Electronic Supplementary Material (ESI) for ChemComm.

Tandem reaction to 3-(2-quinolyl) chromones from ynones and quinoline *N*-oxides under transition metal- and additive-free conditions

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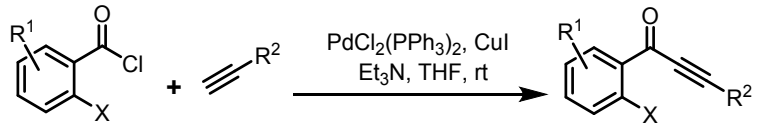
1. General Information

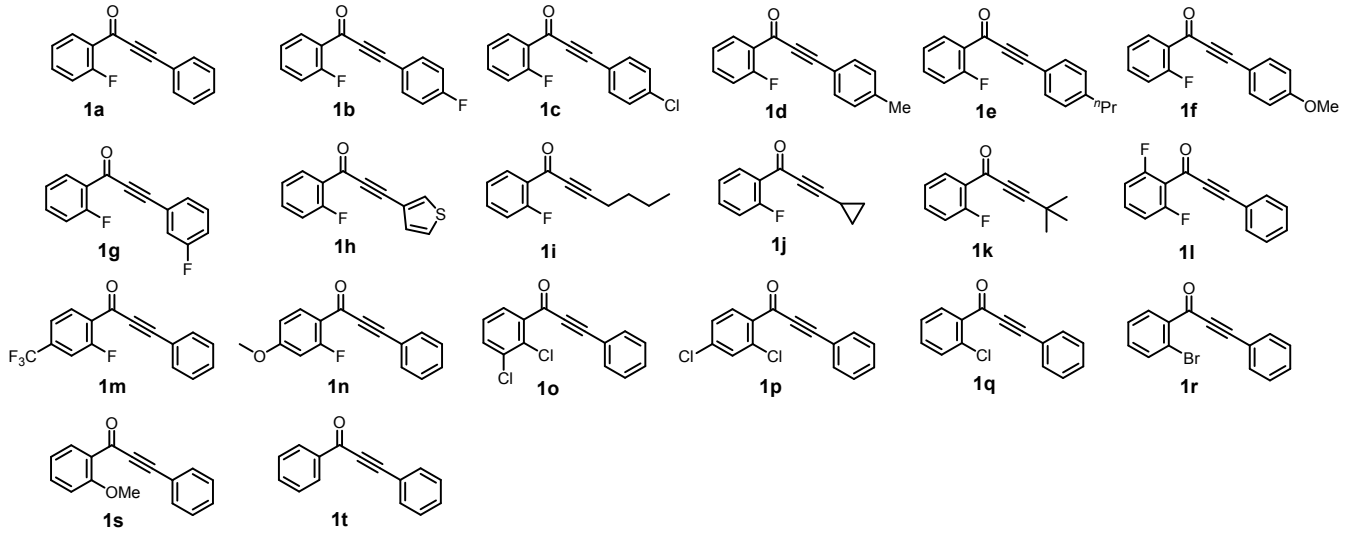
All the solvents were used without further purification. the other commercial chemicals were used without further purification. All reactions were performed under an inert atmosphere of nitrogen in flame-dried glassware, unless otherwise stated. Analytical thin layer chromatography was performed on 0.25 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 Bruker DRX-500 instrument (500 MHz). ^{13}C NMR spectra were recorded on Bruker DRX-500 instrument (126 MHz) were fully decoupled by broad band proton decoupling. High-resolution mass spectra (HRMS) were recorded on an Agilent 1290 Mass spectrometer using using EI or 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 in Hertz (Hz). Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

2. Experimental Section

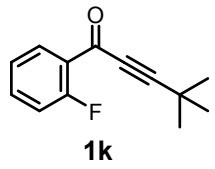
2.1 Procedure for the Preparation of 1[1]



X=F, Cl, Br, OMe

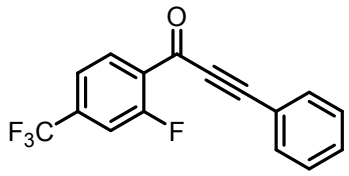


To a solution of the acyl chloride (1.0 mmol) and terminal alkyne (1.1 mmol) in an anhydrous THF (5 mL) under N_2 protection, was added $PdCl_2(PPh_3)_2$ (14 mg, 2 mol %) and CuI (7.6 mg, 4 mol %). After stirring for 1 min, Et_3N (1.5 mmol) was added and the mixture was stirred for 15 h at r.t. When the reaction was complete (Monitored by TLC), distilled H_2O was added. The mixture was extracted with CH_2Cl_2. The organic phase was collected, dried (Na_2SO_4), and concentrated. The residue was purified by column chromatography [silica gel, PE/EtOAc (50:1)].



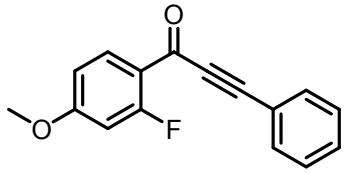
1k

1-(2-fluorophenyl)-4,4-dimethylpent-2-yn-1-one (1k). (15.6 mg, 75%). Yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 – 7.94 (m, 1H), 7.57 – 7.46 (m, 1H), 7.25 – 7.17 (m, 1H), 7.15 – 7.05 (m, 1H), 1.34 – 1.31 (m, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.6 , 161.9 (d, J = 261.8 Hz), 135.2 (d, J = 9.3 Hz), 131.8 , 125.7 (d, J = 8.1 Hz), 124.0 (d, J = 4.0 Hz), 116.9 (d, J = 21.9 Hz), 103.8 (d, J = 2.8 Hz), 79.7 , 29.9 , 27.9; ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.6 , 161.9 (d, J = 261.8 Hz), 135.2 (d, J = 9.3 Hz), 131.8 , 125.7 (d, J = 8.1 Hz), 124.0 (d, J = 4.0 Hz), 116.9 (d, J = 21.9 Hz), 103.8 (d, J = 2.8 Hz), 79.7 , 29.9 , 27.9 . HRMS (ESI-TOF) m/z: calcd for $C_{13}H_{13}FNaO^+$ $(M+Na)^+$: calculated 227.0843, found 227.0839.



1m

1-(2-fluoro-4-(trifluoromethyl)phenyl)-3-phenylprop-2-yn-1-one (1m). (25.6 mg, 86%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (t, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 7.3 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.47 – 7.38 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.7 , 161.5 (d, *J* = 263.4 Hz), 136.6 (qd, *J* = 33.8, 8.5 Hz), 133.3 , 132.4 , 131.3 , 128.7 , 122.5 (qd, *J* = 273.7, 2.3 Hz), 121.5 (d, *J* = 2.3 Hz), 121.0 (p, *J* = 3.8 Hz), 119.6 , 114.7 (dq, *J* = 25.4, 3.8 Hz), 94.4 (d, *J* = 3.2 Hz), 88.2. HRMS (ESI-TOF) m/z: calcd for $C_{16}H_8F_4NaO^+$ $(M+Na)^+$: calculated 315.0403, found 315.0404.

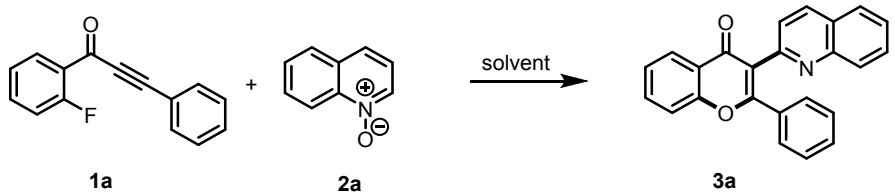


1n

1-(2-fluoro-4-methoxyphenyl)-3-phenylprop-2-yn-1-one (1n). (20.1 mg, 79%)^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (t, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 7.1 Hz, 2H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 6.81 – 6.72 (m, 1H), 6.69 – 6.61 (m, 1H), 3.87 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.9 , 165.5 (d, *J* = 11.8 Hz), 163.8 (d, *J* = 262.3 Hz), 133.4 (d, *J* = 2.3 Hz), 133.0 , 130.6 , 128.5 , 120.2 , 118.8 (d, *J* = 8.0 Hz), 110.4 (d, *J* = 2.8 Hz), 102.2 (d, *J* = 25.4 Hz), 92.0 (d, *J* = 3.2 Hz), 88.3 , 55.9. HRMS (ESI-TOF) m/z: calcd for $C_{16}H_{11}FNaO^+$ $(M+Na)^+$: calculated 277.0635, found 277.0631.

2.2 Optimization of the Reaction Conditions

2.2.1 Table S1 Screening of the reaction conditions (Condition A)[a]

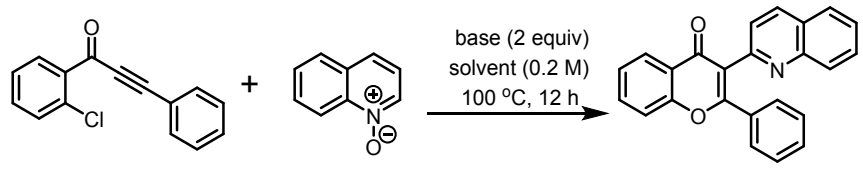


1a 2a 3a

Entry	Solvent	Temp °C	Yield (%)[b]
1	DMF	120	90
2	CH_3CN	120	82
3	*tert*-butanol	120	82
4	MTBE	120	80
5	DCE	120	80
6	1,4-dioxane	120	90
7	toluene	120	92
8	H_2O	120	0
9	toluene	100	70
10[c]	toluene	120	92
11[d]	toluene	120	83
12[e]	toluene	120	90

[a] Reaction condition: **1a** (0.1 mmol), **2a** (0.15 mmol), solvent (0.5 mL) at a corresponding temperature under an air atmosphere. [b] Isolated yield based on **1a**. [c] **2a** (0.2 mmol) was used. [d] **2a** (0.1 mmol) was used. [e] Under nitrogen atmosphere. DMF = *N*,*N*-Dimethyl formamide. MTBE = Methyl tertiary butyl ether. DCE = 1,2-Dichloroethane.

2.2.2 Table S2 Screening of the reaction conditions (Condition B)[a]



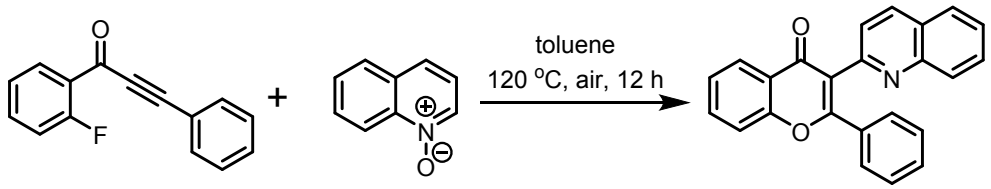
1o **2a**, 1.5 equiv **3a**

Entry	Solvent	Base	Yield (%)[b]
1	DMF	Li_2CO_3	50
2	DMF	Na_2CO_3	30
3	DMF	K_2CO_3	44
4	DMF	Cs_2CO_3	43
5	DMF	$NaHCO_3$	25
6	DMF	$KHCO_3$	30
7	**DMF**	**Na_3PO_4**	**75**
8	DMF	K_3PO_4	64
9	DMF	KOAc	0
10	DMF	LiOH	65
11	DMF	KO^{t}Bu	5
12	DMF	Et_3N	10
13	DMF	DBU	trace
14	DMF	-	trace
15	DMSO	Na_3PO_4	39
16	DMA	Na_3PO_4	50
17	NMP	Na_3PO_4	55
18	THF	Na_3PO_4	20
19	CH_3CN	Na_3PO_4	30
20	*tert*-butanol	Na_3PO_4	35
21	MTBE	Na_3PO_4	25
22	toluene	Na_3PO_4	15
23	DMPU	Na_3PO_4	70
24[c]	DMF	Na_3PO_4	74

[a] **1o** (0.1 mmol), **2a** (0.15 mmol), solvent (0.5 mL), base (2 equiv), under air atmosphere for 12 h. [b] Isolated yield. [c] at 120 °C.

2.3 Procedure for the Synthesis of 3a

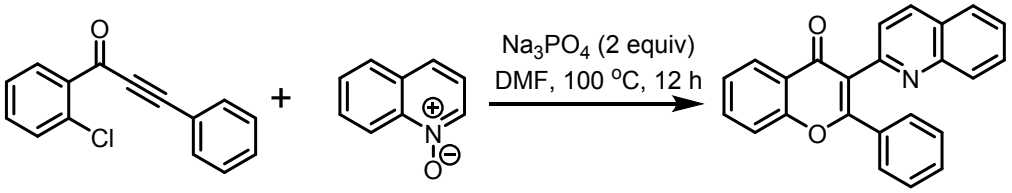
2.3.1 Condition A



1a, 1 equiv **2a**, 2 equiv **3a**

A dried 10 mL Schlenk tube was charged with 1-(2-fluorophenyl)-3-phenylprop-2-yn-1-one **1a** (22.4 mg, 0.1 mmol, 1 equiv), quinoline *N*-oxide **2a** (21.8 mg, 0.15 mmol, 1.5 equiv), and toluene (0.5 mL). The reaction mixture was heated to 120 °C for 12 hours under vigorous stirring. Upon completion, the reaction mixture was cooled to room temperature. The solvent was concentrated under vacuum, and the resulting residue was purified by preparative thin layer chromatograpy (PTLC) with acetate : hexane = 1 : 4 to give the corresponding products **2-phenyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3a)** (32.1mg, 92%) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 – 8.28 (m, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.76 – 7.69 (m, 1H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.47 – 7.38 (m, 3H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.20 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.32 , 163.26 , 156.09 , 153.63 , 148.07 , 136.13 , 133.89 , 132.78 , 130.28 , 129.43 , 129.33 , 129.27 , 128.10 , 127.48 , 127.11 , 126.69 , 126.21 , 125.27 , 124.15 , 123.75 , 123.07 , 117.97; HRMS (EI) for $C_{24}H_{16}NO_2^+$ $(M+H)^+$: calculated 350.1176, found 350.1176.

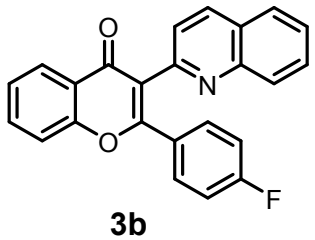
2.3.2 Condition B



1o, 1 equiv **2a**, 1.5 equiv **3a**

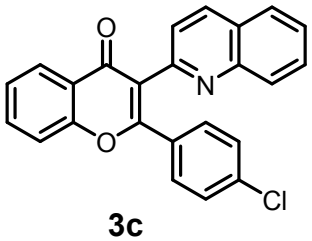
A dried 10 mL Schlenk tube was charged with 1-(2-fluorophenyl)-3-phenylprop-2-yn-1-one **1o** (24.1 mg, 0.1 mmol, 1 equiv), quinoline *N*-oxide **2a** (21.8 mg, 0.15 mmol, 1.5 equiv), Na_3PO_4 (32.6 mg, 0.2 mmol, 2 equiv), and DMF (0.5 mL). The reaction mixture was heated to 100 °C for 12 hours under 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 chromatograpy (PTLC) with acetate : hexane = 1 :

4 to give the corresponding product **2-phenyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3a)** (26.2 mg, 75%) as a white solid.



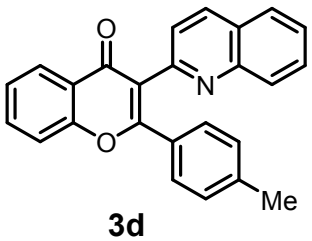
3b

2-(4-fluorophenyl)-3-(quinolin-2-yl)-4*H*-chromen-4-one (3b). (31.6 mg, 86%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 – 8.31 (m, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.77 – 7.73 (m, 1H), 7.71 – 7.66 (m, 1H), 7.60 – 7.55 (m, 2H), 7.53 (d, J = 8.4 Hz, 1H), 7.48 (d, J = 8.0 Hz, 1H), 7.46 – 7.41 (m, 2H), 6.91 (t, J = 8.6 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.2 , 163.5 (d, *J* = 252.3 Hz), 162.2 , 156.0 , 153.4 , 148.1 , 136.3 , 134.0 , 131.5 (d, *J* = 8.7 Hz), 129.5 , 129.4 , 128.9 (d, *J* = 3.4 Hz), 127.5 , 127.1 , 126.8 , 126.2 , 125.4 , 124.1 , 123.7 , 123.0 , 117.9 , 115.3 (d, *J* = 21.9 Hz); HRMS (EI) for $C_{24}H_{15}NO_2^+$ $(M+H)^+$: calculated 368.1081, found 368.1081. (**Condition A**).



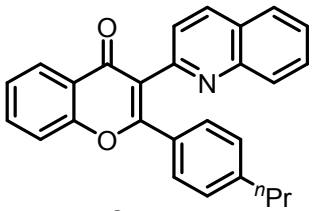
3c

2-(4-chlorophenyl)-3-(quinolin-2-yl)-4*H*-chromen-4-one (3c). (30.0 mg, 78%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 – 8.28 (m, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 7.98 – 7.94 (m, 1H), 7.85 – 7.80 (m, 1H), 7.76 – 7.71 (m, 1H), 7.70 – 7.65 (m, 1H), 7.58 – 7.53 (m, 2H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.37 – 7.33 (m, 2H), 7.19 – 7.15 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.2 , 162.0 , 156.0 , 153.3 , 148.1 , 136.5 , 136.3 , 134.0 , 131.3 , 130.6 , 129.5 , 129.4 , 128.5 , 127.5 , 127.2 , 126.9 , 126.2 , 125.4 , 124.0 , 123.7 , 123.2 , 117.9; HRMS (EI) for $C_{24}H_{15}ClNO_2^+$ $(M+H)^+$: calculated 384.0786, found 384.0785. (**Condition A**).



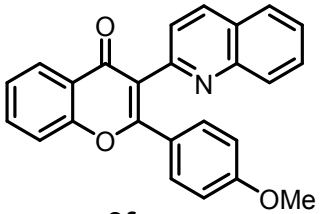
3d

3-(quinolin-2-yl)-2-(*p*-tolyl)-4*H*-chromen-4-one (3d). (29.8 mg, 82%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 – 8.28 (m, 1H), 8.15 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.69 – 7.64 (m, 1H), 7.58 – 7.50 (m, 2H), 7.48 – 7.41 (m, 2H), 7.31 (d, J = 8.3 Hz, 2H), 7.00 (d, J = 8.1 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.3 , 163.3 , 156.1 , 153.9 , 148.1 , 140.7 , 136.2 , 133.8 , 129.9 , 129.5 , 129.3 , 129.2 , 128.8 , 127.5 , 127.1 , 126.6 , 126.2 , 125.2 , 124.2 , 123.7 , 122.7 , 117.9 , 21.3; HRMS (EI) for $C_{25}H_{18}NO_2^+$ $(M+H)^+$: calculated 364.1332, found 364.1329. (**Condition A**).



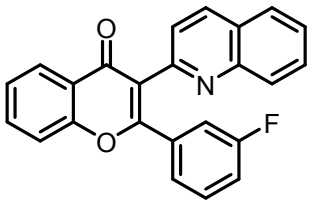
3e

2-(4-propylphenyl)-3-(quinolin-2-yl)-4*H*-chromen-4-one (3e). (31.3 mg, 80%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 – 8.20 (m, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 8.2 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.60 – 7.55 (m, 1H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 2.44 – 2.37 (m, 2H), 1.46 (h, *J* = 7.3 Hz, 2H), 0.77 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.34 , 163.34 , 156.07 , 153.90 , 148.11 , 145.42 , 136.11 , 133.76 , 130.07 , 129.47 , 129.24 , 129.20 , 128.22 , 127.46 , 127.12 , 126.62 , 126.18 , 125.14 , 124.21 , 123.75 , 122.70 , 117.92 , 37.68 , 23.98 , 13.60; HRMS (EI) for $C_{27}H_{22}NO_2^+$ $(M+H)^+$: calculated 392.1645, found 392.1643. (**Condition A**).



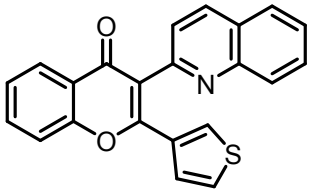
3f

2-(4-methoxyphenyl)-3-(quinolin-2-yl)-4*H*-chromen-4-one (3f). (31.9 mg, 84%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 – 8.19 (m, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.6 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.65 – 7.56 (m, 2H), 7.49 – 7.43 (m, 2H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.27 (d, *J* = 8.9 Hz, 2H), 6.61 (d, *J* = 8.9 Hz, 2H), 3.63 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.3 , 162.9 , 161.1 , 156.0 , 154.1 , 148.1 , 136.2 , 133.7 , 131.3 , 131.0 , 129.5 , 129.3 , 127.5 , 127.1 , 126.7 , 126.1 , 125.1 , 124.9 , 124.2 , 123.7 , 117.8 , 113.6 , 55.2; HRMS (EI) for $C_{25}H_{18}NO_3^+$ $(M+H)^+$: calculated 380.1281, found 380.1282. (**Condition A**).



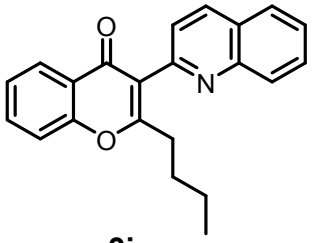
3g

2-(3-fluorophenyl)-3-(quinolin-2-yl)-4*H*-chromen-4-one (3g). (30.1 mg, 82%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 – 8.28 (m, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.86 – 7.80 (m, 1H), 7.78 – 7.71 (m, 1H), 7.70 – 7.64 (m, 1H), 7.60 – 7.51 (m, 3H), 7.49 – 7.45 (m, 1H), 7.26 – 7.22 (m, 1H), 7.16 – 7.07 (m, 2H), 7.02 – 6.97 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.2 , 162.2 (d, *J* = 247.0 Hz), 161.7 , 156.0 , 153.1 , 136.3 , 134.9 (d, *J* = 8.1 Hz), 134.1 , 129.7 (d, *J* = 8.1 Hz), 129.5 , 129.4 , 127.6 , 127.2 , 126.9 , 126.3 , 125.5 , 125.2 (d, *J* = 3.1 Hz), 124.0 , 123.7 , 118.0 , 117.3 (d, *J* = 21.2 Hz), 116.3 (d, *J* = 23.8 Hz), 100.0; HRMS (EI) for $C_{24}H_{15}FNO_2^+$ $(M+H)^+$: calculated 368.1081, found 368.1081. (**Condition A**).



3h

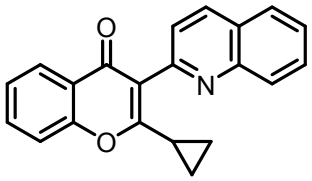
3-(quinolin-2-yl)-2-(thiophen-3-yl)-4H-chromen-4-one (3h). (34.8 mg, 98%). White solid. ethyl acetate : hexane = 1 : 4; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 – 8.23 (m, 2H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.91 – 7.86 (m, 1H), 7.75 – 7.69 (m, 2H), 7.61 – 7.55 (m, 2H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.48 – 7.46 (m, 1H), 7.45 – 7.40 (m, 1H), 7.12 – 7.07 (m, 1H), 6.80 – 6.76 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.53 , 157.85 , 155.83 , 153.80 , 148.26 , 136.71 , 133.87 , 133.68 , 129.64 , 129.57 , 127.61 , 127.41 , 127.31 , 126.95 , 126.07 , 125.55 , 125.16 , 123.95 , 123.64 , 121.84 , 117.82; HRMS (EI) for $C_{22}H_{14}NO_2S^+$ $(M+H)^+$: calculated 356.0740, found 356.0740. (**Condition A**).



3i

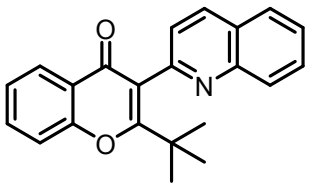
2-butyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3i). (18.4 mg, 56%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 – 8.25 (m, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.75 – 7.70 (m, 1H), 7.70 – 7.66 (m, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.60 –

7.54 (m, 1H), 7.50 (d, J = 8.2 Hz, 1H), 7.43 – 7.37 (m, 1H), 2.78 – 2.71 (m, 2H), 1.79 – 1.70 (m, 2H), 1.34 – 1.24 (m, 2H), 0.82 (t, J = 7.4 Hz, 3H).; ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.8 , 169.3 , 156.0 , 153.7 , 148.1 , 135.7 , 133.5 , 129.4 , 129.3 , 127.6 , 127.3 , 126.6 , 126.1 , 125.0 , 124.2 , 123.8 , 123.1 , 117.7 , 32.3 , 29.5 , 22.3 , 13.6; HRMS (EI) for $C_{22}H_{20}NO_2^+$ $(M+H)^+$: calculated 330.1489, found 330.1491. (**Condition A**).



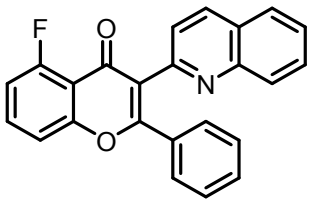
3j

2-cyclopropyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3j). (27.3 mg, 87%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 – 8.16 (m, 2H), 8.08 (d, J = 8.3 Hz, 1H), 7.83 – 7.79 (m, 1H), 7.68 – 7.64 (m, 1H), 7.62 (d, J = 8.5 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.54 – 7.48 (m, 1H), 7.35 – 7.29 (m, 2H), 2.17 – 2.09 (m, 1H), 1.34 – 1.28 (m, 2H), 0.98 – 0.91 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.0 , 168.7 , 155.4 , 153.8 , 136.0 , 133.4 , 129.4 , 129.3 , 127.6 , 127.3 , 126.7 , 126.2 , 125.0 , 124.6 , 123.8 , 122.8 , 117.3 , 12.9 , 9.5; HRMS (EI) for $C_{24}H_{16}NO_2^+$ $(M+H)^+$: calculated 314.1176, found 314.1177. (**Condition A**).



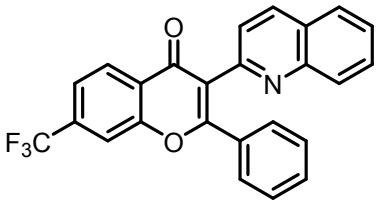
3k

2-(*tert*-butyl)-3-(quinolin-2-yl)-4*H*-chromen-4-one (3k). (9.9 mg, 30%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 – 8.09 (m, 2H), 8.03 (d, J = 8.6 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.67 – 7.63 (m, 1H), 7.63 – 7.59 (m, 1H), 7.53 – 7.48 (m, 1H), 7.46 – 7.40 (m, 1H), 7.39 (d, J = 8.4 Hz, 1H), 7.34 – 7.29 (m, 1H), 1.14 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6 , 172.2 , 155.9 , 155.1 , 147.7 , 135.6 , 133.6 , 129.6 , 129.4 , 127.6 , 127.3 , 126.7 , 125.9 , 124.9 , 124.8 , 123.1 , 123.0 , 117.6 , 39.2 , 29.5; HRMS (EI) for $C_{22}H_{20}NO_2^+$ $(M+H)^+$: calculated 330.1489, found 330.1490. (**Condition A**).



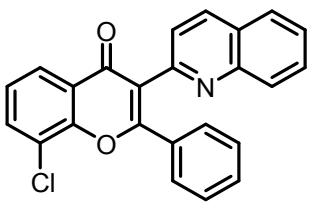
3l

5-fluoro-2-phenyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3l). (28.0 mg, 76%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.83 – 7.79 (m, 1H), 7.67 – 7.60 (m, 2H), 7.55 – 7.48 (m, 2H), 7.41 – 7.35 (m, 3H), 7.31 – 7.26 (m, 1H), 7.22 – 7.16 (m, 2H), 7.11 – 7.03 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.6 (d, *J* = 1.8 Hz), 162.4 , 160.9 (d, *J* = 265.9 Hz), 157.1 (d, *J* = 3.5 Hz), 153.1 , 148.0 , 136.1 , 133.9 (d, *J* = 10.7 Hz), 132.2 , 130.4 , 129.4 , 129.2 , 128.1 , 127.5 , 127.2 , 126.8 , 124.2 , 123.8 , 114.2 (d, *J* = 10.1 Hz), 113.9 (d, *J* = 4.5 Hz), 112.1 (d, *J* = 20.6 Hz); HRMS (EI) for $C_{24}H_{15}FNO_2^+$ $(M+H)^+$: calculated 368.1081, found 368.1081. (**Condition A**).



3m

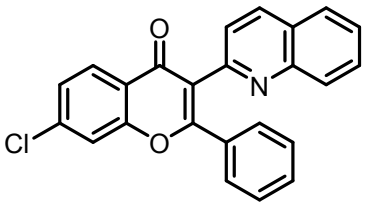
2-phenyl-3-(quinolin-2-yl)-7-(trifluoromethyl)-4*H*-chromen-4-one. (3m). (30 mg, 72%). Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.2 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.91 (s, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.68 (t, *J* = 8.4 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.43 (d, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.21 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.3 , 163.9 , 155.4 , 152.9 , 148.1 , 136.3 , 135.3 (q, *J* = 33.3 Hz), 132.1 , 130.6 , 129.4 , 129.4 , 129.2 , 128.1 , 127.5 , 127.5 , 127.1 , 126.8 , 125.9 , 123.8 , 123.6 , 123.0 (q, *J* = 273.0 Hz), 121.5 (q, *J* = 3.3 Hz), 115.9 (q, *J* = 4.1 Hz). HRMS (EI) for $C_{25}H_{15}F_3NO_2^+$ $(M+H)^+$: calculated 418.1049, found 418.1049



3o

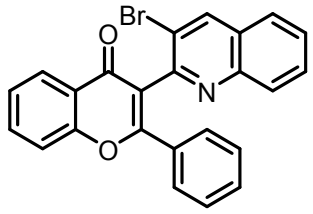
8-chloro-2-phenyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3o). (33.9 mg, 89%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 – 8.11 (m, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.91

(d, J = 8.4 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.72 – 7.69 (m, 1H), 7.62 – 7.57 (m, 1H), 7.49 – 7.45 (m, 1H), 7.42 – 7.37 (m, 3H), 7.30 (t, J = 7.9 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.13 (t, J = 7.7 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.9 , 163.0 , 153.2 , 151.8 , 148.1 , 136.4 , 134.0 , 132.2 , 130.7 , 129.8 , 129.5 , 128.7 , 128.2 , 127.5 , 127.2 , 126.9 , 125.3 , 125.1 , 124.8 , 124.0 , 123.1 , 122.9; HRMS (EI) for $C_{24}H_{15}ClNO_2^+$ $(M+H)^+$: calculated 384.0786, found 384.0787. (**Condition B**).



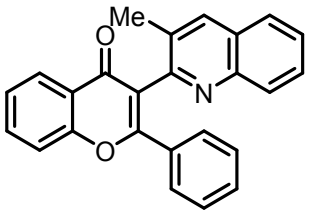
3p

7-chloro-2-phenyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3p). (30.3 mg, 79%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, J = 8.5 Hz, 1H), 8.16 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 8.5 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.61 (d, J = 1.9 Hz, 1H), 7.57 – 7.52 (m, 1H), 7.46 (d, J = 8.4 Hz, 1H), 7.43 – 7.40 (m, 1H), 7.40 – 7.36 (m, 2H), 7.32 – 7.27 (m, 1H), 7.22 – 7.17 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.5 , 163.4 , 156.2 , 153.2 , 148.1 , 139.9 , 136.3 , 132.4 , 130.5 , 129.5 , 129.4 , 129.3 , 128.2 , 127.7 , 127.5 , 127.2 , 126.8 , 126.2 , 124.0 , 123.3 , 122.3 , 118.1; HRMS (EI) for $C_{24}H_{15}ClNO_2^+$ $(M+H)^+$: calculated 384.0786, found 384.0785. (**Condition B**).



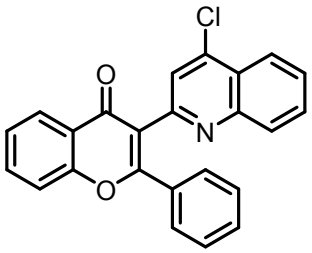
4a

3-(3-bromoquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4a). (26.6 mg, 62%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.33 – 8.28 (m, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.77 – 7.71 (m, 2H), 7.71 – 7.66 (m, 1H), 7.61 – 7.53 (m, 2H), 7.52 – 7.48 (m, 2H), 7.48 – 7.42 (m, 1H), 7.33 – 7.27 (m, 1H), 7.25 – 7.19 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.7 , 162.7 , 156.2 , 153.5 , 146.6 , 139.1 , 134.0 , 132.6 , 130.5 , 129.8 , 129.5 , 128.7 , 128.5 , 128.2 , 127.7 , 126.6 , 126.2 , 125.3 , 123.5 , 122.9 , 119.8 , 118.0; HRMS (EI) for $C_{24}H_{14}BrKNO_2^+$ $(M+K)^+$: calculated 465.9839, found 465.9834. (**Condition A**).



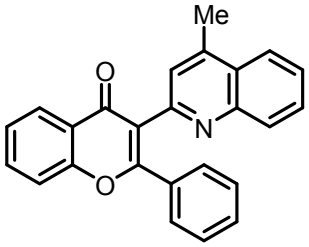
4b

3-(3-methylquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4b). (21.8 mg, 60%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 – 8.27 (m, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.97 (s, 1H), 7.79 – 7.71 (m, 2H), 7.65 – 7.57 (m, 2H), 7.54 – 7.48 (m, 1H), 7.48 – 7.39 (m, 3H), 7.31 – 7.24 (m, 1H), 7.19 (t, *J* = 7.7 Hz, 2H), 2.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.2 , 162.1 , 156.2 , 154.7 , 146.7 , 136.3 , 133.9 , 132.6 , 131.3 , 130.4 , 129.2 , 128.7 , 128.5 , 128.2 , 128.0 , 126.8 , 126.7 , 126.2 , 125.2 , 123.6 , 122.6 , 118.0 , 19.0; HRMS (EI) for $C_{25}H_{18}NO_2^+$ $(M+H)^+$: calculated 364.1332, found 364.1334. (**Condition A**).



4c

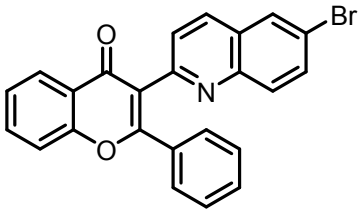
3-(4-chloroquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4c). (29.0 mg, 76%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 – 8.19 (m, 1H), 8.17 – 8.11 (m, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.69 – 7.62 (m, 1H), 7.65 – 7.57 (m, 1H), 7.57 (s, 1H), 7.58 – 7.50 (m, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.41 – 7.32 (m, 3H), 7.27 – 7.19 (m, 1H), 7.15 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.06 , 163.75 , 156.07 , 153.49 , 148.74 , 142.41 , 134.04 , 132.60 , 130.48 , 130.21 , 129.74 , 129.23 , 128.22 , 127.68 , 126.19 , 125.43 , 125.41 , 124.21 , 123.91 , 123.64 , 122.23 , 118.01; HRMS (EI) for $C_{24}H_{15}ClNO_2^+$ $(M+H)^+$: calculated 384.0786, found 384.0786. (**Condition A**).



4d

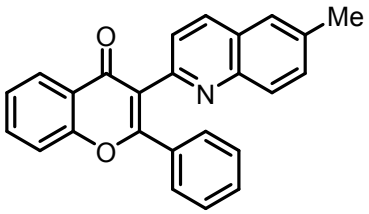
3-(4-methylquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4d). (34.2 mg, 94%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 – 8.20 (m, 1H), 7.93 – 7.87 (m, 1H), 7.85 (d,

J = 8.3 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.57 – 7.52 (m, 1H), 7.51 – 7.43 (m, 2H), 7.38 – 7.34 (m, 3H), 7.29 (s, 1H), 7.22 – 7.18 (m, 1H), 7.11 (t, *J* = 7.6 Hz, 2H), 2.61 (d, *J* = 1.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.5 , 163.1 , 156.1 , 153.3 , 147.8 , 144.3 , 133.8 , 132.9 , 130.2 , 130.0 , 129.2 , 129.0 , 128.1 , 127.3 , 126.4 , 126.2 , 125.2 , 124.7 , 123.7 , 123.6 , 123.1 , 117.9 , 18.8; HRMS (EI) for $C_{25}H_{18}NO_2^+$ $(M+H)^+$: calculated 364.1332, found 364.1334. (**Condition A**).



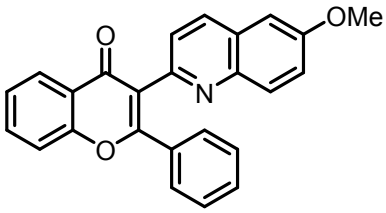
4e

3-(6-bromoquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4e). (37.7 mg, 88%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 – 8.20 (m, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 2.1 Hz, 1H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.68 – 7.60 (m, 2H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.44 (d, *J* = 8.5 Hz, 1H), 7.40 – 7.35 (m, 1H), 7.32 – 7.28 (m, 2H), 7.26 – 7.20 (m, 1H), 7.15 – 7.10 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.15 , 163.55 , 156.09 , 154.15 , 146.59 , 135.04 , 134.00 , 132.84 , 132.70 , 131.10 , 130.40 , 129.52 , 129.24 , 128.19 , 128.16 , 126.21 , 125.38 , 125.10 , 123.69 , 122.72 , 120.64 , 118.01; HRMS (EI) for $C_{24}H_{25}BrNO_2^+$ $(M+H)^+$: calculated 428.0281, found 428.0281. (**Condition A**).



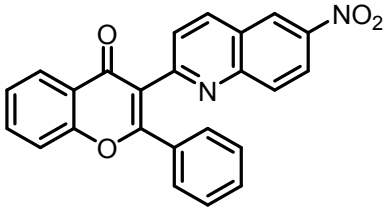
4f

3-(6-methylquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4f). (31.3, 86%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 – 8.21 (m, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.50 – 7.46 (m, 2H), 7.41 – 7.38 (m, 1H), 7.36 (d, *J* = 8.3 Hz, 2H), 7.36 – 7.30 (m, 2H), 7.22 – 7.17 (m, 1H), 7.13 – 7.07 (m, 2H), 2.44 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.3 , 163.2 , 156.1 , 152.6 , 146.7 , 136.6 , 135.4 , 133.8 , 132.9 , 131.6 , 130.2 , 129.2 , 129.1 , 128.0 , 127.1 , 126.3 , 126.2 , 125.2 , 124.1 , 123.8 , 123.1 , 117.9 , 21.6; HRMS (EI) for $C_{25}H_{18}NO_2^+$ $(M+H)^+$: calculated 364.1332, found 364.1331. (**Condition A**).



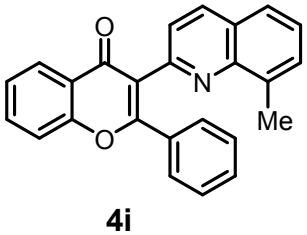
4g

3-(6-methoxyquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4g). (32.6 mg, 86%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 – 8.21 (m, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 9.2 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.48 (d, *J* = 8.3 Hz, 1H), 7.37 – 7.31 (m, 4H), 7.24 – 7.17 (m, 2H), 7.11 (t, *J* = 7.7 Hz, 2H), 6.99 (d, *J* = 2.7 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.4 , 163.2 , 157.9 , 156.1 , 150.9 , 144.2 , 134.9 , 133.8 , 132.9 , 130.8 , 130.2 , 129.6 , 129.3 , 128.2 , 128.0 , 126.2 , 125.2 , 124.4 , 123.8 , 122.1 , 117.9 , 105.0 , 55.5; HRMS (EI) for $C_{25}H_{18}NO_3^+$ $(M+H)^+$: calculated 380.1281, found 380.1283. (**Condition A**).



4h

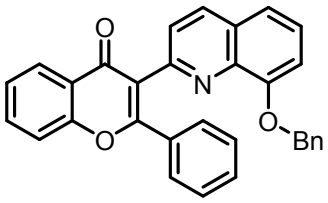
3-(6-nitroquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4h). (30.0 mg, 76%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 2.5 Hz, 1H), 8.35 – 8.32 (m, 1H), 8.28 – 8.23 (m, 2H), 7.97 (d, *J* = 9.2 Hz, 1H), 7.72 – 7.67 (m, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.53 (d, *J* = 8.3 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.34 – 7.29 (m, 2H), 7.29 – 7.23 (m, 1H), 7.16 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.0 , 164.2 , 157.7 , 156.1 , 149.9 , 145.6 , 137.7 , 134.3 , 132.5 , 131.1 , 130.7 , 129.3 , 128.3 , 126.2 , 125.8 , 125.6 , 124.3 , 123.6 , 122.9 , 122.3 , 118.1; HRMS (EI) for $C_{24}H_{15}N_2O_4^+$ $(M+H)^+$: calculated 395.1026, found 395.1025. (**Condition A**).



4i

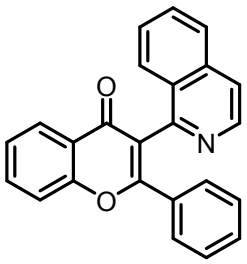
3-(8-methylquinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4i). (31.3 mg, 86%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 – 8.23 (m, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 8.3 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.34 (d, *J* = 6.7 Hz, 1H), 7.31 – 7.28 (m, 3H), 7.22 – 7.17 (m, 1H), 7.10 (t, *J* = 7.7 Hz, 2H), 2.29

(s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.3 , 164.4 , 156.1 , 151.9 , 146.9 , 137.4 , 135.8 , 133.8 , 133.7 , 129.9 , 129.3 , 129.1 , 127.9 , 127.1 , 126.3 , 126.2 , 125.4 , 125.2 , 124.0 , 123.9 , 123.2 , 118.0 , 17.6; HRMS (EI) for $C_{25}H_{18}NO_2^+$ $(M+H)^+$: calculated 364.1332, found 364.1331. (**Condition A**).



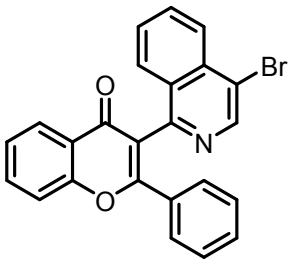
4j

3-(8-(benzyloxy)quinolin-2-yl)-2-phenyl-4*H*-chromen-4-one (4j). (40.1 mg, 88%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 7.9 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 8.6 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 1H), 7.38 – 7.31 (m, 3H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.23 – 7.17 (m, 4H), 7.16 (d, *J* = 5.8 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 4H), 6.82 (d, *J* = 7.6 Hz, 1H), 5.09 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.4 , 163.8 , 156.0 , 154.1 , 152.2 , 140.5 , 137.2 , 135.7 , 133.8 , 133.3 , 129.9 , 129.5 , 128.5 , 128.3 , 127.9 , 127.4 , 126.8 , 126.6 , 126.1 , 125.2 , 124.8 , 123.8 , 123.3 , 119.9 , 117.9 , 111.3 , 70.7; HRMS (EI) for $C_{31}H_{22}NO_3^+$ $(M+H)^+$: calculated 456.1594, found 456.1590. (**Condition A**).



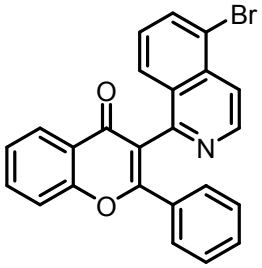
4k

3-(isoquinolin-1-yl)-2-phenyl-4*H*-chromen-4-one (4k). (17.5mg, 50%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (d, *J* = 5.7 Hz, 1H), 8.33 – 8.27 (m, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.3 Hz, 1H), 7.80 – 7.73 (m, 1H), 7.68 – 7.60 (m, 3H), 7.53 – 7.44 (m, 2H), 7.36 – 7.30 (m, 2H), 7.25 (t, *J* = 7.4 Hz, 1H), 7.14 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.3 , 163.2 , 156.3 , 154.6 , 142.5 , 136.2 , 134.0 , 132.7 , 130.4 , 130.2 , 128.7 , 128.6 , 128.1 , 127.6 , 127.1 , 126.5 , 126.3 , 125.4 , 123.5 , 121.6 , 120.8 , 118.0; HRMS (EI) for $C_{24}H_{16}NO_2^+$ $(M+H)^+$: calculated 350.1176, found 350.1177. (**Condition B**).



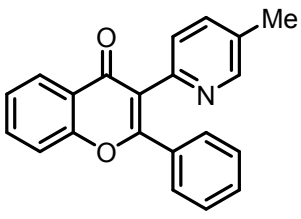
4l

3-(4-bromoisoquinolin-1-yl)-2-phenyl-4*H*-chromen-4-one (4l). (32.9 mg, 75%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.23 – 8.19 (m, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.41 – 7.36 (m, 1H), 7.29 – 7.24 (m, 2H), 7.22 – 7.17 (m, 1H), 7.10 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.1 , 163.4 , 156.3 , 154.2 , 144.2 , 135.0 , 134.1 , 132.5 , 131.5 , 130.6 , 129.8 , 128.6 , 128.3 , 127.0 , 126.4 , 126.3 , 125.5 , 123.4 , 121.0 , 119.8 , 118.1; HRMS (EI) for $C_{24}H_{25}BrNNaO_2^+$ $(M+Na)^+$: calculated 450.0100, found 450.0095. (**Condition B**).



4m

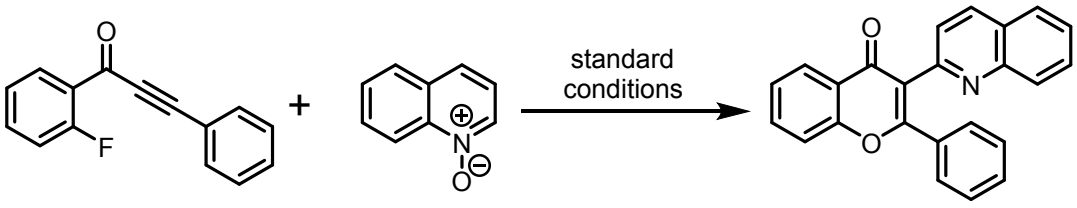
3-(5-bromoisoquinolin-1-yl)-2-phenyl-4*H*-chromen-4-one (4m). (18.1 mg, 43%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, *J* = 5.9 Hz, 1H), 8.24 – 8.18 (m, 1H), 7.93 (d, *J* = 5.9 Hz, 1H), 7.86 (d, *J* = 7.4 Hz, 1H), 7.80 (d, *J* = 8.3 Hz, 1H), 7.72 – 7.66 (m, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.29 – 7.22 (m, 3H), 7.19 (d, *J* = 6.4 Hz, 1H), 7.09 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.2 , 163.5 , 156.3 , 155.2 , 143.8 , 135.4 , 134.1 , 134.0 , 132.5 , 130.6 , 129.8 , 128.6 , 128.3 , 128.0 , 126.4 , 126.3 , 125.5 , 123.4 , 122.0 , 121.3 , 119.8 , 118.1; HRMS (EI) for $C_{24}H_{25}BrNO_2^+$ $(M+H)^+$: calculated 428.0281, found 428.0281. (**Condition B**).



4n

3-(5-methylpyridin-2-yl)-2-phenyl-4*H*-chromen-4-one (4n). (10.7 mg, 34%). White solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 4.7 Hz, 1H), 8.31 – 8.27 (m, 1H), 7.75 – 7.71 (m, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.53 – 7.50 (m, 1H), 7.48 – 7.42 (m, 1H), 7.41 – 7.33 (m, 3H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.20 – 7.16 (m, 1H), 2.12 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.96 , 162.19 , 156.20 , 152.67 , 147.24 , 137.92 , 133.84 , 133.80 , 132.82 , 130.41 , 128.69 , 128.17 , 126.24 , 125.19 , 123.55 , 123.01 , 122.38 , 117.98 , 18.68; HRMS (EI) for $C_{21}H_{16}NO_2^+$ $(M+H)^+$: calculated 314.1176, found 314.1177. (**Condition B**).

2.4 Procedure for the Gram-Scale Preparation of 3a

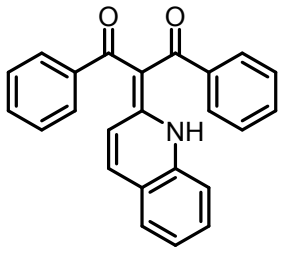


1a, 5 mmol **2a**, 1.5 equiv **3a**, 1.59 g, 91%

A dried 100 mL Schlenk tube was charged with **1-(2-fluorophenyl)-3-phenylprop-2-yn-1-one 1a** (1.12 g, 5 mmol, 1 equiv), quinoline *N*-oxide **2a** (1.09 g, 7.5 mmol, 1.5 equiv), and toluene (25 mL). The reaction mixture was heated to 120 °C for 12 hours under vigorous stirring. Upon completion, the reaction mixture was cooled to room temperature. The solvent was concentrated under vacuum, and the resulting residue was purified by flash chromatograpy with acetate : hexane = 1 : 4 to give the corresponding products **2-phenyl-3-(quinolin-2-yl)-4*H*-chromen-4-one (3a)** (1.59 g, 91%) as a white solid.

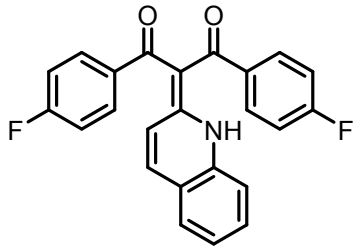
2.5 Procedure for the Preparation of 5

A dried 10 mL Schlenk tube was charged with 1,3-diphenylprop-2-yn-1-one **1r** (20.7 mg, 0.1 mmol, 1 equiv), quinoline *N*-oxide **2a** (21.8 mg, 0.15 mmol, 1.5 equiv), and toluene (0.5 mL). The reaction mixture was heated to 120 °C for 12 hours under vigorous stirring. Upon completion, the reaction mixture was cooled to room temperature. The solvent was concentrated under vacuum, and the resulting residue was purified by preparative thin layer chromatograpy (PTLC) with acetate : hexane = 1 : 4 to give the corresponding products **1,3-diphenyl-2-(quinolin-2(1*H*)-ylidene)propane-1,3-dione (5a)** (31.6 mg, 90%) as a yellow solid.



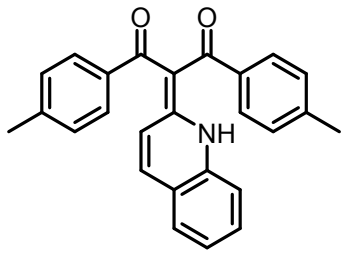
5a

1,3-diphenyl-2-(quinolin-2(1*H*)-ylidene)propane-1,3-dione (5a). (31.6 mg, 90%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 1.7 Hz, 2H), 7.72 – 7.65 (m, 3H), 7.61 (d, *J* = 7.3 Hz, 2H), 7.45 – 7.37 (m, 3H), 7.21 (d, *J* = 7.0 Hz, 1H), 7.12 (q, *J* = 7.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.65 , 192.79 , 154.43 , 142.56 , 142.15 , 138.33 , 136.41 , 131.65 , 131.42 , 129.77 , 129.29 , 128.14 , 127.74 , 127.71 , 125.07 , 123.69 , 119.79 , 118.62 , 106.10; HRMS (EI) for $C_{24}H_{17}NO_2^+$ $(M+H)^+$: calculated 352.1332, found 352.1333.



5b

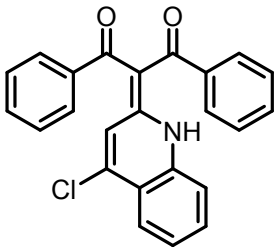
1,3-bis(4-fluorophenyl)-2-(quinolin-2(1*H*)-ylidene)propane-1,3-dione (5b). (32.9 mg, 85%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.9 (q, *J* = 9.5 Hz, 2H), 7.7 – 7.6 (m, 5H), 7.5 – 7.4 (m, 3H), 6.8 (t, *J* = 7.9 Hz, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.8 , 191.1 , 164.5 (d, *J* = 254.5 Hz), , 163.4 (d, *J* = 257.0 Hz), 154.3 , 138.7, 138.5, 138.3, 136.2 , 131.7, 131.6, 130.2, 127.7 , 125.2 , 123.7 , 119.5 , 118.5, 114.8 (d, *J* = 21.7 Hz). HRMS (EI) for $C_{24}H_{16}F_2NO_2^+$ $(M+H)^+$: calculated 388.1144, found 388.1145.



5c

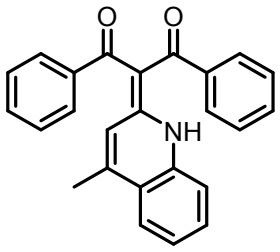
2-(quinolin-2(1*H*)-ylidene)-1,3-di-p-tolylpropane-1,3-dione (5c). (18.1 mg, 48%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 9.5 Hz, 1H), 7.74 (d, *J* = 9.5 Hz, 1H), 7.64 (d, *J* = 6.9 Hz, 3H), 7.58 (d, *J* = 7.7 Hz, 2H), 7.41 – 7.35 (m, 1H), 7.34 (d, *J* = 7.6 Hz, 2H), 6.99 –

6.88 (m, 4H), 2.22 (d, J = 21.2 Hz, 6H).; ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.3 , 191.8 , 154.2 , 142.2 , 139.9 , 139.6 , 139.1 , 137.8 , 136.6 , 131.5 , 129.5 , 129.1 , 128.5 , 128.4 , 128.1 , 127.6 , 124.8 , 123.5 , 119.8 , 118.5 , 106.1 , 21.4 , 21.3 . HRMS (EI) for $C_{26}H_{22}NO_2^+$ $(M+H)^+$: calculated 380.1645, found 380.1644.



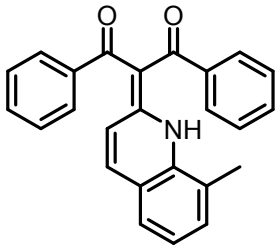
5d

2-(4-chloroquinolin-2(1*H*)-ylidene)-1,3-diphenylpropane-1,3-dione (5d). (17.2 mg, 45%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (s, 1H), 8.06 (d, J = 8.1 Hz, 1H), 7.72 (t, J = 7.6 Hz, 1H), 7.65 (d, J = 8.2 Hz, 1H), 7.59 (d, J = 7.4 Hz, 2H), 7.48 (t, J = 7.6 Hz, 1H), 7.39 (d, J = 6.8 Hz, 2H), 7.21 (t, J = 7.0 Hz, 1H), 7.16 – 7.01 (m, 5H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.1 , 189.8 , 154.7 , 142.2 , 140.9 , 138.6 , 136.1 , 131.7 , 131.3 , 131.1 , 129.7 , 129.3 , 128.5 , 127.7 (d, J = 2.1 Hz), 125.9 , 125.4 , 123.8 , 120.0 , 118.8 , 107.6 . HRMS (EI) for $C_{24}H_{17}ClNO_2^+$ $(M+H)^+$: calculated 386.0942, found 386.0943.



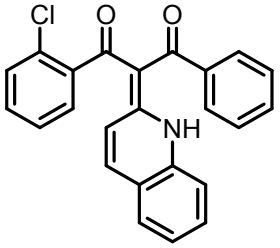
5e

2-(4-methylquinolin-2(1*H*)-ylidene)-1,3-diphenylpropane-1,3-dione (5e). (20.1 mg, 55%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 9.3 Hz, 2H), 7.67 (d, J = 5.9 Hz, 2H), 7.60 (s, 2H), 7.47 – 7.42 (m, 1H), 7.39 (s, 2H), 7.20 (s, 1H), 7.10 (s, 5H), 2.62 (s, 3H) ; ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.9 , 192.9 , 153.9 , 147.5 , 142.8 , 142.4 , 136.1 , 131.3 , 129.6 , 129.3 , 128.1 , 127.7 , 124.9 , 124.2 , 124.0 , 119.1 , 119.0 , 105.5 , 19.6 . HRMS (EI) for $C_{25}H_{20}NO_2^+$ $(M+H)^+$: calculated 366.1489, found 366.1487.



5f

2-(8-methylquinolin-2(1*H*)-ylidene)-1,3-diphenylpropane-1,3-dione (5f). (22.3 mg, 60%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (s, 2H), 7.62 (d, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.3 Hz, 2H), 7.44 – 7.38 (m, 2H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.11 (m, *J* = 6.8, 5.8 Hz, 5H), 2.79 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.7 , 192.7 , 154.1 , 142.7 , 142.2 , 138.8 , 135.6 , 132.2 , 131.3 , 129.6 , 129.3 , 128.2 , 127.7 , 127.7 , 126.8 , 125.5 , 124.8 , 123.7 , 119.3 , 106.3 , 17.2 . HRMS (EI) for $C_{25}H_{20}NO_2^+$ $(M+H)^+$: calculated 366.1489, found 366.1488.

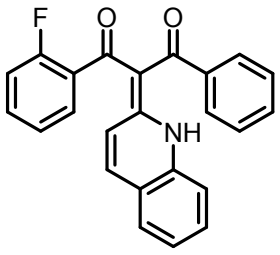


5g

(*E*)-1-(2-chlorophenyl)-3-phenyl-2-(quinolin-2(1*H*)-ylidene)propane-1,3-dione (5g). (26.6 mg, 69%). Yellow solid. ethyl acetate : hexane = 1 : 4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.4 Hz, 1H), 7.82 (s, 1H), 7.70 (t, *J* = 5.6 Hz, 3H), 7.59 (s, 2H), 7.48 – 7.41 (m, 1H), 7.30 – 7.10 (m, 4H), 7.05 – 6.92 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.1 , 189.8 , 154.7 , 142.2 , 140.9 , 138.6 , 136.1 , 131.7 , 131.3 , 131.1 , 129.7 , 129.3 , 128.5 , 127.7 , 125.9 , 125.4 , 123.8 , 120.0 , 118.8 , 107.6. HRMS (EI) for $C_{24}H_{17}ClNO_2^+$ $(M+H)^+$: calculated 386.0942, found 386.0944.

2.6 Procedure for the Preparation of 6

A dried 50 mL Schlenk tube was charged with 20 mL of H_2O were added sequentially the ynone **1a** (224.3 mg, 1 mmol, 1 equiv), qunoline *N*-oxide **2a** (218 mg, 1.5 mmol, 1.5 equiv). The resulting mixture was stirred at 100 ºC, and the progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was extracted by ethyl acetate and dried by Na_2SO_4 and then concentrated under vacuum. The residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired product **1-(2-fluorophenyl)-3-phenyl-2-(quinolin-2-yl)propane-1,3-dione (6)** (296 mg) in 80% yield as a yellow solid.

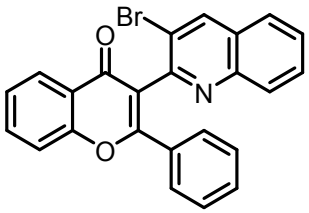


6

(*E*)-1-(2-fluorophenyl)-3-phenyl-2-(quinolin-2(1*H*)-ylidene)propane-1,3-dione (6). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.88 (s, 1H), 7.77 – 7.55 (m, 5H), 7.48 – 7.39 (m, 1H), 7.24 (s, 2H), 7.16 (d, *J* = 6.7 Hz, 2H), 7.06 (q, *J* = 6.7, 6.1 Hz, 1H), 6.88 (t, *J* = 7.2 Hz, 1H), 6.69 (t, *J* = 9.2 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.88 , 188.10 , 158.46 (d, *J* = 248.9 Hz), 154.47 , 142.04 , 138.61 , 136.07 , 131.71 , 131.40 , 130.91 , 129.39 , 128.77 , 127.71 , 127.67 , 125.32 , 123.81 , 123.34 (d, *J* = 2.5 Hz), 119.83 , 118.68 , 115.43 (d, *J* = 22.7 Hz), 107.50; HRMS (EI) for $C_{24}H_{17}FNO_2^+$ $(M+H)^+$: calculated 370.1238, found 370.1237.

2.7 Crystal Data and structure Refinement for 4a

Crystal structure and data of 4a (CCDC 1940117, Displacement ellipsoids are drawn at the 50% probability level.)



4a

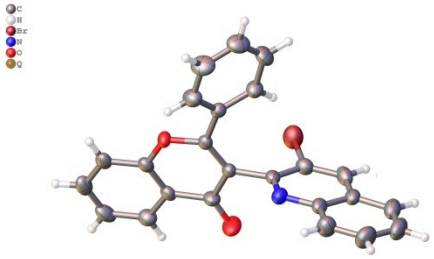


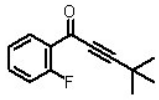
Table S3 Crystal data and structure refinement for exp_7038.

Identification code	exp_7038
Empirical formula	$C_{24}H_{14}NO_2Br$
Formula weight	428.27
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	6.7672(7)
b/Å	9.2017(10)
c/Å	15.1089(11)
α/°	81.431(7)
β/°	82.868(7)
γ/°	80.818(9)
Volume/Å^3	913.54(15)
Z	2
ρ_{calc}g/cm^3	1.557
μ/mm^{-1}	2.270
F(000)	432.0
Crystal size/mm^3	0.10 × 0.10 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.14 to 52
Index ranges	$-6 \le h \le 8$, $-11 \le k \le 11$, $-15 \le l \le 18$
Reflections collected	6979
Data/restraints/parameters	3582/0/253
Goodness-of-fit on F^2	0.952
Final R indexes [I>=2σ (I)]	R_1 = 0.0710, wR_2 = 0.1675
Final R indexes [all data]	R_1 = 0.1014, wR_2 = 0.1868
Largest diff. peak/hole / e Å^{-3}	0.70/-1.22

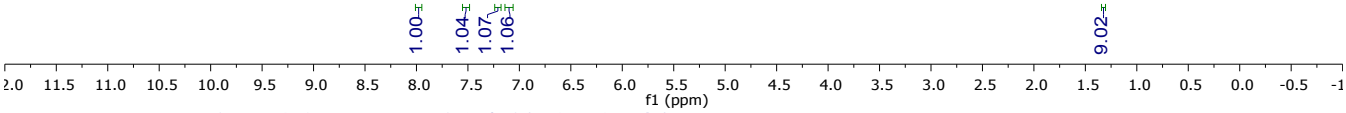
Reference:

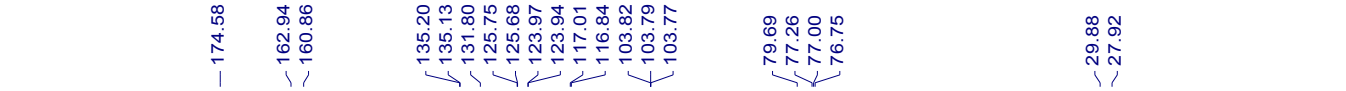
1. (a) X. Wang, G. Cheng, and X. Cui *Chem.Commun*. 2013, **50**, 652-654; (b) J. Liu, D. Ba, W. Lv, Y. Chen, Z. Zhao, and G. Cheng *Adv. Synth. Catal.* 2019, DOI: 10.1002/adsc.201900960.

3. ^{1}H and ^{13}C NMR Spectra

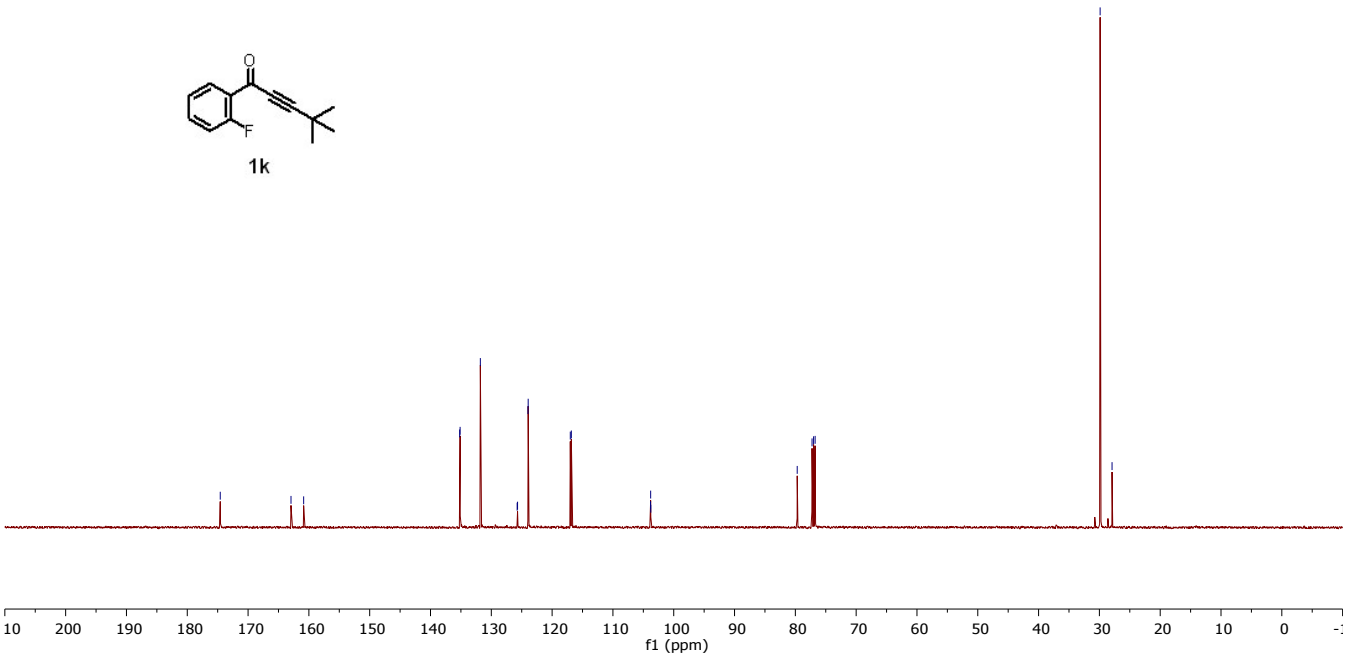


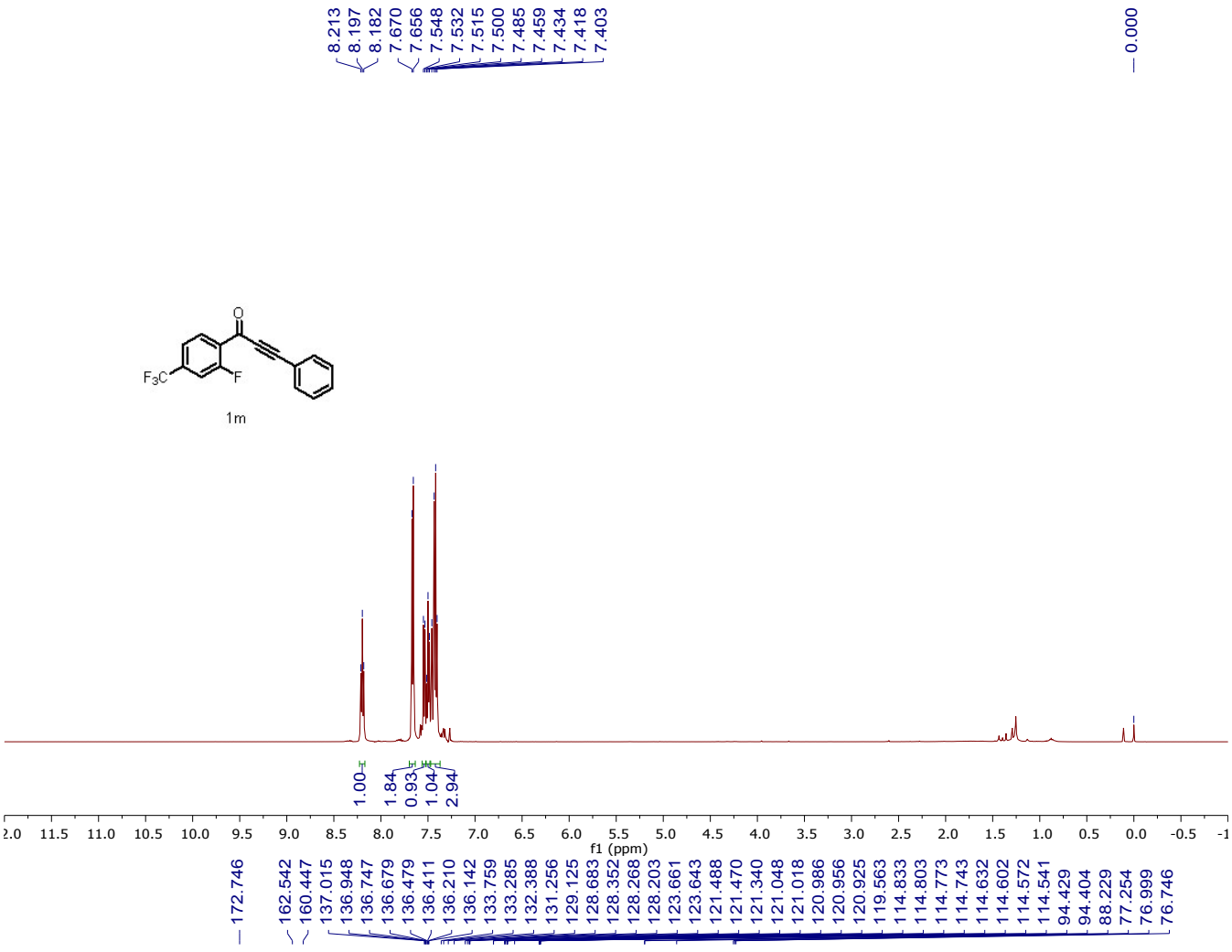
1k





1k

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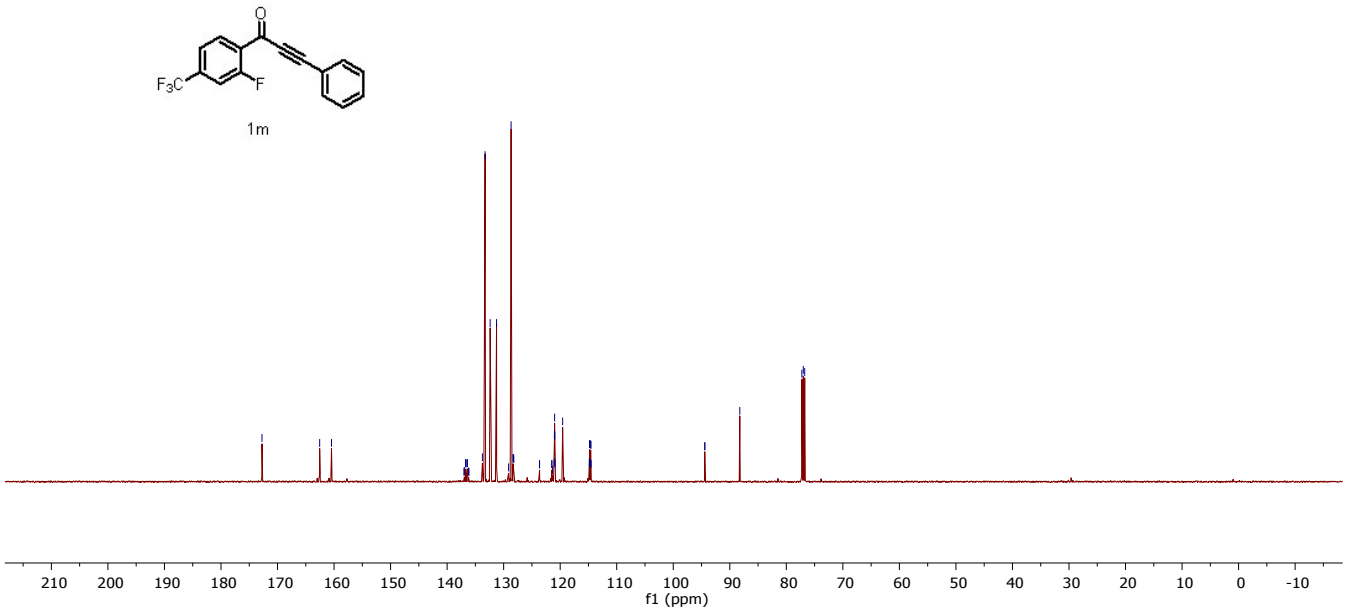
8.197
8.182
7.670
7.656
7.548
7.532
7.515
7.500
7.485
7.459
7.434
7.418
7.403
0.000
F3C
F
O
1m
1.00
1.84
0.93
1.04
2.94
f1 (ppm)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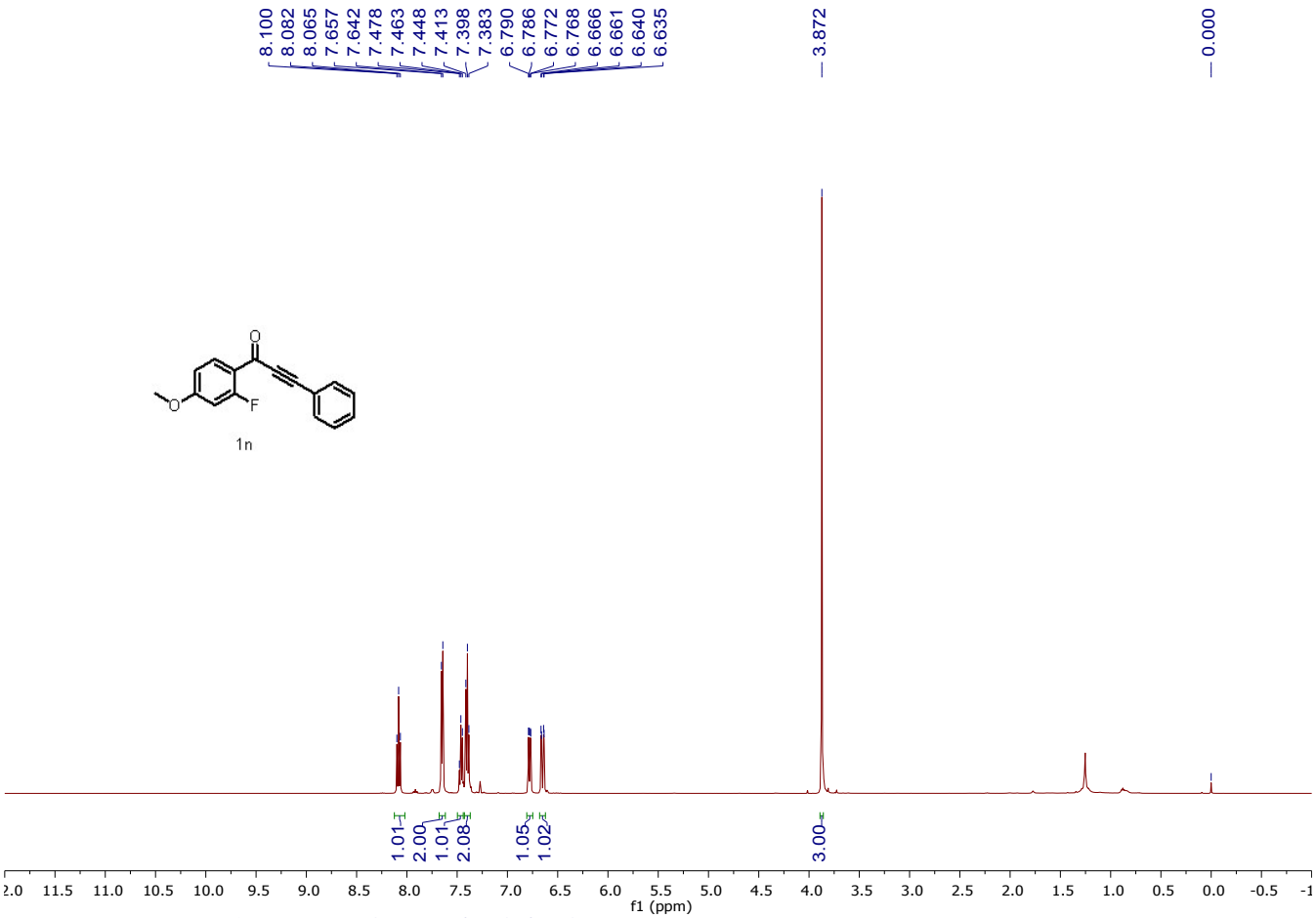
162.542
160.447
137.015
136.948
136.747
136.679
136.479
136.411
136.210
136.142
133.759
133.285
132.388
131.256
129.125
128.683
128.352
128.268
128.203
123.661
123.643
121.488
121.470
121.340
121.048
121.018
120.986
120.956
120.925
119.563
114.833
114.803
114.773
114.743
114.632
114.602
114.572
114.541
94.429
94.404
88.229
77.254
76.999
76.746
F3C
F
O
1m
f1 (ppm)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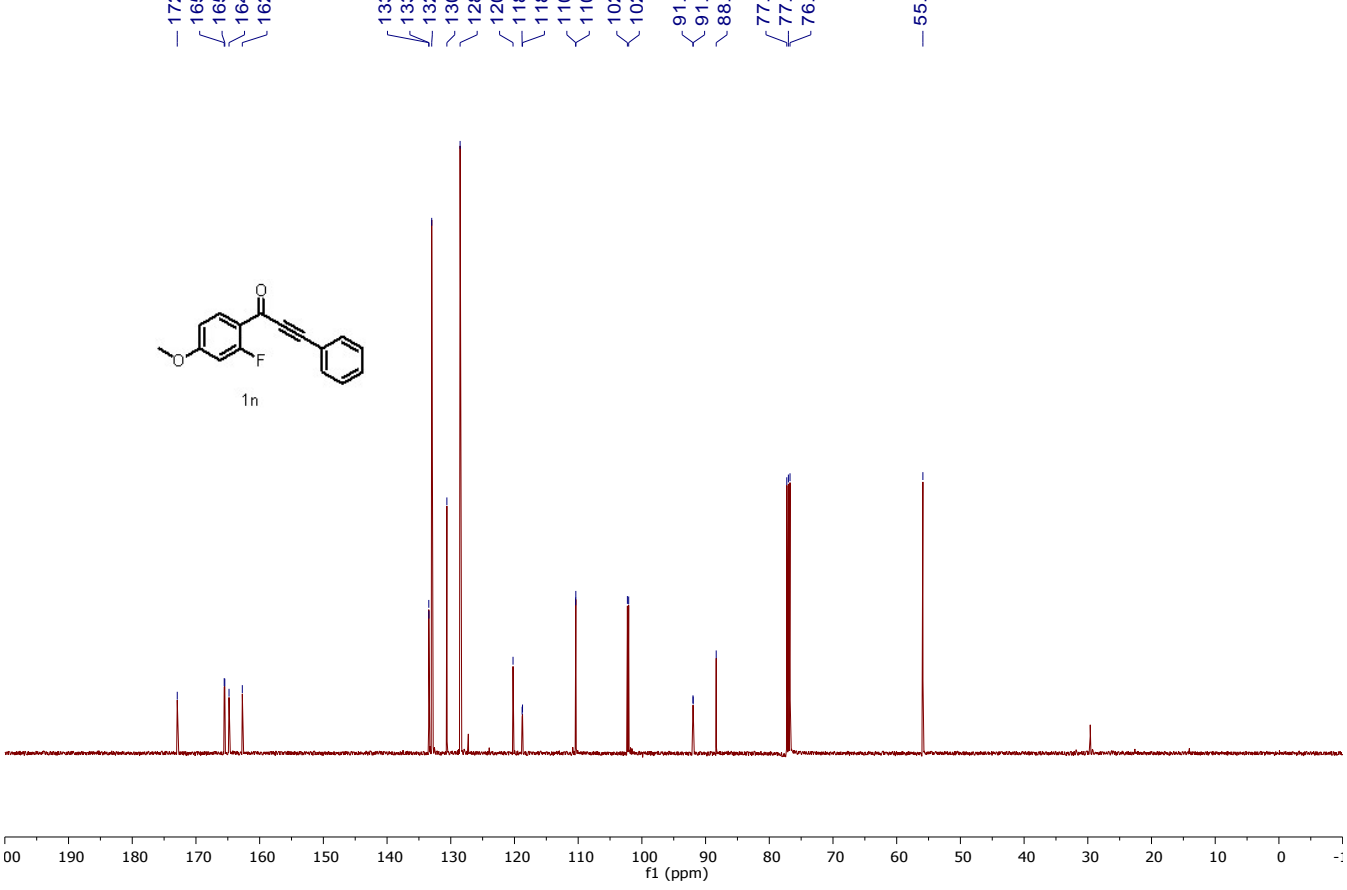
8.082
8.065
7.657
7.642
7.478
7.463
7.448
7.413
7.398
7.383
6.790
6.786
6.772
6.768
6.666
6.661
6.640
6.635
3.872
0.000
1n
1.01
2.00
1.01
2.08
1.05
1.02
3.00
f1 (ppm)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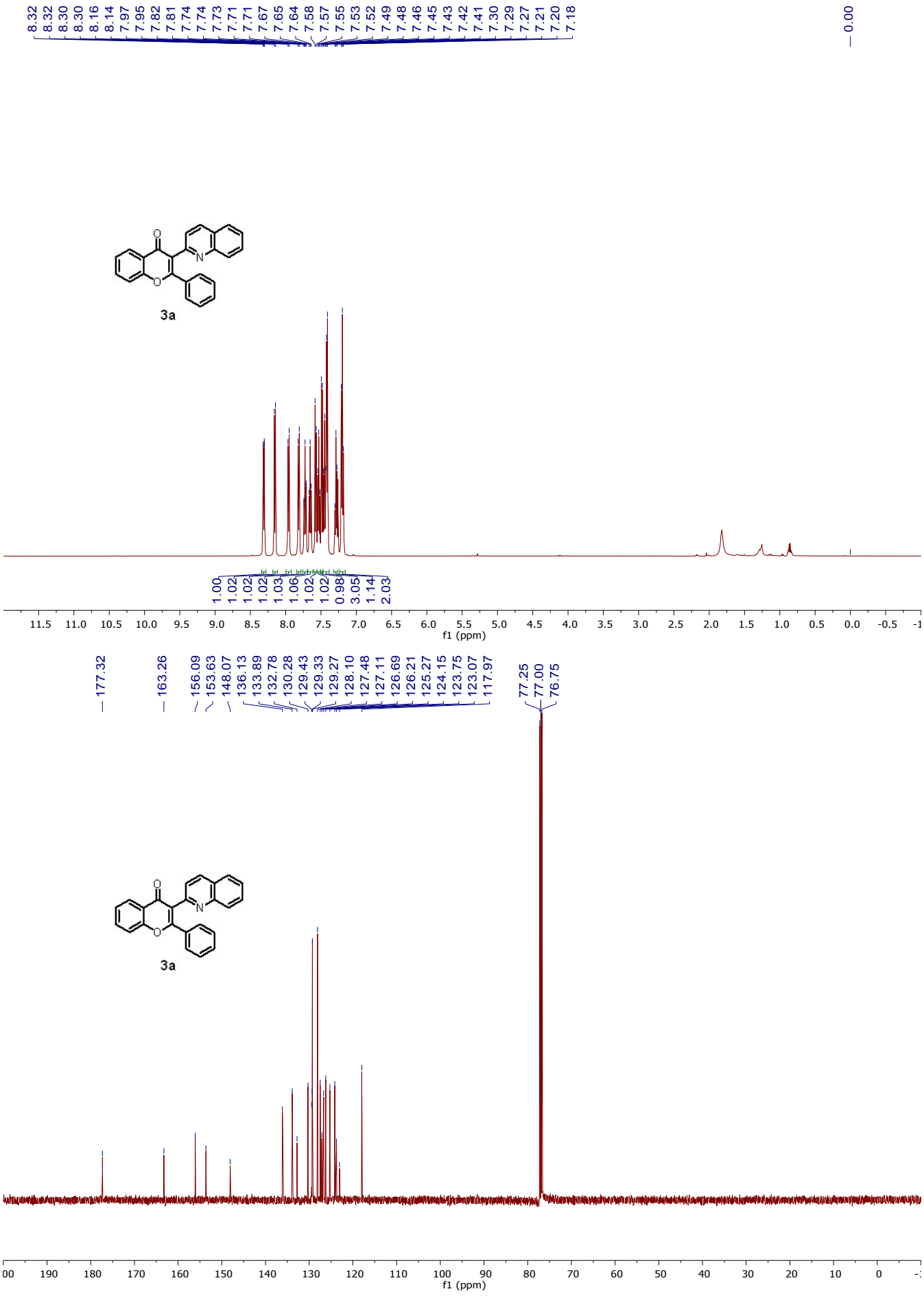
165.564
165.471
164.808
162.722
133.449
133.431
132.991
130.611
128.535
120.226
118.799
118.735
110.392
110.369
102.274
102.072
91.976
91.950
88.332
77.254
77.000
76.745
55.888
1n
f1 (ppm)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8.32
8.30
8.30
8.16
8.14
7.97
7.95
7.82
7.81
7.74
7.74
7.73
7.71
7.71
7.67
7.65
7.64
7.58
7.57
7.55
7.53
7.52
7.49
7.48
7.46
7.45
7.43
7.42
7.41
7.30
7.29
7.27
7.21
7.20
7.18
0.00
3a
1.00
1.02
1.02
1.02
1.03
1.06
1.02
1.02
0.98
3.05
1.14
2.03
f1 (ppm)
177.32
163.26
156.09
153.63
148.07
136.13
133.89
132.78
130.28
129.43
129.33
129.27
128.10
127.48
127.11
126.69
126.21
125.27
124.15
123.75
123.07
117.97
77.25
77.00
76.75
3a
f1 (ppm)


8.230
8.226
8.214
8.211
8.104
8.087
7.883
7.866
7.755
7.752
7.738
7.735
7.663
7.659
7.648
7.645
7.642
7.631
7.628
7.601
7.598
7.588
7.585
7.581
7.571
7.568
7.491
7.475
7.462
7.448
7.431
7.414
7.383
7.367
7.353
7.346
7.342
7.336
7.332
7.329
7.323
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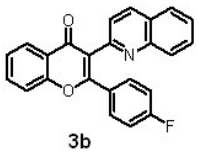
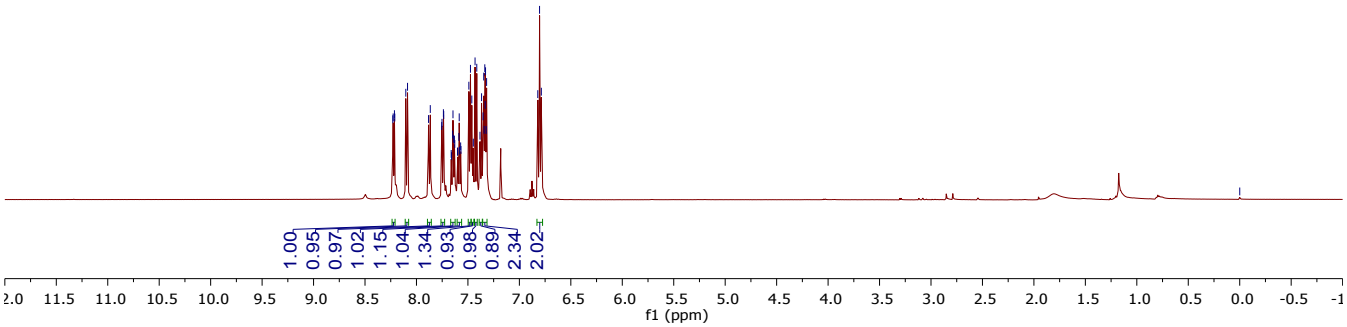
6.821
6.804
6.787
-0.000


O
N
O
F

3b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0.97
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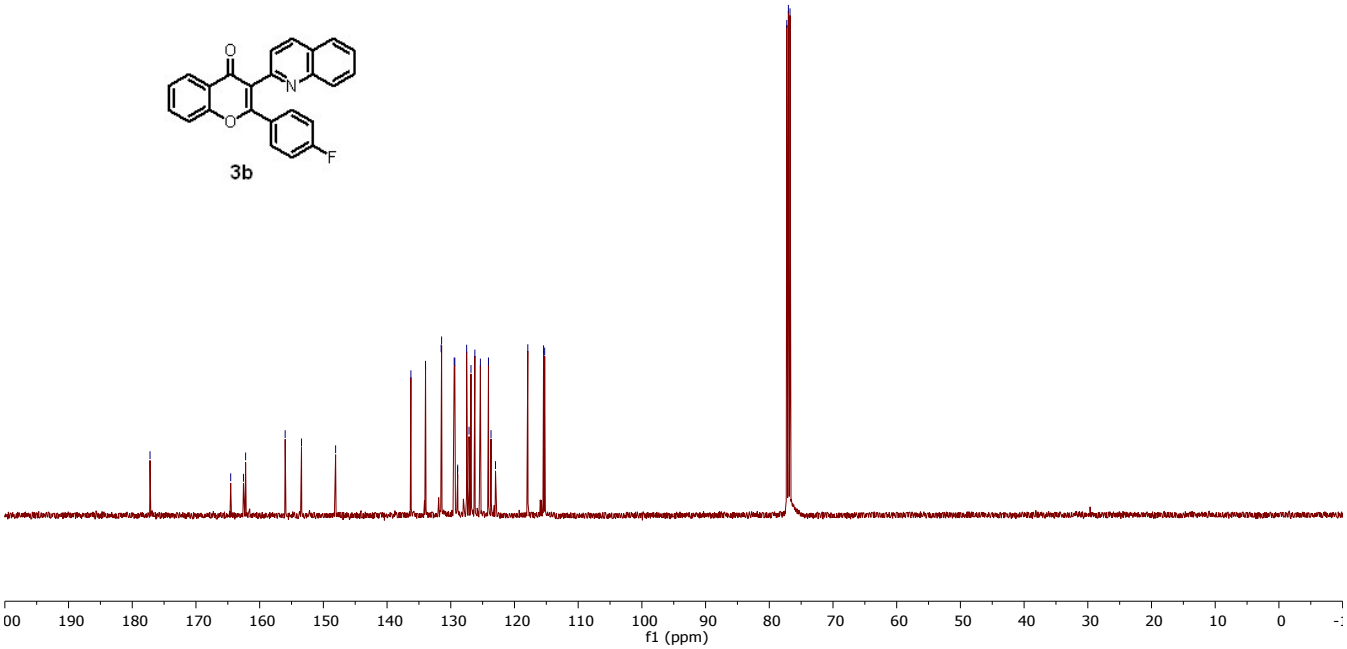
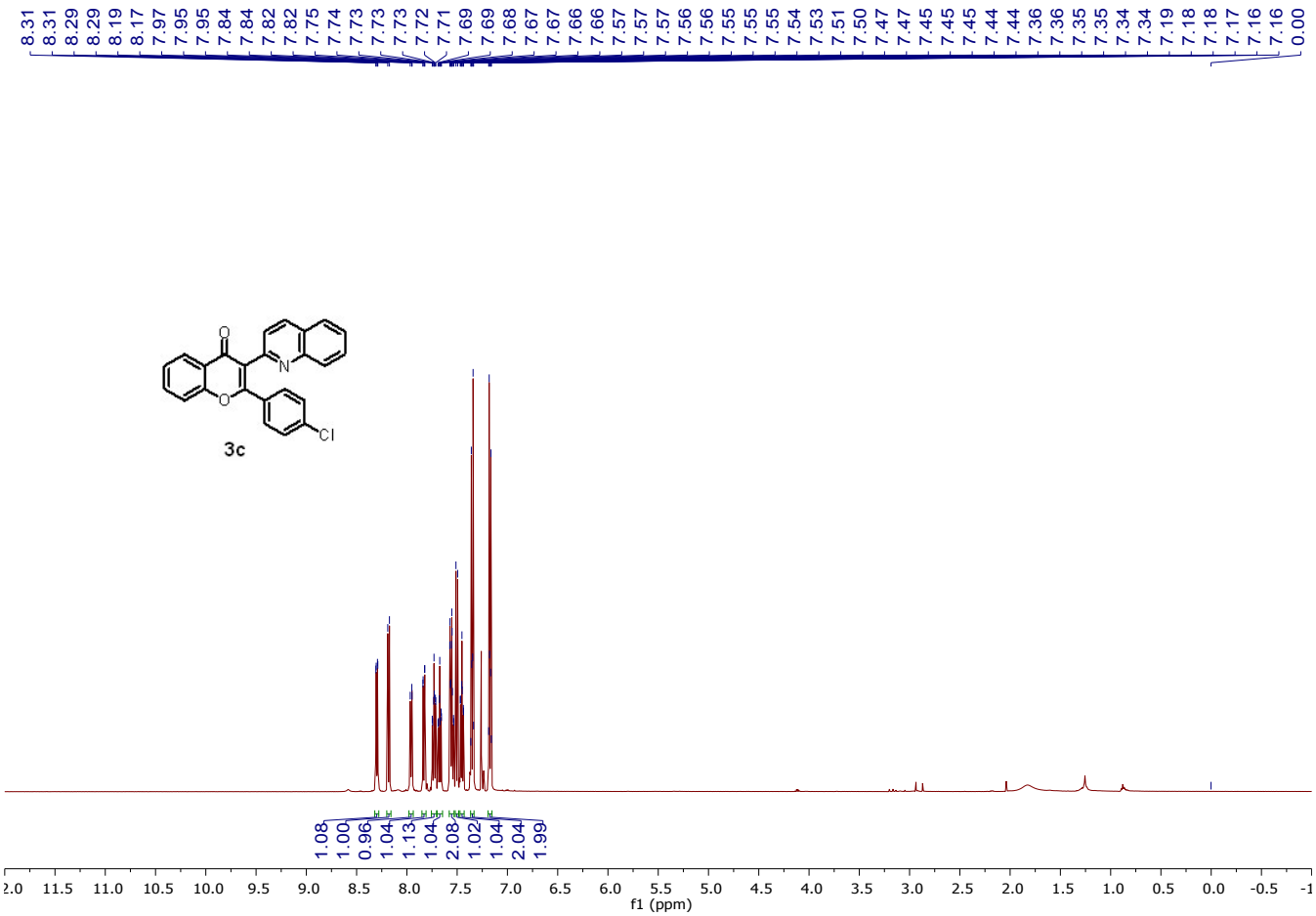
1.15
1.04
1.34
0.93
0.98
0.89
2.34
2.02
f1 (ppm)


177.21
164.55
162.54
162.20
156.00
153.43
148.08
136.26
133.96
131.51
131.44
129.46
129.36
128.94
128.91
127.51
127.13
126.83
126.22
125.35
124.08
123.68
122.98
117.91
115.43
115.26
77.25
77.00
76.75

O
N
O
F

3b


f1 (ppm)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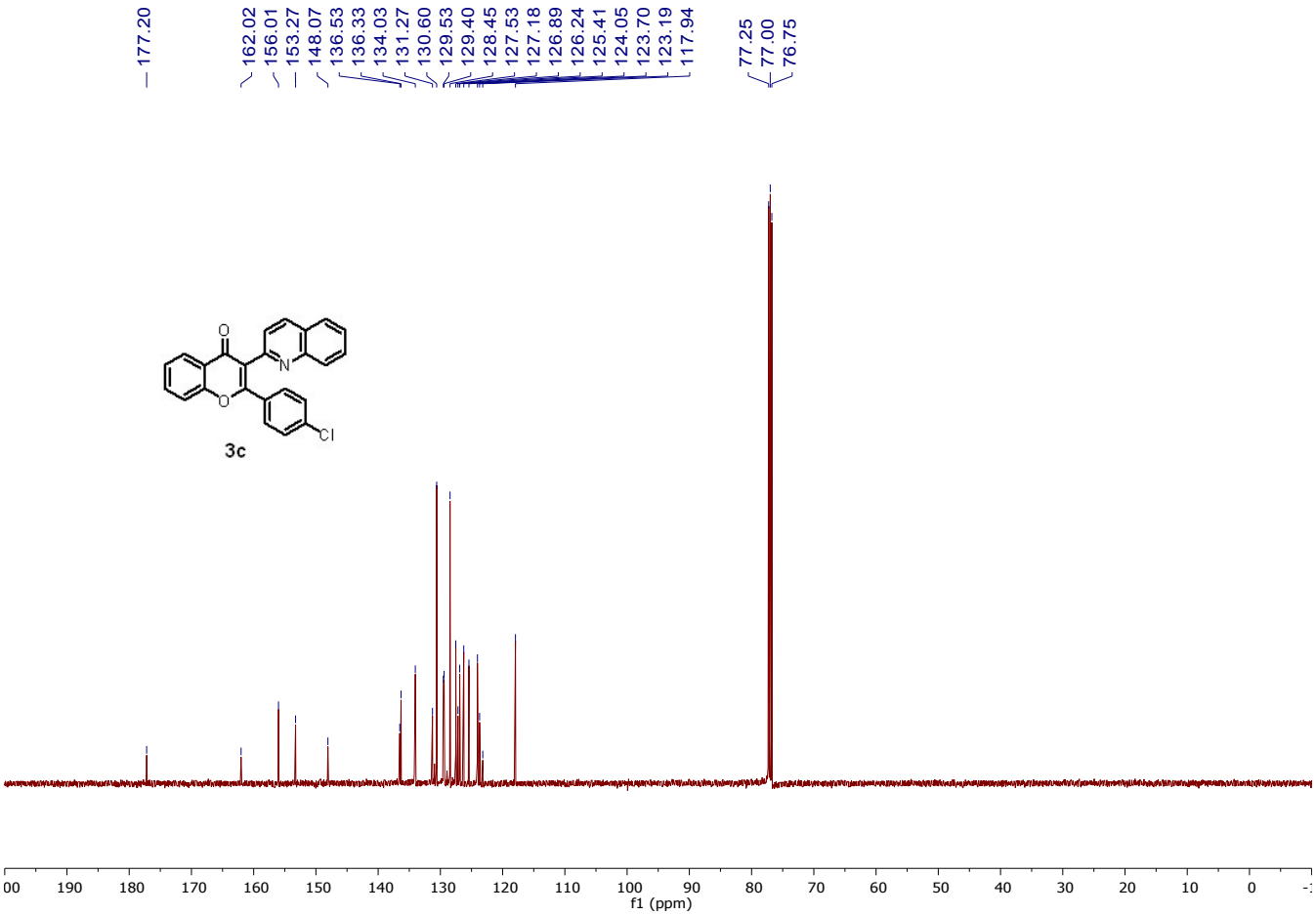
3c
1.08 1.00 0.96 1.04 1.13 1.04 2.08 1.02 1.04 2.04 1.99
f1 (ppm)


177.20
162.02 156.01 153.27 148.07 136.53 136.33 134.03 131.27 130.60 129.53 129.40 128.45 127.53 127.18 126.89 126.24 125.41 124.05 123.70 123.19 117.94
77.25 77.00 76.75
3c
f1 (ppm)


8.31
8.30
8.29
8.29
8.16
8.14
8.01
7.99
7.82
7.81
7.73
7.72
7.71
7.71
7.71
7.70
7.69
7.68
7.68
7.66
7.65
7.65
7.57
7.55
7.55
7.55
7.53
7.52
7.52
7.47
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7.45
7.45
7.43
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7.42
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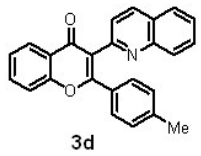
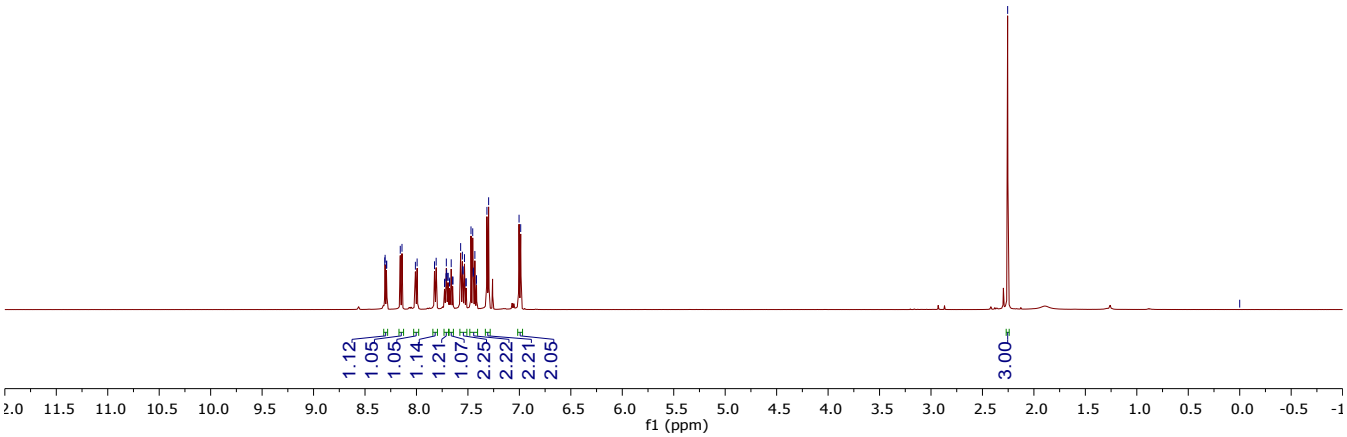
7.30
7.00
6.99
2.26
0.00


O
N
O
Me

3d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1.05
1.14
1.21
1.07
2.25
2.22
2.21
2.05
3.00
f1 (ppm)


177.35
163.28
156.08
153.91
148.11
140.75
136.15
133.77
129.87
129.49
129.28
129.20
128.85
127.48
127.12
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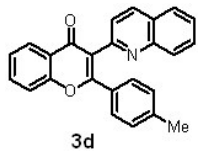
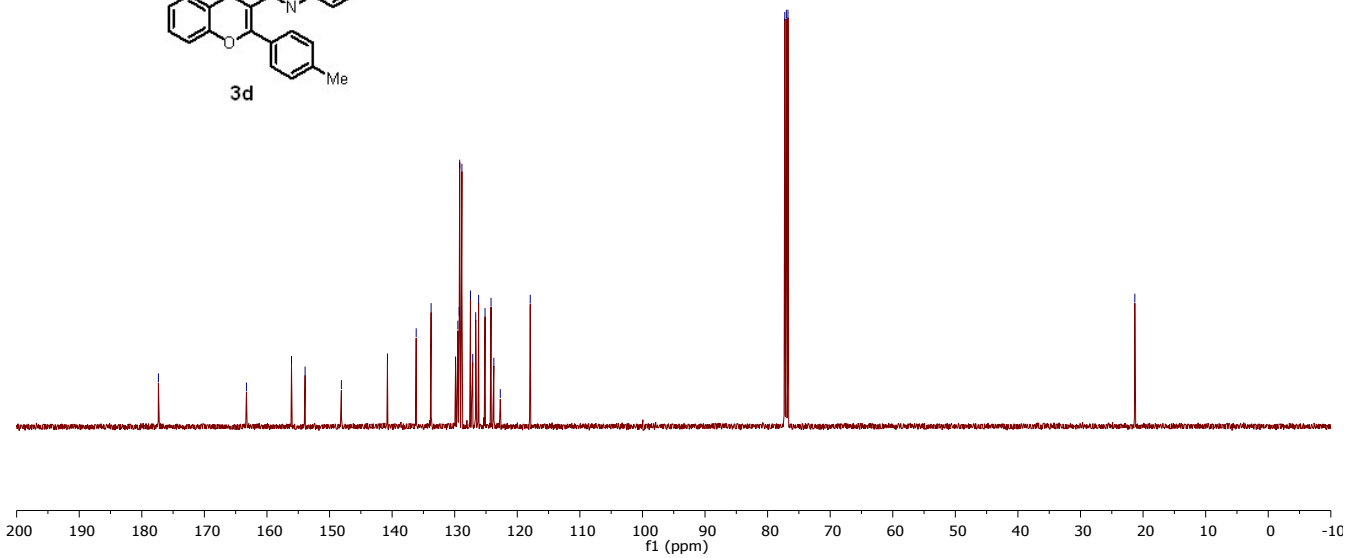
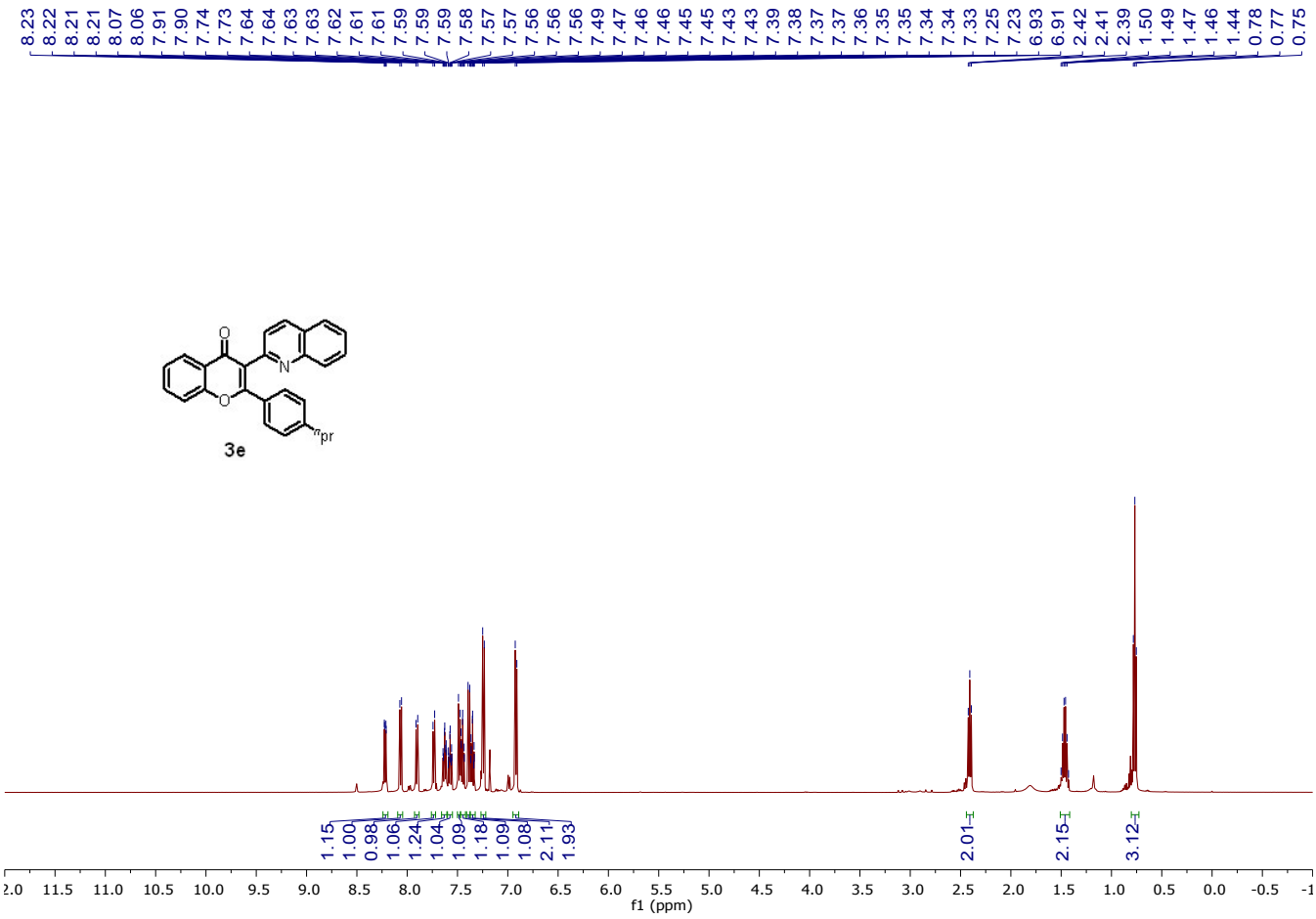
126.18
125.15
124.20
123.75
122.71
117.93
77.25
77.00
76.75
21.32


O
N
O
Me

3d


f1 (ppm)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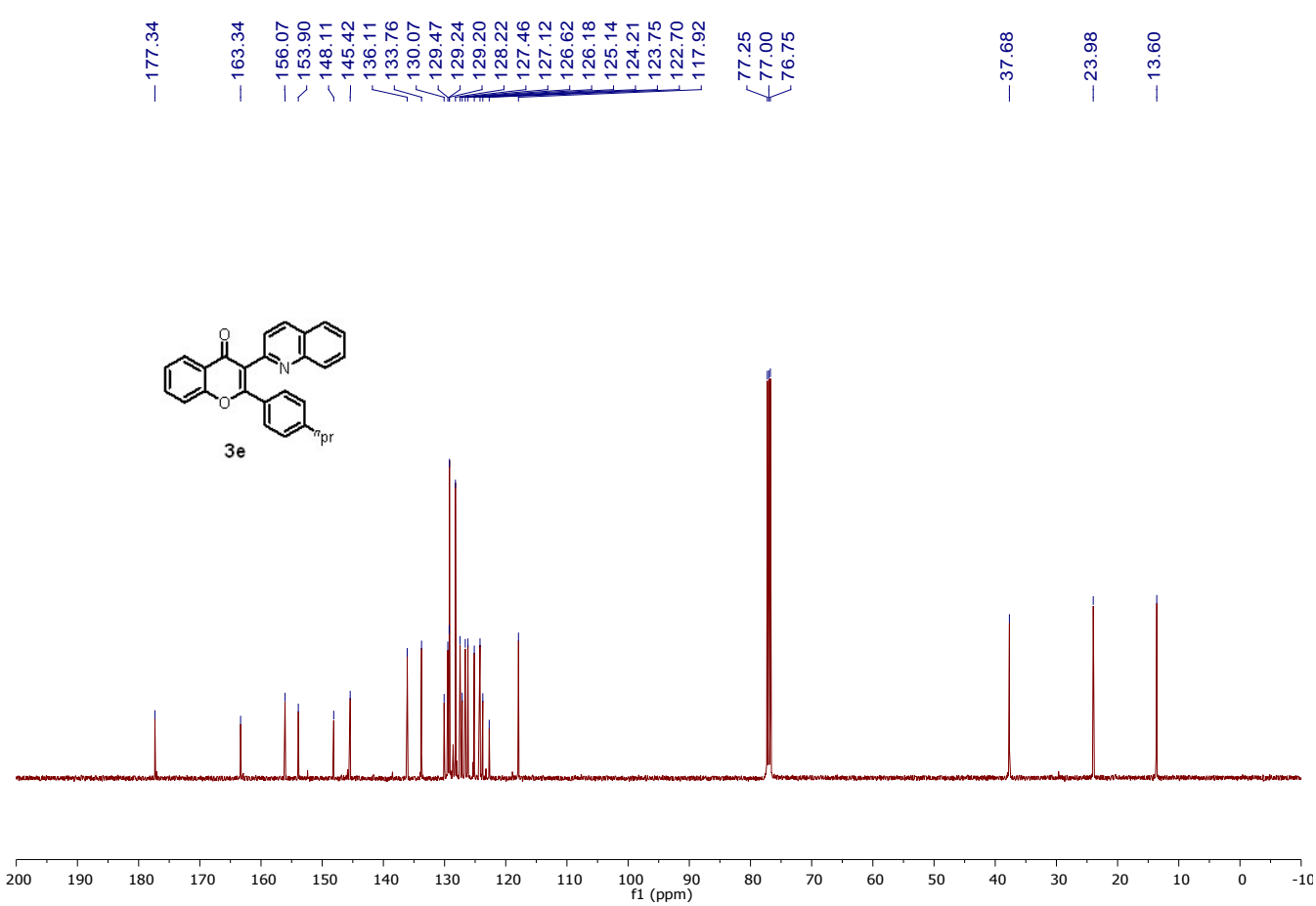
O
N
O
nPr
3e
1.15 1.00 0.98 1.06 1.24 1.04 1.09 1.18 1.09 1.08 2.11 1.93 2.01 2.15 3.12
f1 (ppm)


177.34 163.34 156.07 153.90 148.11 145.42 136.11 133.76 130.07 129.47 129.24 129.20 128.22 127.46 127.12 126.62 126.18 125.14 124.21 123.75 122.70 117.92 77.25 77.00 76.75 37.68 23.98 13.60
O
N
O
nPr
3e
f1 (ppm)


8.22
8.21
8.20
8.20
8.08
8.07
7.93
7.75
7.75
7.73
7.73
7.62
7.62
7.60
7.59
7.48
7.47
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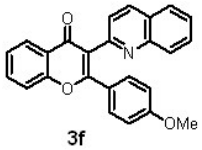
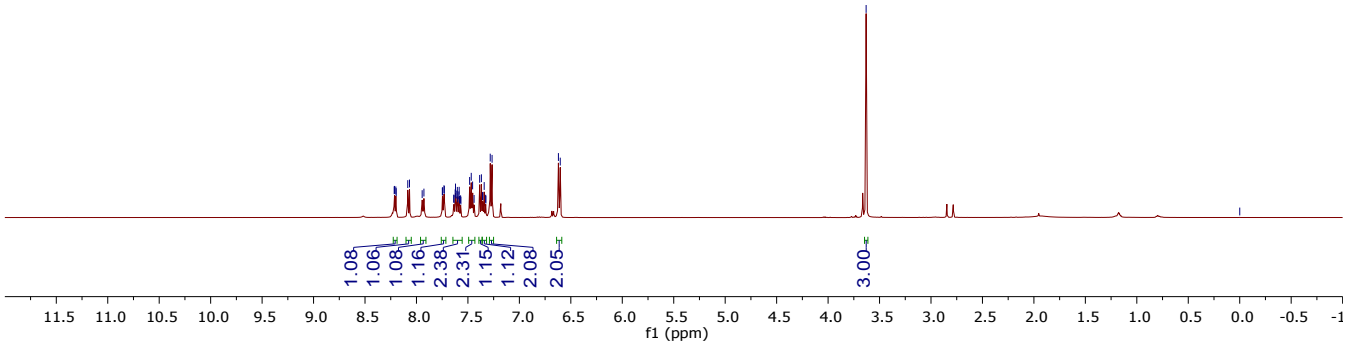
7.27
6.62
6.60
3.63
-0.00


O
N
O
OMe

3f


1.08
1.06
1.08
1.16
2.38
2.31
1.15
1.12
2.08
2.05
3.00
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)


177.33
162.93
161.11
155.99
154.09
148.15
136.23
133.71
131.35
130.99
129.49
129.30
127.48
127.11
126.65
126.15
125.10
124.89
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123.69
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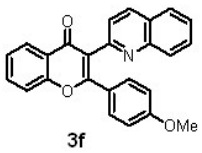
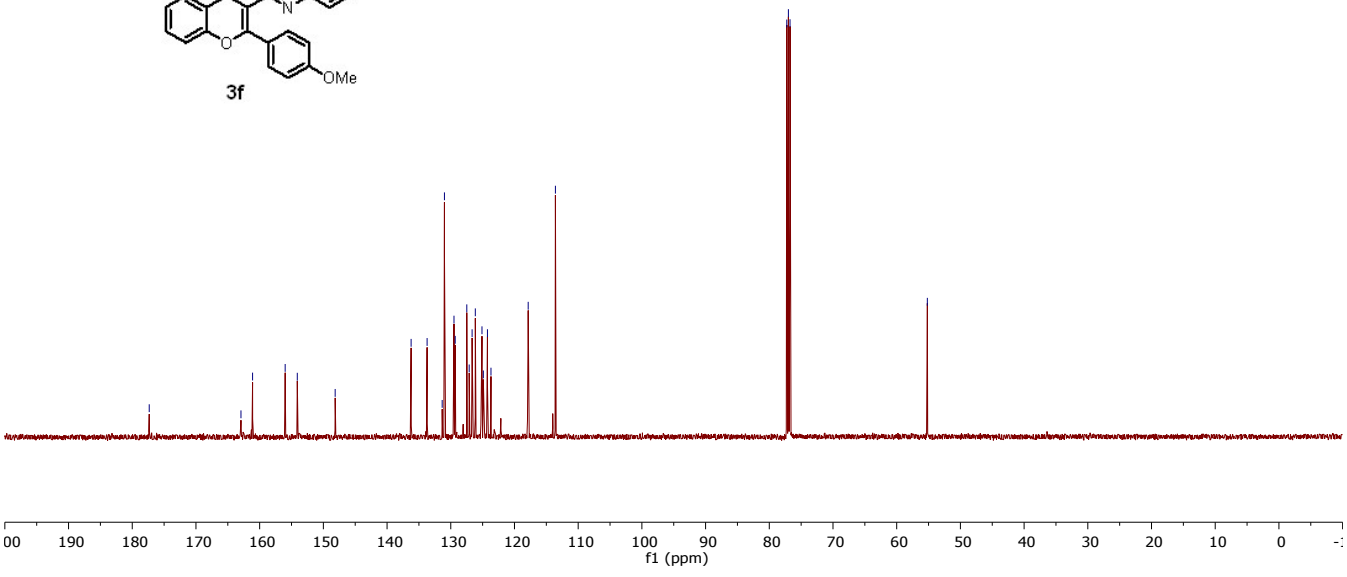
113.57
77.25
77.00
76.75
55.19


O
N
O
OMe

3f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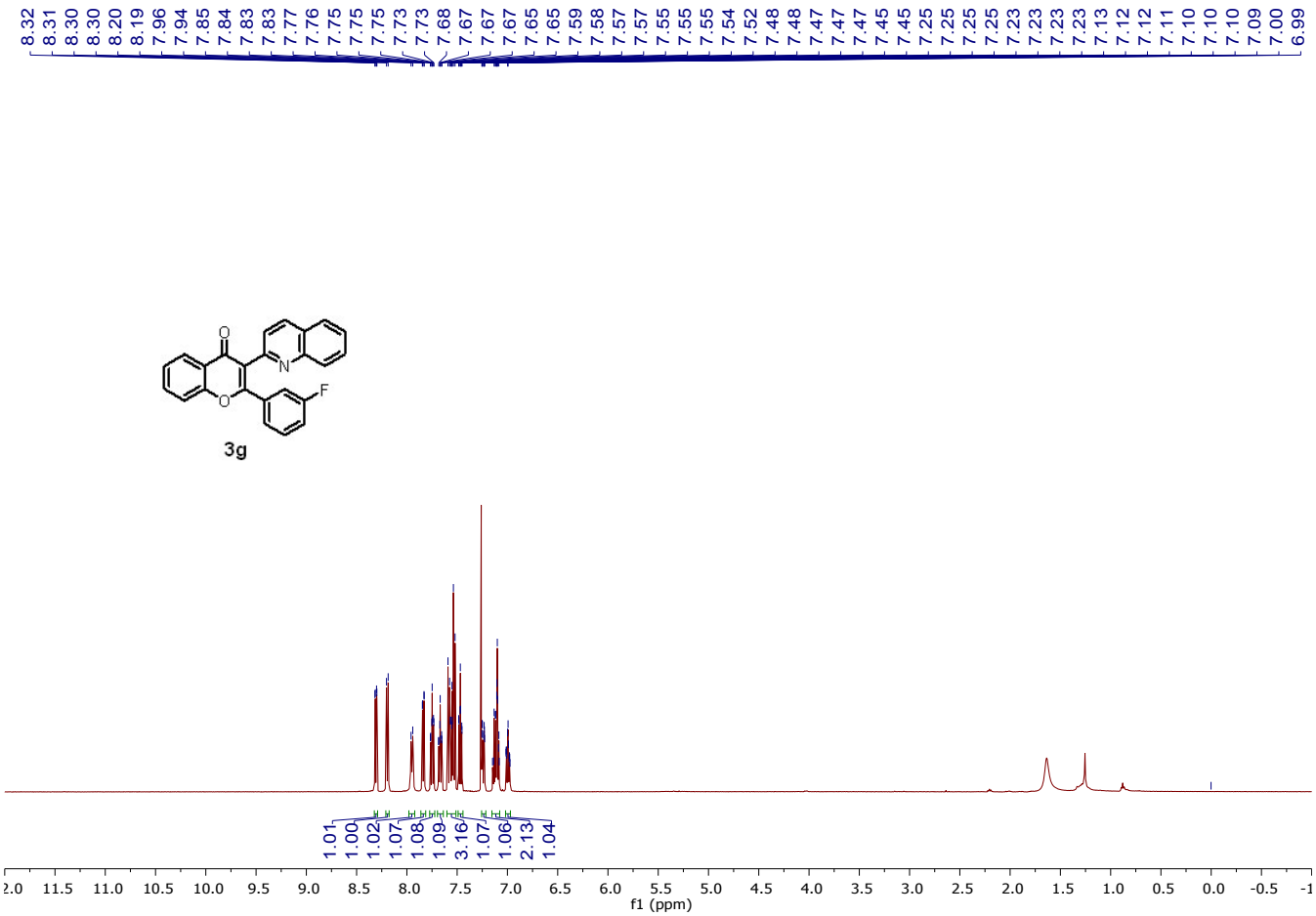
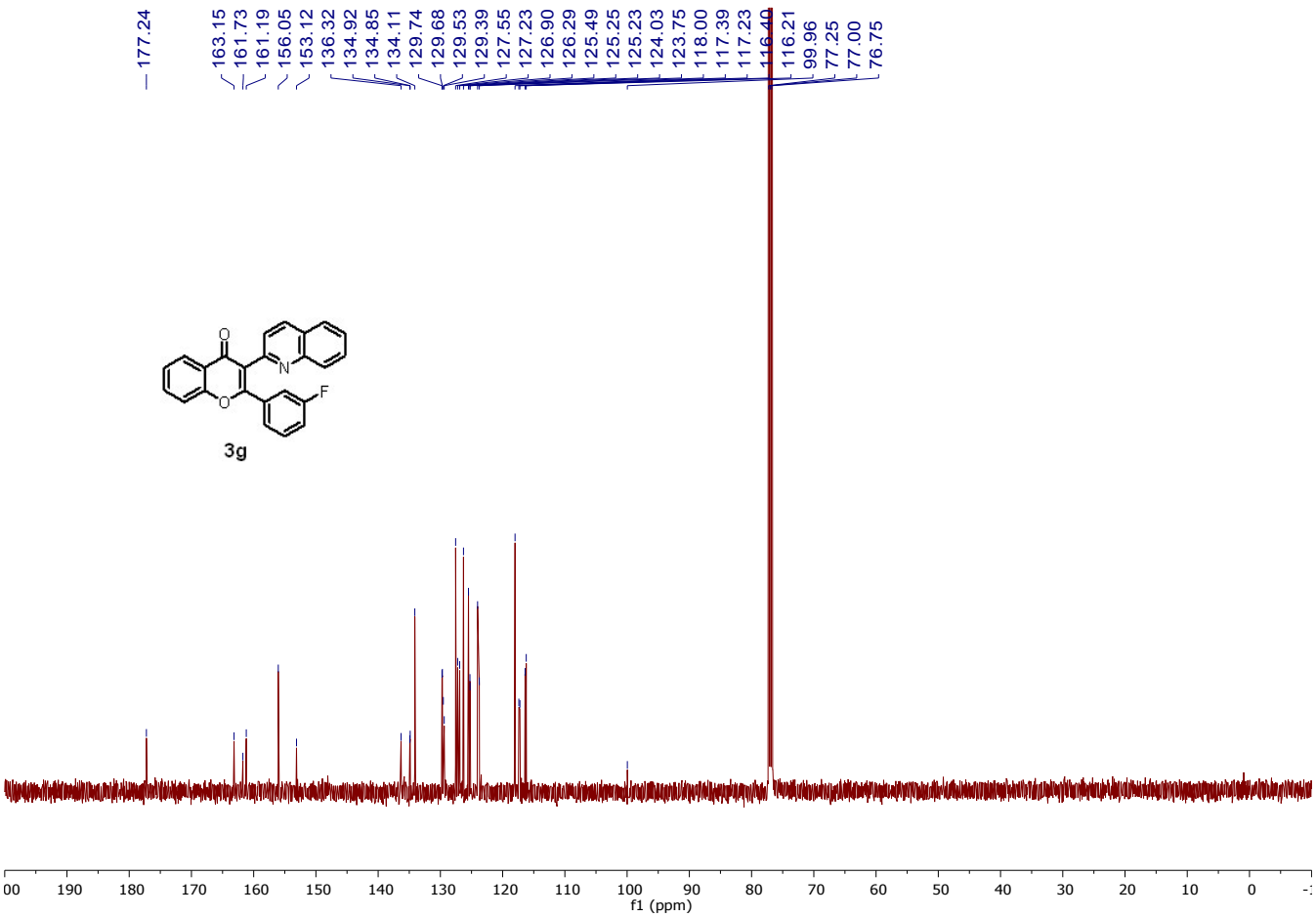
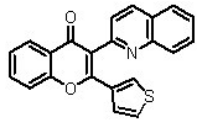
f1 (ppm)

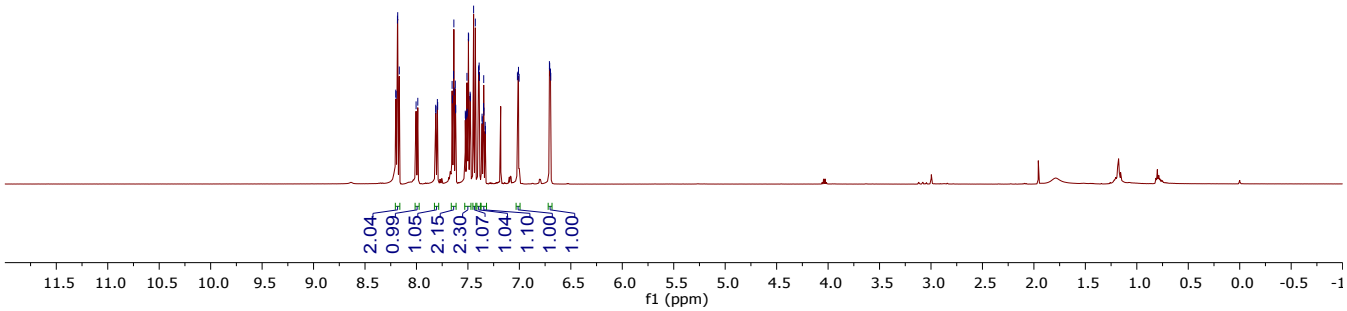

8.32 8.31 8.30 8.30 8.20 8.19 7.96 7.94 7.85 7.84 7.83 7.83 7.77 7.76 7.75 7.75 7.75 7.73 7.73 7.68 7.67 7.67 7.67 7.65 7.65 7.59 7.58 7.57 7.57 7.55 7.55 7.55 7.54 7.52 7.48 7.48 7.47 7.47 7.47 7.45 7.45 7.25 7.25 7.25 7.25 7.23 7.23 7.23 7.23 7.13 7.12 7.12 7.11 7.10 7.10 7.10 7.09 7.00 6.99
O
N
O
F
3g
1.01 1.00 1.02 1.07 1.08 1.09 3.16 1.07 1.06 2.13 1.04
f1 (ppm)


177.24
163.15 161.73 161.19 156.05 153.12 136.32 134.92 134.85 134.11 129.74 129.68 129.53 129.39 127.55 127.23 126.90 126.29 125.49 125.25 125.23 124.03 123.75 118.00 117.39 117.23 116.40 116.21 99.96 77.25 77.00 76.75
O
N
O
F
3g
f1 (ppm)


8.20
8.20
8.18
8.18
8.17
8.00
7.99
7.81
7.81
7.80
7.79
7.65
7.65
7.64
7.64
7.63
7.62
7.62
7.62
7.53
7.52
7.51
7.51
7.51
7.50
7.49
7.48
7.48
7.44
7.43
7.40
7.39
7.39
7.39
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.02
7.01
7.01
7.00
6.71
6.71
6.70
6.70

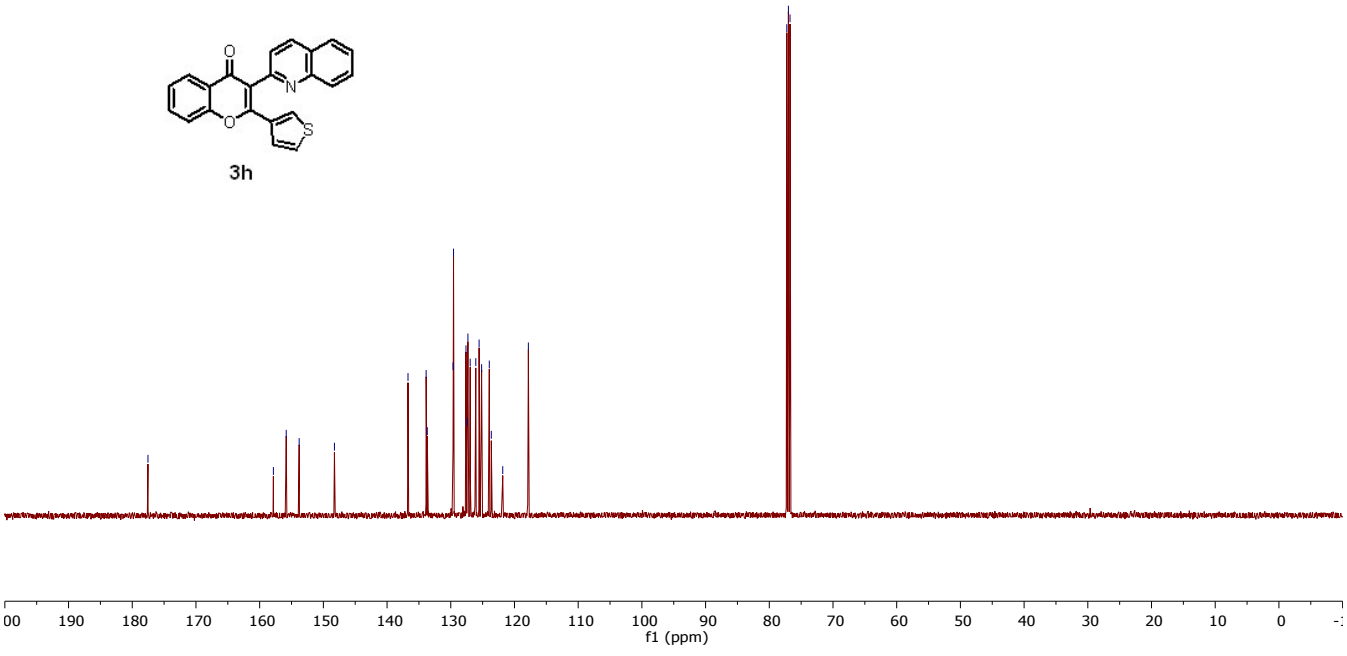


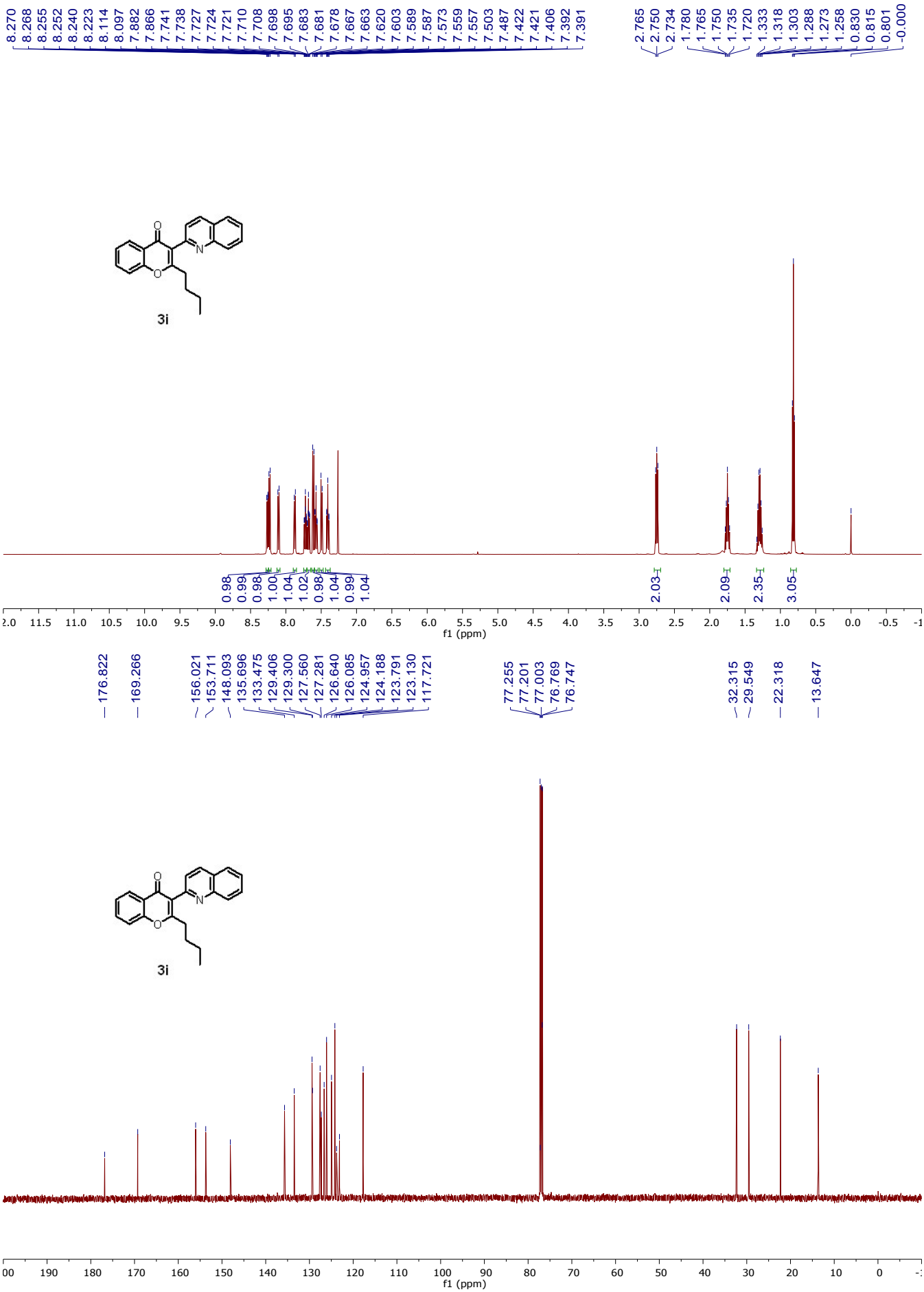
3h


2.04
0.99
1.05
2.15
2.30
1.07
1.04
1.10
1.00
1.00
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)


177.53
157.85
155.83
153.80
148.26
136.71
133.87
133.68
129.64
129.57
127.61
127.41
127.31
126.95
126.07
125.55
125.16
123.95
123.64
121.84
117.82
77.25
77.00
76.75

3h


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.270
8.268
8.255
8.252
8.240
8.223
8.114
8.097
7.882
7.866
7.741
7.738
7.727
7.724
7.721
7.710
7.708
7.698
7.695
7.683
7.681
7.678
7.667
7.663
7.620
7.603
7.589
7.587
7.573
7.559
7.557
7.503
7.487
7.422
7.421
7.406
7.392
7.391
2.765
2.750
2.734
1.780
1.765
1.750
1.735
1.720
1.333
1.318
1.303
1.288
1.273
1.258
0.830
0.815
0.801
-0.000
3i
0.98
0.99
0.98
1.00
1.04
1.02
0.98
1.04
0.99
1.04
2.03
2.09
2.35
3.05
f1 (ppm)
176.822
169.266
156.021
153.711
148.093
135.696
133.475
129.406
129.300
127.560
127.281
126.640
126.085
124.957
124.188
123.791
123.130
117.721
77.255
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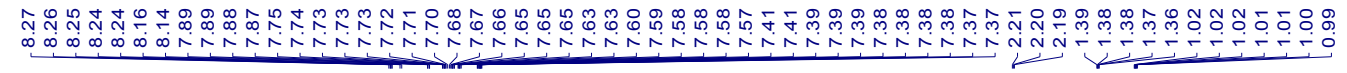
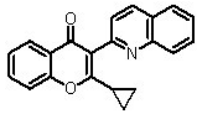
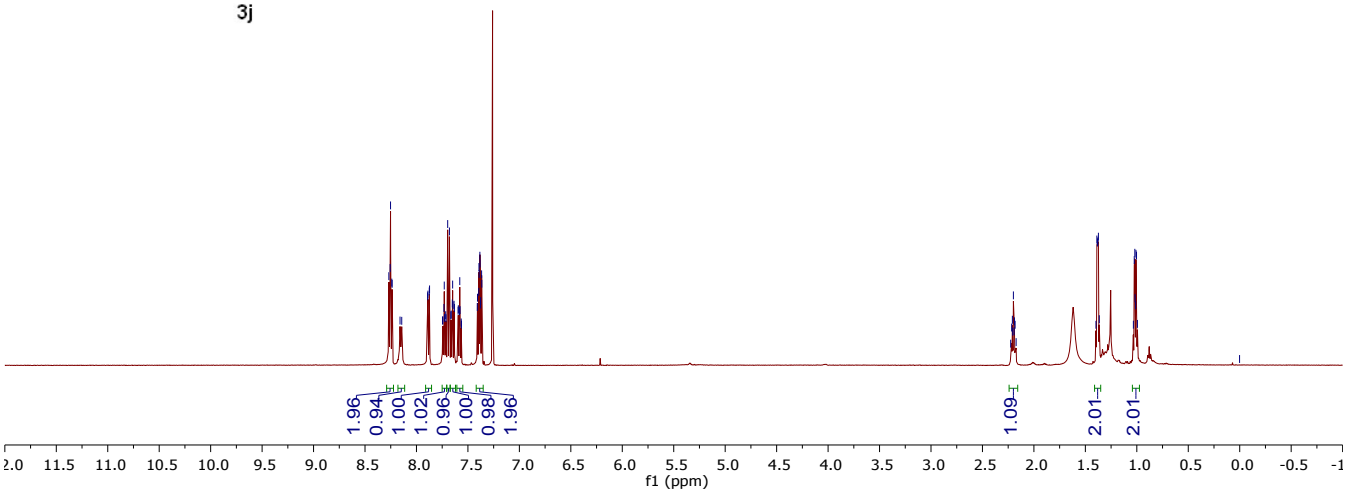
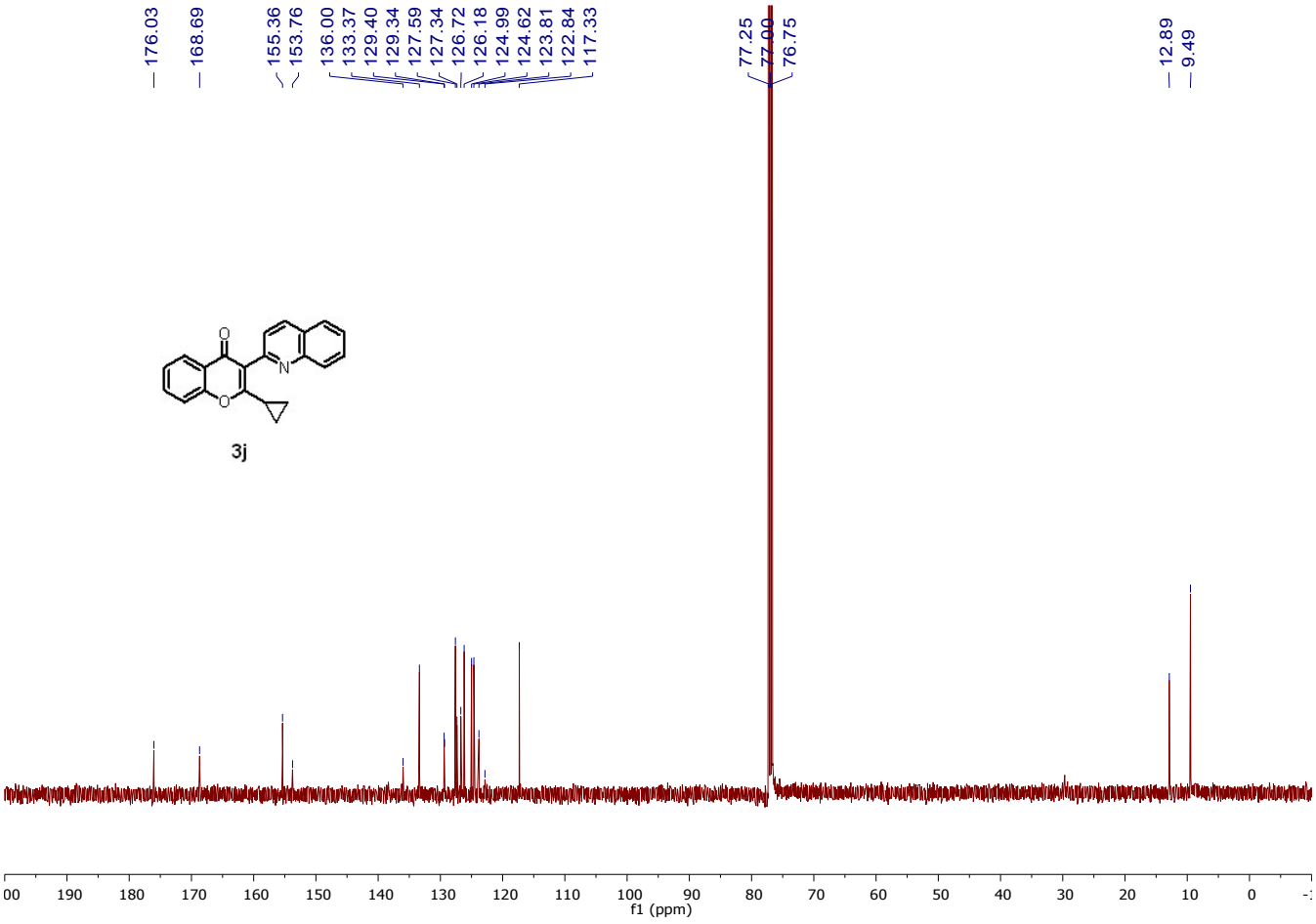
77.003
76.769
76.747
32.315
29.549
22.318
13.647
3i
f1 (ppm)


8.27 8.26 8.25 8.24 8.24 8.16 8.14 7.89 7.89 7.88 7.87 7.75 7.74 7.73 7.73 7.73 7.72 7.71 7.70 7.68 7.67 7.66 7.65 7.65 7.65 7.63 7.63 7.60 7.59 7.58 7.58 7.58 7.57 7.41 7.41 7.39 7.39 7.39 7.38 7.38 7.38 7.38 7.37 7.37 2.21 2.20 2.19 1.39 1.38 1.38 1.37 1.36 1.02 1.02 1.02 1.01 1.01 1.00 0.99

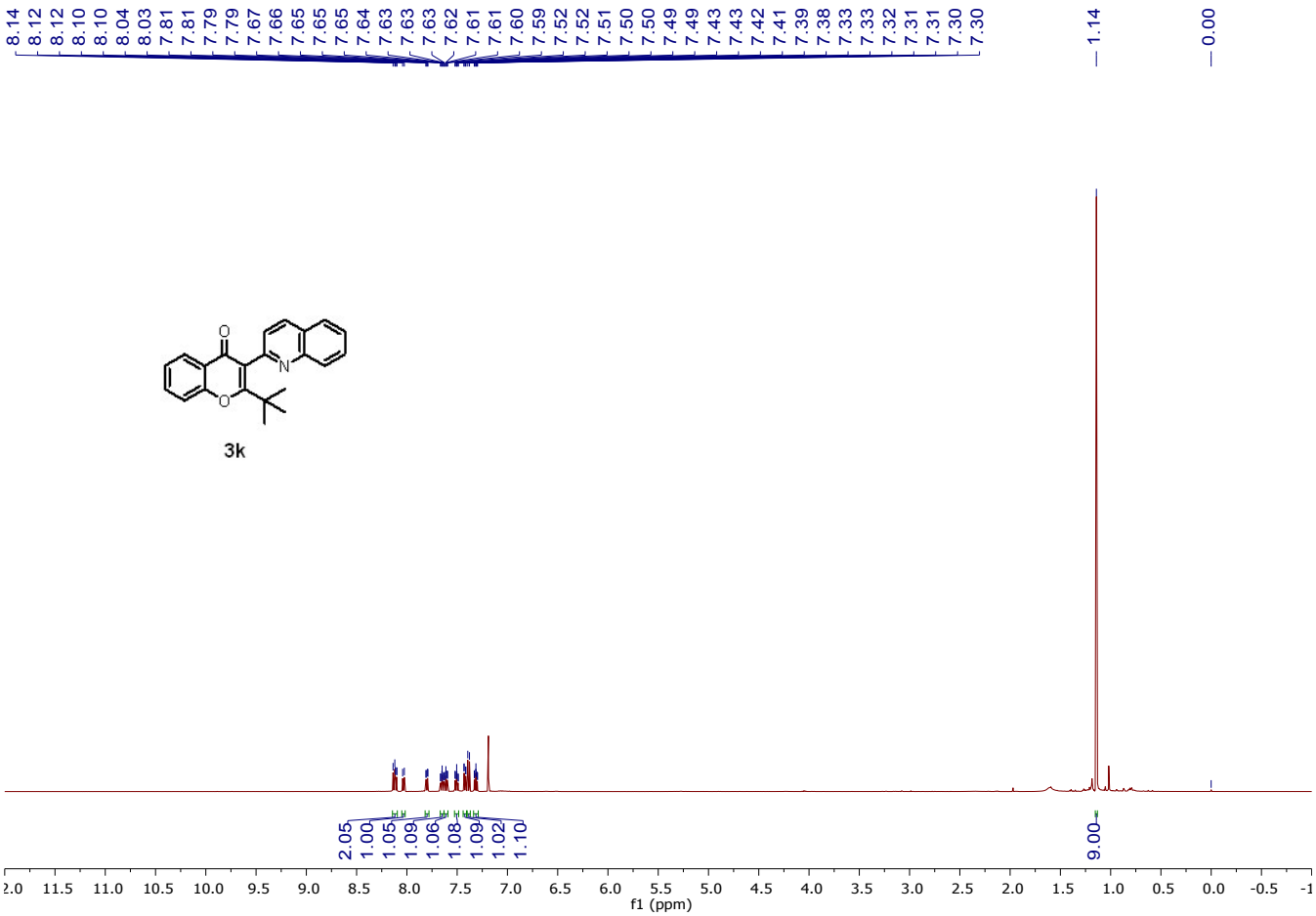


3j


1.96 0.94 1.00 1.02 0.96 1.00 0.98 1.96 1.09 2.01 2.01
f1 (ppm)


176.03 168.69 155.36 153.76 136.00 133.37 129.40 129.34 127.59 127.34 126.72 126.18 124.99 124.62 123.81 122.84 117.33 77.25 77.00 76.75 12.89 9.49
f1 (ppm)

3j


8.14 8.12 8.12 8.10 8.10 8.04 8.03 7.81 7.81 7.79 7.79 7.67 7.66 7.65 7.65 7.65 7.64 7.63 7.63 7.63 7.62 7.61 7.61 7.60 7.59 7.52 7.52 7.51 7.50 7.50 7.49 7.49 7.43 7.43 7.42 7.41 7.39 7.38 7.33 7.33 7.32 7.31 7.31 7.30 7.30
1.14
0.00
O
N
O
3k
2.05 1.00 1.05 1.09 1.06 1.08 1.09 1.02 1.10
9.00
f1 (ppm)
178.57 172.18 155.95 155.10 147.73 135.57 133.59 129.57 129.39 127.60 127.28 126.73 125.86 124.89 124.76 123.08 123.03 117.60
77.25 77.00 76.75
39.15 29.47
O
N
O
3k
f1 (ppm)


8.16
8.15
7.94
7.92
7.82
7.82
7.81
7.80
7.66
7.65
7.64
7.64
7.64
7.63
7.63
7.63
7.61
7.54
7.54
7.53
7.53
7.52
7.51
7.49
7.40
7.39
7.38
7.38
7.38
7.36
7.30
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.20
7.20
7.19
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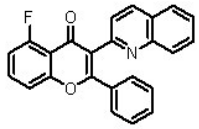
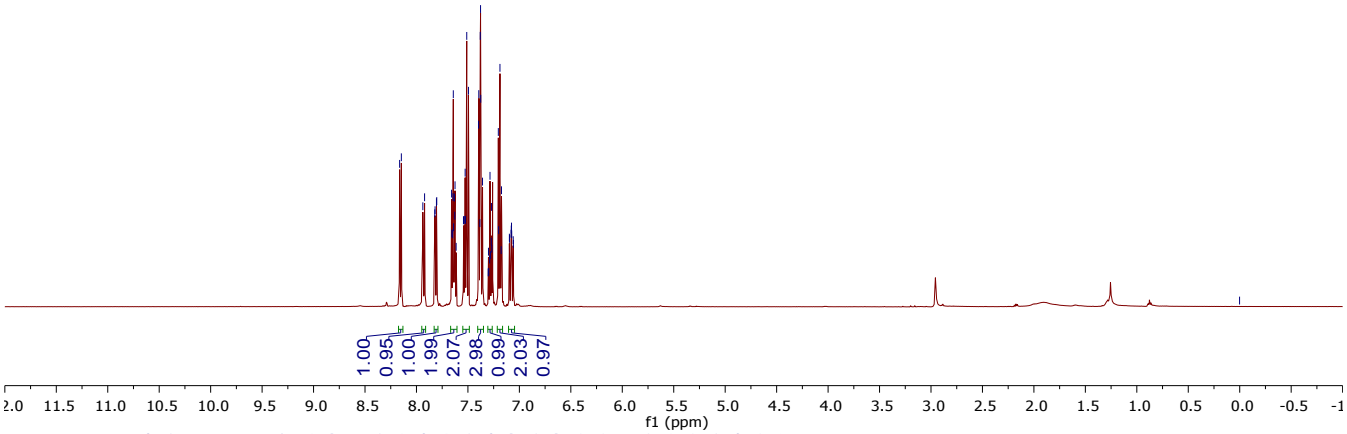
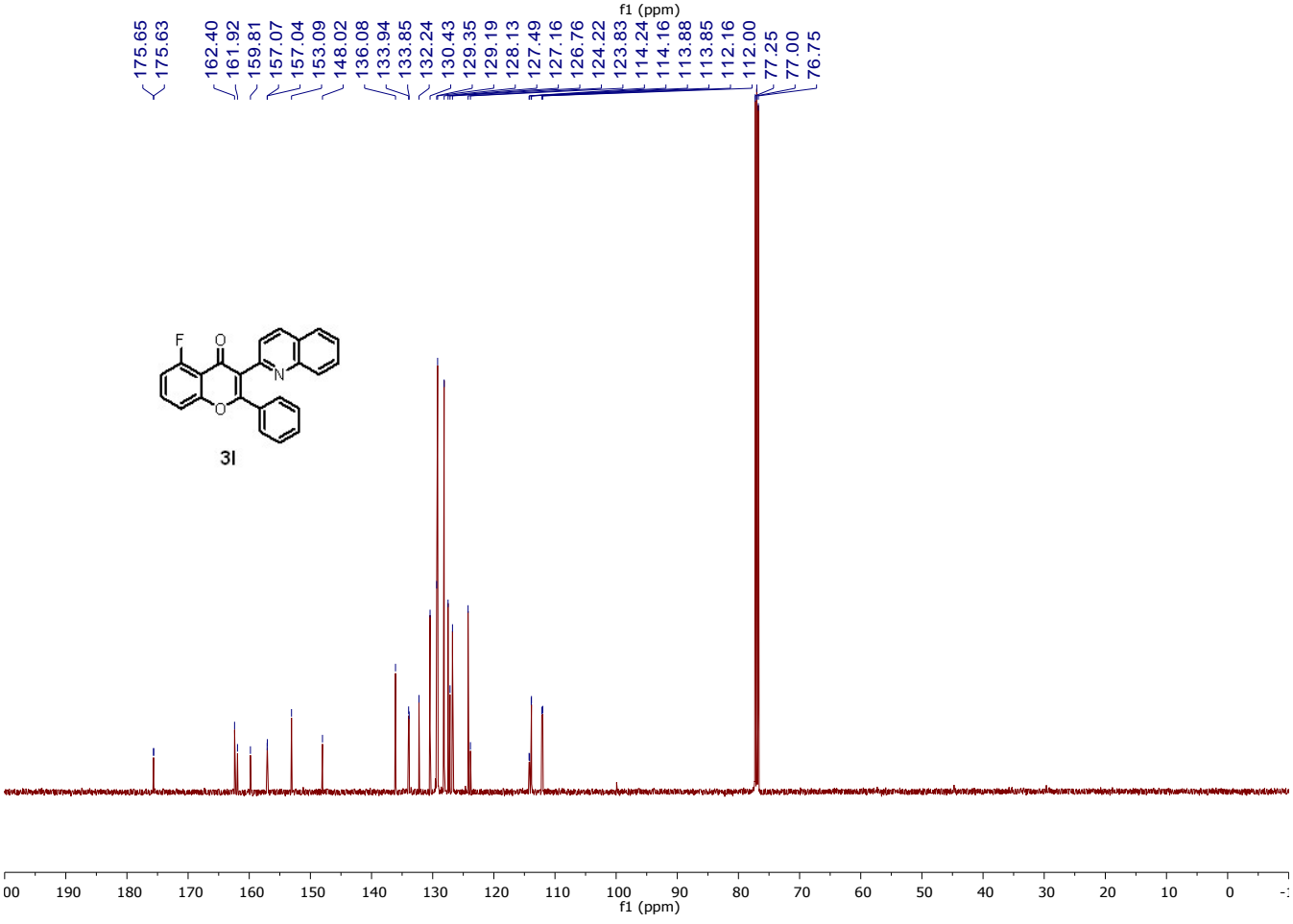
7.17
7.10
7.10
7.08
7.08
7.08
7.07
7.06
7.06
0.00


F
O
N
O

3l


1.00
0.95
1.00
1.99
2.07
2.98
0.99
2.03
0.97
2.0 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)


175.65
175.63
162.40
161.92
159.81
157.07
157.04
153.09
148.02
136.08
133.94
133.85
132.24
130.43
129.35
129.19
128.13
127.49
127.16
126.76
124.22
123.83
114.24
114.16
113.88
113.85
112.16
112.00
77.25
77.00
76.75
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

F
O
N
O

3l


8.452
8.436
8.177
8.160
8.001
7.984
7.907
7.835
7.819
7.695
7.679
7.662
7.563
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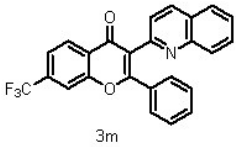
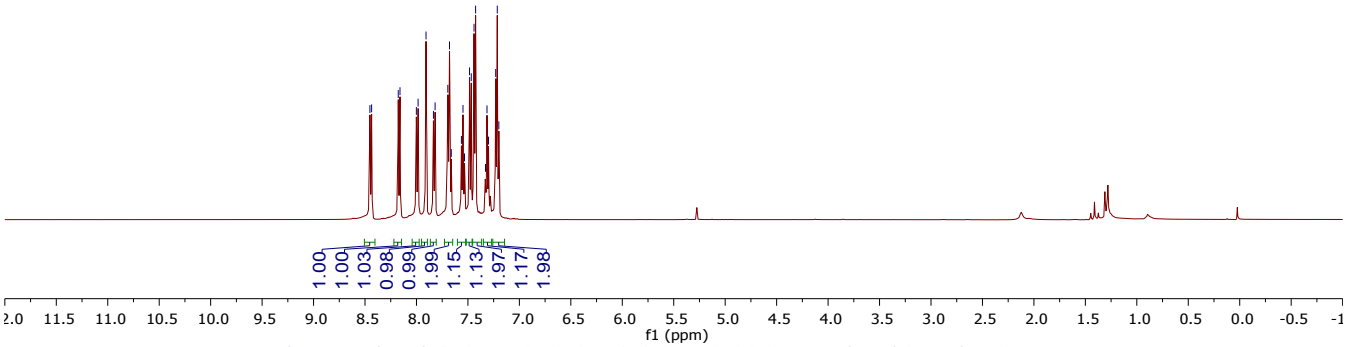
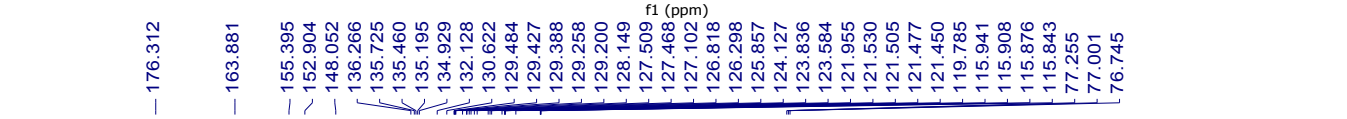
7.329
7.315
7.300
7.230
7.215
7.199


O
N
F3C
O

3m


1.00
1.00
1.03
0.98
0.99
1.99
1.15
1.13
1.97
1.17
1.98
f1 (ppm)


176.312
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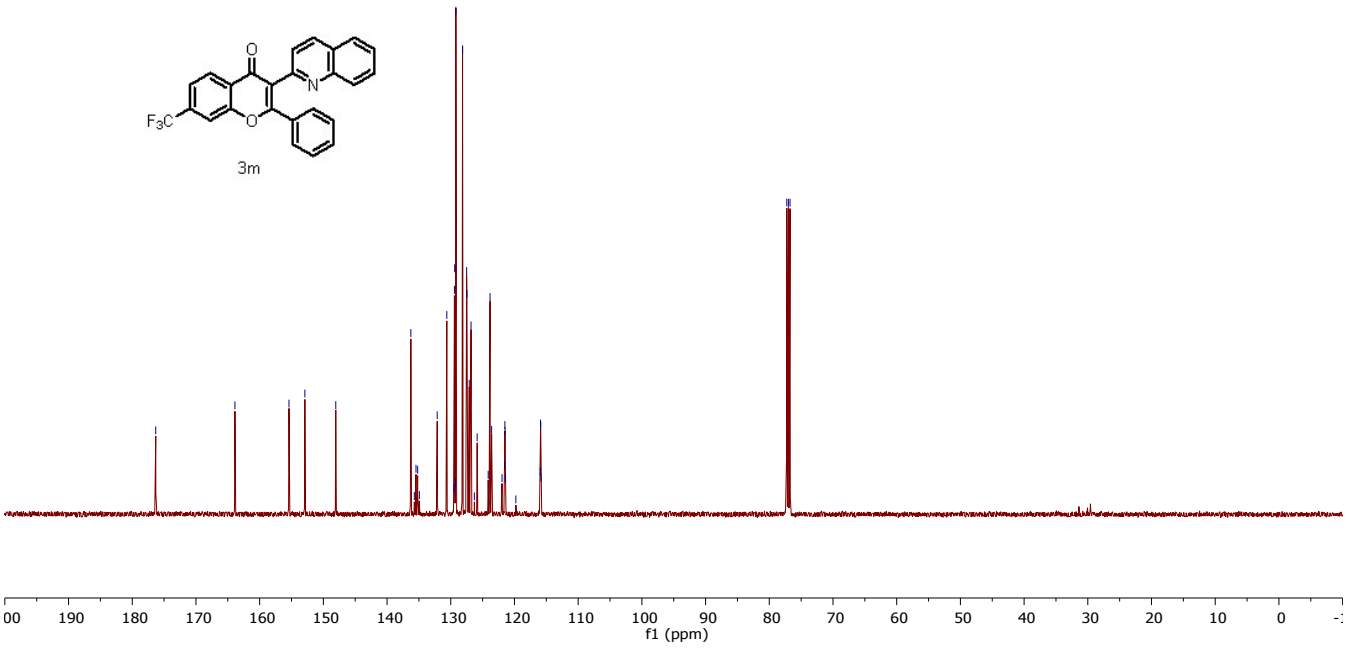
152.904
148.052
136.266
135.725
135.460
135.195
134.929
132.128
130.622
129.484
129.427
129.388
129.258
129.200
128.149
127.509
127.468
127.102
126.818
126.298
125.857
124.127
123.836
123.584
121.955
121.530
121.505
121.477
121.450
119.785
115.941
115.908
115.876
115.843
77.255
77.001
76.745

O
N
F3C
O

3m


f1 (ppm)


8.13
8.13
8.12
8.11
8.11
8.09
7.92
7.90
7.76
7.74
7.72
7.71
7.70
7.70
7.61
7.61
7.60
7.59
7.59
7.58
7.58
7.49
7.49
7.48
7.47
7.47
7.46
7.46
7.41
7.40
7.40
7.39
7.38
7.38
7.31
7.30
7.28
7.25
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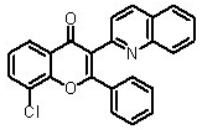
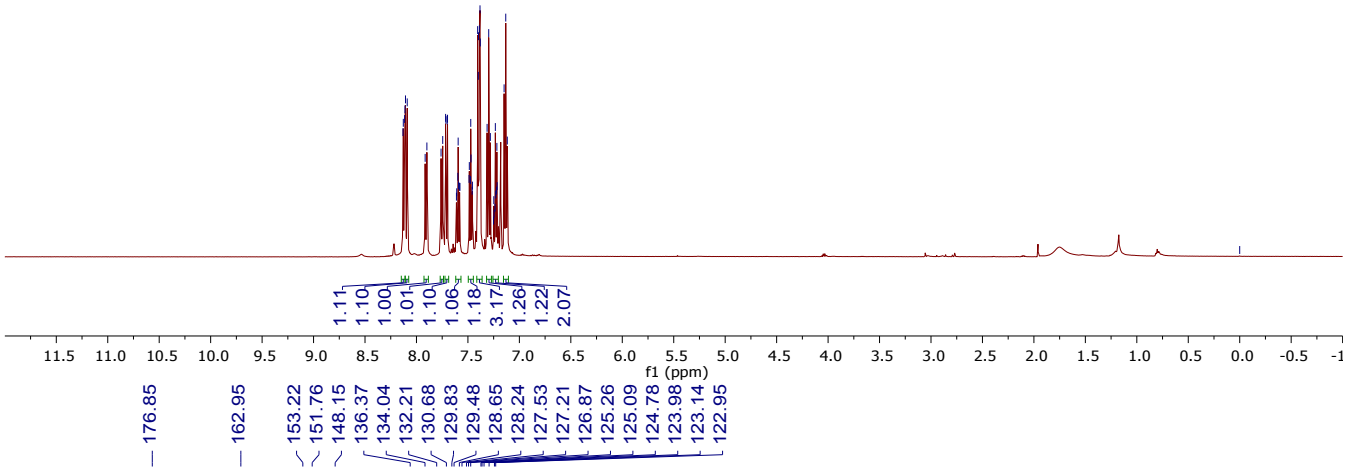
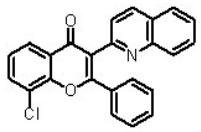
7.22
7.22
7.15
7.13
7.12
0.00



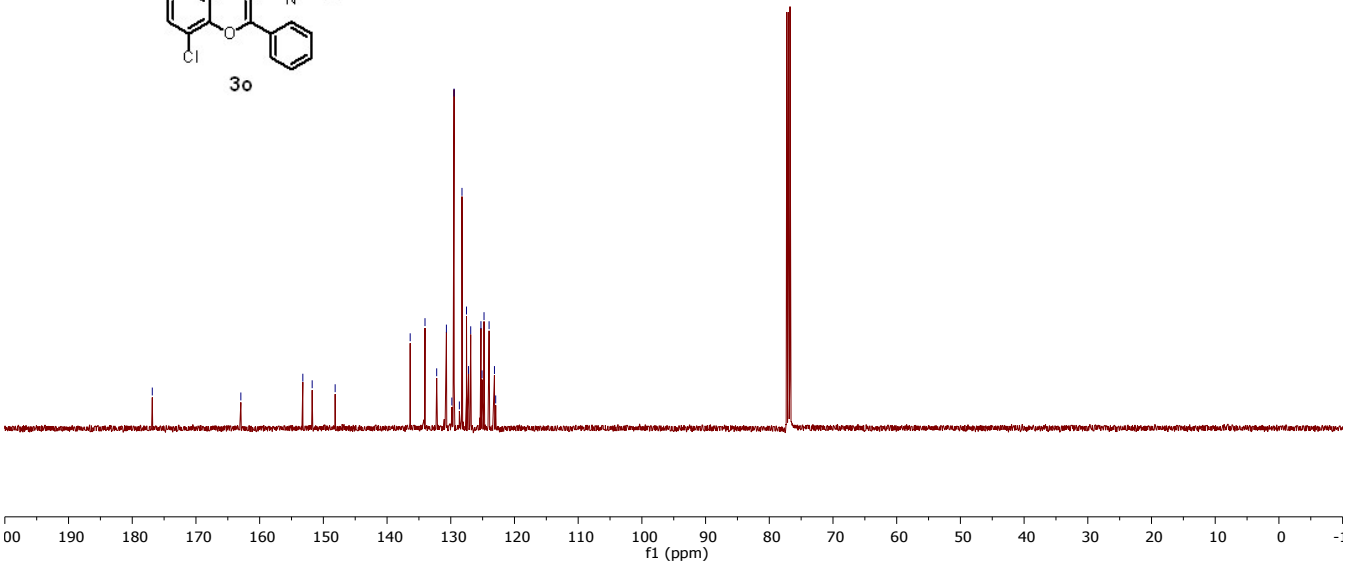
3o


1.11
1.10
1.00
1.01
1.10
1.06
1.18
3.17
1.26
1.22
2.07
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)

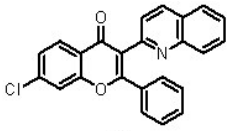
176.85
162.95
153.22
151.76
148.15
136.37
134.04
132.21
130.68
129.83
129.48
128.65
128.24
127.53
127.21
126.87
125.26
125.09
124.78
123.98
123.14
122.95



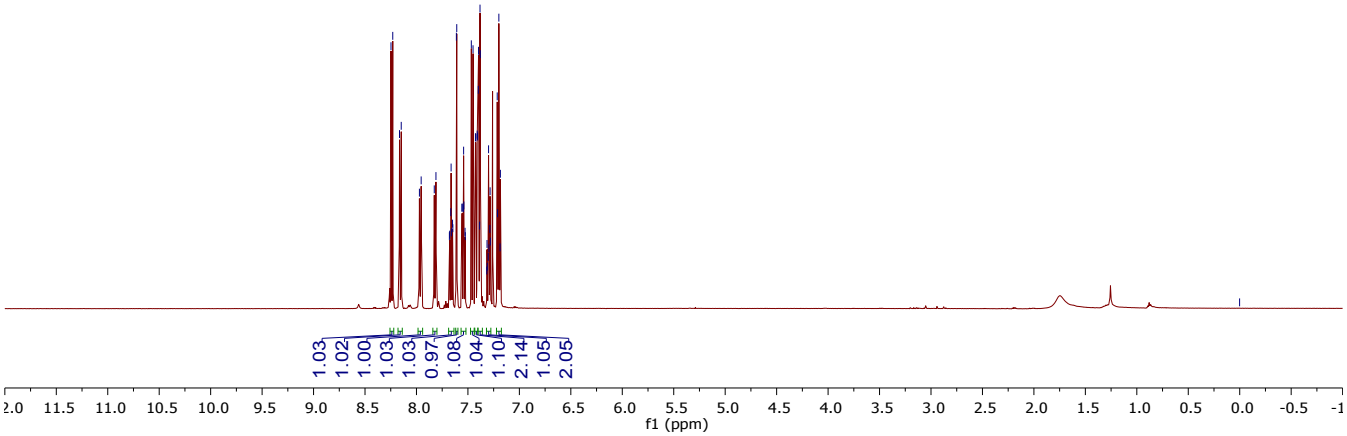
3o

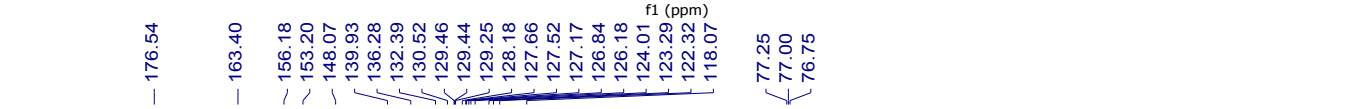

00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.25 8.23 8.16 8.15 7.97 7.95 7.83 7.81 7.68 7.68 7.67 7.66 7.66 7.65 7.65 7.61 7.61 7.56 7.56 7.54 7.54 7.54 7.53 7.53 7.47 7.45 7.43 7.42 7.41 7.41 7.40 7.40 7.39 7.38 7.38 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.28 7.28 7.22 7.21 7.20 7.19 7.18
0.00


O
N
Cl
O

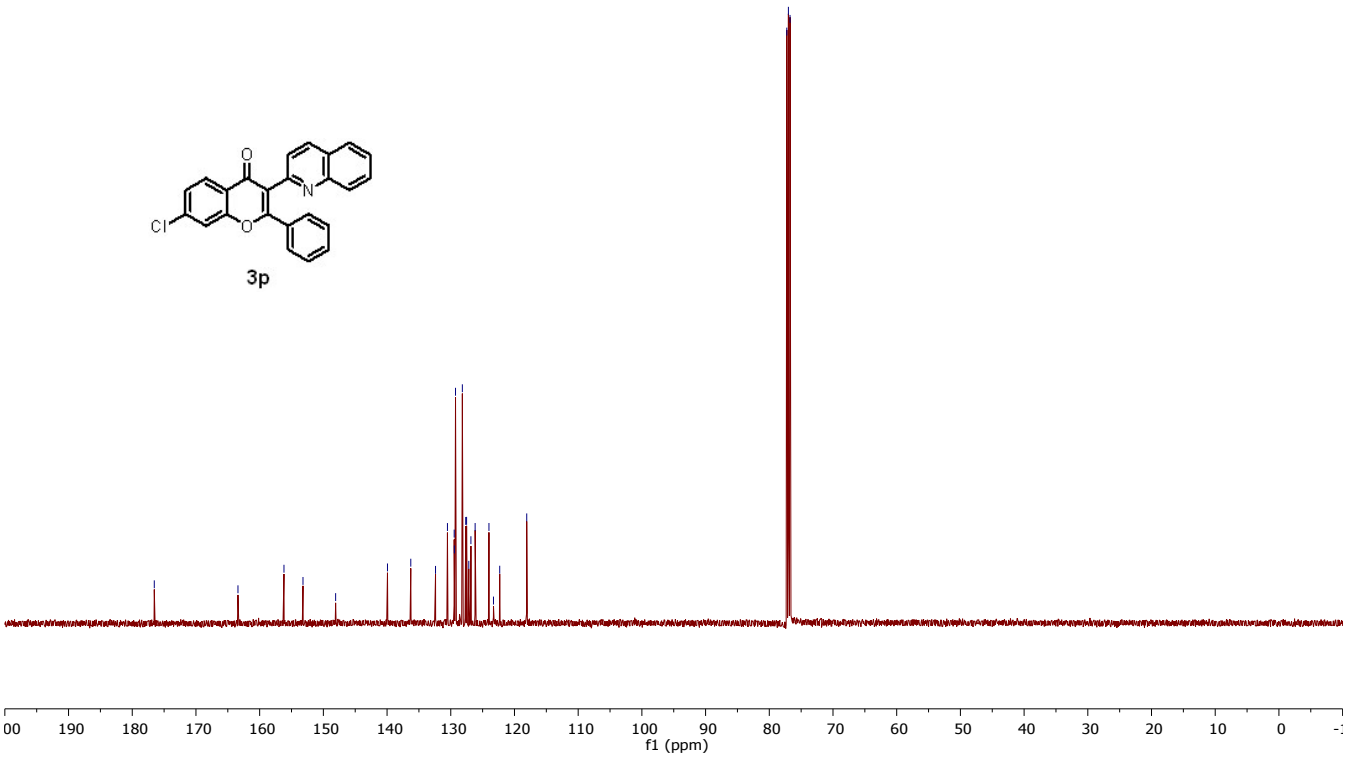
3p

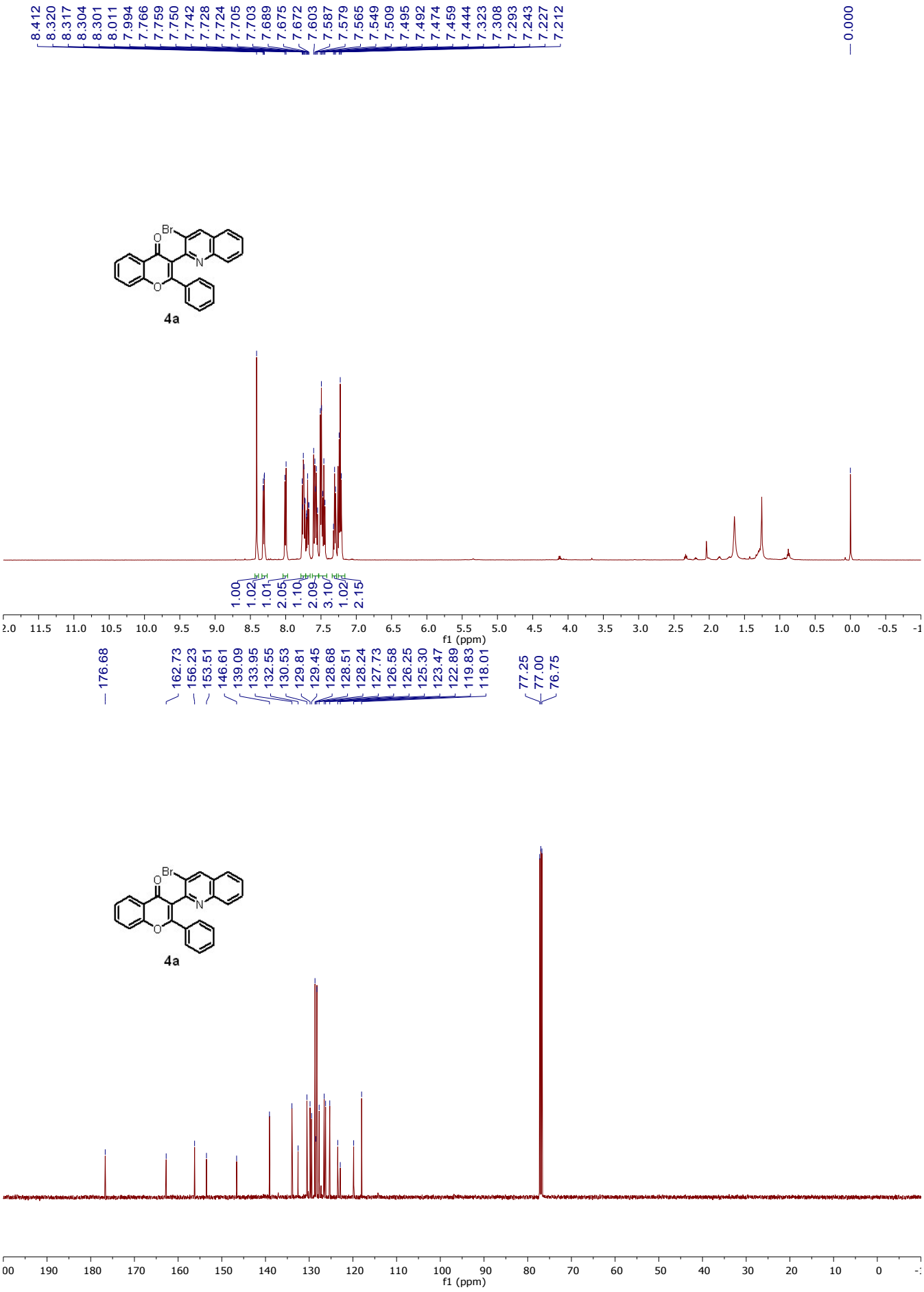

1.03 1.02 1.00 1.03 1.03 0.97 1.08 1.04 1.10 2.14 1.05 2.05
f1 (ppm)


176.54 163.40 156.18 153.20 148.07 139.93 136.28 132.39 130.52 129.46 129.44 129.25 128.18 127.66 127.52 127.17 126.84 126.18 124.01 123.29 122.32 118.07 77.25 77.00 76.75

O
N
Cl
O

3p


f1 (ppm)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8.011
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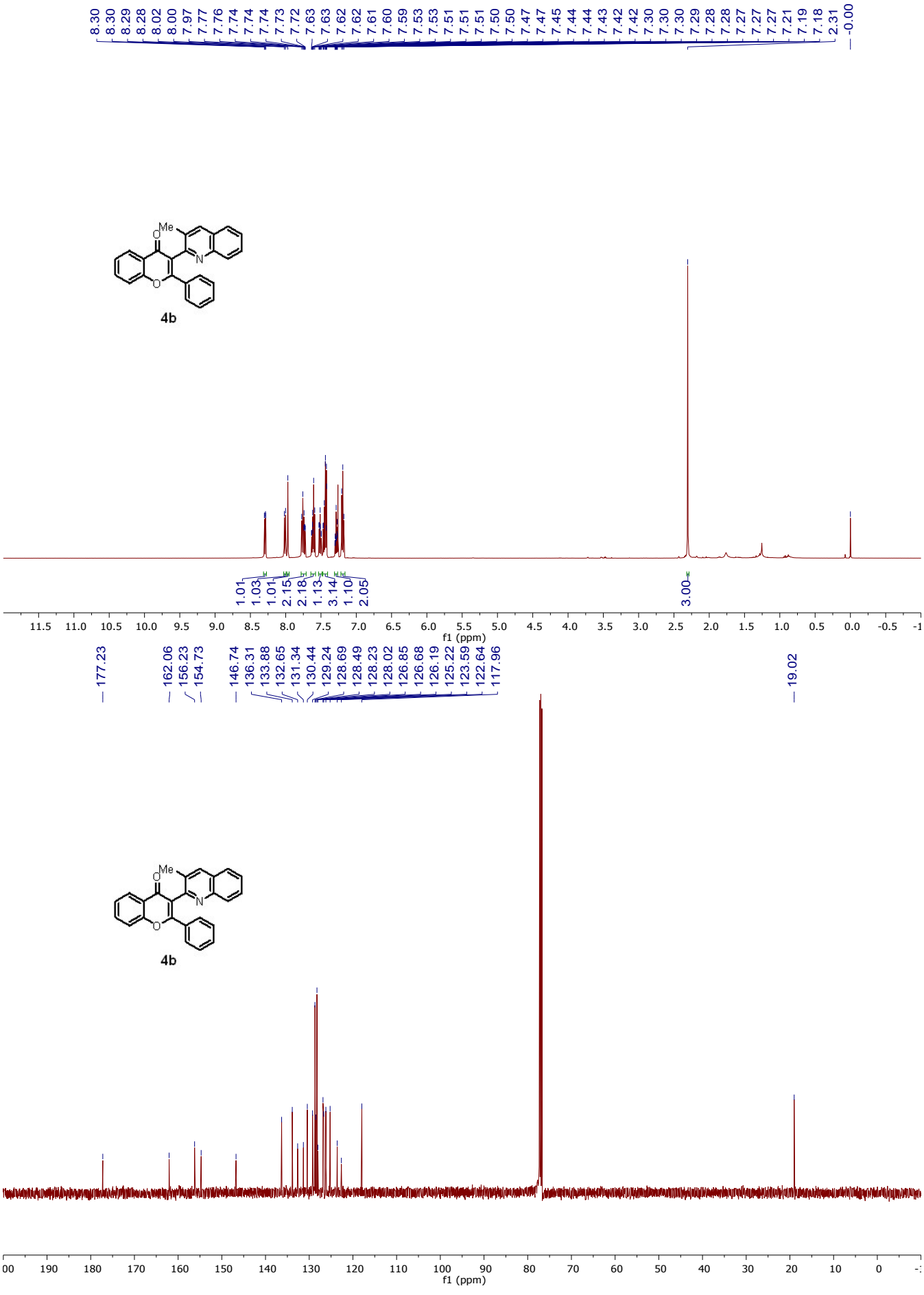
7.759
7.750
7.742
7.728
7.724
7.705
7.703
7.689
7.675
7.672
7.603
7.587
7.579
7.565
7.549
7.509
7.495
7.492
7.474
7.459
7.444
7.323
7.308
7.293
7.243
7.227
7.212
0.000
Br
O
N
O
4a
1.00
1.02
1.01
2.05
1.10
2.09
3.10
1.02
2.15
f1 (ppm)
176.68
162.73
156.23
153.51
146.61
139.09
133.95
132.55
130.53
129.81
129.45
128.68
128.51
128.24
127.73
126.58
126.25
125.30
123.47
122.89
119.83
118.01
77.25
77.00
76.75
Br
O
N
O
4a
f1 (ppm)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8.02
8.00
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7.77
7.76
7.74
7.74
7.74
7.73
7.72
7.63
7.63
7.62
7.62
7.61
7.60
7.59
7.53
7.53
7.51
7.51
7.51
7.50
7.50
7.47
7.47
7.45
7.44
7.44
7.43
7.42
7.42
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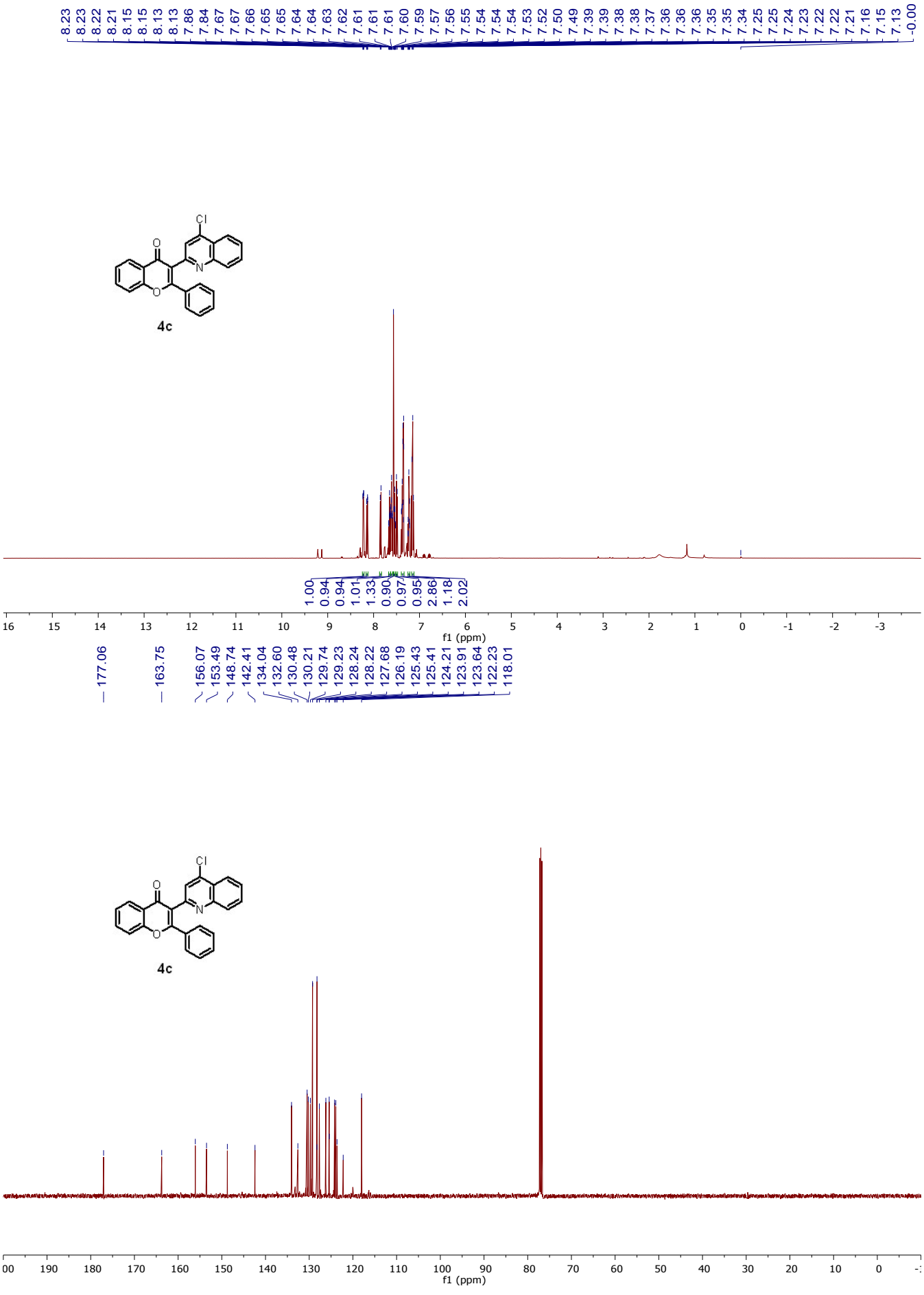
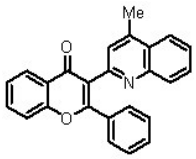
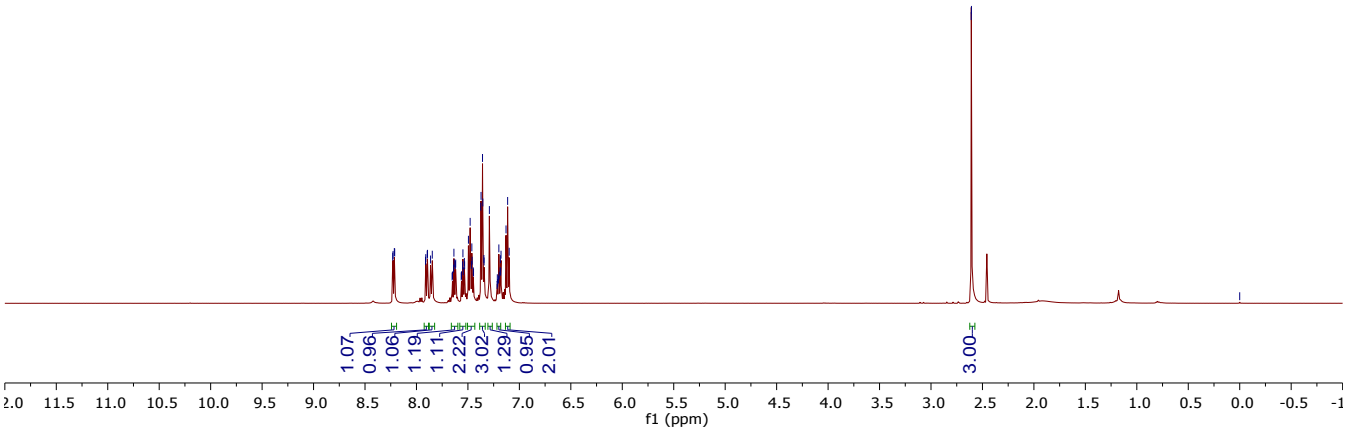
7.30
7.30
7.29
7.28
7.27
7.27
7.27
7.21
7.19
7.18
2.31
-0.00
Me
O
N
O
4b
1.01
1.03
1.01
2.15
2.18
1.13
3.14
1.10
2.05
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)
177.23
162.06
156.23
154.73
146.74
136.31
133.88
132.65
131.34
130.44
129.24
128.69
128.49
128.23
128.02
126.85
126.68
126.19
125.22
123.59
122.64
117.96
19.02
Me
O
N
O
4b
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.23 8.23 8.22 8.21 8.15 8.15 8.13 8.13 7.86 7.84 7.67 7.67 7.66 7.65 7.65 7.64 7.64 7.63 7.62 7.61 7.61 7.61 7.60 7.59 7.57 7.56 7.55 7.54 7.54 7.54 7.53 7.52 7.50 7.49 7.39 7.39 7.38 7.38 7.37 7.36 7.36 7.36 7.35 7.35 7.34 7.25 7.25 7.24 7.23 7.22 7.22 7.21 7.16 7.15 7.13 -0.00
Cl
O
N
O
4c
1.00 0.94 0.94 1.01 1.33 0.90 0.97 0.95 2.86 1.18 2.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)
177.06 163.75 156.07 153.49 148.74 142.41 134.04 132.60 130.48 130.21 129.74 129.23 128.24 128.22 127.68 126.19 125.43 125.41 124.21 123.91 123.64 122.23 118.01
Cl
O
N
O
4c
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

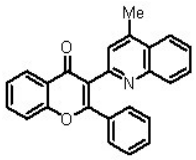

8.23 8.23 8.22 8.21 7.91 7.91 7.90 7.89 7.86 7.85 7.65 7.65 7.64 7.64 7.63 7.62 7.62 7.57 7.56 7.55 7.55 7.55 7.53 7.53 7.50 7.48 7.46 7.46 7.46 7.45 7.45 7.37 7.37 7.36 7.36 7.34 7.34 7.29 7.22 7.21 7.21 7.20 7.20 7.20 7.19 7.18 7.18 7.18 7.13 7.11 7.10 2.61 2.61 0.00


Me
O
N
O

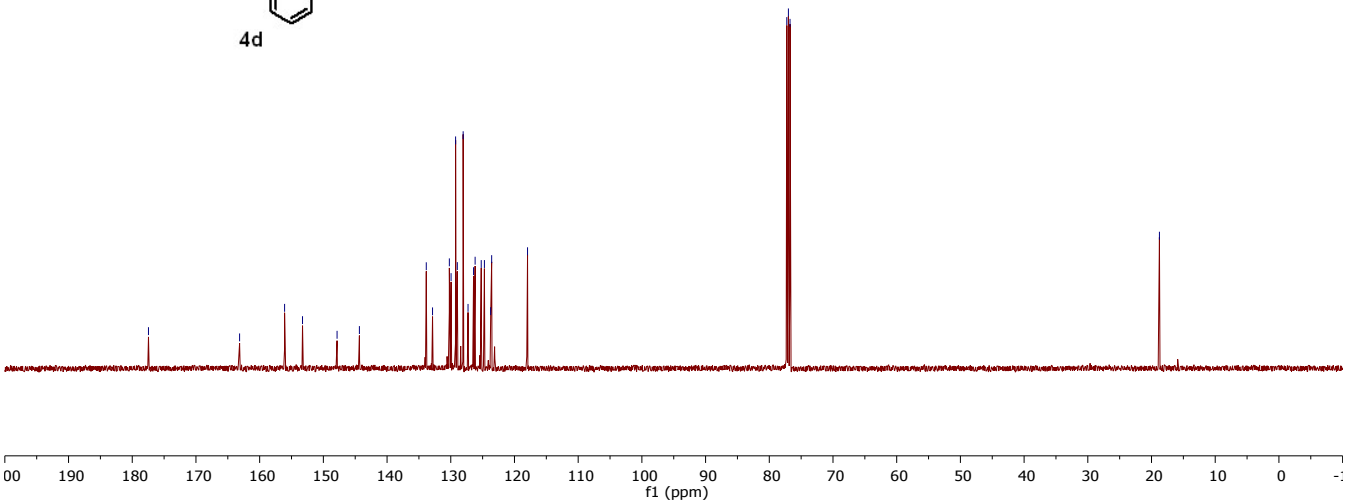
4d


1.07 0.96 1.06 1.19 1.11 2.22 3.02 1.29 0.95 2.01
3.00
f1 (ppm)

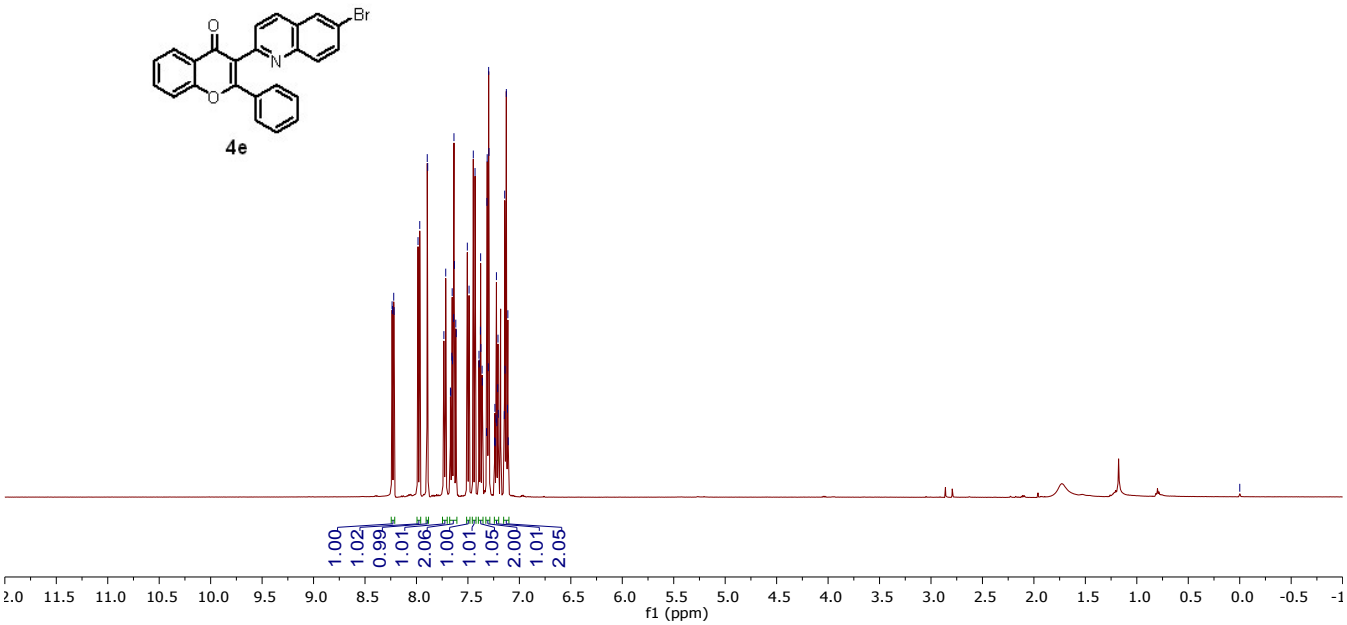

177.45 163.15 156.09 153.27 147.85 144.34 133.84 132.86 130.22 129.95 129.24 128.97 128.06 127.29 126.42 126.18 125.22 124.72 123.74 123.58 117.95
77.25 77.00 76.75
18.76

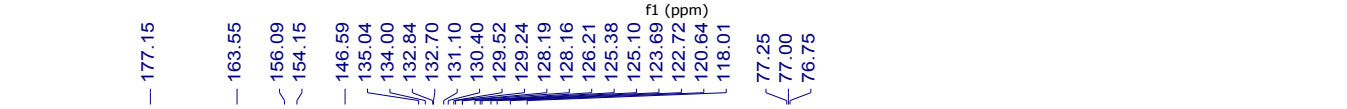

Me
O
N
O

4d


f1 (ppm)


8.24 8.23 8.22 8.22 7.98 7.97 7.90 7.89 7.73 7.72 7.67 7.67 7.66 7.65 7.65 7.64 7.64 7.63 7.62 7.61 7.51 7.49 7.45 7.43 7.39 7.39 7.38 7.38 7.37 7.36 7.36 7.32 7.31 7.31 7.30 7.30 7.30 7.24 7.24 7.23 7.22 7.22 7.21 7.21 7.21 7.15 7.14 7.14 7.13 7.12 7.11 7.11
-0.00


Br
O
N
O
4e
1.00 1.02 0.99 1.01 2.06 1.00 1.01 1.05 2.00 1.01 2.05
f1 (ppm)


177.15
163.55
156.09
154.15
146.59
135.04
134.00
132.84
132.70
131.10
130.40
129.52
129.24
128.19
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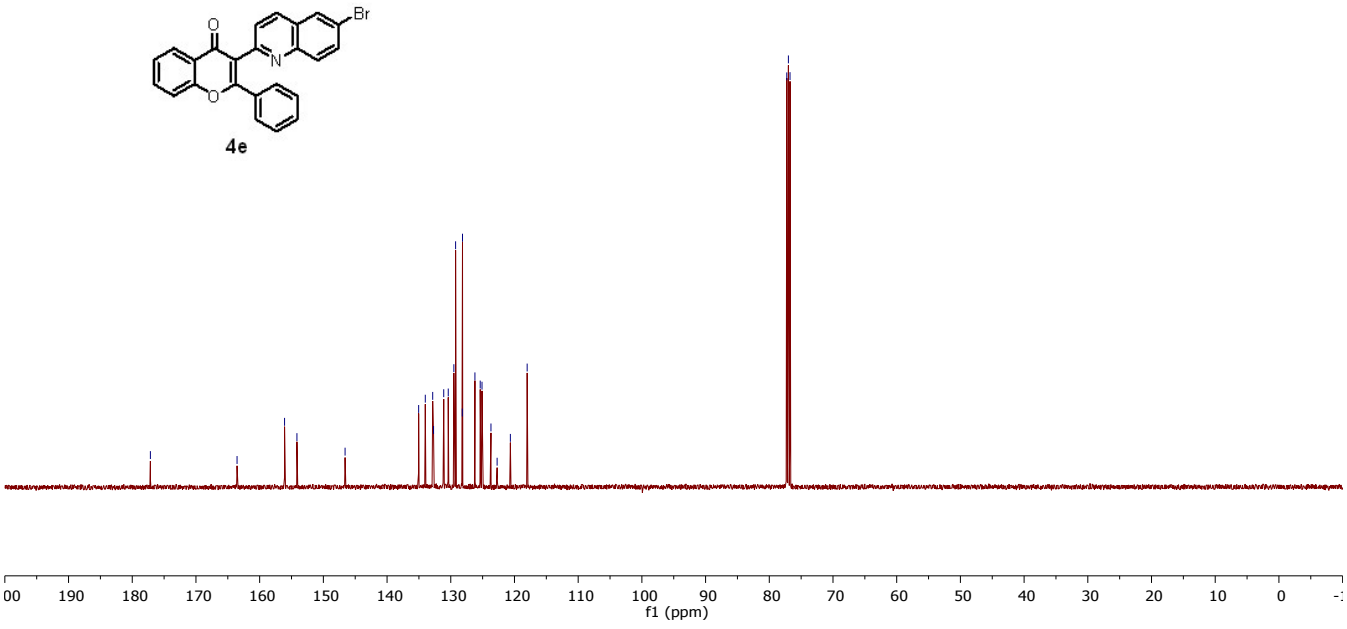
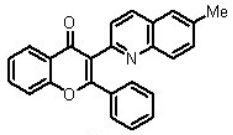
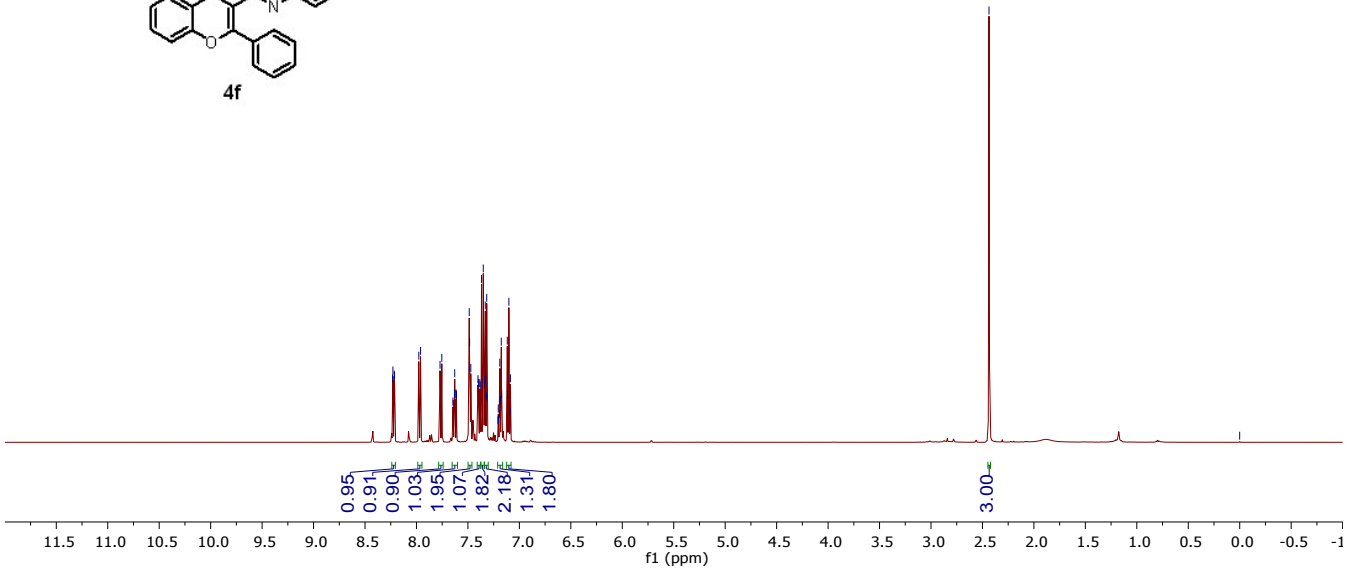
123.69
122.72
120.64
118.01
77.25
77.00
76.75

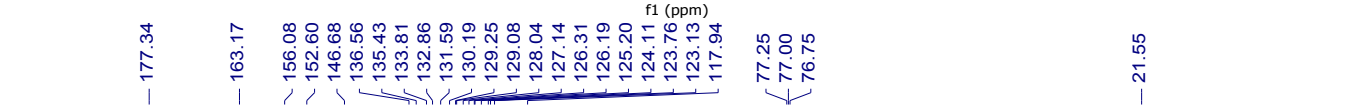

Br
O
N
O
4e
f1 (ppm)

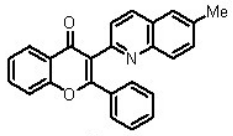

8.23
8.23
8.22
8.21
7.98
7.96
7.77
7.75
7.65
7.64
7.63
7.63
7.63
7.61
7.61
7.49
7.48
7.47
7.40
7.40
7.38
7.38
7.37
7.35
7.34
7.34
7.33
7.32
7.21
7.21
7.20
7.19
7.19
7.19
7.18
7.17
7.12
7.11
7.10
7.09
7.09
2.44
0.00


O
N
O
Me

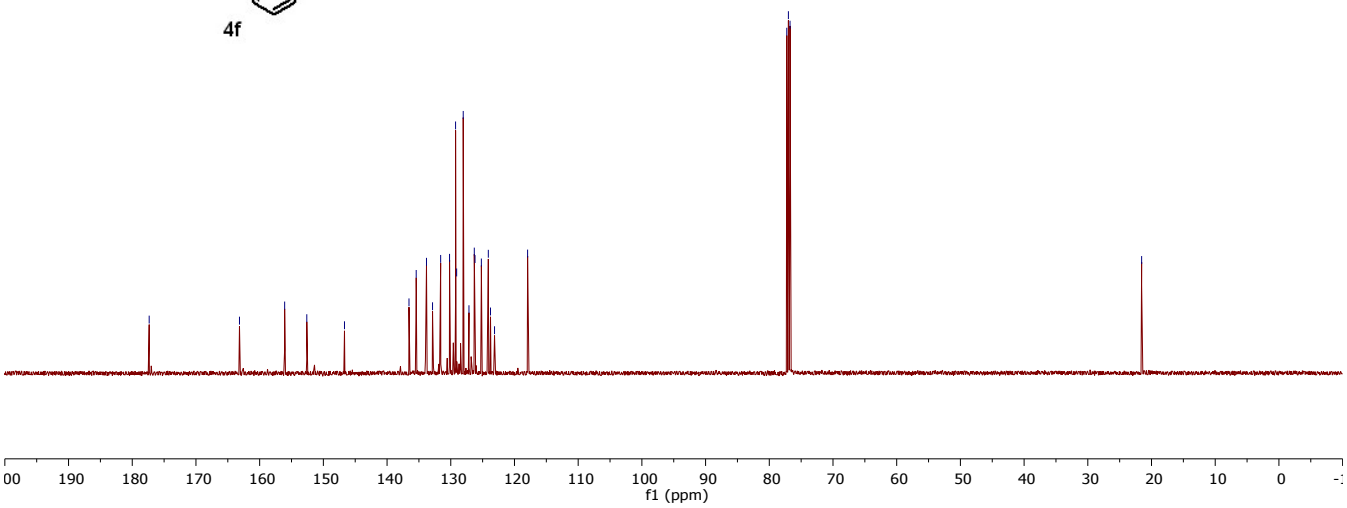
4f

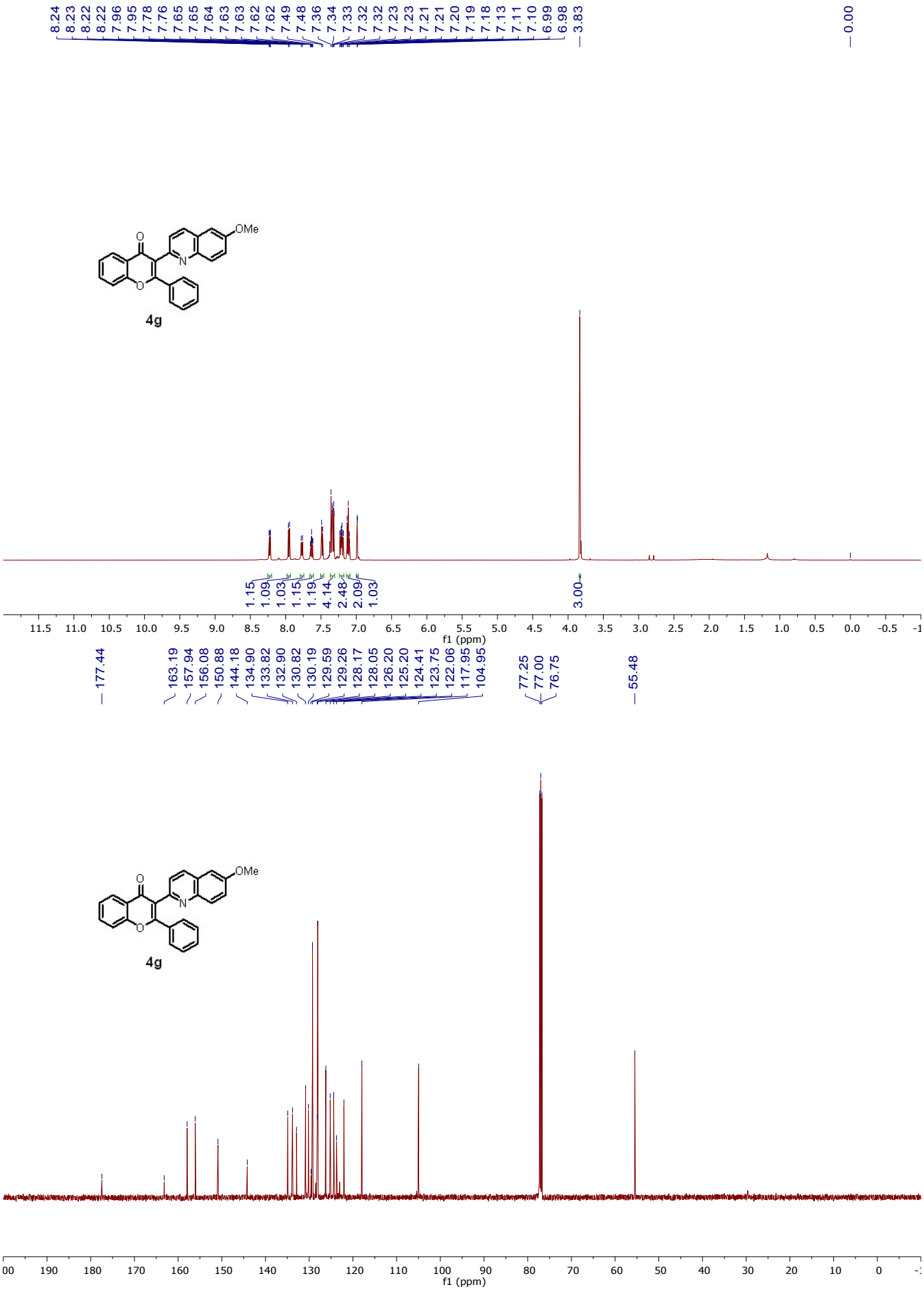

0.95
0.91
0.90
1.03
1.95
1.07
1.82
2.18
1.31
1.80
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


177.34
163.17
156.08
152.60
146.68
136.56
135.43
133.81
132.86
131.59
130.19
129.25
129.08
128.04
127.14
126.31
126.19
125.20
124.11
123.76
123.13
117.94
77.25
77.00
76.75
21.55

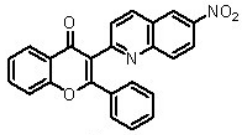

O
N
O
Me

4f

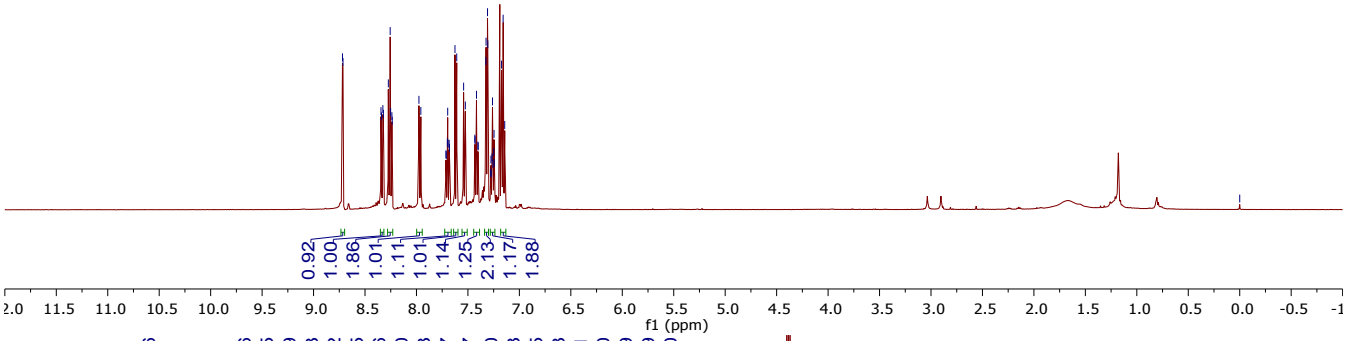

00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

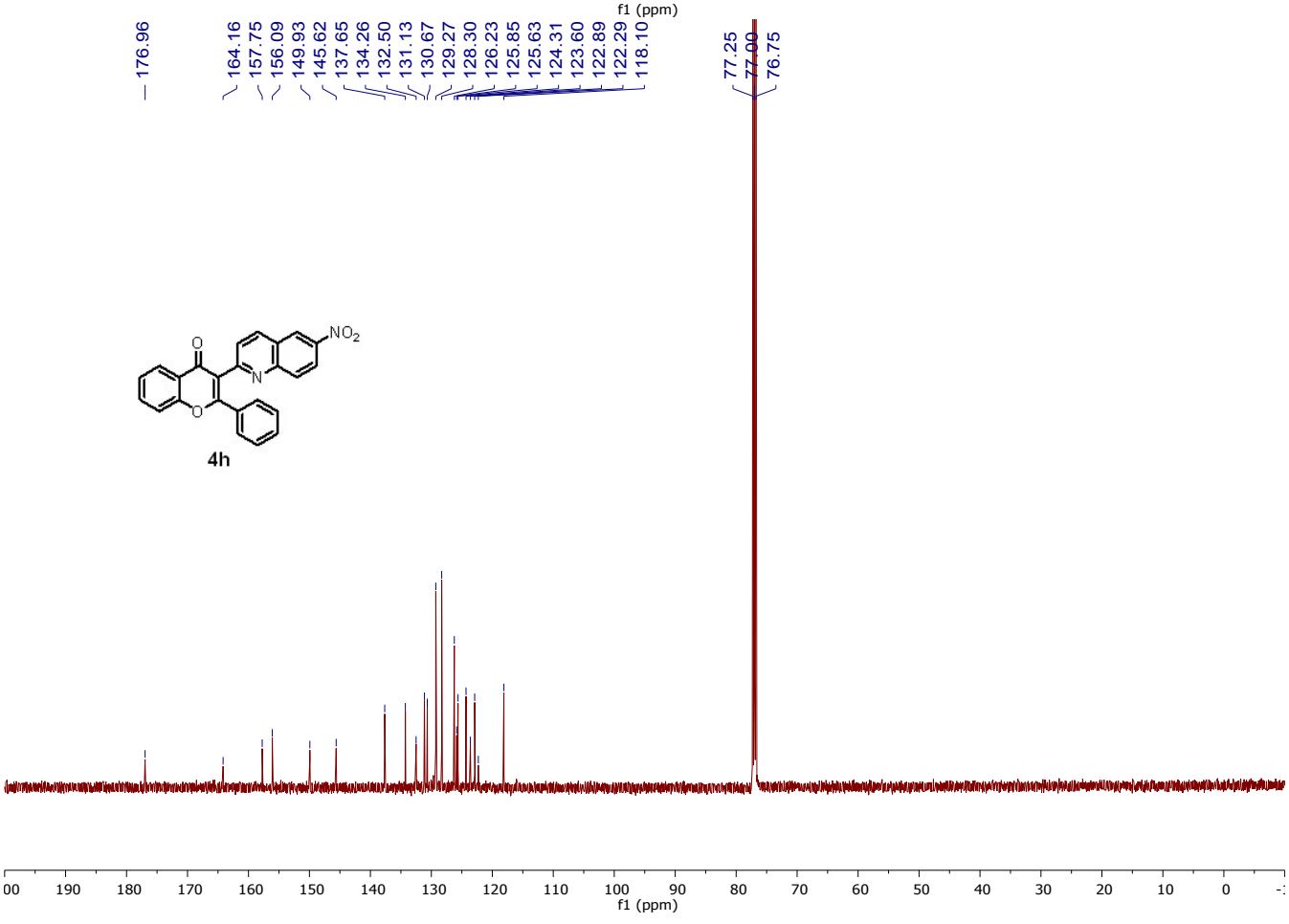

8.24
8.23
8.22
8.22
7.96
7.95
7.78
7.76
7.65
7.65
7.64
7.63
7.63
7.62
7.62
7.49
7.48
7.36
7.34
7.33
7.32
7.32
7.23
7.23
7.21
7.21
7.20
7.19
7.18
7.13
7.11
7.10
6.99
6.98
3.83
0.00
OMe
O
N
O
4g
1.15
1.09
1.03
1.15
1.19
4.14
2.48
2.09
1.03
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 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)
177.44
163.19
157.94
156.08
150.88
144.18
134.90
133.82
132.90
130.82
130.19
129.59
129.26
128.17
128.05
126.20
125.20
124.41
123.75
122.06
117.95
104.95
77.25
77.00
76.75
55.48
OMe
O
N
O
4g
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


8.72
8.71
8.34
8.34
8.33
8.32
8.27
8.26
8.25
8.24
8.24
7.98
7.96
7.71
7.71
7.70
7.70
7.69
7.68
7.68
7.63
7.61
7.54
7.53
7.43
7.43
7.42
7.40
7.40
7.33
7.32
7.31
7.31
7.28
7.28
7.27
7.26
7.26
7.26
7.25
7.25
7.24
7.17
7.16
7.14
-0.00


O
N
O
NO2

4h

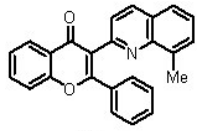

0.92
1.00
1.86
1.01
1.11
1.01
1.14
1.25
2.13
1.17
1.88
f1 (ppm)


176.96
164.16
157.75
156.09
149.93
145.62
137.65
134.26
132.50
131.13
130.67
129.27
128.30
126.23
125.85
125.63
124.31
123.60
122.89
122.29
118.10
77.25
77.00
76.75
f1 (ppm)

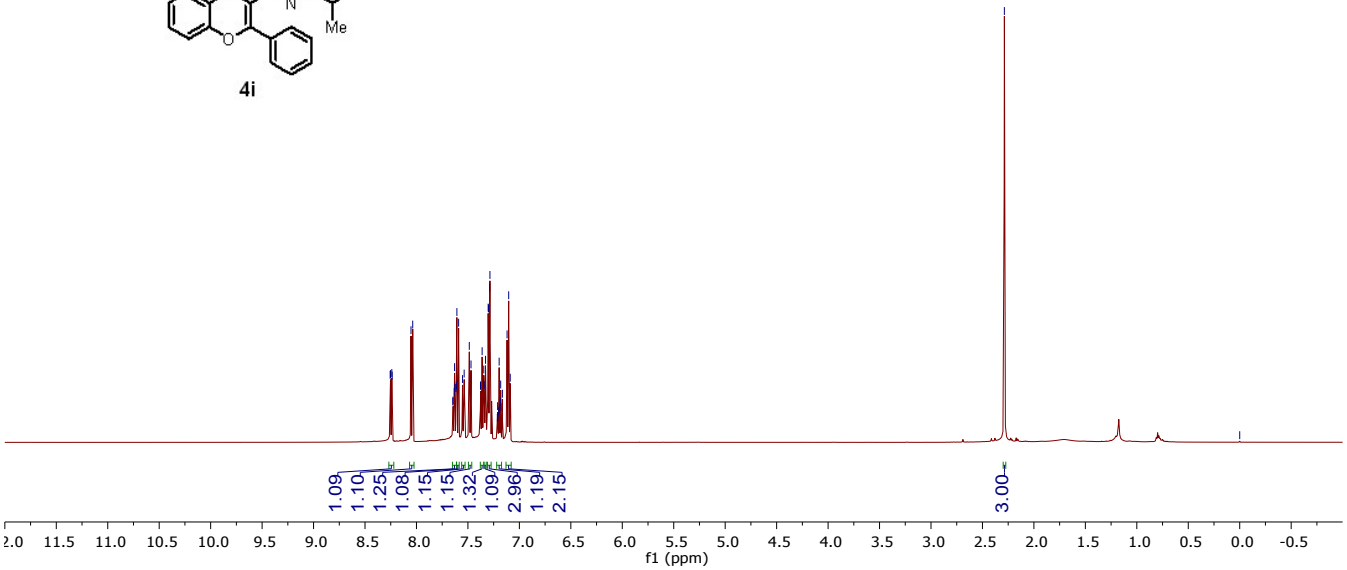
O
N
O
NO2

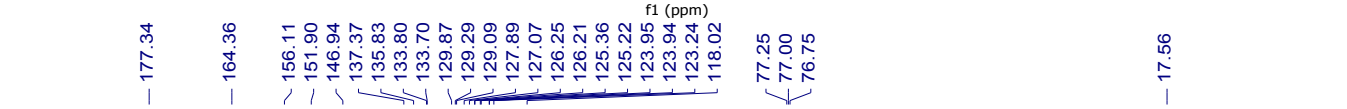
4h

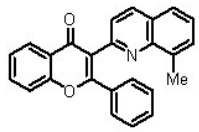

8.26
8.25
8.24
8.24
8.05
8.04
7.65
7.64
7.63
7.63
7.63
7.62
7.61
7.61
7.59
7.55
7.54
7.49
7.47
7.38
7.38
7.36
7.35
7.35
7.34
7.33
7.30
7.30
7.29
7.29
7.21
7.21
7.21
7.20
7.20
7.19
7.18
7.18
7.18
7.17
7.12
7.10
7.09
2.29
-0.00


O
N
Me
O

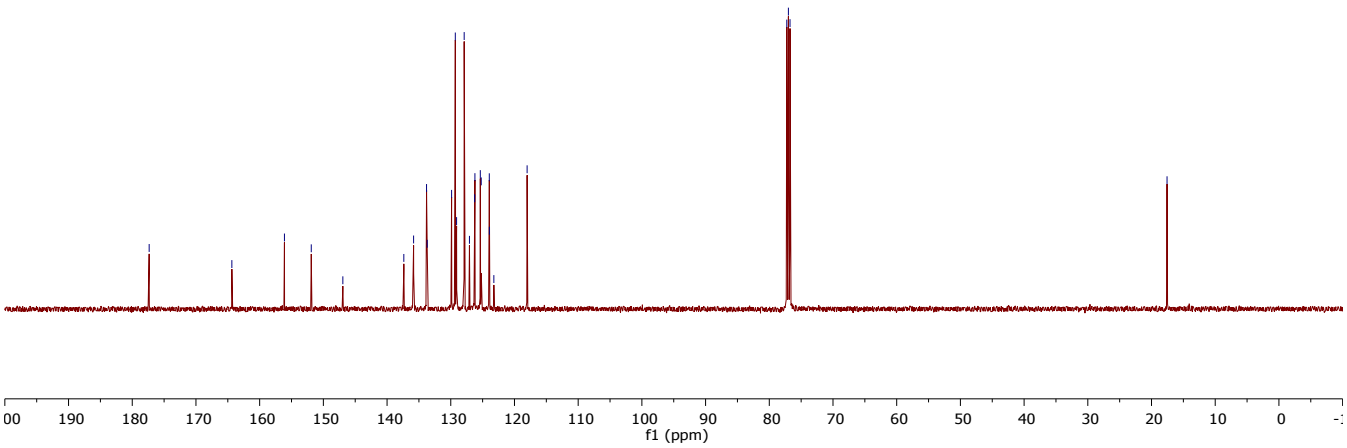
4i


1.09
1.10
1.25
1.08
1.15
1.15
1.32
1.09
2.96
1.19
2.15
3.00
2.0 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
f1 (ppm)

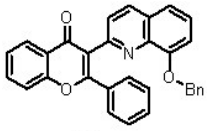

177.34
164.36
156.11
151.90
146.94
137.37
135.83
133.80
133.70
129.87
129.29
129.09
127.89
127.07
126.25
126.21
125.36
125.22
123.95
123.94
123.24
118.02
77.25
77.00
76.75
17.56


O
N
Me
O

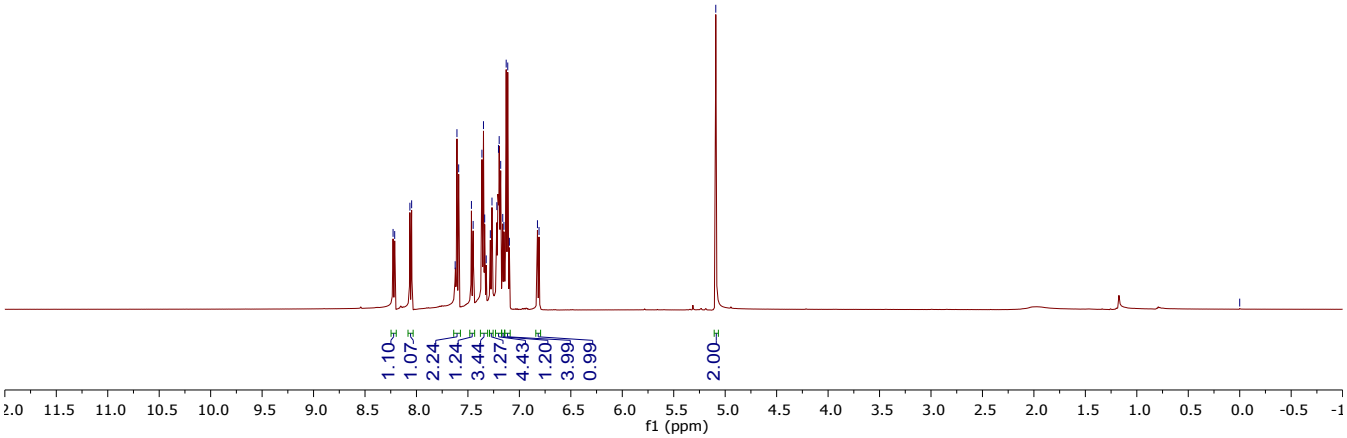
4i


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

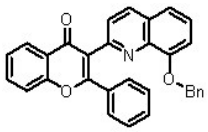

8.23
8.21
8.06
8.05
7.62
7.61
7.59
7.47
7.45
7.36
7.35
7.34
7.32
7.28
7.27
7.22
7.20
7.20
7.18
7.16
7.15
7.13
7.11
7.10
6.82
6.81
5.09
0.00


O
N
O
O
Bn

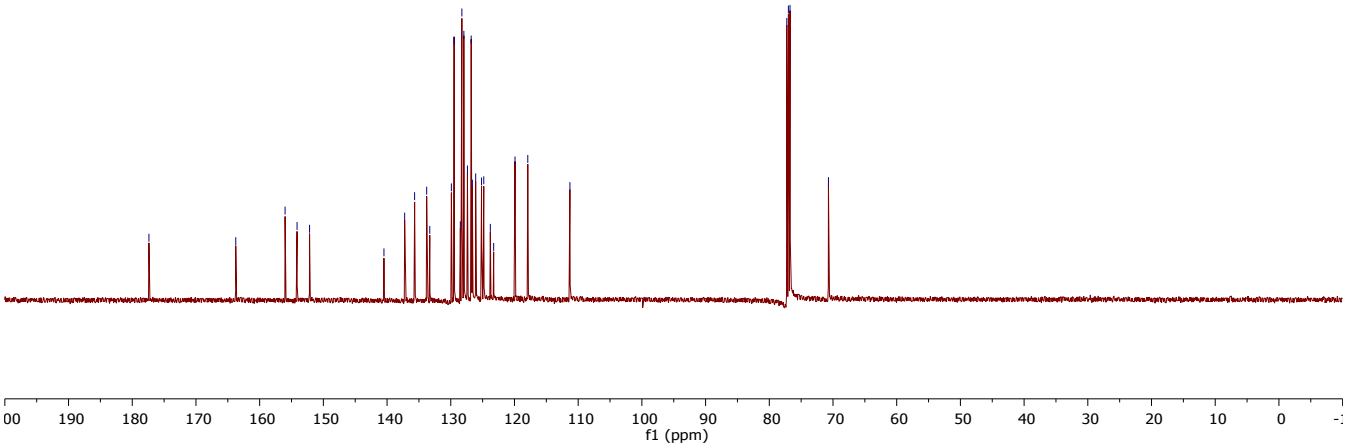
4j


1.10
1.07
2.24
1.24
3.44
1.27
4.43
1.20
3.99
0.99
2.00
f1 (ppm)


177.38
163.75
156.01
154.13
152.17
140.49
137.24
135.68
133.78
133.29
129.90
129.48
128.50
128.26
127.95
127.38
126.79
126.61
126.09
125.17
124.82
123.79
123.27
119.92
117.91
111.30
77.25
77.00
76.74
70.71


O
N
O
O
Bn

4j


f1 (ppm)


8.53
8.51
8.31
8.31
8.29
8.29
7.89
7.87
7.85
7.83
7.78
7.78
7.77
7.76
7.76
7.75
7.75
7.66
7.65
7.64
7.64
7.64
7.63
7.62
7.51
7.51
7.49
7.49
7.48
7.48
7.47
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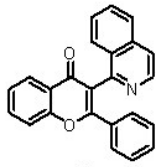
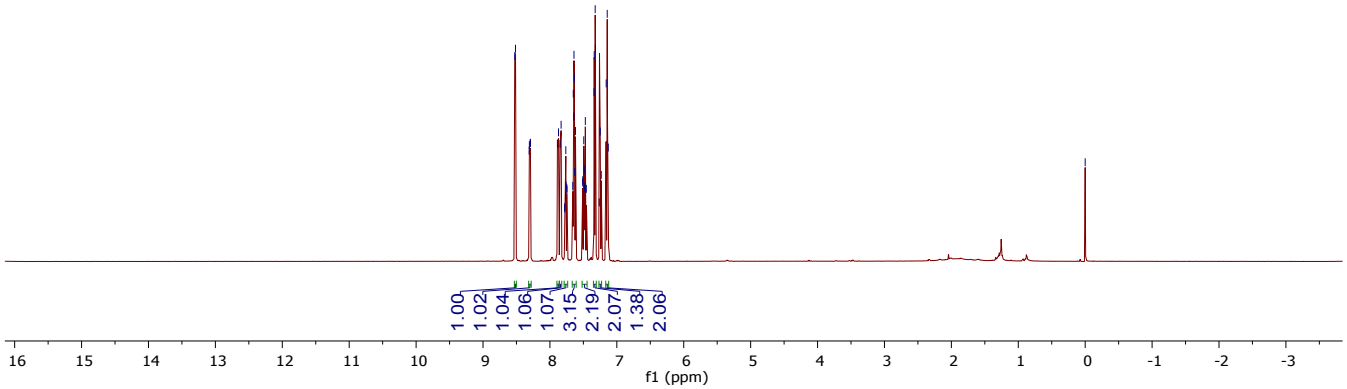
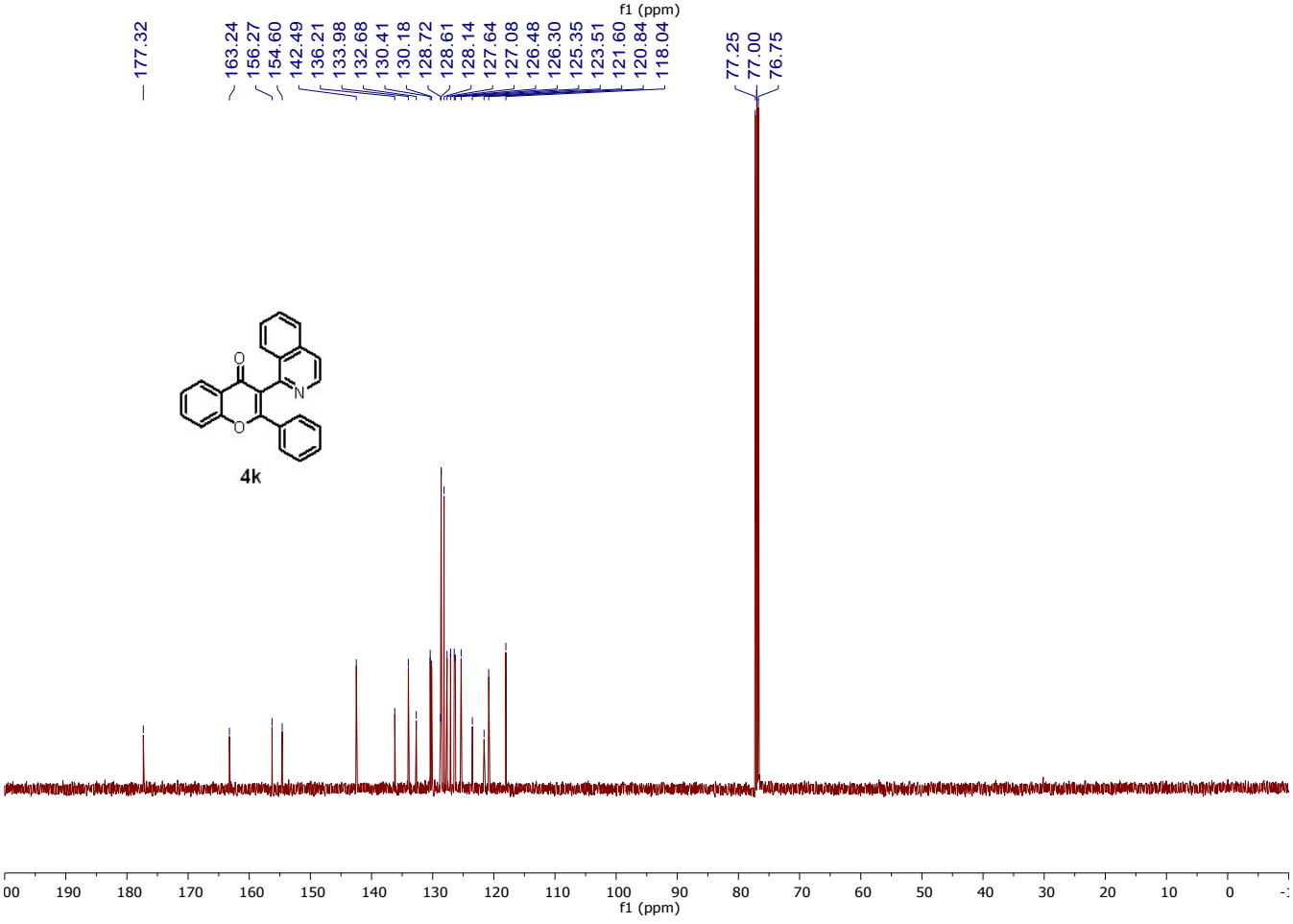
7.25
7.23
7.16
7.14
7.13
0.00



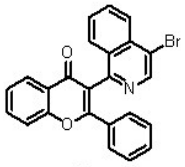
4k


1.00
1.02
1.04
1.06
1.07
3.15
2.19
2.07
1.38
2.06
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

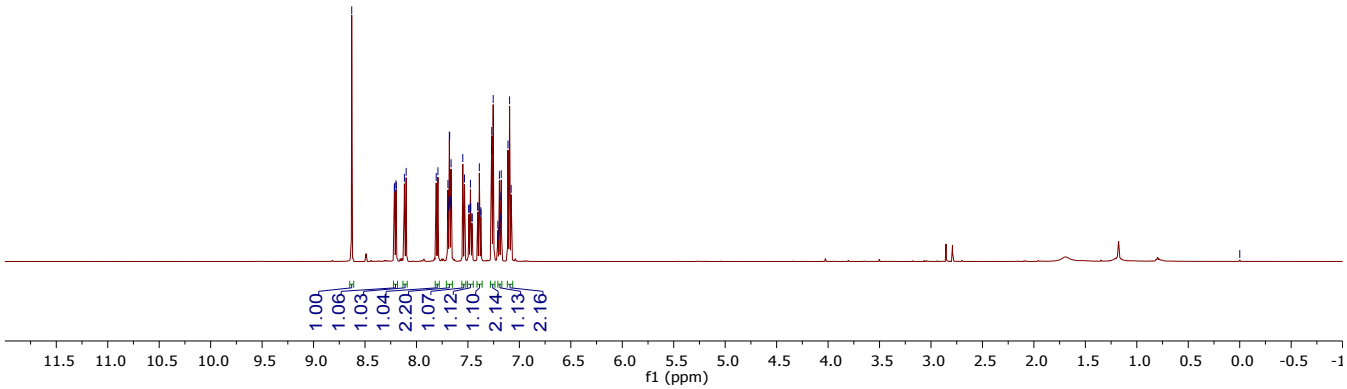

177.32
163.24
156.27
154.60
142.49
136.21
133.98
132.68
130.41
130.18
128.72
128.61
128.14
127.64
127.08
126.48
126.30
125.35
123.51
121.60
120.84
118.04
77.25
77.00
76.75
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

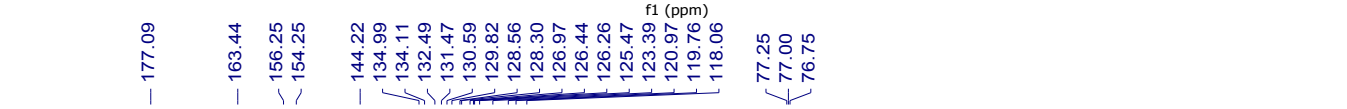
4k

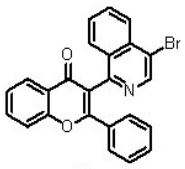

8.63 8.21 8.21 8.20 8.20 8.12 8.10 7.81 7.79 7.70 7.69 7.69 7.68 7.68 7.68 7.67 7.67 7.66 7.66 7.55 7.53 7.49 7.49 7.48 7.48 7.47 7.46 7.46 7.40 7.40 7.39 7.37 7.37 7.27 7.27 7.25 7.25 7.21 7.21 7.21 7.20 7.19 7.19 7.18 7.18 7.18 7.11 7.09 7.08
-0.00


O
N
O
Br

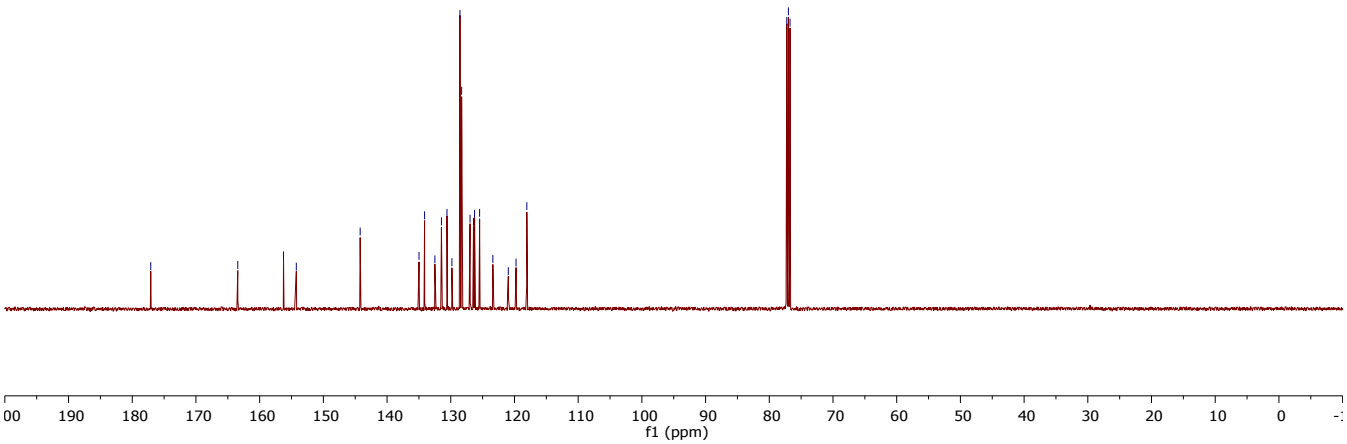
4l


1.00 1.06 1.03 1.04 2.20 1.07 1.12 1.10 2.14 1.13 2.16
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)

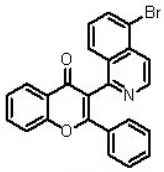

177.09
163.44
156.25
154.25
144.22
134.99
134.11
132.49
131.47
130.59
129.82
128.56
128.30
126.97
126.44
126.26
125.47
123.39
120.97
119.76
118.06
77.25
77.00
76.75


O
N
O
Br

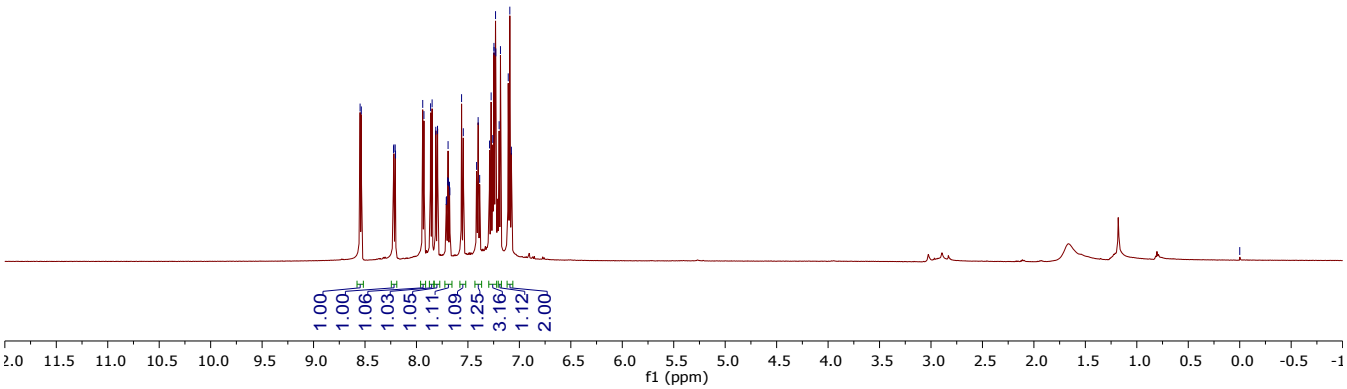
4i


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.55
8.54
8.22
8.22
8.21
8.20
7.94
7.93
7.86
7.85
7.81
7.80
7.71
7.71
7.70
7.69
7.69
7.68
7.68
7.56
7.54
7.42
7.40
7.39
7.29
7.27
7.26
7.25
7.25
7.23
7.23
7.20
7.18
7.11
7.09
7.08
-0.00


Br
O
N
O

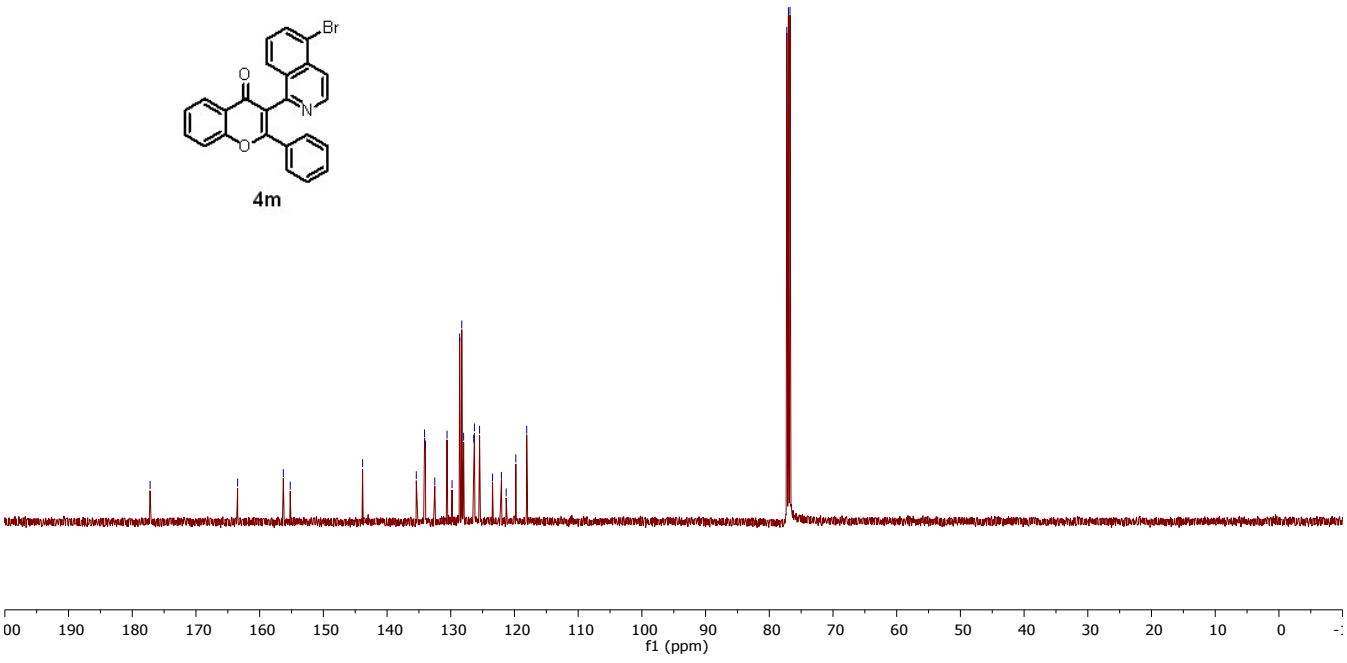
4m

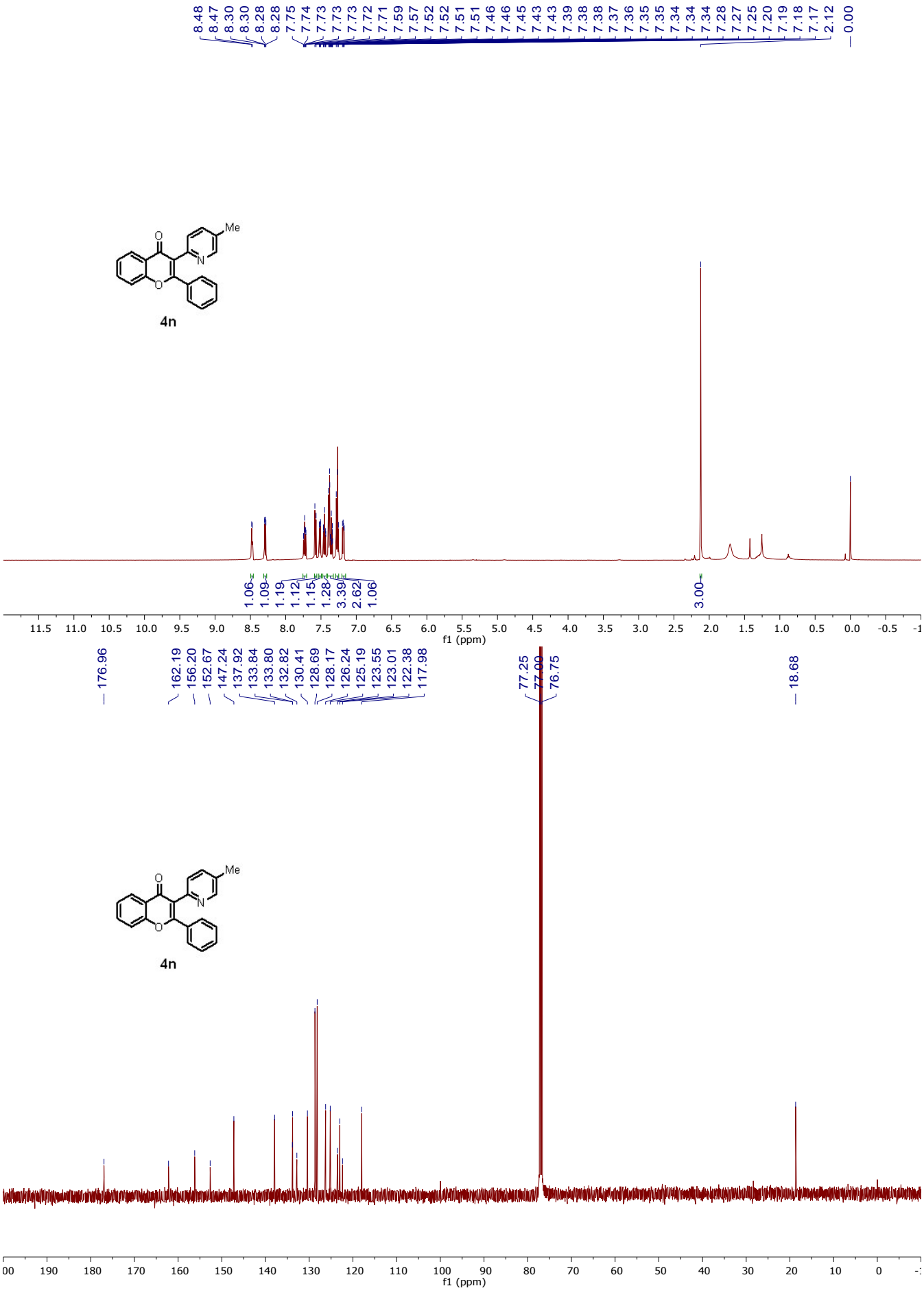

1.00
1.00
1.06
1.03
1.05
1.11
1.09
1.25
3.16
1.12
2.00
f1 (ppm)

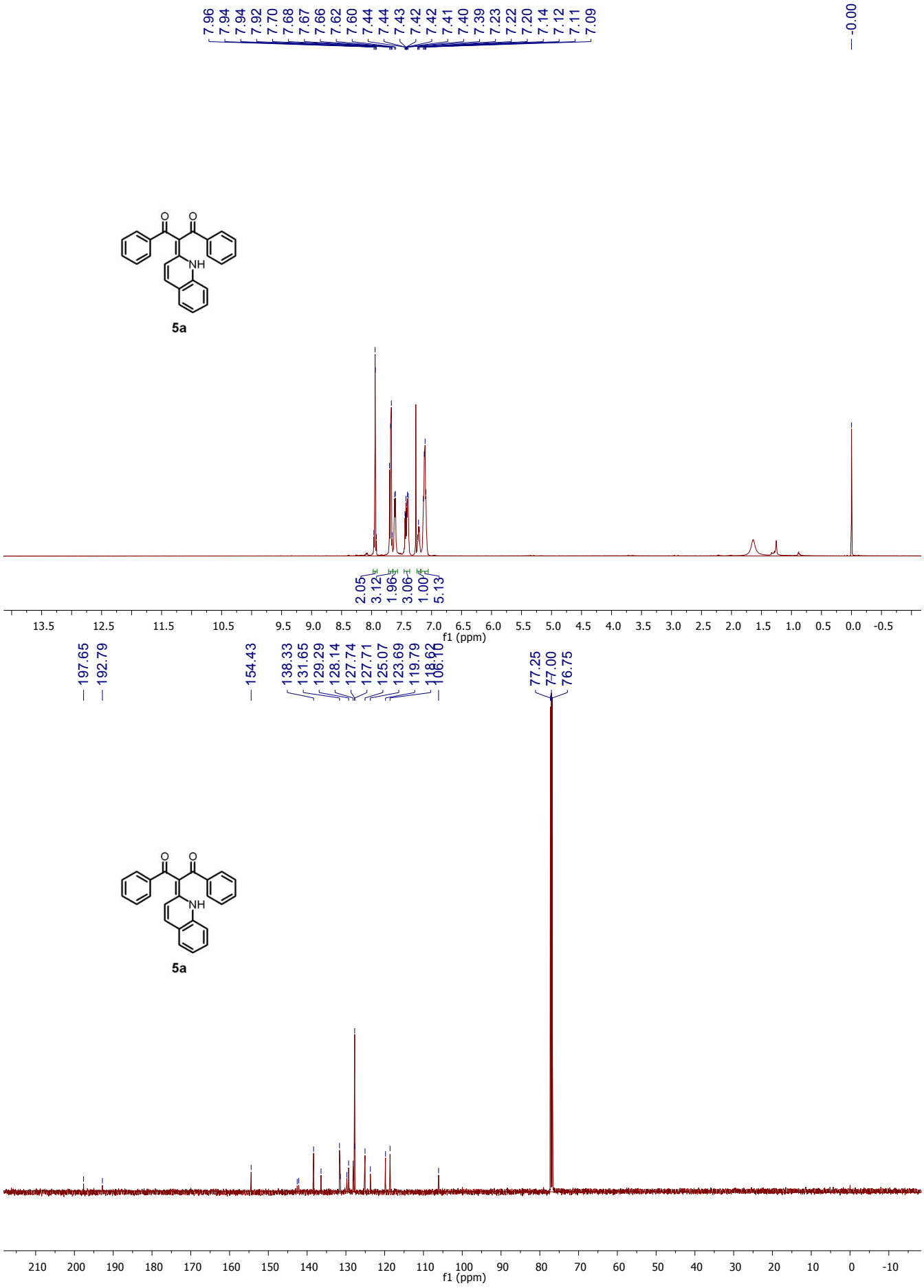

177.20
163.46
156.28
155.20
143.84
135.41
134.11
133.98
132.51
130.59
129.80
128.60
128.27
127.98
126.39
126.28
125.48
123.44
122.05
121.30
119.79
118.08
77.25
77.00
76.75

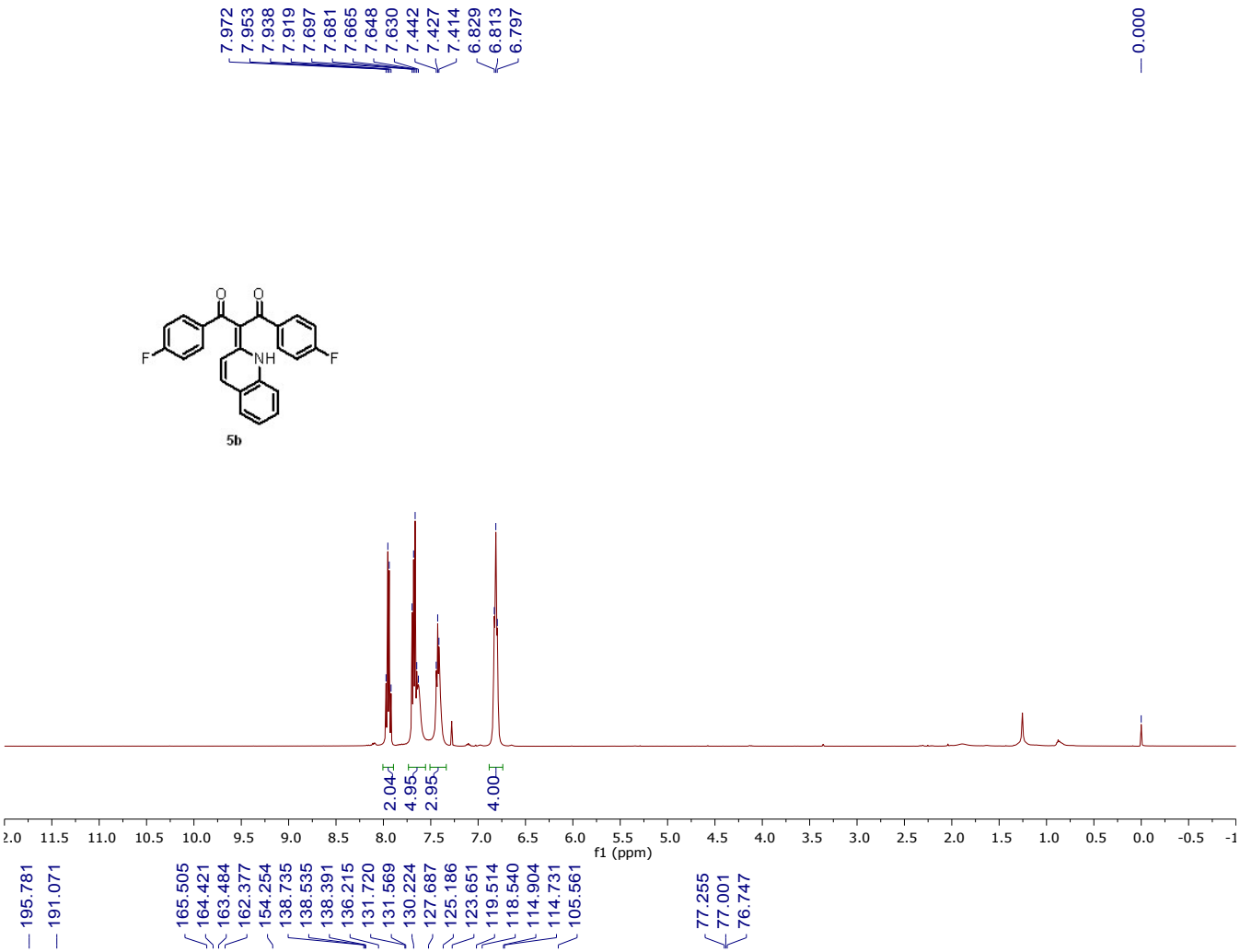
Br
O
N
O

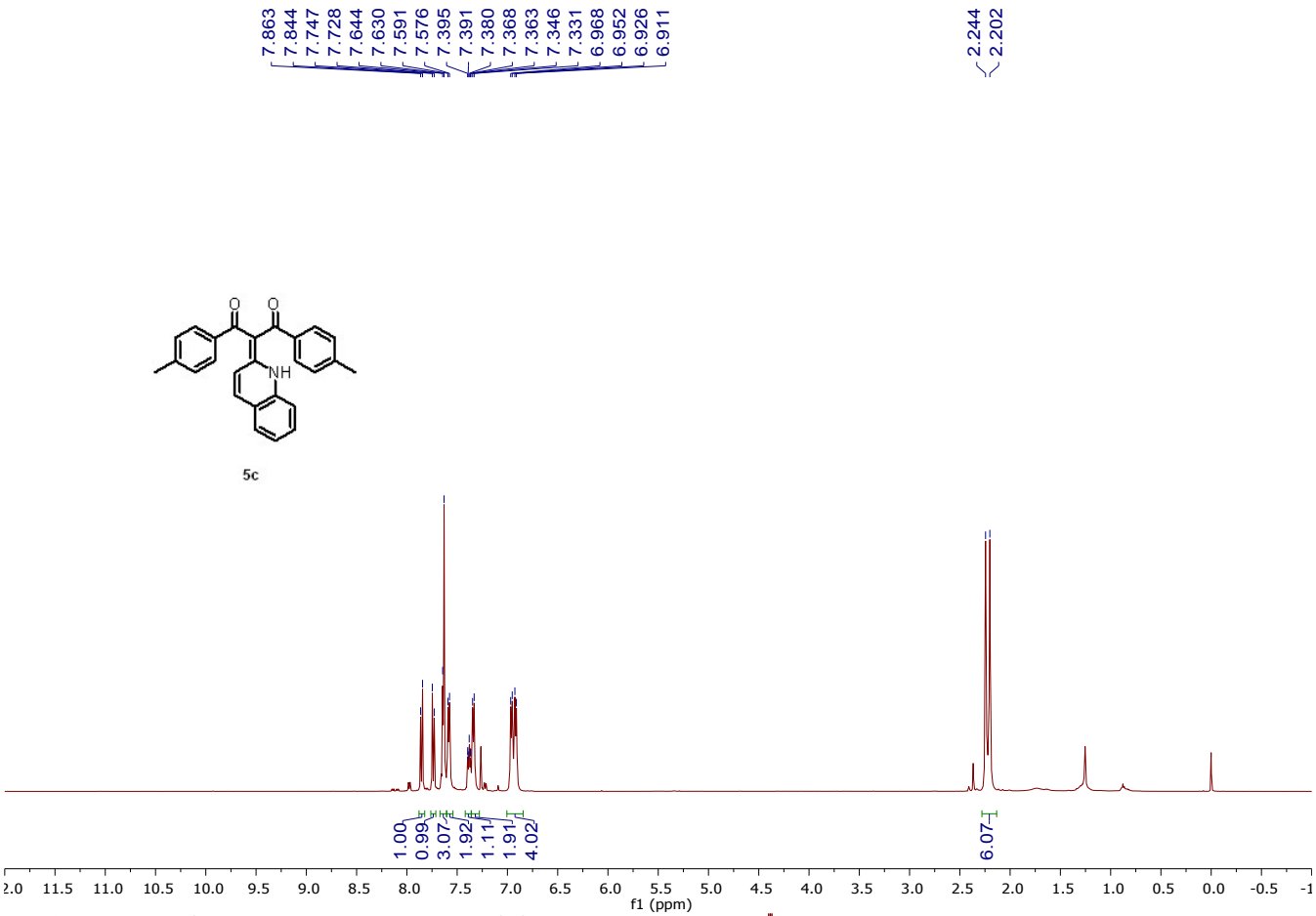
4m

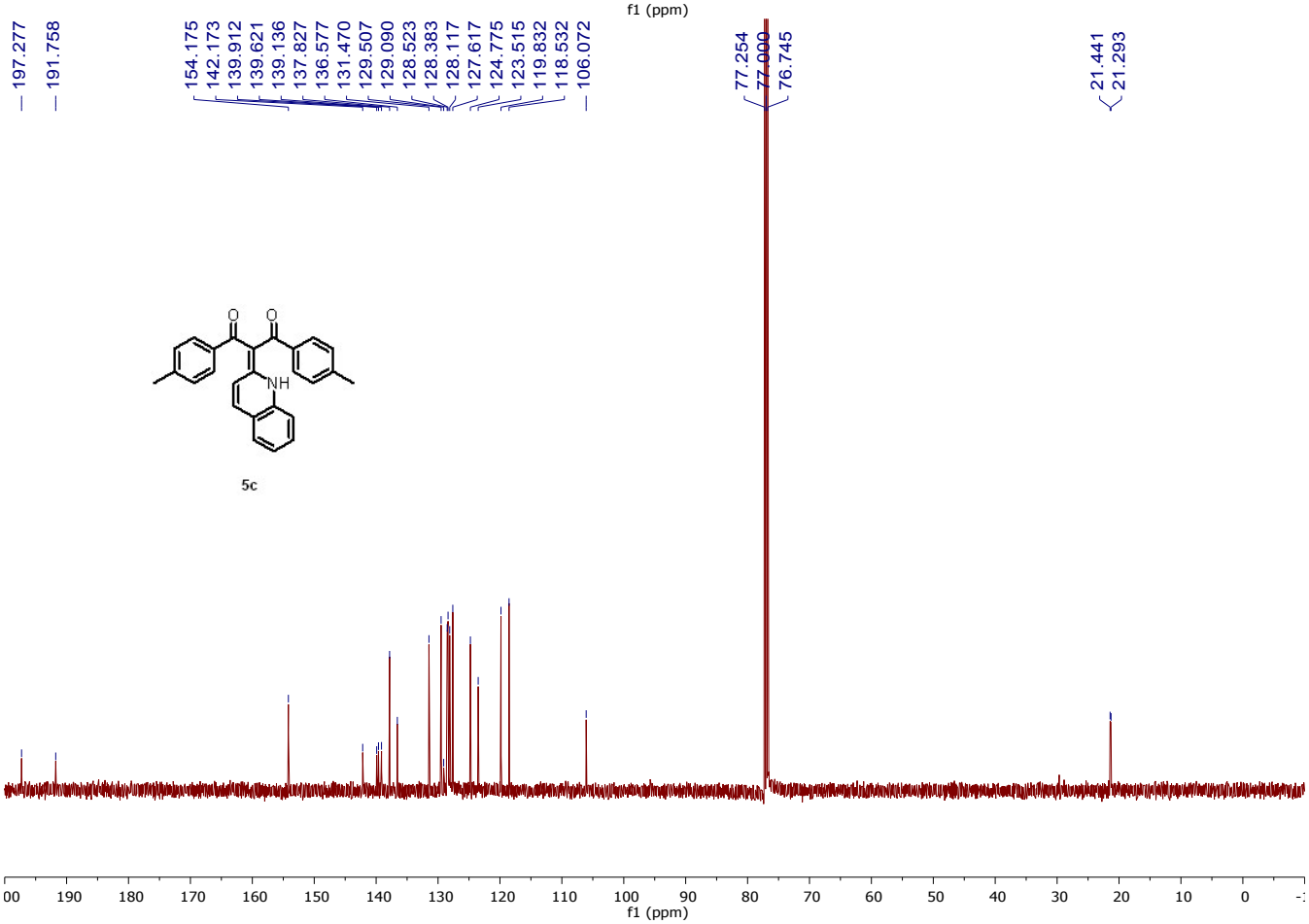

f1 (ppm)

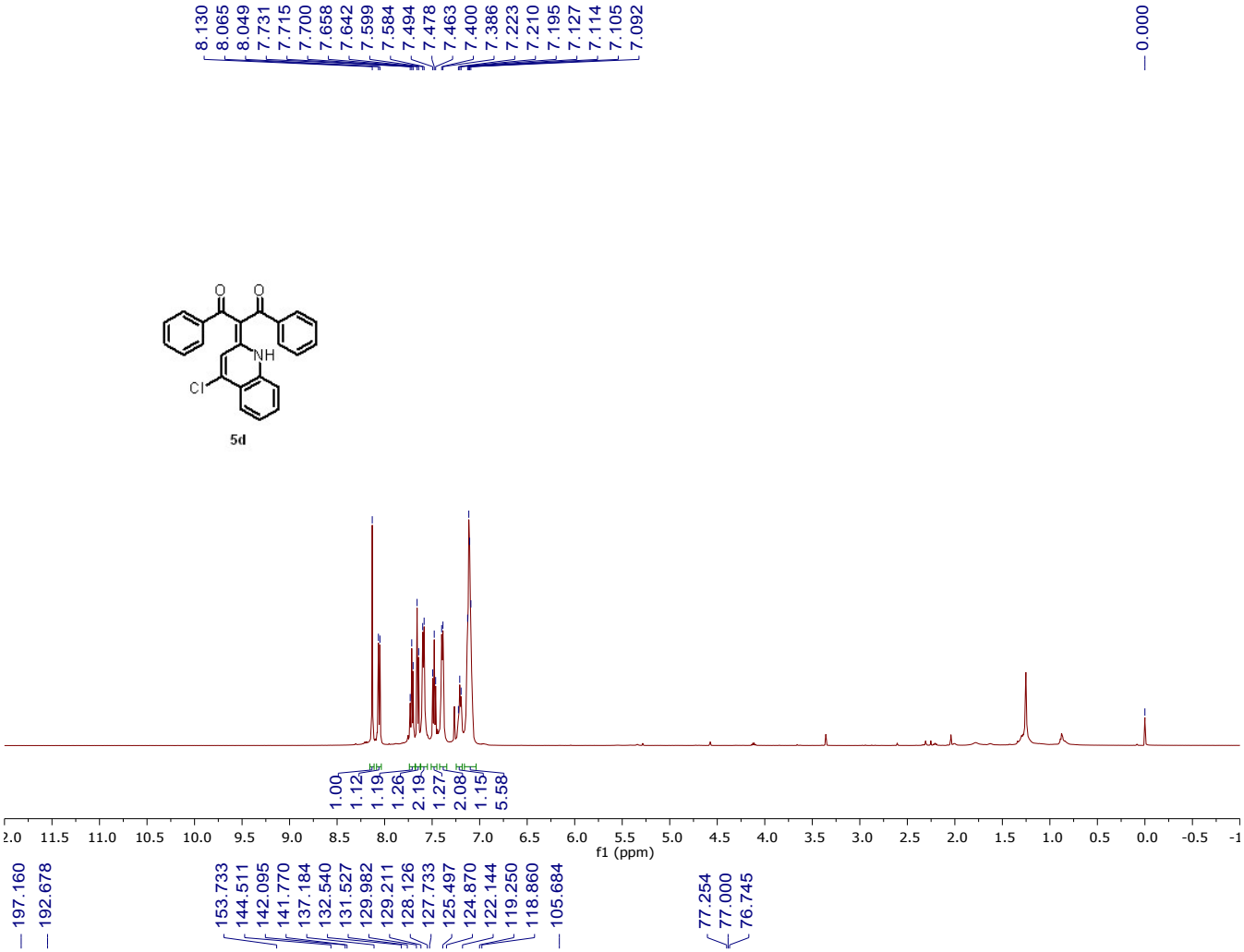

8.48
8.47
8.30
8.30
8.28
8.28
7.75
7.74
7.73
7.73
7.73
7.72
7.71
7.59
7.57
7.52
7.52
7.51
7.51
7.46
7.46
7.45
7.43
7.43
7.39
7.38
7.38
7.37
7.36
7.35
7.35
7.34
7.34
7.28
7.27
7.25
7.20
7.19
7.18
7.17
2.12
0.00
Me
O
N
O
4n
1.06
1.09
1.19
1.12
1.15
1.28
3.39
2.62
1.06
3.00
f1 (ppm)
176.96
162.19
156.20
152.67
147.24
137.92
133.84
133.80
132.82
130.41
128.69
128.17
126.24
125.19
123.55
123.01
122.38
117.98
77.25
77.00
76.75
18.68
Me
O
N
O
4n
f1 (ppm)

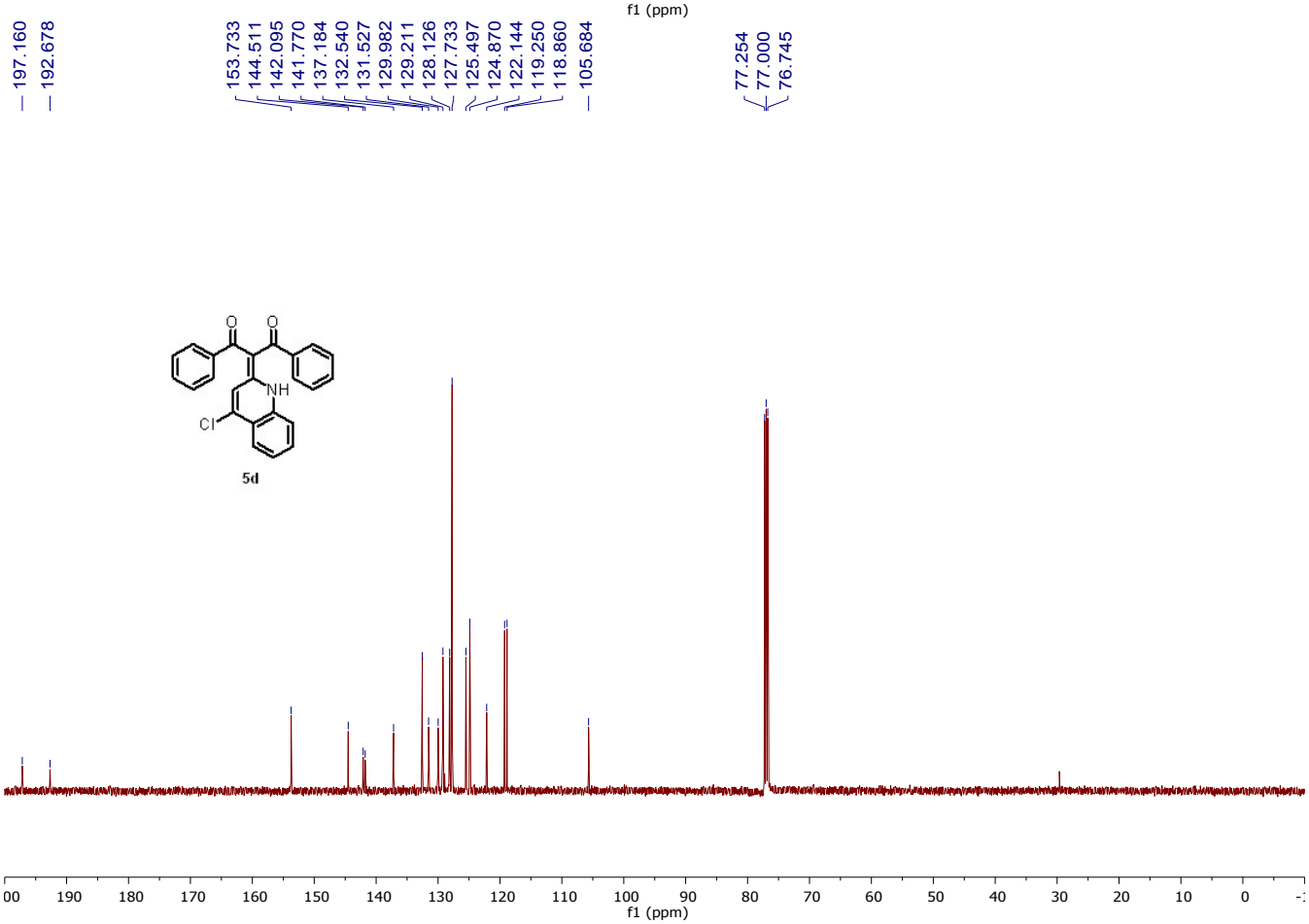

7.96
7.94
7.94
7.92
7.70
7.68
7.67
7.66
7.62
7.60
7.44
7.44
7.43
7.42
7.42
7.41
7.40
7.39
7.23
7.22
7.20
7.14
7.12
7.11
7.09
-0.00
5a
2.05
3.12
1.96
3.06
1.00
5.13
f1 (ppm)
197.65
192.79
154.43
138.33
131.65
129.29
128.14
127.74
127.71
125.07
123.69
119.79
77.25
77.00
76.75
5a
f1 (ppm)

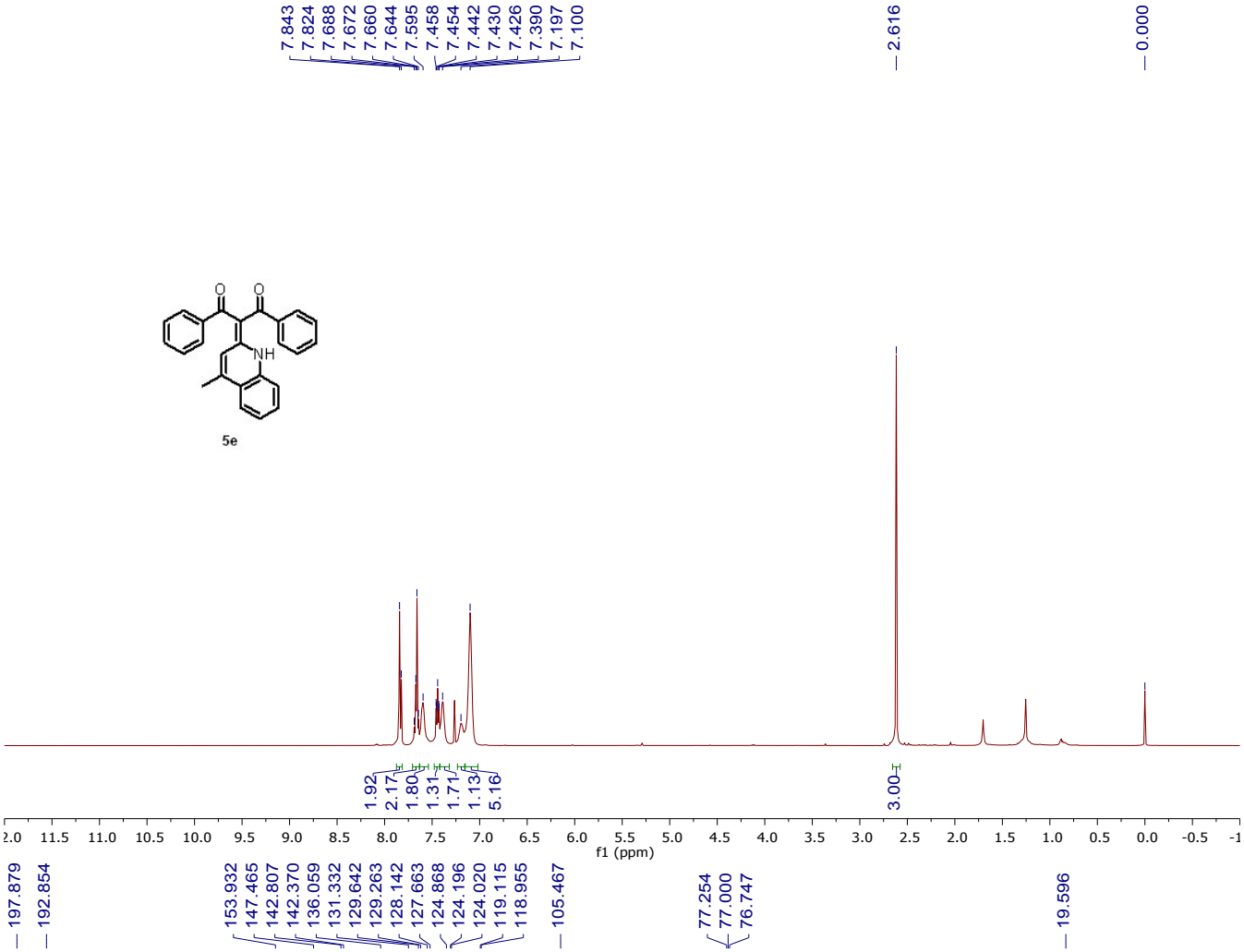

7.972
7.953
7.938
7.919
7.697
7.681
7.665
7.648
7.630
7.442
7.427
7.414
6.829
6.813
6.797
0.000
5b
2.04
4.95
2.95
4.00
f1 (ppm)
195.781
191.071
165.505
164.421
163.484
162.377
154.254
138.735
138.535
138.391
136.215
131.720
131.569
130.224
127.687
125.186
123.651
119.514
118.540
114.904
114.731
105.561
77.255
77.001
76.747
5b
f1 (ppm)

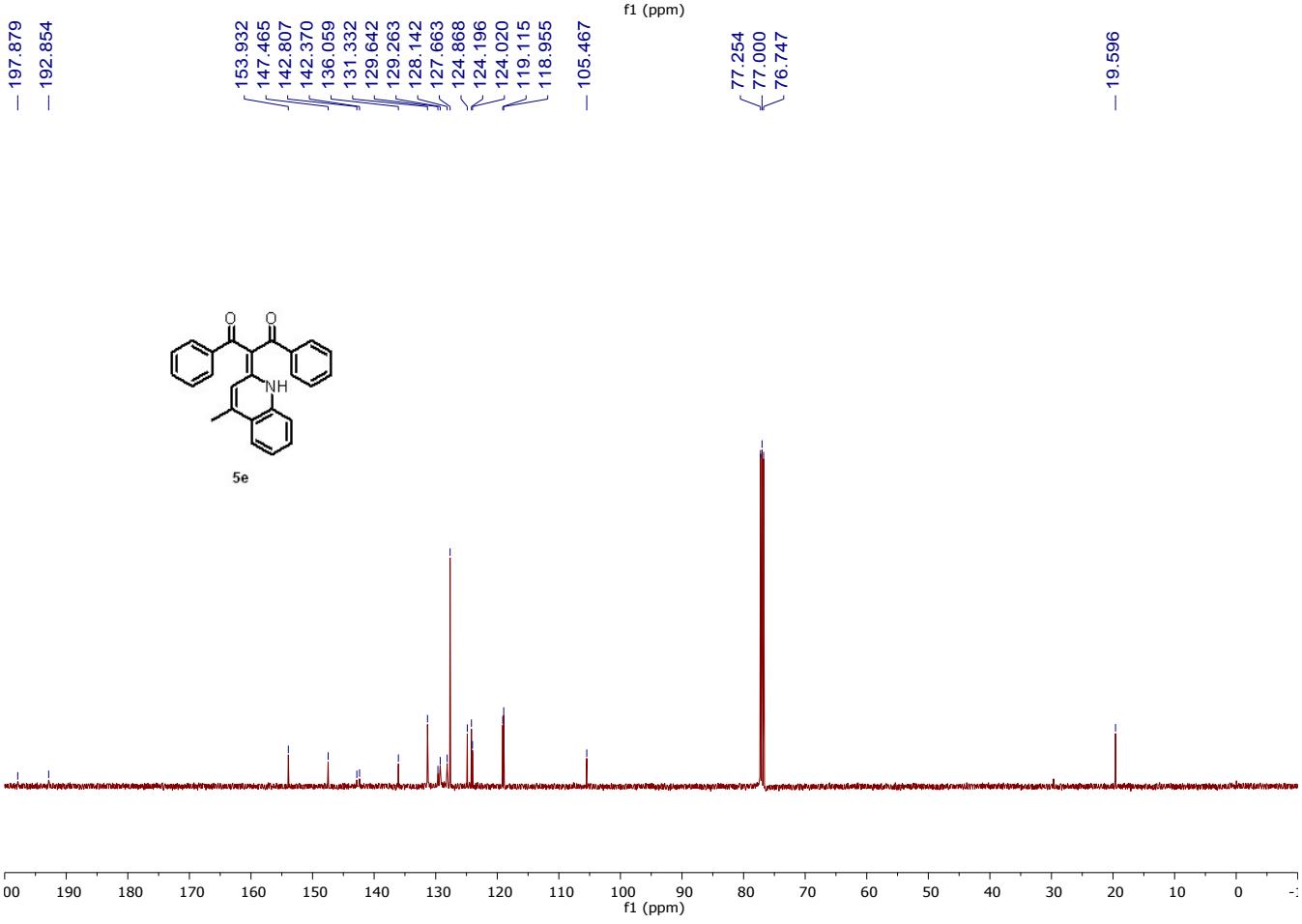

7.863
7.844
7.747
7.728
7.644
7.630
7.591
7.576
7.395
7.391
7.380
7.368
7.363
7.346
7.331
6.968
6.952
6.926
6.911
2.244
2.202
5c
1.00
0.99
3.07
1.92
1.11
1.91
4.02
6.07
f1 (ppm)

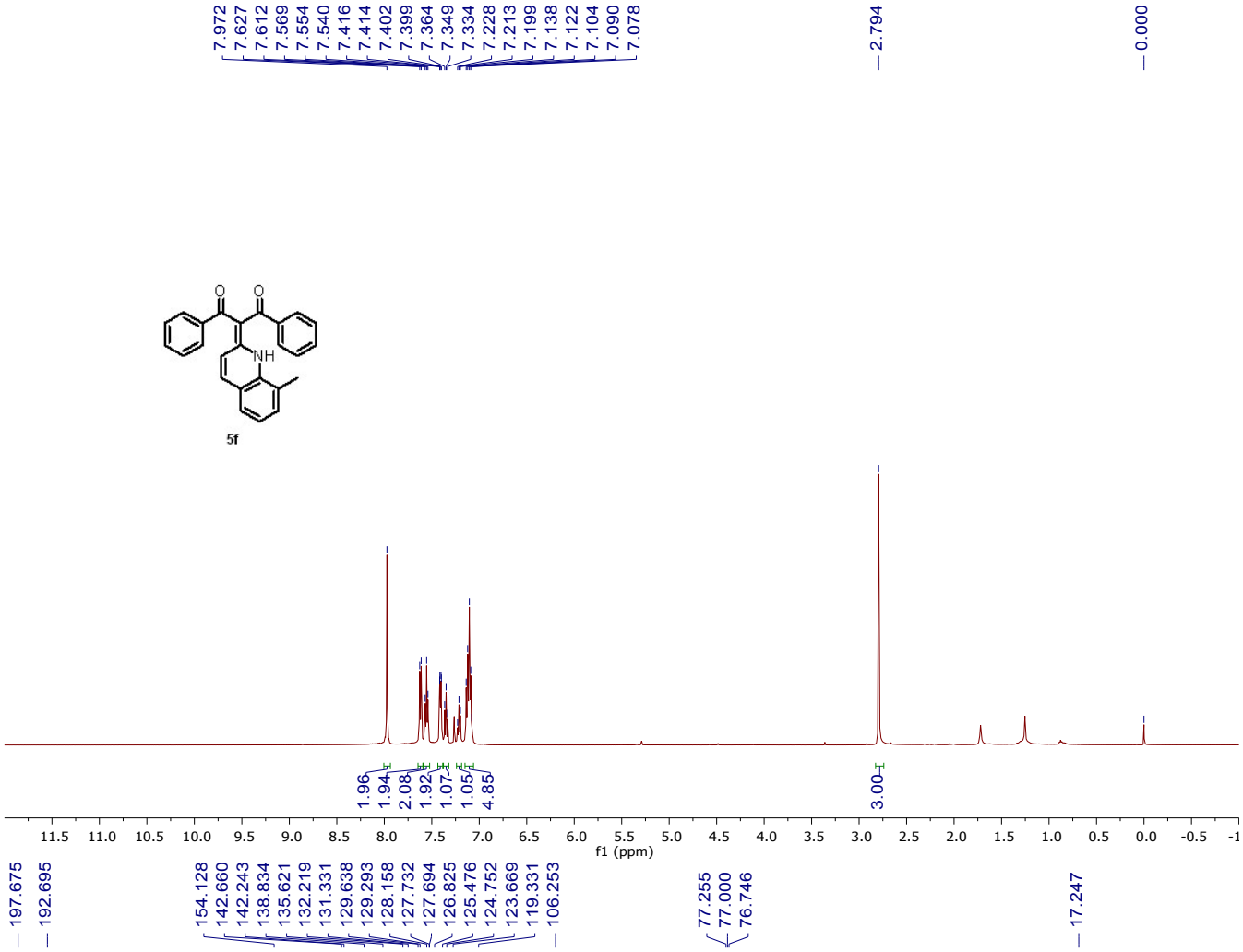

197.277
191.758
154.175
142.173
139.912
139.621
139.136
137.827
136.577
131.470
129.507
129.090
128.523
128.383
128.117
127.617
124.775
123.515
119.832
118.532
106.072
77.254
77.000
76.745
21.441
21.293
5c
f1 (ppm)

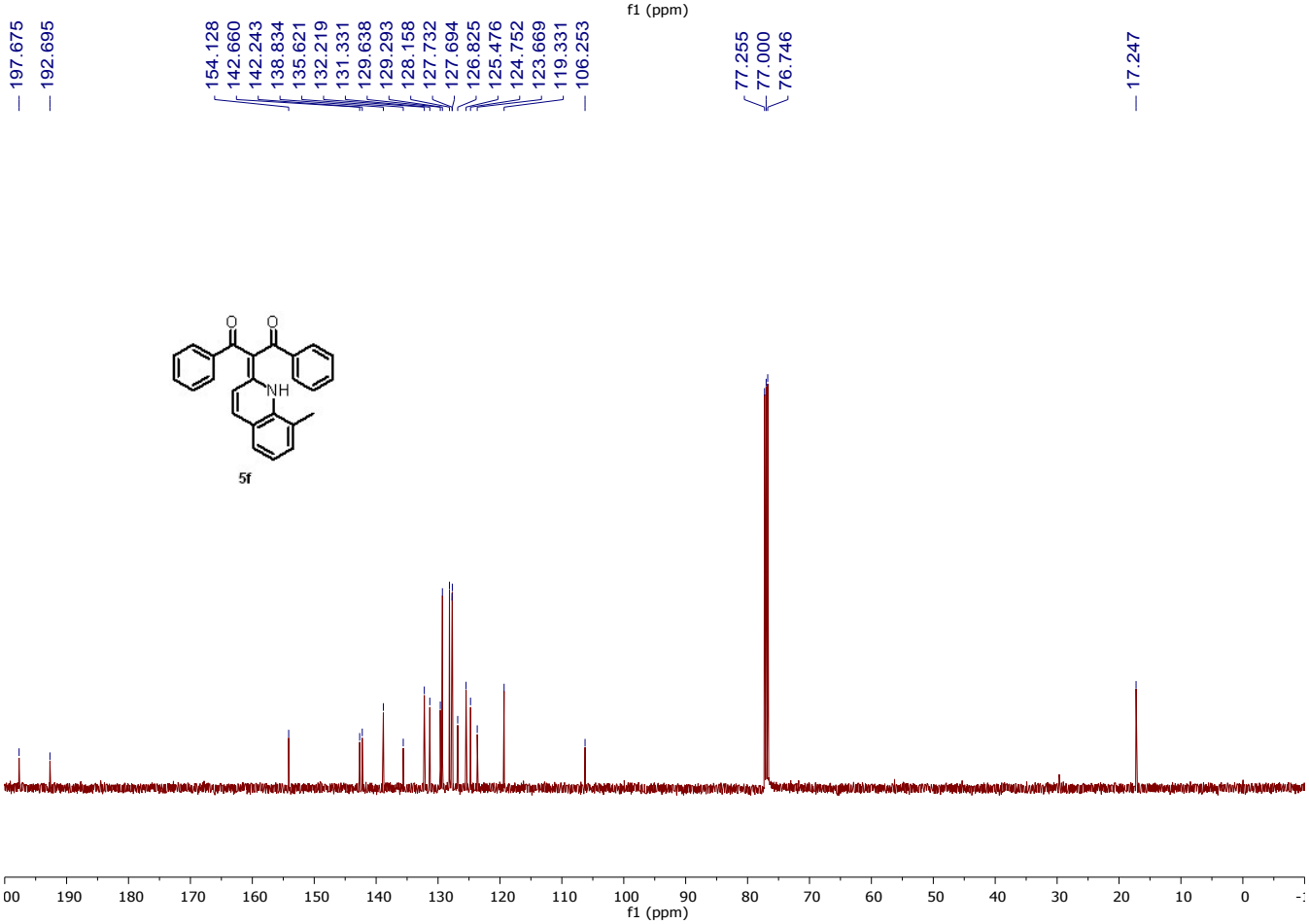

8.130
8.065
8.049
7.731
7.715
7.700
7.658
7.642
7.599
7.584
7.494
7.478
7.463
7.400
7.386
7.223
7.210
7.195
7.127
7.114
7.105
7.092
0.000
O
O
NH
Cl
5d
1.00
1.12
1.19
1.26
2.19
1.27
2.08
1.15
5.58
f1 (ppm)

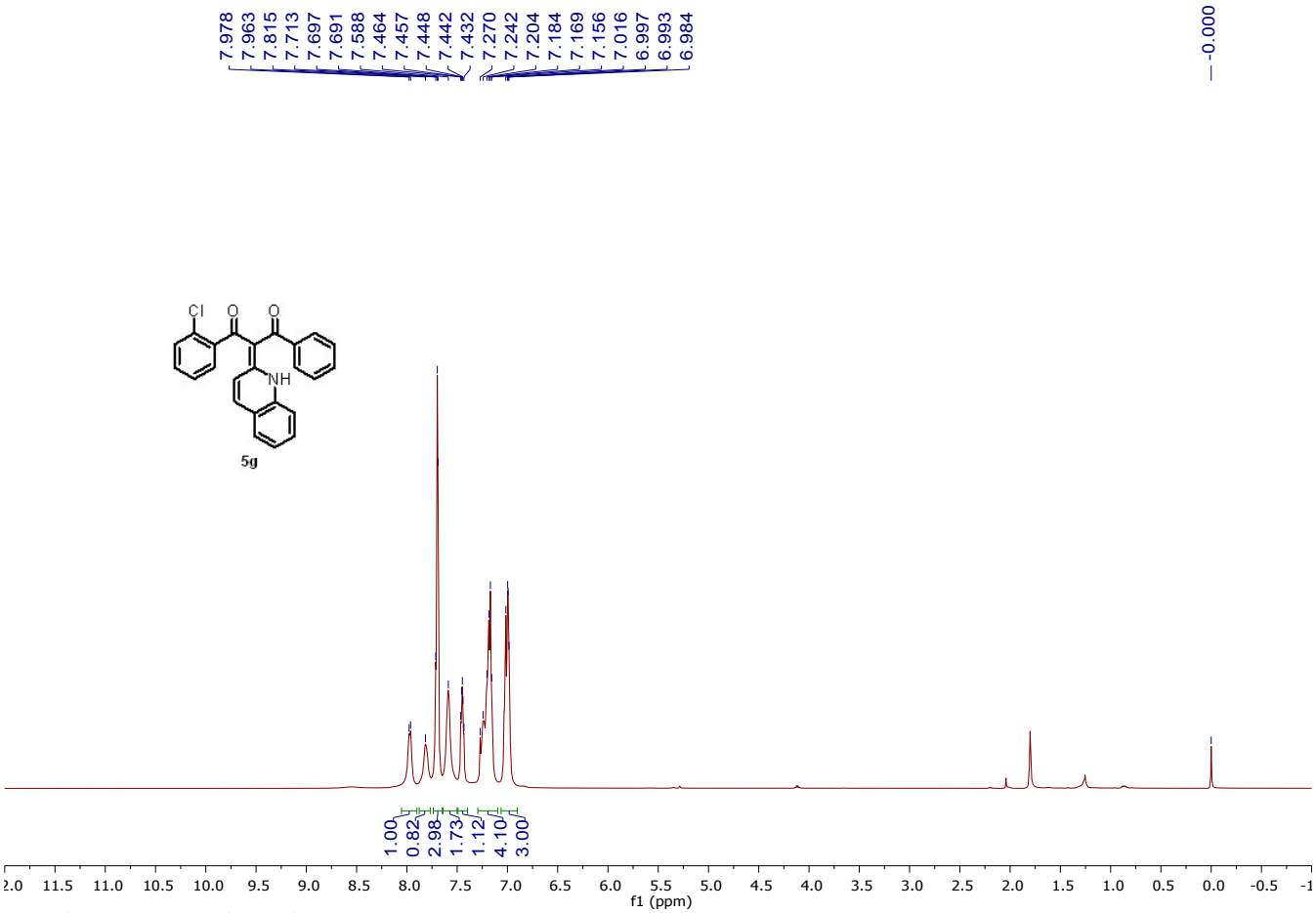

197.160
192.678
153.733
144.511
142.095
141.770
137.184
132.540
131.527
129.982
129.211
128.126
127.733
125.497
124.870
122.144
119.250
118.860
105.684
77.254
77.000
76.745
O
O
NH
Cl
5d
f1 (ppm)

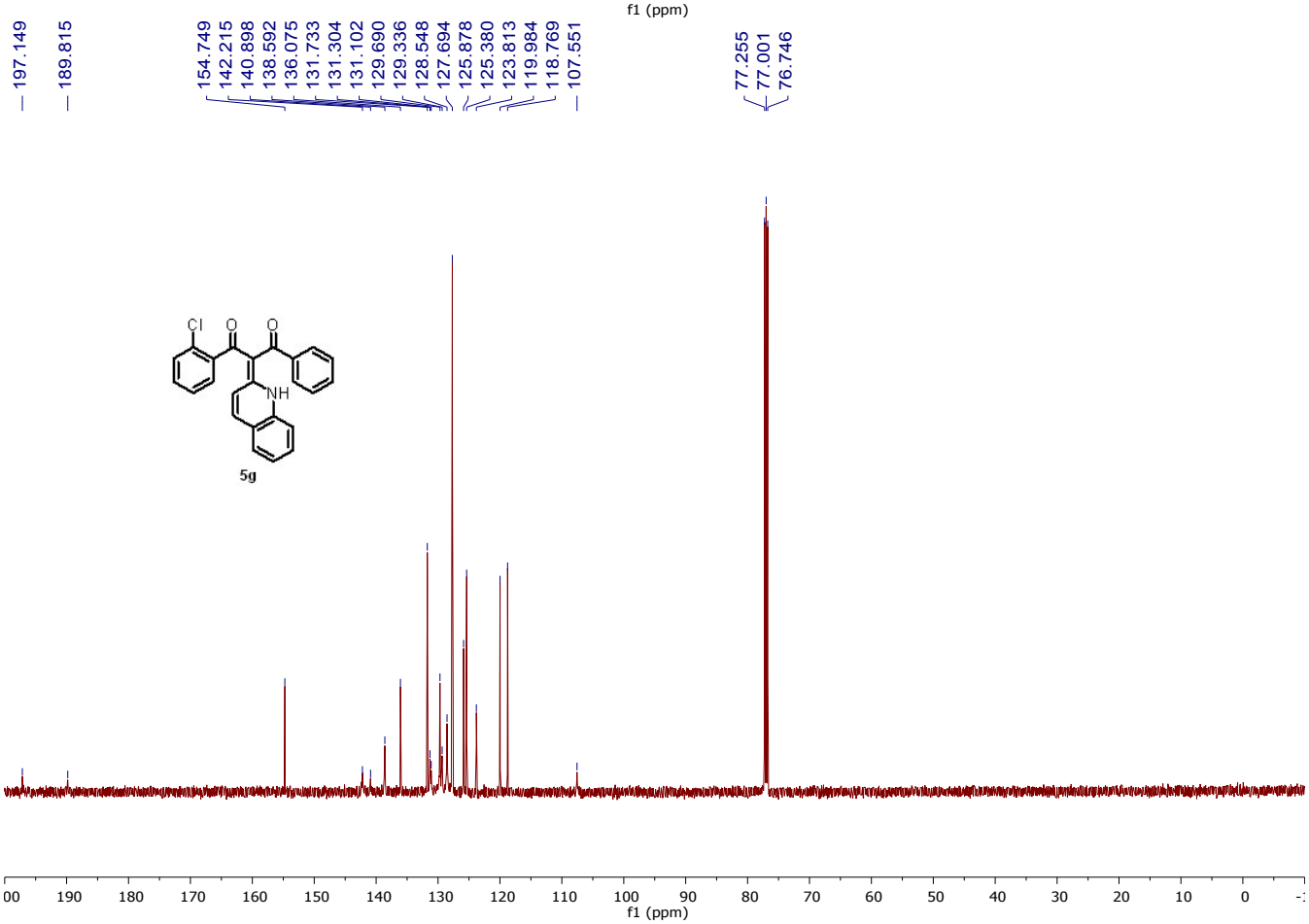

7.843
7.824
7.688
7.672
7.660
7.644
7.595
7.458
7.454
7.442
7.430
7.426
7.390
7.197
7.100
2.616
0.000
O
O
NH
5e
1.92
2.17
1.80
1.31
1.71
1.13
5.16
3.00
f1 (ppm)

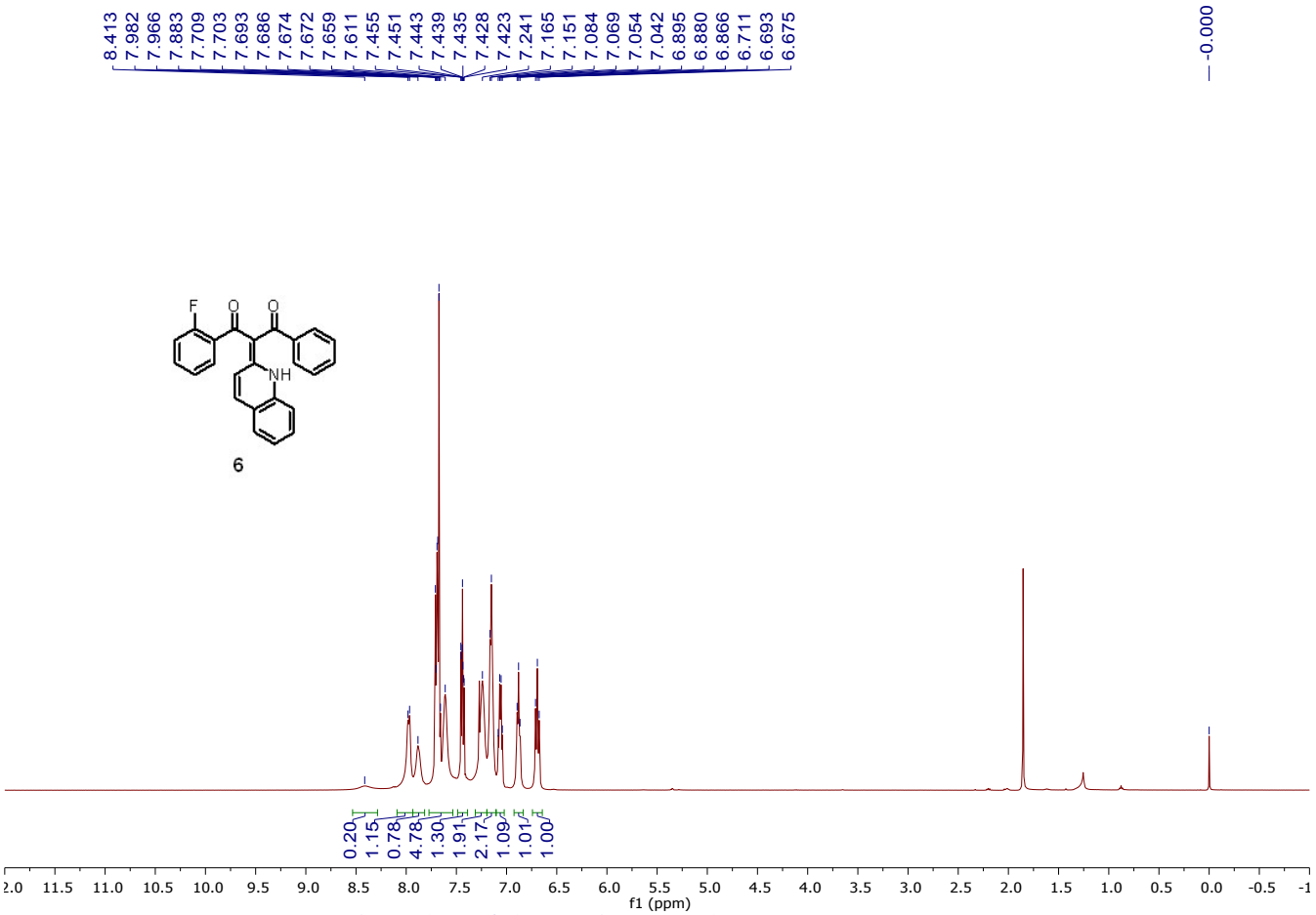

197.879
192.854
153.932
147.465
142.807
142.370
136.059
131.332
129.642
129.263
128.142
127.663
124.868
124.196
124.020
119.115
118.955
105.467
77.254
77.000
76.747
19.596
O
O
NH
5e
f1 (ppm)

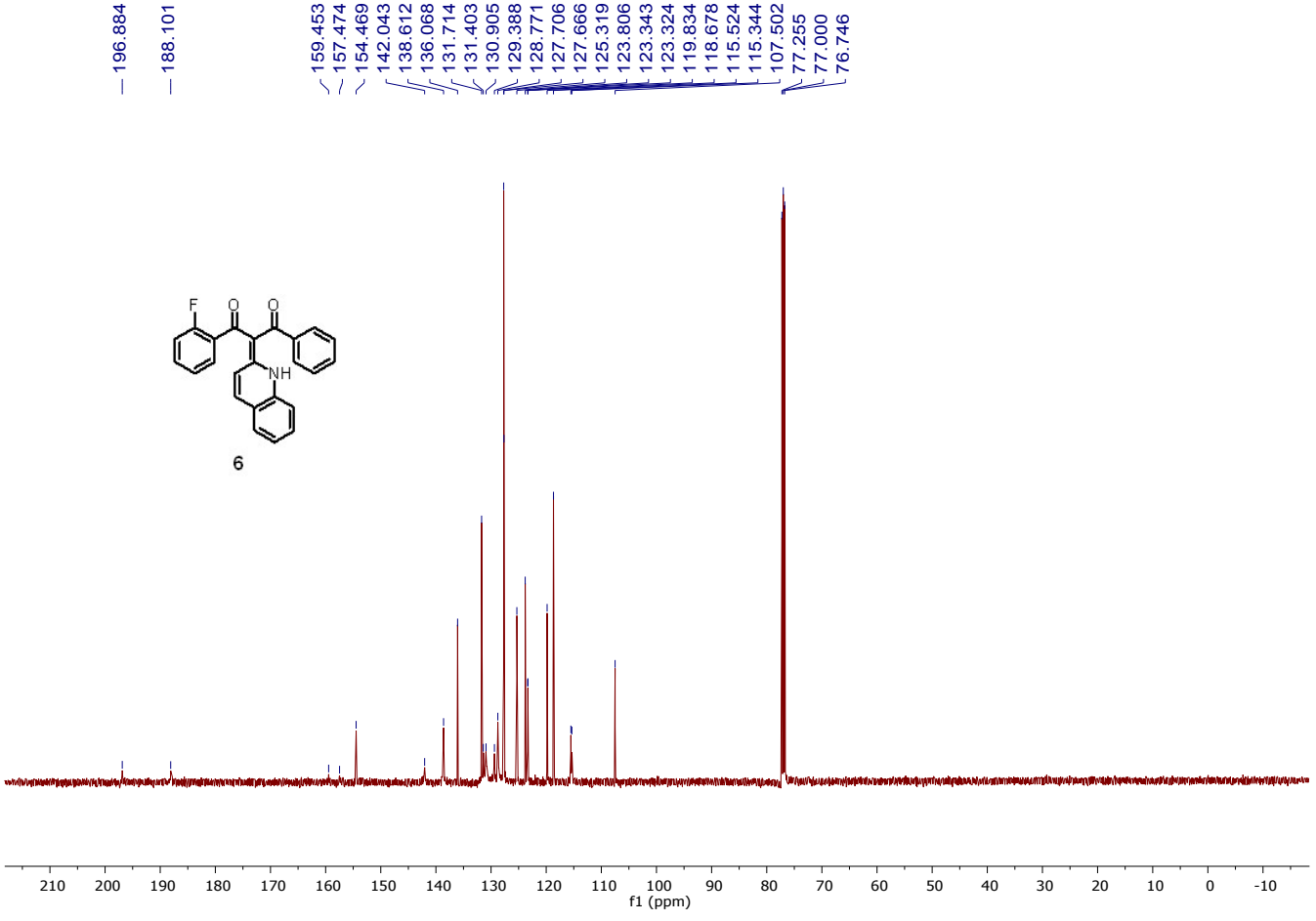

7.972
7.627
7.612
7.569
7.554
7.540
7.416
7.414
7.402
7.399
7.364
7.349
7.334
7.228
7.213
7.199
7.138
7.122
7.104
7.090
7.078
2.794
0.000
5f
1.96
1.94
2.08
1.92
1.07
1.05
4.85
3.00
f1 (ppm)


197.675
192.695
154.128
142.660
142.243
138.834
135.621
132.219
131.331
129.638
129.293
128.158
127.732
127.694
126.825
125.476
124.752
123.669
119.331
106.253
77.255
77.000
76.746
17.247
5f
f1 (ppm)


7.978
7.963
7.815
7.713
7.697
7.691
7.588
7.464
7.457
7.448
7.442
7.432
7.270
7.242
7.204
7.184
7.169
7.156
7.016
6.997
6.993
6.984
-0.000
Cl
O
O
NH
5g
1.00
0.82
2.98
1.73
1.12
4.10
3.00
f1 (ppm)


197.149
189.815
154.749
142.215
140.898
138.592
136.075
131.733
131.304
131.102
129.690
129.336
128.548
127.694
125.878
125.380
123.813
119.984
118.769
107.551
77.255
77.001
76.746
Cl
O
O
NH
5g
f1 (ppm)


8.413
7.982
7.966
7.883
7.709
7.703
7.693
7.686
7.674
7.672
7.659
7.611
7.455
7.451
7.443
7.439
7.435
7.428
7.423
7.241
7.165
7.151
7.084
7.069
7.054
7.042
6.895
6.880
6.866
6.711
6.693
6.675
-0.000
F
O
O
NH
6
0.20
1.15
0.78
4.78
1.30
1.91
2.17
1.09
1.01
1.00
f1 (ppm)


196.884
188.101
159.453
157.474
154.469
142.043
138.612
136.068
131.714
131.403
130.905
129.388
128.771
127.706
127.666
125.319
123.806
123.343
123.324
119.834
118.678
115.524
115.344
107.502
77.255
77.000
76.746
F
O
O
NH
6
f1 (ppm)