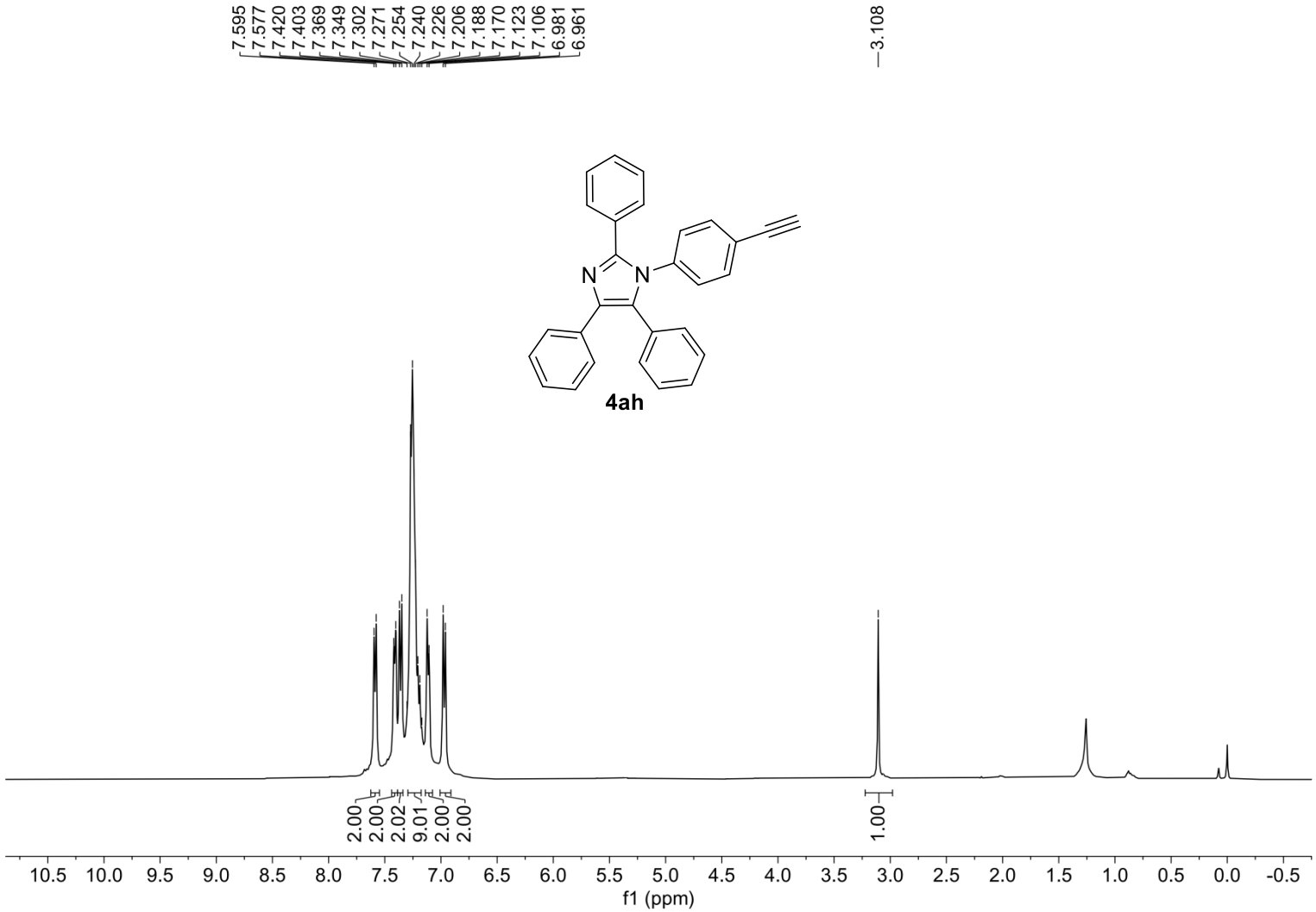
f1 (ppm)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7.240
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7.188
7.170
7.123
7.106
6.981
6.961
3.108
N
N
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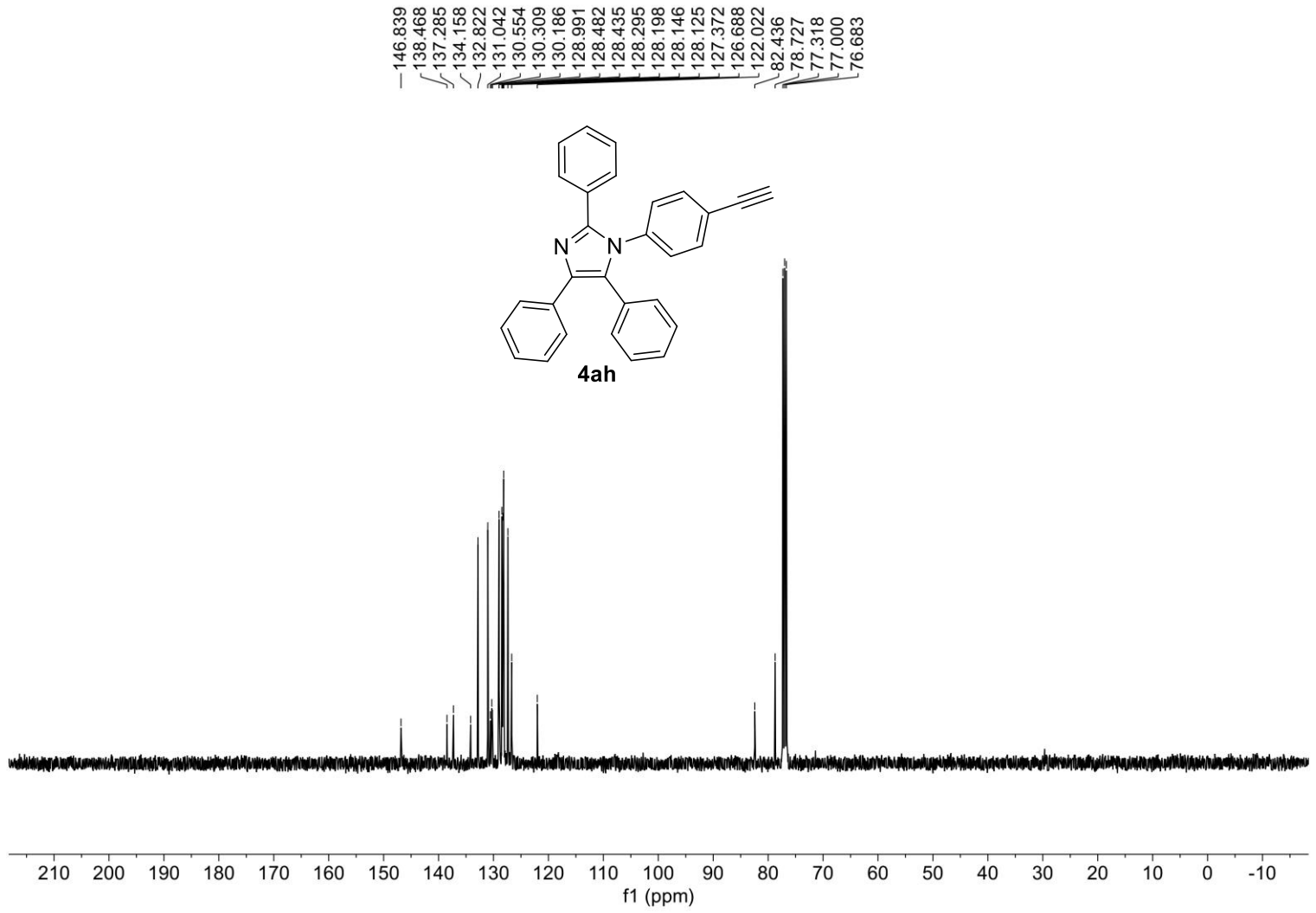
2.00
2.02
9.01
2.00
2.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.435
128.295
128.198
128.146
128.125
127.372
126.688
122.022
82.436
78.727
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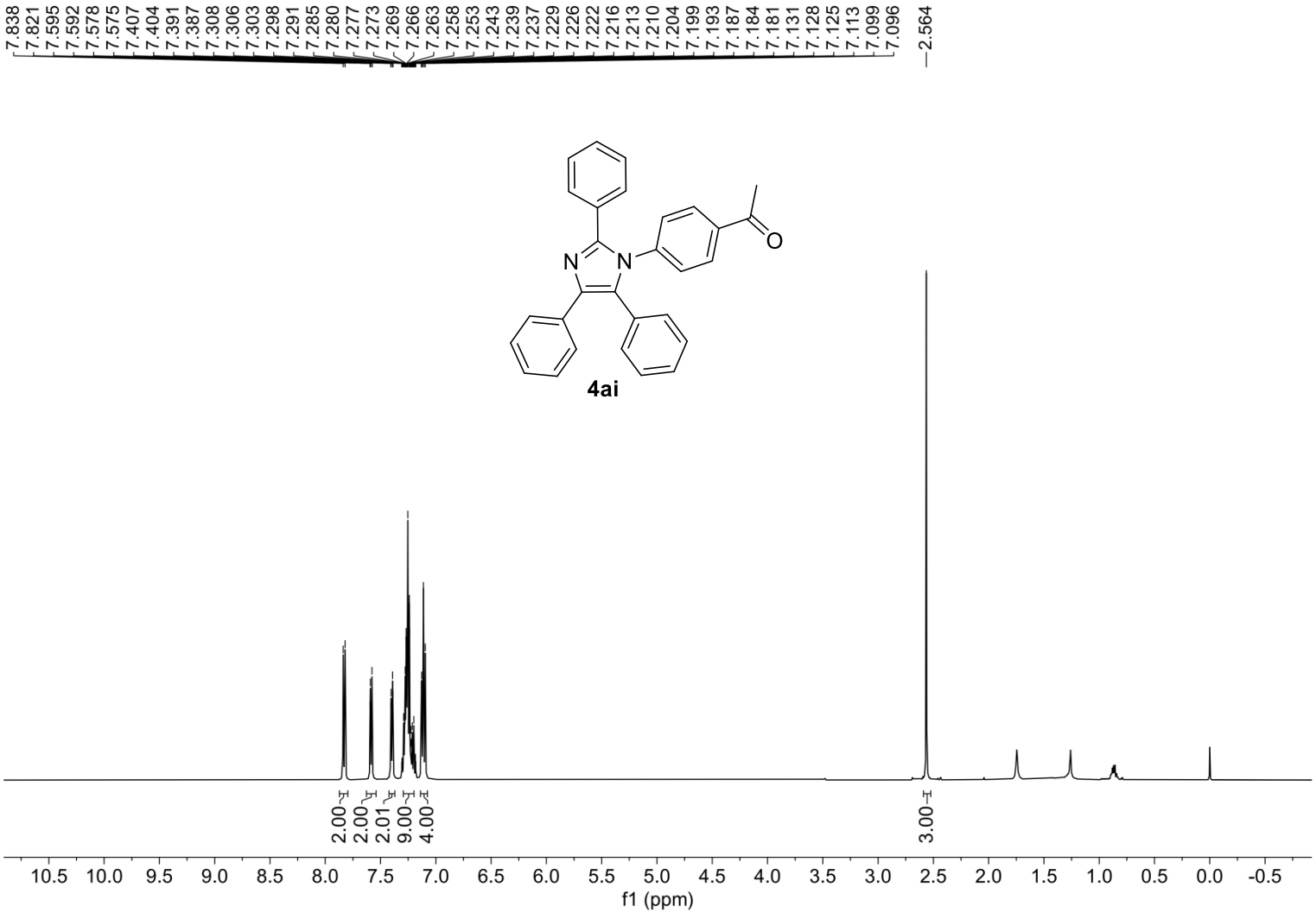
76.683
N
N
4ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.303
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7.291
7.285
7.280
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7.273
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7.253
7.243
7.239
7.237
7.229
7.226
7.222
7.216
7.213
7.210
7.204
7.199
7.193
7.187
7.184
7.181
7.131
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7.125
7.113
7.099
7.096
2.564
N
N
O
4ai
2.00
2.00
2.01
9.00
4.00
3.00
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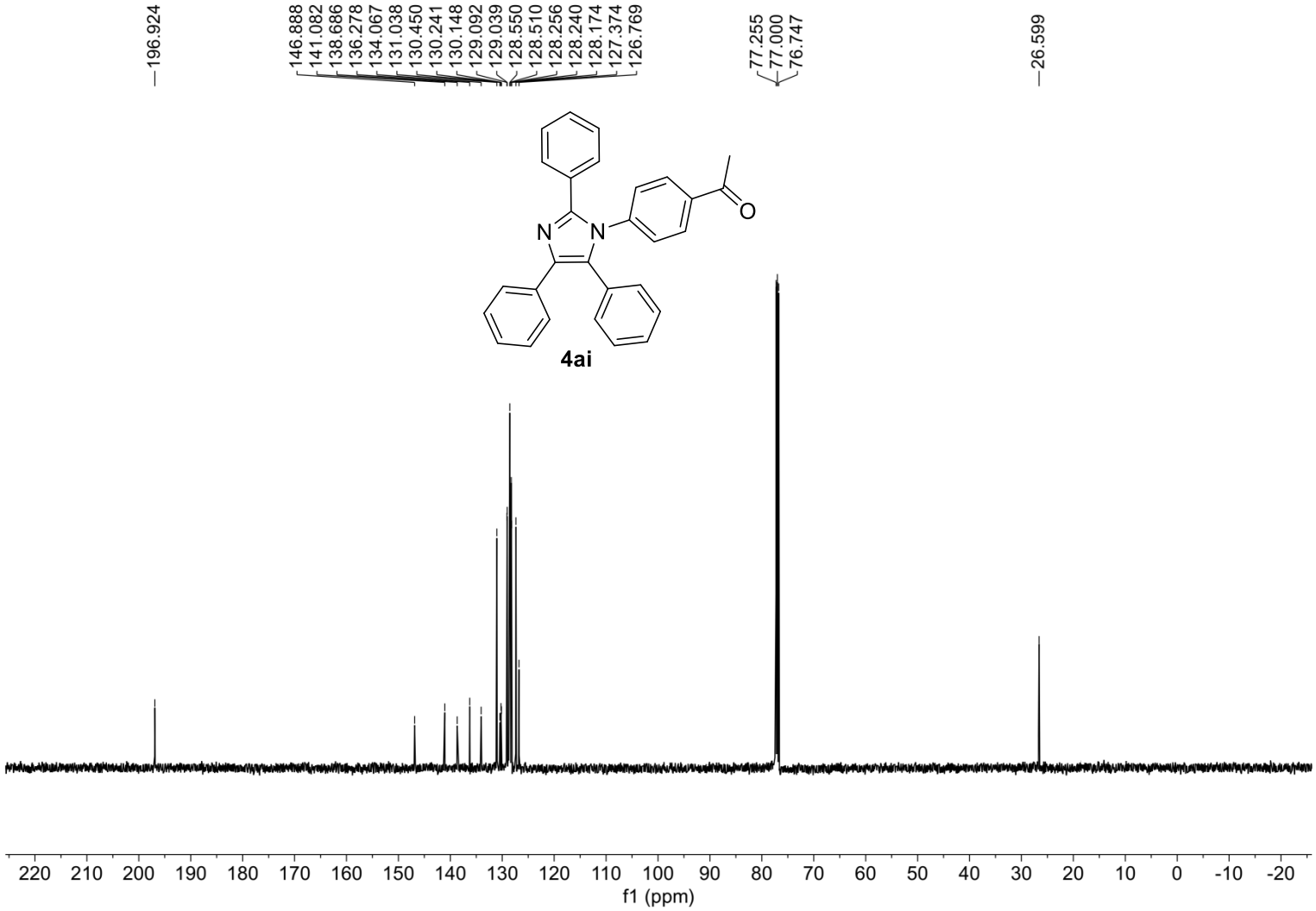
f1 (ppm)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129.039
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128.510
128.256
128.240
128.174
127.374
126.769
77.255
77.000
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N
N
O
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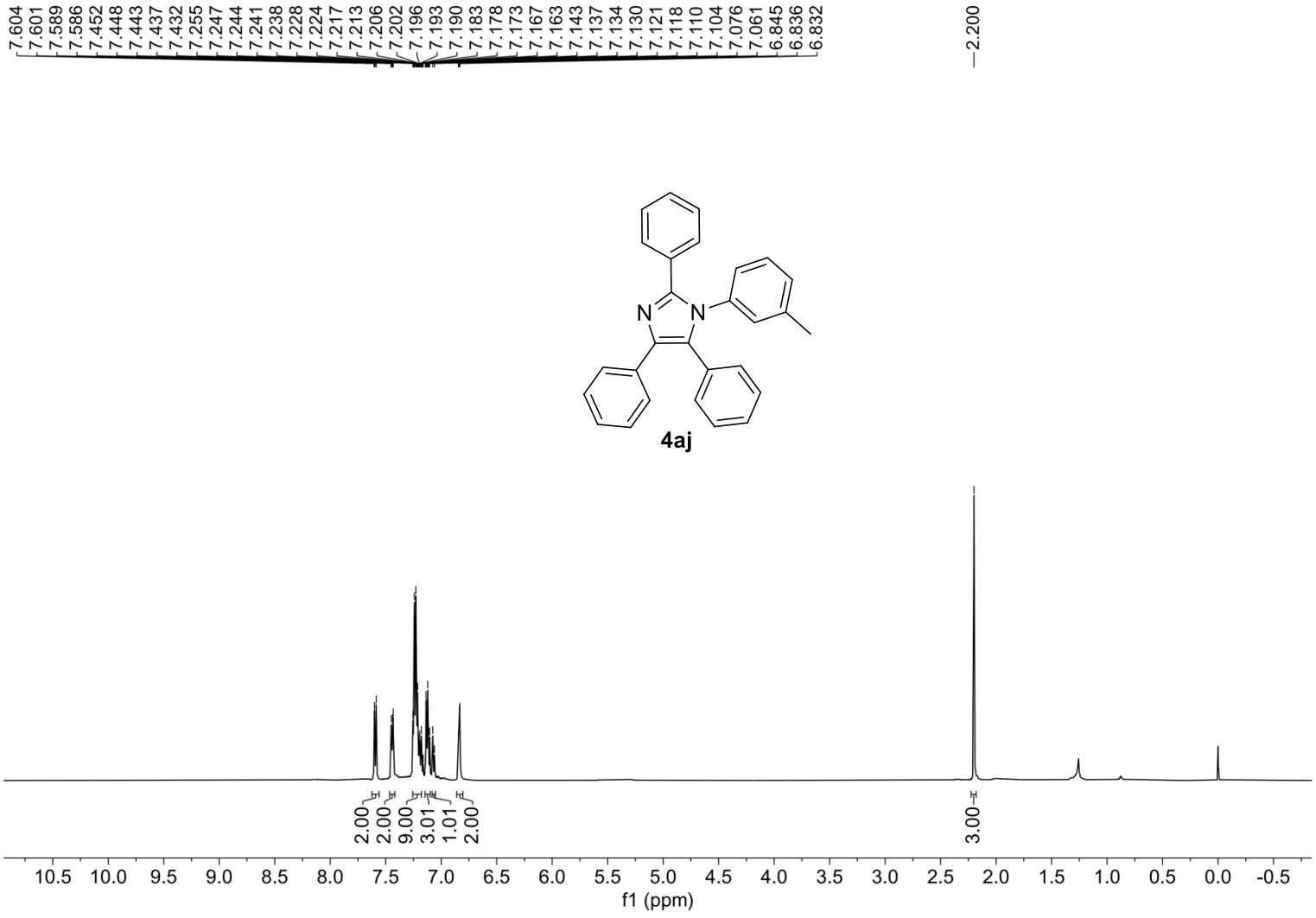
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.241
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7.228
7.224
7.217
7.213
7.206
7.202
7.196
7.193
7.190
7.183
7.178
7.173
7.167
7.163
7.143
7.137
7.134
7.130
7.121
7.118
7.110
7.104
7.076
7.061
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6.836
6.832
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N
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2.00
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1.01
2.00
3.00
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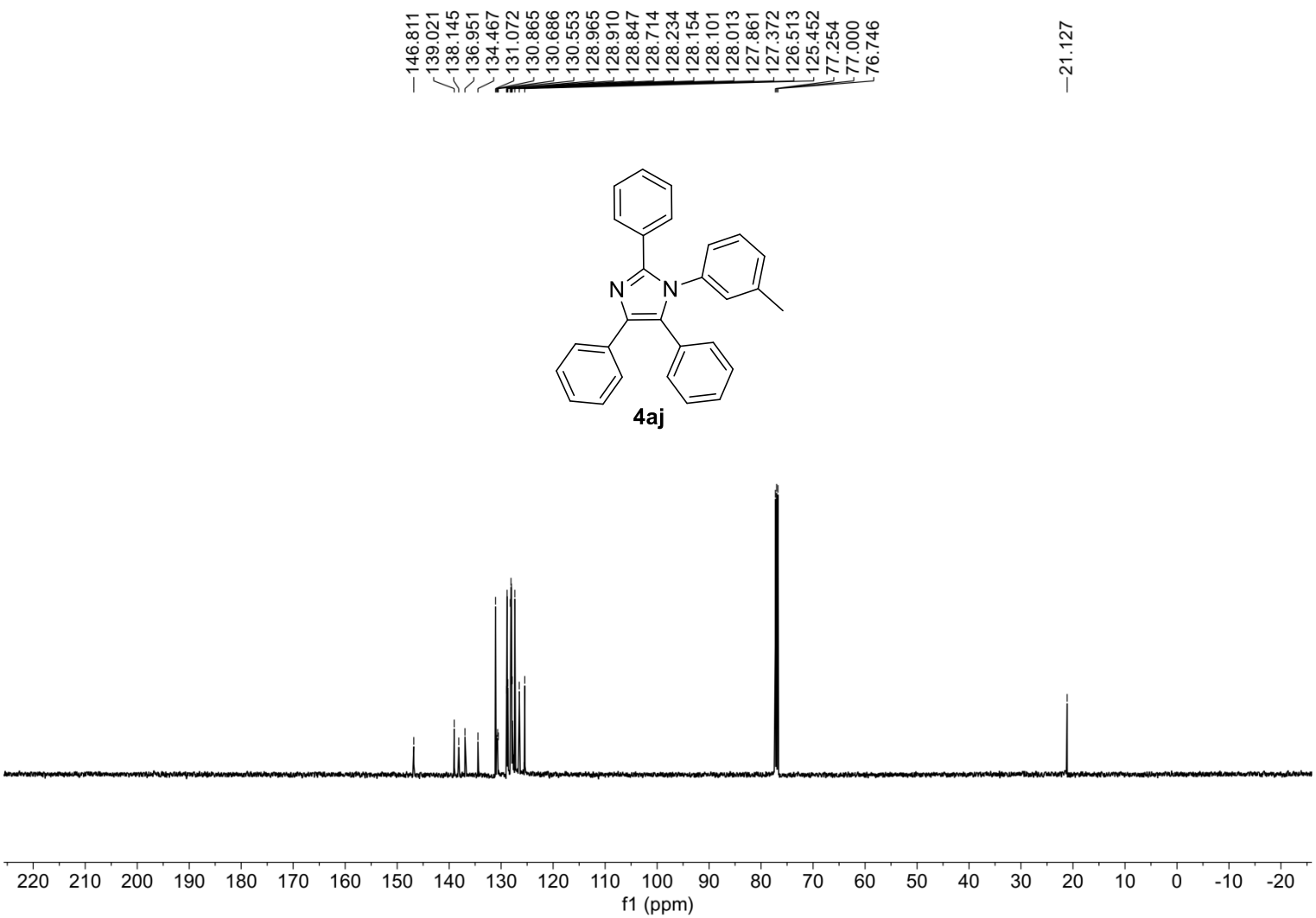
f1 (ppm)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128.714
128.234
128.154
128.101
128.013
127.861
127.372
126.513
125.452
77.254
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76.746
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N
N
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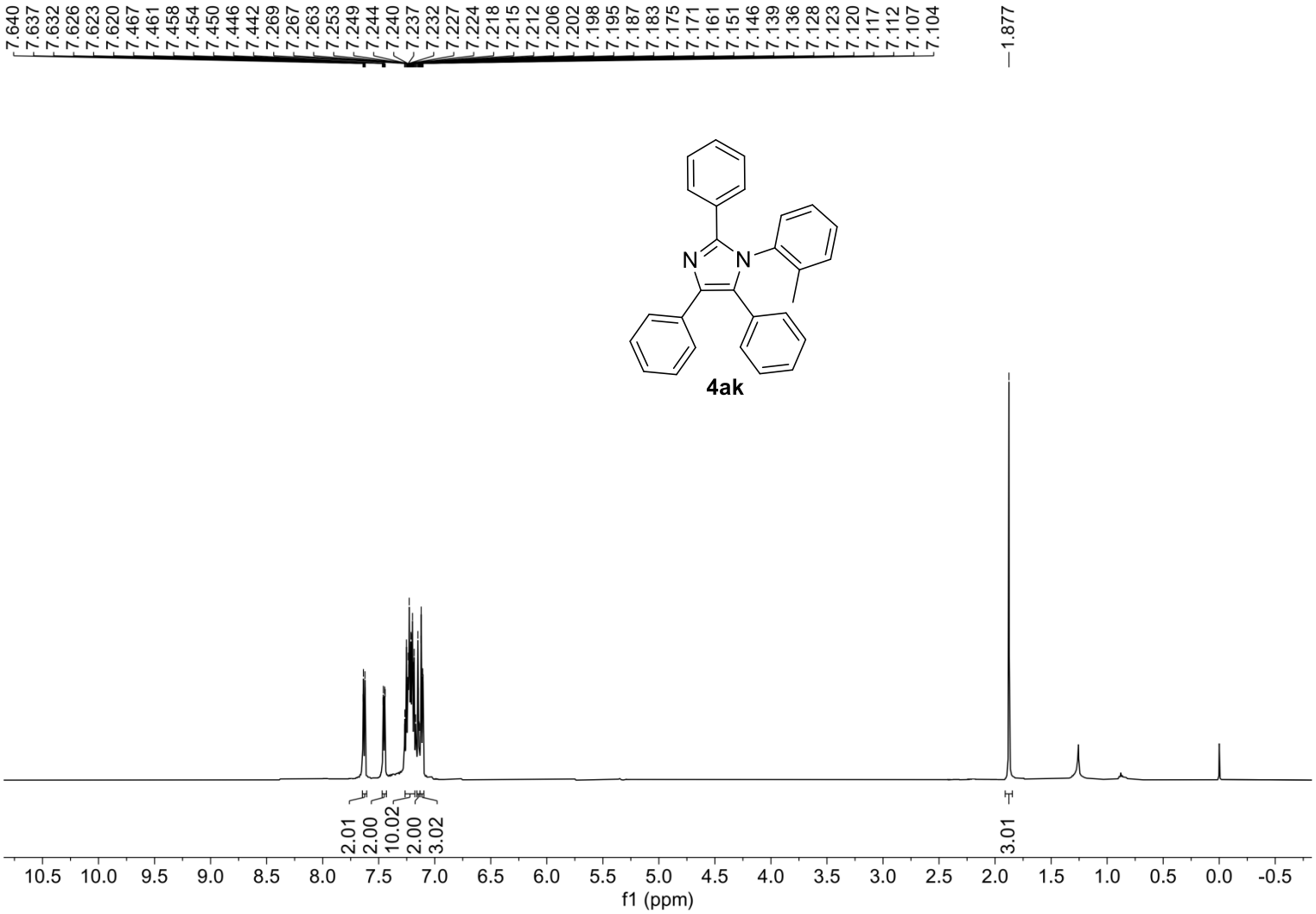
f1 (ppm)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7.267
7.263
7.253
7.249
7.244
7.240
7.237
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7.227
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7.218
7.215
7.212
7.206
7.202
7.198
7.195
7.187
7.183
7.175
7.171
7.161
7.151
7.146
7.139
7.136
7.128
7.123
7.120
7.117
7.112
7.107
7.104
1.877
N
N
4ak
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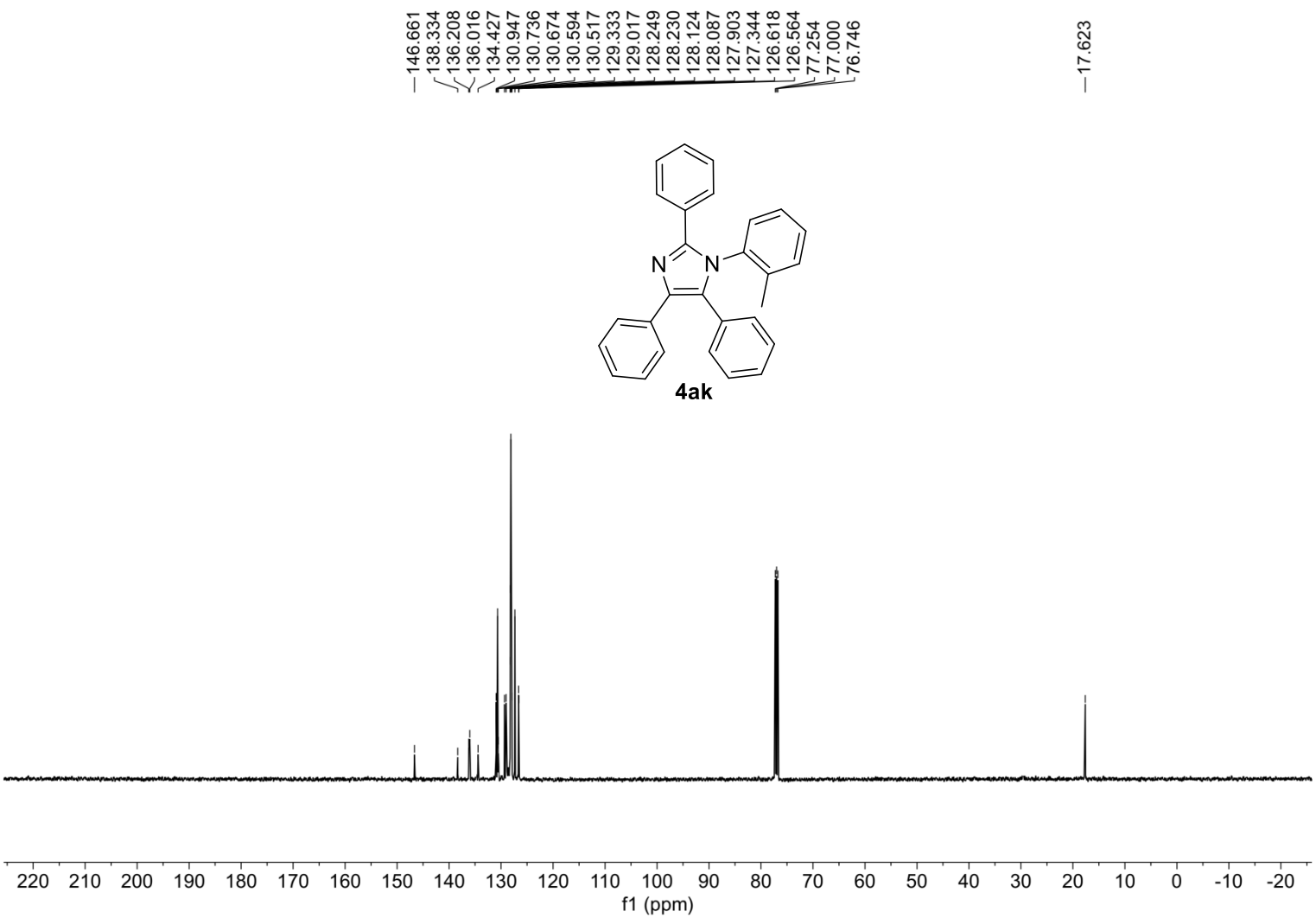
2.00
10.02
2.00
3.02
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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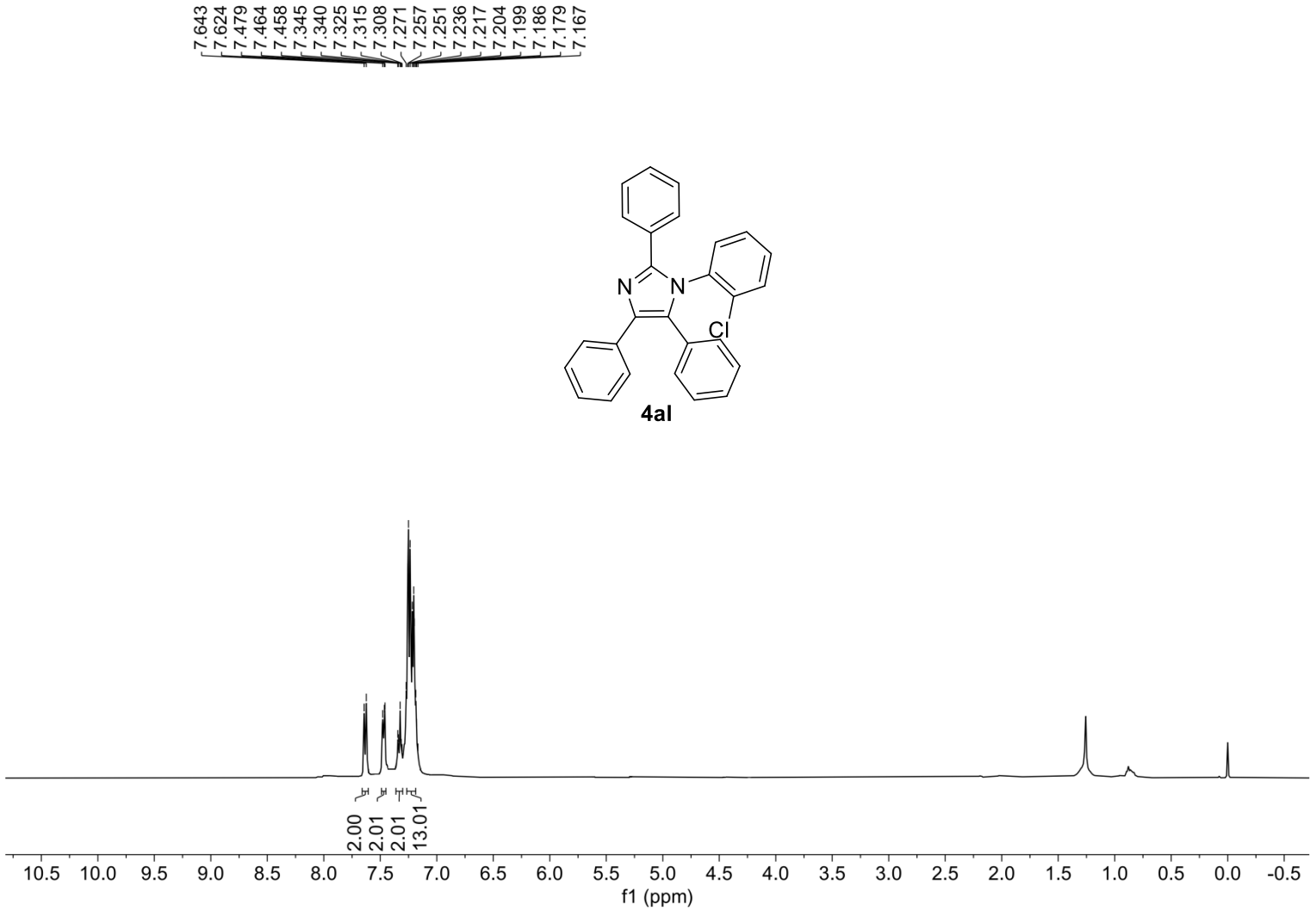
129.017
128.249
128.230
128.124
128.087
127.903
127.344
126.618
126.564
77.254
77.000
76.746
17.623
N
N
4ak
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.186
7.179
7.167
N
N
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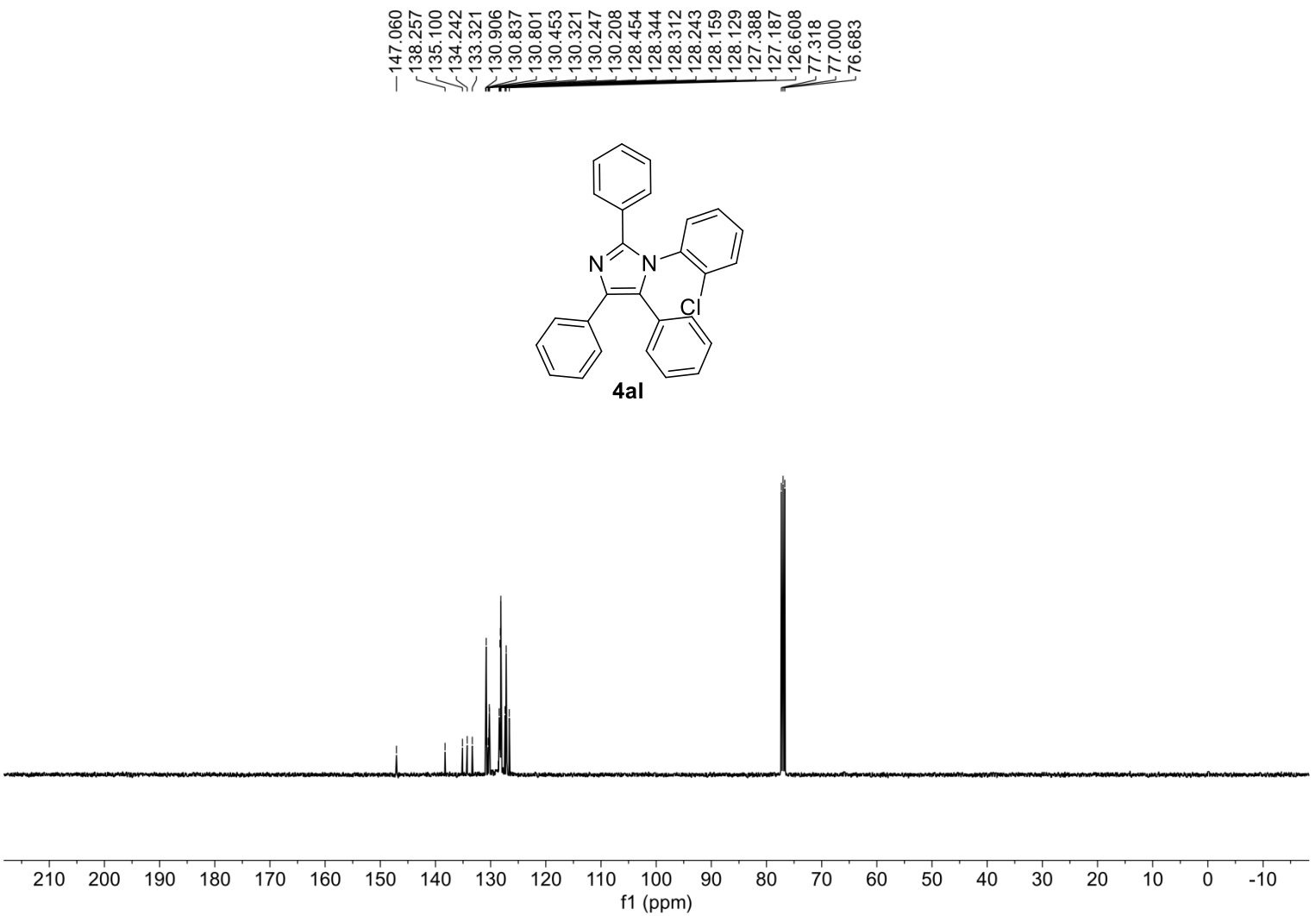
2.01
2.01
13.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.242
133.321
130.906
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130.801
130.453
130.321
130.247
130.208
128.454
128.344
128.312
128.243
128.159
128.129
127.388
127.187
126.608
77.318
77.000
76.683
N
N
Cl
4al
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.404
7.607
7.602
7.589
7.585
7.582
7.402
7.398
7.394
7.382
7.377
7.283
7.280
7.275
7.265
7.262
7.257
7.248
7.244
7.239
7.232
7.229
7.225
7.218
7.203
7.198
7.186
7.181
7.176
7.164
7.147
7.142
7.099
7.095
7.091
7.079
7.074
7.038
7.033
7.021
7.017
2.599
2.592
2.563
2.265
2.259
2.247
2.241
2.229
2.223
2.211
2.204
2.197
2.188
2.179
2.166
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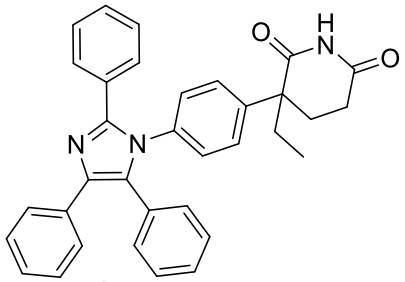
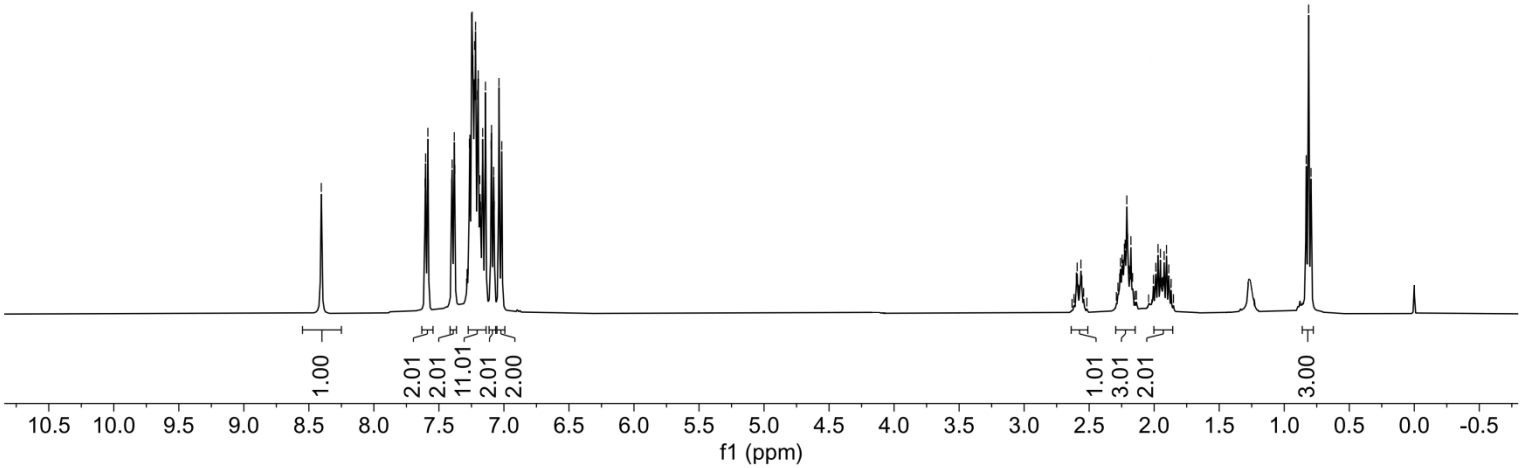
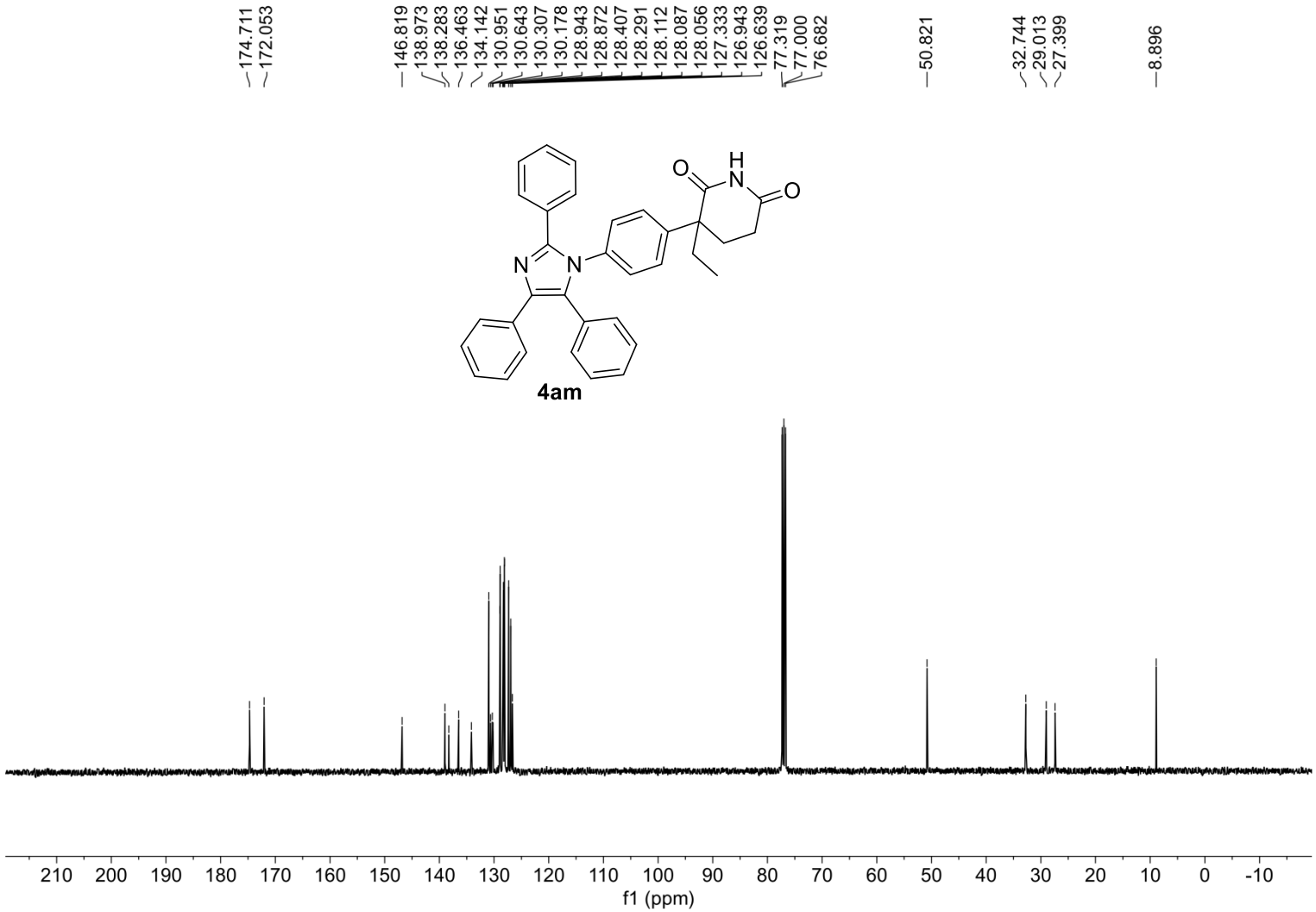
1.970
1.952
1.923
1.905
1.888
0.831
0.812
0.794


O
H
N
O
N
N

4am


1.00
2.01
2.01
11.01
2.01
2.00
1.01
3.01
2.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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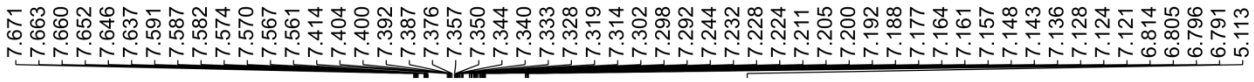
172.053
146.819
138.973
138.283
136.463
134.142
130.951
130.643
130.307
130.178
128.943
128.872
128.407
128.291
128.112
128.087
128.056
127.333
126.943
126.639
77.319
77.000
76.682
50.821
32.744
29.013
27.399
8.896
O
H
N
O
N
N
4am
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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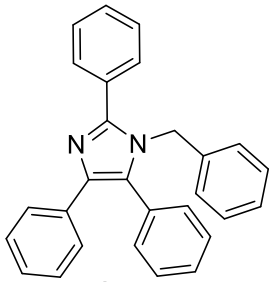
7.663
7.660
7.652
7.646
7.637
7.591
7.587
7.582
7.574
7.570
7.567
7.561
7.414
7.404
7.400
7.392
7.387
7.376
7.357
7.350
7.344
7.340
7.333
7.328
7.319
7.314
7.302
7.298
7.292
7.244
7.232
7.228
7.224
7.211
7.205
7.200
7.192
7.188
7.177
7.164
7.161
7.157
7.148
7.143
7.136
7.128
7.124
7.121
6.814
6.805
6.796
6.791
5.113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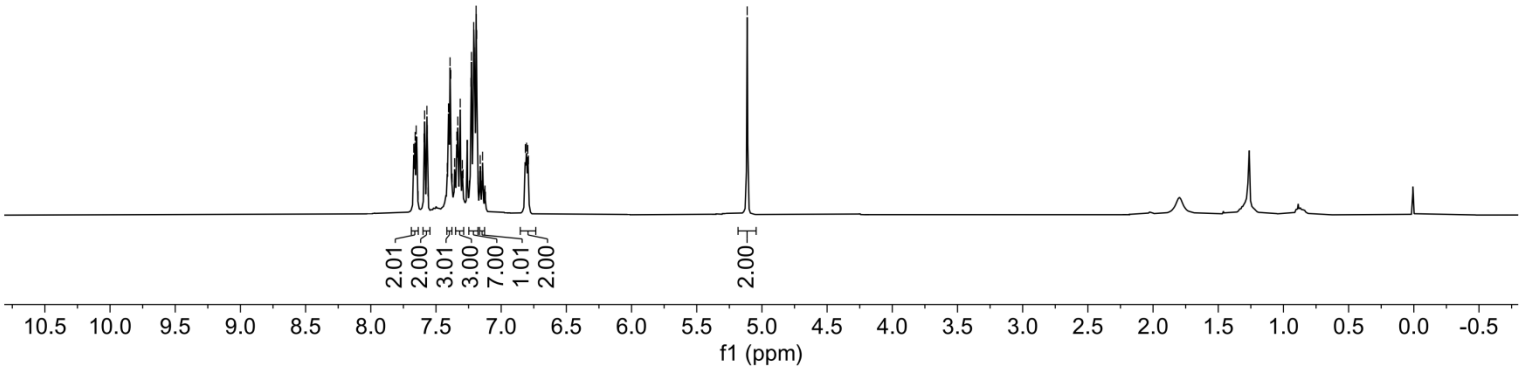
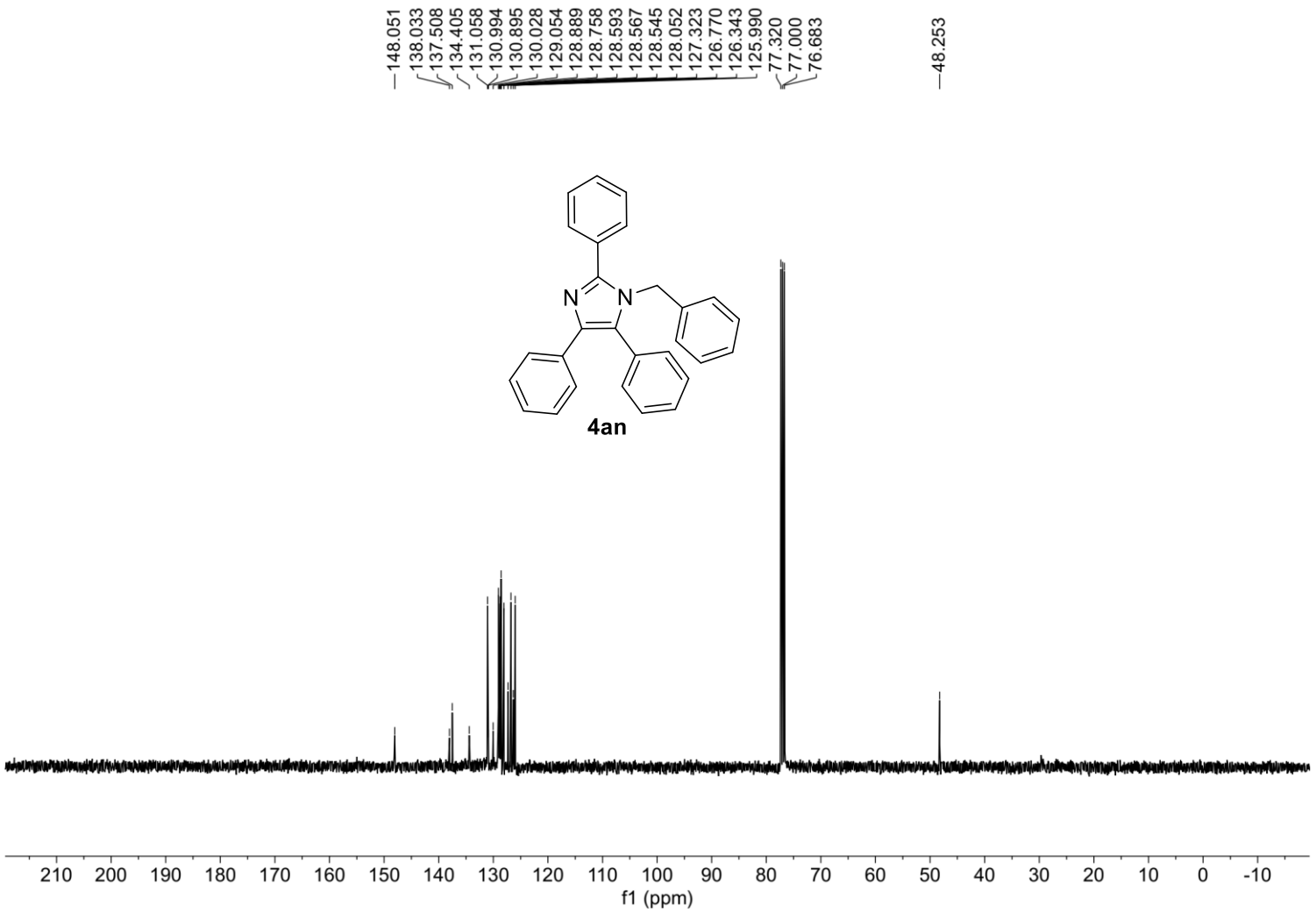
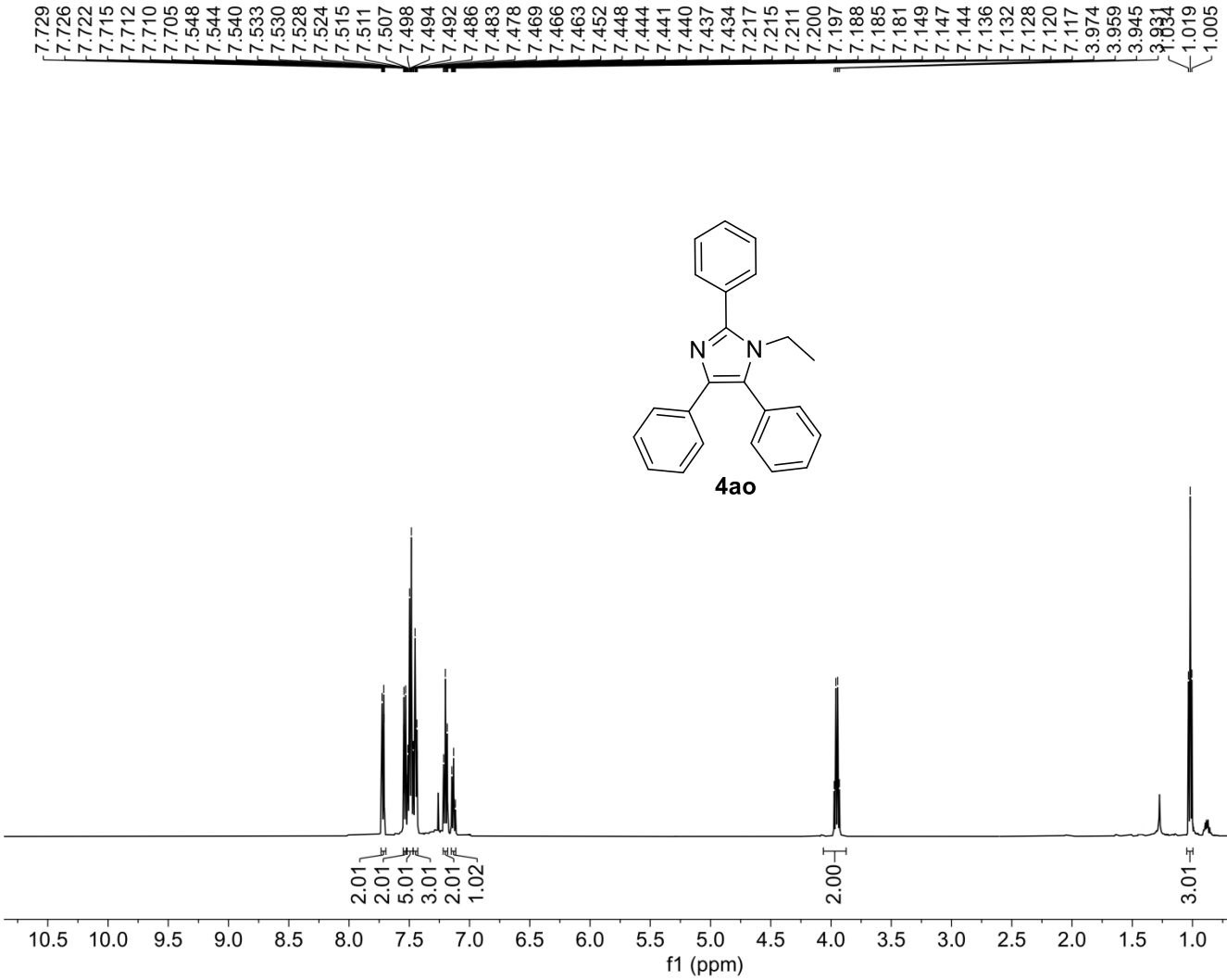
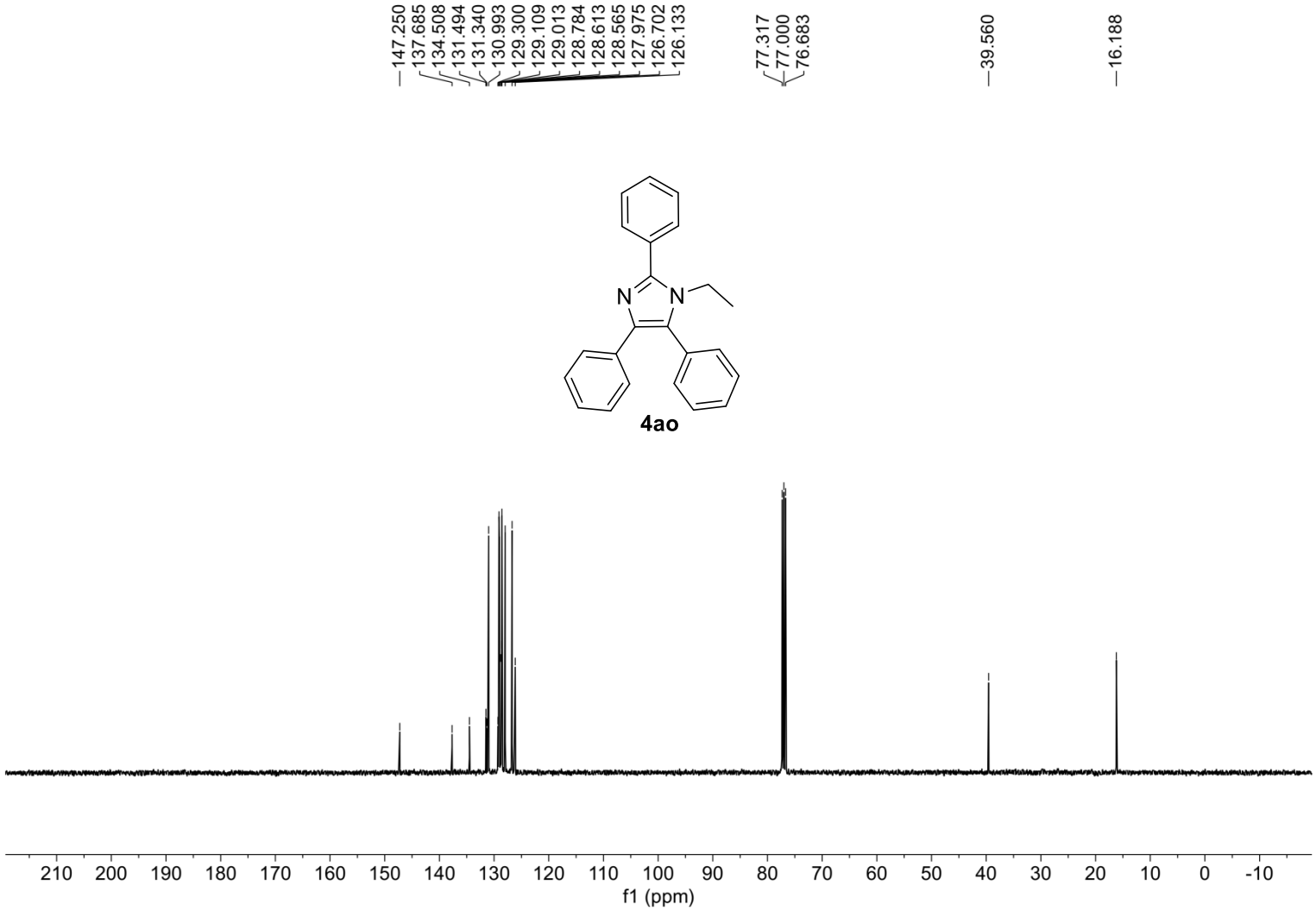
N

4an


2.01
2.00
3.01
3.00
7.00
1.01
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


148.051
138.033
137.508
134.405
131.058
130.994
130.895
130.028
129.054
128.889
128.758
128.593
128.567
128.545
128.052
127.323
126.770
126.343
125.990
77.320
77.000
76.683
48.253
N
N
4an
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.729
7.726
7.722
7.715
7.712
7.710
7.705
7.548
7.544
7.540
7.533
7.530
7.528
7.524
7.515
7.511
7.507
7.498
7.494
7.492
7.486
7.483
7.478
7.469
7.466
7.463
7.452
7.448
7.444
7.441
7.440
7.437
7.434
7.217
7.215
7.211
7.200
7.197
7.188
7.185
7.181
7.149
7.147
7.144
7.136
7.132
7.128
7.120
7.117
3.974
3.959
3.945
1.019
1.005
N
N
4ao
2.01
2.01
5.01
3.01
2.01
1.02
2.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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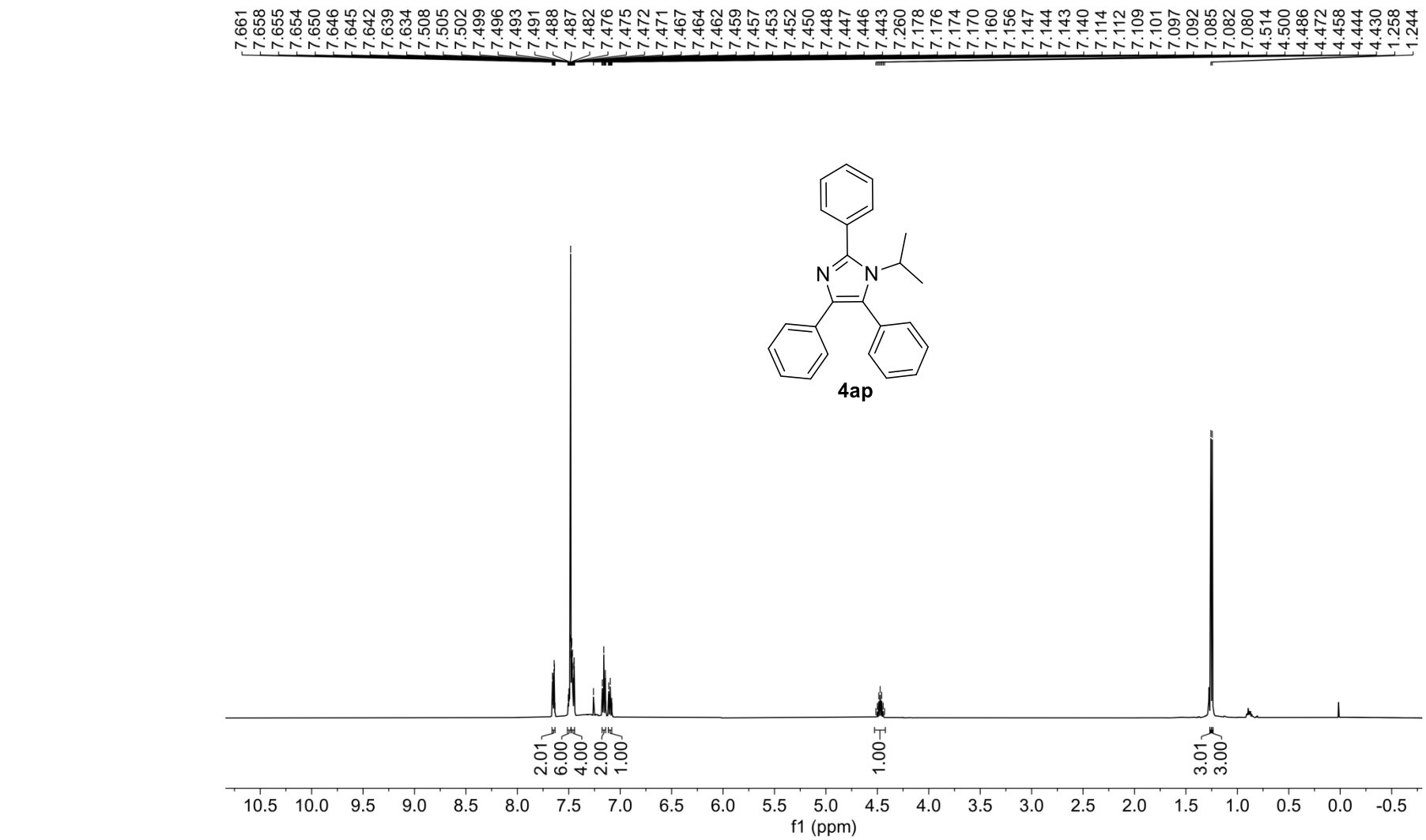
131.340
130.993
129.300
129.109
129.013
128.784
128.613
128.565
127.975
126.702
126.133
77.317
77.000
76.683
39.560
16.188
N
N
4ao
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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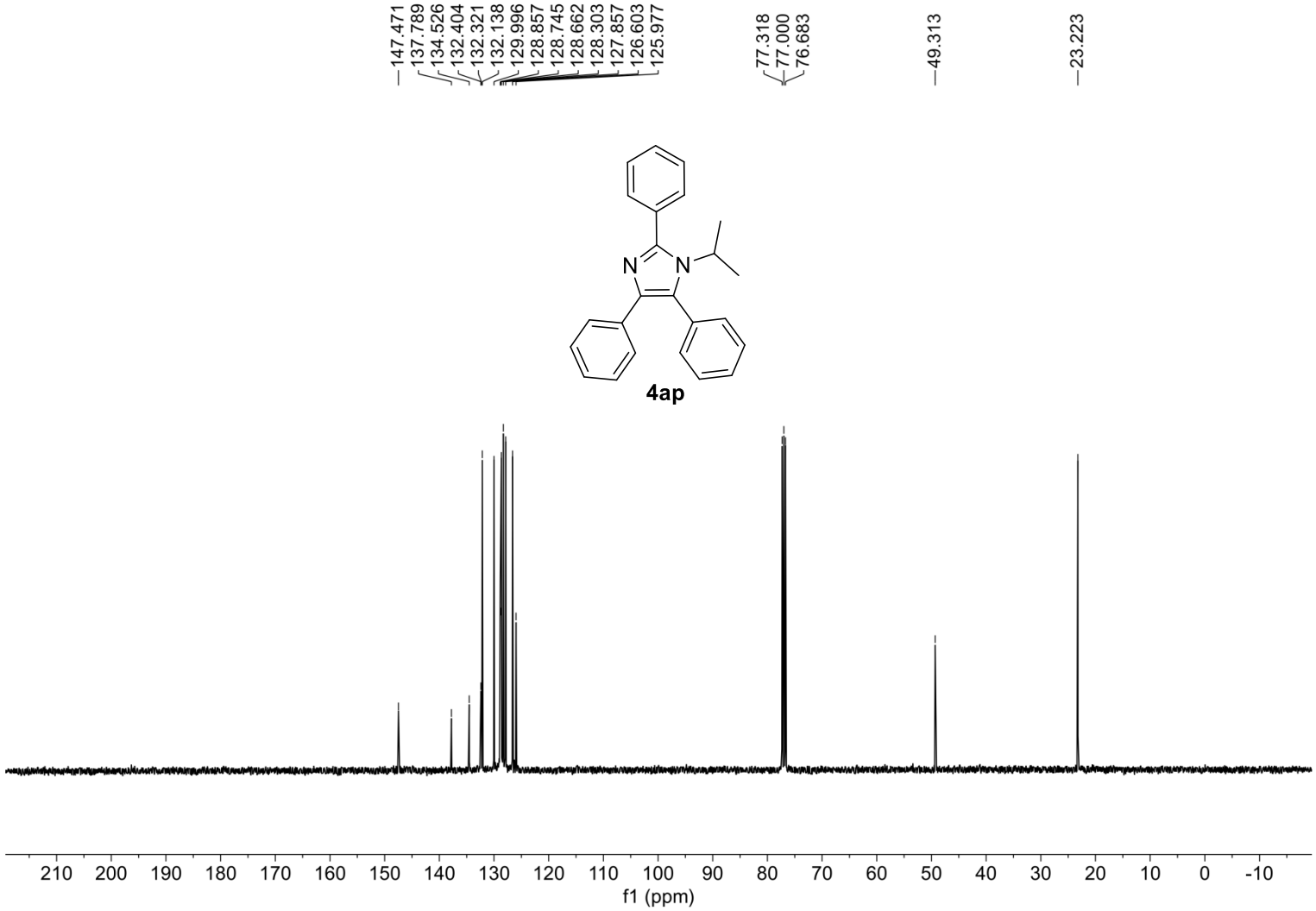
7.658
7.655
7.654
7.650
7.646
7.645
7.642
7.639
7.634
7.508
7.505
7.502
7.499
7.496
7.493
7.491
7.488
7.487
7.482
7.476
7.475
7.472
7.471
7.467
7.464
7.462
7.459
7.457
7.453
7.452
7.450
7.448
7.447
7.446
7.443
7.260
7.178
7.176
7.174
7.170
7.160
7.156
7.147
7.144
7.143
7.140
7.114
7.112
7.109
7.101
7.097
7.092
7.085
7.082
7.080
4.514
4.500
4.486
4.472
4.458
4.444
4.430
1.258
1.244
N
N
4ap
2.01
6.00
4.00
2.00
1.00
1.00
3.01
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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132.321
132.138
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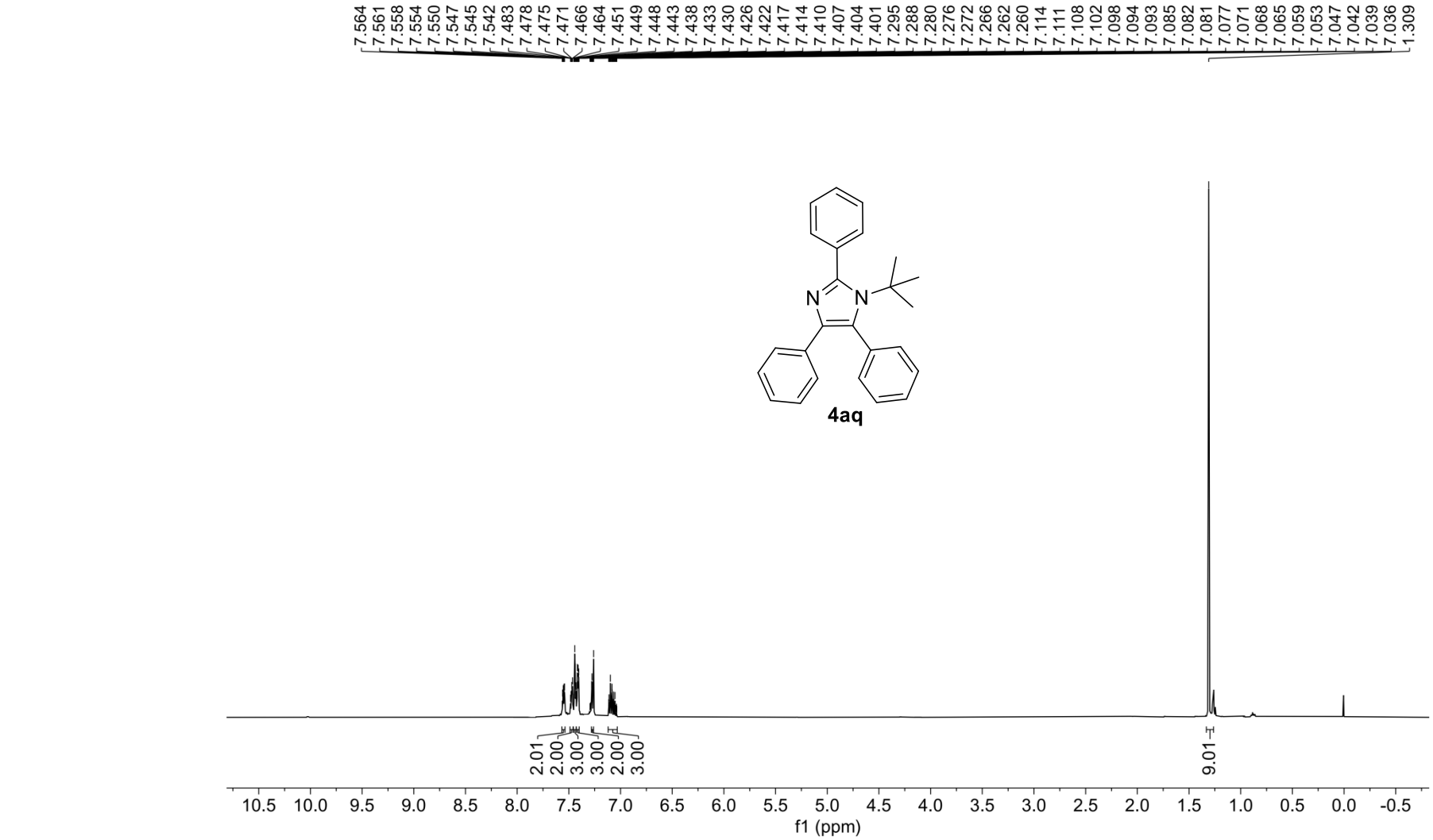
128.857
128.745
128.662
128.303
127.857
126.603
125.977
77.318
77.000
76.683
49.313
23.223
N
N
4ap
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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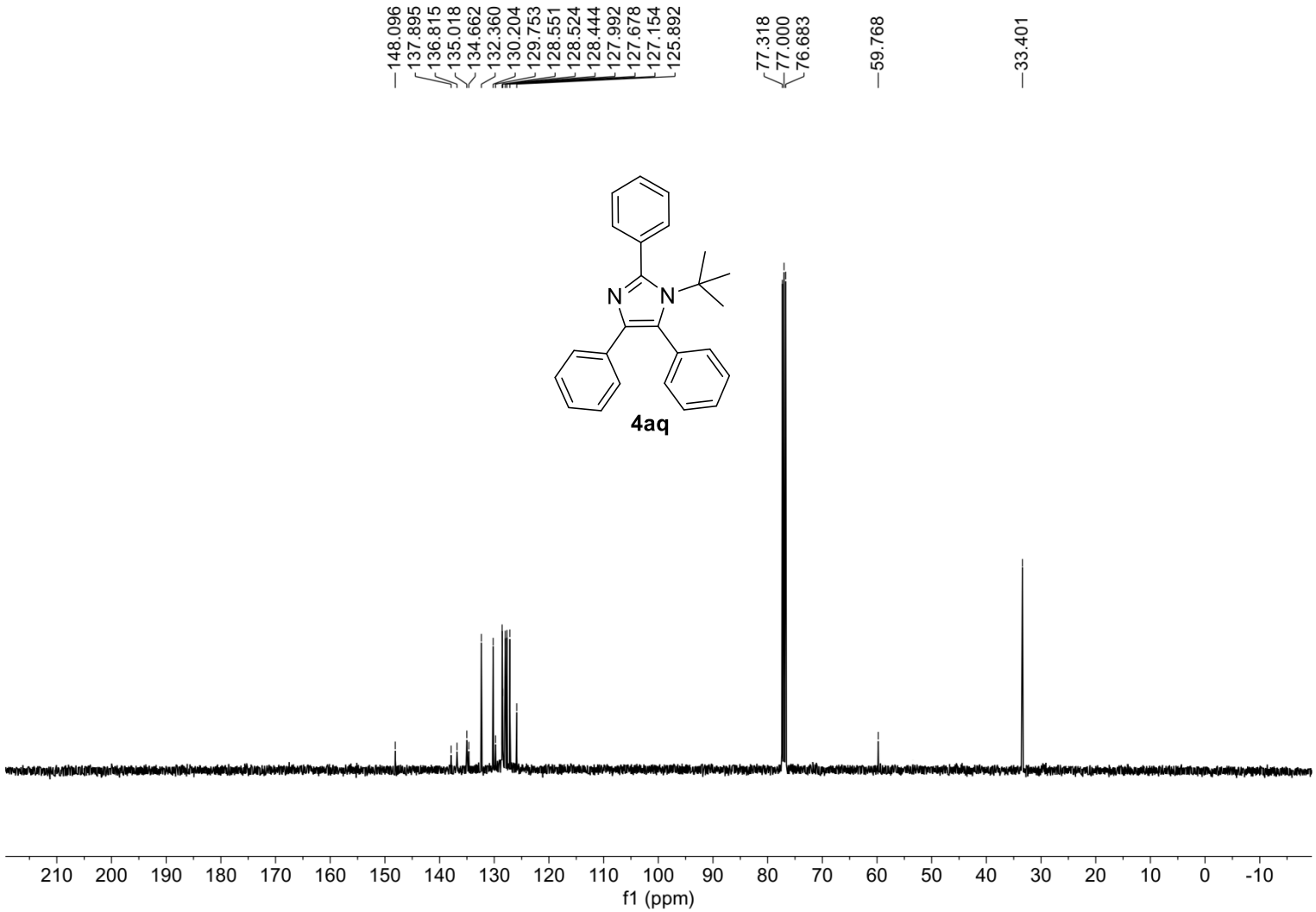
7.561
7.558
7.554
7.550
7.547
7.545
7.542
7.483
7.478
7.475
7.471
7.466
7.464
7.451
7.449
7.448
7.443
7.438
7.433
7.430
7.426
7.422
7.417
7.414
7.410
7.407
7.404
7.401
7.295
7.288
7.280
7.276
7.272
7.266
7.262
7.260
7.114
7.111
7.108
7.102
7.098
7.094
7.093
7.085
7.082
7.081
7.077
7.071
7.068
7.065
7.059
7.053
7.047
7.042
7.039
7.036
1.309
N
N
4aq
2.01
2.00
3.00
3.00
2.00
3.00
9.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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136.815
135.018
134.662
132.360
130.204
129.753
128.551
128.524
128.444
127.992
127.678
127.154
125.892
77.318
77.000
76.683
59.768
33.401
N
N
4aq
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)