Ruthenium(II)-catalyzed chemoselective deacylative annulation of 1,3-diones with sulfoxonium ylides *via* C–C bond activation

Si Wen, Weiwei Lv, Dan Ba, Jing Liu, and Guolin Cheng*

College of Materials Science & Engineering, Huaqiao University, Xiamen 361021, China.

E-mail: glcheng@hqu.edu.cn

Table of Contents

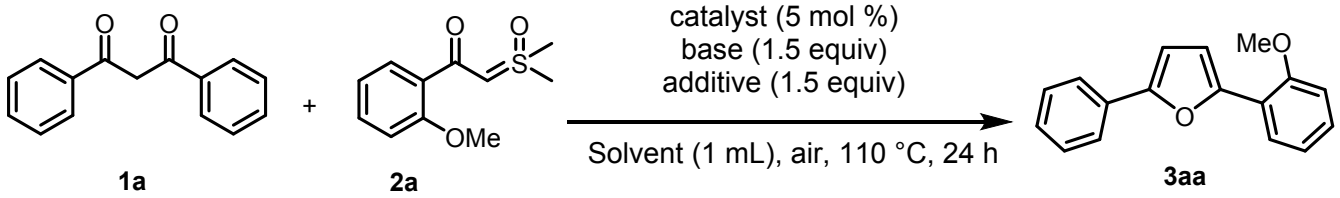
1. General Information

All the solvents were used without further purification. the other commercial chemicals were used without further purification. All reactions were performed under an inert atmosphere of nitrogen in flame-dried glassware, unless otherwise stated. Analytical thin-layer chromatography was performed on 0.25 mm silica gel, 60-F254. Visualization was carried out with UV light and Vogel's permanganate. Preparative TLC was performed on 1.0 mm silica gel. ^{1}H NMR spectra were recorded on a Bruker DRX-500 instrument (500 MHz). ^{13}C NMR spectra were recorded on a Bruker DRX-500 instrument (126 MHz) and were fully decoupled by broad band proton decoupling. High-resolution mass spectra (HRMS) were recorded on an Agilent 1290 mass spectrometer using ESI-TOF (electrospray ionization time-of-flight). NMR spectra were recorded in $CDCl_3$. ^{1}H NMR spectra were referenced to residual $CHCl_3$ at 7.26 ppm, and ^{13}C NMR spectra were referenced to the central peak of $CDCl_3$ at 77.0 ppm. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are reported in hertz (Hz). Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

2. Experimental Section

2.1 Optimization of the Reaction Conditions

2.1.1 Table S1 Optimization of the Reaction Conditions[a]



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

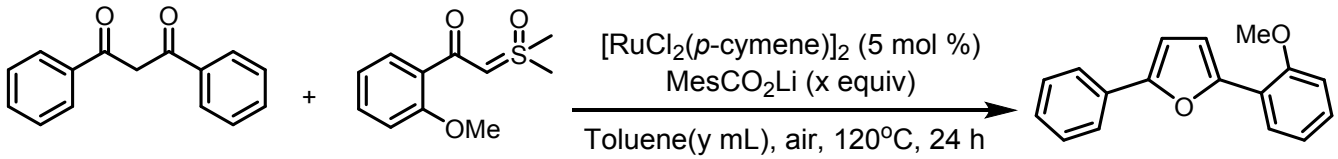
Entry	Catalyst	Solvent	Base	Additive	Yield (%)[b]
1	$[RuCl_2(p\text{-cymene})]_2$	HFIP	Na_3PO_4	$MesCO_2H$	23
2	$[RuCl_2(p\text{-cymene})]_2$	DCE	Na_3PO_4	$MesCO_2H$	15
3	$[RuCl_2(p\text{-cymene})]_2$	^{i}PrOH	Na_3PO_4	$MesCO_2H$	26
4	$[RuCl_2(p\text{-cymene})]_2$	DMF	Na_3PO_4	$MesCO_2H$	30
5	$[RuCl_2(p\text{-cymene})]_2$	CH_3CN	Na_3PO_4	$MesCO_2H$	25
6	$[RuCl_2(p\text{-cymene})]_2$	toluene	Na_3PO_4	$MesCO_2H$	35
7	$[RuCl_2(p\text{-cymene})]_2$	toluene	$NaHCO_3$	$MesCO_2H$	24
8	$[RuCl_2(p\text{-cymene})]_2$	toluene	K_2CO_3	$MesCO_2H$	20
9	$[RuCl_2(p\text{-cymene})]_2$	toluene	$KHCO_3$	$MesCO_2H$	22
10	$[RuCl_2(p\text{-cymene})]_2$	toluene	Cs_2CO_3	$MesCO_2H$	25
11	$[RuCl_2(p\text{-cymene})]_2$	toluene	NaOAc	$MesCO_2H$	30
12	$[RuCl_2(p\text{-cymene})]_2$	toluene	NaOH	$MesCO_2H$	26
13	$[RuCl_2(p\text{-cymene})]_2$	toluene	KOAc	$MesCO_2H$	15
14	$[RuCl_2(p\text{-cymene})]_2$	toluene	KOH	$MesCO_2H$	15
15	$[RuCl_2(p\text{-cymene})]_2$	toluene	K_2HPO_4	$MesCO_2H$	52
16	$[RuCl_2(p\text{-cymene})]_2$	toluene	K_3PO_4	$MesCO_2H$	15
17	$[RuCl_2(p\text{-cymene})]_2$	toluene	KH_2PO_4	$MesCO_2H$	40
18	$[RuCl_2(p\text{-cymene})]_2$	toluene	HCOONa	$MesCO_2H$	25
19	$[RuCl_2(p\text{-cymene})]_2$	toluene	CH_3ONa	$MesCO_2H$	25
20	$[RuCl_2(p\text{-cymene})]_2$	toluene	Na_2CO_3	$MesCO_2H$	30
21	$[RuCl_2(p\text{-cymene})]_2$	toluene	NaH_2PO_4	$MesCO_2H$	25
22	$[RuCl_2(p\text{-cymene})]_2$	toluene	^{t}BuOK	$MesCO_2H$	10
23	$[RuCl_2(p\text{-cymene})]_2$	toluene	^{t}BuONa	$MesCO_2H$	20

24	$[RuCl_2(p\text{-cymene})]_2$	toluene	LiOH	$MesCO_2H$	15
25	$[RuCl_2(p\text{-cymene})]_2$	toluene	CH_3OK	$MesCO_2H$	10
26	$[RuCl_2(p\text{-cymene})]_2$	toluene	Li_2CO_3	$MesCO_2H$	10
27	$[RuCl_2(p\text{-cymene})]_2$	toluene	CsOAc	$MesCO_2H$	12
28	$[RuCl_2(p\text{-cymene})]_2$	toluene	^{t}BuOLi	$MesCO_2H$	72
29	$[RuCl_2(p\text{-cymene})]_2$	toluene	-	$MesCO_2H$	10
30	$[RuCl_2(p\text{-cymene})]_2$	toluene	^{t}BuOLi	-	trace
31	$[RuCl_2(p\text{-cymene})]_2$	toluene	^{t}BuOLi	AcOH	20
32	$[RuCl_2(p\text{-cymene})]_2$	toluene	^{t}BuOLi	Ac-Gly-OH	10
33	$[RuCl_2(p\text{-cymene})]_2$	toluene	^{t}BuOLi	Val-Boc-OH	10
34	$[RuCl_2(p\text{-cymene})]_2$	toluene	$MesCO_2Li$	-	71
35	$[RuCl_2(p\text{-cymene})]_2$	DCE	$MesCO_2Li$	-	20
36	$[RuCl_2(p\text{-cymene})]_2$	NMP	$MesCO_2Li$	-	trace
37	$[RuCl_2(p\text{-cymene})]_2$	1,4-dioxane	$MesCO_2Li$	-	20
38	$[RuCl_2(p\text{-cymene})]_2$	THF	$MesCO_2Li$	-	58
39	$[RuCl_2(p\text{-cymene})]_2$	HFIP	$MesCO_2Li$	-	10
40	$[RuCl_2(p\text{-cymene})]_2$	^{t}AmOH	$MesCO_2Li$	-	15
41	$[RuCl_2(p\text{-cymene})]_2$	DME	$MesCO_2Li$	-	62
42	$[RuCl_2(p\text{-cymene})]_2$	DMSO	$MesCO_2Li$	-	N.R.
43	$[RuCl_2(p\text{-cymene})]_2$	DMF	$MesCO_2Li$	-	10
44	$[RuCl_2(p\text{-cymene})]_2$	^{i}PrOH	$MesCO_2Li$	-	15
45	$[RuCl_2(p\text{-cymene})]_2$	TMBE	$MesCO_2Li$	-	60
46	$[RuCl_2(p\text{-cymene})]_2$	CH_3CN	$MesCO_2Li$	-	10
47[c]	$[RuCl_2(p\text{-cymene})]_2$	toluene	$MesCO_2Li$	-	12

48[d]	$[RuCl_2(p\text{-cymene})]_2$	toluene	$MesCO_2Li$	-	66
49[e]	$[RuCl_2(p\text{-cymene})]_2$	toluene	$MesCO_2Li$	-	78
50[f]	$[RuCl_2(p\text{-cymene})]_2$	toluene	$MesCO_2Li$	-	40
51[g]	$[RuCl_2(p\text{-cymene})]_2$	toluene	$MesCO_2Li$	-	30
52	$Pd(OAc)_2$	toluene	$MesCO_2Li$	-	0
53	$[Cp^*RhCl_2]_2$	toluene	$MesCO_2Li$	-	0
54	$Cu(OAc)_2$	toluene	$MesCO_2Li$	-	0
55	AgOAc	toluene	$MesCO_2Li$	-	0

[a] **1a** (0.1 mmol), **2a** (0.2 mmol), solvent (1 mL), base (1.5 equiv), catalyst (5 mol%), additive (1.5 equiv) at 110 °C under air for 24 h. [b] The yields were determined by ^1H NMR analysis of the crude product using CH_2Br_2 as the internal standard. [c] At 80°C. [d] At 100°C. [e] At 120°C. [f] At 130°C. [g] At 140°C.

2.1.2 Table S2 Optimization of the Reaction Conditions[a]



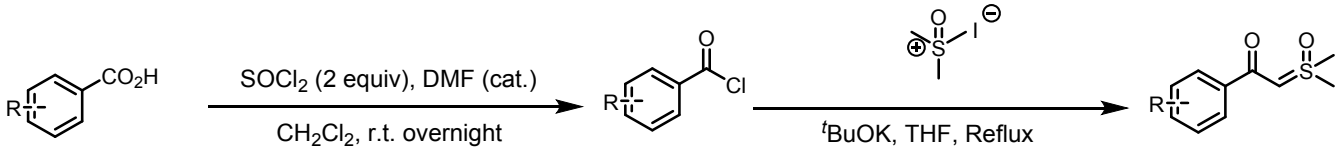
1a **2a** **3aa**

Entry	Solvent	Base	Yield (%)[b]
1	toluene	$MesCO_2Li$ (1.0 equiv)	66
2	toluene	$MesCO_2Li$ (2.0 equiv)	72
3	toluene (0.5 mL)	$MesCO_2Li$	72
4	toluene (2 mL)	$MesCO_2Li$	85
5	toluene (3 mL)	$MesCO_2Li$	66

[a] **1a** (0.1 mmol), **2a** (0.2 mmol), $MesCO_2Li$, $[RuCl_2(p\text{-cymene})]_2$ (5 mol%), in toluene at 120 °C for 24 h. [b] The yields were determined by ^1H NMR analysis of the crude product using CH_2Br_2 as the internal standard.

2.2 Procedure for the Synthesis of 2

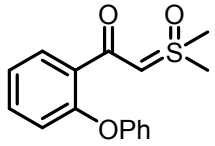
Method 1: Under N_2, trimethylsulfoxonium iodide (3.3 g, 15 mmol, 3.0 equiv) was suspended in THF (50 mL) in a flame-dried 100 mL round bottom flask, ^{t}BuOK (1.7 g, 15 mmol, 3.0 equiv) was added and the mixture was stirred at room temperature for 2 hours. After, benzoyl chloride (5 mmol, 1.0 equiv) was added. The mixture was stirred at room temperature for 3 hours and then filtered through a plug of celite beofre all volatiles were removed under vacuum. Purification by flash chromatography (DCM/MeOH = 50 :1) afforded products[1].



Method 2: Sulfurous dichloride (10 mmol, 2.0 equiv) was added to a mixture of the carboxylic acid (5 mmol, 1.0 equiv), *N,N*-dimethylformamide 3 drops in CH_2Cl_2 (30 mL) under N_2 atmosphere at 0 °C. The mixture was stirred at at room temperature overnight. Then, the excess of sulfurous dichloride and CH_2Cl_2 were removed in vacuo, obtain crude benzoyl chloride[2].

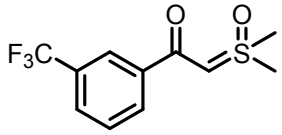
Under N_2, trimethylsulfoxonium iodide (3.3 g, 15 mmol, 3.0 equiv) was suspended in THF (50 mL) in a flame-dried 100 mL round bottom flask, ^{t}BuOK (1.7 g, 15 mmol, 3.0 equiv) was added and the mixture was stirred at room temperature for 2 hours. After, crude benzoyl chloride (5 mmol, 1.0 equiv) was added. The mixture was stirred at room temperature for 3 hours and then filtered through a plug of celite beofre all volatiles were removed under vacuum. Purification by flash chromatography (DCM/MeOH = 50 :1) afforded products [1].

Method 3: 2az was synthesized following a literature procedure[3]



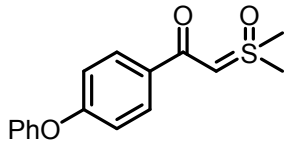
2ac

2-(dimethyl(oxo)-λ⁶-sulfanylidene)-1-(2-phenoxyphenyl)ethan-1-one (**2ac**) as cream solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.88 (d, J = 7.7 Hz, 1H), 7.32 (t, J = 7.7 Hz, 1H), 7.27 (t, J = 7.8 Hz, 2H), 7.18 (t, J = 7.5 Hz, 1H), 7.01 (t, J = 7.4 Hz, 1H), 6.91 (t, J = 8.5 Hz, 3H), 5.20 (s, 1H), 3.25 (s, 6H); ^{13}C NMR (126 MHz, Chloroform-d) δ 179.3, 157.3, 153.3, 131.7, 131.0, 129.7, 129.3, 123.7, 122.2, 120.15, 117.2, 73.9, 41.1; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{17}O_3S^+$: 289.0893 $(M + H)^+$, found: 289.0891.



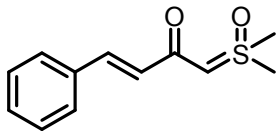
2al

2-(dimethyl(oxo)-λ⁶-sulfanylidene)-1-(3-(trifluoromethyl)phenyl)ethan-1-one (**2al**) as beige solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.06 (s, 1H), 7.98 – 7.92 (m, 1H), 7.66 (t, J = 6.2 Hz, 1H), 7.48 (q, J = 7.3 Hz, 1H), 5.19 (d, J = 2.7 Hz, 1H), 3.54 (d, J = 3.6 Hz, 6H); ^{13}C NMR (126 MHz, Chloroform-d) δ 180.2, 139.4, 130.1 (q, J = 32.3 Hz), 129.6, 128.5, 126.9 (q, J = 3.7 Hz), 123.8 (q, J = 272.4 Hz), 123.2 (q, J = 3.9 Hz), 70.2, 41.6; HRMS (ESI-TOF) m/z: calcd for $C_{11}H_{12}F_3O_2S^+$: 265.0505 $(M + H)^+$, found: 265.0507.



2ao

2-(dimethyl(oxo)-λ⁶-sulfanylidene)-1-(4-phenoxyphenyl)ethan-1-one (**2ao**) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 (d, J = 8.8 Hz, 2H), 7.35 (t, J = 8.0 Hz, 2H), 7.13 (t, J = 7.5 Hz, 1H), 7.05 – 7.01 (m, 2H), 6.99 – 6.94 (m, 2H), 5.00 (s, 1H), 3.49 (s, 6H); ^{13}C NMR (126 MHz, Chloroform-d) δ 181.3, 159.5, 156.1, 133.5, 129.7, 128.3, 123.7, 119.4, 117.5, 68.2, 42.1; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{17}O_3S^+$: 289.0893 $(M + H)^+$, found: 289.0895.



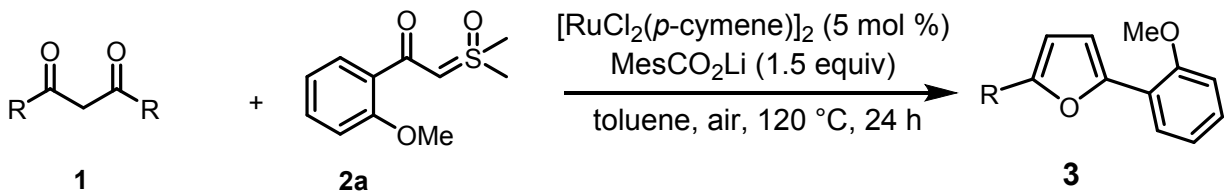
2ba

(*E*)-1-(dimethyl(oxo)-λ⁶-sulfanylidene)-4-phenylbut-3-en-2-one (**2ba**) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.54 – 7.47 (m, 2H), 7.46 – 7.41 (m, 1H), 7.39 – 7.27 (m, 3H), 6.63 – 6.55 (m, 1H), 4.59 (d, J = 1.7 Hz, 1H), 3.51 – 3.46 (m, 6H); ^{13}C NMR (126 MHz, Chloroform-d) δ 179.9, 136.4, 135.5, 129.0, 128.6, 127.6, 126.8 (d, J = 1.7 Hz), 71.8, 71.7, 42.3 (d, J = 4.5 Hz); HRMS (ESI-TOF) m/z: calcd for $C_{12}H_{15}O_2S^+$: 223.0787 $(M + H)^+$, found: 223.0789.

2.3 Procedure for the Synthesis of 3

1 was synthesized following a literature procedure[4].

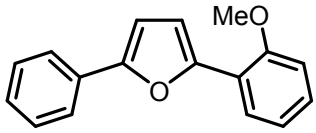
2.3.1 Procedure for Synthesis of 3aa-3aq



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

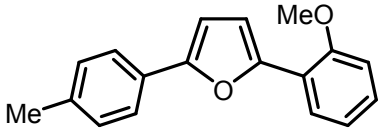
A dried 10 mL Schlenk tube was charged with **1,3-diphenylpropane-1,3-dione 1** (0.1 mmol, 1 equiv), **2-(dimethyl(oxo)-λ⁶-sulfanylidene)-1-(2-methoxyphenyl)ethan-1-one 2a** (45.3 mg, 0.2 mmol, 2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (3.1 mg, 0.005 mmol, 5 mol %), $MesCO_2Li$ (25.5 mg, 0.15 mmol, 1.5 equiv), and toluene (2 mL). The reaction mixture was heated to 120 °C for 24 hours under vigorous

stirring. Upon completion, the reaction mixture was cooled to room temperature, diluted with ethyl acetate, and filtered through a pad of celite. The filtrate was concentrated under vacuum, and the resulting residue was purified by preparative thin layer chromatography (PTLC) with hexane to give the corresponding products.



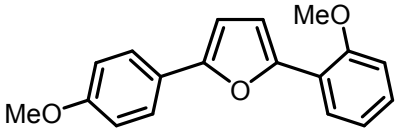
3aa

2-(2-methoxyphenyl)-5-phenylfuran （**3aa**） (20.4 mg, 82%) as a white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ8.00 – 7.97 (m, 1H), 7.76 (d, J = 7.5 Hz, 2H), 7.40 (t, J = 7.8 Hz, 2H), 7.29 – 7.22 (m, 2H), 7.06 (d, J = 7.7 Hz, 1H), 7.03 (d, J = 3.4 Hz, 1H), 6.97 (d, J = 8.2 Hz, 1H), 6.76 (d, J = 3.4 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.4, 152.2, 149.7, 130.9, 128.6, 128.0, 127.1, 125.8, 123.7, 120.7, 119.8, 112.2, 110.9, 107.4, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{15}O_2^+$: 251.1067 $(M + H)^+$, found: 251.1068.



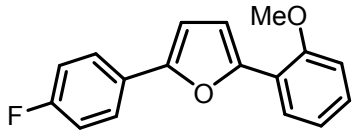
3ab

2-(2-methoxyphenyl)-5-(*p*-tolyl)furan (**3ab**) (16.9 mg, 64%) was prepared from typical procedure (hexane) as yellowish solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 – 7.96 (m, 1H), 7.65 (d, J = 8.1 Hz, 2H), 7.26 – 7.22 (m, 1H), 7.20 (d, J = 7.9 Hz, 2H), 7.05 (t, J = 7.6 Hz, 1H), 7.02 (d, J = 3.4 Hz, 1H), 6.96 (d, J = 8.2 Hz, 1H), 6.70 (d, J = 3.4 Hz, 1H), 3.95 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.4, 152.5, 149.3, 137.0, 129.3, 128.2, 127.8, 125.7, 123.7, 120.7, 119.9, 112.2, 110.9, 106.6, 55.4, 21.3; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{17}O_2^+$: 265.1223 $(M + H)^+$, found: 265.1227.



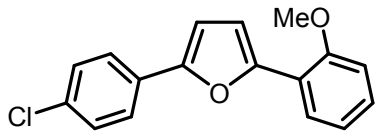
3ac

2-(2-methoxyphenyl)-5-(4-methoxyphenyl)furan (**3ac**) (13.5 mg, 48%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ7.97 – 7.95 (m, 1H), 7.72 – 7.65 (m, 2H), 7.25 – 7.21 (m, 1H), 7.06 – 7.02 (m, 1H), 7.01 (d, J = 3.4 Hz, 1H), 6.97 – 6.92 (m, 3H), 6.62 (d, J = 3.4 Hz, 1H), 3.94 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 158.9, 155.3, 152.3, 149.1, 127.7, 125.6, 125.2, 124.0, 120.7, 119.9, 114.1, 112.2, 110.9, 105.8, 55.3 (d, J = 3.4 Hz); HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{17}O_3^+$: 281.1172 $(M + H)^+$, found: 281.1177.



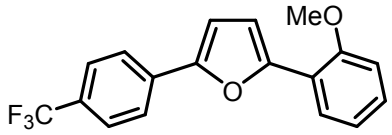
3ad

2-(4-fluorophenyl)-5-(2-methoxyphenyl)furan (**3ad**) (20.1 mg, 75%) was prepared from typical procedure (hexane) as yellowish solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.97 – 7.93 (m, 1H), 7.74 – 7.67 (m, 2H), 7.27 – 7.22 (m, 1H), 7.11 – 7.07 (m, 2H), 7.07 – 7.03 (m, 1H), 7.01 (d, J = 3.4 Hz, 1H), 6.96 (d, J = 8.3 Hz, 1H), 6.68 (d, J = 3.4 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ162.0 (d, *J* = 246.9 Hz), 155.4, 151.4, 149.8, 128.0, 127.3 (d, *J* = 3.3 Hz), 125.7, 125.4 (d, *J* = 7.9 Hz), 120.7, 119.7, 115. 7 (d, *J* = 21.9 Hz), 112.2, 111.0, 107.0 (d, *J* = 1.7 Hz), 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{14}FO_2^+$: 269.0972 $(M + H)^+$, found: 269.0977.



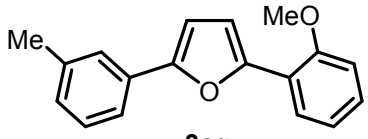
3ae

2-(4-chlorophenyl)-5-(2-methoxyphenyl)furan (**3ae**) (17 mg, 60%) was prepared from typical procedure (hexane) as colorless solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.98 – 7.92 (m, 1H), 7.69 – 7.64 (m, 2H), 7.37 – 7.33 (m, 2H), 7.27 – 7.23 (m, 1H), 7.07 – 7.03 (m, 1H), 7.02 (d, J = 3.4 Hz, 1H), 6.97 (d, J = 8.2 Hz, 1H), 6.74 (d, J = 3.5 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.5, 151.1, 150.1, 132.7, 129.4, 128.8, 128.2, 125.8, 124.9, 120.7, 119.5, 112.3, 111.0, 107.8, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{14}ClO_2^+$: 285.0677 $(M + H)^+$, found: 285.0679.



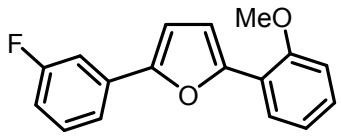
3af

2-(2-methoxyphenyl)-5-(4-(trifluoromethyl)phenyl)furan (**3af**) (24.2 mg, 76%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 – 7.94 (m, 1H), 7.85 – 7.79 (m, 2H), 7.63 (d, J = 8.2 Hz, 2H), 7.31 – 7.26 (m, 1H), 7.09 – 7.06 (m, 1H), 7.05 (d, J = 3.4 Hz, 1H), 6.98 (d, J = 8.2 Hz, 1H), 6.86 (d, J = 3.5 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.7, 150.9, 150.7, 133.9, 128.6 (q, J = 32.3 Hz), 128.5, 125.9, 125.7 (q, J = 3.9 Hz), 124.2 (q, J = 271.7 Hz), 123.6, 123.1, 120.8, 119.3, 112.4, 111.0, 109.4, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{14}F_3O_2^+$: 319.0940 $(M + H)^+$, found: 319.0944.



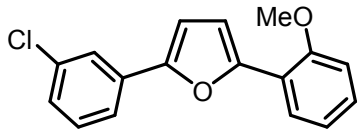
3ag

2-(2-methoxyphenyl)-5-(*m*-tolyl)furan (**3ag**) (16.7 mg, 63%) was prepared from typical procedure (hexane) as yellow solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.02 – 7.97 (m, 1H), 7.56 (d, J = 11.4 Hz, 2H), 7.28 (t, J = 7.6 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.09 – 7.05 (m, 2H), 7.02 (d, J = 3.5 Hz, 1H), 6.96 (d, J = 8.3 Hz, 1H), 6.75 – 6.73 (m, 1H), 3.94 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 155.4, 152.4, 149.6, 138.2, 130.8, 128.6, 128.0, 127.9, 125.8, 124.3, 121.0, 120.7, 119.8, 112.2, 111.0, 107.3, 55.3, 21.5. HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{17}O_2^+$: 265.1223 $(M + H)^+$, found: 265.1227.



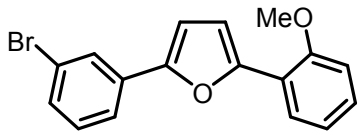
3ah

2-(3-fluorophenyl)-5-(2-methoxyphenyl)furan (**3ah**) (20.3 mg, 76%) was prepared from typical procedure (hexane) as colorless solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 – 7.93 (m, 1H), 7.53 – 7.49 (m, 1H), 7.47 – 7.40 (m, 1H), 7.37 – 7.31 (m, 1H), 7.30 – 7.22 (m, 1H), 7.09 – 7.04 (m, 1H), 7.03 (d, J = 3.5 Hz, 1H), 6.96 (d, J = 8.5 Hz, 1H), 6.97 – 6.90 (m, 1H), 6.77 (d, J = 3.5 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 163.2 (d, J = 244.9 Hz), 155.6, 151.0 (d, J = 3.1 Hz), 150.3, 133.0 (d, *J* = 8.5 Hz), 130.2 (d, *J* = 8.6 Hz), 128.3, 125.9, 120.8, 119.5, 119.3 (d, J = 2.7 Hz), 113.8 (d, *J* = 21.5 Hz), 112.2, 111.0, 110.5 (d, *J* = 23.5 Hz), 108.4, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{14}FO_2^+$: 269.0972 $(M + H)^+$, found: 269.0975.



3ai

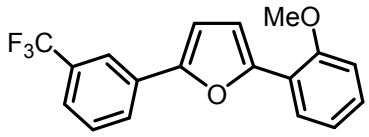
2-(3-chlorophenyl)-5-(2-methoxyphenyl)furan (**3ai**) (20 mg, 70%) was prepared from typical procedure (hexane) as cream solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.99 – 7.95 (m, 1H), 7.72 (t, J = 1.8 Hz, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.31 (t, J = 7.9 Hz, 1H), 7.28 – 7.23 (m, 1H), 7.23 – 7.19 (m, 1H), 7.06 (t, J = 7.5 Hz, 1H), 7.03 (d, J = 3.5 Hz, 1H), 6.97 (d, J = 8.0 Hz, 1H), 6.77 (d, J = 3.4 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.6, 150.7, 150.4, 134.7, 132.5, 129.9, 128.3, 127.0, 125.9, 123.6, 121.7, 120.8, 119.4, 112.3, 111.0, 108.5, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{14}ClO_2^+$: 285.0677 $(M + H)^+$, found: 285.0678.



3aj

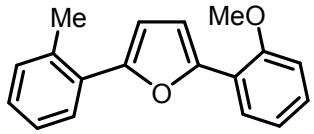
2-(3-bromophenyl)-5-(2-methoxyphenyl)furan (**3aj**) (12.1 mg, 37%) was prepared from typical procedure (hexane) as colorless solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.99 – 7.95 (m, 1H), 7.88 (t, J = 1.8 Hz, 1H), 7.68 – 7.63 (m, 1H), 7.38 – 7.35 (m, 1H), 7.26 (q, J = 7.9, 7.3 Hz, 2H), 7.09 – 7.05 (m,

1H), 7.03 (d, J = 3.5 Hz, 1H), 6.97 (d, J = 8.3 Hz, 1H), 6.77 (d, *J* = 3.5 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.6, 150.5, 150.4, 132.8, 130.2, 129.9, 128.3, 126.5, 125.9, 122.9, 122.2, 120.8, 119.4, 112.3, 111.0, 108.5, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{14}BrO_2^+$: 329.0172 $(M + H)^+$, found: 329.0175.



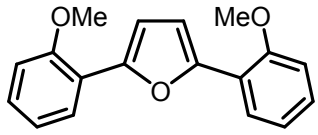
3ak

2-(2-methoxyphenyl)-5-(3-(trifluoromethyl)phenyl)furan (**3ak**) (25 mg, 79%) was prepared from typical procedure (hexane) as colorless solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.01 – 7.94 (m, 2H), 7.92 – 7.86 (m, 1H), 7.52 – 7.47 (m, 2H), 7.29 – 7.25 (m, 1H), 7.09 – 7.06 (m, 1H), 7.05 (d, J = 3.5 Hz, 1H), 6.97 (d, J = 8.2 Hz, 1H), 6.83 (d, J = 3.5 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.6, 150.64, 150.61, 131.5, 131.2 (q, J = 32.3 Hz), 129.1, 128.4, 126.6, 125.9, 124.0 (q, J = 272.4 Hz), 123.5 (q, J = 3.9 Hz), 120.8, 120.3 (q, J = 4.0 Hz), 119.4, 112.3, 111.0, 108.7, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{14}F_3O_2^+$: 319.0940 $(M + H)^+$, found: 319.0943.



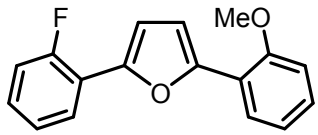
3al

2-(2-methoxyphenyl)-5-(*o*-tolyl)furan (**3al**) (13.9 mg, 53%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.97 – 7.94 (m, 1H), 7.83 – 7.77 (m, 1H), 7.29 – 7.24 (m, 3H), 7.24 – 7.18 (m, 1H), 7.06 – 7.03 (m, 2H), 6.98 (d, J = 8.2 Hz, 1H), 6.66 (d, J = 3.5 Hz, 1H), 3.96 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.5, 152.0, 149.4, 134.4, 131.2, 130.2, 128.0, 127.3, 126.9, 126.0, 125.8, 120.8, 119.8, 111.9, 110.9, 110.8, 55.4, 22.1; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{17}O_2^+$: 265.1223 $(M + H)^+$, found: 265.1227.



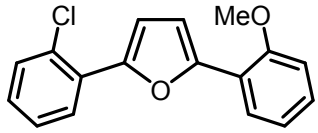
3am

2,5-bis(2-methoxyphenyl)furan (**3am**) (8.9 mg, 32%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.02 – 7.98 (m, 2H), 7.27 – 7.21 (m, 2H), 7.09 – 7.02 (m, 4H), 6.97 (d, J = 8.2 Hz, 2H), 3.96 (s, 6H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.5, 148.7, 127.8, 125.9, 120.7, 119.9, 112.4, 111.0, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{17}O_3^+$: 281.1172 $(M + H)^+$, found: 281.1176.



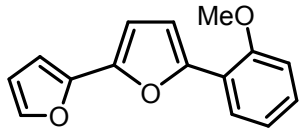
3an

2-(2-fluorophenyl)-5-(2-methoxyphenyl)furan (**3an**) (15 mg, 56%) was prepared from typical procedure (hexane) as cream solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.99 – 7.97 (m, 1H), 7.97 – 7.92 (m, 1H), 7.30 – 7.24 (m, 1H), 7.24 – 7.18 (m, 2H), 7.14 – 7.09 (m, 1H), 7.09 – 7.02 (m, 2H), 6.97 (d, J = 8.3 Hz, 1H), 6.95 (t, J = 3.7 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 158.7 (d, J = 250.7 Hz), 155.6, 149.6, 146.4 (d, J = 3.0 Hz), 128.2, 128.0 (d, J = 8.2 Hz), 125.92, 125.91 (d, J = 4.2 Hz), 124.3 (d, J = 3.5 Hz), 120.7, 119.6, 119.2 (d, J = 12.1 Hz), 125.9 (d, J = 21.6 Hz), 112.5 (d, J = 11.8 Hz),, 112.4 (d, J = 1.7 Hz), 111.0, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{14}FO_2^+$: 269.0972 $(M + H)^+$, found: 269.0974.



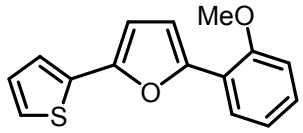
3ao

2-(2-chlorophenyl)-5-(2-methoxyphenyl)furan (**3ao**) (17.4 mg, 61%) was prepared from typical procedure (hexane) as orange solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.02 – 7.94 (m, 2H), 7.48 – 7.41 (m, 1H), 7.38 – 7.30 (m, 1H), 7.29 – 7.26 (m, 1H), 7.26 – 7.23 (m, 1H), 7.21 – 7.17 (m, 1H), 7.10 – 7.02 (m, 2H), 6.98 (d, J = 8.2 Hz, 1H), 3.97 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.7, 149.8, 148.5, 130.8, 130.0, 129.2, 128.3, 127.8, 127.7, 126.8, 126.0, 120.7, 119.5, 113.3, 112.2, 111.0, 55.4. HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{14}ClO_2^+$: 285.0677 $(M + H)^+$, found: 285.0678.



3ap

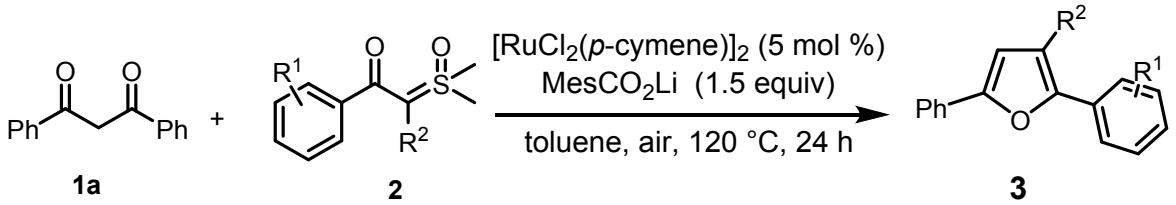
5-(2-methoxyphenyl)-2,2'-bifuran (**3ap**) (9.5 mg, 40%) was prepared from typical procedure (hexane) as black solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.97 – 7.90 (m, 1H), 7.43 (d, J = 2.0 Hz, 1H), 7.28 – 7.22 (m, 1H), 7.07 – 7.02 (m, 1H), 7.01 (d, J = 3.3 Hz, 1H), 6.96 (d, J = 8.4 Hz, 1H), 6.68 – 6.61 (m, 2H), 6.51 – 6.45 (m, 1H), 3.94 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.4, 149.5, 146.8, 145.0, 141.7, 128.1, 125.8, 120.7, 119.5, 111.8, 111.4, 110.9, 107.4, 105.0, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{15}H_{13}O_3^+$: 241.0859 $(M + H)^+$, found: 241.0860.



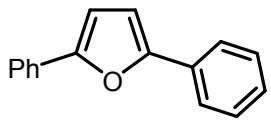
3aq

2-(2-methoxyphenyl)-5-(thiophen-2-yl)furan (**3aq**) (15.4 mg, 60%) was prepared from typical procedure (hexane) as dark brown solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.95 – 7.91 (m, 1H), 7.33 – 7.31 (m, 1H), 7.26 – 7.24 (m, 1H), 7.23 – 7.21 (m, 1H), 7.07 – 7.03 (m, 2H), 7.00 (d, J = 3.5 Hz, 1H), 6.96 (d, J = 8.2 Hz, 1H), 6.60 (d, J = 3.4 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 155.4, 149.3, 147.9, 134.0, 128.0, 127.6, 125.7, 123.9, 122.4, 120.7, 119.5, 112.1, 110.9, 107.3, 55.4; HRMS (ESI-TOF) m/z: calcd for $C_{15}H_{13}O_2S^+$: 257.0631 $(M + H)^+$, found: 257.0635.

2.3.2 Procedure for Synthesis of 3ba-3bz

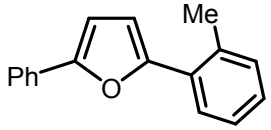


A dried 10 mL Schlenk tube was charged with **1,3-diphenylpropane-1,3-dione 1a** (22.4 mg, 0.1 mmol, 1 equiv), **sulfoxonium ylide 2** (0.2 mmol, 2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (3.1 mg, 0.005 mmol, 5 mol %), $MesCO_2Li$ (25.5 mg, 0.15 mmol, 1.5 equiv), and toluene (2 mL). The reaction mixture was heated to 120 °C for 24 hours under vigorous stirring. Upon completion, the reaction mixture was cooled to room temperature, diluted with ethyl acetate, and filtered through a pad of celite. The filtrate was concentrated under vacuum, and the resulting residue was purified by preparative thin layer chromatography (PTLC) with hexane to give the corresponding products.



3ba

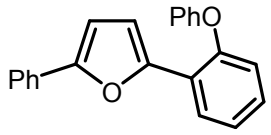
2,5-diphenylfuran (**3ba**) (9.2 mg, 42%) was prepared from typical procedure (hexane) as beige solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.79 – 7.74 (m, 4H), 7.42 (t, J = 7.8 Hz, 4H), 7.30 – 7.26 (m, 2H), 6.75 (s, 2H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.3, 130.7, 128.7, 127.3, 123.7, 107.2; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{13}O^+$: 221.0961 $(M + H)^+$, found: 221.0957.



3bb

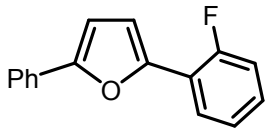
2-phenyl-5-(*o*-tolyl)furan (**3bb**) (17 mg, 73%) was prepared from typical procedure (hexane) as yellow oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.81 (d, J = 7.8 Hz, 1H), 7.78 – 7.75 (m, 2H), 7.42 (t, J = 7.8 Hz, 2H), 7.31 (d, J = 6.7 Hz, 1H), 7.28 (d, J = 7.4 Hz, 2H), 7.25 – 7.21 (m, 1H), 6.79 (d, J = 3.5 Hz, 1H), 6.66 (d, J = 3.4 Hz, 1H), 2.59 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.1, 153.0,

134.4, 131.3, 130.8, 130.0, 128.7, 127.4, 127.3, 126.8, 126.0, 123.7, 110.6, 106.9, 22.1; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{15}O^+$: 235.1117 $(M + H)^+$, found: 235.1117.



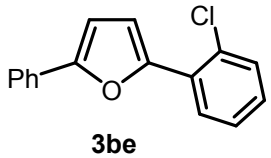
3bc

2-(2-phenoxyphenyl)-5-phenylfuran (**3bc**) (16.4 mg, 53%) was prepared from typical procedure (hexane) as yellow oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.13 – 8.08 (m, 1H), 7.79 – 7.74 (m, 2H), 7.43 (t, J = 7.8 Hz, 2H), 7.41 – 7.36 (m, 2H), 7.32 – 7.28 (m, 1H), 7.28 – 7.23 (m, 2H), 7.17 – 7.12 (m, 1H), 7.10 – 7.06 (m, 2H), 7.02 (d, J = 3.5 Hz, 1H), 7.01 – 6.98 (m, 1H), 6.75 (d, J = 3.5 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 156.9, 152.7, 152.4, 149.0, 130.7, 129.8, 128.7, 128.0, 127.3, 126.2, 123.9, 123.8, 123.2, 122.8, 119.8, 118.3, 112.5, 107.5; HRMS (ESI-TOF) m/z: calcd for $C_{22}H_{17}O_2^+$: 313.1223 $(M + H)^+$, found: 313.1226.



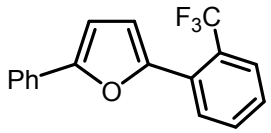
3bd

2-(2-fluorophenyl)-5-phenylfuran (**3bd**) (14.2 mg, 60%) was prepared from typical procedure (hexane) as yellow oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 – 7.91 (m, 1H), 7.80 – 7.74 (m, 2H), 7.43 (t, J = 7.8 Hz, 2H), 7.32 – 7.28 (m, 1H), 7.26 – 7.21 (m, 2H), 7.17 – 7.11 (m, 1H), 6.95 (t, J = 3.6 Hz, 1H), 6.79 (d, J = 3.5 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 158.7 (d, J = 250.7 Hz), 153.2, 147.4 (d, J = 3.1 Hz), 130.5, 128.7, 128.2 (d, J = 8.4Hz), 127.5, 125.8 (d, J = 3.2 Hz), 124.3 (d, J = 3.5 Hz), 123.9, 119.0 (d, J = 12.0 Hz), 115.9 (d, J = 21.4 Hz), 112.4 (d, J = 12.1 Hz), 107.5 (d, J = 1.8 Hz); HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}FO^+$: 239.0867 $(M + H)^+$, found: 239.0866.



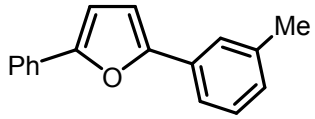
3be

2-(2-chlorophenyl)-5-phenylfuran (**3be**) (10.6 mg, 42%) was prepared from typical procedure (hexane) as yellow white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ8.01 – 7.97 (m, 1H), 7.79 – 7.75 (m, 2H), 7.47 – 7.45 (m, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.38 – 7.33 (m, 1H), 7.32 – 7.28 (m, 1H), 7.24 (d, J = 3.5 Hz, 1H), 7.23 – 7.19 (m, 1H), 6.80 (d, J = 3.6 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.3, 149.5, 130.8, 130.5, 130.0, 129.1, 128.7, 127.9, 127.7, 127.6, 126.9, 123.9, 113.2, 107.2; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}ClO^+$: 255.0571 $(M + H)^+$, found: 255.0572.



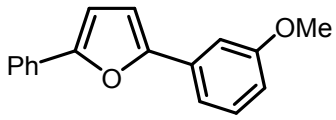
3bf

2-phenyl-5-(2-(trifluoromethyl)phenyl)furan (**3bf**) (13.5 mg, 47%) was prepared from typical procedure (hexane) as yellow oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.84 (d, J = 7.9 Hz, 1H), 7.79 (d, J = 8.1 Hz, 1H), 7.79 – 7.73 (m, 2H), 7.60 (t, J = 7.6 Hz, 1H), 7.46 – 7.38 (m, 3H), 7.30 (t, J = 7.4 Hz, 1H), 6.82 (d, J = 3.5 Hz, 1H), 6.78 (d, J = 3.5 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ154.5, 150.0, 131.7, 130.5, 129.6, 129.5 (d, *J* = 2.1 Hz), 128.7, 127.8, 127.5, 127.3, 126.2 (d, *J* = 31.3 Hz), 124.1 (q, J = 273.3 Hz), 123.9, 112.2 (q, *J* = 3.1 Hz), 107.0; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{12}F_3O^+$: 289.0835 $(M + H)^+$, found: 289.0838.



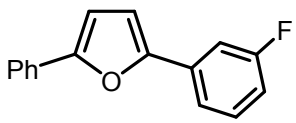
3bg

2-phenyl-5-(*m*-tolyl)furan (**3bg**) (12.1 mg, 52%) was prepared from typical procedure (hexane) as cream solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.79 – 7.73 (m, 2H), 7.60 – 7.53 (m, 2H), 7.42 (t, J = 7.8 Hz, 2H), 7.34 – 7.24 (m, 2H), 7.10 (d, J = 7.5 Hz, 1H), 6.74 (q, J = 3.4 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.5, 153.2, 138.3, 130.8, 130.7, 128.7, 128.6, 128.2, 127.3, 124.3, 123.7, 120.9, 107.2, 107.1, 21.5; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{15}O^+$: 235.1117 $(M + H)^+$, found: 235.1120.



3bh

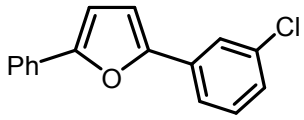
2-(3-methoxyphenyl)-5-phenylfuran (**3bh**) (9.4 mg, 38%) was prepared from typical procedure (hexane) as yellow oil. ^{1}H NMR (500 MHz, Chloroform-d) δ7.77 – 7.74 (m, 2H), 7.44 – 7.39 (m, 2H), 7.37 – 7.32 (m, 2H), 7.32 – 7.26 (m, 2H), 6.86 – 6.82 (m, 1H), 6.75 (s, 2H), 3.89 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 159.9, 153.4, 153.1, 132.0, 130.7, 129.8, 128.7, 127.4, 123.7, 116.4, 112.9, 109.2, 107.6, 107.2, 55.3; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{15}O_2^+$: 251.1067 $(M + H)^+$, found: 251.1070.



3bi

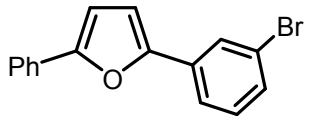
2-(3-fluorophenyl)-5-phenylfuran (**3bi**) (8.8 mg, 37%) was prepared from typical procedure (hexane) as cream solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.79 – 7.72 (m, 2H), 7.51 (d, J = 7.8 Hz, 1H), 7.48 – 7.39 (m, 3H), 7.39 – 7.34 (m, 1H), 7.33 – 7.27 (m, 1H), 7.00 – 6.92 (m, 1H), 6.78 – 6.74 (m, 2H); ^{13}C

NMR (126 MHz, Chloroform-d) δ163.2 (d, J = 245.1 Hz), 153.8, 152.0 (d, J = 3.1 Hz), 132.8 (d, J = 8.5 Hz), 130.5, 130.3 (d, J = 8.5 Hz), 128.7, 127.6, 123.8, 119.3 (d, J = 2.9 Hz), 114.0 (d, J = 21.5 Hz), 110.5 (d, J = 23.5 Hz), 108.3, 107.3; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}FO^+$: 239.0867 $(M + H)^+$, found: 239.0868.



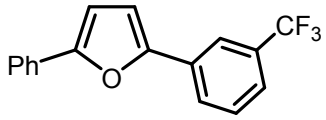
3bj

2-(3-chlorophenyl)-5-phenylfuran (**3bj**) (11.9 mg, 47%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ7.77 – 7.74 (m, 2H), 7.73 (t, J = 1.9 Hz, 1H), 7.61 (m, 1H), 7.45 – 7.40 (m, 2H), 7.33 (t, J = 7.9 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.25 – 7.22 (m, 1H), 6.78 – 6.74 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.9, 151.8, 134.7, 132.4, 130.4, 130.0, 128.7, 127.6, 127.1, 123.8, 123.6, 121.7, 108.3, 107.3; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}ClO^+$: 255.0571 $(M + H)^+$, found: 255.0573.



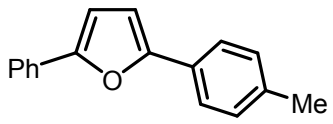
3bk

2-(3-bromophenyl)-5-phenylfuran (**3bk**) (16.8 mg, 56%) was prepared from typical procedure (hexane) as cream solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.88 (t, J = 1.8 Hz, 1H), 7.79 – 7.72 (m, 2H), 7.67 – 7.64 (m, 1H), 7.45 – 7.40 (m, 2H), 7.40 – 7.37 (m, 1H), 7.32 – 7.28 (m, 1H), 7.27 – 7.25 (m, 1H), 6.77 – 6.74 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-d) δ 154.0, 151.6, 132.6, 130.4, 130.2, 130.1, 128.7, 127.6, 126.5, 123.8, 122.9, 122.1, 108.3, 107.2; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}BrO^+$: 299.0066 $(M + H)^+$, found: 299.0065.



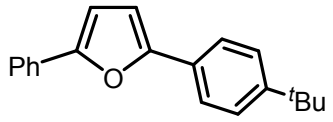
3bl

2-phenyl-5-(3-(trifluoromethyl)phenyl)furan (**3bl**) (18.1 mg, 63%) was prepared from typical procedure (hexane) as yellowish solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.97 (s, 1H), 7.93 – 7.87 (m, 1H), 7.77 (d, J = 7.4 Hz, 2H), 7.57 – 7.48 (m, 2H), 7.44 (t, J = 7.8 Hz, 2H), 7.31 (t, J = 7.5 Hz, 1H), 6.83 (d, J = 3.5 Hz, 1H), 6.77 (d, J = 3.5 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ154.2, 151.7, 131.4, 131.2 (q, J = 32.3 Hz), 130.3, 129.2, 128.8, 127.7, 126.6, 124.1 (q, J = 272.4 Hz), 123.9, 123.7 (d, J = 4.9 Hz), 120.3 (d, J = 4.0 Hz), 108.6, 107.3; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{12}F_3O^+$: 289.0835 $(M + H)^+$, found: 289.0836.



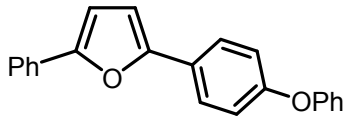
3bm

2-phenyl-5-(*p*-tolyl)furan (**3bm**) (11.9 mg, 51%) was prepared from typical procedure (hexane) as pale yellow solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.64 – 7.60 (m, 2H), 7.52 (d, J = 8.1 Hz, 2H), 7.27 (t, J = 7.7 Hz, 2H), 7.16 – 7.11 (m, 1H), 7.09 (d, J = 7.9 Hz, 2H), 6.62 – 6.59 (m, 1H), 6.57 – 6.53 (m, 1H), 2.25 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.6, 152.9, 137.2, 130.8, 129.4, 128.7, 128.1, 127.2, 123.7, 123.6, 107.2, 106.5, 21.3; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{15}O^{+}$: 235.1117 $(M + H)^{+}$, found: 235.1121.



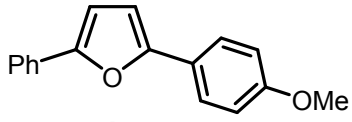
3bn

2-(4-(*tert*-butyl)phenyl)-5-phenylfuran (**3bn**) (14.4 mg, 52%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 – 7.74 (m, 2H), 7.71 – 7.67 (m, 2H), 7.46 – 7.43 (m, 2H), 7.42 (t, J = 7.9 Hz, 2H), 7.30 – 7.25 (m, 1H), 6.76 – 6.73 (m, 1H), 6.71 – 6.68 (m, 1H), 1.36 (s, 9H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.5, 153.0, 150.4, 130.9, 128.7, 128.1, 127.2, 125.6, 123.6, 123.5, 107.2, 106.6, 34.6, 31.3; HRMS (ESI-TOF) m/z: calcd for $C_{20}H_{21}O^{+}$: 277.1587 $(M + H)^{+}$, found: 277.1586.



3bo

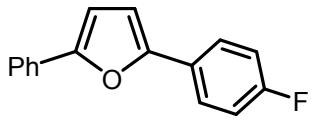
2-(4-phenoxyphenyl)-5-phenylfuran (**3bo**) (14.1 mg, 45%) was prepared from typical procedure (hexane) as yellowish solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.78 – 7.69 (m, 4H), 7.41 (t, J = 7.8 Hz, 2H), 7.39 – 7.35 (m, 2H), 7.30 – 7.25 (m, 1H), 7.14 (t, J = 7.4 Hz, 1H), 7.10 – 7.03 (m, 4H), 6.74 (d, J = 3.5 Hz, 1H), 6.67 (d, J = 3.4 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 157.0, 156.6, 153.1, 153.0, 130.7, 129.8, 128.7, 127.2, 126.2, 125.2, 123.6, 123.4, 119.1, 118.9, 107.2, 106.5; HRMS (ESI-TOF) m/z: calcd for $C_{22}H_{17}O_{2}^{+}$: 313.1223 $(M + H)^{+}$, found: 313.1228.



3bp

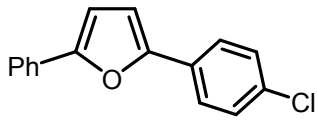
2-(4-methoxyphenyl)-5-phenylfuran (**3bp**) (13.8 mg, 55%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ7.75 – 7.72 (m, 2H), 7.71 – 7.67 (m, 2H), 7.40 (t, J = 7.8 Hz, 2H), 7.30 – 7.22 (m, 1H), 6.97 – 6.94 (m, 2H), 6.72 (d, J = 3.4 Hz, 1H), 6.61 (d, J = 3.4 Hz, 1H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-d) δ 159.0, 153.4, 152.6, 130.9, 128.6,

127.1, 125.2, 123.9, 123.5, 114.1, 107.2, 105.6, 55.3; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{15}O_2^+$: 251.1067 $(M + H)^+$, found: 251.1070.



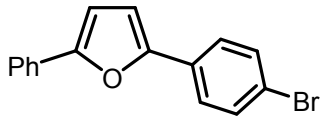
3bq

2-(4-fluorophenyl)-5-phenylfuran (**3bq**) (13.8 mg, 58%) was prepared from typical procedure (hexane) as cream solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.79 – 7.68 (m, 4H), 7.42 (t, J = 7.8 Hz, 2H), 7.32 – 7.25 (m, 1H), 7.14 – 7.08 (m, 2H), 6.75 – 6.72 (m, 1H), 6.68 – 6.66 (m, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 162.1 (d, J = 247.1 Hz), 153.3, 152.5, 130.6, 128.7, 127.4, 127.3, 127.1 (d, J = 3.5 Hz), 125.4 (d, J = 7.9 Hz), 123.7, 123.6, 115.7 (d, J = 21.9 Hz), 107.2, 106.8 (d, J = 1.6 Hz); HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}FO^+$: 239.0867 $(M + H)^+$, found: 239.0869.



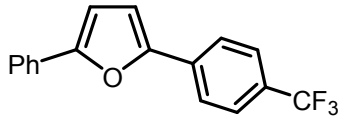
3br

2-(4-chlorophenyl)-5-phenylfuran (**3br**) (12.9 mg, 51%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.79 – 7.71 (m, 2H), 7.70 – 7.62 (m, 2H), 7.42 (t, J = 7.7 Hz, 2H), 7.37 (d, J = 8.6 Hz, 2H), 7.29 (t, J = 7.4 Hz, 1H), 6.74 (q, J = 3.5 Hz, 2H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.6, 152.2, 132.9, 130.5, 129.2, 128.9, 128.7, 127.5, 124.9, 123.7, 107.7, 107.3; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}ClO^+$: 255.0571 $(M + H)^+$, found: 255.0570.



3bs

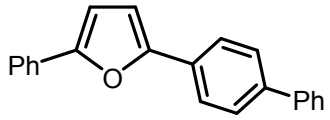
2-(4-bromophenyl)-5-phenylfuran (**3bs**) (13.2 mg, 44%) was prepared from typical procedure (hexane) as white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 – 7.71 (m, 2H), 7.62 – 7.59 (m, 2H), 7.54 – 7.51 (m, 2H), 7.42 (t, J = 7.8 Hz, 2H), 7.31 – 7.27 (m, 1H), 6.75 – 6.72 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.7, 152.2, 131.8, 130.5, 129.6, 128.7, 127.5, 125.1, 123.7, 121.0, 107.8, 107.3; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{12}BrO^+$: 299.0066 $(M + H)^+$, found: 299.0067.



3bt

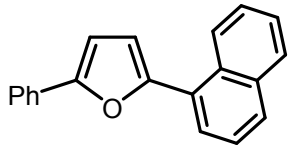
2-phenyl-5-(4-(trifluoromethyl)phenyl)furan (**3bt**) (15.2 mg, 53%) was prepared from typical procedure (hexane) as light yellow solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.83 (d, J = 8.1 Hz, 2H), 7.79 – 7.73 (m, 2H), 7.65 (d, J = 8.2 Hz, 2H), 7.43 (t, J = 7.8 Hz, 2H), 7.34 – 7.29 (m, 1H), 6.86 (d, J = 3.5 Hz, 1H), 6.77 (d, J = 3.5 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ154.4, 151.7, 133.8, 130.3,

128.81 (q, *J* = 31.5 Hz), 128.78, 127.8, 125.7 (q, *J* = 3.9 Hz), 124.2 (q, *J* = 271.8 Hz), 123.9, 123.6, 109.2, 107.4; HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{12}F_3O^+$: 289.0835 $(M + H)^+$, found: 289.0839.



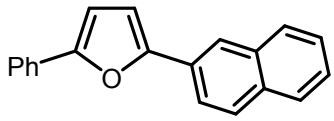
3bu

2-([1,1'-biphenyl]-4-yl)-5-phenylfuran (**3bu**) (17.7 mg, 60%) was prepared from typical procedure (hexane) as colorless solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.86 – 7.82 (m, 2H), 7.81 – 7.75 (m, 2H), 7.70 – 7.62 (m, 4H), 7.47 (t, J = 7.7 Hz, 2H), 7.43 (t, J = 7.8 Hz, 2H), 7.37 (t, J = 7.4 Hz, 1H), 7.29 (t, J = 7.4 Hz, 1H), 6.81 – 6.76 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.4, 153.1, 140.6, 139.9, 130.7, 129.7, 128.8, 128.7, 127.4, 126.9, 124.1, 123.7, 107.4, 107.3; HRMS (ESI-TOF) m/z: calcd for $C_{22}H_{17}O^+$: 297.1274 $(M + H)^+$, found: 297.1274.



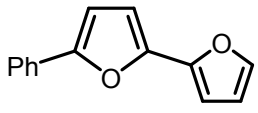
3bv

2-(naphthalen-1-yl)-5-phenylfuran (**3bv**) (9.2 mg, 34%) was prepared from typical procedure (hexane) as yellow oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.54 (d, J = 8.6 Hz, 1H), 7.93 – 7.90 (m, 1H), 7.86 (d, J = 8.3 Hz, 1H), 7.85 – 7.83 (m, 1H), 7.83 – 7.77 (m, 2H), 7.60 – 7.56 (m, 1H), 7.56 – 7.52 (m, 2H), 7.46 – 7.41 (m, 2H), 7.32 – 7.28 (m, 1H), 6.87 (d, J = 3.4 Hz, 1H), 6.84 (d, J = 3.4 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.8, 152.9, 134.0, 130.8, 130.2, 128.7, 128.6, 128.5, 128.4, 127.4, 126.6, 126.0, 125.9, 125.5, 125.3, 123.7, 111.4, 106.9; HRMS (ESI-TOF) m/z: calcd for $C_{20}H_{15}O^+$: 271.1117 $(M + H)^+$, found: 271.1115.



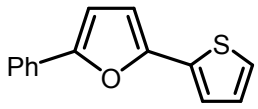
3bw

2-(naphthalen-2-yl)-5-phenylfuran (**3bw**) (12.1 mg, 45%) was prepared from typical procedure (hexane) as yellow solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.23 (s, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.87 (d, J = 8.6 Hz, 1H), 7.87 – 7.79 (m, 4H), 7.53 – 7.47 (m, 2H), 7.47 – 7.43 (m, 2H), 7.33 – 7.29 (m, 1H), 6.87 (d, J = 3.5 Hz, 1H), 6.80 (d, J = 3.5 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.6, 153.4, 133.6, 132.7, 130.7, 128.7, 128.4, 128.1, 128.0, 127.8, 127.4, 126.5, 125.9, 123.8, 122.2, 121.9, 107.9, 107.4; HRMS (ESI-TOF) m/z: calcd for $C_{20}H_{15}O^+$: 271.1117 $(M + H)^+$, found: 271.1118.



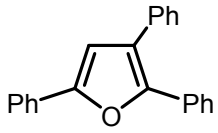
3bx

5-phenyl-2,2'-bifuran (**3bx**) (11.4 mg, 54%) was prepared from typical procedure (hexane) as reddish black oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.75 – 7.69 (m, 2H), 7.44 (s, 1H), 7.40 (t, J = 7.8 Hz, 2H), 7.31 – 7.24 (m, 1H), 6.72 (d, J = 3.5 Hz, 1H), 6.65 – 6.63 (m, 2H), 6.52 – 6.46 (m, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.1, 146.5, 146.0, 141.8, 130.4, 128.7, 127.4, 123.7, 111.5, 107.2, 106.8, 105.2; HRMS (ESI-TOF) m/z: calcd for $C_{14}H_{11}O_2^+$: 211.0754 $(M + H)^+$, found: 211.0759.



3by

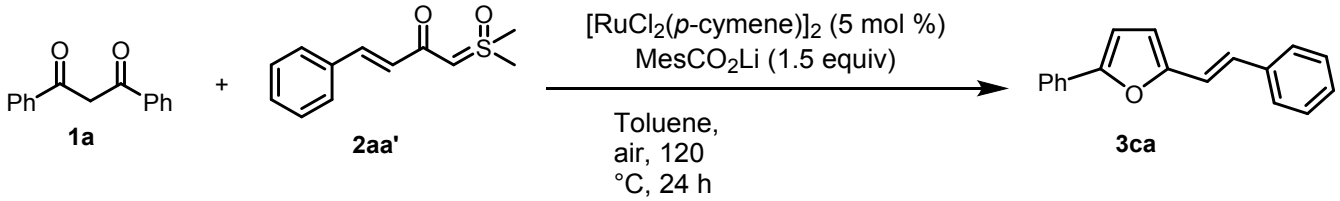
2-phenyl-5-(thiophen-2-yl)furan (**3by**) (12.5 mg, 55%) was prepared from typical procedure (hexane) as black solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.76 – 7.69 (m, 2H), 7.41 (t, J = 7.8 Hz, 2H), 7.34 – 7.31 (m, 1H), 7.30 – 7.26 (m, 1H), 7.26 – 7.23 (m, 1H), 7.10 – 7.04 (m, 1H), 6.71 (d, J = 3.4 Hz, 1H), 6.59 (d, J = 3.5 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-d) δ 152.9, 148.9, 133.7, 130.5, 128.7, 127.7, 127.4, 124.1, 123.7, 122.5, 107.2, 107.1; HRMS (ESI-TOF) m/z: calcd for $C_{14}H_{11}OS^+$: 227.0525 $(M + H)^+$, found: 227.0529.



3bz

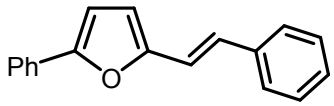
2,3,5-triphenylfuran (**3bz**) (7.9 mg, 27%) as a white solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.80 – 7.73 (m, 2H), 7.63 – 7.59 (m, 2H), 7.49 – 7.46 (m, 2H), 7.44 – 7.37 (m, 4H), 7.35 – 7.28 (m, 4H), 7.28 – 7.23 (m, 1H), 6.82 (s, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 152.5, 147.9, 134.3, 131.1, 130.5, 128.7, 128.7, 128.7, 128.4, 127.5, 127.5, 127.3, 126.1, 124.5, 123.8, 109.4; HRMS (ESI-TOF) m/z: calcd for $C_{22}H_{17}O^+$: 297.1274 $(M + H)^+$, found: 297.1275.

2.3.3 Procedure for Synthesis of 3ca



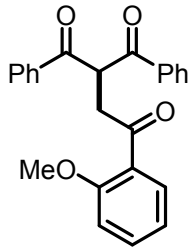
A dried 10 mL Schlenk tube was charged with **1,3-diphenylpropane-1,3-dione 1a** (22.4 mg, 0.1 mmol, 1 equiv), **(*E*)-1-(dimethyl(oxo)-λ^6-sulfanylidene)-4-phenylbut-3-en-2-one 2aa'** (44.5mg, 0.2 mmol), $[RuCl_2(p\text{-cymene})]_2$ (3.1 mg, 0.005 mmol, 5 mol %), $MesCO_2Li$ (25.5 mg, 0.15 mmol, 1.5 equiv), and toluene (2 mL). The reaction mixture was heated to 120 °C for 24 hours under vigorous stirring. Upon completion, the reaction mixture was cooled to room temperature, diluted with ethyl acetate, and filtered through a pad of celite. The filtrate was concentrated under vacuum, and the resulting residue

was purified by preparative thin layer chromatography (PTLC) with hexane to give the corresponding products (**3ca**).

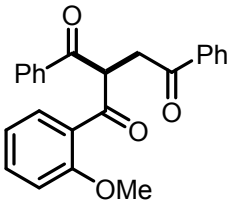


3ca

(*E*)-2-phenyl-5-styrylfuran (**3ca**) (6.7 mg, 27%) as a pale yellow solid. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 – 7.71 (m, 2H), 7.50 (d, J = 7.3 Hz, 2H), 7.40 (t, J = 7.8 Hz, 2H), 7.36 (t, J = 7.7 Hz, 2H), 7.31 – 7.21 (m, 2H), 7.13 (d, J = 16.2 Hz, 1H), 6.92 (d, J = 16.3 Hz, 1H), 6.70 (d, J = 3.5 Hz, 1H), 6.44 (d, J = 3.5 Hz, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 153.5, 152.8, 137.1, 130.6, 128.7, 127.5, 127.4, 126.9, 126.3, 123.8, 116.4, 111.1, 107.3; HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{15}O^{+}$: 247.1117 $(M + H)^{+}$, found: 247.1115.

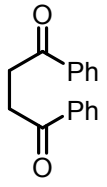


4a



5a

^{1}H NMR (500 MHz, Chloroform-d) δ 8.10 – 8.05 (m, 2H), 8.05 – 7.98 (m, 3H), 7.96 – 7.90 (m, 2H), 7.62 – 7.55 (m, 3H), 7.53 – 7.42 (m, 6H), 7.02 (t, J = 7.6 Hz, 1H), 6.88 (d, J = 8.7 Hz, 1H), 6.18 – 6.09 (m, 1H), 4.03 – 3.97 (m, 1H), 3.86 (s, 0.5H), 3.80 (d, J = 6.4 Hz, 0.37H), 3.47 (s, 3H), 3.37 – 3.31 (m, 1H); ^{13}C NMR (126 MHz, Chloroform-d) δ 197.0, 196.8, 195.2, 158.6, 136.3, 135.6, 134.6, 133.3, 133.2, 131.5, 128.9, 128.8, 128.6, 128.6, 128.2, 125.6, 121.0, 111.4, 55.6, 54.9, 37.4; HRMS (ESI-TOF) m/z: calcd for $C_{24}H_{21}O_{4}^{+}$: 373.1434 $(M + H)^{+}$, found: 373.1436. (**4a:5a**=1:6)



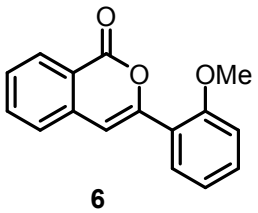
9

1,4-diphenylbutane-1,4-dione[5] (**9**) ^{1}H NMR (500 MHz, Chloroform-d) δ 8.07 – 8.03 (m, 4H), 7.61 – 7.56 (m, 2H), 7.49 (t, J = 7.7 Hz, 4H), 3.48 (s, 4H); ^{13}C NMR (126 MHz, Chloroform-d) δ 198.7, 136.7, 133.2, 128.6, 128.1, 32.6.

3.Procedure for Gram-Scale Experiment of 3aa

A dried 150 mL Schlenk tube was charged with **1,3-diphenylpropane-1,3-dione 1a** (1.0 g, 4.5 mmol, 1 equiv), **2-(dimethyl(oxo)-λ^{6}-sulfanylidene)-1-(2-methoxyphenyl)ethan-1-one 2a** (2.0 g, 9.0 mmol, 2

equiv), $[RuCl_2(p\text{-Cymene})]_2$ (137.8 mg, 0.225 mmol, 5 mol %), $MesCO_2Li$ (1.1g, 6.75 mmol, 1.5 equiv), and toluene (90 mL). The reaction mixture was heated to 120 °C for 48 hours under vigorous stirring. Upon completion, the reaction mixture was cooled to room temperature, diluted with ethyl acetate, and filtered through a pad of celite. The filtrate was concentrated under vacuum, and the resulting residue was purified by preparative thin layer chromatography (PTLC) with hexane to give the corresponding products **2-(2-methoxyphenyl)-5-phenylfuran** (**3aa**) (0.686 g, 61%) as a white solid.



6

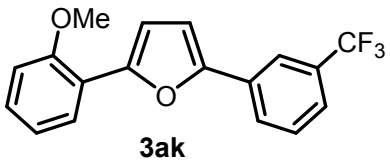
3-(2-methoxyphenyl)-*1H*-isochromen-1-one (**6**) (147.6 mg 13%) was also isolated as a yellow solid. ^1H NMR (500 MHz, Chloroform-d) δ 8.31 (d, J = 7.9 Hz, 1H), 8.01 – 7.96 (m, 1H), 7.75 – 7.67 (m, 1H), 7.53 – 7.46 (m, 2H), 7.41 – 7.37 (m, 2H), 7.08 (t, J = 7.6 Hz, 1H), 7.02 (d, J = 8.3 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 162.7, 157.1, 150.4, 138.0, 134.6, 130.7, 129.4, 128.8, 128.0, 126.3, 120.8, 120.7, 120.6, 111.3, 107.0, 55.6; HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{13}O_3^+$: 253.0859 $(M + H)^+$, found: 253.0857.

4.Procedure for Gram-Scale Experiment of 3ad

A dried 150 mL Schlenk tube was charged with **1,3-bis(4-fluorophenyl)propane-1,3-dione 1d** (1.3 g, 5.0 mmol, 1 equiv), **2-(dimethyl(oxo)-λ⁶-sulfanylidene)-1-(2-methoxyphenyl)ethan-1-one 2a** (2.3 g, 10.0 mmol, 2 equiv), $[RuCl_2(p\text{-Cymene})]_2$ (153.1 mg, 0.25 mmol, 5 mol %), $MesCO_2Li$ (1.3g, 7.5 mmol, 1.5 equiv), and toluene (100 mL). The reaction mixture was heated to 120 °C for 48 hours under vigorous stirring. Upon completion, the reaction mixture was cooled to room temperature, diluted with ethyl acetate, and filtered through a pad of celite. The filtrate was concentrated under vacuum, and the resulting residue was purified by preparative thin layer chromatography (PTLC) with hexane to give the corresponding products **2-(4-fluorophenyl)-5-(2-methoxyphenyl)furan** (**3ad**) (0.890 g, 66%) as a white solid.

5. X-Ray Crystallographic Data of 3ak

Crystal structure and data of 2-(2-methoxyphenyl)-5-(3-(trifluoromethyl)phenyl)furan (**3ak**) (CCDC 1918495, Displacement ellipsoids are drawn at the 50% probability level.)



3ak

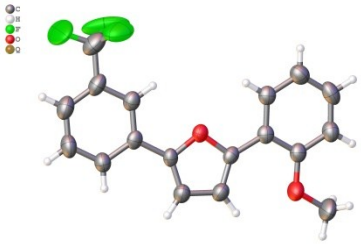


Table S3 Crystal data and structure refinement for 3ak.

Empirical formula	$C_{18}H_{13}F_3O_2$
Formula weight	318.28
Temperature/K	295.5(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.501(3)
b/Å	16.731(5)
c/Å	9.633(2)
α/°	90.00
β/°	99.37(3)
γ/°	90.00
Volume/Å^3	1510.8(7)
Z	4
ρ_{calc}g/cm^3	1.346
μ/mm^{-1}	0.112
F(000)	632.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.42 to 50
Index ranges	$-10 \le h \le 11$, $-19 \le k \le 19$, $-11 \le l \le 11$
Reflections collected	8734
Independent reflections	2659 [R_{int} = 0.1477, R_{sigma} = 0.1036]
Data/restraints/parameters	2659/34/237
Goodness-of-fit on F^2	0.971
Final R indexes [I>=2σ (I)]	R_1 = 0.0932, wR_2 = 0.2108
Final R indexes [all data]	R_1 = 0.1319, wR_2 = 0.2718
Largest diff. peak/hole/e Å^{-3}	0.43/-0.64

Reference

1 (*a*) R. M. P. Dias and A. C. B. Burtoloso, *Org. Lett.*, 2016, **18**, 3034; (*b*) A. M. Phelps, V. S. Chan, J. G. Napolitano, S. W. Krabbe, J. M. Schomaker and S. Shekhar, *J. Org. Chem.*, 2016, **81**, 4158; (*c*) M. Barday, C. Janot, N. R. Halcovitch, J. Muir and C. Aissa, *Angew. Chem. Int. Ed.*, 2017, **56**, 13117.

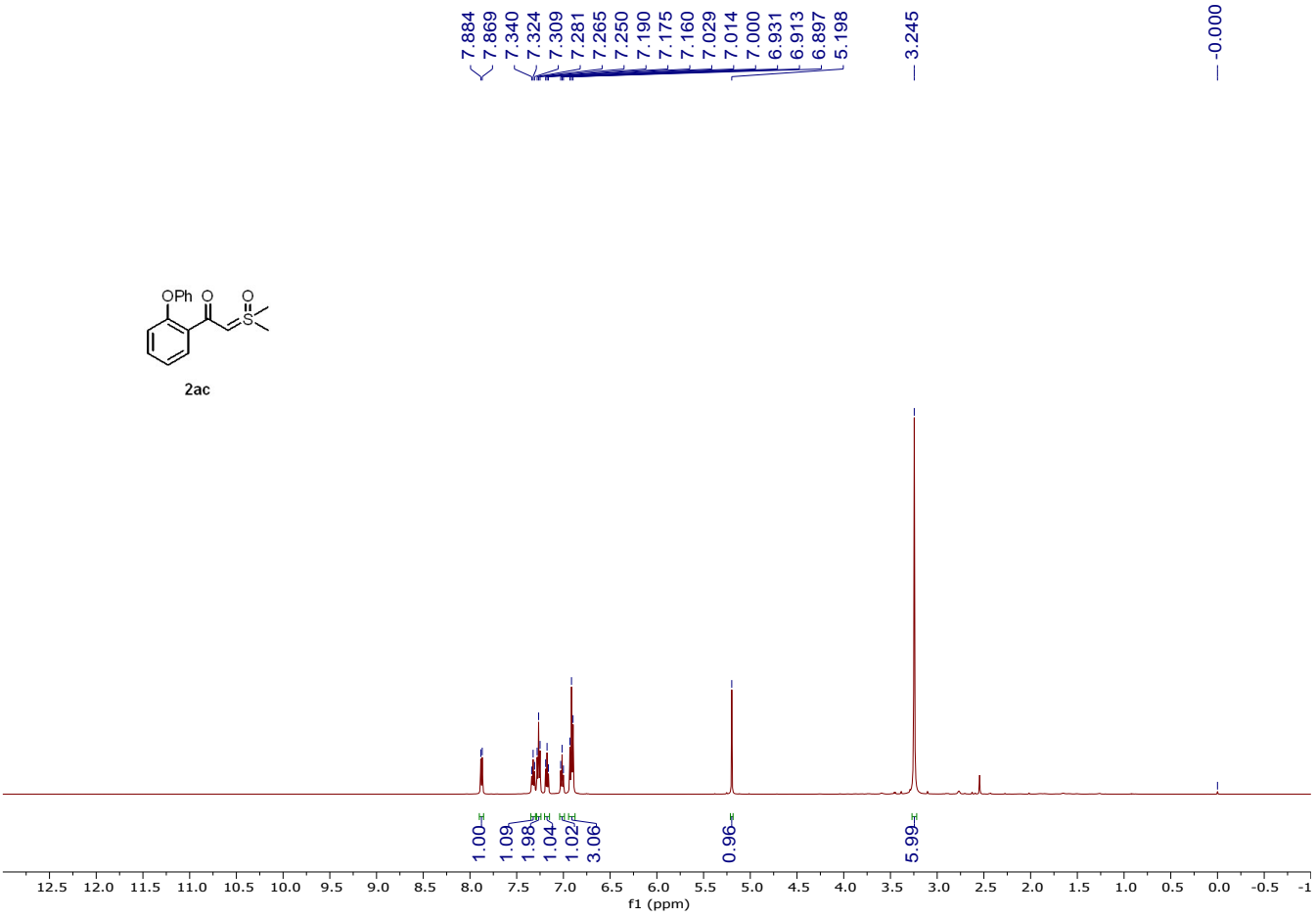
2 S.-S. Zhang, J.-Q. Wu, Y.-X. Lao, X.-G. Liu, Y. Liu, W.-X. Lv, D.-H. Tan, Y.-F. Zeng and H. Wang, *Org. Lett.*, 2014, **16**, 6412.

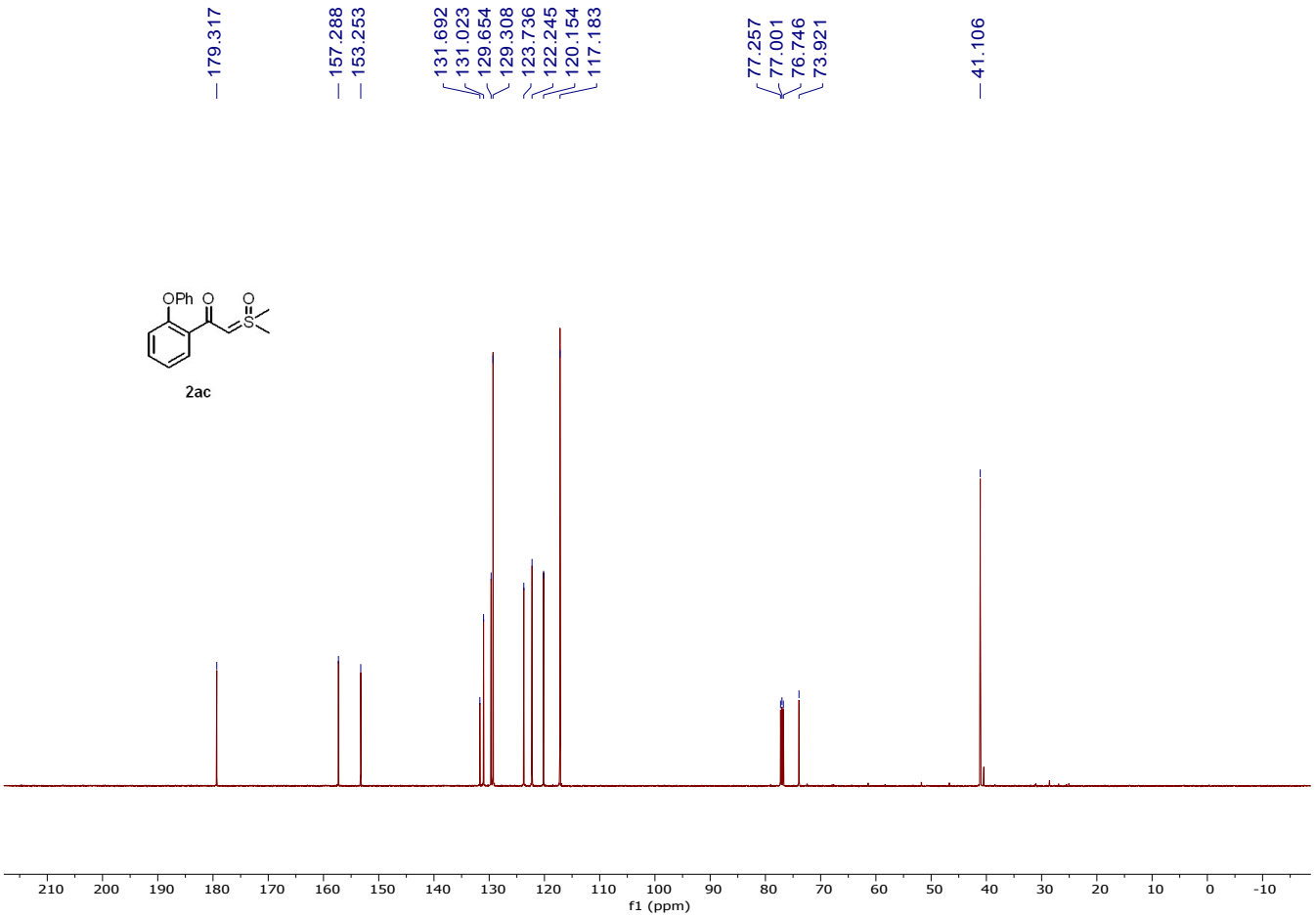
3 A. G. Talero, B. S. Martins and A. C. B. Burtoloso, *Org. Lett.*, 2018, **20**, 7206.

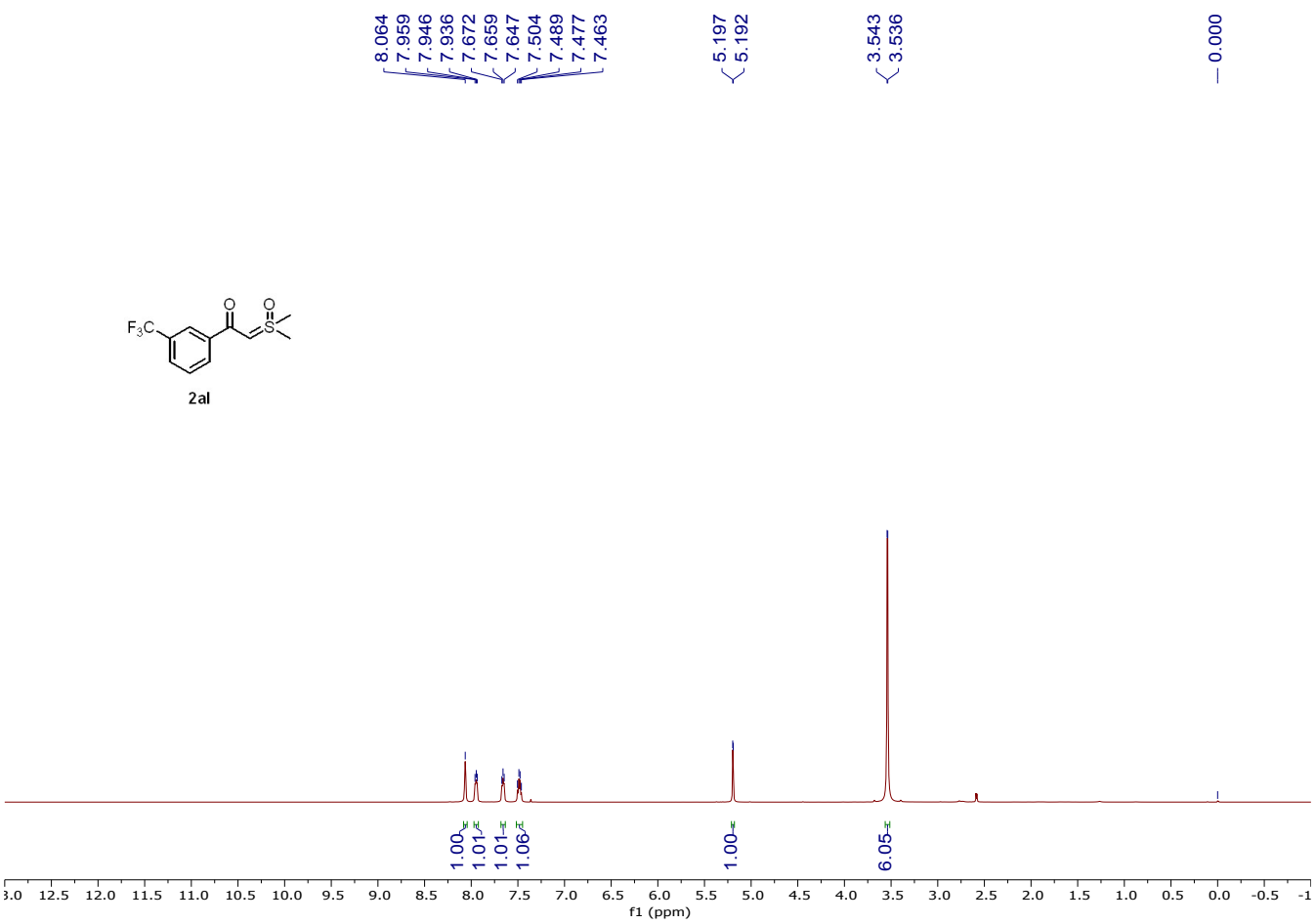
4 D. Lim, F. Fang, G. Zhou and D. M. Coltart, *Org. Lett.*, 2007, **9**, 4139.

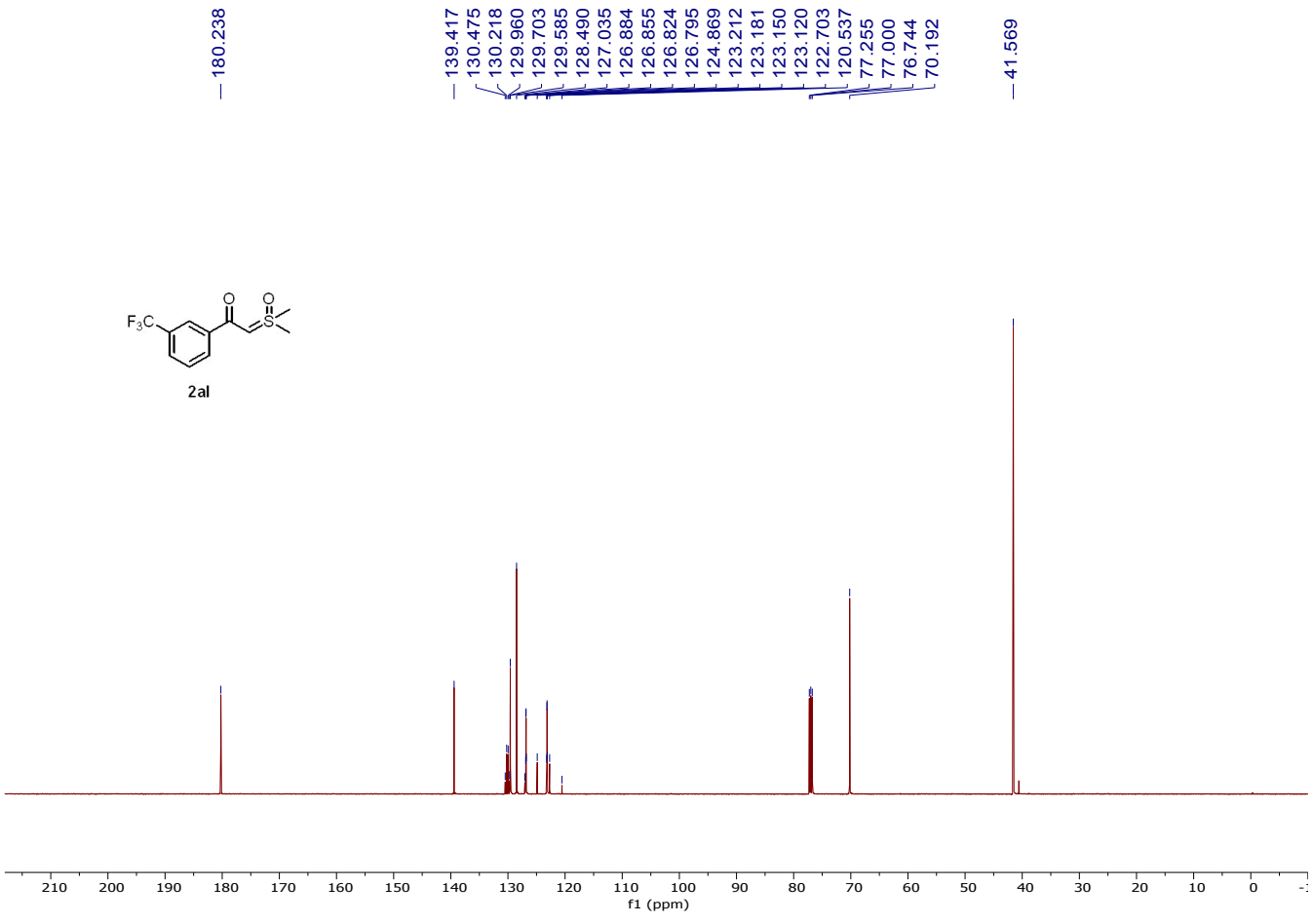
5 Y. Peng, L. Luo, C.-S. Yan, J.-J. Zhang and Y.-W. Wang, *J. Org. Chem.*, 2013, **78**, 10960.

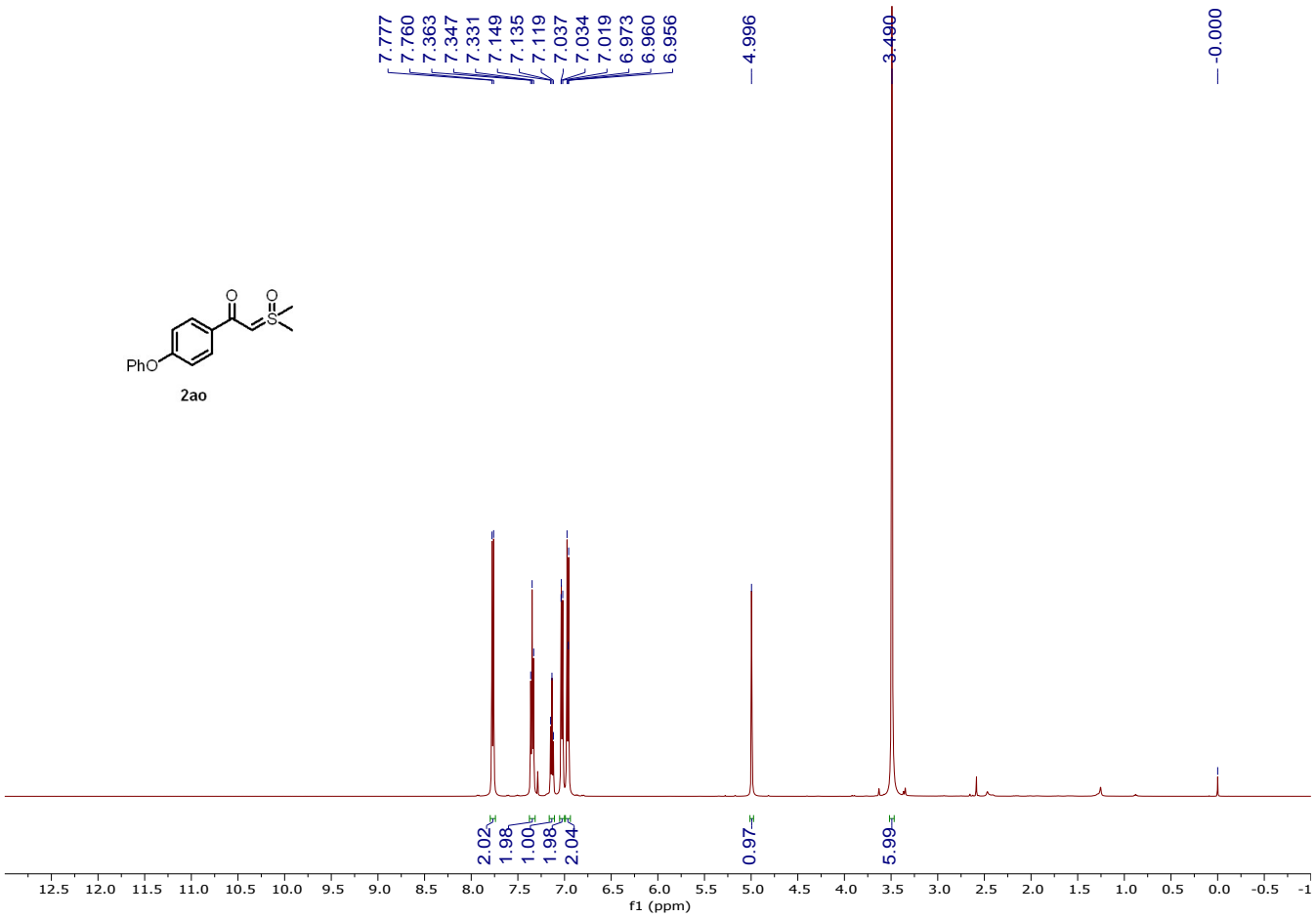
6. ^{1}H and ^{13}C NMR Spectra

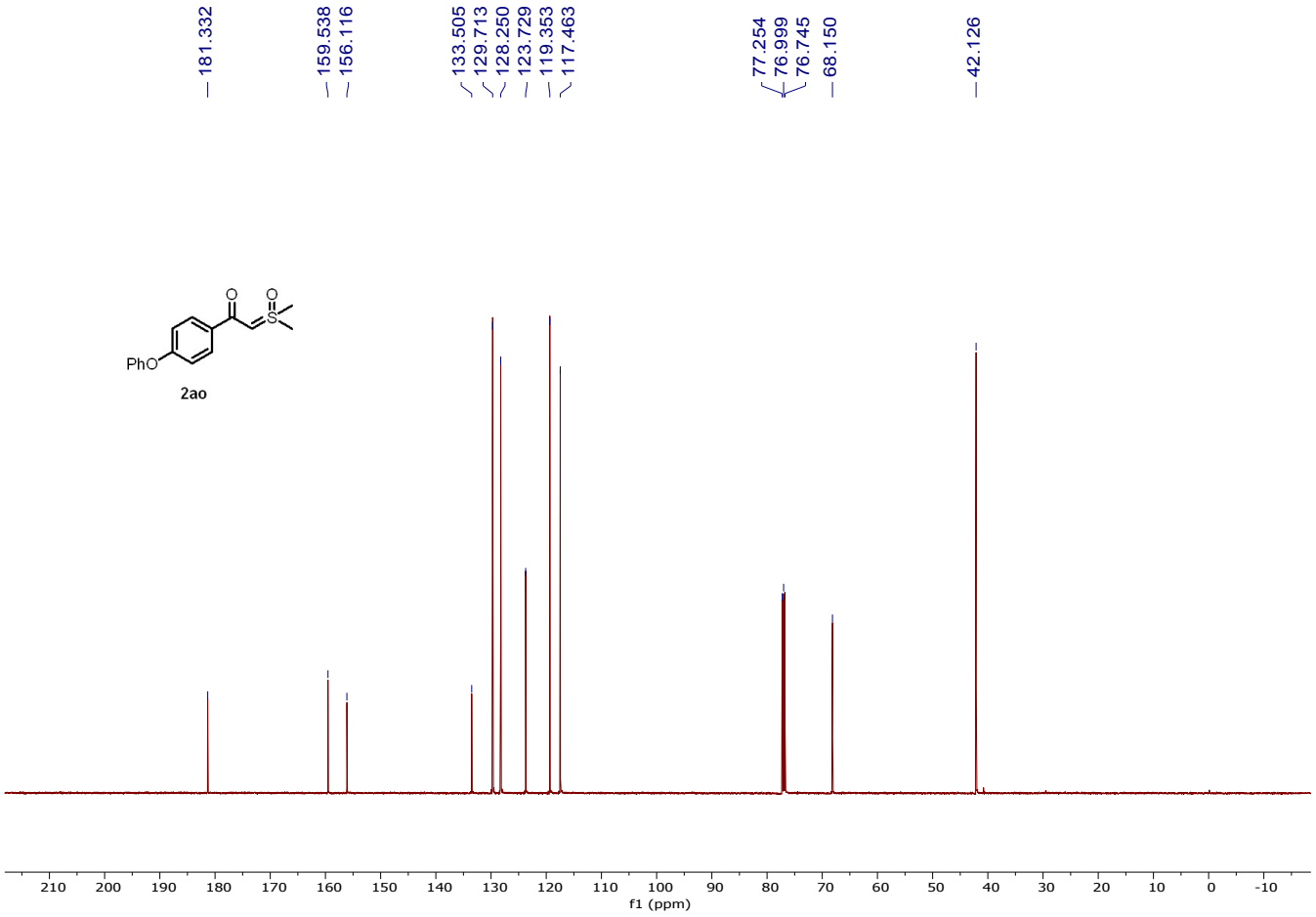




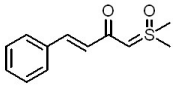

8.064
7.959
7.946
7.936
7.672
7.659
7.647
7.504
7.489
7.477
7.463
5.197
5.192
3.543
3.536
0.000
F3C
O
O
S
2al
1.00
1.01
1.01
1.06
1.00
6.05
f1 (ppm)


180.238
139.417
130.475
130.218
129.960
129.703
129.585
128.490
127.035
126.884
126.855
126.824
126.795
124.869
123.212
123.181
123.150
123.120
122.703
120.537
77.255
77.000
76.744
70.192
41.569
F3C
O
O
S
2al
f1 (ppm)

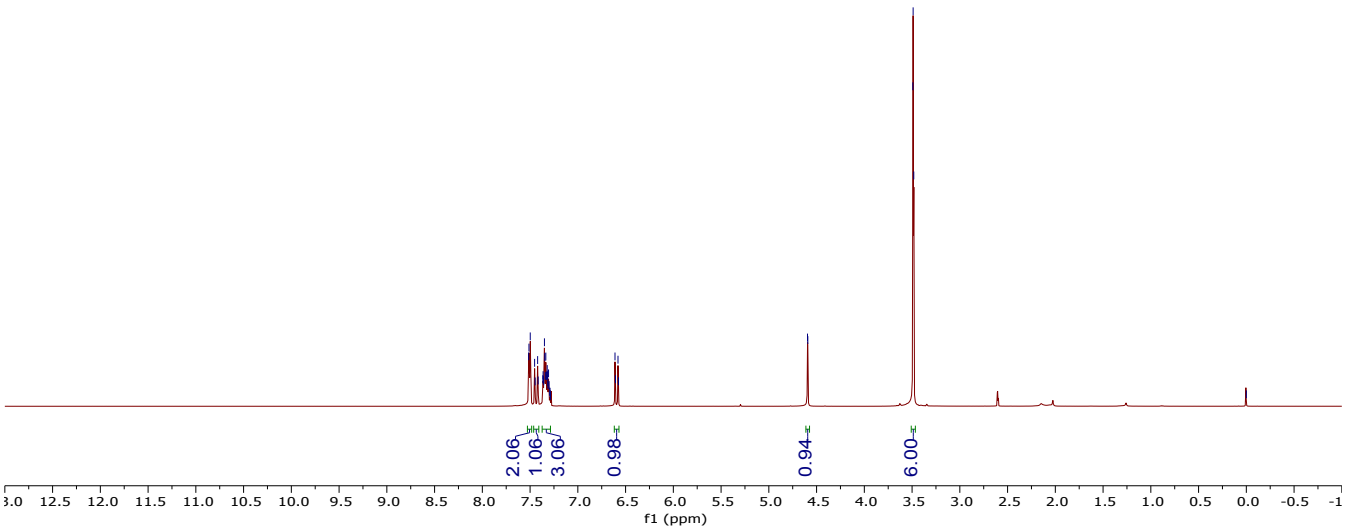

7.777
7.760
7.363
7.347
7.331
7.149
7.135
7.119
7.037
7.034
7.019
6.973
6.960
6.956
4.996
3.490
-0.000
PhO
2ao
2.02
1.98
1.00
1.98
2.04
0.97
5.99
f1 (ppm)


181.332
159.538
156.116
133.505
129.713
128.250
123.729
119.353
117.463
77.254
76.999
76.745
68.150
42.126
PhO
2ao
f1 (ppm)

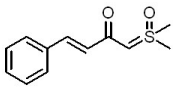

7.515
7.512
7.498
7.453
7.447
7.421
7.416
7.367
7.364
7.361
7.358
7.350
7.346
7.340
7.335
7.329
7.323
7.321
7.318
7.315
7.312
7.307
7.301
7.295
7.292
6.611
6.605
6.579
6.574
4.595
4.592
3.492
3.489
3.482
-0.000



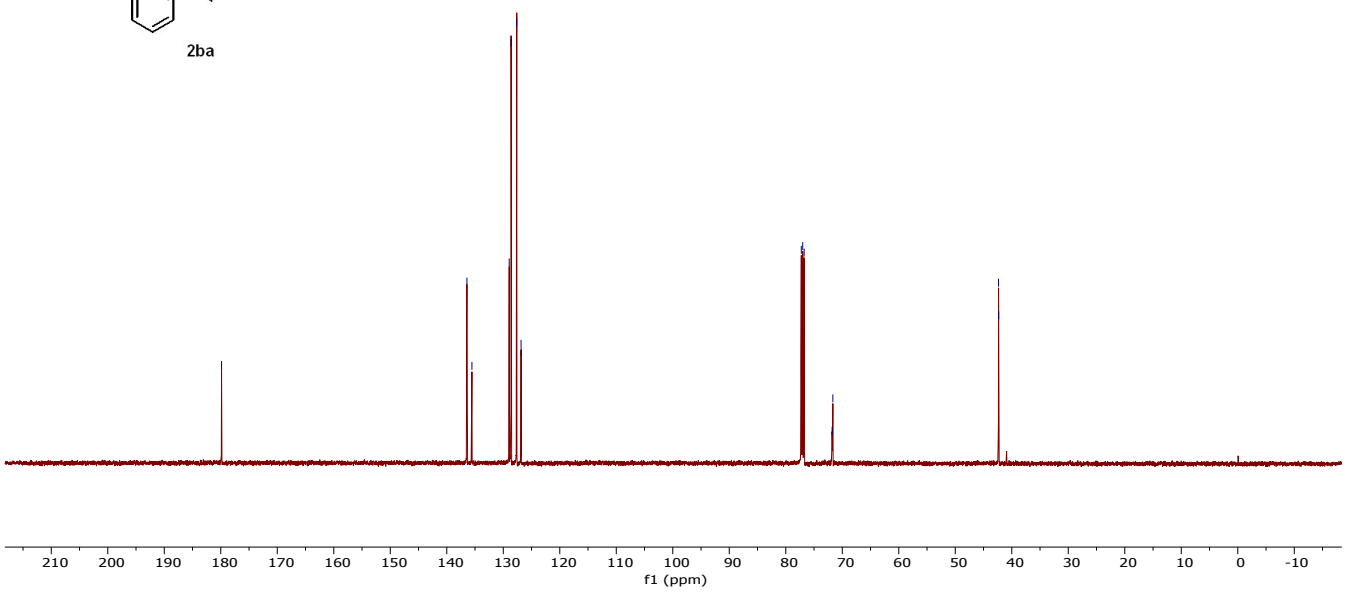
2ba

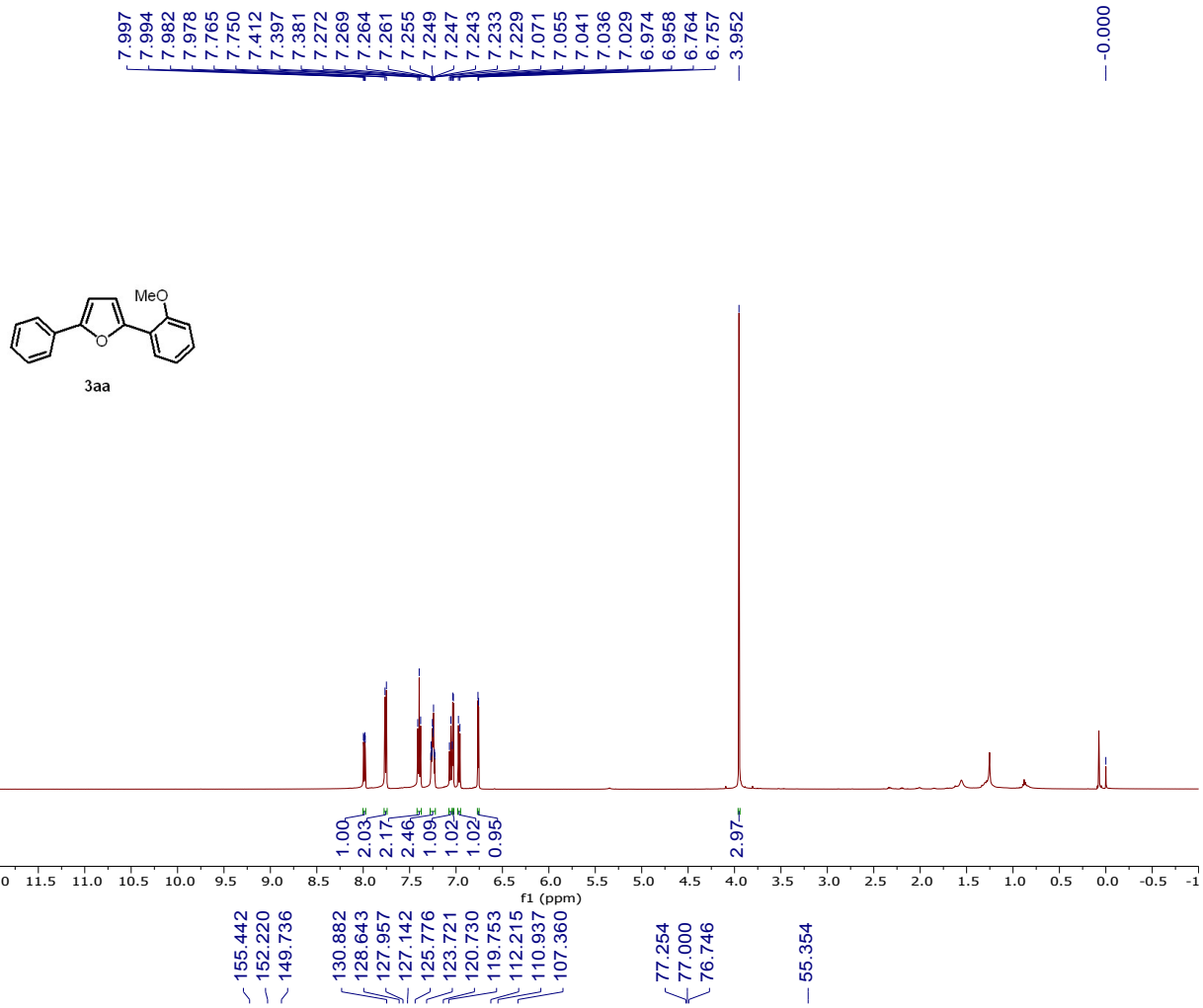

2.06
1.06
3.06
0.98
0.94
6.00
f1 (ppm)

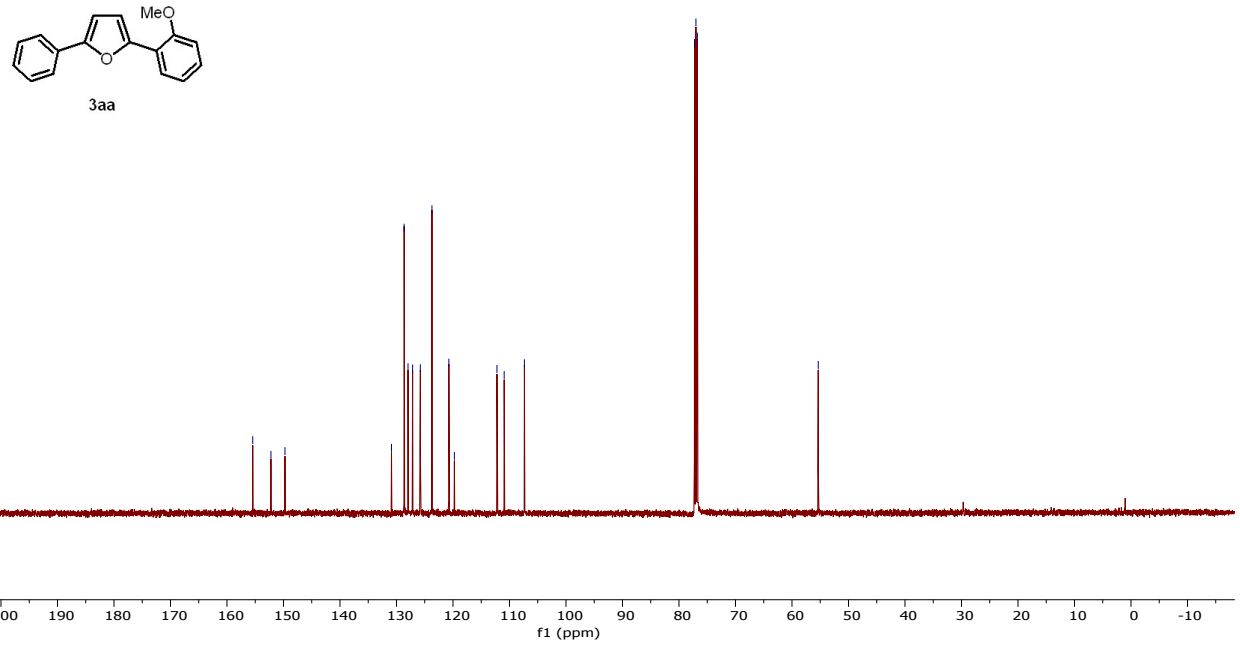

179.865
136.435
135.549
128.951
128.618
127.613
126.850
126.836
77.254
77.000
76.746
71.797
71.667
42.344
42.308

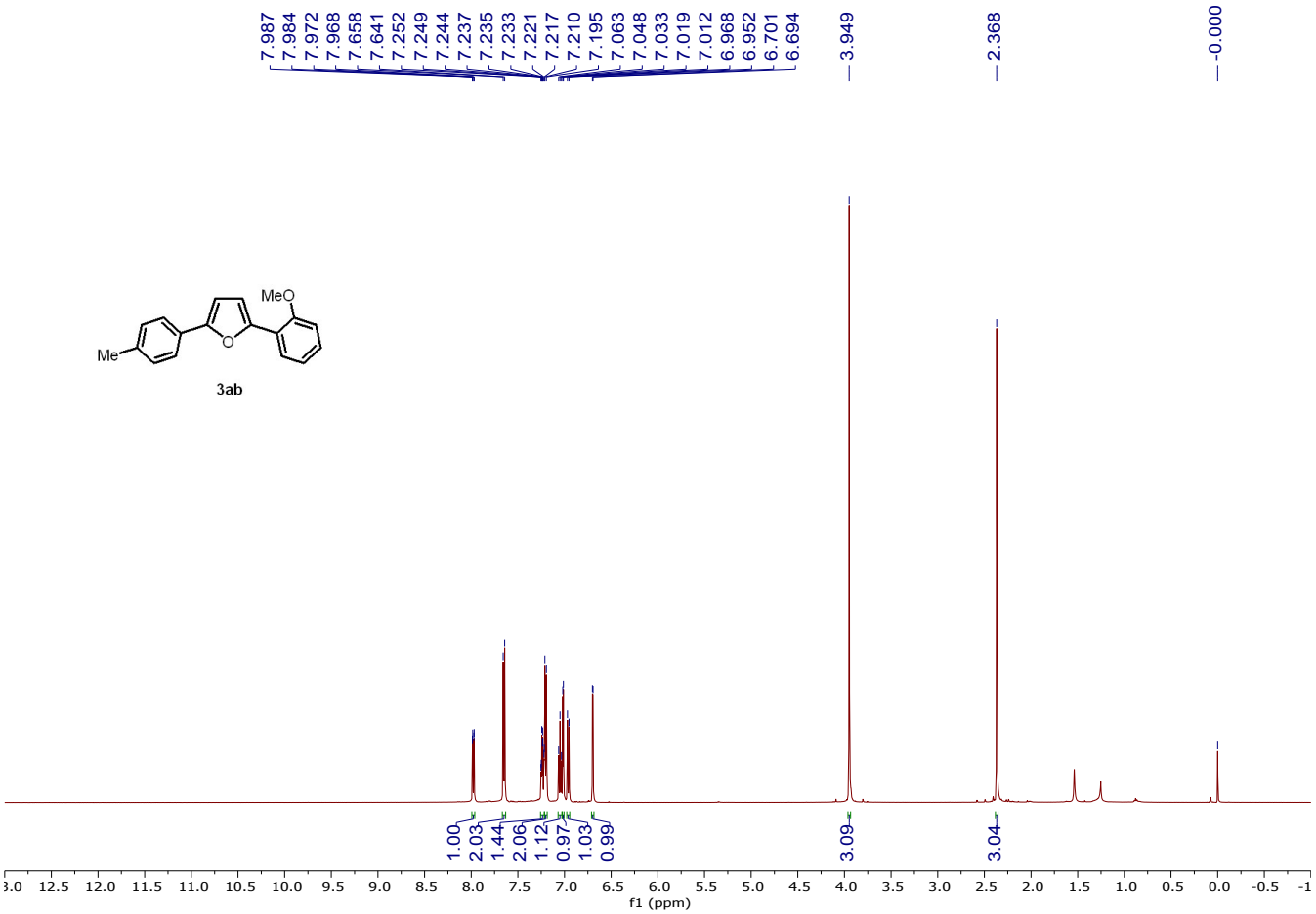


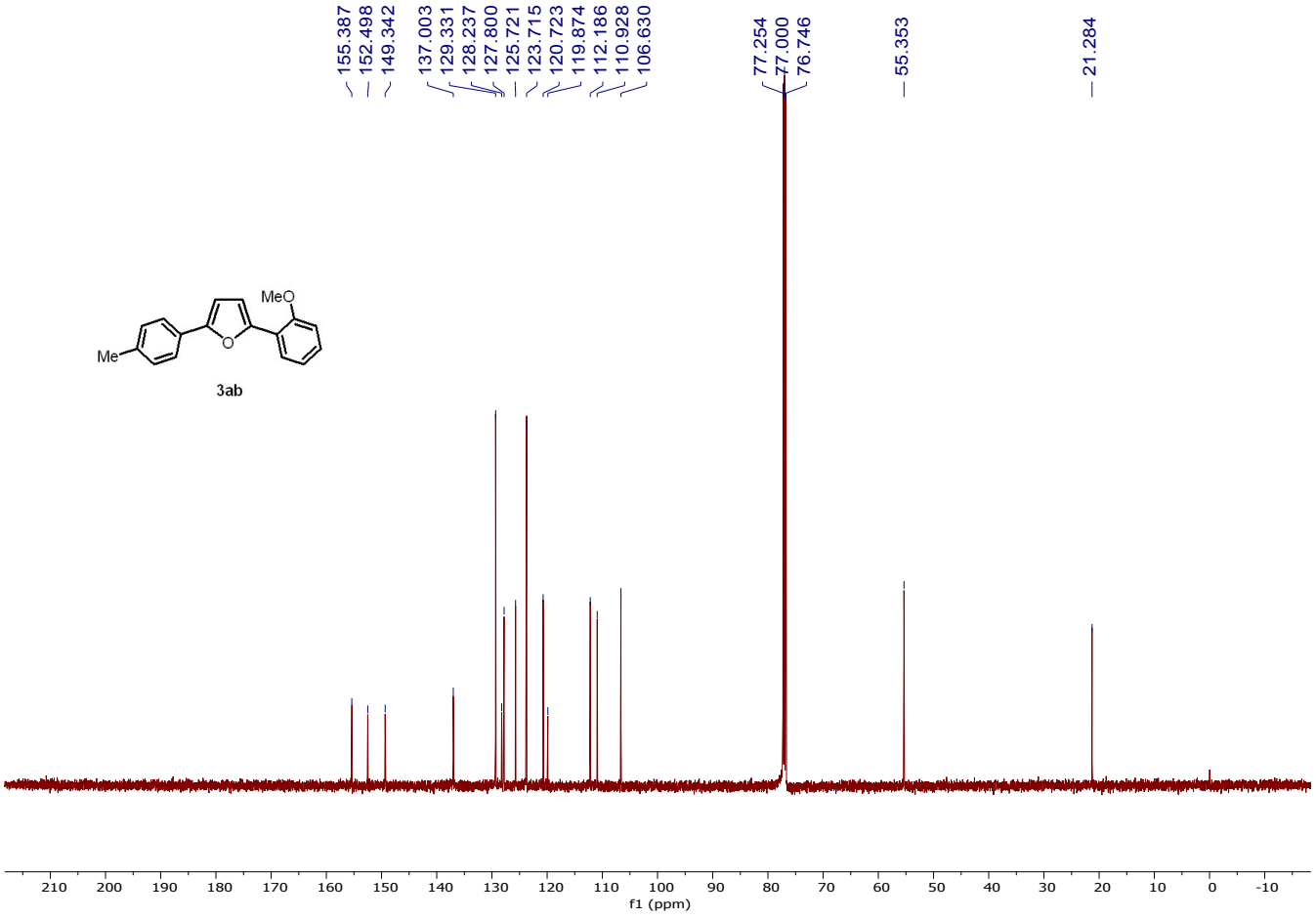
2ba


f1 (ppm)

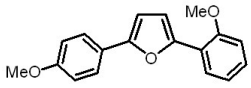

7.997
7.994
7.982
7.978
7.765
7.750
7.412
7.397
7.381
7.272
7.269
7.264
7.261
7.255
7.249
7.247
7.243
7.233
7.229
7.071
7.055
7.041
7.036
7.029
6.974
6.958
6.764
6.757
3.952
-0.000
MeO
3aa
1.00
2.03
2.17
2.46
1.09
1.02
1.02
0.95
2.97
f1 (ppm)


155.442
152.220
149.736
130.882
128.643
127.957
127.142
125.776
123.721
120.730
119.753
112.215
110.937
107.360
77.254
77.000
76.746
55.354
MeO
3aa
f1 (ppm)

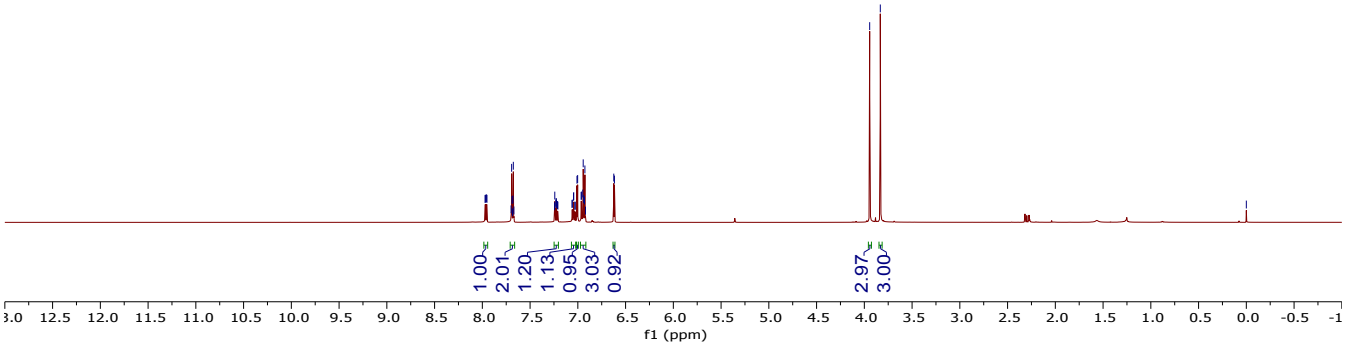

7.987
7.984
7.972
7.968
7.658
7.641
7.252
7.249
7.244
7.237
7.235
7.233
7.221
7.217
7.210
7.195
7.063
7.048
7.033
7.019
7.012
6.968
6.952
6.701
6.694
3.949
2.368
-0.000
MeO
Me
O
3ab
1.00
2.03
1.44
2.06
1.12
0.97
1.03
0.99
3.09
3.04
f1 (ppm)


155.387
152.498
149.342
137.003
129.331
128.237
127.800
125.721
123.715
120.723
119.874
112.186
110.928
106.630
77.254
77.000
76.746
55.353
21.284
MeO
Me
O
3ab
f1 (ppm)

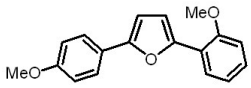

7.971
7.968
7.956
7.952
7.699
7.693
7.689
7.684
7.680
7.676
7.670
7.244
7.241
7.229
7.227
7.226
7.224
7.213
7.209
7.060
7.058
7.045
7.043
7.030
7.028
7.009
7.002
6.965
6.963
6.948
6.944
6.939
6.930
6.926
6.920
6.624
6.617
3.944
3.833
-0.000


MeO
MeO
O

3ac

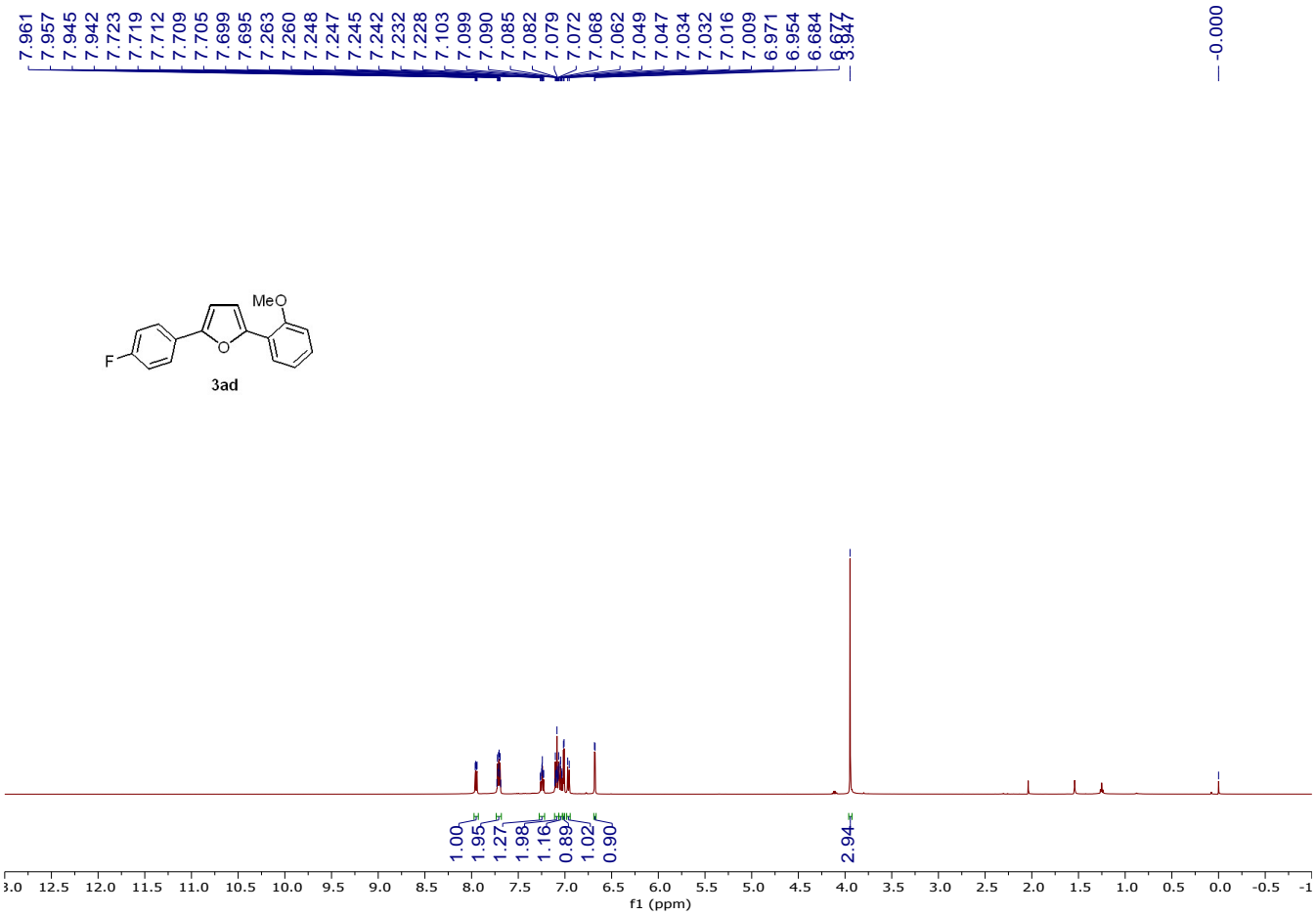

1.00
2.01
1.20
1.13
0.95
3.03
0.92
2.97
3.00
f1 (ppm)

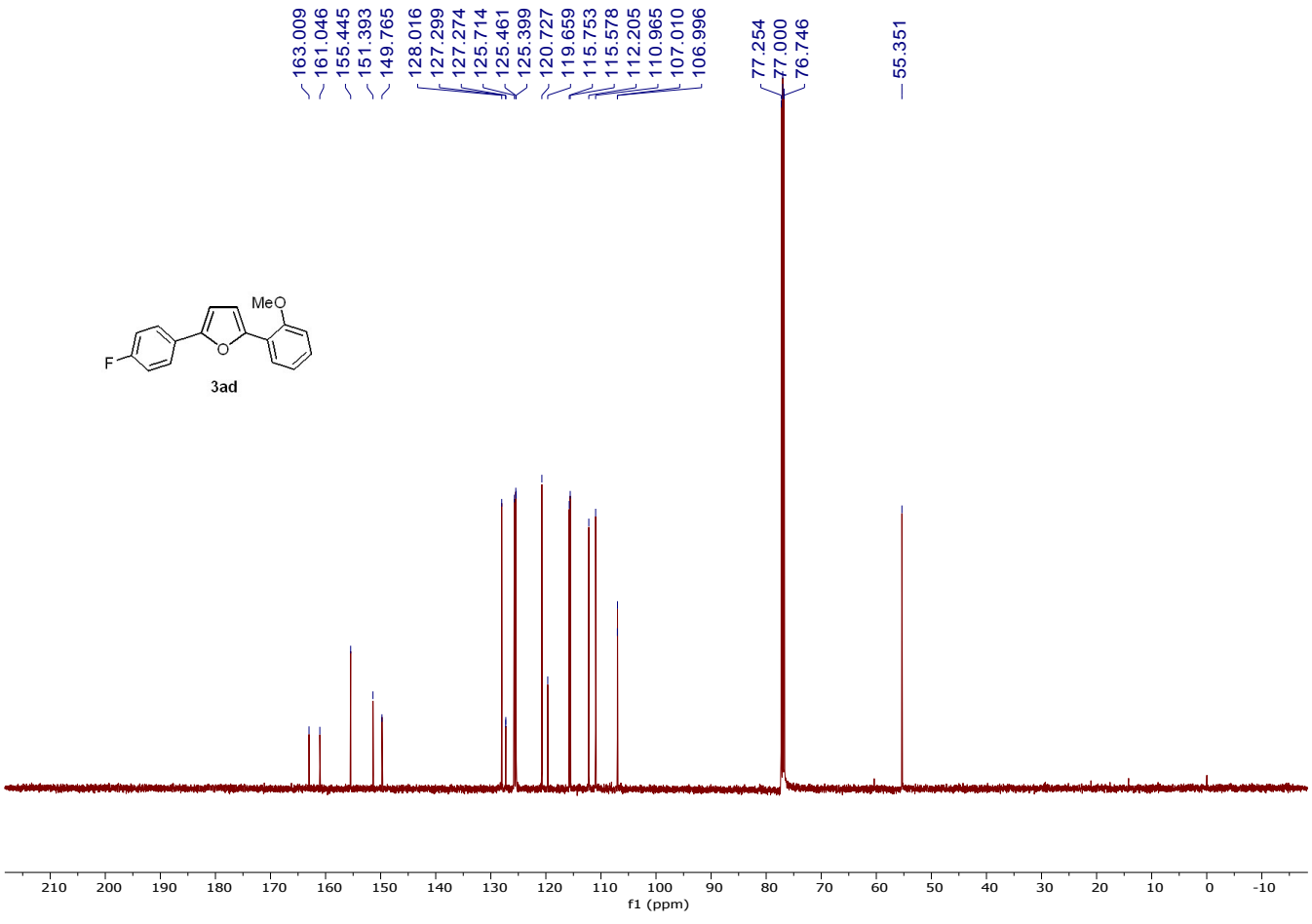

158.944
155.316
152.344
149.069
127.672
125.602
125.183
124.042
120.707
119.909
114.124
112.207
110.915
105.786
77.254
77.000
76.746
55.337
55.310

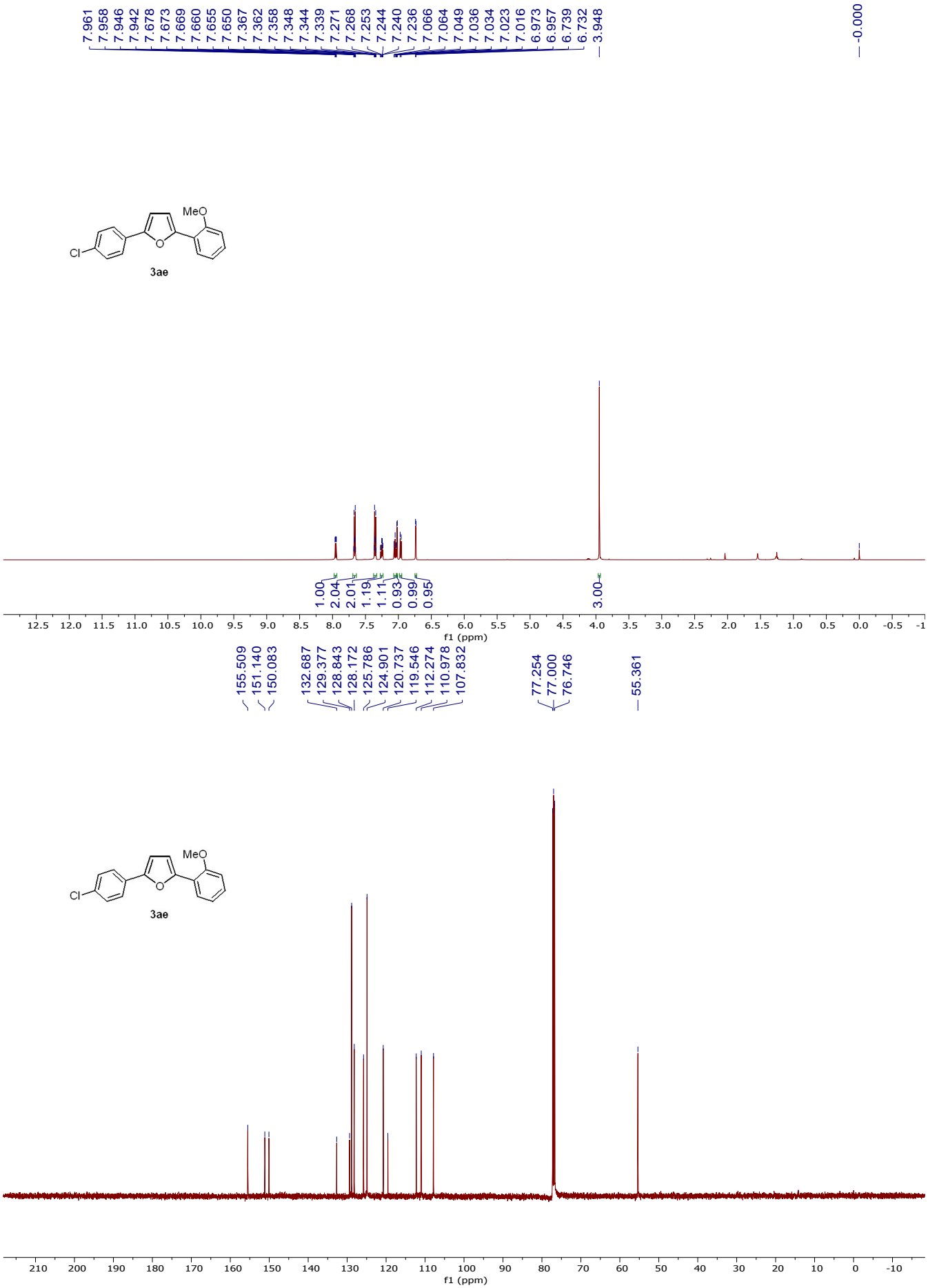

MeO
MeO
O

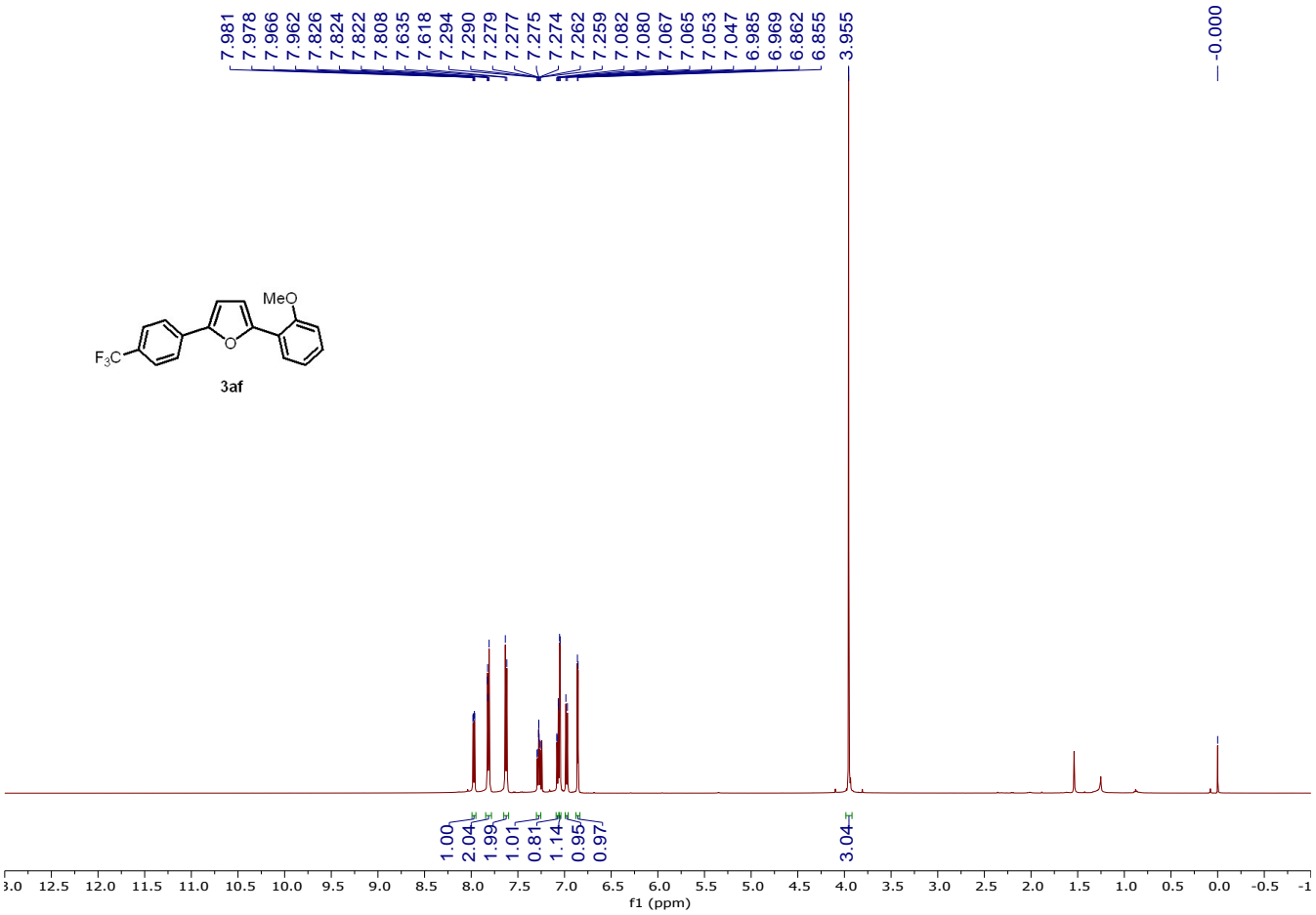
3ac

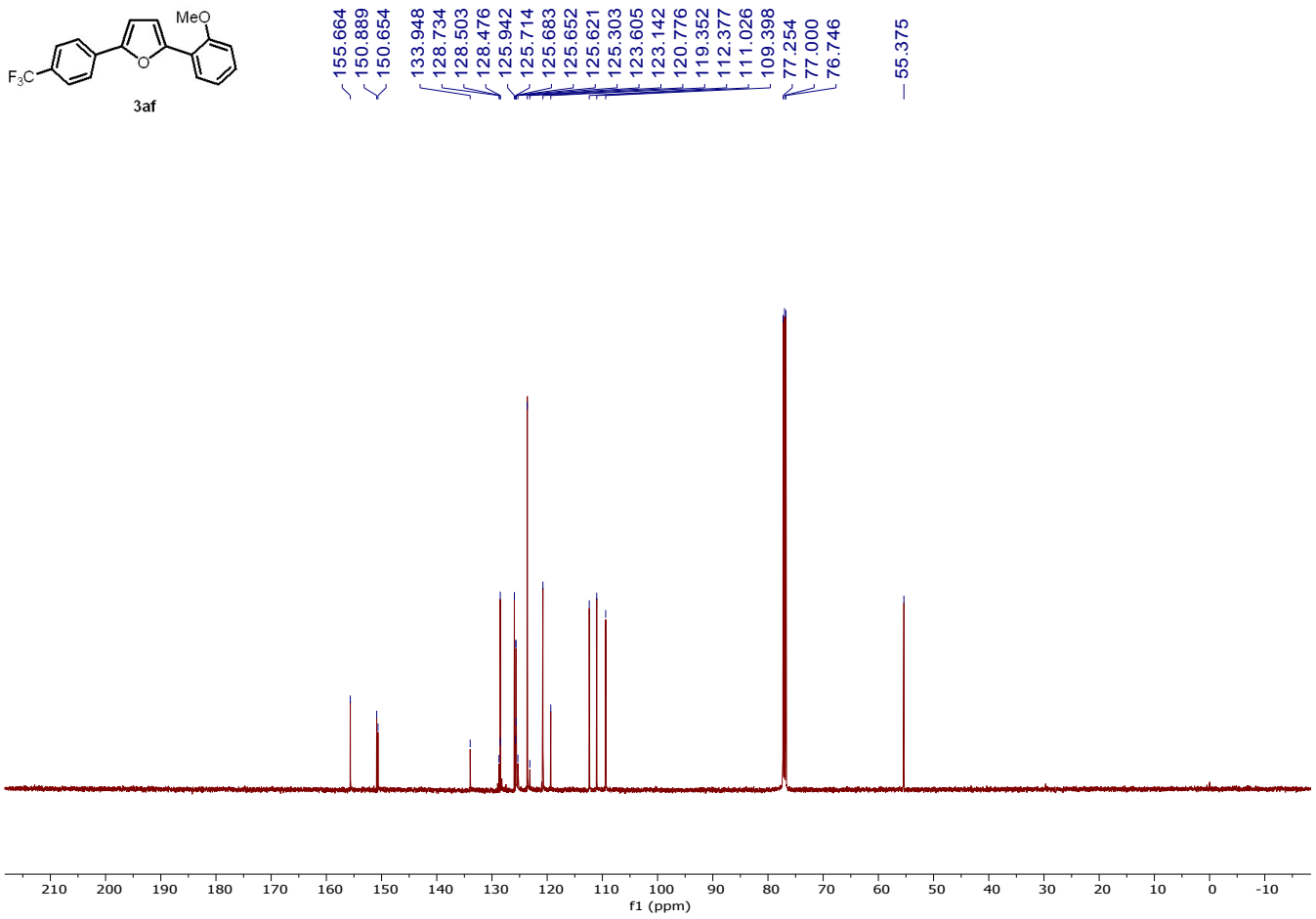
f1 (ppm)


7.961
7.957
7.945
7.942
7.723
7.719
7.712
7.709
7.705
7.699
7.695
7.263
7.260
7.248
7.247
7.245
7.242
7.232
7.228
7.103
7.099
7.090
7.085
7.082
7.079
7.072
7.068
7.062
7.049
7.047
7.034
7.032
7.016
7.009
6.971
6.954
6.684
6.677
3.947
-0.000
MeO
F
O
3ad
1.00
1.95
1.27
1.98
1.16
0.89
1.02
0.90
2.94
f1 (ppm)

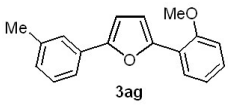

163.009
161.046
155.445
151.393
149.765
128.016
127.299
127.274
125.714
125.461
125.399
120.727
119.659
115.753
115.578
112.205
110.965
107.010
106.996
77.254
77.000
76.746
55.351
MeO
F
O
3ad
f1 (ppm)


7.961
7.958
7.946
7.942
7.678
7.673
7.669
7.660
7.655
7.650
7.367
7.362
7.358
7.348
7.344
7.339
7.271
7.268
7.253
7.244
7.240
7.236
7.066
7.064
7.049
7.036
7.034
7.023
7.016
6.973
6.957
6.739
6.732
3.948
-0.000
MeO
Cl
O
3ae
1.00
2.04
2.01
1.19
1.11
0.93
0.99
0.95
3.00
f1 (ppm)
155.509
151.140
150.083
132.687
129.377
128.843
128.172
125.786
124.901
120.737
119.546
112.274
110.978
107.832
77.254
77.000
76.746
55.361
MeO
Cl
O
3ae
f1 (ppm)

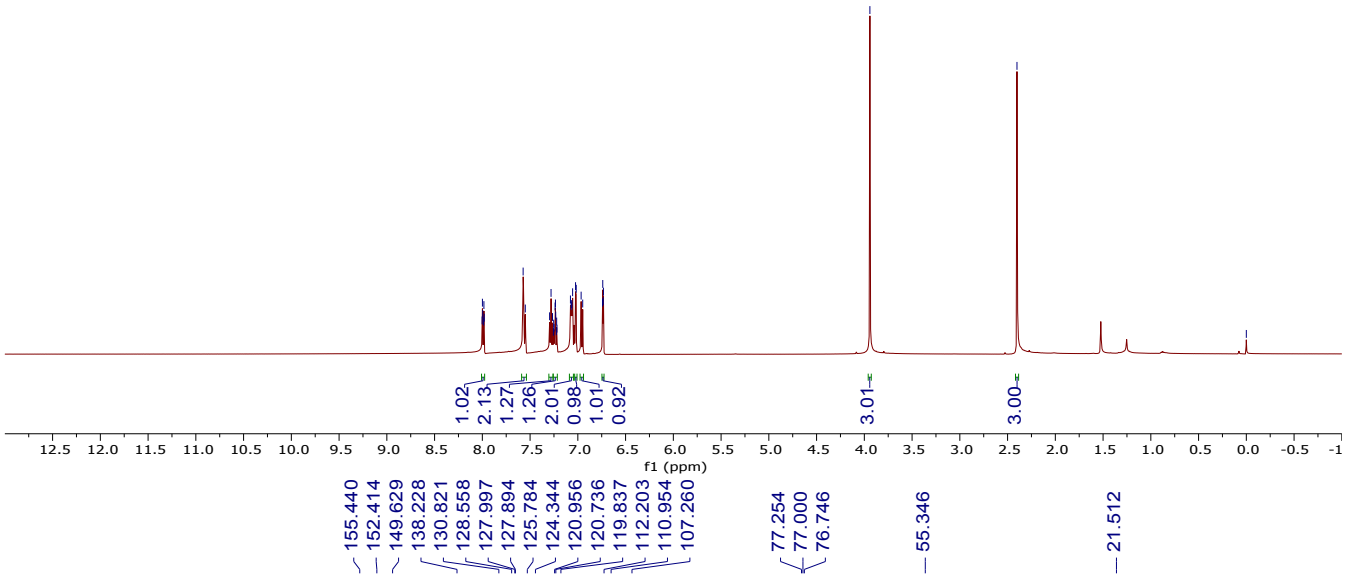

7.981
7.978
7.966
7.962
7.826
7.824
7.822
7.808
7.635
7.618
7.294
7.290
7.279
7.277
7.275
7.274
7.262
7.259
7.082
7.080
7.067
7.065
7.053
7.047
6.985
6.969
6.862
6.855
3.955
-0.000
MeO
F3C
O
3af
1.00
2.04
1.99
1.01
0.81
1.14
0.95
0.97
3.04
f1 (ppm)


MeO
F3C
O
3af
155.664
150.889
150.654
133.948
128.734
128.503
128.476
125.942
125.714
125.683
125.652
125.621
125.303
123.605
123.142
120.776
119.352
112.377
111.026
109.398
77.254
77.000
76.746
55.375
f1 (ppm)

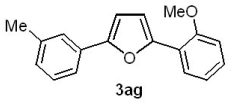

8.002
7.999
7.996
7.986
7.984
7.980
7.573
7.550
7.296
7.281
7.265
7.256
7.253
7.250
7.238
7.234
7.232
7.225
7.222
7.219
7.077
7.070
7.068
7.062
7.055
7.024
7.017
6.966
6.949
6.741
6.739
6.734
6.732
3.942
2.402
0.000


Me
MeO
O

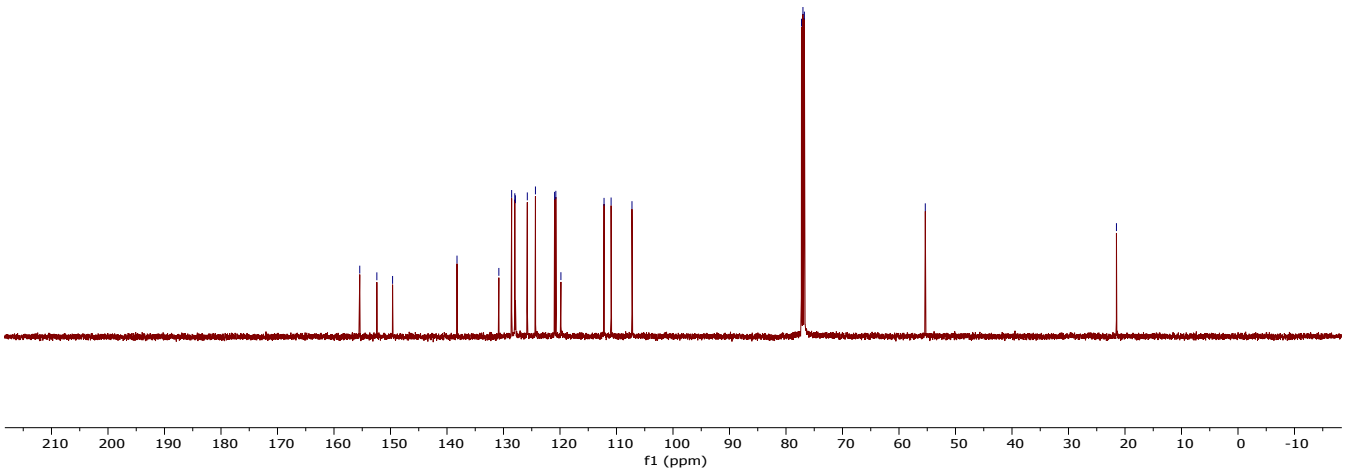
3ag

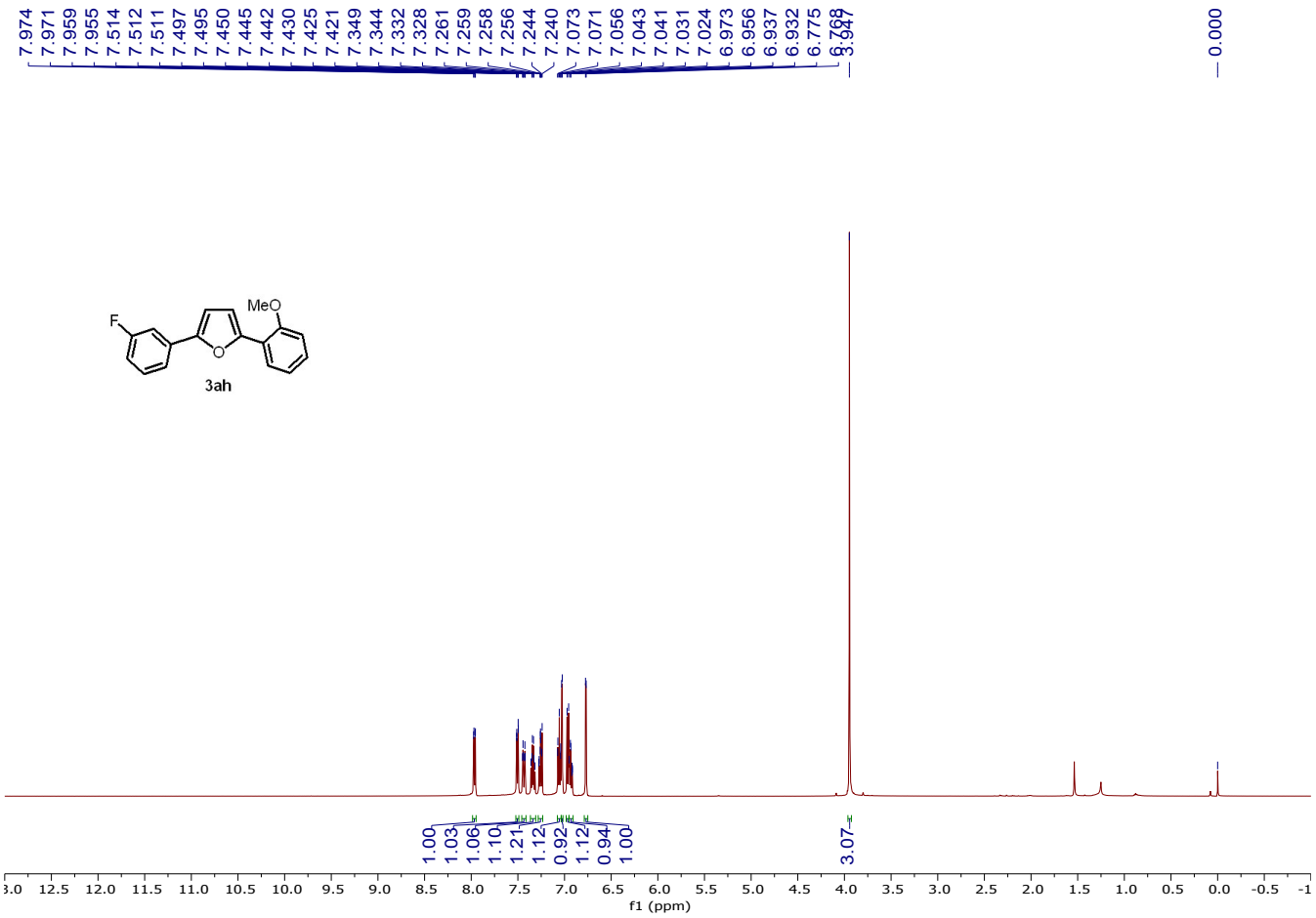

1.02
2.13
1.27
1.26
2.01
0.98
1.01
0.92
3.01
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

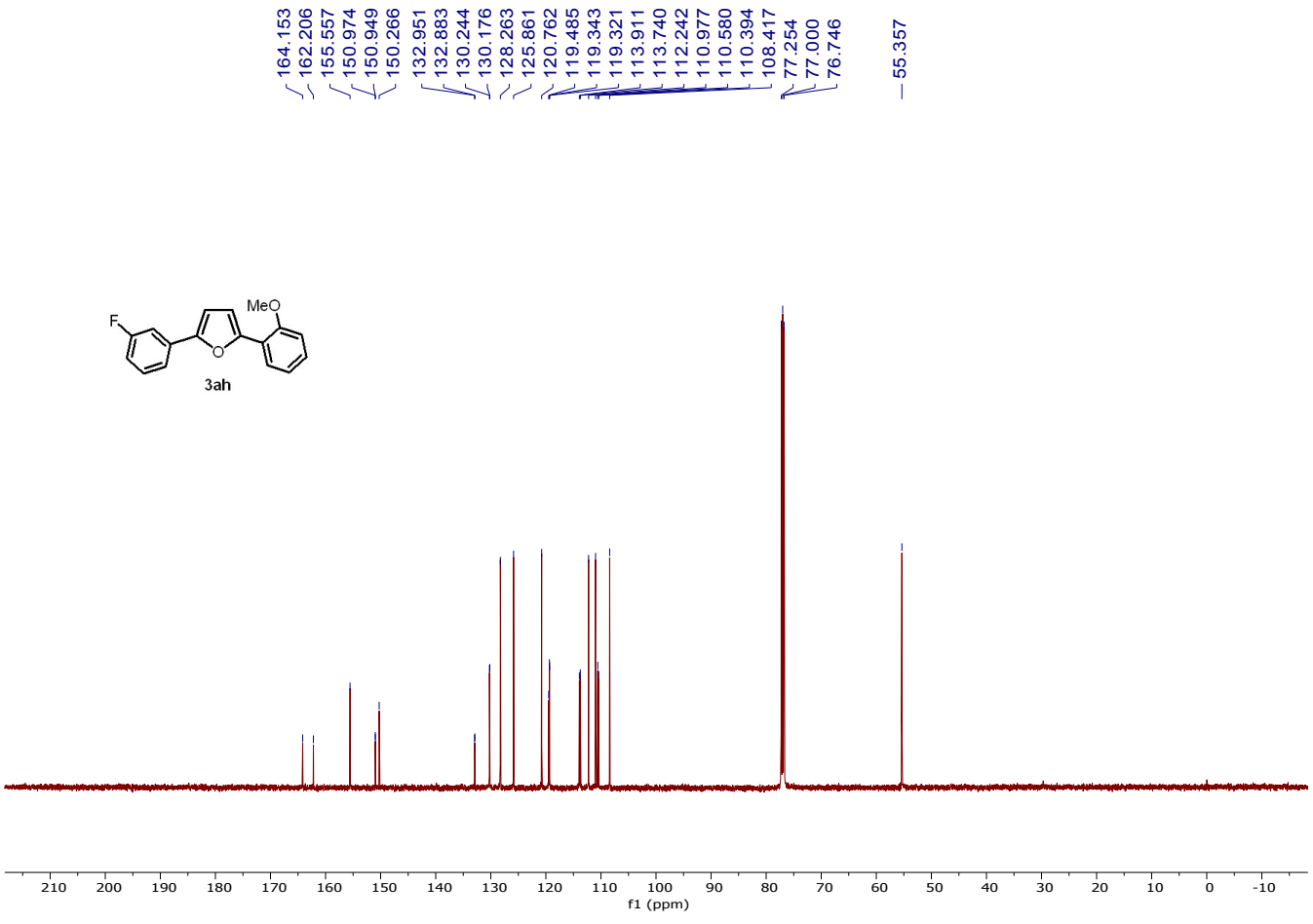
155.440
152.414
149.629
138.228
130.821
128.558
127.997
127.894
125.784
124.344
120.956
120.736
119.837
112.203
110.954
107.260
77.254
77.000
76.746
55.346
21.512

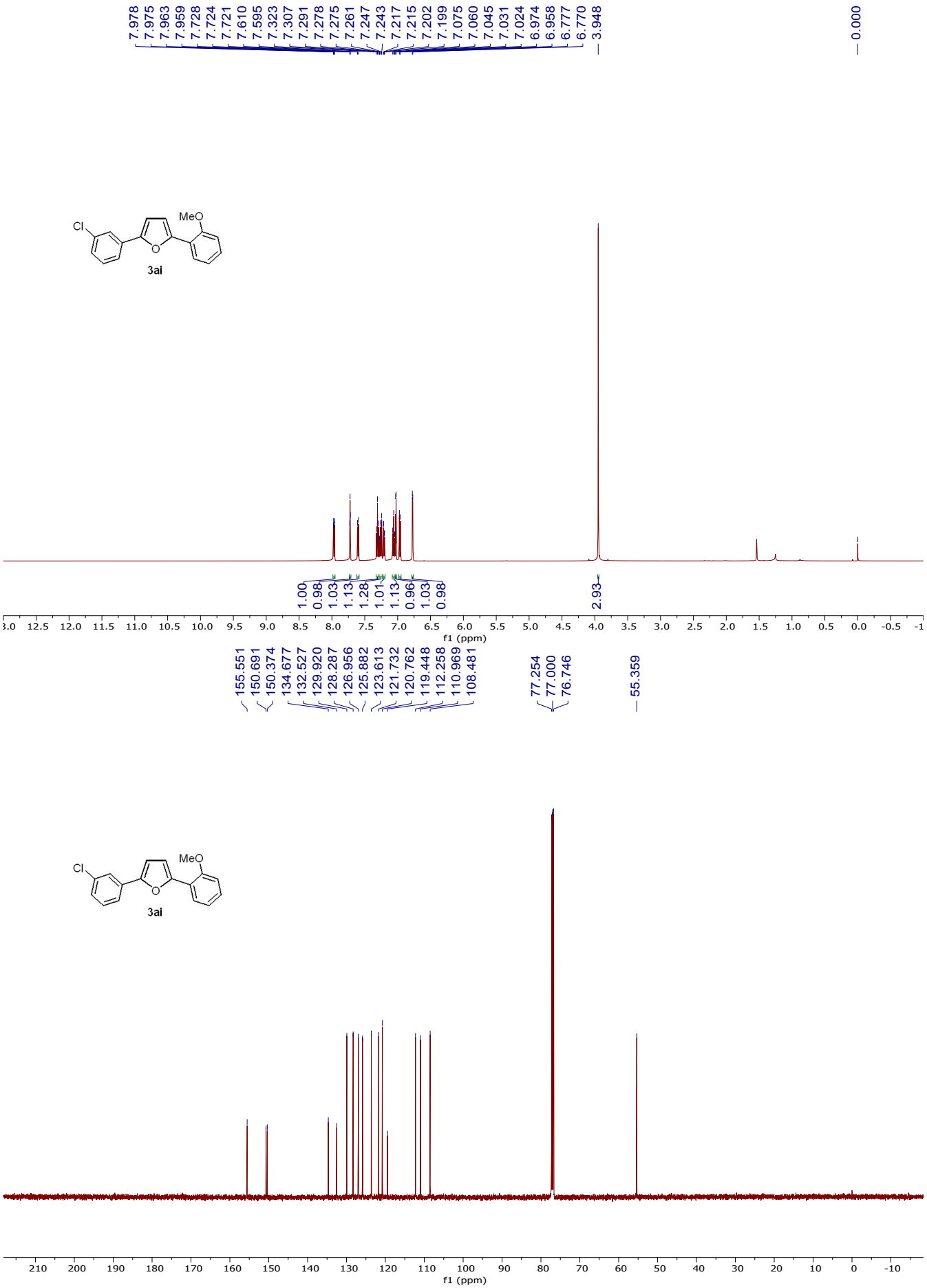

Me
MeO
O

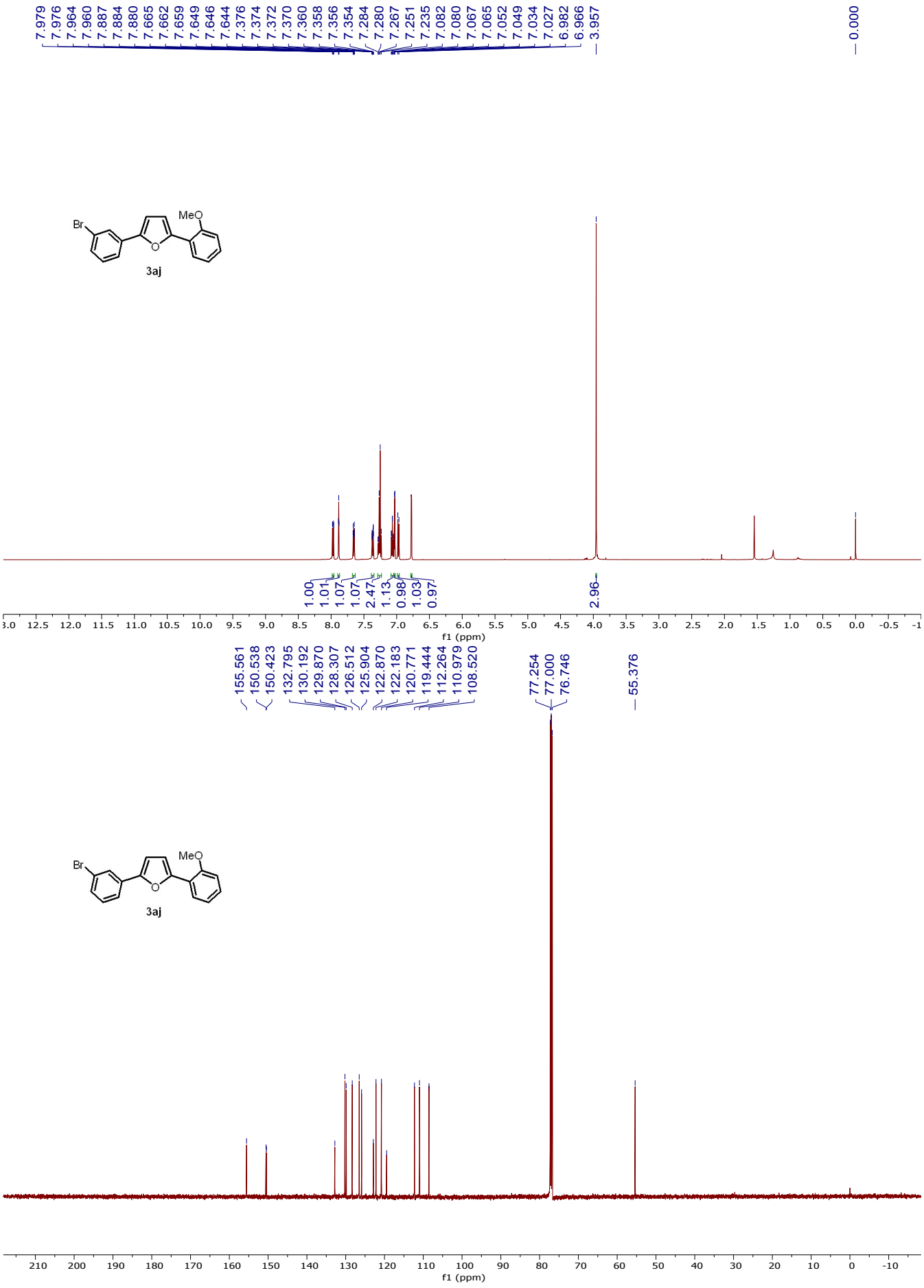
3ag

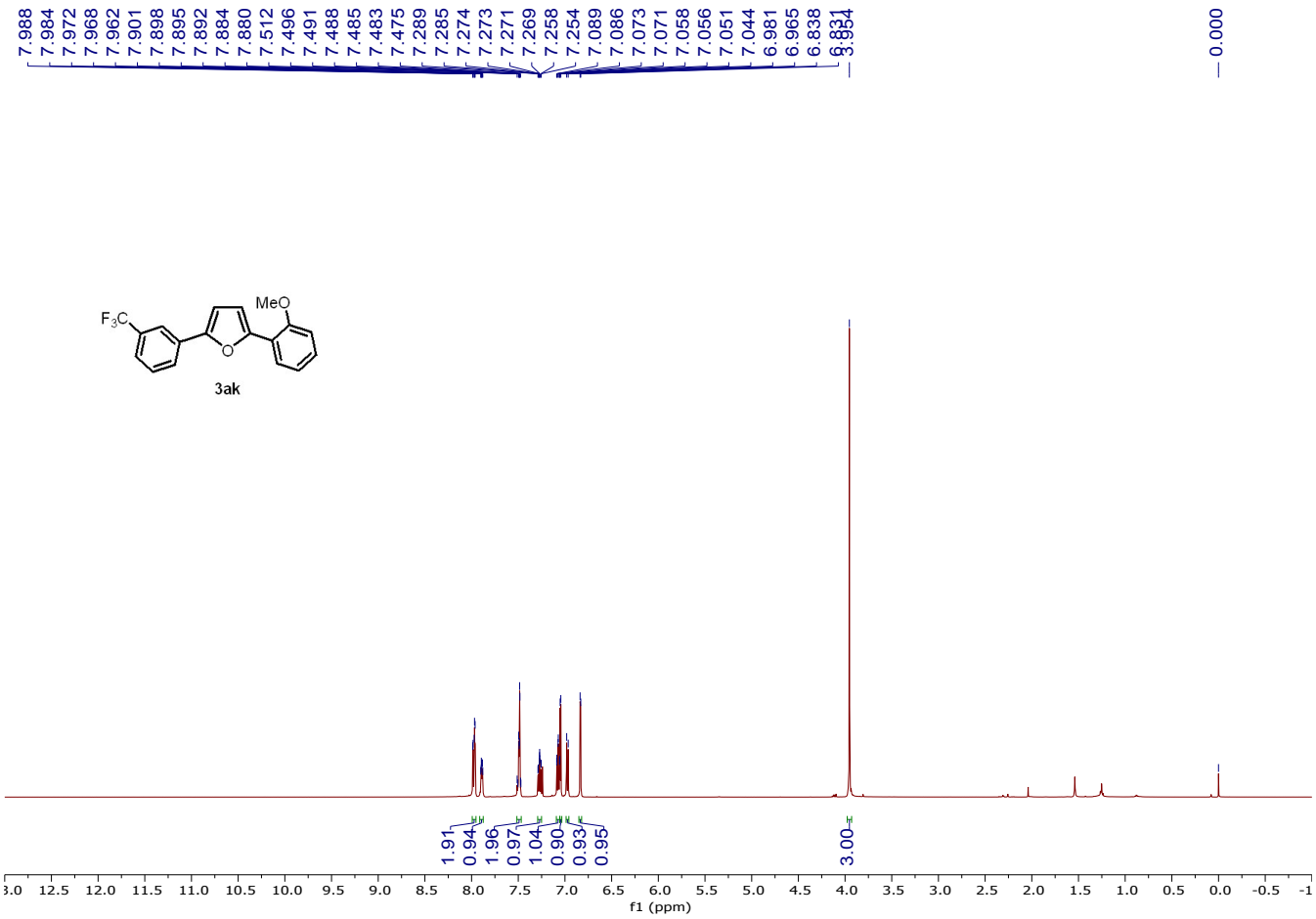

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

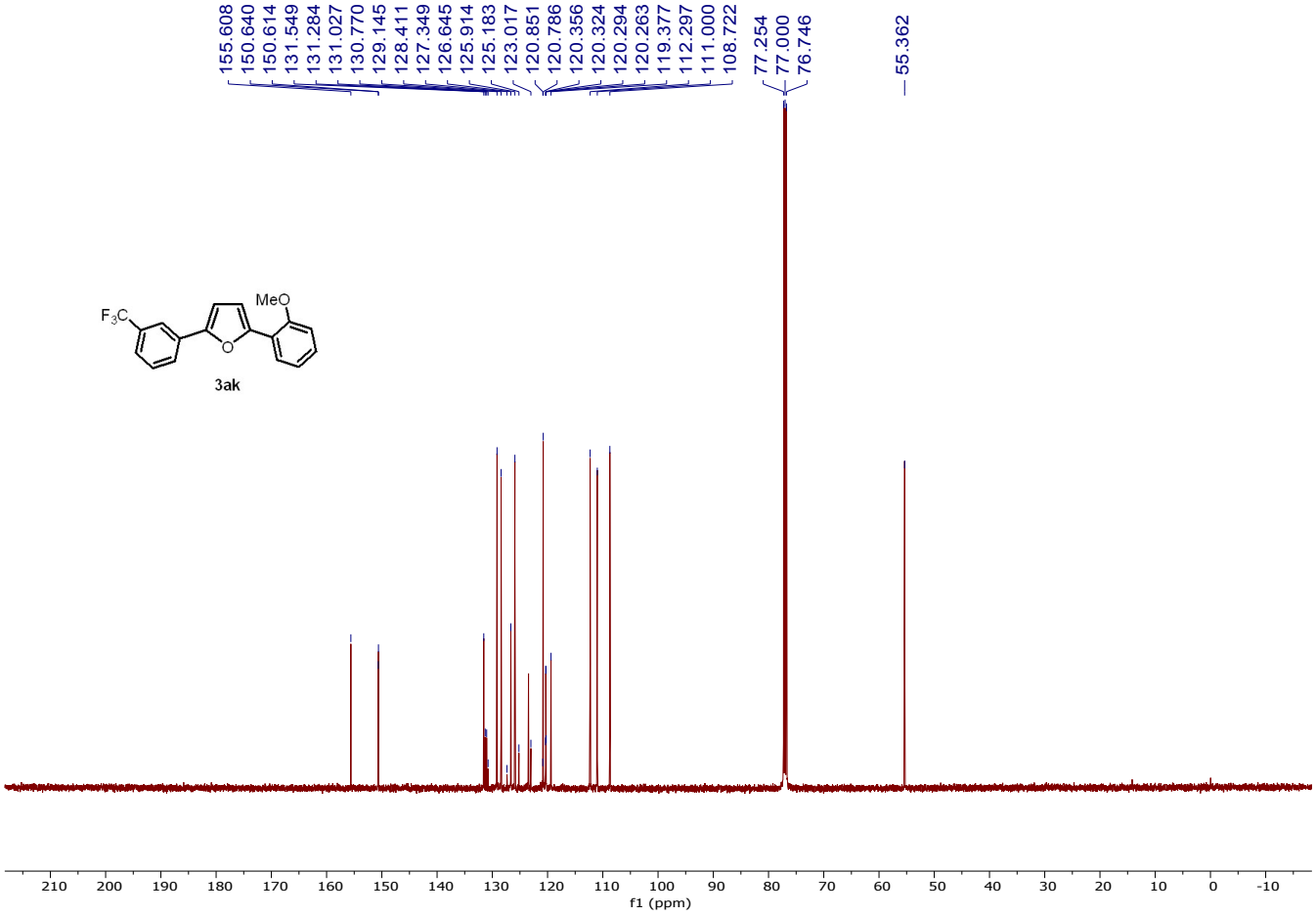

7.974
7.971
7.959
7.955
7.514
7.512
7.511
7.497
7.495
7.450
7.445
7.442
7.430
7.425
7.421
7.349
7.344
7.332
7.328
7.261
7.259
7.258
7.256
7.244
7.240
7.073
7.071
7.056
7.043
7.041
7.031
7.024
6.973
6.956
6.937
6.932
6.775
6.768
3.947
0.000
MeO
F
O
3ah
1.00
1.03
1.06
1.10
1.21
1.12
0.92
1.12
0.94
1.00
3.07
f1 (ppm)

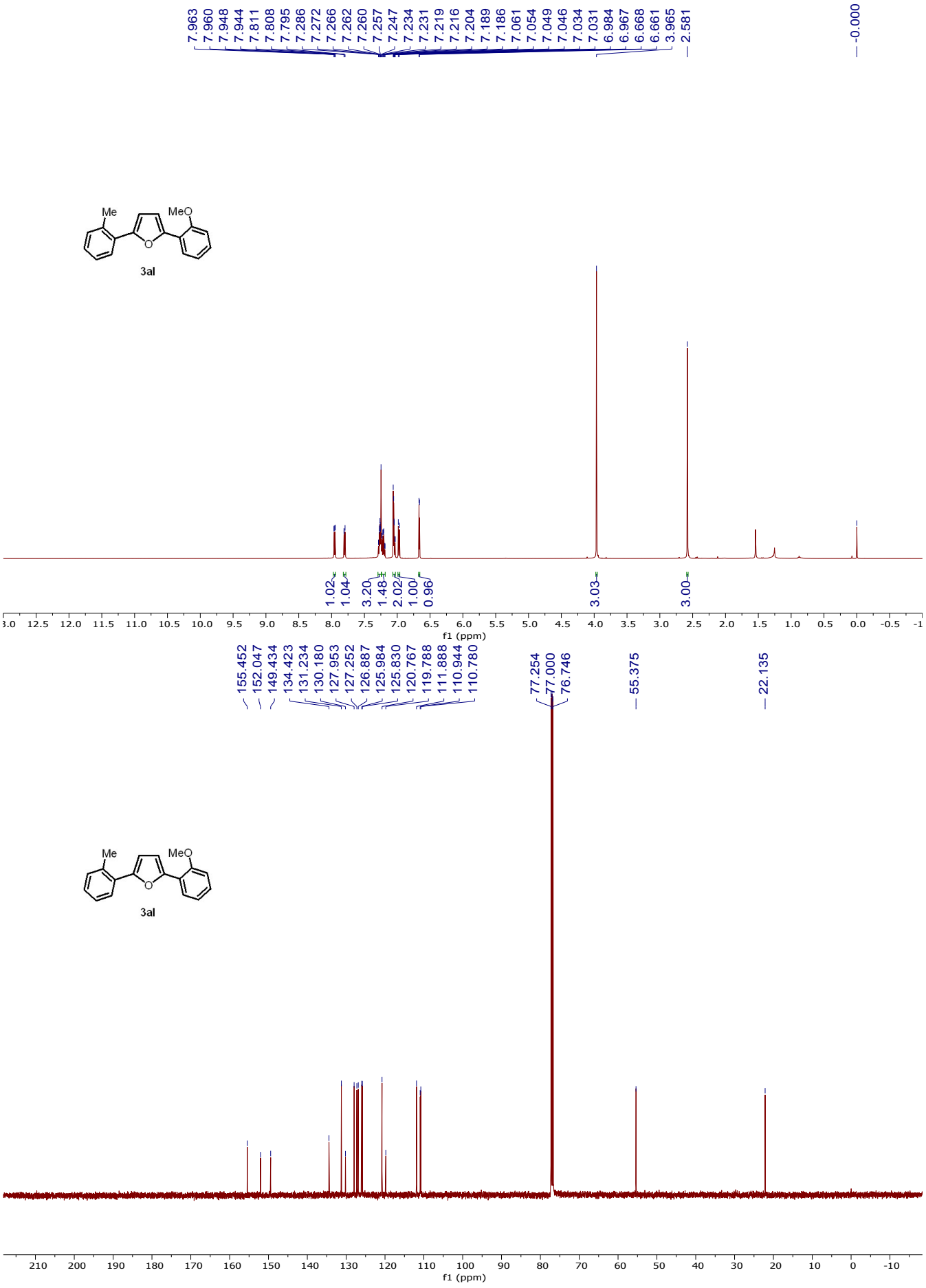

164.153
162.206
155.557
150.974
150.949
150.266
132.951
132.883
130.244
130.176
128.263
125.861
120.762
119.485
119.343
119.321
113.911
113.740
112.242
110.977
110.580
110.394
108.417
77.254
77.000
76.746
55.357
MeO
F
O
3ah
f1 (ppm)

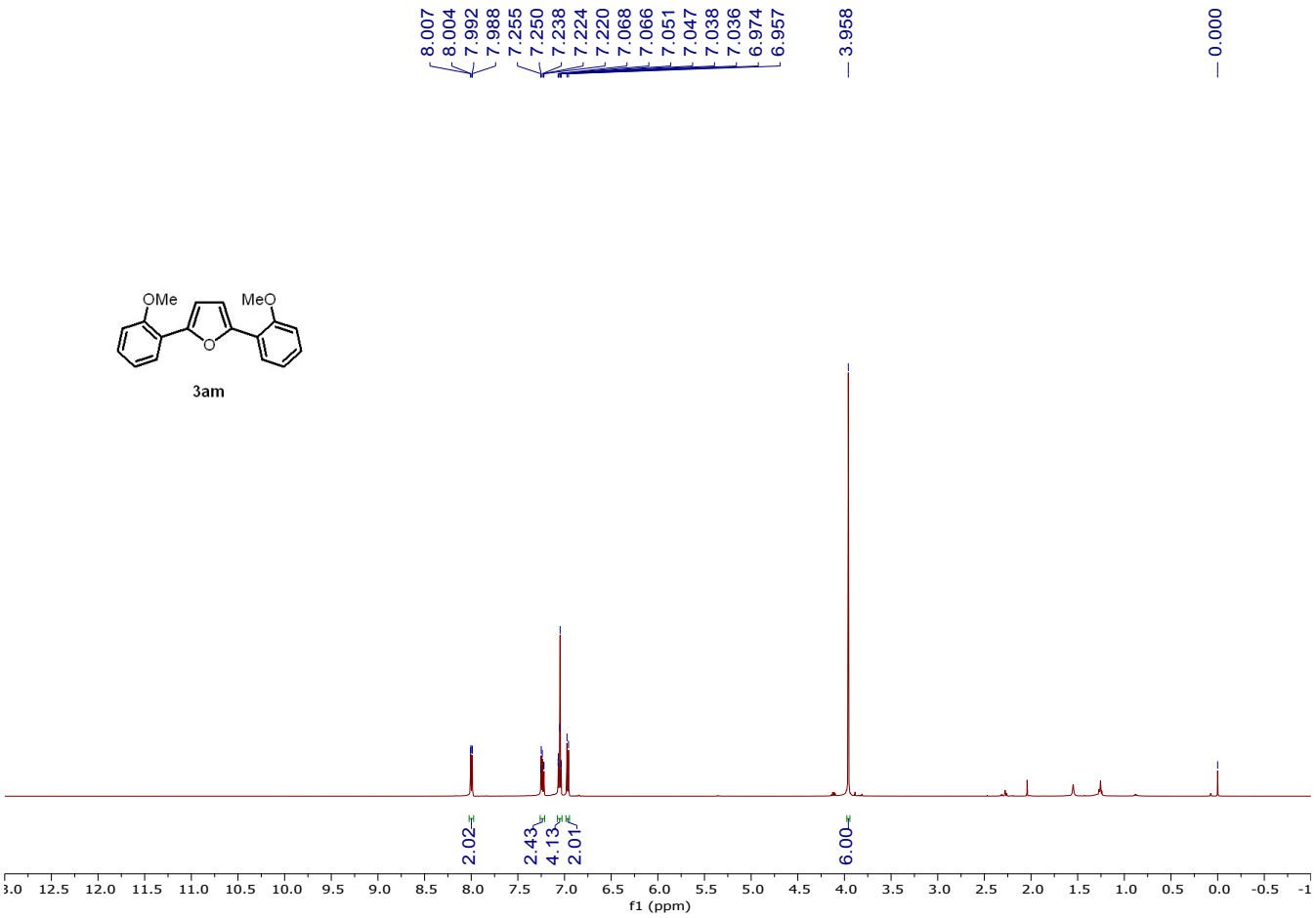

7.978
7.975
7.963
7.959
7.728
7.724
7.721
7.610
7.595
7.323
7.307
7.291
7.278
7.275
7.261
7.247
7.243
7.217
7.215
7.202
7.199
7.075
7.060
7.045
7.031
7.024
6.974
6.958
6.777
6.770
3.948
0.000
Cl
MeO
O
3ai
1.00
0.98
1.03
1.13
1.28
1.01
1.13
0.96
1.03
0.98
2.93
f1 (ppm)
155.551
150.691
150.374
134.677
132.527
129.920
128.287
126.956
125.882
123.613
121.732
120.762
119.448
112.258
110.969
108.481
77.254
77.000
76.746
55.359
f1 (ppm)

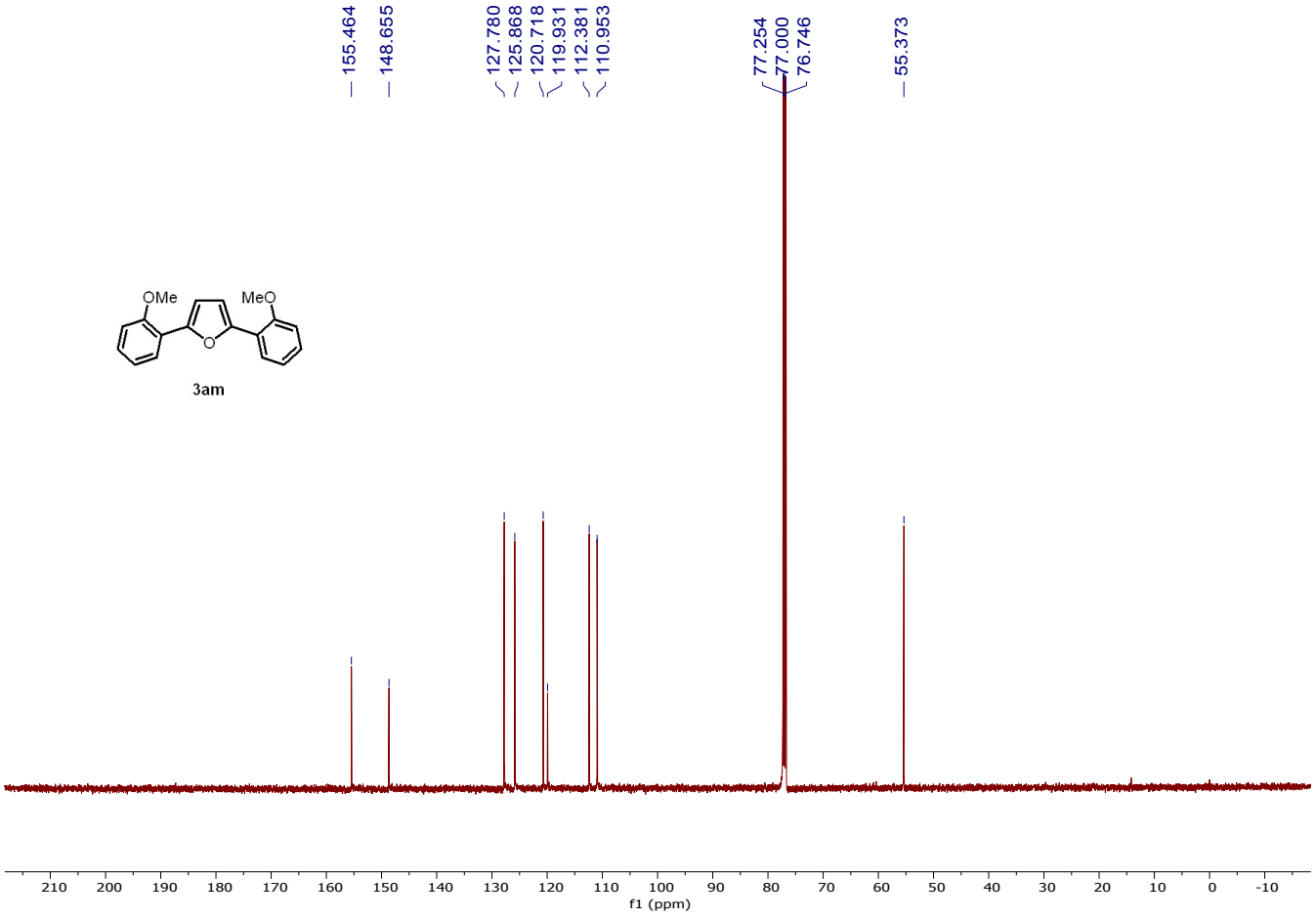

7.979
7.976
7.964
7.960
7.887
7.884
7.880
7.665
7.662
7.659
7.649
7.646
7.644
7.376
7.374
7.372
7.370
7.360
7.358
7.356
7.354
7.284
7.280
7.267
7.251
7.235
7.082
7.080
7.067
7.065
7.052
7.049
7.034
7.027
6.982
6.966
3.957
0.000
Br
MeO
3aj
1.00
1.01
1.07
1.07
2.47
1.13
0.98
1.03
0.97
2.96
f1 (ppm)
155.561
150.538
150.423
132.795
130.192
129.870
128.307
126.512
125.904
122.870
122.183
120.771
119.444
112.264
110.979
108.520
77.254
77.000
76.746
55.376
Br
MeO
3aj
f1 (ppm)

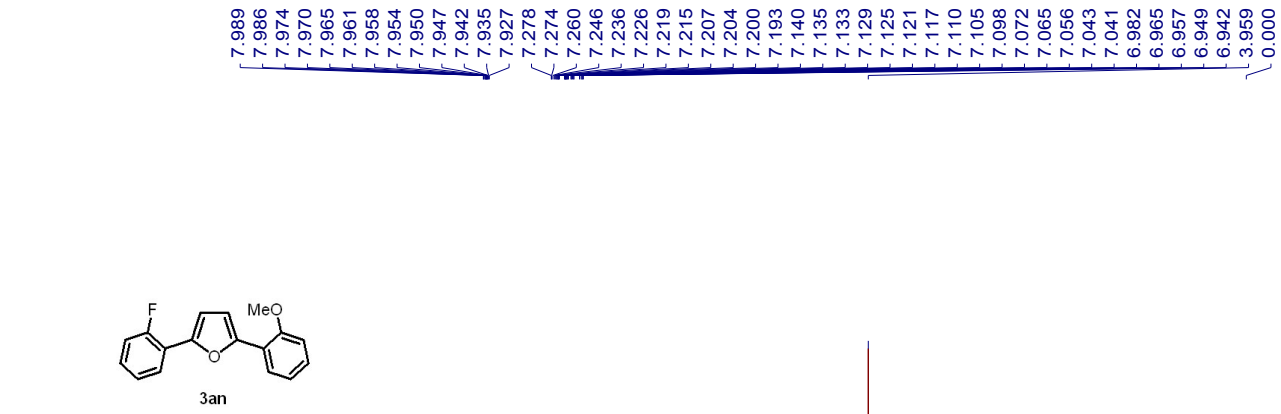

7.988
7.984
7.972
7.968
7.962
7.901
7.898
7.895
7.892
7.884
7.880
7.512
7.496
7.491
7.488
7.485
7.483
7.475
7.289
7.285
7.274
7.273
7.271
7.269
7.258
7.254
7.089
7.086
7.073
7.071
7.058
7.056
7.051
7.044
6.981
6.965
6.838
6.831
3.954
0.000
MeO
F3C
O
3ak
1.91
0.94
1.96
0.97
1.04
0.90
0.93
0.95
3.00
f1 (ppm)


155.608
150.640
150.614
131.549
131.284
131.027
130.770
129.145
128.411
127.349
126.645
125.914
125.183
123.017
120.851
120.786
120.356
120.324
120.294
120.263
119.377
112.297
111.000
108.722
77.254
77.000
76.746
55.362
MeO
F3C
O
3ak
f1 (ppm)


7.963
7.960
7.948
7.944
7.811
7.808
7.795
7.286
7.272
7.266
7.262
7.260
7.257
7.247
7.234
7.231
7.219
7.216
7.204
7.189
7.186
7.061
7.054
7.049
7.046
7.034
7.031
6.984
6.967
6.668
6.661
3.965
2.581
-0.000
Me
MeO
3al
1.02
1.04
3.20
1.48
2.02
1.00
0.96
3.03
3.00
f1 (ppm)
155.452
152.047
149.434
134.423
131.234
130.180
127.953
127.252
126.887
125.984
125.830
120.767
119.788
111.888
110.944
110.780
77.254
77.000
76.746
55.375
22.135
Me
MeO
3al
f1 (ppm)


8.007
8.004
7.992
7.988
7.255
7.250
7.238
7.224
7.220
7.068
7.066
7.051
7.047
7.038
7.036
6.974
6.957
3.958
0.000
OMe
MeO
3am
2.02
2.43
4.13
2.01
6.00
f1 (ppm)


155.464
148.655
127.780
125.868
120.718
119.931
112.381
110.953
77.254
77.000
76.746
55.373
OMe
MeO
3am
f1 (ppm)

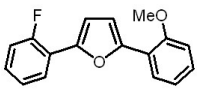

7.989
7.986
7.974
7.970
7.965
7.961
7.958
7.954
7.950
7.947
7.942
7.935
7.927
7.278
7.274
7.260
7.246
7.236
7.226
7.219
7.215
7.207
7.204
7.200
7.193
7.140
7.135
7.133
7.129
7.125
7.121
7.117
7.110
7.105
7.098
7.072
7.065
7.056
7.043
7.041
6.982
6.965
6.957
6.949
6.942
3.959
0.000

F
MeO
O

3an

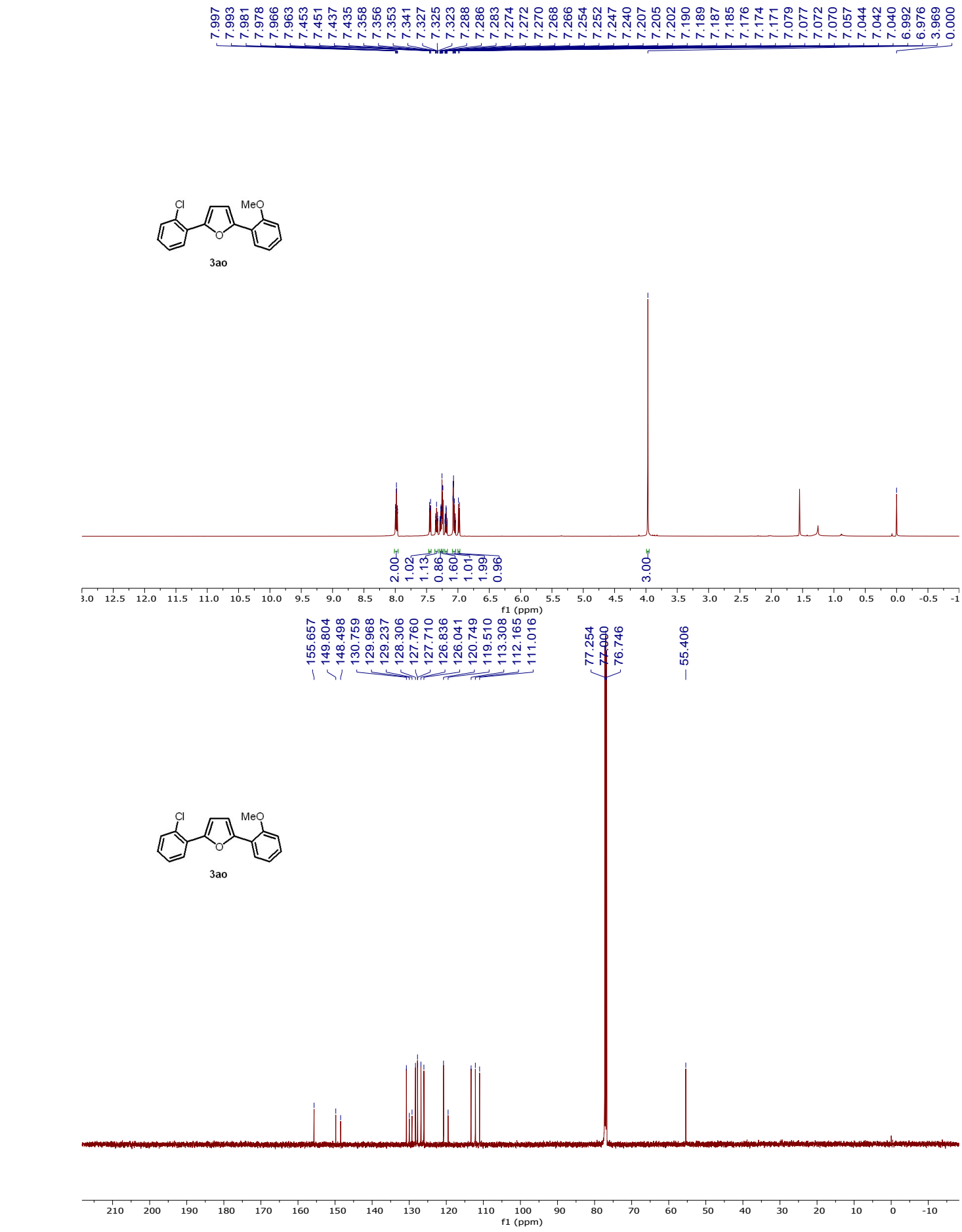
1.10
0.88
1.37
2.09
1.09
1.96
1.02
0.97
3.00
f1 (ppm)

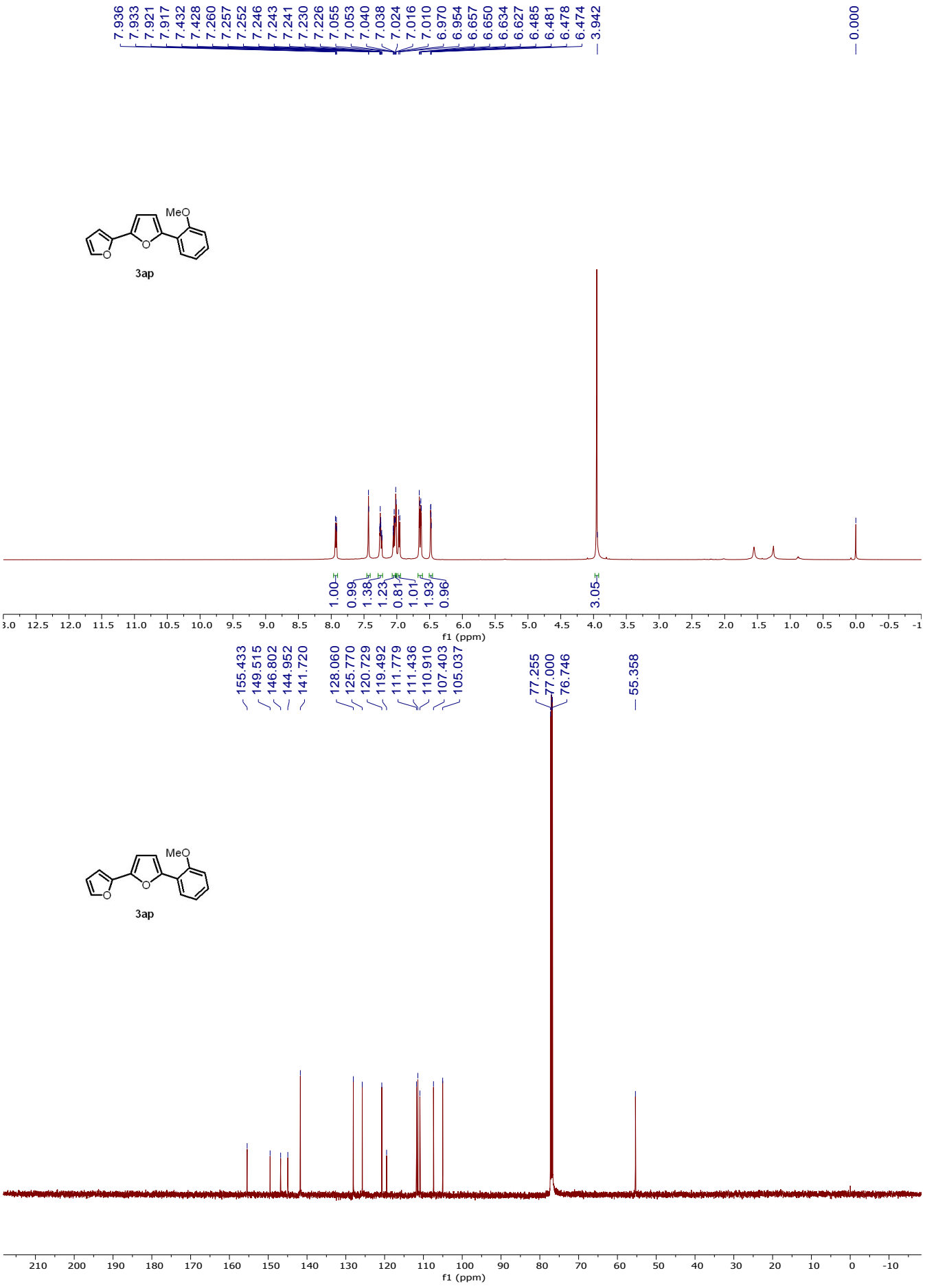

159.672
157.678
155.581
149.632
146.370
146.346
128.209
128.002
127.937
125.927
125.894
124.267
124.239
120.729
119.560
119.217
119.120
115.963
115.791
112.587
112.493
112.455
112.442
110.996
77.254
77.000
76.746
55.378

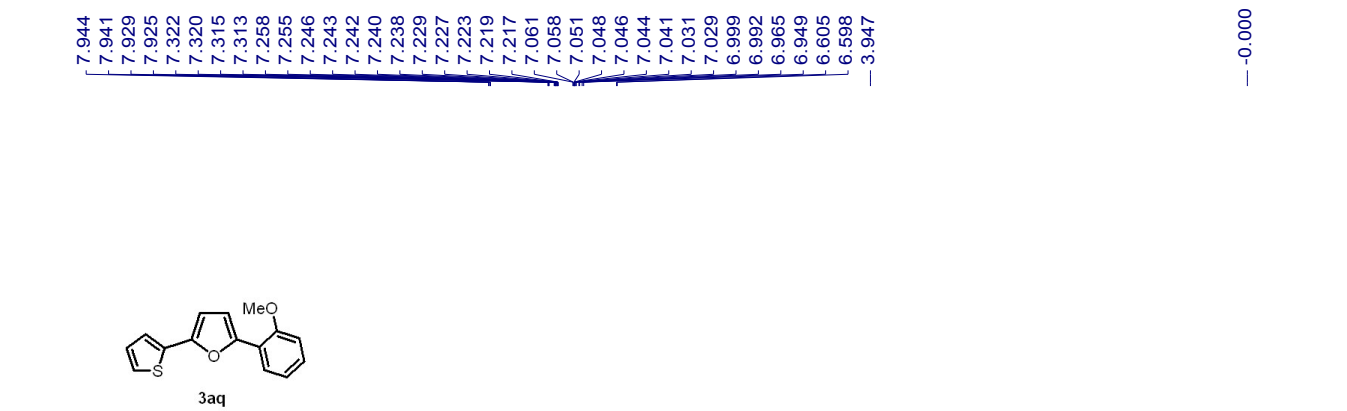

F
MeO
O

3an

f1 (ppm)

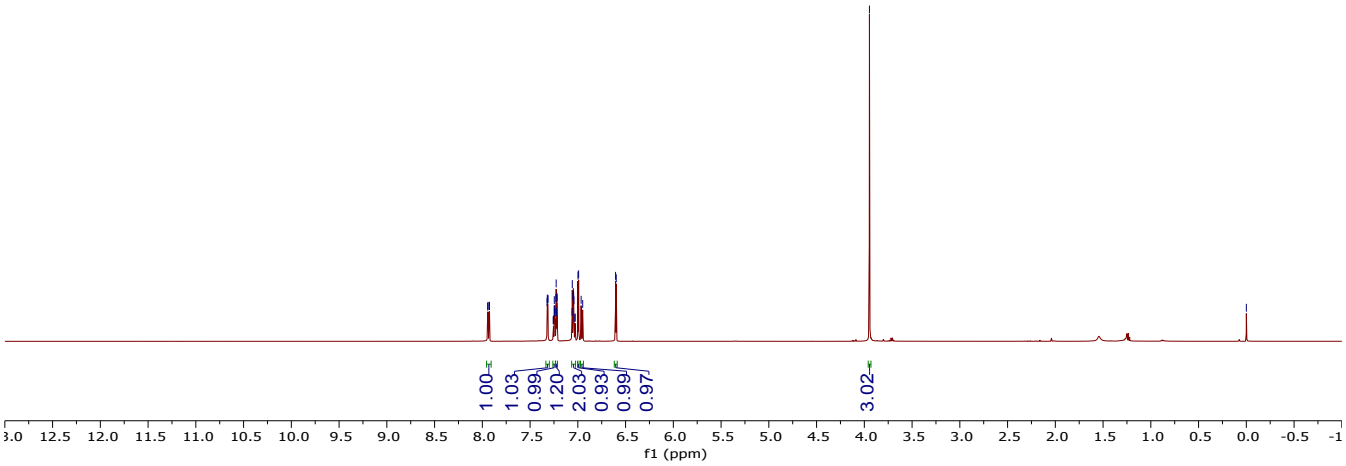

7.997
7.993
7.981
7.978
7.966
7.963
7.453
7.451
7.437
7.435
7.358
7.356
7.353
7.341
7.327
7.325
7.323
7.288
7.286
7.283
7.274
7.272
7.270
7.268
7.266
7.254
7.252
7.247
7.240
7.207
7.205
7.202
7.190
7.189
7.187
7.185
7.176
7.174
7.171
7.079
7.077
7.072
7.070
7.057
7.044
7.042
7.040
6.992
6.976
3.969
0.000
Cl
MeO
O
3ao
2.00
1.02
1.13
0.86
1.60
1.01
1.99
0.96
3.00
f1 (ppm)
155.657
149.804
148.498
130.759
129.968
129.237
128.306
127.760
127.710
126.836
126.041
120.749
119.510
113.308
112.165
111.016
77.254
77.000
76.746
55.406
Cl
MeO
O
3ao
f1 (ppm)

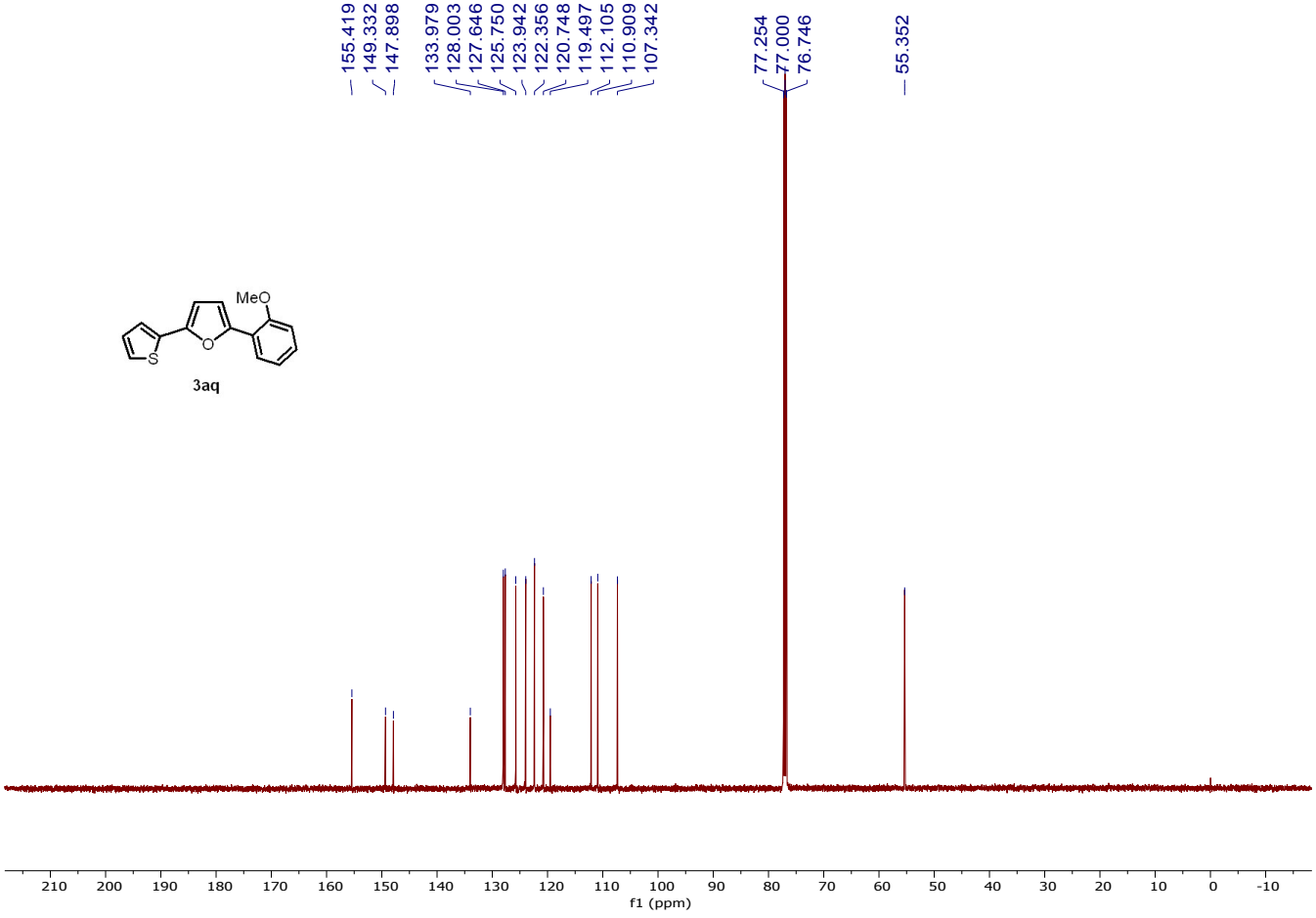

7.936
7.933
7.921
7.917
7.432
7.428
7.260
7.257
7.252
7.246
7.243
7.241
7.230
7.226
7.055
7.053
7.040
7.038
7.024
7.016
7.010
6.970
6.954
6.657
6.650
6.634
6.627
6.485
6.481
6.478
6.474
3.942
0.000
MeO
3ap
1.00
0.99
1.38
1.23
0.81
1.01
1.93
0.96
3.05
f1 (ppm)
155.433
149.515
146.802
144.952
141.720
128.060
125.770
120.729
119.492
111.779
111.436
110.910
107.403
105.037
77.255
77.000
76.746
55.358
MeO
3ap
f1 (ppm)


7.944
7.941
7.929
7.925
7.322
7.320
7.315
7.313
7.258
7.255
7.246
7.243
7.242
7.240
7.238
7.229
7.227
7.223
7.219
7.217
7.061
7.058
7.051
7.048
7.046
7.044
7.041
7.031
7.029
6.999
6.992
6.965
6.949
6.605
6.598
3.947
-0.000

MeO
S
O

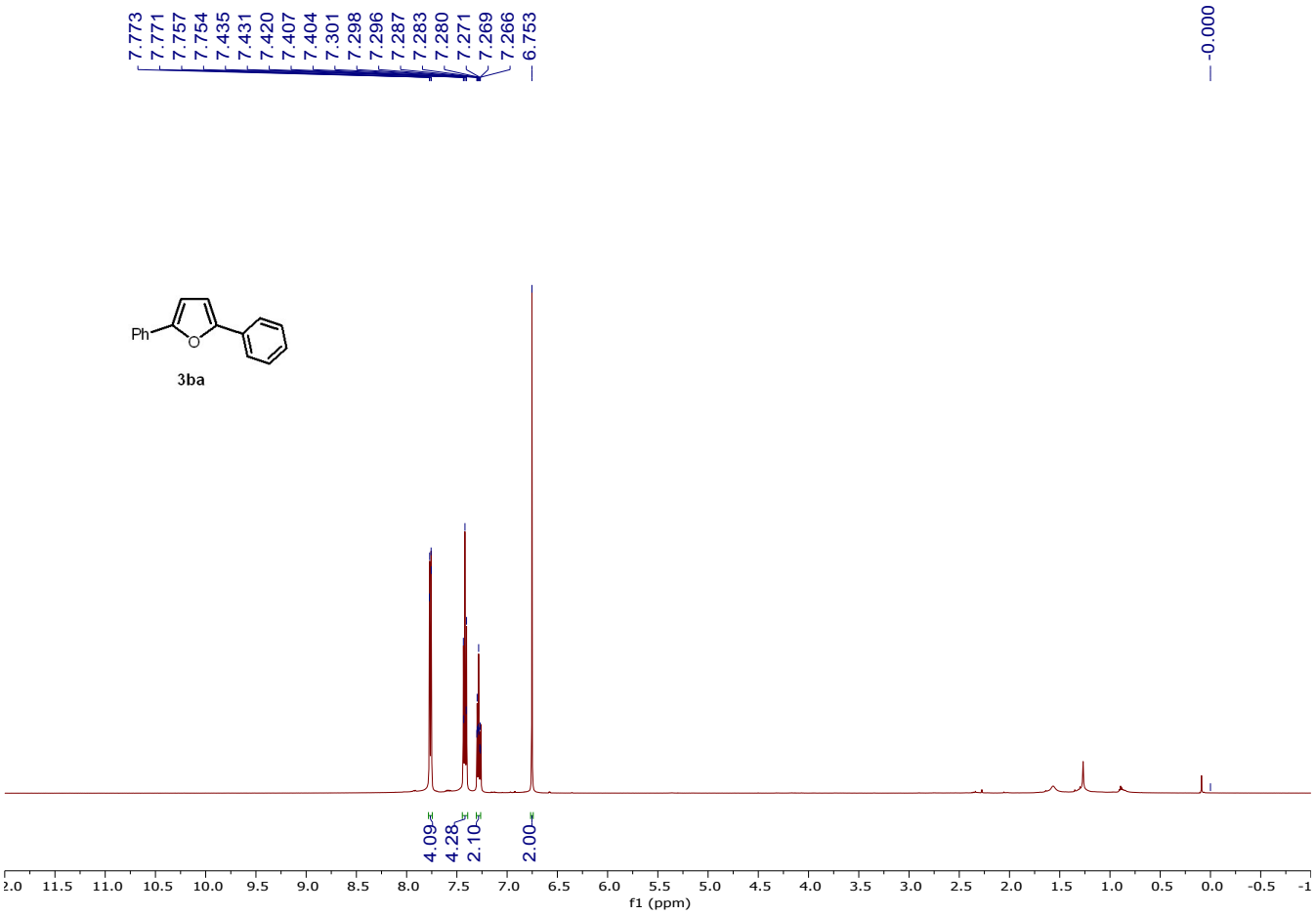
3aq

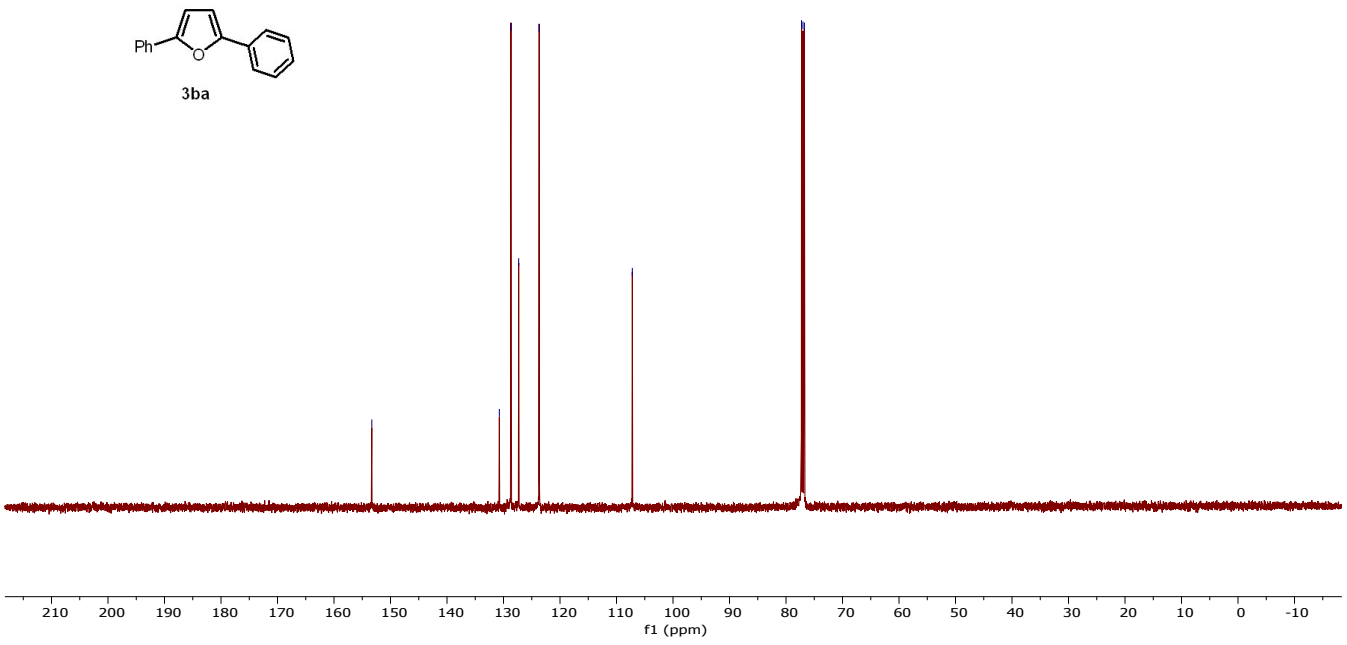

1.00
1.03
0.99
1.20
2.03
0.93
0.99
0.97
3.02
f1 (ppm)

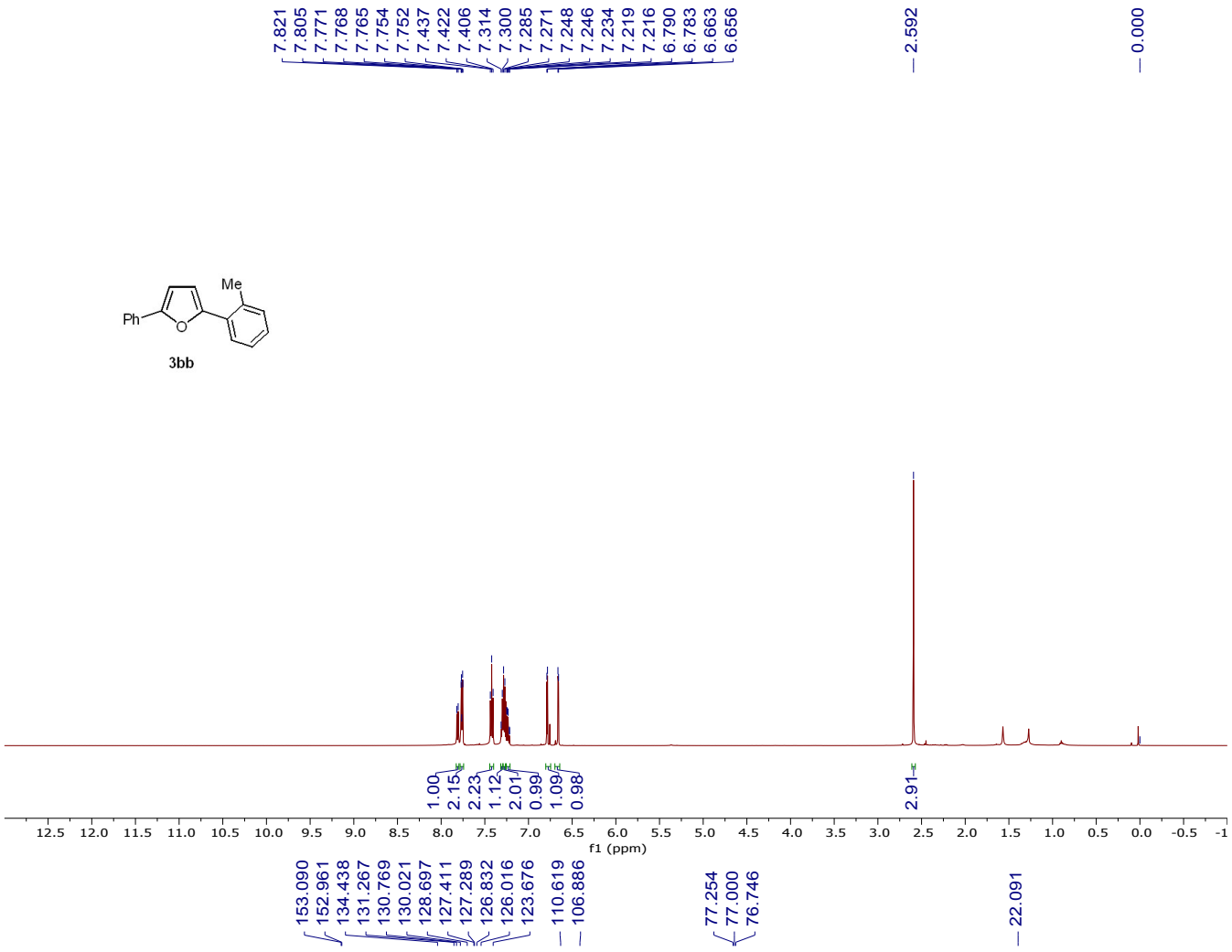

155.419
149.332
147.898
133.979
128.003
127.646
125.750
123.942
122.356
120.748
119.497
112.105
110.909
107.342
77.254
77.000
76.746
55.352
f1 (ppm)

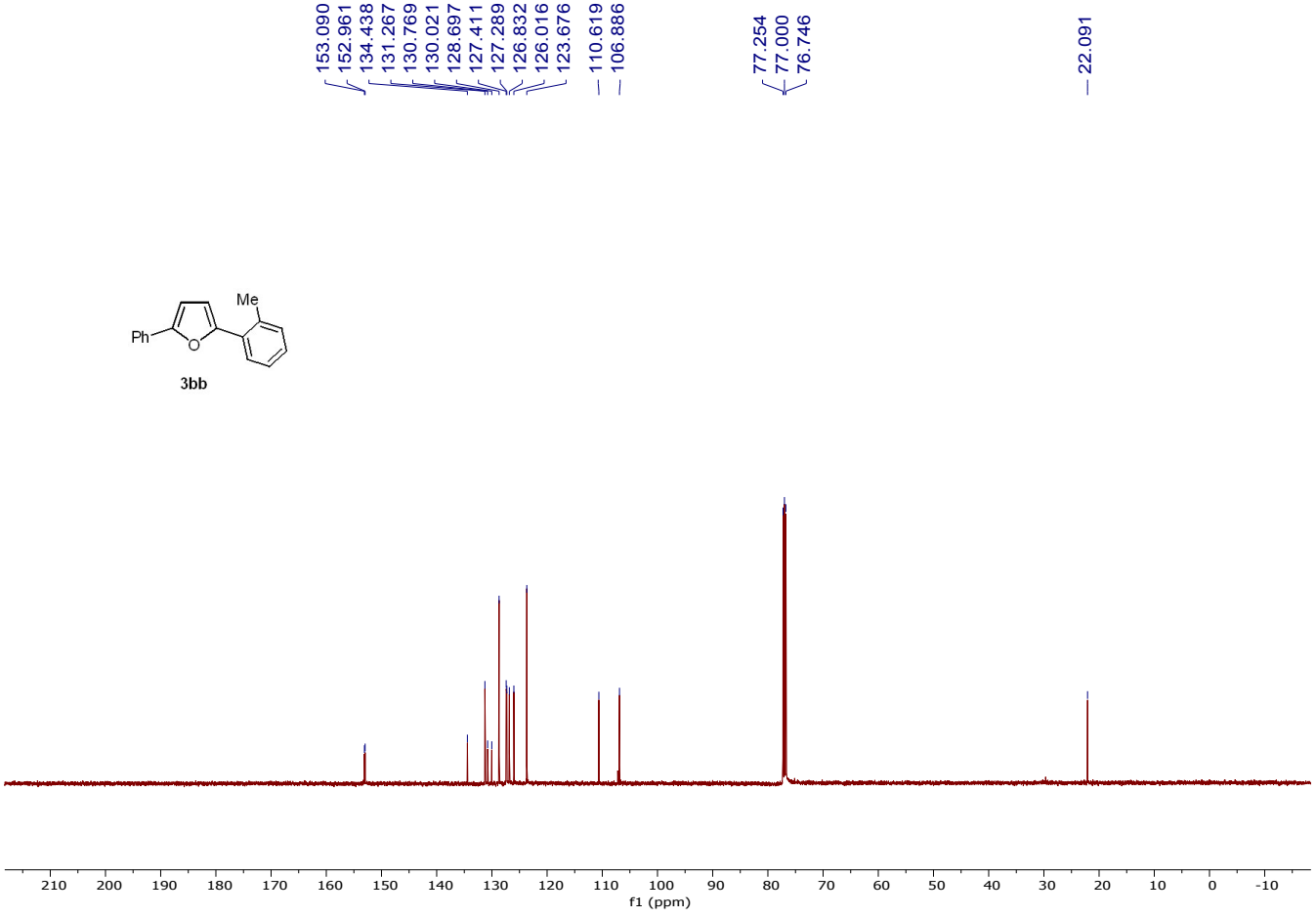
MeO
S
O

3aq

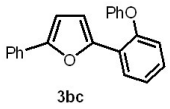

7.773
7.771
7.757
7.754
7.435
7.431
7.420
7.407
7.404
7.301
7.298
7.296
7.287
7.283
7.280
7.271
7.269
7.266
6.753
-0.000
Ph
O
3ba
4.09
4.28
2.10
2.00
f1 (ppm)


153.307
130.736
128.684
127.315
123.683
107.201
77.254
77.000
76.746
Ph
O
3ba
f1 (ppm)

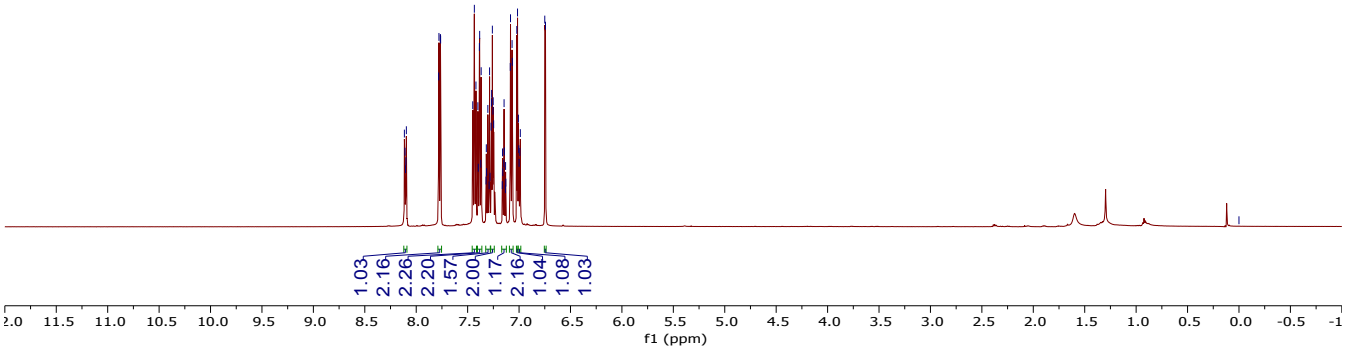

7.821
7.805
7.771
7.768
7.765
7.754
7.752
7.437
7.422
7.406
7.314
7.300
7.285
7.271
7.248
7.246
7.234
7.219
7.216
6.790
6.783
6.663
6.656
2.592
0.000
Me
Ph
O
3bb
1.00
2.15
2.23
1.12
2.01
0.99
1.09
0.98
2.91
f1 (ppm)


153.090
152.961
134.438
131.267
130.769
130.021
128.697
127.411
127.289
126.832
126.016
123.676
110.619
106.886
77.254
77.000
76.746
22.091
Me
Ph
O
3bb
f1 (ppm)

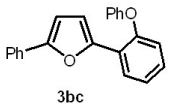

8.115
8.109
8.103
8.100
8.096
7.782
7.779
7.765
7.763
7.450
7.435
7.419
7.400
7.396
7.386
7.383
7.372
7.368
7.321
7.318
7.316
7.304
7.291
7.287
7.283
7.272
7.268
7.267
7.260
7.254
7.252
7.247
7.163
7.161
7.158
7.148
7.146
7.143
7.133
7.131
7.129
7.086
7.083
7.068
7.066
7.022
7.015
7.006
7.003
7.000
6.992
6.988
6.750
6.743
0.000


PhO
Ph
O

3bc

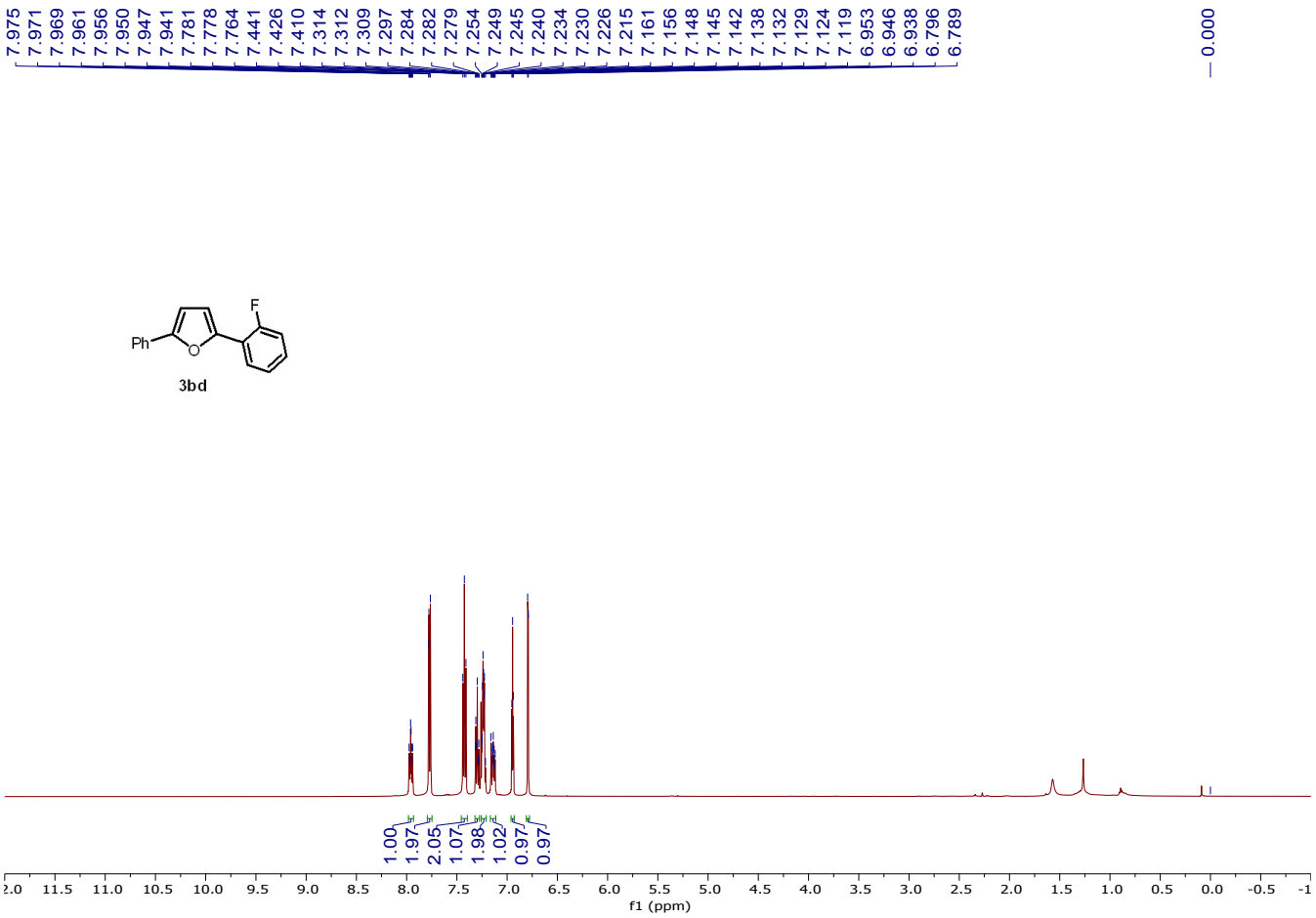

1.03
2.16
2.26
2.20
1.57
2.00
1.17
2.16
1.04
1.08
1.03
f1 (ppm)


156.914
152.719
152.426
148.993
130.690
129.820
128.663
128.019
127.327
126.237
123.910
123.788
123.151
122.824
119.782
118.265
112.550
107.533
77.254
77.000
76.746

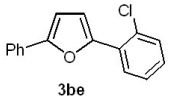

PhO
Ph
O

3bc

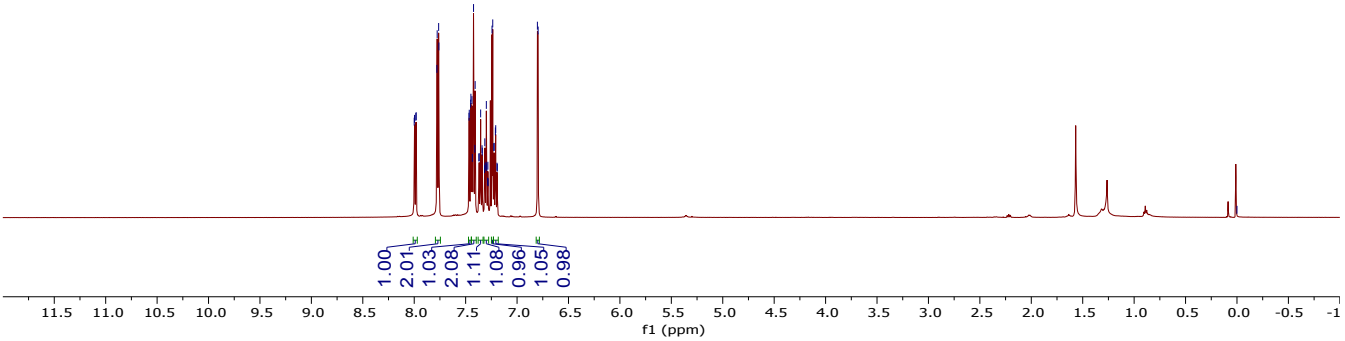
f1 (ppm)

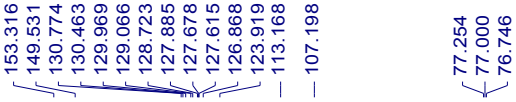

7.975
7.971
7.969
7.961
7.956
7.950
7.947
7.941
7.781
7.778
7.764
7.441
7.426
7.410
7.314
7.312
7.309
7.297
7.284
7.282
7.279
7.254
7.249
7.245
7.240
7.234
7.230
7.226
7.215
7.161
7.156
7.148
7.145
7.142
7.138
7.132
7.129
7.124
7.119
6.953
6.946
6.938
6.796
6.789
0.000
F
Ph
O
3bd
1.00
1.97
2.05
1.07
1.98
1.02
0.97
0.97
f1 (ppm)
159.660
157.666
153.178
147.438
147.414
130.521
128.716
128.199
128.132
127.536
125.838
125.813
124.304
124.276
123.852
119.068
118.972
115.995
115.825
112.434
112.338
107.490
107.475
77.254
77.000
76.746
F
Ph
O
3bd
f1 (ppm)

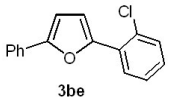

8.000
7.997
7.984
7.981
7.780
7.777
7.762
7.760
7.467
7.465
7.451
7.449
7.439
7.435
7.423
7.411
7.408
7.371
7.369
7.354
7.341
7.338
7.316
7.313
7.311
7.302
7.299
7.295
7.286
7.284
7.281
7.244
7.237
7.226
7.223
7.211
7.208
7.195
7.192
6.802
6.795
-0.000


Cl
Ph
O

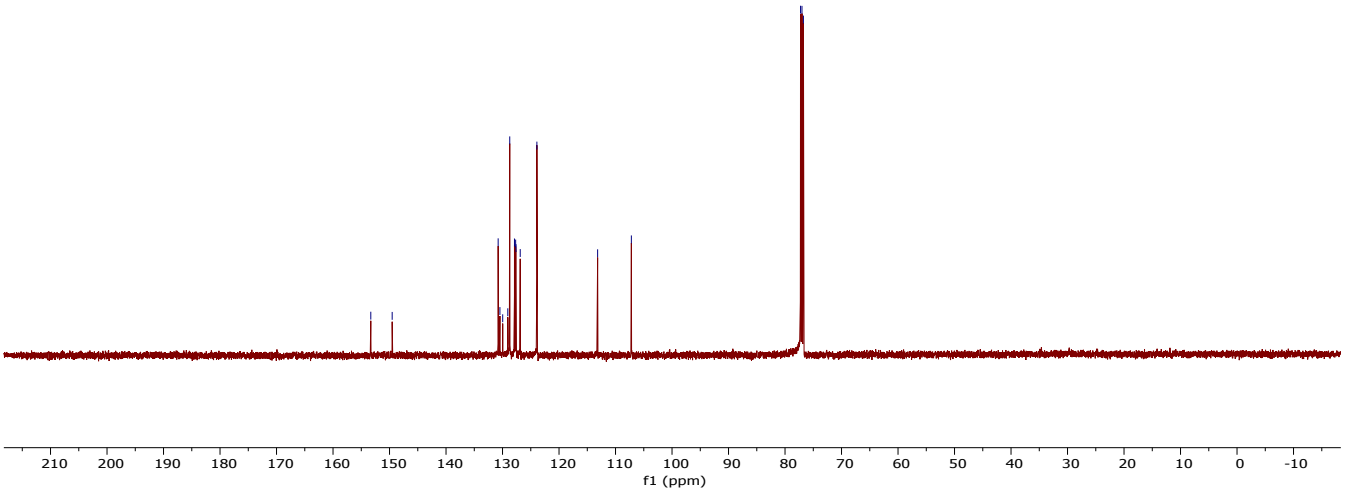
3be

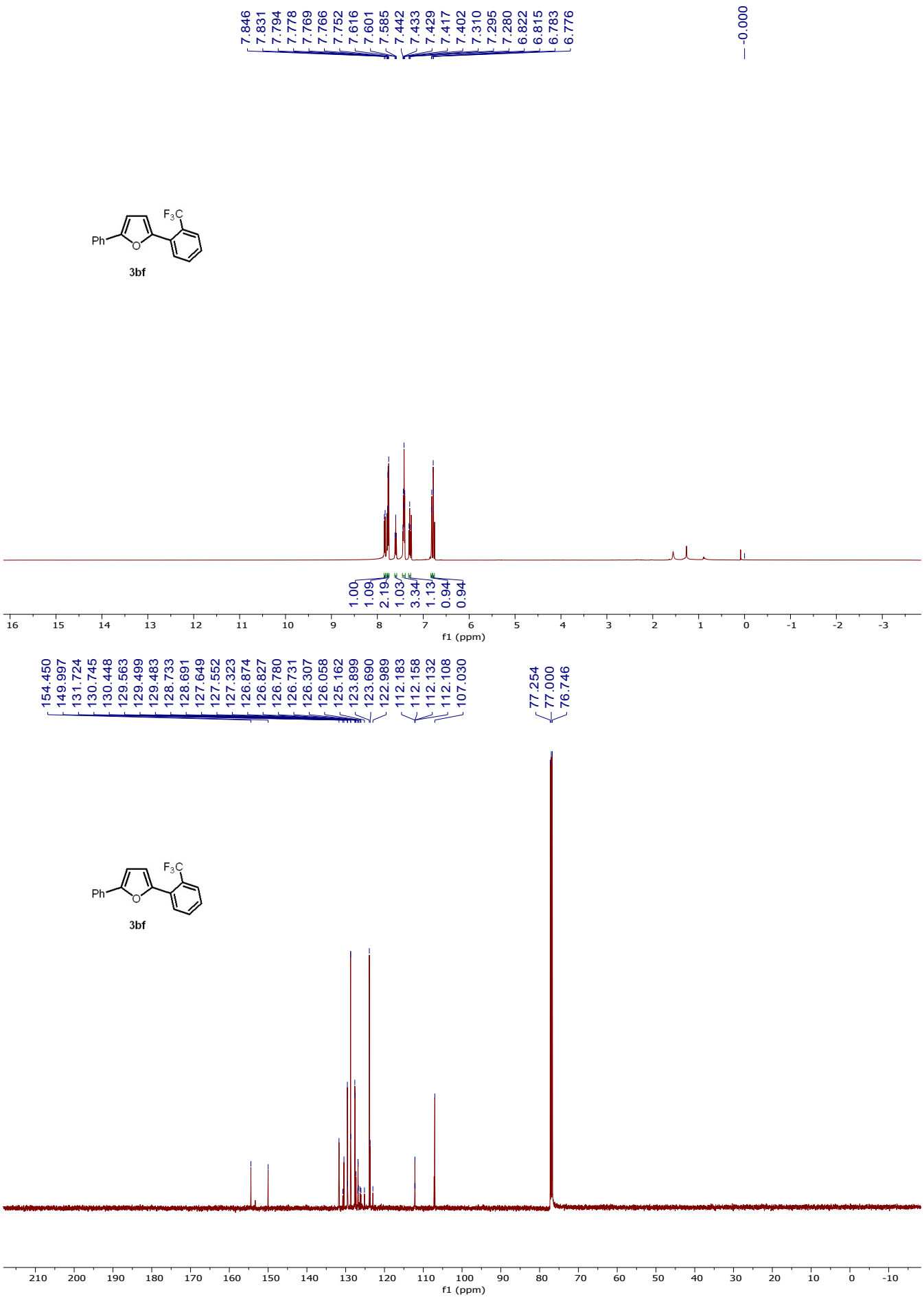

1.00
2.01
1.03
2.08
1.11
1.08
0.96
1.05
0.98
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

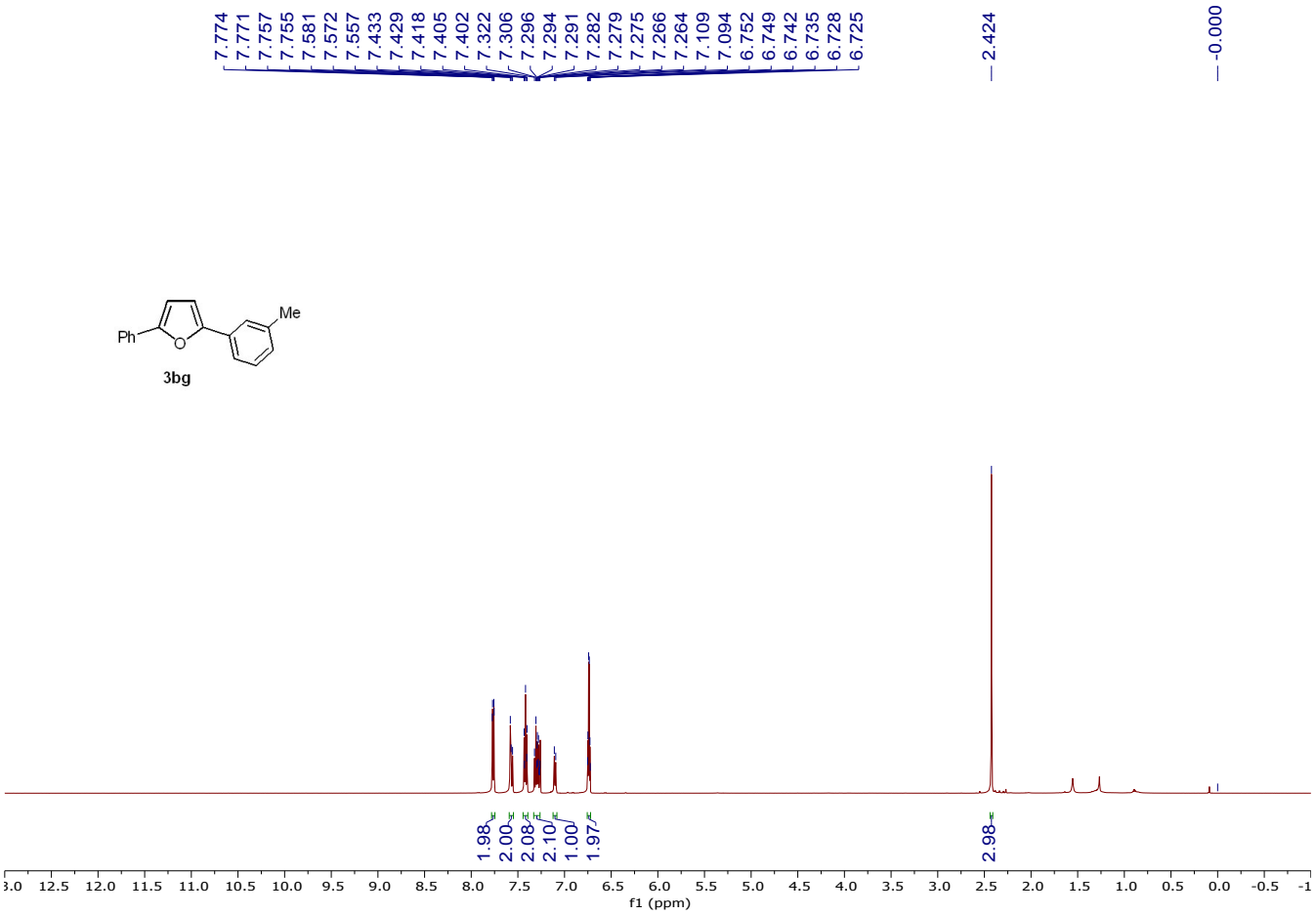

153.316
149.531
130.774
130.463
129.969
129.066
128.723
127.885
127.678
127.615
126.868
123.919
113.168
107.198
77.254
77.000
76.746

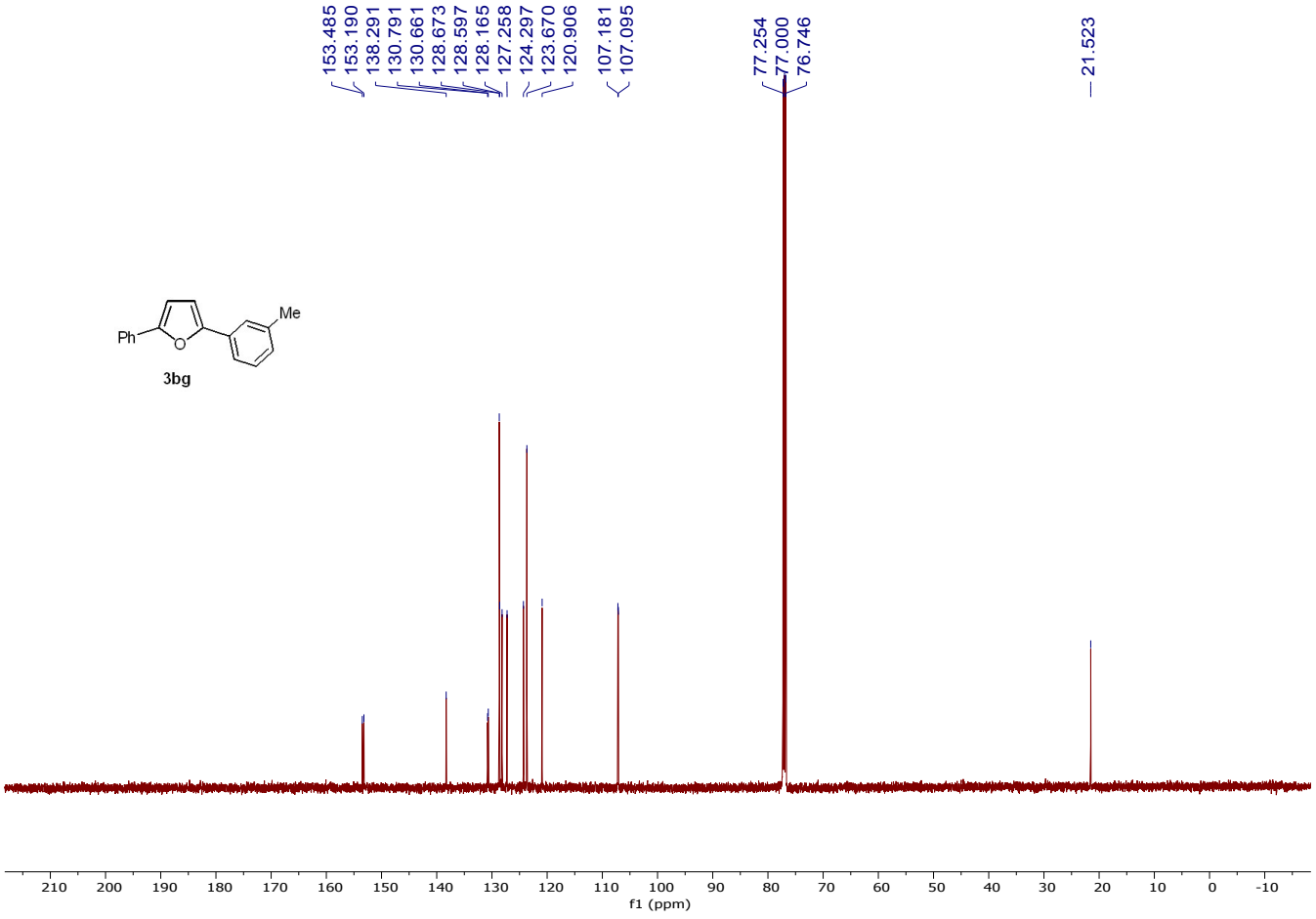

Cl
Ph
O

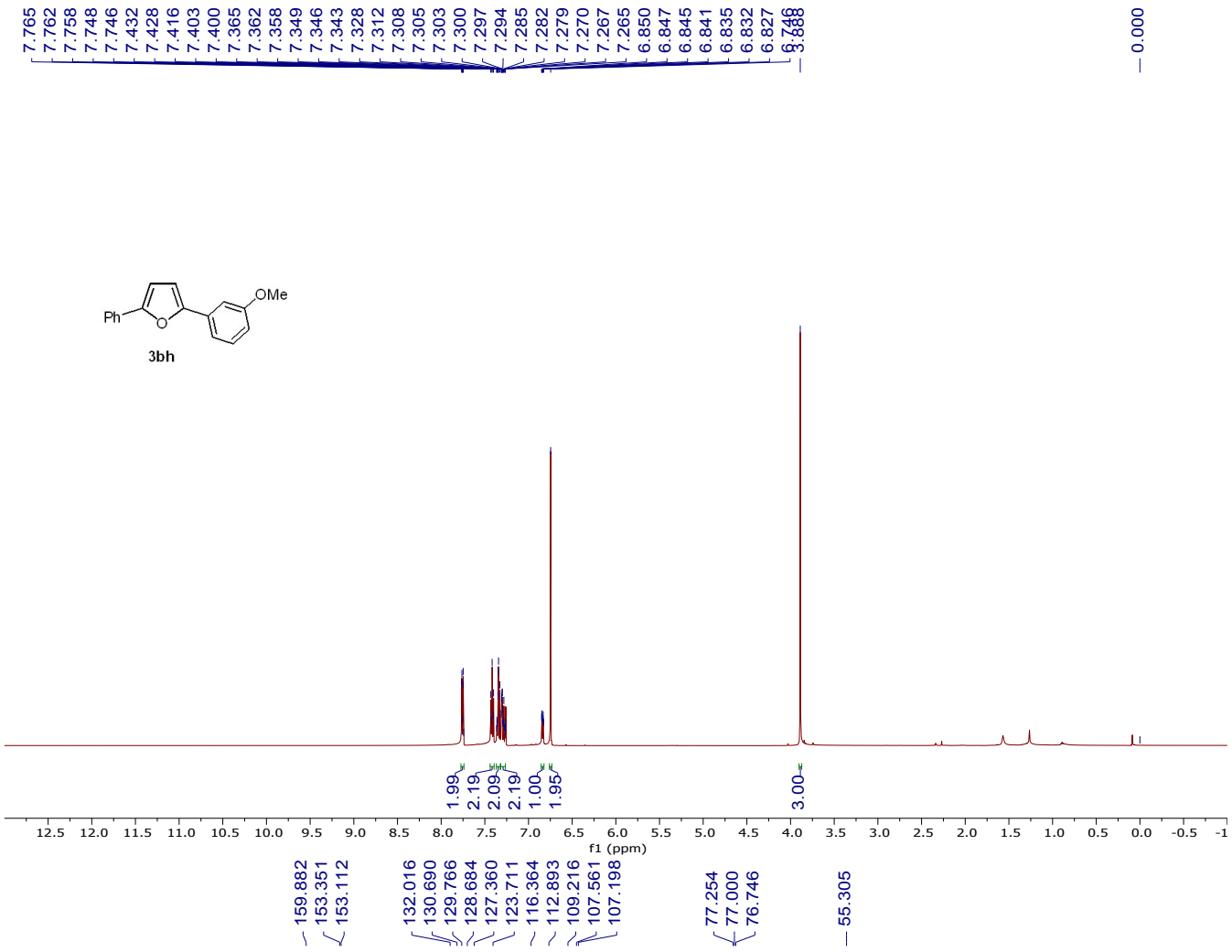
3be

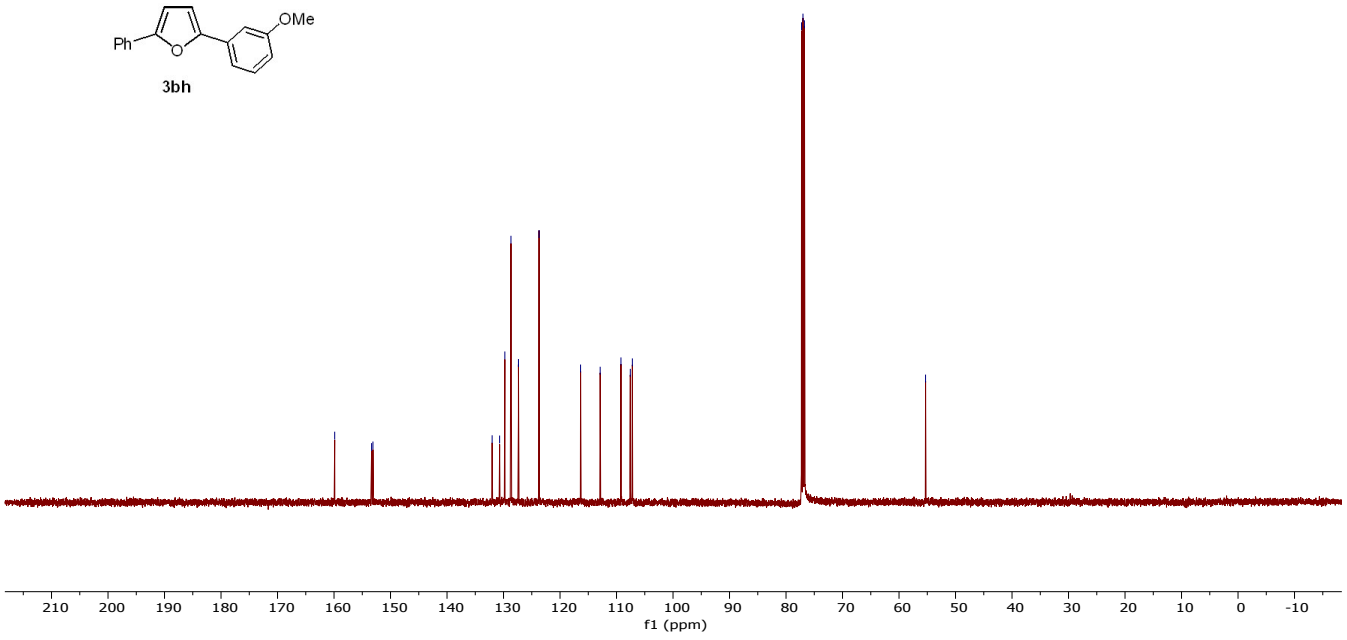

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.846
7.831
7.794
7.778
7.769
7.766
7.752
7.616
7.601
7.585
7.442
7.433
7.429
7.417
7.402
7.310
7.295
7.280
6.822
6.815
6.783
6.776
-0.000
F3C
Ph
O
3bf
1.00
1.09
2.19
1.03
3.34
1.13
0.94
0.94
f1 (ppm)
154.450
149.997
131.724
130.745
130.448
129.563
129.499
129.483
128.733
128.691
127.649
127.552
127.323
126.874
126.827
126.780
126.731
126.307
126.058
125.162
123.899
123.690
122.989
112.183
112.158
112.132
112.108
107.030
77.254
77.000
76.746
F3C
Ph
O
3bf
f1 (ppm)

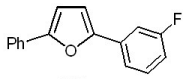

7.774
7.771
7.757
7.755
7.581
7.572
7.557
7.433
7.429
7.418
7.405
7.402
7.322
7.306
7.296
7.294
7.291
7.282
7.279
7.275
7.266
7.264
7.109
7.094
6.752
6.749
6.742
6.735
6.728
6.725
2.424
-0.000
Ph
Me
O
3bg
1.98
2.00
2.08
2.10
1.00
1.97
2.98
f1 (ppm)


153.485
153.190
138.291
130.791
130.661
128.673
128.597
128.165
127.258
124.297
123.670
120.906
107.181
107.095
77.254
77.000
76.746
21.523
Ph
Me
O
3bg
f1 (ppm)

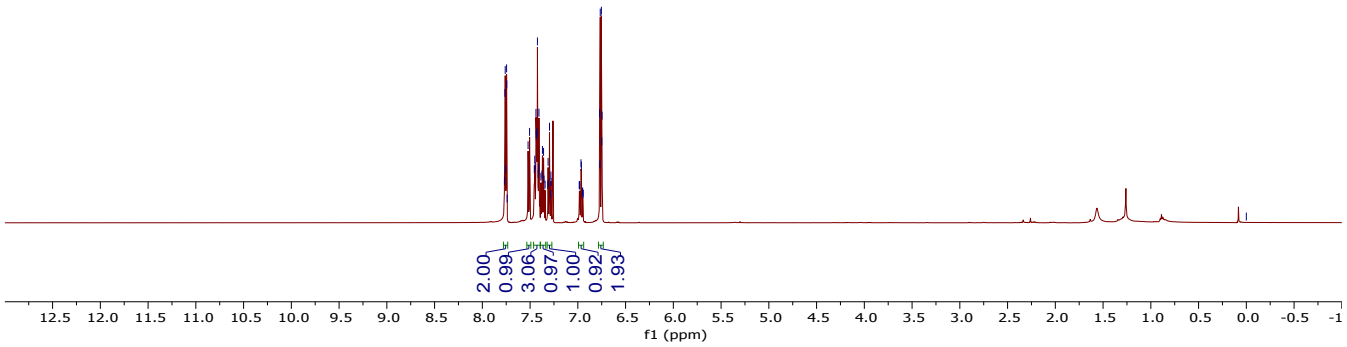

7.765
7.762
7.758
7.748
7.746
7.432
7.428
7.416
7.403
7.400
7.365
7.362
7.358
7.349
7.346
7.343
7.328
7.312
7.308
7.305
7.303
7.300
7.297
7.294
7.285
7.282
7.279
7.270
7.267
7.265
6.850
6.847
6.845
6.841
6.835
6.832
6.827
3.888
0.000
OMe
Ph
O
3bh
1.99
2.19
2.09
2.19
1.00
1.95
3.00
f1 (ppm)


159.882
153.351
153.112
132.016
130.690
129.766
128.684
127.360
123.711
116.364
112.893
109.216
107.561
107.198
77.254
77.000
76.746
55.305
OMe
Ph
O
3bh
f1 (ppm)

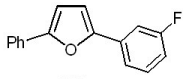

7.769
7.763
7.760
7.756
7.746
7.744
7.740
7.521
7.505
7.456
7.451
7.448
7.439
7.435
7.431
7.427
7.423
7.415
7.411
7.407
7.387
7.375
7.371
7.359
7.355
7.343
7.314
7.311
7.309
7.297
7.284
7.282
7.279
6.985
6.983
6.980
6.967
6.963
6.951
6.950
6.946
6.945
6.772
6.769
6.765
6.753
6.749
6.746
0.000


Ph
O
F

3bi


2.00
0.99
3.06
0.97
1.00
0.92
1.93
12.5 12.0 11.5 11.0 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 -1
f1 (ppm)

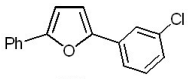

164.151
162.202
153.812
152.059
152.035
132.790
132.723
130.463
130.308
130.240
128.736
127.603
123.801
119.314
119.291
114.118
113.948
110.584
110.397
108.259
107.252
77.254
77.000
76.746


Ph
O
F

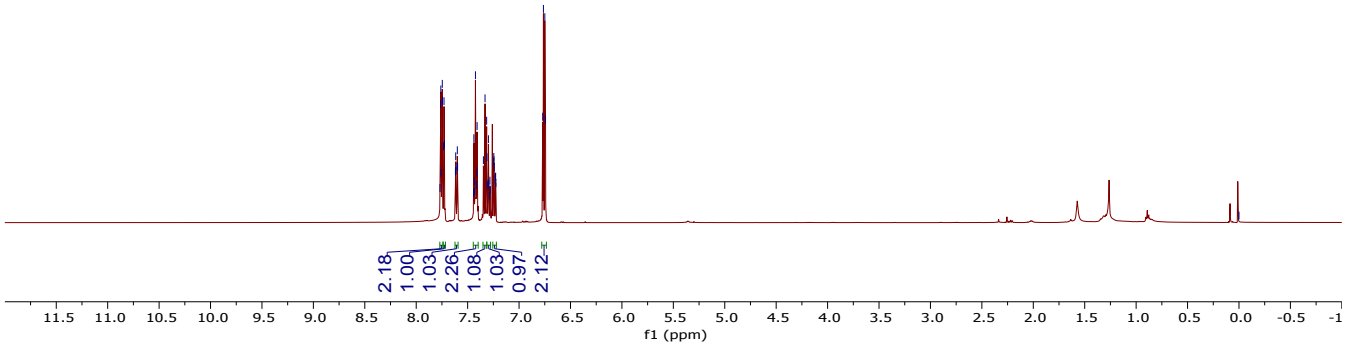
3bi

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)

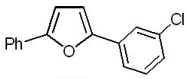

7.769
7.763
7.761
7.757
7.746
7.744
7.733
7.730
7.726
7.619
7.616
7.613
7.603
7.600
7.598
7.442
7.439
7.435
7.431
7.424
7.416
7.411
7.408
7.347
7.331
7.315
7.313
7.310
7.301
7.298
7.295
7.286
7.283
7.280
7.248
7.246
7.244
7.242
7.232
7.230
7.228
7.226
6.770
6.763
6.750
6.743
-0.000


Ph
O
Cl

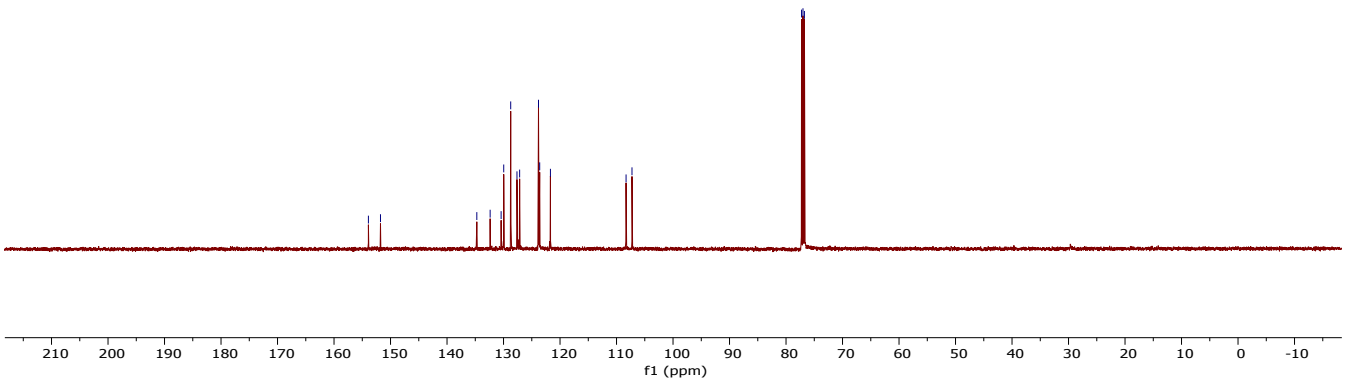
3bj


2.18
1.00
1.03
2.26
1.08
1.03
0.97
2.12
11.5 11.0 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 -1
f1 (ppm)

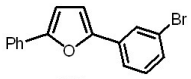

153.914
151.777
134.728
132.369
130.426
129.964
128.730
127.620
127.148
123.811
123.599
121.699
108.311
107.263
77.254
77.000
76.746


Ph
O
Cl

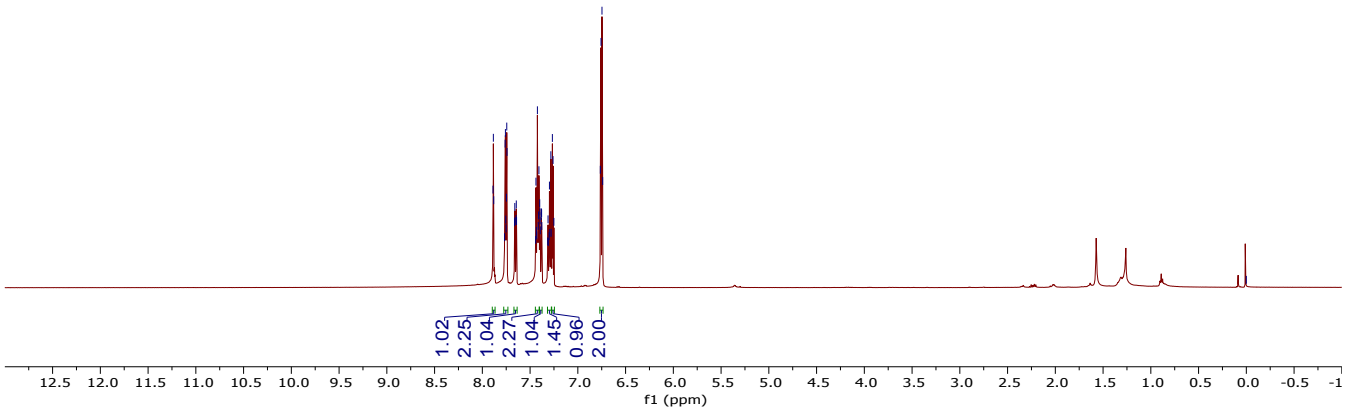
3bj


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)

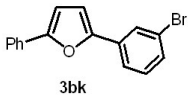

7.888
7.885
7.881
7.761
7.758
7.748
7.744
7.742
7.660
7.647
7.644
7.438
7.423
7.411
7.407
7.399
7.397
7.383
7.381
7.379
7.312
7.297
7.282
7.267
7.260
6.764
6.757
6.747
6.740
-0.000


Ph
Br
O

3bk


1.02
2.25
1.04
2.27
1.04
1.45
0.96
2.00
12.5 12.0 11.5 11.0 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 -1
f1 (ppm)

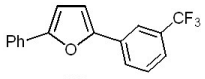

153.953
151.611
132.622
130.410
130.387
130.223
130.051
128.730
128.681
127.629
127.312
126.612
126.484
123.818
123.681
122.898
122.141
108.393
108.346
107.269
107.198
77.254
77.000
76.746


Ph
Br
O

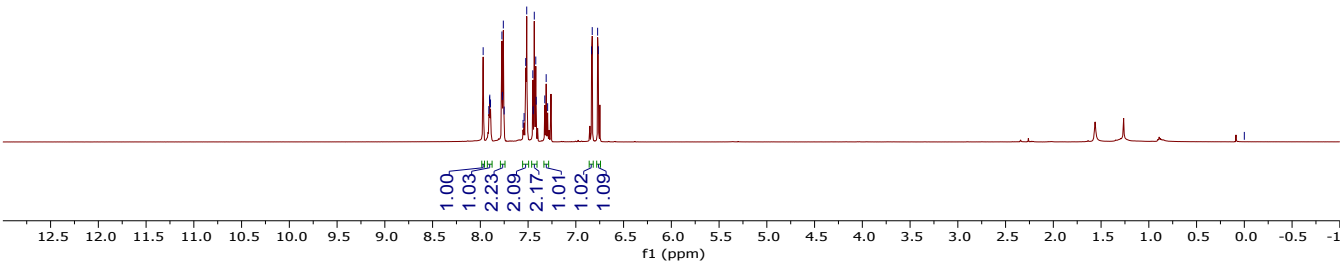
3bk

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)

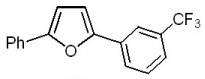

7.970
7.911
7.904
7.901
7.893
7.774
7.769
7.759
7.751
7.552
7.542
7.525
7.514
7.451
7.447
7.435
7.419
7.415
7.325
7.311
7.295
6.835
6.828
6.772
6.765
0.000


Ph
CF3

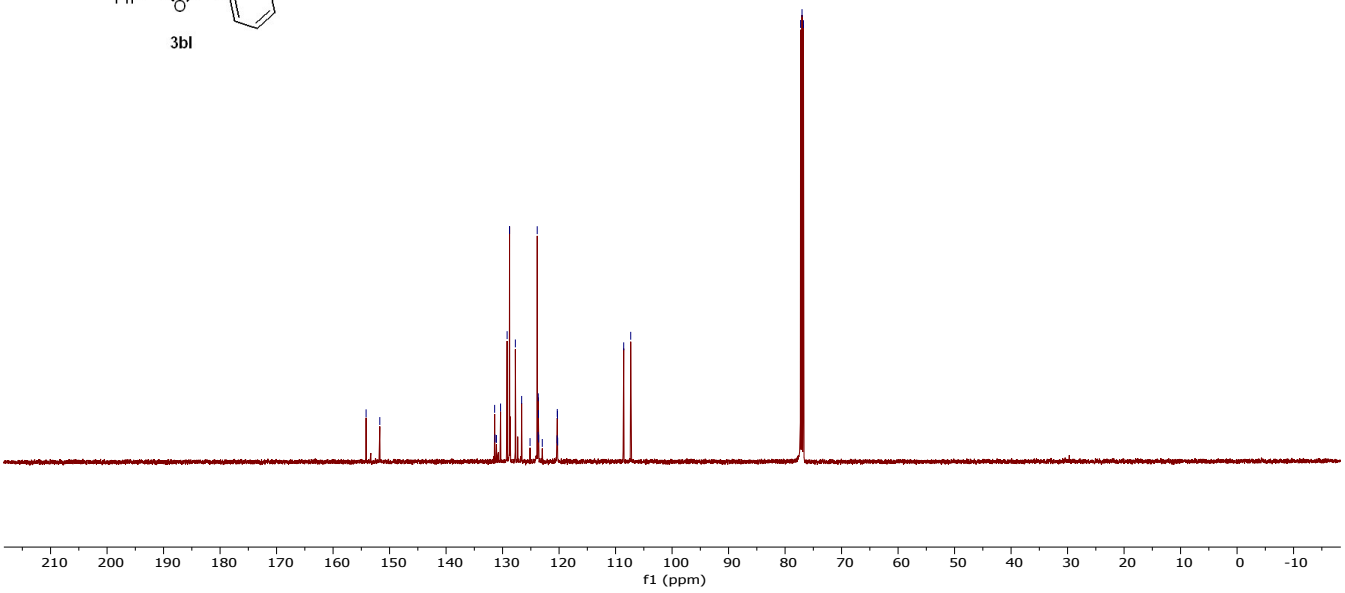
3bl

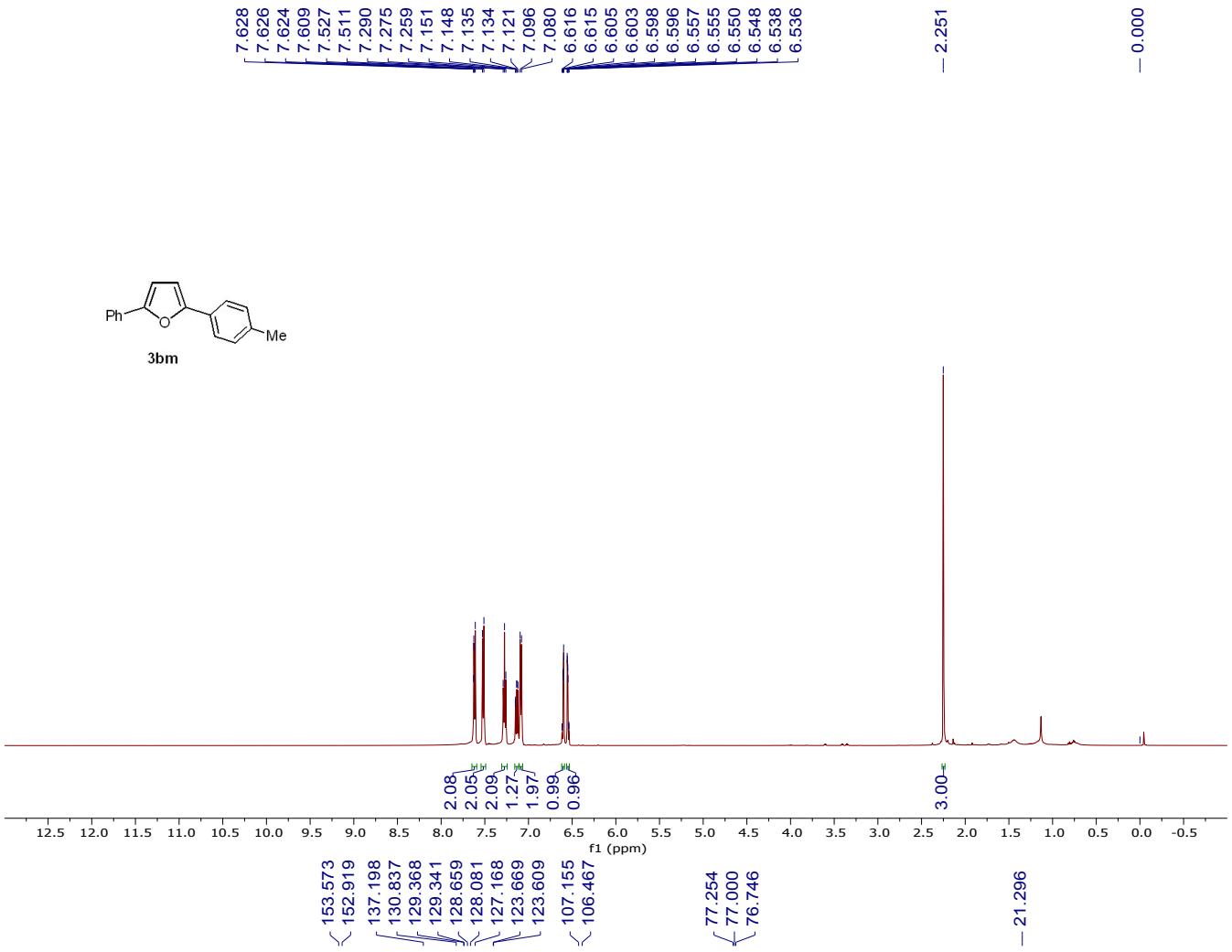

1.00
1.03
2.23
2.09
2.17
1.01
1.02
1.09
f1 (ppm)

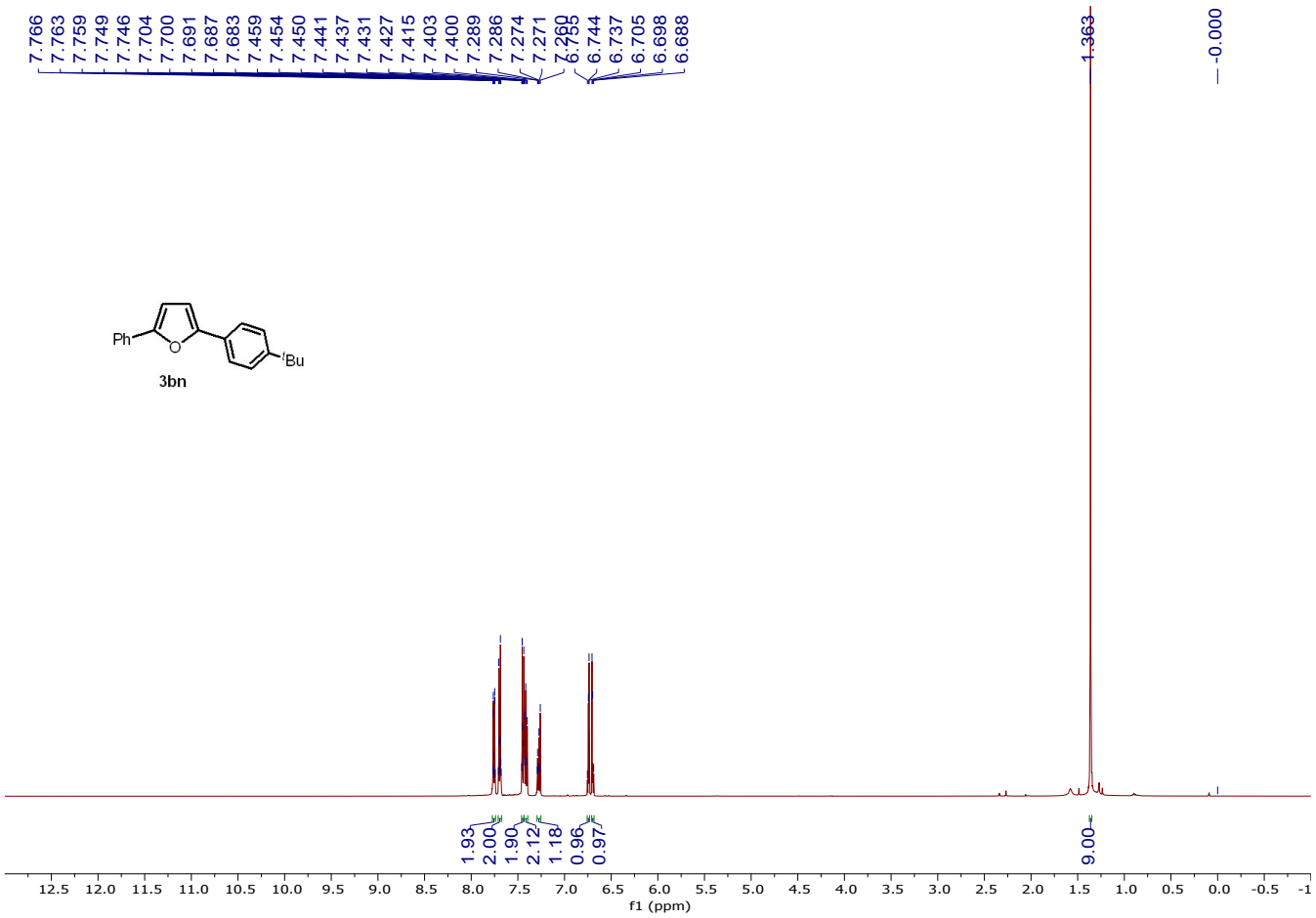

154.157
151.730
131.402
131.342
131.085
130.354
129.197
128.765
127.738
126.623
125.138
123.869
123.709
123.685
123.646
123.615
122.973
120.348
120.318
120.286
120.255
108.562
107.319
77.254
77.000
76.746

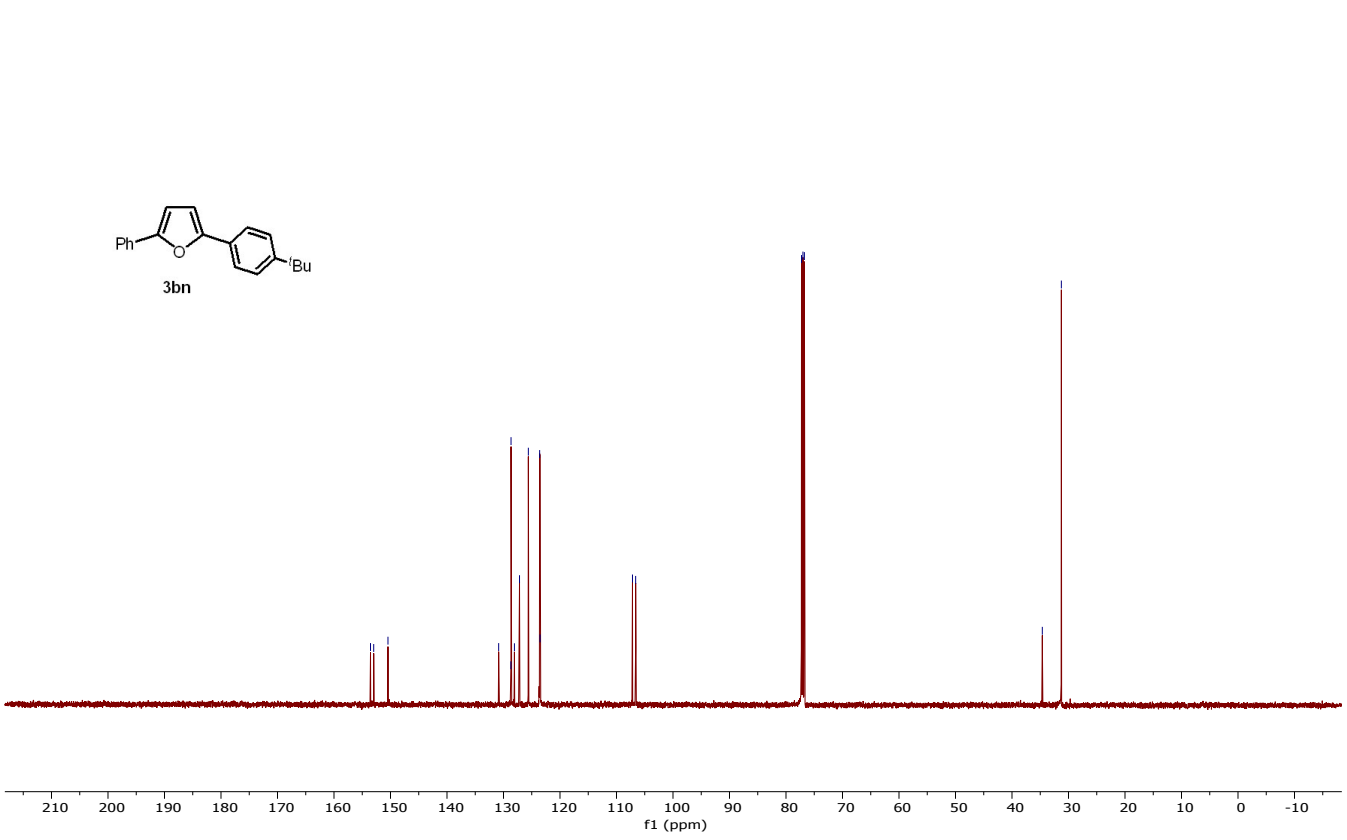

Ph
CF3

3bl

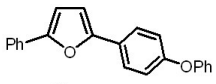

f1 (ppm)


7.628
7.626
7.624
7.609
7.527
7.511
7.290
7.275
7.259
7.151
7.148
7.135
7.134
7.121
7.096
7.080
6.616
6.615
6.605
6.603
6.598
6.596
6.557
6.555
6.550
6.548
6.538
6.536
2.251
0.000
Ph
O
Me
3bm
2.08
2.05
2.09
1.27
1.97
0.99
0.96
3.00
f1 (ppm)
153.573
152.919
137.198
130.837
129.368
129.341
128.659
128.081
127.168
123.669
123.609
107.155
106.467
77.254
77.000
76.746
21.296
Ph
O
Me
3bm
f1 (ppm)

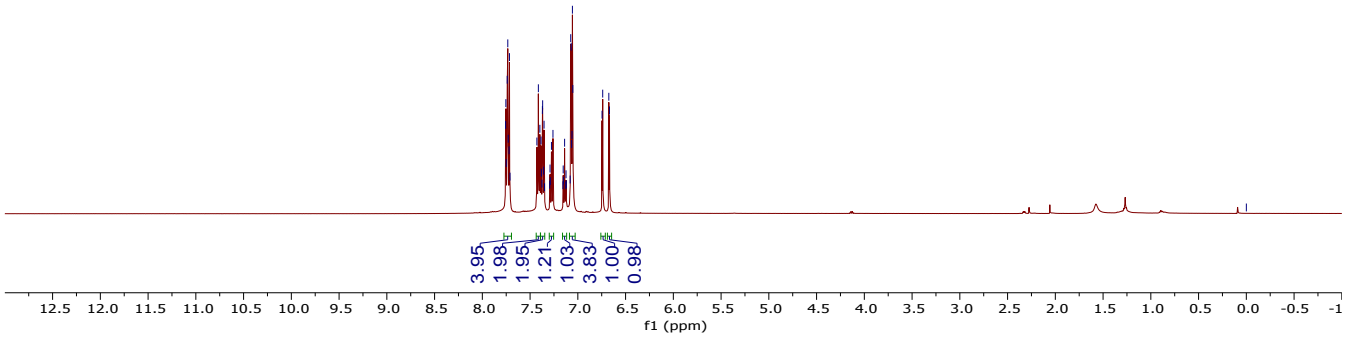

7.766
7.763
7.759
7.749
7.746
7.704
7.700
7.691
7.687
7.683
7.459
7.454
7.450
7.441
7.437
7.431
7.427
7.415
7.403
7.400
7.289
7.286
7.274
7.271
7.260
6.755
6.744
6.737
6.705
6.698
6.688
1.363
-0.000
Ph
tBu
3bn
1.93
2.00
1.90
2.12
1.18
0.96
0.97
9.00
f1 (ppm)

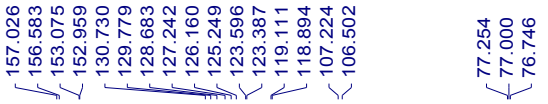

153.537
152.970
150.446
130.854
128.687
128.666
128.066
127.163
125.600
123.601
123.532
107.170
106.608
77.254
77.000
76.746
34.635
31.265
Ph
tBu
3bn
f1 (ppm)

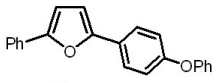

7.756
7.754
7.750
7.739
7.733
7.729
7.720
7.716
7.710
7.429
7.413
7.398
7.386
7.382
7.376
7.371
7.368
7.358
7.354
7.349
7.294
7.291
7.288
7.276
7.260
7.156
7.153
7.151
7.138
7.126
7.124
7.121
7.080
7.074
7.070
7.065
7.061
7.057
7.052
6.747
6.740
6.675
6.669
-0.000


Ph
O
OPh

3bo

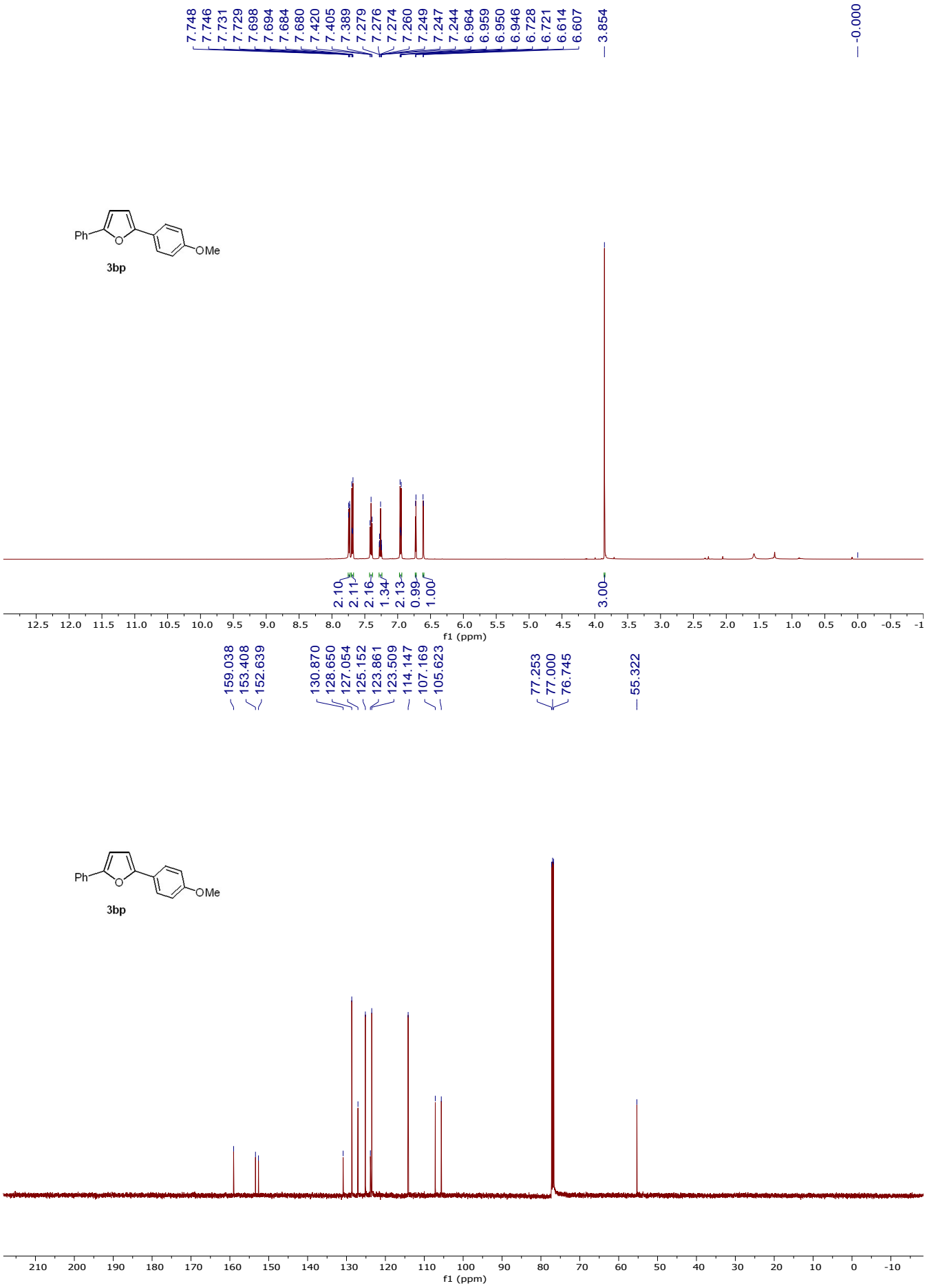

3.95
1.98
1.95
1.21
1.03
3.83
1.00
0.98
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

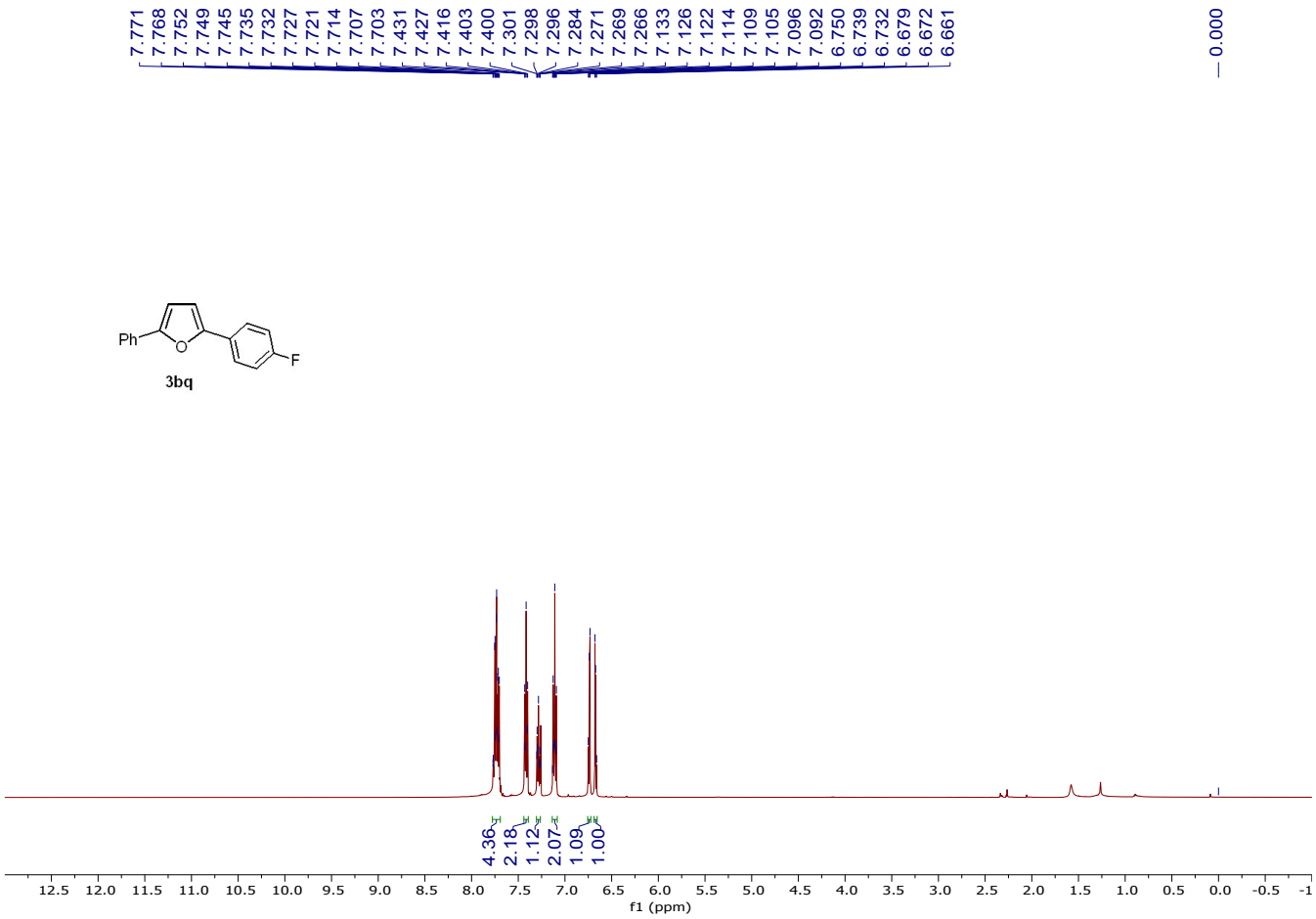

157.026
156.583
153.075
152.959
130.730
129.779
128.683
127.242
126.160
125.249
123.596
123.387
119.111
118.894
107.224
106.502
77.254
77.000
76.746

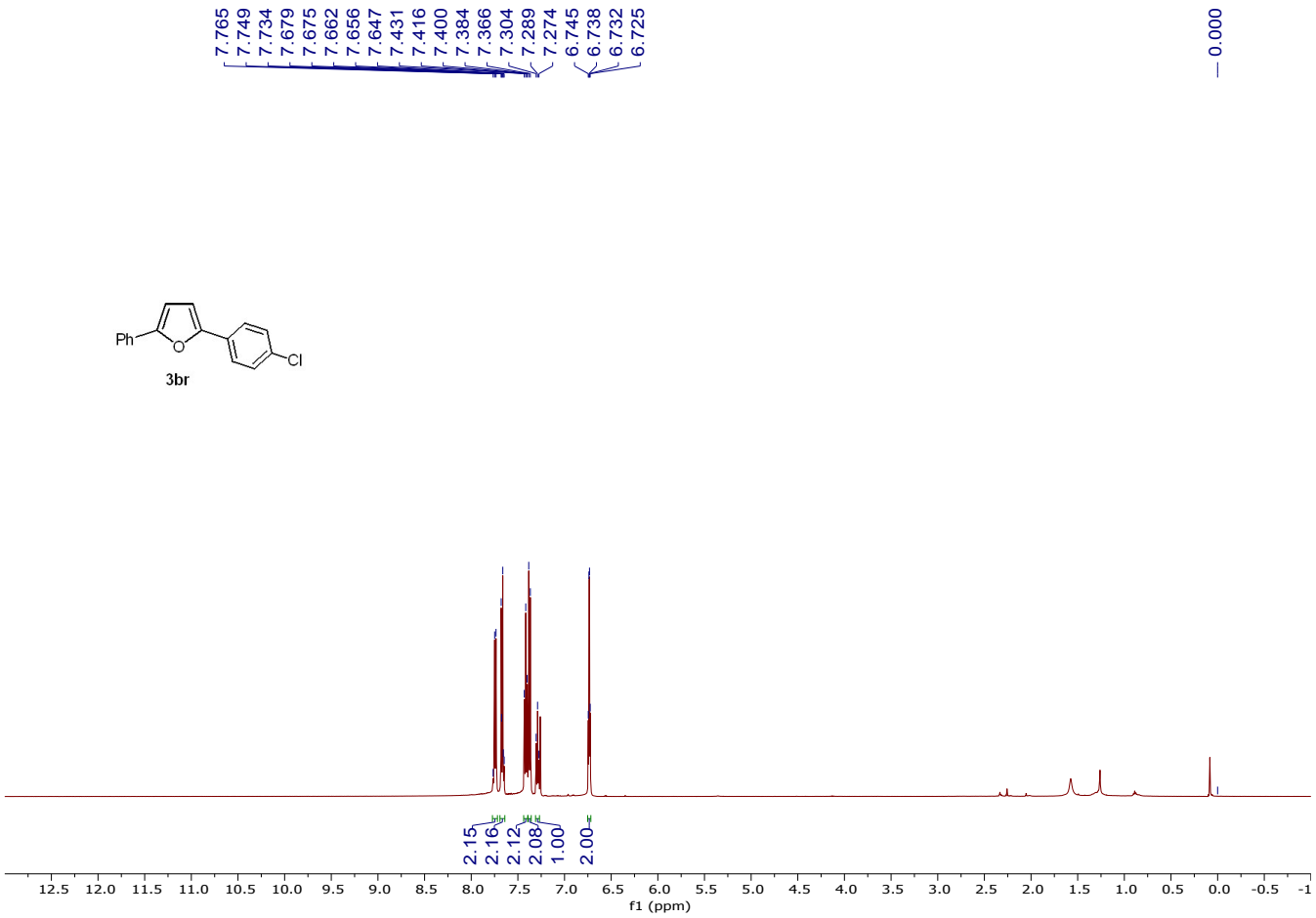

Ph
O
OPh

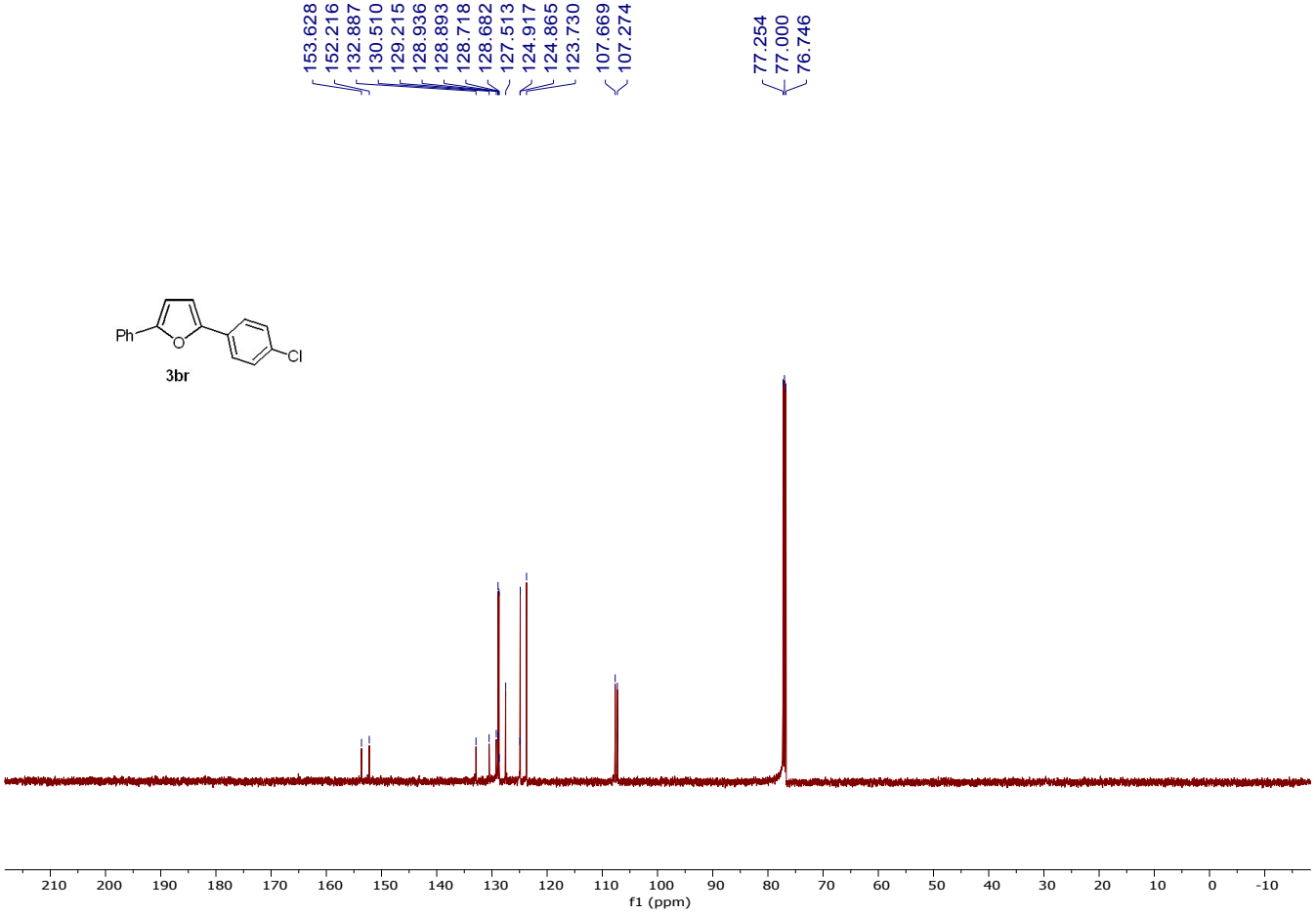
3bo

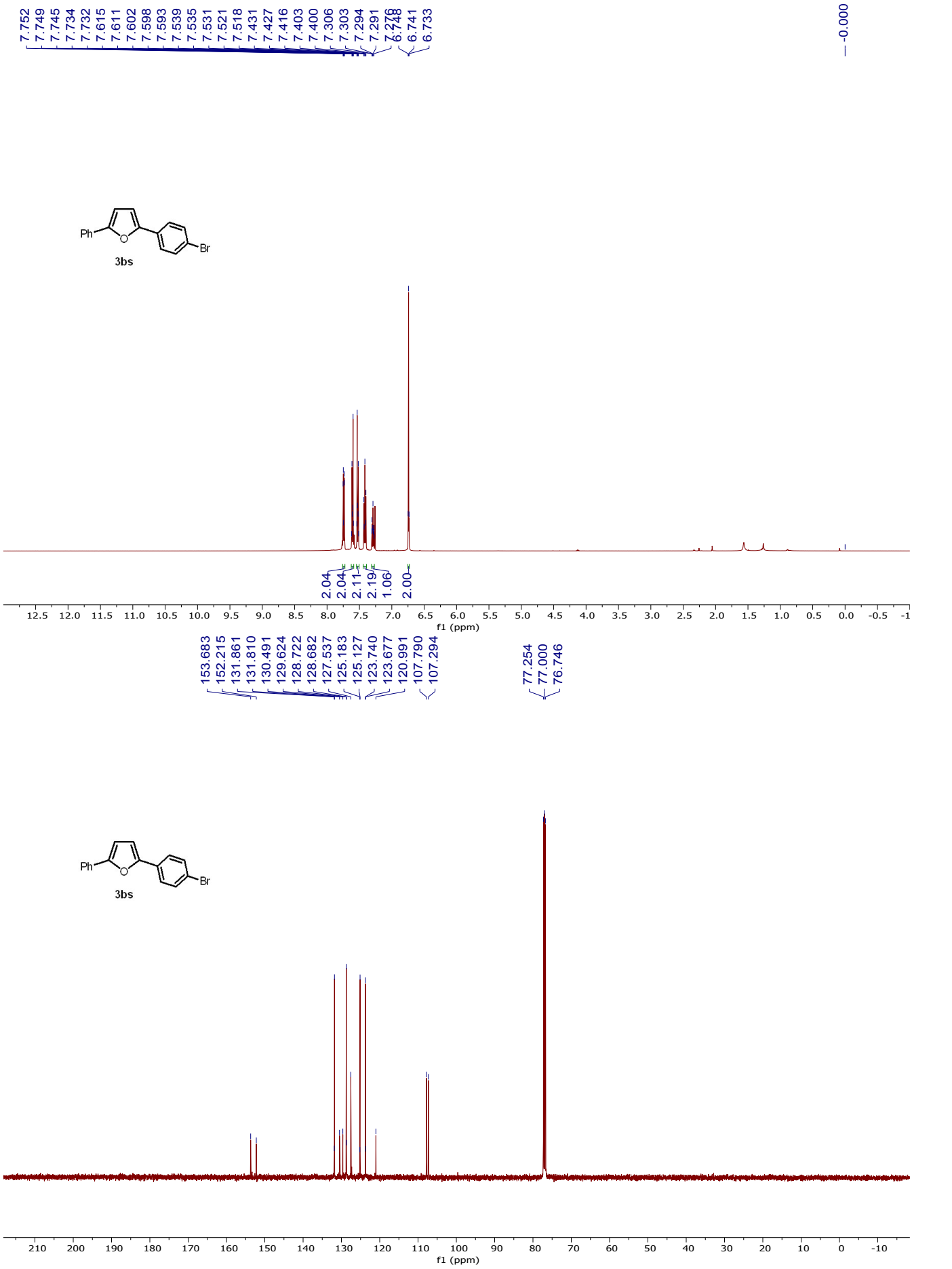
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

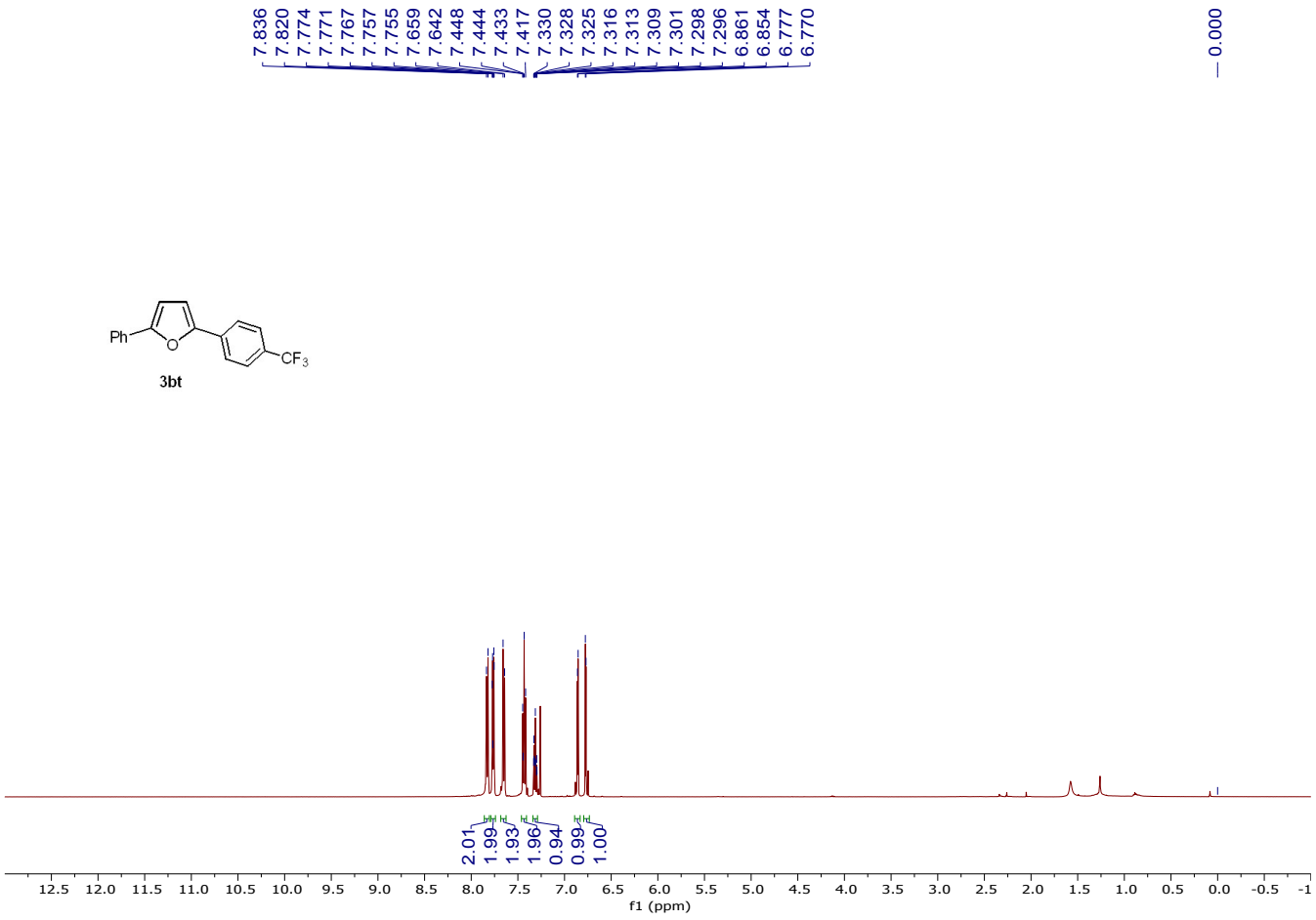

7.748
7.746
7.731
7.729
7.698
7.694
7.684
7.680
7.420
7.405
7.389
7.279
7.276
7.274
7.260
7.249
7.247
7.244
6.964
6.959
6.950
6.946
6.728
6.721
6.614
6.607
3.854
-0.000
Ph
O
OMe
3bp
2.10
2.11
2.16
1.34
2.13
0.99
1.00
3.00
f1 (ppm)
159.038
153.408
152.639
130.870
128.650
127.054
125.152
123.861
123.509
114.147
107.169
105.623
77.253
77.000
76.745
55.322
Ph
O
OMe
3bp
f1 (ppm)

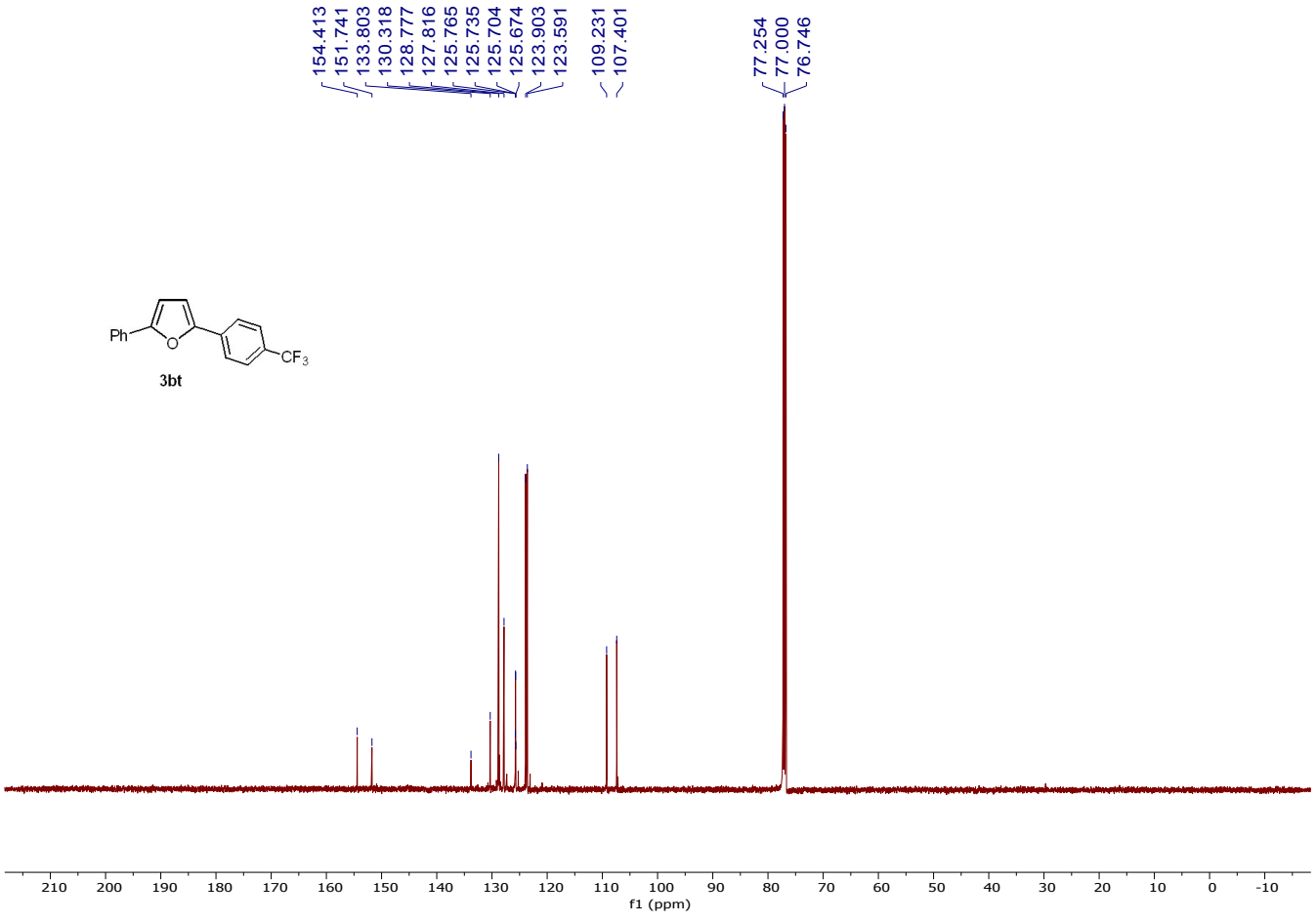

7.771
7.768
7.752
7.749
7.745
7.735
7.732
7.727
7.721
7.714
7.707
7.703
7.431
7.427
7.416
7.403
7.400
7.301
7.298
7.296
7.284
7.271
7.269
7.266
7.133
7.126
7.122
7.114
7.109
7.105
7.096
7.092
6.750
6.739
6.732
6.679
6.672
6.661
0.000
Ph
O
F
3bq
4.36
2.18
1.12
2.07
1.09
1.00
f1 (ppm)
163.083
161.118
153.320
152.456
130.623
128.701
127.371
127.314
127.134
127.106
125.442
125.379
123.679
123.650
115.812
115.637
107.196
106.856
106.843
77.254
77.000
76.746
Ph
O
F
3bq
f1 (ppm)

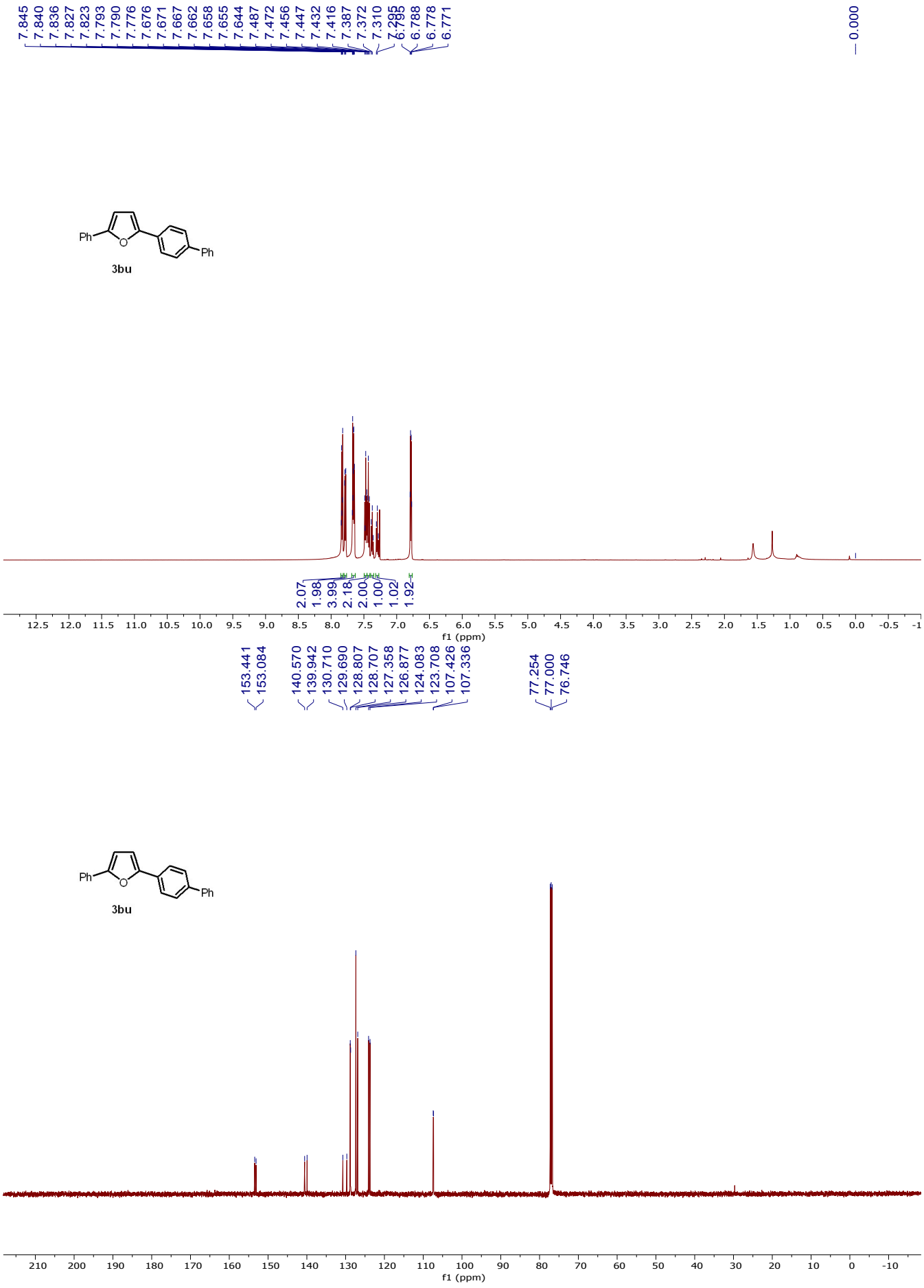

7.765
7.749
7.734
7.679
7.675
7.662
7.656
7.647
7.431
7.416
7.400
7.384
7.366
7.304
7.289
7.274
6.745
6.738
6.732
6.725
0.000
Ph
O
Cl
3br
2.15
2.16
2.12
2.08
1.00
2.00
f1 (ppm)

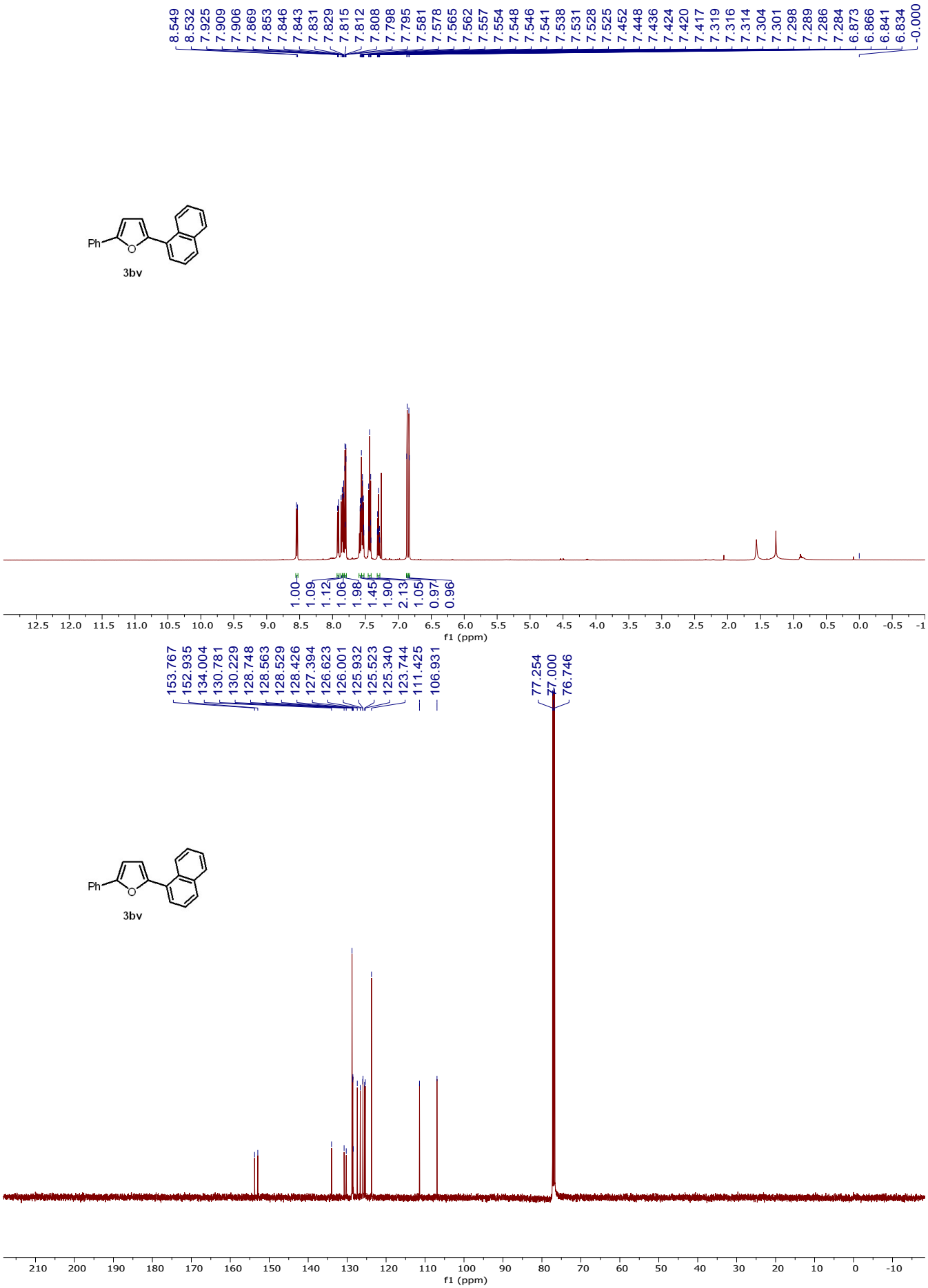

153.628
152.216
132.887
130.510
129.215
128.936
128.893
128.718
128.682
127.513
124.917
124.865
123.730
107.669
107.274
77.254
77.000
76.746
Ph
O
Cl
3br
f1 (ppm)


7.752
7.749
7.745
7.734
7.732
7.615
7.611
7.602
7.598
7.593
7.539
7.535
7.531
7.521
7.518
7.431
7.427
7.416
7.403
7.400
7.306
7.303
7.294
7.291
7.276
6.748
6.741
6.733
-0.000
Ph
O
Br
3bs
2.04
2.04
2.11
2.19
1.06
2.00
f1 (ppm)
153.683
152.215
131.861
131.810
130.491
129.624
128.722
128.682
127.537
125.183
125.127
123.740
123.677
120.991
107.790
107.294
77.254
77.000
76.746
Ph
O
Br
3bs
f1 (ppm)

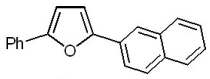

7.836
7.820
7.774
7.771
7.767
7.757
7.755
7.659
7.642
7.448
7.444
7.433
7.417
7.330
7.328
7.325
7.316
7.313
7.309
7.301
7.298
7.296
6.861
6.854
6.777
6.770
0.000
Ph
CF3
3bt
2.01
1.99
1.93
1.96
0.94
0.99
1.00
f1 (ppm)


154.413
151.741
133.803
130.318
128.777
127.816
125.765
125.735
125.704
125.674
123.903
123.591
109.231
107.401
77.254
77.000
76.746
Ph
CF3
3bt
f1 (ppm)

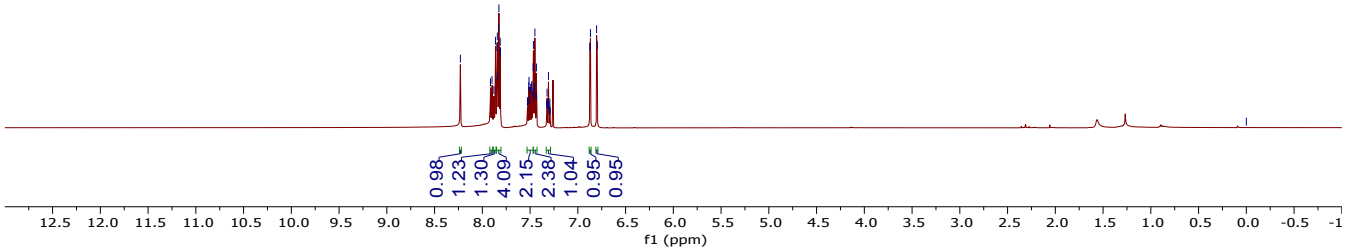

7.845
7.840
7.836
7.827
7.823
7.793
7.790
7.776
7.676
7.671
7.667
7.662
7.658
7.655
7.644
7.487
7.472
7.456
7.447
7.432
7.416
7.387
7.372
7.310
6.795
6.788
6.778
6.771
0.000
Ph
O
Ph
3bu
2.07
1.98
3.99
2.18
2.00
1.00
1.02
1.92
f1 (ppm)
153.441
153.084
140.570
139.942
130.710
129.690
128.807
128.707
127.358
126.877
124.083
123.708
107.426
107.336
77.254
77.000
76.746
Ph
O
Ph
3bu
f1 (ppm)


8.549
8.532
7.925
7.909
7.906
7.869
7.853
7.846
7.843
7.831
7.829
7.815
7.812
7.808
7.798
7.795
7.581
7.578
7.565
7.562
7.557
7.554
7.548
7.546
7.541
7.538
7.531
7.528
7.525
7.452
7.448
7.436
7.424
7.420
7.417
7.319
7.316
7.314
7.304
7.301
7.298
7.289
7.286
7.284
6.873
6.866
6.841
6.834
-0.000
Ph
O
3bv
1.00
1.09
1.12
1.06
1.98
1.45
1.90
2.13
1.05
0.97
0.96
f1 (ppm)
153.767
152.935
134.004
130.781
130.229
128.748
128.563
128.529
128.426
127.394
126.623
126.001
125.932
125.523
125.340
123.744
111.425
106.931
77.254
77.000
76.746
Ph
O
3bv
f1 (ppm)

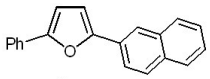

8.230
7.915
7.899
7.879
7.862
7.847
7.843
7.839
7.830
7.827
7.813
7.810
7.528
7.525
7.514
7.511
7.508
7.498
7.495
7.484
7.481
7.470
7.468
7.465
7.461
7.454
7.450
7.437
7.434
7.325
7.322
7.320
7.311
7.308
7.304
7.295
7.293
7.290
6.875
6.868
6.804
6.797
0.000


Ph
O

3bw

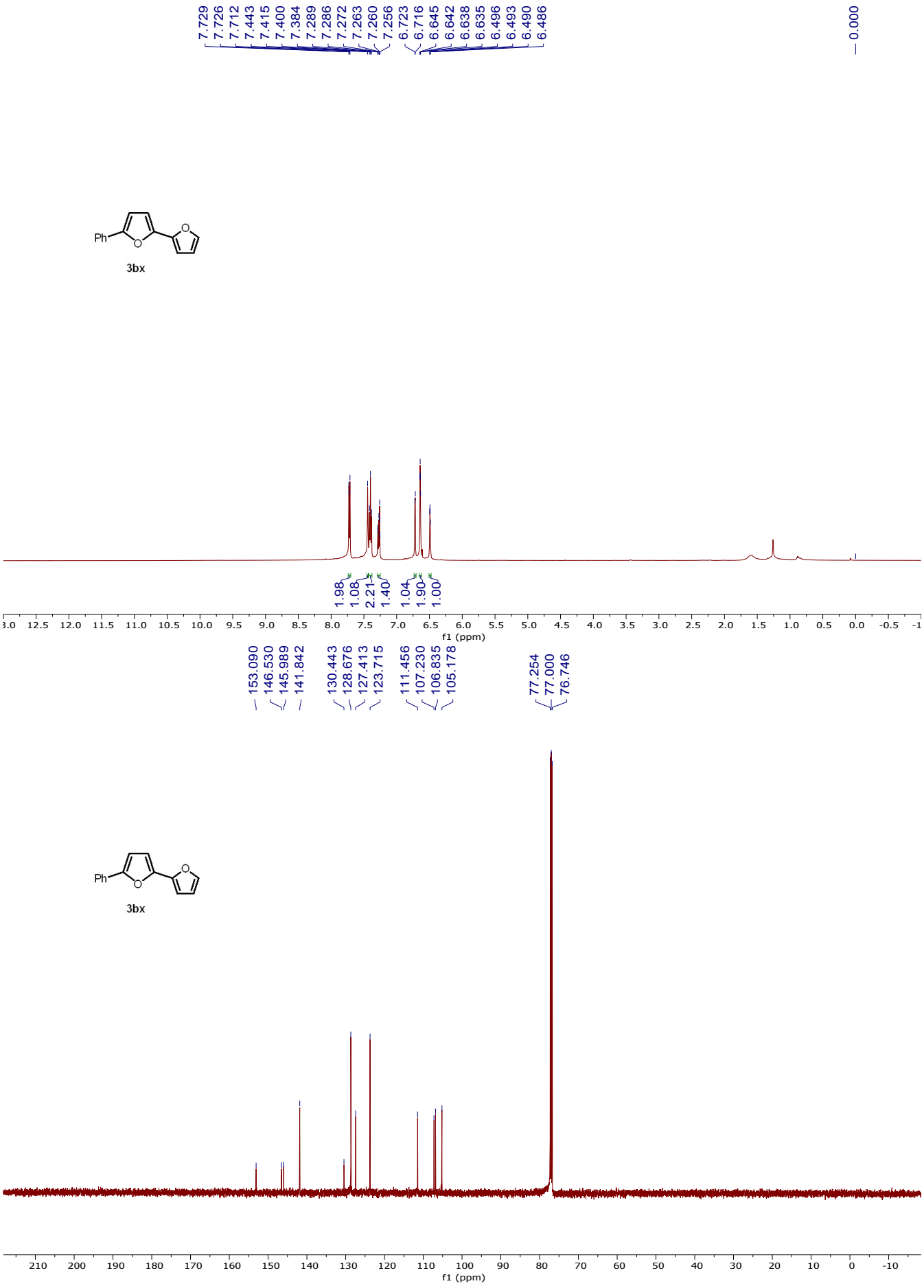

0.98
1.23
1.30
4.09
2.15
2.38
1.04
0.95
0.95
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


153.611
153.391
133.560
132.653
130.704
128.721
128.379
128.122
128.109
128.044
127.757
127.407
126.500
125.872
123.771
122.222
121.921
107.894
107.385
77.254
77.000
76.746

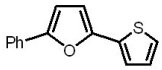

Ph
O

3bw

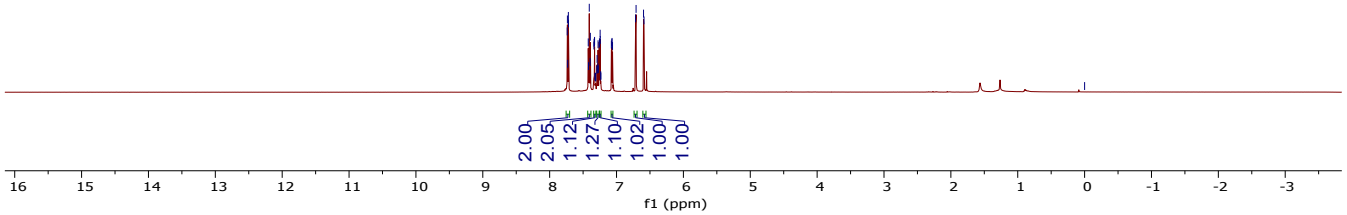
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.729
7.726
7.712
7.443
7.415
7.400
7.384
7.289
7.286
7.272
7.263
7.260
7.256
6.723
6.716
6.645
6.642
6.638
6.635
6.496
6.493
6.490
6.486
0.000
Ph
O
O
3bx
1.98
1.08
2.21
1.40
1.04
1.90
1.00
f1 (ppm)
153.090
146.530
145.989
141.842
130.443
128.676
127.413
123.715
111.456
107.230
106.835
105.178
77.254
77.000
76.746
Ph
O
O
3bx
f1 (ppm)

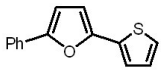

7.737
7.734
7.731
7.720
7.718
7.423
7.419
7.408
7.395
7.392
7.338
7.336
7.331
7.328
7.321
7.318
7.313
7.311
7.293
7.291
7.288
7.279
7.276
7.273
7.255
7.253
7.245
7.243
7.237
7.234
7.077
7.070
7.067
7.060
6.715
6.708
6.596
6.589
-0.000


Ph
O
S

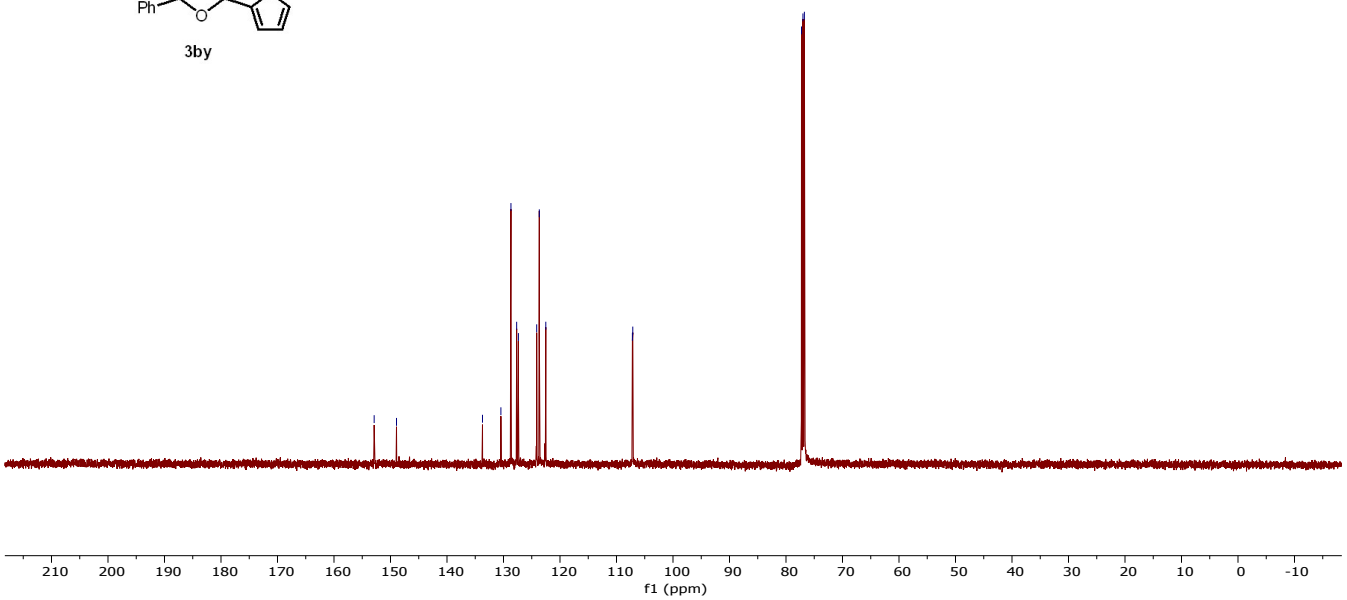
3by

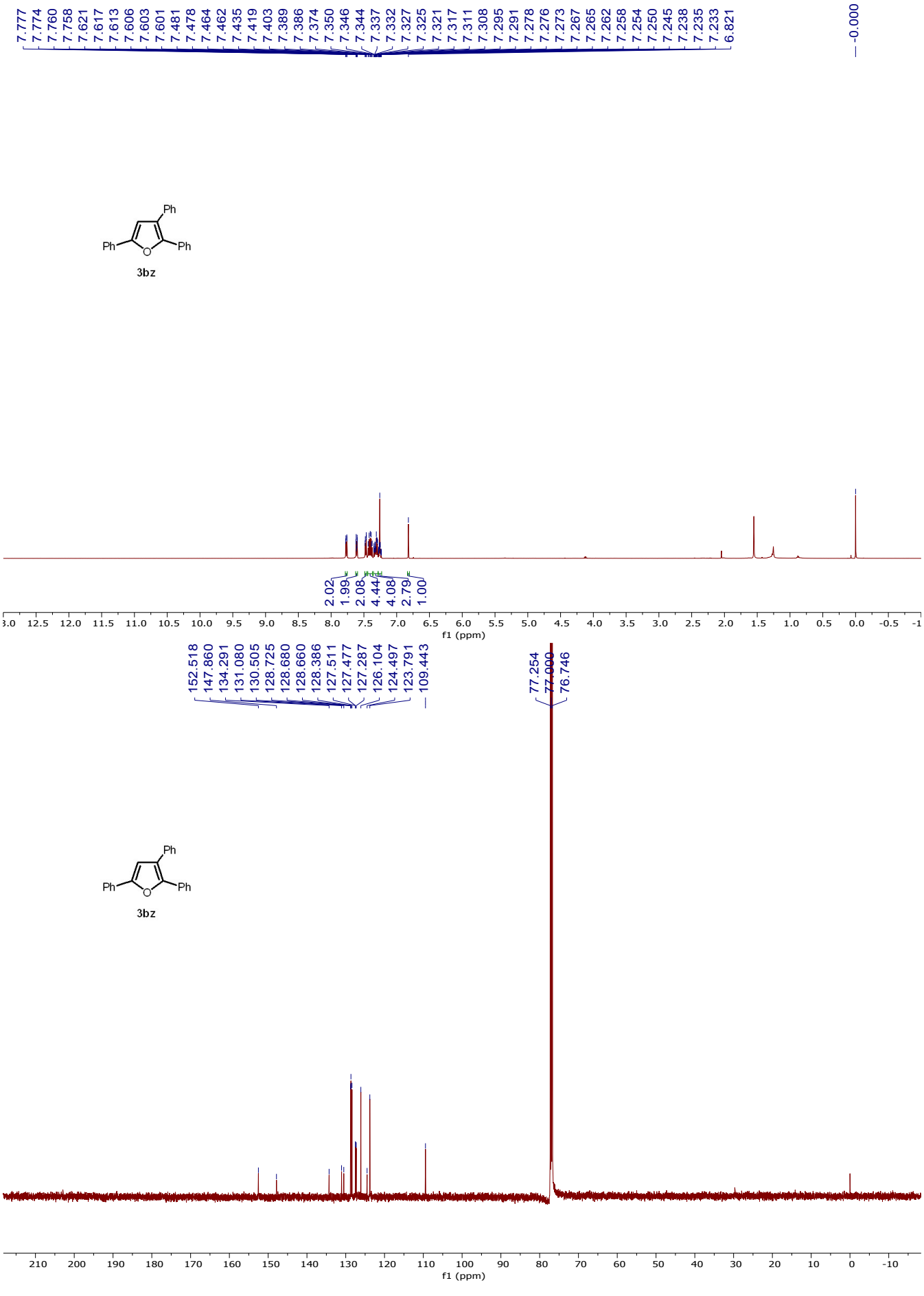

2.00
2.05
1.12
1.27
1.10
1.02
1.00
1.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

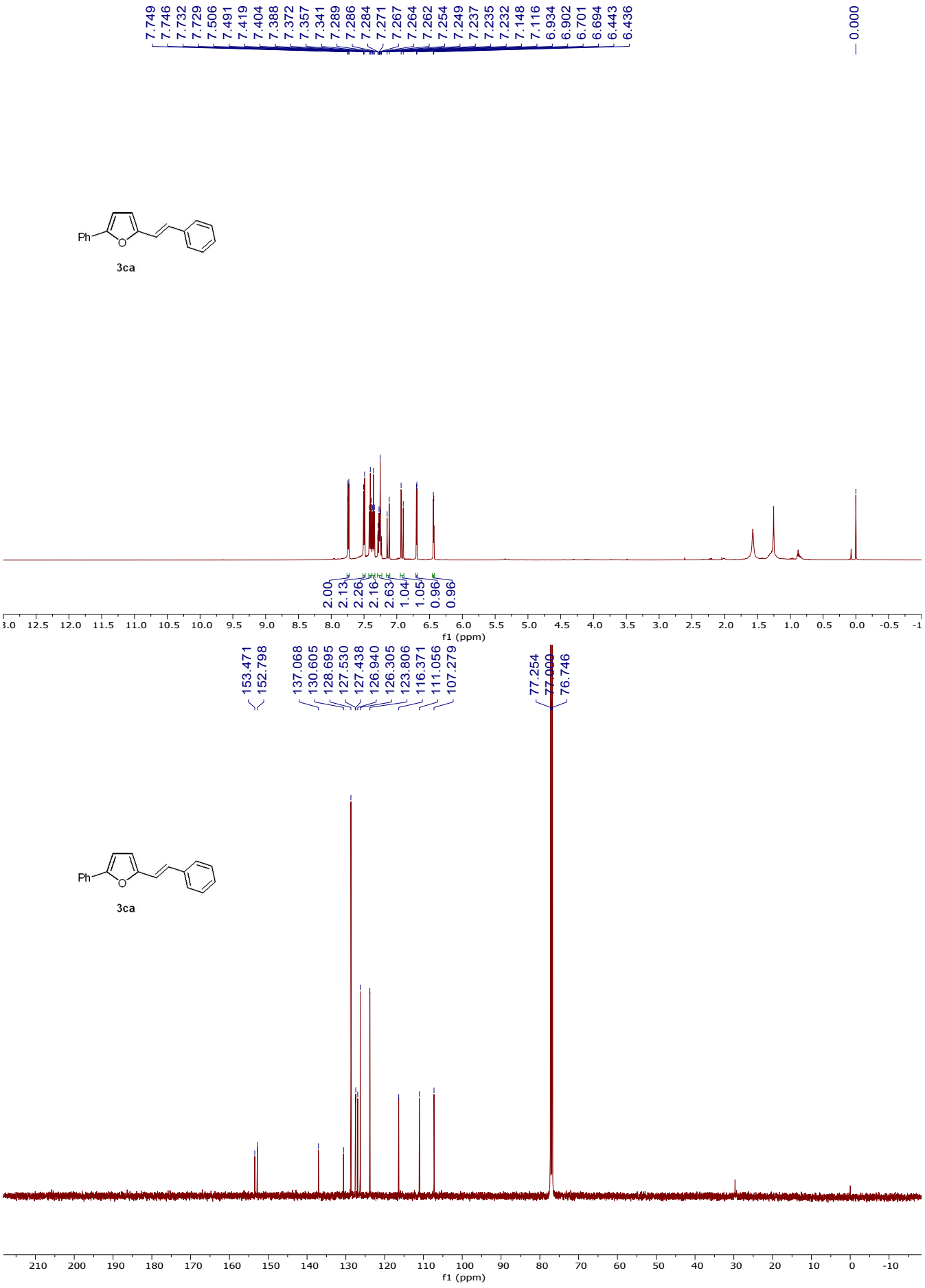

152.891
148.936
133.717
130.460
128.681
127.670
127.360
124.123
123.660
122.512
107.186
107.117
77.254
77.000
76.746


Ph
O
S

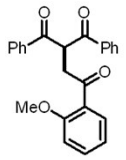
3by


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)

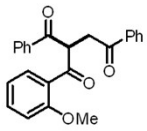

7.777
7.774
7.760
7.758
7.621
7.617
7.613
7.606
7.603
7.601
7.481
7.478
7.464
7.462
7.435
7.419
7.403
7.389
7.386
7.374
7.350
7.346
7.344
7.337
7.332
7.327
7.325
7.321
7.317
7.311
7.308
7.295
7.291
7.278
7.276
7.273
7.267
7.265
7.262
7.258
7.254
7.250
7.245
7.238
7.235
7.233
6.821
-0.000
Ph
Ph
Ph
O
3bz
2.02
1.99
2.08
4.44
4.08
2.79
1.00
f1 (ppm)
152.518
147.860
134.291
131.080
130.505
128.725
128.680
128.660
128.386
127.511
127.477
127.287
126.104
124.497
123.791
109.443
77.254
77.000
76.746
Ph
Ph
Ph
O
3bz
f1 (ppm)


7.749
7.746
7.732
7.729
7.506
7.491
7.419
7.404
7.388
7.372
7.357
7.341
7.289
7.286
7.284
7.271
7.267
7.264
7.262
7.254
7.249
7.237
7.235
7.232
7.148
7.116
6.934
6.902
6.701
6.694
6.443
6.436
0.000
Ph
O
3ca
2.00
2.13
2.26
2.16
2.63
1.04
1.05
0.96
0.96
f1 (ppm)
153.471
152.798
137.068
130.605
128.695
127.530
127.438
126.940
126.305
123.806
116.371
111.056
107.279
77.254
77.000
76.746
Ph
O
3ca
f1 (ppm)

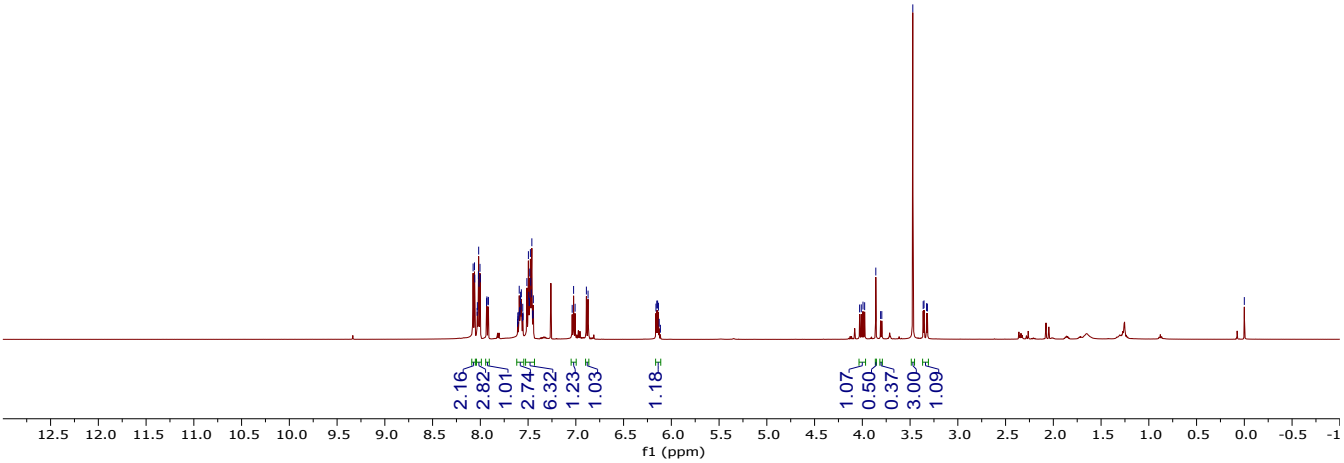

8.076
8.061
8.058
8.033
8.031
8.020
8.017
8.014
8.004
8.001
7.935
7.932
7.920
7.916
7.597
7.593
7.589
7.585
7.581
7.578
7.575
7.570
7.556
7.553
7.513
7.497
7.493
7.489
7.486
7.482
7.476
7.472
7.467
7.461
7.451
7.449
7.445
7.038
7.023
7.008
6.889
6.872
6.161
6.153
6.144
6.135
4.028
4.011
3.993
3.976
3.859
3.809
3.796
3.471
3.363
3.354
3.327
3.319
0.000

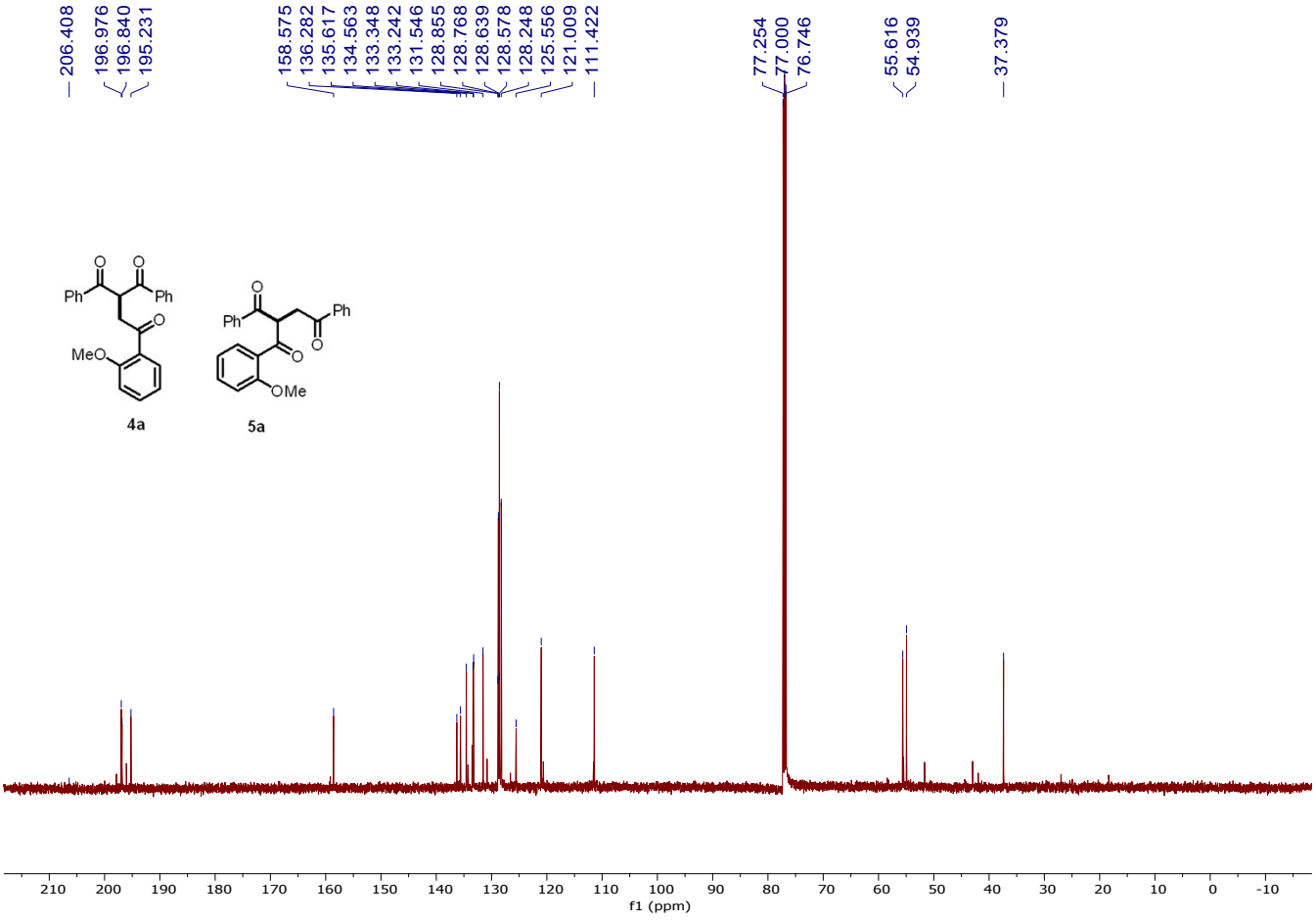

Ph
Ph
MeO

4a


Ph
Ph
OMe

5a


2.16
2.82
1.01
2.74
6.32
1.23
1.03
1.18
1.07
0.50
0.37
3.00
1.09
12.5 12.0 11.5 11.0 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 -1
f1 (ppm)

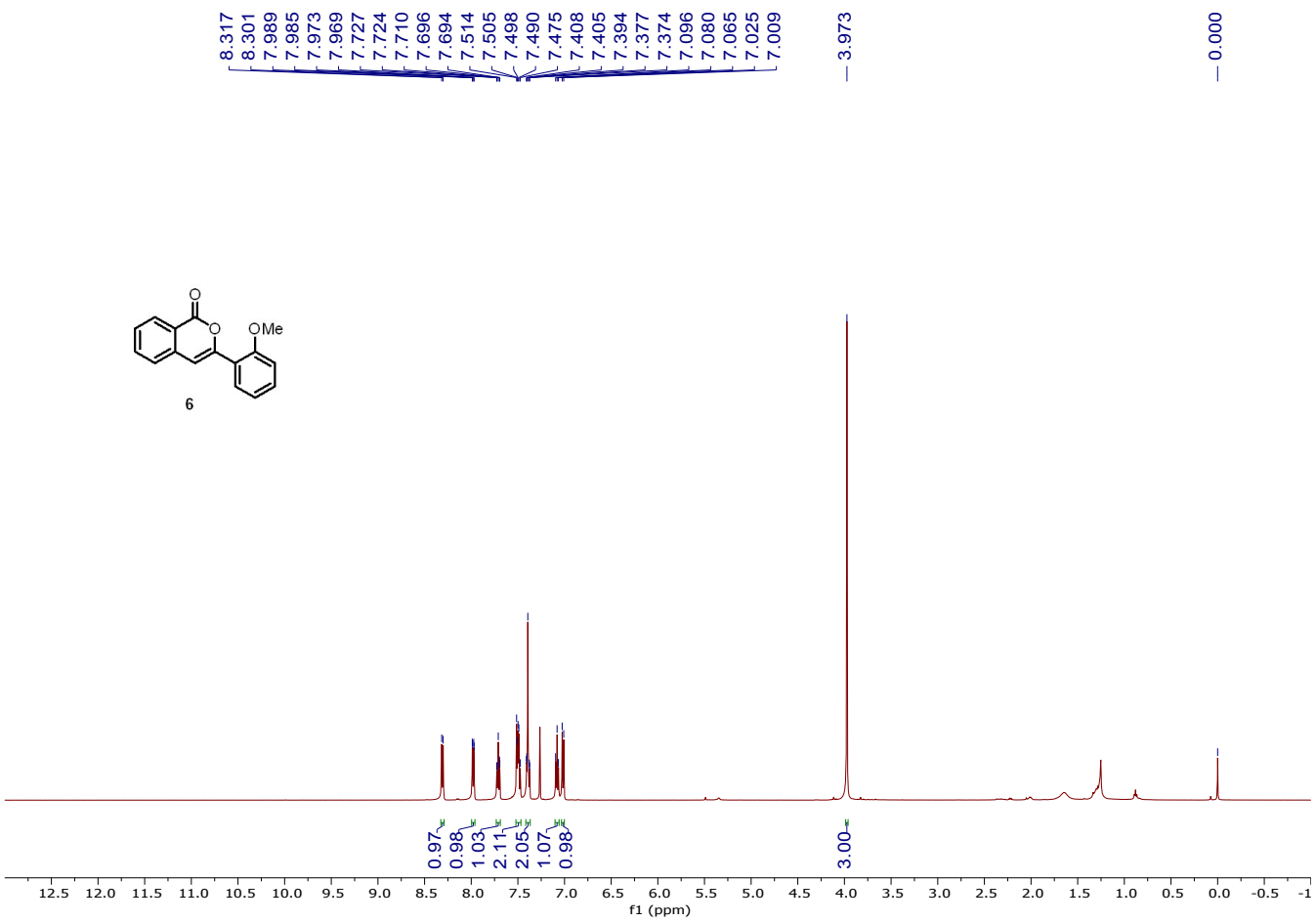

206.408
196.976
196.840
195.231
158.575
136.282
135.617
134.563
133.348
133.242
131.546
128.855
128.768
128.639
128.578
128.248
125.556
121.009
111.422
77.254
77.000
76.746
55.616
54.939
37.379
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

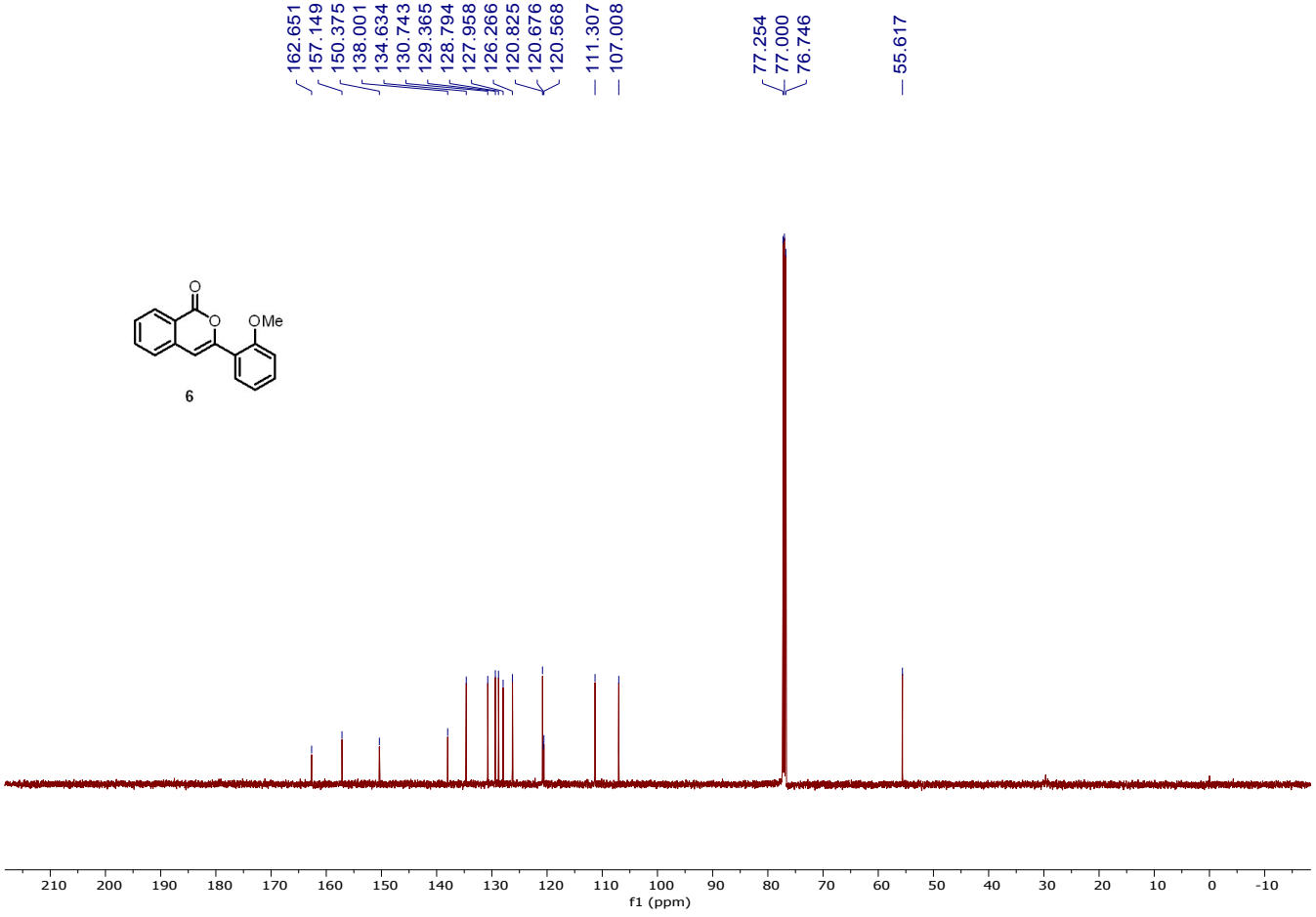
Ph
Ph
MeO

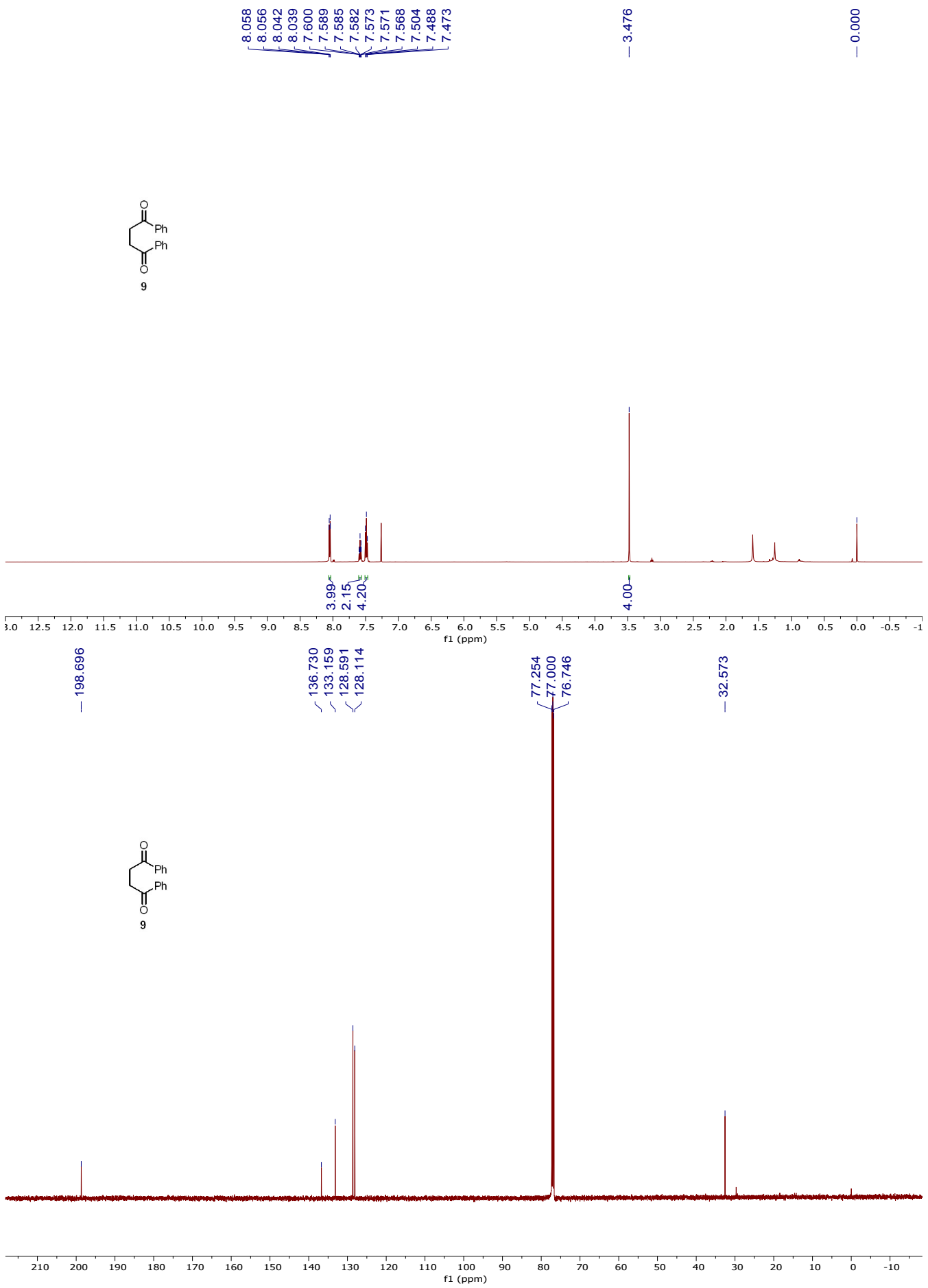
4a

Ph
Ph
OMe

5a


8.317
8.301
7.989
7.985
7.973
7.969
7.727
7.724
7.710
7.696
7.694
7.514
7.505
7.498
7.490
7.475
7.408
7.405
7.394
7.377
7.374
7.096
7.080
7.065
7.025
7.009
3.973
0.000
O
O
OMe
6
0.97
0.98
1.03
2.11
2.05
1.07
0.98
3.00
12.5 12.0 11.5 11.0 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 -1
f1 (ppm)


162.651
157.149
150.375
138.001
134.634
130.743
129.365
128.794
127.958
126.266
120.825
120.676
120.568
111.307
107.008
77.254
77.000
76.746
55.617
O
O
OMe
6
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)


8.058
8.056
8.042
8.039
7.600
7.589
7.585
7.582
7.573
7.571
7.568
7.504
7.488
7.473
3.476
0.000
Ph
Ph
O
O
9
3.99
2.15
4.20
4.00
f1 (ppm)
198.696
136.730
133.159
128.591
128.114
77.254
77.000
76.746
32.573
Ph
Ph
O
O
9
f1 (ppm)