Supporting Information for Publication

I_2 promoted domino oxidative cyclization for one-pot synthesis of 2-acylbenzothiazoles via metal-free sp^3 C-H functionalization

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1. General

All aryl methyl ketones (**1a-1n**) and other reagents were obtained from commercial suppliers and used without further purification. Dimethyl Sulphoxide (DMSO) was distilled from calcium hydride (CaH_2). TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200-300 mesh). IR spectra were recorded on a Perkin-Elmer PE-983 infrared spectrometer as KBr pellets with absorption in cm^{-1}. ^1H NMR spectra were recorded on a Varian Mercury 400 or 600 MHz spectrometer Chemical shifts are reported in ppm, relative to the internal standard of tetramethylsilane (TMS). HRMS were obtained on an Apex-Ultra MS equipped with an electrospray source. Melting points were determined using XT-4 apparatus and not corrected.

2. Synthesis of 3 and 5

2.1. General procedure for preparation of 3 and 5 (3a as an example). A sealed tube was charged with acetophenone **1a** (120 mg, 1 mmol), 2-aminobenzenethiol **2a** (150.2 mg, 1.2 mmol), and iodine (380.7 mg, 1.5 mmol) at room temperature, and then dried solvent DMSO (3 mL) was added. The resulting mixture was stirred at 100 ℃ for 1 h, after disappearance of the reactant (monitored by TLC), and added 50mL water to the mixture, then extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% $Na_2S_2O_3$ solution (V/V), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **3a** as a yellow solid (205.8 mg, 86% yield).

2.2. Reaction condition screenings and optimizations.[a]

Entry	I_2 (mmol)	CuO (mmol)	Temperature (℃)	Solvent	Time (h)	Yield (%)[b]
1	1.1	1.1	80	DMSO	2.0	50

2	1.1	1.1	90	DMSO	2.0	53
3	1.1	1.1	100	DMSO	1.5	62
4	1.5	1.1	100	DMSO	1.5	72
5	2.0	1.1	100	DMSO	1.5	75
6	2.0	-	100	DMSO	1.0	80
7	-	1.1	100	DMSO	12	n.r.
8	-	-	100	DMSO	12	n.r.
9	2.0	-	100	DMSO	1.0	83
10	2.0	-	110	DMSO	1.0	60
11	0.8	-	100	DMSO	2.5	65
12	1.0	-	100	DMSO	2.0	75
13	1.2	-	100	DMSO	1.5	78
14	1.5	-	100	DMSO	1.0	86
15	1.5	-	100	DMF	12	n.r.
16	1.5	-	66	THF	12	n.r.
17	1.5	-	110	Toluene	12	n.r.
18	1.5	-	101	1,4-dioxane	12	n.r.
19	1.5	-	78	MeOH	12	n.r.
20	1.5	-	81	MeCN	12	n.r.

[a] Reaction conditions: 1.0 mmol **1a**, 3 mL solvent, monitored by TLC. [b] Isolated yield. n.r. = no reaction.

3. The reaction process and kinetic profile.

3.1 The ^{1}H NMR titration experiments of 3a with HI.

The spectral copies of ^{1}H NMR were listed in the following (Figure S1). The experiments clearly indicated that compound **3a** and HI easily formed inner salt. In addition, it was found that the chemical shift of HI moved toward down field with the addition of HI, obviously. The results effectively testified that the intermediacy of byproduct HI in the reaction of **1a** with **2a**.

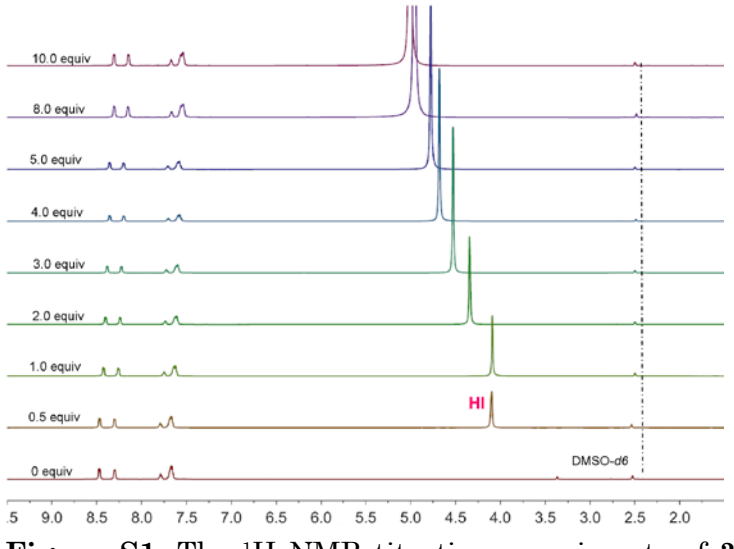

Figure S1. The ^{1}H NMR titration experiments of **3a** with HI. Partial ^{1}H NMR spectra (600 MHz in DMSO-d_6 at 298 +/-0.5 K) of **3a** upon addition of 0-10.0 equiv of HI.

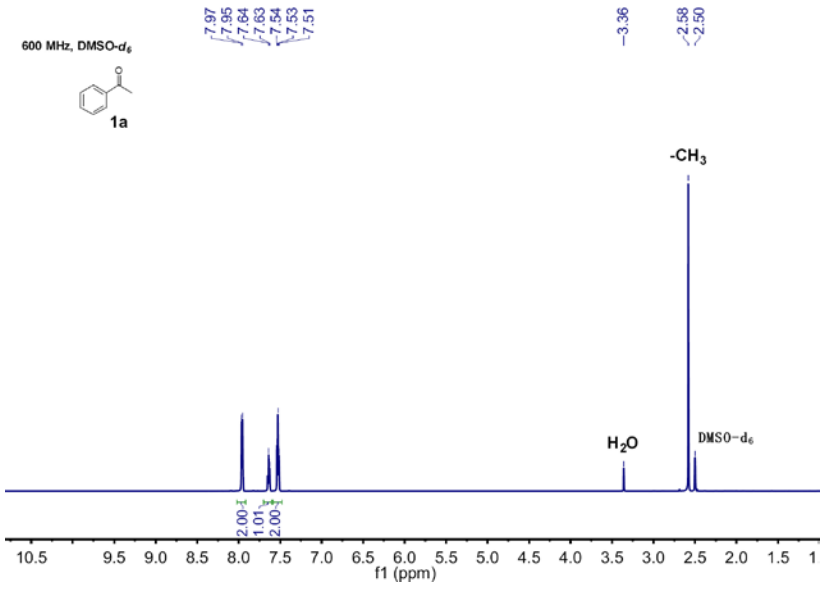

Figure S2. The ^{1}H NMR spectra of authentic sample of acetophenone (**1a**) (600 MHz, DMSO-d_6, 298 +/-0.5 K).

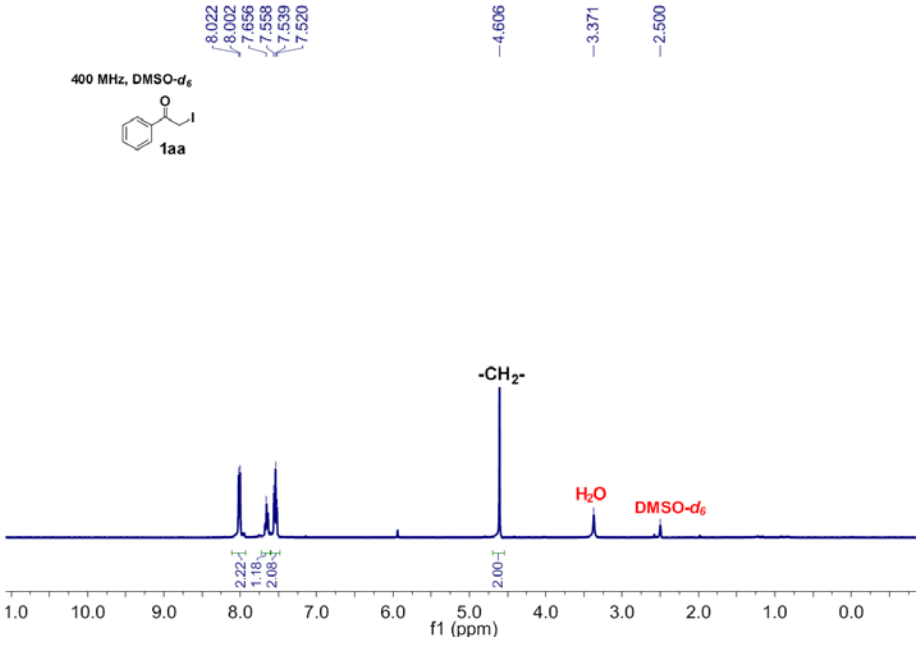

Figure S3. The ^{1}H NMR spectra of authentic sample of 2-iodo-1-phenylethanone (**1aa**) (400 MHz, DMSO-d_6, 298 +/-0.5 K).

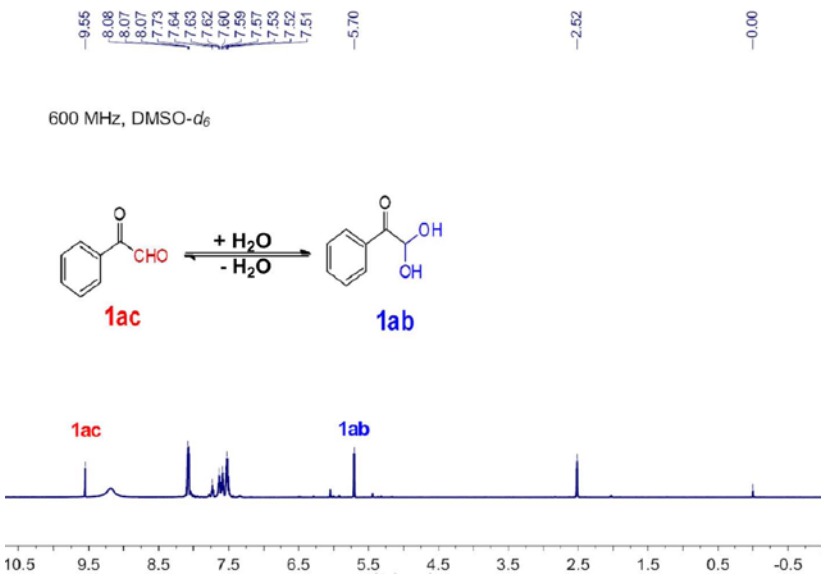

Figure S4. The ^{1}H NMR spectra of phenylglyoxal aldehyde group (**1ac**) and the hemiacetal group (**1ab**).

3.2 Reaction profiles of 1a with 2a

To probe the accelerating affect of I_2 on the reactions of **1a** with **2a,** the kinetics of **1a** with **2a** in the presence of different amounts of I_2 (0.8-1.4 equiv.) were further monitored by ^{1}H NMR spectroscopy. Figure S5 shows the profile of the decay and conversion of **1a** over time. The reaction of **1a** with **2a** to afford **3a** occurred to 90% conversion after about 10 min in the presence of 1.4 equivalent of I_2 (Figure S5B). In contrast, the same reaction only occurred to 47% conversion in the presence of 0.8 equivalent of I_2 for the same time. In addition, Figure S5A and S5B show that the reaction of **1a** with **2a** added 1.0-1.4 equivalent of I_2 occurred faster than that with 0.8 equivalent of I_2. 0.8 equivalent of I_2 did not efficiently promote the transformation. However, the reaction performed very well when 1.0-1.4 equivalent of I_2 was added.

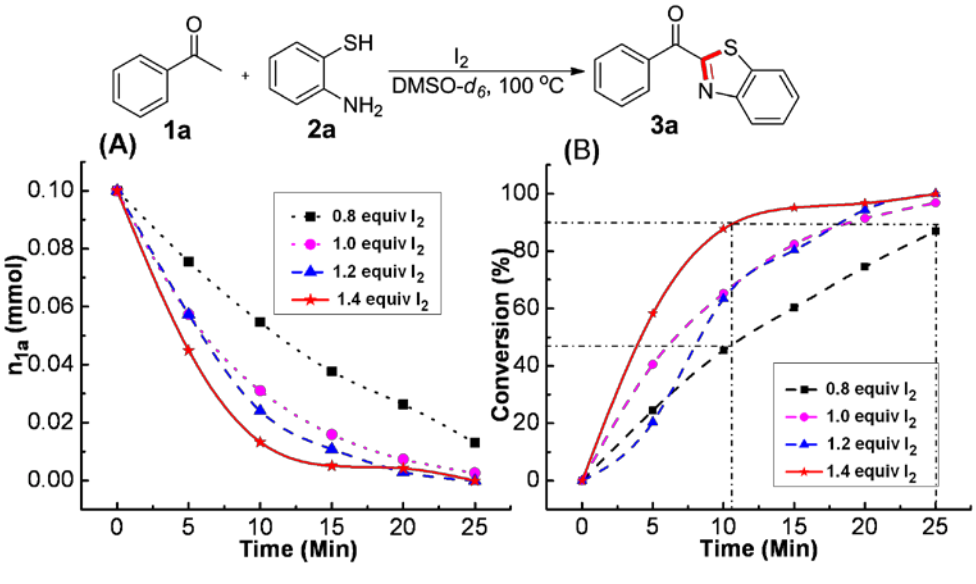

Figure S5. Reaction profiles of **1a** (12 mg, 0.1 mmol) with **2a** (15 mg, 0.12 mmol) in the presence of different amounts of I_2 (0.8-1.4 equivalent). (A) The amount of **1a**

over time. (B) The conversion of **1a** over time. (a) Reaction performed in the presence of 0.8 equiv. I_2 (black squares). (b) Reaction performed in the presence of 1.0 equiv. I_2 (pink circles). (c) Reaction performed in the presence of 1.2 equiv. I_2 （blue triagels）. (d) Reaction performed in the presence of 1.4 equiv. I_2 （red pentacles）.

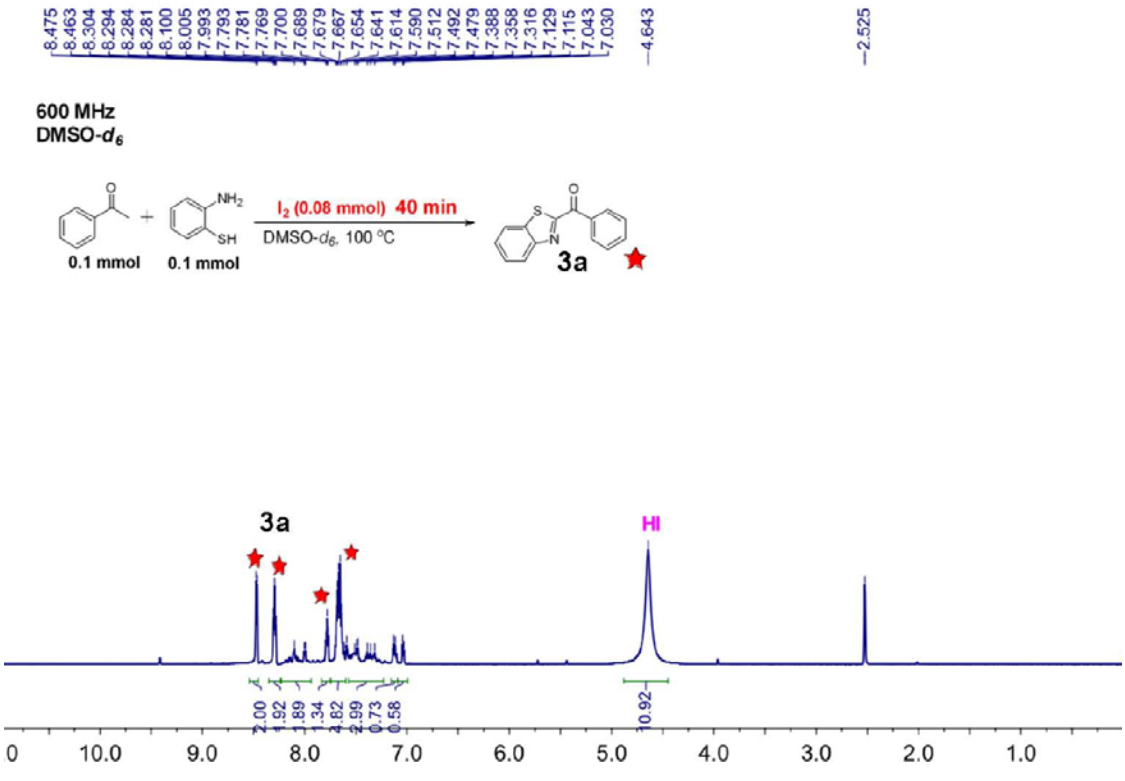

Figure S6. The ^{1}H NMR spectra of reaction **1a** with **2a** in the presence of I_2 (0.08 mmol) at 40 min.

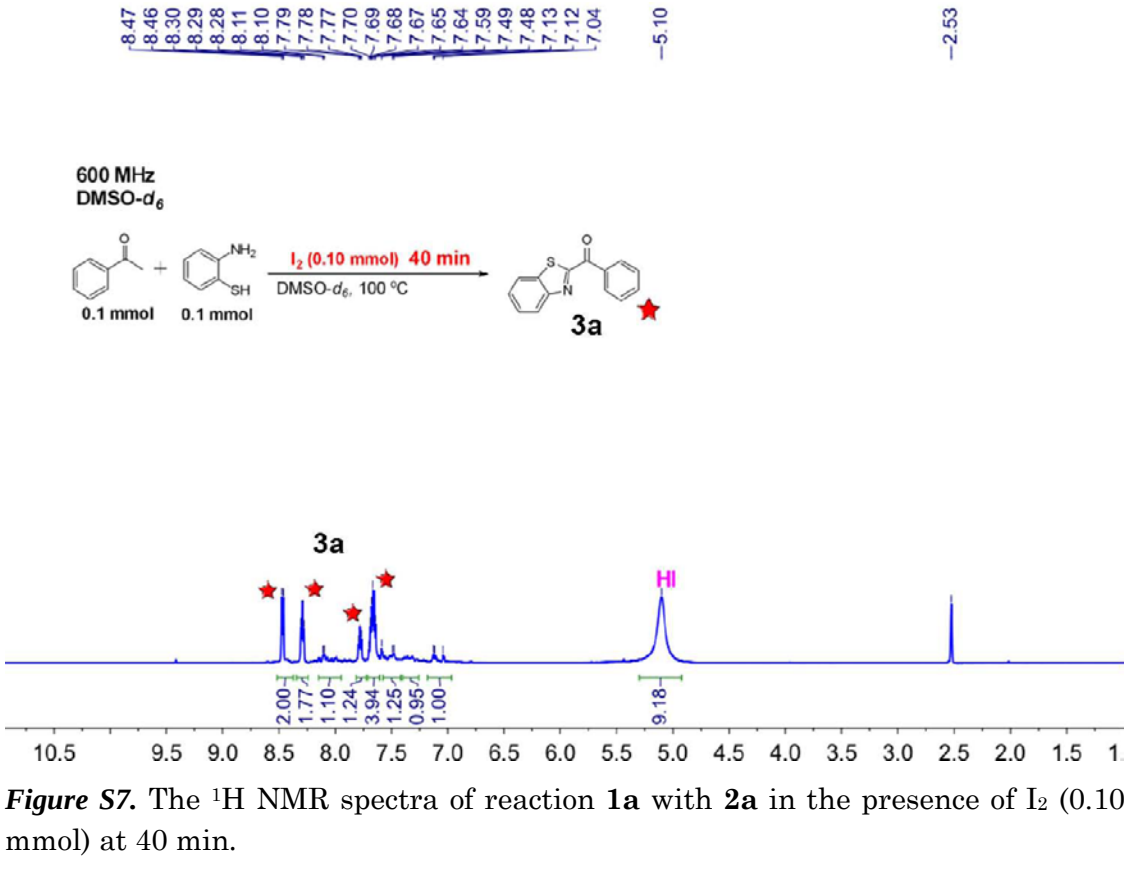

Figure S7. The ^{1}H NMR spectra of reaction **1a** with **2a** in the presence of I_2 (0.10 mmol) at 40 min.

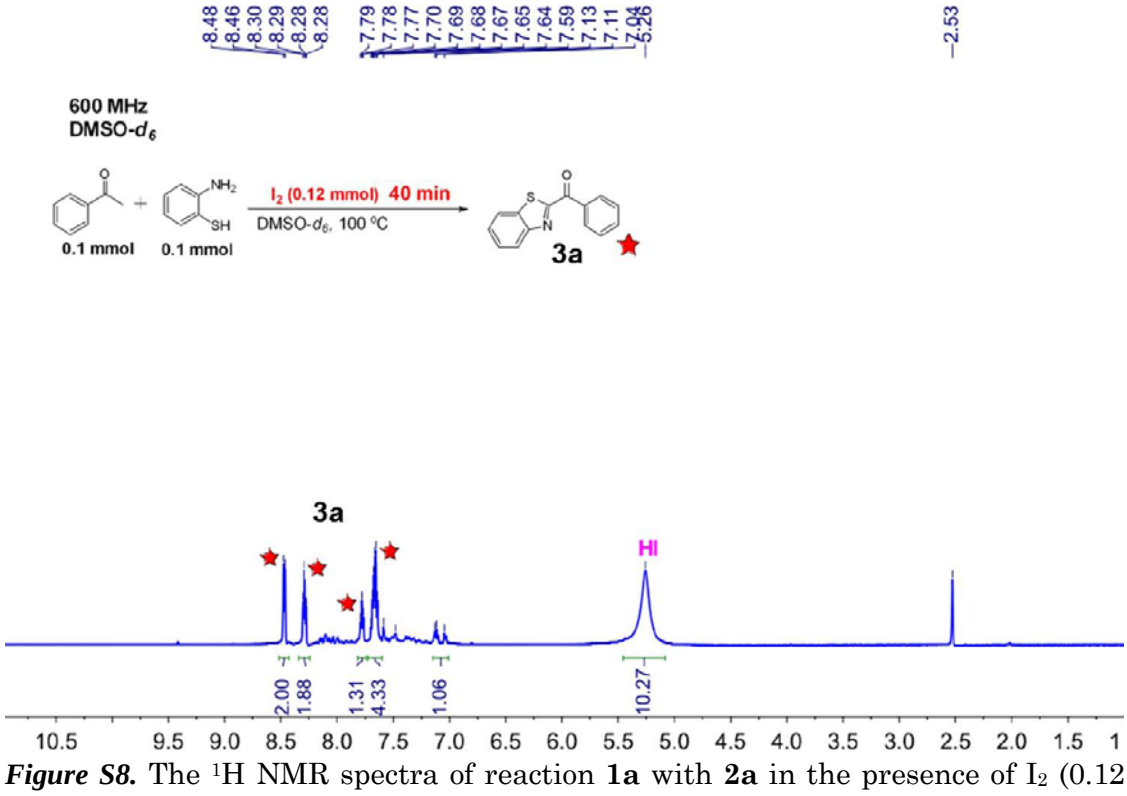

Figure S8. The ^{1}H NMR spectra of reaction **1a** with **2a** in the presence of I_2 (0.12 mmol) at 40 min.

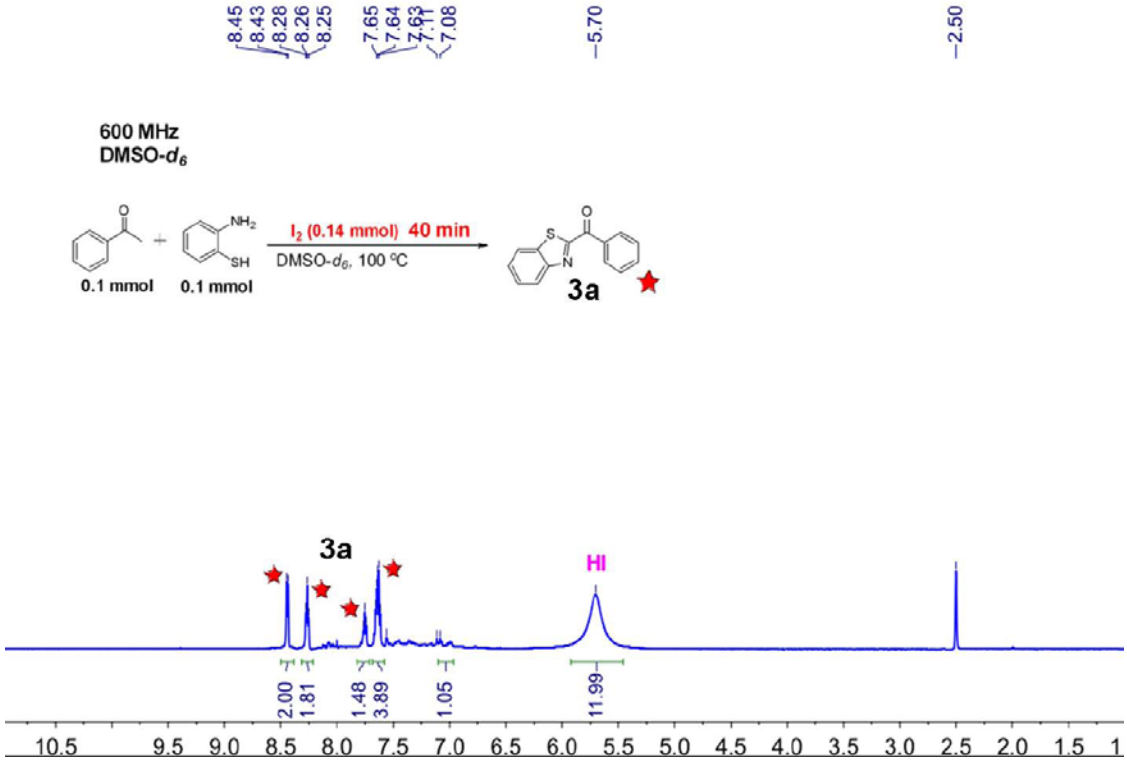

Figure S7. The ^{1}H NMR spectra of reaction **1a** with **2a** in the presence of I_2 (0.14 mmol) at 40 min.

3.3 The kinetic profile of the reaction 1ab with 2a.

To gain insight into the autocatalytic process, the kinetics of **1ab** with **2a** were also studied at 0-30 mins by ^{1}H NMR spectroscopy, anisole was selected as an internal standard for the integration of the ^{1}H NMR signals. The rate of formation of product **3aa** was very slow in the absence of additive, and the yield was also very low (only 27% at 30 min). When this reaction was proceed with iodide, however, the rate was greatly accelerated: from 27% yield at 30 min in the absence of additive to 76% yield at 30 min when added 30% mmol or 50% mmol iodide (Figure S9). The results clearly proved that molecular I_2 promoted the heterocyclization step of **1ac** to **3a.**

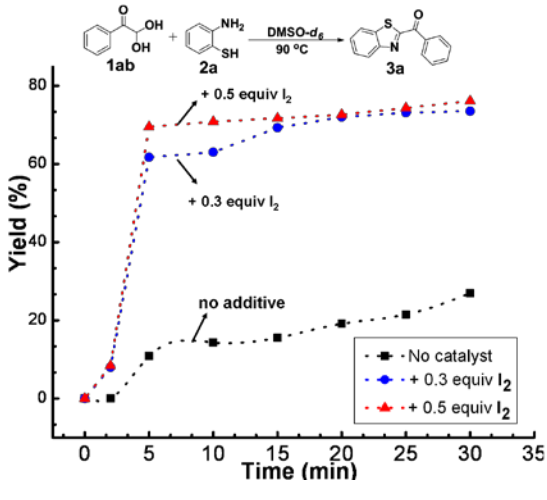

Figure S9. Kinetics of reaction **1ab** (0.1 mmol) with **2a** (0.1 mmol) in DMSO-d_6 at 298+/-0.5 K, as monitored by ^{1}H NMR spectroscopy (anisole as internal

standard). (a) Reaction performed in the absence of additive (black squares). (b) Reaction performed in the presence of 0.03 mmol I_2 (blue circles). (c) Reaction performed in the presence of 0.05 mmol I_2 （red triagels）.

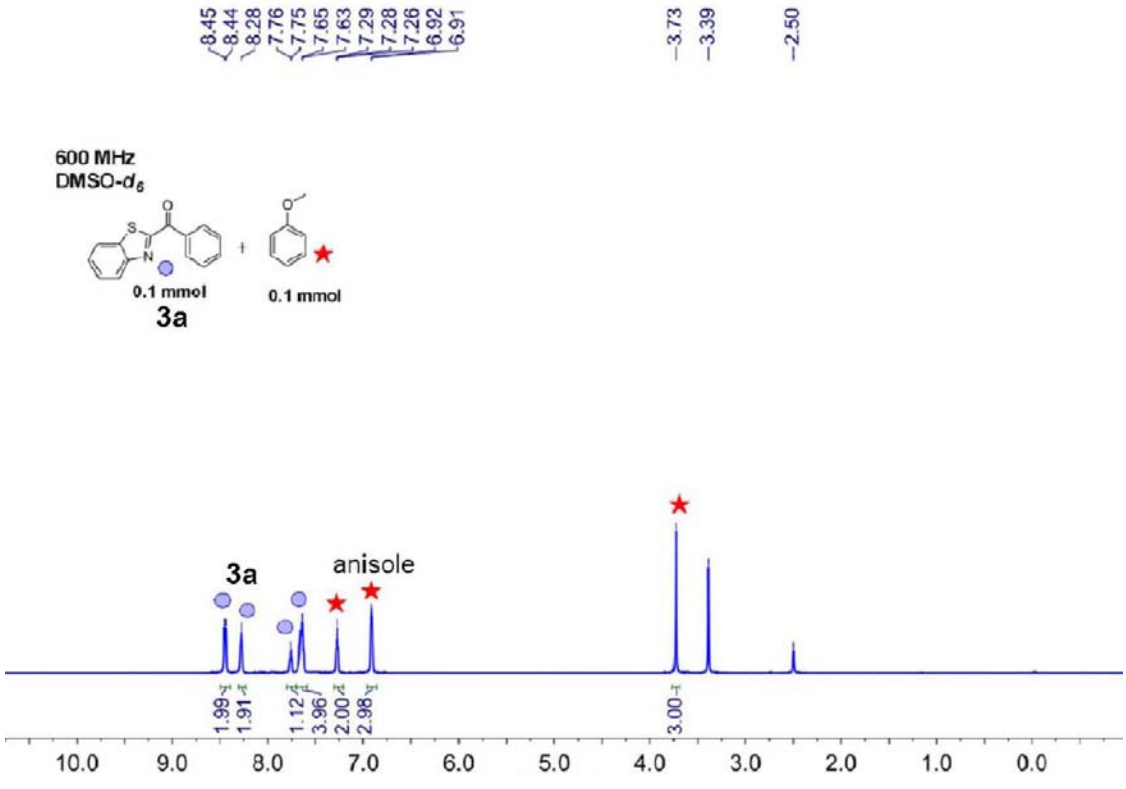

Figure S10. The ^{1}H NMR spectra of **1a** (0.1 mmol) with internal standard anisole (0.1 mmol).

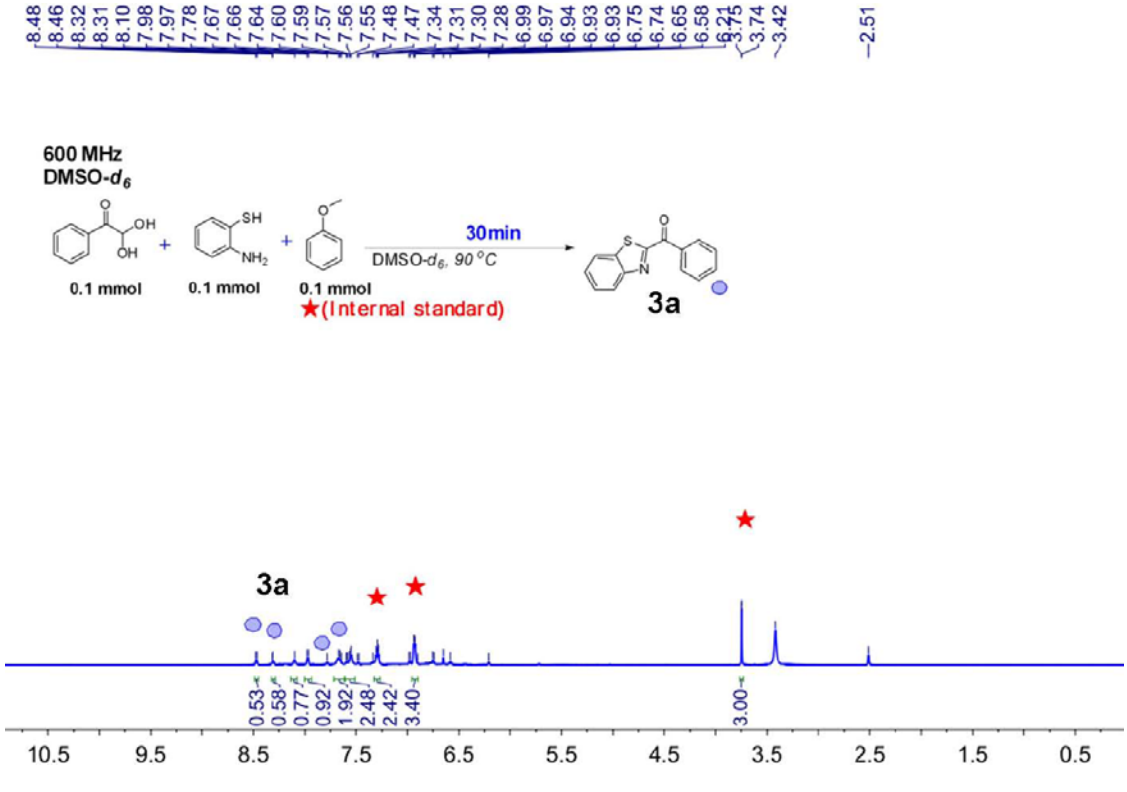

Figure S11. The ^{1}H NMR spectra of reaction **1ab** (0.1 mmol) with **2a** (0.1 mmol), and anisole (0.1 mmol) without I_2 at 30 min.

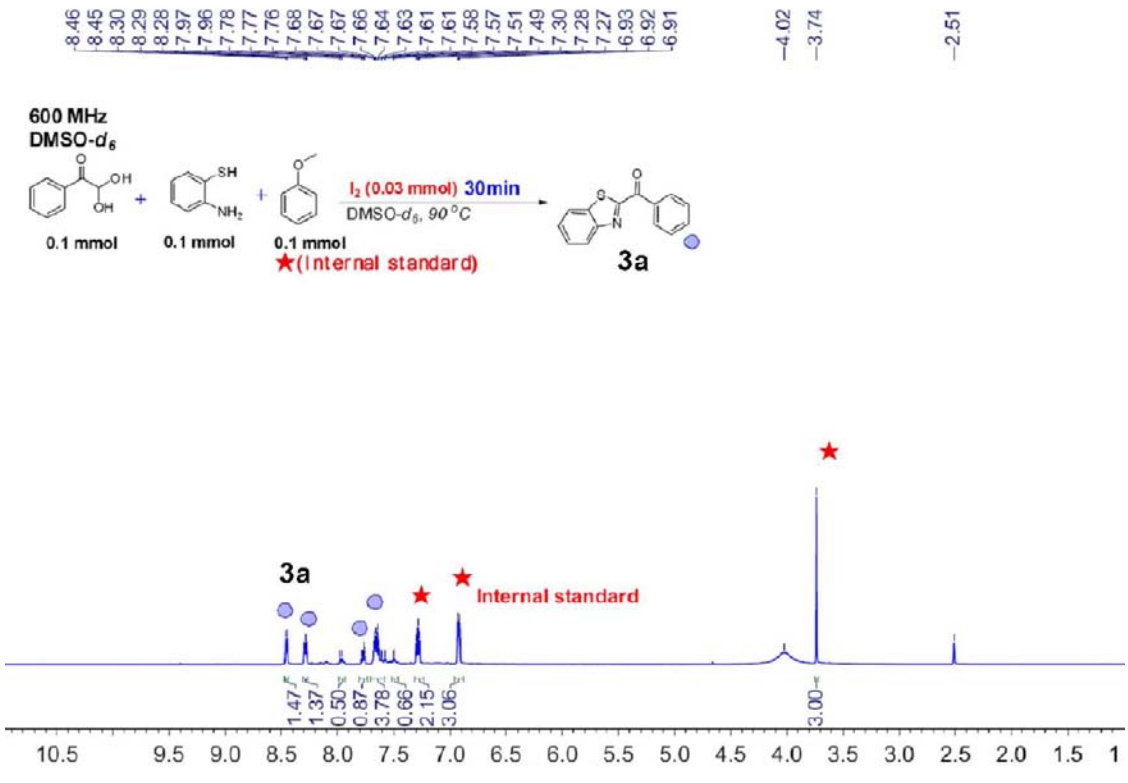

Figure S12. The ^{1}H NMR spectra of the reaction **1ab** (0.1 mmol) with **2a** (0.1 mmol), and anisole (0.1 mmol) in the presence of I_2 (0.03 mmol) at 30 min.

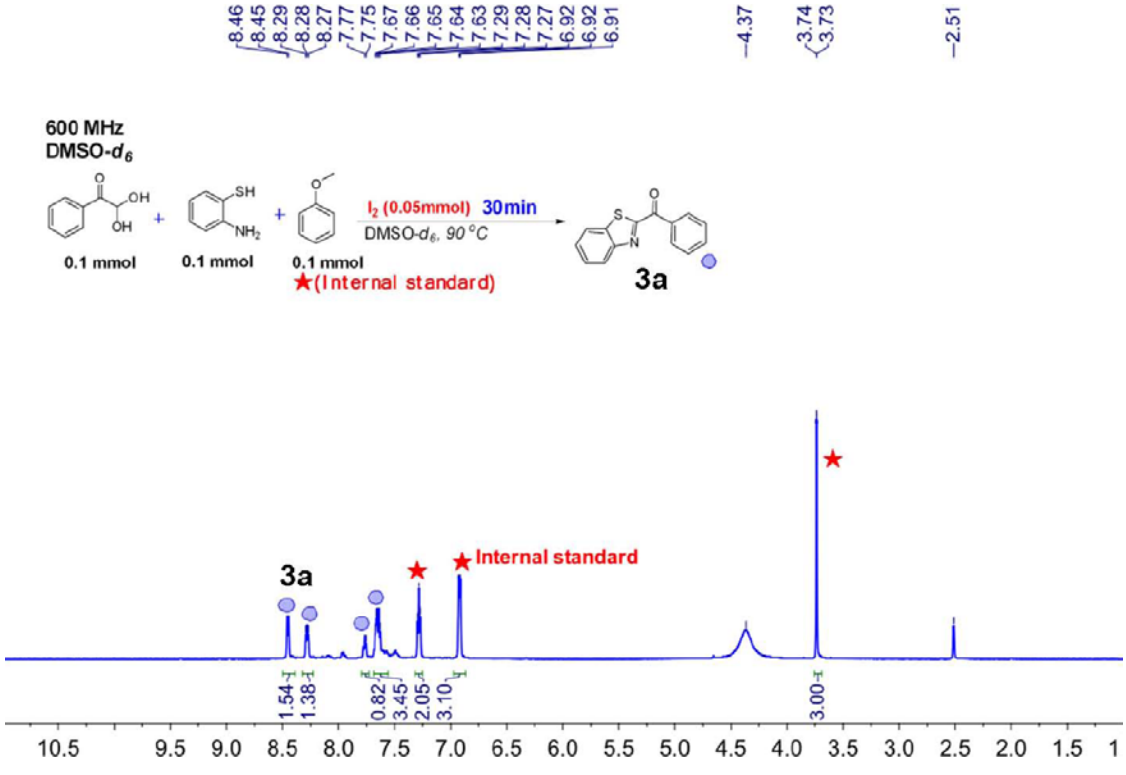

Figure S13. The ^{1}H NMR spectra of the reaction **1ab** (0.1 mmol) with **2a** (0.1 mmol), and anisole (0.1 mmol) in the presence of I_2 (0.05 mmol) at 30 min.

3.4 The control experiments.

It was found that phenacyl iodine **1aa** (0.5 mmol) reacted with **2a** (0.5 mmol) and I_2 (0.5 mmol) to provide the desired product **3a** in 85% yield. The reaction of intermediate (**1ab)** with **2a** also performed smoothly in excellent yield (> 95%). These results clearly confirmed intermediacy of phenacyl iodine (**1aa)** and phenylglyoxal (**1ac)** in the transformation.

Scheme S1 The control experiments.

4. Spectral data of compound 3a-3y, 5a-5i

benzo[d]thiazol-2-yl(phenyl)methanone (**3a):** 205.8 mg, 86% yield; yellow solid; mp 97-99 °C (lit.[1] 98-99 ℃); IR (KBr): 350, 1667, 1596, 1574, 1485, 1419, 1324, 1292, 1272, 1183, 1124, 946, 890 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56 (d, J = 8.4 Hz, 2H), 8.22 (d, J = 7.6 Hz, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.65 (t, J = 7.6 Hz, 1H), 7.46-7.59 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ =185.2, 167.0, 153.8, 136.9, 134.9, 133.8, 131.2, 128.4, 127.5, 126.8, 125.6, 122.1; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{14}H_{10}NOS$: 240.04776; found: 240.04727.

benzo[d]thiazol-2-yl(p-tolyl)methanone (**3b**): 207.7 mg, 82% yield; colorless crystal; mp 95-97 °C (lit.[2] 96-98 ℃; IR (KBr): 3452, 1640, 1604, 1482, 1419, 1290, 1184, 1117 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.37 (d, J = 8.0 Hz, 2H), 8.11 (d, J = 7.6 Hz, 1H), 7.88 (d, J = 7.2 Hz, 1H), 7.40-7.45 (m, 2H), 7.23 (d, J = 8.0 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 184.7, 167.4, 153.8, 144.9, 136.9, 132.3, 131.3, 129.2, 127.4, 126.7, 125.6, 122.0, 21.8; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{15}H_{12}$ NOS: 254.06341; found: 254.06302.

benzo[d]thiazol-2-yl(4-methoxyphenyl)methanone (**3c**): 228.9 mg, 85% yield; white solid; mp 118-121 °C (lit.[1] 122-123 ℃); IR (KBr): 3454, 3054, 1628, 1602, 1569, 1492, 1425, 1322, 1302, 1261, 1179, 1116, 1064, 1025 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.54-8.57 (m, 2H), 8.13 (d, J = 7.6 Hz, 1H), 7.90 (d, J =

8.4 Hz, 1H), 7.41-7.49 (m, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 183.3, 167.9, 164.3, 153.8, 136.8, 133.8, 127.7, 127.3, 126.7, 125.5, 122.1, 113.8, 55.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{15}H_{12}NO_2S$: 270.05833; found: 270.05807.

benzo[d]thiazol-2-yl(2,4-dimethoxyphenyl)methanone (**3d**):233.5 mg, 78% yield; yellow solid; mp 122-125 ℃; IR (KBr): 3451, 2933, 1646, 1604, 1458, 1271, 1210, 1160, 1107, 1027 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.15 (d, *J* = 7.6 Hz, 1H), 7.98 (t, *J* = 8.4 Hz, 2H), 7.47-7.54 (m, 2H), 6.55-6.70 (m, 2H), 3.87 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 185.6, 168.3, 164.7, 161.4, 153.5, 137.0, 134.3, 127.1, 126.6, 125.3, 122.1, 118.7, 104.7, 99.2, 55.9, 55.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{16}H_{14}NO_3S$: 300.06889; found: 300.06853.

benzo[d]thiazol-2-yl(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)methanone (**3e**): 237.9 mg, 80% yield; yellow solid; mp 140-142 ℃; IR (KBr): 3443, 2947, 1629, 1593, 1575, 1494, 1453, 1431, 1327, 1302, 1197, 1131, 1100, 1063 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.16-8.24 (m, 3H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.49-7.57 (m, 2H), 7.99 (d, *J* = 8.4 Hz, 1H), 4.34-4.36 (m, 2H), 4.31-4.29 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 183.1, 167.5, 153.8, 149.0, 143.1, 136.8, 128.3, 127.3, 126.7, 125.7, 125.5, 122.0, 120.9, 117.3, 64.8, 64.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{16}H_{12}NO_3S$: 298.05324; found: 298.05309.

benzo[d]thiazol-2-yl(4-chlorophenyl)methanone (**3f**): 196.8 mg, 72% yield; white solid; mp 99-102 ℃ (lit.[2] 102-103 ℃); IR (KBr): 3443, 1639, 1586, 1480, 1398, 1320, 1293, 1175, 1116, 1089, 1010 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.55 (d, *J* = 8.4 Hz, 2H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.52-7.61 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 183.9, 166.7, 153.7, 140.5, 137.0, 133.2, 132.7, 128.8, 127.7, 127.0, 125.7, 122.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{14}H_9ClNOS$: 274.00879; found: 274.00862.

benzo[d]thiazol-2-yl(4-bromophenyl)methanone (**3g**): 222.7 mg, 70% yield; yellow solid; mp 121-123 ℃ (lit.[3] 123-124 ℃); IR (KBr): 3453, 1641, 1581, 1561, 1477, 1421, 1392, 1291, 1273, 1178, 1115, 1068, 1009 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.45 (d, *J* = 6.8 Hz, 2H), 8.21 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.51-7.59 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 184.0, 166.7, 153.7, 137.0, 133.5, 132.7, 131.8, 129.4, 127.7, 127.0, 125.7, 122.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{14}H_9BrNOS$: 317.95827; found: 317.95814.

benzo[d]thiazol-2-yl(4-nitrophenyl)methanone (**3h**): 184.8 Mg, 65% yield; yellow solid; mp 174-177 ℃ (lit.[3] 177-178 ℃); IR (KBr): 3451, 3108, 1643,

1597, 1524, 1482, 1419, 1350, 1319, 1293, 1269, 1240, 1115, 1011 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.73 (d, J = 8.8 Hz, 2H), 8.39 (d, J = 8.8 Hz, 2H), 8.25 (d, J = 7.6 Hz, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.57-7.65 (m, 2H),; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 183.8, 165.8, 150.5, 153.7, 139.6, 137.1, 132.2, 128.2, 127.3, 125.9, 123.4, 122.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{14}H_9N_2O_3S$: 285.03284; found: 285.03276.

benzo[d]thiazol-2-yl(3,4-dichlorophenyl)methanone (**3i**): 209.6 mg, 68% yield; yellow solid; mp 109-112 ℃; IR (KBr): 3454, 3093, 1642, 1580, 1552, 1487, 1464, 1421, 1374, 1297, 1273, 1251, 1144, 1116, 1033 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.72 (s, 1H), 8.46 (d, J = 8.8 Hz, 1H), 8.24 (d, J = 7.2 Hz, 1H), 8.01 (d, J = 7.6 Hz, 1H), 7.56-7.64 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 183.0, 166.4, 153.9, 138.8, 137.3, 134.6, 133.3, 130.8, 130.5, 128.2, 127.3, 126.1, 122.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{14}H_8Cl_2NOS$: 307.96982; found: 307.96969.

benzo[d]thiazol-2-yl(4-hydroxyphenyl)methanone (**3j**): 140.4 mg, 55% yield; yellow solid; mp 179-182 ℃; IR (KBr): 3423, 2257, 1628, 1597, 1572, 1487, 1379, 1290, 1239, 1167, 1115, 999 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 10.74, (s, 1H), 8.49 (d, J = 8.4 Hz, 2H), 8.25 (s, 2H), 7.63 (s, 2H), 6.99 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 182.2, 167.8, 163.4, 153.3, 136.0, 133.8, 127.7, 127.2, 125.5, 125.1, 122.7, 115.6; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{14}H_{10}NO_2S$: 256.04268; found: 256.04227.

benzo[d]thiazol-2-yl(naphthalen-2-yl)methanone (**3k**): 231.5 mg, 80% yield; yellow solid; mp 164-166 ℃; IR (KBr): 3445, 1632, 1618, 1485, 1386, 1348, 1291, 1235, 1192, 1149, 1131, 1096 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 9.35 (s, 1H), 8.44 (d, J = 8.4 Hz, 1H), 8.30 (d, J = 8.0 Hz, 1H), 7.89-798 (m, 4H), 7.54-7.66 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 184.8, 167.1, 153.7, 136.8, 135.7, 134.1, 132.2, 131.9, 130.0, 128.8, 128.1, 127.5, 127.3, 126.7, 126.5, 125.6, 125.5, 121.9; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{12}NOS$: 290.06341; found: 290.06326.

benzo[d]thiazol-2-yl(naphthalen-1-yl)methanone (**3l**): 237.0 mg, 82% yield; yellow solid; mp 141-143 ℃; yellow solid; IR (KBr): 3447, 1653, 1593, 1509, 1481, 1293, 1254, 1202, 1147, 1031 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.52 (d, J = 8.0 Hz, 1H), 8.35 (d, J = 7.2 Hz, 1H), 8.17-8.19 (m, 1H), 8.09 (d, J = 8.4 Hz, 1H), 8.02-8.04 (m, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.54-7.63 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 188.2, 168.0, 153.7, 137.3, 133.9, 133.6, 132.2, 131.9, 131.1, 128.6, 128.0, 127.7, 126.9, 126.5, 125.8, 125.4, 124.3, 122.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{12}NOS$: 290.06341; found: 290.06325.

[1,1'-biphenyl]-4-yl(benzo[d]thiazol-2-yl)methanone (**3m**): 239.7 mg, 76% yield; yellow solid; mp 104-107 ℃; IR (KBr): 3447, 1636, 1600, 1553, 1484, 1405, 1294, 1270, 1193, 1115, 1006 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.63 (d, J = 6.4 Hz, 2H), 8.24 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 6.8 Hz, 2H), 7.65 (d, J = 7.6 Hz, 2H), 7.44-7.57 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 184.6, 167.2, 153.8, 146.4, 139.7, 136.9, 133.5, 131.8, 128.9, 128.3, 127.5, 127.2, 127.0, 126.8, 125.6, 122.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{20}H_{14}NOS$: 316.07906; found: 316.07899.

benzo[d]thiazol-2-yl(furan-2-yl)methanone (**3n**): 155.9 mg, 68% yield; yellow solid; mp 149-151 ℃; IR (KBr): 3452, 1640, 1554, 1493, 1308, 1230, 1185, 1164, 1142, 1066, 1021 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.36 (d, J = 3.6 Hz, 1H), 8.20 (d, J = 7.6 Hz, 1H), 7.99 (d, J = 7.6 Hz, 1H), 7.82 (s, 1H), 7.52-7.57 (m, 2H), 6.68 （d, J = 3.6 Hz, 1H）; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 172.3, 166.3, 153.7, 149.7, 148.9, 136.8, 127.5, 126.9, 125.5, 125.0, 122.2, 112.9; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{12}H_8NO_2S$: 230.02703; found: 230.02652.

benzo[d]thiazol-2-yl(thiophen-2-yl)methanone (**3o**): 184.0 mg, 75% yield; yellow solid; mp 104-106 ℃; IR (KBr): 3444, 3096, 1618, 1459, 1409, 1356, 1295, 1227, 1115, 1038 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.75 (d, J = 3.6 Hz, 1H), 8.23 (d, J = 8.4 Hz, 1H), 7.99 (d, J = 7.6 Hz, 1H), 7.83 (d, J = 5.2 Hz, 1H), 7.53-7.58 (m, 2H), 7.25 (d, J = 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 176.9, 166.5, 153.6, 139.6, 137.3, 136.9, 136.7, 128.4, 127.5, 126.9, 125.5, 122.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{12}H_8NOS_2$: 246.00418; found: 246.00377.

benzo[d]thiazol-2-yl(thiophen-3-yl)methanone (**3p**): 171.7 mg, 70% yield; yellow solid; mp 100-102 ℃; IR (KBr): 3450, 3123, 1630, 1511, 1491, 1420, 1385, 1319, 1287, 1269, 1122 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 9.29 (s, 1H), 8.23 (d, J = 8.4 Hz,1H), 8.00 (d, J = 7.2 Hz, 2H), 7.51-7.60 (m, 2H), 7.39 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 178.2, 167.5, 153.8, 138.4, 138.0, 136.9, 128.8, 127.5, 126.9, 125.8, 125.5, 122.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{12}H_8NOS_2$: 246.00418; found: 246.00373.

benzo[d]thiazol-2-yl(1-methyl-1H-pyrrol-2-yl)methanone (**3q**): 152.6 mg, 63% yield; black solid; mp 109-111 ℃; IR (KBr): 3446, 1626, 1525, 1491, 1417, 1332, 1225, 1107 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 8.42 (s, 1H), 8.18 (d, J = 7.2 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.51 (d, J = 7.6 Hz, 1H), 7.28 (s, 2H), 3.73 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ = 177.6, 168.5, 153.8, 136.8,

133.8, 127.0, 126.6, 125.2, 123.7, 122.2, 121.2, 73.4, 39.0; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{13}H_{11}N_2OS$: 243.05866; found: 243.05817.

benzo[d]thiazol-2-yl(benzofuran-2-yl)methanone (**3r**): 209.5 mg, 75% yield; yellow solid; mp 123-125 ℃; IR (KBr): 3425, 2921, 2364, 1637, 1542, 1488, 1305, 1215, 1186, 1101, 1028 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.81 (s, 1H), 8.29-8.35 (m, 2H), 8.02 (d, J = 7.6 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.61-7.73 (m, 3H), 7.44 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 173.1, 165.7, 155.6, 153.2, 149.1, 136.1, 129.7, 128.1, 127.6, 126.9, 125.3, 124.6, 124.4, 123.0, 120.9, 112.3; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{16}H_{10}NO_2S$: 280.04268; found: 280.04247.

benzo[d]thiazol-2-yl(1H-indol-2-yl)methanone (**3s**): 194.8 mg, 70% yield; yellow solid; mp 242-244 ℃; IR (KBr): 3453, 3223, 1572, 1512, 1439, 1380, 1312, 1241, 1195, 1129, 1103, 1078, 1042 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.41 (s, 1H), 9.26 (s, 1H), 8.36 (s, 1H), 8.26 (s, 2H), 7.62 (s, 3H), 7.32 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 177.9, 153.5, 136.5, 135.9, 127.2, 127.1, 126.5, 124.9, 123.7, 122.8, 121.5, 112.8, 112.6, 109.4; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{16}H_{11}N_2OS$: 279.05866; found: 279.05849.

benzo[d]thiazol-2-yl(4-morpholinophenyl)methanone (**3t**): 253.0 mg, 82% yield; yellow solid; mp 150-152 ℃; IR (KBr): 3452, 2961, 1603, 1490, 1437, 1381, 1302, 1244, 1197, 1116 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.61 (d, J = 8.8 Hz, 2H), 8.21 (d, J = 8.0 Hz, 1H), 7.99 (d, J = 7.6 Hz, 1H), 7.51-7.56 (m, 2H), 6.94 (d, J = 9.2 Hz, 2H), 3.86 (s, 4H), 3.38 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.5, 168.5, 154.7, 153.9, 136.8, 136.6, 127.1, 126.6, 125.3, 125.0, 122.1, 113.0, 66.5, 47.1; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{18}H_{17}N_2O_2S$: 325.10052; found: 325.10026.

(5-chlorobenzo[d]thiazol-2-yl)(phenyl)methanone (**3u**): 221.7 mg, 81% yield; yellow solid; mp 127-130 ℃; (lit.[4] 133-136 ℃); IR (KBr): 3449, 2922, 1643, 1592, 1536, 1489, 1432, 1283, 1225, 1184, 1117, 1056 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.54 (d, J = 7.6 Hz, 2H), 8.19 (s, 1H), 7.88 (d, J = 8.8 Hz, 1H), 7.65 (d, J = 7.2 Hz, 1H), 7.46-7.56 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 184.8, 169.0, 154.6, 135.3, 134.7, 134.2, 133.1, 131.4, 128.6, 128.3, 125.3, 123.0; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{14}H_9ClNOS$: 274.00879; found: 274.00853

(5-chlorobenzo[d]thiazol-2-yl)(4-methoxyphenyl)methanone (**3v**): 252.1 mg, 83% yield; yellow solid; mp 140-142 ℃; IR (KBr): 3451, 1631, 1602, 1570, 1487, 1433, 1303, 1265, 1178, 1117, 1064, 1022 cm^{-1}; ^{1}H NMR (400 MHz,

$CDCl_3$): δ = 8.62 (d, J = 8.8 Hz, 2H), 8.18 (s, 1H), 7.89 (d, J = 8.8 Hz, 1H), 7.47 (d, J = 8.4 Hz, 1H), 7.02 (d, J = 8.4 Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.7, 169.7, 164.5, 154.5, 135.0, 133.8, 132.7, 127.9, 127.4, 125.0, 122.8, 113.9, 55.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{15}H_{11}ClNO_2S$: 304.01935; found: 304.01919.

(4-bromophenyl)(5-chlorobenzo[d]thiazol-2-yl)methanone (**3w**)**:** 253.9 mg, 72% yield; yellow solid; mp 184-186 ℃; IR (KBr): 3441, 3093, 2959, 1731, 1640, 1583, 1540, 1495, 1434, 1396, 1291, 1115, 1070, 1009 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.46 (d, J = 8.4 Hz, 2H), 8.23 (s, 1H), 7.94 (d, J = 9.2 Hz, 1H), 7.71 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 183.8, 169.8, 164.2, 135.2, 133.3, 133.2, 132.8, 131.9, 129.8, 128.4, 125.3, 123.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{14}H_8BrClNOS$: 351.91930; found: 391.91902.

(5-chlorobenzo[d]thiazol-2-yl)(thiophen-2-yl)methanone (**3x**): 173.5 mg, 62% yield; yellow solid; mp 141-143 ℃; IR (KBr): 3456, 2355, 1631, 1568, 1415, 1261, 1121, 1069 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.69 (s, 1H), 8.31 (d, J = 8.4 Hz, 3H), 7.66 (d, J = 8.4 Hz, 1H), 7.41 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 175.9, 168.2, 153.7, 138.7, 138.6, 137.8, 134.8, 132.1, 129.1, 128.0, 124.5, 124.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{12}H_7ClNOS_2$: 279.96521; found: 279.96506.

1,3-phenylenebis(benzo[d]thiazol-2-ylmethanone) (**3y**): 260.3 mg, 65% yield; yellow solid; mp 158-161 ℃; IR (KBr): 3445, 2925, 1727, 1650, 1592, 1552, 1486, 1421, 1288, 1262, 1111 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.46 (s, 1H), 8.81 (d, J = 7.6 Hz, 2H), 8.25-8.31 (m, 4H), 8.68 (s, 5H); ^{13}C NMR (150 MHz, DMSO-d_6): δ = 184.2, 166.4, 153.2, 136.4, 135.9, 134.8, 129.1, 128.6, 128.2, 127.5, 125.4, 123.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{22}H_{13}N_2O_2S_2$: 401.04130; found: 401.04099.

(E)-1-(benzo[d]thiazol-2-yl)-3-phenylprop-2-en-1-one (**5a**): 95.5 mg, 72% yield; yellow solid; mp 151-153 ℃; IR (KBr): 3444, 1660, 1597, 1571, 1485, 1447, 1341, 1311, 1286, 1212, 1122, 1071 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.22 (d, J = 8.0 Hz, 1H), 8.06 (dd, J_1 = 16.0 Hz, J_2 = 4.8Hz, 2H), 7.97 (d, J = 8.0 Hz, 1H), 7.73 (s, 2H), 7.49-7.59 (m, 2H), 7.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.9, 168.0, 153.6, 146.1, 137.4, 134.5, 131.1, 129.0, 128.9, 127.5, 126.9, 125.4, 122.3, 120.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{16}H_{12}NOS$: 266.06341; found: 266.06315.

(E)-1-(benzo[d]thiazol-2-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (**5b**): 103.4 mg, 70% yield; yellow solid; mp 146-149 ℃; IR (KBr): 3453, 1649, 1587, 1512, 1487, 1425, 1309, 1264, 1215, 1175, 1026, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.21 (d, J = 8.0 Hz, 1H), 7.92-8.04 (m, 3H), 7.71 (d, J = 7.6 Hz, 2H), 7.57 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 6.94 (d, J = 7.6 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.7, 168.5, 162.2, 153.7, 146.0, 137.4, 131.0, 127.4, 126.8, 125.3, 122.4, 117.9, 114.4, 55.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{17}H_{14}NO_2S$: 296.07398; found: 296.07377

(E)-1-(benzo[d]thiazol-2-yl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (**5c**): 102.5 mg, 63% yield; yellow solid; mp 194-197 ℃; IR (KBr): 3449, 2961, 2927, 1726, 1661, 1592, 1511, 1474, 1415, 1357, 1307, 1265, 1206, 1155, 1134, 1015 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.22 (d, J = 8.0 Hz, 1H), 7.90-8.22 (m, 3H), 7.52-7.58 (q, J = 11.8 Hz, 2H), 7.32 (d, J = 8.4 Hz, 1H), 7.28 (s, 1H), 6.91 (d, J = 8.0 Hz, 1H), 3.99 (s, 3H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.7, 168.5, 153.7, 152.1, 149.3, 146.4, 137.4, 127.6, 127.4, 126.9, 125.2, 124.5, 122.4, 118.0, 111.0, 110.2, 56.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{16}NO_3S$: 326.08454; found: 326.08437.

(E)-1-(benzo[d]thiazol-2-yl)-3-(3-(benzyloxy)-4-methoxyphenyl)p rop-2-en-1-one (**5d**): 130.5 mg, 65% yield; yellow solid; mp 163-166 ℃; IR (KBr): 3450, 3054, 2945, 1656, 1590, 1508, 1425, 1387, 1354, 1311, 1263, 1204, 1144, 1072, 1028 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.23 (d, J = 8.4 Hz, 1H), 8.01 (t, J = 7.6 Hz, 2H), 7.94 (s, 1H), 7.55-7.61 (m, 2H), 7.52 (d, J = 7.2 Hz, 2H), 7.45 (d, J = 7.2 Hz, 2H), 7.39 (t, J = 7.2 Hz, 2H), 7.34-7.27 (m, 1H), 6.93 (d, J = 8.0 Hz, 1H), 5.23 (s, 2H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.7, 171.6, 168.5, 152.9, 151.2, 149.8, 146.4, 137.4, 136.4, 128.7, 128.1, 127.5, 127.2, 126.9, 125.3, 124.2, 122.4, 118.1, 113.3, 110.9, 70.8, 56.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{24}H_{20}NO_3S$: 402.11584; found: 402.11560.

(E)-1-(benzo[d]thiazol-2-yl)-3-(3-nitrophenyl)prop-2-en-1-one (**5e**): 149.0 mg, 48% yield; yellow solid; mp 191-192 ℃; IR (KBr): 3442, 1660, 1605, 1530, 1486, 1353, 1312, 1270, 1215, 1123, 1071 cm^{-1}; ^1H NMR (400 MHz, d_6-DMSO): δ = 8.66 (s, 1H), 8.26-8.35 (m, 4H), 8.13 (br, 2H), 7.75-7.79 (t, J = 8.0 Hz, 1H), 7.68 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.5, 167.1, 142.7, 140.0, 137.4, 136.3, 134.5, 130.0, 127.9, 127.1, 125.5, 125.1, 123.2, 123.0, 122.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{16}H_{11}N_2O_3S$: 311.04849; found: 311.04832.

(E)-1-(5-chlorobenzo[d]thiazol-2-yl)-3-phenylprop-2-en-1-one (**5f**): 101.9 mg, 68% yield; yellow solid; mp 133-136 ℃; IR (KBr): 3446, 1663, 1607, 1596, 1575, 1539, 1484, 1448, 1435, 1338, 1305, 1205, 1122, 1062 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.17 (s, 1H), 7.96-8.05 (q, J = 17.8 Hz, 2H), 7.87 (d, J = 8.8 Hz, 1H), 7.72 (br, 2H), 7.47 (s, 1H), 7.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.5, 169.7, 154.3, 146.5, 135.6, 134.4, 132.9, 131.2, 129.0, 128.9, 128.1, 124.9, 123.1, 120.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{16}H_{11}ClNOS$: 300.02444; found: 300.02441.

(E)-1-(5-chlorobenzo[d]thiazol-2-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (**5g**): 115.4 mg, 70% yield; yellow solid; mp 164-166 ℃; IR (KBr): 3445, 3091, 1650, 1586, 1569, 1514, 1488, 1434, 1343, 1325, 1307, 1268, 1212, 1178, 1122, 1066, 1024 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.18 (s, 1H), 7.91 (s, 1H), 7.87-7.91 (m, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.4 Hz, 1H), 6.95 (d, J = 8.4 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.4, 170.2, 162.4, 154.4, 146.5, 136.0, 132.9, 131.1, 127.9, 127.3, 124.8, 123.1, 117.6, 114.5, 55.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{17}H_{13}ClNO_2S$: 330.03500; found: 330.03487.

(E)-1-(5-chlorobenzo[d]thiazol-2-yl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (**5h**): 116.9 mg, 65% yield; yellow solid; mp 158-160 ℃; IR (KBr): 3447, 1652, 1575, 1514, 1482, 1423, 1271, 1208, 1144, 1065, 1016 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = ^1H NMR (400 MHz, $CDCl_3$): δ = 8.18 (s, 1H), 7.97 (s, 1H), 7.81-7.89 (q, J = 16.6 Hz, 2H), 7.47 (d, J = 8.4 Hz, 1H), 7.28-7.31 (t, J = 6.8 Hz, 1H), 7.24 (s, 1H), 6.90 (d, J = 8.0 Hz, 1H), 3.98(s, 3H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.2, 170.2, 162.3, 154.3, 152.1, 149.2, 146.8, 135.5, 132.8, 127.9, 127.5, 124.8, 123.1, 117.6, 111.0, 110.2, 56.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{15}ClNO_3S$: 360.04557; found: 360.04520.

(E)-1-(5-chlorobenzo[d]thiazol-2-yl)-3-(3-nitrophenyl)prop-2-en-1-one (**5i**): 86.2 mg, 50% yield; yellow solid; mp 183-185 ℃; IR (KBr): 3445, 1663, 1611, 1529, 1482, 1434, 1353, 1340, 1309, 1272, 1212, 1065 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.59 (s, 1H), 8.30 (d, J = 7.2 Hz, 1H), 8.23 (s, 1H), 8.03-8.17 (m, 3H), 7.90-7.94 (t, J = 8.4 Hz, 1H), 7.64-7.71 (m, 1H), 7.58 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 182.4, 168.9, 154.3, 148.8, 143.9, 143.1, 136.2, 134.5, 133.3, 130.1, 128.5, 125.3, 125.1, 123.2, 123.1, 130.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{16}H_{10}ClN_2O_3S$: 345.00952; found: 345.00928.

5. Reference

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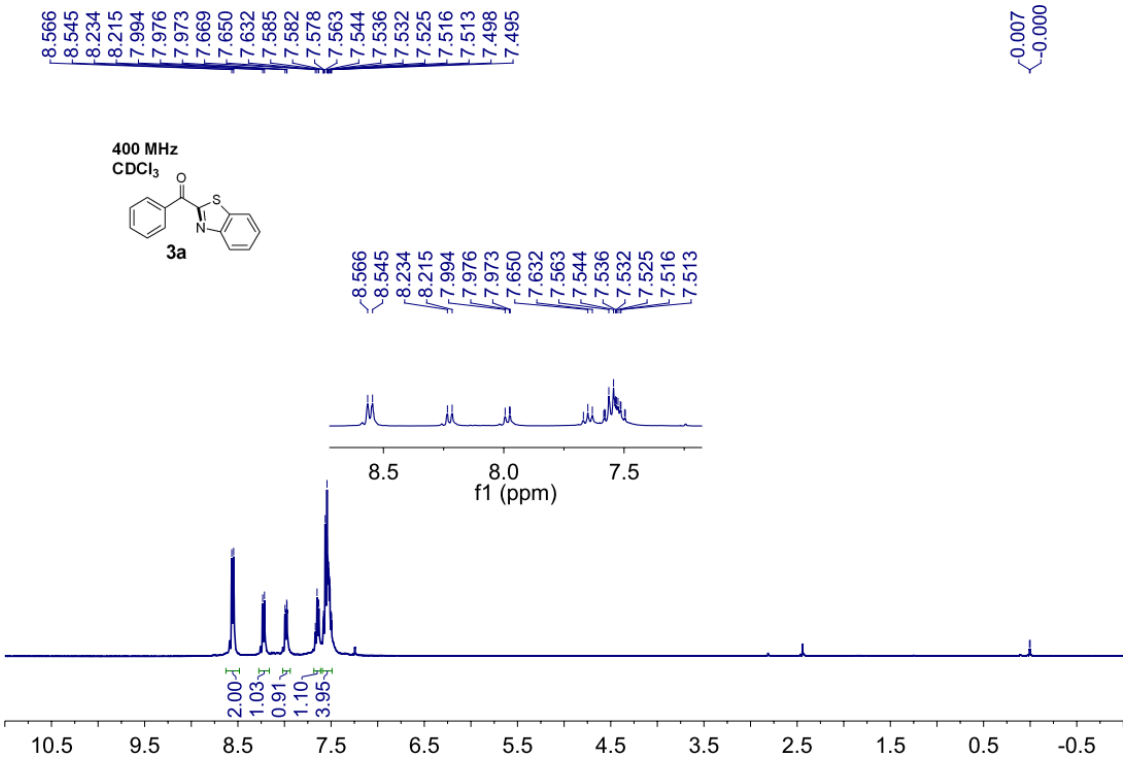
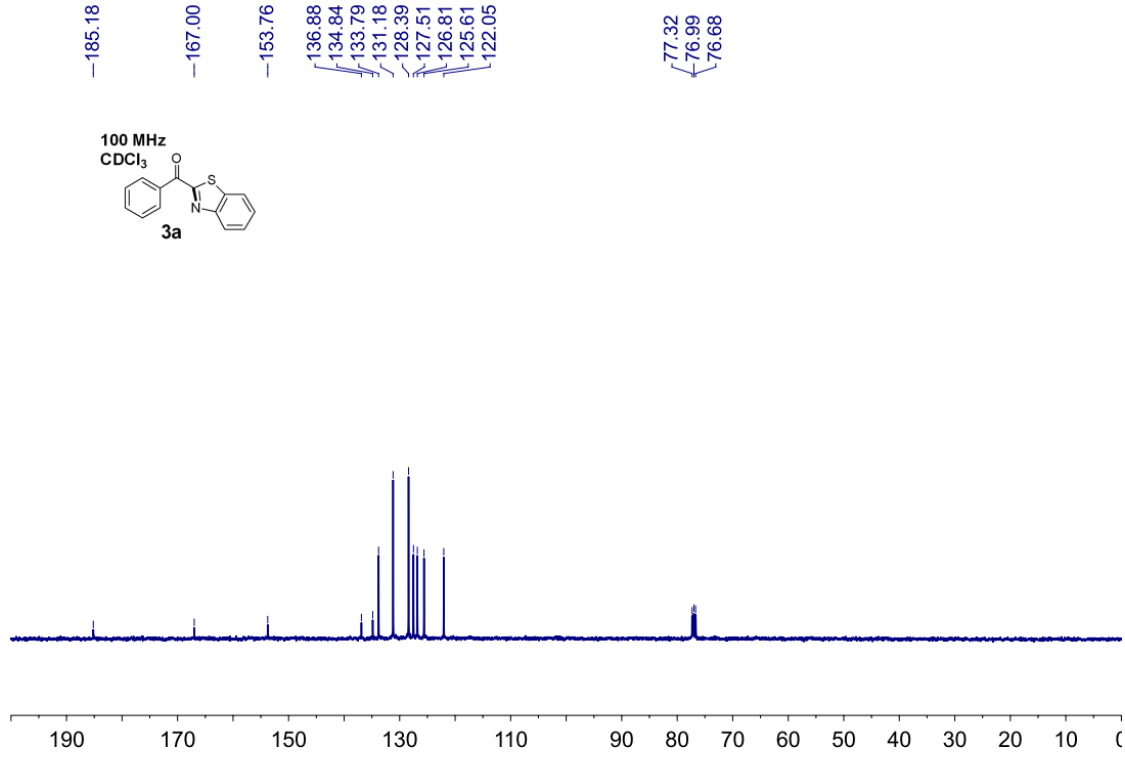
(3) C. Boga, R. Stengel, R. Abdayem, E. D. Vecchio, L. Forlani and P. E. Todesco, *J. Org. Chem.* 2004, **69**, 8903.
(4) X. S. Fan, Y. He, S. H. Guo and X. Y. Zhang, *Aust. J. Chem.* 2011, **64**, 1568-1573.

6. Appendix: spectral Copies of ^{1}H NMR and ^{13}C NMR of compounds obtained in this Study

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125.61
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77.32
76.99
76.68
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150
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80
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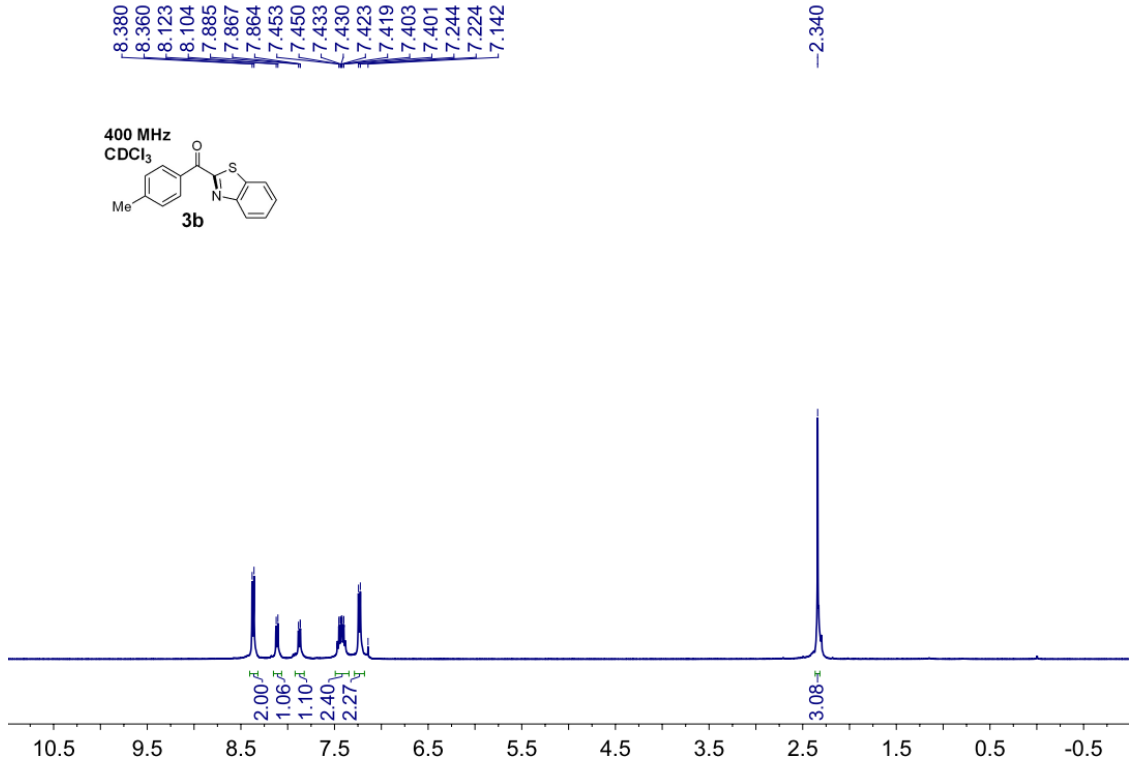
20
10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7.403
7.401
7.244
7.224
7.142
2.340
400 MHz
CDCl3
Me
3b
2.00
1.06
1.10
2.40
2.27
3.08
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6.5
5.5
4.5
3.5
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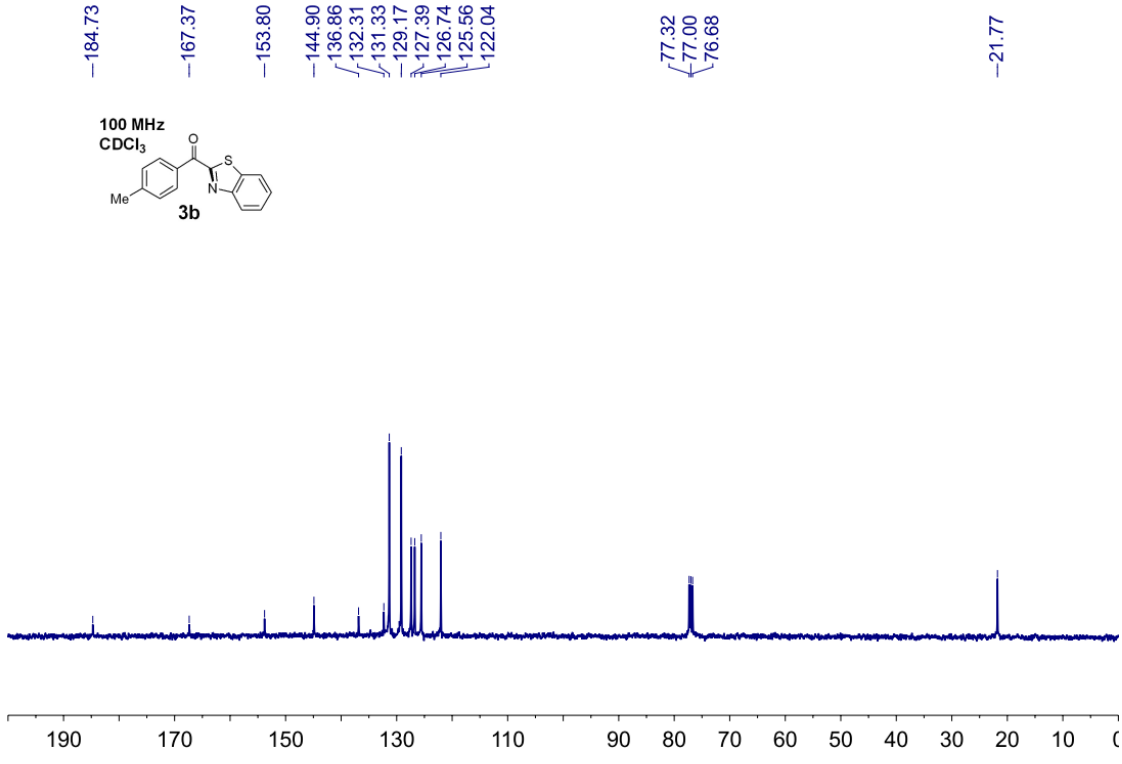
0.5
-0.5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77.00
76.68
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Me
3b
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150
130
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80
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40
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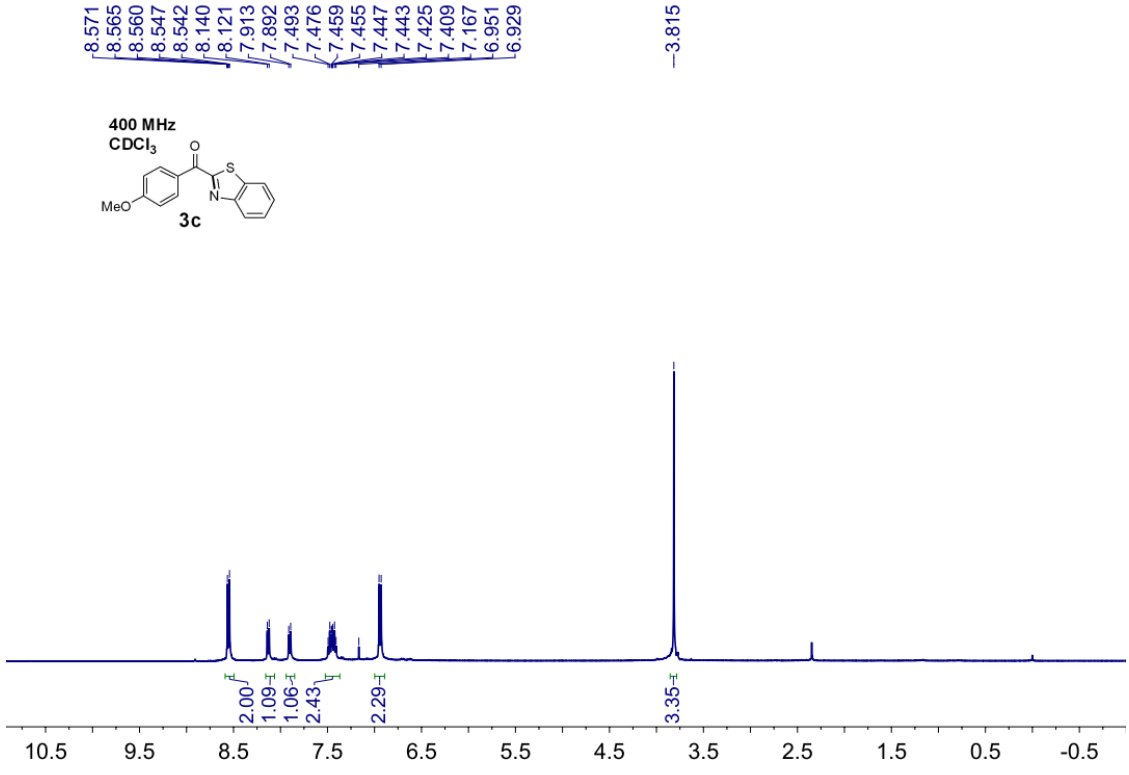
20
10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7.455
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7.443
7.425
7.409
7.167
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6.929
3.815
400 MHz
CDCl3
MeO
3c
2.00
1.09
1.06
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2.29
3.35
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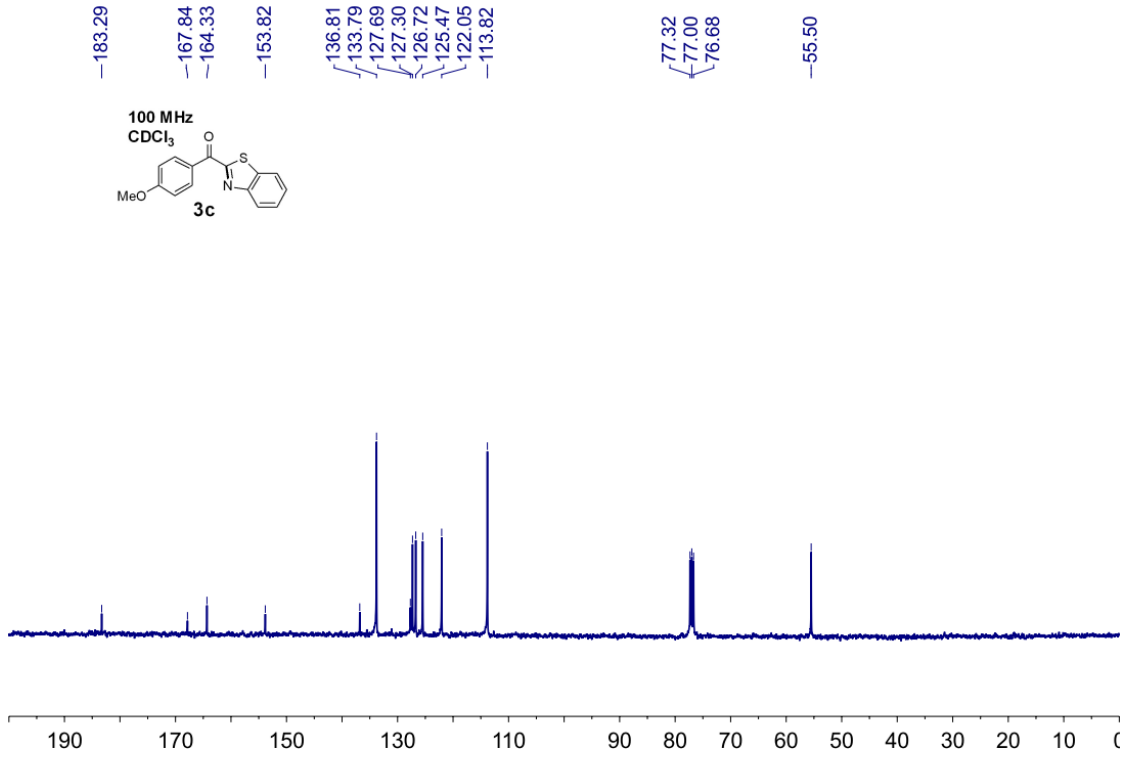
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77.00
76.68
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3c
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150
130
110
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80
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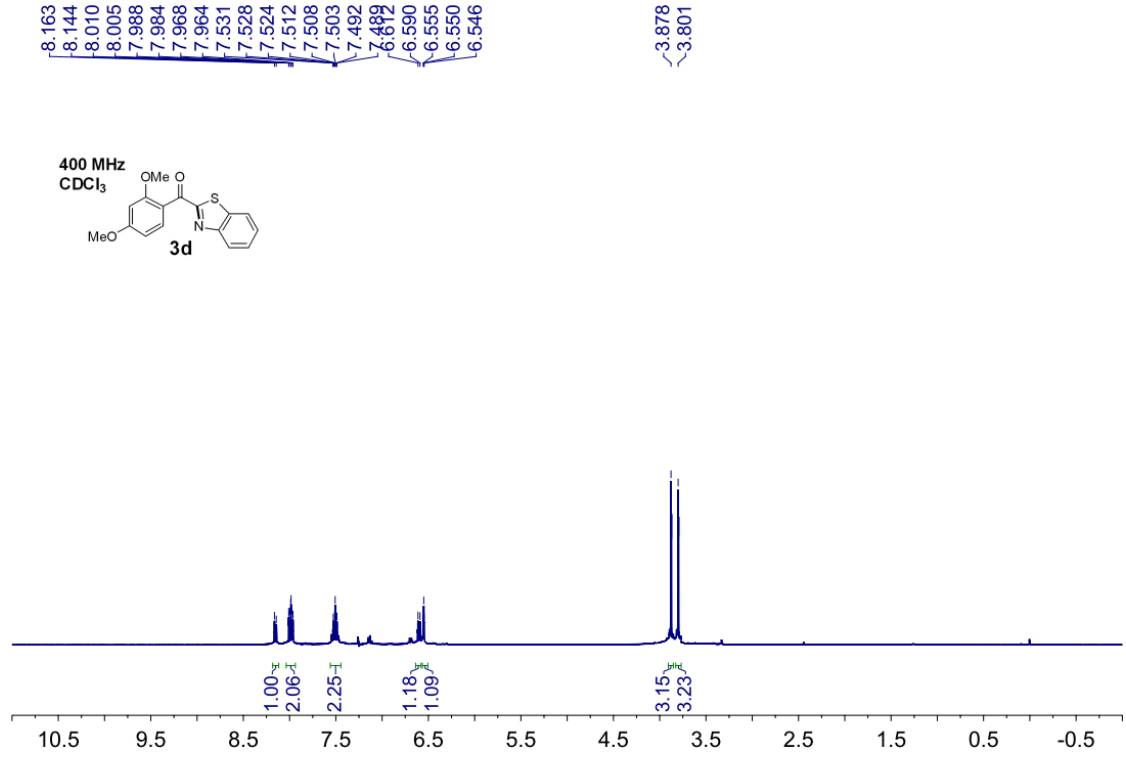
50
40
30
20
10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7.503
7.492
6.590
6.555
6.550
6.546
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MeO
3d
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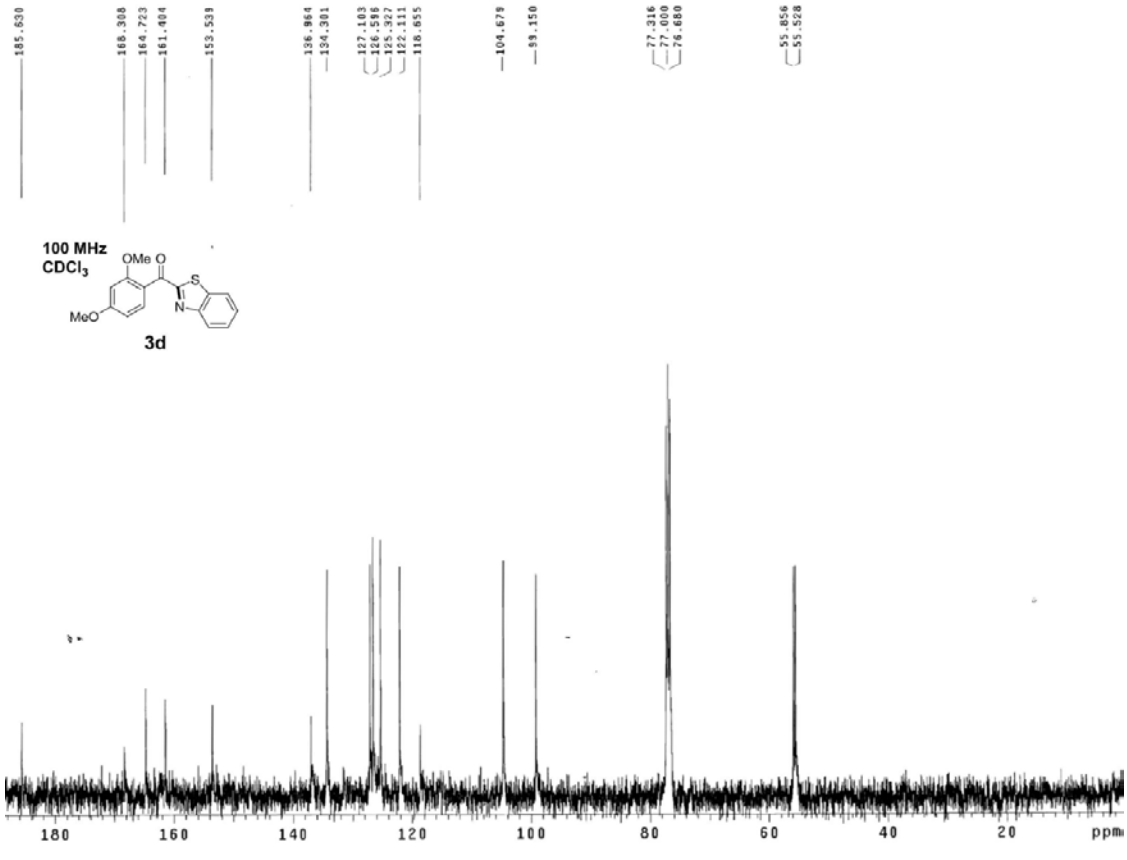
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104.679
89.150
77.316
77.000
76.680
55.856
55.528
100 MHz
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OMe O
S
N
MeO
3d
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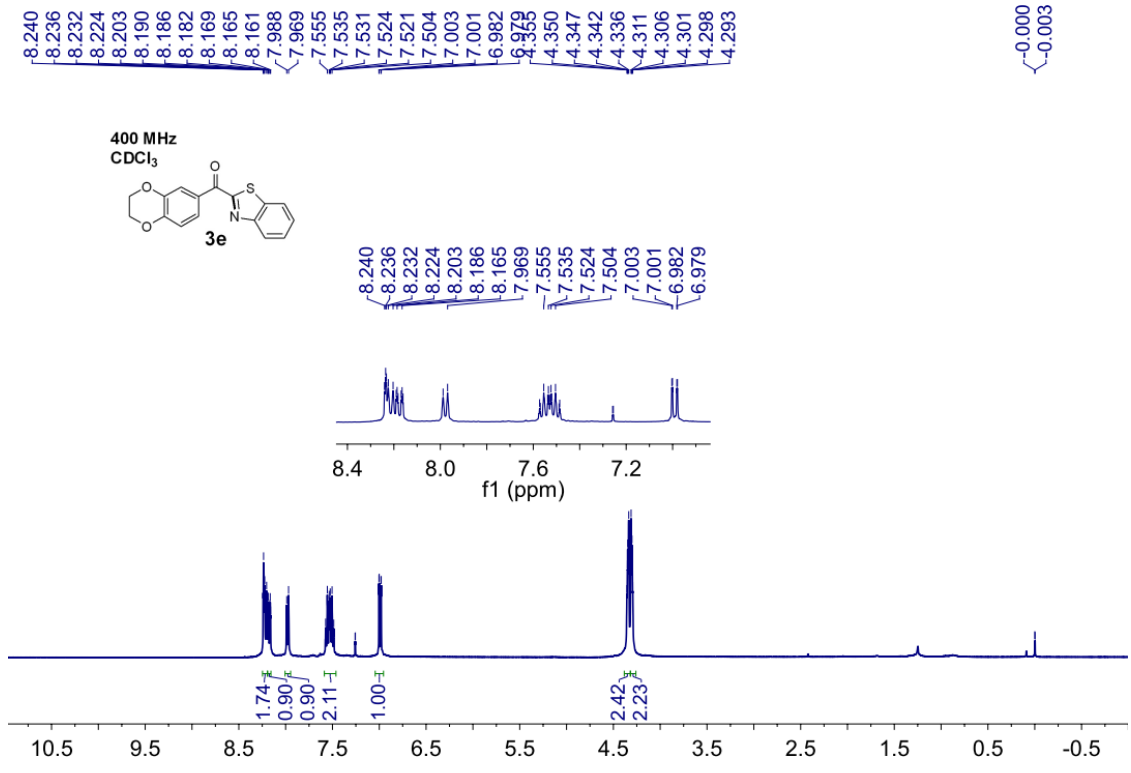
140
120
100
80
60
40
20
ppm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7.531
7.524
7.521
7.504
7.003
7.001
6.982
6.979
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4.336
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4.301
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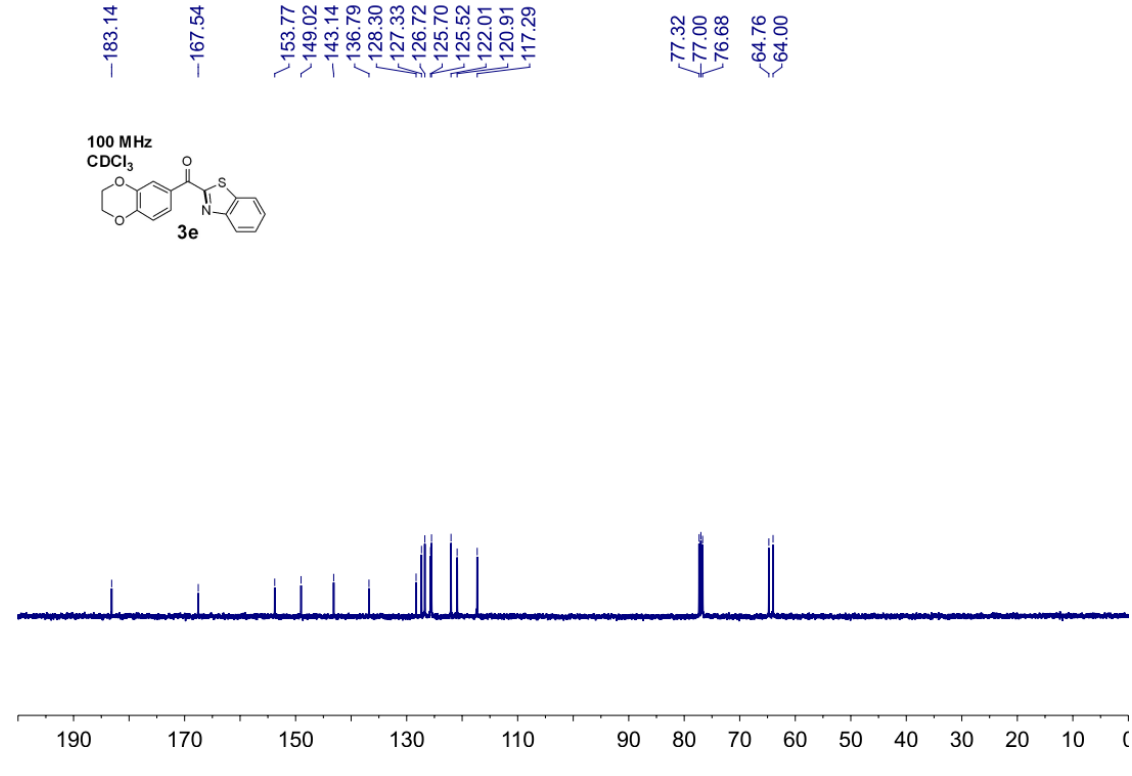
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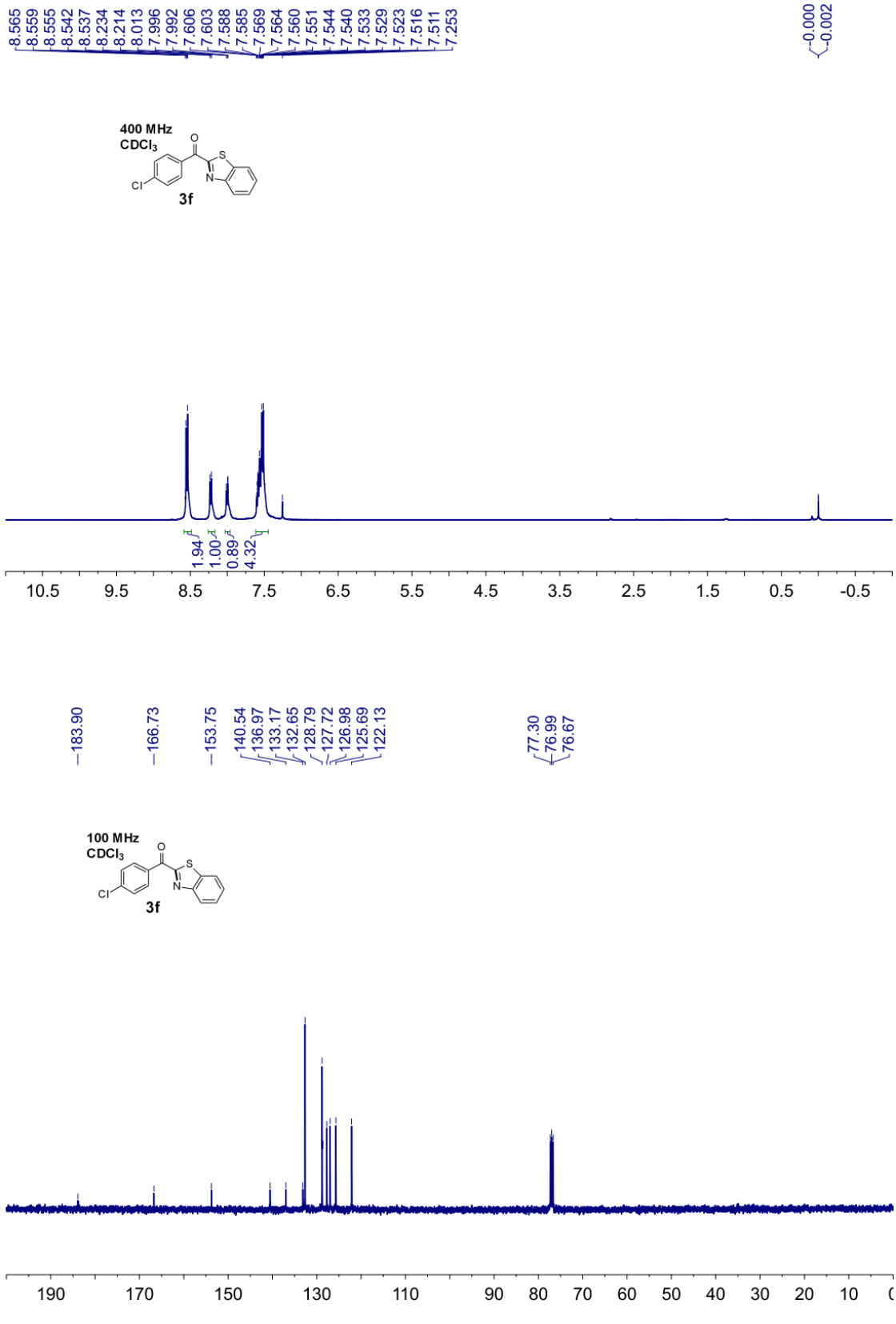
CDCl3
3e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7.569
7.564
7.560
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7.544
7.540
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7.529
7.523
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7.511
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8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
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153.75
140.54
136.97
133.17
132.65
128.79
127.72
126.98
125.69
122.13
77.30
76.99
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3f
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170
150
130
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80
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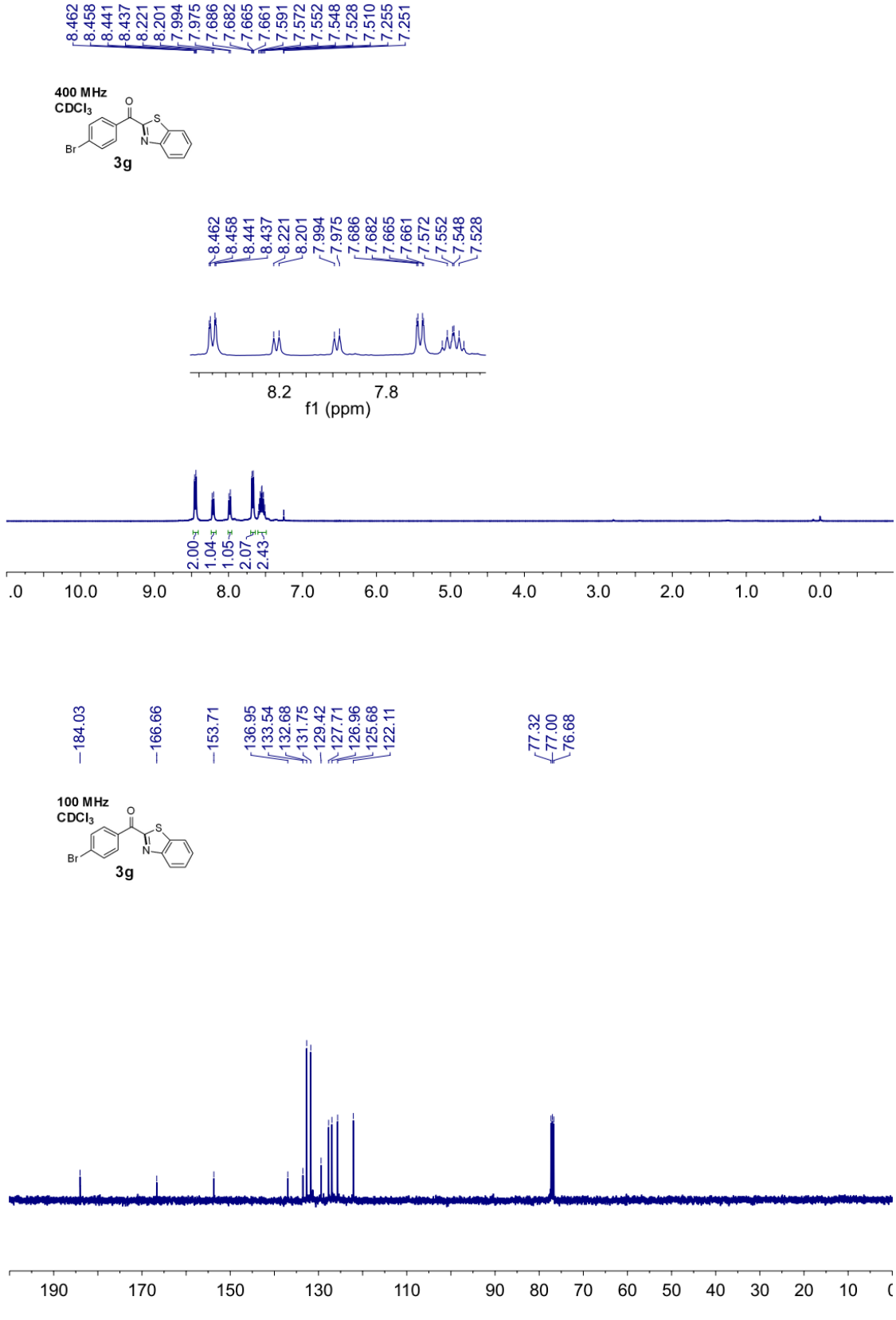
50
40
30
20
10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7.682
7.665
7.661
7.591
7.572
7.552
7.548
7.528
7.510
7.255
7.251
400 MHz
CDCl3
O
S
N
Br
3g
8.462
8.458
8.441
8.437
8.221
8.201
7.994
7.975
7.686
7.682
7.665
7.661
7.572
7.552
7.548
7.528
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7.8
f1 (ppm)
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7.0
6.0
5.0
4.0
3.0
2.0
1.0
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129.42
127.71
126.96
125.68
122.11
77.32
77.00
76.68
100 MHz
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S
N
Br
3g
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150
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110
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80
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40
30
20
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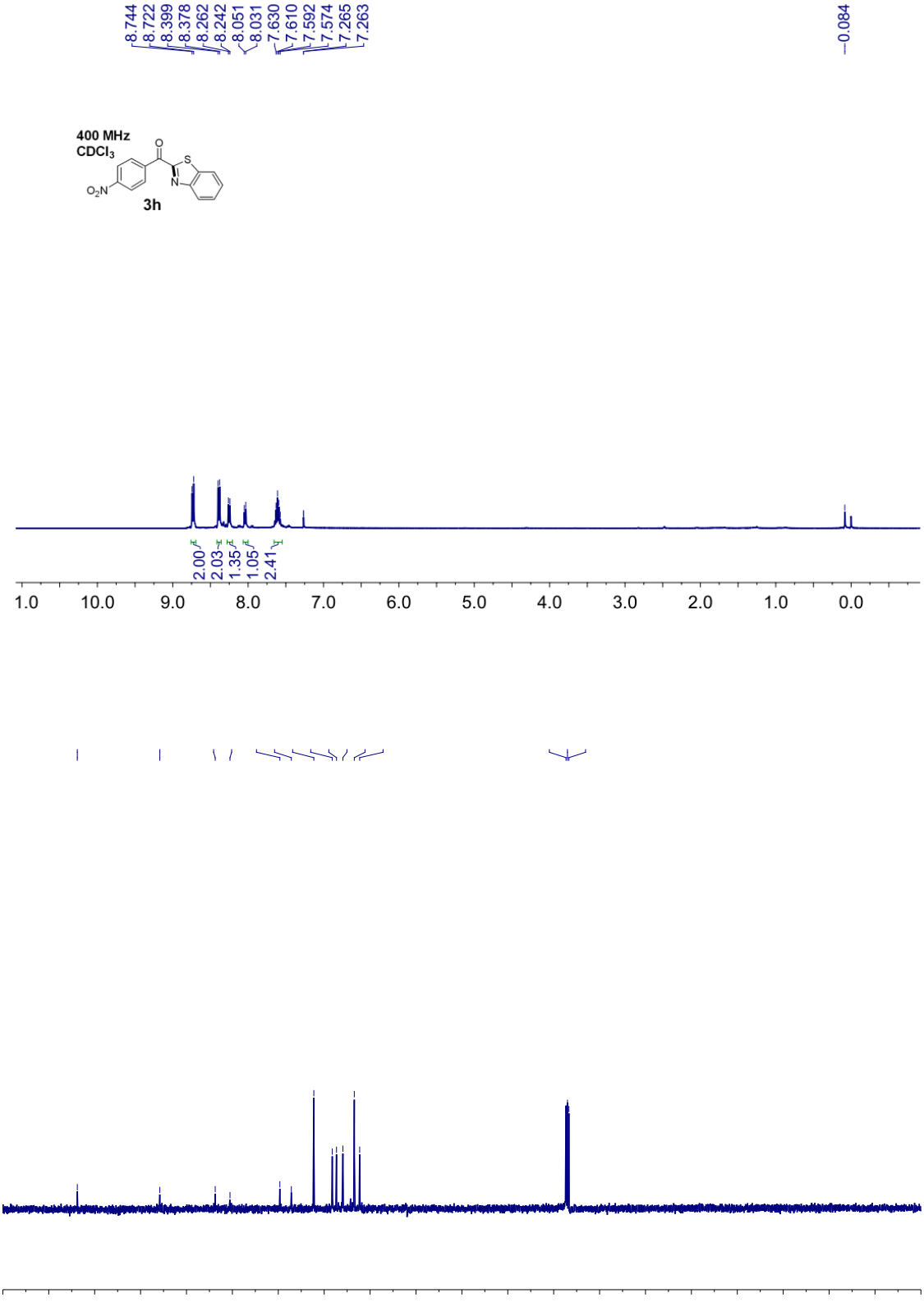
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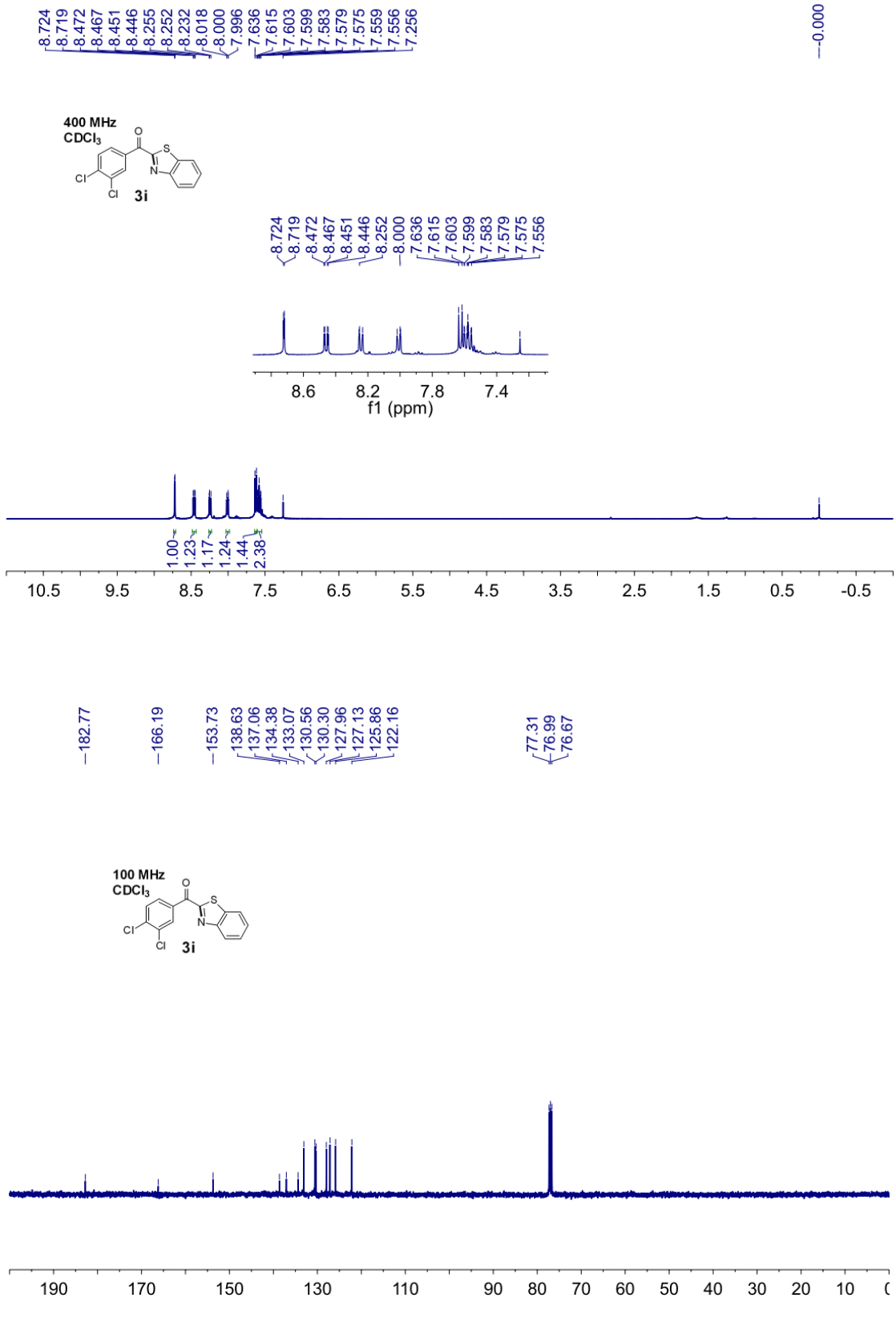
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400 MHz
CDCl3
3i
8.724
8.719
8.472
8.467
8.451
8.446
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8.000
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8.6
8.2
7.8
7.4
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7.5
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125.86
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3i
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20
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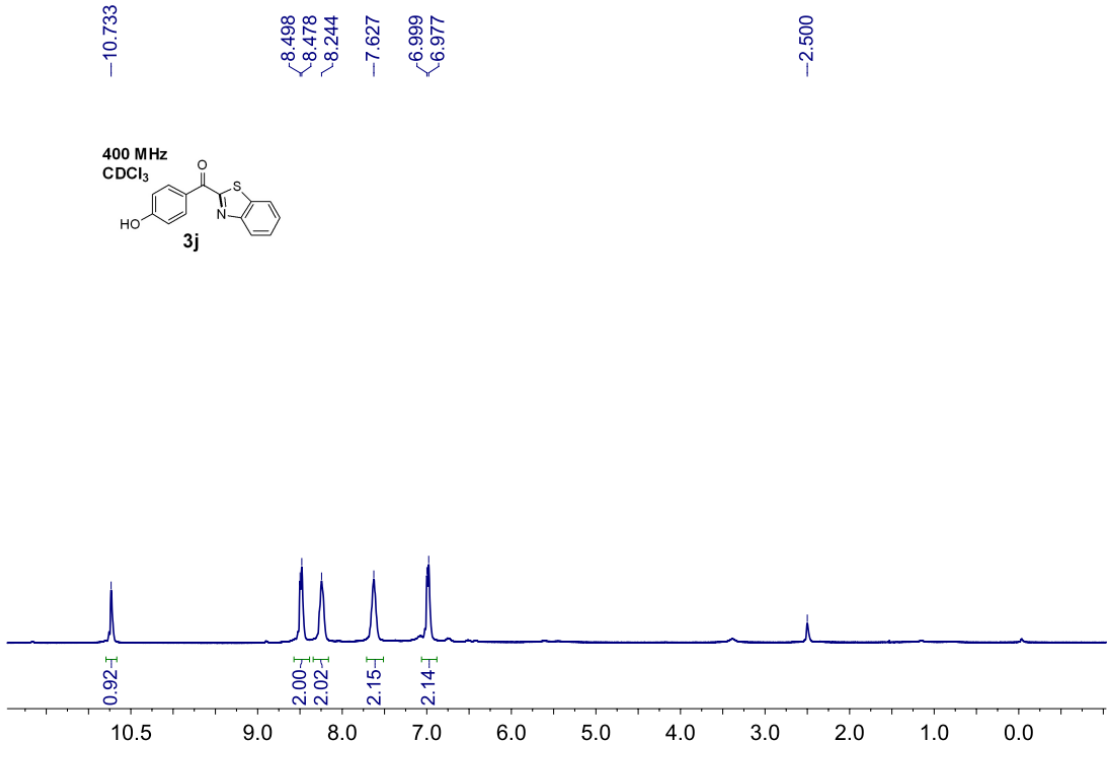
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3j
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2.02
2.15
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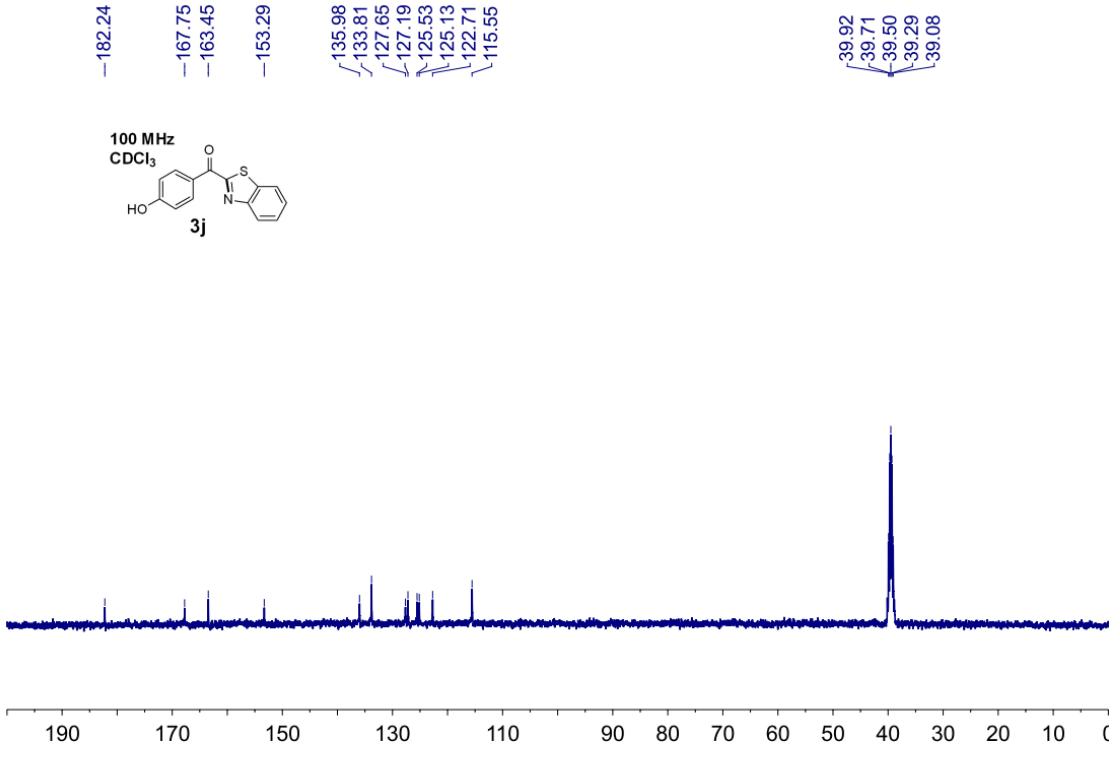
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39.29
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20
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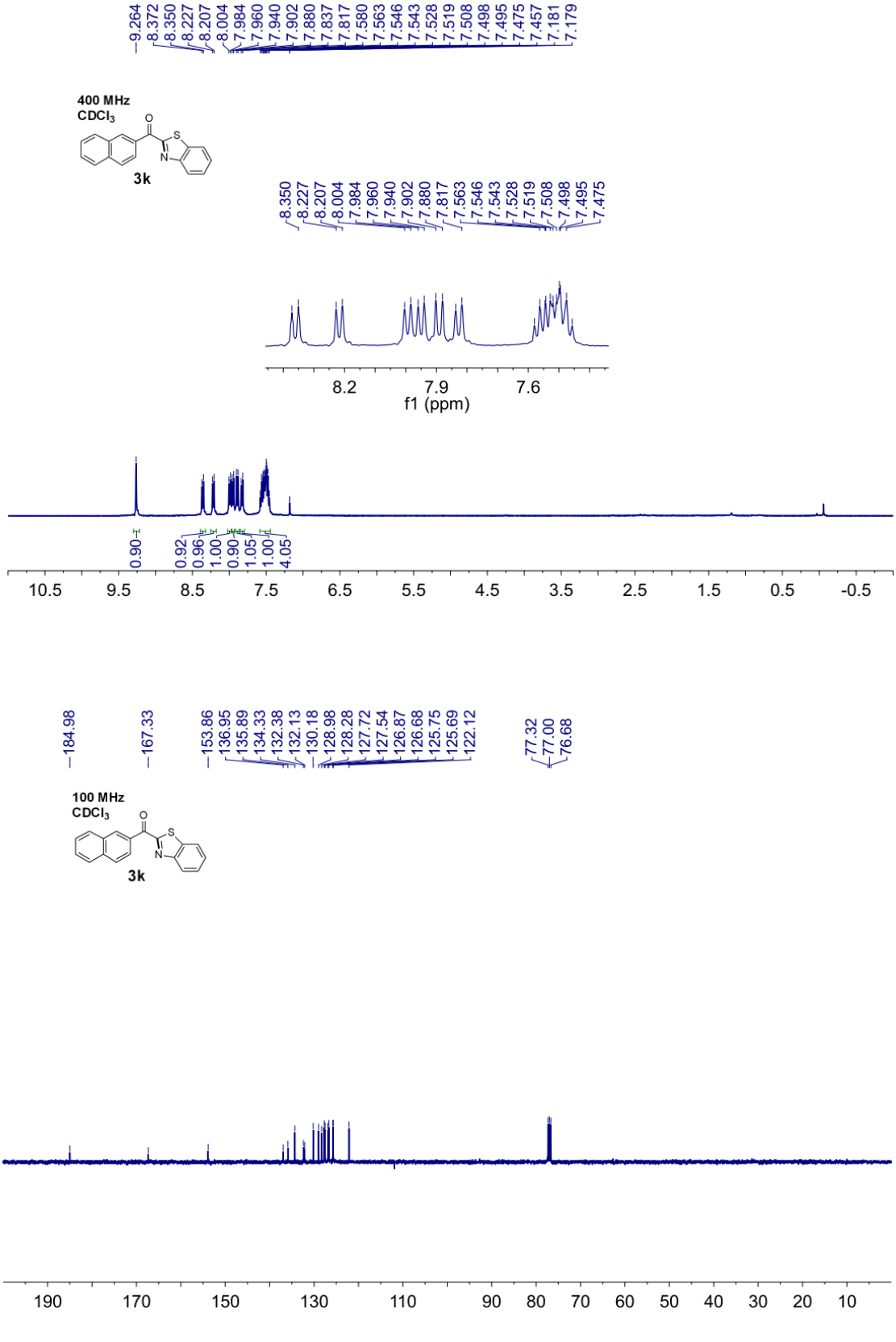
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7.580
7.563
7.546
7.543
7.528
7.519
7.508
7.498
7.495
7.475
7.457
7.181
7.179
400 MHz
CDCl3
3k
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8.227
8.207
8.004
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7.902
7.880
7.817
7.563
7.546
7.543
7.528
7.519
7.508
7.498
7.495
7.475
8.2
7.9
7.6
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1.00
0.90
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1.00
4.05
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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127.72
127.54
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126.68
125.75
125.69
122.12
77.32
77.00
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40
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20
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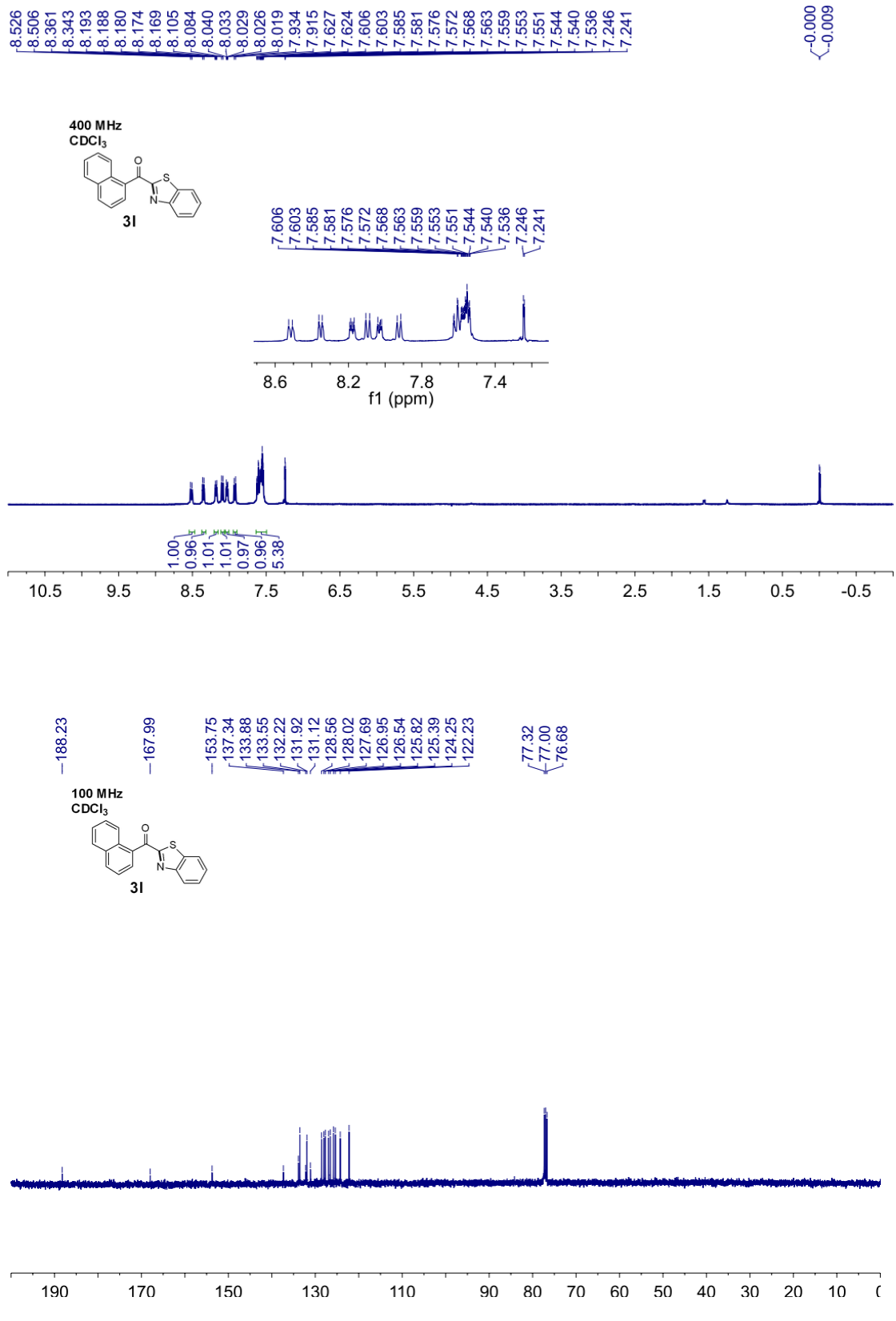
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3l
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7.8
7.4
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6.5
5.5
4.5
3.5
2.5
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-0.5
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133.55
132.22
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128.02
127.69
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125.39
124.25
122.23
77.32
77.00
76.68
100 MHz
CDCl3
3l
190
170
150
130
110
90
80
70
60
50
40
30
20
10


8.646
8.641
8.625
8.620
8.244
8.224
7.979
7.959
7.773
7.756
7.751
7.735
7.730
7.678
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7.530
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7.517
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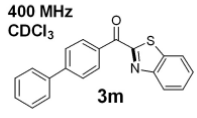
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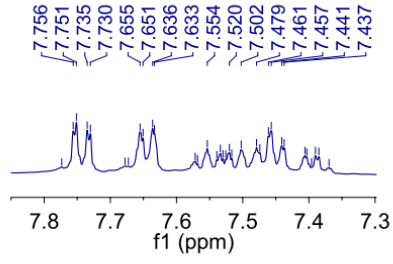
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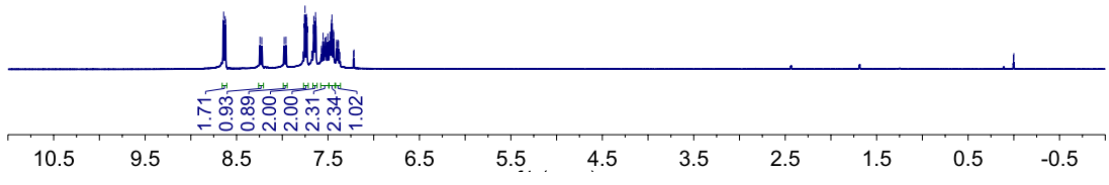
f1 (ppm)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6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


184.58
167.22
153.78
146.37
139.72
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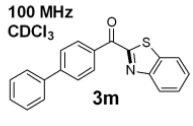
76.68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CDCl3
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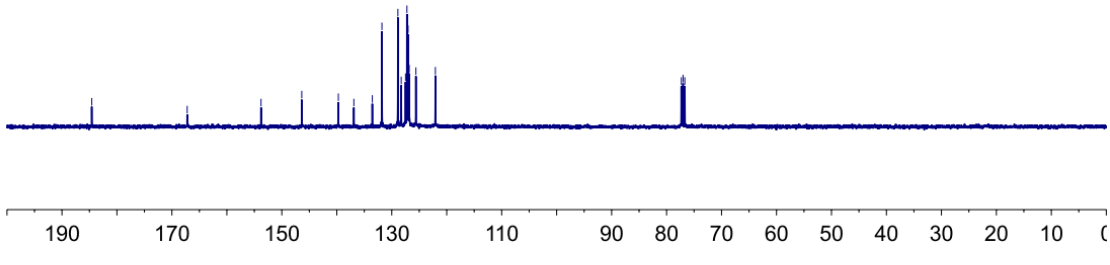
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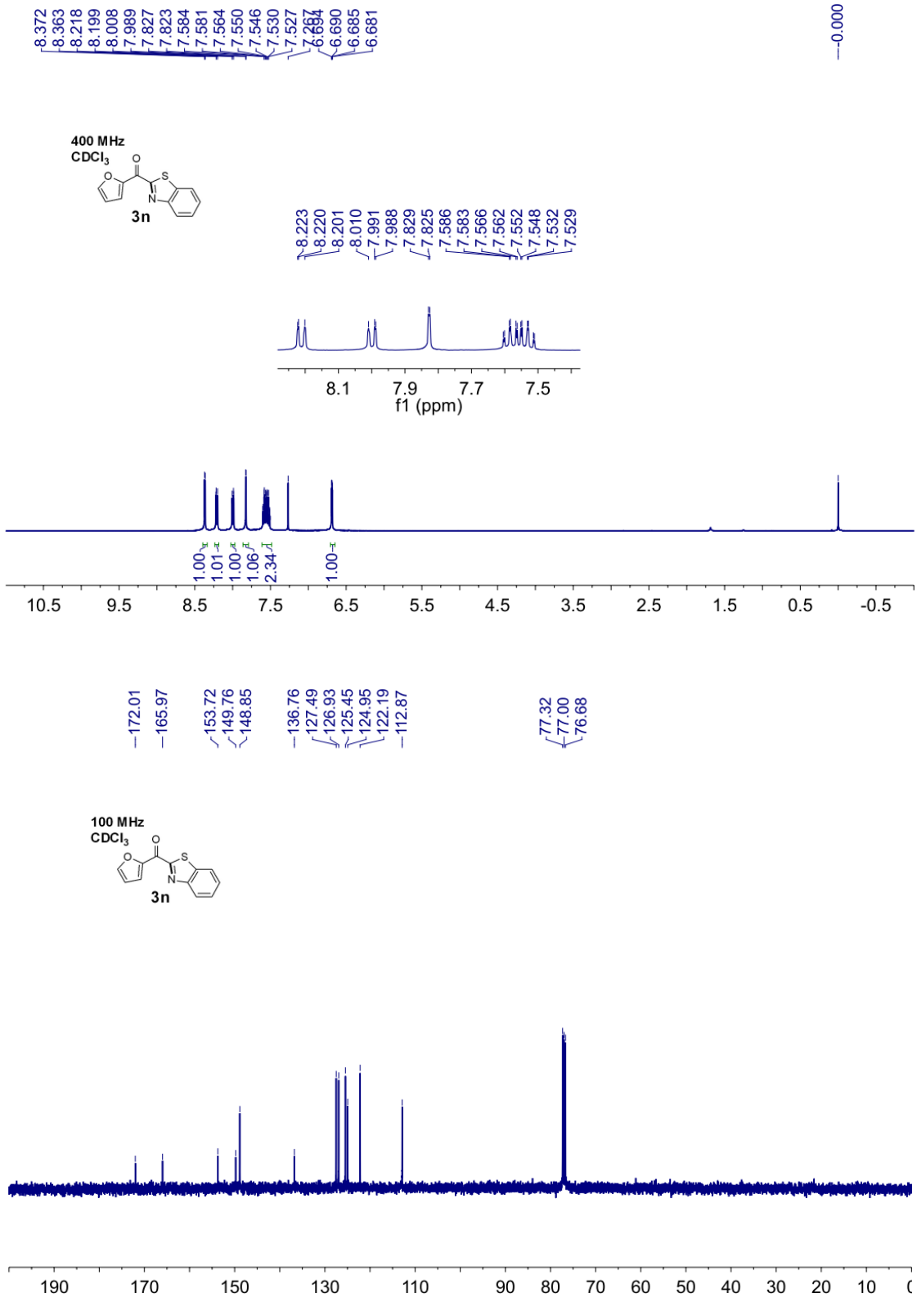
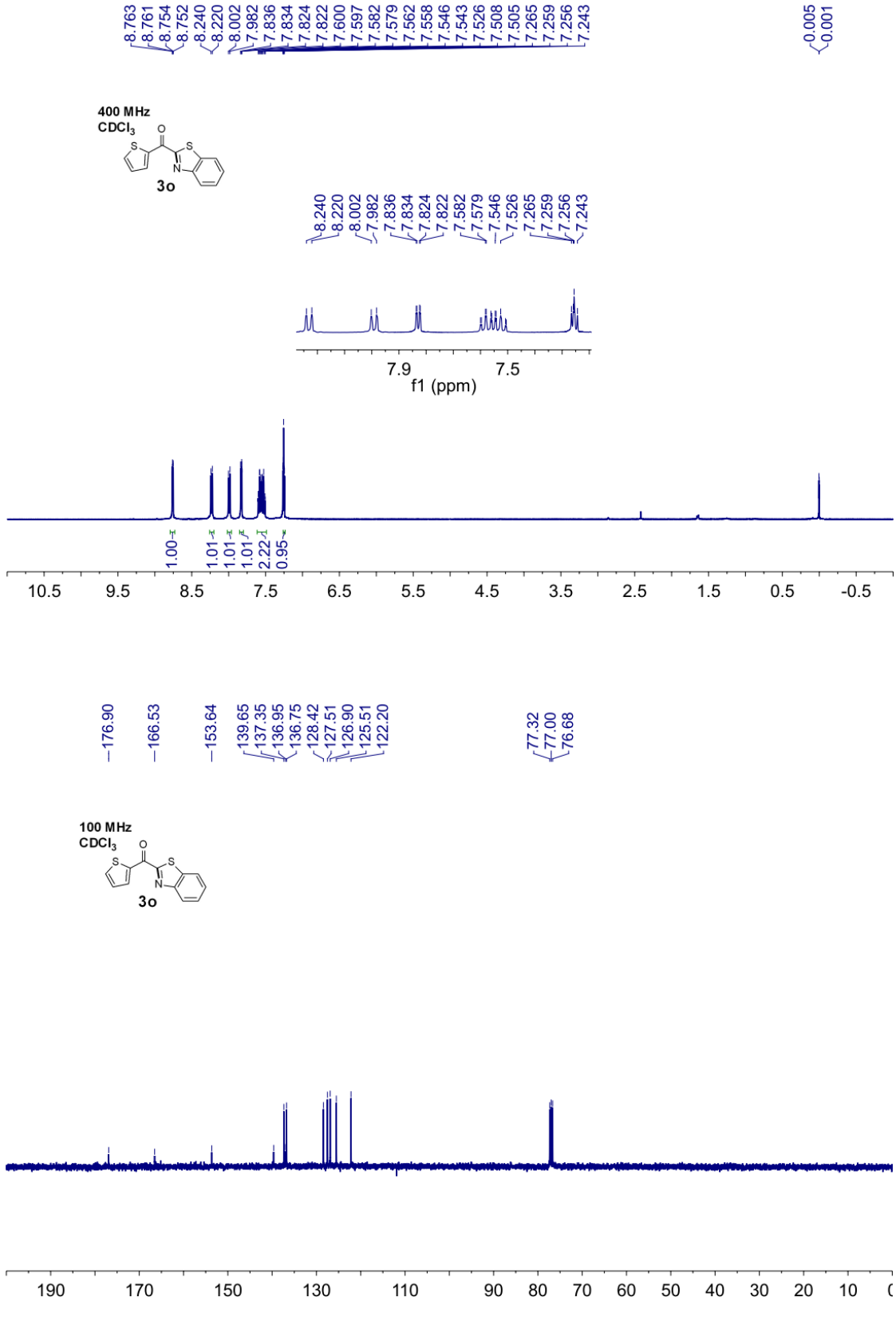
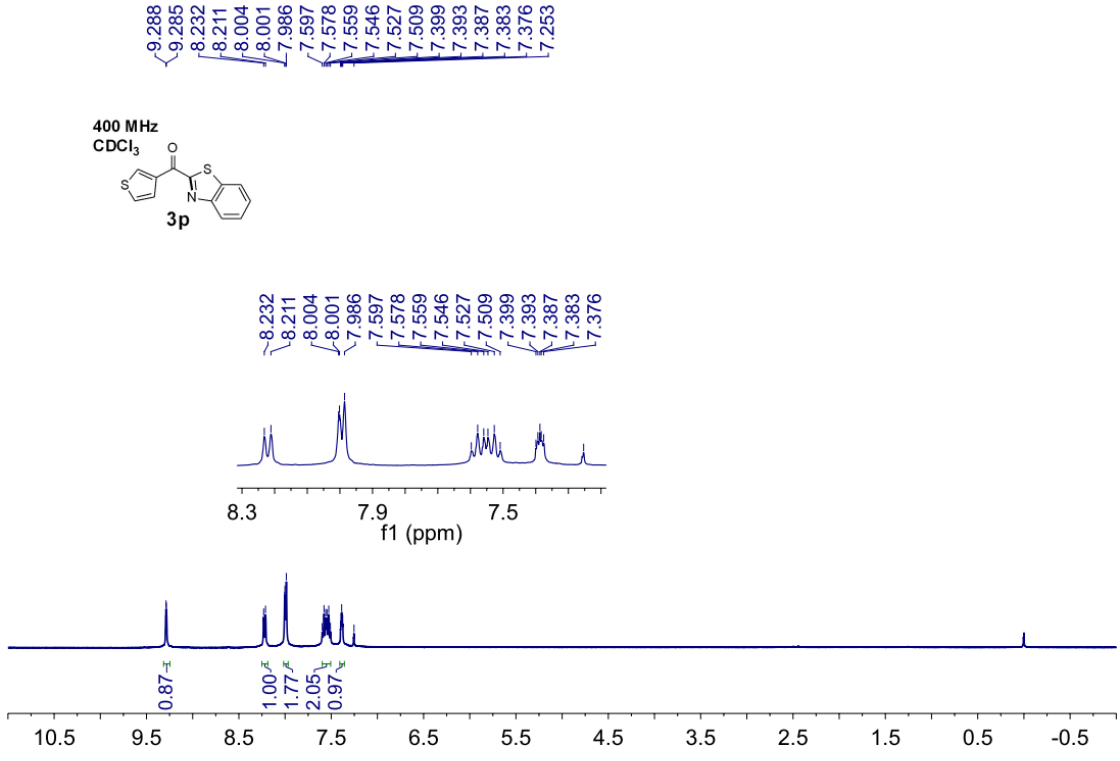
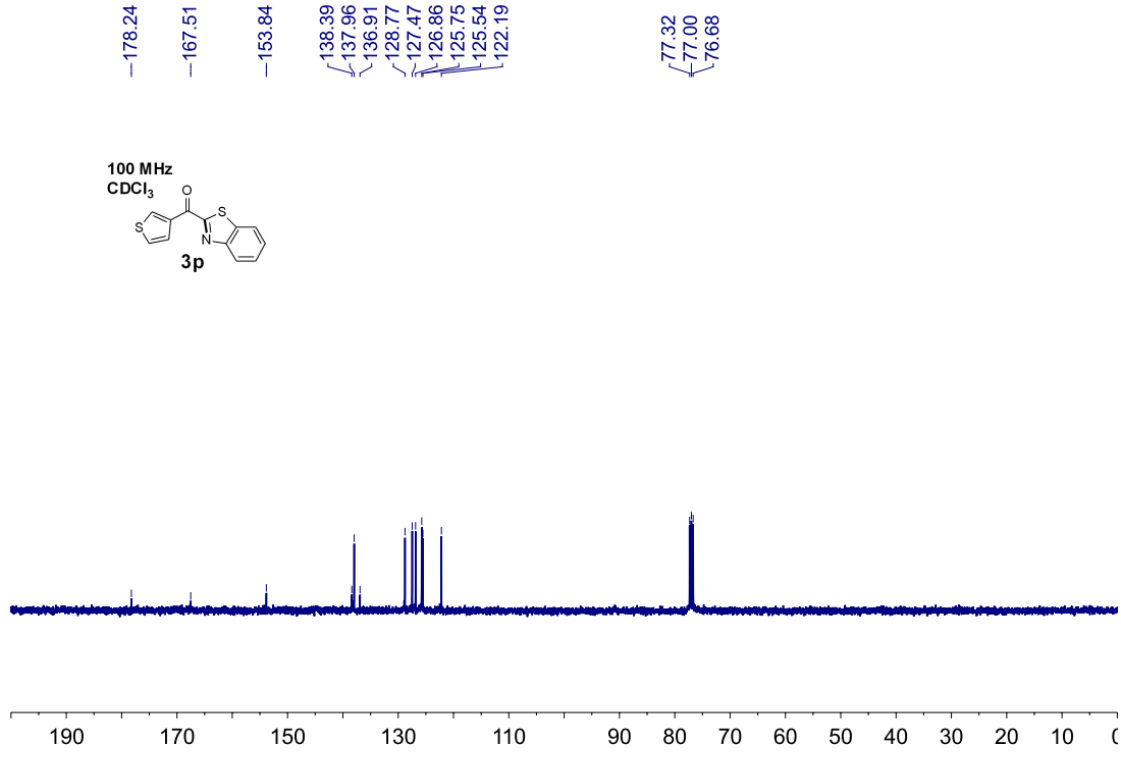
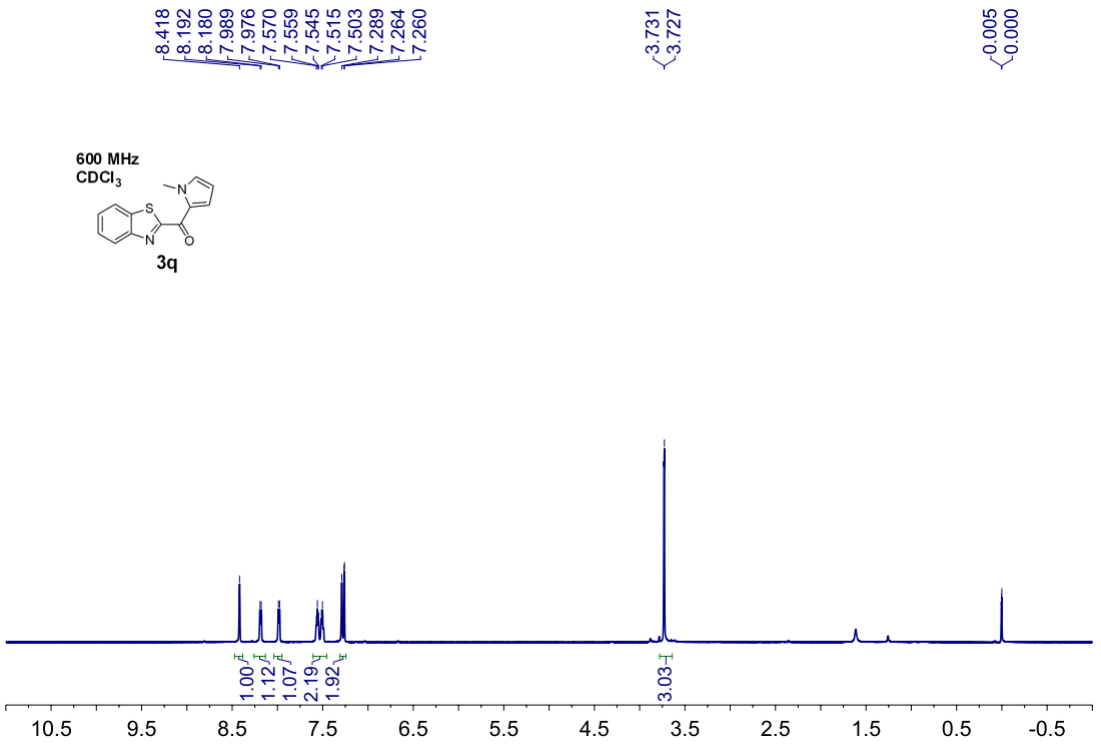
50
40
30
20
10

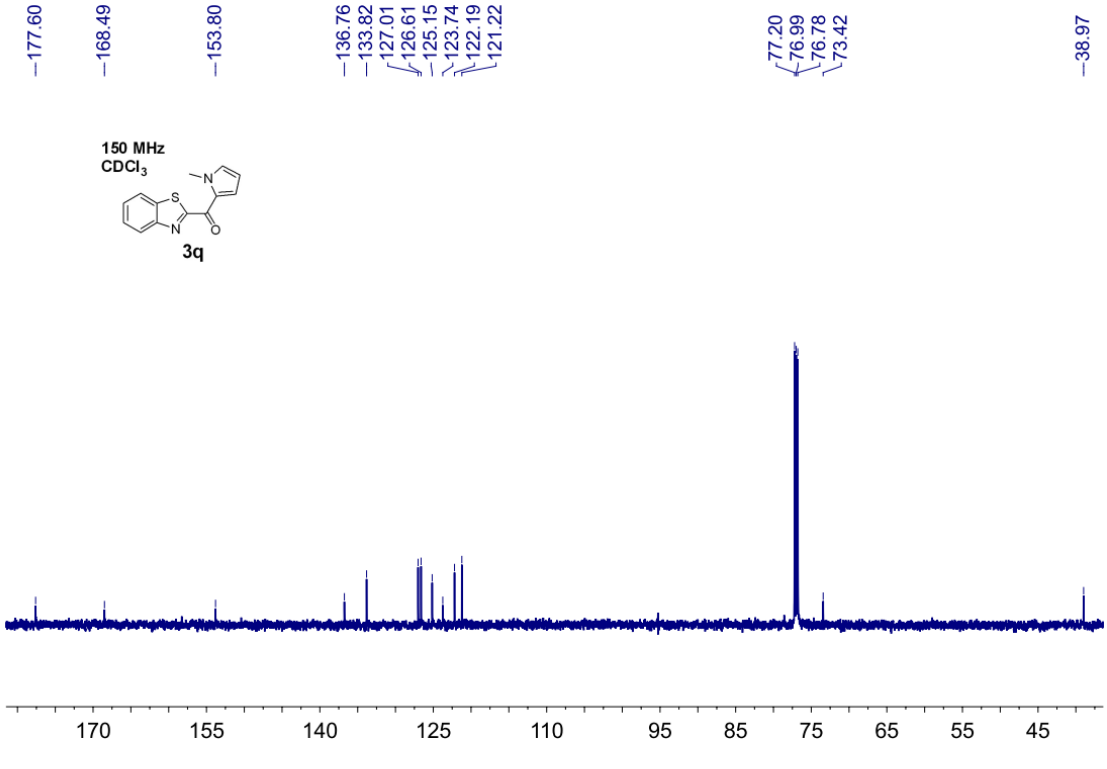

8.372
8.363
8.218
8.199
8.008
7.989
7.827
7.823
7.584
7.581
7.564
7.550
7.546
7.530
7.527
6.690
6.685
6.681
-0.000
400 MHz
CDCl3
3n
8.223
8.220
8.201
8.010
7.991
7.988
7.829
7.825
7.586
7.583
7.566
7.562
7.552
7.548
7.532
7.529
8.1
7.9
7.7
7.5
f1 (ppm)
1.00
1.01
1.00
1.06
2.34
1.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
172.01
165.97
153.72
149.76
148.85
136.76
127.49
126.93
125.45
124.95
122.19
112.87
77.32
77.00
76.68
100 MHz
CDCl3
3n
190
170
150
130
110
90
80
70
60
50
40
30
20
10

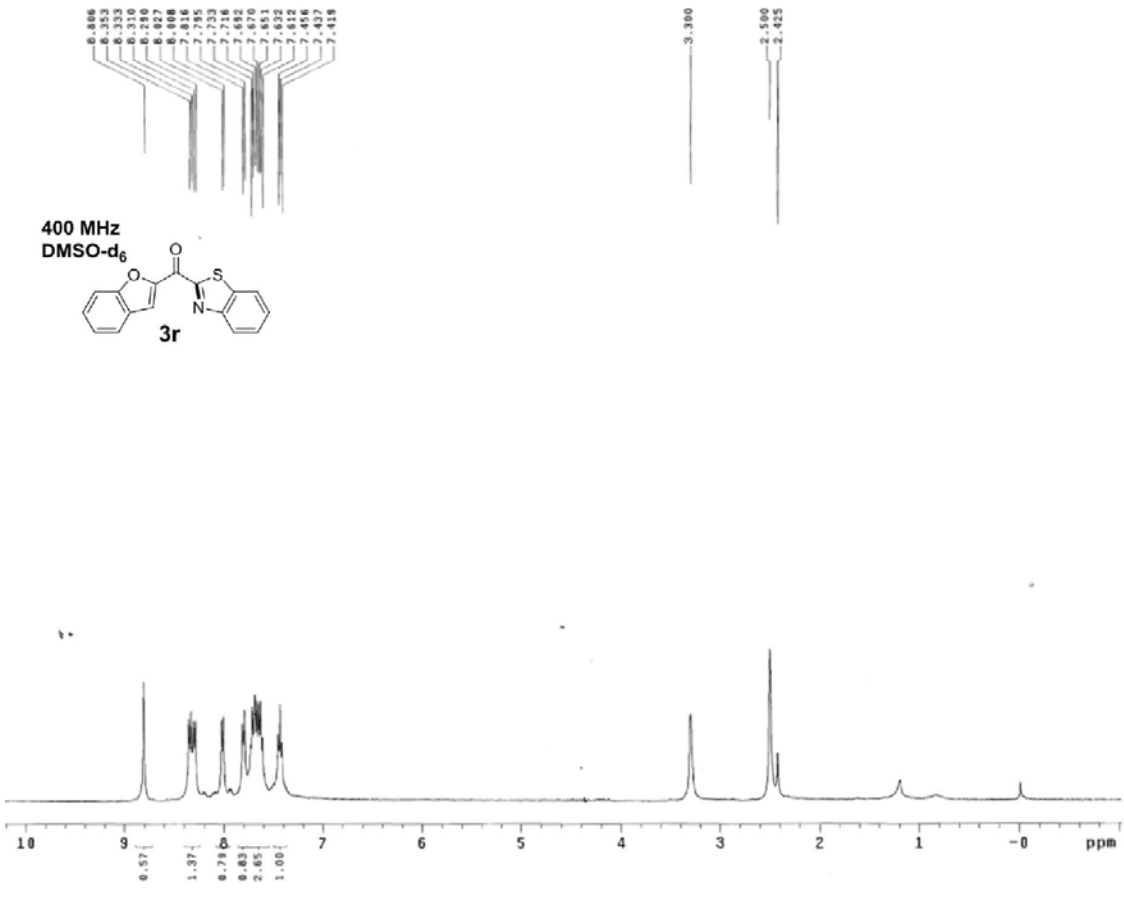

8.763
8.761
8.754
8.752
8.240
8.220
8.002
7.982
7.836
7.834
7.824
7.822
7.600
7.597
7.582
7.579
7.562
7.558
7.546
7.543
7.526
7.508
7.505
7.265
7.259
7.256
7.243
0.005
0.001
400 MHz
CDCl3
3o
7.9
7.5
f1 (ppm)
1.00
1.01
1.01
1.01
2.22
0.95
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
176.90
166.53
153.64
139.65
137.35
136.95
136.75
128.42
127.51
126.90
125.51
122.20
77.32
77.00
76.68
100 MHz
CDCl3
3o
190
170
150
130
110
90
80
70
60
50
40
30
20
10

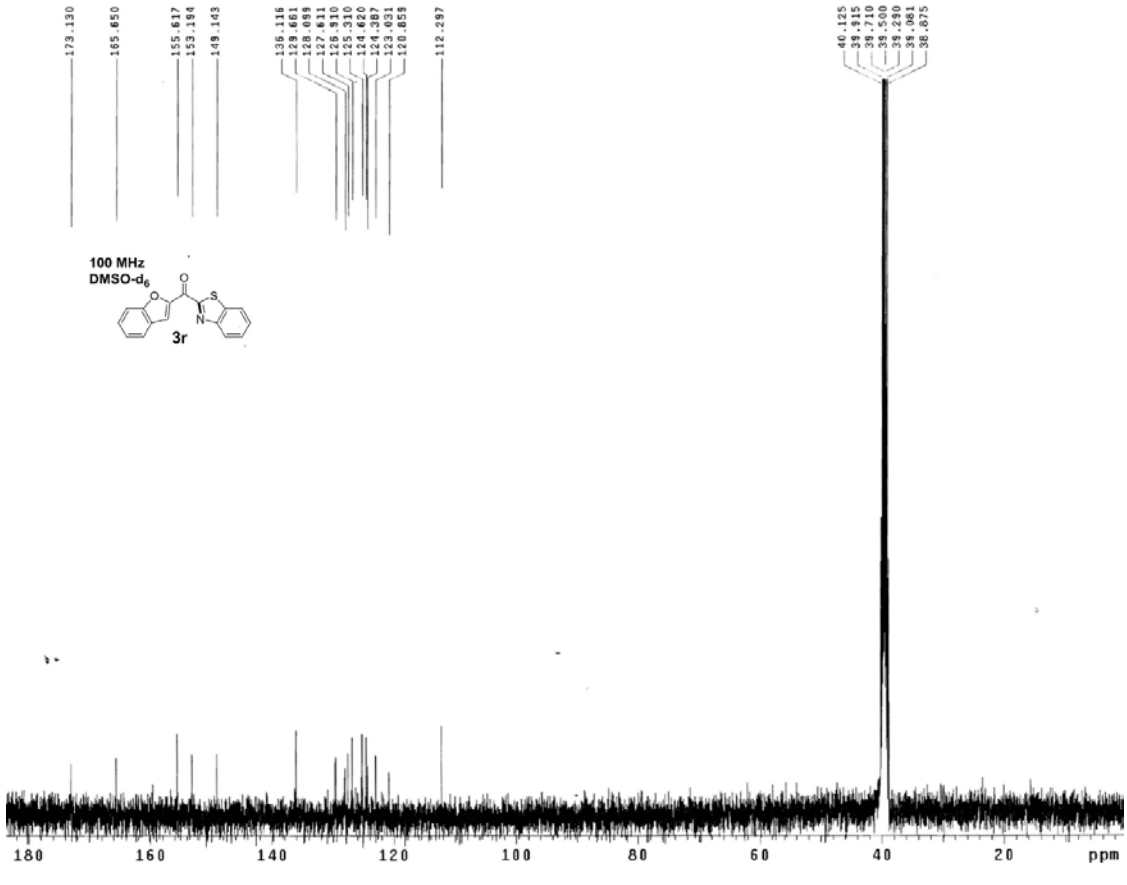

9.288
9.285
8.232
8.211
8.004
8.001
7.986
7.597
7.578
7.559
7.546
7.527
7.509
7.399
7.393
7.387
7.383
7.376
7.253
400 MHz
CDCl3
3p
8.232
8.211
8.004
8.001
7.986
7.597
7.578
7.559
7.546
7.527
7.509
7.399
7.393
7.387
7.383
7.376
8.3
7.9
7.5
f1 (ppm)
0.87
1.00
1.77
2.05
0.97
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

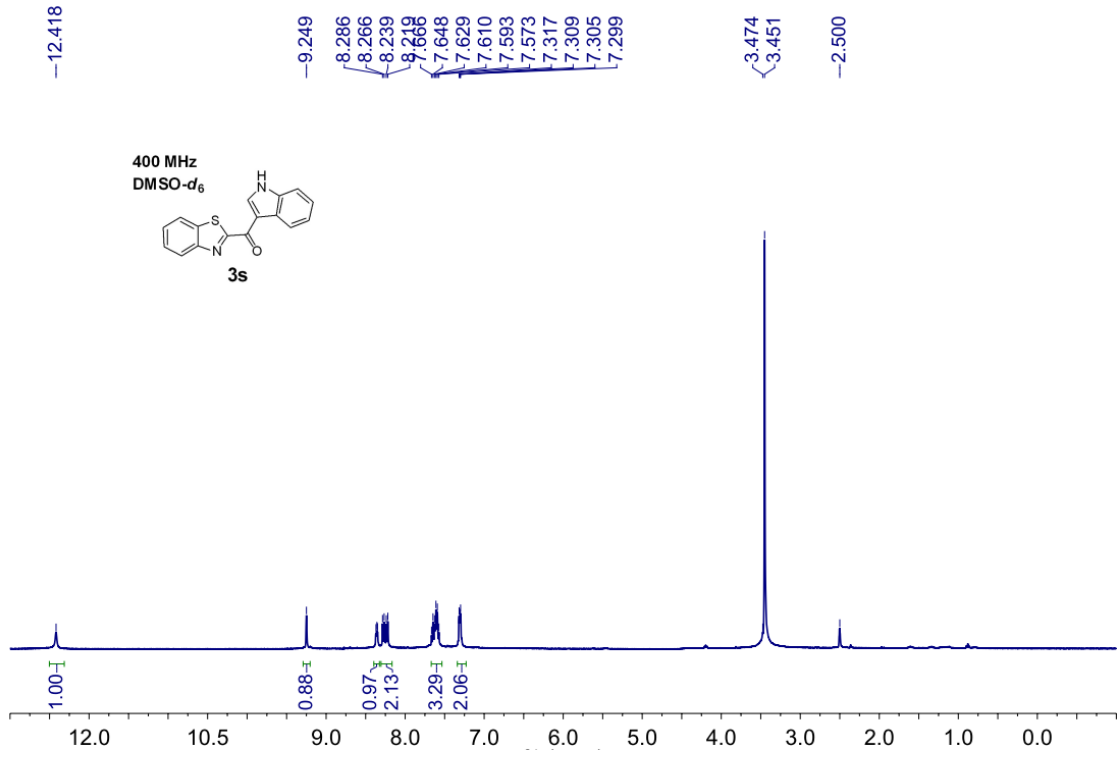

178.24
167.51
153.84
138.39
137.96
136.91
128.77
127.47
126.86
125.75
125.54
122.19
77.32
77.00
76.68
100 MHz
CDCl3
3p
190
170
150
130
110
90
80
70
60
50
40
30
20
10

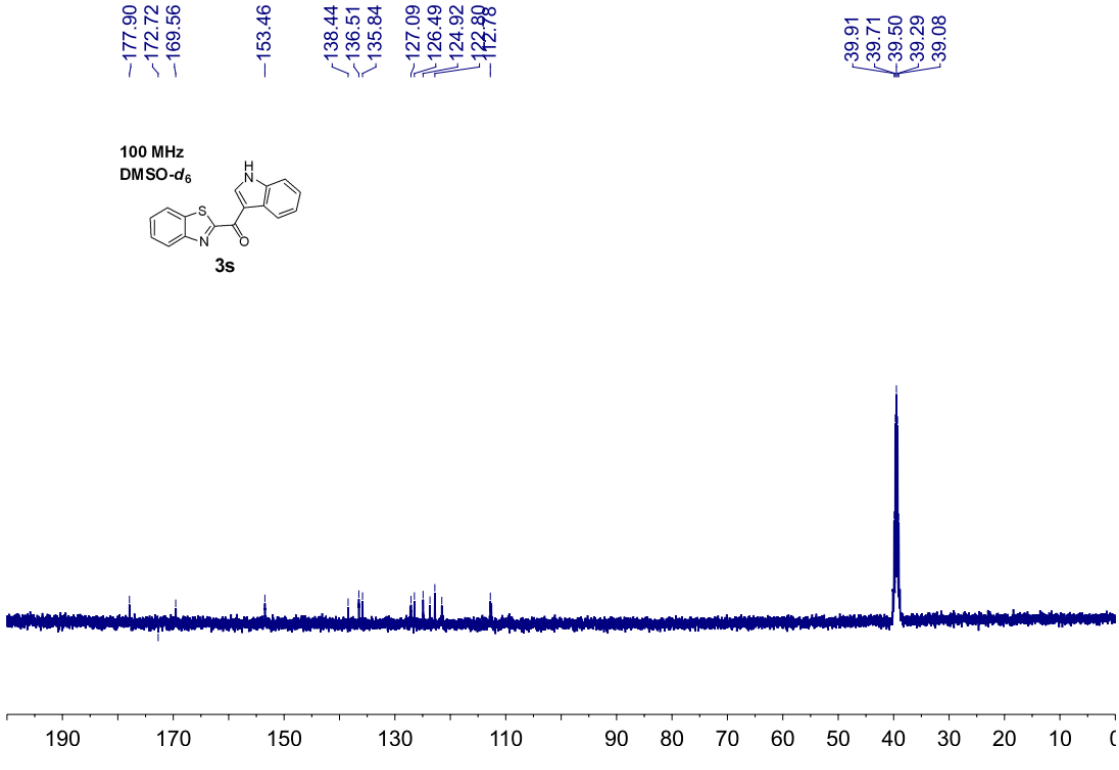

8.418
8.192
8.180
7.989
7.976
7.570
7.559
7.545
7.515
7.503
7.289
7.264
7.260
3.731
3.727
0.005
0.000
600 MHz
CDCl3
3q
1.00
1.12
1.07
2.19
1.92
3.03
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

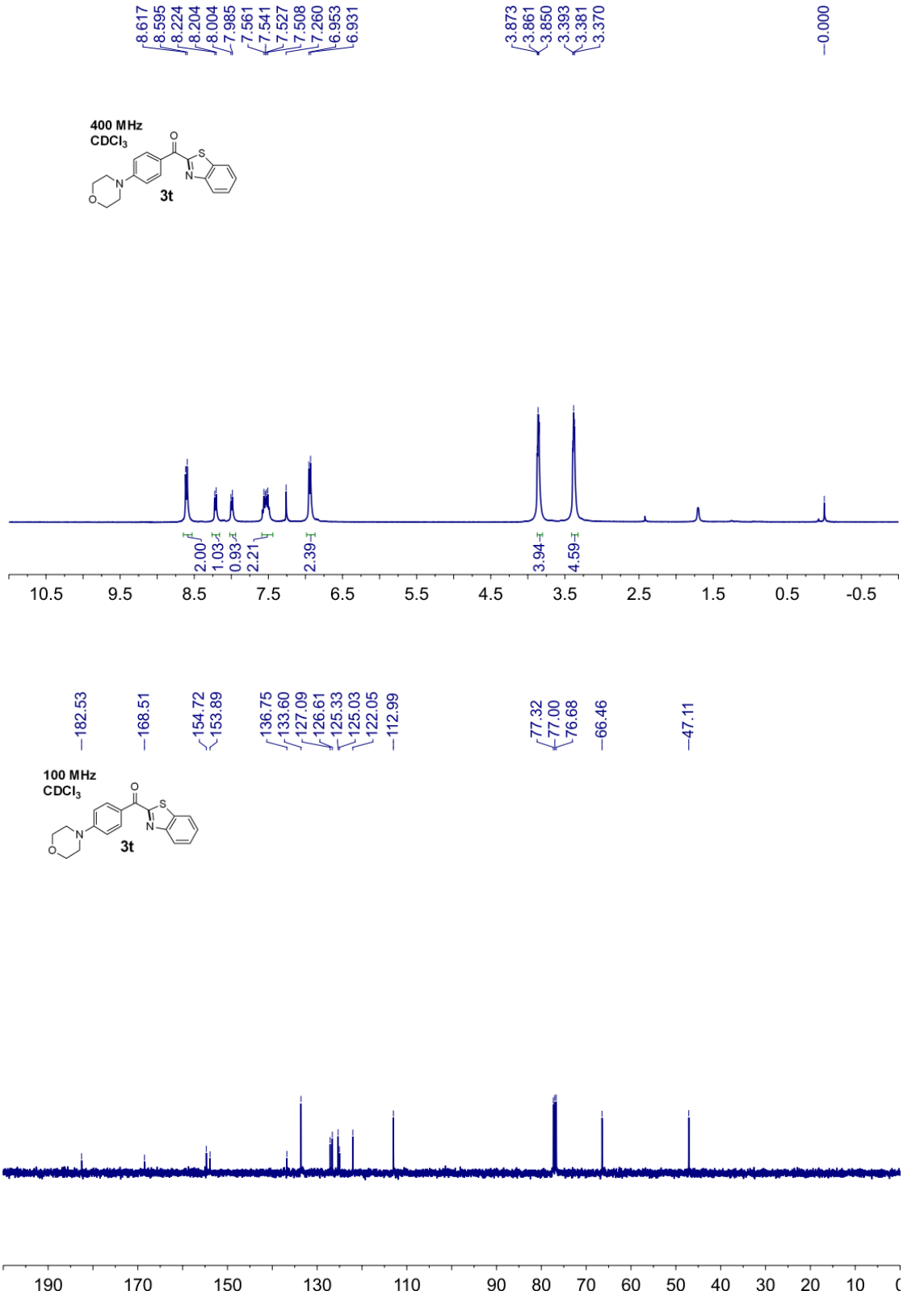

177.60
168.49
153.80
136.76
133.82
127.01
126.61
125.15
123.74
122.19
121.22
77.20
76.99
76.78
73.42
38.97
150 MHz
CDCl3
3q
170
155
140
125
110
95
85
75
65
55
45

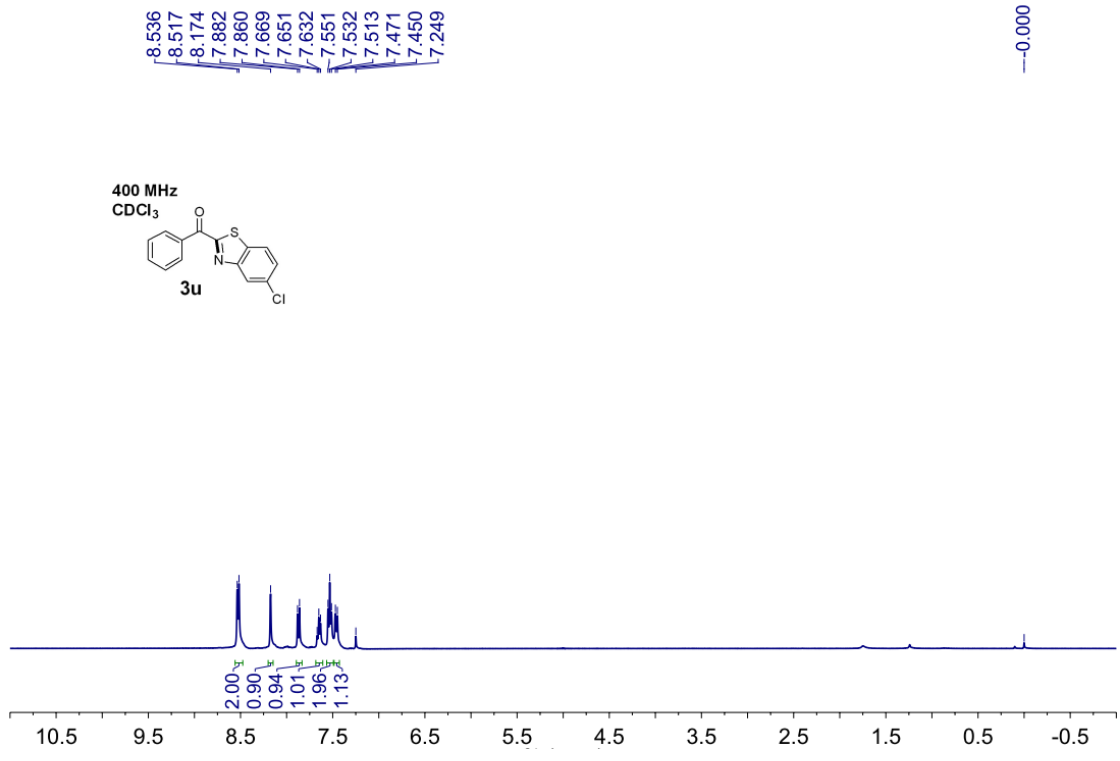

400 MHz
DMSO-d6
3r
ppm

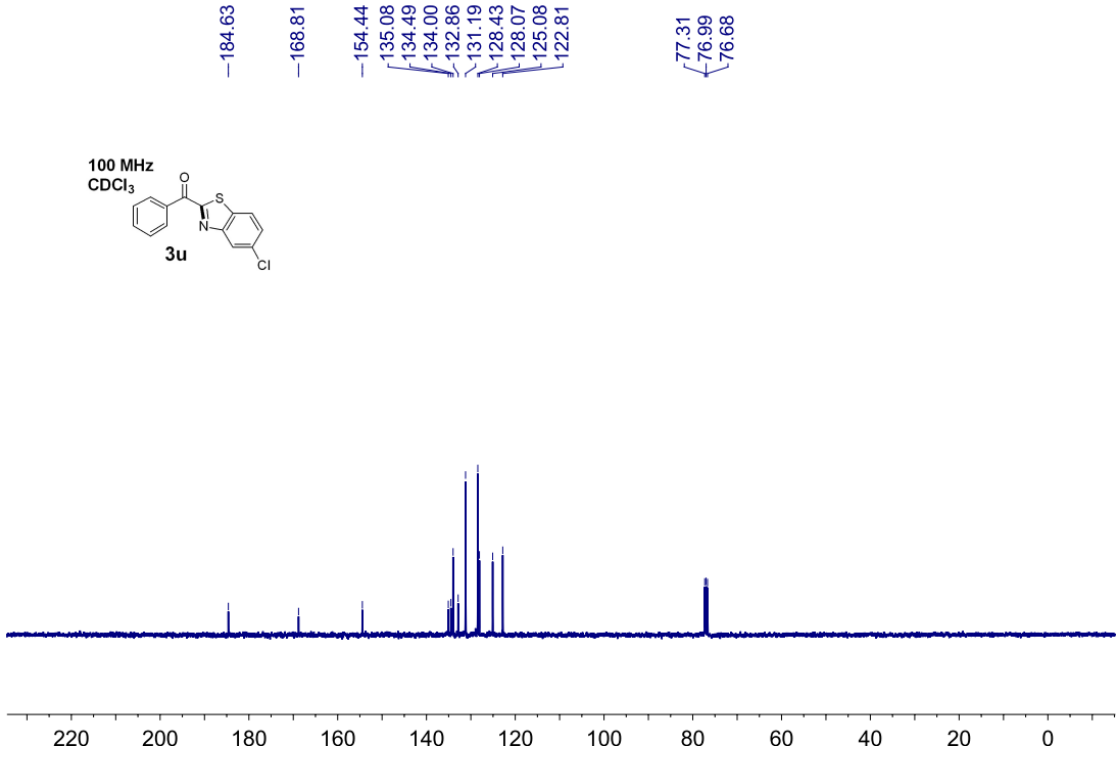

100 MHz
DMSO-d6
3r
ppm

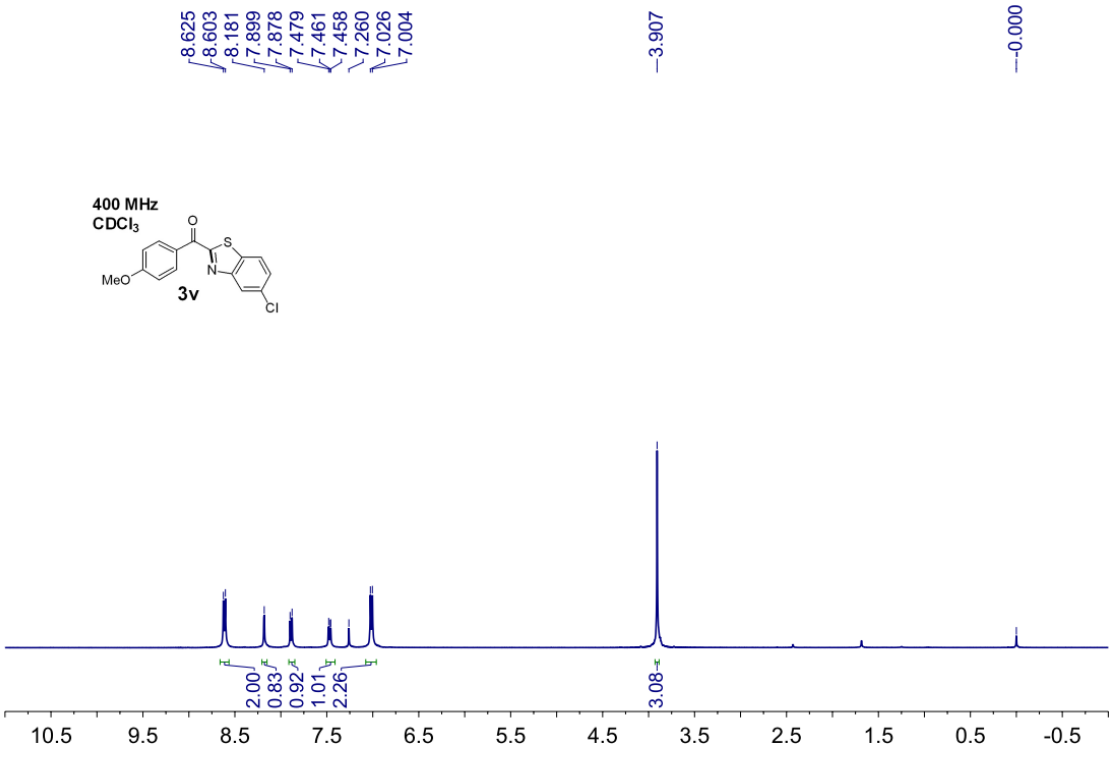

12.418
9.249
8.286
8.266
8.239
7.666
7.648
7.629
7.610
7.593
7.573
7.317
7.309
7.305
7.299
3.474
3.451
2.500
400 MHz
DMSO-d_6
3s
1.00
0.88
0.97
2.13
3.29
2.06
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

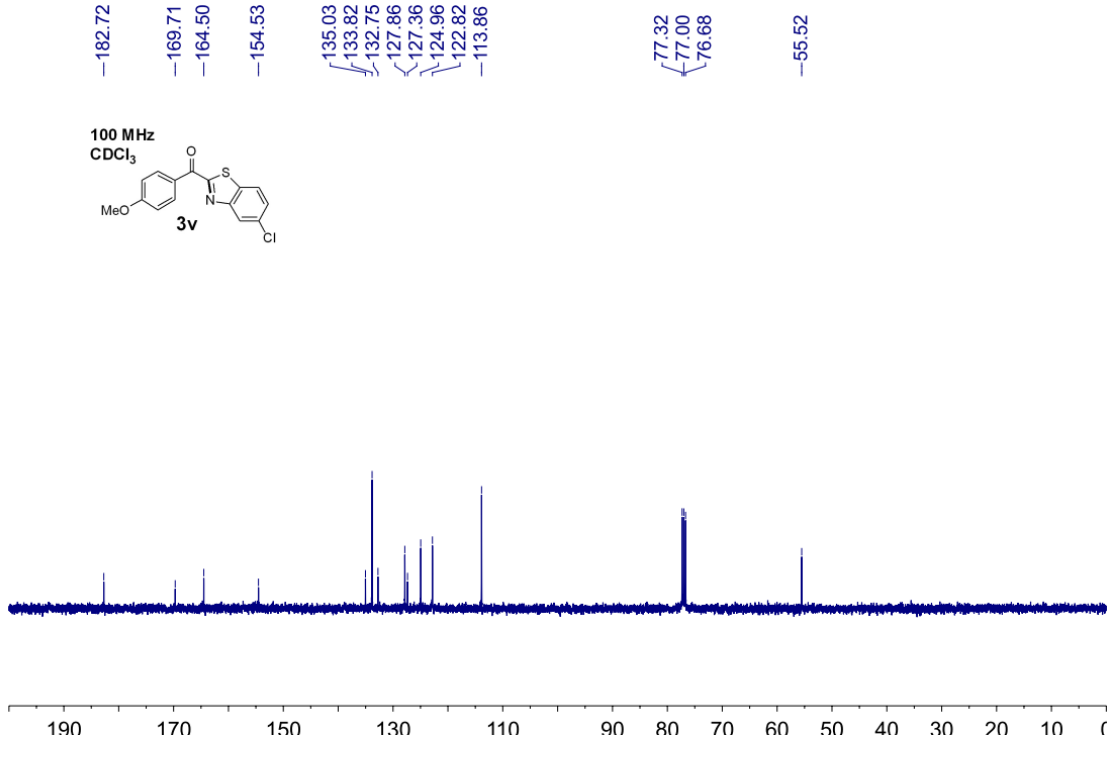

177.90
172.72
169.56
153.46
138.44
136.51
135.84
127.09
126.49
124.92
122.80
112.78
39.91
39.71
39.50
39.29
39.08
100 MHz
DMSO-d_6
3s
190
170
150
130
110
90
80
70
60
50
40
30
20
10

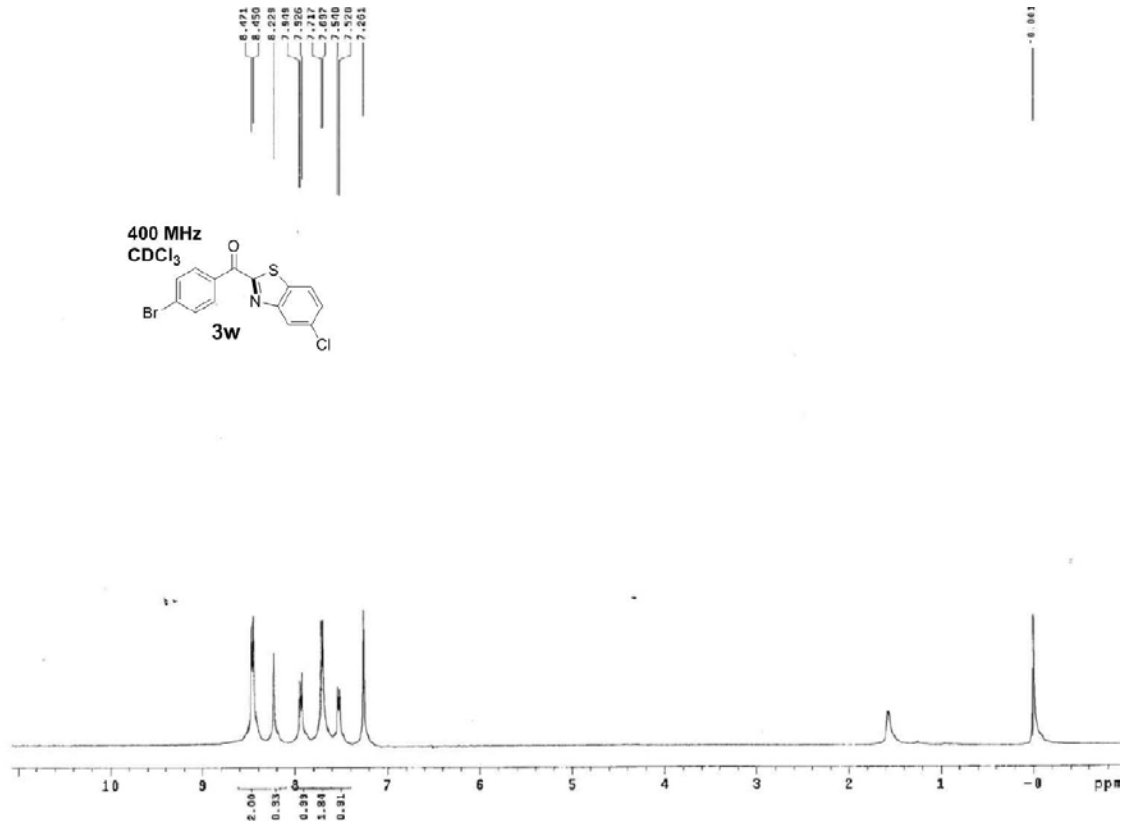

8.617
8.595
8.224
8.204
8.004
7.985
7.561
7.541
7.527
7.508
7.260
6.953
6.931
3.873
3.861
3.850
3.393
3.381
3.370
0.000
400 MHz
CDCl3
3t
2.00
1.03
0.93
2.21
2.39
3.94
4.59
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
182.53
168.51
154.72
153.89
136.75
133.60
127.09
126.61
125.33
125.03
122.05
112.99
77.32
77.00
76.68
66.46
47.11
100 MHz
CDCl3
3t
190
170
150
130
110
90
80
70
60
50
40
30
20
10

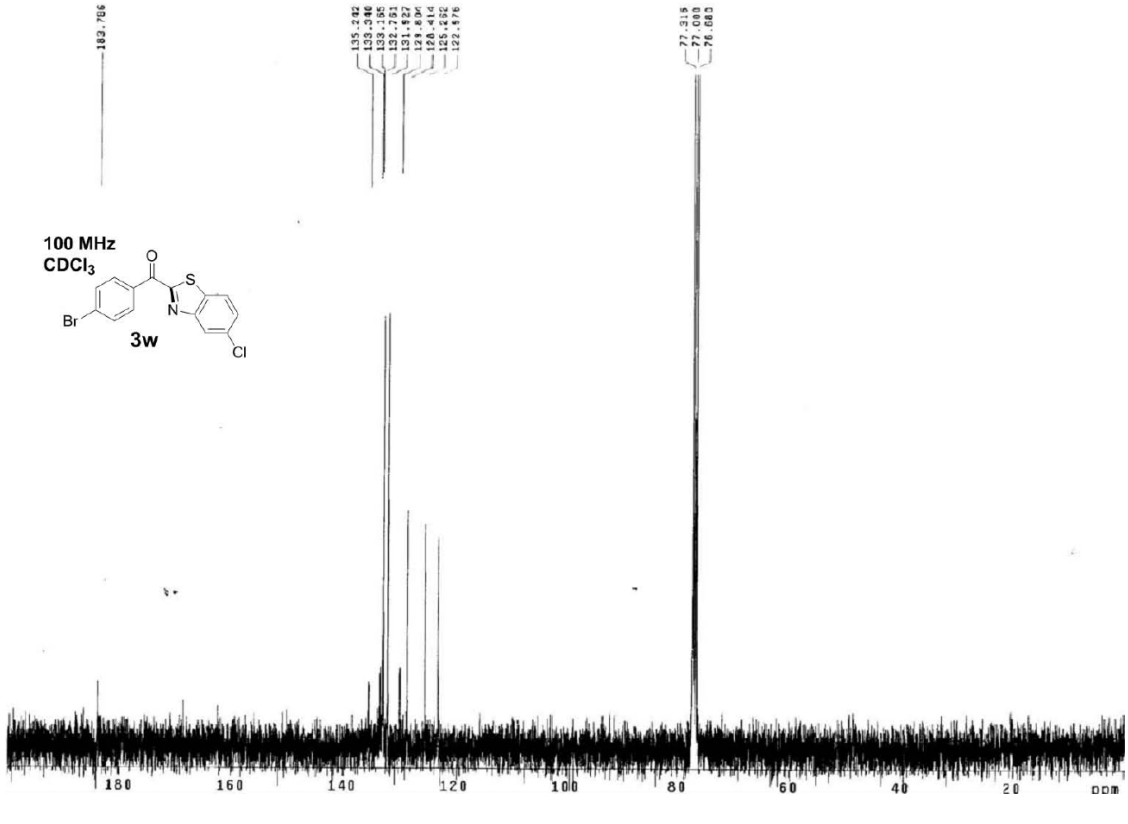

8.536
8.517
8.174
7.882
7.860
7.669
7.651
7.632
7.551
7.532
7.513
7.471
7.450
7.249
0.000
400 MHz
CDCl3
3u
2.00
0.90
0.94
1.01
1.96
1.13
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


184.63
168.81
154.44
135.08
134.49
134.00
132.86
131.19
128.43
128.07
125.08
122.81
77.31
76.99
76.68
100 MHz
CDCl3
3u
220
200
180
160
140
120
100
80
60
40
20
0


8.625
8.603
8.181
7.899
7.878
7.479
7.461
7.458
7.260
7.026
7.004
3.907
0.000
400 MHz
CDCl3
MeO
3v
Cl
2.00
0.83
0.92
1.01
2.26
3.08
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

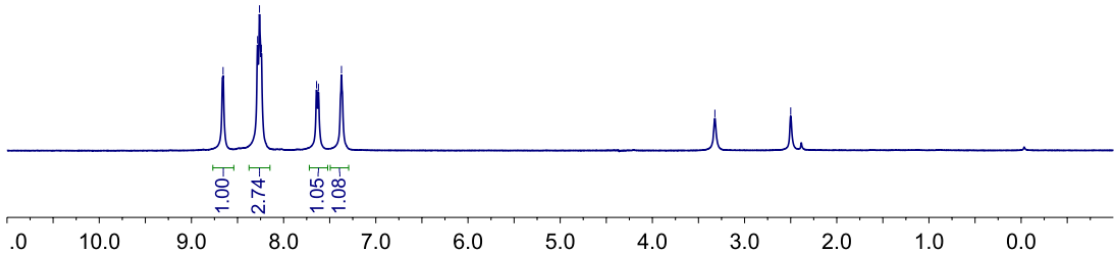

182.72
169.71
164.50
154.53
135.03
133.82
132.75
127.86
127.36
124.96
122.82
113.86
77.32
77.00
76.68
55.52
100 MHz
CDCl3
MeO
3v
Cl
190
170
150
130
110
90
80
70
60
50
40
30
20
10


400 MHz
CDCl3
3w
Br
Cl
ppm

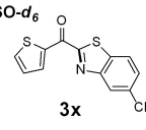

100 MHz
CDCl3
3w
Br
Cl
ppm

400 MHz
DMSO-d_6

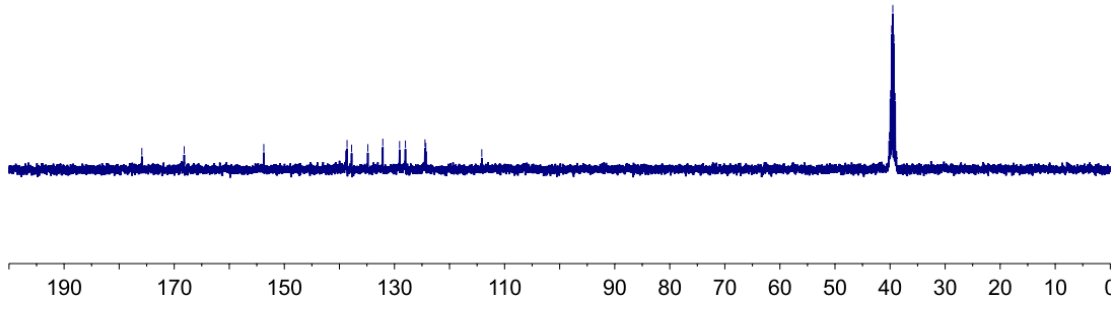
3x

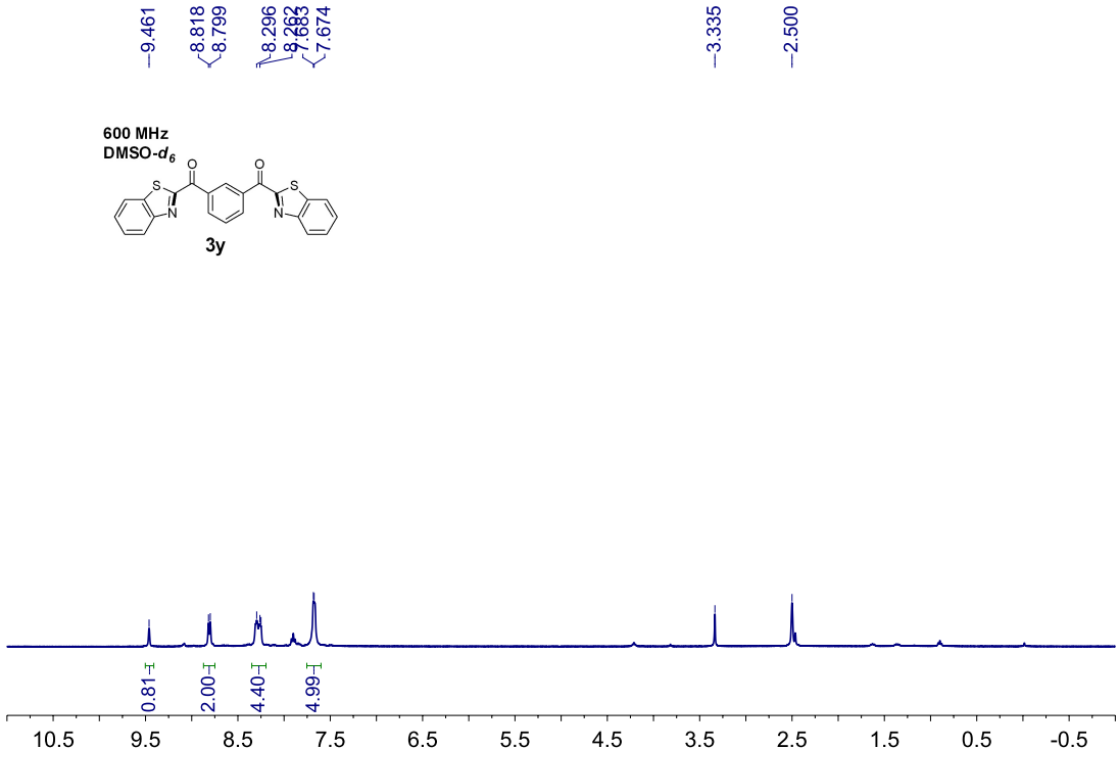


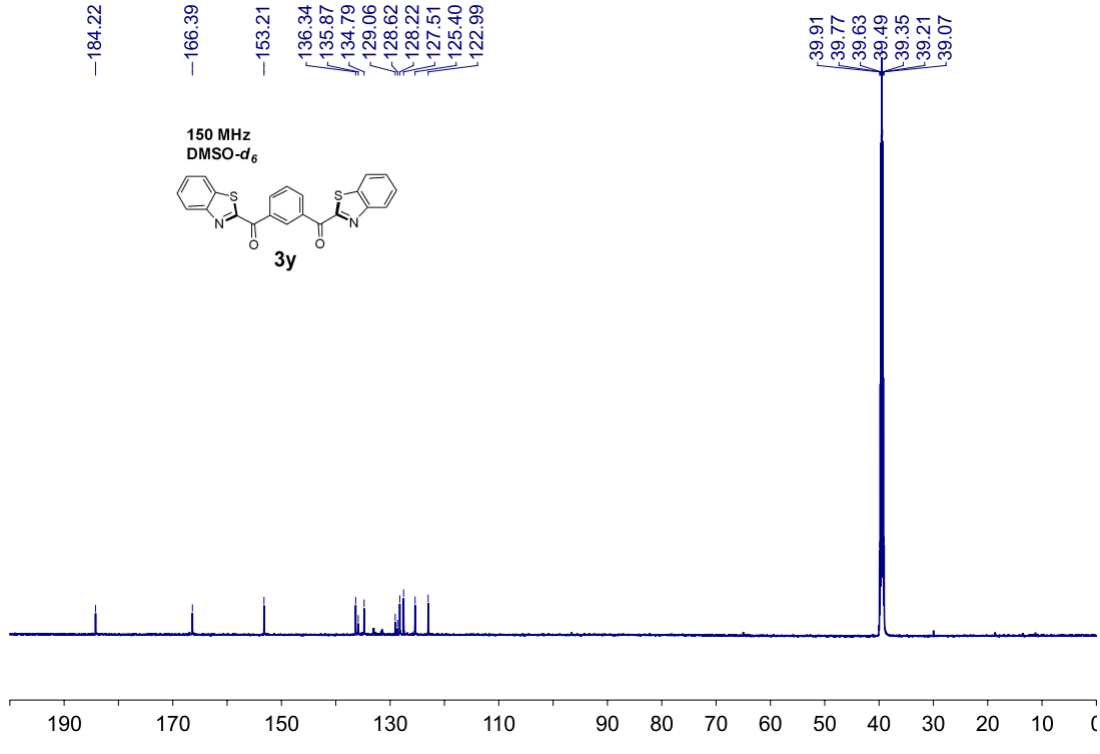
100 MHz
DMSO-d_6

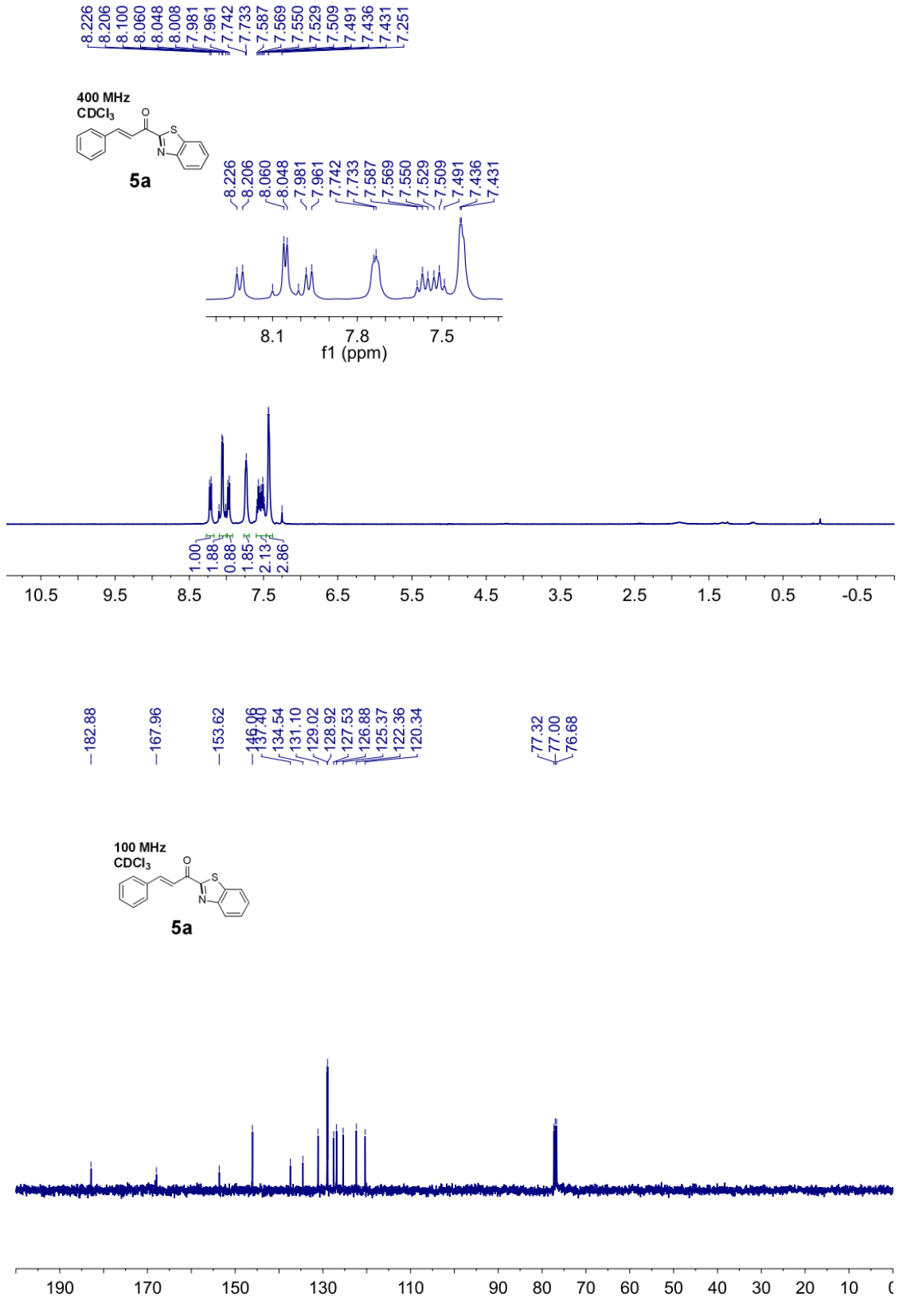


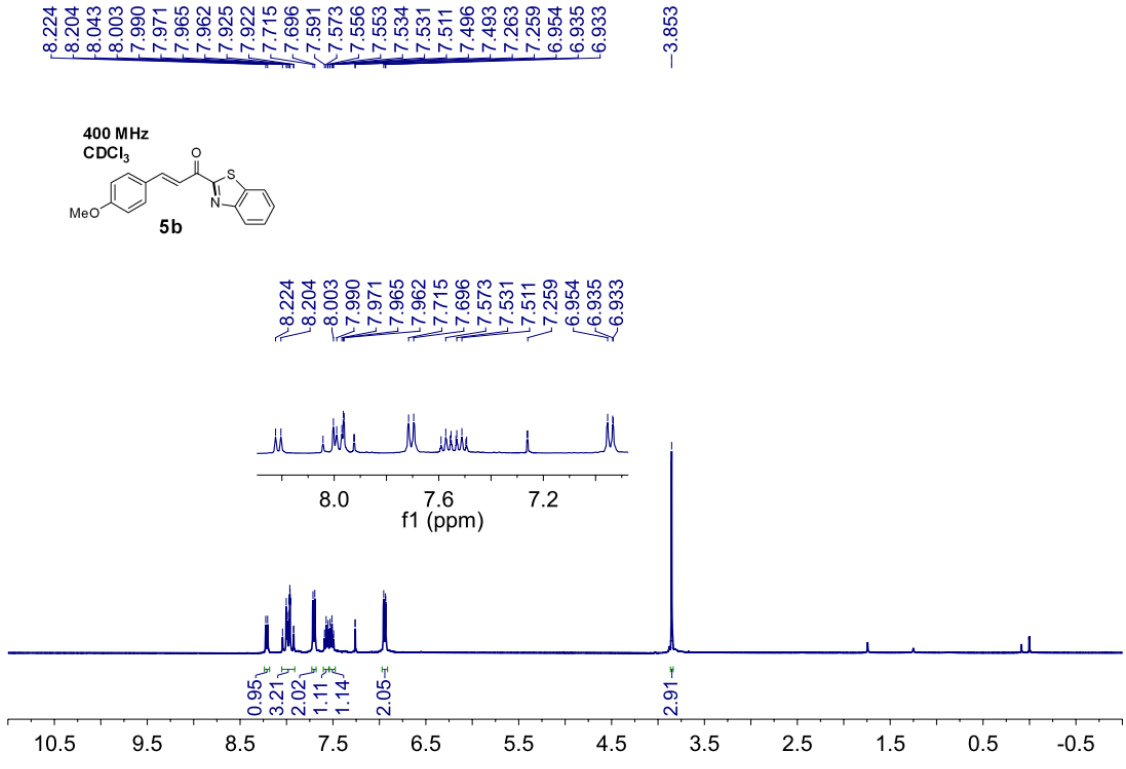
3x

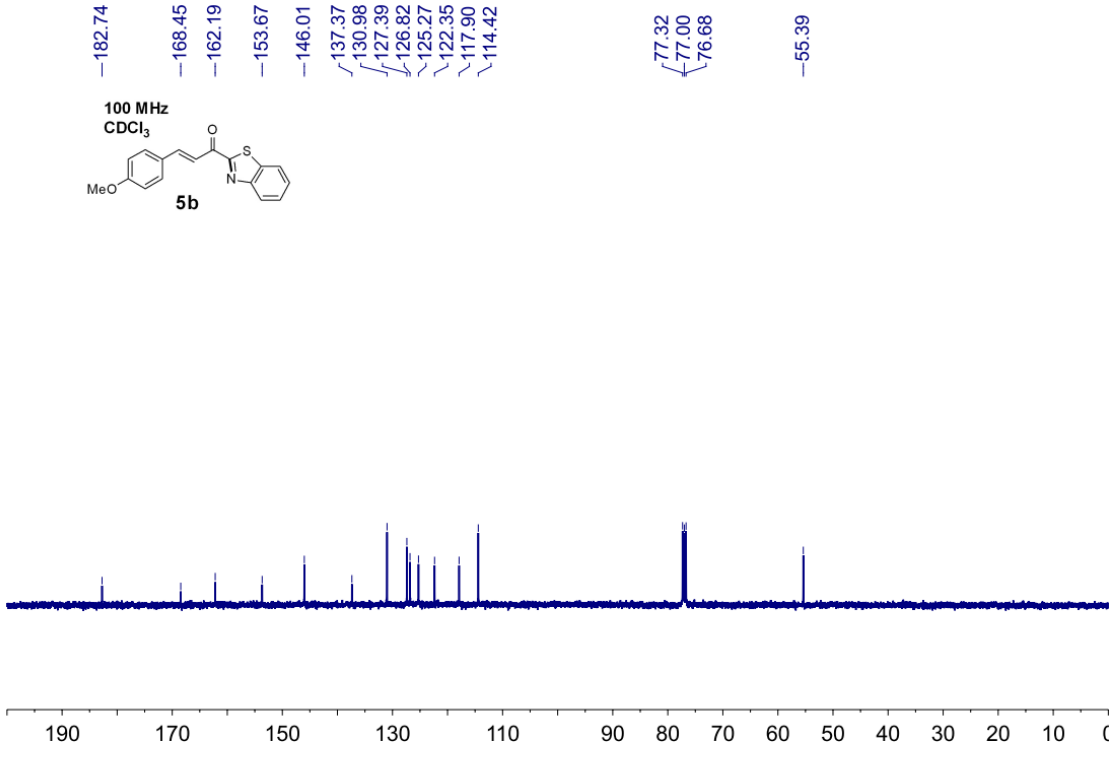


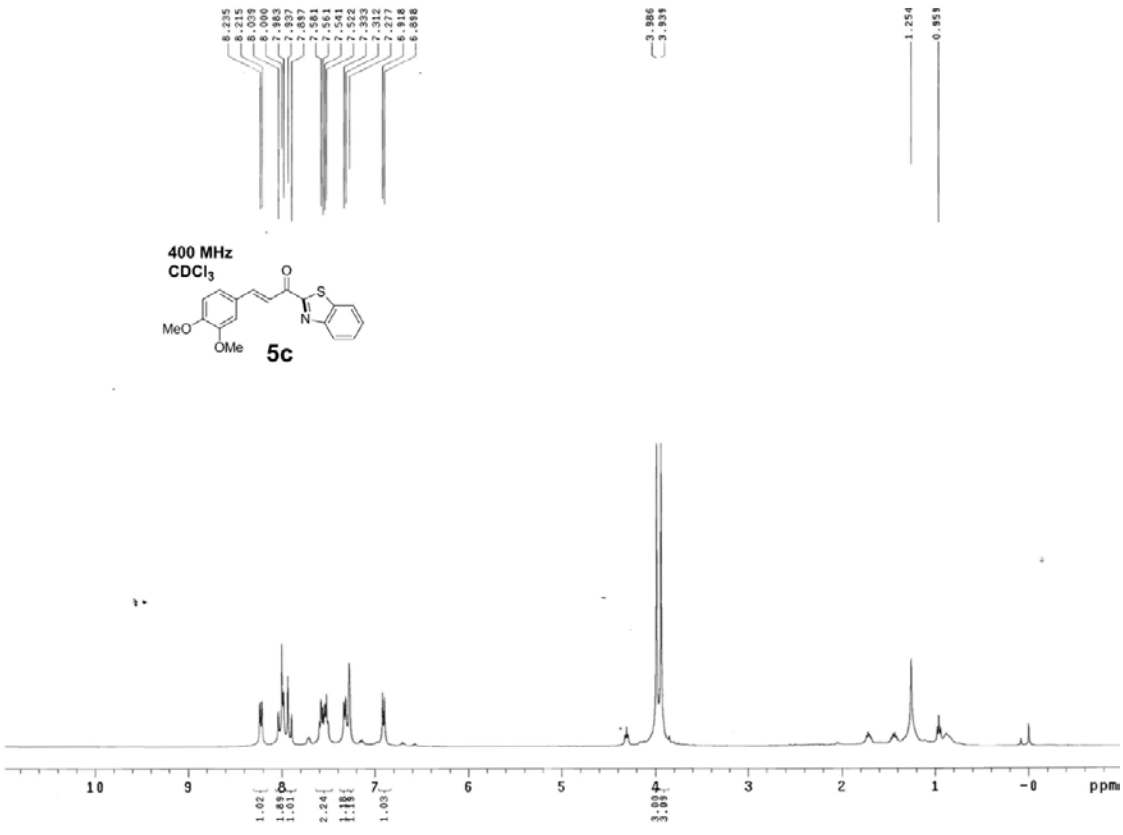

9.461
8.818
8.799
8.296
8.262
7.683
7.674
3.335
2.500
600 MHz
DMSO-d_6
3y
0.81
2.00
4.40
4.99
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

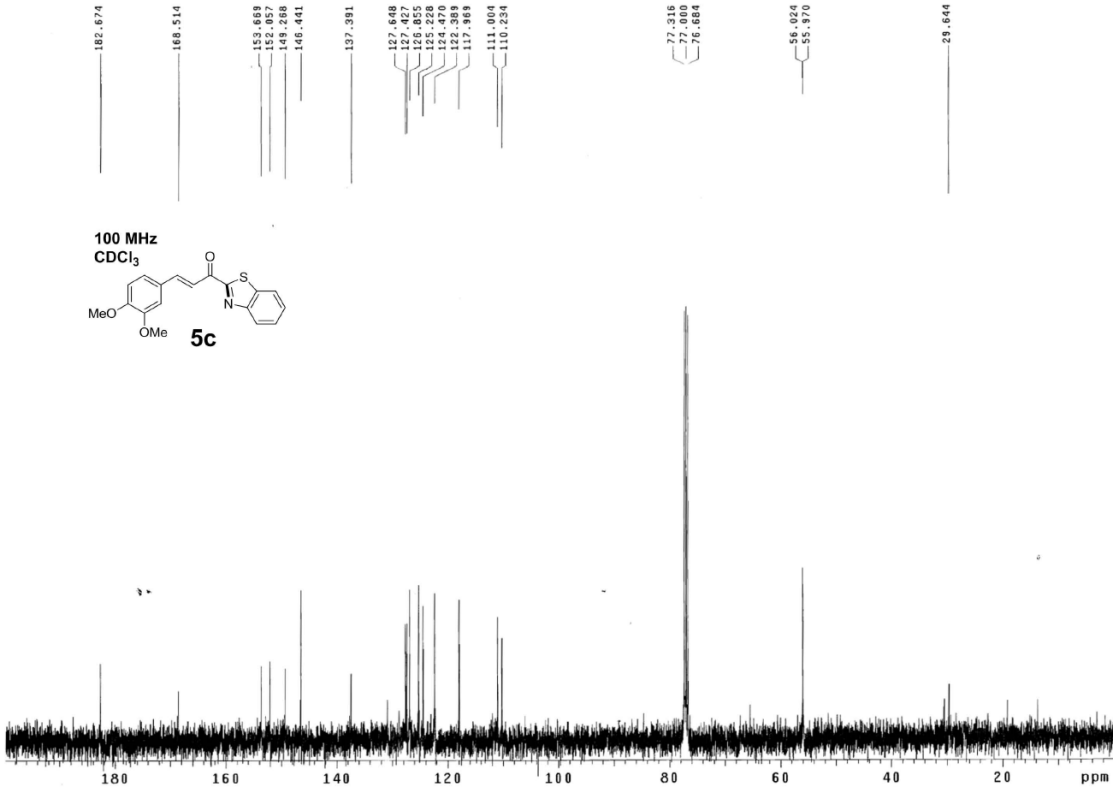

184.22
166.39
153.21
136.34
135.87
134.79
129.06
128.62
128.22
127.51
125.40
122.99
39.91
39.77
39.63
39.49
39.35
39.21
39.07
150 MHz
DMSO-d_6
3y
190
170
150
130
110
90
80
70
60
50
40
30
20
10

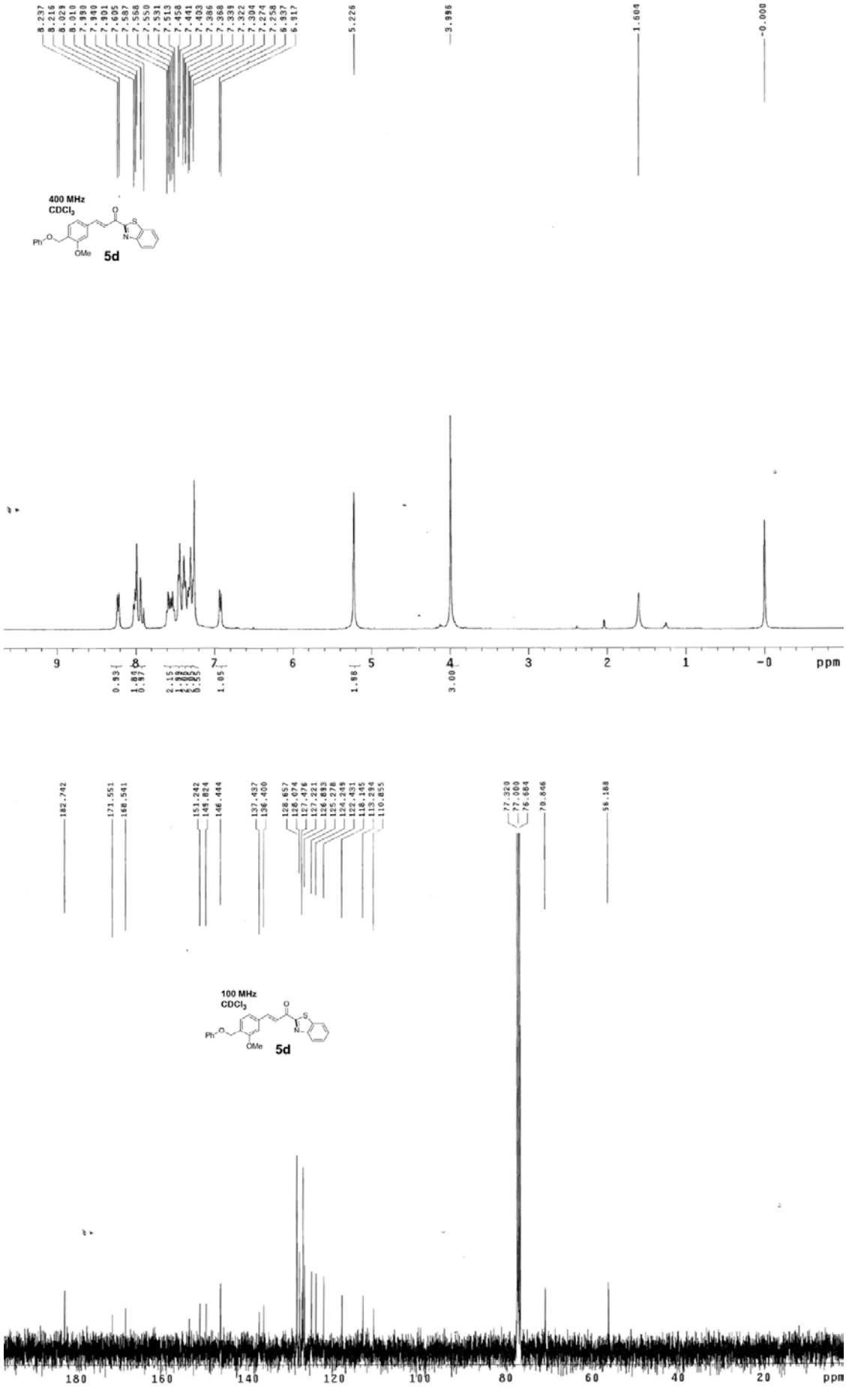

8.226
8.206
8.100
8.060
8.048
8.008
7.981
7.961
7.742
7.733
7.587
7.569
7.550
7.529
7.509
7.491
7.436
7.431
7.251
400 MHz
CDCl3
5a
f1 (ppm)
1.00
1.88
0.88
1.85
2.13
2.86
182.88
167.96
153.62
146.06
137.40
134.54
131.10
129.02
128.92
127.53
126.88
125.37
122.36
120.34
77.32
77.00
76.68
100 MHz
CDCl3
5a

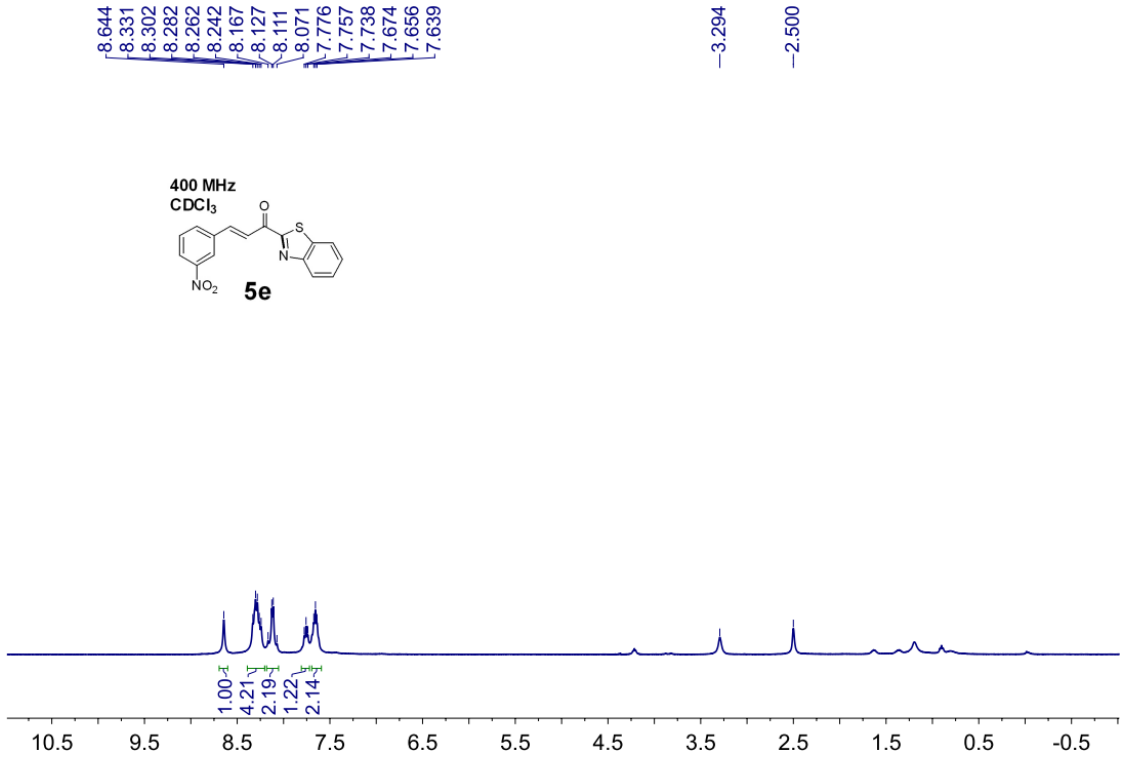

8.224
8.204
8.043
8.003
7.990
7.971
7.965
7.962
7.925
7.922
7.715
7.696
7.591
7.573
7.556
7.553
7.534
7.531
7.511
7.496
7.493
7.263
7.259
6.954
6.935
6.933
3.853
400 MHz
CDCl3
MeO
5b
8.0
7.6
7.2
f1 (ppm)
0.95
3.21
2.02
1.11
1.14
2.05
2.91
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

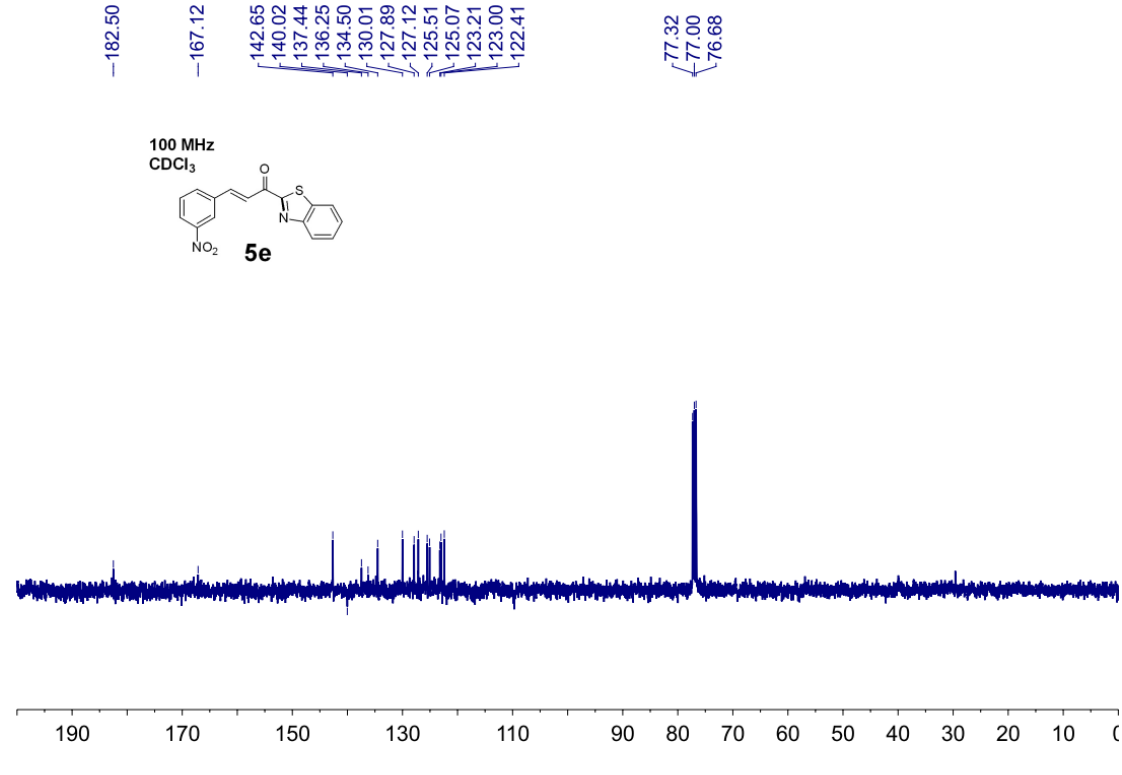

182.74
168.45
162.19
153.67
146.01
137.37
130.98
127.39
126.82
125.27
122.35
117.90
114.42
77.32
77.00
76.68
55.39
100 MHz
CDCl3
MeO
5b
190
170
150
130
110
90
80
70
60
50
40
30
20
10

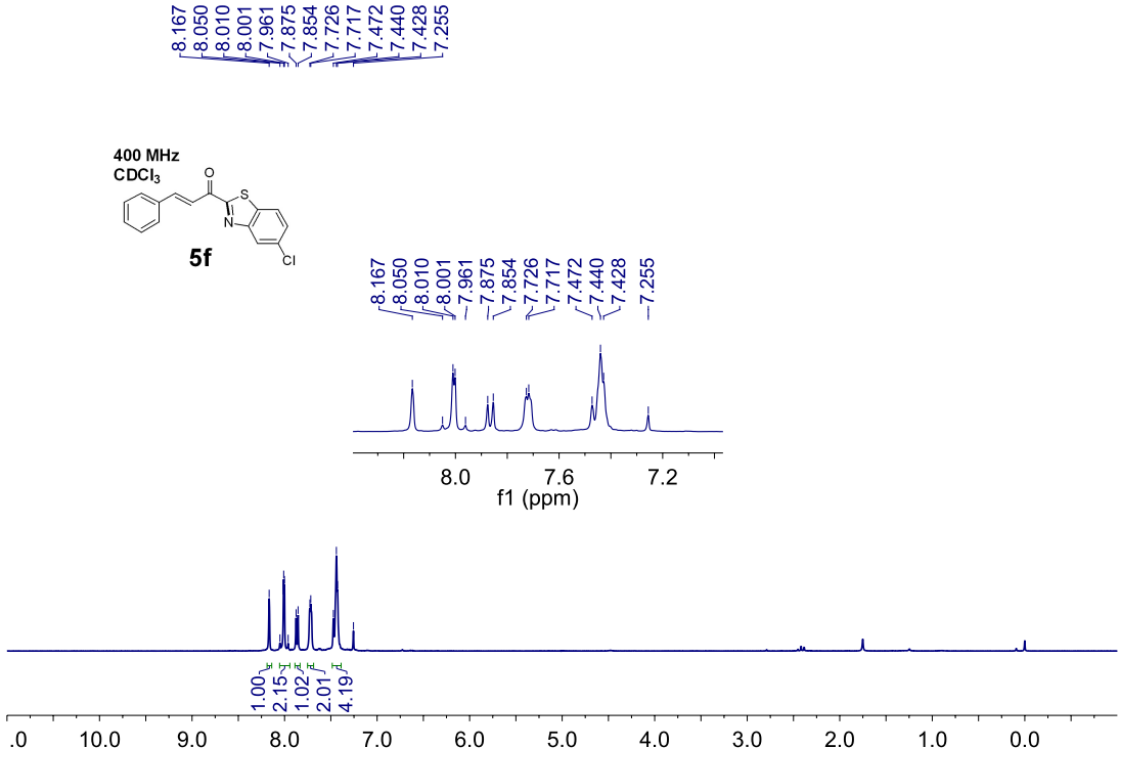

400 MHz
CDCl3
MeO
OMe
5c
ppm

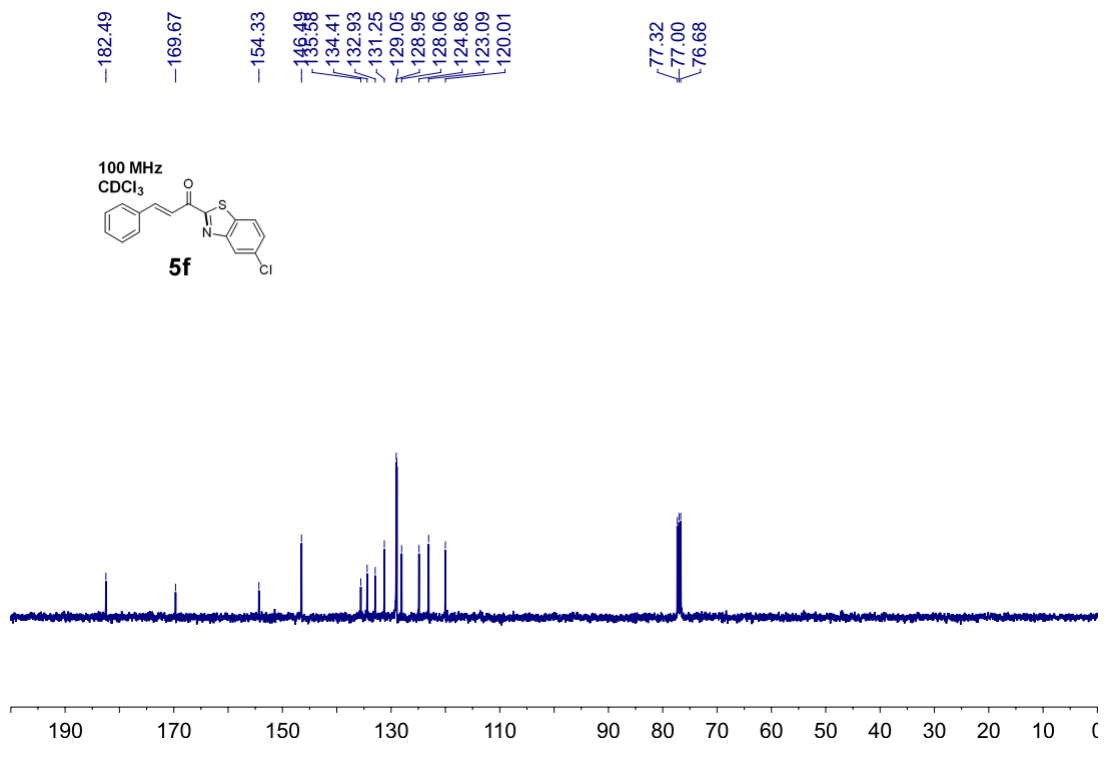

100 MHz
CDCl3
MeO
OMe
5c
ppm

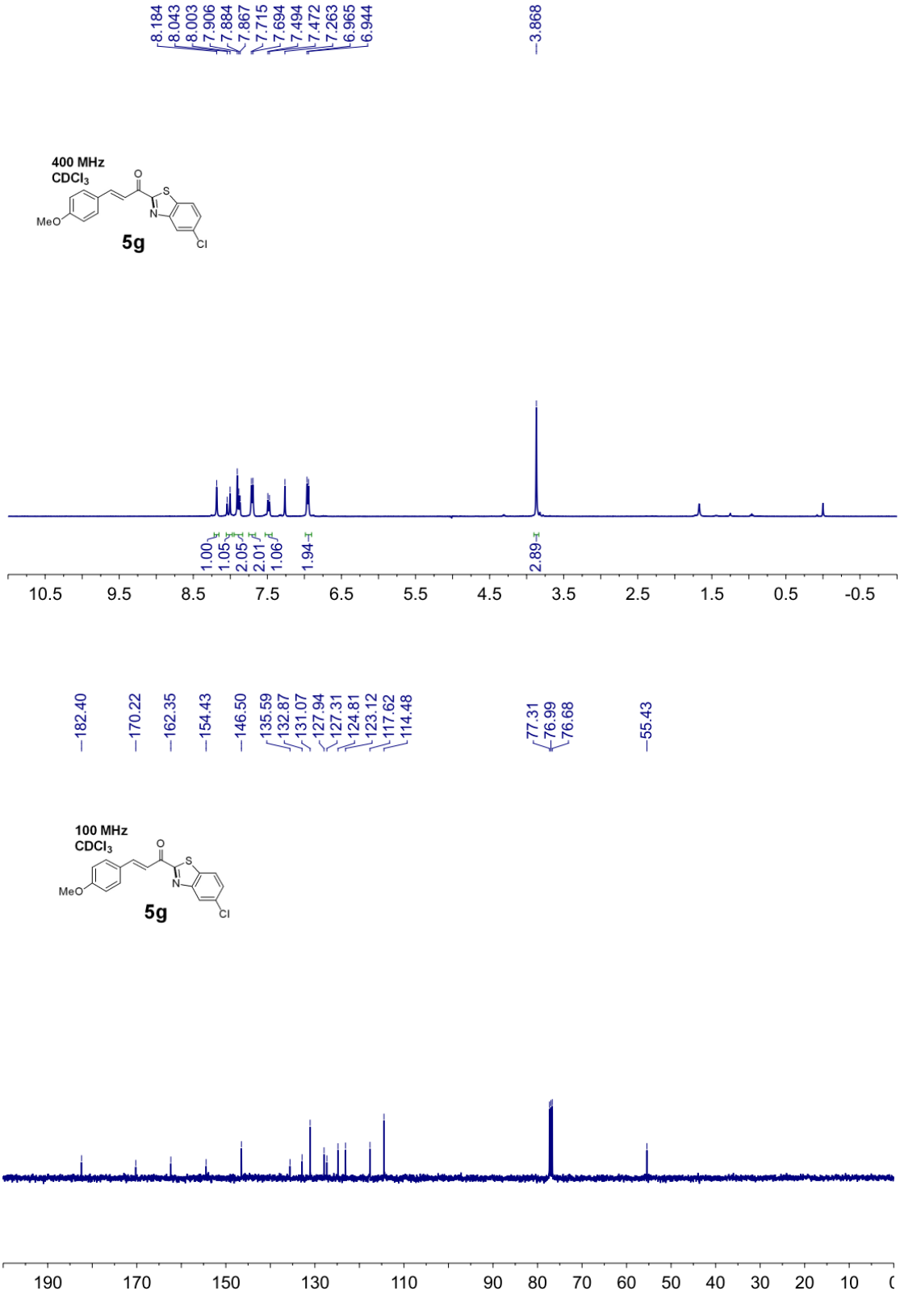

400 MHz
CDCl3
5d
100 MHz
CDCl3
5d
ppm

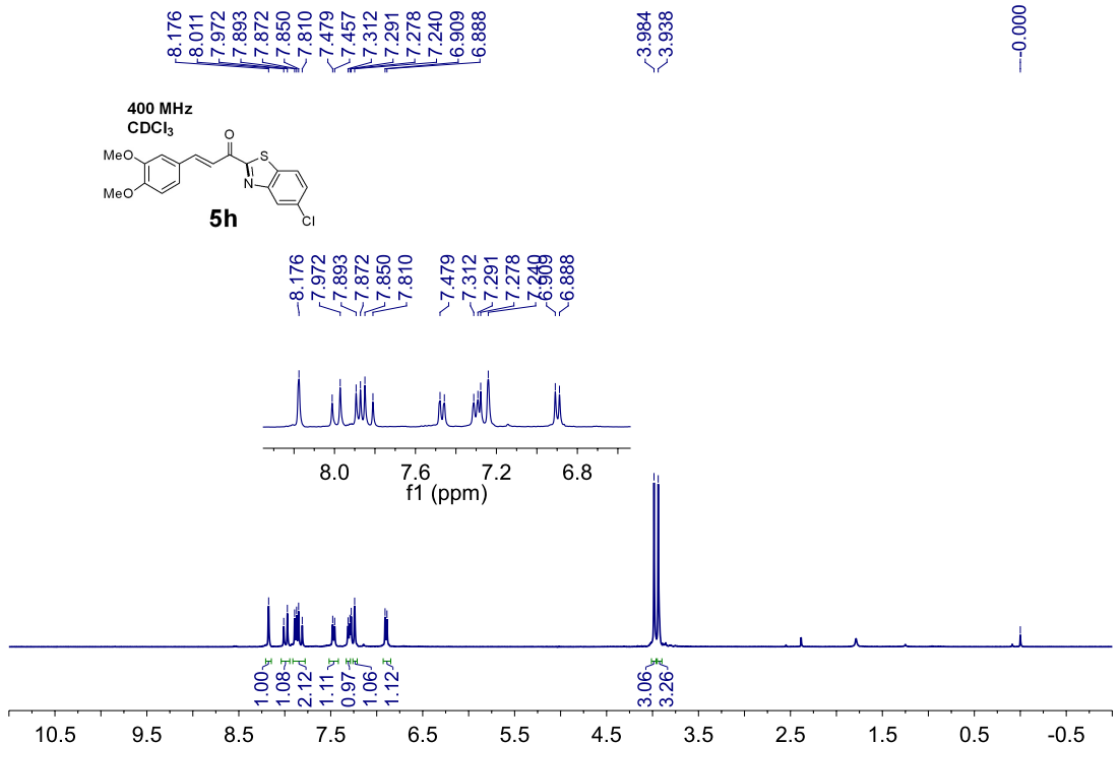

8.644
8.331
8.302
8.282
8.262
8.242
8.167
8.127
8.111
8.071
7.776
7.757
7.738
7.674
7.656
7.639
3.294
2.500
400 MHz
CDCl3
5e
1.00
4.21
2.19
1.22
2.14
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

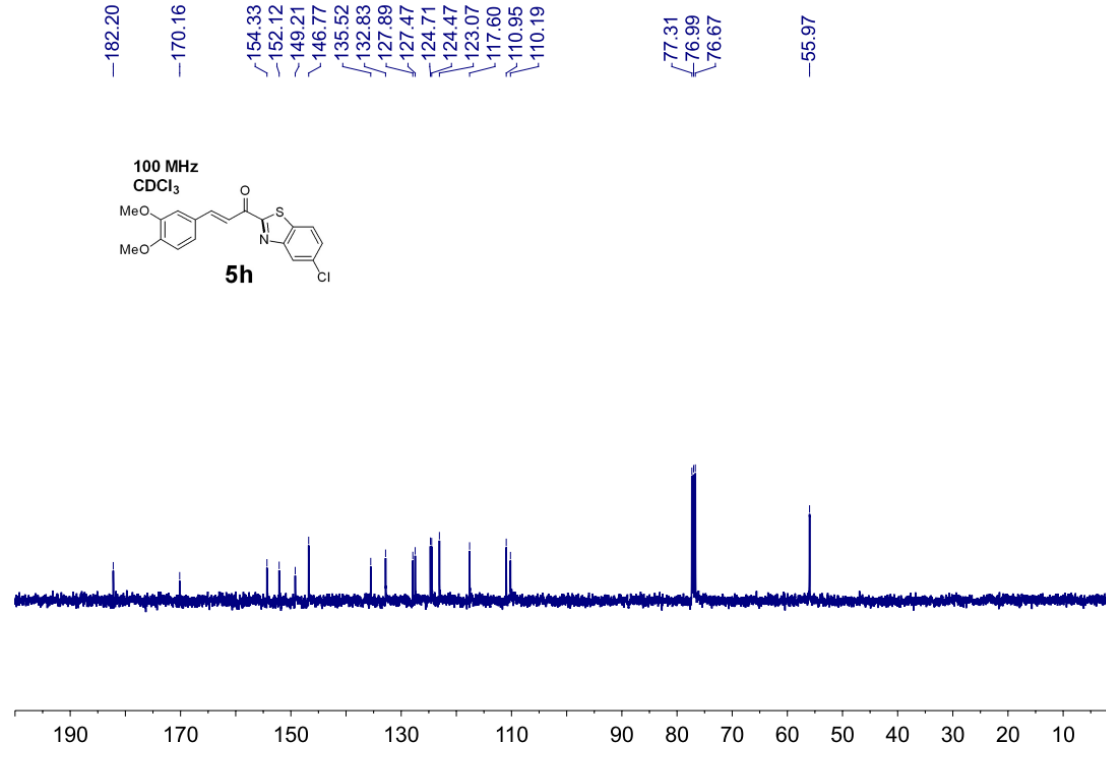

182.50
167.12
142.65
140.02
137.44
136.25
134.50
130.01
127.89
127.12
125.51
125.07
123.21
123.00
122.41
77.32
77.00
76.68
100 MHz
CDCl3
5e
190
170
150
130
110
90
80
70
60
50
40
30
20
10

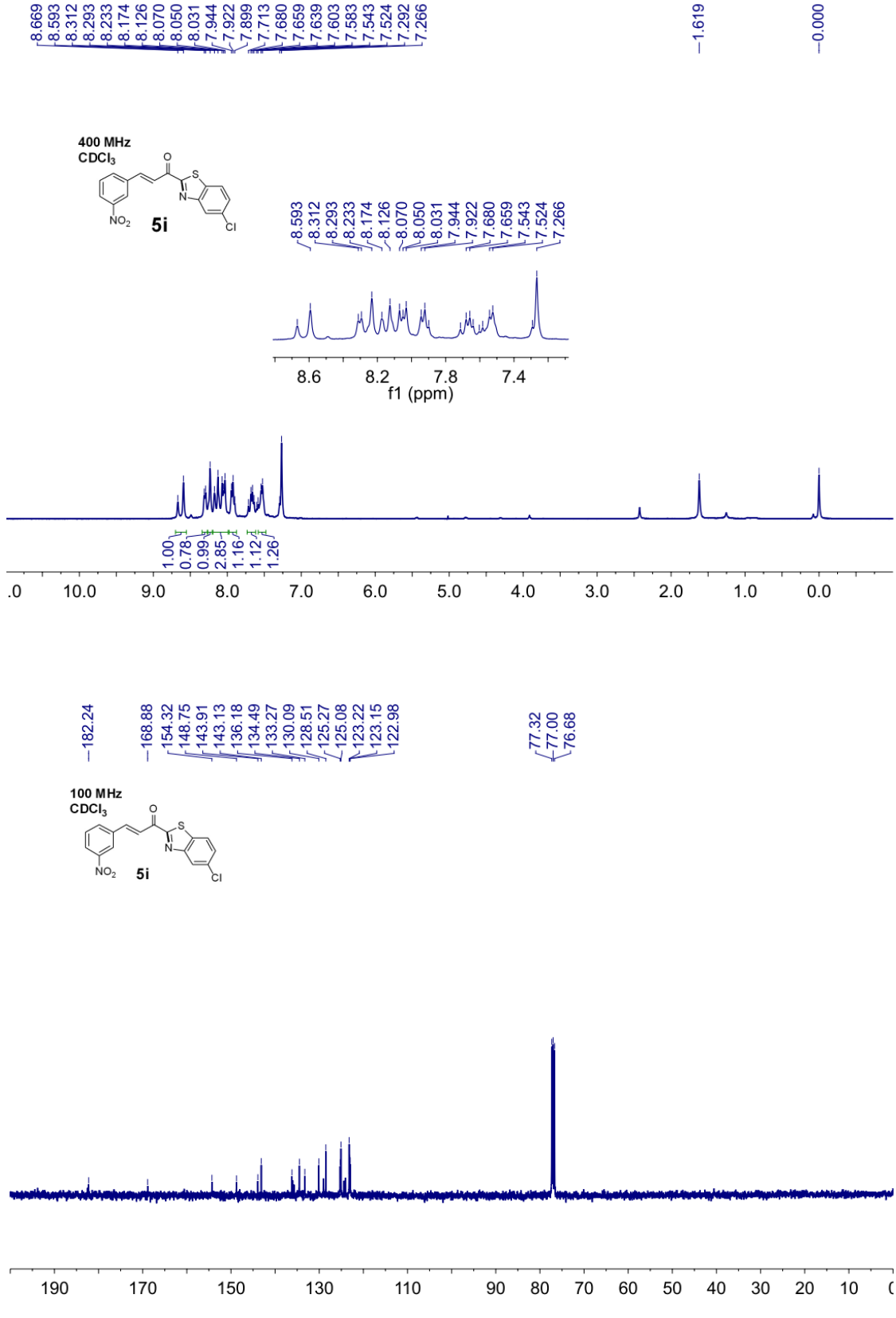

8.167
8.050
8.010
8.001
7.961
7.875
7.854
7.726
7.717
7.472
7.440
7.428
7.255
400 MHz
CDCl3
5f
f1 (ppm)
1.00
2.15
1.02
2.01
4.19


182.49
169.67
154.33
146.49
135.58
134.41
132.93
131.25
129.05
128.95
128.06
124.86
123.09
120.01
77.32
77.00
76.68
100 MHz
CDCl3
5f


8.184
8.043
8.003
7.906
7.884
7.867
7.715
7.694
7.494
7.472
7.263
6.965
6.944
3.868
400 MHz
CDCl3
MeO
Cl
5g
1.00
1.05
2.05
2.01
1.06
1.94
2.89
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
182.40
170.22
162.35
154.43
146.50
135.59
132.87
131.07
127.94
127.31
124.81
123.12
117.62
114.48
77.31
76.99
76.68
55.43
100 MHz
CDCl3
MeO
Cl
5g
190
170
150
130
110
90
80
70
60
50
40
30
20
10


8.176
8.011
7.972
7.893
7.872
7.850
7.810
7.479
7.457
7.312
7.291
7.278
7.240
6.909
6.888
3.984
3.938
-0.000
400 MHz
CDCl3
MeO
MeO
O
S
N
Cl
5h
8.176
7.972
7.893
7.872
7.850
7.810
7.479
7.312
7.291
7.278
6.909
6.888
8.0
7.6
7.2
6.8
f1 (ppm)
1.00
1.08
2.12
1.11
0.97
1.06
1.12
3.06
3.26
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


182.20
170.16
154.33
152.12
149.21
146.77
135.52
132.83
127.89
127.47
124.71
124.47
123.07
117.60
110.95
110.19
77.31
76.99
76.67
55.97
100 MHz
CDCl3
MeO
MeO
O
S
N
Cl
5h
190
170
150
130
110
90
80
70
60
50
40
30
20
10


8.669
8.593
8.312
8.293
8.233
8.174
8.126
8.070
8.050
8.031
7.944
7.922
7.899
7.713
7.680
7.659
7.639
7.603
7.583
7.543
7.524
7.292
7.266
1.619
0.000
400 MHz
CDCl3
5i
f1 (ppm)
1.00
0.78
0.99
2.85
1.16
1.12
1.26
182.24
168.88
154.32
148.75
143.91
143.13
136.18
134.49
133.27
130.09
128.51
125.27
125.08
123.22
123.15
122.98
77.32
77.00
76.68
100 MHz
CDCl3
5i