SUPPORTING INFORMATION

A One-Pot Domino C-H, C-C Activation in Coumarins: A fast track to 2,3-diaryl substituted benzo[b]furans

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Contents

1. General Methods and Materials

All commercially available reagents were used without further purification. Coumarins, catalysts and other reagents were purchased from Acros Organics. Column chromatography was carried out on silica gel. TLC was conducted on silica gel 250 micron, F254 plates. ^{1}H NMR spectra were recorded at room temperature on a Bruker 500 MHz spectrometer, using $CDCl_3$ as solvent. Chemical shifts are reported in ppm with TMS as an internal standard (TMS: δ 0.0 ppm). ^{13}C NMR spectra are referenced from the solvent central peak (77.23 ppm). Chemical shifts are given in ppm.

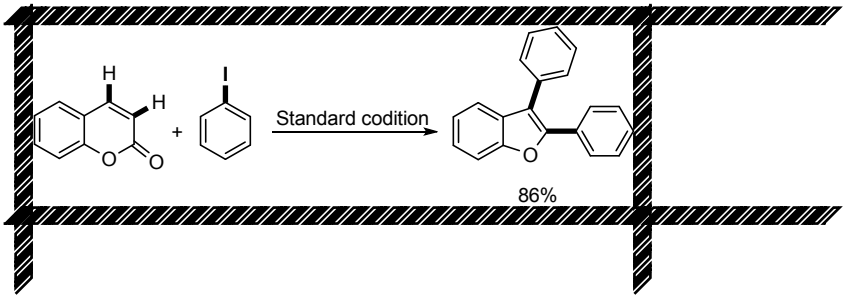
2. Experimental Procedures

A vial equipped with a stir bar was charged with coumarin (0.1 mmol, 1.0 equiv), arylbromide (2.5 equiv), $Pd(OAc)_2$ (20 mol%), Cs_2CO_3 (2.5 eqiuv.), 1,10-Phenanthroline (20 mol %), Mesitylene (0.5 mL), and capped. The resulting mixture was heated in an oil bath at 160 °C for 18 h. Removal of the solvent gave a crude mixture which was purified by flash column chromatography (hexane/EtOAc gradient).

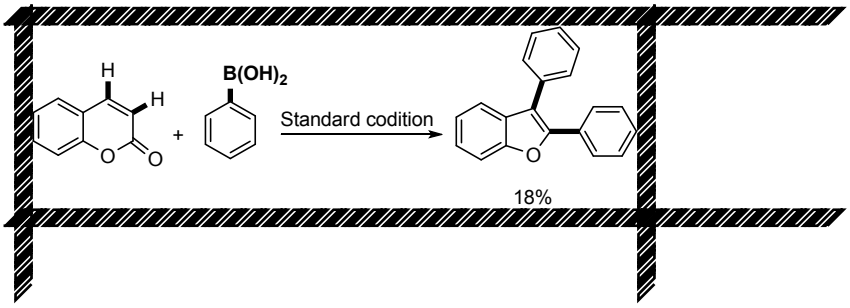
3. Further Experiments

Other experiments being tested are as follows: iodobenzene was allowed to react with coumarin under standard reaction condition generating higher yield than did bromobenzene (**Scheme S1**). In another attempt, phenylboronic acid (**Scheme S2**) and phenyl tosylate (**Scheme S3**) were used in place of bromobenzene which both led to far lower yields (20%). In this context, neither phenyl triflate nor chlorobenzene furnished the product (**Scheme S4**). Besides, using coumarin-3-carboxylic acid as model substrate diminished the yield to a good deal (20%) (**Scheme S5**). It was also observed that use of 4A° molecular sieve had a negligible effect on the reaction yield.

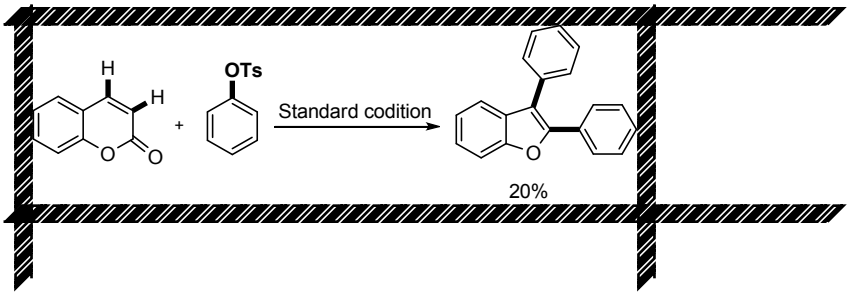
Scheme S1: Reaction of Coumarin with Iodobenzene



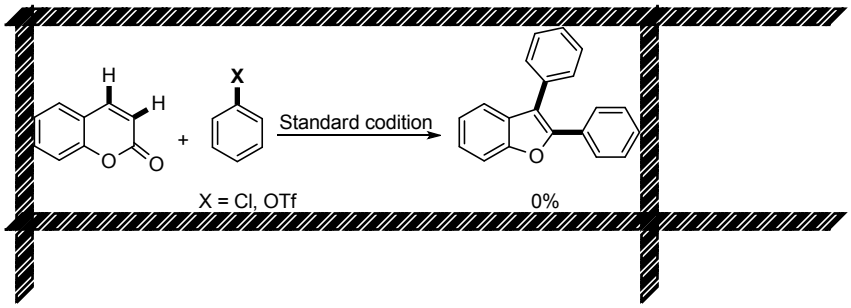
Scheme S2: Reaction of Coumarin with Phenylboronic acid



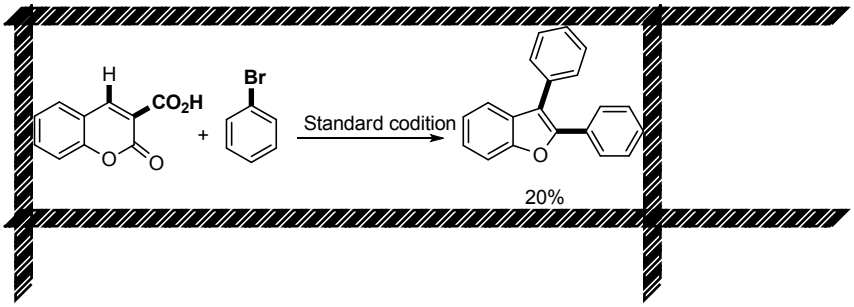
Scheme S3: Reaction of Coumarin with Phenyltosylate



Scheme S4: Reaction of Coumarin with Chlorobenzene and Phenyltriflate

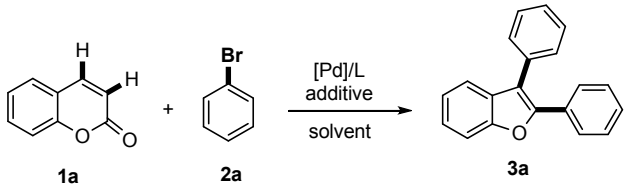


Scheme S5: Reaction of Coumarin-3-carboxylic acid with Bromobenzene



4. Monitoring Reaction Condition:

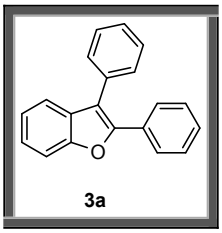
Table S1: Optimization of Reaction of Coumarin (1a) and Bromobenzene (2a)[a]



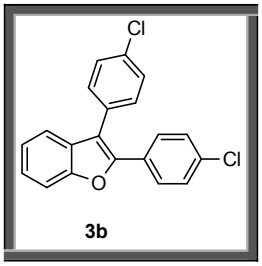
entry	catalyst	ligand	base	solvent	temp. (°C)	yield (%)[b]
1	$Pd(OAc)_2$	PPh_3	Cs_2CO_3	Mesitylene	160	30
2	$Pd(OAc)_2$	PCy_3	Cs_2CO_3	Mesitylene	160	28
3	$Pd(OAc)_2$	Neocuproine	Cs_2CO_3	Mesitylene	160	25
4	$Pd(OAc)_2$	Bipy.	Cs_2CO_3	Mesitylene	160	25
5	***$Pd(OAc)_2$***	***Phen.***	***Cs_2CO_3***	***Mesitylene***	***160***	***76***
6	$Pd(OAc)_2$	DMAP	Cs_2CO_3	Mesitylene	160	30
7	$Pd(OAc)_2$	2,3-Lutidine	Cs_2CO_3	Mesitylene	160	0
8	$Pd(OAc)_2$	4-Methylbenzene-1,2-diamine	Cs_2CO_3	Mesitylene	160	0
9	$Pd(OAc)_2$	1,3-Dimethyl thiourea	Cs_2CO_3	Mesitylene	160	0
10	$Pd(OAc)_2$	Phen.	K_2CO_3	Mesitylene	160	20
11	$Pd(OAc)_2$	Phen.	KO^tBu	Mesitylene	160	5
12	$Pd(OAc)_2$	Phen.	KF	Mesitylene	160	0
13	$Pd(OAc)_2$	Phen.	Cs_2CO_3	1,4-Dioxane	160	15
14	$Pd(OAc)_2$	Phen.	Cs_2CO_3	Dimethylether	160	10
15	$Pd(OAc)_2$	Phen.	Cs_2CO_3	CH_3CN	160	25
16	$Pd(OAc)_2$	Phen.	Cs_2CO_3	DMF	160	69
17	$PdCl_2$	Phen.	Cs_2CO_3	DMF	160	30
18	$Pd(dba)_2$	Phen.	Cs_2CO_3	DMF	160	40
19	$Pd(acac)_2$	Phen.	Cs_2CO_3	DMF	160	14
20	$Pd(PPh_3)_4$	Phen.	Cs_2CO_3	DMF	160	58
21	$Pd(OAc)_2$	-	Cs_2CO_3	Mesitylene	160	20
22	$Pd(OAc)_2$	Phen.	-	Mesitylene	160	0
23	$Pd(OAc)_2$	Phen.	Cs_2CO_3	Mesitylene	120	0
24	$Pd(OAc)_2$	Phen.	Cs_2CO_3	Mesitylene	180	70

[a] Reaction conditions: Coumarin (0.1 mmol, 1.0 equiv), bromobenzene (2.5 equiv), palladium catalyst (20 mol%), Phen. (20 mol%), base (2.5 equiv), solvent (0.2 M), 160 °C, 18 h. [b]Isolated yields.

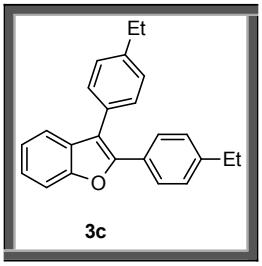
5. Characterization Data



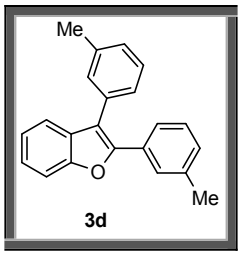
2,3- Diphenylbenzofuran (3a). White crystal, 21 mg, Yield 76%, mp 111-114 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.0 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.52 – 7.41 (m, 7H), 7.37 – 7.24 (m, 4H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 153.5, 150.0, 132.4, 130.2, 129.8, 129.3, 128.5, 128.3, 127.9, 127.8, 127.1, 126.5, 124.2, 122.4, 119.5, 117.0, 110.6; Anal. Calcd for $C_{20}H_{14}O$ (270.10): C, 88.86; H, 5.22. Found: C, 88.61; H, 5.43.



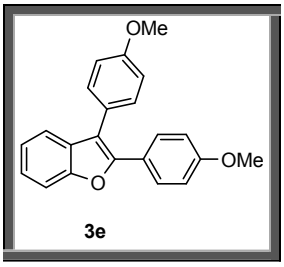
2,3-Bis(4-chlorophenyl)benzofuran (3b). White crystal, 27 mg, Yield 79%, mp 109-113 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 3H), 7.48 – 7.43 (m, 5H), 7.37 (t, *J* = 7.21 Hz, 1H), 7.33 – 7.25 (m, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 153.5, 149.1, 133.9, 133.3, 130.5, 129.2, 128.9, 128.3, 127.7, 124.6, 122.7, 119.3, 116.3, 110.7; MS *m/z* (%) 338 (M•+,100), 302 (19), 268 (55), 239 (56), 134 (29); Anal. Calcd for $C_{20}H_{12}Cl_2O$ (338.02): C, 70.81; H, 3.57. Found: C, 70.99; H, 3.75.



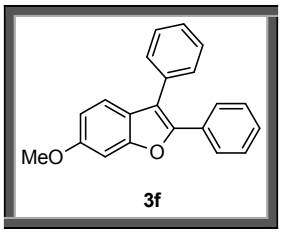
2,3-Bis(4-ethylphenyl)benzofuran (3c). White crystal, 25 mg, Yield 78%, mp 76 – 79 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.9 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.35 – 7.32 (m, 3H), 7.26 (t, *J* = 7.5 Hz, 1H), 7.19 (d, *J* = 7.9 Hz, 2H), 2.76 (q, *J* = 7.5 Hz, 2H), 2.67 (q, *J* = 7.5 Hz, 2H), 1.35 (t, *J* = 7.5 Hz, 3H), 1.27 (t, *J* = 7.5 Hz, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 153.4, 150.1, 144.0, 143.0, 130.0, 129.6, 129.1, 127.9, 127.7, 127.4, 126.5, 123.8, 122.2, 119.5, 116.3, 110.5, 28.2, 14.9; MS *m/z* (%) 326 (M•+,100), 296 (14), 268 (25), 252 (17), 148 (29), 57 (10); Anal. Calcd for $C_{24}H_{22}O$ (326.16): C, 88.31; H, 6.79. Found: C, 88.61; H, 6.97.



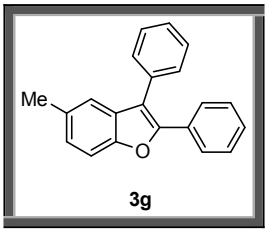
2,3-Di-*m*-tolylbenzofuran (3d). White crystal, 23 mg, Yield 76%, mp 112-116 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.60 – 7.57 (m, 2H), 7.53(d, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.38 – 7.31 (m, 4H), 7.28 – 7.19 (m, 3H), 7.13 (d, *J* = 7.2 Hz, 1H), 2.42 (s, 3H), 2.35 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 153.4, 150.1, 138.0, 137.5, 132.2, 130.1, 129.8, 128.6, 128.2, 127.8, 127.7, 127.0, 126.3, 124.0, 123.7, 122.3, 119.5, 117.0, 110.5, 20.9; MS *m/z* (%) 298 (M•+,100), 281 (15), 255 (23), 238(16); Anal. Calcd for $C_{22}H_{18}O$ (298.13): C, 88.56; H, 6.08. Found: C, 88.71; H, 6.33.



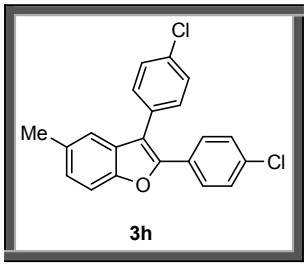
2,3-Bis(4-methoxyphenyl)benzofuran (3e). White crystal, 26 mg, Yield 79%, mp 146-148 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.23 (t, *J* = 7.3 Hz, 1H) , 7.02 (d, *J* = 8.0 Hz, 2H) , 6.87 (d, *J* = 8.2 Hz, 2H), 3.90 (s, 3H), 3.83 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 159.6, 159.0, 153.8, 150.49, 130.9, 130.6, 128.4, 124.2, 123.5, 122.7, 119.7, 115.7, 114.5, 113.9, 110.9, 55.3; MS *m/z* (%) 330 (M•+,100), 315 (61), 255 (30), 215 (15), 149 (16); Anal. Calcd for $C_{22}H_{18}O_3$ (330.12): C, 79.98; H, 5.49. Found: C, 79.61; H, 5.23.



6-Methoxy-2,3-diphenylbenzofuran (3f). White crystal, 25 mg, Yield 83%, mp 117-120 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 6.6 Hz, 2H), 7.51 – 7.48 (m, 4H), 7.42 – 7.38 (m, 2H), 7.32 – 7.28 (m, 3H) , 7.12 (s, 1H) , 6.89 (d, *J* = 7.7 Hz, 1H), 3.91 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 157.9, 154.4, 149.1, 132.4, 130.3, 129.1, 128.4, 127.8, 127.4, 127.0, 126.0, 123.2, 119.7, 116.9, 111.4, 95.1, 55.3; Anal. Calcd for $C_{21}H_{16}O_2$ (300.11): C, 83.98; H, 5.37. Found: C, 83.64; H, 5.03.

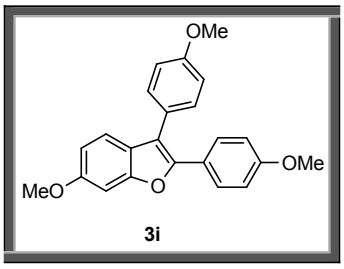


5-Methyl-2,3-diphenylbenzofuran (3g). White crystal, 22 mg, Yield 77%, mp 105-107 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 6.7 Hz, 2H), 7.51 – 7.43 (m, 6H), 7.32 – 7.27 (m, 4H), 7.16 (d, *J* = 7.9 Hz, 1H), 2.44 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 151.9, 150.1, 132.5, 131.9, 130.2, 129.8, 129.2, 128.4, 127.8, 127.7, 127.0, 126.4, 125.4, 119.2, 110.1, 20.8; MS *m/z* (%) 284 (M•+,100), 255 (42), 239 (42), 178 (20), 134 (24), 77 (14); Anal. Calcd for $C_{21}H_{16}O$ (284.35): C, 88.70; H, 5.67. Found: C, 88.91; H, 5.93.



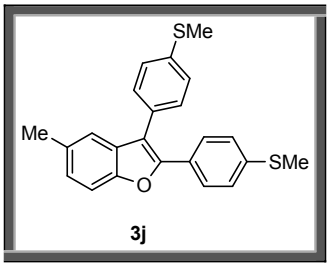
3h

2,3-Bis(4-chlorophenyl)-5-methylbenzofuran (3h). White crystal, 26 mg, Yield 74%, mp 151-153 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.5 Hz, 2H), 7.47 – 7.42 (m, 5H), 7.31 (d, *J* = 8.5 Hz, 2H), 7.24 (s, 1H), 7.17 (d, *J* = 8.1Hz, 1H), 2.44 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 151.9, 149.2, 133.8, 133.2, 132.3, 130.7, 130.5, 129.3, 128.9, 128.4, 128.2, 127.6, 125.9, 119.0, 116.0, 110.2, 20.8; MS *m/z* (%) 352 (M•+,100), 282 (24), 252 (18), 141 (7); Anal. Calcd for $C_{21}H_{14}Cl_2O$ (354.24): C, 71.40; H, 3.99. Found: C, 71.68; H, 4.23.



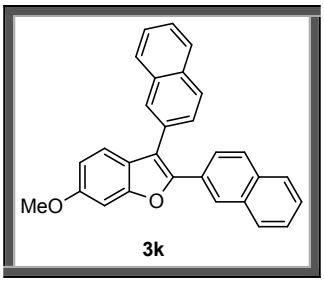
3i

6-Methoxy-2,3-bis(4-methoxyphenyl)benzofuran (3i). White crystal, 33 mg, Yield 91%, mp 263 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.7 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.09 (d, *J* = 1.7 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 2H), 6.88 – 6.86 (m, 3H), 3.89 (s, 6H), 3.82 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 158.7, 158.4, 157.5, 154.2, 149.0, 130.2, 127.4, 124.7, 123.5, 123.2, 119.3, 115.0, 113.8, 113.3, 111.0, 95.2, 55.3, 54.7; MS *m/z* (%) 360 (M•+,100), 345 (81), 326 (68), 311 (27), 202 (12), 180 (19); Anal. Calcd for $C_{23}H_{20}O_4$ (360.40): C, 76.65; H, 5.59. Found: C, 76.98; H, 5.88.



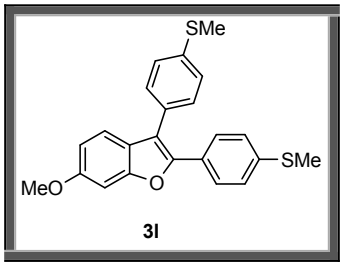
3j

5-Methyl-2,3-bis(4-(methylthio)phenyl)benzofuran (3j). White crystal, 33 mg, Yield 89%, mp 137-139 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.37 – 7.32 (m, 3H), 7.19 (d, *J* = 8.3 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 1H) , 2.57 (s, 3H) , 2.50 (s, 3H), 2.43 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 151.8, 149.8, 138.5, 137.3, 131.9, 129.6, 129.1, 126.8, 126.6, 126.5, 126.3, 125.4, 125.3, 119.0, 115.8, 110.0, 20.8, 15.1, 14.8; MS *m/z* (%) 376 (M•+,100), 326 (88), 311 (29), 282 (21), 69 (25); Anal. Calcd for $C_{23}H_{20}OS_2$ (376.53): C, 73.37; H, 5.35. Found: C, 73.68; H, 5.63.



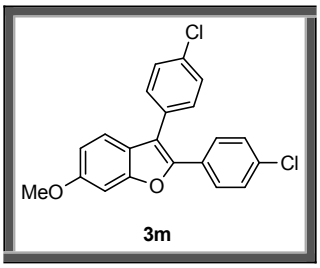
3k

6-Methoxy-2,3-di(naphthalen-2-yl)benzofuran (3k). White crystal, 34 mg, Yield 85%, mp 161-164 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 8.25 (s, 1H), 8.09 (s, 1H), 7.94 – 7.87 (m, 3H), 7.80 – 7.76 (m, 2H), 7.69 – 7.56 (m, 5H), 7.49 – 7.47 (m, 3H) , 7.19 (s, 1H) , 6.94 (d, *J* = 6.8 Hz, 1H), 3.94 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 158.1, 154.7, 149.5, 133.3, 132.8, 132.3, 132.3, 129.9, 128.1, 128.0, 127.9, 127.8, 127.6, 127.4, 127.3, 127.2, 125.9, 125.7, 125.3, 123.9, 123.4, 119.8, 117.3, 111.6, 95.3, 55.3; MS *m/z* (%) 400 (M•+,71), 274 (27), 155 (27), 83 (66), 57 (100); Anal. Calcd for $C_{29}H_{20}O_2$ (400.46): C, 86.98; H, 5.03. Found: C, 86.63; H, 4.78.



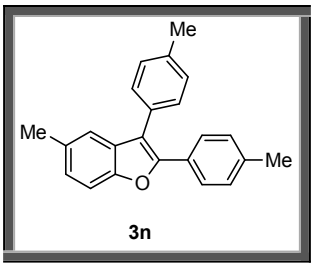
3l

6-Methoxy-2,3-bis(4-(methylthio)phenyl)benzofuran (3l). White crystal, 30 mg, Yield 88%, mp 115-118 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.34 (m, 3H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 2.0 Hz, 1H), 6.88 (dd, *J* = 2.0, 8.4 Hz, 1H), 3.89 (s, 3H), 2.56 (s, 3H), 2.50 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 157.8, 154.4, 148.8, 138.0, 137.3, 129.5, 129.0, 126.9, 126.5, 126.3, 126.2, 125.5, 123.1, 119.5, 115.9, 111.4, 95.2, 55.3, 15.1, 14.9; MS *m/z* (%) 392 (M•+,100), 317 (9), 226 (18), 196 (30), 149 (34), 57 (16); Anal. Calcd for $C_{23}H_{20}O_2S_2$ (392.53): C, 70.38; H, 5.14. Found: C, 70.68; H, 5.40.



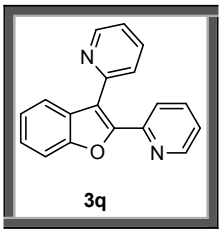
3m

2,3-Bis(4-chlorophenyl)-6-methoxybenzofuran (3m). White crystal, 28 mg, Yield 78%, mp 93-95 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.42 (m, 4H), 7.33 – 7.29 (m, , 3H), 7.09 (d, *J* = 2.0 Hz, 1H), 6.88 (dd, *J* = 2.0, 8.4 Hz, 1H), 3.90 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 158.2, 154.5, 148.2, 133.4, 133.2, 130.6, 130.4, 128.8, 128.5, 128.2, 127.2, 122.6, 119.5, 116.2, 111.8, 95.2, 55.3; MS *m/z* (%) 368 (M•+,100), 262 (23), 226 (33), 139 (33), 113 (30); Anal. Calcd for $C_{21}H_{14}Cl_2O_2$ (369.24): C, 68.31; H, 3.82. Found: C, 68.72; H, 3.97.



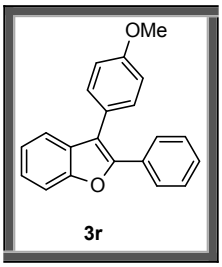
3n

5-Methyl-2,3-di-p-tolylbenzofuran (3n). White crystal, 24 mg, Yield 76%, mp 84-87 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.9 Hz, 2H), 7.44 – 7.39 (m, 3H), 7.30 – 7.28 (m, 3H), 7.14 – 7.13 (m, 3H), 2.46 (s, 3H), 2.43 (s, 3H), 2.36 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 151.8, 150.2, 137.6, 136.6, 131.7, 130.0, 129.5, 129.1, 128.6, 127.6, 126.3, 125.1, 119.1, 116.0, 110.0, 20.8; MS *m/z* (%) 312 (M•+,100), 269 (18), 252 (11), 141 (8); Anal. Calcd for $C_{23}H_{20}O$ (312.40): C, 88.43; H, 6.45. Found: C, 88.72; H, 6.23.



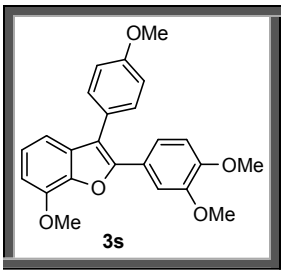
3q

2,2'-(Benzofuran-2,3-diyl)dipyridine (3q). Pale yellow solid, 19 mg, Yield 72%, mp 120-122 ˚C; ^{1}HNMR (500 MHz, $CDCl_3$) δ 8.56 (d, *J* = 3.7 Hz, 1H), 8.21 (d, *J* = 3.4 Hz, 1H), 7.81 – 7.76 (m, 1H), 7.70 (t, *J* = 7.1 Hz, 1H), 7.63 (t, *J* = 7.1 Hz, 1H), 7.40 – 7.33 (m, 2H) , 7.28 – 7.26 (m, 1H) , 7.14 – 7.10 (m, 2H) , 7.00 – 6.96 (m, 2H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 163.2, 154.9, 151.6, 148.2, 147.4, 139.0, 136.4, 135.8, 129.0, 126.9, 124.7, 121.7, 121.6, 121.2, 118.0, 110.9; MS *m/z* (%) 271 (M•+,29), 196 (26), 180 (100), 152 (29), 78 (75), 51 (60); Anal. Calcd for $C_{18}H_{12}N_2O$ (272.09): C, 79.39; H, 4.44; N, 10.29. Found: C, 79.61; H, 4.63; N, 10.51.



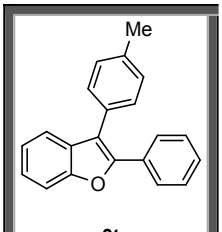
3r

2-phenyl-3-(p-tolyl)benzofuran (3r). White crystals, 21mg, Yield 70%, ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.69 – 7.67 (m, 2H), 7.55 (d, *J* = 8 Hz, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.44 – 7.42 (m, 2H), 7.35 – 7.22 (m, 5H), 7.03 – 7.00 (m, 2H) , 3.89 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 159.1, 153.9, 150.2, 130.9, 130.5, 128.4, 128.2, 126.9, 124.9, 124.6, 122.8, 120.0, 117.1, 114.4, 111.0, 55.3; MS *m/z* (%) 300 (M•+, 100), 278 (15), 255 (13), 228 (13), 149 (14), 125 (23); Anal. Calcd for $C_{21}H_{16}O$ (300.12): C, 83.98; H, 5.3. Found: C, 84.03; H, 5.33.



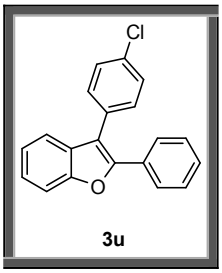
3s

2-(3,4-dimethoxyphenyl)-7-methoxy-3-(4-methoxyphenyl)benzofuran (3s). oil, 26mg, Yield 68%, ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.43 – 7.42 (m, 2H) , 7.17 – 7.13 (m, 4H) , 7.07 – 7.00 (m, 3H), 6.83 – 6.81 (m, 2H), 4.07 (s, 3H), 3.89 (s, 3H), 3.87 (s, 3H), 3.71 (s, 3H); MS *m/z* (%) 390 (M•+, 86), 369 (7), 316 (5), 195 (9), 172 (13), 151 (15), 125 (22); Anal. Calcd for $C_{24}H_{22}O_5$ (390.43): C, 73.83; H, 5.68. Found: C, 73.97; H, 5.73.



3t

2-phenyl-3-(p-tolyl)benzofuran (3t). White crystals, 19mg, Yield 68%, ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.69 – 7.67 (m, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 7.1 Hz , 1H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 8 Hz, 2H), 7.34 – 7.22 (m, 7H), 2,44 (s, 3H); ^{13}CNMR (125 MHz, $CDCl_3$) δ 154.0 , 137.4, 129.7, 129.6, 128.4, 128.2, 127.0, 124.6, 122.8, 120.1, 111.1, 29.7; MS *m/z* (%) 284 (M•+, 100), 239 (19), 134 (13), 85 (20), 57 (40); Anal. Calcd for $C_{21}H_{16}O$ (390.43): C, 73.83; H, 5.68. Found: C, 73.87; H, 5.77.



3u

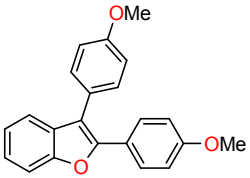
3-(4-chlorophenyl)-2-phenylbenzofuran (3u). White crystals, 20mg, Yield 66%, ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.65 – 7.63 (m, 2H), 7.57 – 7.56 (m,1H), 7.48– 7.44 (m,5H), 7.36– 7.32 (m, 4H), 7.27– 7.26 (m, 1H); MS *m/z* (%) 306 (M•+2, 33), 305 (M•+1,22), 304 (M•+,100), 268 (28), 239 (32), 194 (11), 149 (22), 119 (17), 85 (10), 57 (19); Anal. Calcd for $C_{20}H_{13}ClO$ (304.07): C, 78.82; H, 4.30. Found: C, 78.91; H, 4.43.

6. ***X-ray crystallography***

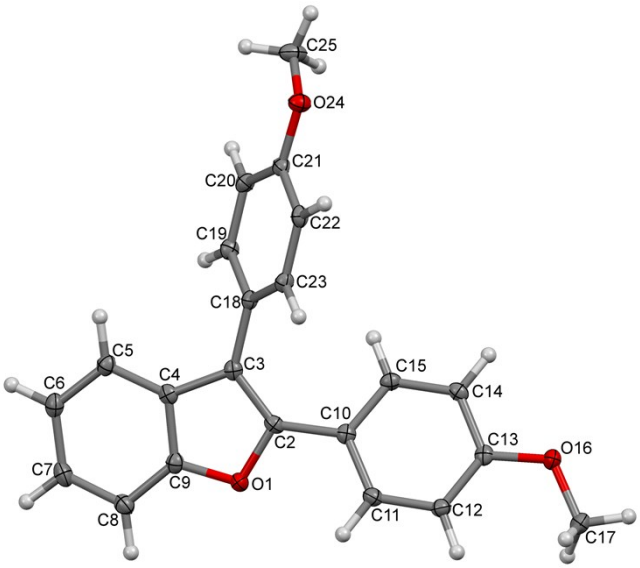
Diffraction data were collected at 100(1)K by the ω-scan technique on Agilent Technologies four-circle XCalibur diffractometer with Eos CCD detector, equipped with graphite-monochromated MoK_α radiation source (λ = 0.71073 Å). The data were corrected for Lorentz-polarization as well as for absorption effects [1]. Precise unit-cell parameters were determined by a least-squares fit of 15846 reflections of the highest intensity, chosen from the whole experiment. The structure was solved with SIR92 [2] and refined with the full-matrix least-squares procedure on F^2 by SHELXL-2013 [3]. The scattering factors incorporated in SHELXL97 were used. All non-hydrogen atoms were refined anisotropically, hydrogen atoms were found in difference Fourier maps, and freely refined with isotropic displacement parameters.

6.1. Crystal Data and ORTEP diagram of compound 3e

Figure S1: ORTEP diagram of 3e (CCDC-1035494).



3e



Crystal data for 3e: $C_{22}H_{18}O_3$, M_r=330.36, monoclinic, $P2_1/c$, a=8.6642(2)Å, b=20.3575(3)Å, c=10.1977(2)Å, β=115.123(3)°, V=1628.53(7)Å^3, Z=4, d_x=1.35g·cm^{-3}, μ=0.089mm^{-1}, F(000)-696, MoK_α, λ=0.71073Å, T=100(1)K, 37859 reflections measured of which 3818 symmetry-independent, R_{int}=2.36%. Final R(all reflections)=3.88%, wR2(all reflections)=8.98%, S=1.036, $\Delta\rho_{max}/\Delta\rho_{min}$=0.29/-0.22 e·Å^{-3}. CCDC-1035494.

CheckCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

No syntax errors found.

Table S2: Crystal data for 3e

Bond precision: C-C = 0.0015 A Wavelength = 0.71070

Cell:	a = 8.6642 (2)	b = 20.3575 (3)	c = 10.1977 (2)
	alpha = 90	beta = 115.123(3)	gamma = 90
Temperature:	100 K		

	Calculated	Reported
Volume	1628.53 (7)	1628.53 (7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H18 O3	C22 H18 O3
Sum formula	C22 H18 O3	C22 H18 O3
Mr	330.36	330.36
Dx,g cm-3	1.347	1.347
Z	4	4
Mu (mm-1)	0.089	0.089
F000	696.0	696.0
F000’	696.34	
h,k,lmax	11,27,13	11,27,13
Nref	4111	3818
Tmin,Tmax	0.968,0.991	0.925,1.000
Tmin’	0.965	

Correction method = MULTI-SCAN

Data completeness = 0.929 Theta (max) = 28.411

R(reflections) = 0.0353 (3500) wR2(reflections) = 0.0898 (3818)

S = 1.036 Npar = 298

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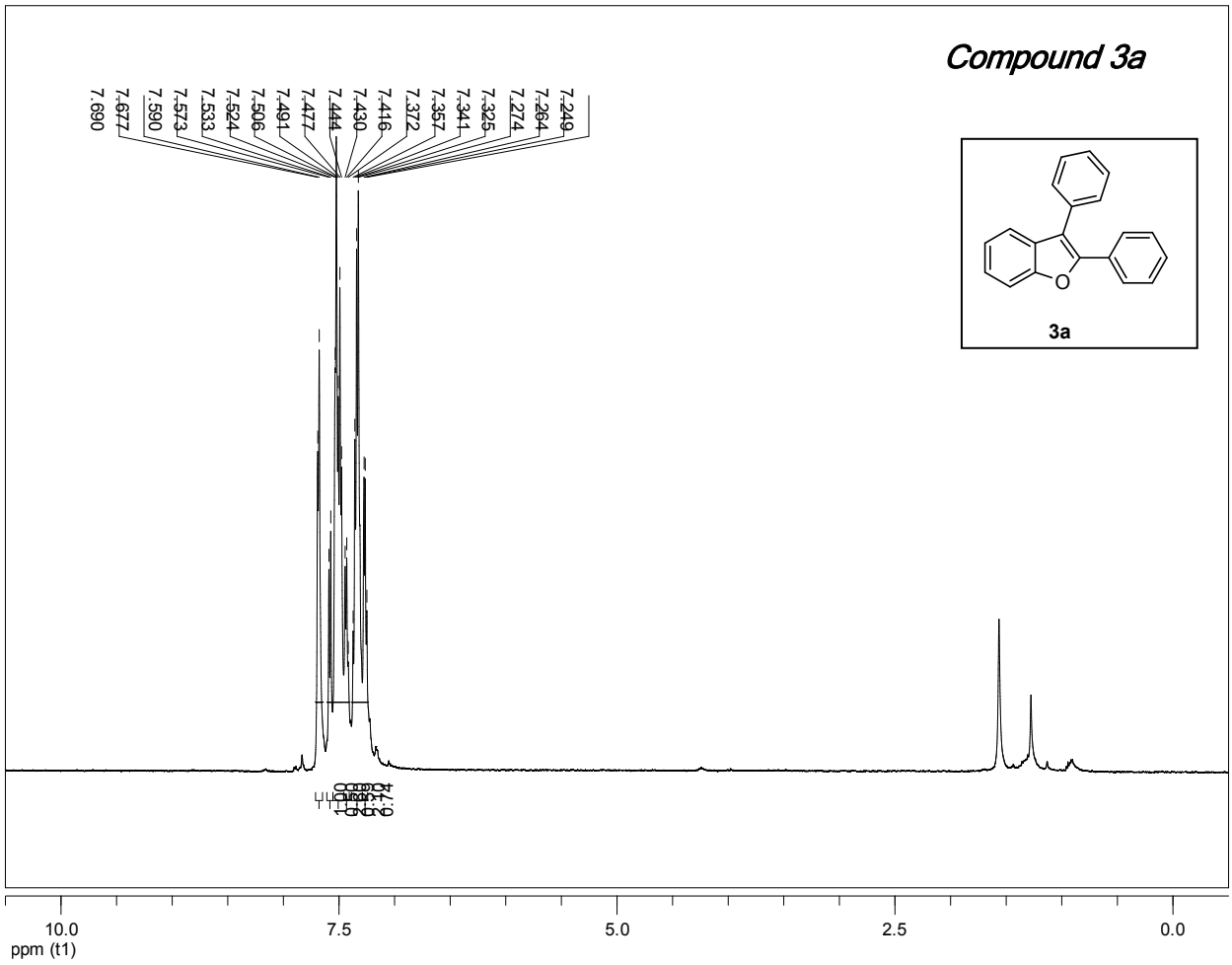
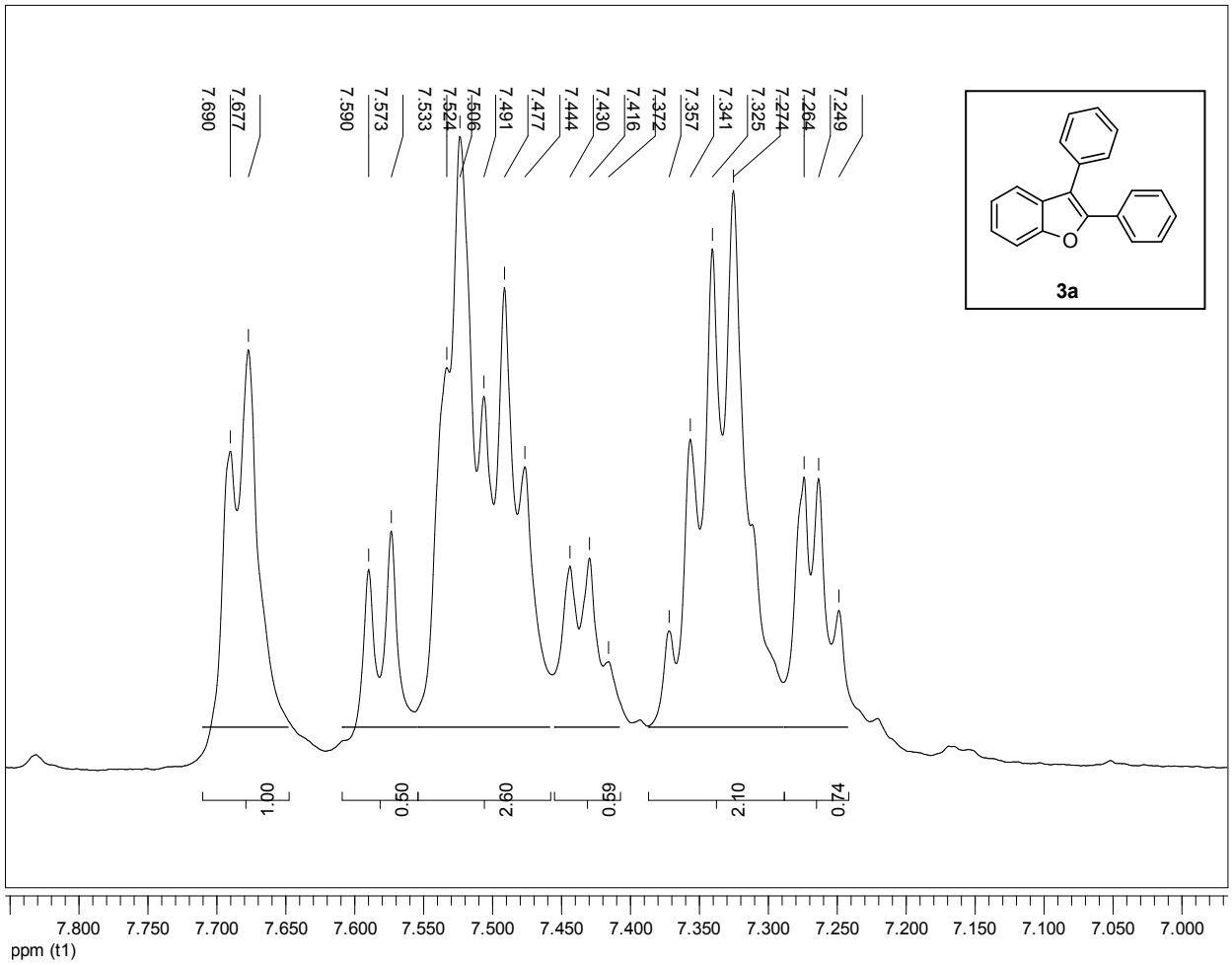
7. Copies of ^{1}H, ^{13}C NMR and Mass Spectra

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7.524
7.506
7.491
7.477
7.444
7.430
7.416
7.372
7.357
7.341
7.325
7.274
7.264
7.249
1.00
0.60
2.60
0.69
2.10
0.74
3a
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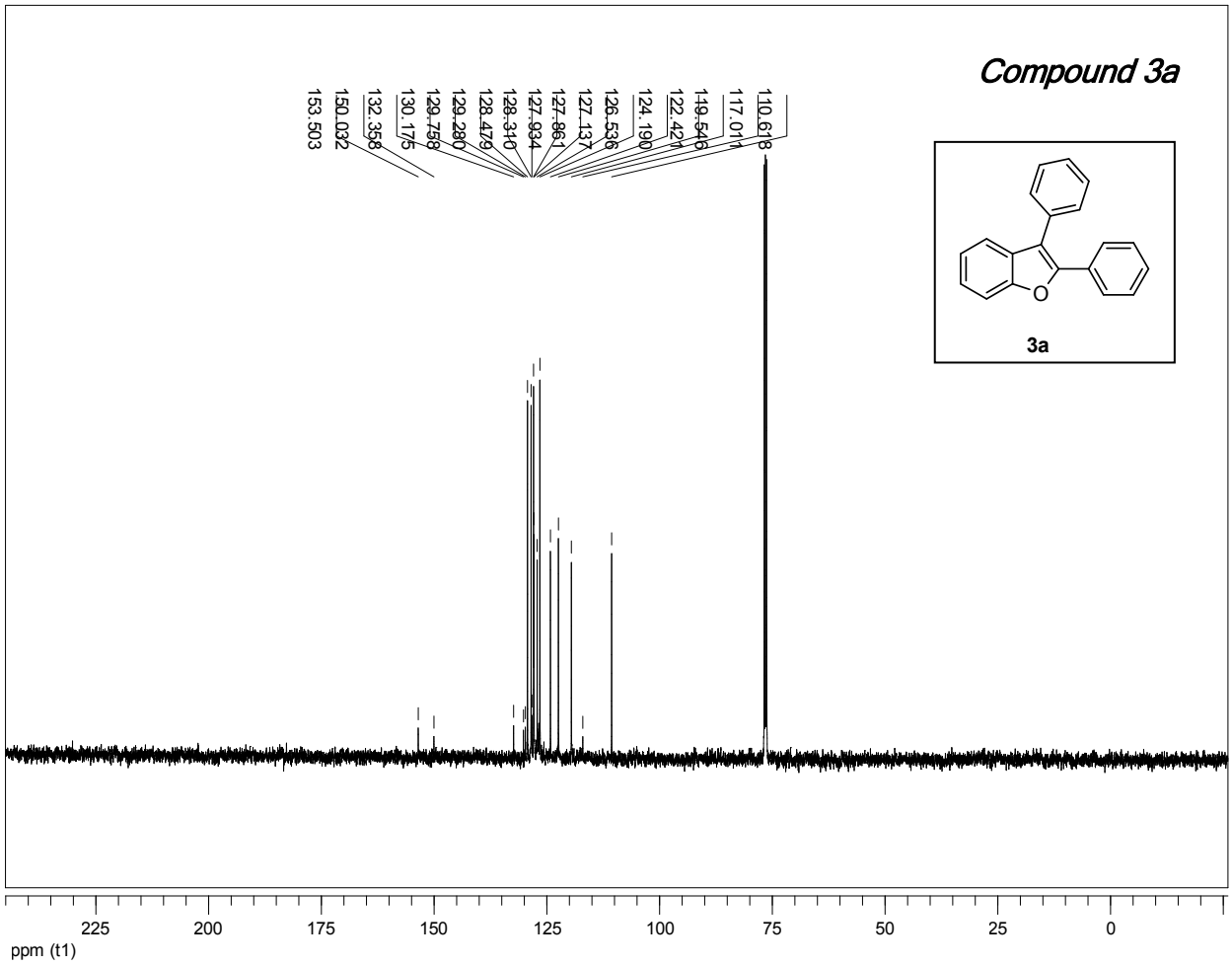
ppm (t1)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129.280
128.479
128.310
127.934
127.861
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126.536
124.190
122.421
119.546
117.011
110.618
3a
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175
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125
100
75
50
25
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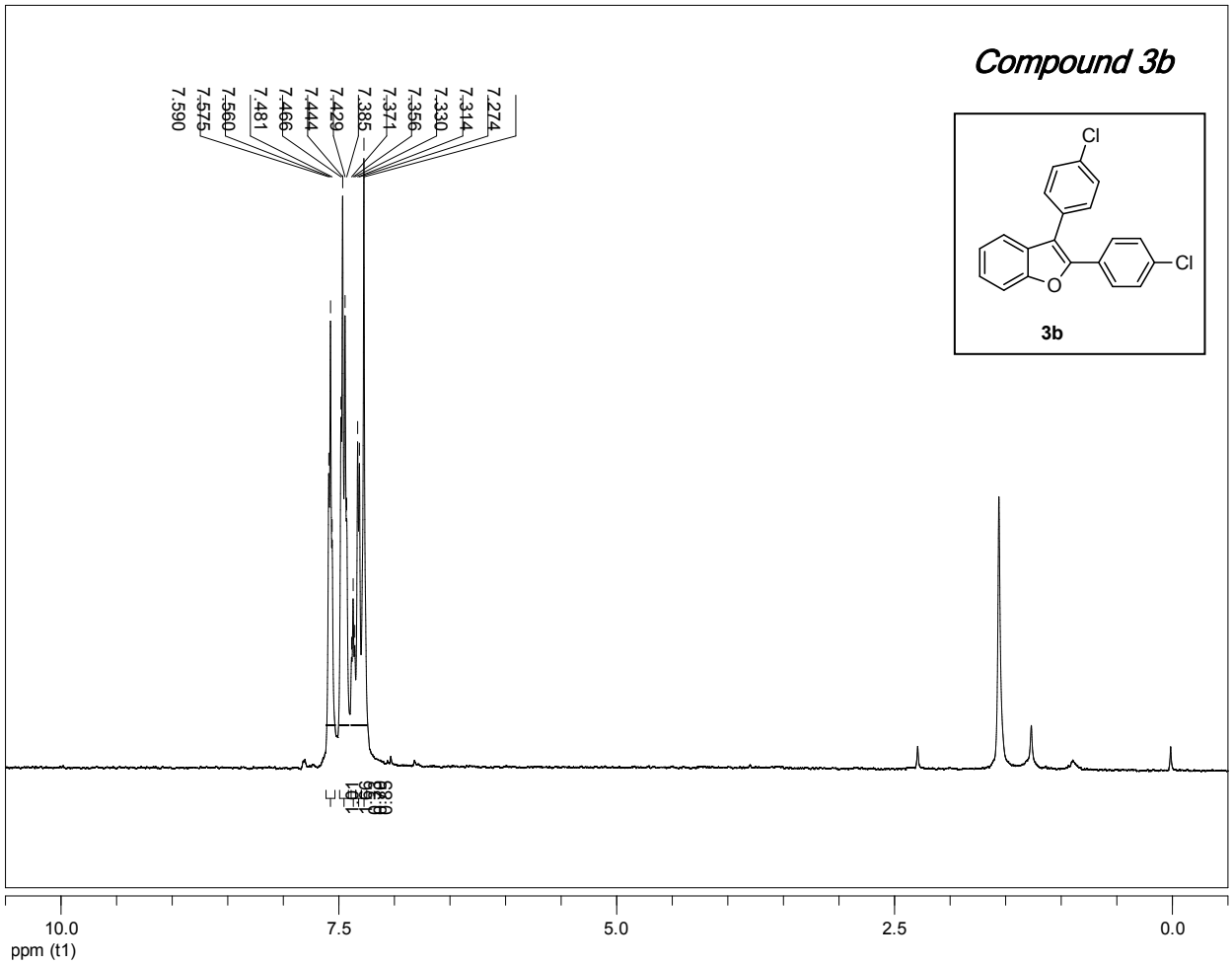
ppm (t1)


Compound 3b
7.590
7.575
7.560
7.481
7.466
7.444
7.429
7.385
7.371
7.356
7.330
7.314
7.274
Cl
Cl
O
3b
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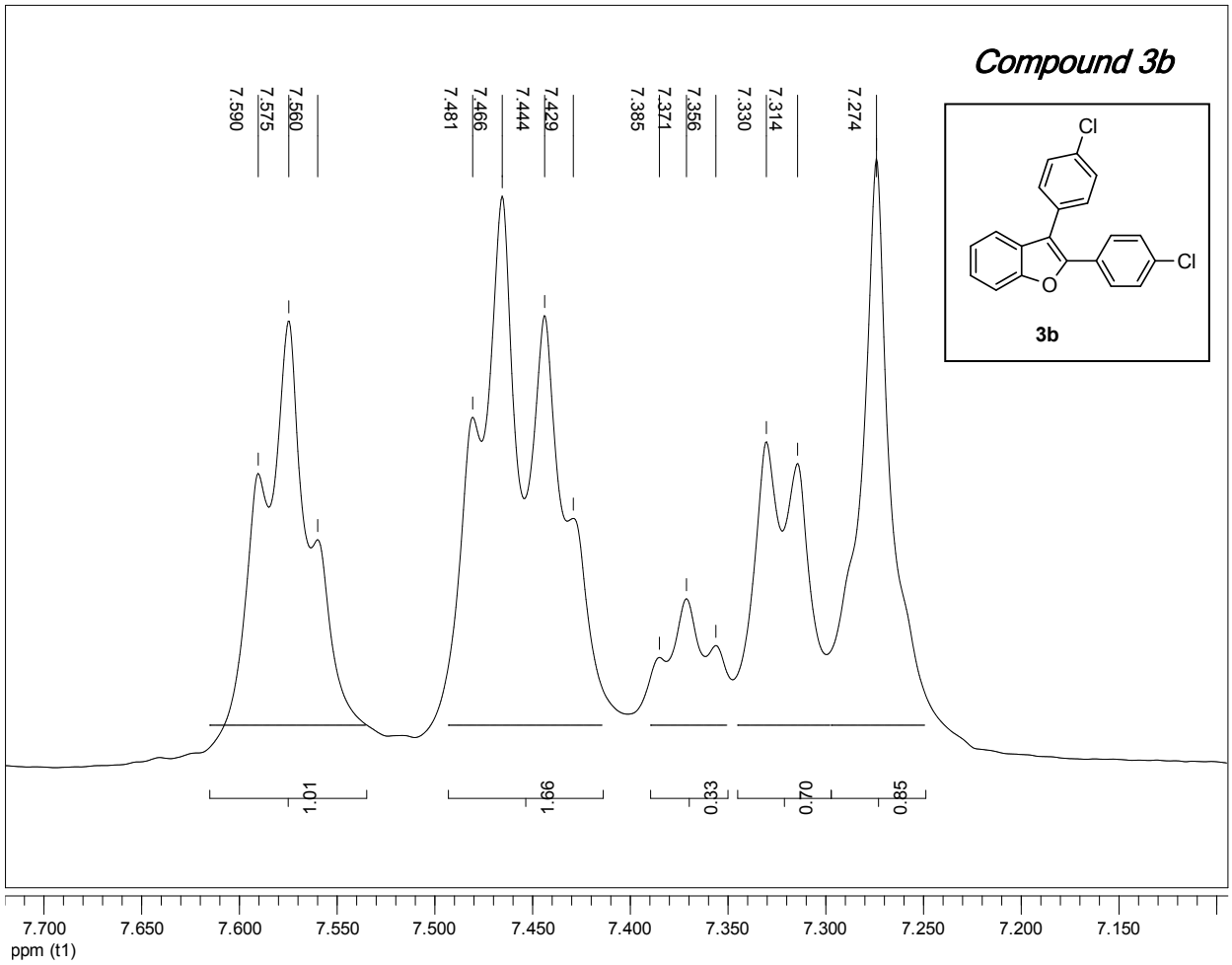
5.0
2.5
0.0
ppm (t1)


Compound 3b
7.590
7.575
7.560
7.481
7.466
7.444
7.429
7.385
7.371
7.356
7.330
7.314
7.274
Cl
Cl
O
3b
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1.96
0.33
0.70
0.85
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7.500
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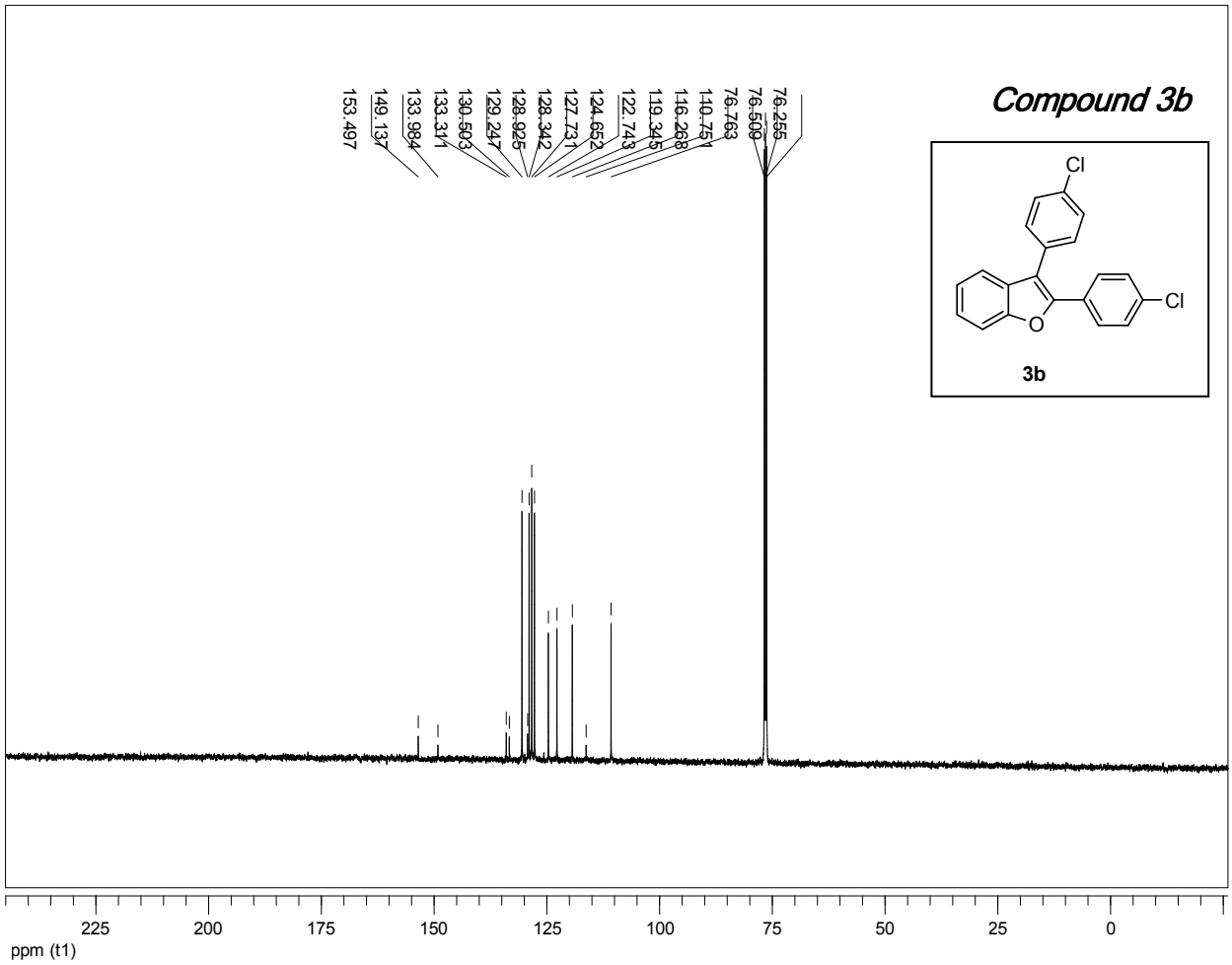
7.250
7.200
7.150
ppm (t1)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110.751
76.763
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76.255
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Cl
O
3b
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200
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150
125
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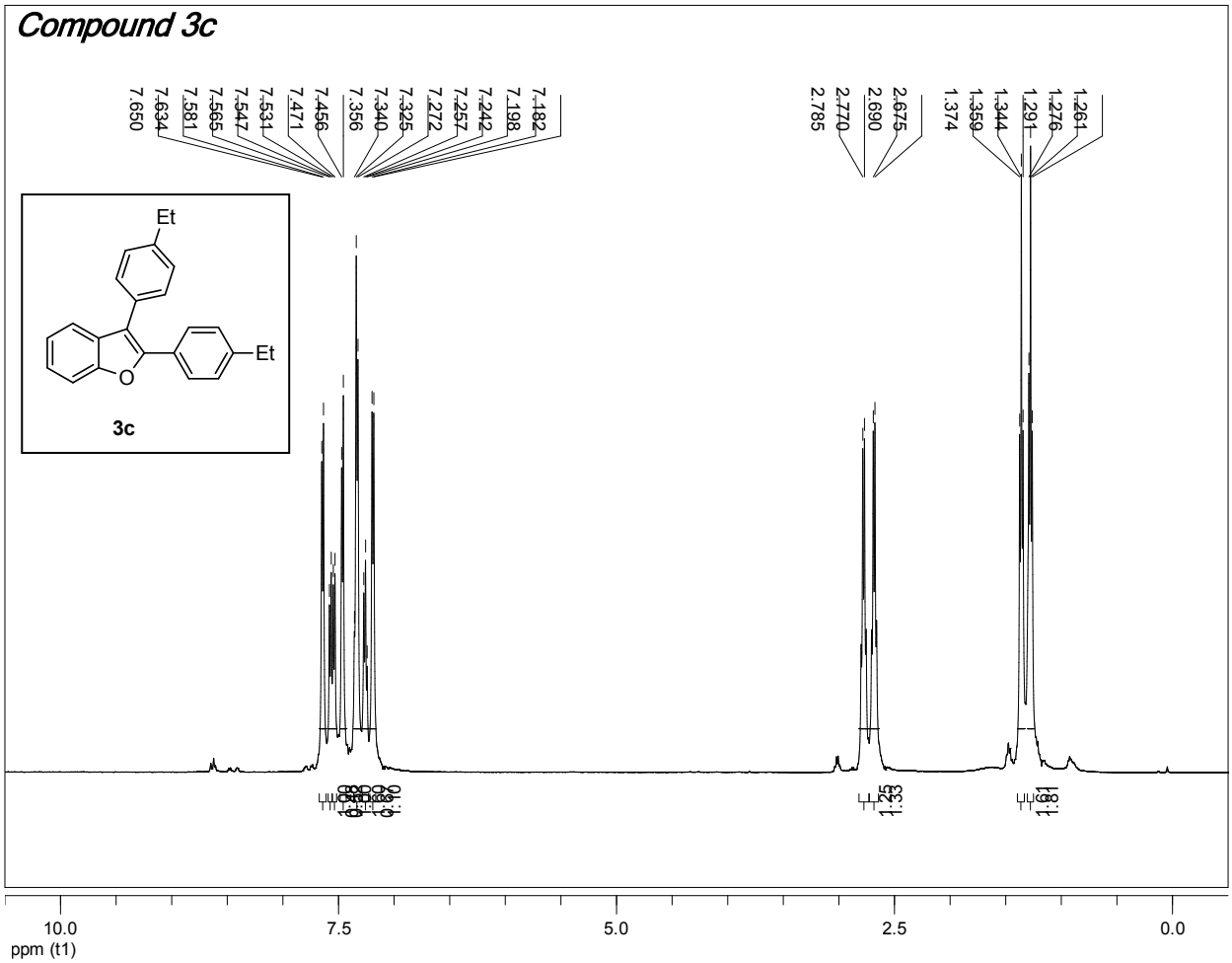
50
25
0
ppm (t1)


Compound 3c
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7.325
7.272
7.257
7.242
7.198
7.182
2.785
2.770
2.690
2.675
1.374
1.359
1.344
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Et
Et
O
3c
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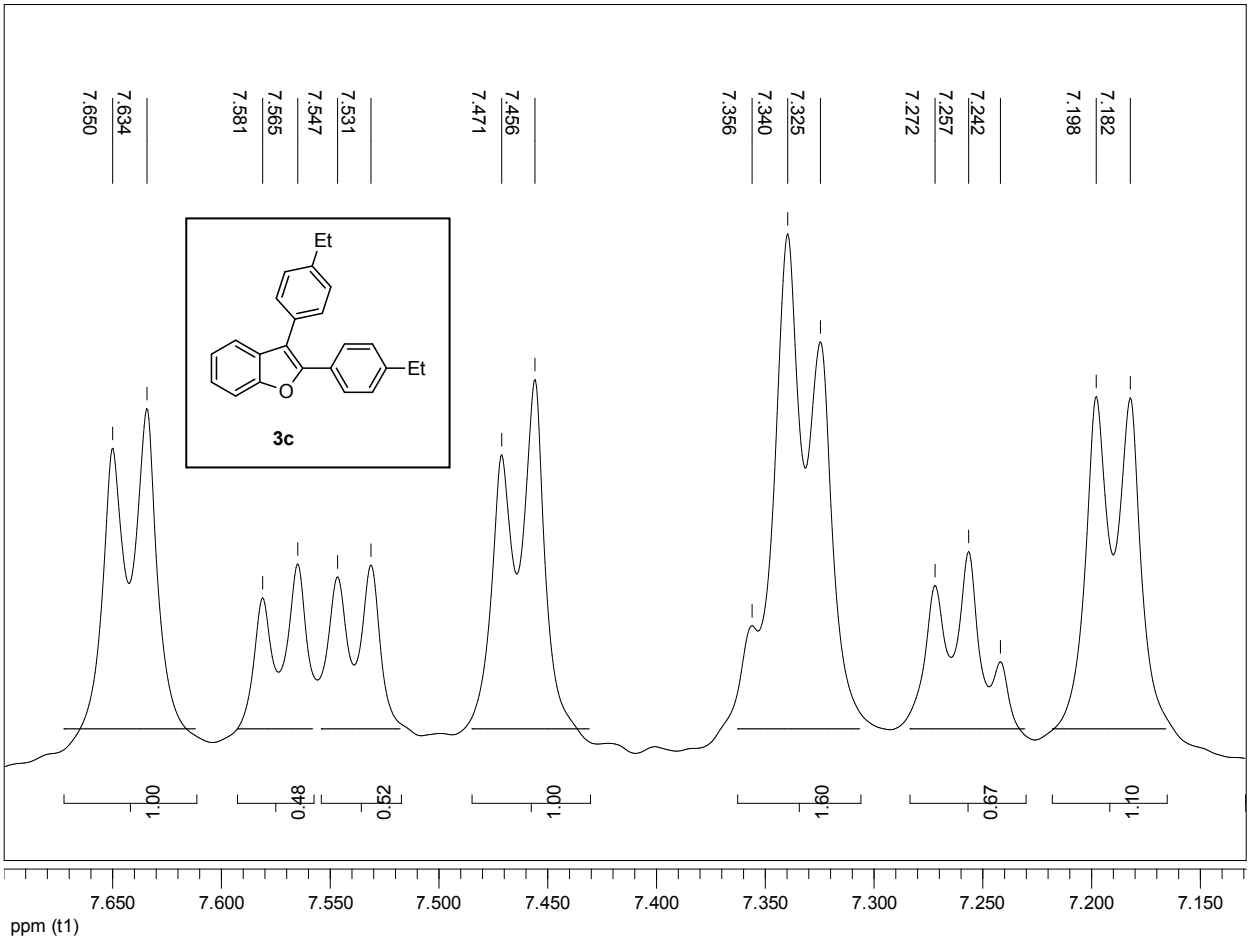
ppm (t1)


7.650
7.634
7.581
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7.547
7.531
7.471
7.456
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7.340
7.325
7.272
7.257
7.242
7.198
7.182
Et
Et
O
3c
1.00
0.48
0.52
1.00
1.60
0.67
1.10
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7.500
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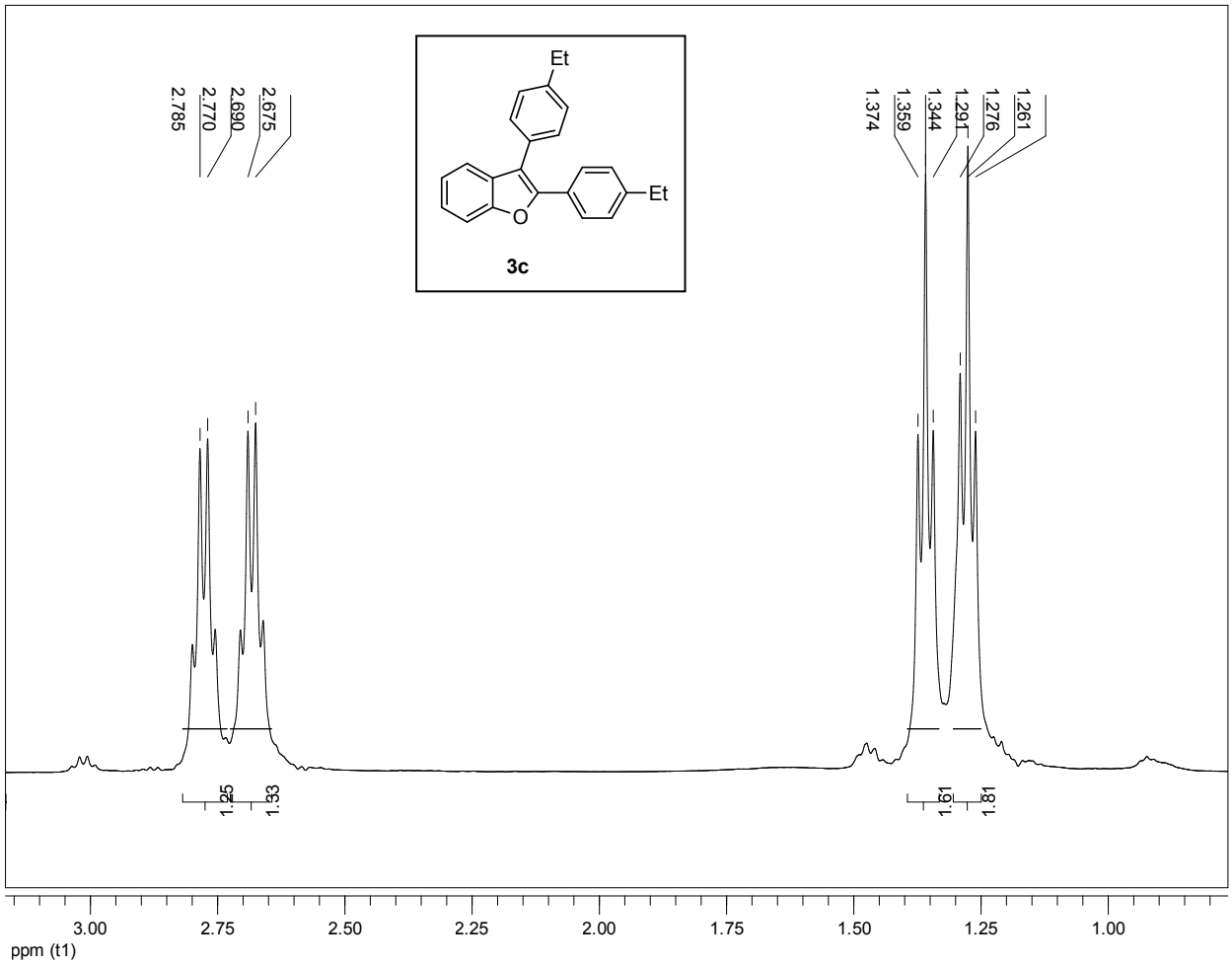
7.400
7.350
7.300
7.250
7.200
7.150
ppm (t1)


Et
Et
O
3c
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1.261
1.26
1.33
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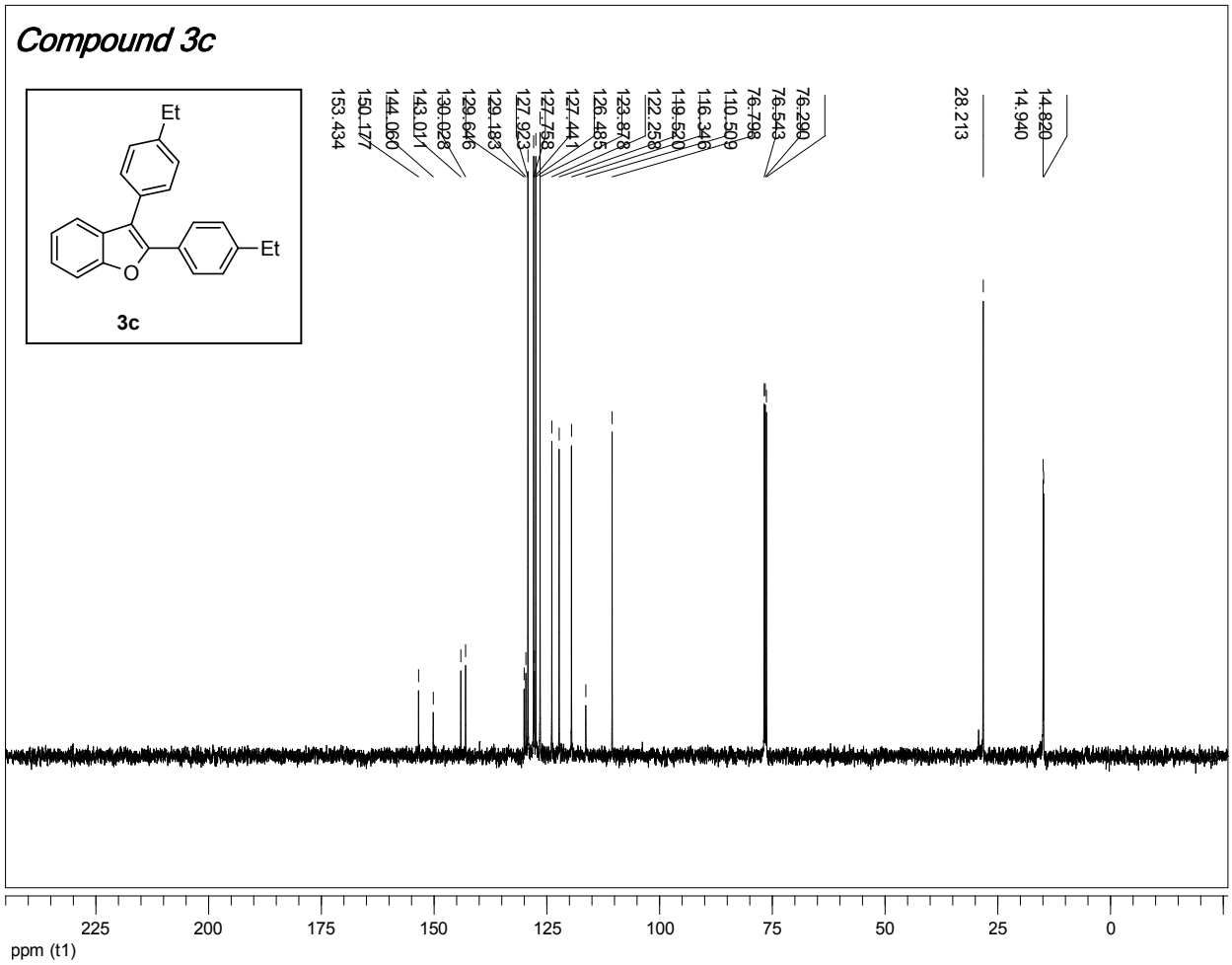
1.00
ppm (t1)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Et
O
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127.441
126.485
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110.509
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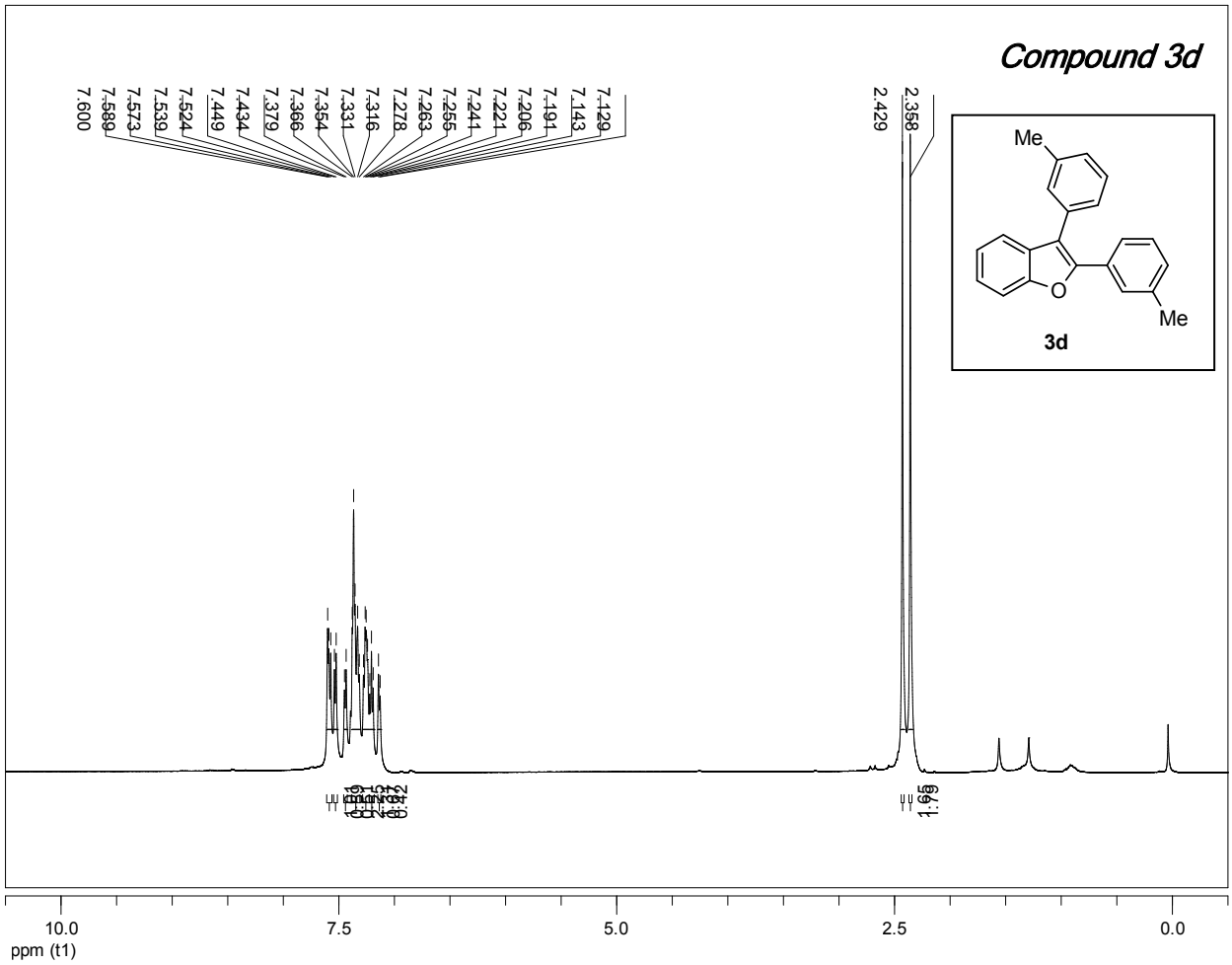
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7.221
7.206
7.191
7.143
7.129
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Me
Me
O
3d
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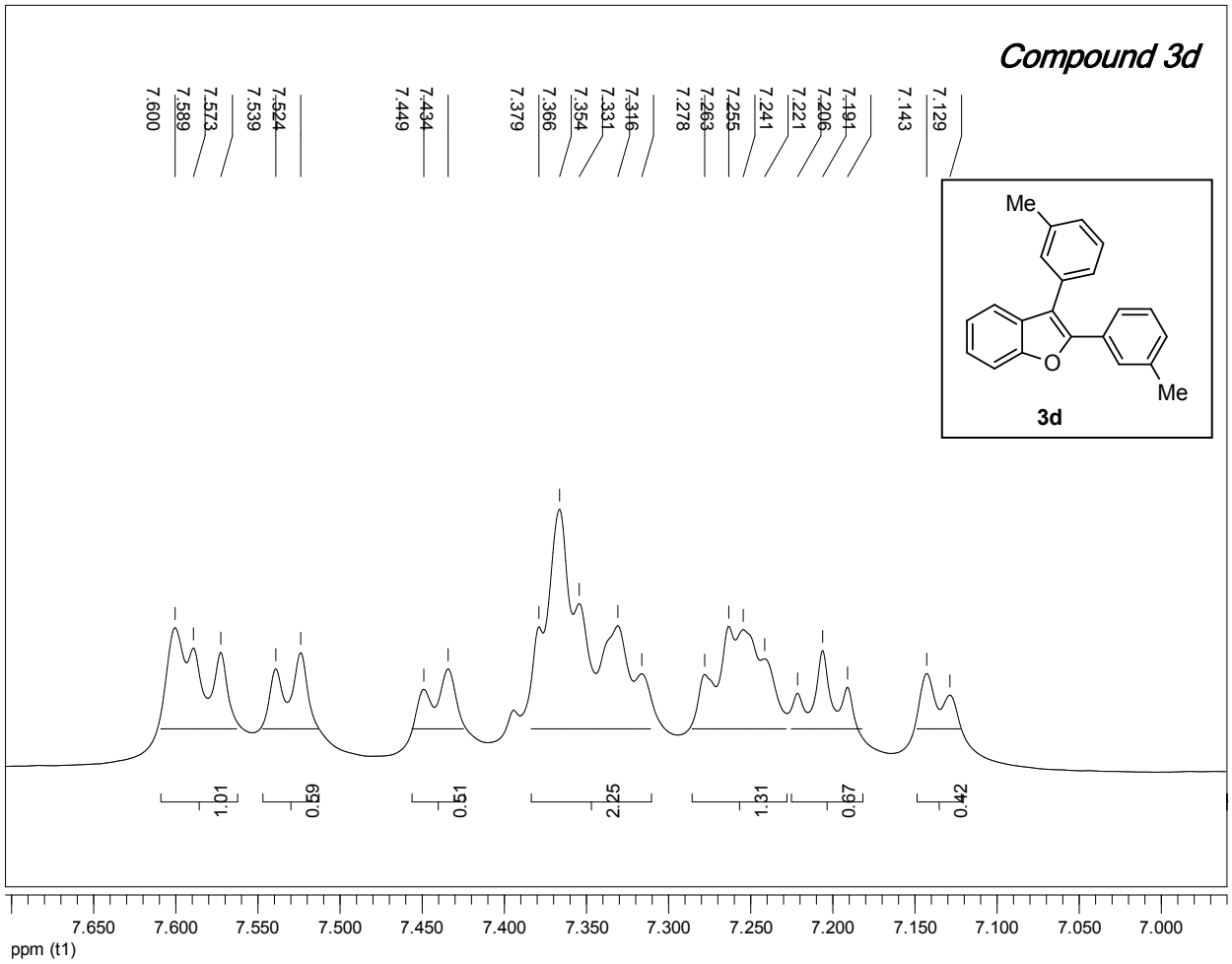
5.0
2.5
0.0
ppm (t1)


Compound 3d
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7.434
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7.366
7.354
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7.255
7.241
7.221
7.206
7.191
7.143
7.129
Me
Me
O
3d
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0.51
2.25
1.31
0.97
0.42
7.650
7.600
7.550
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7.100
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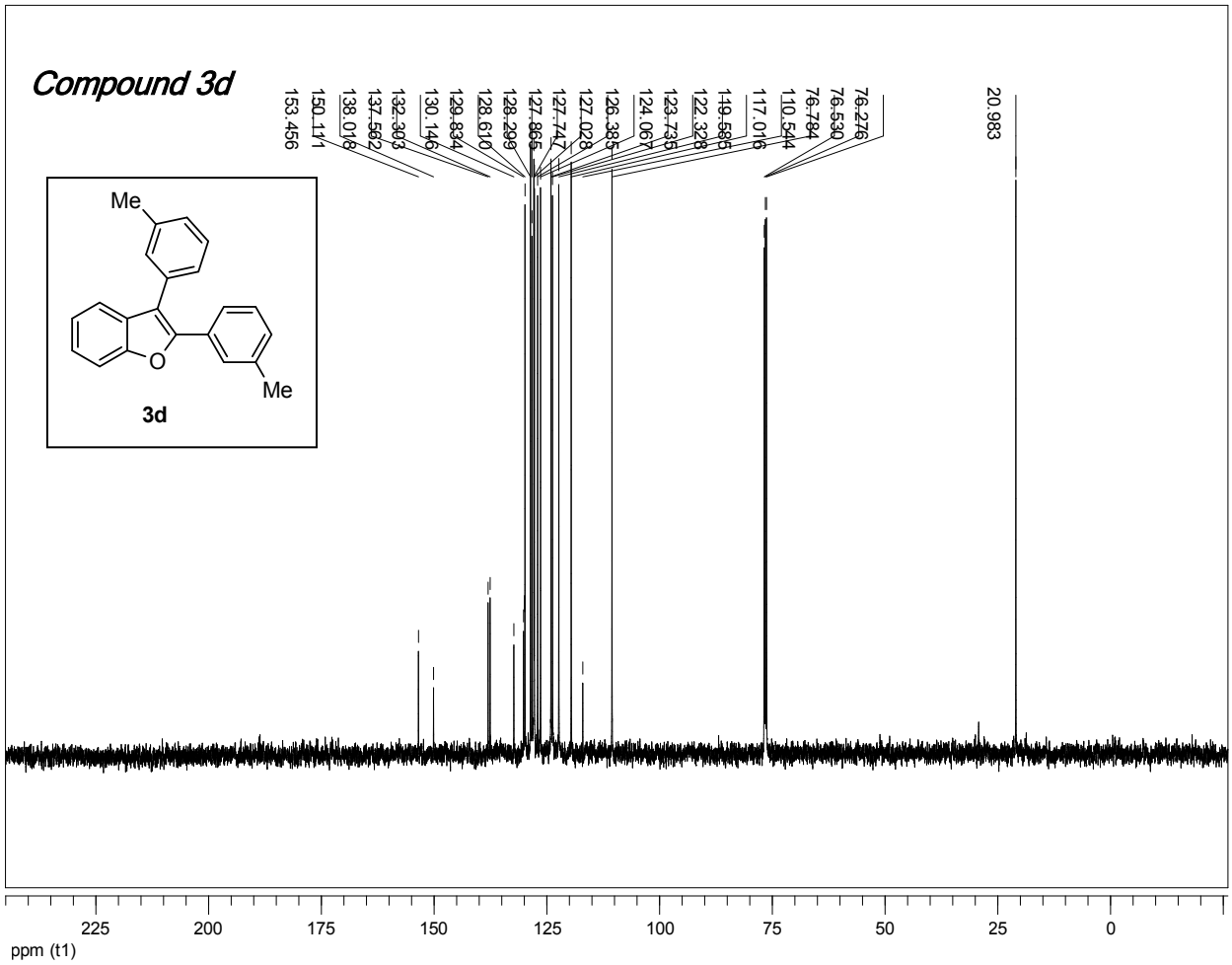
7.000
ppm (t1)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119.585
117.016
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76.530
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O
Me
3d
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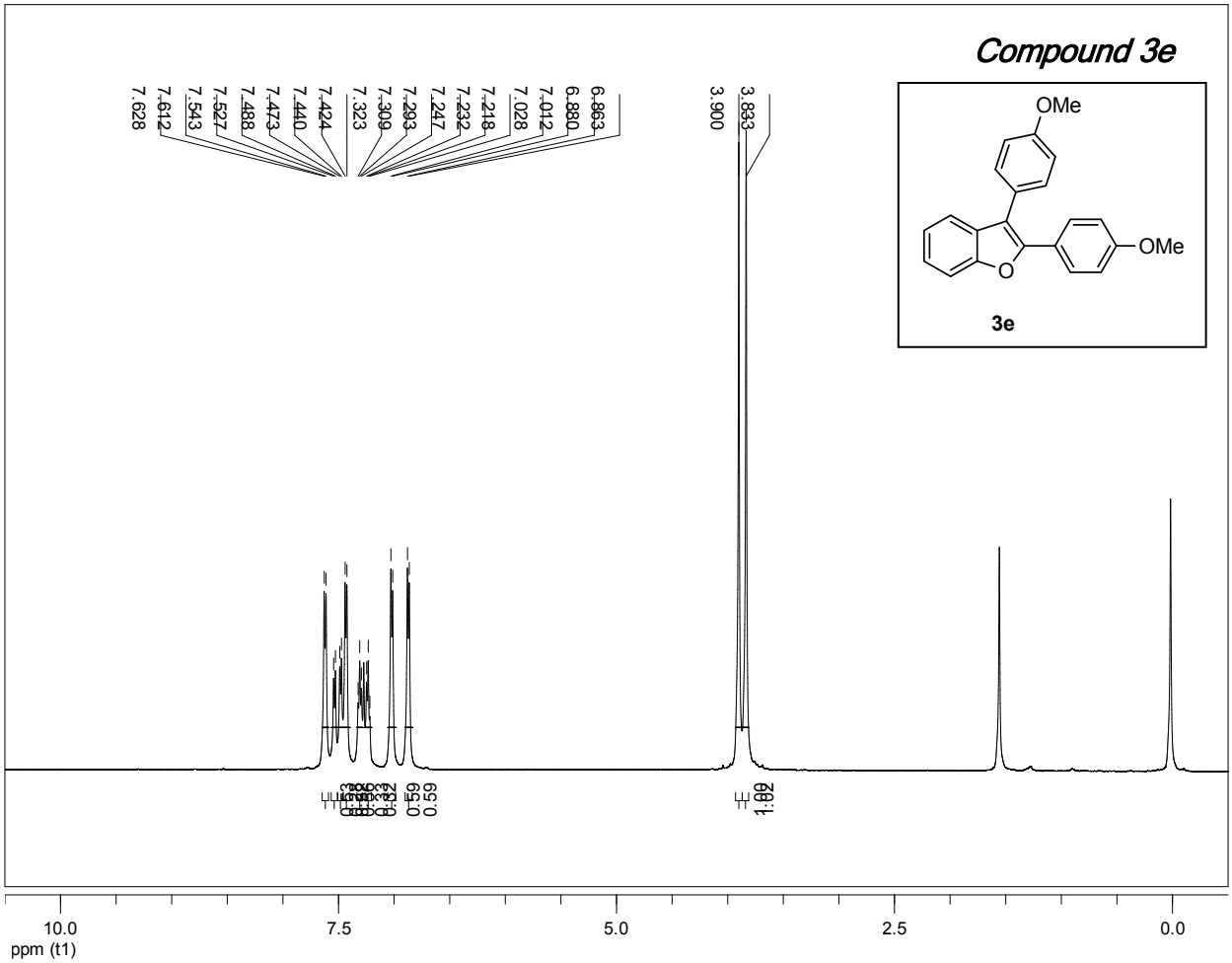
ppm (t1)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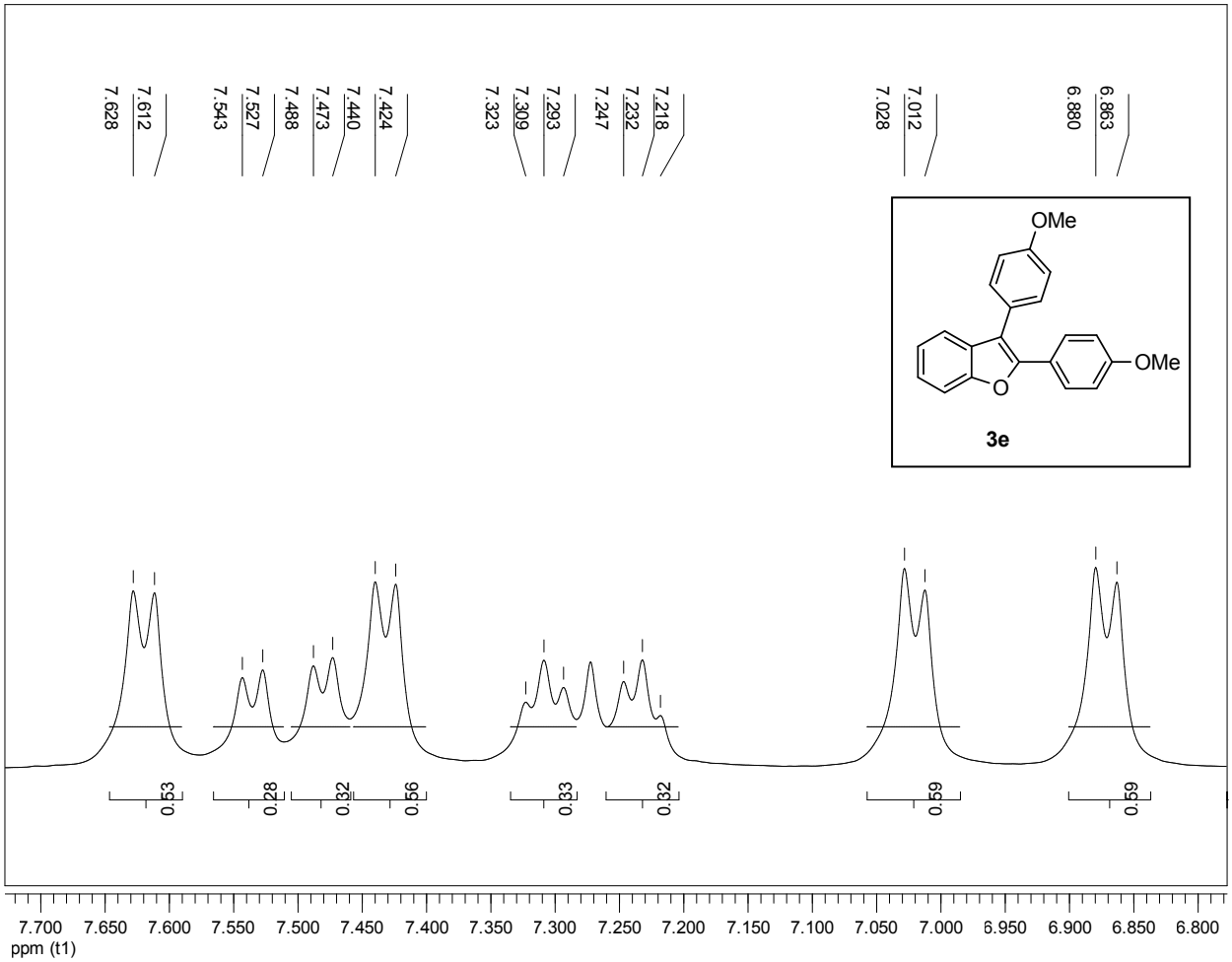
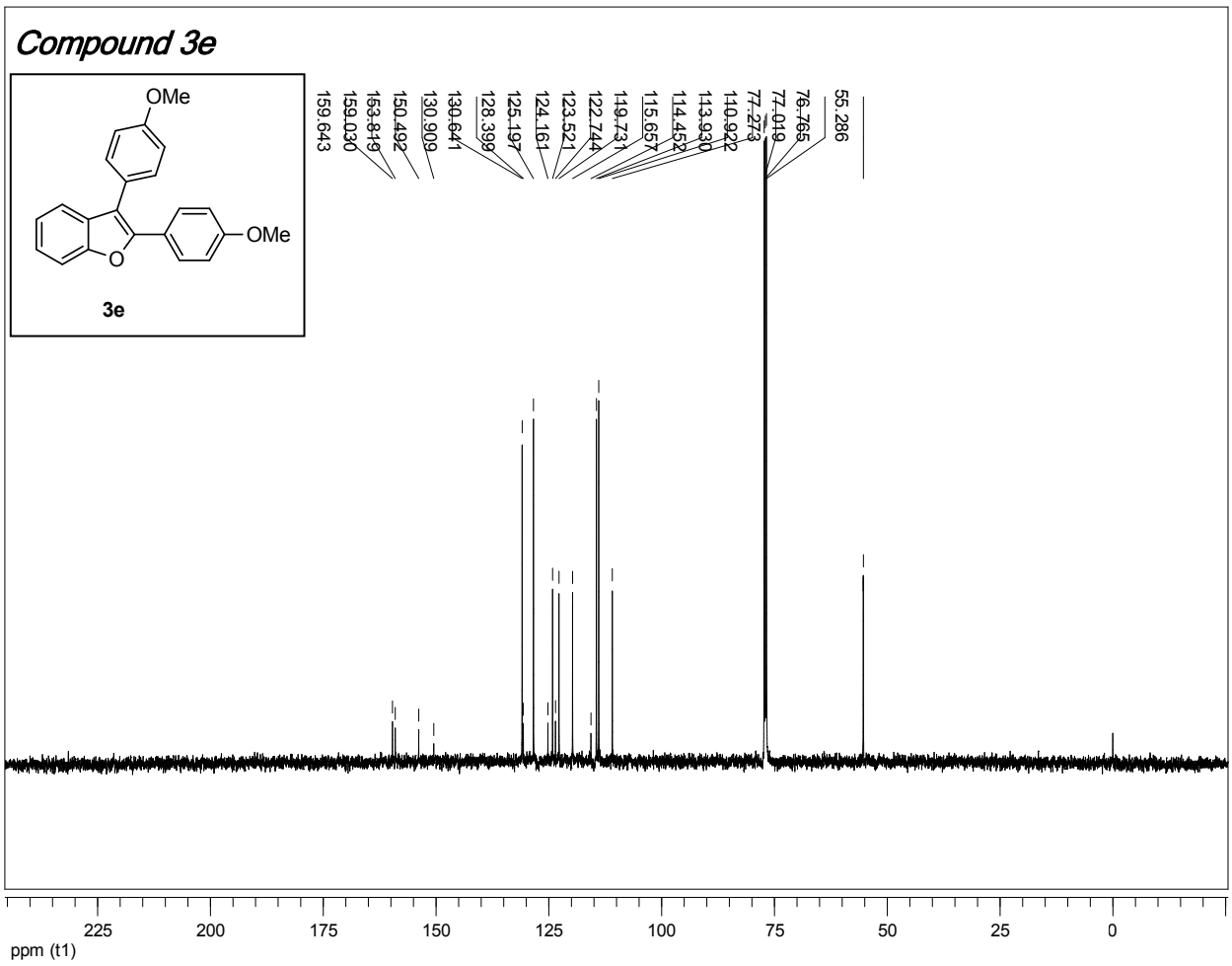
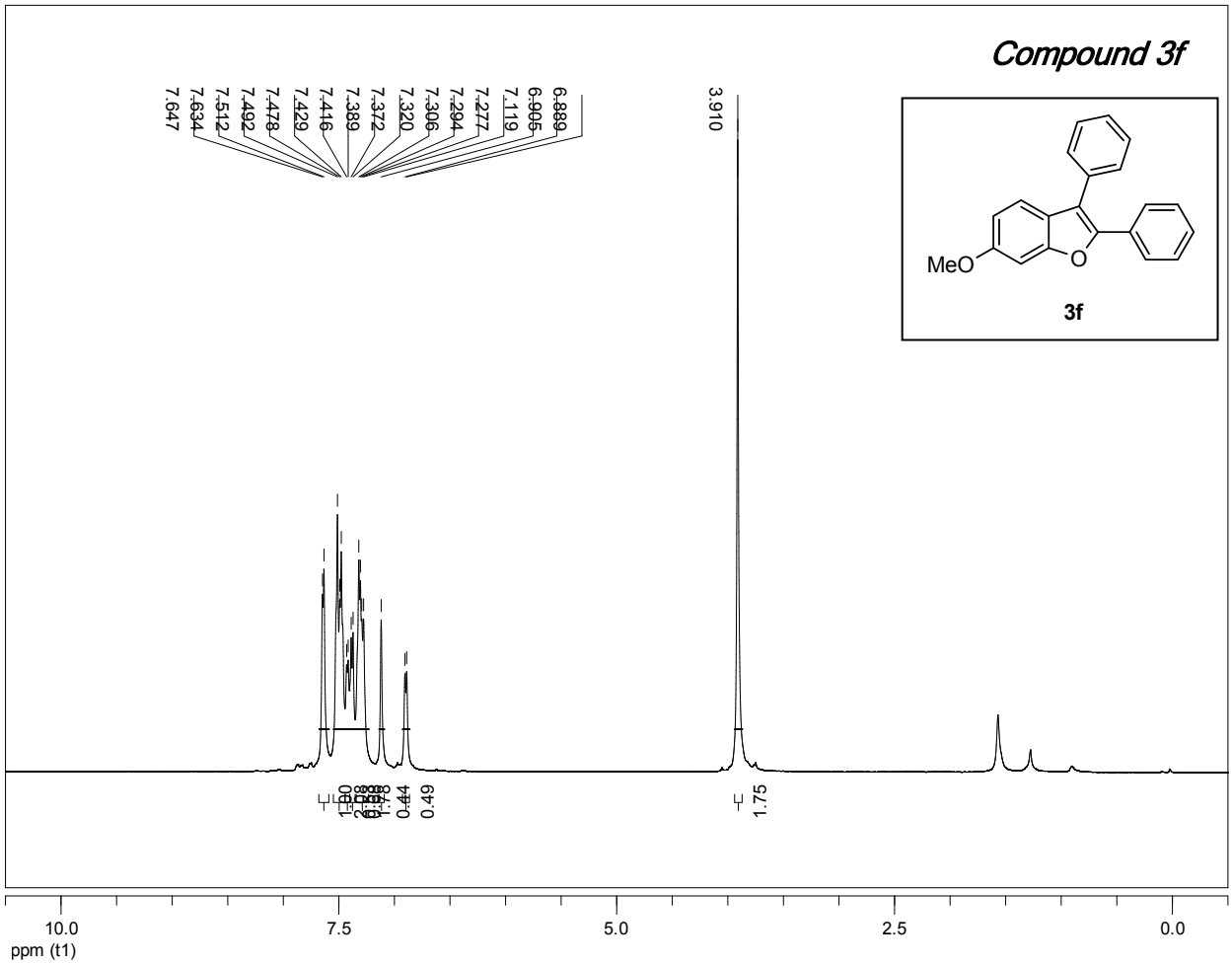
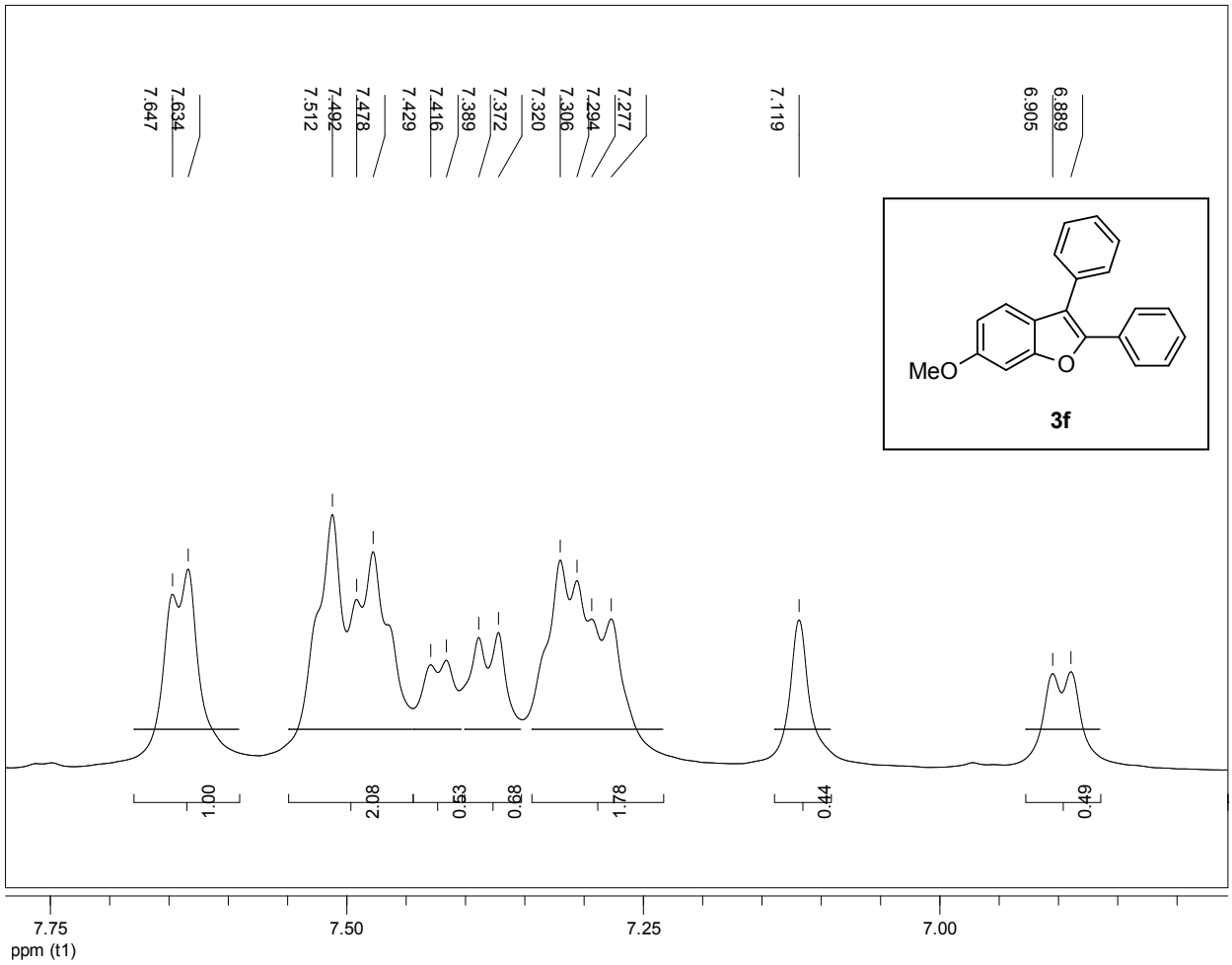
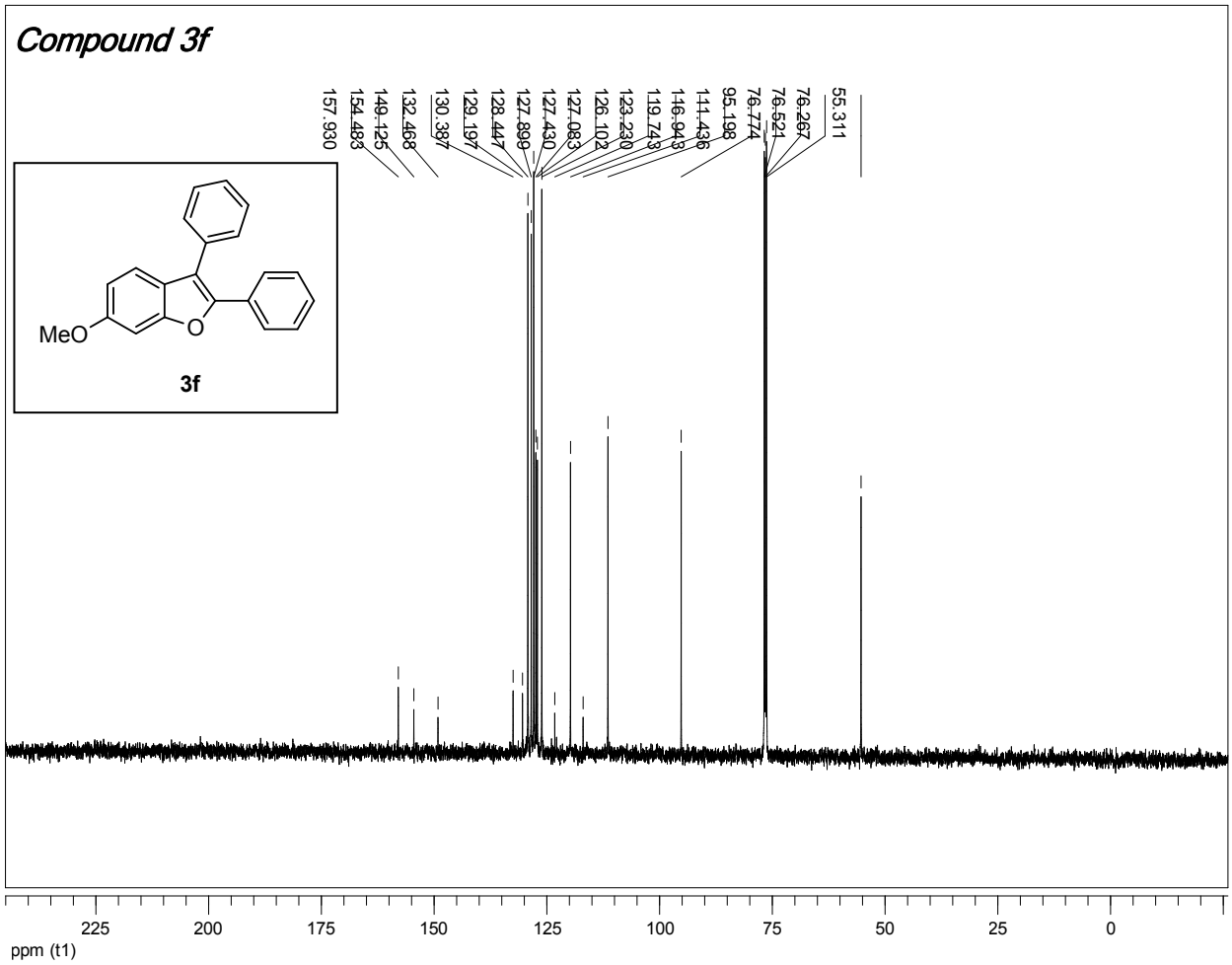
7.028
7.012
6.880
6.863
3.900
3.883
OMe
OMe
3e
10.0
7.5
5.0
2.5
0.0
ppm (t1)

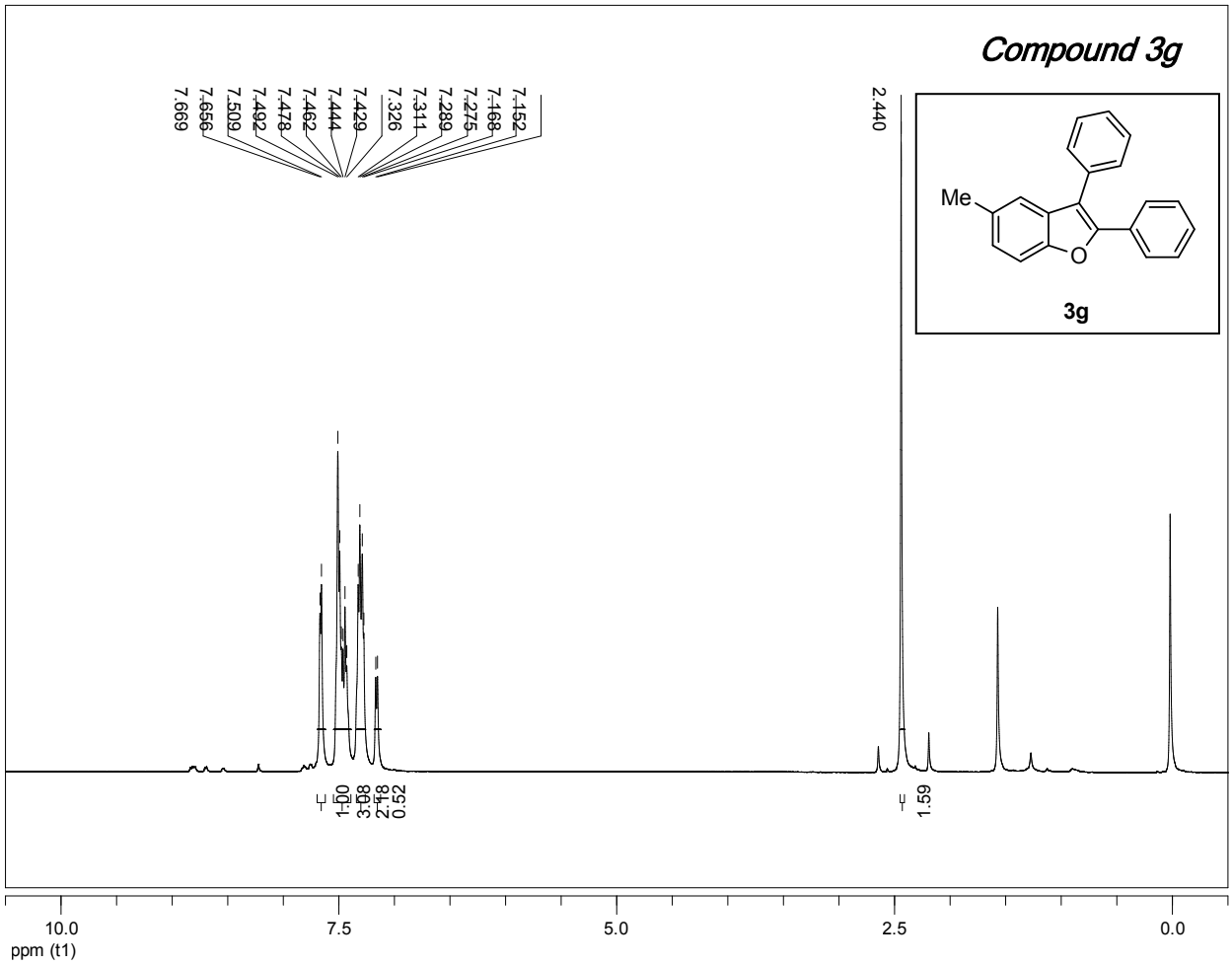

7.628
7.612
7.543
7.527
7.488
7.473
7.440
7.424
7.323
7.309
7.293
7.247
7.232
7.218
7.028
7.012
6.880
6.863
OMe
OMe
O
3e
0.53
0.28
0.32
0.66
0.33
0.32
0.69
0.69
7.700 7.650 7.600 7.550 7.500 7.450 7.400 7.350 7.300 7.250 7.200 7.150 7.100 7.050 7.000 6.950 6.900 6.850 6.800
ppm (t1)

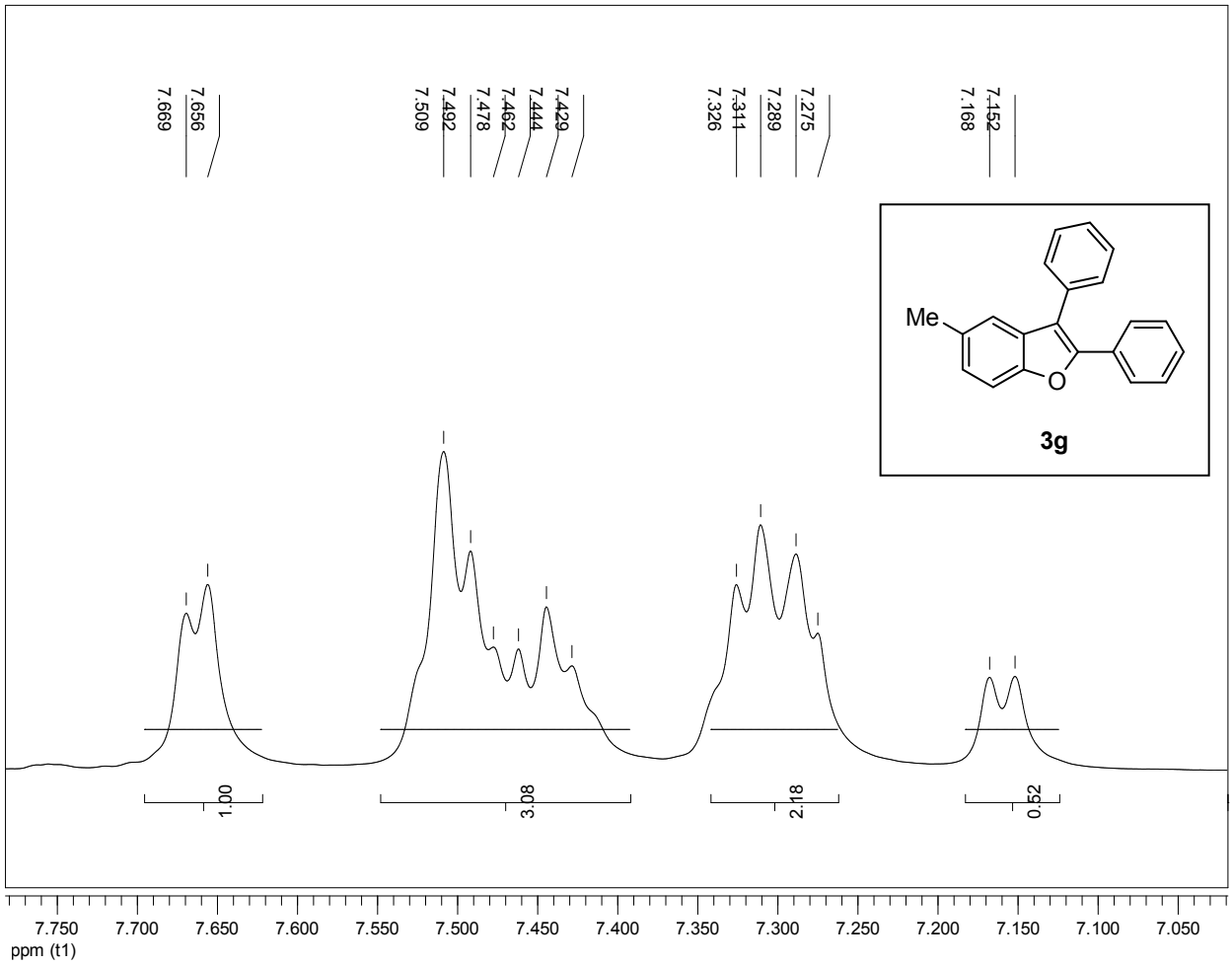

Compound 3e
OMe
OMe
O
3e
159.643
159.030
153.819
150.492
130.909
130.641
128.399
125.197
124.161
123.521
122.744
119.731
115.657
114.452
113.930
110.922
77.273
77.019
76.765
55.286
225
200
175
150
125
100
75
50
25
0
ppm (t1)

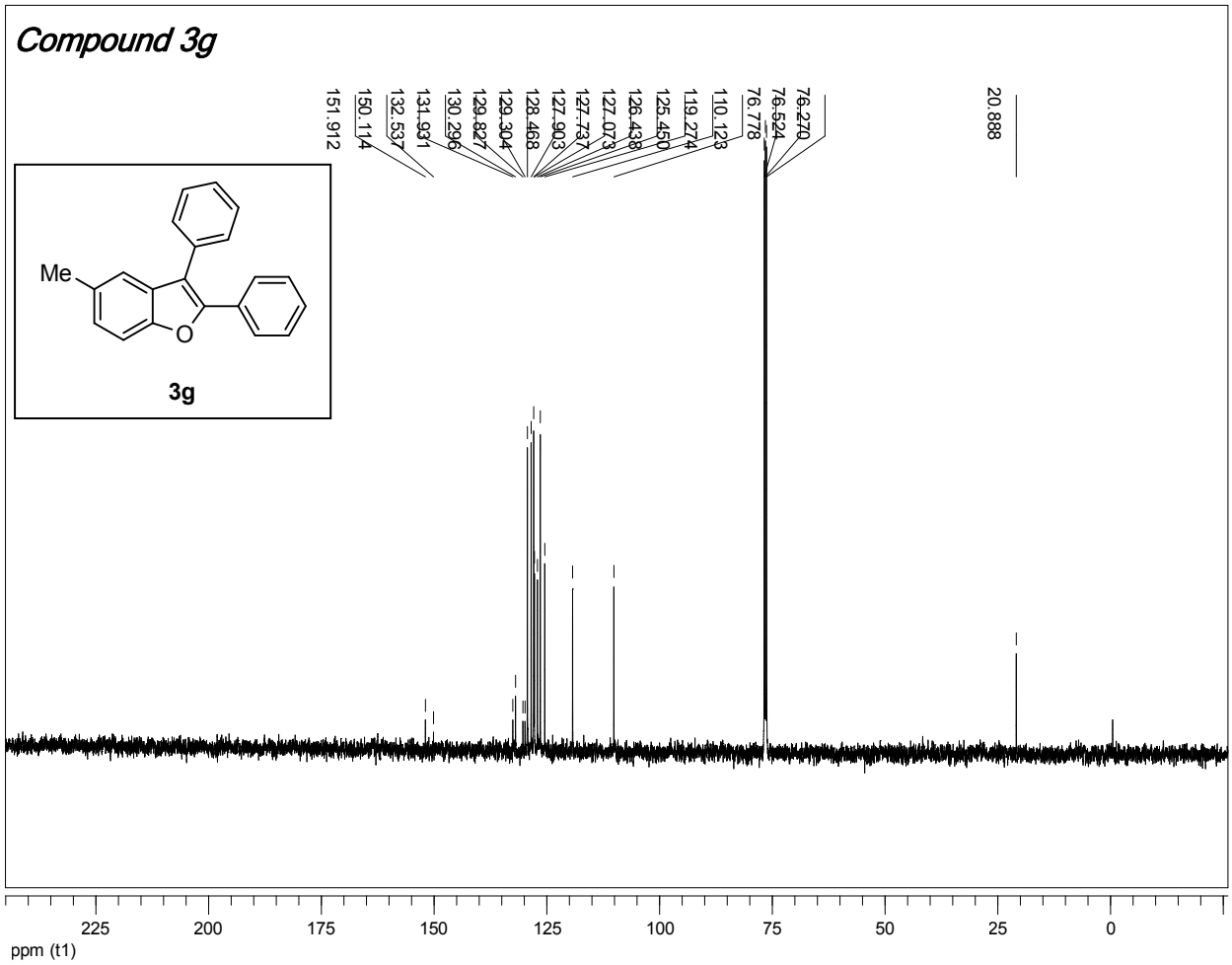

Compound 3f
7.647
7.634
7.512
7.492
7.478
7.429
7.416
7.389
7.372
7.320
7.306
7.294
7.277
7.119
6.905
6.889
3.910
MeO
O
3f
1.75
10.0
7.5
5.0
2.5
0.0
ppm (t1)

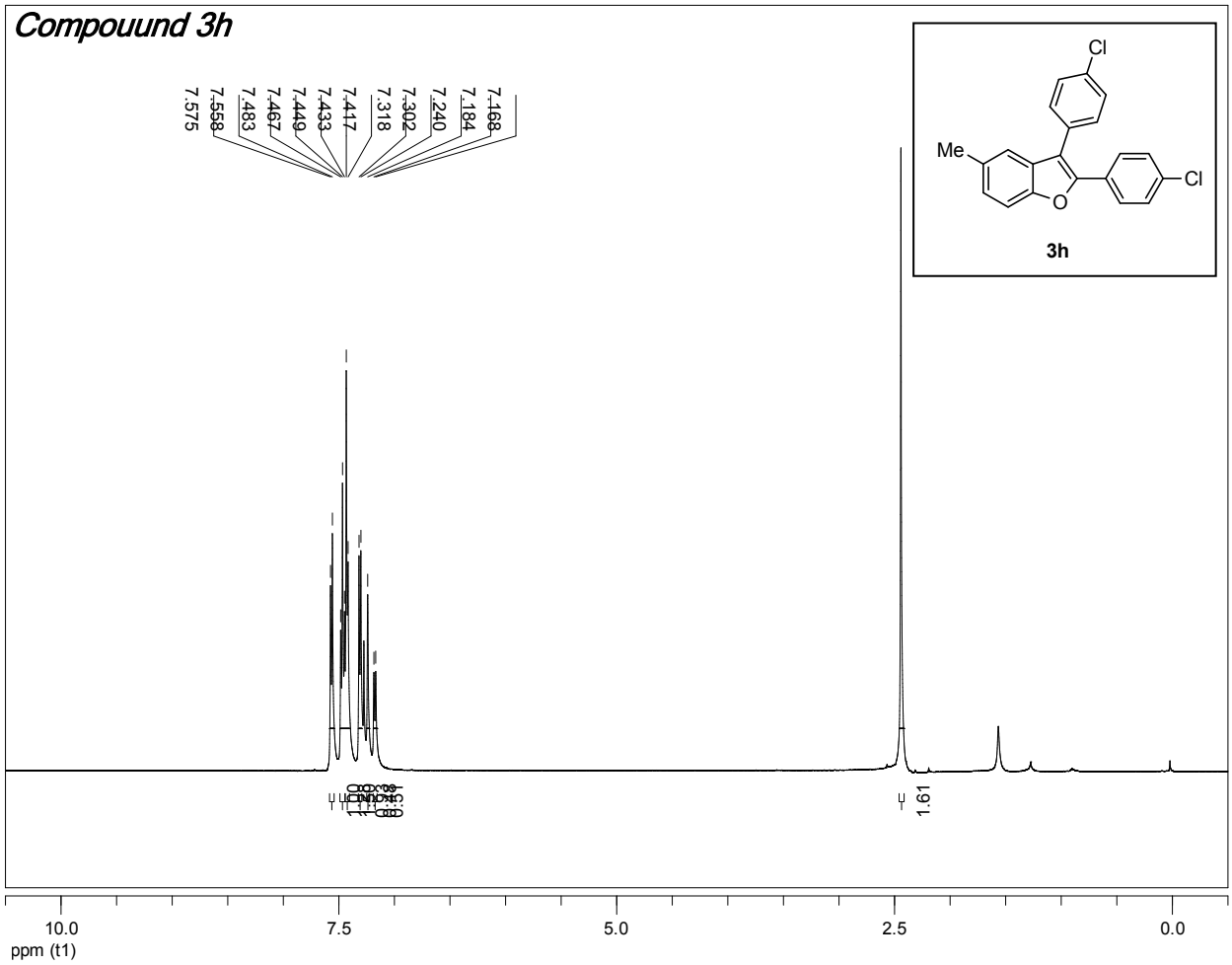

7.647
7.634
7.512
7.492
7.478
7.429
7.416
7.389
7.372
7.320
7.306
7.294
7.277
7.119
6.905
6.889
MeO
O
3f
1.00
2.08
0.53
0.98
1.78
0.44
0.49
7.75
7.50
7.25
7.00
ppm (t1)

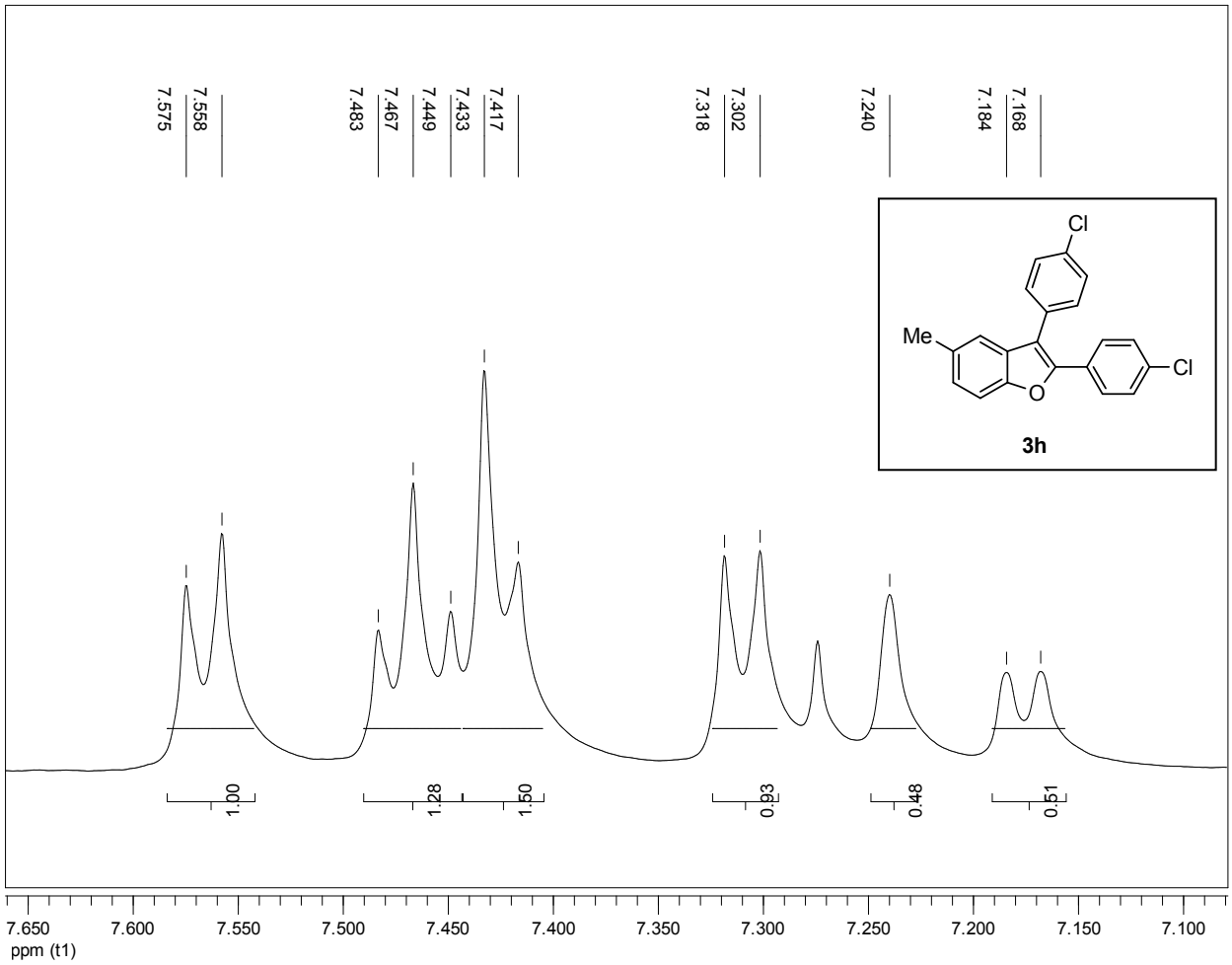

Compound 3f
157.930
154.483
149.125
132.468
130.387
129.197
128.447
127.899
127.430
127.083
126.102
123.230
119.743
116.943
111.436
95.198
76.774
76.521
76.267
55.311
MeO
O
3f
225
200
175
150
125
100
75
50
25
0
ppm (t1)

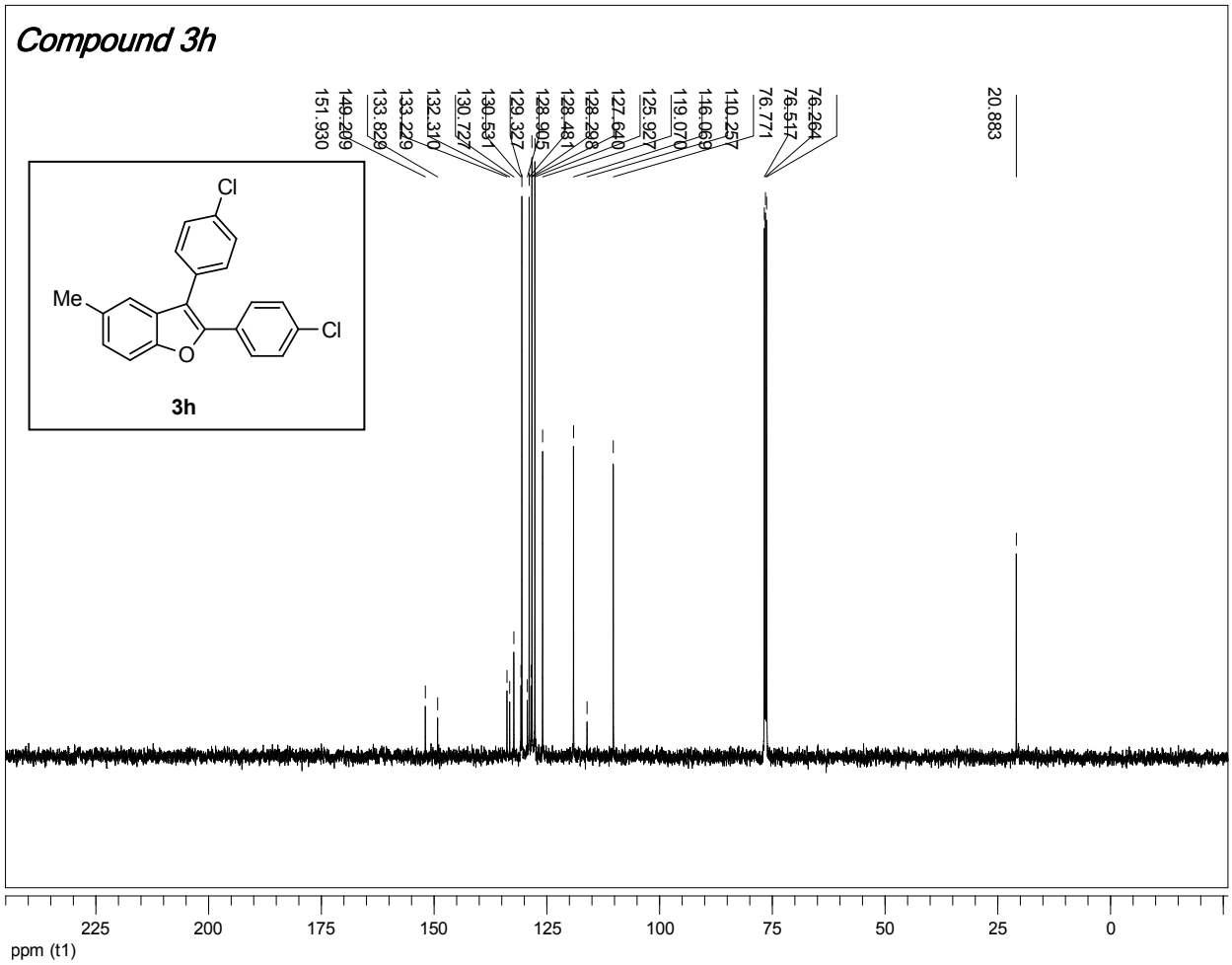

Compound 3g
7.669
7.656
7.509
7.492
7.478
7.462
7.444
7.429
7.326
7.311
7.289
7.275
7.168
7.152
2.440
Me
O
3g
1.00
3.08
2.18
0.52
1.59
10.0
7.5
5.0
2.5
0.0
ppm (t1)

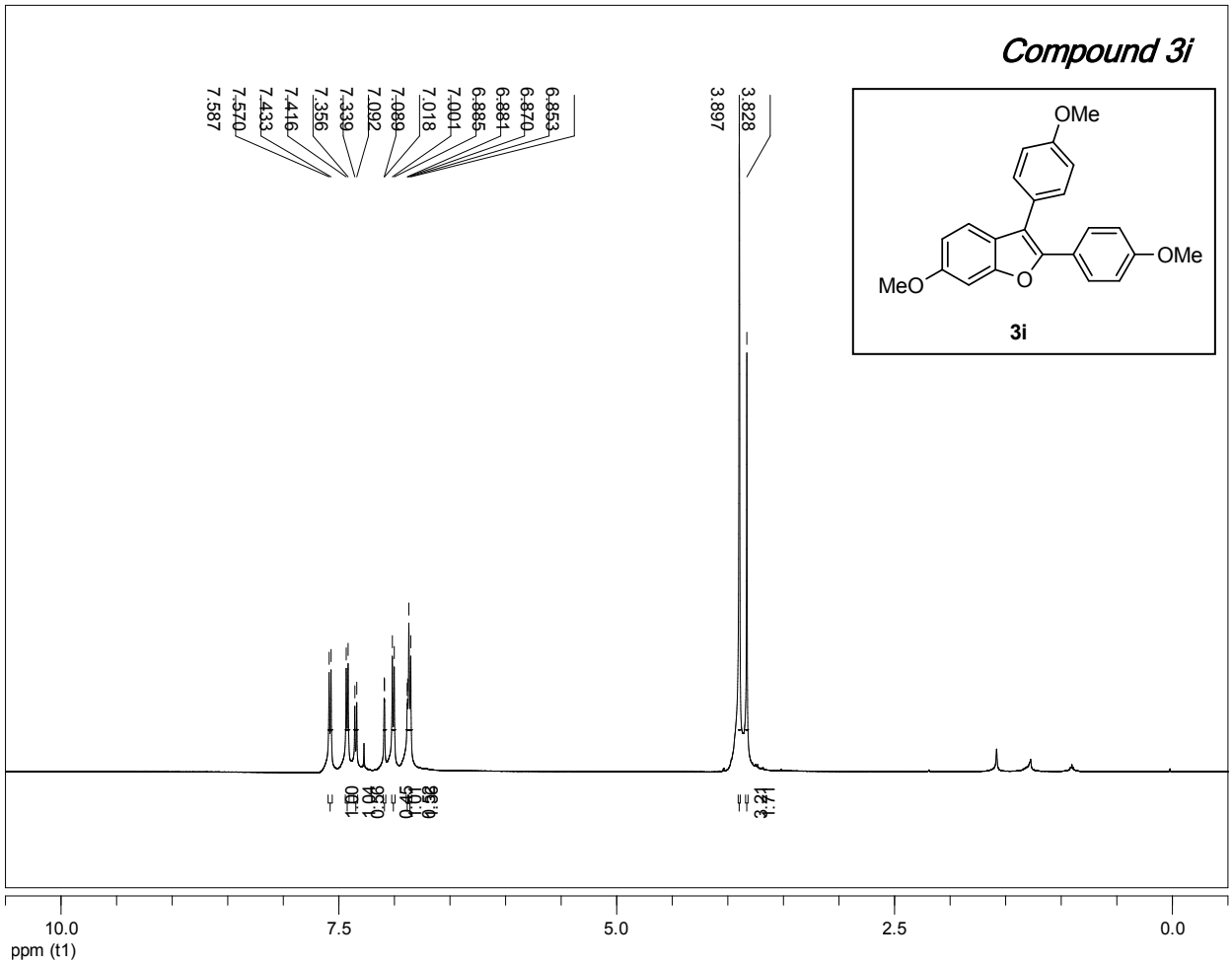

7.669
7.656
7.509
7.492
7.478
7.462
7.444
7.429
7.326
7.311
7.289
7.275
7.168
7.152
Me
O
3g
1.00
3.08
2.18
0.62
7.750
7.700
7.650
7.600
7.550
7.500
7.450
7.400
7.350
7.300
7.250
7.200
7.150
7.100
7.050
ppm (t1)

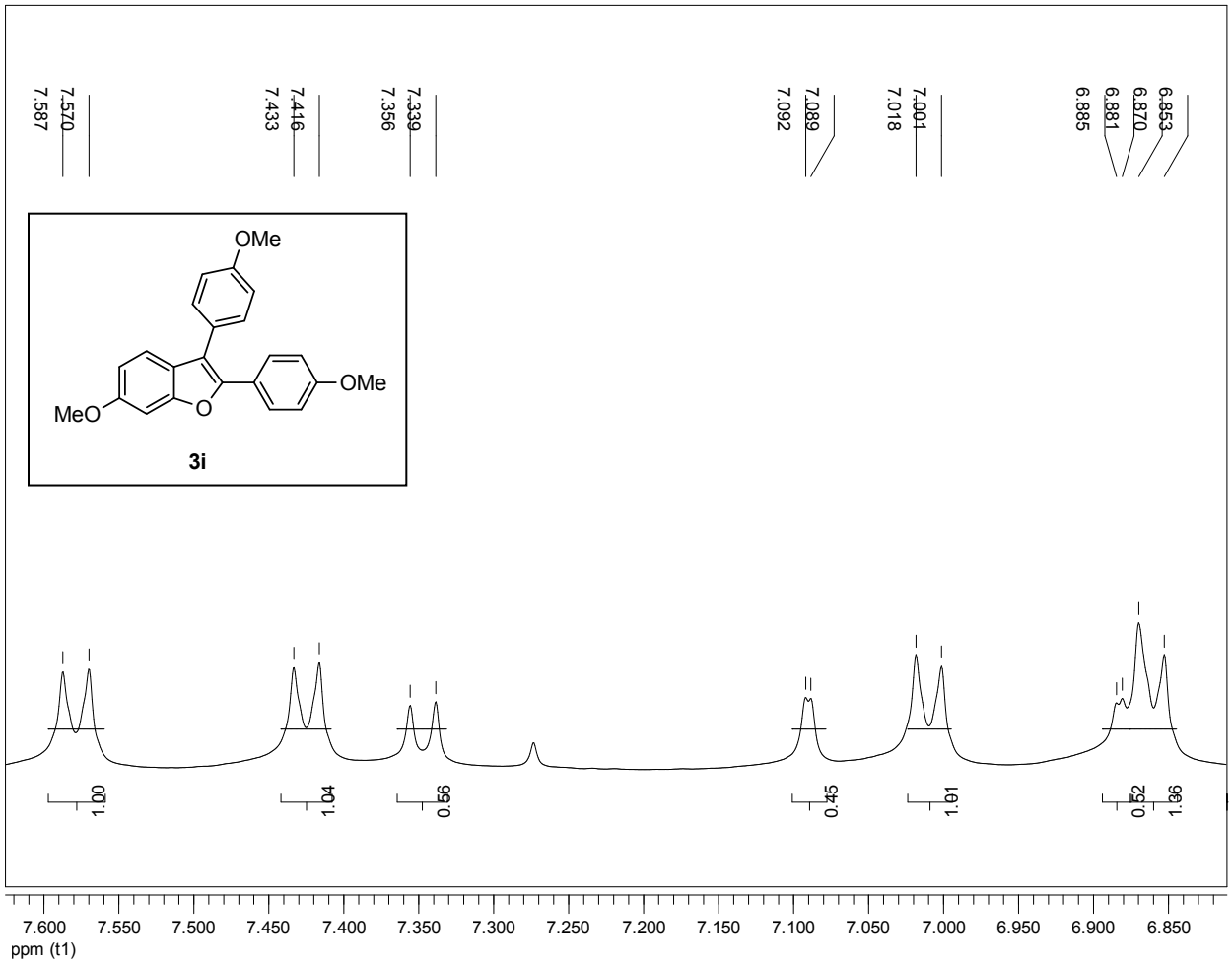

Compound 3g
151.912
150.114
132.537
131.931
130.296
129.827
129.304
128.468
127.903
127.737
127.073
126.438
125.450
119.274
110.123
76.778
76.524
76.270
20.888
Me
O
3g
225
200
175
150
125
100
75
50
25
0
ppm (t1)

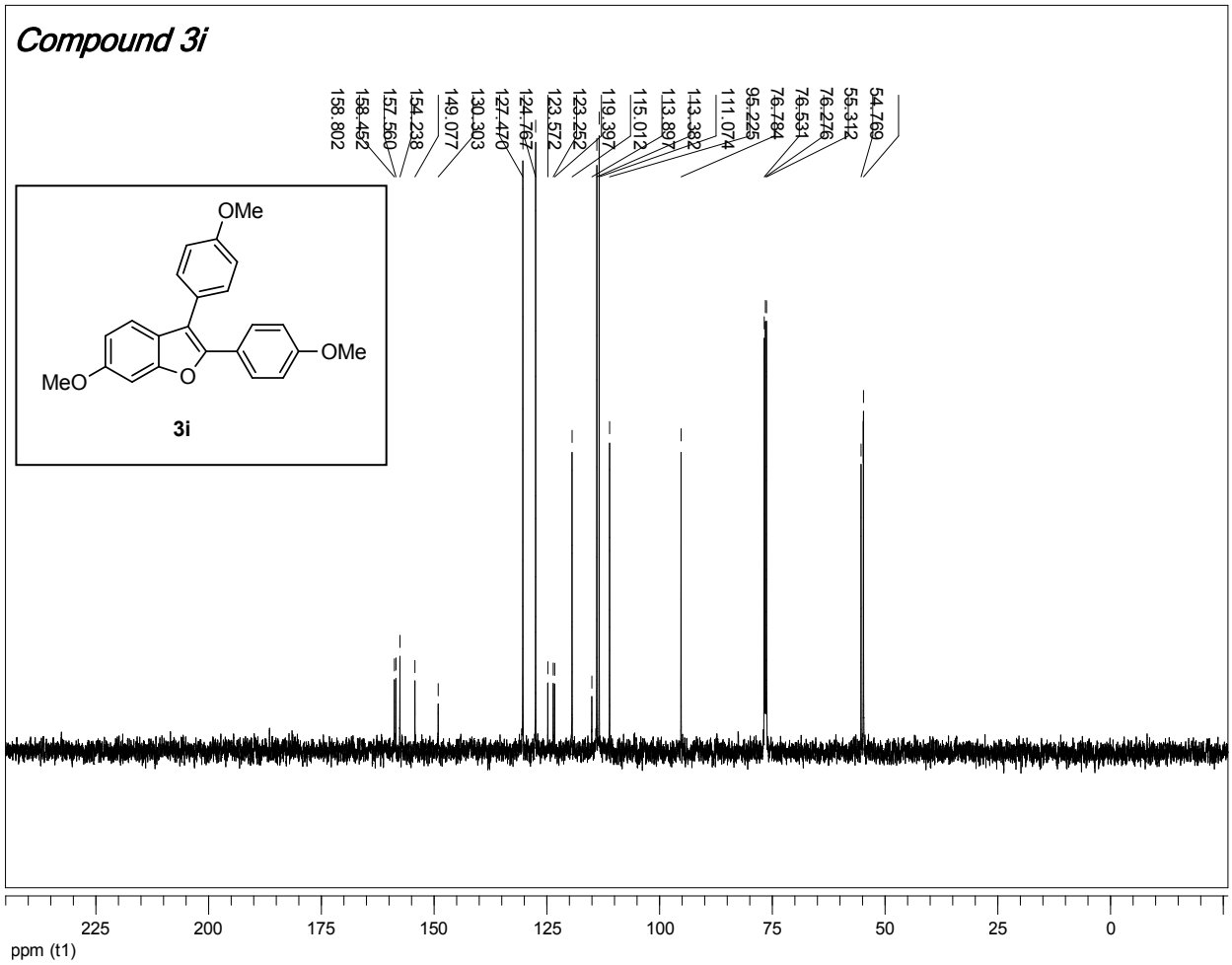

Compouund 3h
7.575
7.558
7.483
7.467
7.449
7.433
7.417
7.318
7.302
7.240
7.184
7.168
Cl
Me
Cl
O
3h
1.61
10.0
7.5
5.0
2.5
0.0
ppm (t1)

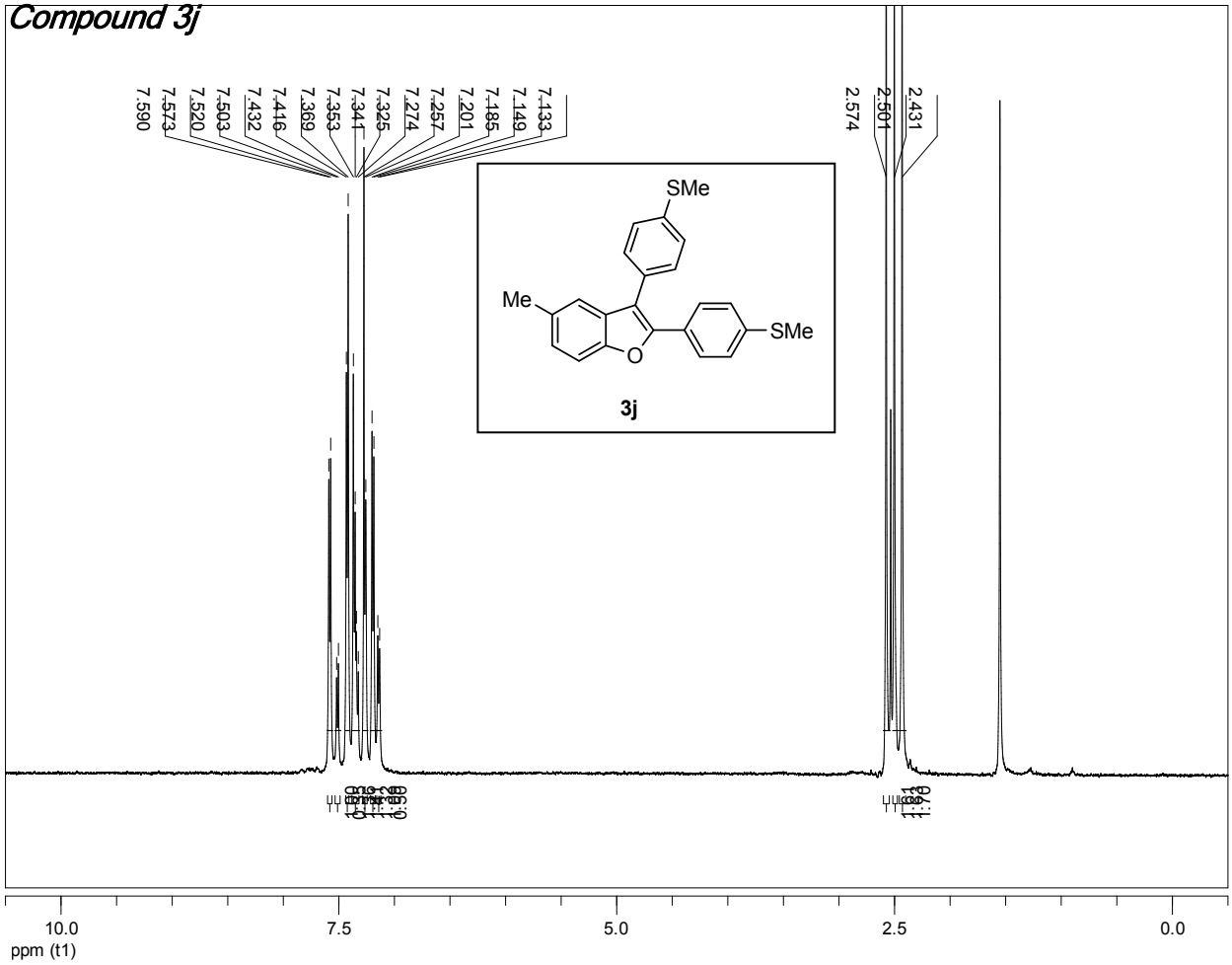

7.575
7.558
7.483
7.467
7.449
7.433
7.417
7.318
7.302
7.240
7.184
7.168
Cl
Me
Cl
O
3h
1.00
1.28
1.90
0.93
0.48
0.51
7.650
7.600
7.550
7.500
7.450
7.400
7.350
7.300
7.250
7.200
7.150
7.100
ppm (t1)

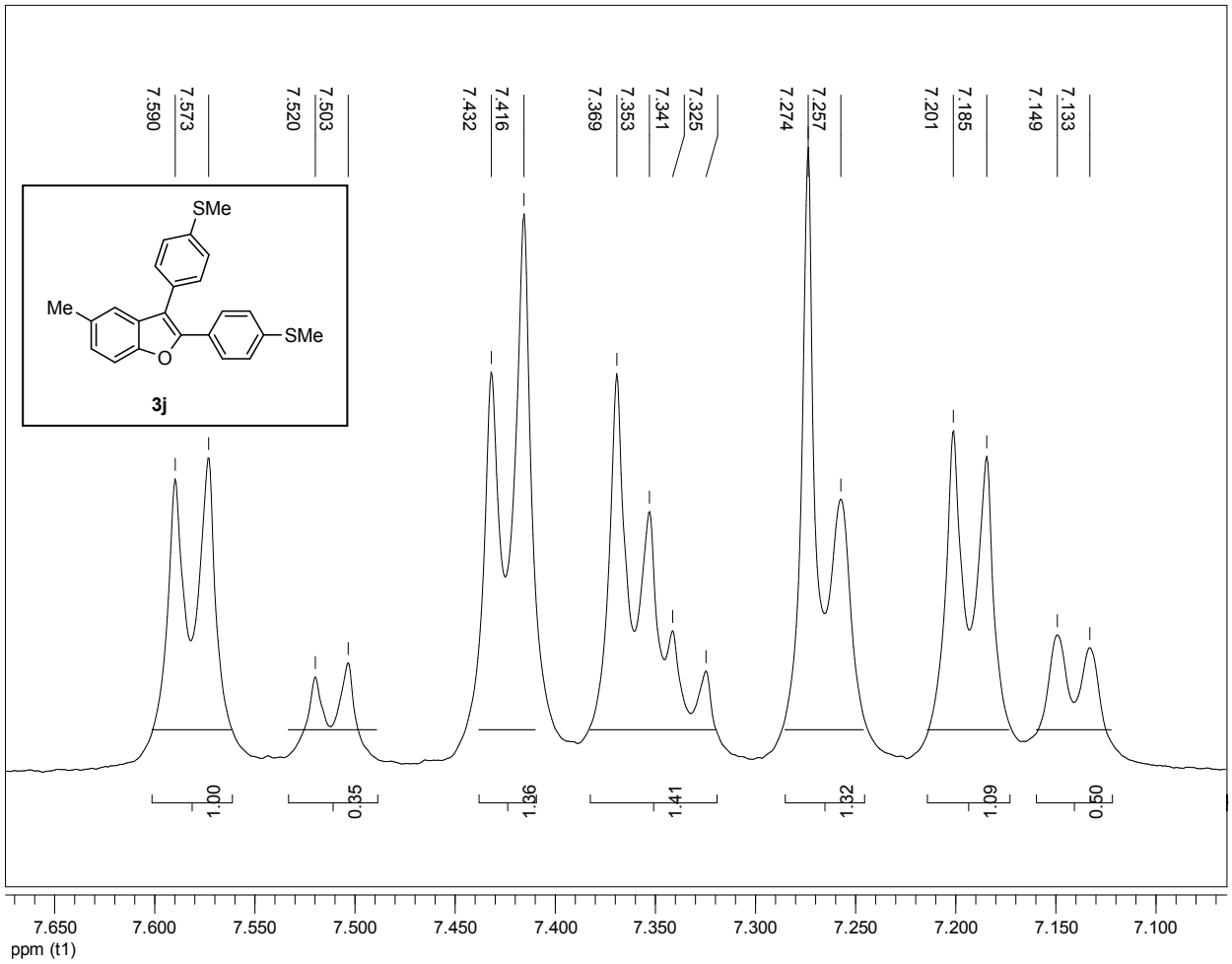

Compound 3h
151.930
149.209
133.829
133.229
132.310
130.727
130.531
129.327
128.905
128.481
128.298
127.640
125.927
119.070
116.069
110.257
76.771
76.517
76.264
20.883
Cl
Me
Cl
O
3h
225
200
175
150
125
100
75
50
25
0
ppm (t1)

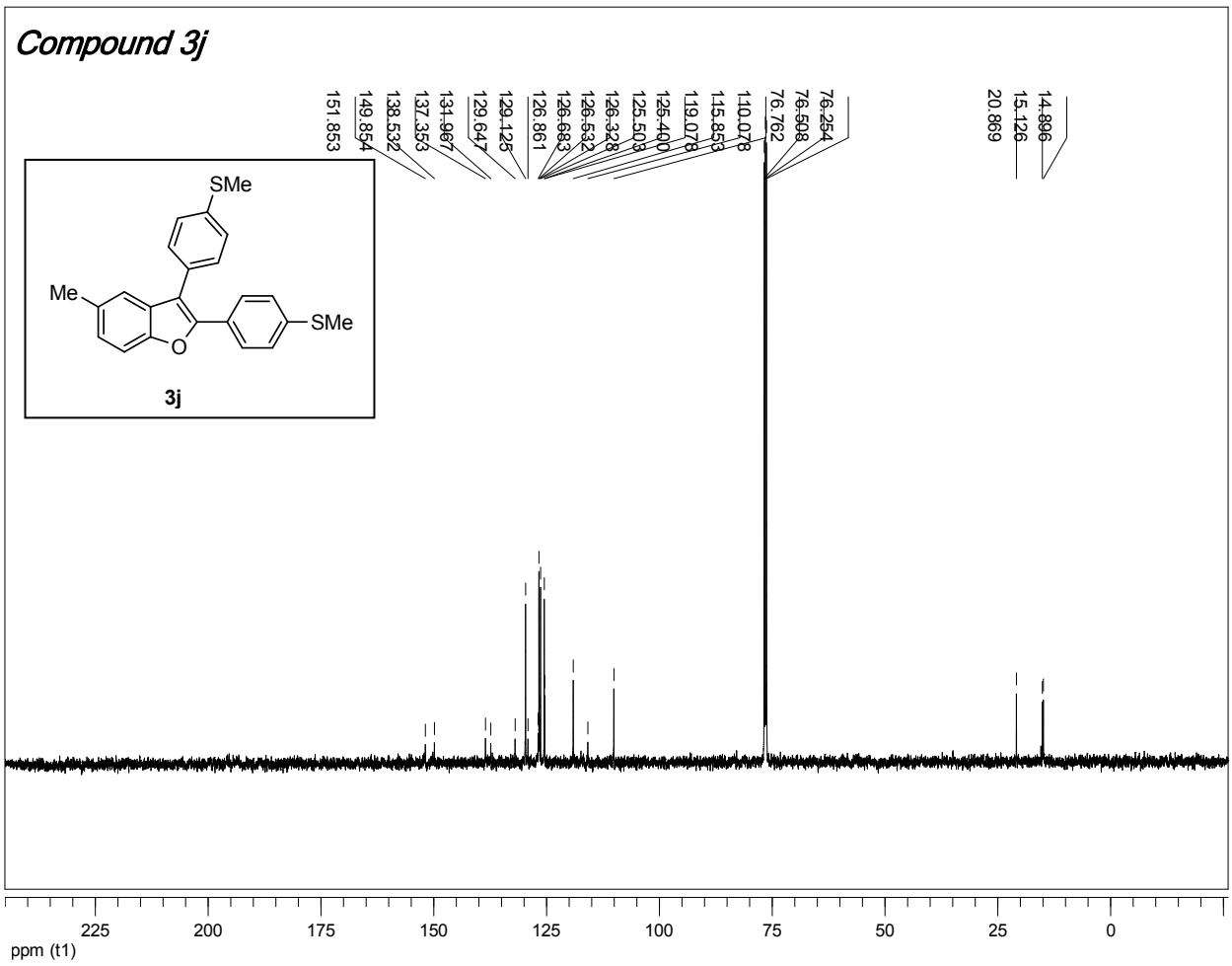

Compound 3i
7.587
7.570
7.433
7.416
7.356
7.339
7.092
7.089
7.018
7.001
6.885
6.881
6.870
6.853
3.897
3.828
OMe
OMe
MeO
O
3i
10.0
7.5
5.0
2.5
0.0
ppm (t1)

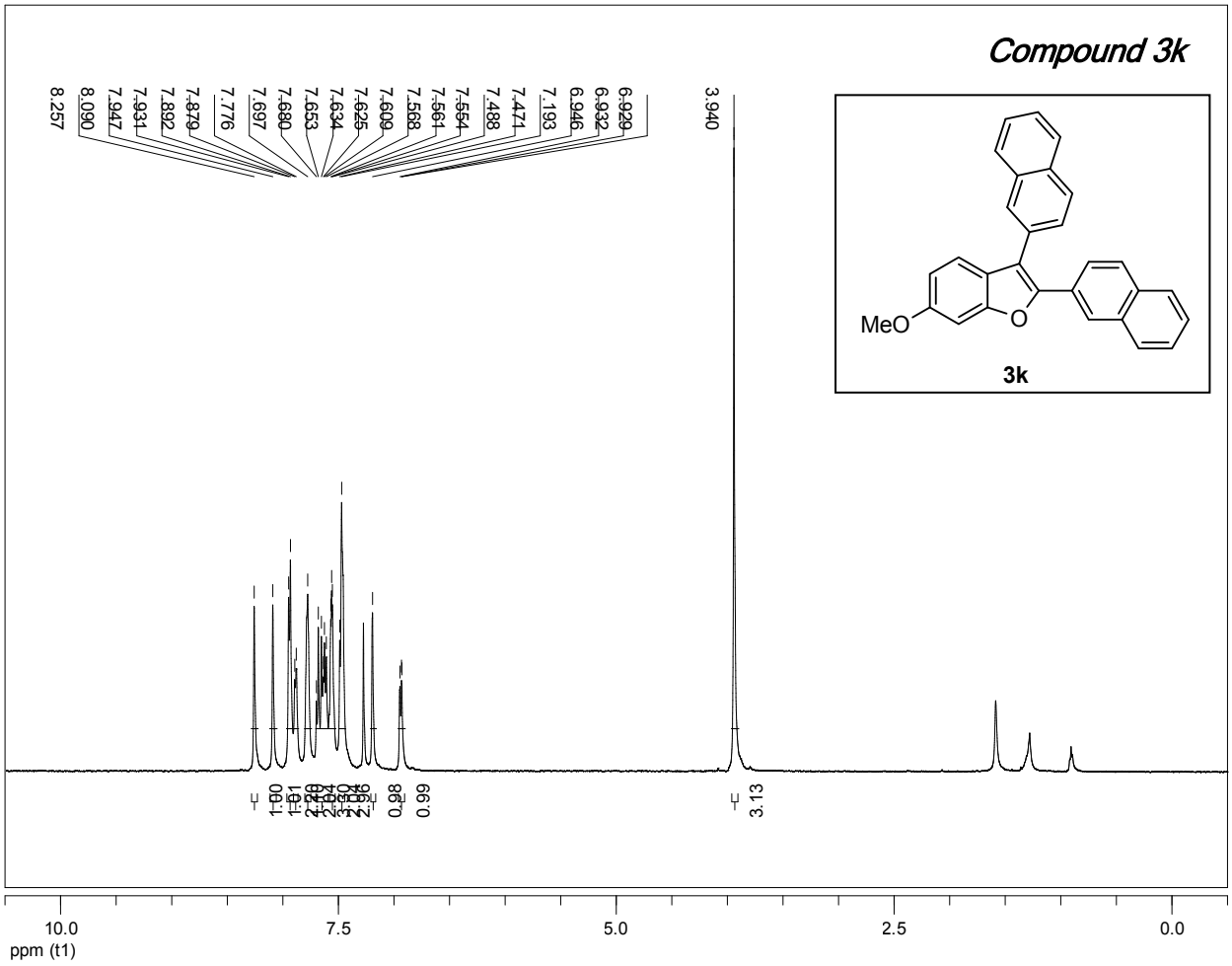

7.587
7.570
7.433
7.416
7.356
7.339
7.092
7.089
7.018
7.001
6.885
6.881
6.870
6.853
OMe
OMe
MeO
O
3i
1.00
1.04
0.56
0.45
1.01
0.52
1.36
7.600
7.550
7.500
7.450
7.400
7.350
7.300
7.250
7.200
7.150
7.100
7.050
7.000
6.950
6.900
6.850
ppm (t1)

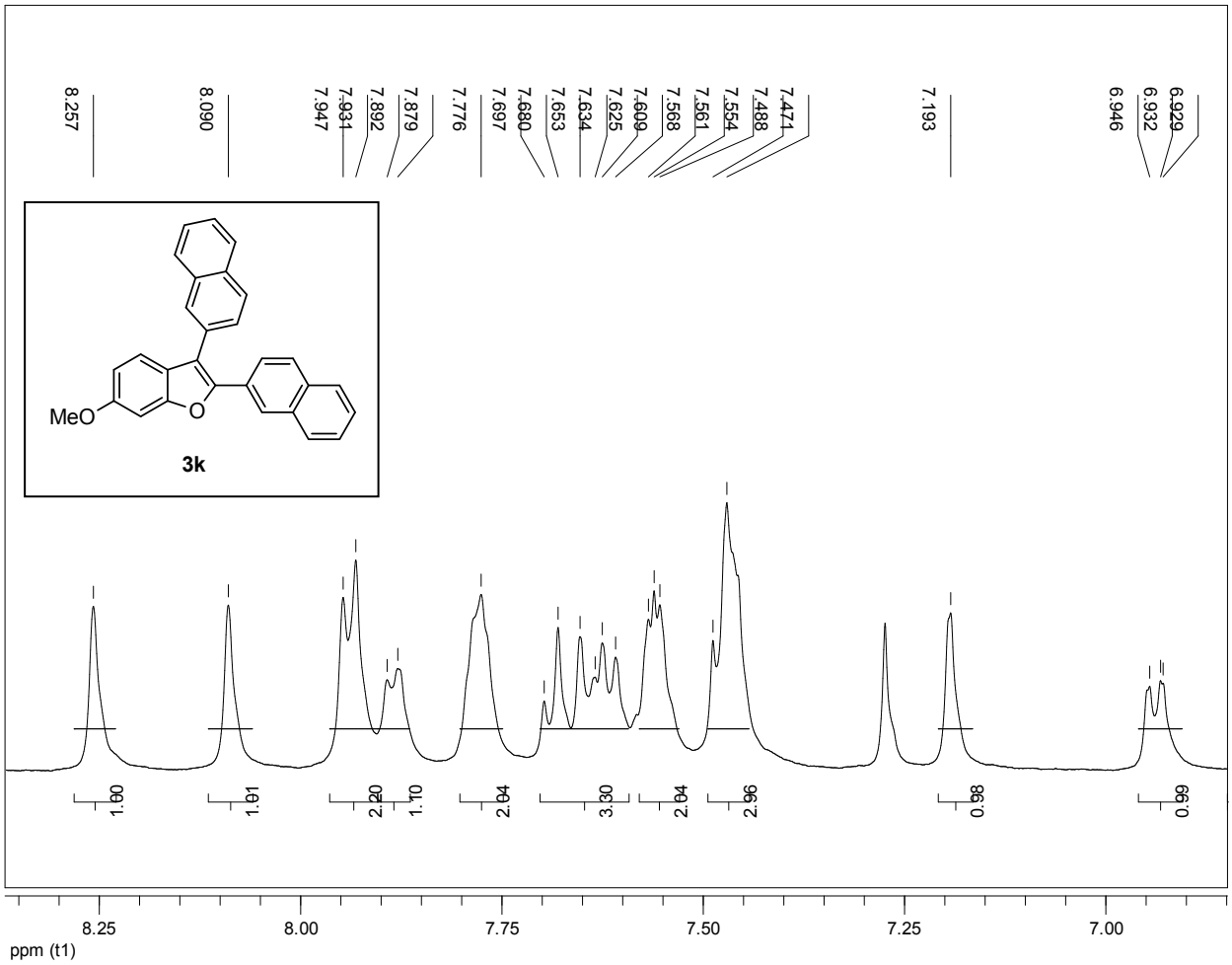

Compound 3i
158.802
158.452
157.560
154.238
149.077
130.303
127.470
124.767
123.572
123.252
119.397
115.012
113.897
113.382
111.074
95.225
76.784
76.531
76.276
55.312
54.769
OMe
MeO
O
OMe
3i
225
200
175
150
125
100
75
50
25
0
ppm (t1)

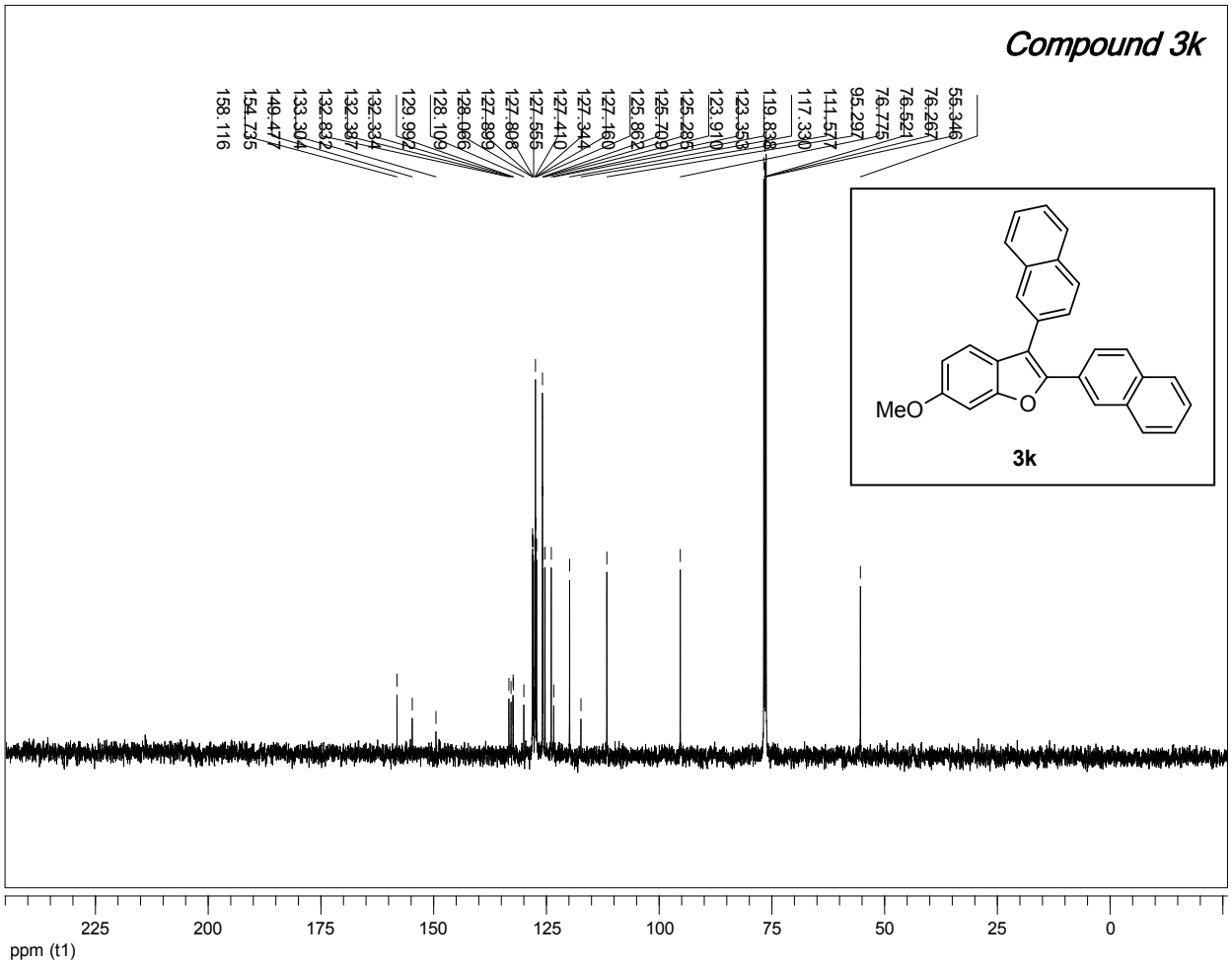

Compound 3j
7.590
7.573
7.520
7.503
7.432
7.416
7.369
7.353
7.341
7.325
7.274
7.257
7.201
7.185
7.149
7.133
2.574
2.501
2.431
SMe
Me
SMe
O
3j
10.0
7.5
5.0
2.5
0.0
ppm (t1)

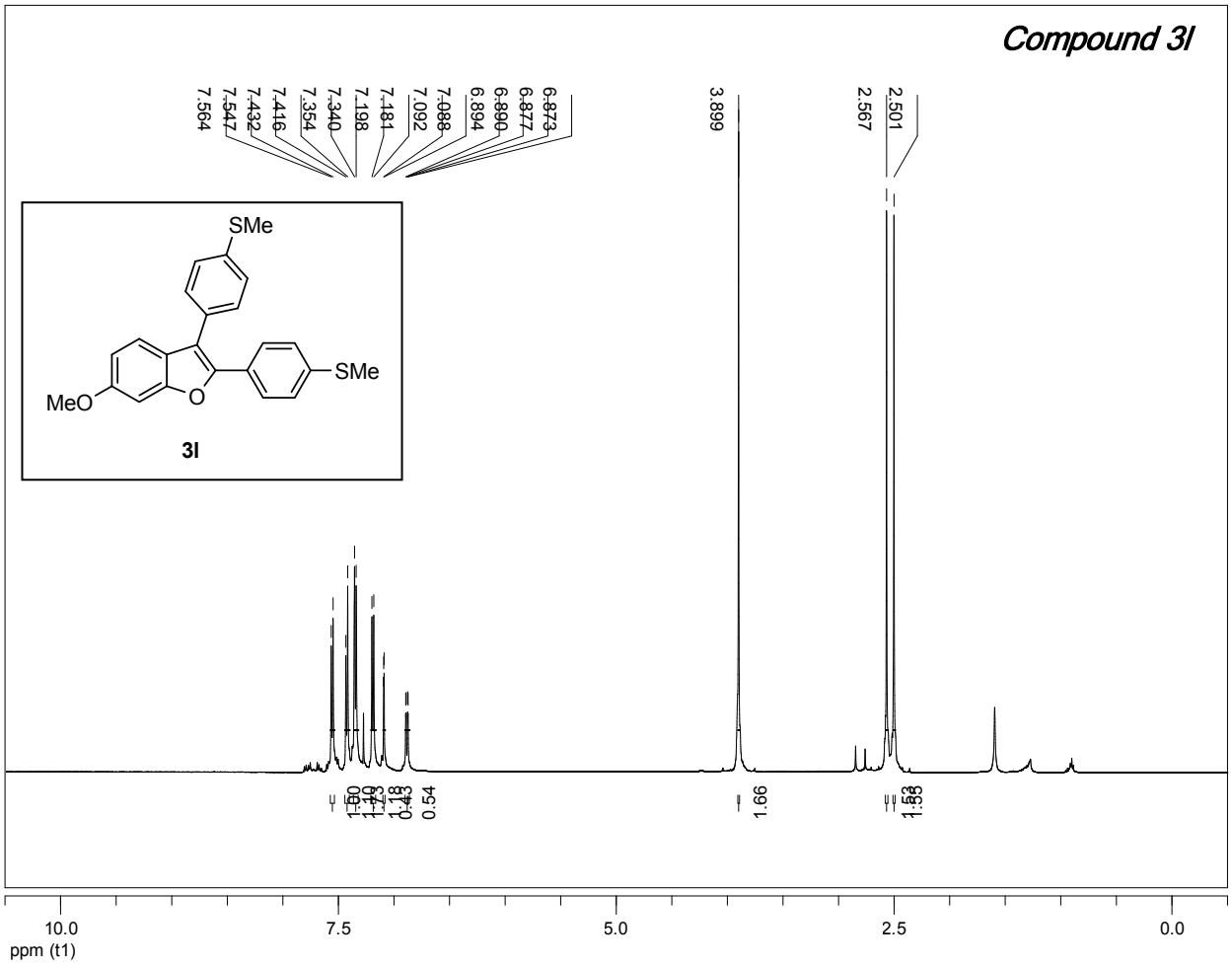

7.590
7.573
7.520
7.503
7.432
7.416
7.369
7.353
7.341
7.325
7.274
7.257
7.201
7.185
7.149
7.133
SMe
Me
SMe
O
3j
1.00
0.35
1.36
1.41
1.32
1.09
0.50
7.650
7.600
7.550
7.500
7.450
7.400
7.350
7.300
7.250
7.200
7.150
7.100
ppm (t1)

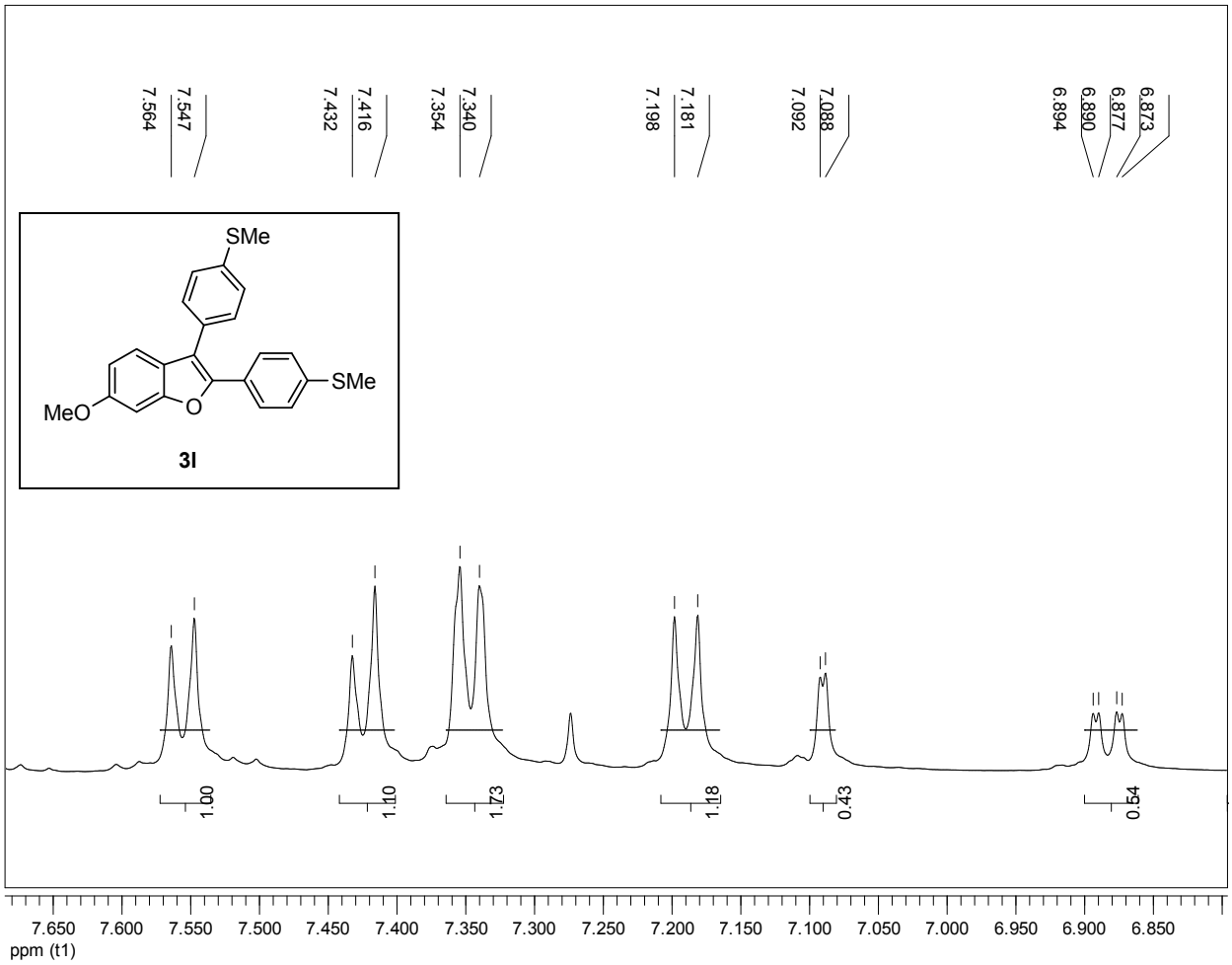

Compound 3j
151.853
149.854
138.532
137.353
131.967
129.647
129.125
126.861
126.683
126.532
126.328
125.503
125.400
119.078
115.853
110.078
76.762
76.508
76.254
20.869
15.126
14.896
SMe
Me
SMe
O
3j
225
200
175
150
125
100
75
50
25
0
ppm (t1)

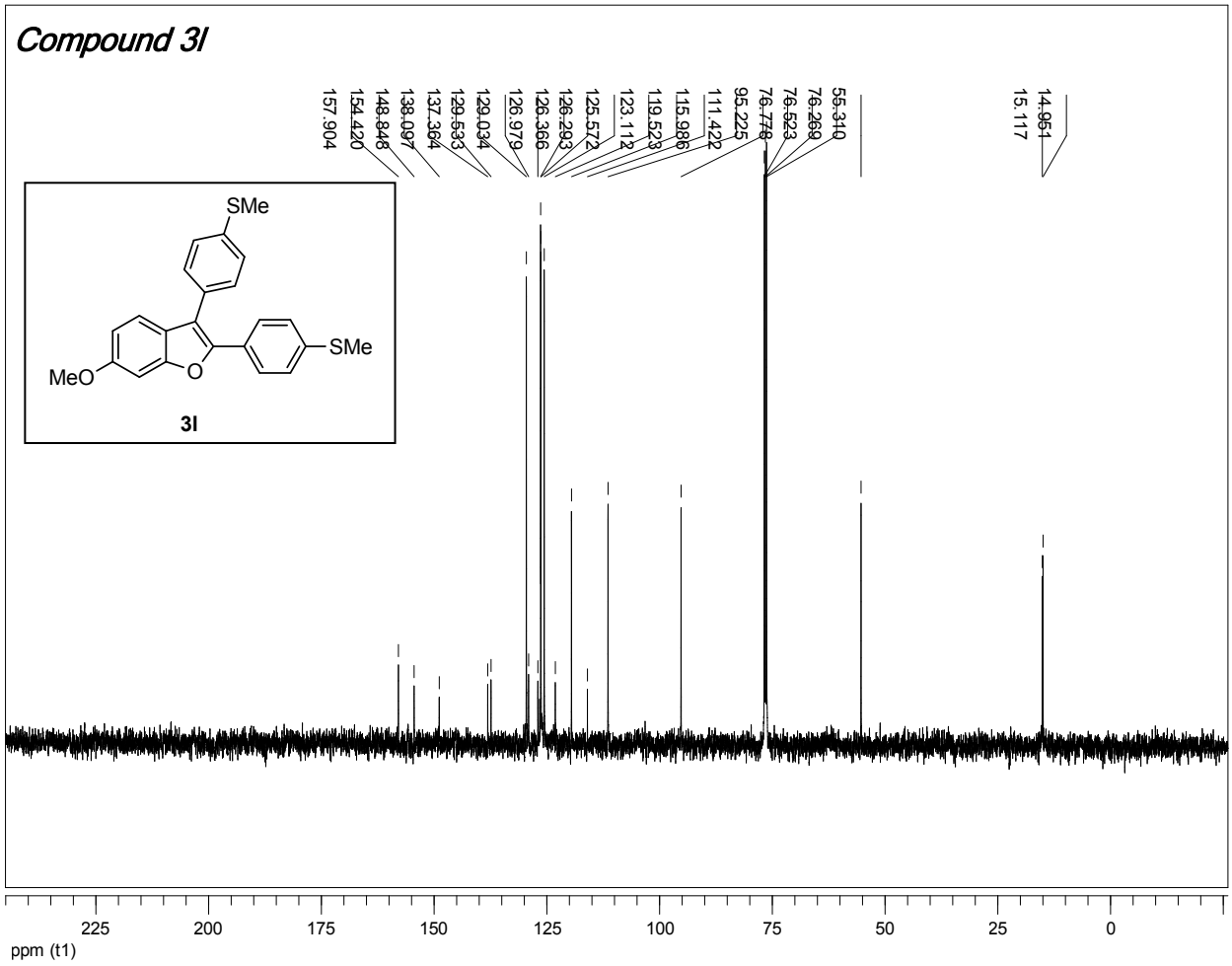

Compound 3k
8.257
8.090
7.947
7.931
7.892
7.879
7.776
7.697
7.680
7.653
7.634
7.625
7.609
7.568
7.561
7.554
7.488
7.471
7.193
6.946
6.932
6.929
3.940
MeO
O
3k
1.00
1.01
1.01
2.04
2.04
3.30
2.06
0.98
0.99
3.13
10.0
7.5
5.0
2.5
0.0
ppm (t1)

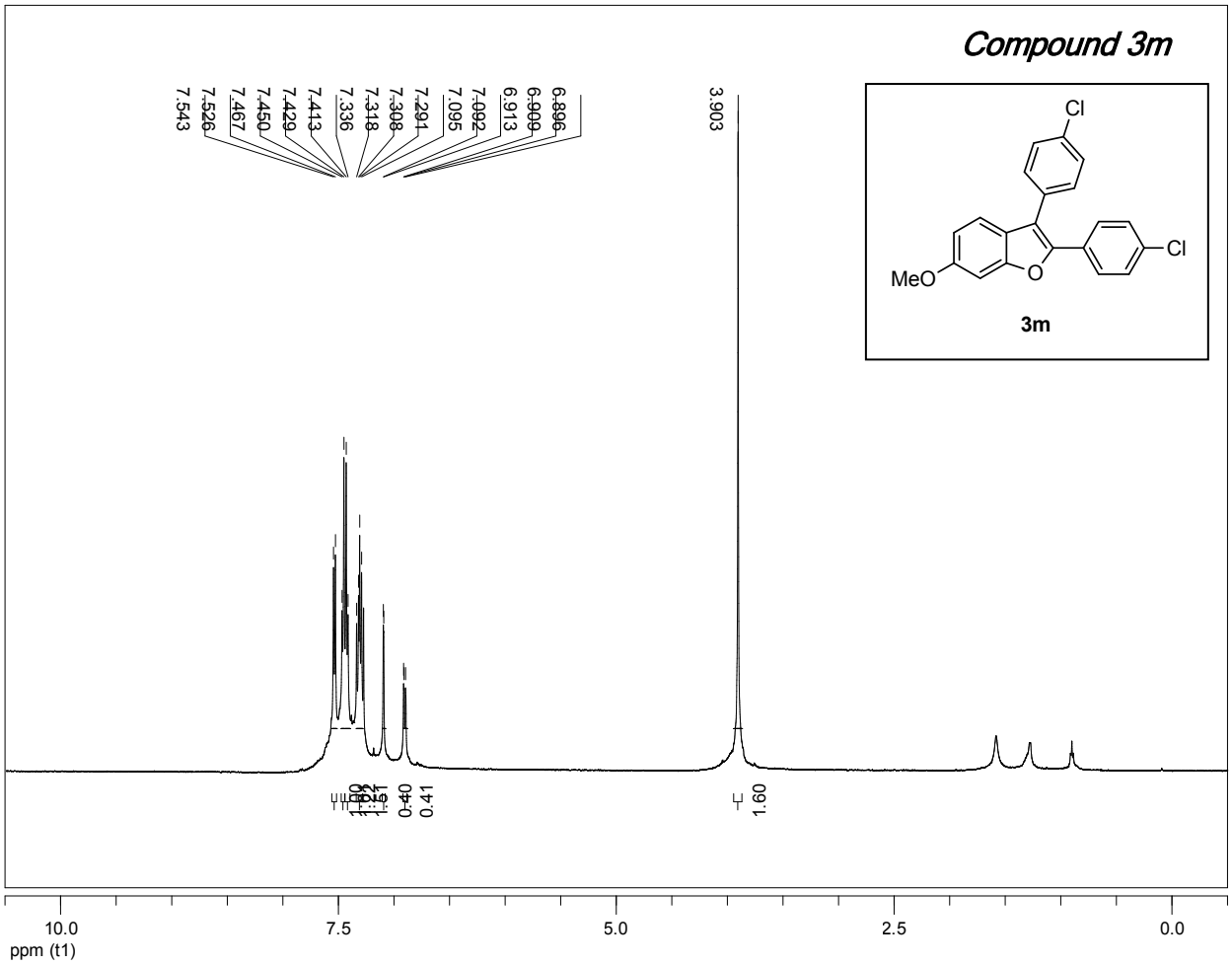

8.257
8.090
7.947
7.931
7.892
7.879
7.776
7.697
7.680
7.653
7.634
7.625
7.609
7.568
7.561
7.554
7.488
7.471
7.193
6.946
6.932
6.929
MeO
O
3k
1.00
1.01
2.20
1.10
2.04
3.30
2.04
2.96
0.98
0.99
8.25
8.00
7.75
7.50
7.25
7.00
ppm (t1)

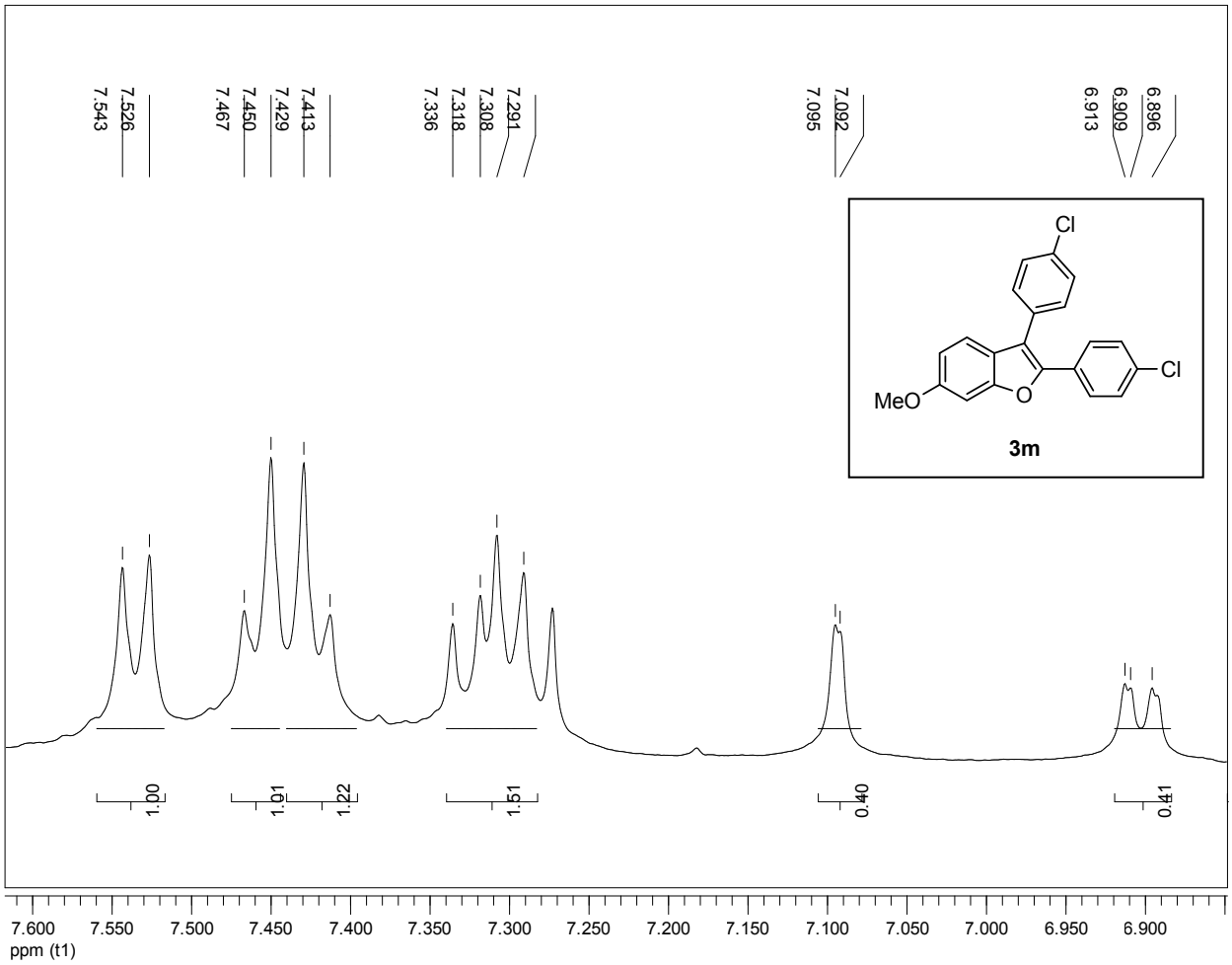

Compound 3k
158.116
154.735
149.477
133.304
132.832
132.387
132.334
129.992
128.109
128.066
127.899
127.808
127.555
127.410
127.344
127.160
125.862
125.709
125.285
123.910
123.353
119.838
117.330
111.577
95.297
76.775
76.521
76.267
55.346
MeO
O
3k
225
200
175
150
125
100
75
50
25
0
ppm (t1)

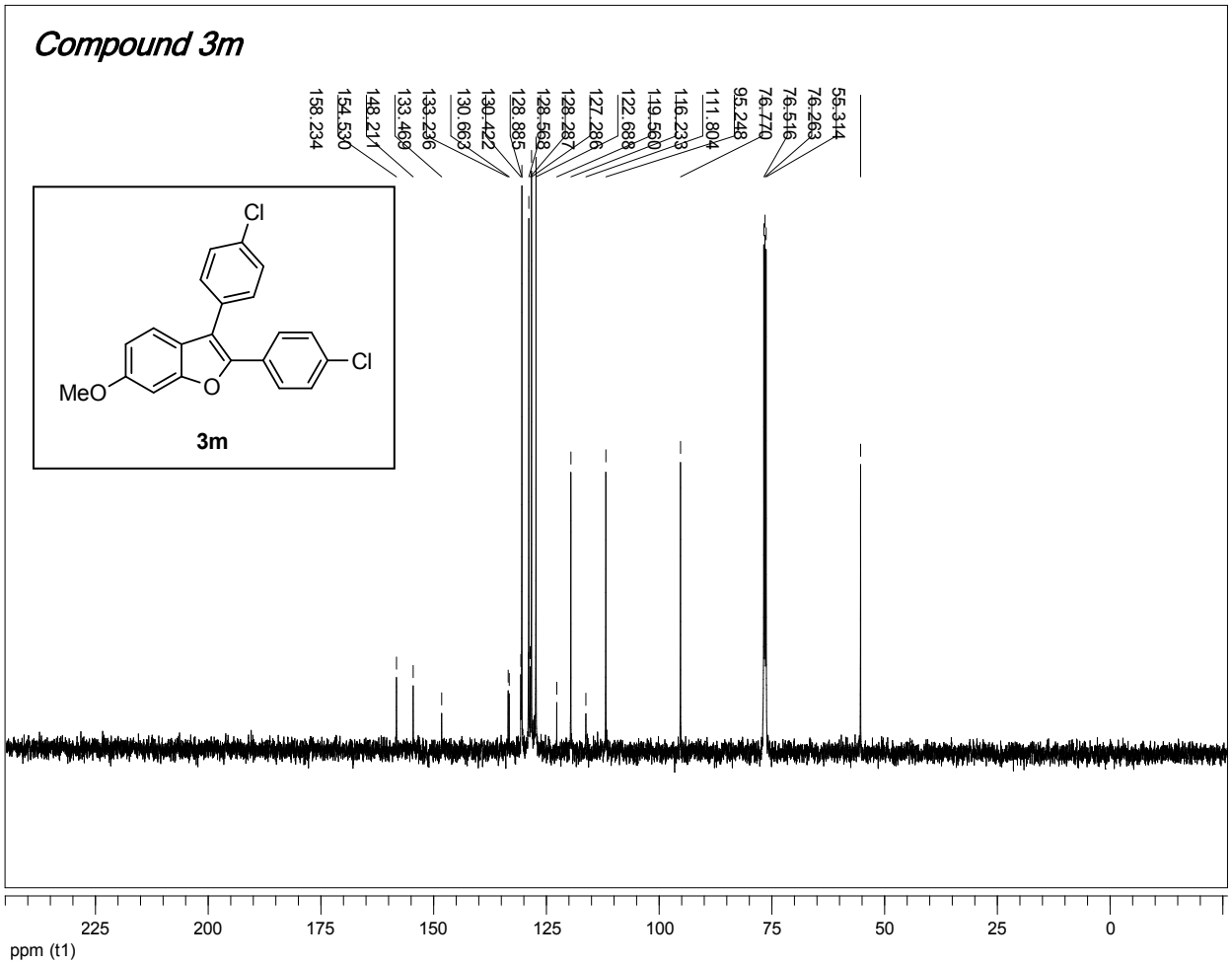

Compound 3l
7.564
7.547
7.432
7.416
7.354
7.340
7.198
7.181
7.092
7.088
6.894
6.890
6.877
6.873
3.899
2.567
2.501
SMe
SMe
MeO
O
3l
1.50
1.40
1.23
1.18
0.43
0.54
1.66
1.53
10.0
7.5
5.0
2.5
0.0
ppm (t1)

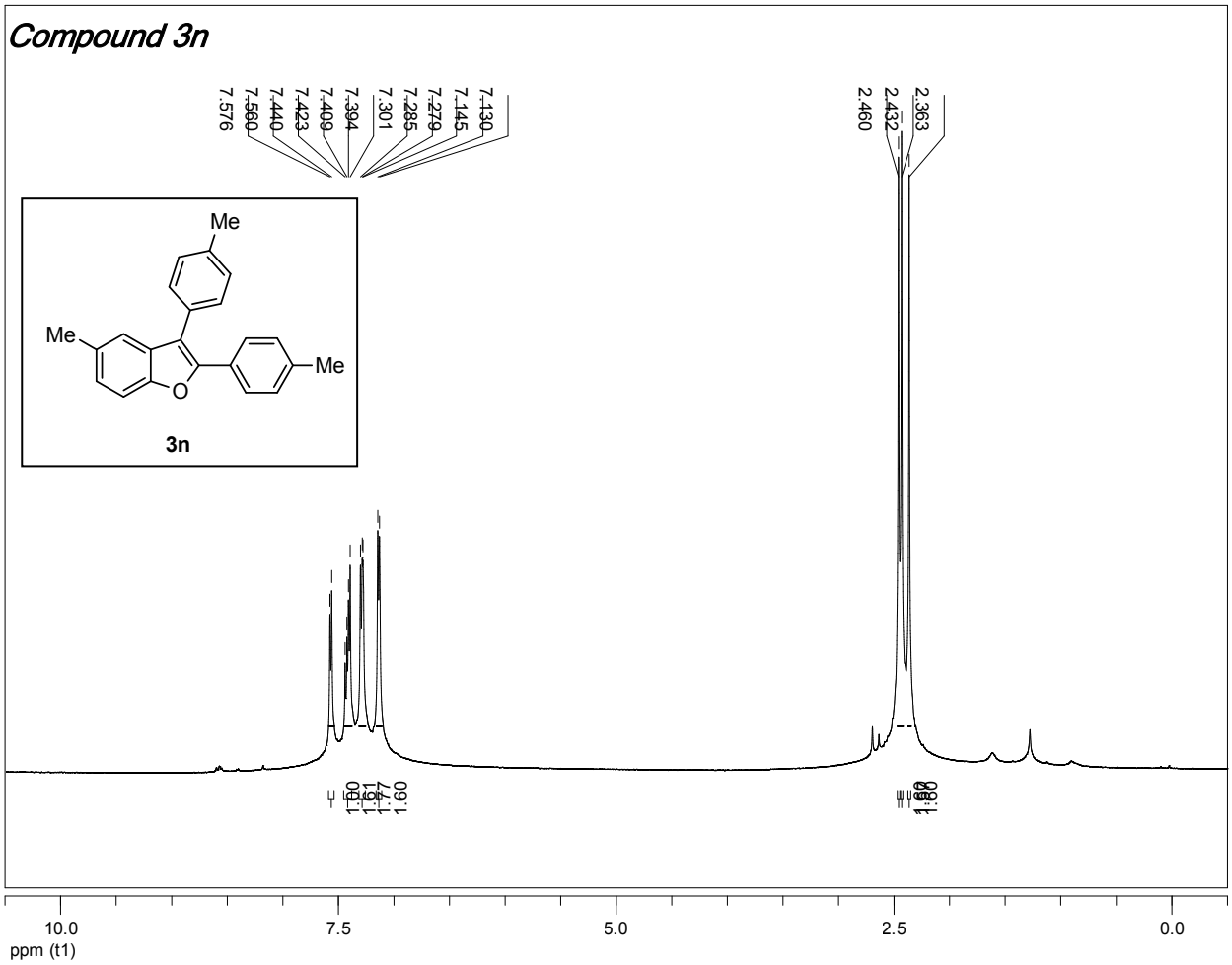

7.564
7.547
7.432
7.416
7.354
7.340
7.198
7.181
7.092
7.088
6.894
6.890
6.877
6.873
SMe
SMe
MeO
O
3l
1.00
1.10
1.73
1.18
0.43
0.54
7.650 7.600 7.550 7.500 7.450 7.400 7.350 7.300 7.250 7.200 7.150 7.100 7.050 7.000 6.950 6.900 6.850
ppm (t1)

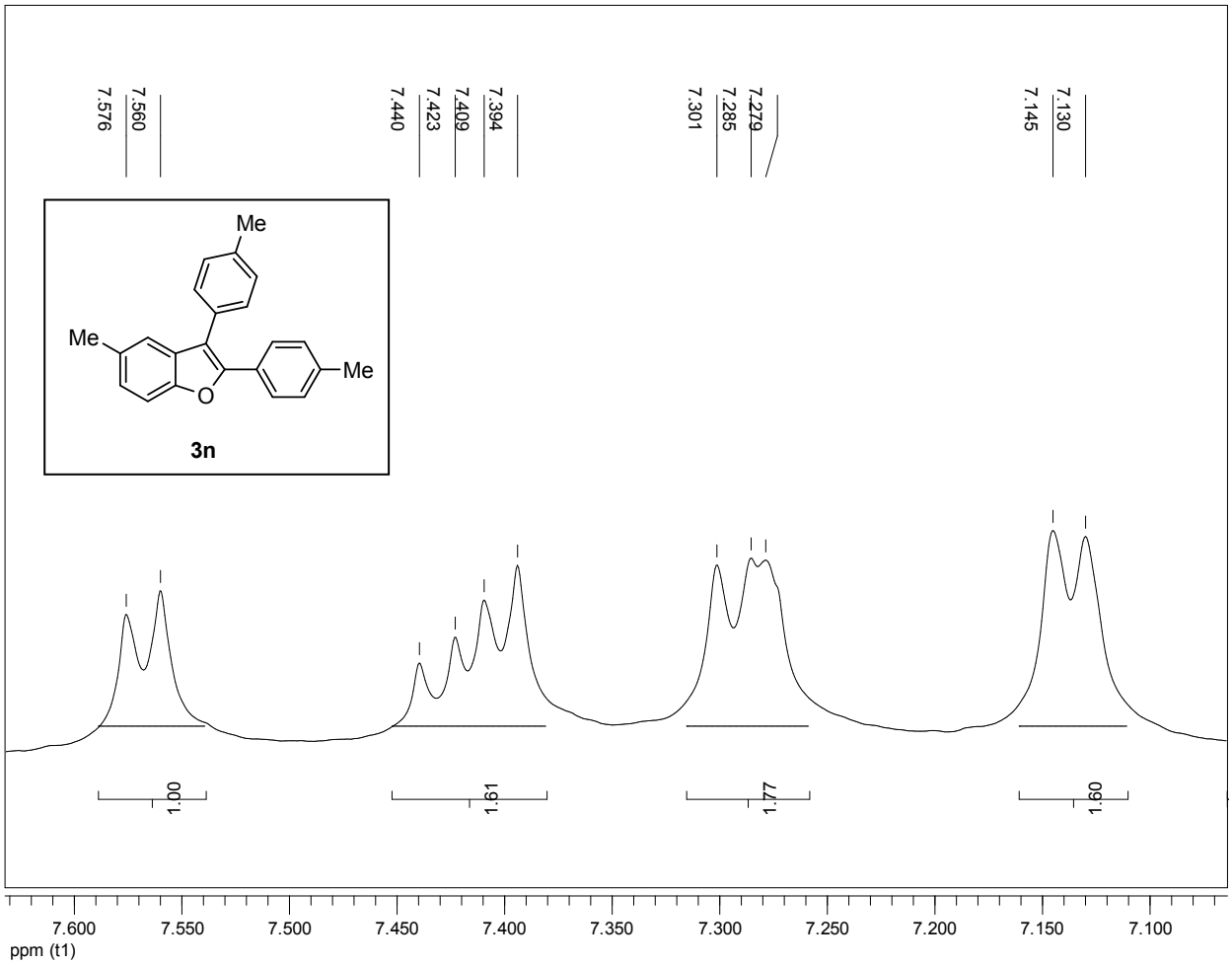

Compound 3l
157.904
154.420
148.848
138.097
137.364
129.533
129.034
126.979
126.366
126.293
125.572
123.112
119.523
115.986
111.422
95.225
76.778
76.523
76.269
55.310
15.117
14.951
SMe
SMe
MeO
O
3l
225
200
175
150
125
100
75
50
25
0
ppm (t1)

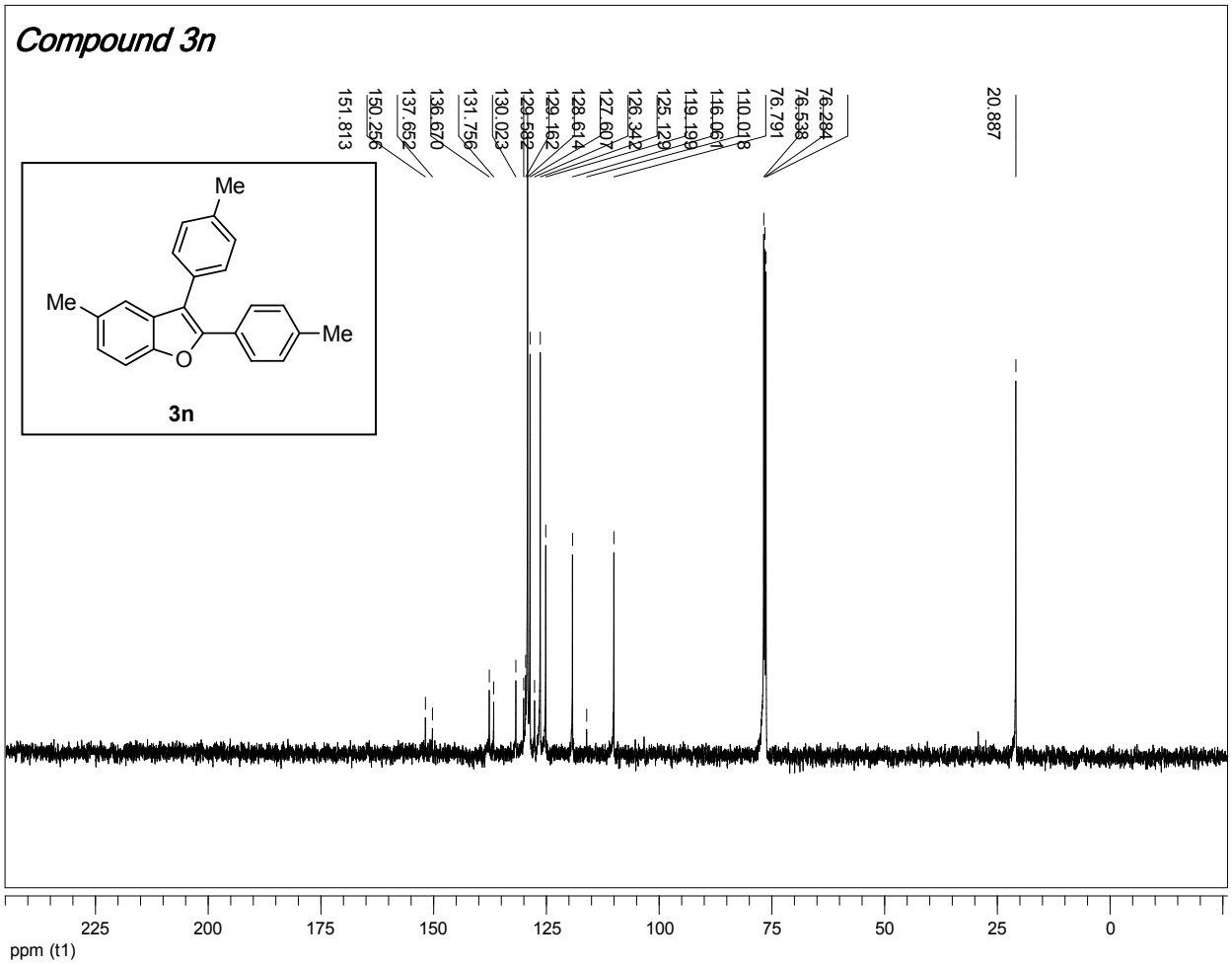

Compound 3m
7.543
7.526
7.467
7.450
7.429
7.413
7.336
7.318
7.308
7.291
7.095
7.092
6.913
6.909
6.896
3.903
Cl
Cl
MeO
O
3m
0.40
0.41
1.60
10.0
7.5
5.0
2.5
0.0
ppm (t1)

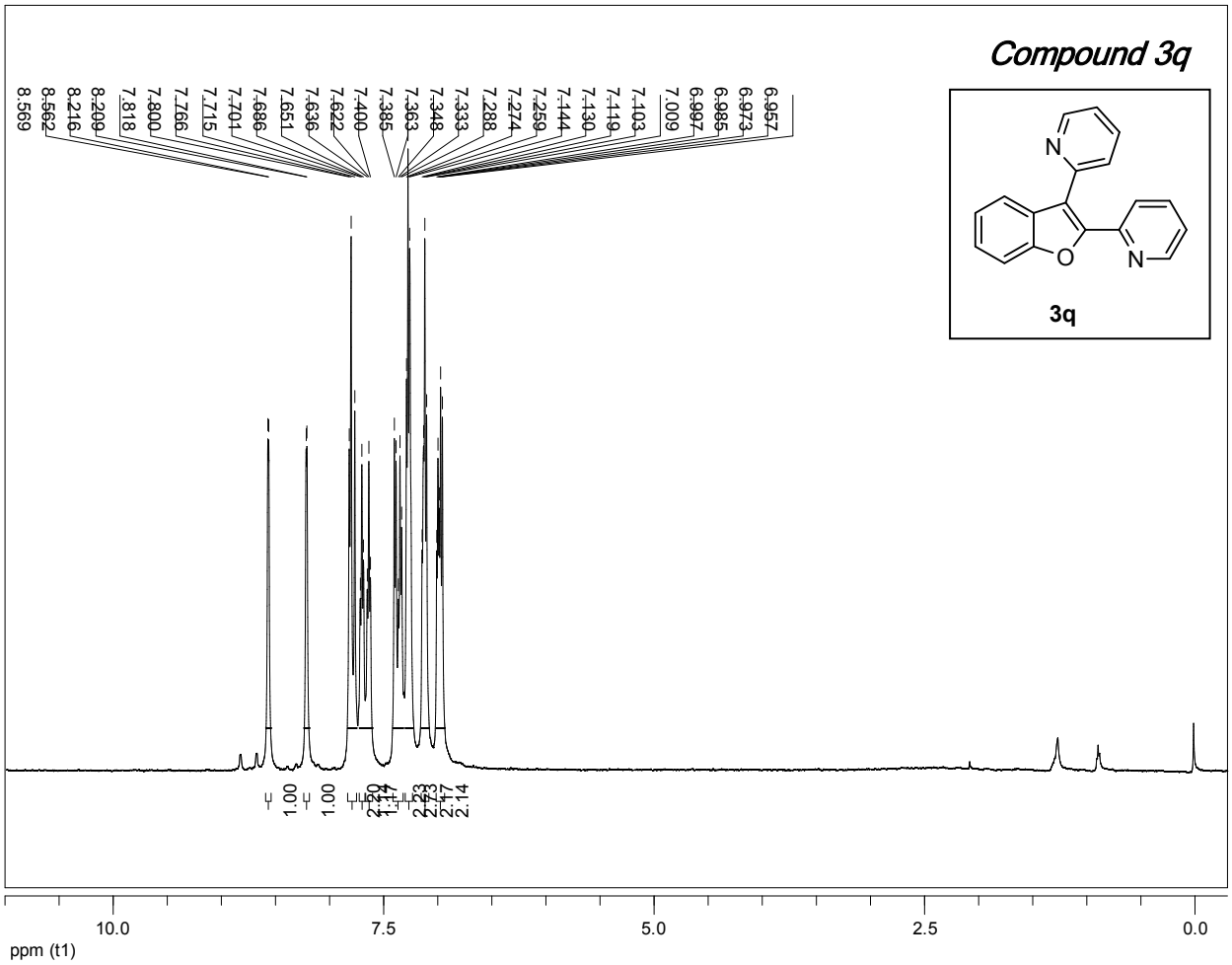

7.543
7.526
7.467
7.450
7.429
7.413
7.336
7.318
7.308
7.291
7.095
7.092
6.913
6.909
6.896
Cl
Cl
MeO
O
3m
1.00
1.01
1.22
1.51
0.40
0.41
7.600
7.550
7.500
7.450
7.400
7.350
7.300
7.250
7.200
7.150
7.100
7.050
7.000
6.950
6.900
ppm (t1)

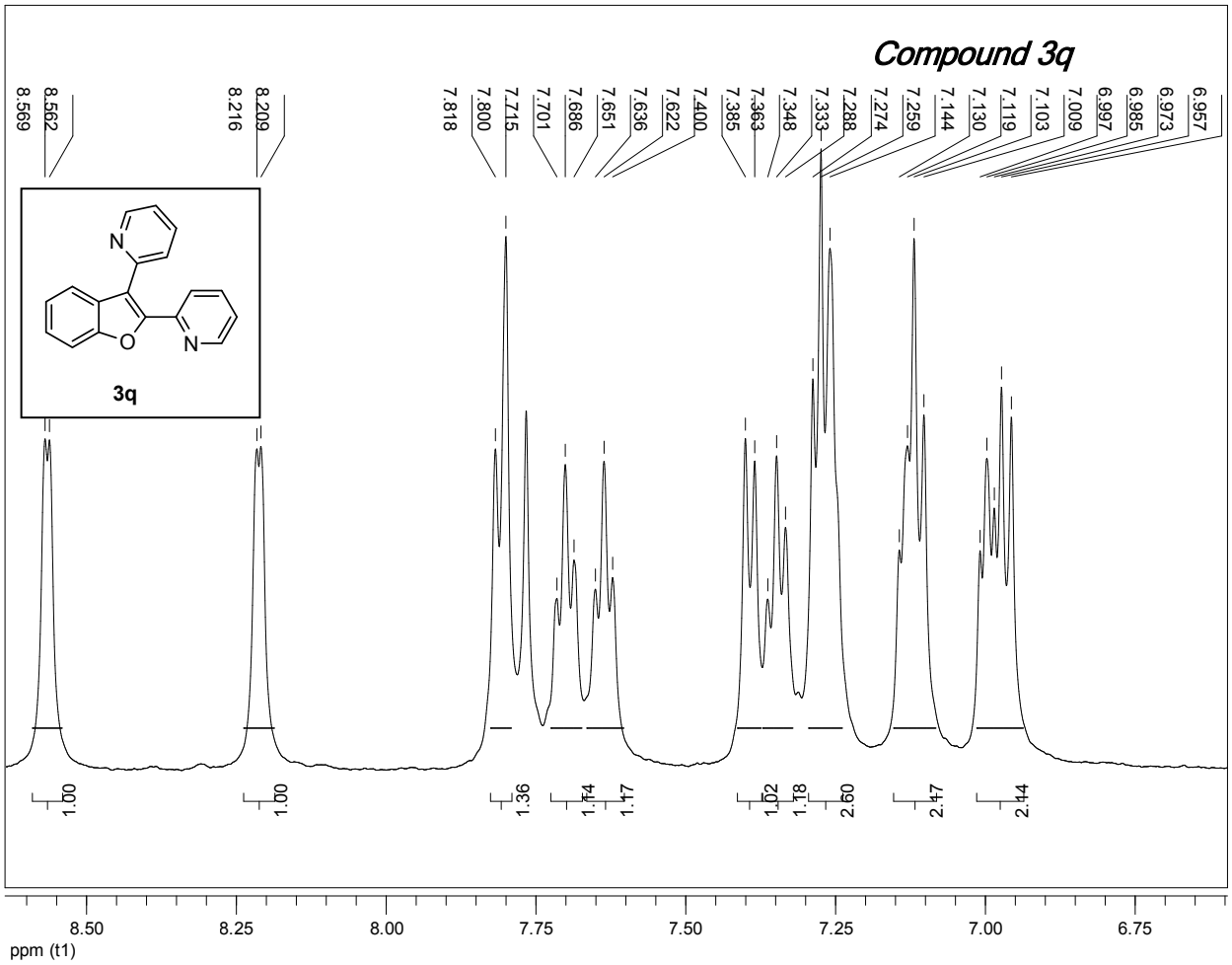

Compound 3m
158.234
154.530
148.211
133.469
133.236
130.663
130.422
128.885
128.568
128.287
127.286
122.688
119.560
116.233
111.804
95.248
76.770
76.516
76.263
55.314
Cl
Cl
MeO
O
3m
225
200
175
150
125
100
75
50
25
0
ppm (t1)

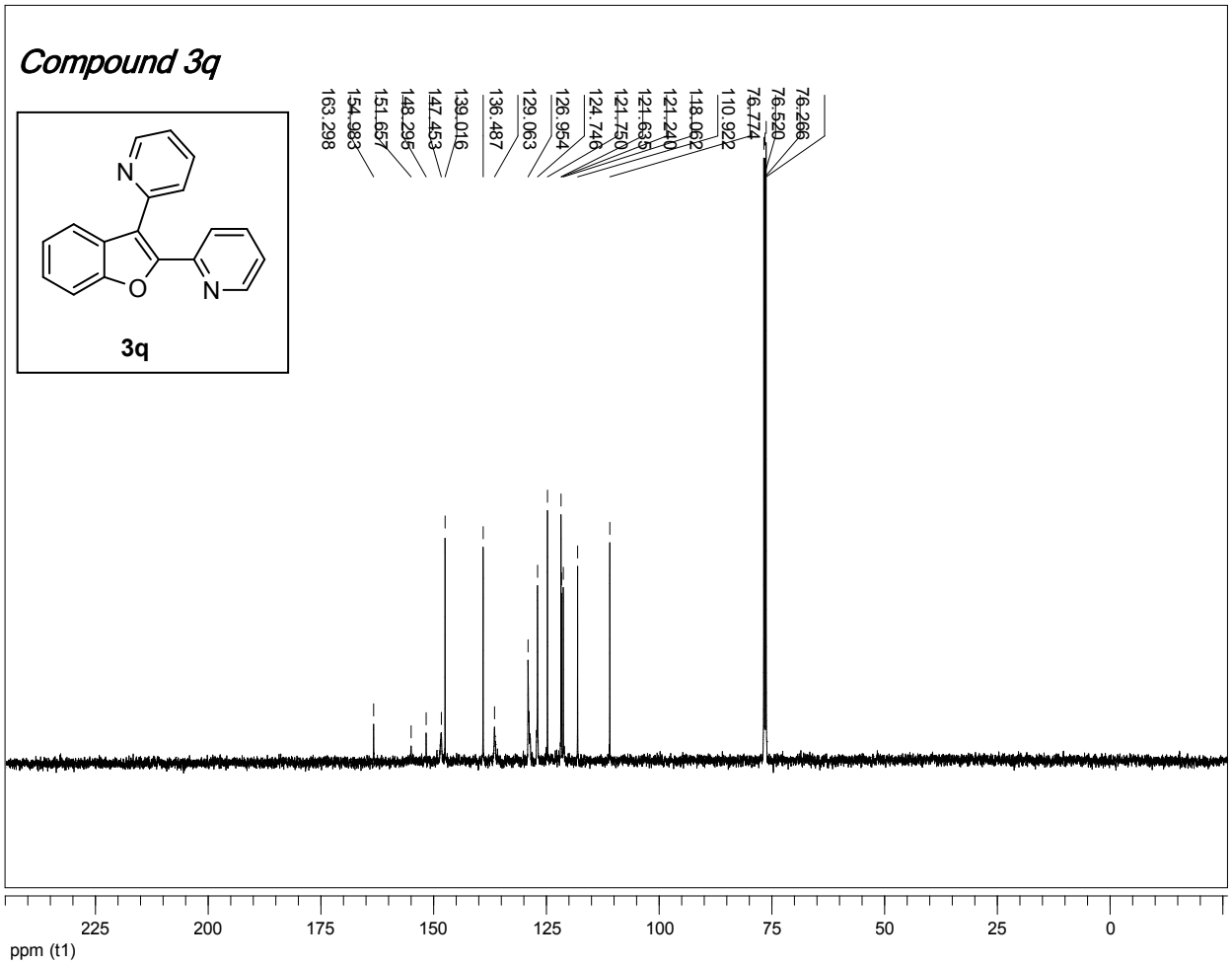

Compound 3n
7.576
7.560
7.440
7.423
7.409
7.394
7.301
7.285
7.279
7.145
7.130
2.460
2.432
2.363
Me
Me
Me
O
3n
10.0
7.5
5.0
2.5
0.0
ppm (t1)

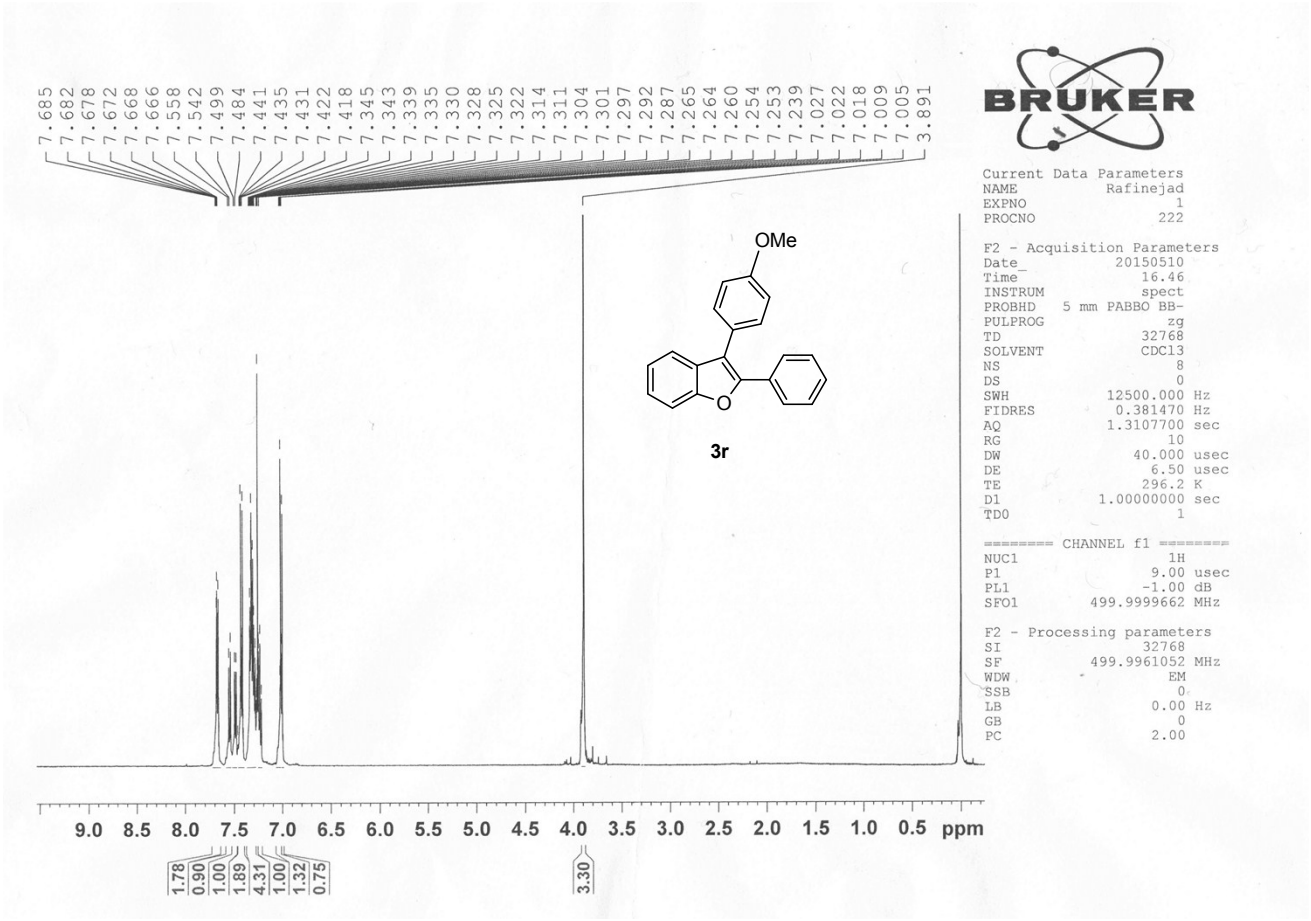

7.576
7.560
7.440
7.423
7.409
7.394
7.301
7.285
7.279
7.145
7.130
Me
Me
Me
O
3n
1.00
1.91
1.77
1.90
7.600
7.550
7.500
7.450
7.400
7.350
7.300
7.250
7.200
7.150
7.100
ppm (t1)

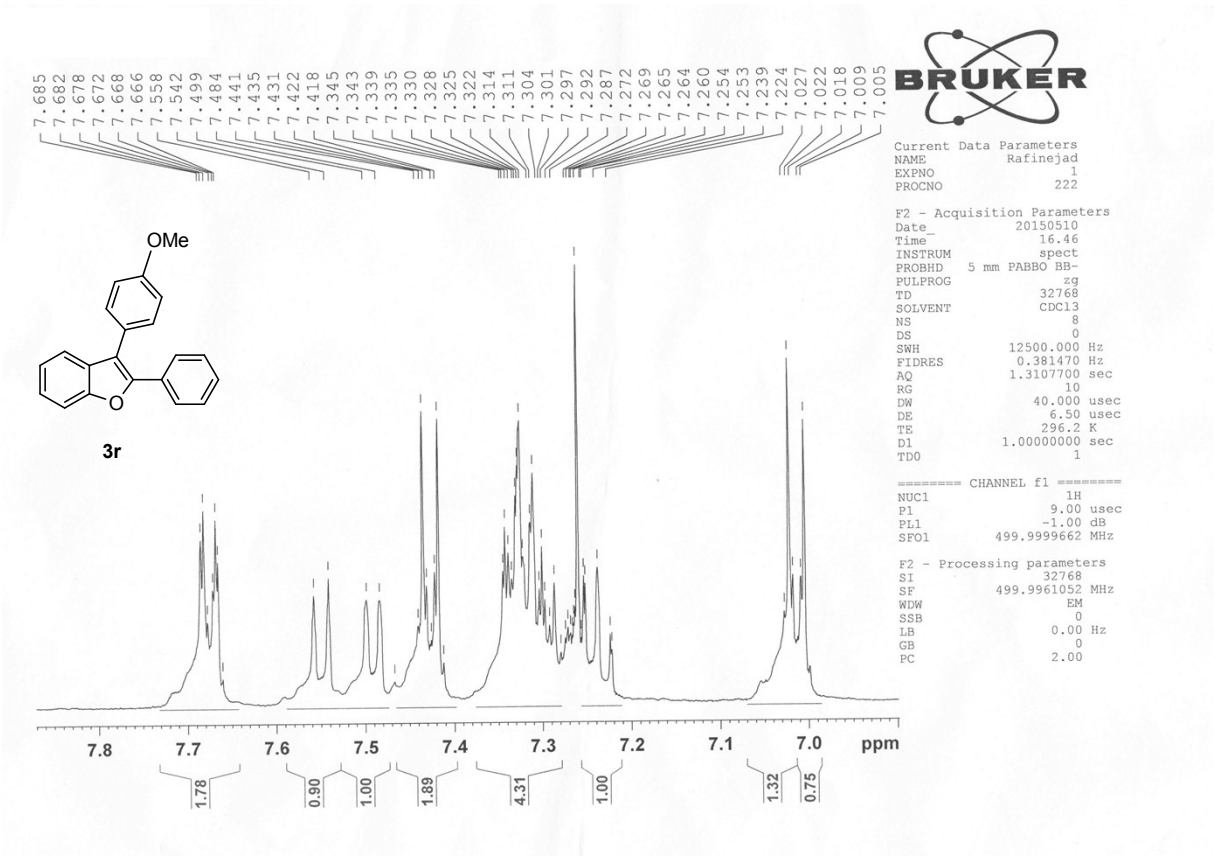

Compound 3n
151.813
150.256
137.652
136.670
131.756
130.023
129.582
129.162
128.614
127.607
126.342
125.129
119.199
116.061
110.018
76.791
76.538
76.284
20.887
Me
Me
Me
O
3n
225
200
175
150
125
100
75
50
25
0
ppm (t1)

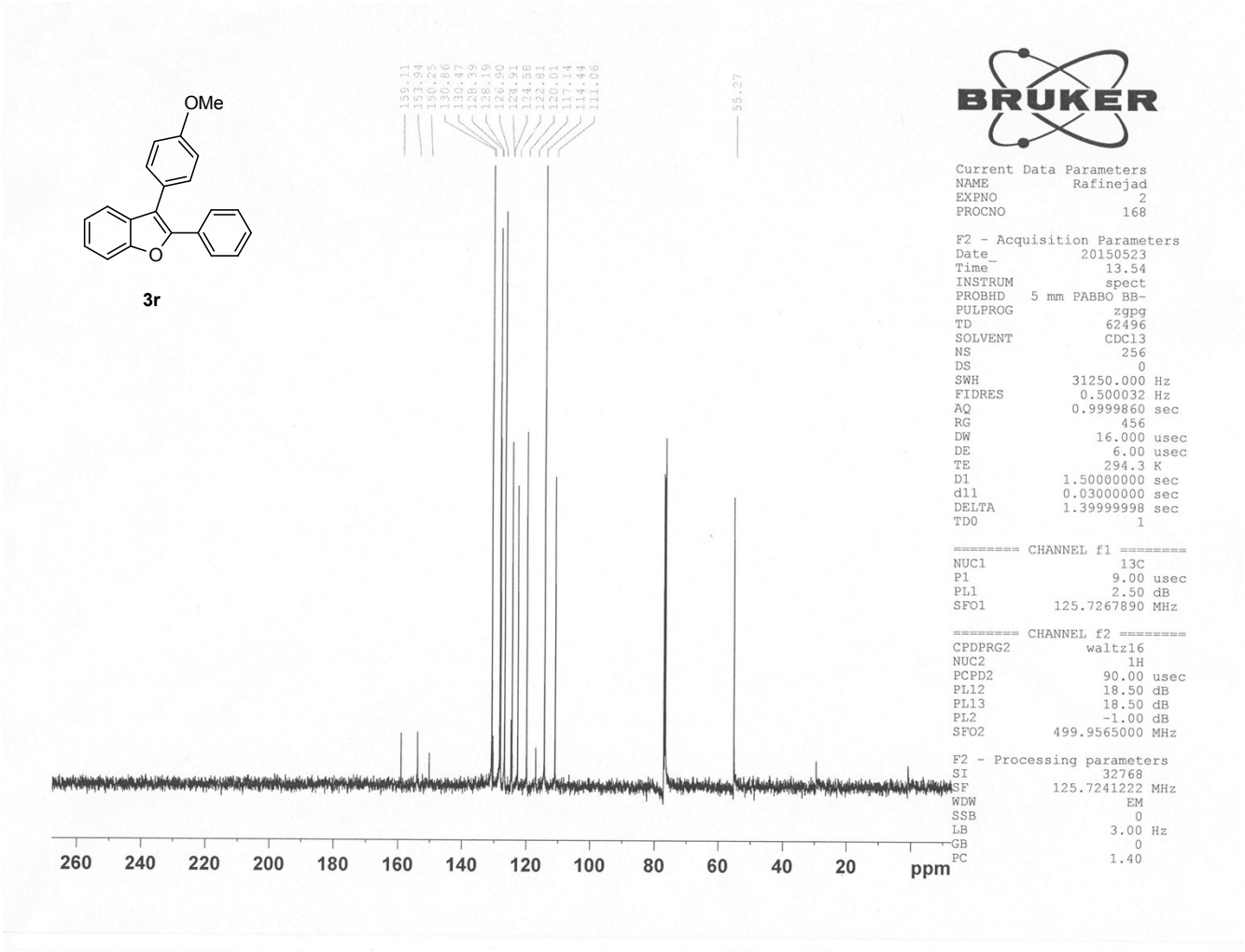

Compound 3q
8.569
8.562
8.216
8.209
7.818
7.800
7.766
7.715
7.701
7.686
7.651
7.636
7.622
7.400
7.385
7.363
7.348
7.333
7.288
7.274
7.259
7.144
7.130
7.119
7.103
7.009
6.997
6.985
6.973
6.957
N
O
N
3q
1.00
1.00
2.20
1.17
2.23
2.17
2.14
10.0
7.5
5.0
2.5
0.0
ppm (t1)

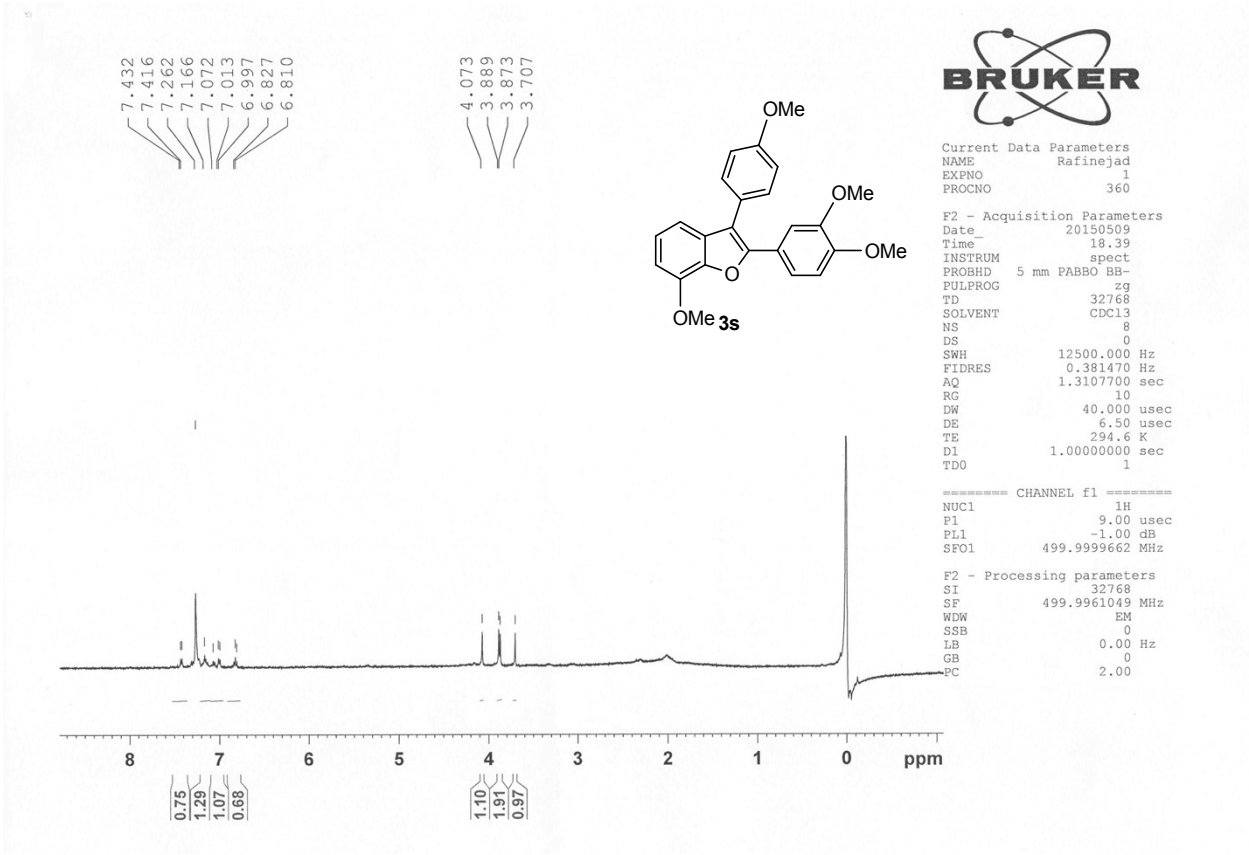

Compound 3q
8.569
8.562
8.216
8.209
7.818
7.800
7.715
7.701
7.686
7.651
7.636
7.622
7.400
7.385
7.363
7.348
7.333
7.288
7.274
7.259
7.144
7.130
7.119
7.103
7.009
6.997
6.985
6.973
6.957
3q
1.00
1.00
1.36
1.14
1.17
1.02
1.18
2.60
2.47
2.44
8.50
8.25
8.00
7.75
7.50
7.25
7.00
6.75
ppm (t1)


Compound 3q
163.298
154.983
151.657
148.295
147.453
139.016
136.487
129.063
126.954
124.746
121.750
121.635
121.240
118.062
110.922
76.774
76.520
76.266
N
O
N
3q
225
200
175
150
125
100
75
50
25
0
ppm (t1)


7.685
7.682
7.678
7.672
7.668
7.666
7.558
7.542
7.499
7.484
7.441
7.435
7.431
7.422
7.418
7.345
7.343
7.339
7.335
7.330
7.328
7.325
7.322
7.314
7.311
7.304
7.301
7.297
7.292
7.287
7.265
7.264
7.260
7.254
7.253
7.239
7.027
7.022
7.018
7.009
7.005
3.891
OMe
O
3r
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.78
0.90
1.00
1.89
4.31
1.00
1.32
0.75
3.30
BRUKER
Current Data Parameters
NAME Rafinejad
EXPNO 1
PROCNO 222
F2 - Acquisition Parameters
Date_ 20150510
Time 16.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 12500.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 10
DW 40.000 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -1.00 dB
SFO1 499.9999662 MHz
F2 - Processing parameters
SI 32768
SF 499.9961052 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

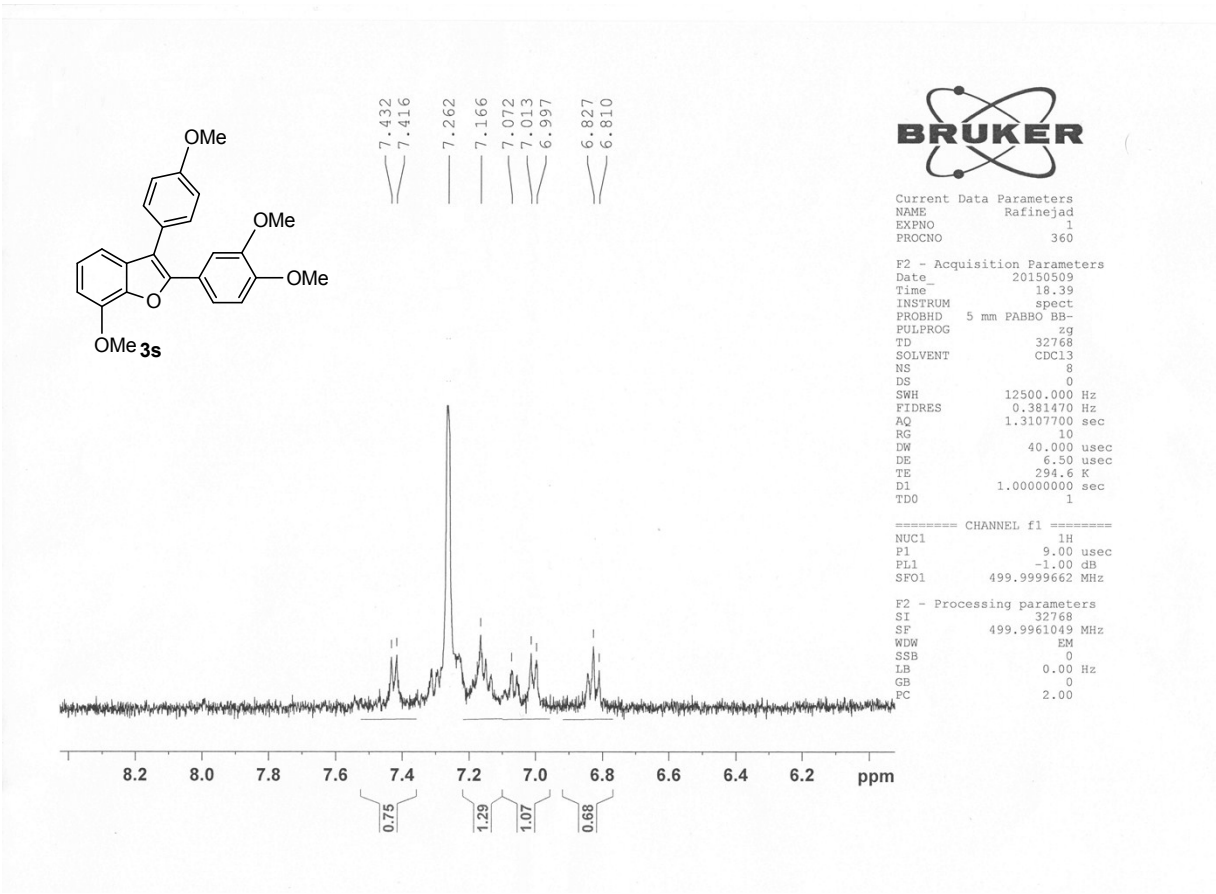

7.685
7.682
7.678
7.672
7.668
7.666
7.558
7.542
7.499
7.484
7.441
7.435
7.431
7.422
7.418
7.345
7.343
7.339
7.335
7.330
7.328
7.325
7.322
7.314
7.311
7.304
7.301
7.297
7.292
7.287
7.272
7.269
7.265
7.264
7.260
7.254
7.253
7.239
7.224
7.027
7.022
7.018
7.009
7.005
OMe
O
3r
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
1.78
0.90
1.00
1.89
4.31
1.00
1.32
0.75
BRUKER
Current Data Parameters
NAME Rafinejad
EXPNO 1
PROCNO 222
F2 - Acquisition Parameters
Date_ 20150510
Time 16.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 12500.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 10
DW 40.000 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -1.00 dB
SFO1 499.9999662 MHz
F2 - Processing parameters
SI 32768
SF 499.9961052 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

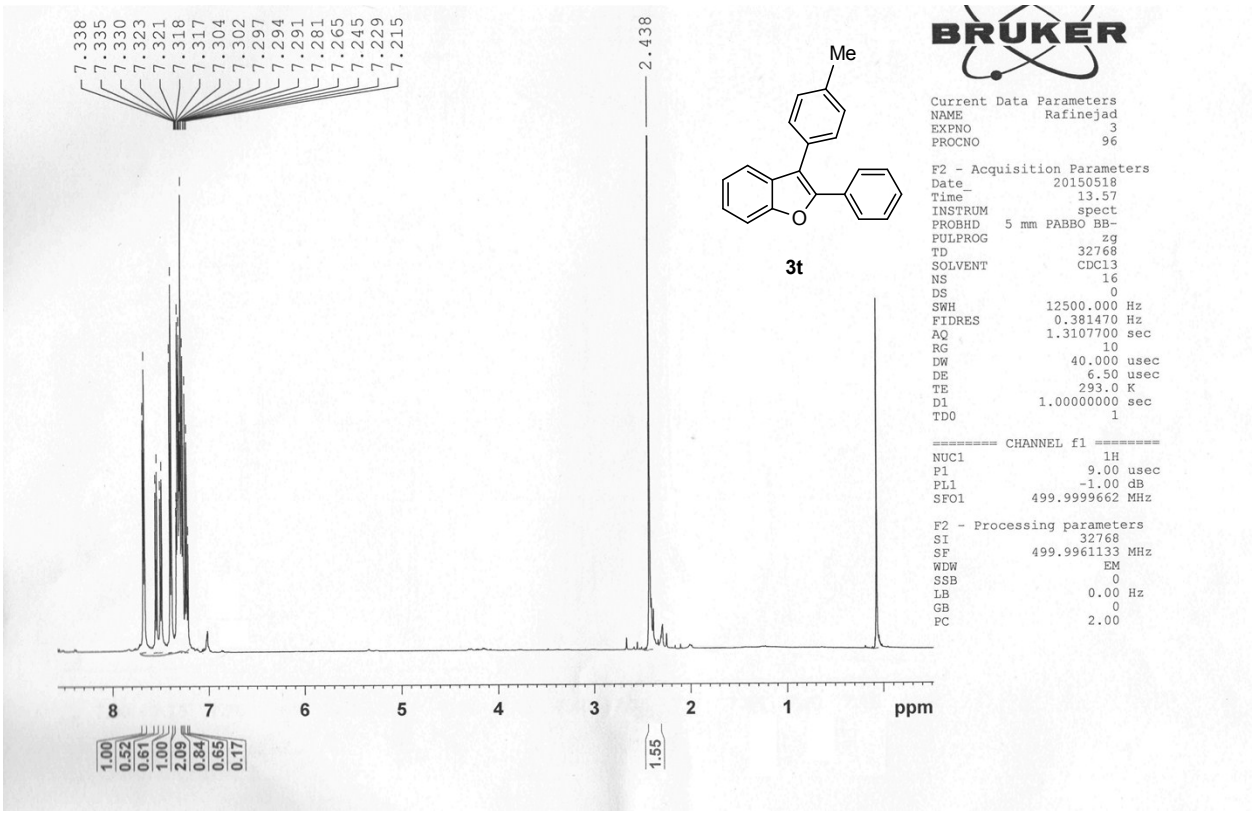

OMe
O
3r
159.11
153.94
150.25
130.86
130.47
128.39
128.19
126.90
124.91
124.58
122.81
120.01
117.14
114.44
111.06
55.27
260
240
220
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME Rafinejad
EXPNO 2
PROCNO 168
F2 - Acquisition Parameters
Date_ 20150523
Time 13.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 62496
SOLVENT CDCl3
NS 256
DS 0
SWH 31250.000 Hz
FIDRES 0.500032 Hz
AQ 0.9999860 sec
RG 456
DW 16.000 usec
DE 6.00 usec
TE 294.3 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 2.50 dB
SFO1 125.7267890 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 18.50 dB
PL13 18.50 dB
PL2 -1.00 dB
SFO2 499.9565000 MHz
F2 - Processing parameters
SI 32768
SF 125.7241222 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

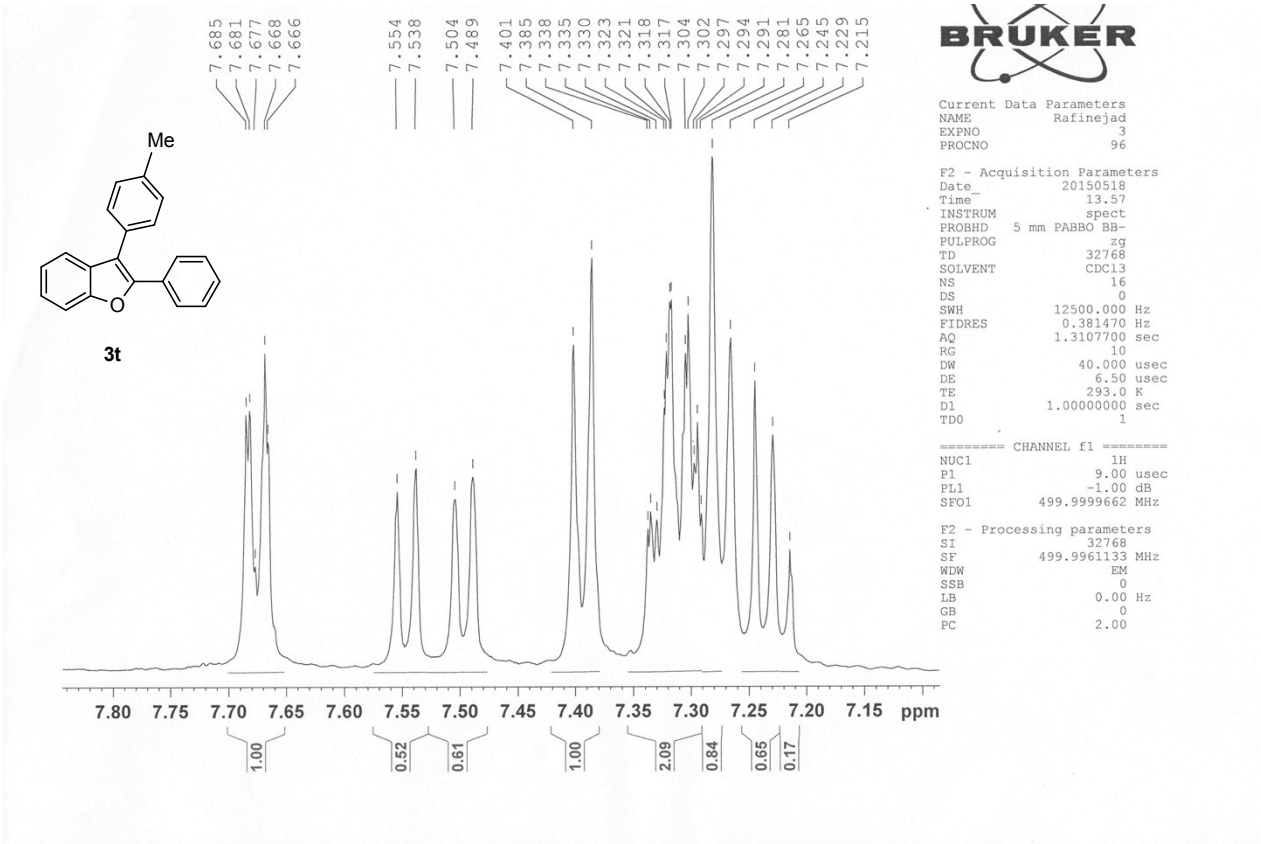


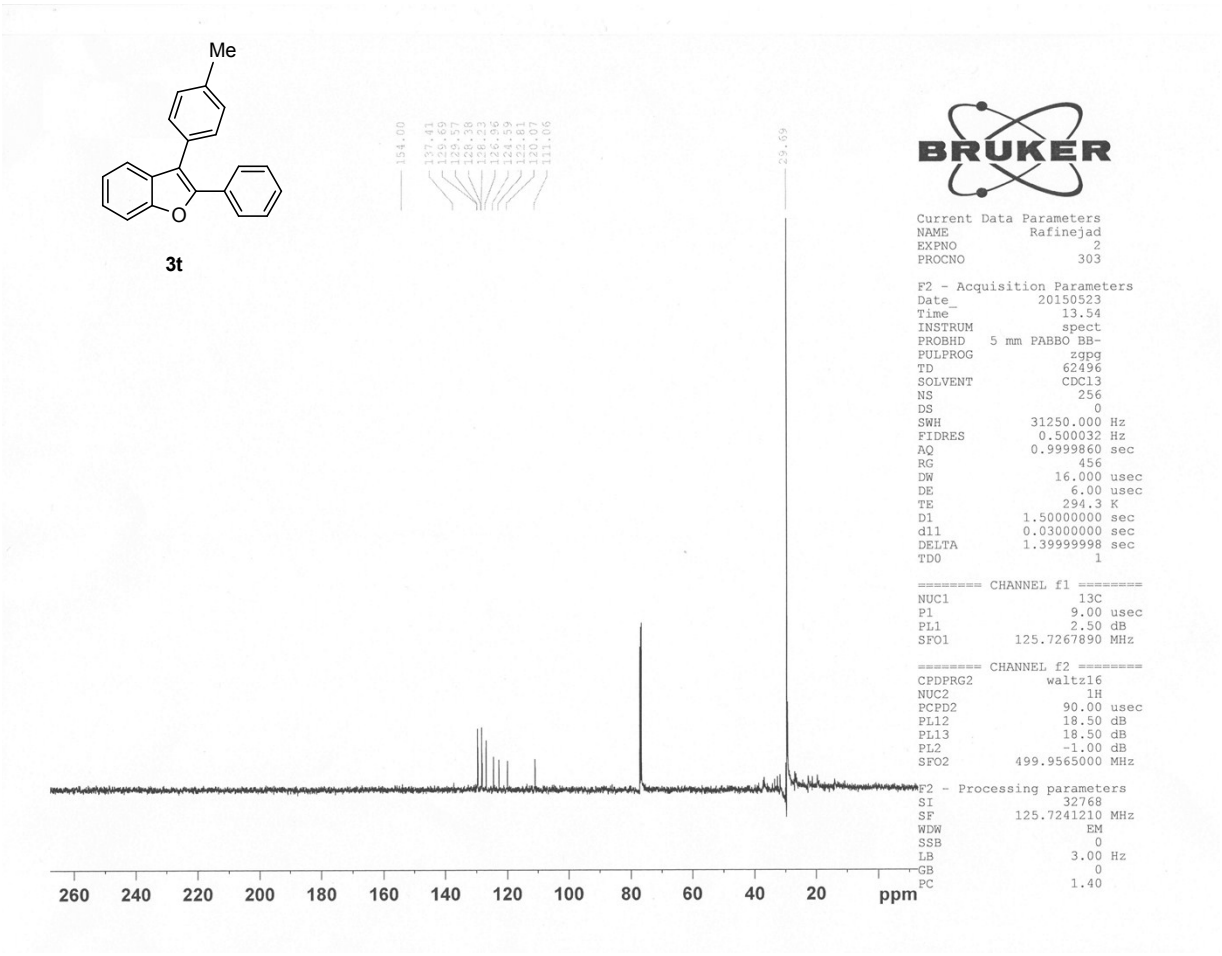
BRUKER

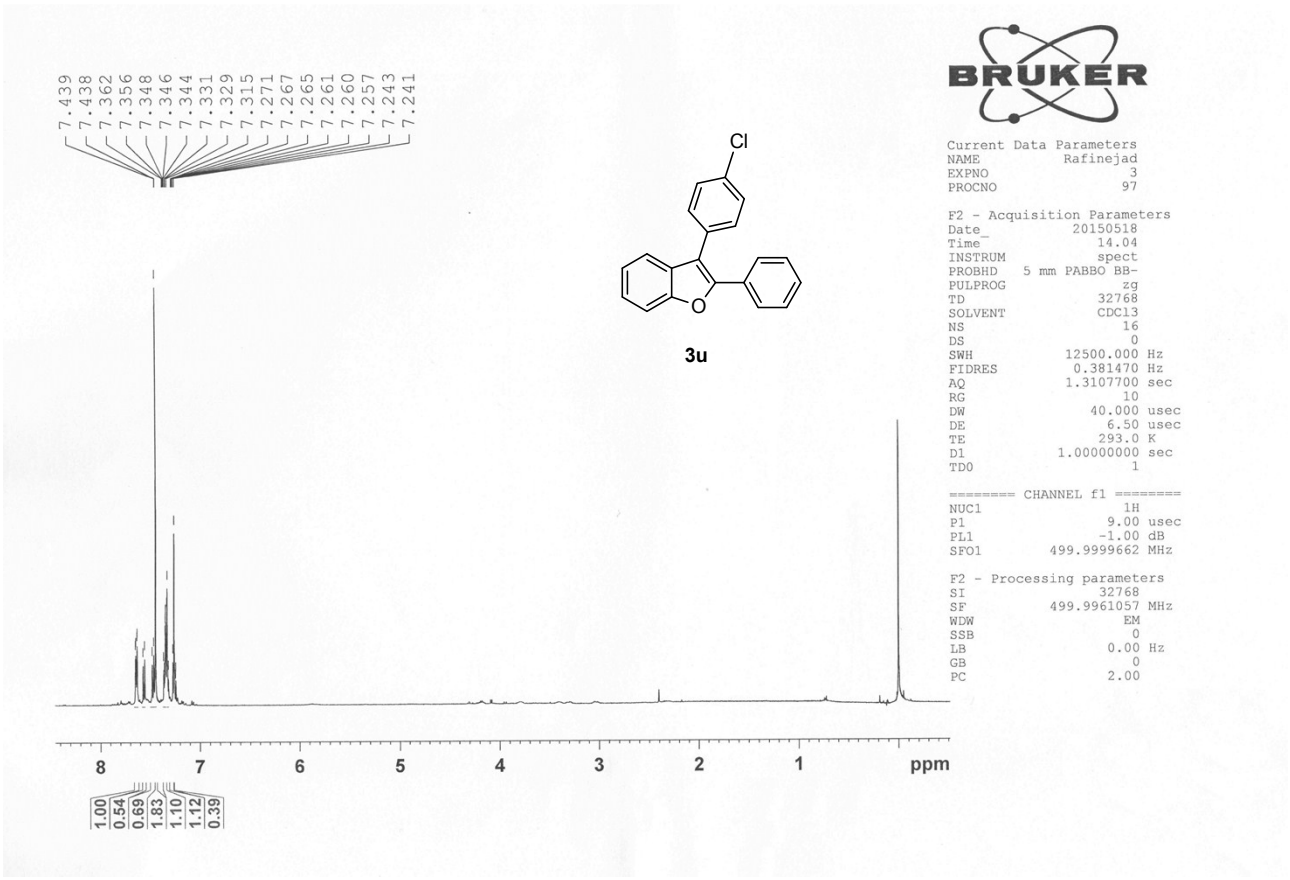
```
Current Data Parameters
NAME                  Rafinejad
EXPNO                         1
PROCNO                      360

F2 - Acquisition Parameters
Date_                  20150509
Time                      18.39
INSTRUM                   spect
PROBHD     5 mm PABBO BB-
PULPROG                      zg
TD                        32768
SOLVENT                   CDCl3
NS                            8
DS                            0
SWH                   12500.000 Hz
FIDRES                0.381470 Hz
AQ                    1.3107700 sec
RG                           10
DW                       40.000 usec
DE                        6.50 usec
TE                       294.6 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        9.00 usec
PL1                      -1.00 dB
SFO1                499.9999662 MHz

F2 - Processing parameters
SI                        32768
SF                  499.9961049 MHz
WDW                          EM
SSB                           0
LB                        0.00 Hz
GB                            0
PC                        2.00
```


OMe
OMe
OMe
OMe
O
3s
7.432
7.416
7.262
7.166
7.072
7.013
6.997
6.827
6.810
BRUKER
Current Data Parameters
NAME Rafinejad
EXPNO 1
PROCNO 360
F2 - Acquisition Parameters
Date_ 20150509
Time 18.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 12500.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 10
DW 40.000 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -1.00 dB
SFO1 499.9999662 MHz
F2 - Processing parameters
SI 32768
SF 499.9961049 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 2.00
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
ppm
0.75
1.29
1.07
0.68


7.338
7.335
7.330
7.323
7.321
7.318
7.317
7.304
7.302
7.297
7.294
7.291
7.281
7.265
7.245
7.229
7.215
2.438
Me
O
3t
BRUKER
Current Data Parameters
NAME Rafinejad
EXPNO 3
PROCNO 96
F2 - Acquisition Parameters
Date_ 20150518
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12500.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 10
DW 40.000 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -1.00 dB
SFO1 499.9999662 MHz
F2 - Processing parameters
SI 32768
SF 499.9961133 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 2.00
8
7
6
5
4
3
2
1
ppm
1.00
0.52
0.61
1.00
2.09
0.84
0.65
0.17
1.55


7.685
7.681
7.677
7.668
7.666
7.554
7.538
7.504
7.489
7.401
7.385
7.338
7.335
7.330
7.323
7.321
7.318
7.317
7.304
7.302
7.297
7.294
7.291
7.281
7.265
7.245
7.229
7.215
Me
O
3t
7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 ppm
1.00
0.52
0.61
1.00
2.09
0.84
0.65
0.17
BRUKER
Current Data Parameters
NAME Rafinejad
EXPNO 3
PROCNO 96
F2 - Acquisition Parameters
Date_ 20150518
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 12500.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 10
DW 40.000 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -1.00 dB
SFO1 499.9999662 MHz
F2 - Processing parameters
SI 32768
SF 499.9961133 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 2.00


Me
O
3t
154.00
137.41
129.69
128.57
128.38
126.33
124.56
124.59
123.81
120.07
111.06
29.69
260
240
220
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Rafinejad
EXPNO 2
PROCNO 303
F2 - Acquisition Parameters
Date_ 20150523
Time 13.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 62496
SOLVENT CDCl3
NS 256
DS 0
SWH 31250.000 Hz
FIDRES 0.500032 Hz
AQ 0.9999860 sec
RG 456
DW 16.000 usec
DE 6.00 usec
TE 294.3 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 2.50 dB
SFO1 125.7267890 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 18.50 dB
PL13 18.50 dB
PL2 -1.00 dB
SFO2 499.9565000 MHz
F2 - Processing parameters
SI 32768
SF 125.7241210 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



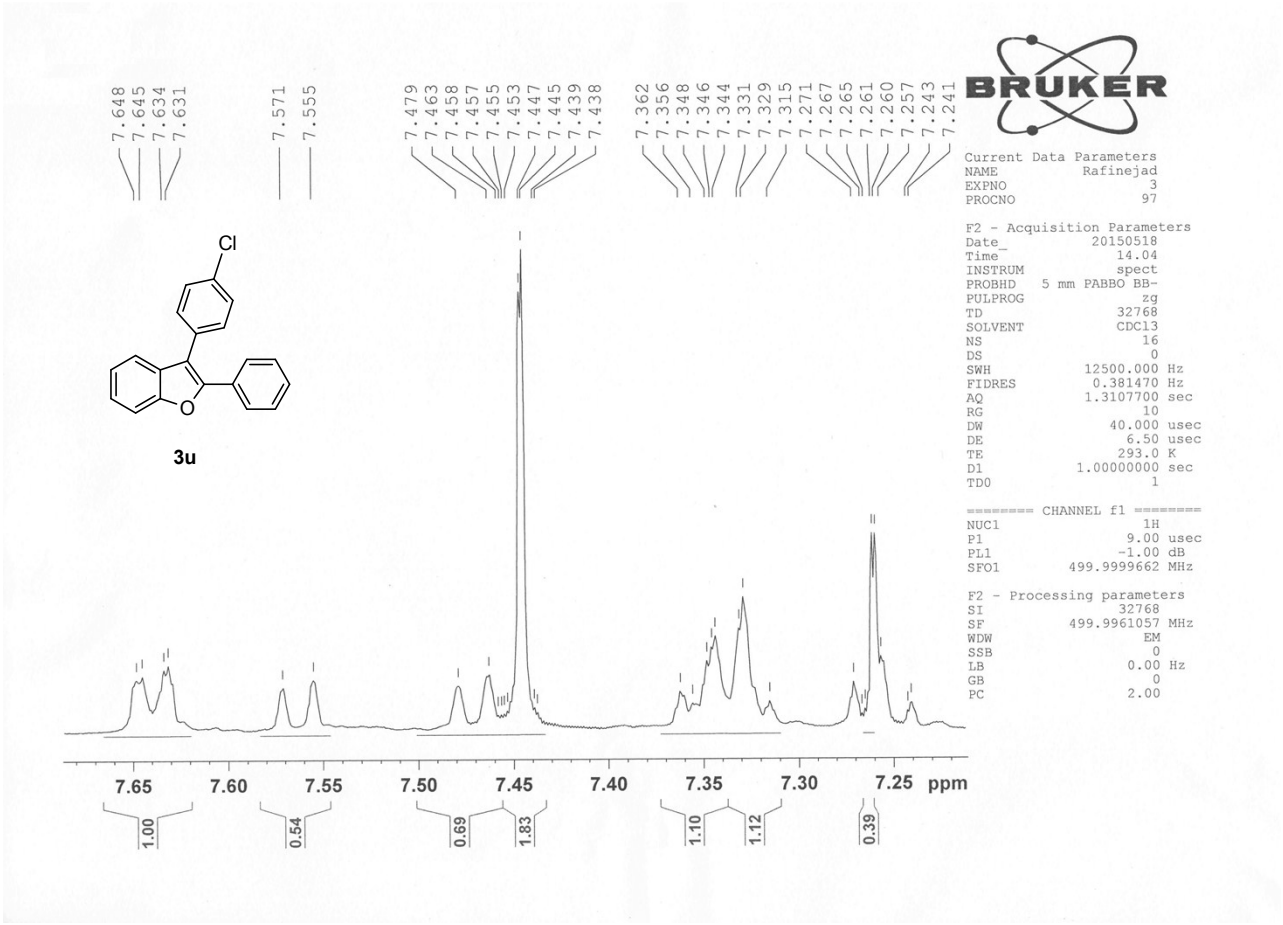
BRUKER

Current Data Parameters
NAME Rafinejad
EXPNO 3
PROCNO 97

F2 - Acquisition Parameters
Date_ 20150518
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12500.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 10
DW 40.000 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -1.00 dB
SFO1 499.9999662 MHz

F2 - Processing parameters
SI 32768
SF 499.9961057 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 2.00


7.648
7.645
7.634
7.631
7.571
7.555
7.479
7.463
7.458
7.457
7.455
7.453
7.447
7.445
7.439
7.438
7.362
7.356
7.348
7.346
7.344
7.331
7.329
7.315
7.271
7.267
7.265
7.261
7.260
7.257
7.243
7.241
Cl
O
3u
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
ppm
1.00
0.54
0.69
1.83
1.10
1.12
0.39
BRUKER
Current Data Parameters
NAME Rafinejad
EXPNO 3
PROCNO 97
F2 - Acquisition Parameters
Date_ 20150518
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12500.000 Hz
FIDRES 0.381470 Hz
AQ 1.3107700 sec
RG 10
DW 40.000 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -1.00 dB
SFO1 499.9999662 MHz
F2 - Processing parameters
SI 32768
SF 499.9961057 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 2.00