Tandem imine generation/N-cyclization/C-alkylation sequence to access N-functionalized indoles featuring an *aza*-quaternary carbon

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Supporting Information

(Part I)

1. General information

Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products was carried out by flash chromatography on silica gel. Chemical yields refer to pure isolated substances. Infrared (IR) spectra were obtained using a Nicolet Nexus 670 FT-IR spectrometer with KBr pellets in the range 4000-400 cmm^{-1}. Low resolution mass spectra are determined on GCMS-QP2010 (Shimadzu) or Agilent 5975C MSD. High resolution mass spectra are determined on Agilent Technologies 6224 TOF LC-MS or Agilent 6545 QTOF LC-MS. ^{1}H, ^{13}C and ^{19}F NMR spectra were obtained using a Bruker DPX-400 and Bruker DPX-300 spectrometer. Chemical shifts are reported in ppm from $CDCl_3$ with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet, br = broad.

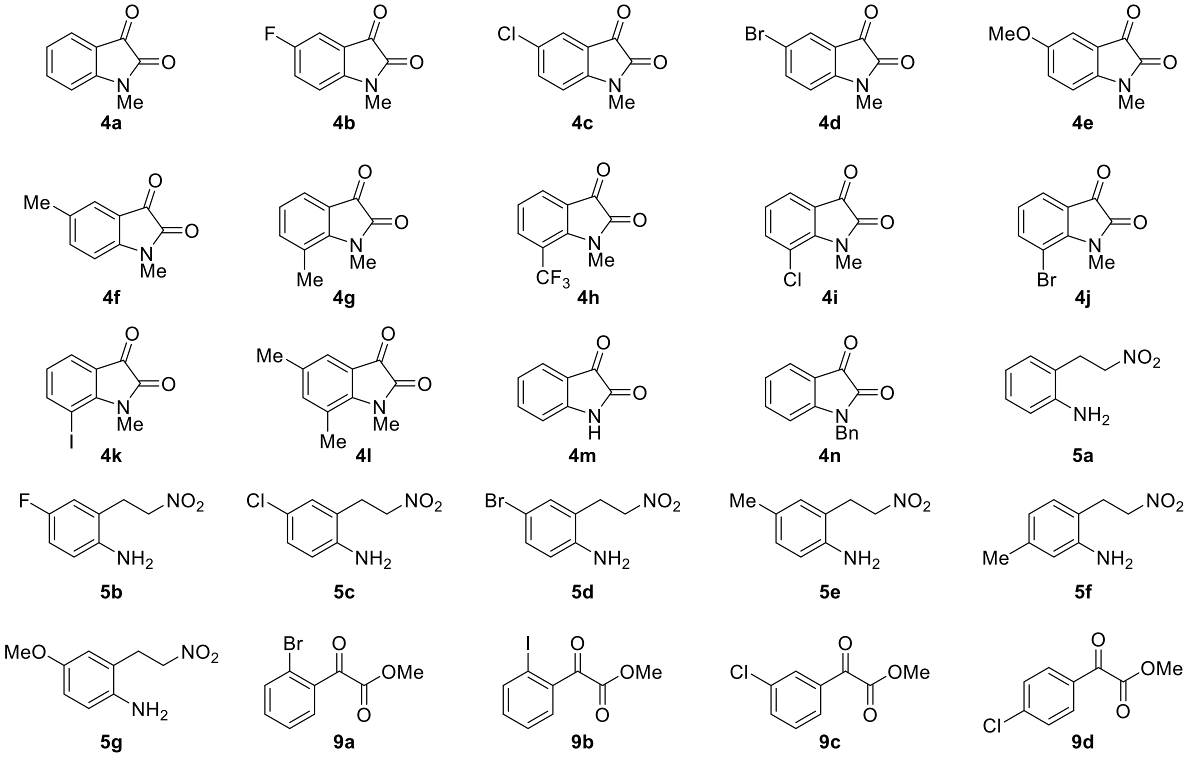
Unless noted, all the reactions were carried out under an atmosphere of N_2. Anhydrous CH_2Cl_2 and MeCN are prepared by first distillation over P_2O_5 and then from CaH_2. Anhydrous THF, dioxane, and toluene are freshly distilled from sodium/benzophenone, and MeOH from Mg. Anhydrous DMSO, DMA and DMF were prepared by drying over Na_2SO_4, distillation again from $CaSO_4$ and storing over MS 4Å.

List of abbreviation:

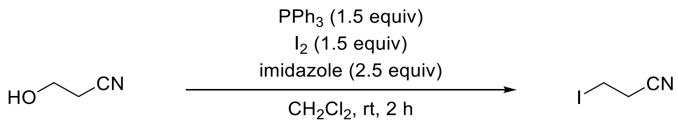
Entry	Chemical name	Abbreviation
1	Petroleum ether	PE
2	Ethyl acetate	EtOAc
3	Tetrahydrofuran	THF
4	Dichloromethane	CH_2Cl_2
5	Acetonitrile	MeCN
6	Dimethylsulfoxide	DMSO
7	*N*,*N*-dimethylacetamide	DMA
8	*N*,*N*-dimethylformamide	DMF
9	Methanol	MeOH
10	Toluene	PhMe

2. General procedure for the synthesis of starting materials

The **4a** and **4m** are commercially available. **4b-4g**,[1] **4h**,[2] **4i**,[3] **4j**,[4] **4k**,[5] **4l**,[2] **4n**,[3] **5a-5g**,[6] **9a**,[7] **9b**,[8] **9c**,[9] and **9d**,[7] are known compounds and synthesized accordingly.



The synthesis of 3-iodopropanenitrile.

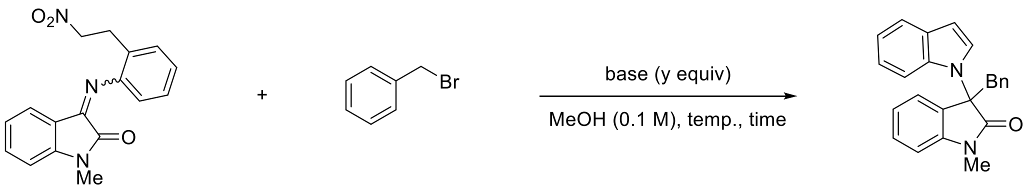


To a solution of PPh_3 (7.87 g, 30.0 mmol) in dry CH_2Cl_2 (90 mL) was added I_2 (7.61 g, 30.0 mmol). The reaction mixture was stirred at room temperature for 10 min and imidazole (3.40 g, 50.0 mmol) was added. After stirred for another 10 min, 3-hydroxypropanenitrile (1.42 g, 20.0 mmol) was added and stirred for 2 h, and then quenched with saturated aqueous $Na_2S_2O_3$ solution (30 mL). Then extracted the aqueous layer with CH_2Cl_2 (3 × 30 mL) followed by drying of the combined organic layers over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by distillation (101 ºC, 23 Torr) to afford 3-iodopropanenitrile as colorless oil in 54% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.28 (t, J = 7.2 Hz, 2H), 3.01 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 118.26, 22.67, 6.74. Spectral data was in agreement with that reported in literature.[10]

3. Condition optimization

The condition optimization for the one-pot tandem *N*-cyclization/*C*-benzylation reaction of isatin ketimine **1a** and BnBr **2a** was conducted as follows. To a 25-mL Schlenk tube were added **1a** (30.9 mg, 0.1 mmol), BnBr **2a** and MeOH (1.0 mL), followed by the addition of specific bases at 0 °C. The resulting mixture was stirred at specific temperature till the full consumption of **1a**, and then filtered through short silica gel and washed with CH_2Cl_2. The filtrate was concentrated and purified by column chromatography (PE/EtOAc, 10/1, v/v) to afford the desired product **3a**.

Table S1 Condition optimization for the *N*-cyclization/*C*-benzylation of isatin ketimine.



1a (0.1 mmol) **2a** (x equiv) **3a**

entry	BnBr (x equiv)	base (y equiv))	temp. (°C)	time (h)	yield (%)[a]
1	2.0	Na_2CO_3 (2.0)	0	24	29
2	2.0	K_2CO_3 (2.0)	0	4	63
3	2.0	Cs_2CO_3 (2.0)	0	3	68
4	2.0	KOH (2.0)	0	2	64
5	2.0	NaOH (2.0)	0	2	61
6	2.0	K_3PO_4 (2.0)	0	24	54
7	2.0	CsOH•H_2O (2.0)	0	3	73
8	2.0	CsOH•H_2O (2.0)	20	1.0	66
9	2.0	CsOH•H_2O (2.0)	-20	6	45
10	2.0	CsOH•H_2O (1.5)	0	24	46
11	2.0	CsOH•H_2O (2.5)	0	2.5	75
12	2.0	CsOH•H_2O (3.0)	0	1.5	66
13	1.0	CsOH•H_2O (2.5)	0	24	65
14	1.2	CsOH•H_2O (2.5)	0	9	72
15	1.5	CsOH•H_2O (2.5)	0	5	75
16[b]	1.5	CsOH•H_2O (2.5)	0	4	72
17[c]	1.5	CsOH•H_2O (2.5)	0	10	79

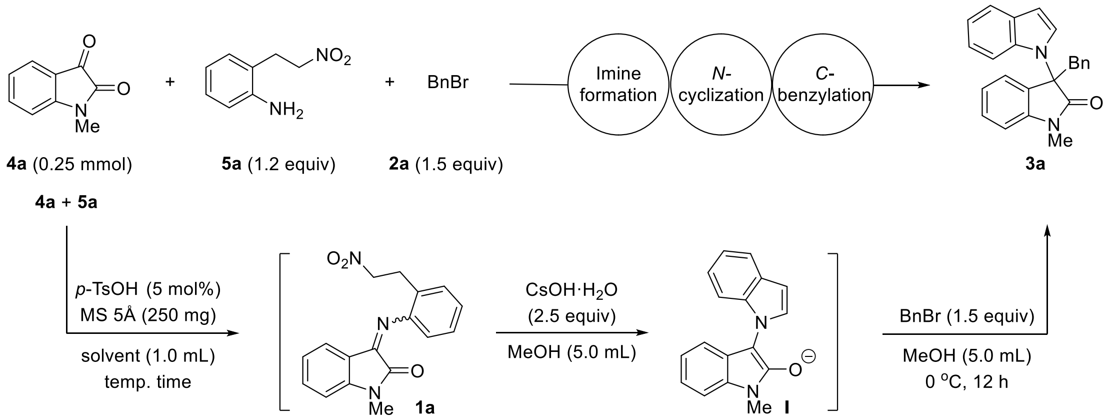
[a]Isolated yield. [b]The reaction mixture was performed at 0.2 M. [c]The reaction mixture was performed at 0.05 M.

As shown in Table S1, the properties of base greatly influenced the reaction outcome, and $CsOH \cdot H_2O$ proved to be the best choice, giving **3a** in 73% yield within 3 hours at 0 ºC (entries 1-7). The influence on reaction temperature was also evaluated, and the best result was obtained by running the reaction at 0 ºC (entries 8-9). The study of the usage of $CsOH \cdot H_2O$ and BnBr (entries 10-15) showed that when 2.5 equivs $CsOH \cdot H_2O$ and 1.5 equivs BnBr were used, product **3a** could be obtained in 75% yield within 5 hours (entry 15), which was further increased to 79% if decreasing the concentration of the reaction from 0.1 to 0.05 M (entry 17).

Based on these results, we further tried extending this protocol to a sequential imine formation/*N*-cyclization/*C*-benzylation process. The reaction of *N*-methylisatin **4a**, 2-(2-nitroethyl)aniline **5a** and BnBr **2a** was selected for condition optimization and conducted as follows. To a 25-mL Schlenk tube were added *N*-methylisatin **4a** (40.3 mg, 0.25 mmol), 2-(2-nitroethyl)aniline **5a** (49.9 mg, 0.3 mmol), MS 5Å (250.0 mg) and anhydrous PhMe (1.0 mL), followed by the addition of *p*-TsOH (2.2 mg, 5 mol%). The reaction mixture was stirred at specific temperature till the full consumption of *N*-methylisatin **4a**, and then cooled down to room temperature and concentrated under vacuum. The residue was dissolved in anhydrous MeOH (5.0 mL) followed by the addition of BnBr **2a** (64.1 mg, 0.375 mmol) and $CsOH \cdot H_2O$ (104.9 mg, 0.625 mmol) at 0 ºC. The resulting mixture was stirred at 0 ºC for 12 h, and then filtered through short silica gel and washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by column chromatography (PE/EtOAc, 10/1, v/v) to afford the desired product **3a**.

As shown in Table S2, We first tried running the condensation of *N*-methylisatin **4a** with 2-(2-nitroethyl)aniline **5a** in MeOH, the solvent for the *N*-cyclization and *C*-benzylation reaction, to simplify the operation. However, by screening the temperature (entries 1-2), the proportion of **4a** and **5a** (entry 3), and the amount of *p*-TsOH (entry 4) and addition of MS 5Å (entry 5), no promising results were obtained. To our delight, the desired product **3a** could be obtained in 64% yield using PhMe as solvent (entry 6). When PhMe is removed after the condensation of **4a** and **5a**, the yield of **3a** could be obtained in 68% yield (entry 7), which was further increased to 73% if lowering the temperature of condensation process to 60 ºC (entry 8).

Table S2 Condition optimization for imine formation/*N*-cyclization/*C*-benzylation of isatin.



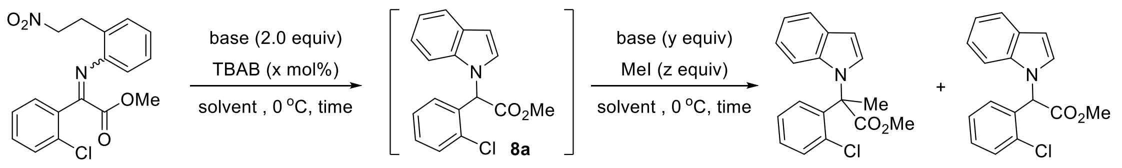
entry	**4a**:**5a**	solvent	temp. (°C)	time (h)	yield (%)[a]
1	1:1.2	MeOH	75	3	56
2	1:1.2	MeOH	90	3	55
3	1.2:1	MeOH	75	3	46
4[b]	1:1.2	MeOH	75	3	51
5[c]	1:1.2	MeOH	75	3	49
6	1:1.2	PhMe	75	3	64
7[d]	1:1.2	PhMe	75	3	68
8[d]	1:1.2	PhMe	60	3	73

[a]Isolated yield. [b]10 mol% of *p*-TsOH was added. [c]500 mg of MS 5Å was added. [d]PhMe was removed in the second step.

The success for the synthesis of C3-quaternary amino-oxindoles encouraged us to probe whether other types of *N*-functionalized indoles could be accessed via this sequence. Accordingly, α-ketoester derived imine **6a** was subjected to the reaction. Considering the steric congestion of the enolate, with a tetrasubstituted carbon–carbon double bond, the less sterically demanding MeI was employed as the alkylating reagent.

The conditions for the reaction of α-ketoester derived imine **6a** and MeI **2b** was conducted as follows. To a 25-mL Schlenk tube were added imine **6a** (34.7 mg, 0.1 mmol), specific solvent (1.0 mL) and TBAB (3.2 mg, 10 mol%), followed by the addition of K_2CO_3 (27.6 mg, 0.2 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 30 min or 12 h, and then concentrated under vacuum. The residue was dissolved in specific solvent, followed by the addition of MeI and specific base at 0 °C. The resulting mixture was stirred at 0 °C for specific time, and then quenched with saturated aqueous NH_4Cl (5 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with water (3 × 20 mL) and brine (20 mL), then dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the desired product **7a**.

Table S3 Condition optimization for *N*-cyclization/*C*-methylation of α-ketoester derived ketimine.



6a (0.1 mmol) **7a** **8a**

entry	N-alkylation				Methylation				Isolated yield	
	base	TBAB (x)	solvent (conc. M)	time (h)	base (y)	MeI (z)	solvent (conc. M)	time (h)	**7a**	**8a**
1	K_2CO_3	0	MeOH (0.1)	0.5	K_2CO_3 (1.0)	1.5	MeOH (0.1)	24	0	65%
2	K_2CO_3	10	PhMe (0.1)	10	^{t}BuOK (1.0)	1.5	PhMe (0.1)	24	0	91%
3	K_2CO_3	10	PhMe (0.1)	10	^{t}BuOK (1.0)	1.5	CH_2Cl_2 (0.1)	24	45%	10%
4	K_2CO_3	10	PhMe (0.1)	10	^{t}BuOK (1.0)	1.5	DMF (0.1)	24	53%	45%
5	K_2CO_3	10	PhMe (0.1)	10	^{t}BuOK (1.0)	1.5	THF (0.1)	24	37%	41%
6	K_2CO_3	10	PhMe (0.1)	10	^{t}BuOK (1.0)	1.5	MeCN (0.1)	24	41%	54%
7	K_2CO_3	10	PhMe (0.1)	10	^{t}BuOK (1.0)	1.5	DMA (0.1)	24	58%	40%
8	K_2CO_3	0	MeOH (0.1)	0.5	Cs_2CO_3 (1.0)	1.5	DMA (0.1)	24	16%	70%
9	K_2CO_3	0	MeOH (0.1)	0.5	CsOH•H_2O (1.0)	1.5	DMA (0.1)	24	73%	trace
10	K_2CO_3	0	MeOH (0.1)	0.5	KOH (1.0)	1.5	DMA (0.1)	24	6%	61%
11	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.0)	1.5	DMA (0.1)	24	80%	trace
12	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.5)	1.5	DMA (0.1)	12	86%	trace
13	K_2CO_3	0	MeOH (0.1)	0.5	NaH (2.0)	1.5	DMA (0.1)	5	87%	0
14	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.5)	2.0	DMA (0.1)	12	90%	0
15	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.5)	2.5	DMA (0.1)	12	90%	0
16	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.5)	2.0	DMA (0.2)	5	83%	0
17	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.5)	2.0	DMA (0.05)	12	93%	0
18[a]	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.5)	2.0	DMA (0.05)	12	69%	0
19[b]	K_2CO_3	0	MeOH (0.1)	0.5	NaH (1.5)	2.0	DMA (0.05)	5	75%	0

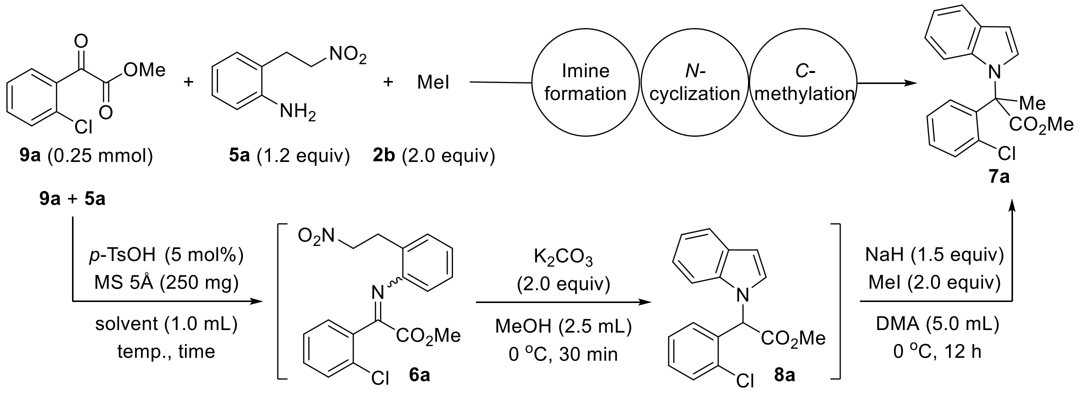
[a]The reaction was performed at -10 °C. [b]The reaction was performed at 10 °C.

As shown in Table S3, the nature of the solvent was found to play a crucial role. If the sequence was run in MeOH or toluene, only the *N*-cyclization product **8a** was formed, with no detectable formation of adduct **7a** (entries 1-2). However, if the solvent was removed after the *N*-cyclization step, and then CH_2Cl_2 and 1.0 equivalent of $KOBu^t$ were added for the following *C*-methylation sequence, the desired product **7a** could be obtained in promising 45% yield (entry 3). Further optimization revealed that DMA was the most suitable solvent for the *C*-methylation, giving **7a** in 58% yield (entries 4-7). Further screening of other bases demonstrated that NaH was the best choice (entries 8-11). Evaluating the amount of NaH and MeI indicated that the desired product **7a** was obtained in 90% yield within 12 hours at 0 ºC, when using 1.5 equivs NaH and 2.0 equivs MeI (entries 12-15). Further decreasing the concentration from 0.1 to 0.05 M resulted in the improved 93% yield of product **7a** (entry 17). Varying the reaction temperature failed to afford better results (entries 18-19).

Next, we tried to combine the imine formation with the aforementioned process to form a sequential imine formation/*N*-cyclization/*C*-methylation sequence. The condition optimization of the reaction of α-ketoester **9a**, 2-(2-nitroethyl)aniline **5a** and MeI **2b** was conducted as follows. To a 25-mL Schlenk tube were added α-ketoester **9a** (0.25 mmol, 1.0 equiv), 2-(2-nitroethyl)aniline **5a** (0.3 mmol, 1.2 equiv), MS 5Å (250.0 mg) and anhydrous PhMe (1.0 mL) or MeOH (1.0 mL), followed by the addition of *p*-TsOH (2.2 mg, 5 mol%). The reaction mixture was stirred at specific temperature till the full consumption of α-ketoester **9a**, and then cooled down to room temperature for concentration under vacuum. The thus obtained residue was dissolved in anhydrous MeOH (2.5 mL), followed by the addition of K_2CO_3 (69.1 mg, 0.5 mmol) at 0 ºC. The resulting mixture was stirred at 0 ºC for 30 min, concentrated in vacuum, and then the residue was dissolved in anhydrous DMA (5.0 mL), followed by the addition of MeI (71. 0 mg, 0.5 mmol) and NaH (15.0 mg, 0.375 mmol) at 0 ºC. The reaction mixture was stirred at 0 ºC for 12 h, and then quenched with saturated aqueous NH_4Cl (5 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with water (3 × 20 mL) and brine (20 mL), then dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the desired product **7a**.

As shown in Table S4, we first performed the condensation of α-ketoester **9a** with 2-(2-nitroethyl)aniline **5a** in MeOH, the solvent previously identified for the *N*-cyclization reaction, to simplify the operation. However, by screening the proportion of **9a** and **5a** (entry 2), and the amount of *p*-TsOH (entry 3) and MS 5Å (entry 4), no satisfactory result was obtained. To our delight, when replacing MeOH by PhMe as the solvent for the condensation, the desired product **7a** could be obtained in 85% isolated yield (entry 5). If lowering the temperature for the imine formation step, the yield of **7a** obviously decreased (entries 6-7).

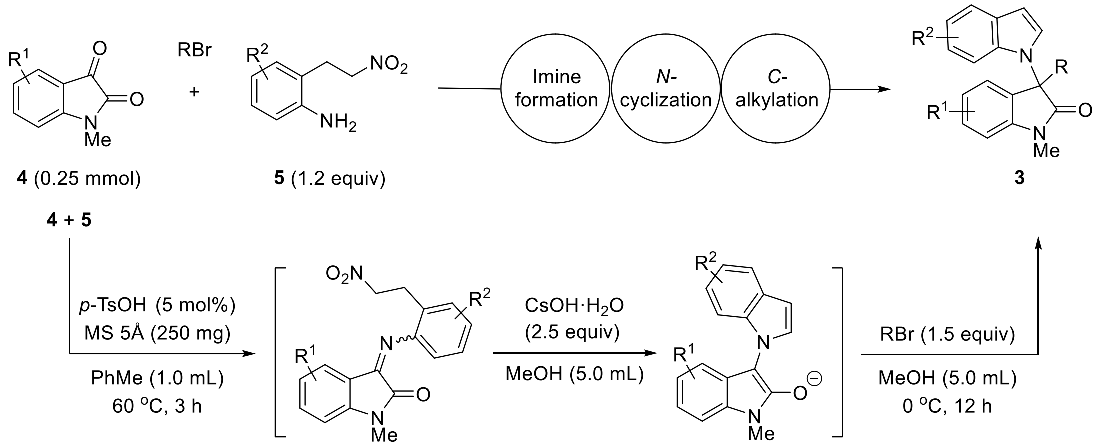
Table S4 Condition optimization for imine formation/*N*-cyclization/*C*-methylation of α-ketoester.



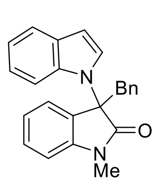
entry	solvent	temp. (°C)	time (h)	yield (%)[a]
1	MeOH	120	6	62
2[b]	MeOH	120	5	72
3[c]	MeOH	120	3	57
4[d]	MeOH	120	6	61
5	PhMe	120	2	85
6	PhMe	100	4	75
7	PhMe	80	5	47

[a]Isolated yield. [b]**9a** (1.2 equivs), **5a** (0.25 mmol). [c]10 mol% of *p*-TsOH was added. [d]500 mg of MS 5Å was added.

4. General procedure for one-pot tandem sequence of isatins.

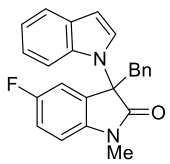


To a 25-mL Schlenk tube were added *N*-methylisatin **4** (0.25 mmol, 1.0 equiv), anilines **5** (0.3 mmol, 1.2 equiv), MS 5Å (250.0 mg) and anhydrous toluene (1.0 mL), followed by the addition of *p*-TsOH (2.2 mg, 5 mol%). The reaction mixture was stirred at 60 ºC for 3 h till the full conversion of *N*-methylisatin **4**, and then cooled down to room temperature and concentrated under vacuum. The residue was dissolved in anhydrous MeOH (5.0 mL), followed by the addition of alkyl bromides (0.375 mmol, 1.5 equiv) and $CsOH{\cdot}H_2O$ (104.9 mg, 0.625 mmol) at 0 ºC. The resulting mixture was stirred at 0 ºC for 12 h, and then filtered through short silica gel and washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by column chromatography (PE/EtOAc, 10/1, v/v) to afford the desired product **3a-3ap**.



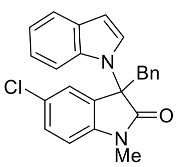
3a

Product **3a** was obtained in 73% yield as white solid; Mp: 179-180 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 3.2 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.28-7.25 (m, 1H), 7.13 (dd, J_1 = 17.2 Hz, J_2 = 7.6 Hz, 2H), 7.06-7.02 (m, 4H), 6.89 (t, J = 8.0 Hz, 1H), 6.79 (d, J = 7.6 Hz, 2H), 6.66 (d, J = 2.8 Hz, 1H), 6.59 (d, J = 8.0 Hz, 1H), 6.49 (d, J = 8.4 Hz, 1H), 3.98, 3.76 (AB, J = 11.6 Hz, 2H), 2.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.21, 143.10, 135.83, 132.46, 130.39, 129.90, 128.37, 127.61, 127.31, 125.26, 124.24, 123.21, 122.00, 121.18, 120.13, 111.24, 108.37, 102.77, 68.00, 43.61, 26.05; IR (neat): 3030, 1720, 1612, 1492, 1469, 1456, 1087, 1020, 752, 733, 698; HRMS (ESI): Exact mass calcd for $C_{24}H_{20}N_2ONa$ $[M+Na]^+$: 375.1468, Found: 375.1476.



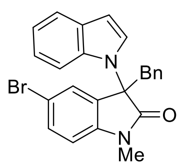
3b

Product **3b** was obtained in 75% yield as white solid; Mp: 180-182 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 3.2 Hz, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.14-7.03 (m, 4H), 6.97-6.90 (m, 3H), 6.83 (d, J = 7.6 Hz, 2H), 6.68 (d, J = 3.2 Hz, 1H), 6.52 (dd, J_1 = 8.4 Hz, J_2 = 4.0 Hz, 1H), 6.44 (d, J = 8.4 Hz, 1H), 3.99, 3.74 (AB, J = 11.6 Hz, 2H), 2.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.97, 159.56 (d, J = 241.0 Hz), 139.00 (d, J = 2.0 Hz), 135.72, 132.02, 130.31, 130.09 (d, J = 7.0 Hz), 129.89, 127.75, 127.51, 125.02, 122.18, 121.33, 120.32, 116.24 (d, J = 23.0 Hz), 112.23 (d, J = 25.0 Hz), 110.85, 109.04 (d, J = 8.0 Hz), 103.10, 68.11, 43.61, 26.19; ^{19}F NMR (376 MHz, $CDCl_3$): δ -118.99; IR (neat): 2929, 1718, 1612, 1492, 1467, 1263, 1236, 1203, 1122, 1099, 1070, 750; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}FN_2ONa$ $[M+Na]^+$: 393.1374, Found: 393.1376.



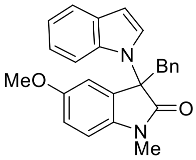
3c

Product **3c** was obtained in 76% yield as yellow solid; Mp: 192-194 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 3.2 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.24 (d, J = 8.4 Hz, 1H), 7.14-7.10 (m, 2H), 7.09-7.03 (m, 3H), 6.92 (t, J = 7.6 Hz, 1H), 6.81 (d, J = 7.6 Hz, 2H), 6.68 (d, J = 2.8 Hz, 1H), 6.51 (d, J = 8.0 Hz, 1H), 6.44 (d, J = 8.4 Hz, 1H), 3.98, 3.75 (AB, J= 11.2 Hz, 2H), 2.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.79, 141.58, 135.69, 131.94, 130.33, 130.17, 129.87, 128.75, 127.80, 127.56, 124.98, 124.45, 122.24, 121.36, 120.35, 110.82, 109.35, 103.15, 67.92, 43.65, 26.17; IR (neat): 2931, 1722, 1610, 1489, 1456, 1234, 1136, 1099, 1018, 734; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}ClN_2ONa$ $[M+Na]^+$: 409.1078, Found: 409.1089.



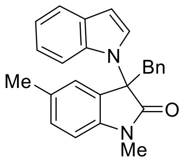
3d

Product **3d** was obtained in 76% yield as white solid; Mp: 214-216 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 3.2 Hz, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.39 (d, J = 8.4 Hz, 1H), 7.27 (d, J = 6.0 Hz, 1H), 7.13-7.06 (m, 4H), 6.94 (t, J = 7.6 Hz, 1H), 6.82 (d, J = 7.6 Hz, 2H), 6.69 (d, J = 3.6 Hz, 1H), 6.46 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 2H), 3.98, 3.75 (AB, J = 11.6 Hz, 2H), 2.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.66, 142.09, 135.71, 132.78, 131.95, 130.52, 130.35, 129.89, 127.81, 127.57, 127.18, 124.98, 122.27, 121.37, 120.37, 115.94, 110.83, 109.81, 103.18, 67.87, 43.70, 26.16; IR (neat): 2929, 1722, 1606, 1516, 1508, 1489, 1456, 1359, 1267, 1234, 1099, 736; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrN_2ONa$ $[M+Na]^+$: 453.0573, Found: 453.0581.



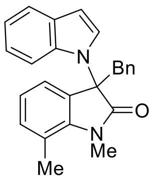
3e

Product **3e** was obtained in 73% yield as yellow solid; Mp: 167-168 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 3.6 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.14-7.12 (m, 1H), 7.09-7.04 (m, 3H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.85-6.76 (m, 4H), 6.67 (d, *J* = 3.2 Hz, 1H), 6.51 (d, *J* = 8.4 Hz, 2H), 3.97, 3.75 (AB, *J* = 11.2 Hz, 2H), 3.72 (s, 3H), 2.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.87, 156.49, 136.55, 135.87, 132.45, 130.39, 129.87, 129.58, 127.64, 127.32, 125.19, 122.04, 121.15, 120.14, 114.48, 111.25, 111.12, 108.91, 102.78, 68.28, 55.89, 43.60, 26.12; IR (neat): 2929, 2835, 1716, 1604, 1496, 1471, 1456, 1236, 1224, 1149, 1132, 1028, 731, 698; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2O_2Na$ $[M+Na]^+$: 405.1573, Found: 405.1584.



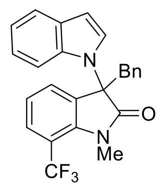
3f

Product **3f** was obtained in 71% yield as white solid; Mp: 166-168 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 3.2 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.12 (t, *J* = 7.2 Hz, 1H), 7.07-7.01 (m, 4H), 6.96 (s, 1H), 6.91 (t, *J* = 7.6 Hz, 1H), 6.79 (d, *J* = 7.6 Hz, 2H), 6.66 (d, *J* = 2.8 Hz, 1H), 6.49 (t, *J* = 8.0 Hz, 2H), 3.96, 3.74 (AB, *J* = 11.6 Hz, 2H), 2.88 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.09, 140.71, 135.81, 132.83, 132.52, 130.39, 130.14, 129.81, 128.31, 127.57, 127.26, 125.23, 124.80, 121.97, 121.12, 120.07, 111.28, 108.12, 102.63, 68.04, 43.60, 26.04, 21.21; IR (neat): 2926, 1718, 1604, 1500, 1456, 1361, 1315, 1265, 1238, 1099, 1018, 731; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$: 389.1624, Found: 389.1626.



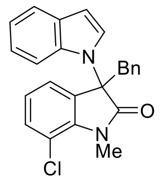
3g

Product **3g** was obtained in 74% yield as white solid; Mp: 153-155 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 3.6 Hz, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.13-7.11 (m, 1H), 7.07-6.99 (m, 3H), 6.97-6.86 (m, 4H), 6.74 (d, *J* = 7.6 Hz, 2H), 6.64 (d, *J* = 3.2 Hz, 1H), 6.50 (d, *J* = 8.4 Hz, 1H), 3.94, 3.67 (AB, *J* = 11.2 Hz, 2H), 3.12 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.93, 140.84, 135.80, 133.41, 132.55, 130.37, 129.82, 129.09, 127.48, 127.31, 125.24, 123.14, 121.94, 121.12, 120.10, 120.06, 111.27, 102.64, 67.59, 44.15, 29.46, 18.80; IR (neat): 2927, 1718, 1602, 1473, 1456, 1363, 1323, 1116, 1064, 738, 700; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$: 389.1624, Found: 389.1630.



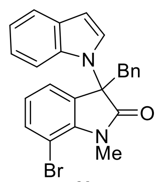
3h

Product **3h** was obtained in 76% yield as yellow solid; Mp: 60-62 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 3.6 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.55 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.28 (dd, J_1 = 7.2 Hz, J_2 = 0.4 Hz, 1H), 7.16-7.12 (m, 1H), 7.10-7.03 (m, 4H), 6.92-6.71 (m, 1H), 6.70-6.69 (m, 3H), 6.36 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1H), 3.99, 3.73 (AB, J = 11.2 Hz, 2H), 3.08 (q, J = 2.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.19, 140.90, 135.58, 131.56, 131.31, 130.04, 129.86, 127.80, 127.78, 127.60 (q, J = 6.0 Hz), 127.20, 125.00, 123.25 (q, J = 270.0 Hz), 122.62, 122.35, 121.38, 120.42, 112.91 (q, J = 33.0 Hz), 110.60, 103.22, 66.62, 44.31, 28.76 (q, J = 7.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ -53.69; IR (neat): 2927, 1732, 1598, 1489, 1473, 1456, 1321, 1122, 1093, 1074, 1056, 732, 698; HRMS (ESI): Exact mass calcd for $C_{25}H_{19}F_3N_2ONa$ $[M+Na]^+$: 443.1342, Found: 443.1352.



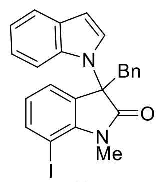
3i

Product **3i** was obtained in 83% yield yellow solid; Mp: 174-176 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 3.6 Hz, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.20-7.18 (m, 2H), 7.11 (t, J = 7.4 Hz, 2H), 7.05-7.00 (m, 2H), 6.94 (q, J = 8.0 Hz, 2H), 6.77 (d, J = 7.6 Hz, 2H), 6.68 (d, J = 3.2 Hz, 1H), 6.48 (d, J = 8.4 Hz, 1H), 3.97, 3.71 (AB, J = 11.2 Hz, 2H), 3.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.56, 138.95, 135.65, 132.01, 131.87, 131.39, 130.22, 129.82, 127.75, 127.72, 125.01, 123.99, 122.46, 122.23, 121.28, 120.31, 115.96, 110.89, 103.03, 67.65, 44.13, 29.47; IR (neat): 2949, 1730, 1608, 1456, 1363, 1321, 1107, 738, 700; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}ClN_2ONa$ $[M+Na]^+$: 409.1078, Found: 409.1088.

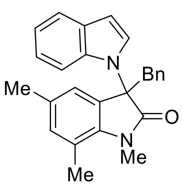


3j

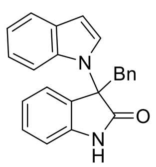
Product **3j** was obtained in 80% yield as white solid; Mp: 150-152 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 3.6 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.20 (t, J = 7.2 Hz, 1H), 7.11 (t, J = 7.6 Hz, 2H), 7.07-7.03 (m, 2H), 6.95 (t, J = 8.0 Hz, 1H), 6.87 (t, J = 8.0 Hz, 1H), 6.76 (d, J = 7.6 Hz, 2H), 6.67 (d, J = 3.2 Hz, 1H), 6.47 (d, J = 8.4 Hz, 1H), 3.97, 3.70 (AB, J = 11.6 Hz, 2H), 3.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.75, 140.46, 135.66, 135.37, 131.86, 131.77, 130.23, 129.84, 127.77, 125.01, 124.38, 122.98, 122.27, 121.30, 120.34, 110.93, 103.07, 102.84, 67.68, 44.26, 29.69; IR (neat): 2927, 1724, 1608, 1577, 1514, 1228, 1101, 1074, 1018, 1006, 731, 700; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrN_2ONa$ $[M+Na]^+$: 453.0573, Found: 453.0579.


3k

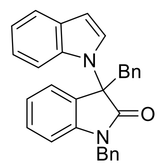
Product **3k** was obtained in 83% yield as yellow solid; Mp: 162-163 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 3.2 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 2H), 7.05 (t, *J* = 5.6 Hz, 2H), 6.95 (t, *J* = 8.0 Hz, 1H), 6.75-6.70 (m, 3H), 6.67 (d, *J* = 3.2 Hz, 1H), 6.45 (d, *J* = 8.4 Hz, 1H), 3.96, 3.69 (AB, *J* = 11.2 Hz, 2H), 3.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.03, 143.50, 142.30, 135.65, 131.86, 131.71, 130.21, 129.83, 127.76, 127.74, 125.03, 124.87, 123.65, 122.26, 121.29, 120.33, 110.95, 103.05, 71.81, 67.60, 44.31, 29.93; IR (neat): 2926, 2854, 1724, 1602, 1571, 1516, 1454, 1317, 1228, 1097, 1072, 734, 700; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}IN_2ONa$ $[M+Na]^+$: 501.0434, Found: 501.0441.


3l

Product **3l** was obtained in 70% yield as yellow solid; Mp: 128-130 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 3.6 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.17-7.16 (m, 1H), 7.12-7.04 (m, 3H), 6.98-6.94 (m, 1H), 6.82-6.78 (m, 4H), 6.69 (d, *J* = 3.2 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 3.96, 3.70 (AB, *J* = 11.2 Hz, 2H), 3.13 (s, 3H), 2.31 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 174.80, 138.41, 135.77, 133.88, 132.67, 132.61, 130.39, 129.74, 129.10, 127.46, 127.27, 125.21, 122.40, 121.94, 121.07, 120.02, 119.79, 111.33, 102.51, 67.65, 44.16, 29.40, 20.91, 18.66; IR (neat): 2924, 1716, 1602, 1508, 1483, 1473, 1456, 1323, 1230, 1099, 738, 700; HRMS (ESI): Exact mass calcd for $C_{26}H_{24}N_2ONa$ $[M+Na]^+$: 403.1781, Found: 403.1790.

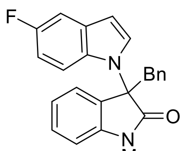

3m

Product **3m** was obtained in 54% yield as white solid; Mp: 218-220 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (s, 1H), 7.70 (d, *J* = 3.6 Hz, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.20 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.16-7.10 (m, 2H), 7.09-6.99 (m, 4H), 6.93-6.84 (m, 3H), 6.70-6.57 (m, 3H), 4.00, 3.80 (AB, *J* = 11.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 176.67, 140.25, 135.85, 132.28, 130.57, 129.94, 129.86, 128.70, 127.89, 127.42, 125.20, 124.65, 123.24, 122.12, 121.21, 120.23, 111.36, 110.63, 102.89, 68.21, 43.42; IR (neat): 2926, 2852, 1722, 1620, 1516, 1489, 1471, 1456, 1263, 1220, 732, 698; HRMS (ESI): Exact mass calcd for $C_{23}H_{18}N_2ONa$ $[M+Na]^+$: 361.1311, Found: 361.1312.



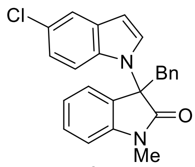
3n

Product **3n** was obtained in 75% yield as white solid; Mp: 148-150 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 3.2 Hz, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.22-7.12 (m, 6H), 7.08-7.00 (m, 4H), 6.88-6.81 (m, 5H), 6.65 (d, J = 3.2 Hz, 1H), 6.46 (dd, J_1 = 14.4 Hz, J_2 = 7.6 Hz, 2H), 4.75, 4.50 (AB, J = 15.6 Hz, 2H), 4.08, 3.80 (AB, J = 11.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.36, 142.72, 135.83, 135.08, 132.58, 130.75, 129.96, 129.92, 128.78, 128.36, 128.01, 127.67, 127.52, 127.41, 125.26, 124.45, 123.27, 121.92, 121.20, 120.16, 111.56, 109.77, 102.81, 67.91, 44.27, 43.31; IR (neat): 2926, 2852, 1722, 1610, 1516, 1489, 1467, 1454, 1193, 1029, 1018, 731, 696; HRMS (ESI): Exact mass calcd for $C_{30}H_{24}N_2ONa$ $[M+Na]^+$: 451.1781, Found: 451.1788.



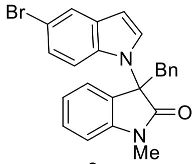
3o

Product **3o** was obtained in 68% yield as white solid; Mp: 192-194 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, J = 3.6 Hz, 1H), 7.30-7.22 (m, 2H), 7.15-7.10 (m, 2H), 7.07-7.03 (m, 3H), 6.78 (d, J = 7.6 Hz, 2H), 6.65-6.59 (m, 3H), 6.40 (dd, J_1 = 9.2 Hz, J_2 = 4.4 Hz, 1H), 3.96, 3.73 (AB, J= 11.6 Hz, 2H), 2.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.05, 159.19 (d, J = 234.0 Hz), 143.03, 132.34, 132.25, 130.34, 130.32 (d, J = 10.0 Hz), 130.09, 128.04, 127.66, 127.40, 126.99, 124.20, 123.32, 111.85 (d, J = 9.0 Hz), 110.30 (d, J = 25.0 Hz), 108.50, 105.93 (d, J = 23.0 Hz), 102.75 (d, J = 5.0 Hz), 68.04, 43.52, 26.10; ^{19}F NMR (376 MHz, $CDCl_3$): δ -124.69; IR (neat): 2927, 2850, 1720, 1612, 1508, 1490, 1448, 1371, 1124, 1020, 1001, 736, 700; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}FN_2ONa$ $[M+Na]^+$: 393.1374, Found: 393.1383.



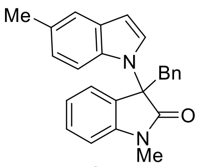
3p

Product **3p** was obtained in 61% yield as yellow solid; Mp: 175-176 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 3.6 Hz, 1H), 7.56 (d, J = 2.0 Hz, 1H), 7.30-7.26 (m, 1H), 7.12 (t, J = 7.6 Hz, 2H), 7.05 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 3H), 6.85 (dd, J_1 = 9.2 Hz, J_2 = 2.4 Hz, 1H), 6.77 (d, J = 7.2 Hz, 2H), 6.61-6.59 (m, 2H), 6.40 (d, J = 8.8 Hz, 1H), 3.95, 3.73 (AB, J = 11.6 Hz, 2H), 2.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.97, 143.07, 134.17, 132.22, 130.98, 130.35, 130.16, 127.98, 127.69, 127.44, 126.73, 125.95, 124.24, 123.34, 122.30, 120.55, 112.26, 108.55, 102.42, 68.07, 43.50, 26.12; IR (neat): 2927, 1720, 1612, 1508, 1492, 1469, 1456, 1126, 1089, 1020, 729, 700; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}ClN_2ONa$ $[M+Na]^+$: 409.1078, Found: 409.1085.



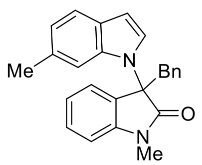
3q

Product **3q** was obtained in 70% yield as yellow solid; Mp: 160-162 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 1.6 Hz, 1H), 7.70 (d, J = 3.6 Hz, 1H), 7.30-7.26 (m, 1H), 7.13-7.11 (m, 2H), 7.05 (t, J = 7.6 Hz, 3H), 6.98 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 1H), 6.78 (d, J = 7.2 Hz, 2H), 6.61-6.59 (m, 2H), 6.36 (d, J = 8.8 Hz, 1H), 3.95, 3.73 (AB, J = 11.2 Hz, 2H), 2.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.91, 143.00, 134.40, 132.15, 131.57, 130.32, 130.16, 127.89, 127.67, 127.43, 126.56, 124.83, 124.19, 123.63, 123.33, 113.56, 112.67, 108.54, 102.30, 68.02, 43.45, 26.11; IR (neat): 2922, 1720, 1612, 1508, 1492, 1469, 1452, 1126, 1089, 1020, 1001, 750, 698; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrN_2ONa$ $[M+Na]^+$: 453.0573, Found: 453.0580.



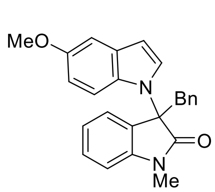
3r

Product **3r** was obtained in 71% yield as yellow solid; Mp: 173-174 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 3.2 Hz, 1H), 7.37 (s, 1H), 7.26-7.22 (m, 1H), 7.14-7.08 (m, 2H), 7.04-6.99 (m, 3H), 6.78 (d, J = 7.6 Hz, 2H), 6.71 (d, J = 8.4 Hz, 1H), 6.58-6.56 (m, 2H), 6.35 (d, J = 8.4 Hz, 1H), 3.96, 3.72 (AB, J = 11.2 Hz, 2H), 2.89 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.25, 143.08, 134.16, 132.51, 130.37, 130.15, 129.84, 129.31, 128.42, 127.58, 127.27, 125.33, 124.22, 123.58, 123.18, 120.89, 110.81, 108.32, 102.24, 67.92, 43.48, 26.02, 21.31; IR (neat): 2924, 2854, 1722, 1612, 1492, 1469, 1456, 1371, 1319, 750, 736, 700; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$: 389.1624, Found: 389.1630.



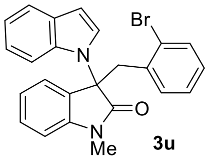
3s

Product **3s** was obtained in 74% yield as yellow solid; Mp: 180-182 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (d, J = 3.6 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.19-7.14 (m, 1H), 7.05-7.00 (m, 2H), 6.97-6.93 (m, 3H), 6.77 (d, J = 8.0 Hz, 1H), 6.70 (d, J = 7.6 Hz, 2H), 6.50-6.49 (m, 2H), 6.19 (s, 1H), 3.87, 3.65 (AB, J = 11.6 Hz, 2H), 2.82 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.29, 143.05, 136.19, 132.53, 131.43, 130.37, 129.83, 128.36, 127.65, 127.57, 127.25, 124.64, 124.27, 123.18, 121.88, 120.72, 111.35, 108.26, 102.51, 67.91, 43.50, 26.03, 22.19; IR (neat): 2927, 2858, 1722, 1612, 1508, 1492, 1469, 1456, 1373, 1325, 1238, 1089, 754, 700; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$: 389.1624, Found: 389.1627.



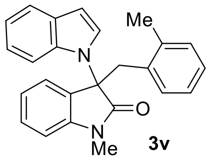
3t

Product **3t** was obtained in 73% yield as yellow solid; Mp: 153-155 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, *J* = 3.2 Hz, 1H), 7.26-7.22 (m, 1H), 7.13-7.08 (m, 2H), 7.04-7.00 (m, 4H), 6.77 (d, *J* = 7.6 Hz, 2H), 6.58-6.53 (m, 3H), 6.37 (d, *J* = 9.2 Hz, 1H), 3.94, 3.73 (AB, *J* = 11.6 Hz, 2H), 3.75 (s, 3H), 2.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.23, 154.28, 143.07, 132.49, 131.05, 130.44, 130.36, 129.91, 128.32, 127.60, 127.28, 125.95, 124.25, 123.20, 112.00, 111.91, 108.38, 102.92, 102.42, 67.95, 55.78, 43.45, 26.05; IR (neat): 2931, 2831, 1722, 1614, 1492, 1473, 1448, 1371, 1247, 767, 750, 700; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2O_2Na$ $[M+Na]^+$: 405.1573, Found: 405.1582.



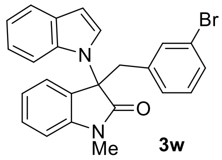
3u

Product **3u** was obtained in 68% yield as yellow solid; Mp: 149-151 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 2.8 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.27-7.23 (m, 1H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.08-7.01 (m, 3H), 6.98-6.89 (m, 3H), 6.66-6.60 (m, 3H), 4.38, 3.98 (AB, *J* = 12.4 Hz, 2H), 3.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.71, 142.86, 135.79, 133.02, 132.95, 131.18, 130.13, 129.02, 126.78, 126.42, 126.31, 125.80, 122.85, 122.02, 121.26, 120.19, 111.87, 108.09, 102.85, 67.87, 40.99, 26.34; IR (neat): 1720, 1612, 1471, 1456, 1263, 1234, 1029, 1020, 702, 538; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrN_2ONa$ $[M+Na]^+$: 453.0573, Found: 453.0579.



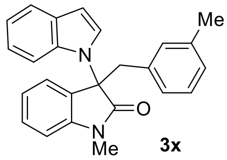
3v

Product **3v** was obtained in 77% yield as yellow solid; Mp: 150-152 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 3.2 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.30-7.26 (m, 1H), 7.07-6.96 (m, 5H), 6.91-6.88 (m, 2H), 6.71 (d, *J* = 7.6 Hz, 1H), 6.67-6.65 (m, 2H), 6.55 (d, *J* = 8.4 Hz, 1H), 3.97 (s, 2H), 3.00 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.87, 143.29, 137.70, 135.82, 131.18, 130.47, 130.36, 130.04, 128.24, 127.40, 125.60, 125.11, 124.92, 122.88, 121.98, 121.21, 120.13, 111.64, 108.36, 102.75, 68.11, 39.04, 26.19, 20.07; IR (neat): 2931, 1722, 1612, 1490, 1469, 1456, 1371, 1328, 1128, 1020, 736, 538; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$: 389.1624, Found: 389.1633.



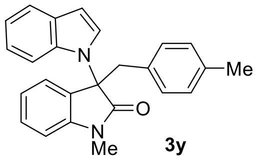
3w

Product **3w** was obtained in 84% yield as yellow solid; Mp: 144-146 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 3.2 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.29-7.22 (m, 2H), 7.10 (d, *J* = 7.2 Hz, 1H), 7.04-6.99 (m, 2H), 6.90-6.88 (m, 3H), 6.74 (d, *J* = 8.0 Hz, 1H), 6.64-6.60 (m, 2H), 6.48 (d, *J* = 8.4 Hz, 1H), 3.91, 3.66 (AB, *J* = 11.6 Hz, 2H), 2.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.91, 142.94, 135.77, 134.82, 133.16, 130.41, 130.19, 129.86, 129.16, 129.07, 127.88, 125.13, 124.21, 123.37, 122.07, 121.51, 121.22, 120.21, 111.21, 108.55, 102.91, 67.75, 43.11, 26.08; IR (neat): 2933, 1720, 1612, 1490, 1471, 1456, 1327, 1263, 1126, 1072, 696, 688; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrN_2ONa$ $[M+Na]^+$: 453.0573, Found: 453.0582.



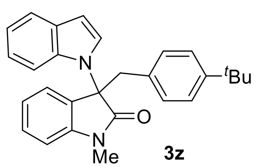
3x

Product **3x** was obtained in 77% yield as yellow solid; Mp: 128-130 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 3.2 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.28-7.23 (m, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 7.05-7.00 (m, 2H), 6.95-6.87 (m, 3H), 6.66 (d, *J* = 3.2 Hz, 1H), 6.61-6.58 (m, 3H), 6.49 (d, *J* = 8.4 Hz, 1H), 3.94, 3.71 (AB, *J*= 11.2 Hz, 2H), 2.92 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.23, 143.21, 137.22, 135.87, 132.36, 131.12, 129.91, 129.82, 128.54, 127.94, 127.50, 127.45, 125.31, 124.31, 123.12, 121.98, 121.18, 120.12, 111.31, 108.31, 102.73, 68.04, 43.61, 26.04, 21.20; IR (neat): 2928, 1720, 1687, 1612, 1490, 1469, 1456, 1328, 1126, 1093, 1018, 700, 692, 538; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$: 389.1624, Found: 389.1631.

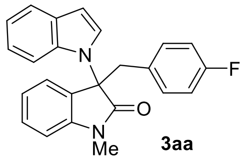


3y

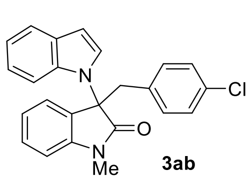
Product **3y** was obtained in 77% yield as yellow solid; Mp: 190-192 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 3.2 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.27-7.23 (m, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 2H), 6.89-6.82 (m, 3H), 6.67-6.60 (m, 4H), 6.48 (d, *J* = 8.4 Hz, 1H), 3.92, 3.70 (AB, *J* = 11.6 Hz, 2H), 2.91 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.28, 143.19, 136.86, 135.84, 130.24, 129.90, 129.83, 129.31, 128.50, 128.33, 125.31, 124.24, 123.14, 121.95, 121.15, 120.09, 111.29, 108.39, 102.69, 67.97, 43.19, 26.08, 21.13; IR (neat): 2926, 1720, 1612, 1514, 1490, 1469, 1456, 1328, 1126, 1020, 702, 692; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$: 389.1624, Found: 389.1630.



Product **3z** was obtained in 71% yield as yellow solid; Mp: 156-158 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 3.2 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.16 (t, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.97-6.92 (m, 4H), 6.80 (t, *J* = 8.0 Hz, 1H), 6.60 (d, *J* = 8.0 Hz, 2H), 6.56 (d, *J* = 3.2 Hz, 1H), 6.46 (d, *J* = 7.6 Hz, 1H), 6.40 (d, *J* = 8.4 Hz, 1H), 3.84, 3.63 (AB, *J* = 11.2 Hz, 2H), 2.76 (s, 3H), 1.13 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.20, 150.32, 143.13, 135.83, 130.00, 129.85, 129.82, 129.29, 128.52, 125.32, 124.35, 124.16, 123.13, 121.92, 121.12, 120.07, 111.24, 108.20, 102.66, 68.06, 43.19, 34.45, 31.36, 25.98; IR (neat): 2960, 2868, 1722, 1612, 1492, 1469, 1456, 1371, 1236, 1128, 1020, 736; HRMS (ESI): Exact mass calcd for $C_{28}H_{28}N_2ONa$ $[M+Na]^+$: 431.2094, Found: 431.2105.

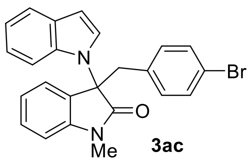


Product **3aa** was obtained in 74% yield as yellow solid; Mp: 228-230 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, *J* = 3.2 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 7.2 Hz, 1H), 7.04 (dd, J_1 = 14.8 Hz, J_2 = 7.2 Hz, 2H), 6.90 (t, *J* = 8.0 Hz, 1H), 6.76-6.72 (m, 4H), 6.66-6.63 (m, 2H), 6.48 (d, *J* = 8.4 Hz, 1H), 3.97, 3.73 (AB, *J* = 11.6 Hz, 2H), 2.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.10, 162.20 (d, *J* = 244.0 Hz), 143.06, 135.81, 131.96 (d, *J* = 8.0 Hz), 130.07, 129.88, 128.24 (d, *J* = 3.0 Hz), 128.18, 125.14, 124.20, 123.34, 122.07, 121.22, 120.20, 114.54 (d, *J* = 21.0 Hz), 111.19, 108.53, 102.88, 67.85, 42.70, 26.09; ^{19}F NMR (376 MHz, $CDCl_3$): δ -115.06; IR (neat): 2918, 2849, 1724, 1610, 1508, 1490, 1469, 1456, 1236, 1219, 1097, 837, 752, 738; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}FN_2ONa$ $[M+Na]^+$: 393.1374, Found: 393.1381.

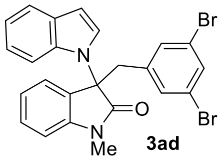


Product **3ab** was obtained in 73% yield as yellow solid; Mp: 230-232 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 3.2 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.06-7.02 (m, 4H), 6.91 (t, *J* = 8.0 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 2H), 6.66-6.65 (m, 2H), 6.50 (d, *J* = 8.4 Hz, 1H), 3.96, 3.73 (AB, *J* = 11.6 Hz, 2H), 2.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.00, 143.08, 135.80, 133.42, 131.72, 131.08, 130.16, 129.91, 128.04, 127.84, 125.13, 124.24, 123.36, 122.10, 121.25, 120.23, 111.23, 108.64, 102.93, 67.75, 42.83, 26.14; IR (neat): 2929, 1612, 1490, 1469, 1456, 1126, 1091, 1082, 1014, 763, 752; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}ClN_2ONa$

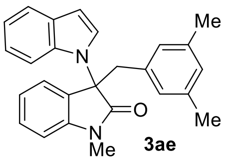
[M+Na]$^+$: 409.1078, Found: 409.1086.


3ac

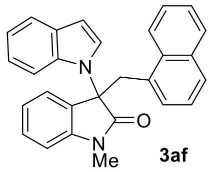
Product **3ac** was obtained in 80% yield as yellow solid; Mp: 210-212 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (d, *J* = 3.2 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.16 (dd, J_1 = 16.8 Hz, J_2 = 8.0 Hz, 3H), 7.04 (dd, J_1 = 12.4 Hz, J_2 = 6.8 Hz, 2H), 6.91 (t, *J* = 8.0 Hz, 1H), 6.67-6.65 (m, 4H), 6.50 (d, *J* = 8.4 Hz, 1H), 3.94, 3.71 (AB, *J* = 11.6 Hz, 2H), 2.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.00, 143.07, 135.79, 132.07, 131.60, 130.80, 130.19, 129.91, 128.01, 125.13, 124.25, 123.38, 122.11, 121.60, 121.25, 120.23, 111.23, 108.67, 102.94, 67.69, 42.88, 26.15; IR (neat): 2933, 1724, 1612, 1508, 1489, 1469, 1456, 1263, 1126, 1093, 808, 522; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrN_2ONa$ [M+Na]$^+$: 453.0573, Found: 453.0581.


3ad

Product **3ad** was obtained in 83% yield as yellow solid; Mp: 178-179 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.60 (m, 2H), 7.45 (s, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 7.2 Hz, 1H), 7.07 (dd, J_1 = 15.2 Hz, J_2 = 7.6 Hz, 2H), 6.93 (t, *J* = 7.6 Hz, 1H), 6.89 (s, 2H), 6.71-6.67 (m, 2H), 6.52 (d, *J* = 8.4 Hz, 1H), 3.90, 3.64 (AB, *J* = 11.6 Hz, 2H), 3.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.65, 142.81, 136.50, 135.72, 132.94, 132.10, 130.45, 129.85, 127.46, 125.01, 124.25, 123.51, 122.15, 121.85, 121.27, 120.31, 111.19, 108.72, 103.05, 67.55, 42.71, 26.14; IR (neat): 2931, 1716, 1612, 1552, 1490, 1469, 1456, 1313, 1126, 1089, 1001, 732; HRMS (ESI): Exact mass calcd for $C_{24}H_{18}Br_2N_2ONa$ [M+Na]$^+$: 530.9678, Found: 530.9684.

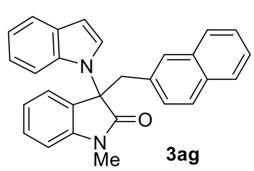

3ae

Product **3ae** was obtained in 73% yield as yellow solid; Mp: 144-146 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 3.6 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.26-7.22 (m, 1H), 7.12 (d, *J* = 7.2 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 2H), 6.88 (t, *J* = 7.6 Hz, 1H), 6.72 (s, 1H), 6.64 (d, *J* = 2.4 Hz, 1H), 6.58 (d, *J* = 8.0 Hz, 1H), 6.48 (d, *J* = 8.4 Hz, 1H), 6.38 (s, 2H), 3.88, 3.65 (AB, *J* = 11.6 Hz, 2H), 2.90 (s, 3H), 2.08 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.24, 143.25, 137.01, 135.88, 132.24, 129.89, 129.72, 128.72, 128.65, 128.23, 125.35, 124.32, 123.00, 121.93, 121.15, 120.09, 111.33, 108.24, 102.66, 68.05, 43.56, 26.00, 21.07; IR (neat): 2920, 2860, 1720, 1610, 1516, 1508, 1490, 1469, 1126, 1018, 702, 690, 538; HRMS (ESI): Exact mass calcd for $C_{26}H_{24}N_2ONa$ [M+Na]$^+$: 403.1781, Found: 403.1790.



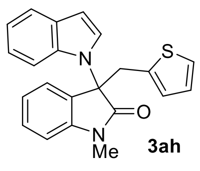
3af

Product **3af** was obtained in 85% yield as yellow solid; Mp: 190-192 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98-7.96 (m, 1H), 7.83 (d, *J* = 3.2 Hz, 1H), 7.72-7.69 (m, 1H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.37-7.35 (m, 2H), 7.15 (dd, J_1 = 14.0 Hz, J_2 = 7.6 Hz, 2H), 7.07-7.01 (m, 3H), 6.91-6.85 (m, 2H), 6.71 (d, *J* = 2.8 Hz, 1H), 6.43 (dd, J_1 = 18.0 Hz, J_2 = 8.4 Hz, 2H), 4.49, 4.36 (AB, *J* = 12.4 Hz, 2H), 2.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.77, 142.92, 135.95, 133.40, 132.26, 129.98, 129.73, 128.98, 128.93, 128.35, 128.20, 128.17, 125.56, 125.41, 124.93, 124.43, 124.21, 122.85, 121.99, 121.21, 120.14, 111.51, 108.09, 102.89, 68.16, 38.77, 25.93; IR (neat): 2933, 1720, 1612, 1514, 1490, 1469, 1454, 1126, 1089, 1016, 702, 692; HRMS (ESI): Exact mass calcd for $C_{28}H_{22}N_2ONa$ $[M+Na]^+$: 425.1624, Found: 425.1631.



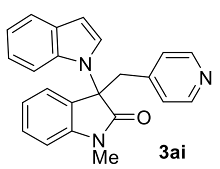
3ag

Product **3ag** was obtained in 83% yield as yellow solid; Mp: 208-210 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71-7.68 (m, 2H), 7.61-7.57 (m, 2H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.39-7.37 (m, 2H), 7.26 (s, 1H), 7.20-7.16 (m, 2H), 7.01 (t, *J* = 7.6 Hz, 2H), 6.90-6.86 (m, 2H), 6.66 (d, *J* = 3.2 Hz, 1H), 6.50 (d, *J* = 8.4 Hz, 1H), 6.43 (d, *J* = 7.6 Hz, 1H), 4.11, 3.87 (AB, *J* = 11.6 Hz, 2H), 2.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.20, 143.06, 135.84, 132.93, 132.43, 130.03, 129.92, 129.45, 128.30 127.76, 127.51, 126.97, 125.97, 125.94, 125.31, 124.29, 123.18, 122.00, 121.19, 120.14, 111.30, 108.46, 102.79, 68.02, 43.63, 26.02; IR (neat): 2931, 1720, 1612, 1508, 1490, 1469, 1456, 1124, 1083, 1016, 1001, 734, 692; HRMS (ESI): Exact mass calcd for $C_{28}H_{22}N_2ONa$ $[M+Na]^+$: 425.1624, Found: 425.1634.

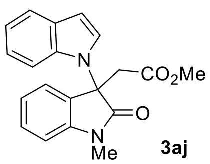


3ah

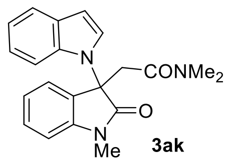
Product **3ah** was obtained in 61% yield as yellow solid; Mp: 178-180 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61-7.60 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.13-7.02 (m, 4H), 6.94 (t, *J* = 7.7 Hz, 1H), 6.79-6.76 (m, 2H), 6.66-6.64 (m, 2H), 6.61 (d, *J* = 3.2 Hz, 1H), 4.19, 4.04 (AB, *J* = 13.2 Hz, 2H), 3.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.03, 143.73, 135.90, 133.99, 130.31, 129.98, 128.35, 128.17, 126.31, 125.48, 125.36, 124.63, 123.40, 122.08, 121.21, 120.21, 111.58, 108.61, 102.92, 67.50, 37.58, 26.30; IR (neat): 2924, 1716, 1610, 1492, 1469, 1456, 1311, 1236, 1122, 1018, 732, 692; HRMS (ESI): Exact mass calcd for $C_{22}H_{18}N_2OSNa$ $[M+Na]^+$: 381.1032, Found: 381.1039.


3ai

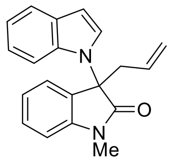
Product **3ai** was obtained in 60% yield as white solid; Mp: 200-202 ºC; ^{1}H NMR (400 MHz, CDCl$_3$)**:** δ 8.30 (d, *J* = 4.8 Hz, 2H), 7.62-7.59 (m, 2H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 7.2 Hz, 1H), 7.05 (dd, J_1 = 15.2 Hz, J_2 = 7.6 Hz, 2H), 6.91 (t, *J* = 8.0 Hz, 1H), 6.72 (d, *J* = 4.8 Hz, 2H), 6.66-6.63 (m, 2H), 6.51 (d, *J* = 8.4 Hz, 1H), 3.96, 3.73 (AB, *J* = 11.2 Hz, 2H), 2.95 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 173.64, 149.18, 142.95, 141.86, 135.68, 130.44, 129.93, 127.51, 125.45, 125.02, 124.29, 123.52, 122.20, 121.31, 120.32, 111.18, 108.76, 103.12, 67.36, 42.77, 26.08; IR (neat): 2929, 1716, 1612, 1600, 1490, 1469, 1456, 1313, 1234, 1126, 736, 692; HRMS (ESI): Exact mass calcd for $C_{23}H_{19}N_3ONa$ [M+Na]$^+$: 376.1420, Found: 376.1423.


3aj

Product **3aj** was obtained in 37% yield as yellow solid; Mp: 110-112 ºC; ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.56 (d, *J* = 7.2 Hz, 1H), 7.45 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.34 (dd, J_1 = 7.2 Hz, J_2 = 0.8 Hz, 1H), 7.28 (d, *J* = 3.6 Hz, 1H), 7.10 (td, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H), 7.04-6.96 (m, 3H), 6.87 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1H), 6.54 (dd, J_1 = 3.2 Hz, J_2 = 0.8 Hz, 1H), 3.83, 3.60 (AB, *J* = 15.2 Hz, 2H), 3.51 (s, 3H), 3.30 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 173.92, 168.58, 144.52, 135.60, 130.82, 130.30, 127.34, 125.85, 125.31, 123.30, 122.11, 121.32, 120.27, 112.18, 109.02, 102.96, 64.05, 52.15, 41.23, 26.77; IR (neat): 2920, 2848, 1724, 1612, 1492, 1469, 1454, 1238, 1199, 1128, 1087, 1018, 738; HRMS (ESI): Exact mass calcd for $C_{20}H_{18}N_2O_3Na$ [M+Na]$^+$: 357.1210, Found: 357.1205.

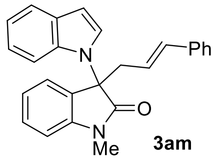

3ak

Product **3ak** was obtained in 27% yield as yellow solid; Mp: 66-68 ºC; ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.58-7.56 (m, 1H), 7.44-7.35 (m, 3H), 7.15 (d, *J* = 3.2 Hz, 1H), 7.11-7.04 (m, 3H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.47 (d, *J* = 3.2 Hz, 1H), 4.01, 3.59 (AB, *J* = 16.0 Hz, 2H), 3.27 (s, 3H), 2.98 (s, 3H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 174.59, 167.46, 145.22, 135.55, 130.44, 130.40, 128.19, 126.34, 124.82, 122.61, 121.89, 121.29, 120.08, 113.23, 108.99, 102.29, 64.97, 39.48, 37.56, 35.57, 26.73; IR (neat): 2929, 1722, 1647, 1610, 1492, 1469, 1452, 1165, 1147, 1126, 1087, 731; HRMS (ESI): Exact mass calcd for $C_{21}H_{21}N_3O_2Na$ [M+Na]$^+$: 370.1526, Found: 370.1527.



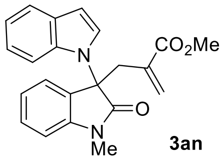
3al

Product **3al** was obtained in 65% yield as yellow solid; Mp: 80-82 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, J = 8.0 Hz, 2H), 7.41 (t, J = 7.6 Hz, 1H), 7.14 (d, J = 7.6 Hz, 1H), 7.08-6.98 (m, 3H), 6.89 (t, J = 7.6 Hz, 1H), 6.60 (d, J = 2.8 Hz, 1H), 6.46 (d, J = 8.4 Hz, 1H), 5.51-5.40 (m, 1H), δ 5.15 (d, J = 17.2 Hz, 1H), 5.07 (d, J = 10.0 Hz, 1H), 3.37-3.25 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.53, 143.27, 135.78, 129.99, 129.94, 129.61, 128.65, 125.60, 124.42, 123.41, 121.94, 121.24, 121.14, 120.07, 111.19, 108.70, 102.70, 66.41, 41.58, 26.45; IR (neat): 2918, 1720, 1610, 1490, 1469, 1456, 1369, 1234, 1078, 1018, 736, 692; HRMS (ESI): Exact mass calcd for $C_{20}H_{18}N_2ONa$ $[M]^+$: 325.1311, Found: 325.1310.



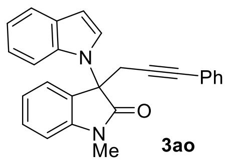
3am

Product **3am** was obtained in 83% yield as yellow solid; Mp: 100-102 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.57 (m, 2H), 7.39 (t, J = 7.6 Hz, 1H), 7.26-7.19 (m, 3H), 7.15-7.14 (m, 3H), 7.08-6.89 (m, 2H), 6.95-6.89 (m, 2H), 6.62 (d, J = 2.8 Hz, 1H), 6.48-6.42 (m, 2H), 5.83-5.76 (m, 1H), 3.49 (dd, J_1 = 12.8 Hz, J_2 = 6.4 Hz, 1H), 3.37 (dd, J_1 = 12.4 Hz, J_2 = 8.4 Hz, 1H), 3.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.57, 143.19, 136.83, 135.97, 135.86, 130.09, 129.95, 128.69, 128.63, 127.78, 126.33, 125.66, 124.48, 123.47, 121.98, 121.18, 120.81, 120.12, 111.23, 108.76, 102.83, 66.80, 40.75, 26.53; IR (neat): 1722, 1612, 1471, 1456, 1265, 1128, 968, 731, 692, 538; HRMS (ESI): Exact mass calcd for $C_{26}H_{22}N_2ONa$ $[M+Na]^+$: 401.1624, Found: 401.1632.

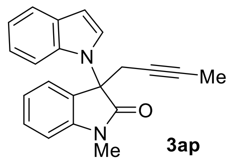


3an

Product **3an** was obtained in 85% yield as yellow solid; Mp: 133-135 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58-7.56 (m, 2H), 7.36 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.13 (dd, J_1 = 7.2 Hz, J_2 = 0.8 Hz, 1H), 7.12-7.00 (m, 2H), 6.92-6.89 (m, 2H), 6.61 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 6.48 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 6.04 (s, 1H), 5.57 (d, J = 0.8 Hz, 1H), 3.97, 3.55 (AB, J = 15.2 Hz, 2H), 3.44 (s, 3H), 3.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.26, 166.98, 143.36, 135.69, 133.83, 130.28, 129.99, 129.42, 126.87, 126.04, 125.43, 123.03, 122.03, 121.23, 120.17, 111.23, 108.71, 102.85, 67.10, 51.91, 37.84, 26.35; IR (neat): 2949, 2931, 1720, 1612, 1516, 1492, 1471, 1456, 1319, 1234, 1126, 1082, 738; HRMS (ESI): Exact mass calcd for $C_{22}H_{20}N_2O_3Na$ $[M+Na]^+$: 383.1366, Found: 383.1371.

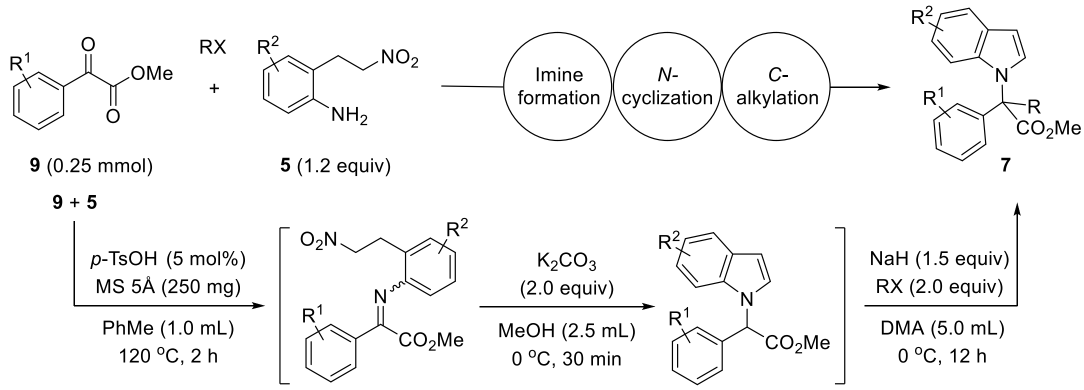

3ao

Product **3ao** was obtained in 84% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 3.2 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.26-7.25 (m, 5H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.05-7.00 (m, 2H), 6.90 (t, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 2.4 Hz, 1H), 6.42 (d, *J* = 8.4 Hz, 1H), 3.78 (d, *J* = 16.4 Hz, 1H), 3.34-3.30 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.18, 143.26, 135.79, 131.70, 130.40, 130.01, 128.45, 128.39, 126.32, 125.20, 123.58, 122.79, 122.06, 121.20, 120.20, 111.05, 108.81, 102.91, 84.92, 82.75, 65.39, 29.20, 26.75; IR (neat): 2933, 1724, 1612, 1490, 1469, 1456, 1369, 1315, 754, 738; HRMS (ESI): Exact mass calcd for $C_{26}H_{20}N_2ONa$ $[M+Na]^+$: 399.1468, Found: 399.1476.

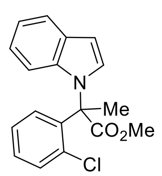

3ap

Product **3ap** was obtained in 64% yield as yellow solid; Mp: 138-140 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 3.2 Hz, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 7.6 Hz, 2H), 6.88 (t, *J* = 7.6 Hz, 1H), 6.62 (d, *J* = 2.8 Hz, 1H), 6.35 (d, *J* = 8.4 Hz, 1H), 3.51 (d, *J* = 16.4 Hz, 1H), 3.33 (s, 3H), 3.01 (d, *J* = 16.8 Hz, 1H), 1.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.35, 143.09, 135.75, 130.22, 129.94, 128.59, 126.52, 125.14, 123.42, 121.94, 121.11, 120.08, 110.95, 108.70, 102.66, 80.71, 72.10, 65.26, 28.57, 26.67, 3.59; IR (neat): 2920, 1722, 1612, 1471, 1456, 1369, 1265, 1074, 731, 702, 536; HRMS (ESI): Exact mass calcd for $C_{21}H_{18}N_2ONa$ $[M+Na]^+$: 337.1311, Found: 337.1305.

5. General procedure for one-pot tandem sequence of keto esters.

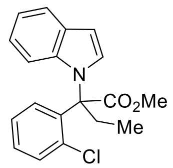


To a 25-mL Schlenk reaction tube were added α-ketoester **9** (0.25 mmol, 1.0 equiv), aniline derivatives **5** (0.3 mmol, 1.2 equiv), MS 5Å (250.0 mg) and anhydrous toluene (1.0 mL), followed by the addition of *p*-TsOH (2.2 mg, 5 mol%). The reaction mixture was stirred at 120 ºC for 2 h, and then cooled down to room temperature for concentration under vacuum. The thus obtained residue was dissolved in anhydrous MeOH (2.5 mL), followed by the addition of K_2CO_3 (69.1 mg, 0.5 mmol) at 0 ºC. The resulting mixture was stirred at 0 ºC for 30 min, concentrated in vacuum, and then the residue was dissolved in anhydrous DMA (5.0 mL), followed by the addition of alkyl iodides (0.5 mmol, 2.0 equiv) or alkyl bromides (0.5 mmol, 2.0 equiv) and NaH (15.0 mg, 0.375 mmol) at 0 ºC. The resulting mixture was stirred at 0 ºC for 12 h, and then quenched with saturated aqueous NH_4Cl (5 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with water (3 × 20 mL) and brine (20 mL), then dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the desired product **7a**-**7t**.



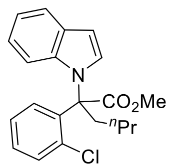
7a

Product **7a** was obtained in 85% yield as white solid; Mp: 93-95 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.46-7.43 (m, 2H), 7.27 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.14-6.98 (m, 4H), 6.77 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 6.64 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 3.71 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.97, 138.12, 136.04, 132.44, 131.54, 130.24, 129.37, 128.91, 127.02, 125.90, 121.40, 120.93, 120.06, 115.33, 103.07, 68.15, 52.88, 25.57; IR (neat): 2951, 2922, 1739, 1517, 1471, 1452, 1292, 1230, 1112, 1091, 1018, 763, 742; HRMS (ESI): Exact mass calcd for $C_{18}H_{16}ClNO_2Na$ $[M+Na]^+$: 336.0762, Found: 336.0760.



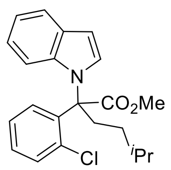
7b

Product **7b** was obtained in 74% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61-7.59 (m, 1H), 7.51 (d, J = 3.6 Hz, 1H), 7.44 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.29 (td, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 1H), 7.16 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.06 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 2H), 6.94-6.91 (m, 2H), 6.63 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 3.64 (s, 3H), 3.04-2.98 (m, 1H), 2.92-2.86 (m, 1H), 0.81 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.93, 135.87, 135.22, 132.73, 131.48, 131.13, 130.10, 129.34, 126.86, 126.16, 121.17, 120.78, 119.99, 115.59, 103.13, 71.31, 52.64, 28.13, 8.98; IR (neat): 2949, 1737, 1508, 1471, 1452, 1433, 1192, 1180, 1018, 1004, 734, 688; HRMS (ESI): Exact mass calcd for $C_{19}H_{18}ClNO_2Na$ $[M+Na]^+$: 350.0918, Found: 350.0917.



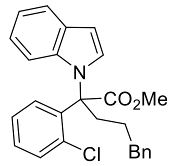
7c

Product **7c** was obtained in 62% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.58 (m, 1H), 7.46 (d, J = 3.6 Hz, 1H), 7.43 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.28 (td, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.15 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.06-7.03 (m, 2H), 6.94-6.91 (m, 2H), 6.62 (dd, J_1 = 3.6 Hz, J_2 = 0.4 Hz, 1H), 3.64 (s, 3H), 2.91-2.87 (m, 2H), 1.35-1.27 (m, 3H), 0.88-0.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.90, 135.92, 135.53, 132.70, 131.44, 130.94, 130.10, 129.30, 126.73, 126.19, 121.18, 120.79, 119.99, 115.60, 103.16, 70.97, 52.64, 34.73, 26.43, 22.81, 13.96; IR (neat): 2929, 1737, 1519, 1469, 1452, 1431, 1193, 1180, 1053, 1018, 763, 738; HRMS (ESI): Exact mass calcd for $C_{21}H_{22}ClNO_2Na$ $[M+Na]^+$: 378.1231, Found: 378.1238.

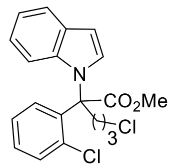


7d

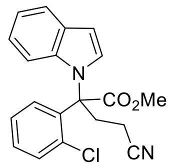
Product **7d** was obtained in 65% yield as yellow solid; Mp: 83-85 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, J = 8.0 Hz, 1H), 7.48 (d, J = 3.6 Hz, 1H), 7.44 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.29 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.15-7.13 (m, 1H), 7.06-7.03 (m, 2H), 6.95-6.92 (m, 2H), 6.63 (d, J = 3.6 Hz, 1H), 3.64 (s, 3H), 2.94-2.87 (m, 2H), 1.62-1.50 (m, 1H), 1.31-1.25 (m, 1H), 0.91 (d, J = 6.8 Hz, 3H), 0.84 (d, J = 6.8 Hz, 3H), 0.76-0.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.92, 135.94, 135.46, 132.67, 131.44, 131.03, 130.11, 129.30, 126.73, 126.15, 121.17, 120.79, 120.00, 115.65, 103.17, 71.04, 52.64, 33.08, 32.92, 28.38, 22.71, 22.40; IR (neat): 2954, 2927, 1737, 1469, 1452, 1431, 1195, 1180, 1055, 1047, 1018, 734, 704; HRMS (ESI): Exact mass calcd for $C_{22}H_{24}ClNO_2Na$ $[M+Na]^+$: 392.1388, Found: 392.1396.


7e

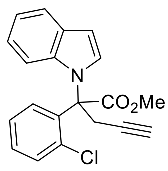
Product **7e** was obtained in 76% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, J = 7.6 Hz, 1H), 7.41 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.28-7.26 (m, 2H), 7.24-7.17 (m, 2H), 7.18-7.10 (m, 2H), 7.09-6.99 (m, 4H), 6.92-6.88 (m, 2H), 6.56 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 3.60 (s, 3H), 2.94-2.87 (m, 2H), 2.59 (t, J = 7.6 Hz, 2H), 1.67-1.64 (m, 1H), 1.28-1.22 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.79, 141.39, 135.89, 135.36, 132.73, 131.48, 130.91, 130.10, 129.40, 128.54, 128.53, 126.63, 126.27, 126.16, 121.21, 120.81, 120.02, 115.57, 103.22, 70.88, 52.66, 35.66, 34.29, 25.93; IR (neat): 2922, 1737, 1517, 1469, 1452, 1431, 1195, 1178, 1037, 1018, 734, 698; HRMS (ESI): Exact mass calcd for $C_{26}H_{24}ClNO_2Na$ $[M+Na]^+$: 440.1388, Found: 440.1398.


7f

Product **7f** was obtained in 53% yield as yellow solid; Mp: 98-100 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, J = 7.6 Hz, 1H), 7.53 (d, J = 3.6 Hz, 1H), 7.45 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.31 (td, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.17 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.07-7.03 (m, 2H), 6.95-6.93 (m, 1H), 6.91-6.90 (m, 1H), 6.64 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 3.66 (s, 3H), 3.55-3.51 (m, 1H), 3.49-3.46 (m, 1H), 3.23-3.13 (m, 1H), 3.03-2.92 (m, 1H), 1.84-1.81 (m, 1H), 1.42-1.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.58, 135.89, 135.17, 132.73, 131.66, 130.73, 130.14, 129.65, 126.56, 126.45, 121.35, 120.92, 120.16, 115.54, 103.56, 70.51, 52.83, 44.74, 32.72, 27.61; IR (neat): 2951, 2920, 1735, 1519, 1469, 1452, 1431, 1197, 1180, 1089, 1018, 763, 736; HRMS (ESI): Exact mass calcd for $C_{20}H_{19}Cl_2NO_2Na$ $[M+Na]^+$: 398.0685, Found: 398.0694.

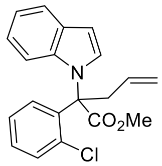

7g

Product **7g** was obtained in 50% yield as white solid; Mp: 58-60 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, J = 7.6 Hz, 1H), 7.47 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.36 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.32 (d, J = 3.6 Hz, 1H), 7.23 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.13-7.04 (m, 2H), 7.01-6.95 (m, 1H), 6.84 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1H), 6.66 (dd, J_1 = 3.2 Hz, J_2 = 0.4 Hz, 1H), 3.71 (s, 3H), 3.46-3.36 (m, 1H), 3.30-3.20 (m, 1H), 2.45-2.35 (m, 1H), 2.08-1.97 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.22, 135.78, 134.02, 132.90, 132.15, 130.39, 130.30, 130.09, 127.01, 125.95, 121.97, 121.31, 120.58, 118.59, 114.80, 104.22, 69.99, 53.26, 31.55, 13.20; IR (neat): 2954, 2254, 1737, 1452, 1433, 1265, 763; HRMS (ESI): Exact mass calcd for $C_{20}H_{17}ClN_2O_2Na$ $[M+Na]^+$: 375.0871, Found: 375.0874.



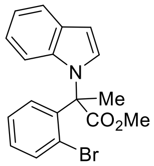
7h

Product **7h** was obtained in 65% yield as yellow solid; Mp: 102-104 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 3.6 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.47 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.32 (td, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.14 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.11-7.06 (m, 1H), 7.03-6.96 (m, 3H), 6.66 (d, J = 3.2 Hz, 1H), 3.94, 3.77 (ABd, J_1 = 18.0 Hz, J_2 = 2.4 Hz, 2H), 3.67 (s, 3H), 1.93 (t, J = 2.4 Hz, 1H); [13]C NMR (100 MHz, $CDCl_3$): δ 168.53, 135.71, 134.33, 132.17, 131.73, 131.12, 130.24, 129.85, 127.06, 126.18, 121.37, 120.89, 120.26, 115.70, 103.44, 78.35, 73.64, 69.86, 52.98, 27.41; IR (neat): 2951, 1735, 1508, 1471, 1454, 1431, 1242, 1193, 1058, 1047, 1020, 734, 690; HRMS (ESI): Exact mass calcd for $C_{20}H_{16}ClNO_2Na$ $[M+Na]^+$: 360.0762, Found: 360.0765.



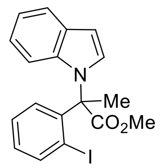
7i

Product **7i** was obtained in 70% yield as yellow oil; [1]H NMR (400 MHz, $CDCl_3$): δ 7.61-7.57 (m, 2H), 7.43 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.30-7.26 (m, 1H), 7.15 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.09-7.04 (m, 1H), 7.00 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 6.98-6.89 (m, 2H), 6.62-6.61 (m, 1H), 5.59-5.52 (m, 1H), 5.11-5.06 (m, 1H), 5.01-4.98 (m, 1H), 3.82-3.73 (m, 1H), 3.67-3.62 (m, 4H); [13]C NMR (100 MHz, $CDCl_3$): δ 169.47, 135.96, 135.20, 132.77, 131.90, 131.49, 131.00, 130.12, 129.49, 127.00, 126.27, 121.26, 120.85, 120.12, 119.70, 115.50, 103.21, 70.66, 52.76, 39.70; IR (neat): 2953, 1737, 1473, 1454, 1433, 1265, 1020, 731, 702; HRMS (ESI): Exact mass calcd for $C_{20}H_{18}ClNO_2Na$ $[M+Na]^+$: 362.0918, Found: 362.0919.



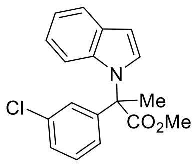
7j

Product **7j** was obtained in 80% yield as white solid; Mp: 127-128 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.65-7.61 (m, 2H), 7.46 (d, J = 3.6 Hz, 1H), 7.18-7.16 (m, 2H), 7.08-7.06 (m, 1H), 6.99-6.96 (m, 2H), 6.82-6.80 (m, 1H), 6.64 (dd, J_1 = 3.6 Hz, J_2 = 0.4 Hz, 1H), 3.71 (s, 3H), 2.39 (s, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 169.91, 139.43, 136.05, 135.21, 130.25, 129.52, 129.21, 127.59, 125.99, 121.88, 121.37, 120.90, 120.06, 115.40, 103.13, 69.21, 52.90, 25.80; IR (neat): 2949, 1737, 1517, 1467, 1452, 1429, 1193, 1111, 1089, 1039, 1018, 761, 740; HRMS (ESI): Exact mass calcd for $C_{18}H_{16}BrNO_2Na$ $[M+Na]^+$: 380.0257, Found: 380.0257.



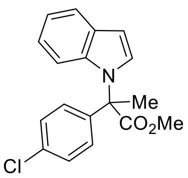
7k

Product **7k** was obtained in 75% yield as yellow solid; Mp: 160-162 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.46 (d, J = 3.6 Hz, 1H), 7.29-7.22 (m, 1H), 7.09-7.04 (m, 1H), 6.99 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 6.96-6.88 (m, 2H), 6.85 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 6.64 (dd, J_1 = 3.2 Hz, J_2 = 0.4 Hz, 1H), 3.71 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.10, 142.89, 141.72, 136.22, 130.20, 129.50, 128.82, 128.36, 126.18, 121.37, 120.85, 120.01, 115.14, 103.21, 95.19, 70.58, 52.95, 26.12; IR (neat): 2922, 1735, 1562, 1517, 1508, 1489, 1452, 1193, 1126, 1087, 1008, 761, 740; HRMS (ESI): Exact mass calcd for $C_{18}H_{16}INO_2Na$ $[M+Na]^+$: 428.0118, Found: 428.0121.



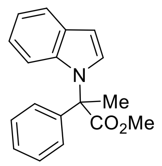
7l

Product **7l** was obtained in 52% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65-7.63 (m, 1H), 7.42 (t, J = 1.6 Hz, 1H), 7.35-7.31 (m, 1H), 7.26 (t, J = 8.0 Hz, 1H), 7.14-7.10 (m, 3H), 7.08-7.04 (m, 1H), 6.78 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 6.58 (dd, J_1 = 3.2 Hz, J_2 = 0.8 Hz, 1H), 3.74 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.86, 142.10, 136.13, 134.66, 129.91, 129.85, 128.66, 127.54, 126.08, 125.41, 121.91, 121.30, 120.09, 112.64, 102.52, 67.14, 53.31, 26.96; IR (neat): 2953, 1737, 1516, 1508, 1475, 1456, 1433, 1263, 1195, 1111, 1072, 763, 702; HRMS (ESI): Exact mass calcd for $C_{18}H_{16}ClNO_2Na$ $[M+Na]^+$: 336.0762, Found: 336.0767.



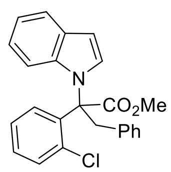
7m

Product **7m** was obtained in 50% yield as yellow solid; Mp: 103-105 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.61 (m, 1H), 7.33-7.27 (m, 2H), 7.26-7.20 (m, 2H), 7.13 (d, J = 3.2 Hz, 1H), 7.08 (td, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.05-6.99 (m, 1H), 6.76 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 6.56 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 3.72 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.05, 138.60, 136.12, 134.42, 129.85, 128.82, 128.68, 126.07, 121.87, 121.29, 120.07, 112.66, 102.44, 67.06, 53.26, 26.98; IR (neat): 2951, 2918, 1735, 1516, 1492, 1456, 1433, 1195, 1095, 1076, 1012, 765, 713; HRMS (ESI): Exact mass calcd for $C_{18}H_{16}ClNO_2Na$ $[M+Na]^+$: 336.0762, Found: 336.0767.



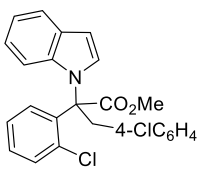
7n

Product **7n** was obtained in 44% yield as yellow solid; Mp: 85-87 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65-7.63 (m, 1H), 7.37 (s, 5H), 7.11-7.08 (m, 2H), 7.07-7.03 (m, 1H), 6.82 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 6.55 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 3.75 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.40, 139.82, 136.25, 129.87, 128.71, 128.50, 127.22, 126.48, 121.63, 121.19, 119.86, 112.84, 102.06, 67.55, 53.13, 26.49; IR (neat): 2951, 2922, 1735, 1514, 1494, 1473, 1454, 1433, 1195, 1107, 1074, 1018, 738, 696; HRMS (ESI): Exact mass calcd for $C_{18}H_{17}NO_2Na$ $[M+Na]^+$: 302.1151, Found: 302.1147.



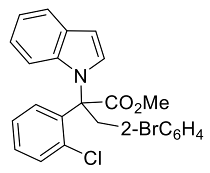
7o

Product **7o** was obtained in 60% yield as yellow solid; Mp: 140-141 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, J = 3.6 Hz, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.28-7.22 (m, 3H), 7.15-7.09 (m, 2H), 7.04 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 3H), 6.87 (t, J = 7.6 Hz, 1H), 6.73 (d, J = 8.4 Hz, 1H), 6.68 (d, J = 7.6 Hz, 2H), 6.55 (d, J = 3.6 Hz, 1H), 4.34, 4.04 (AB, J = 13.6 Hz, 2H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.31, 135.81, 135.45, 134.72, 133.80, 131.59, 130.94, 130.73, 129.92, 129.48, 127.94, 127.70, 127.15, 126.25, 121.11, 120.89, 119.89, 114.21, 102.47, 71.42, 52.80, 42.00; IR (neat): 2922, 1739, 1496, 1473, 1452, 1431, 1288, 1224, 1193, 1176, 1082, 1020, 740, 700; HRMS (ESI): Exact mass calcd for $C_{24}H_{20}ClNO_2Na$ $[M+Na]^+$: 412.1075, Found: 412.1084.



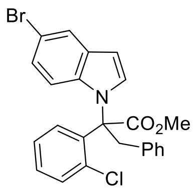
7p

Product **7p** was obtained in 51% yield as white solid; Mp: 151-153 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, J = 3.6 Hz, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.29-7.24 (m, 3H), 7.18-7.16 (m, 1H), 7.07-7.02 (m, 3H), 6.93-6.86 (m, 1H), 6.73 (d, J = 8.4 Hz, 1H), 6.63 (d, J = 8.4 Hz, 2H), 6.57 (d, J = 3.6 Hz, 1H), 4.34, 4.00 (AB, J = 13.6 Hz, 2H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.30, 135.85, 135.26, 133.83, 133.25, 133.21, 132.13, 131.72, 130.85, 129.96, 129.66, 128.07, 127.42, 126.45, 121.25, 120.99, 120.01, 114.24, 102.76, 71.37, 52.84, 41.49; IR (neat): 1743, 1735, 1508, 1490, 1452, 1433, 1274, 1259, 1193, 1016, 763, 748; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}Cl_2NO_2Na$ $[M+Na]^+$: 446.0685, Found: 446.0695.



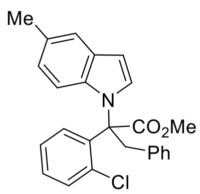
7q

Product **7q** was obtained in 41% yield as white solid; Mp: 150-152 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, J = 3.6 Hz, 1H), 7.78-7.71 (m, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.47 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.36-7.26 (m, 3H), 7.07-6.99 (m, 2H), 6.96-6.86 (m, 2H), 6.78 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1H), 6.50 (dd, J_1 = 3.6 Hz, J_2 = 0.4 Hz, 1H), 6.29-6.19 (m, 1H), 4.50, 4.37 (AB, J = 14.4 Hz, 2H), 3.71 (s, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 169.01, 136.79, 135.68, 134.64, 134.41, 132.77, 131.80, 131.72, 130.01, 129.93, 129.61, 128.83, 127.12, 126.37, 126.34, 121.26, 121.12, 119.88, 113.23, 101.76, 70.24, 53.20, 40.79; IR (neat): 2951, 1745, 1473, 1452, 1433, 1253, 1197, 1178, 1066, 1022, 758, 738; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrClNO_2Na$ $[M+Na]^+$: 490.0180, Found: 490.0193.



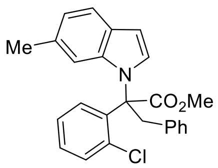
7r

Product **7r** was obtained in 57% yield as yellow solid; Mp: 118-120 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, J = 3.6 Hz, 1H), 7.71 (d, J = 2.0 Hz, 1H), 7.31-7.26 (m, 3H), 7.20-7.13 (m, 2H), 7.07 (t, J = 7.6 Hz, 2H), 6.95 (dd, J_1 = 9.2 Hz, J_2 = 2.0 Hz, 1H), 6.66 (d, J = 7.6 Hz, 2H), 6.58 (d, J = 8.8 Hz, 1H), 6.48 (d, J = 3.6 Hz, 1H), 4.29, 4.03 (AB, J = 13.2 Hz, 2H), 3.70 (s, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 169.10, 135.25, 134.43, 134.40, 133.88, 131.75, 131.62, 130.64, 129.73, 129.07, 128.03, 127.31, 126.45, 123.95, 123.36, 115.30, 113.34, 101.88, 71.43, 52.93, 42.08; IR (neat): 2951, 1739, 1564, 1516, 1508, 1496, 1471, 1446, 1192, 1082, 1056, 1026, 736, 700; HRMS (ESI): Exact mass calcd for $C_{24}H_{19}BrClNO_2Na$ $[M+Na]^+$: 490.0180, Found: 490.0189.



7s

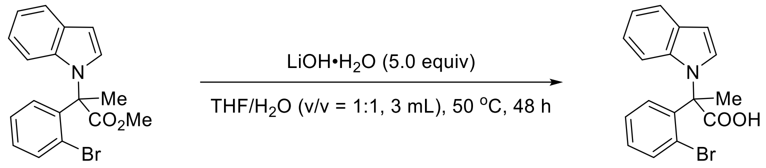
Product **7s** was obtained in 65% yield as yellow solid; Mp: 120-122 ºC; [1]H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 3.6 Hz, 1H), 7.40 (s, 1H), 7.32-7.24 (m, 3H), 7.16-7.13 (m, 2H), 7.09-7.05 (m, 2H), 6.73-6.72 (m, 3H), 6.66-6.64 (m, 1H), 6.51-6.50 (m, 1H), 4.35, 4.06 (AB, J= 13.6 Hz, 2H), 3.70 (s, 3H), 2.40 (s, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 169.33, 135.54, 134.78, 134.15, 133.79, 131.52, 130.97, 130.75, 130.22, 129.42, 129.06, 127.91, 127.76, 127.11, 126.20, 122.74, 120.63, 113.89, 102.00, 71.35, 52.74, 41.95, 21.32; IR (neat): 2920, 2856, 1737, 1496, 1471, 1456, 1431, 1225, 1192, 1176, 1082, 1028, 731, 700; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}ClNO_2Na$ $[M+Na]^+$: 426.1231, Found: 426.1239.



7t

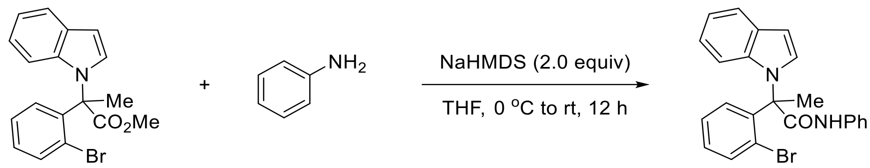
Product **7t** was obtained in 72% yield as white solid; Mp: 60-62 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 3.6 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.32 (td, J_1 = 8.0 Hz , J_2 = 1.2 Hz, 2H), 7.25 (td, J_1 = 7.2 Hz , J_2 = 1.6 Hz, 1H), 7.19-7.12 (m, 2H), 7.09-7.05 (m, 2H), 6.90 (dd, J_1 = 8.0 Hz , J_2 = 0.8 Hz, 1H), 6.72 (d, *J* = 7.2 Hz, 2H), 6.55 (s, 1H), 6.52 (dd, J_1 = 3.6 Hz , J_2 = 0.4 Hz, 1H), 4.35, 4.08 (AB, *J* = 13.6 Hz, 2H), 3.71 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.31, 136.25, 135.57, 134.83, 133.81, 131.58, 130.97, 130.72, 130.60, 129.40, 127.91, 127.75, 127.25, 127.11, 126.15, 121.64, 120.40, 114.23, 102.20, 71.37, 52.77, 41.97, 22.13; IR (neat): 2920, 1737, 1516, 1496, 1471, 1456, 1433, 1192, 1176, 1082, 752, 700; HRMS (ESI): Exact mass calcd for $C_{25}H_{22}ClNO_2Na$ $[M]^+$: 426.1231, Found: 426.1243.

6. Product transformation



7j (0.3 mmol) **10** (84% yield)

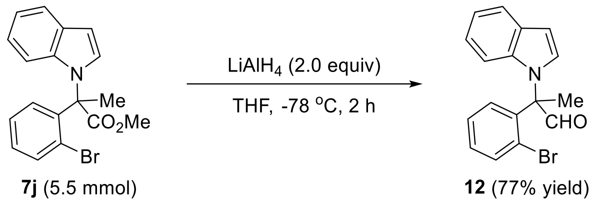
To a solution of methyl 2-(2-bromophenyl)-2-(1H-indol-1-yl)propanoate **7j** (107.5 mg, 0.3 mmol) in THF/H_2O (v/v = 1:1, 3 mL) was added LiOH·H_2O (63.0 mg, 1.5 mmol). The reaction mixture was stirred at 50 °C for 48 h, and then cooled down to room temperature, acidified with HCl (2 M, 10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (CH_2Cl_2/MeOH, 20/1, v/v) to afford the title compound **10** in 84% yield as white solid; Mp: 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64-7.61 (m, 2H), 7.44 (d, J = 3.6 Hz, 1H), 7.20-7.18 (m, 2H), 7.09-7.06 (m, 1H), 6.97-6.90 (m, 3H), 6.60-6.65 (m, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.55, 138.56, 136.02, 135.34, 130.18, 129.70, 129.18, 127.61, 125.89, 121.94, 121.49, 120.93, 120.18, 115.36, 103.39, 69.12, 25.42; IR (neat): 2922, 1708, 1608, 1517, 1467, 1452, 1230, 1193, 1114, 1089, 1020, 738; HRMS (ESI): Exact mass calcd for $C_{17}H_{14}BrNO_2Na$ $[M+Na]^+$: 366.0100, Found: 366.0091.



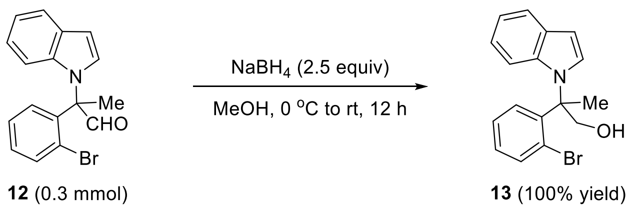
7j (0.3 mmol) (2.5 equiv) **11** (68% yield)

To a solution of $PhNH_2$ (69.8 mg, 0.75 mmol) in dry THF (2 mL) was added NaHMDS (0.6 mL, 1.0 M in THF, 0.6 mmol) dropwise at 0 °C. Then the reaction mixture was stirred for 20 min before methyl 2-(2-bromophenyl)-2-(1H-indol-1-yl)propanoate **7j** (107.5 mg, 0.3 mmol) in THF (1 mL) was added dropwise. The resulting mixture was allowed to warm to room temperature and stirred for 12 h, and then quenched with saturated aqueous NH_4Cl solution (10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the title compound **11** in 68% yield as yellow solid; Mp: 78-80 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.55 (dd, J_1 =

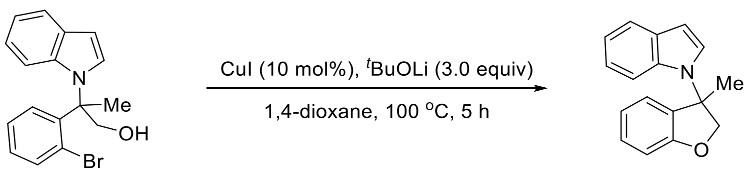
7.6 Hz, J_2 = 1.2 Hz, 1H), 7.47 (s, 1H), 7.43 (d, J = 3.6 Hz, 1H), 7.41-7.36 (m, 1H), 7.25-7.21 (m, 5H), 7.11-7.09 (m, 2H), 6.97-6.91 (m, 1H), 6.71 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 6.57 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.39, 138.52, 137.13, 136.44, 135.70, 130.42, 129.97, 129.72, 129.10, 128.09, 126.88, 125.10, 122.67, 122.56, 121.80, 120.71, 120.33, 112.11, 103.93, 71.08, 25.12; IR (neat): 2924, 1683, 1597, 1498, 1465, 1440, 1313, 1242, 1138, 1078, 1020, 752, 692; HRMS (ESI): Exact mass calcd for $C_{23}H_{19}BrN_2ONa$ $[M+Na]^+$: 441.0573, Found: 441.0580.



To a solution of methyl 2-(2-bromophenyl)-2-(1H-indol-1-yl)propanoate **7j** (1.97 g, 5.5 mmol) in dry THF (55 mL) was added $LiAlH_4$ (418.0 mg, 11.0 mmol) at -78 ºC. The reaction mixture was stirred at -78 ºC for 2 h, and then quenched with saturated aqueous NH_4Cl solution (20 mL), extracted with EtOAc (2 × 30 mL), dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the aldehyde **12** in 77% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.36 (s, 1H), 7.66-7.64 (m, 2H), 7.32-7.25 (m, 3H), 7.10-7.06 (m, 2H), 7.01-6.94 (m, 1H), 6.78 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 6.66 (dd, J_1 = 3.2 Hz, J_2 = 0.4 Hz, 1H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.30, 138.40, 135.44, 130.30, 130.26, 129.41, 128.32, 125.39, 121.89, 121.55, 121.24, 120.35, 112.69, 103.66, 70.47, 22.10; IR (neat): 1726, 1516, 1452, 1427, 1292, 1265, 1234, 1022, 731, 702; HRMS (ESI): Exact mass calcd for $C_{17}H_{14}BrNONa$ $[M+Na]^+$: 350.0151, Found: 350.0145.

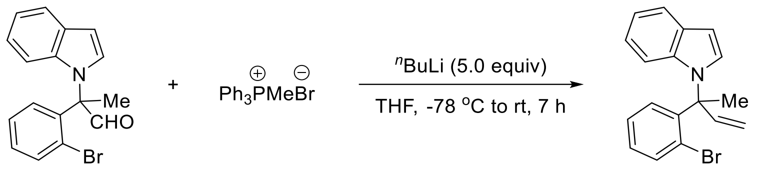


To a solution of methyl 2-(2-bromophenyl)-2-(1H-indol-1-yl)propanal **12** (98.5 mg, 0.3 mmol) in dry MeOH (3 mL) was added $NaBH_4$ (28.4 mg, 0.75 mmol) at 0 ºC. The reaction mixture was then allowed to warm to room temperature and stirred for 12 h before saturated aqueous solution of NH_4Cl (10 mL) was added. The aqueous layer was separated and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 5/1, v/v) to afford the title compound **13** in 100% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, J = 8.0 Hz, 1H), 7.52 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 2H), 7.46-7.41 (m, 2H), 7.17 (td, J_1 = 8.0 Hz , J_2 = 1.6 Hz, 1H), 7.04-7.00 (m, 1H), 6.86-6.82 (m, 1H), 6.59 (dd, J_1 = 3.2 Hz, J_2 = 0.8 Hz, 1H), 6.52 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1H), 4.52 (d, J = 11.2 Hz, 1H), 4.32-4.30 (m, 1H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.76, 136.30, 135.19, 129.98, 129.27, 127.96, 127.76, 127.17, 122.51, 121.21, 121.13, 119.65, 111.90, 101.69, 68.03, 64.41, 23.65; IR (neat): 3502, 2981, 2887, 1512, 1473, 1454, 1055, 1037, 1018, 734; HRMS (ESI): Exact mass calcd for $C_{17}H_{16}BrNONa$ [M+Na]$^+$: 352.0307, Found: 352.0298.



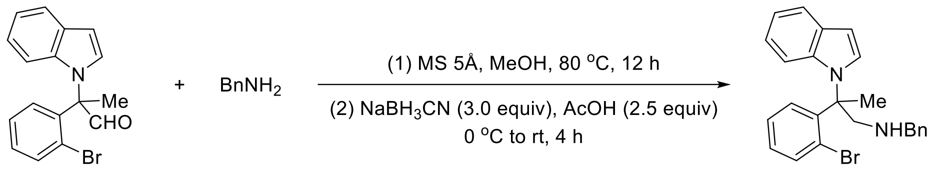
13 (0.3 mmol) **14** (93% yield)

To a 10-mL sealed tube were added 2-(2-bromophenyl)-2-(1H-indol-1-yl)propan-1-ol **13** (99.1 mg, 0.3 mmol) , CuI (5.7 mg, 0.03 mmol), ^{t}BuOLi (72.1 mg, 0.9 mmol) and 1,4-dioxane (3 mL). The reaction mixture was stirred at room temperature for 5 min and then at 100 °C for 5 h, and then filtered through celite and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the title compound **14** in 93% yield as yellow solid; Mp: 68-70 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65-7.63 (m, 1H), 7.36-7.31 (m, 1H), 7.21-7.18 (m, 2H), 7.11-7.07 (m, 3H), 7.01-6.96 (m, 2H), 6.48 (d, J = 3.2 Hz, 1H), 5.04, 4.57 (AB, J = 9.6 Hz, 2H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.77, 134.67, 130.52, 130.13, 126.03, 124.48, 121.55, 121.43, 121.39, 119.78, 112.05, 110.97, 101.22, 81.76, 65.69, 27.30; IR (neat): 2933, 1598, 1479, 1454, 1244, 1220, 1199, 1178, 1149, 1107, 736, 711; HRMS (ESI): Exact mass calcd for $C_{17}H_{15}NONa$ [M+Na]$^+$: 272.1046, Found: 272.1049.



12 (0.3 mmol) (6.0 equiv) **15** (70% yield)

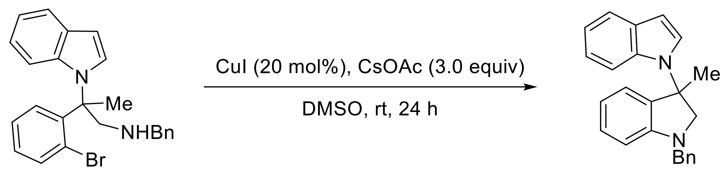
To a solution of methyltriphenylphosphonium bromide (643.0 mg, 1.8 mmol) in dry THF (2 mL) was added ^{n}BuLi (0.6 mL, 2.5 M in hexane, 1.5 mmol) dropwise at -78 °C, and then allowed to warm to room temperature and stirred for 1 h before aldehyde **12** (98.5 mg, 0.3 mmol) in THF (1 mL) was added dropwise at -78 °C. The resulting mixture was allowed to warm to room temperature and stirred for 7 h, and then quenched with saturated aqueous NH_4Cl solution (10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the title compound **15** in 70% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.52 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.42-7.38 (m, 2H), 7.17 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.04-7.00 (m, 1H), 6.88-6.81 (m, 2H), 6.58-6.55 (m, 2H), 5.31 (d, J = 10.8 Hz, 1H), 5.08 (d, J = 17.2 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.81, 140.15, 136.23, 135.42, 129.92, 129.27, 128.77, 127.83, 126.31, 122.58, 121.05, 120.99, 119.34, 115.32, 112.24, 101.49, 65.03, 25.42; IR (neat): 2987, 1512, 1467, 1454, 1425, 1292, 1263, 1230, 1018, 732, 702; HRMS (ESI): Exact mass calcd for $C_{18}H_{16}BrNNa$ [M+Na]$^+$: 348.0358, Found: 348.0351.



12 (0.3 mmol) (3.0 equiv) **16** (85% yield)

To a solution of methyl 2-(2-bromophenyl)-2-(1H-indol-1-yl)propanal **12** (98.5 mg, 0.3 mmol) in dry MeOH (3 mL) were added $BnNH_2$ (96.5 mg, 0.9 mmol) and MS 5Å (600 mg). The reaction mixture was stirred at 80 °C for 12 h before $NaBH_3CN$ (56.5 mg, 0.9 mmol) and AcOH (45.1 mg, 0.75 mmol) were added at 0 °C. The resulting mixture was allowed to warm to room temperature and stirred for 4 h, and then quenched with saturated aqueous $NaHCO_3$ solution (10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography

(PE/EtOAc, 10/1, v/v) to afford the title compound **16** in 85% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.0 Hz, 1H), 7.53 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.48-7.45 (m, 2H), 7.37 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.25-7.19 (m, 3H), 7.15-7.10 (m, 3H), 7.02-6.98 (m, 1H), 6.81-6.77 (m, 1H), 6.55 (dd, J_1 = 3.2 Hz, J_2 = 0.8 Hz, 1H), 6.49 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1H), 3.70-3.64 (m, 3H), 3.48 (d, *J* = 11.2 Hz, 1H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.93, 140.28, 136.19, 135.11, 129.98, 128.99, 128.44, 127.99, 127.88, 127.74, 127.35, 126.99, 122.45, 120.97, 120.90, 119.45, 111.88, 101.12, 63.58, 55.89, 53.75, 25.06; IR (neat): 2981, 1606, 1512, 1494, 1473, 1454, 1363, 1116, 1018, 734, 696; HRMS (ESI): Exact mass calcd for $C_{24}H_{24}BrN_2$ $[M+H]^+$: 419.1117, Found: 419.1125.



16 (0.3 mmol) **17** (98% yield)

To a solution of *N*-benzyl-2-(2-bromophenyl)-2-(1H-indol-1-yl)propan-1-amine **16** (125.8 mg, 0.3 mmol) in dry DMSO (3 mL) were added CuI (11.4 mg, 0.06 mmol) and CsOAc (115.2 mg, 0.9 mmol). The reaction mixture was stirred at room temperature for 24 h and filtered through celite, then extracted with saturated aqueous NaCl solution (10 mL) and EtOAc (3 × 10 mL). The organic layers were washed three times with H_2O (3 × 10 mL), dried over anhydrous Na_2SO_4 and concentrated. The resulting residue was purified by column chromatography (PE/EtOAc, 20/1, v/v) to afford the title compound **17** in 98% yield as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.58 (m, 1H), 7.29-7.21 (m, 7H), 7.03-6.94 (m, 4H), 6.72-6.68 (m, 2H), 6.44 (d, *J* = 3.2 Hz, 1H), 4.49, 4.30 (AB, *J* = 15.2 Hz, 2H), 3.94, 3.45 (AB, *J* = 9.6 Hz, 2H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.83, 137.85, 134.93, 132.36, 130.49, 129.72, 128.74, 127.94, 127.49, 126.35, 124.15, 121.20, 120.97, 119.40, 118.20, 112.97, 107.95, 100.76, 65.02, 64.44, 52.54, 27.60; IR (neat): 2924, 1606, 1508, 1489, 1473, 1454, 1313, 1292, 1220, 1159, 1026, 1018, 736, 698; HRMS (ESI): Exact mass calcd for $C_{24}H_{22}N_2Na$ $[M+Na]^+$: 361.1675, Found: 361.1666.

7. X-ray crystallography data of 7o

Single-Crystal X-ray Crystallography of 7o (CCDC: 2235158)

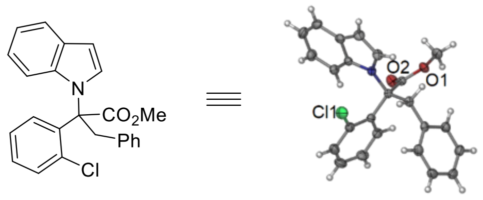


Table 5 Crystal data and structure refinement for 7o.

Identification code	**7o**
Empirical formula	$C_{24}H_{20}ClNO_2$
Formula weight	389.86
Temperature/K	190(20)
Crystal system	triclinic
Space group	P-1
a/Å	6.8922(2)
b/Å	10.1765(3)
c/Å	14.9016(4)
α/°	109.628(2)
β/°	97.057(2)
γ/°	93.235(2)
Volume/Å^3	971.63(5)
Z	2
ρ_{calc}g/cm^3	1.333
μ/mm^{-1}	1.892
F(000)	408.0
Crystal size/mm^3	0.32 × 0.25 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.37 to 134.158
Index ranges	-8 ≤ h ≤ 8, -11 ≤ k ≤ 12, -17 ≤ l ≤ 17
Reflections collected	19351
Independent reflections	3432 [R_{int} = 0.0370, R_{sigma} = 0.0224]
Data/restraints/parameters	3432/0/254
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1 = 0.0346, wR_2 = 0.0913
Final R indexes [all data]	R_1 = 0.0356, wR_2 = 0.0920
Largest diff. peak/hole / e Å^{-3}	0.54/-0.34

Table 6 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 7o. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cl1	9635.2(6)	1359.6(4)	6677.7(3)	39.90(14)
O1	6809.6(14)	5888.4(11)	9173.3(7)	27.8(2)
O2	4282.2(15)	4558.3(12)	8118.9(8)	36.3(3)
N1	7866.4(16)	2978.8(12)	8366.2(8)	22.3(3)
C7	9603.1(19)	5856.7(15)	7425.7(10)	24.4(3)
C15	9597.3(19)	4915.4(15)	8020.0(10)	24.0(3)
C2	6930.8(19)	3273.2(15)	6775.0(10)	22.8(3)
C13	6016.0(19)	4849.6(15)	8364.5(10)	22.7(3)
C17	6525(2)	1847.0(14)	8269.1(10)	22.7(3)
C16	7620.6(19)	4000.1(14)	7860.2(9)	20.8(3)
C22	7289(2)	1205.3(15)	8925.9(10)	26.7(3)
C8	8688(2)	7091.6(16)	7657.3(11)	29.5(3)
C24	9416(2)	3041.6(16)	9074.0(11)	29.0(3)
C18	4712(2)	1352.9(16)	7680.5(11)	28.1(3)
C3	5552(2)	3848.0(17)	6285.8(11)	28.9(3)
C23	9119(2)	1990.6(17)	9422.2(11)	32.0(3)
C12	10566(2)	5511.4(17)	6626.0(11)	32.7(3)
C21	6202(2)	40.5(16)	8989.1(11)	32.4(3)
C14	5412(2)	6688.9(17)	9726.7(12)	33.8(4)
C6	7008(3)	1440.0(18)	5227.9(12)	37.2(4)
C19	3690(2)	196.3(17)	7761.0(12)	35.0(4)
C10	9671(2)	7570.0(17)	6301.2(12)	35.2(4)
C20	4422(2)	-452.4(17)	8406.3(12)	36.2(4)
C9	8707(2)	7935.3(17)	7096.6(12)	34.1(4)
C1	7704(2)	2085.3(16)	6209.4(11)	28.3(3)
C11	10614(3)	6360.0(18)	6071.5(12)	37.9(4)
C4	4887(2)	3229.3(19)	5307.6(12)	37.5(4)
C5	5585(3)	2004(2)	4784.3(12)	41.4(4)

Table 7 Anisotropic Displacement Parameters (Å^2×10^3) for 7o. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	42.3(2)	36.8(2)	44.8(2)	14.14(18)	13.94(18)	21.17(17)
O1	25.5(5)	28.7(5)	25.4(5)	2.9(4)	6.5(4)	5.2(4)
O2	18.5(5)	43.7(7)	39.8(6)	5.5(5)	3.4(4)	6.1(5)
N1	19.9(6)	22.7(6)	23.8(6)	8.4(5)	0.3(4)	3.4(4)
C7	18.1(6)	22.8(7)	28.6(7)	5.5(6)	1.5(5)	-2.0(5)
C15	16.2(6)	23.8(7)	29.7(7)	6.9(6)	1.9(5)	2.4(5)
C2	20.3(6)	23.8(7)	23.9(7)	8.5(6)	3.1(5)	-1.3(5)
C13	20.9(7)	23.6(7)	25.2(7)	10.2(6)	3.0(5)	4.6(5)
C17	24.5(7)	21.1(7)	22.0(7)	5.4(5)	6.5(5)	5.5(5)
C16	17.9(6)	20.8(7)	23.4(7)	7.4(5)	1.7(5)	3.8(5)
C22	30.8(7)	25.8(7)	25.2(7)	8.1(6)	8.3(6)	10.6(6)
C8	30.8(8)	26.4(8)	31.4(8)	8.2(6)	9.2(6)	4.4(6)
C24	23.6(7)	30.7(8)	30.3(8)	10.3(6)	-4.8(6)	3.9(6)
C18	26.5(7)	29.0(8)	27.9(7)	10.0(6)	2.3(6)	0.4(6)
C3	25.9(7)	30.8(8)	30.0(8)	12.2(6)	0.3(6)	1.5(6)
C23	32.2(8)	33.7(9)	31.3(8)	14.4(7)	-2.4(6)	9.1(6)
C12	29.5(8)	28.2(8)	38.0(8)	6.1(7)	12.2(6)	1.9(6)
C21	41.1(9)	28.6(8)	33.8(8)	15.2(7)	13.4(7)	11.6(7)
C14	37.7(9)	29.8(8)	35.0(8)	7.3(7)	17.5(7)	11.4(7)
C6	45.0(9)	31.7(9)	32.3(8)	5.0(7)	14.8(7)	-0.2(7)
C19	30.0(8)	32.9(9)	38.9(9)	10.3(7)	2.9(7)	-4.1(6)
C10	41.2(9)	30.8(8)	32.7(8)	12.7(7)	2.0(7)	-7.9(7)
C20	40.5(9)	27.6(8)	44.2(9)	14.8(7)	14.2(7)	1.7(7)
C9	38.1(9)	26.6(8)	38.4(9)	12.1(7)	6.3(7)	3.2(6)
C1	29.2(8)	26.0(8)	30.3(8)	9.2(6)	9.2(6)	1.7(6)
C11	42.7(9)	36.2(9)	31.8(8)	6.4(7)	14.3(7)	-4.9(7)
C4	34.7(8)	46.7(10)	31.1(8)	17.0(7)	-2.5(7)	-0.3(7)
C5	45.7(10)	48.6(11)	24.6(8)	8.9(7)	1.8(7)	-5.8(8)

Table 8 Bond Lengths for 7o.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C1	1.7414(16)	C17	C18	1.395(2)
O1	C13	1.3365(17)	C22	C23	1.427(2)
O1	C14	1.4503(17)	C22	C21	1.403(2)
O2	C13	1.1956(17)	C8	C9	1.385(2)
N1	C17	1.3918(18)	C24	C23	1.352(2)
N1	C16	1.4807(17)	C18	C19	1.385(2)
N1	C24	1.3883(18)	C3	C4	1.385(2)
C7	C15	1.507(2)	C12	C11	1.383(2)
C7	C8	1.396(2)	C21	C20	1.374(2)
C7	C12	1.387(2)	C6	C1	1.395(2)
C15	C16	1.5519(18)	C6	C5	1.374(3)
C2	C16	1.5350(18)	C19	C20	1.400(2)
C2	C3	1.398(2)	C10	C9	1.382(2)
C2	C1	1.398(2)	C10	C11	1.385(3)
C13	C16	1.5527(18)	C4	C5	1.379(3)
C17	C22	1.415(2)			

Table 9 Bond Angles for 7o.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C13	O1	C14	115.20(11)	C2	C16	C13	111.44(11)
C17	N1	C16	126.23(11)	C17	C22	C23	106.96(13)
C24	N1	C17	107.82(12)	C21	C22	C17	119.37(14)
C24	N1	C16	125.81(12)	C21	C22	C23	133.65(14)
C8	C7	C15	122.28(13)	C9	C8	C7	121.14(14)
C12	C7	C15	119.75(13)	C23	C24	N1	110.31(13)
C12	C7	C8	117.97(14)	C19	C18	C17	117.08(14)
C7	C15	C16	114.27(11)	C4	C3	C2	122.20(15)
C3	C2	C16	120.18(12)	C24	C23	C22	107.46(13)
C1	C2	C16	123.49(12)	C11	C12	C7	121.13(15)
C1	C2	C3	116.19(13)	C20	C21	C22	118.95(15)
O1	C13	C16	111.20(11)	C5	C6	C1	120.07(15)
O2	C13	O1	123.25(13)	C18	C19	C20	121.96(15)
O2	C13	C16	125.27(13)	C9	C10	C11	119.58(15)
N1	C17	C22	107.45(12)	C21	C20	C19	120.87(15)
N1	C17	C18	130.77(13)	C10	C9	C8	119.96(15)
C18	C17	C22	121.76(13)	C2	C1	Cl1	122.09(11)
N1	C16	C15	109.60(10)	C6	C1	Cl1	116.22(12)

Table 9 Bond Angles for 7o.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C16	C2	112.00(11)	C6	C1	C2	121.66(14)
N1	C16	C13	101.60(10)	C12	C11	C10	120.21(15)
C15	C16	C13	112.67(11)	C5	C4	C3	119.94(16)
C2	C16	C15	109.37(11)	C6	C5	C4	119.69(15)

Table 10 Torsion Angles for 7o.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C13	C16	N1	85.37(13)	C22	C21	C20	C19	-0.3(2)
O1	C13	C16	C15	-31.81(15)	C8	C7	C15	C16	76.36(17)
O1	C13	C16	C2	-155.19(11)	C8	C7	C12	C11	-0.2(2)
O2	C13	C16	N1	-88.64(16)	C24	N1	C17	C22	-0.53(15)
O2	C13	C16	C15	154.18(14)	C24	N1	C17	C18	178.18(14)
O2	C13	C16	C2	30.79(19)	C24	N1	C16	C15	15.68(18)
N1	C17	C22	C23	0.34(15)	C24	N1	C16	C2	137.26(13)
N1	C17	C22	C21	178.91(12)	C24	N1	C16	C13	-103.70(14)
N1	C17	C18	C19	-178.95(14)	C18	C17	C22	C23	-178.51(13)
N1	C24	C23	C22	-0.32(18)	C18	C17	C22	C21	0.1(2)
C7	C15	C16	N1	171.88(11)	C18	C19	C20	C21	0.0(3)
C7	C15	C16	C2	48.74(15)	C3	C2	C16	N1	140.99(13)
C7	C15	C16	C13	-75.79(15)	C3	C2	C16	C15	-97.31(14)
C7	C8	C9	C10	-1.0(2)	C3	C2	C16	C13	27.93(17)
C7	C12	C11	C10	-0.8(2)	C3	C2	C1	Cl1	172.43(11)
C15	C7	C8	C9	-179.72(14)	C3	C2	C1	C6	-5.5(2)
C15	C7	C12	C11	-179.38(14)	C3	C4	C5	C6	-3.1(3)
C2	C3	C4	C5	0.1(2)	C23	C22	C21	C20	178.41(16)
C17	N1	C16	C15	-169.28(12)	C12	C7	C15	C16	-104.53(15)
C17	N1	C16	C2	-47.70(17)	C12	C7	C8	C9	1.2(2)
C17	N1	C16	C13	71.34(15)	C21	C22	C23	C24	-178.29(16)
C17	N1	C24	C23	0.54(17)	C14	O1	C13	O2	-2.2(2)
C17	C22	C23	C24	-0.02(17)	C14	O1	C13	C16	-176.39(11)
C17	C22	C21	C20	0.3(2)	C9	C10	C11	C12	1.0(2)
C17	C18	C19	C20	0.4(2)	C1	C2	C16	N1	-43.45(17)
C16	N1	C17	C22	-176.31(12)	C1	C2	C16	C15	78.25(16)
C16	N1	C17	C18	2.4(2)	C1	C2	C16	C13	-156.51(13)
C16	N1	C24	C23	176.34(13)	C1	C2	C3	C4	4.1(2)
C16	C2	C3	C4	180.00(14)	C1	C6	C5	C4	1.7(3)
C16	C2	C1	Cl1	-3.3(2)	C11	C10	C9	C8	-0.1(2)

Table 10 Torsion Angles for 7o.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C16	C2	C1	C6	178.73(14)	C5	C6	C1	Cl1	-175.29(13)
C22	C17	C18	C19	-0.4(2)	C5	C6	C1	C2	2.8(2)

Table 11 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 7o.

Atom	*x*	*y*	*z*	U(eq)
H15A	9911.97	5503.59	8710.19	29
H15B	10650.62	4289.84	7865.42	29
H8	8040.02	7358.08	8208.86	35
H24	10526.5	3725.34	9283.81	35
H18	4201.15	1790.7	7243.59	34
H3	5055.15	4691.25	6636.27	35
H23	9972.82	1808.48	9908.09	38
H12	11204.36	4677.57	6456.18	39
H21	6689.46	-400.62	9428.1	39
H14A	4625.95	7127.09	9333.73	51
H14B	6122.57	7418.22	10306.07	51
H14C	4544.62	6062.28	9914.4	51
H6	7518.25	609.65	4866.07	45
H19	2454.57	-167.75	7366.67	42
H10	9686.63	8145.27	5914.37	42
H20	3678.8	-1243.79	8441.5	43
H9	8058.58	8764.55	7258.73	41
H11	11296.33	6112.18	5531.32	45
H4	3950.91	3648.63	4997.52	45
H5	5084.9	1552.45	4120.14	50

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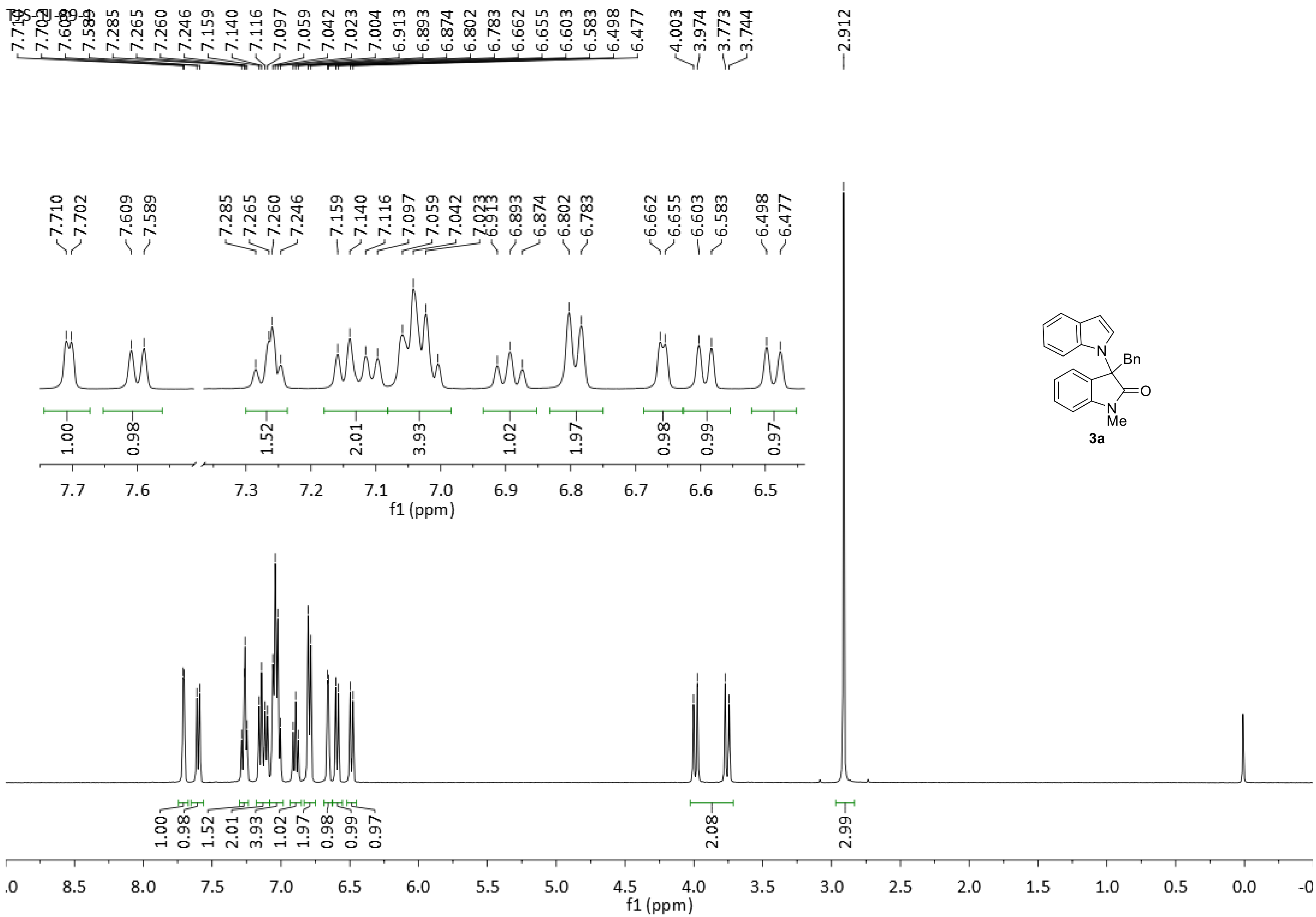
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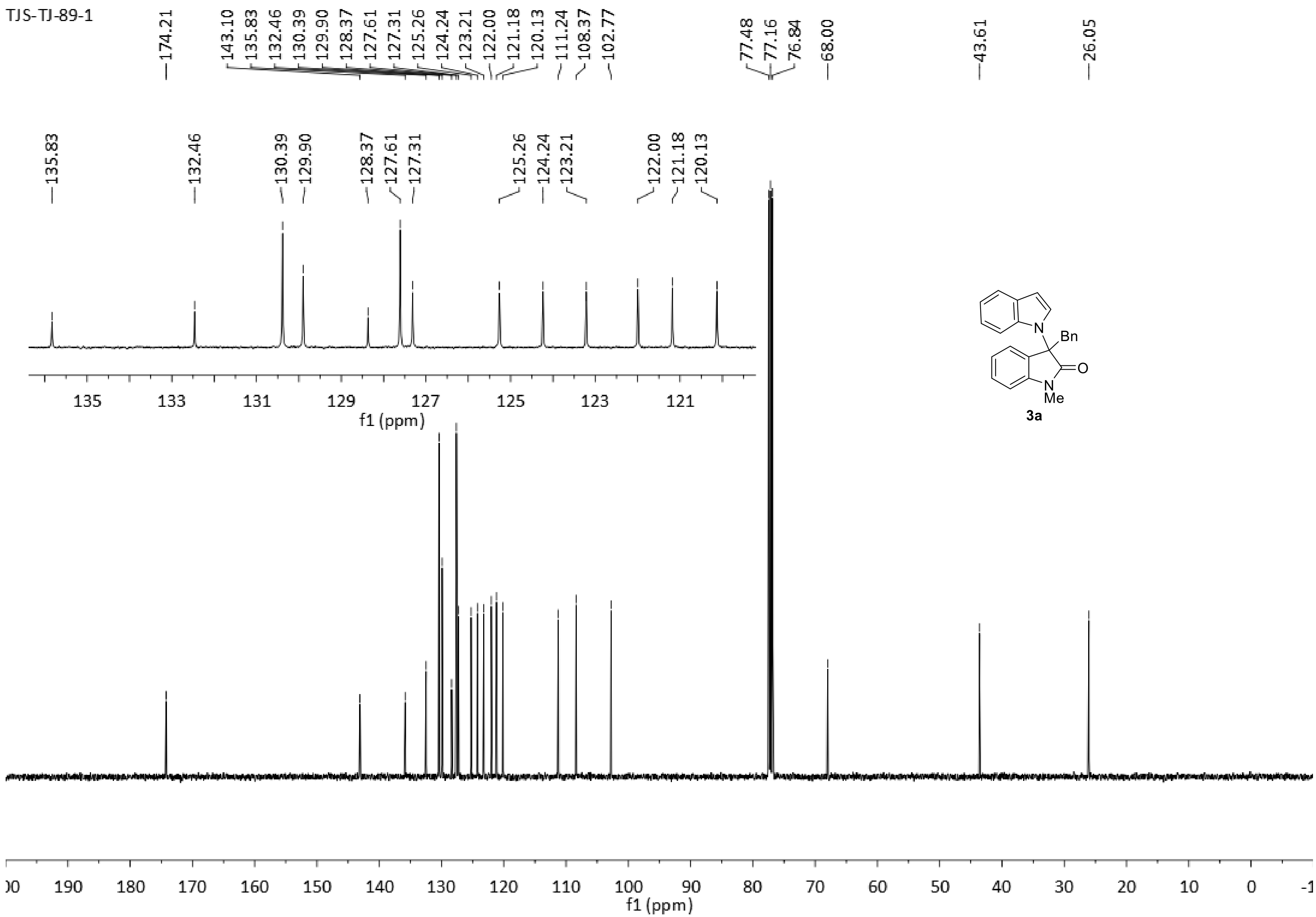
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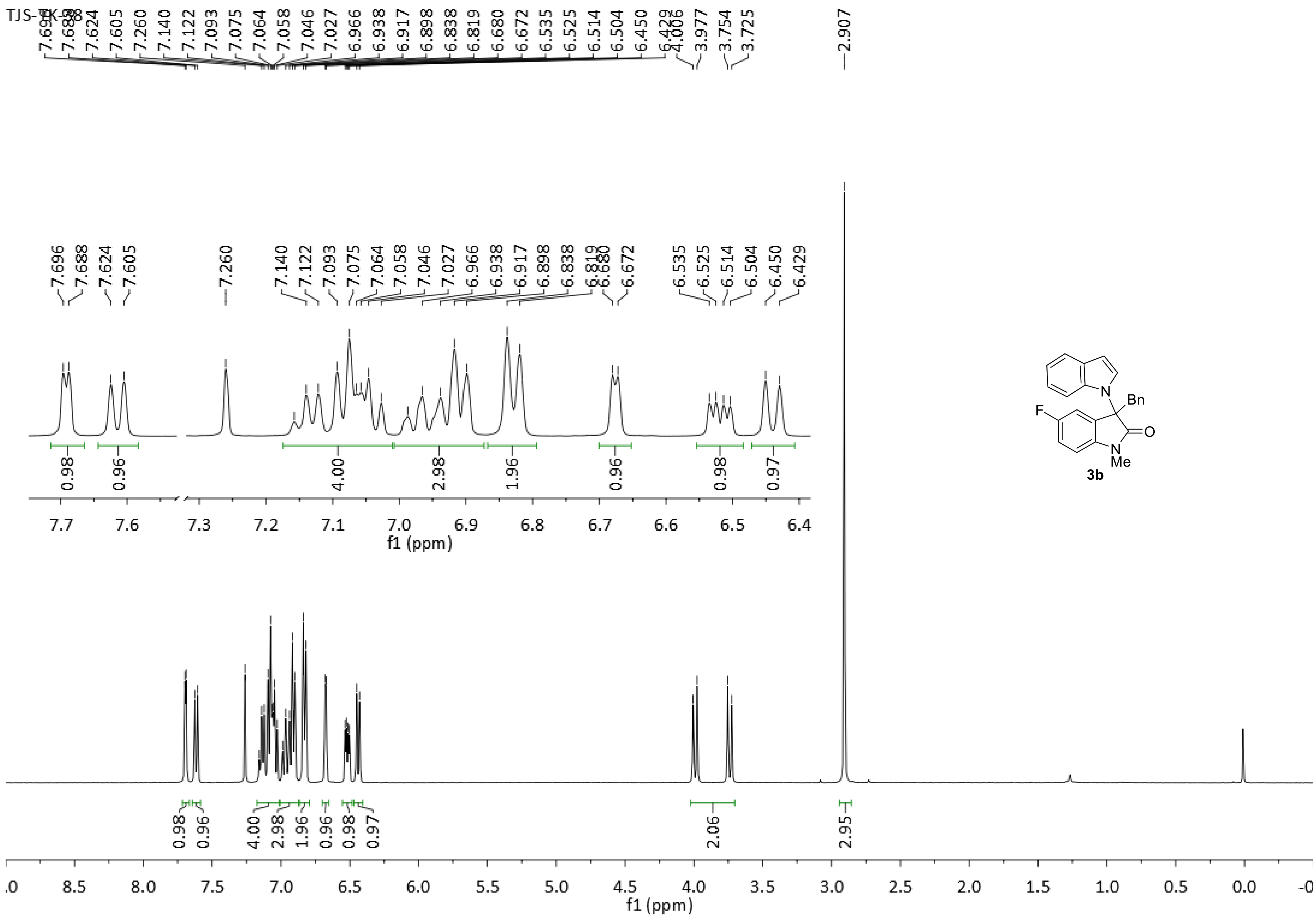
f1 (ppm)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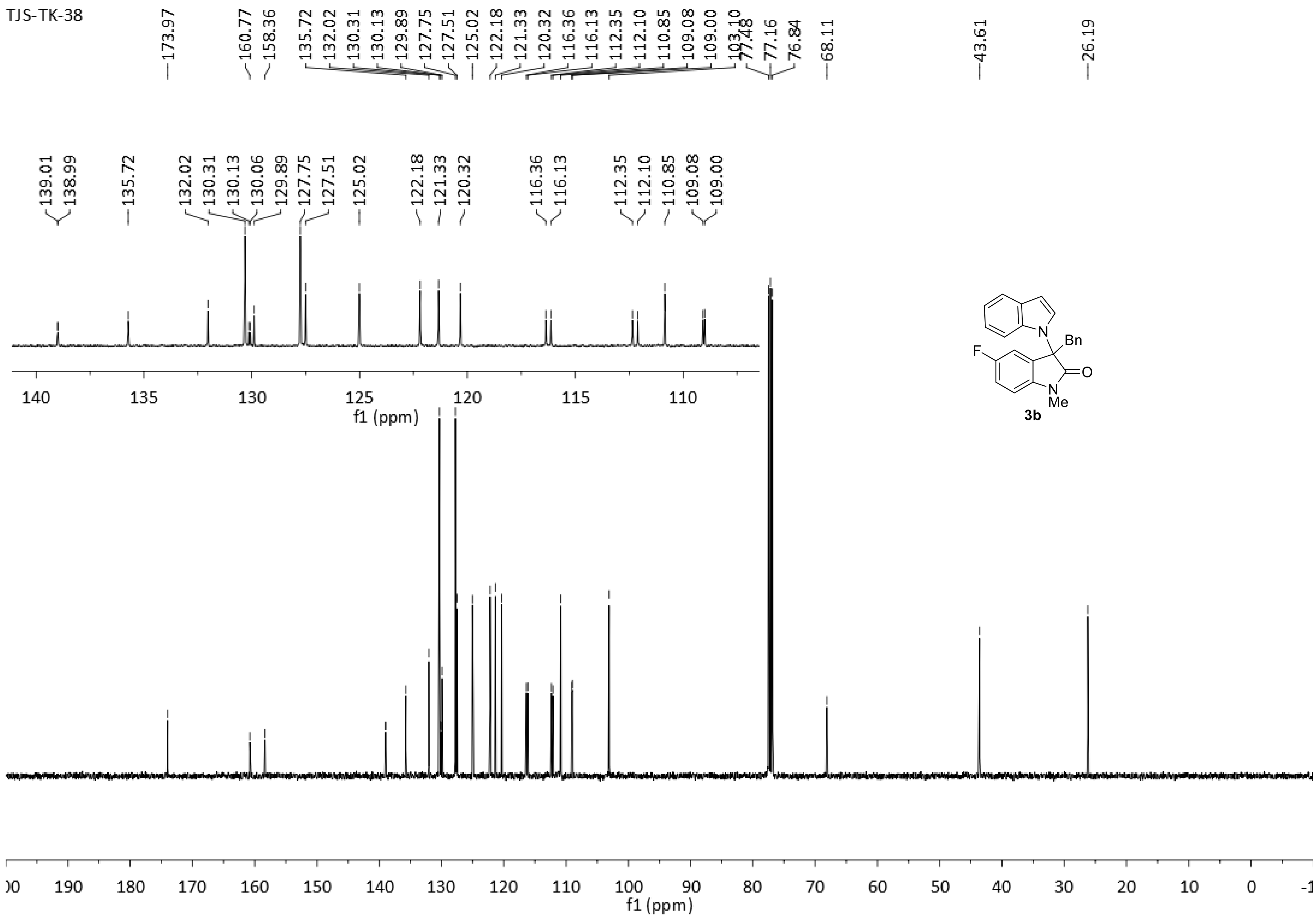

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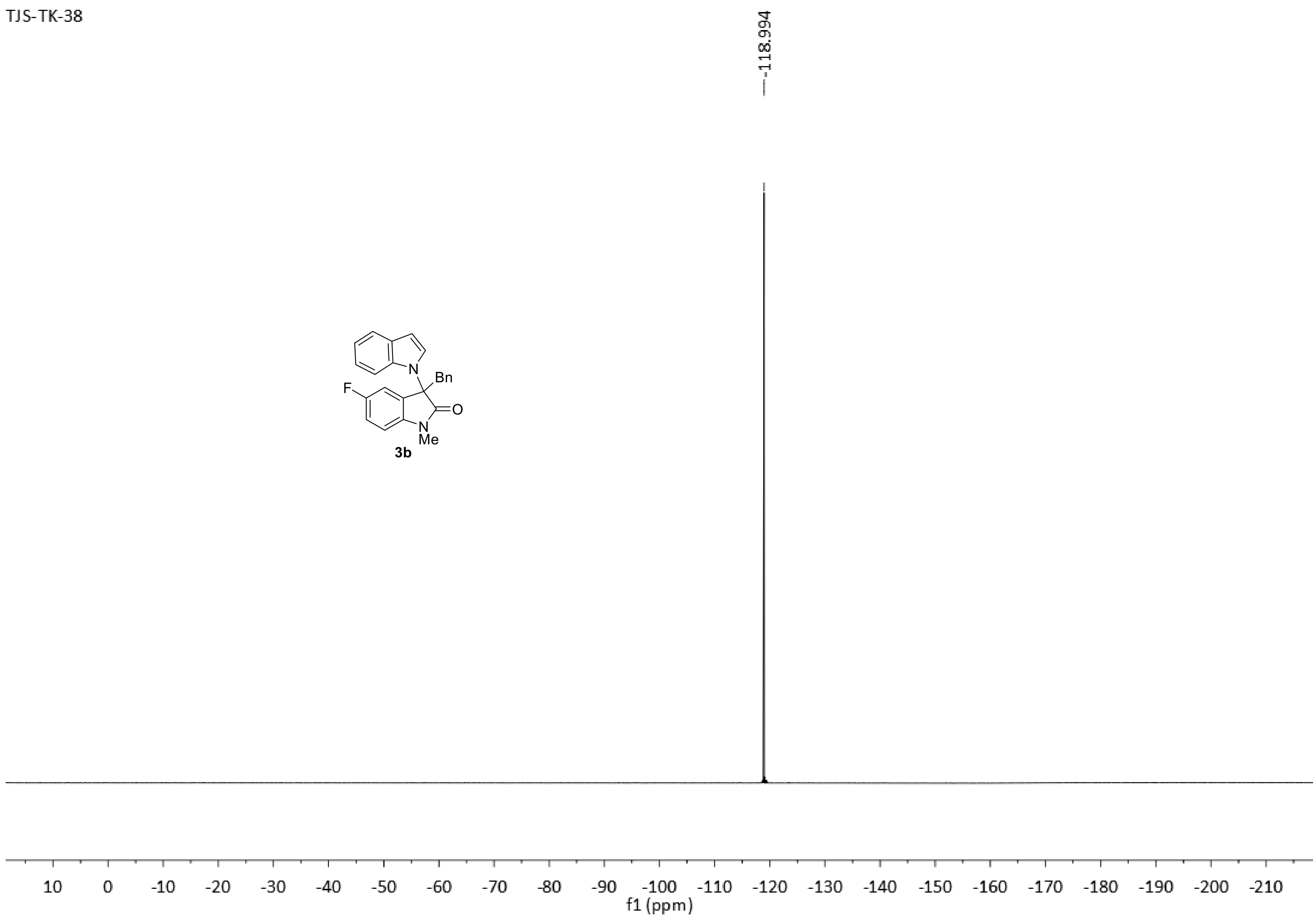
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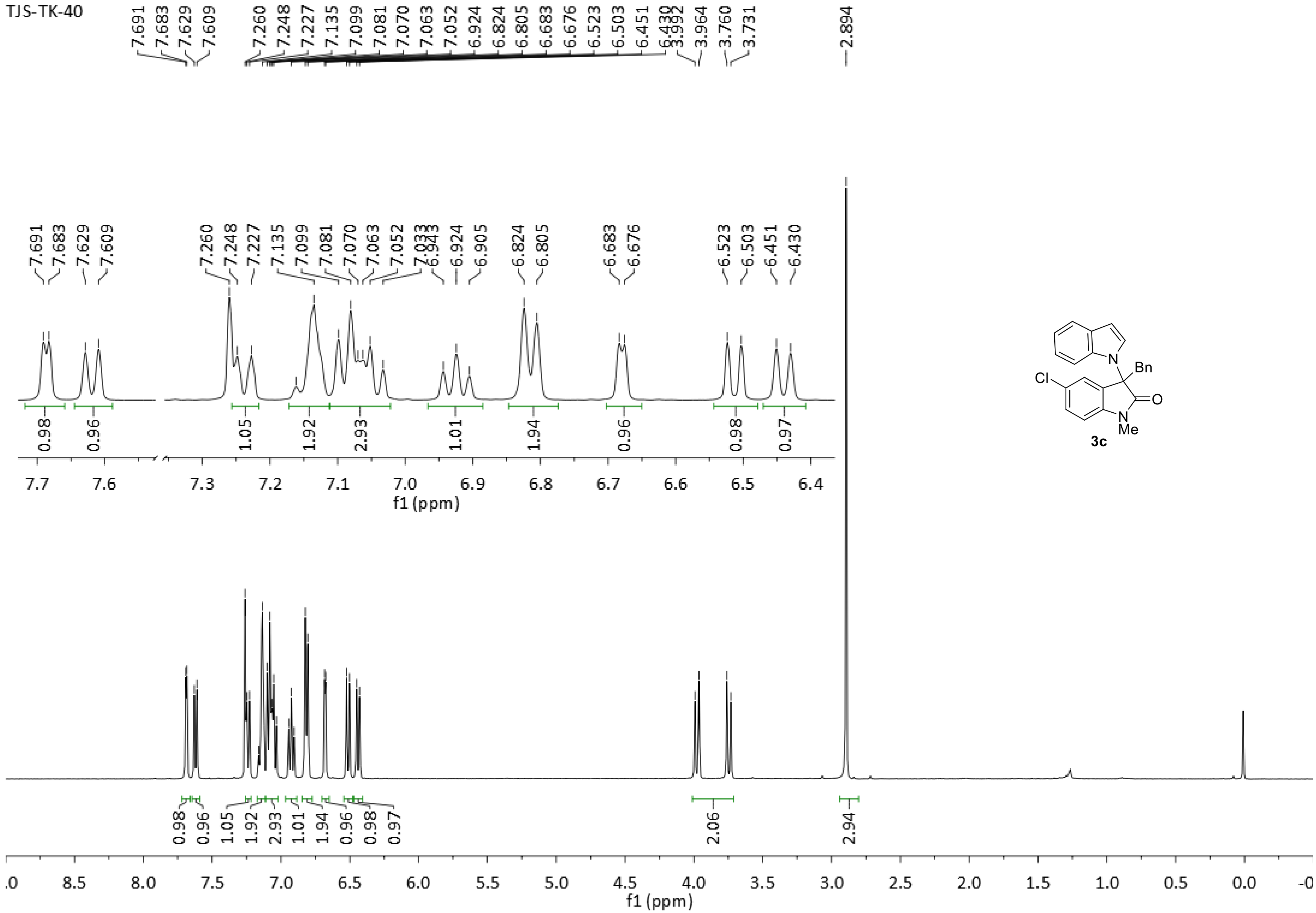
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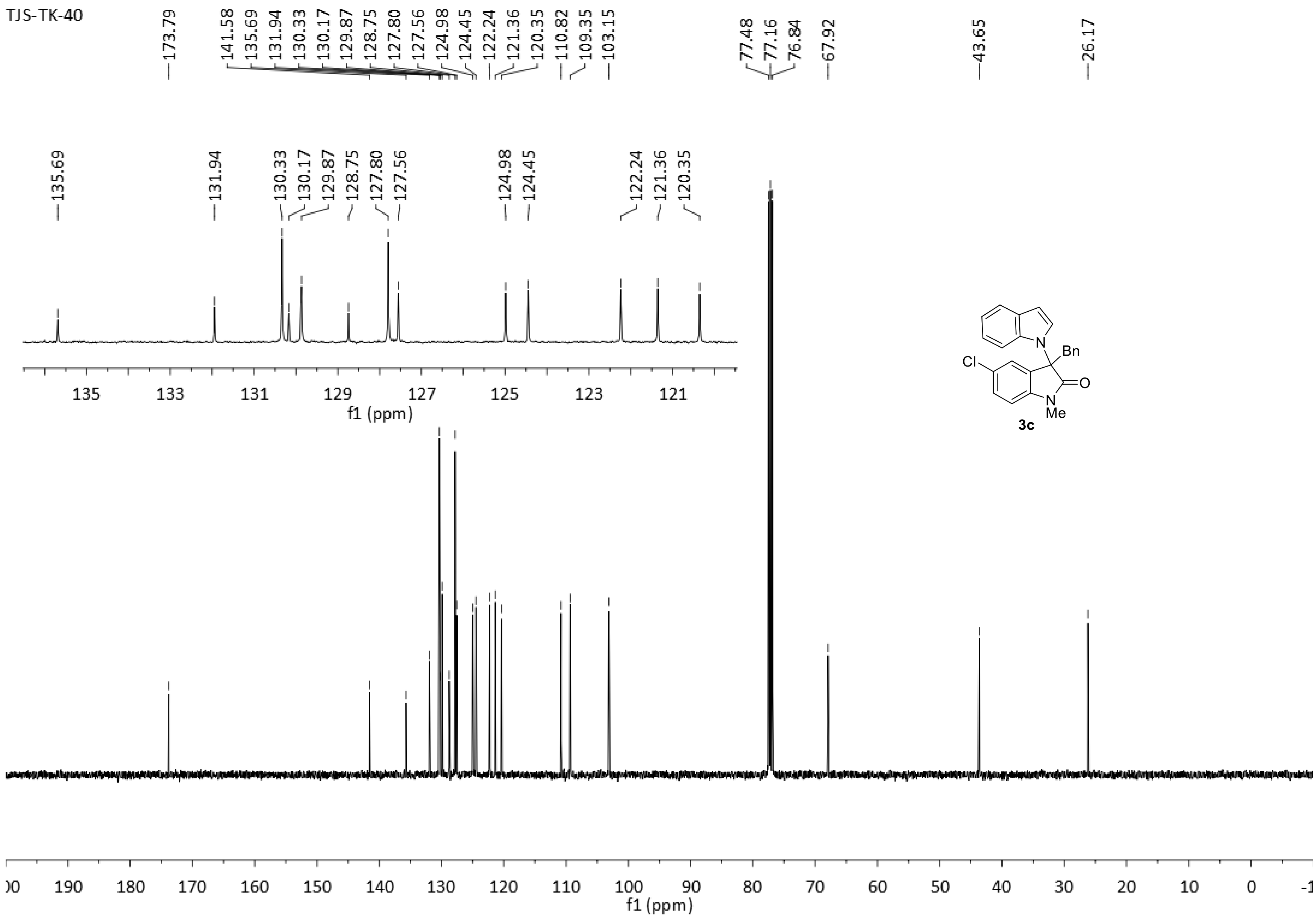
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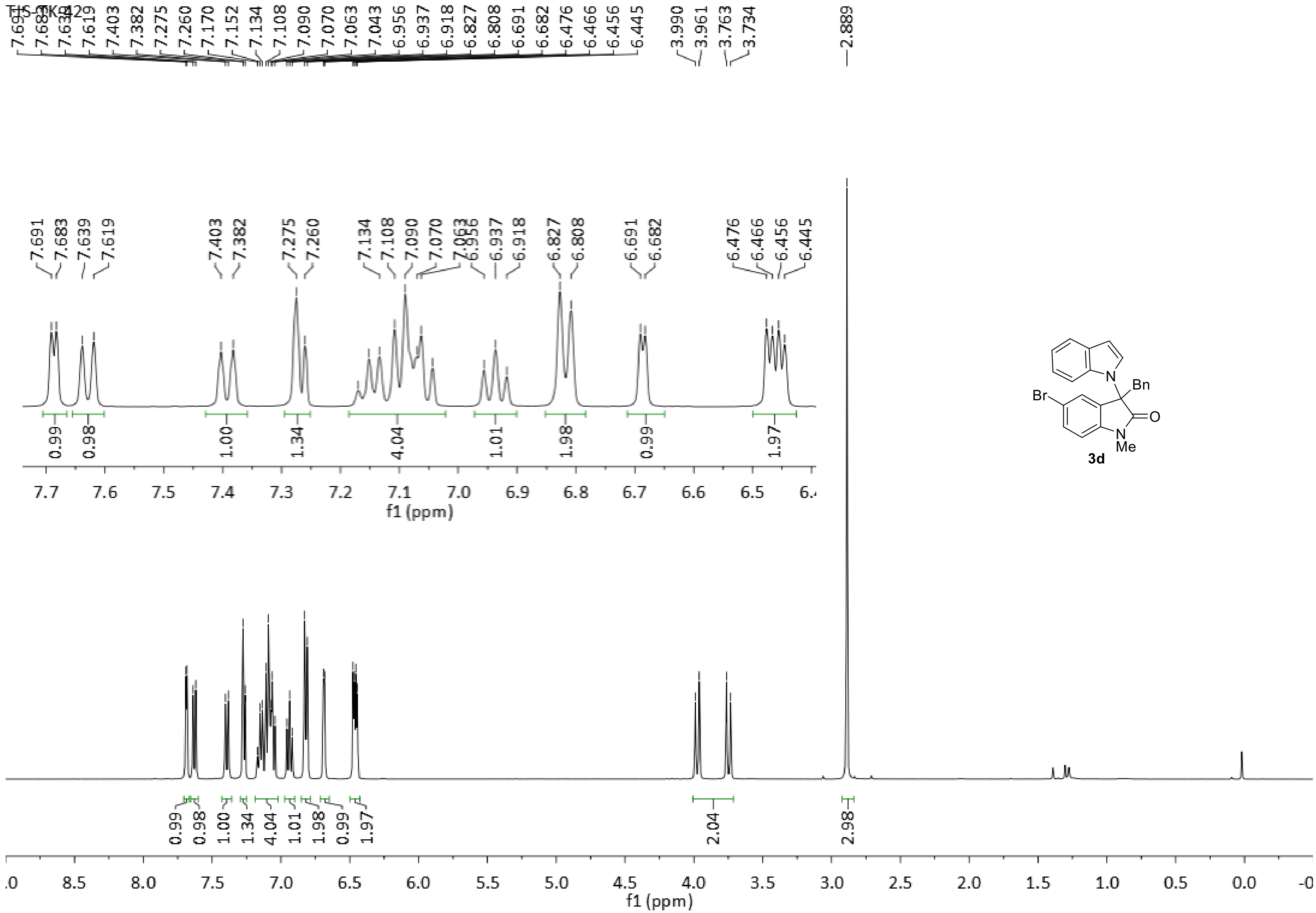
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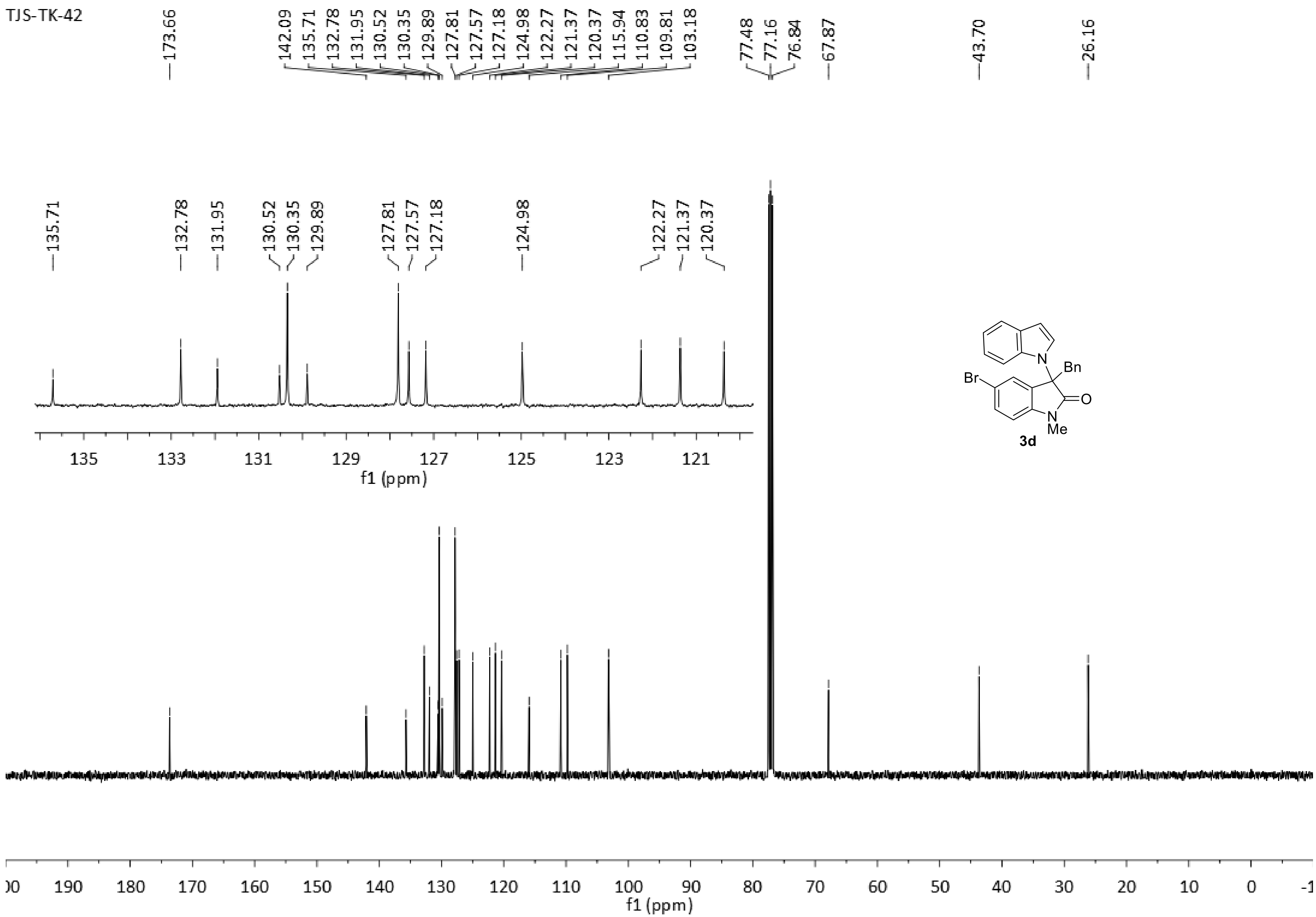
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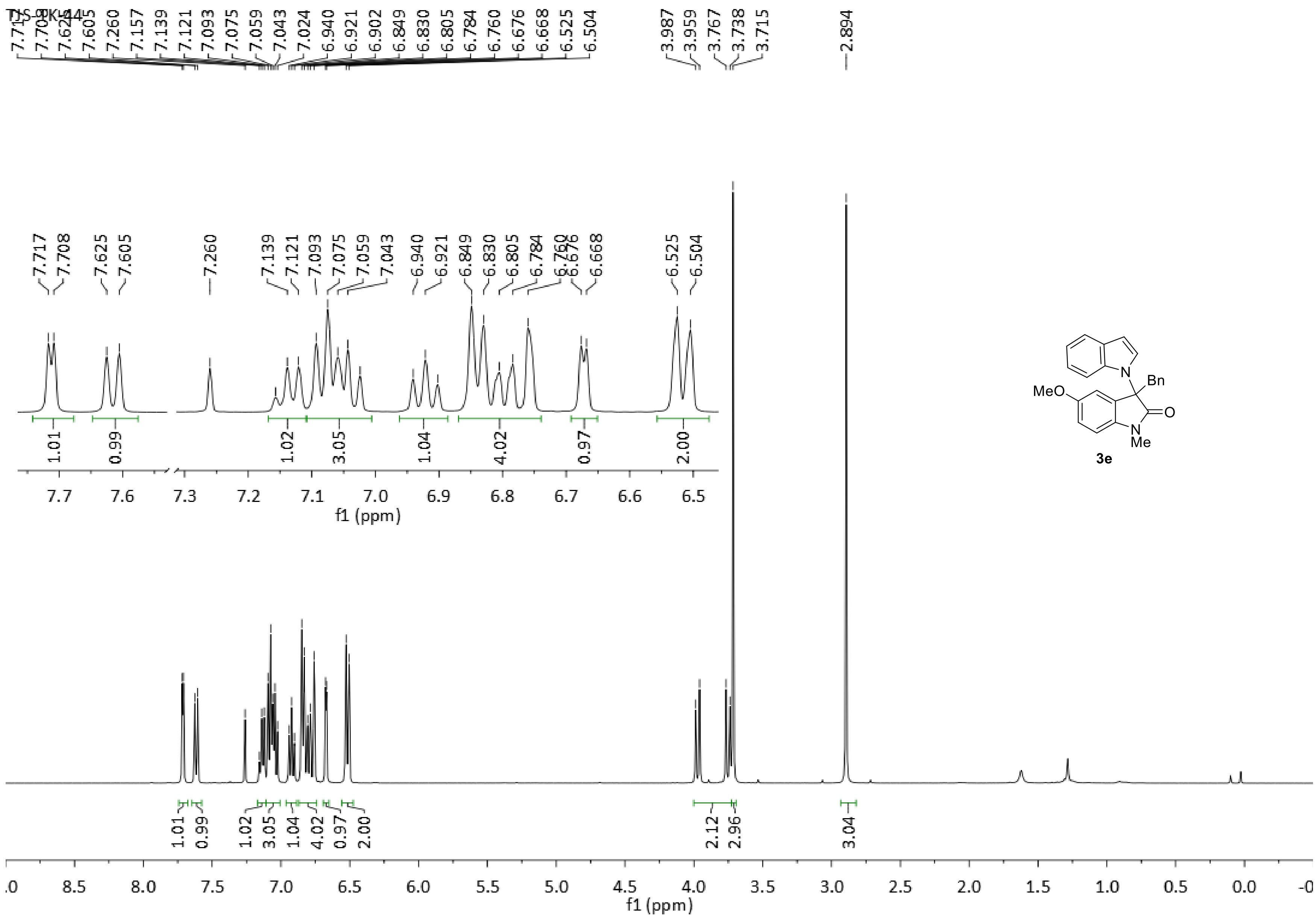
f1 (ppm)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Me
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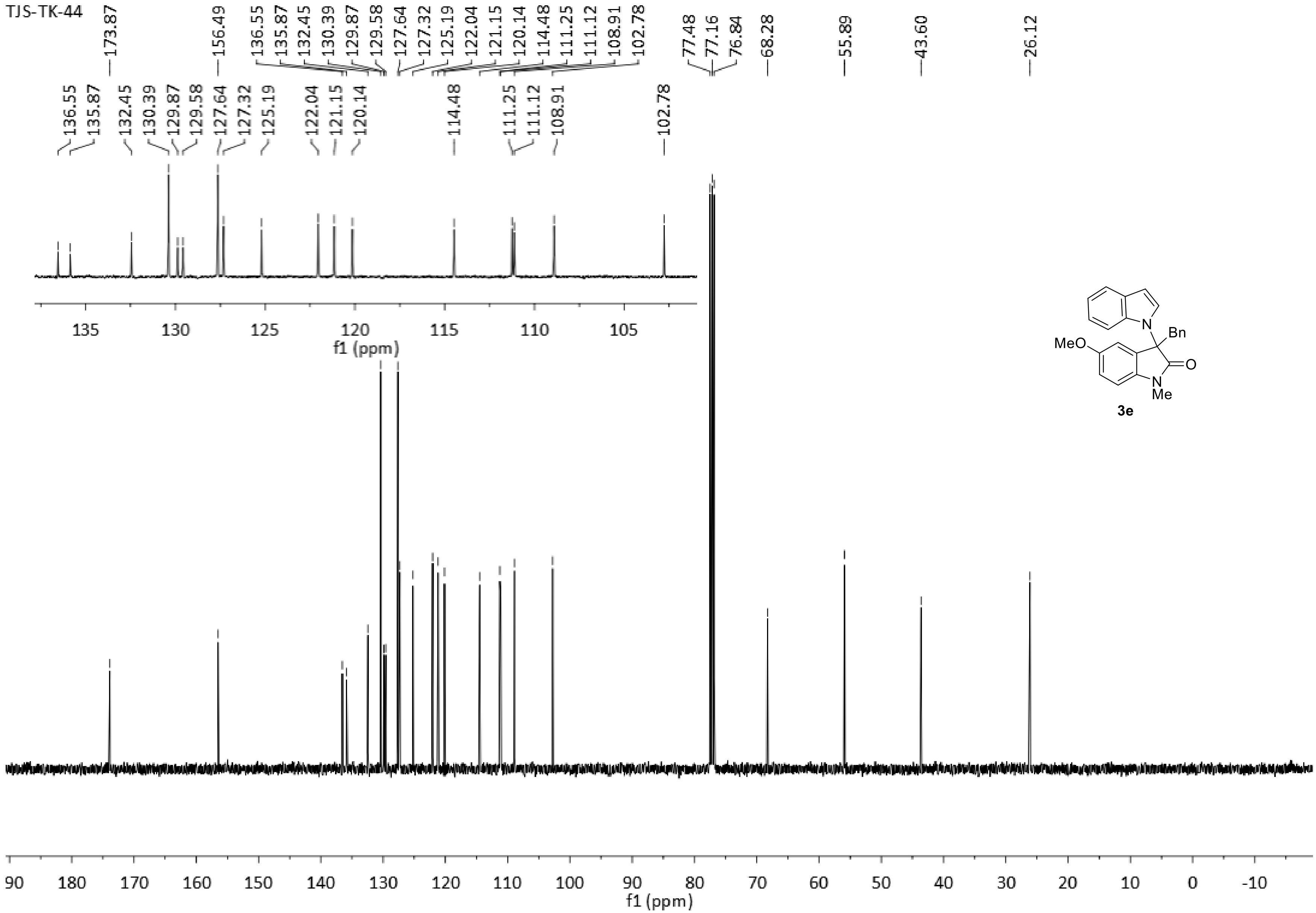
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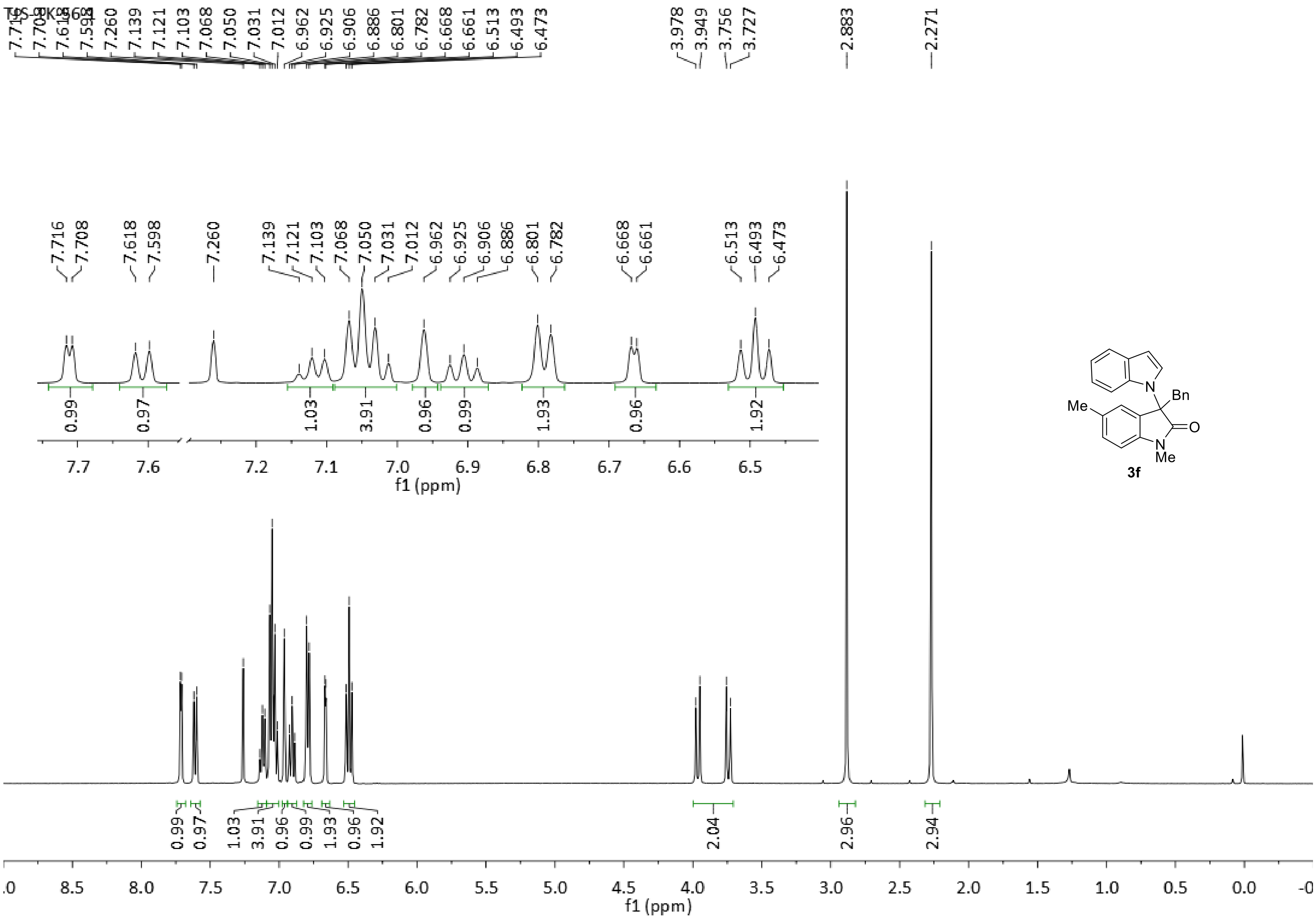
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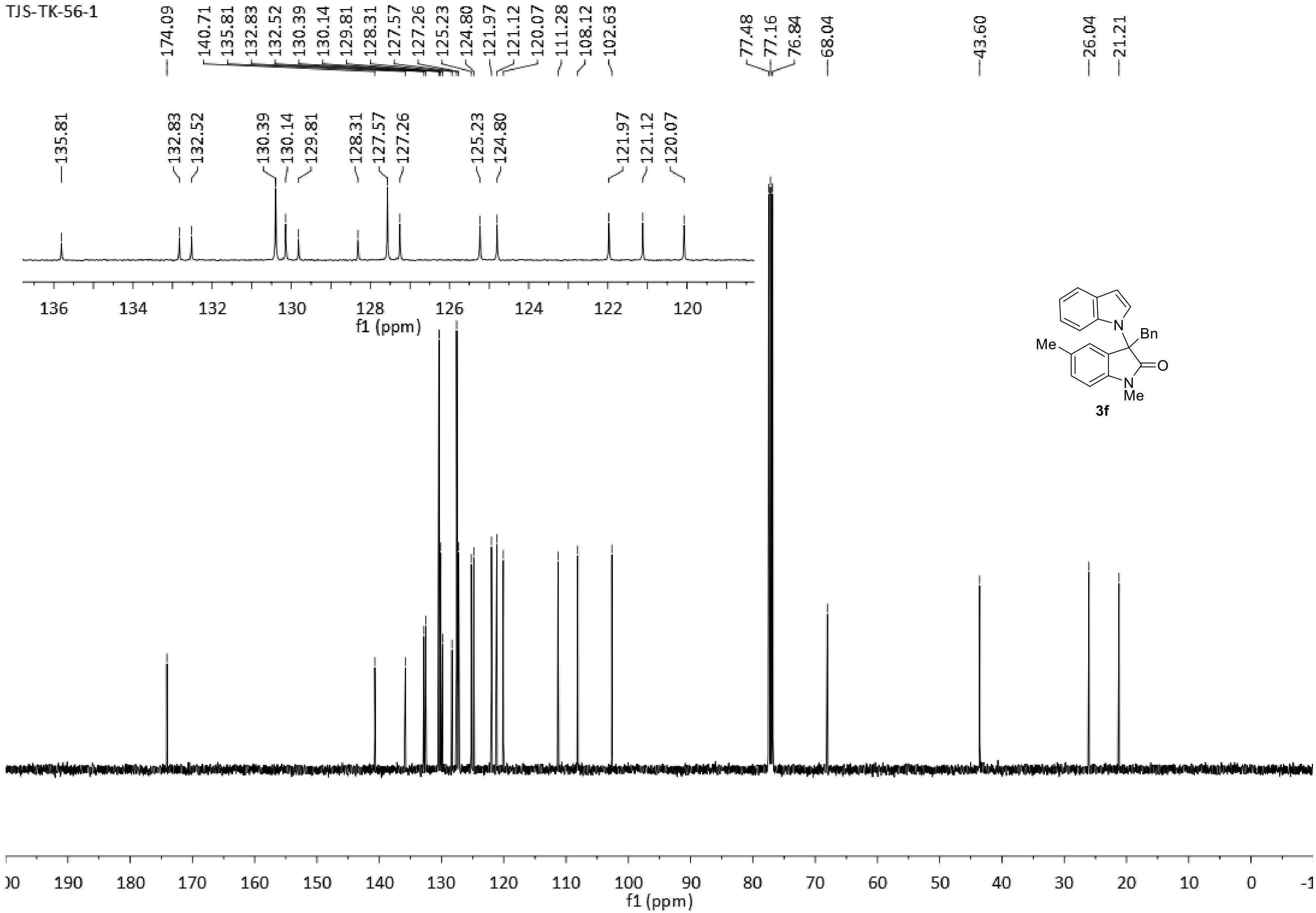
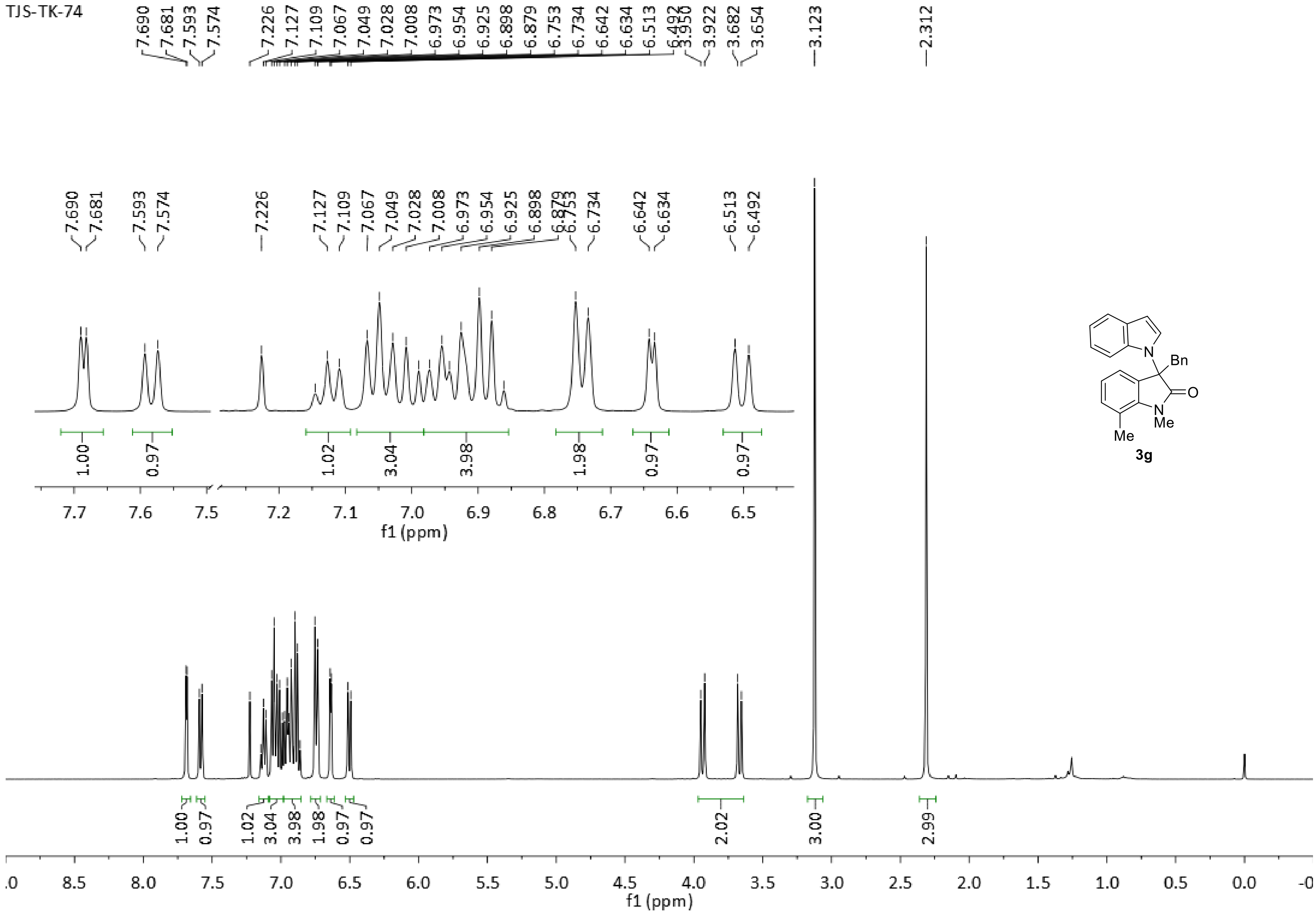
6.513
6.493
6.473
3.978
3.949
3.756
3.727
2.883
2.271
0.99
0.97
1.03
3.91
0.96
0.99
1.93
0.96
1.92
2.04
2.96
2.94
f1 (ppm)
Me
Bn
N
O
N
Me
3f

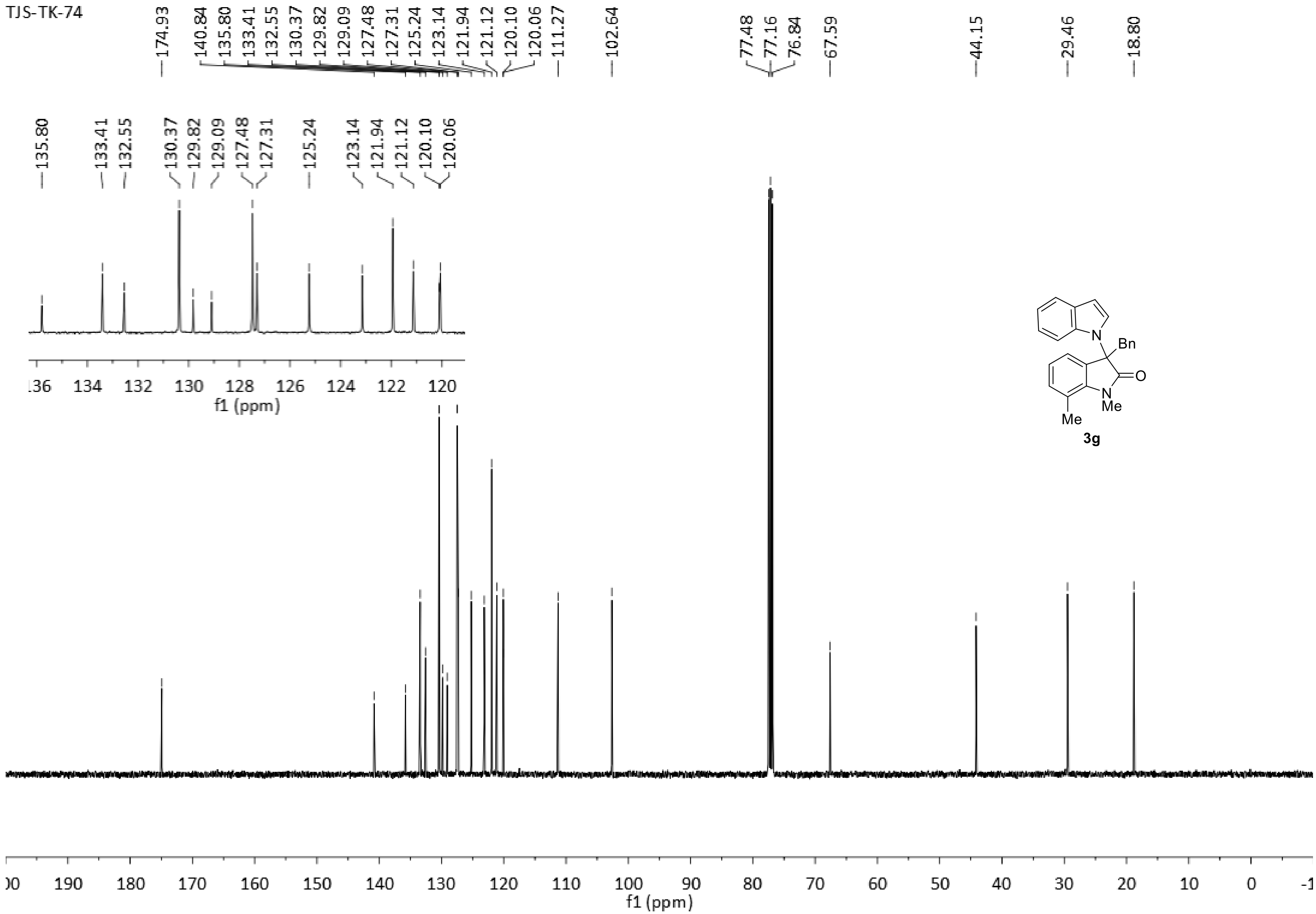

TJS-TK-56-1
174.09
140.71
135.81
132.83
132.52
130.39
130.14
129.81
128.31
127.57
127.26
125.23
124.80
121.97
121.12
120.07
111.28
108.12
102.63
77.48
77.16
76.84
68.04
43.60
26.04
21.21
f1 (ppm)
Me
Bn
N
O
Me
3f

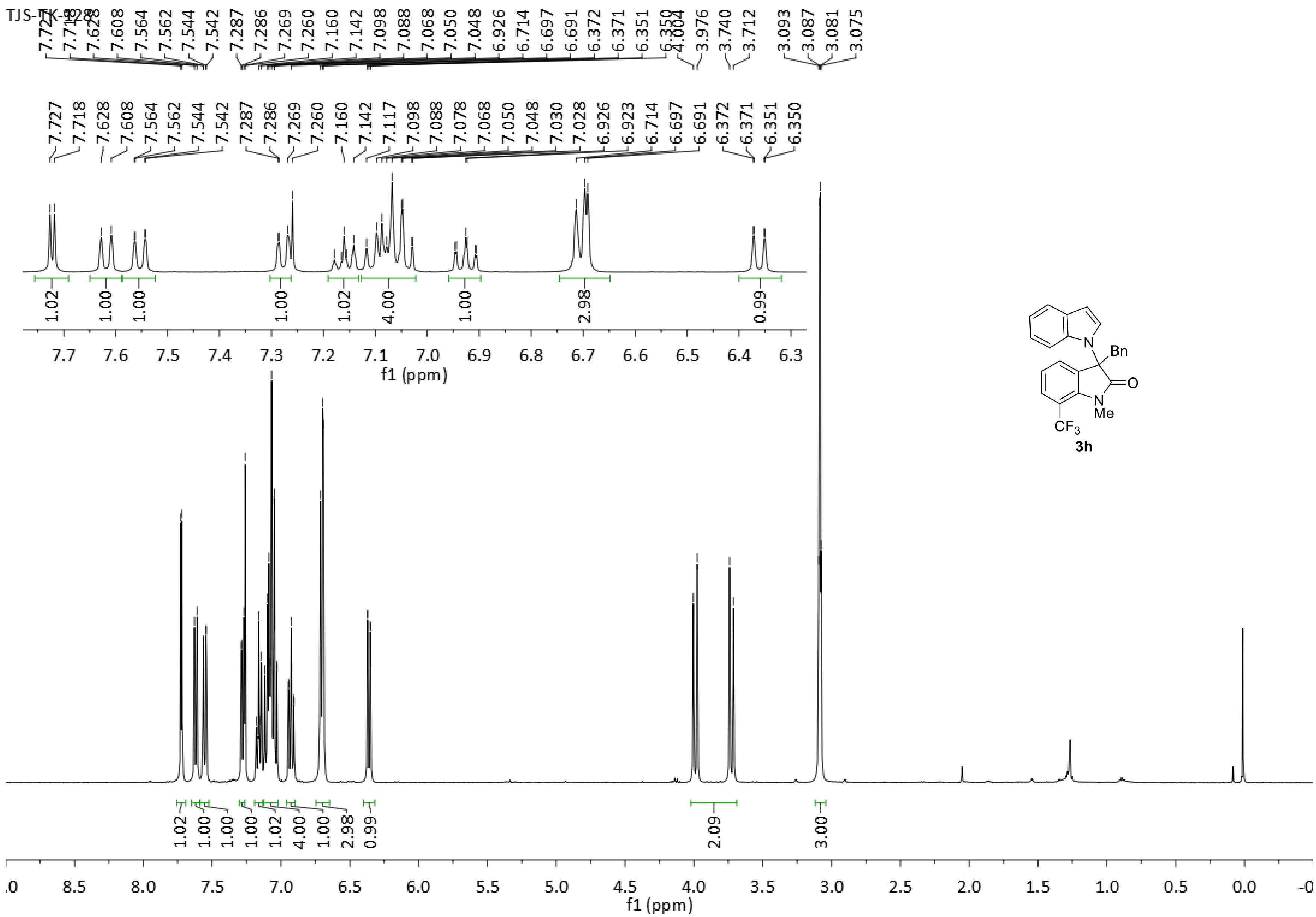
TJS-TK-74

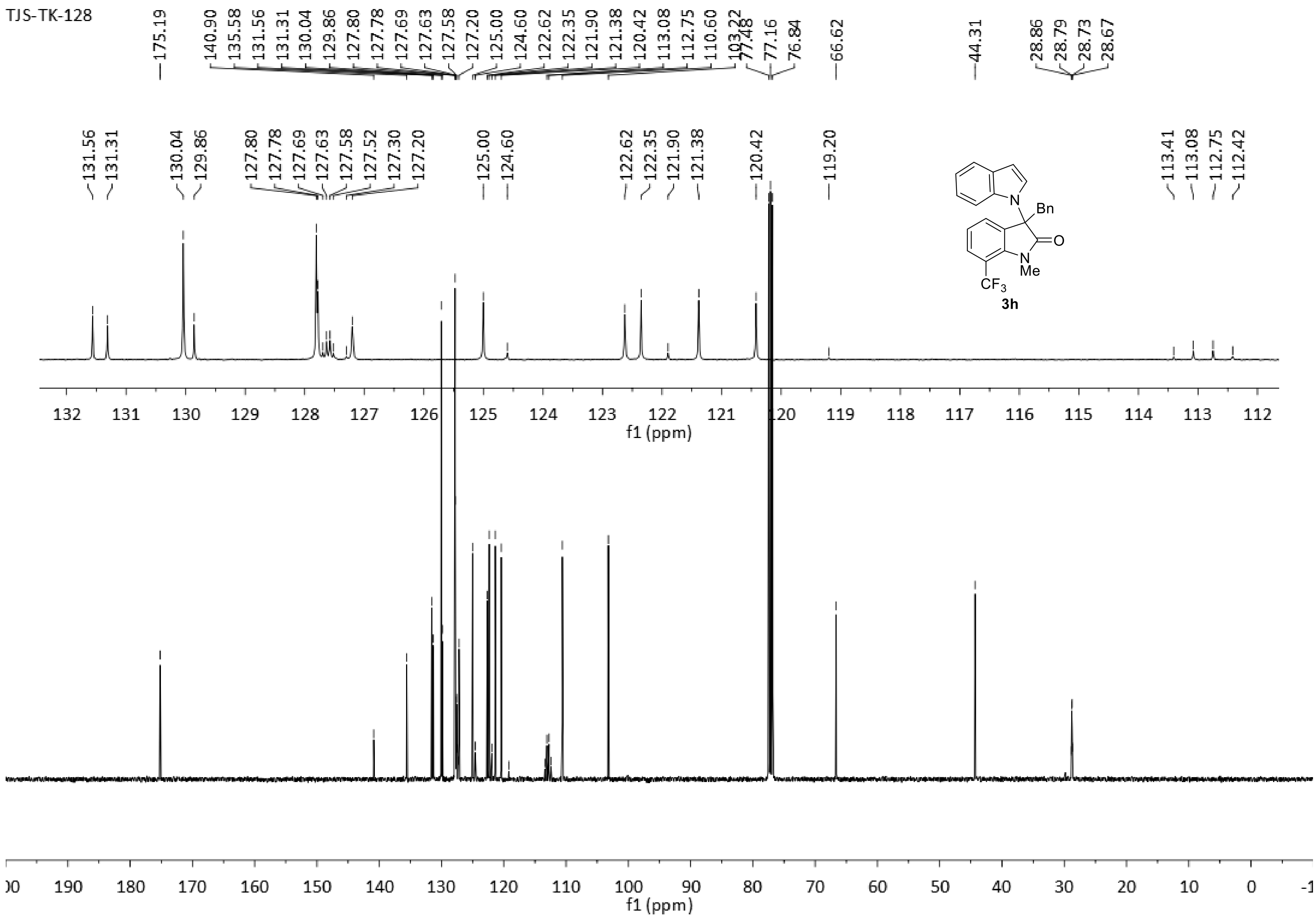


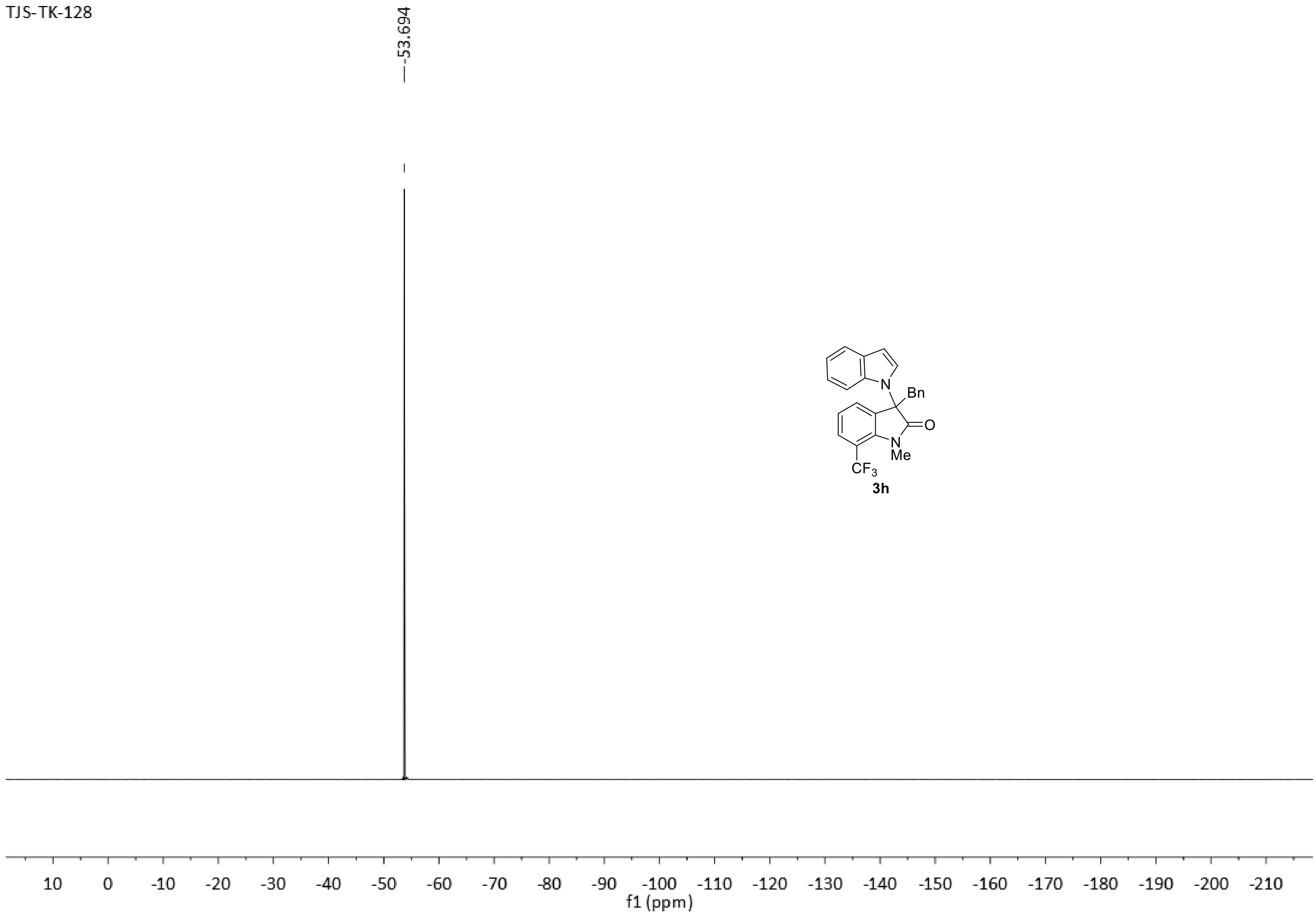
7.690
7.681
7.593
7.574
7.226
7.127
7.109
7.067
7.049
7.028
7.008
6.973
6.954
6.925
6.898
6.879
6.753
6.734
6.642
6.634
6.513
6.492
3.950
3.922
3.682
3.654
3.123
2.312
1.00
0.97
1.02
3.04
3.98
1.98
0.97
0.97
2.02
3.00
2.99
f1 (ppm)
N
Bn
O
N
Me
Me

3g

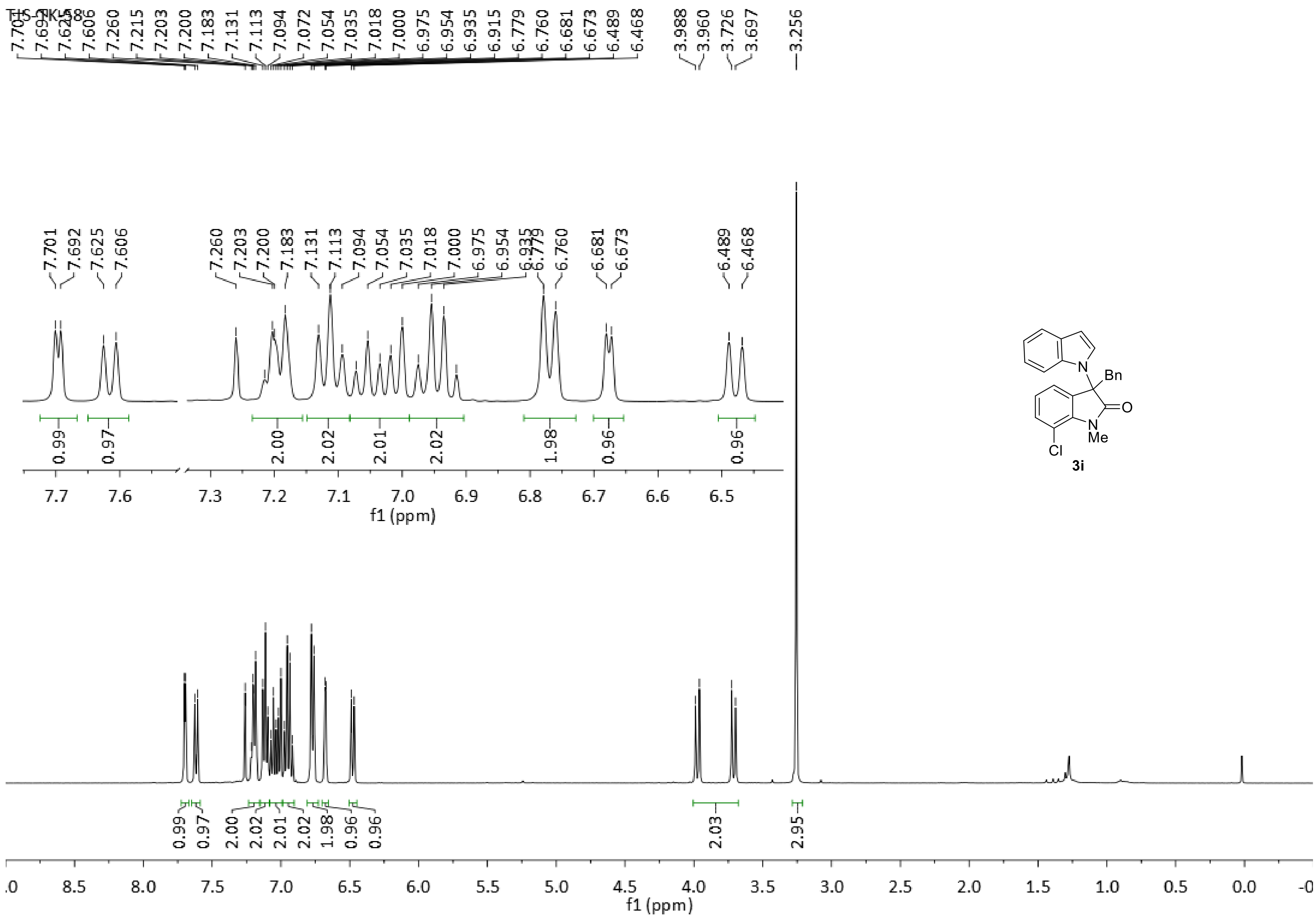

TJS-TK-74
174.93
140.84
135.80
133.41
132.55
130.37
129.82
129.09
127.48
127.31
125.24
123.14
121.94
121.12
120.10
120.06
111.27
102.64
77.48
77.16
76.84
67.59
44.15
29.46
18.80
Bn
N
O
Me
Me
3g
f1 (ppm)

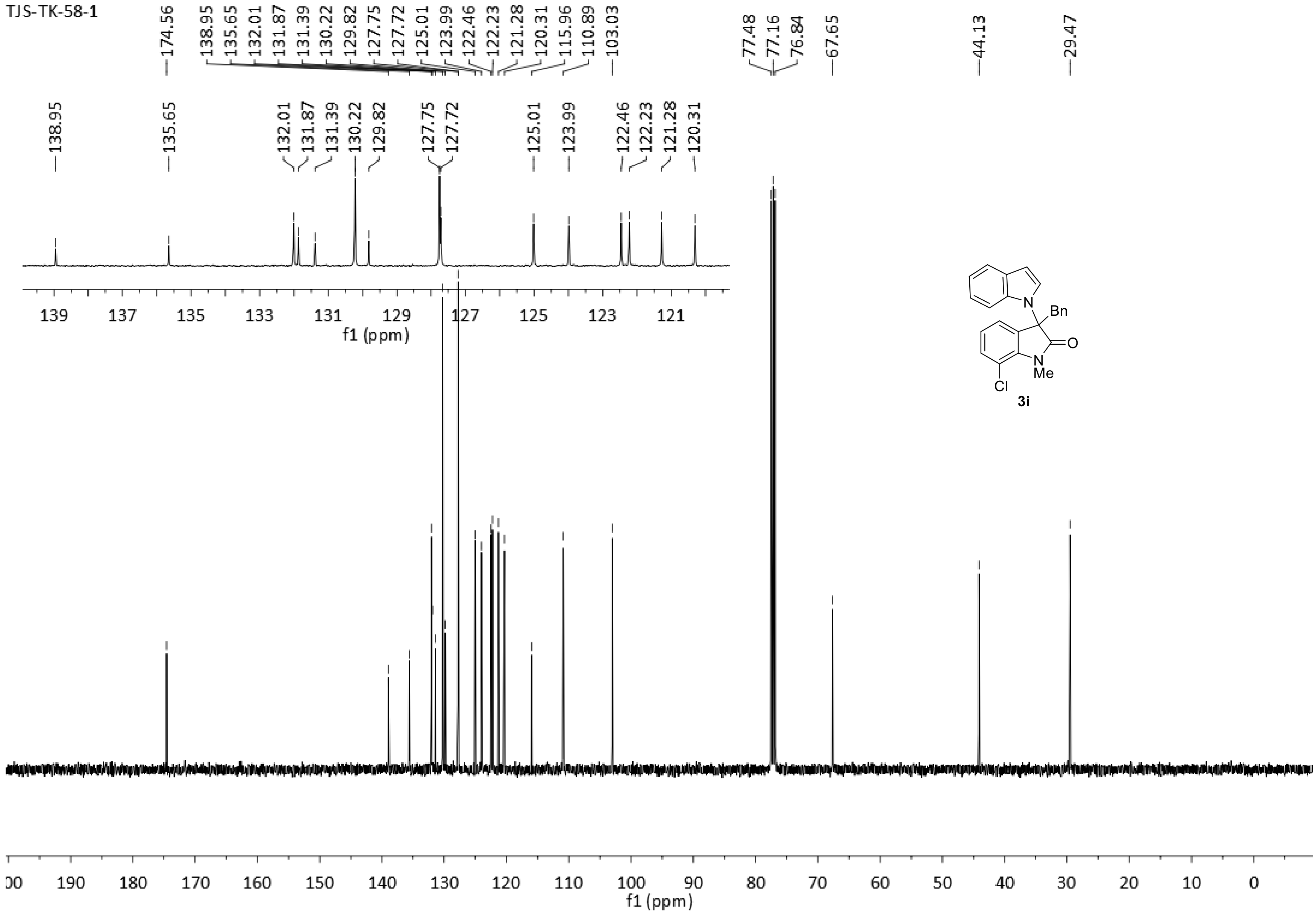

TJS-TK-128
f1 (ppm)
Bn
O
N
Me
CF3
3h

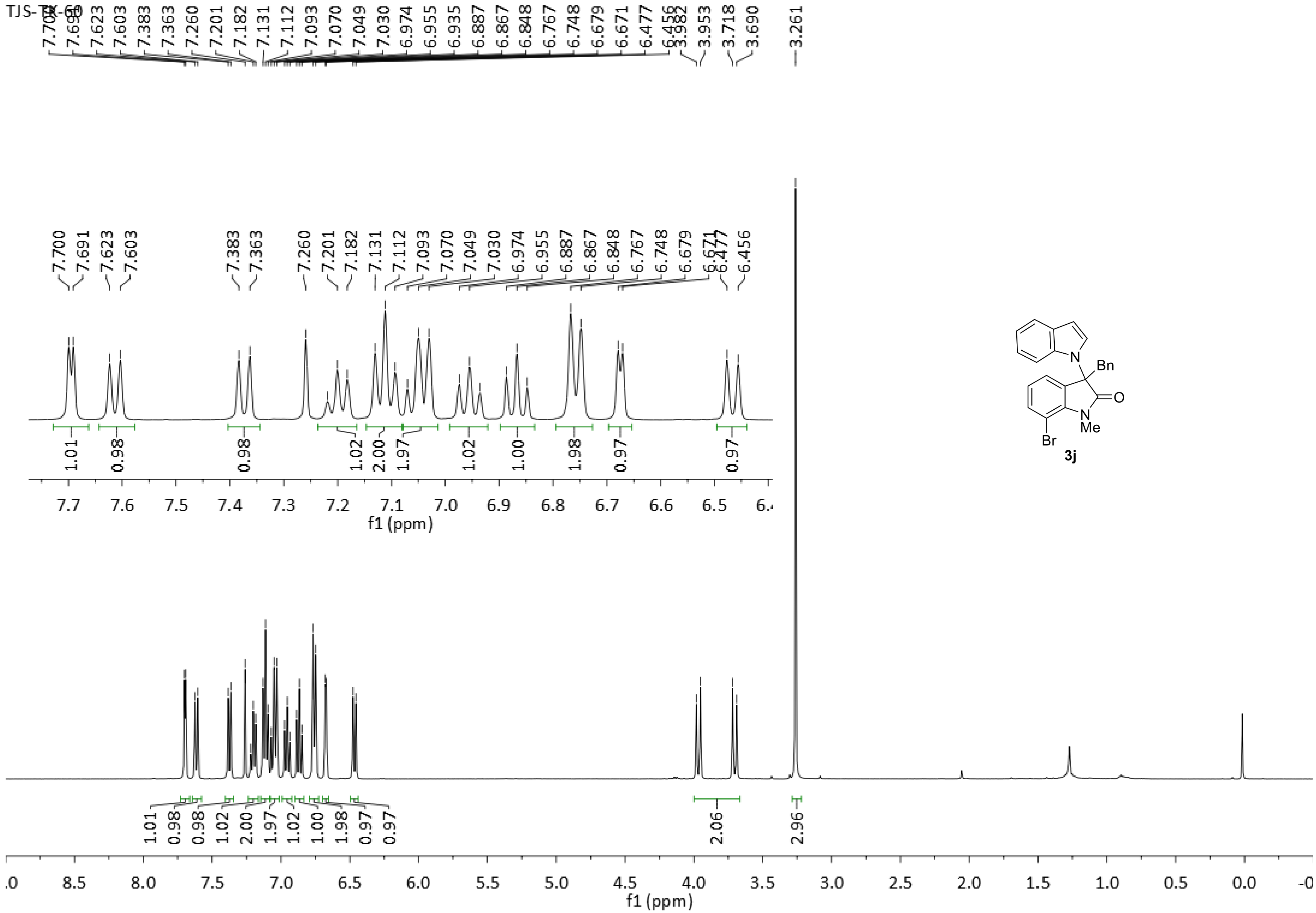

TJS-TK-128
175.19
140.90
135.58
131.56
131.31
130.04
129.86
127.80
127.78
127.69
127.63
127.58
127.20
125.00
124.60
122.62
122.35
121.90
121.38
120.42
113.08
112.75
110.60
103.22
77.48
77.16
76.84
66.62
44.31
28.86
28.79
28.73
28.67
131.56
131.31
130.04
129.86
127.80
127.78
127.69
127.63
127.58
127.52
127.30
127.20
125.00
124.60
122.62
122.35
121.90
121.38
120.42
119.20
113.41
113.08
112.75
112.42
N
Bn
O
N
Me
CF_3
3h
f1 (ppm)
f1 (ppm)

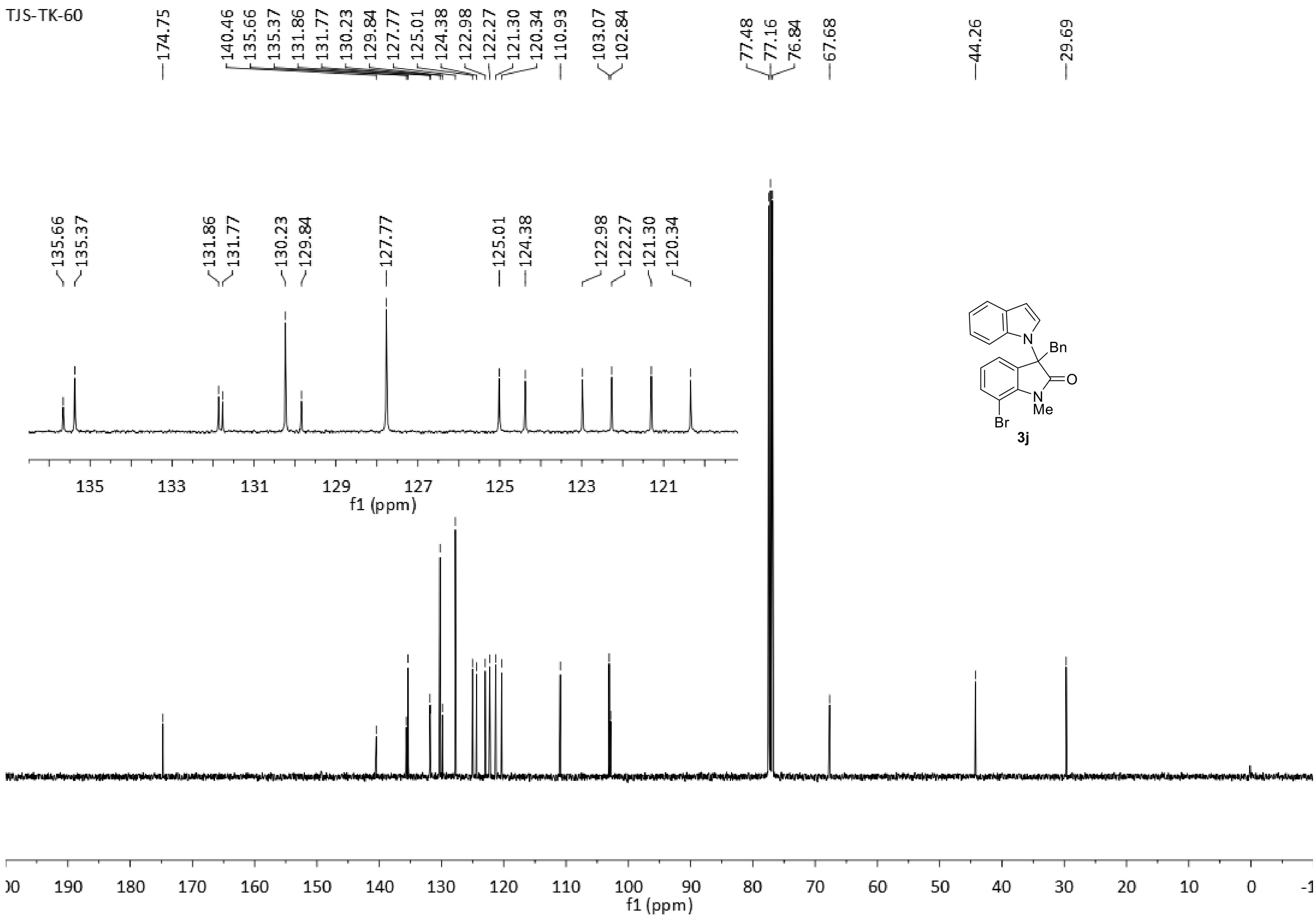

TJS-TK-128
-53.694
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
N
Bn
O
N
Me
CF_3

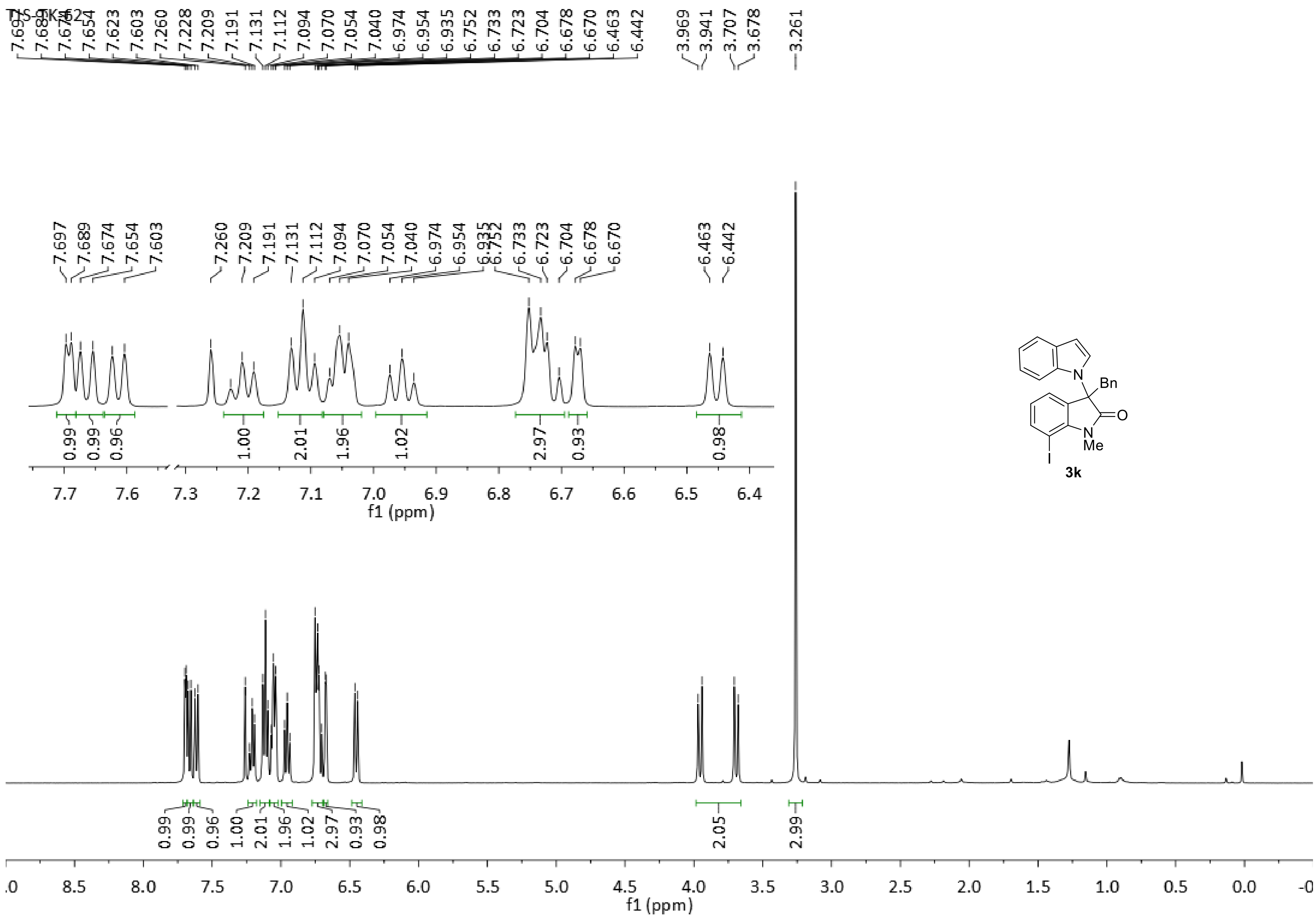
3h


THS-TK-58
f1 (ppm)
Bn
O
N
Me
Cl
3i

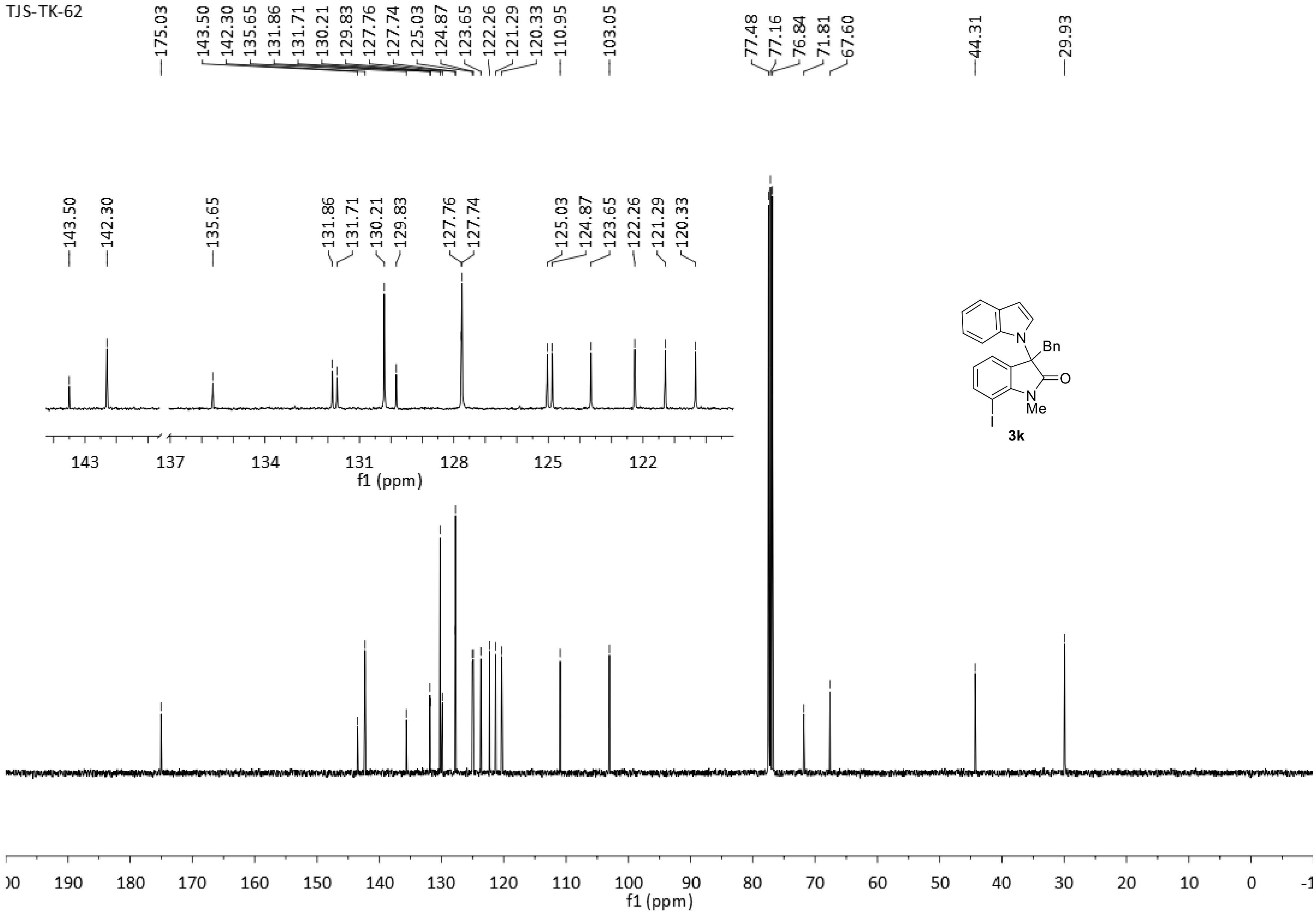

TJS-TK-58-1
174.56
138.95
135.65
132.01
131.87
131.39
130.22
129.82
127.75
127.72
125.01
123.99
122.46
122.23
121.28
120.31
115.96
110.89
103.03
77.48
77.16
76.84
67.65
44.13
29.47
f1 (ppm)
N
Bn
O
N
Me
Cl
3i

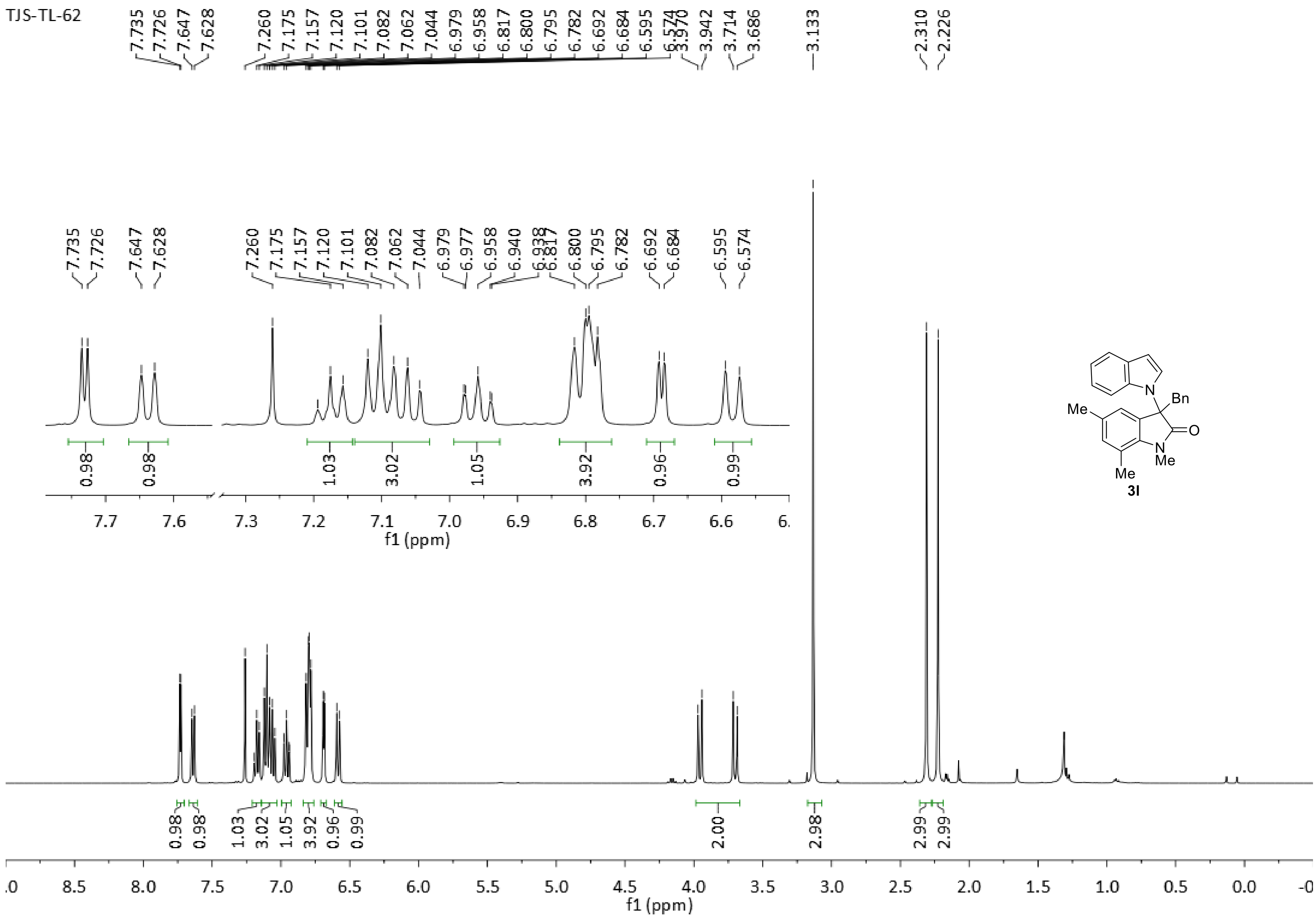

TJS-TX-60
Bn
O
N
Me
Br
3j
f1 (ppm)

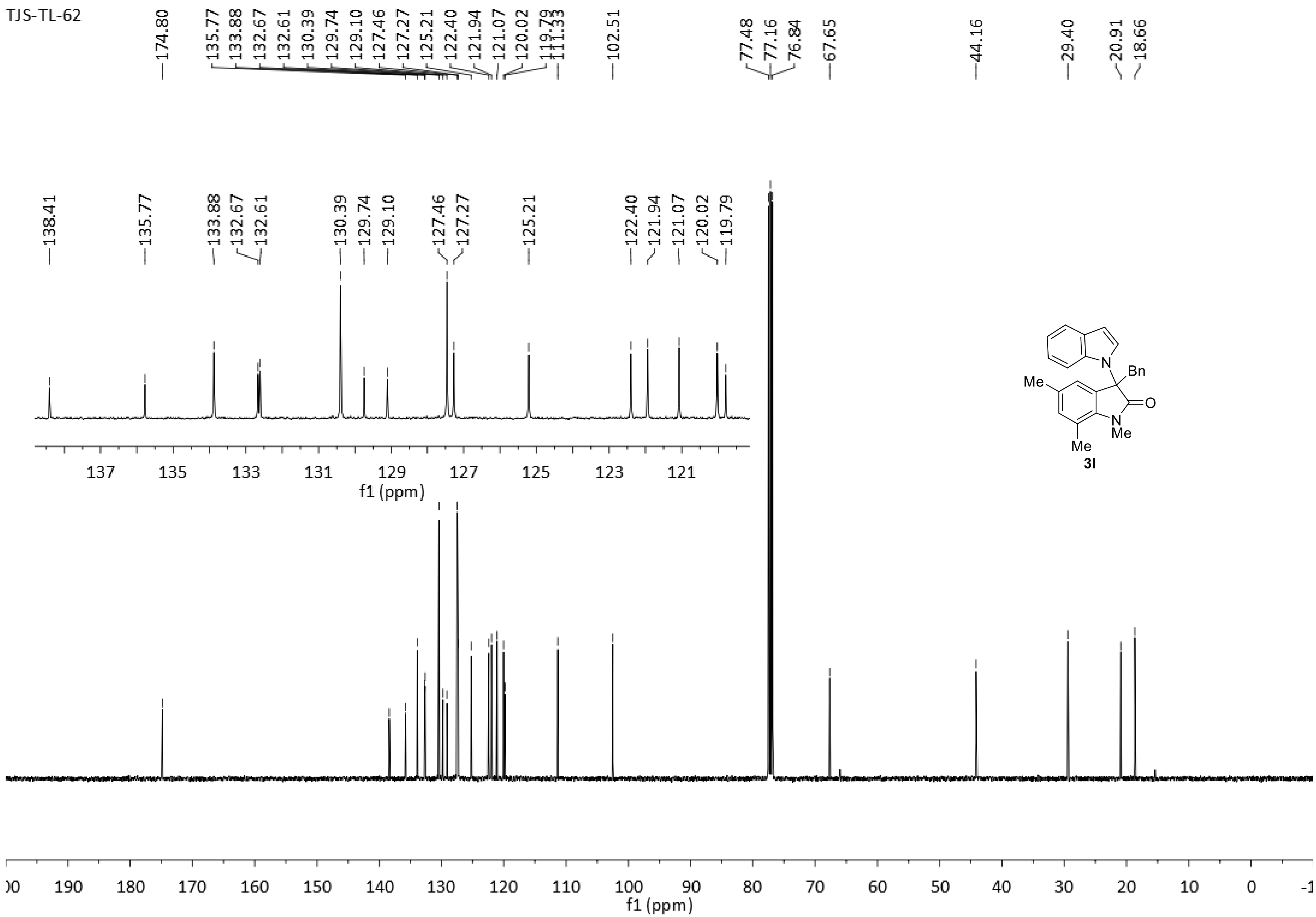

TJS-TK-60
174.75
140.46
135.66
135.37
131.86
131.77
130.23
129.84
127.77
125.01
124.38
122.98
122.27
121.30
120.34
110.93
103.07
102.84
77.48
77.16
76.84
67.68
44.26
29.69
Bn
O
N
Me
Br
3j
f1 (ppm)



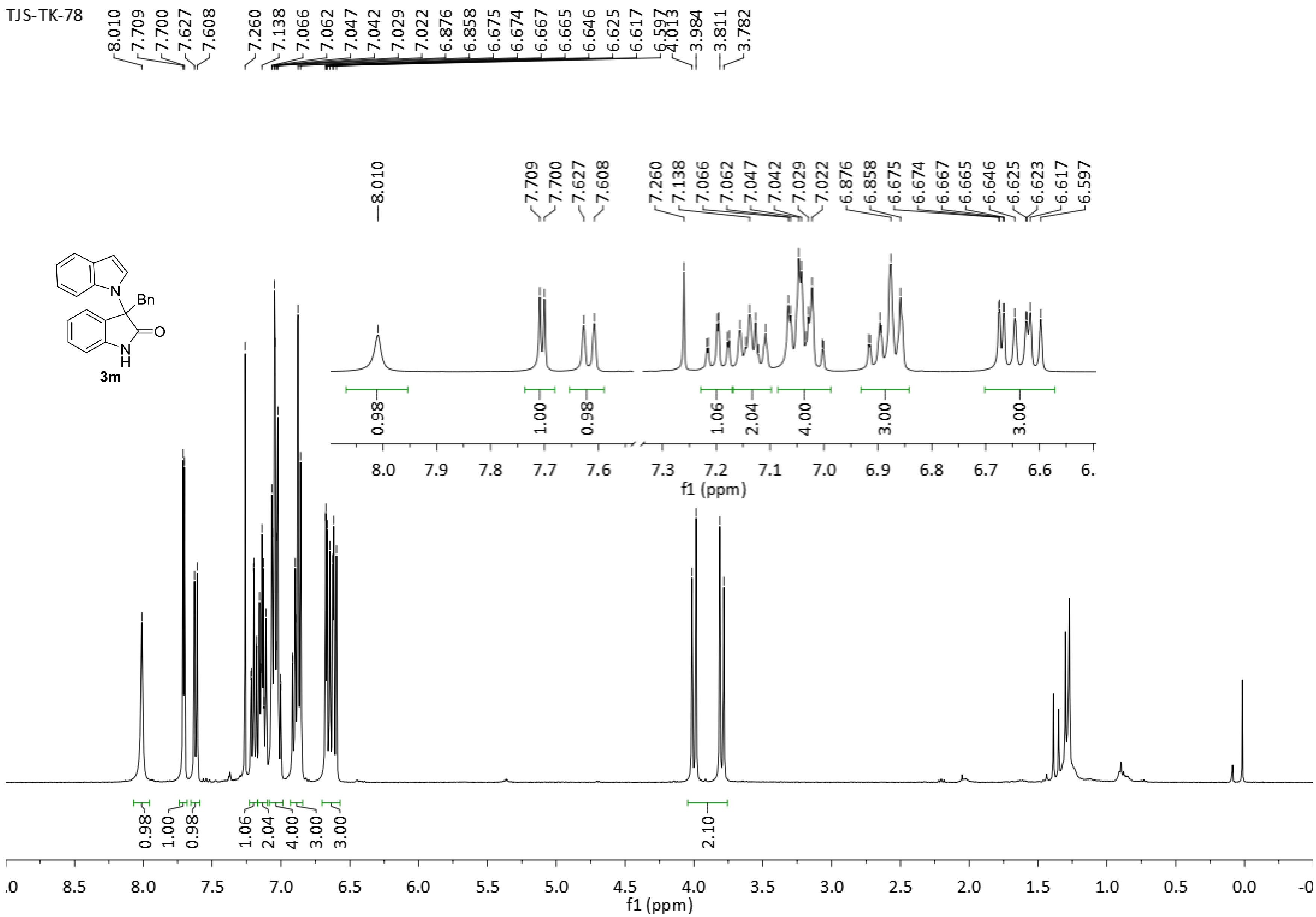
f1 (ppm)
Bn
N
O
Me
I
3k


TJS-TK-62
175.03
143.50
142.30
135.65
131.86
131.71
130.21
129.83
127.76
127.74
125.03
124.87
123.65
122.26
121.29
120.33
110.95
103.05
77.48
77.16
76.84
71.81
67.60
44.31
29.93
143 137 134 131 128 125 122
f1 (ppm)
N
Bn
O
N
Me
I
3k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

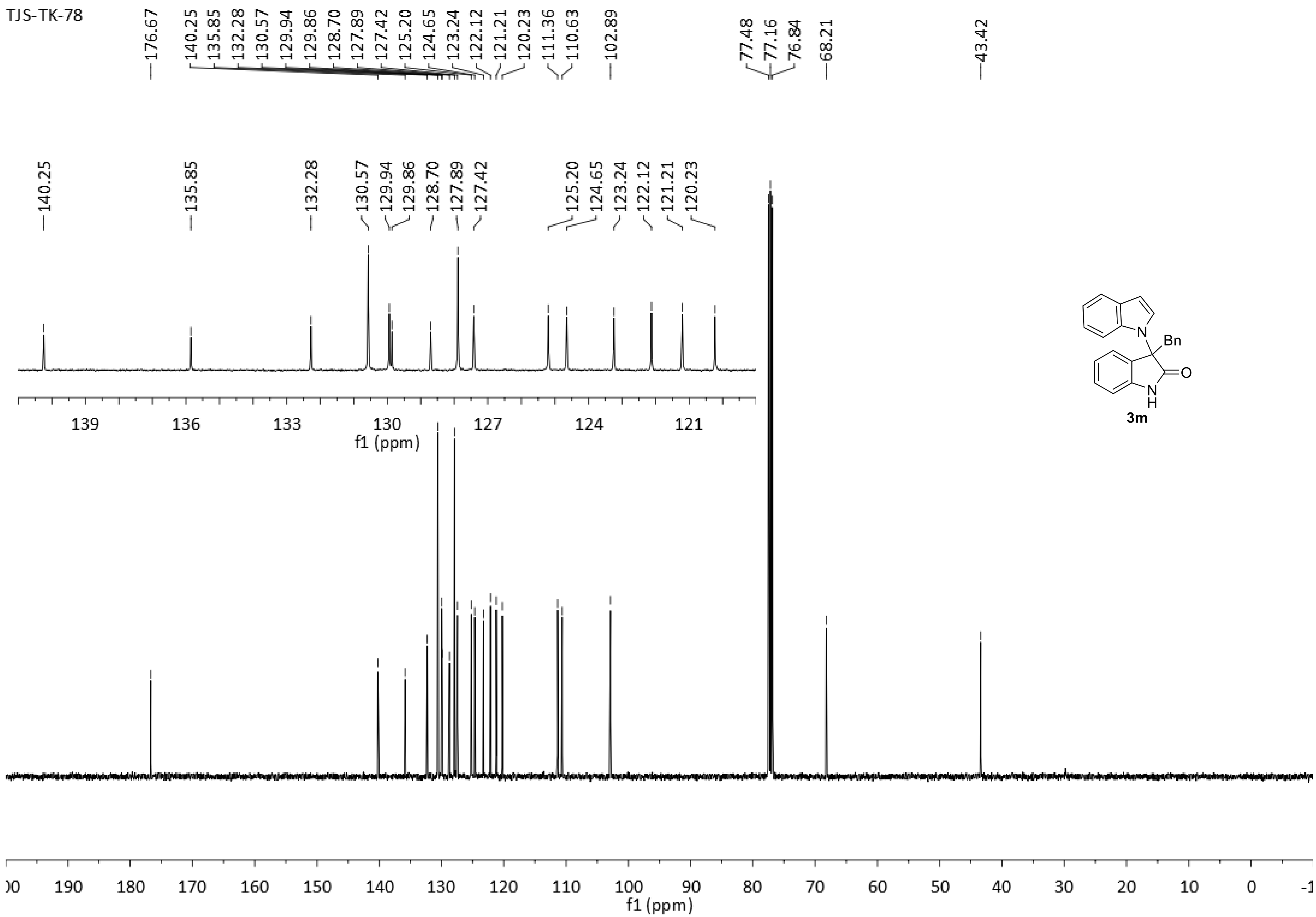

TJS-TL-62
Me
Bn
N
O
Me
3l
f1 (ppm)


TJS-TL-62
174.80
135.77
133.88
132.67
132.61
130.39
129.74
129.10
127.46
127.27
125.21
122.40
121.94
121.07
120.02
119.79
111.33
102.51
77.48
77.16
76.84
67.65
44.16
29.40
20.91
18.66
138.41
135.77
133.88
132.67
132.61
130.39
129.74
129.10
127.46
127.27
125.21
122.40
121.94
121.07
120.02
119.79
137
135
133
131
129
127
125
123
121
f1 (ppm)
Me
N
Bn
O
N
Me
Me
3l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

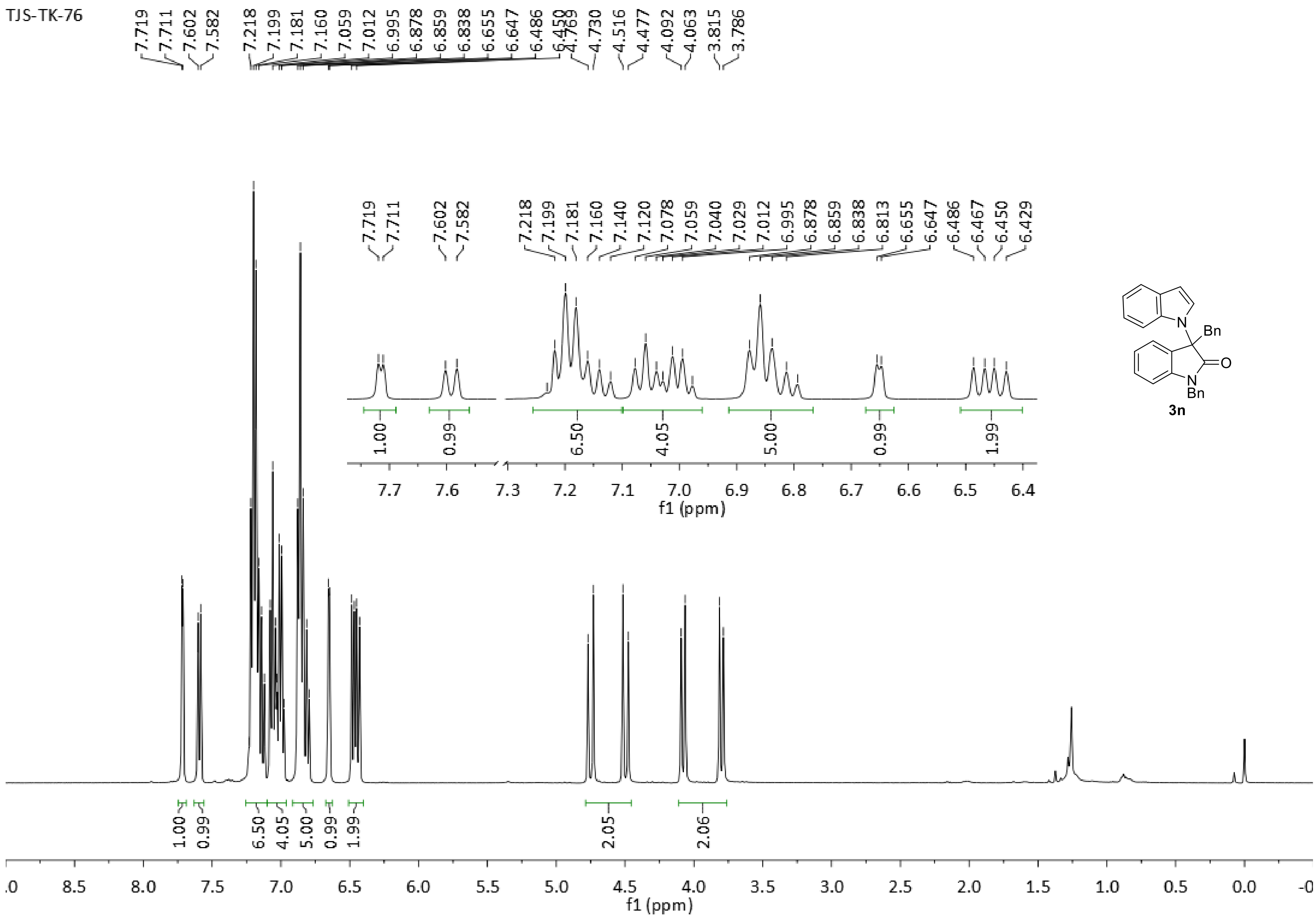
TJS-TK-78



8.010
7.709
7.700
7.627
7.608
7.260
7.138
7.066
7.062
7.047
7.042
7.029
7.022
6.876
6.858
6.675
6.674
6.667
6.665
6.646
6.625
6.623
6.617
6.597
4.013
3.984
3.811
3.782
Bn
N
O
H
3m
0.98
1.00
0.98
1.06
2.04
4.00
3.00
3.00
2.10
f1 (ppm)

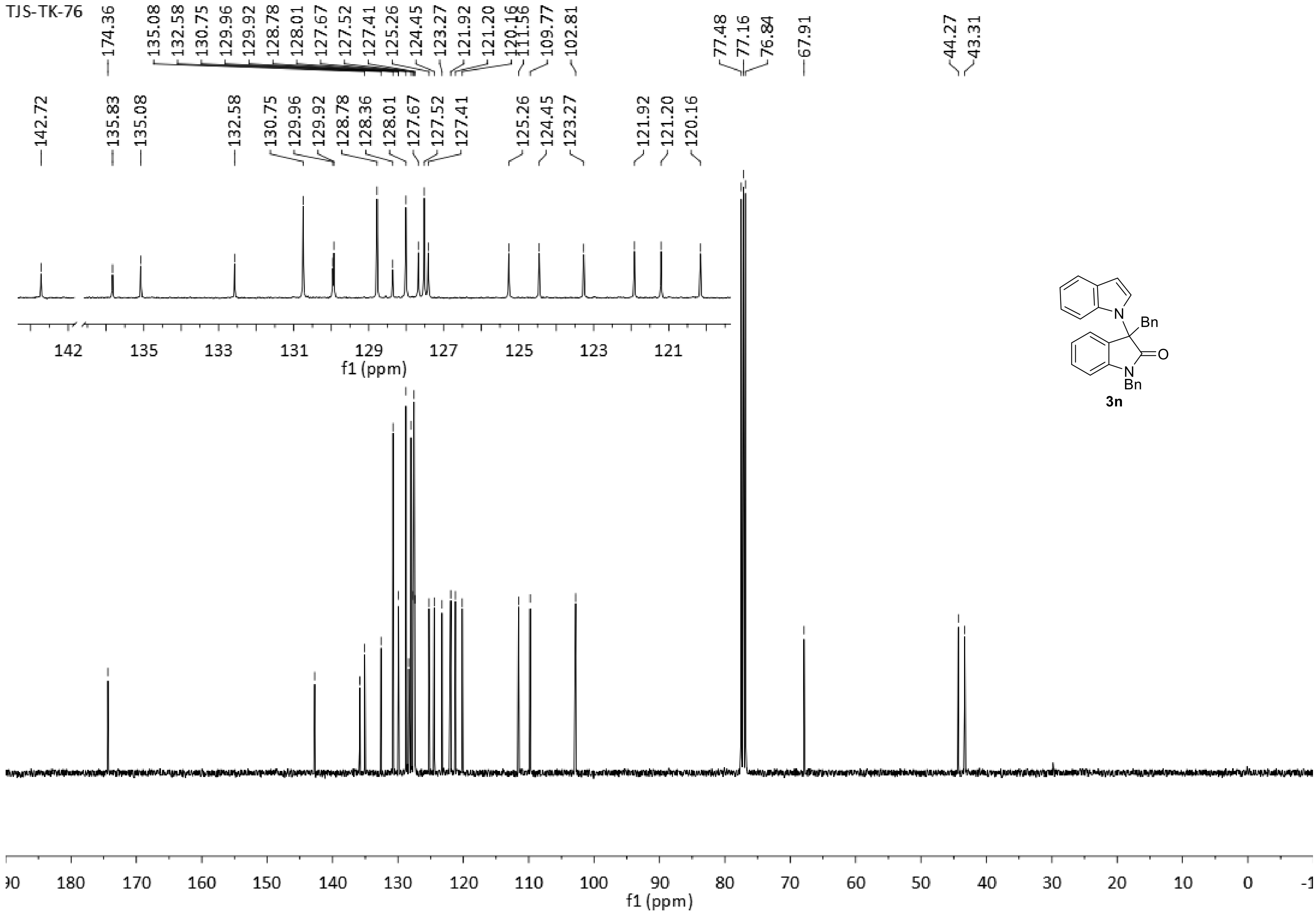

TJS-TK-78
176.67
140.25
135.85
132.28
130.57
129.94
129.86
128.70
127.89
127.42
125.20
124.65
123.24
122.12
121.21
120.23
111.36
110.63
102.89
77.48
77.16
76.84
68.21
43.42
f1 (ppm)
N
Bn
O
N
H

3m


TJS-TK-76
7.719
7.711
7.602
7.582
7.218
7.199
7.181
7.160
7.140
7.120
7.078
7.059
7.040
7.029
7.012
6.995
6.878
6.859
6.838
6.813
6.655
6.647
6.486
6.467
6.450
6.429
4.769
4.730
4.516
4.477
4.092
4.063
3.815
3.786
1.00
0.99
6.50
4.05
5.00
0.99
1.99
2.05
2.06
f1 (ppm)
Bn
O
N
Bn

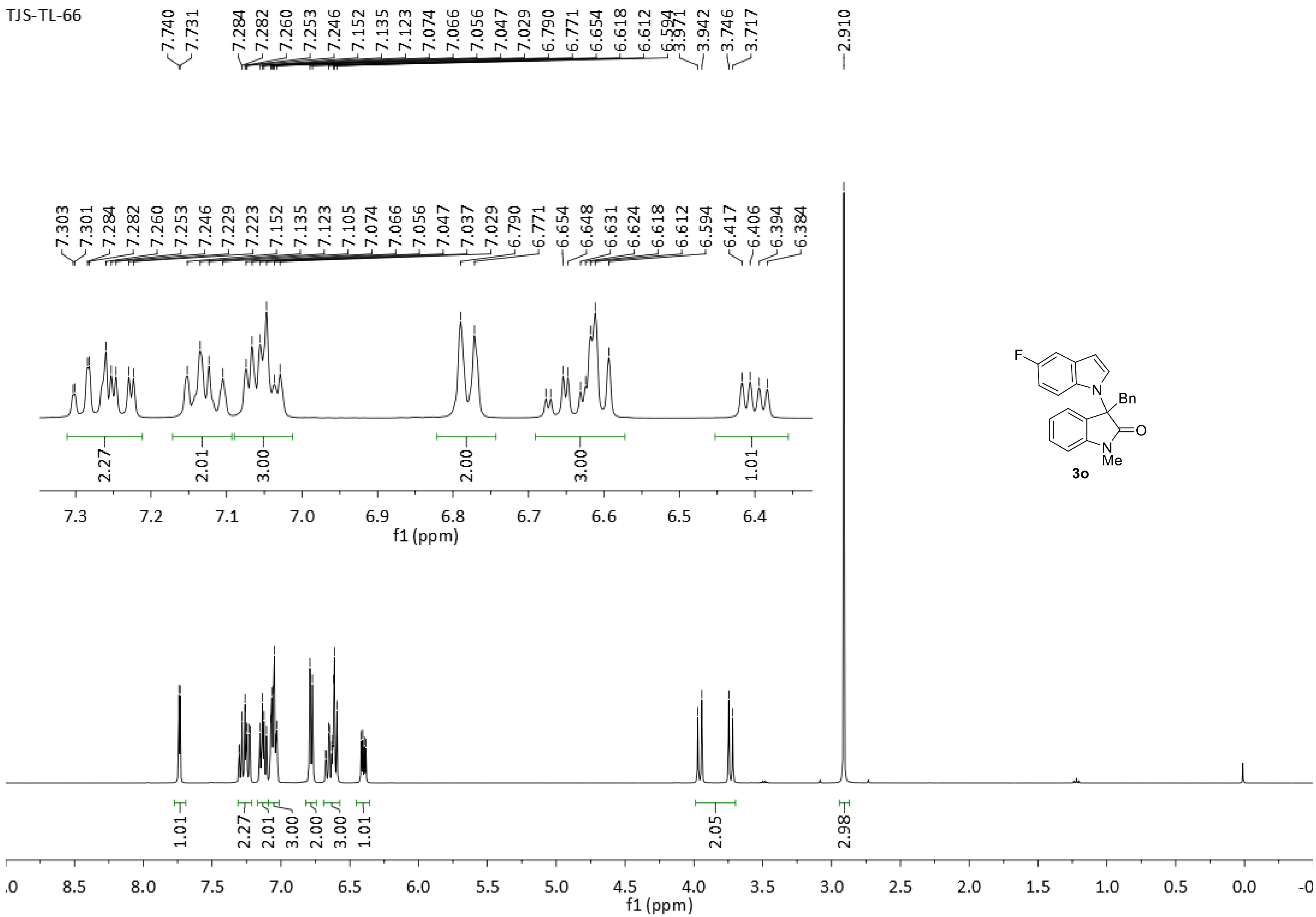
3n

TJS-TK-76

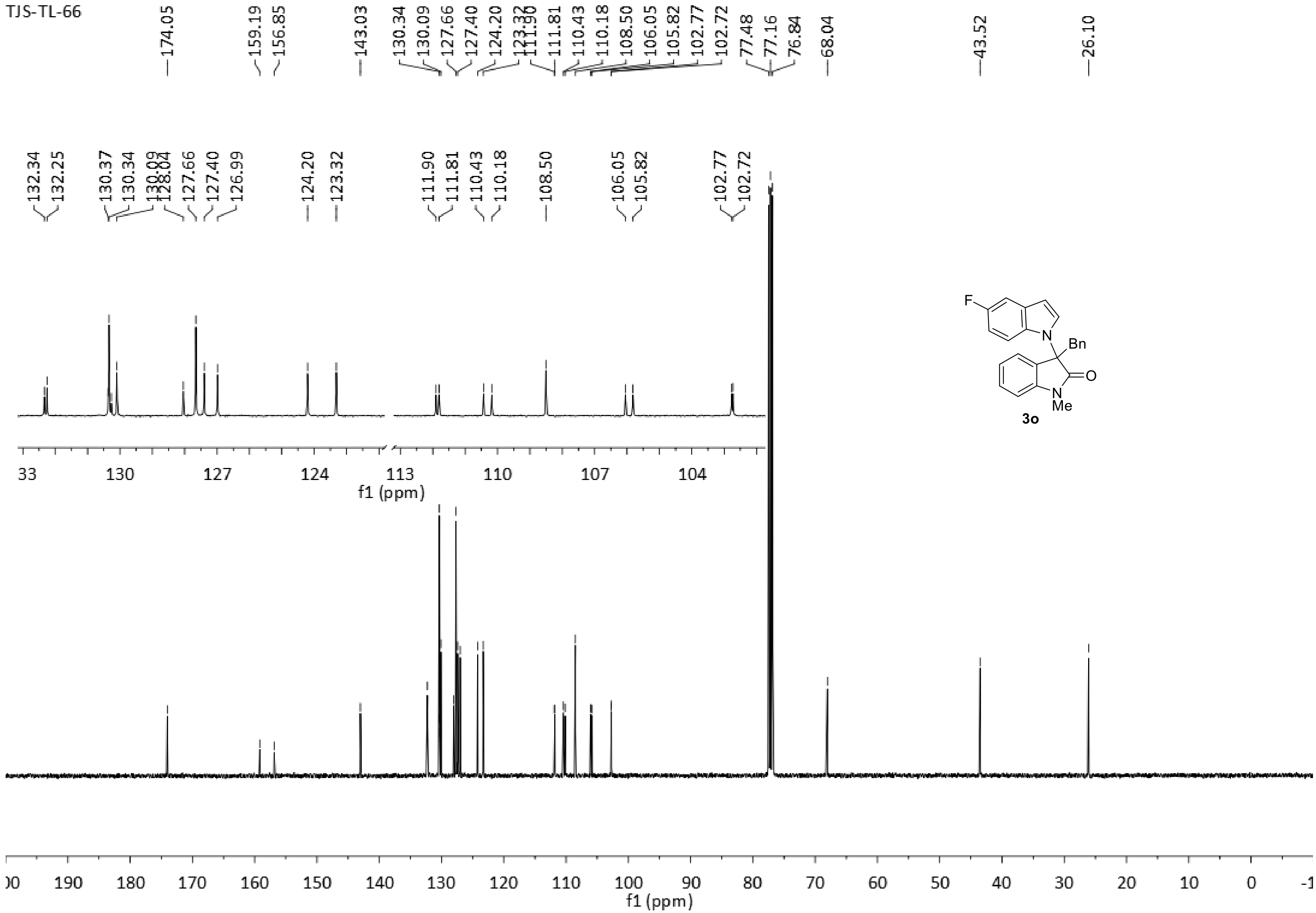


174.36
135.08
132.58
130.75
129.96
129.92
128.78
128.01
127.67
127.52
127.41
125.26
124.45
123.27
121.92
121.20
120.16
111.56
109.77
102.81
77.48
77.16
76.84
67.91
44.27
43.31
142.72
135.83
135.08
132.58
130.75
129.96
129.92
128.78
128.36
128.01
127.67
127.52
127.41
125.26
124.45
123.27
121.92
121.20
120.16
f1 (ppm)
f1 (ppm)
N
Bn
O
N
Bn

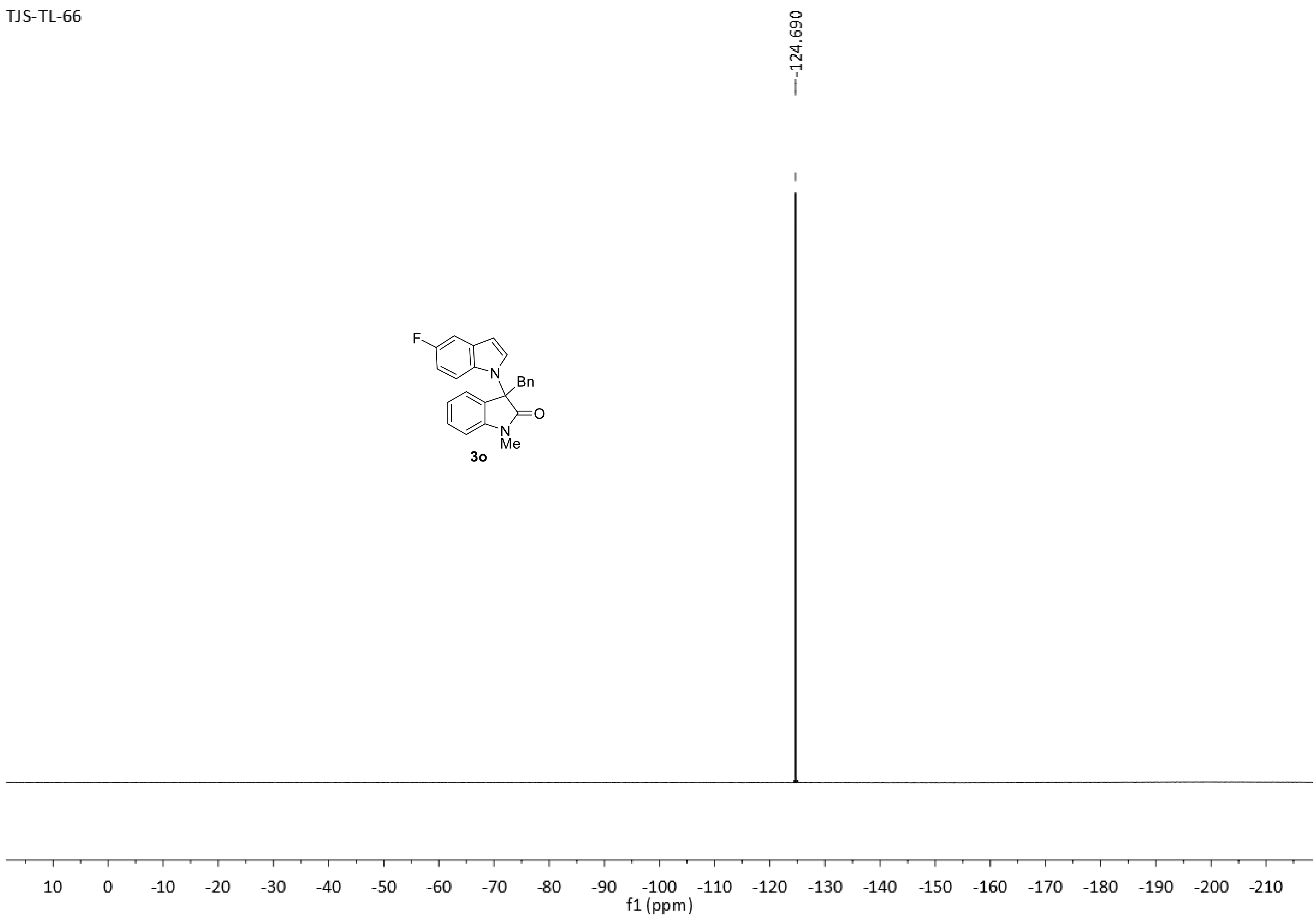
3n

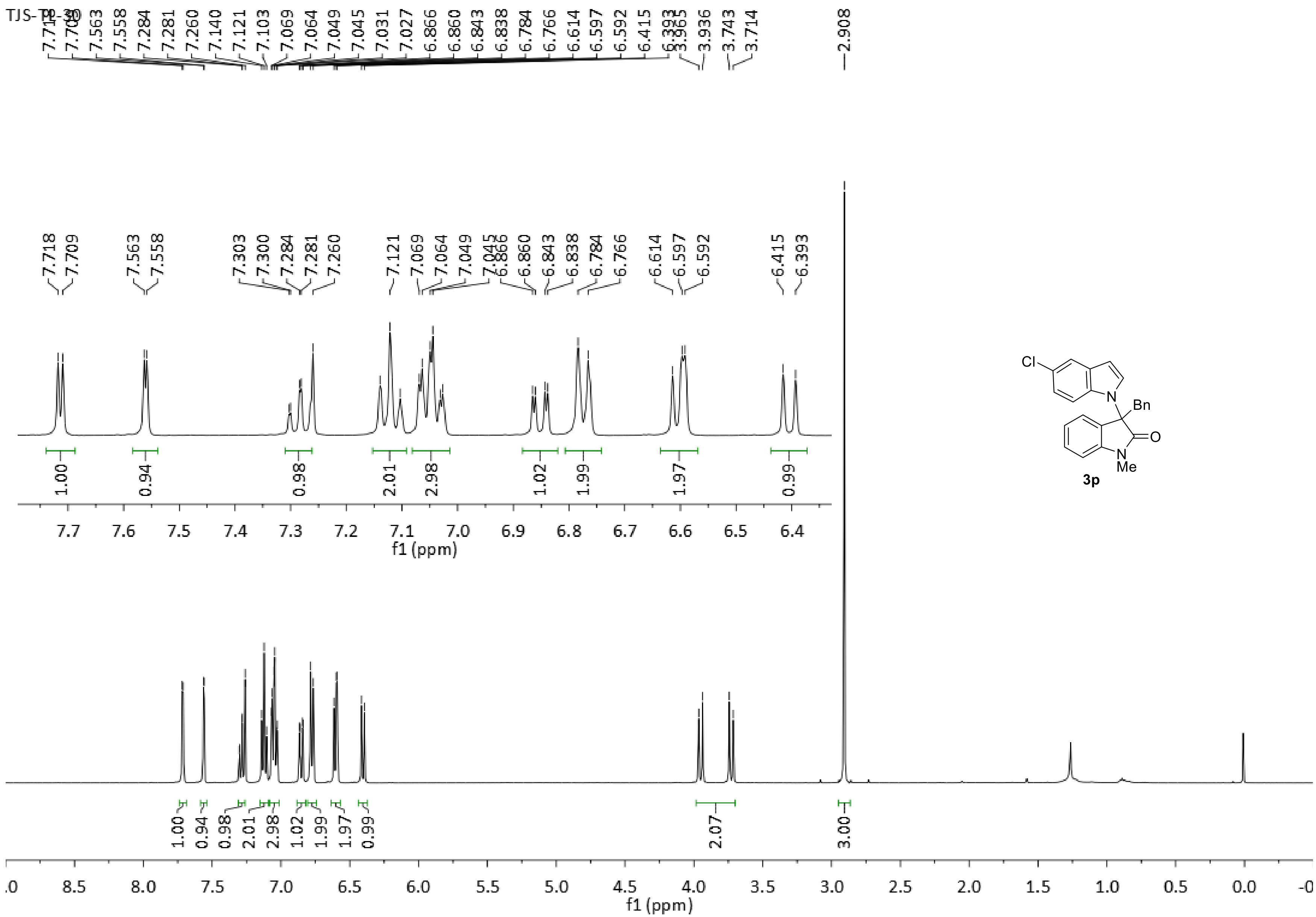

TJS-TL-66
7.740
7.731
7.284
7.282
7.260
7.253
7.246
7.152
7.135
7.123
7.074
7.066
7.056
7.047
7.029
6.790
6.771
6.654
6.618
6.612
6.594
3.971
3.942
3.746
3.717
2.910
7.303
7.301
7.284
7.282
7.260
7.253
7.246
7.229
7.223
7.152
7.135
7.123
7.105
7.074
7.066
7.056
7.047
7.037
7.029
6.790
6.771
6.654
6.648
6.631
6.624
6.618
6.612
6.594
6.417
6.406
6.394
6.384
2.27
2.01
3.00
2.00
3.00
1.01
f1 (ppm)
F
N
Bn
O
N
Me
1.01
2.27
2.01
3.00
2.00
3.00
1.01
2.05
2.98
f1 (ppm)
3o

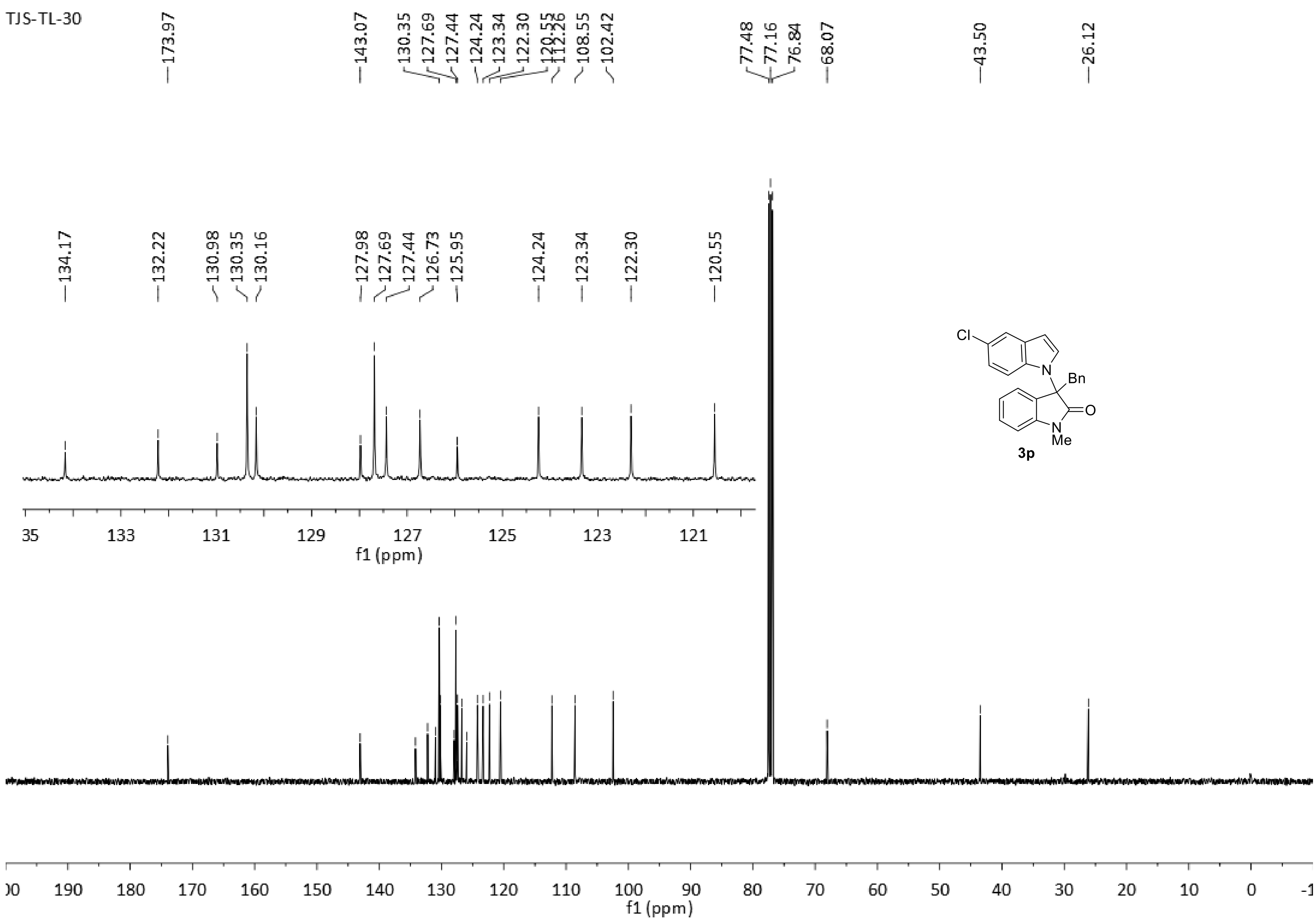
TJS-TL-66

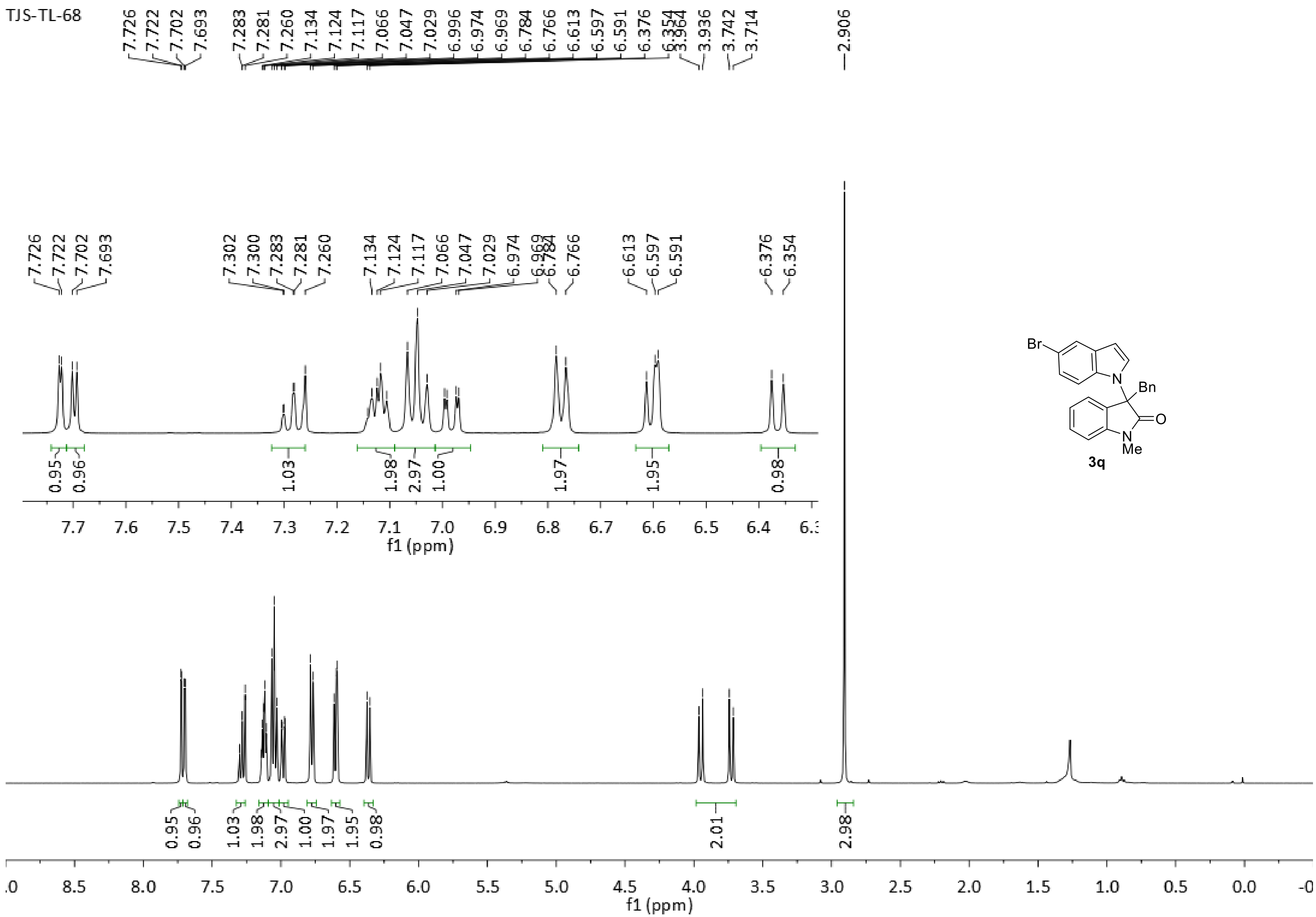

174.05
159.19
156.85
143.03
130.34
130.09
127.66
127.40
124.20
123.32
111.90
111.81
110.43
110.18
108.50
106.05
105.82
102.77
102.72
77.48
77.16
76.84
68.04
43.52
26.10
132.34
132.25
130.37
130.34
130.09
128.04
127.66
127.40
126.99
124.20
123.32
111.90
111.81
110.43
110.18
108.50
106.05
105.82
102.77
102.72
33
130
127
124
113
110
107
104
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
F
N
Bn
O
N
Me

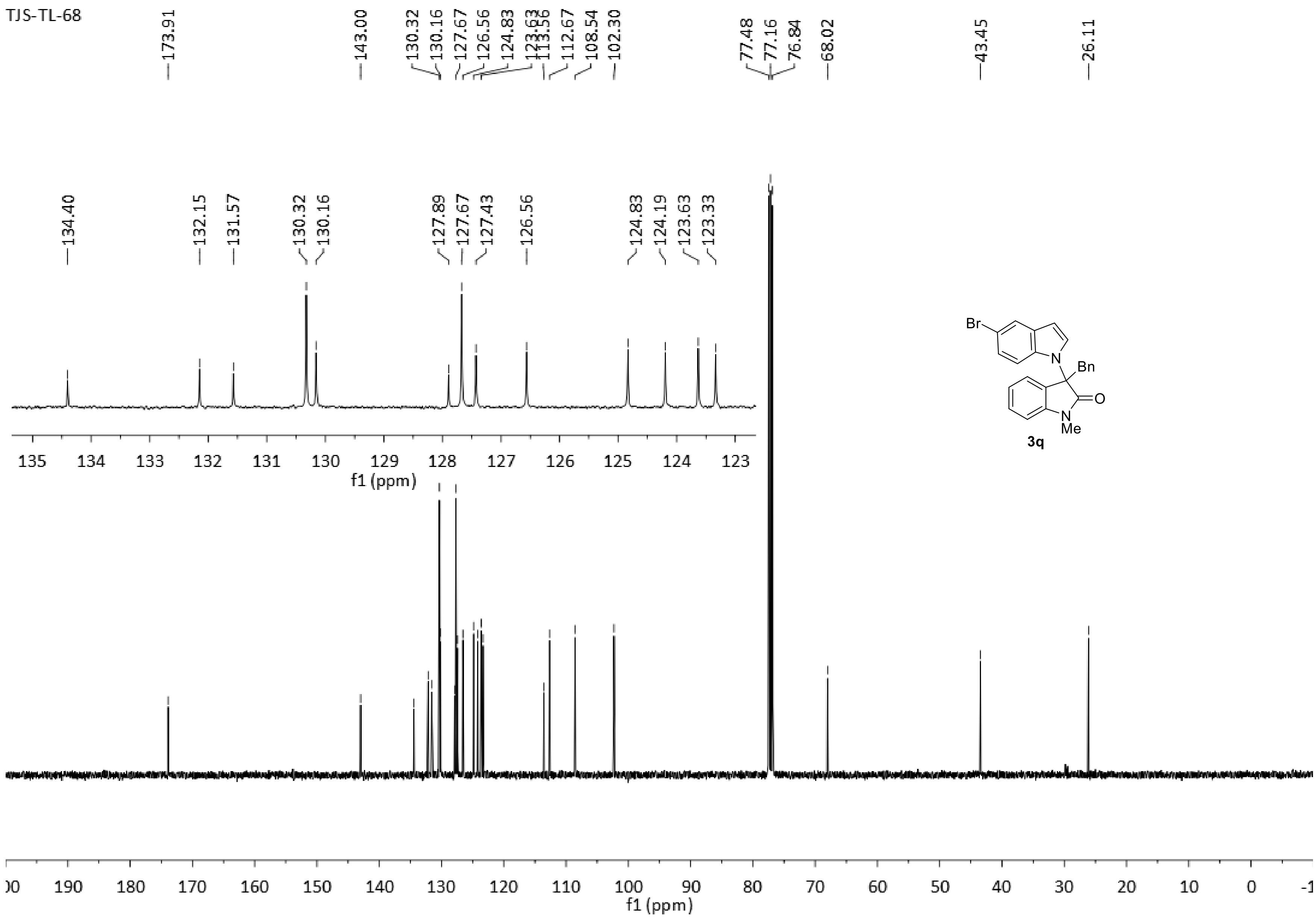
3o

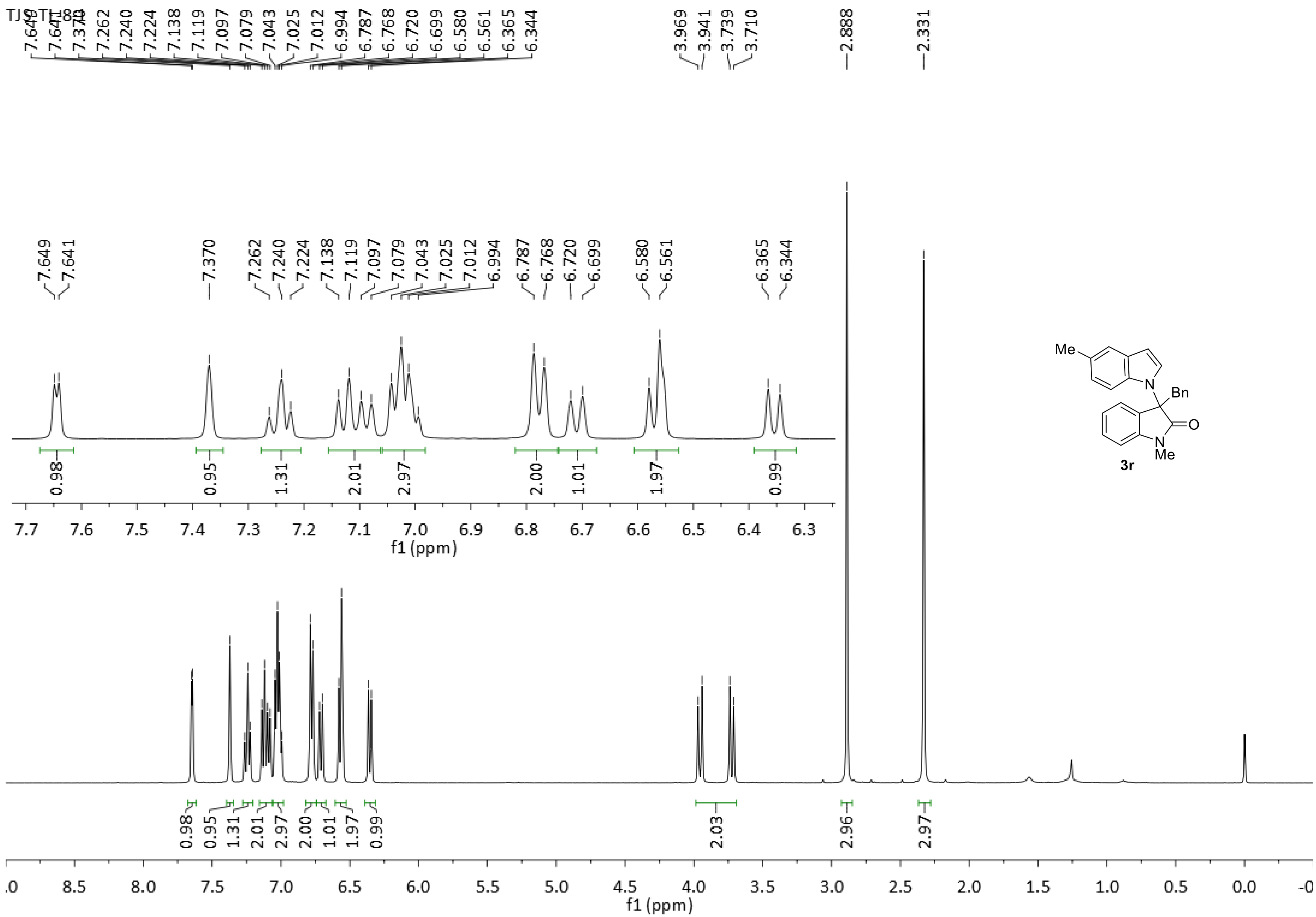

TJS-TL-66
-124.690
F
N
Bn
O
N
Me
3o
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

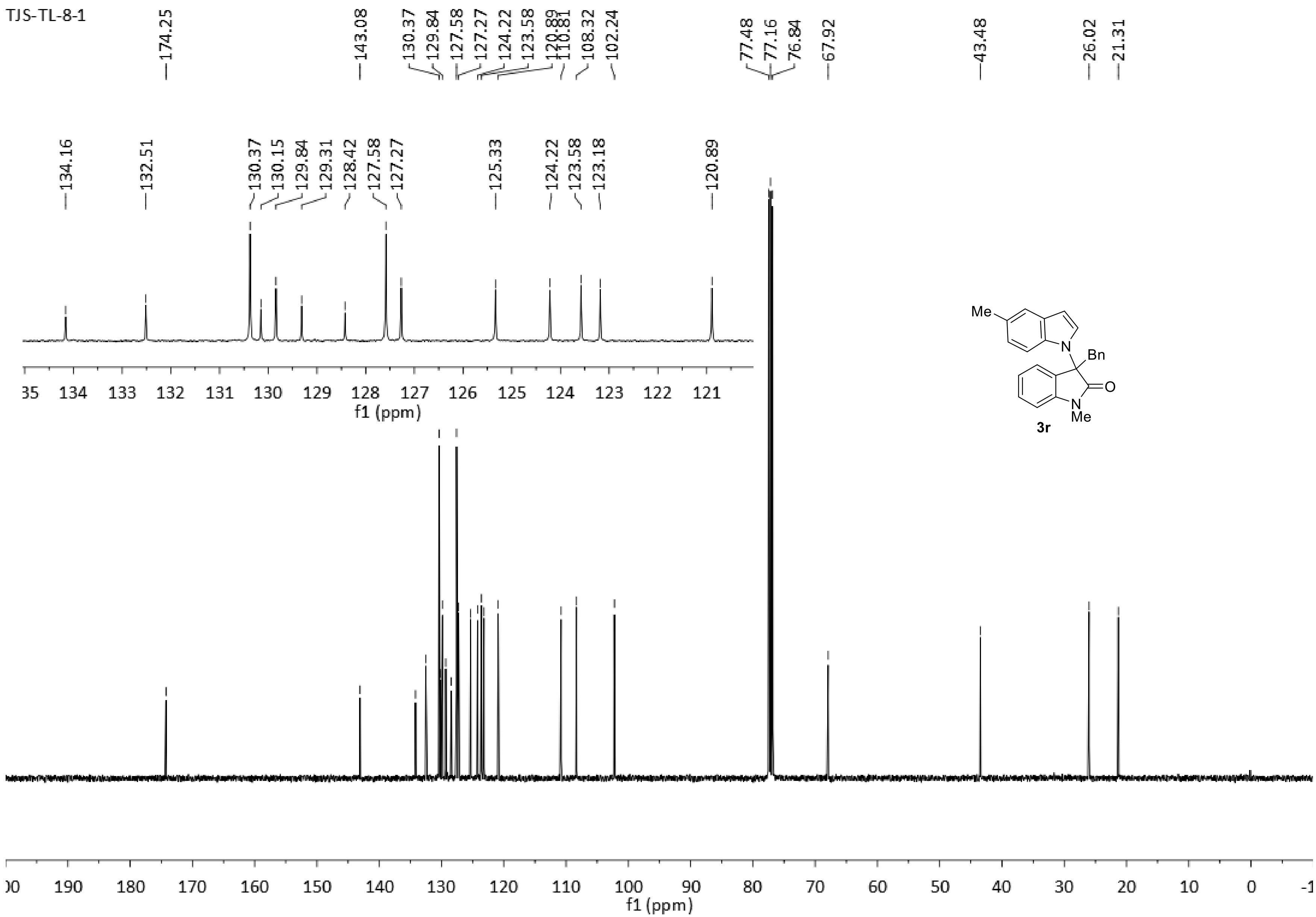

7.718
7.709
7.563
7.558
7.284
7.281
7.260
7.140
7.121
7.103
7.069
7.064
7.049
7.045
7.031
7.027
6.866
6.860
6.843
6.838
6.784
6.766
6.614
6.597
6.592
6.415
6.393
3.965
3.936
3.743
3.714
2.908
7.303
7.300
1.00
0.94
0.98
2.01
2.98
1.02
1.99
1.97
0.99
2.07
3.00
f1 (ppm)
Cl
N
Bn
O
N
Me
3p


TJS-TL-30
173.97
143.07
130.35
127.69
127.44
124.24
123.34
122.30
120.55
112.26
108.55
102.42
77.48
77.16
76.84
68.07
43.50
26.12
134.17
132.22
130.98
130.35
130.16
127.98
127.69
127.44
126.73
125.95
124.24
123.34
122.30
120.55
f1 (ppm)
Cl
N
Bn
O
N
Me
3p
f1 (ppm)

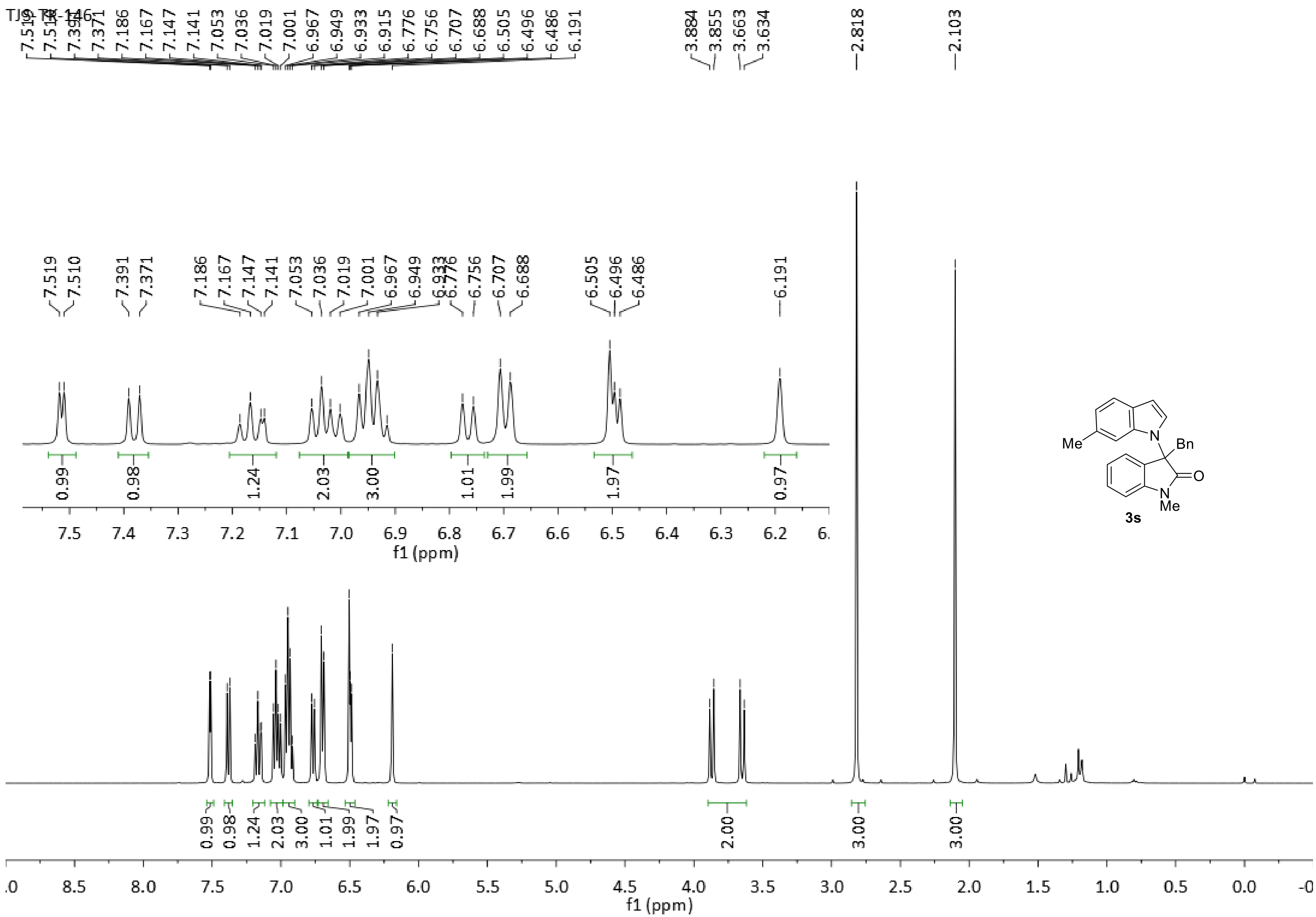

TJS-TL-68
7.726
7.722
7.702
7.693
7.283
7.281
7.260
7.134
7.124
7.117
7.066
7.047
7.029
6.996
6.974
6.969
6.784
6.766
6.613
6.597
6.591
6.376
6.354
3.964
3.936
3.742
3.714
2.906
7.302
7.300
0.95
0.96
1.03
1.98
2.97
1.00
1.97
1.95
0.98
2.01
2.98
f1 (ppm)
Br
N
Bn
O
N
Me
3q

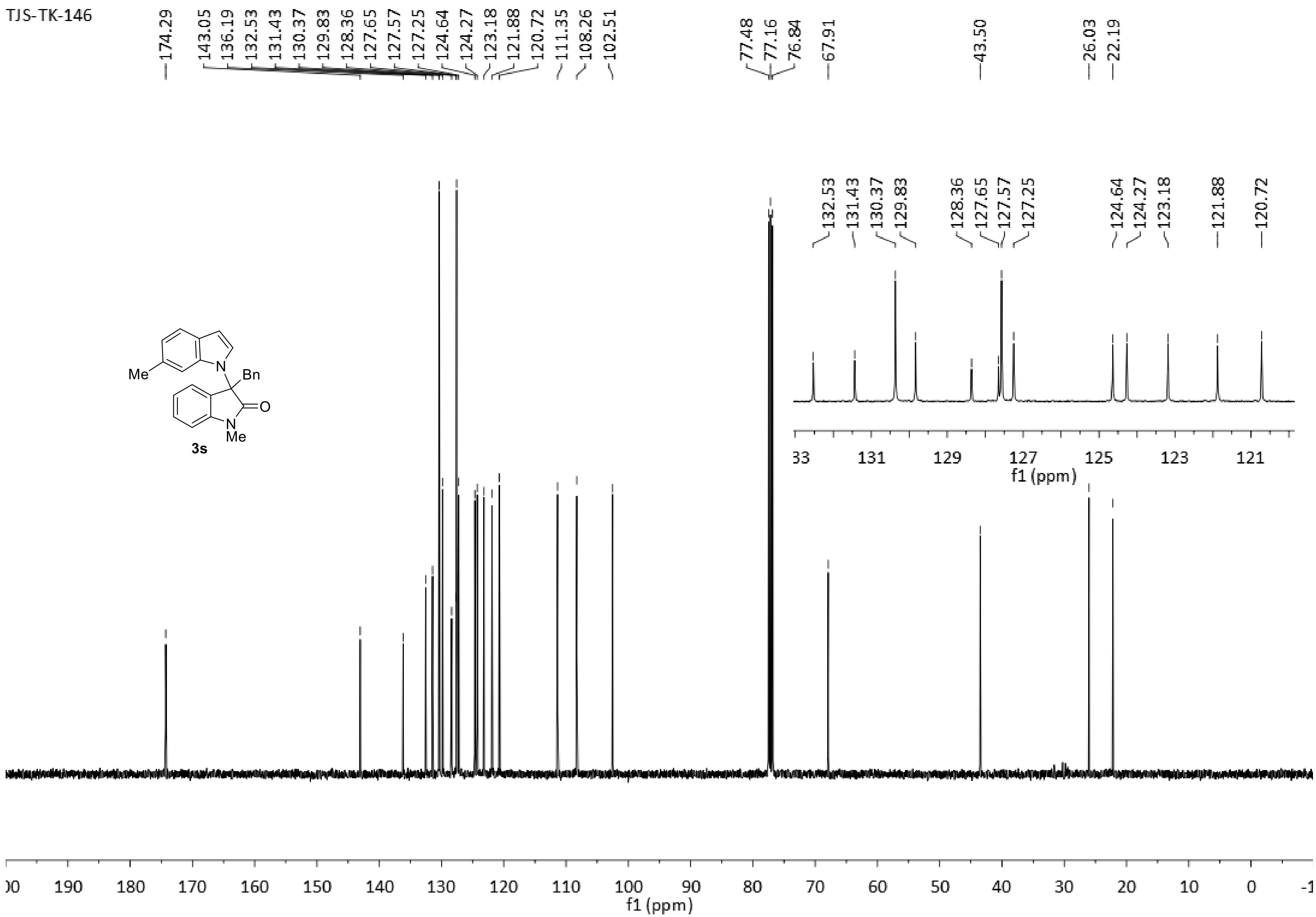

TJS-TL-68
173.91
143.00
130.32
130.16
127.67
126.56
124.83
123.63
113.56
112.67
108.54
102.30
77.48
77.16
76.84
68.02
43.45
26.11
134.40
132.15
131.57
130.32
130.16
127.89
127.67
127.43
126.56
124.83
124.19
123.63
123.33
f1 (ppm)
Br
N
Bn
O
N
Me
3q
f1 (ppm)

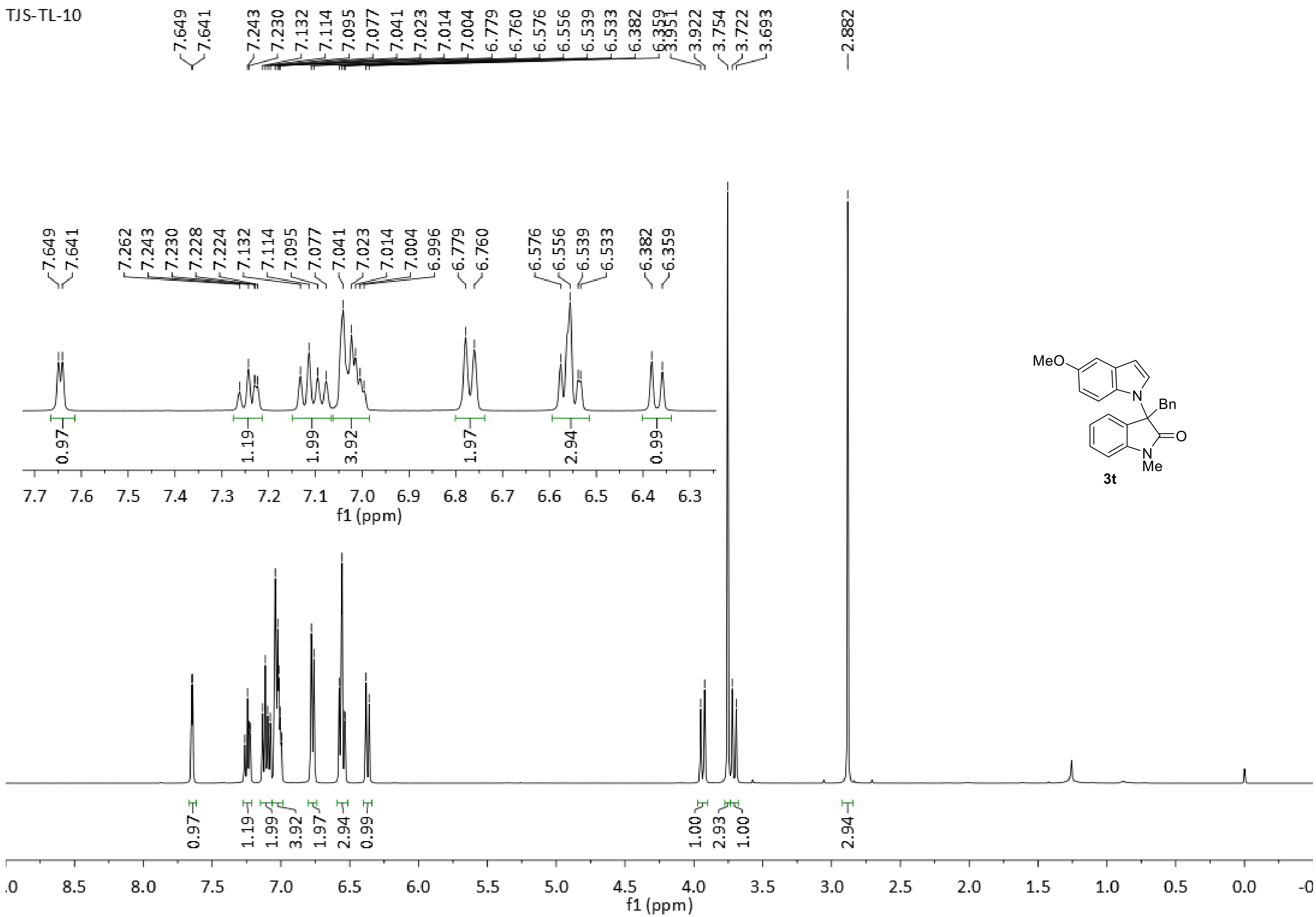

TJS-TH-84
Me
N
Bn
O
N
Me
3r
f1 (ppm)



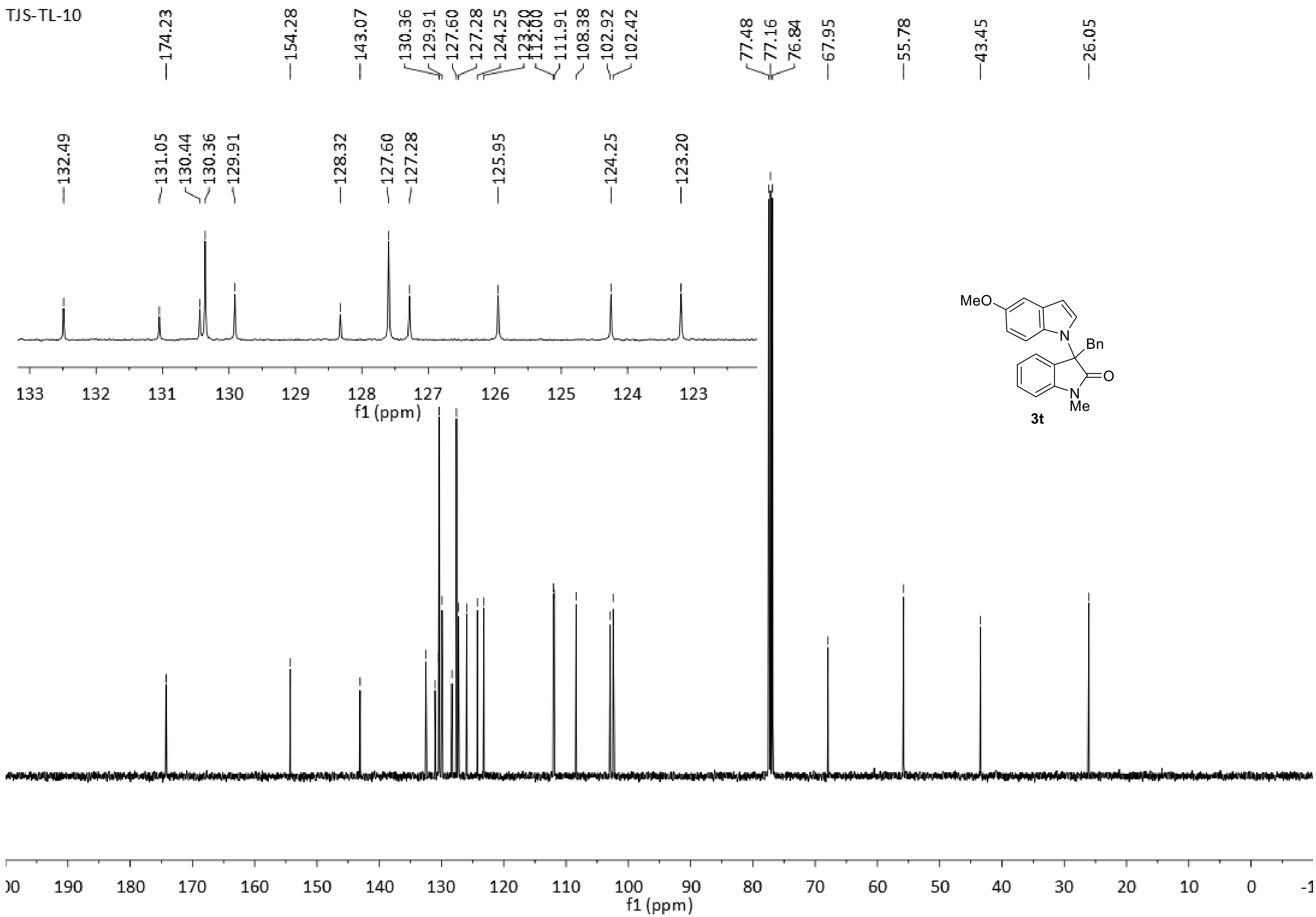
TJS-TL-8-1
174.25
143.08
130.37
129.84
127.58
127.27
124.22
123.58
120.89
110.81
108.32
102.24
77.48
77.16
76.84
67.92
43.48
26.02
21.31
134.16
132.51
130.37
130.15
129.84
129.31
128.42
127.58
127.27
125.33
124.22
123.58
123.18
120.89
f1 (ppm)
Me
N
Bn
O
N
Me
3r
f1 (ppm)


TJS-TK-146
7.519
7.510
7.391
7.371
7.186
7.167
7.147
7.141
7.053
7.036
7.019
7.001
6.967
6.949
6.933
6.915
6.776
6.756
6.707
6.688
6.505
6.496
6.486
6.191
3.884
3.855
3.663
3.634
2.818
2.103
0.99
0.98
1.24
2.03
3.00
1.01
1.99
1.97
0.97
2.00
3.00
3.00
f1 (ppm)
Me
N
Bn
O
N
Me
3s

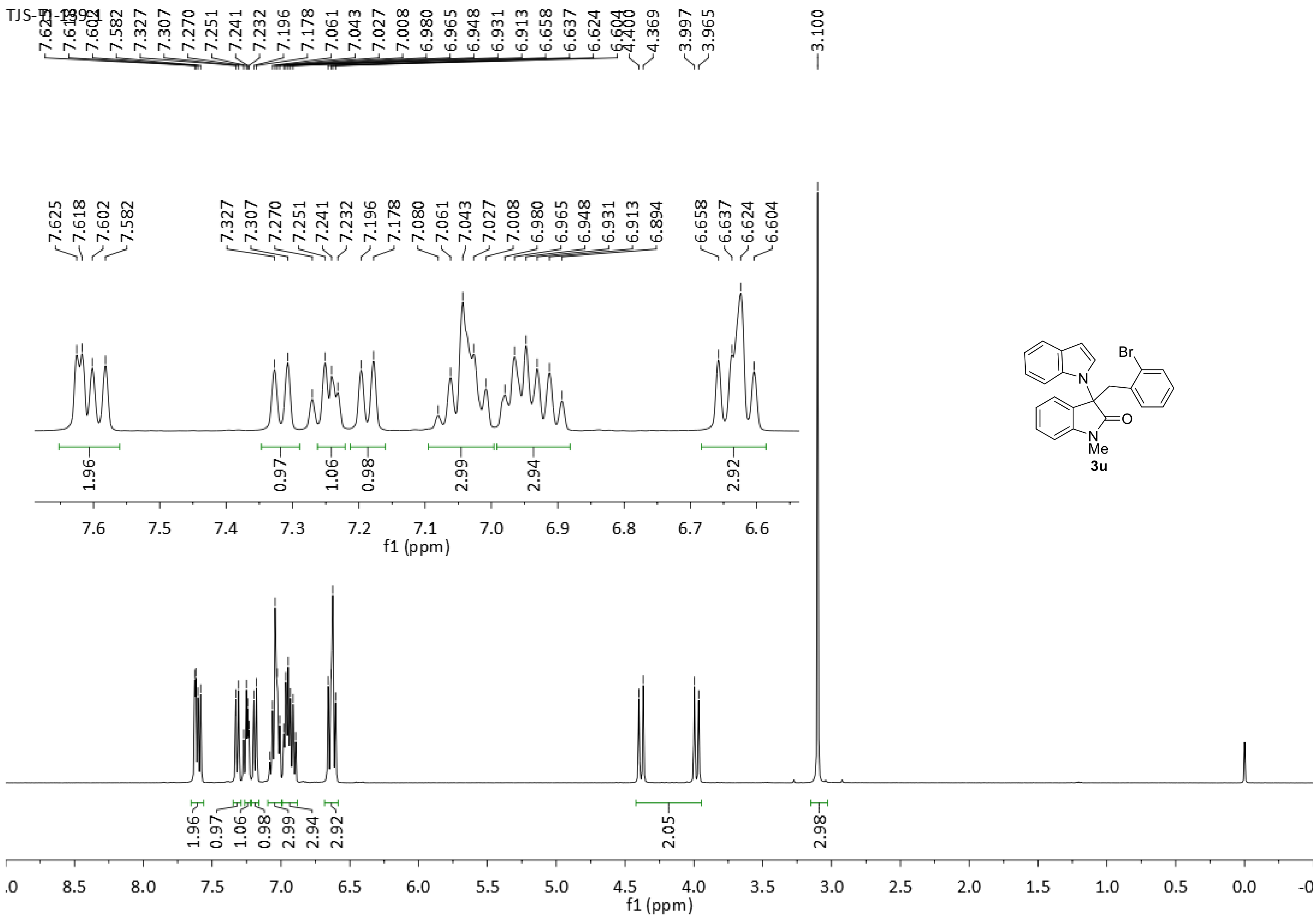

TJS-TK-146
174.29
143.05
136.19
132.53
131.43
130.37
129.83
128.36
127.65
127.57
127.25
124.64
124.27
123.18
121.88
120.72
111.35
108.26
102.51
77.48
77.16
76.84
67.91
43.50
26.03
22.19
Me
N
Bn
O
N
Me
3s
f1 (ppm)

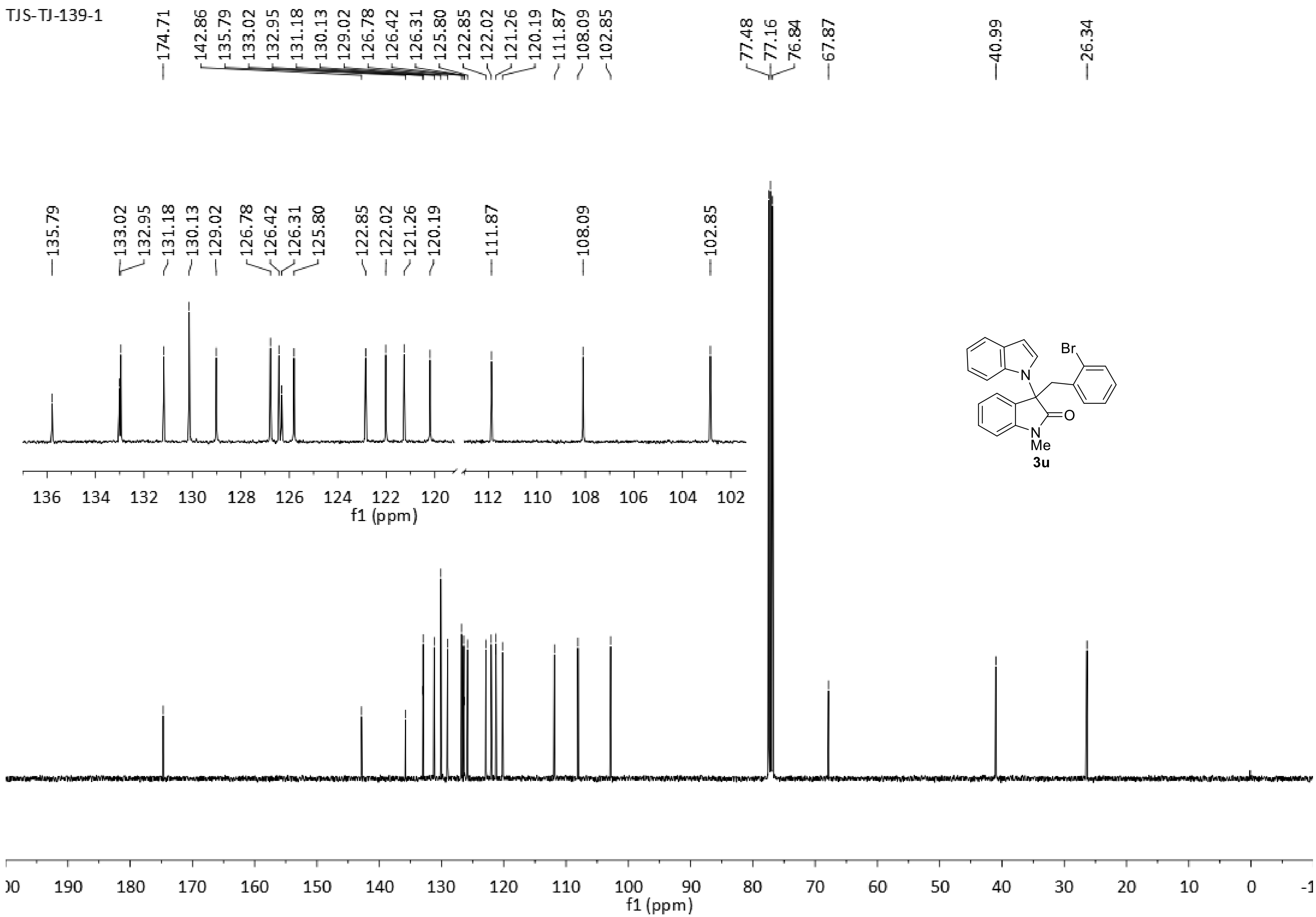


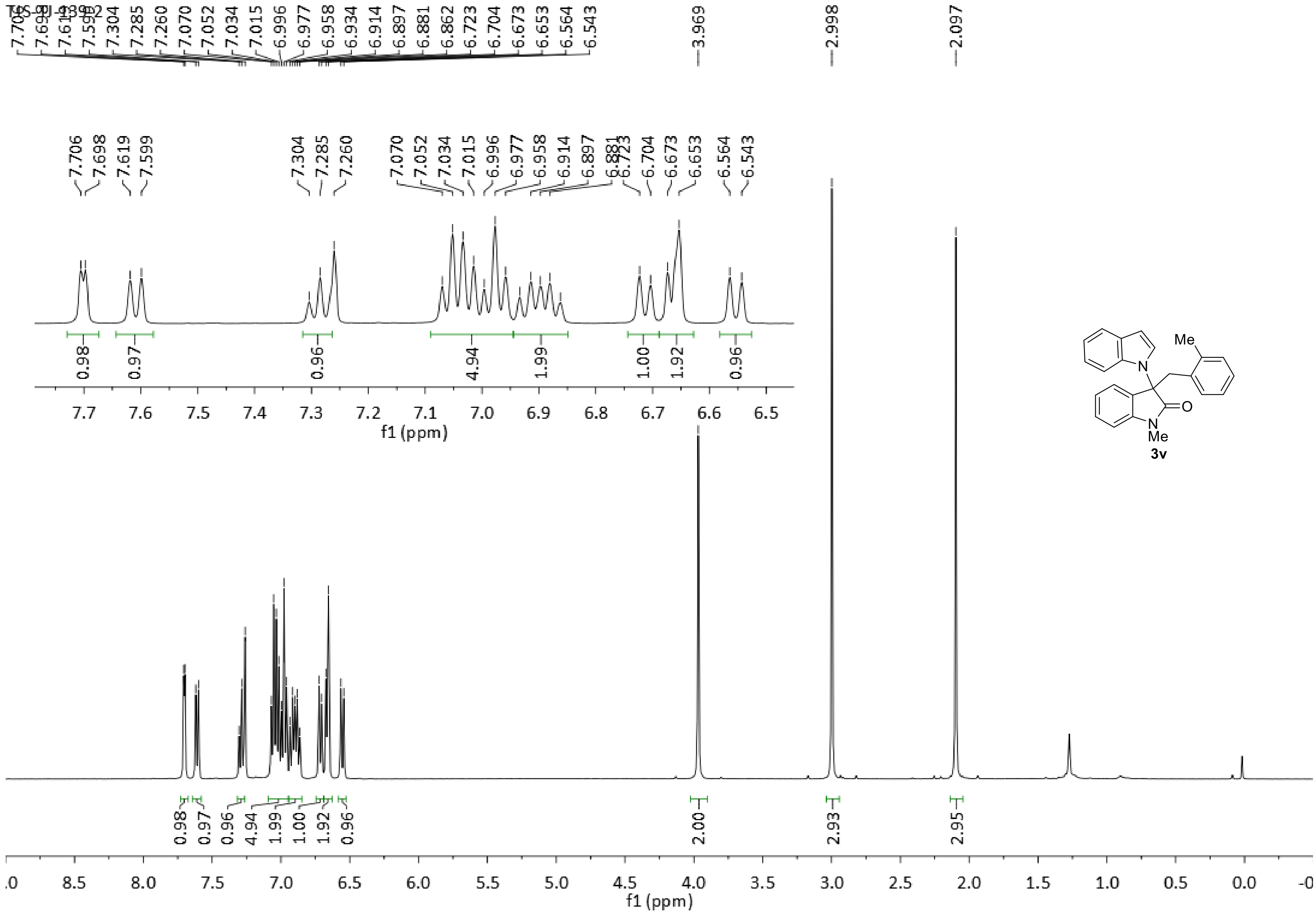
TJS-TL-10
7.649
7.641
7.243
7.230
7.132
7.114
7.095
7.077
7.041
7.023
7.014
7.004
6.779
6.760
6.576
6.556
6.539
6.533
6.382
6.359
3.951
3.922
3.754
3.722
3.693
2.882
7.262
7.228
7.224
6.996
0.97
1.19
1.99
3.92
1.97
2.94
0.99
1.00
2.93
1.00
2.94
f1 (ppm)
MeO
N
Bn
O
N
Me
3t

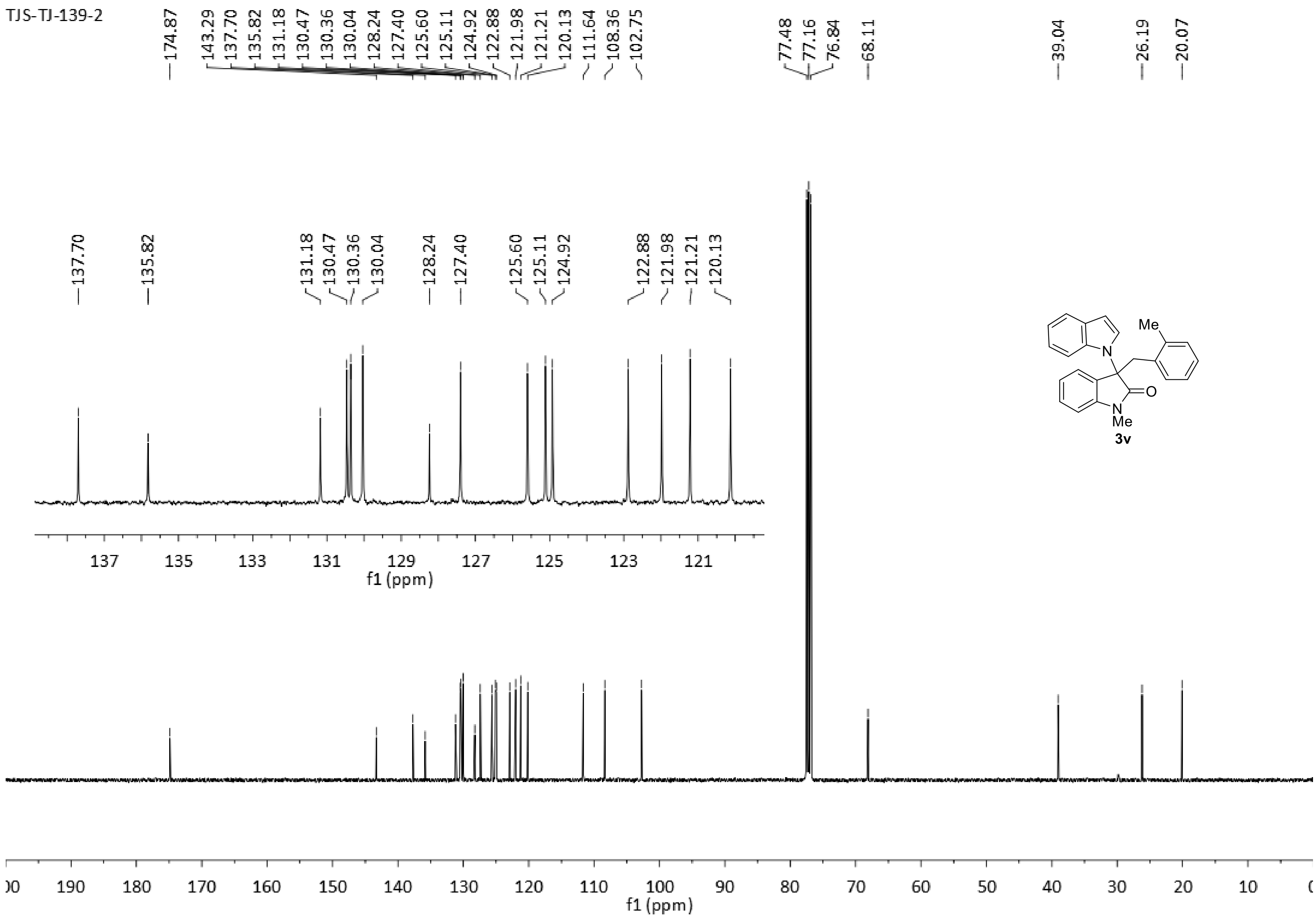


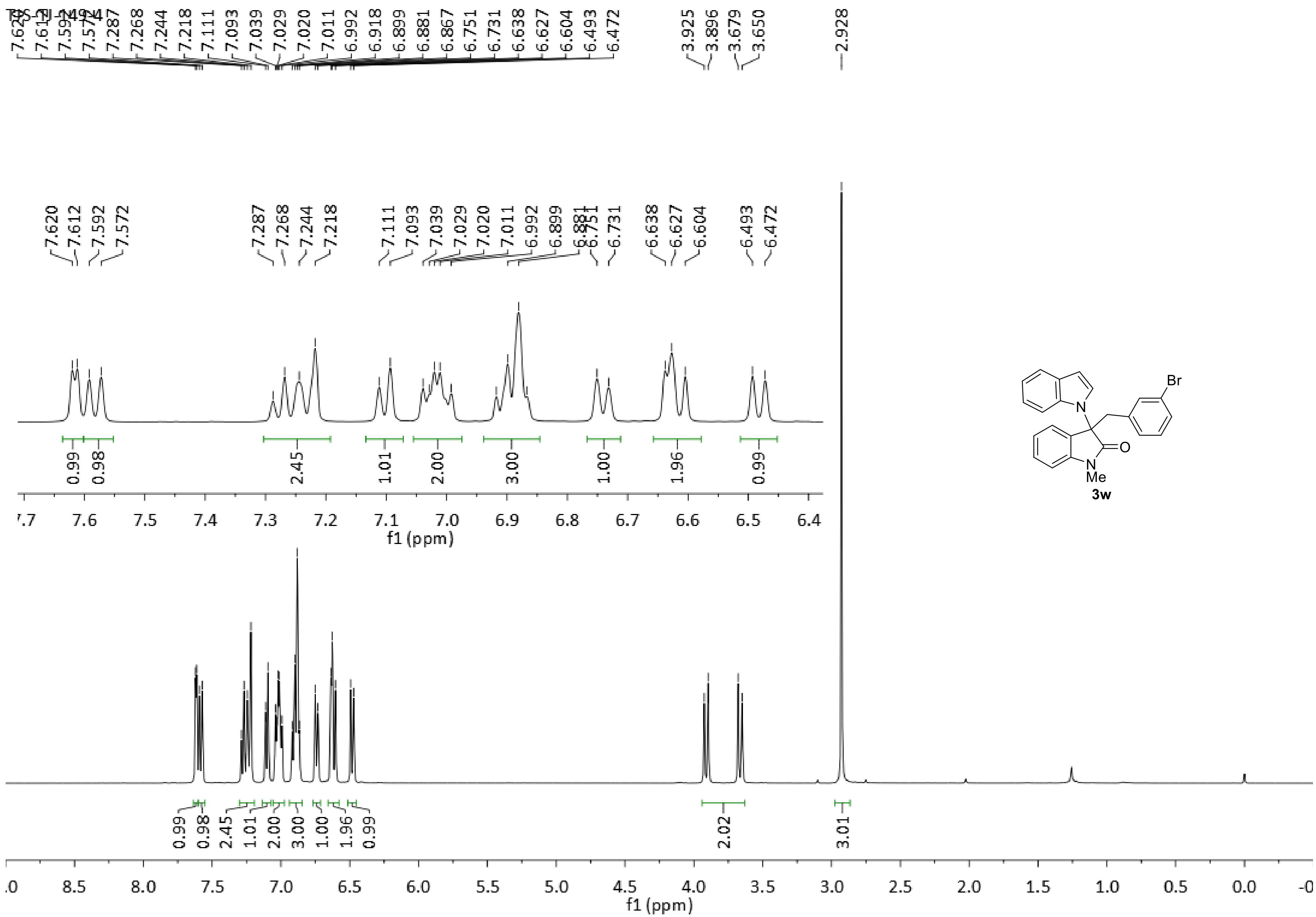
TJS-TL-10
174.23
154.28
143.07
130.36
129.91
127.60
127.28
124.25
123.20
112.00
111.91
108.38
102.92
102.42
77.48
77.16
76.84
67.95
55.78
43.45
26.05
132.49
131.05
130.44
130.36
129.91
128.32
127.60
127.28
125.95
124.25
123.20
f1 (ppm)
MeO
N
Bn
O
N
Me
3t
f1 (ppm)

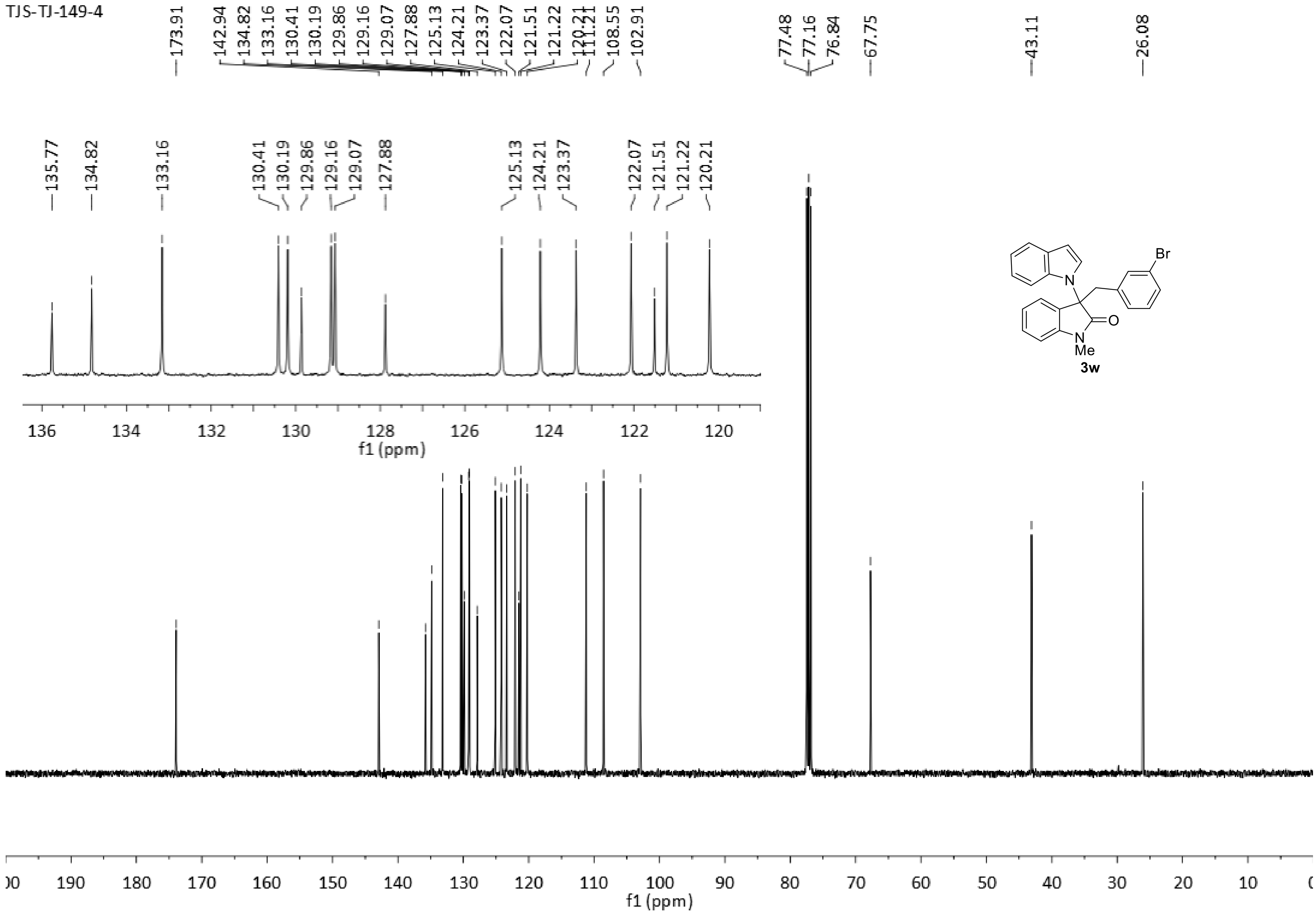

7.625 7.618 7.602 7.582 7.327 7.307 7.270 7.251 7.241 7.232 7.196 7.178 7.080 7.061 7.043 7.027 7.008 6.980 6.965 6.948 6.931 6.913 6.894 6.658 6.637 6.624 6.604
1.96 0.97 1.06 0.98 2.99 2.94 2.92
4.400 4.369 3.997 3.965 3.100
2.05 2.98
f1 (ppm)
Br
N
O
Me
3u

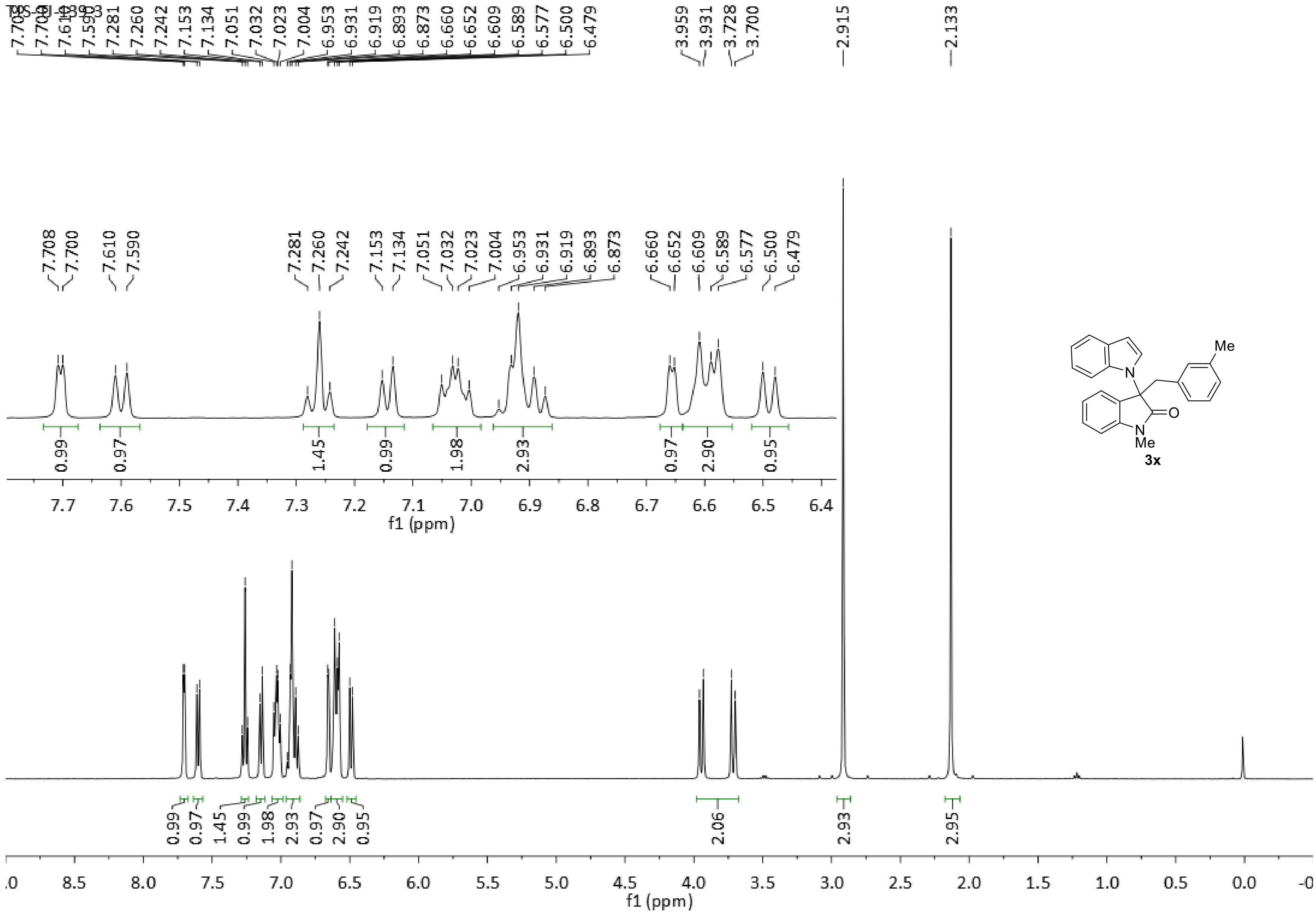

TJS-TJ-139-1
174.71
142.86
135.79
133.02
132.95
131.18
130.13
129.02
126.78
126.42
126.31
125.80
122.85
122.02
121.26
120.19
111.87
108.09
102.85
77.48
77.16
76.84
67.87
40.99
26.34
Br
N
O
N
Me
3u
f1 (ppm)
f1 (ppm)

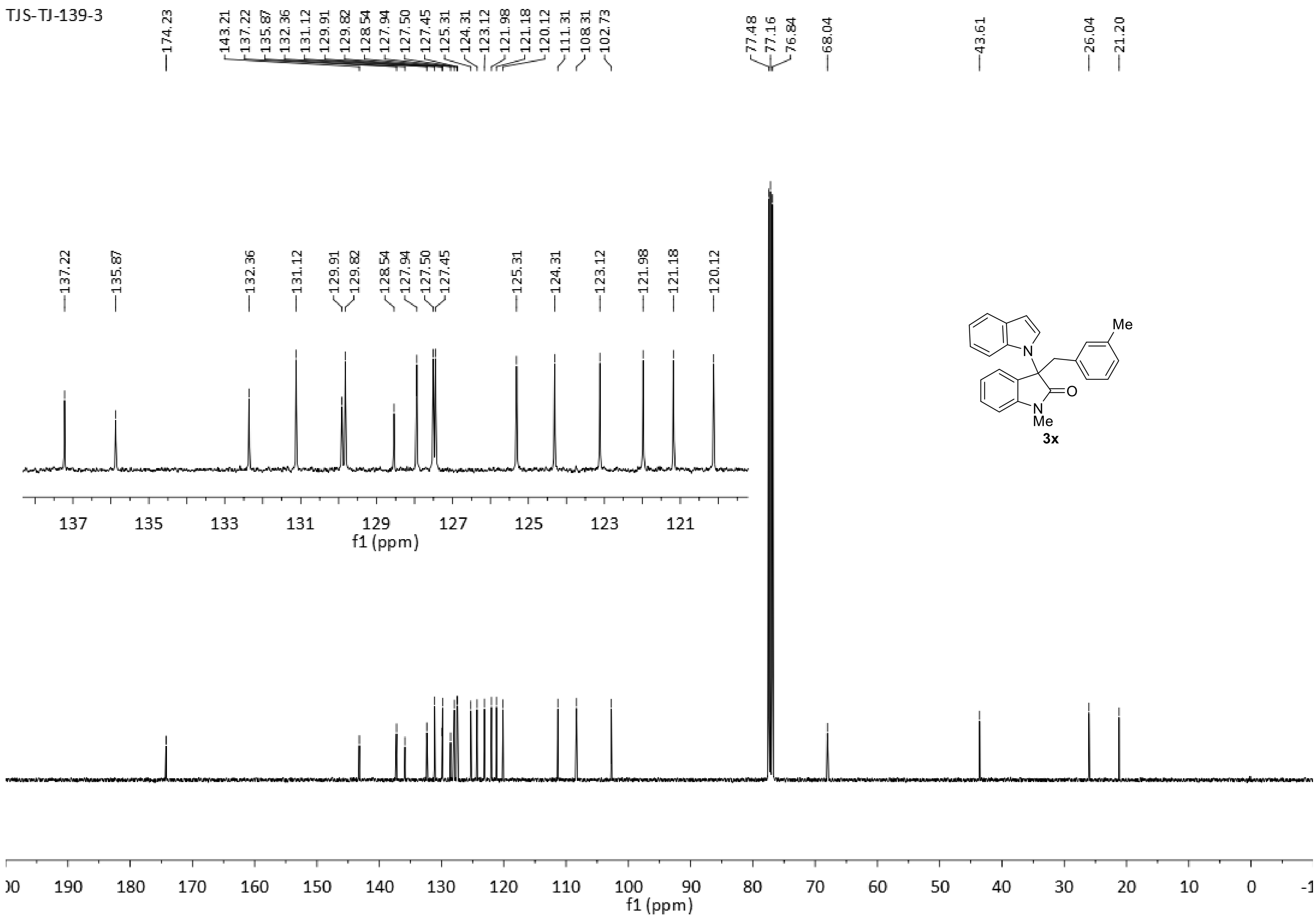

f1 (ppm)
3v

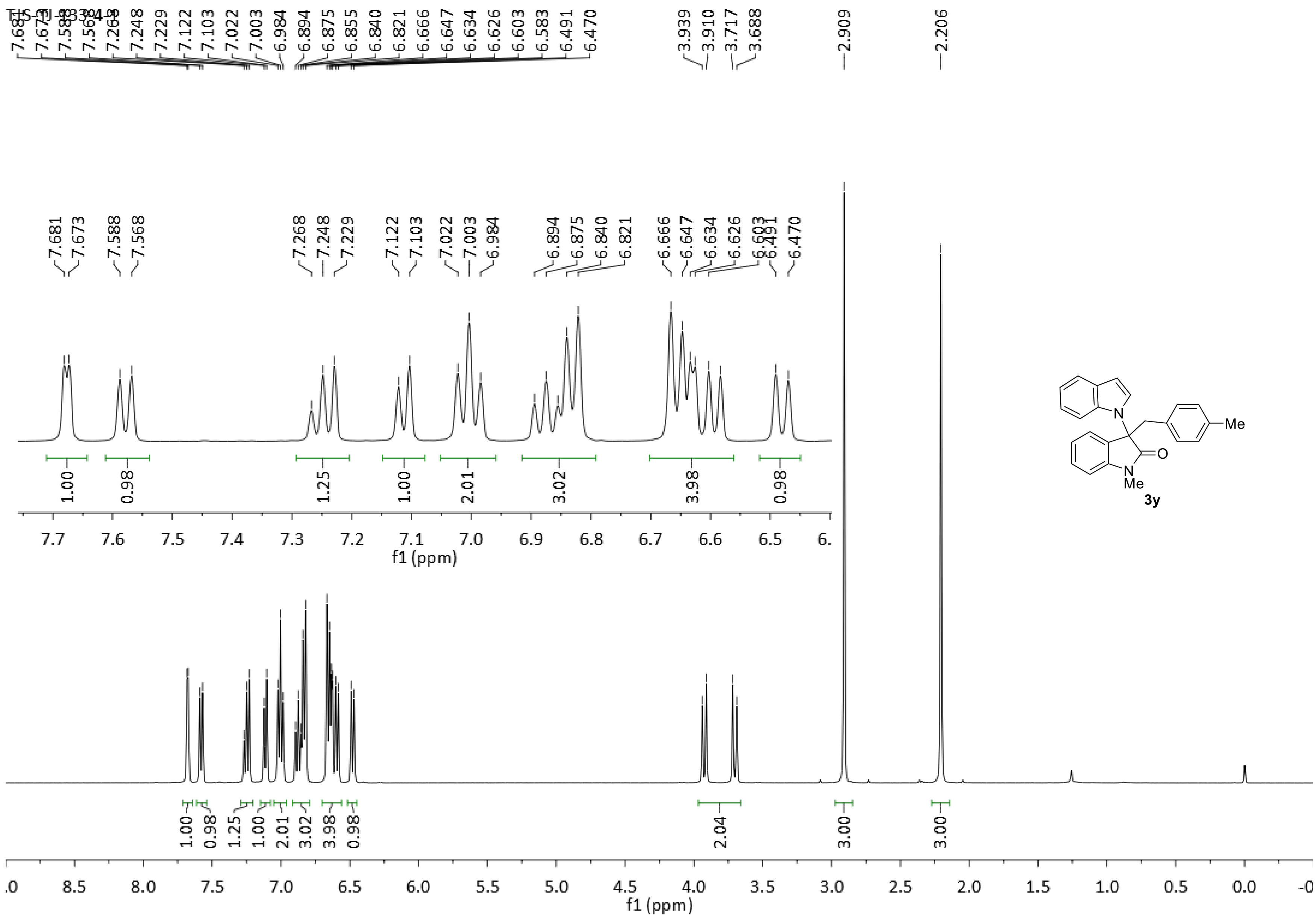

TJS-TJ-139-2
174.87
143.29
137.70
135.82
131.18
130.47
130.36
130.04
128.24
127.40
125.60
125.11
124.92
122.88
121.98
121.21
120.13
111.64
108.36
102.75
77.48
77.16
76.84
68.11
39.04
26.19
20.07
Me
N
O
N
Me
3v
f1 (ppm)
f1 (ppm)


TIS-TI-149-4
f1 (ppm)
Br
N
O
Me
3w


TJS-TJ-149-4
173.91
142.94
134.82
133.16
130.41
130.19
129.86
129.16
129.07
127.88
125.13
124.21
123.37
122.07
121.51
121.22
120.21
111.21
108.55
102.91
77.48
77.16
76.84
67.75
43.11
26.08
135.77
Br
N
O
N
Me
3w
f1 (ppm)
f1 (ppm)

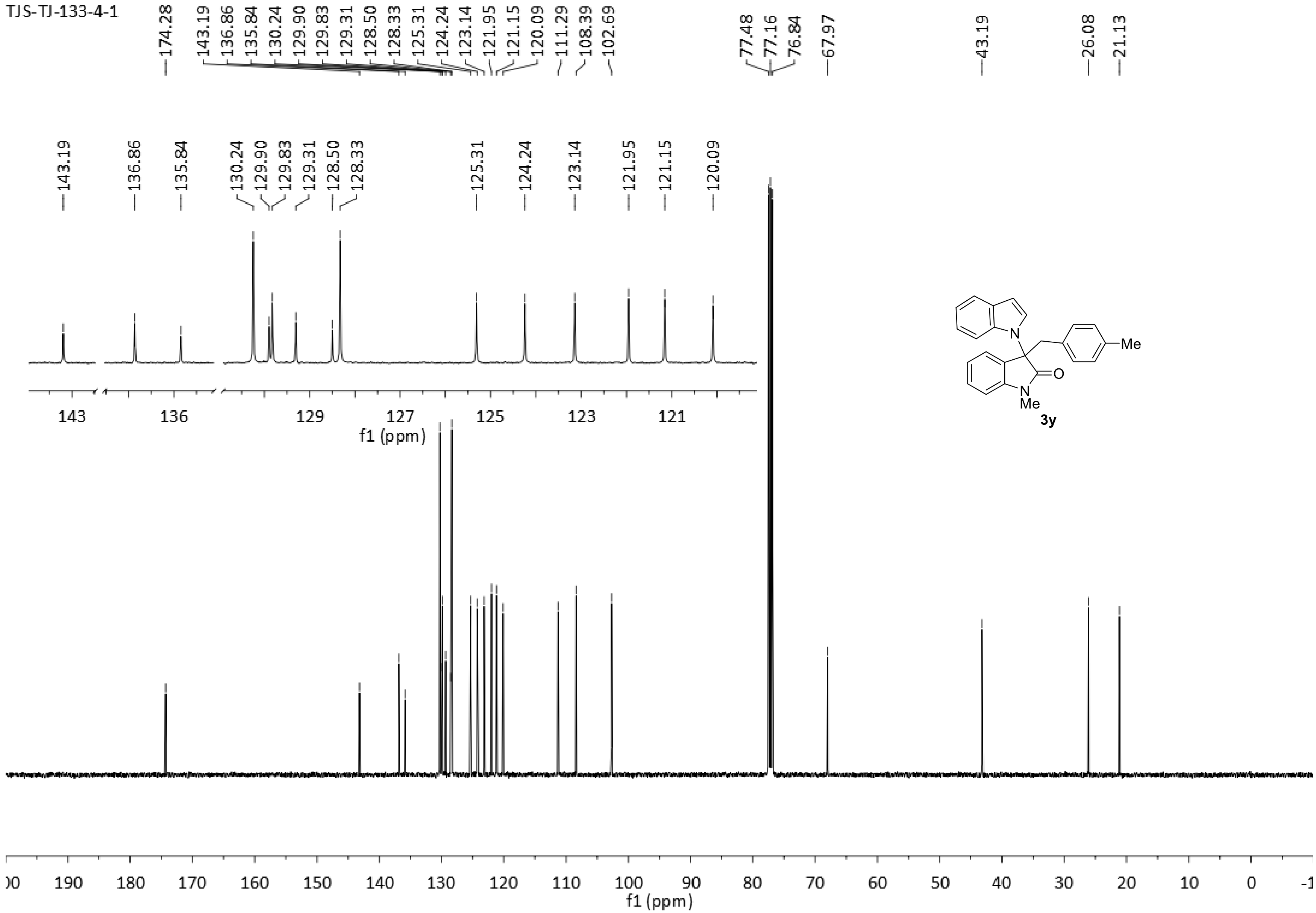

7.708
7.700
7.610
7.590
7.281
7.260
7.242
7.153
7.134
7.051
7.032
7.023
7.004
6.953
6.931
6.919
6.893
6.873
6.660
6.652
6.609
6.589
6.577
6.500
6.479
3.959
3.931
3.728
3.700
2.915
2.133
0.99
0.97
1.45
0.99
1.98
2.93
0.97
2.90
0.95
2.06
2.93
2.95
f1 (ppm)
Me
N
O
Me
3x


TJS-TJ-139-3
174.23
143.21
137.22
135.87
132.36
131.12
129.91
129.82
128.54
127.94
127.50
127.45
125.31
124.31
123.12
121.98
121.18
120.12
111.31
108.31
102.73
77.48
77.16
76.84
68.04
43.61
26.04
21.20
f1 (ppm)
Me
N
O
N
Me
3x

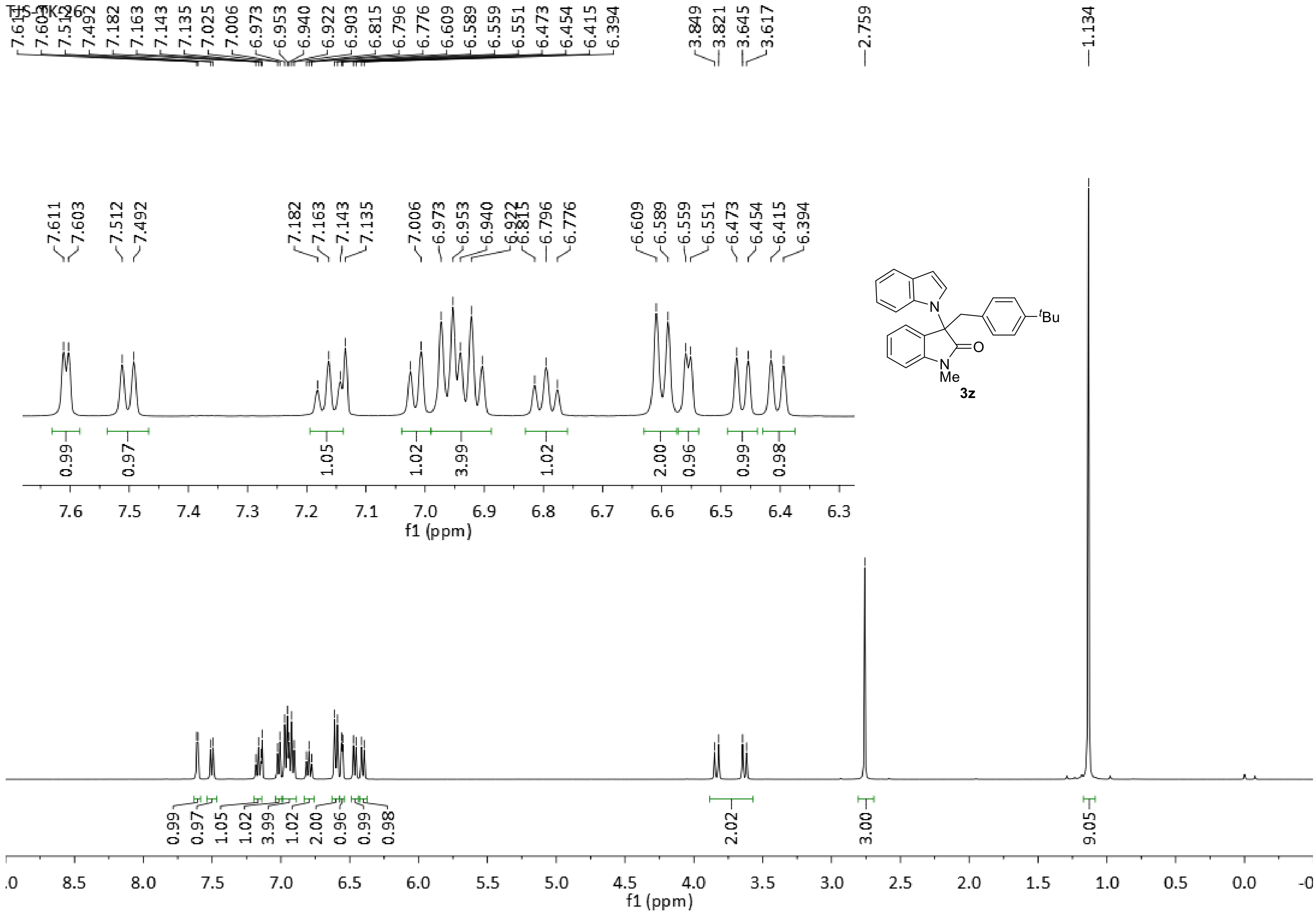


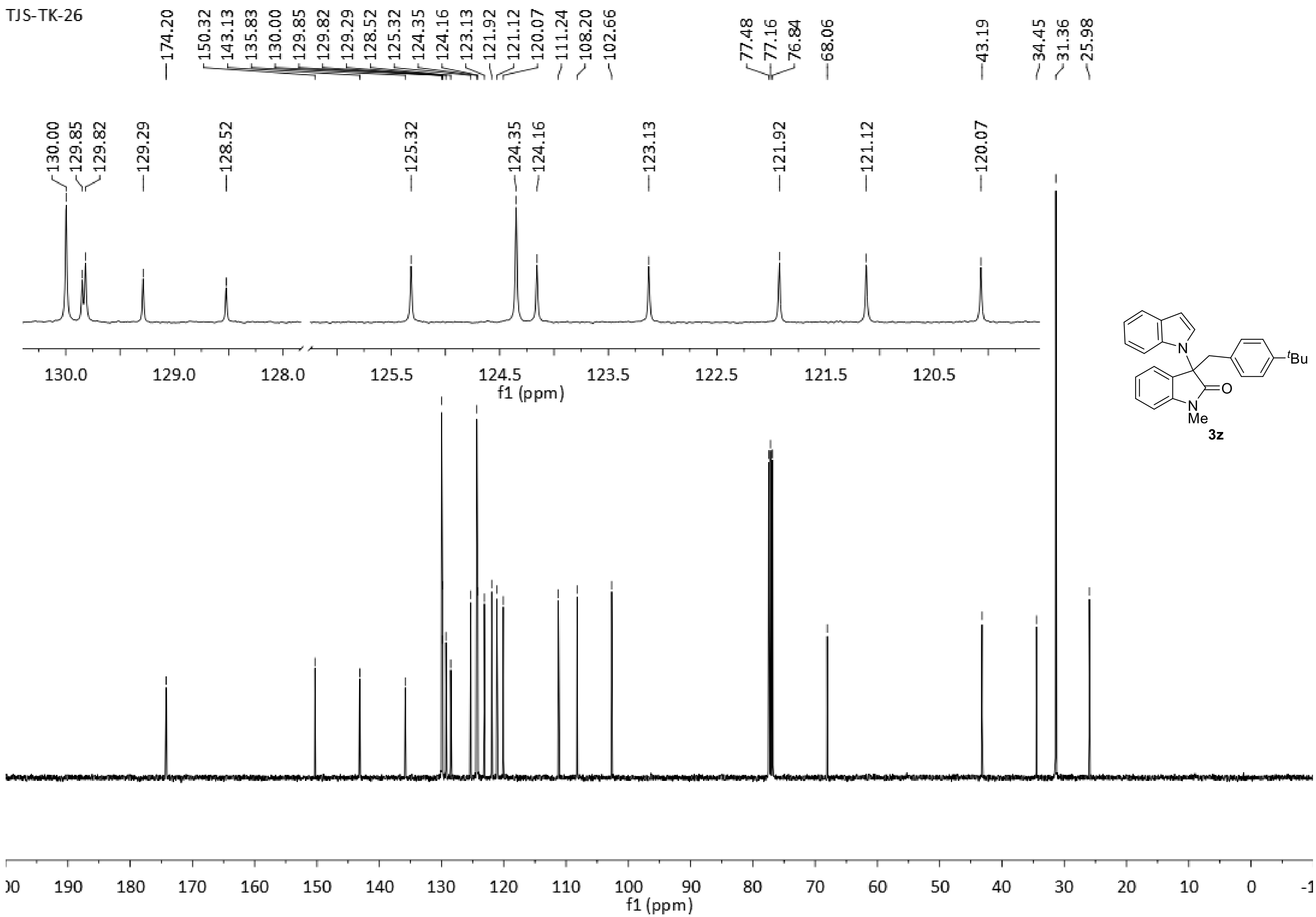
7.681
7.673
7.588
7.568
7.268
7.248
7.229
7.122
7.103
7.022
7.003
6.984
6.894
6.875
6.840
6.821
6.666
6.647
6.634
6.626
6.603
6.491
6.470
3.939
3.910
3.717
3.688
2.909
2.206
1.00
0.98
1.25
1.00
2.01
3.02
3.98
0.98
2.04
3.00
3.00
f1 (ppm)
f1 (ppm)
N
Me
O
N
Me
3y

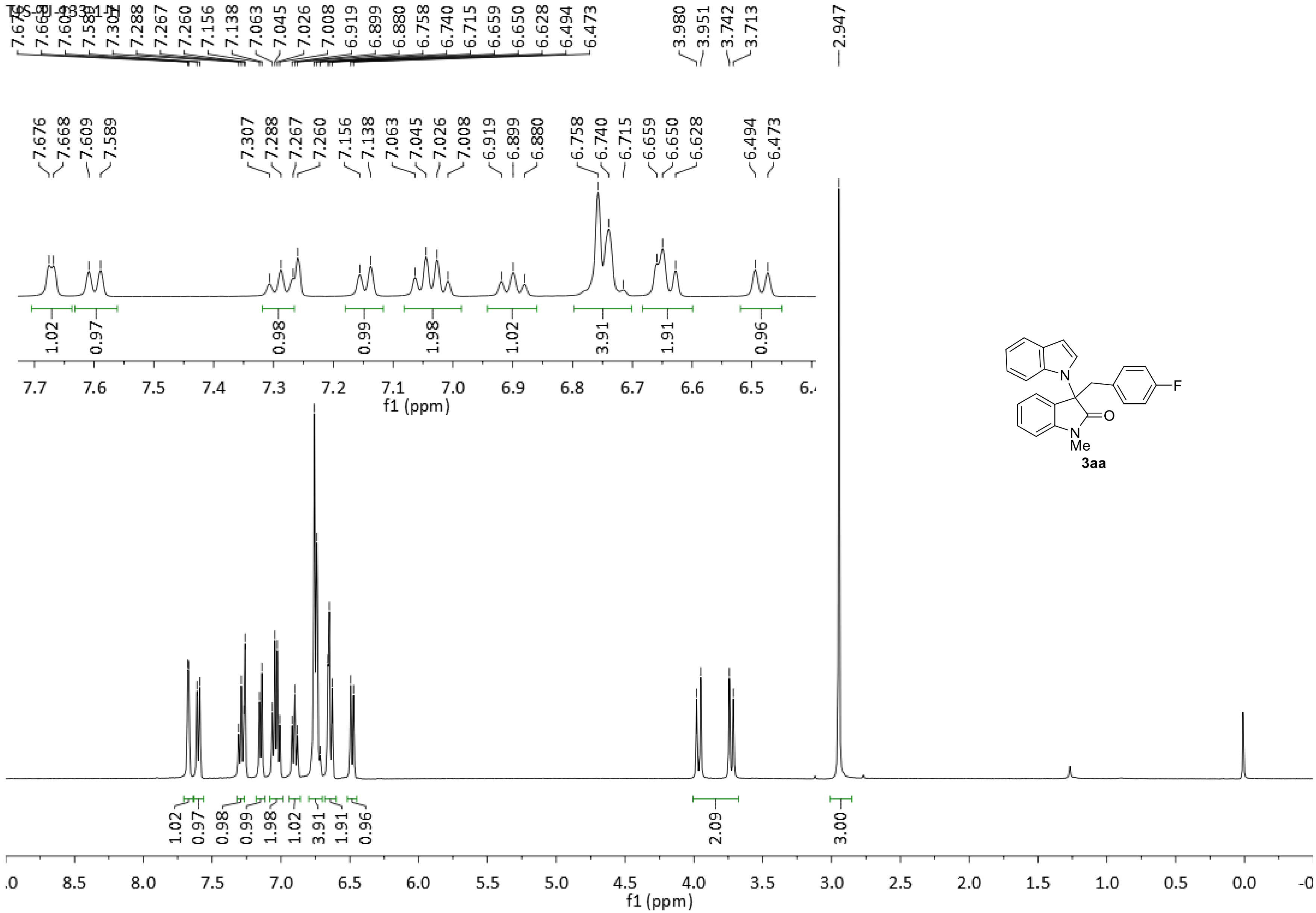
TJS-TJ-133-4-1

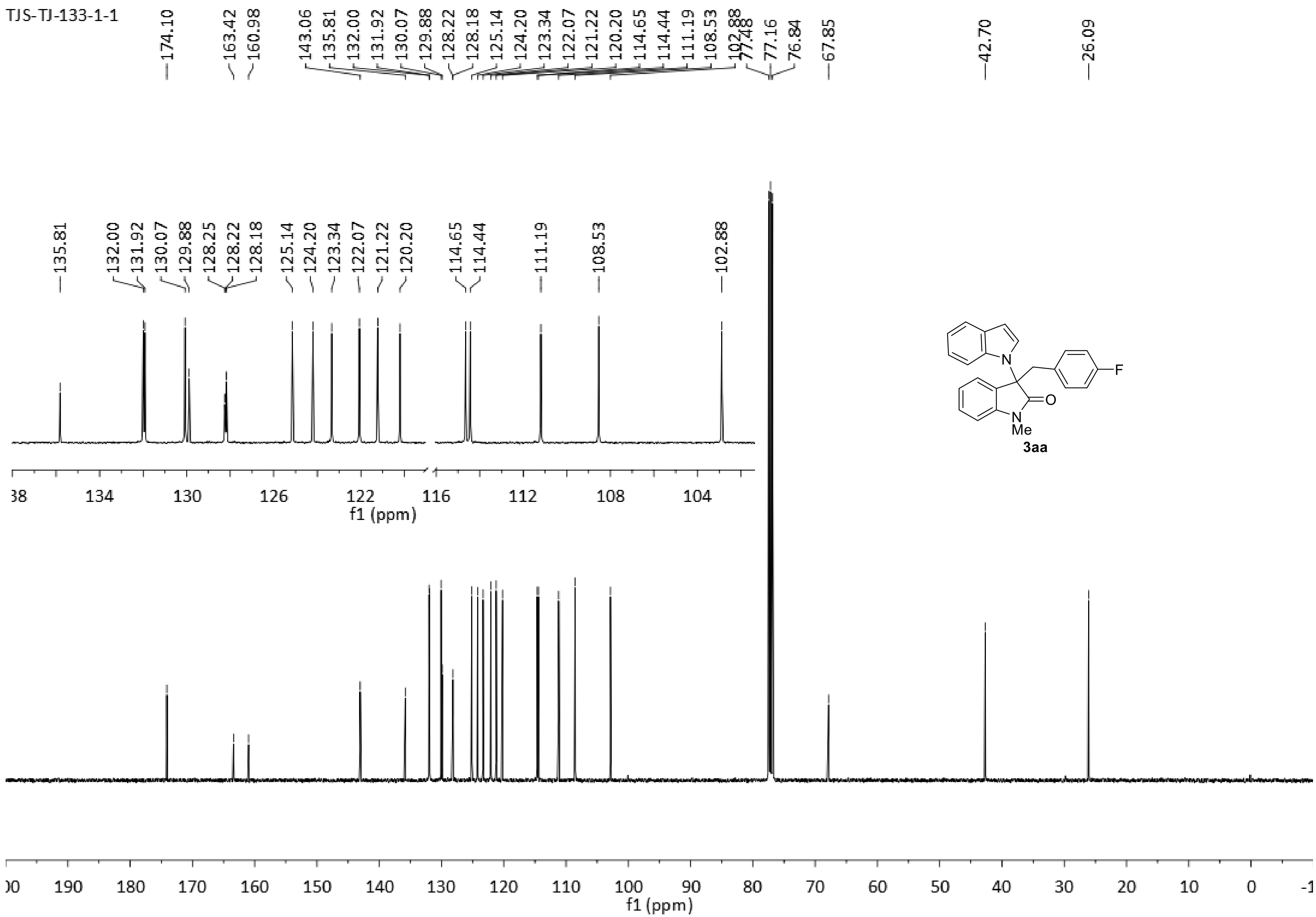


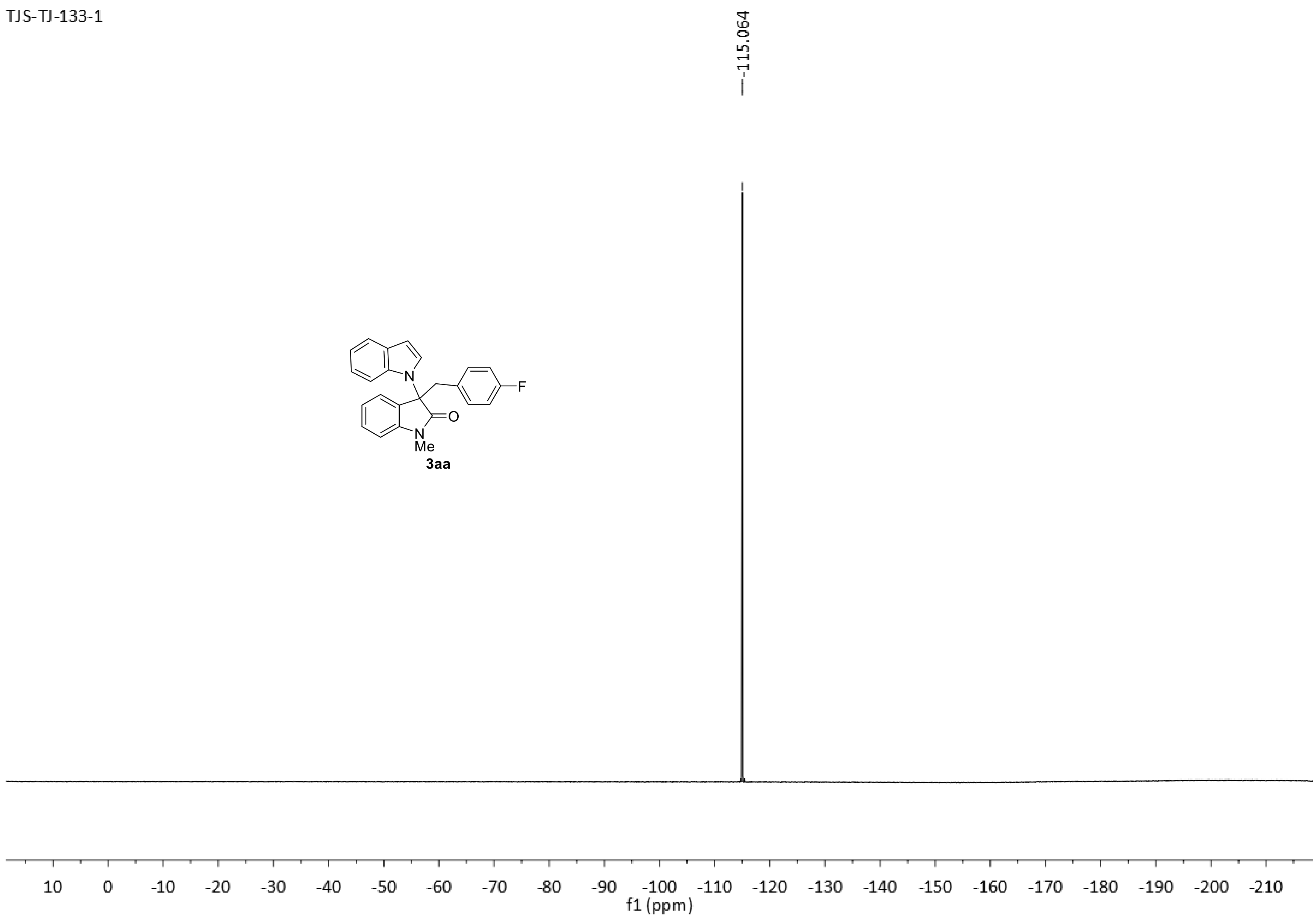
3y

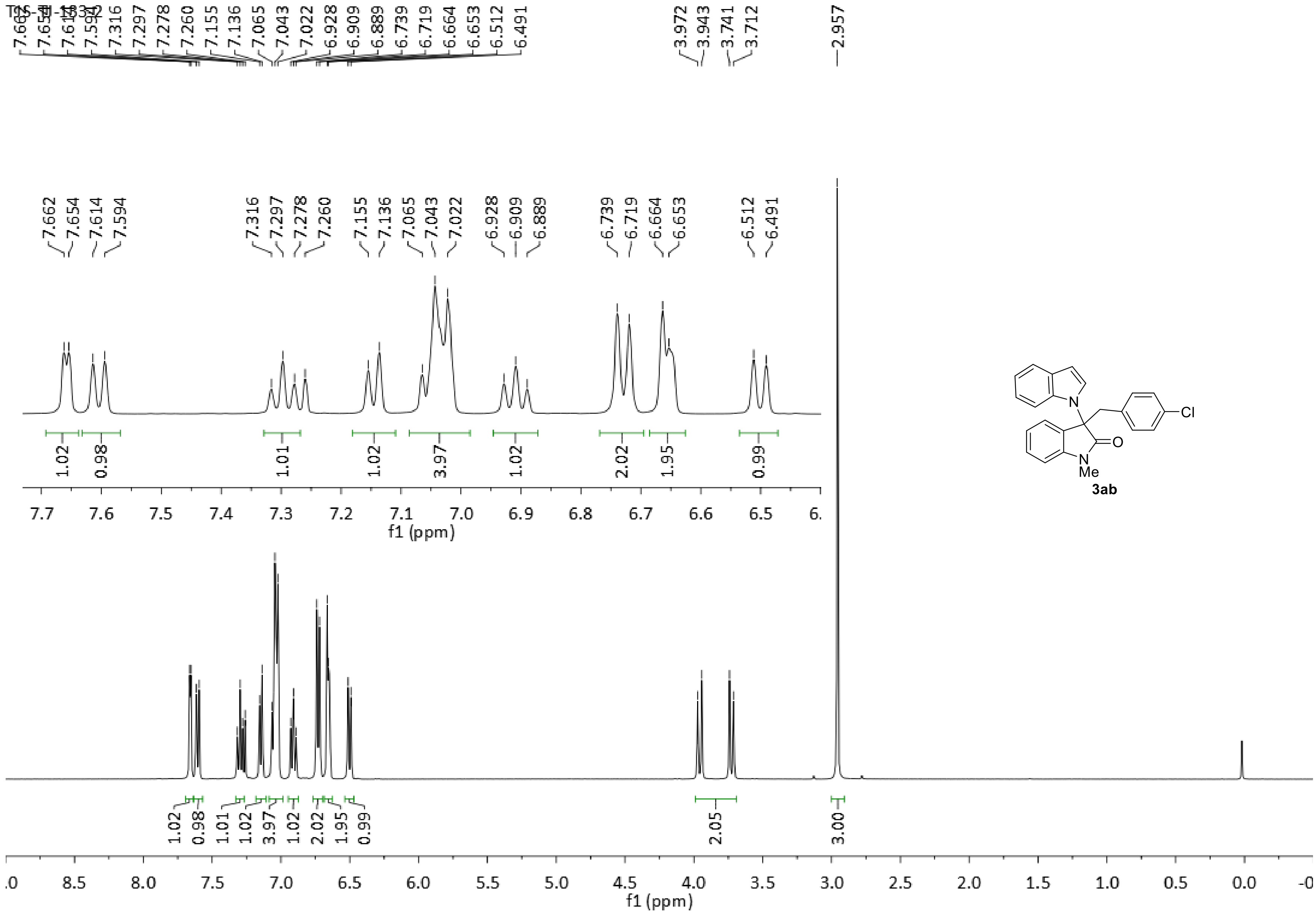

TJS-TK-26
7.611
7.603
7.512
7.492
7.182
7.163
7.143
7.135
7.025
7.006
6.973
6.953
6.940
6.922
6.903
6.815
6.796
6.776
6.609
6.589
6.559
6.551
6.473
6.454
6.415
6.394
3.849
3.821
3.645
3.617
2.759
1.134
0.99
0.97
1.05
1.02
3.99
1.02
2.00
0.96
0.99
0.98
2.02
3.00
9.05
f1 (ppm)
N
tBu
O
N
Me
3z

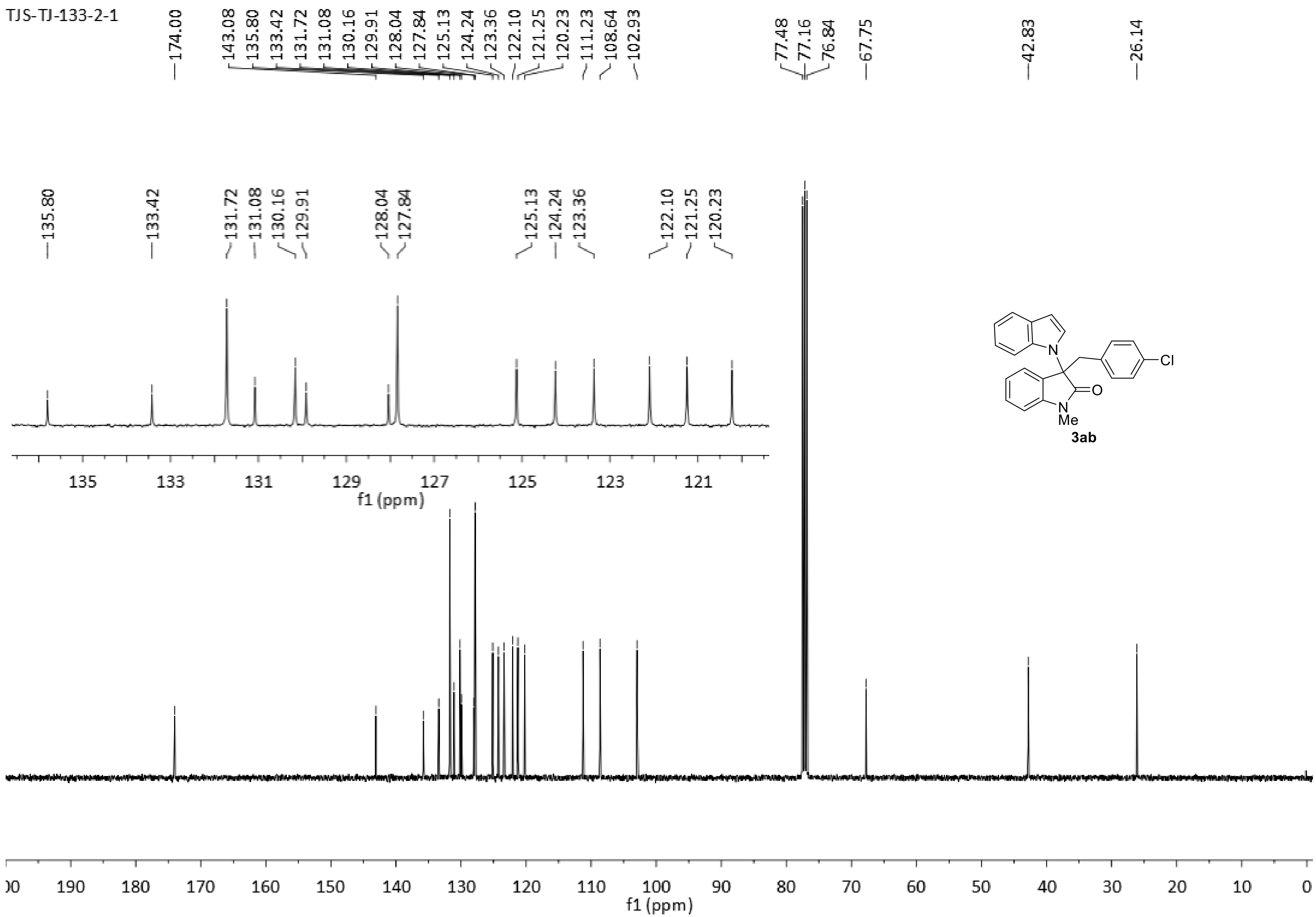

TJS-TK-26
174.20
150.32
143.13
135.83
130.00
129.85
129.82
129.29
128.52
125.32
124.35
124.16
123.13
121.92
121.12
120.07
111.24
108.20
102.66
77.48
77.16
76.84
68.06
43.19
34.45
31.36
25.98
130.00
129.85
129.82
129.29
128.52
125.32
124.35
124.16
123.13
121.92
121.12
120.07
130.0 129.0 128.0 125.5 124.5 123.5 122.5 121.5 120.5
f1 (ppm)
N
^{t}Bu
O
N
Me
3z
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

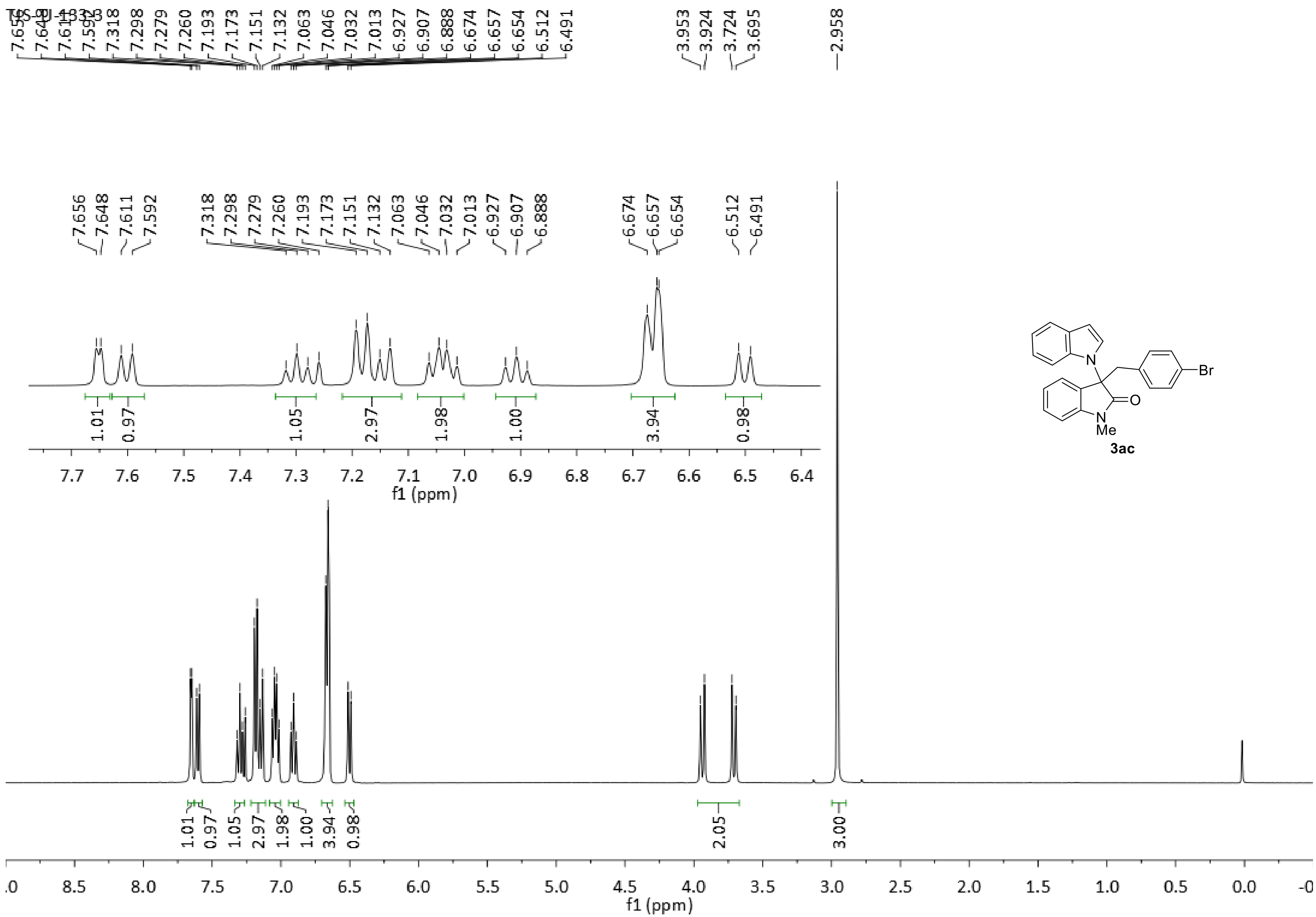

TJS-TJ-133-1-1
7.676 7.668 7.609 7.589 7.307 7.288 7.267 7.260 7.156 7.138 7.063 7.045 7.026 7.008 6.919 6.899 6.880 6.758 6.740 6.715 6.659 6.650 6.628 6.494 6.473
3.980 3.951 3.742 3.713
2.947
1.02 0.97 0.98 0.99 1.98 1.02 3.91 1.91 0.96
2.09
3.00
f1 (ppm)
N
F
O
N
Me
3aa

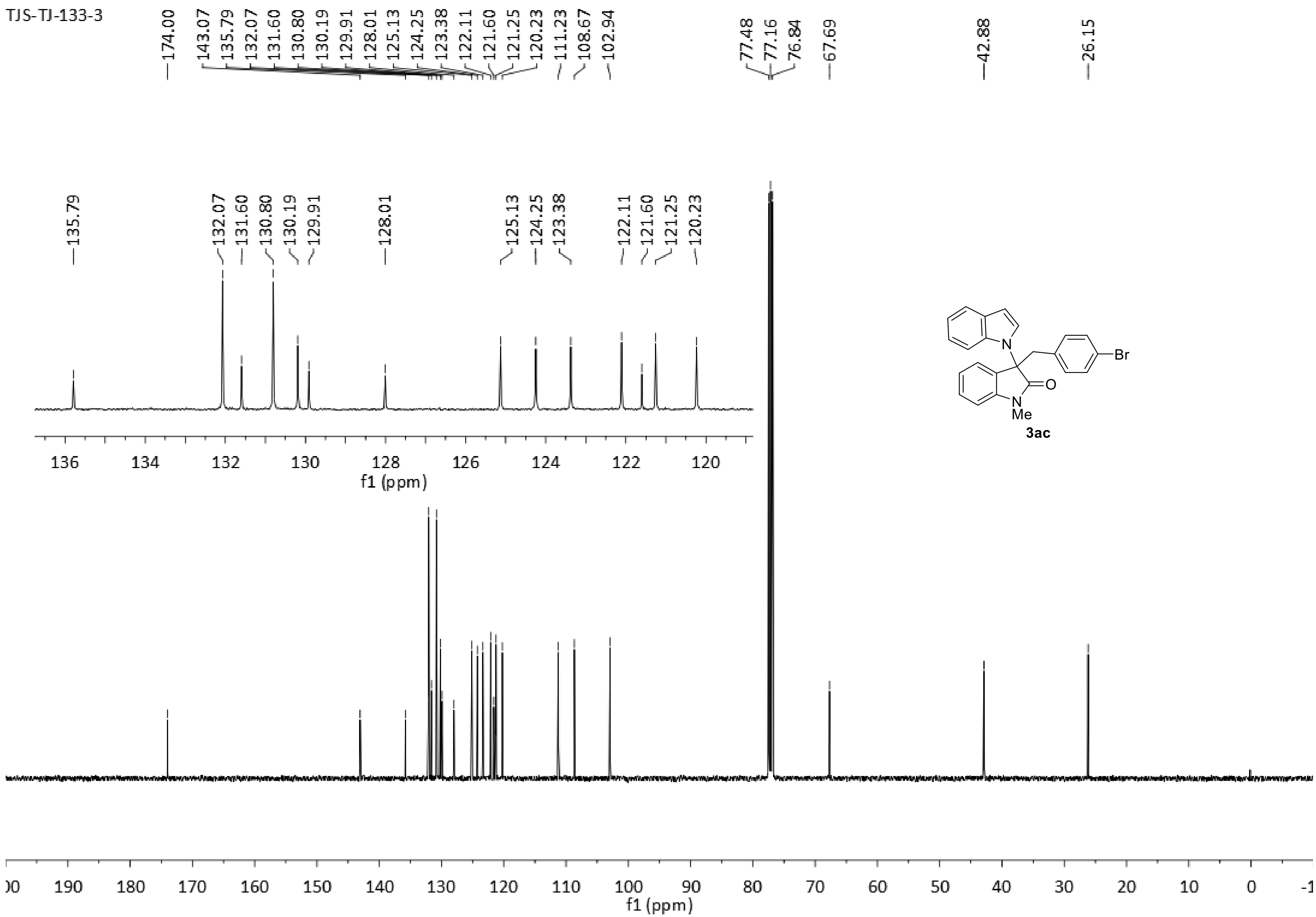

TJS-TJ-133-1-1
174.10
163.42
160.98
143.06
135.81
132.00
131.92
130.07
129.88
128.22
128.18
125.14
124.20
123.34
122.07
121.22
120.20
114.65
114.44
111.19
108.53
102.88
77.48
77.16
76.84
67.85
42.70
26.09
135.81
132.00
131.92
130.07
129.88
128.25
128.22
128.18
125.14
124.20
123.34
122.07
121.22
120.20
114.65
114.44
111.19
108.53
102.88
f1 (ppm)
N
F
O
N
Me
3aa
f1 (ppm)

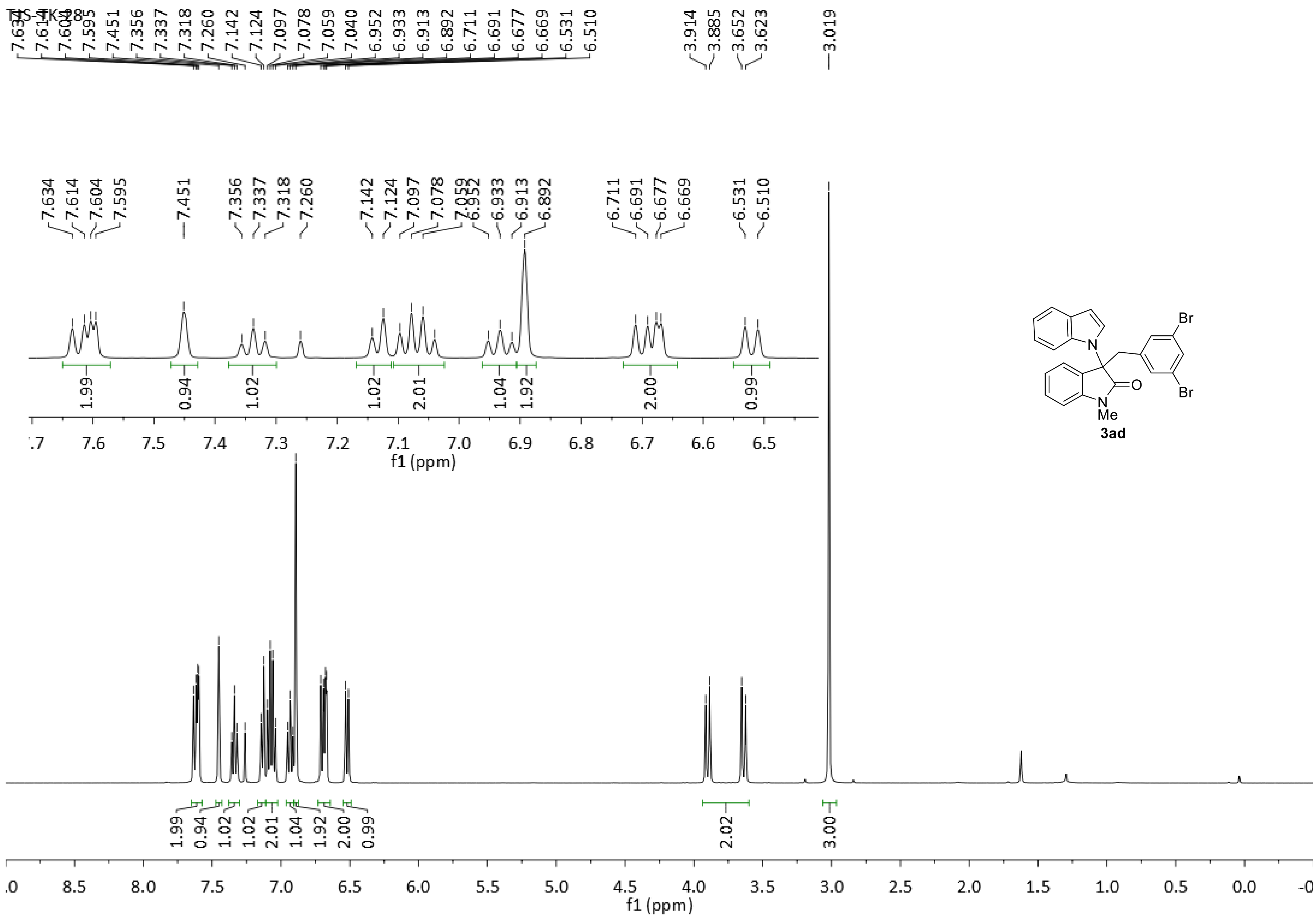

TJS-TJ-133-1
-115.064
N
F
O
N
Me
3aa
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.662
7.654
7.614
7.594
7.316
7.297
7.278
7.260
7.155
7.136
7.065
7.043
7.022
6.928
6.909
6.889
6.739
6.719
6.664
6.653
6.512
6.491
3.972
3.943
3.741
3.712
2.957
1.02
0.98
1.01
1.02
3.97
1.02
2.02
1.95
0.99
2.05
3.00
f1 (ppm)
N
Cl
O
N
Me
3ab

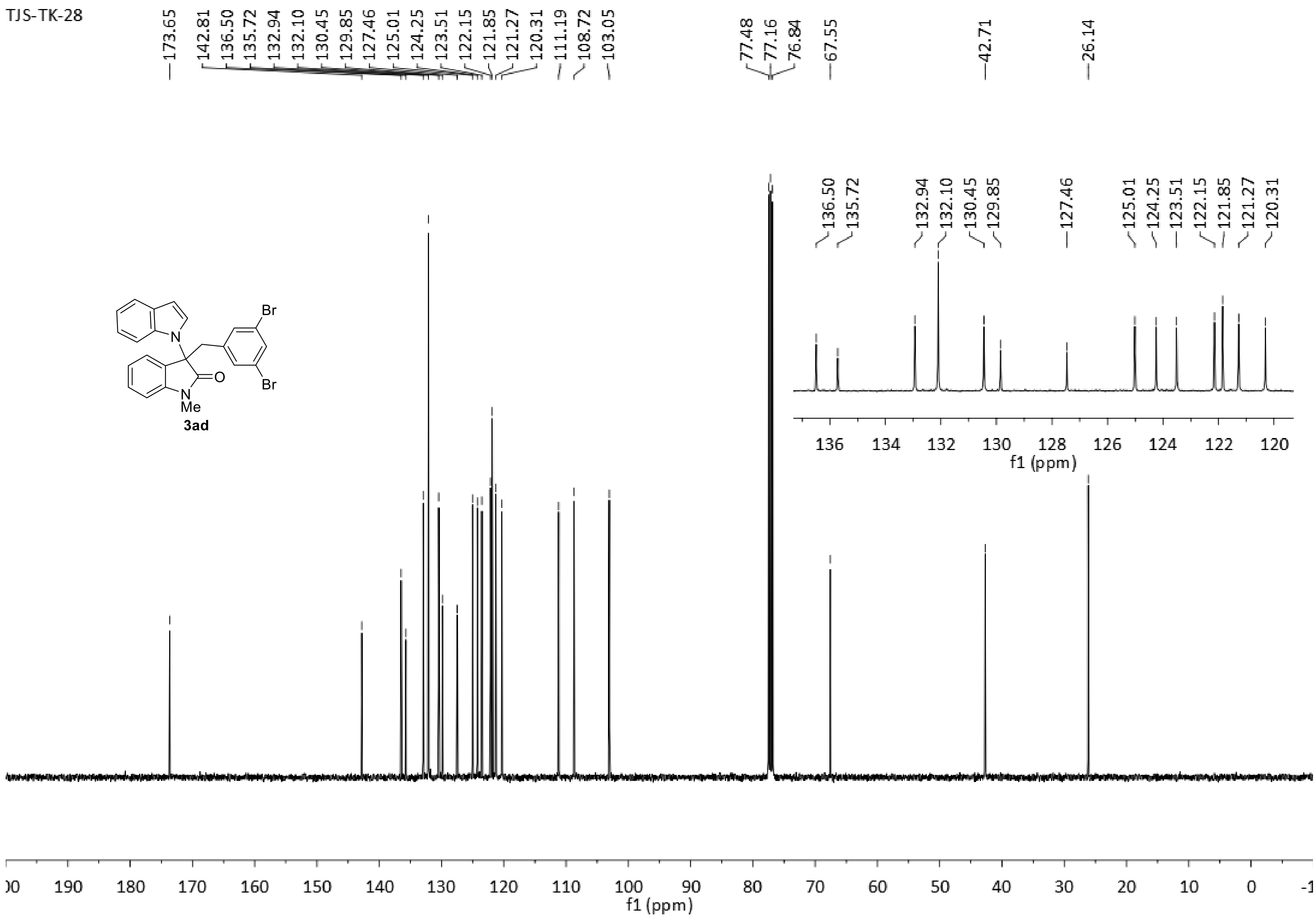

TJS-TJ-133-2-1
174.00
143.08
135.80
133.42
131.72
131.08
130.16
129.91
128.04
127.84
125.13
124.24
123.36
122.10
121.25
120.23
111.23
108.64
102.93
77.48
77.16
76.84
67.75
42.83
26.14
N
Cl
O
N
Me
3ab
f1 (ppm)
f1 (ppm)

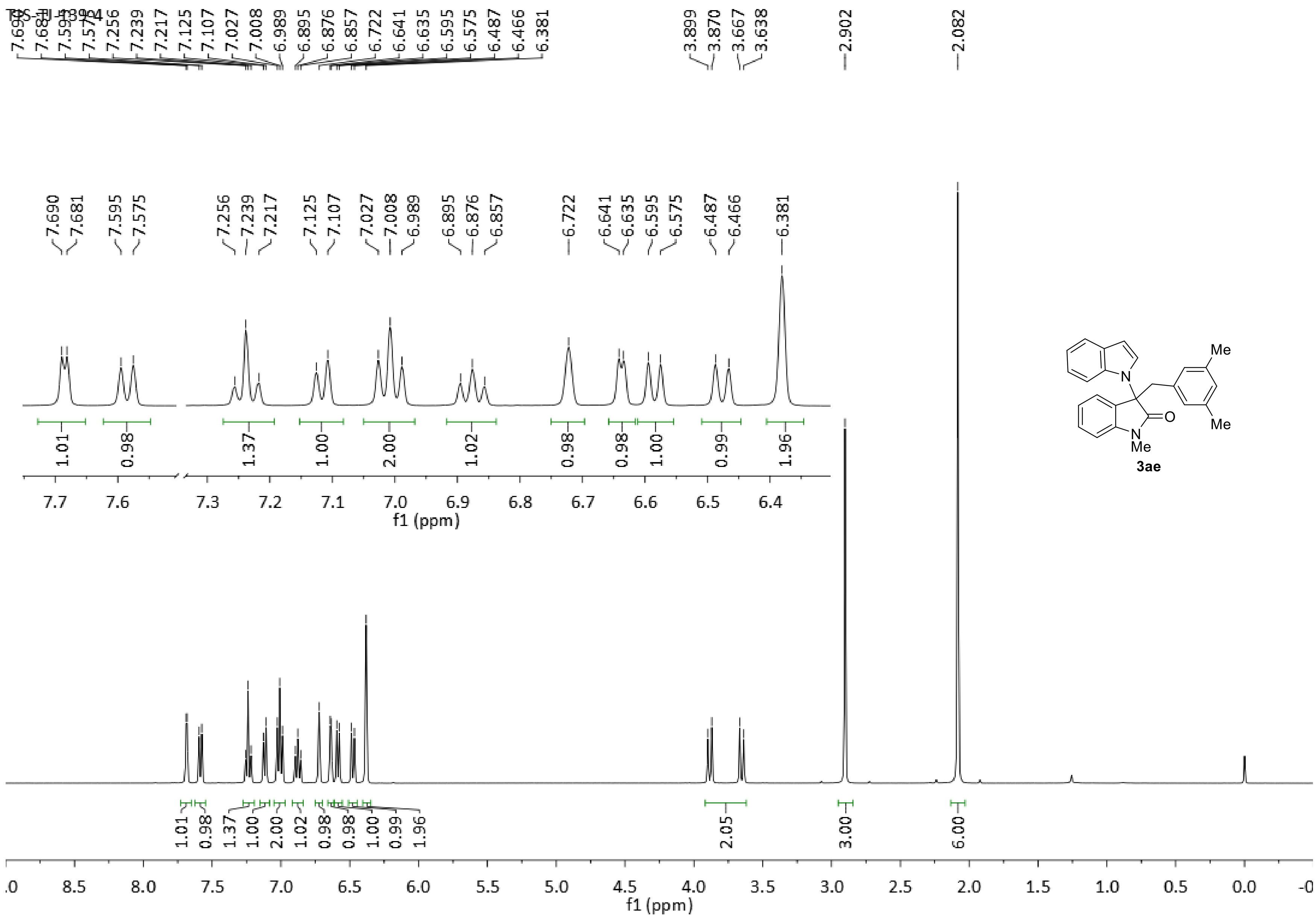

7.656 7.648 7.611 7.592 7.318 7.298 7.279 7.260 7.193 7.173 7.151 7.132 7.063 7.046 7.032 7.013 6.927 6.907 6.888 6.674 6.657 6.654 6.512 6.491
3.953 3.924 3.724 3.695
2.958
1.01 0.97 1.05 2.97 1.98 1.00 3.94 0.98
2.05
3.00
f1 (ppm)
N
Br
O
N
Me
3ac

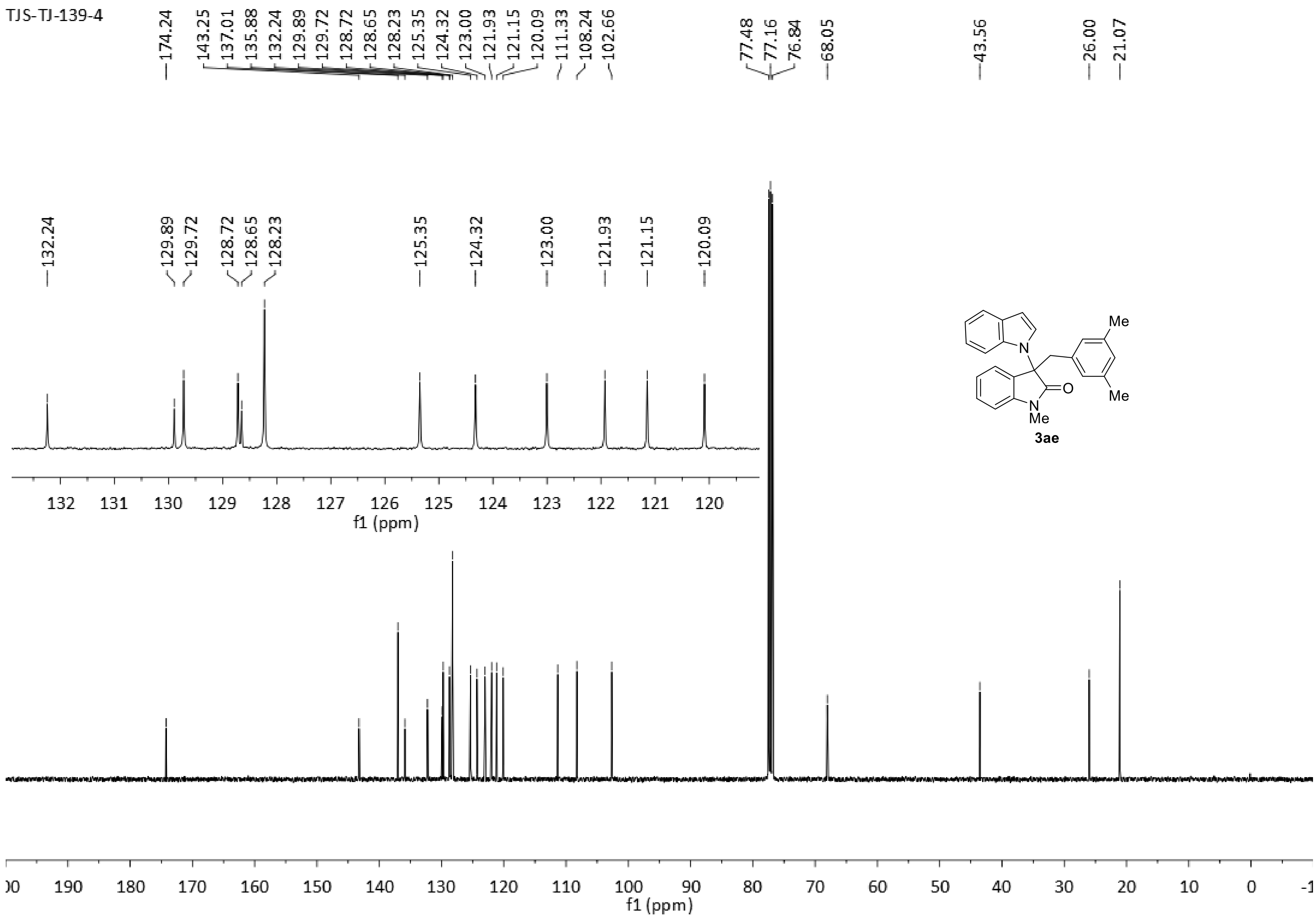

TJS-TJ-133-3
174.00
143.07
135.79
132.07
131.60
130.80
130.19
129.91
128.01
125.13
124.25
123.38
122.11
121.60
121.25
120.23
111.23
108.67
102.94
77.48
77.16
76.84
67.69
42.88
26.15
Br
O
N
Me
3ac
f1 (ppm)
f1 (ppm)

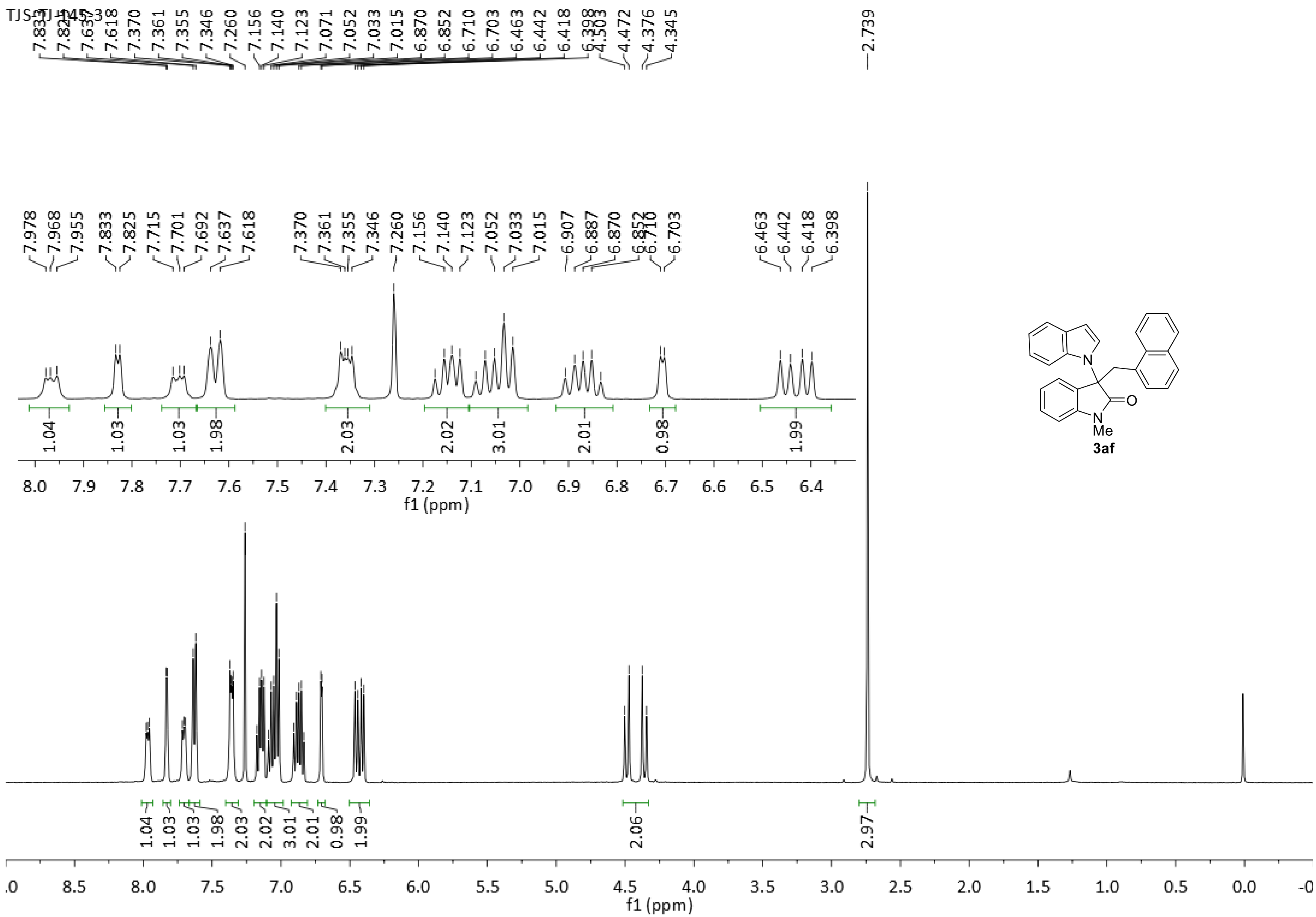


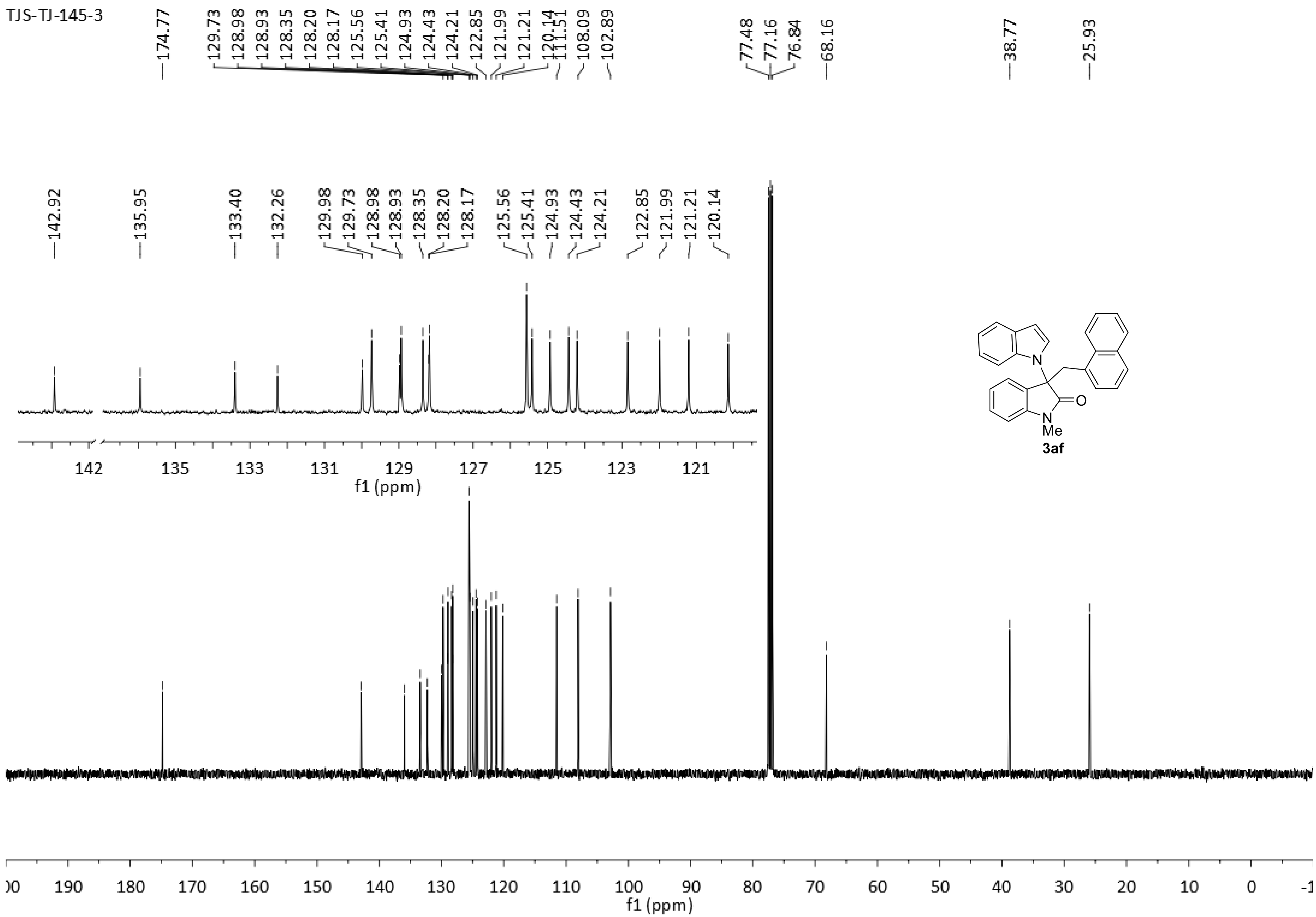
3ad

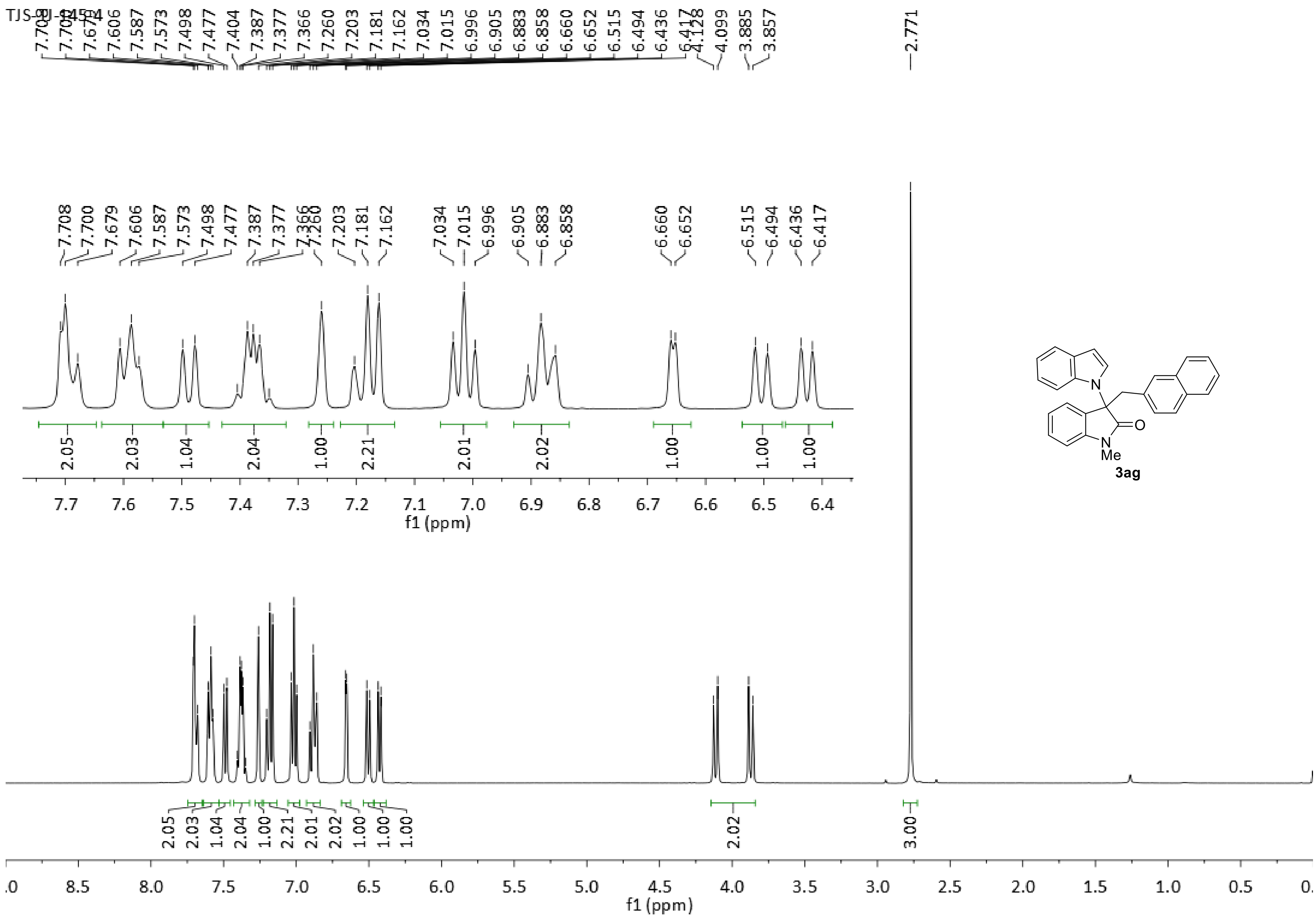

TJS-TK-28
173.65
142.81
136.50
135.72
132.94
132.10
130.45
129.85
127.46
125.01
124.25
123.51
122.15
121.85
121.27
120.31
111.19
108.72
103.05
77.48
77.16
76.84
67.55
42.71
26.14
Br
N
O
Br
N
Me
3ad
136.50
135.72
132.94
132.10
130.45
129.85
127.46
125.01
124.25
123.51
122.15
121.85
121.27
120.31
f1 (ppm)
f1 (ppm)


7.690 7.681 7.595 7.575 7.256 7.239 7.217 7.125 7.107 7.027 7.008 6.989 6.895 6.876 6.857 6.722 6.641 6.635 6.595 6.575 6.487 6.466 6.381
3.899 3.870 3.667 3.638
2.902
2.082
1.01 0.98 1.37 1.00 2.00 1.02 0.98 0.98 1.00 0.99 1.96
2.05 3.00 6.00
f1 (ppm)
Me
Me
N
N
O
Me
3ae

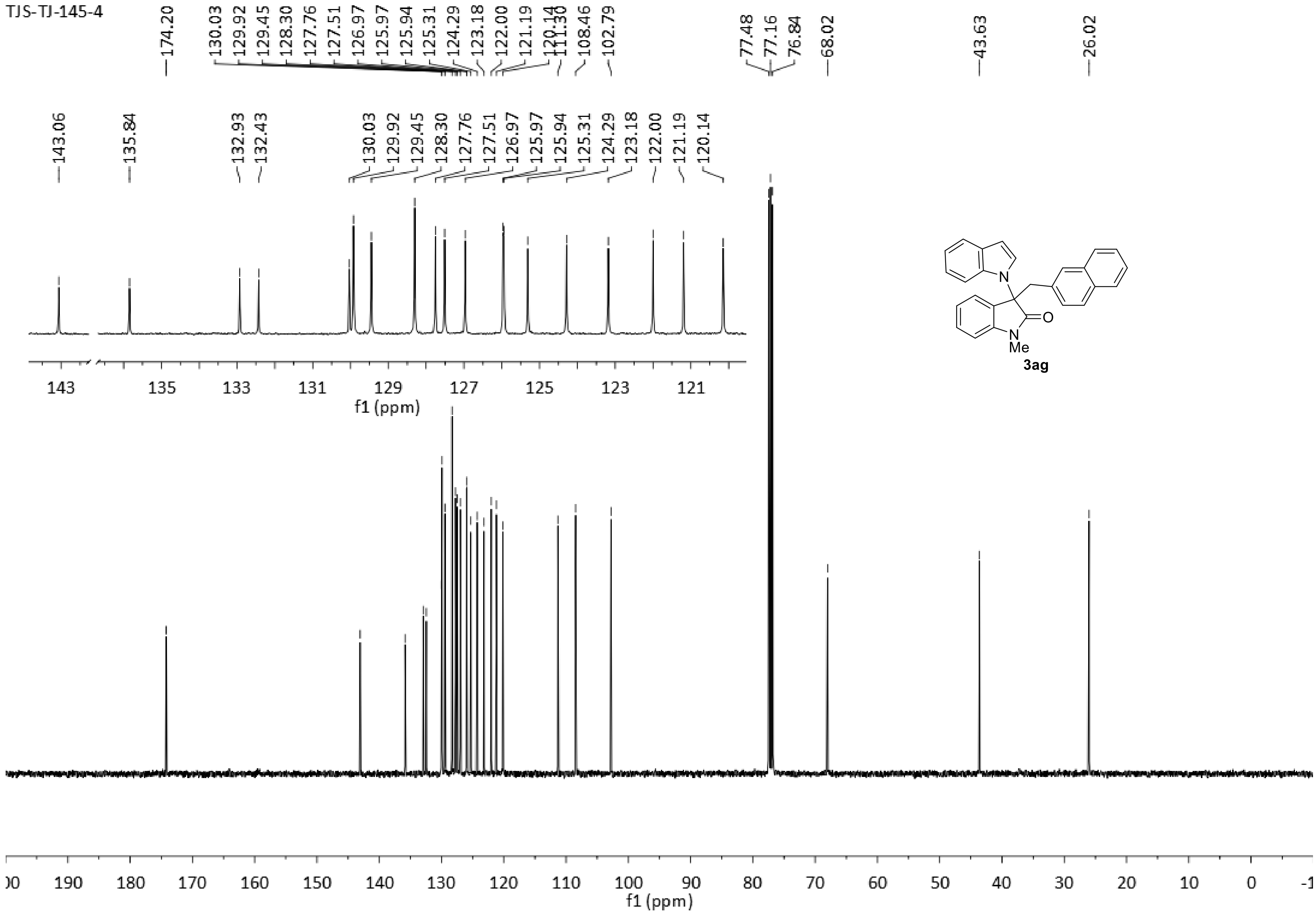

TJS-TJ-139-4
174.24
143.25
137.01
135.88
132.24
129.89
129.72
128.72
128.65
128.23
125.35
124.32
123.00
121.93
121.15
120.09
111.33
108.24
102.66
77.48
77.16
76.84
68.05
43.56
26.00
21.07
f1 (ppm)
Me
N
O
3ae


TJS-TJ-145-3
7.833
7.825
7.637
7.618
7.370
7.361
7.355
7.346
7.260
7.156
7.140
7.123
7.071
7.052
7.033
7.015
6.870
6.852
6.710
6.703
6.463
6.442
6.418
6.398
4.503
4.472
4.376
4.345
2.739
7.978
7.968
7.955
7.715
7.701
7.692
6.907
6.887
1.04
1.03
1.03
1.98
2.03
2.02
3.01
2.01
0.98
1.99
2.06
2.97
f1 (ppm)
N
O
Me
3af

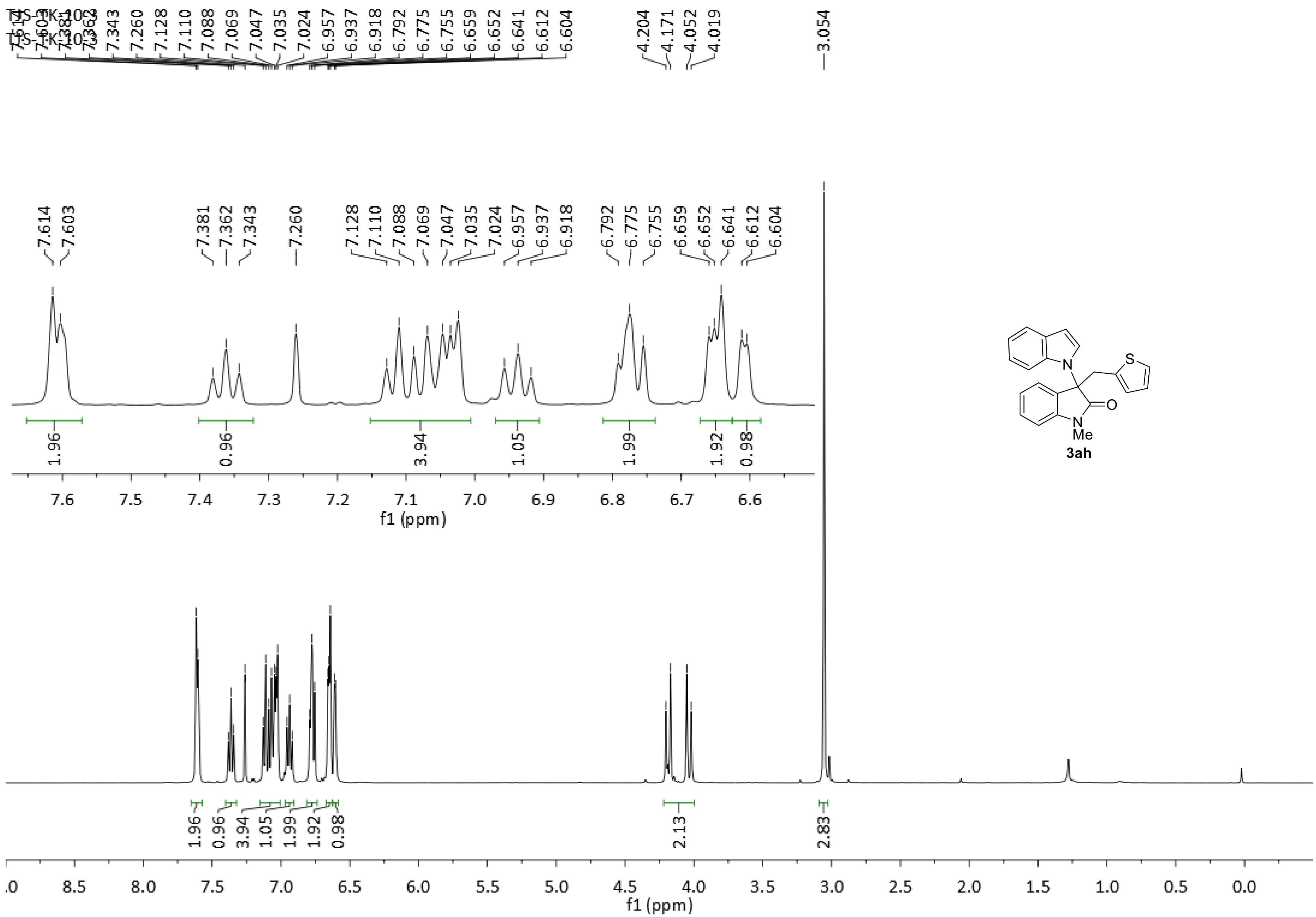

TJS-TJ-145-3
174.77
129.73
128.98
128.93
128.35
128.20
128.17
125.56
125.41
124.93
124.43
124.21
122.85
121.99
121.21
120.14
111.51
108.09
102.89
77.48
77.16
76.84
68.16
38.77
25.93
142.92
135.95
133.40
132.26
129.98
129.73
128.98
128.93
128.35
128.20
128.17
125.56
125.41
124.93
124.43
124.21
122.85
121.99
121.21
120.14
142
135
133
131
129
127
125
123
121
f1 (ppm)
N
O
N
Me
3af
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


f1 (ppm)
2.771
3.885
3.857
4.099
2.02
3.00
N
O
N
Me
3ag

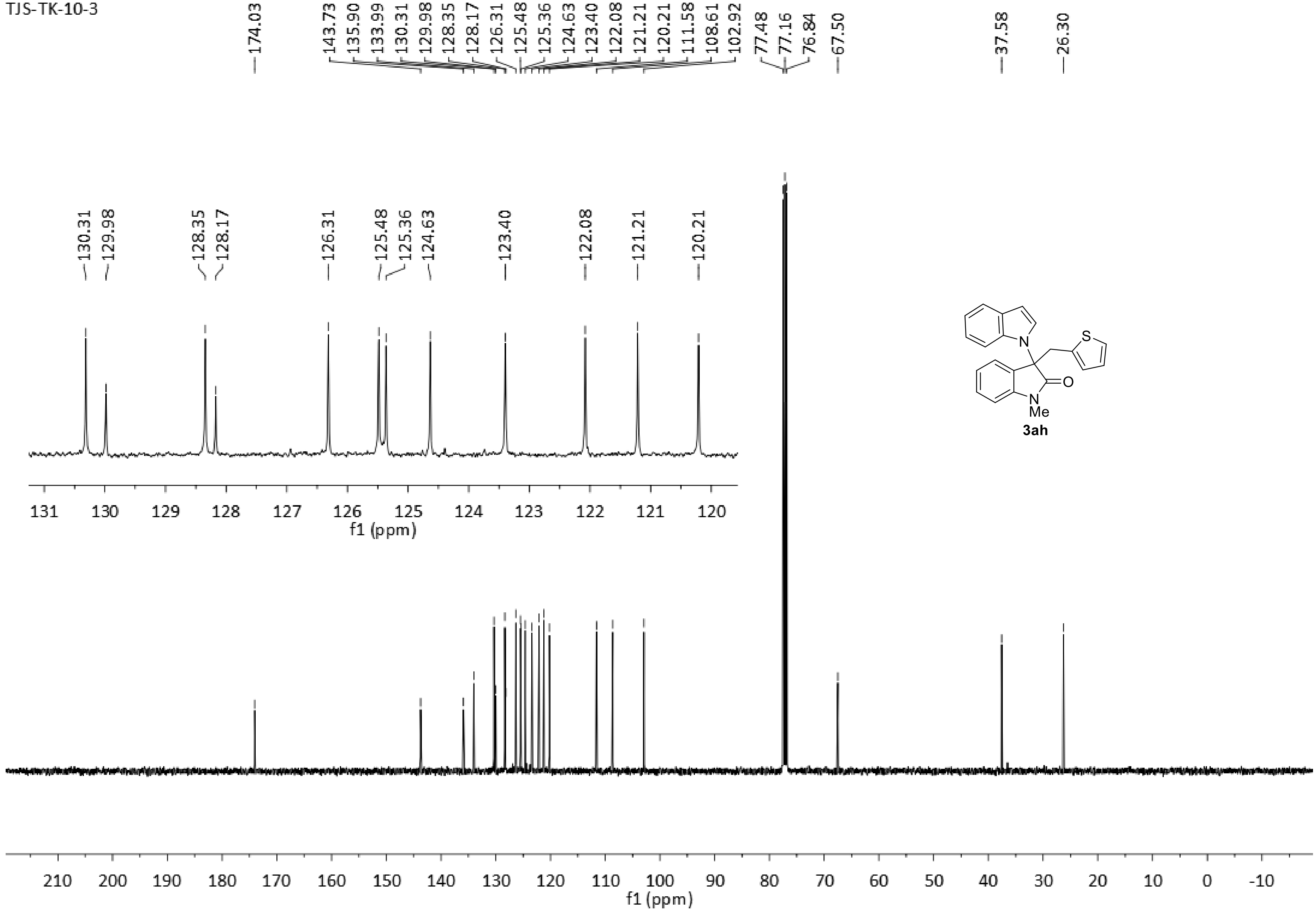
TJS-TJ-145-4



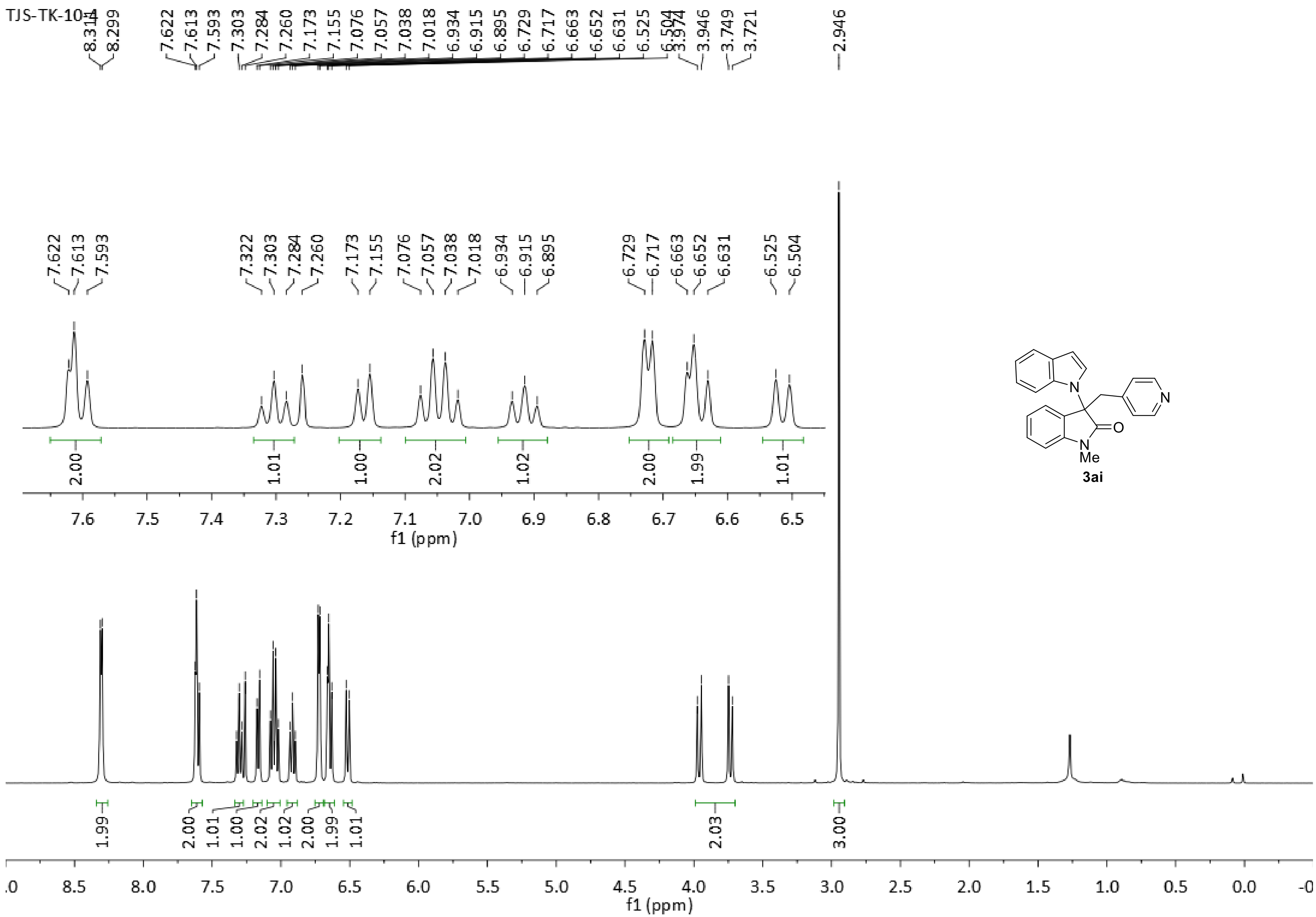
3ag

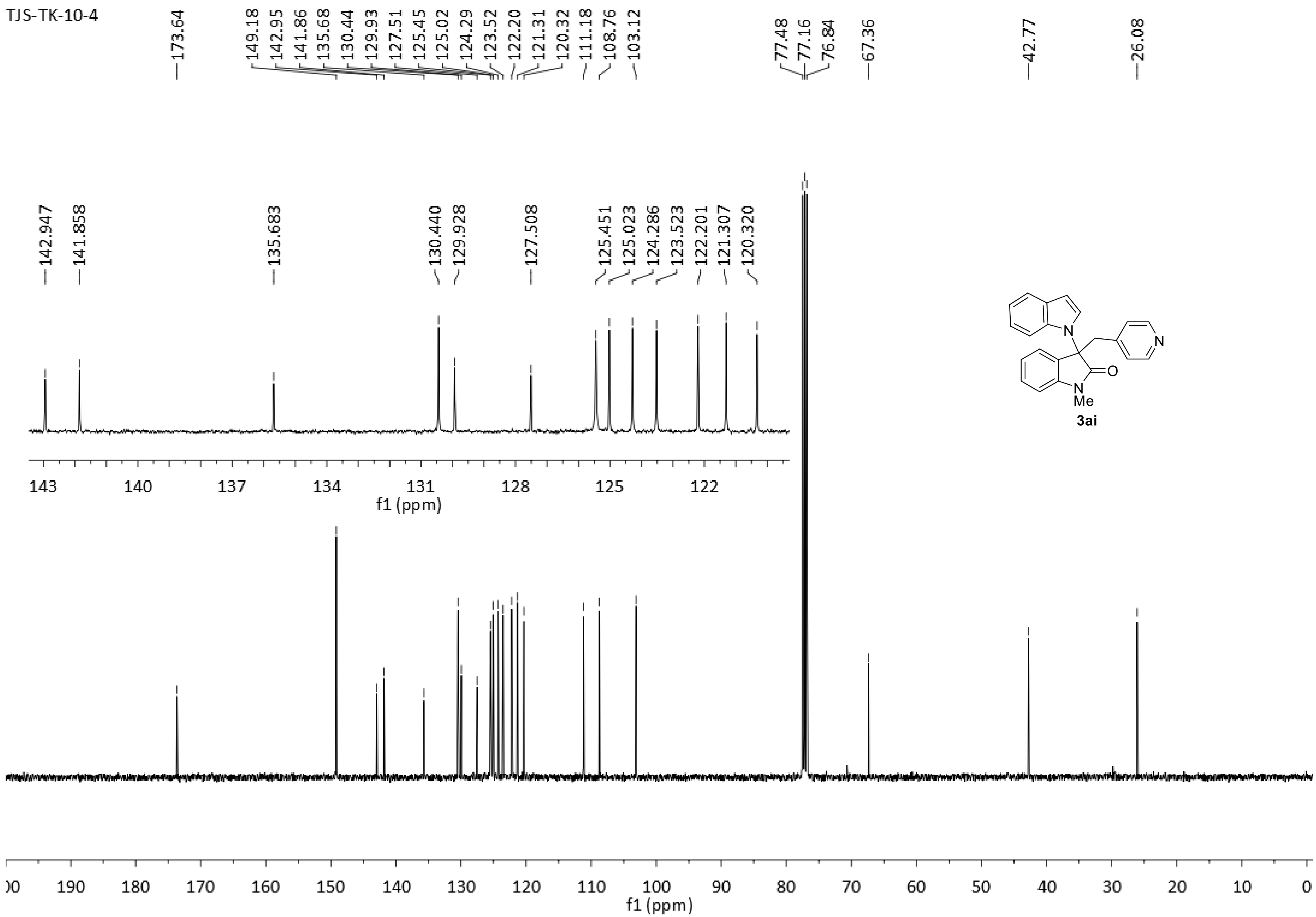

TJS-TK-10-3
7.614
7.603
7.381
7.362
7.343
7.260
7.128
7.110
7.088
7.069
7.047
7.035
7.024
6.957
6.937
6.918
6.792
6.775
6.755
6.659
6.652
6.641
6.612
6.604
4.204
4.171
4.052
4.019
3.054
1.96
0.96
3.94
1.05
1.99
1.92
0.98
2.13
2.83
f1 (ppm)
S
N
O
N
Me
3ah

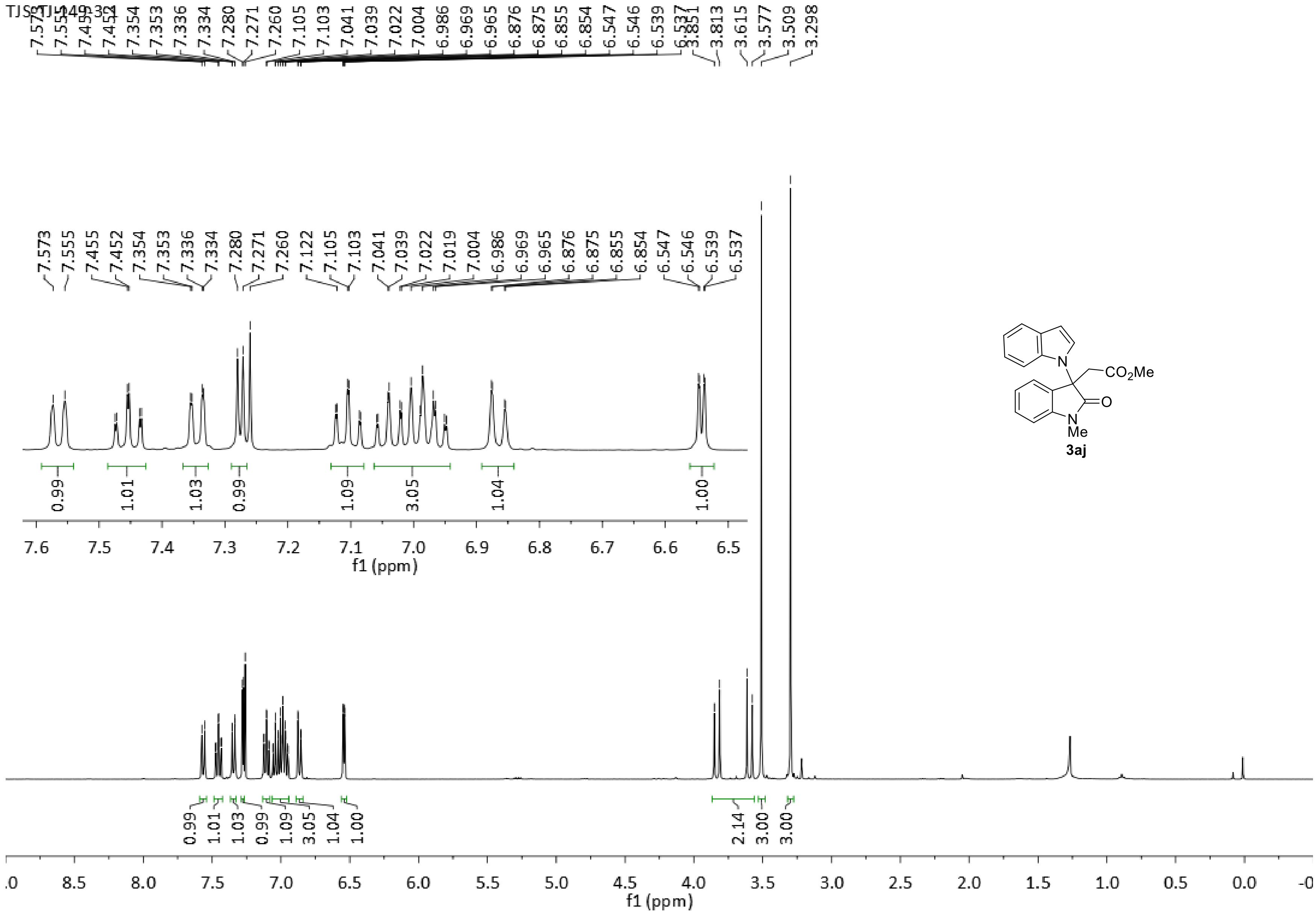
TJS-TK-10-3

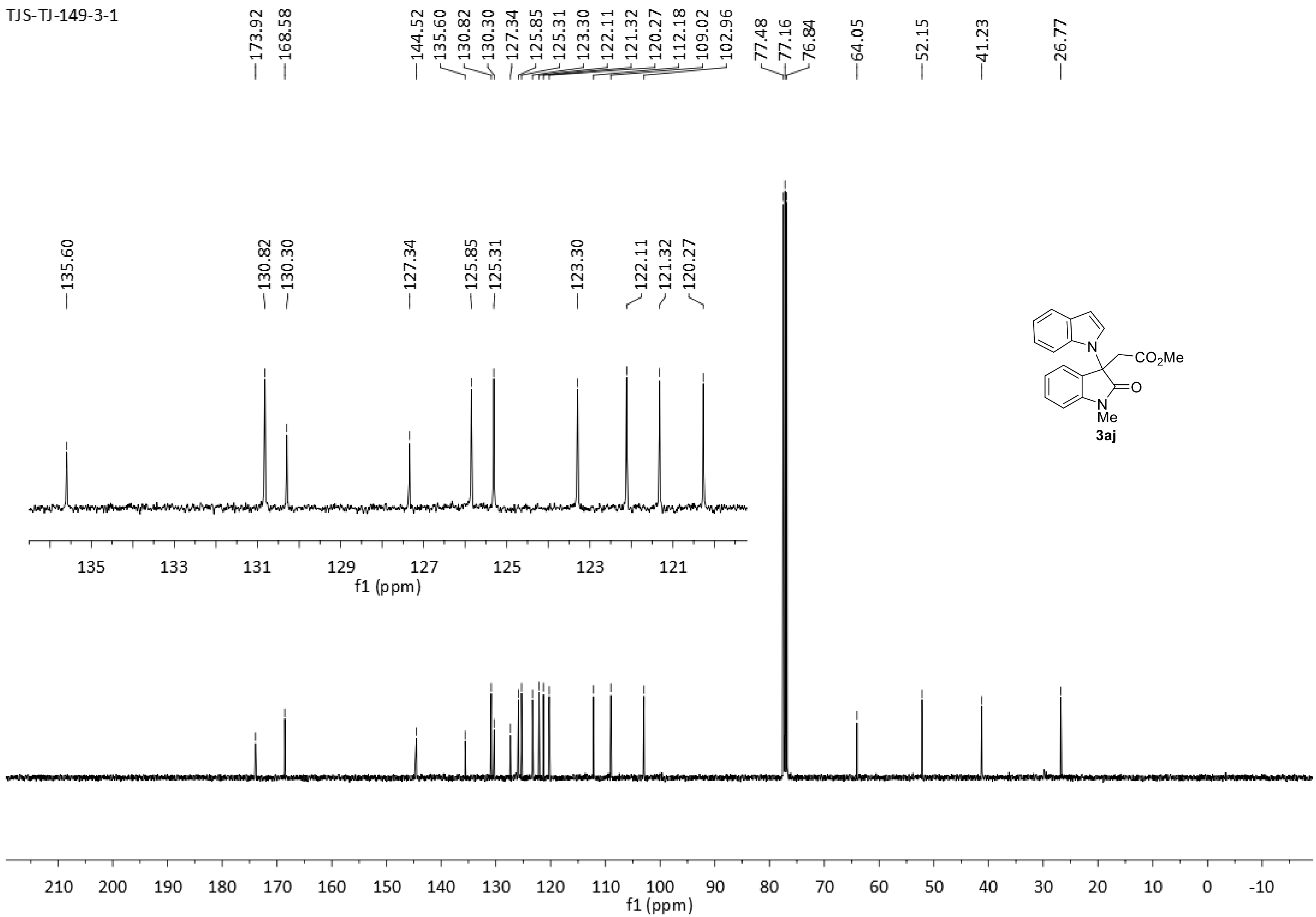


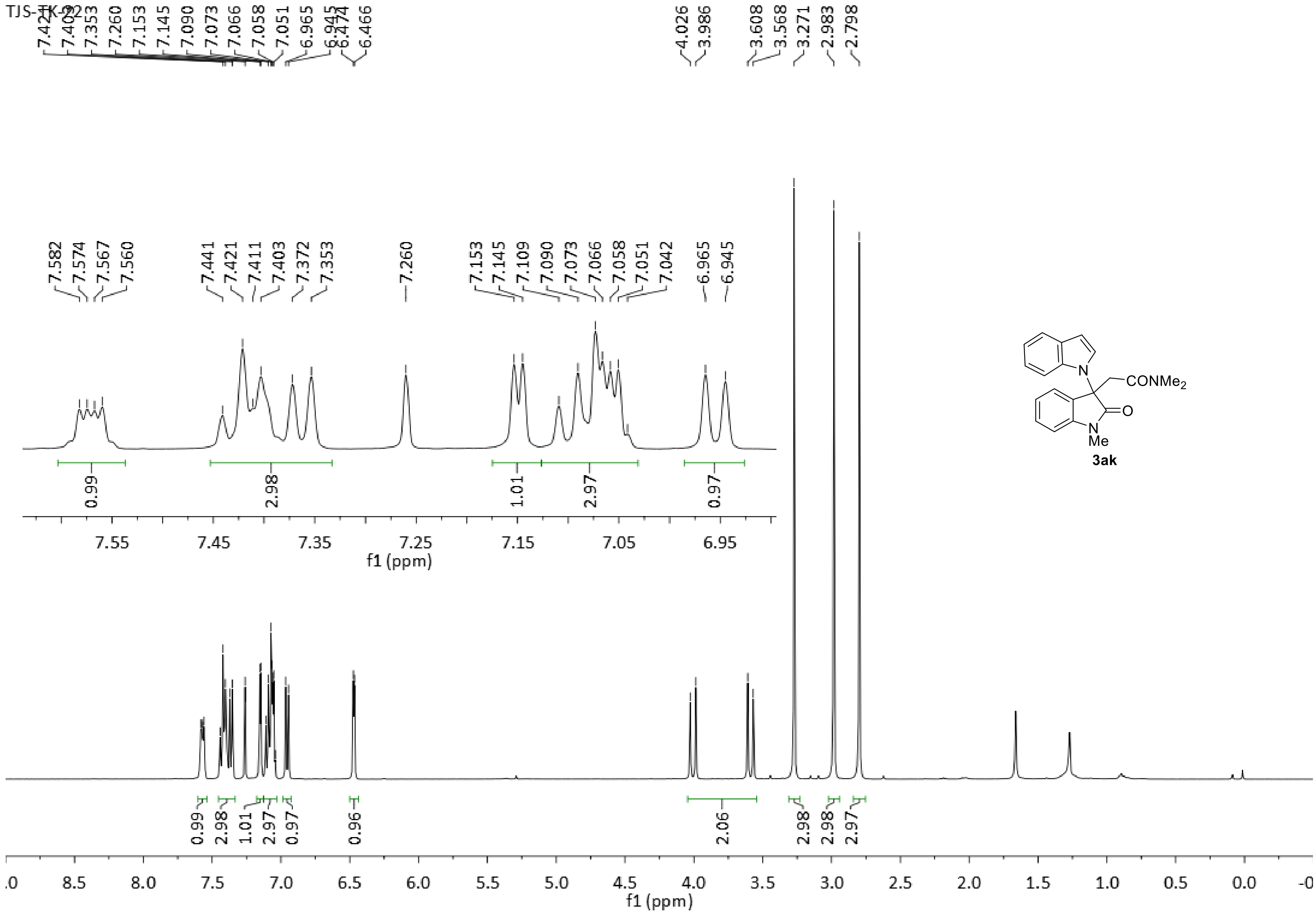
3ah

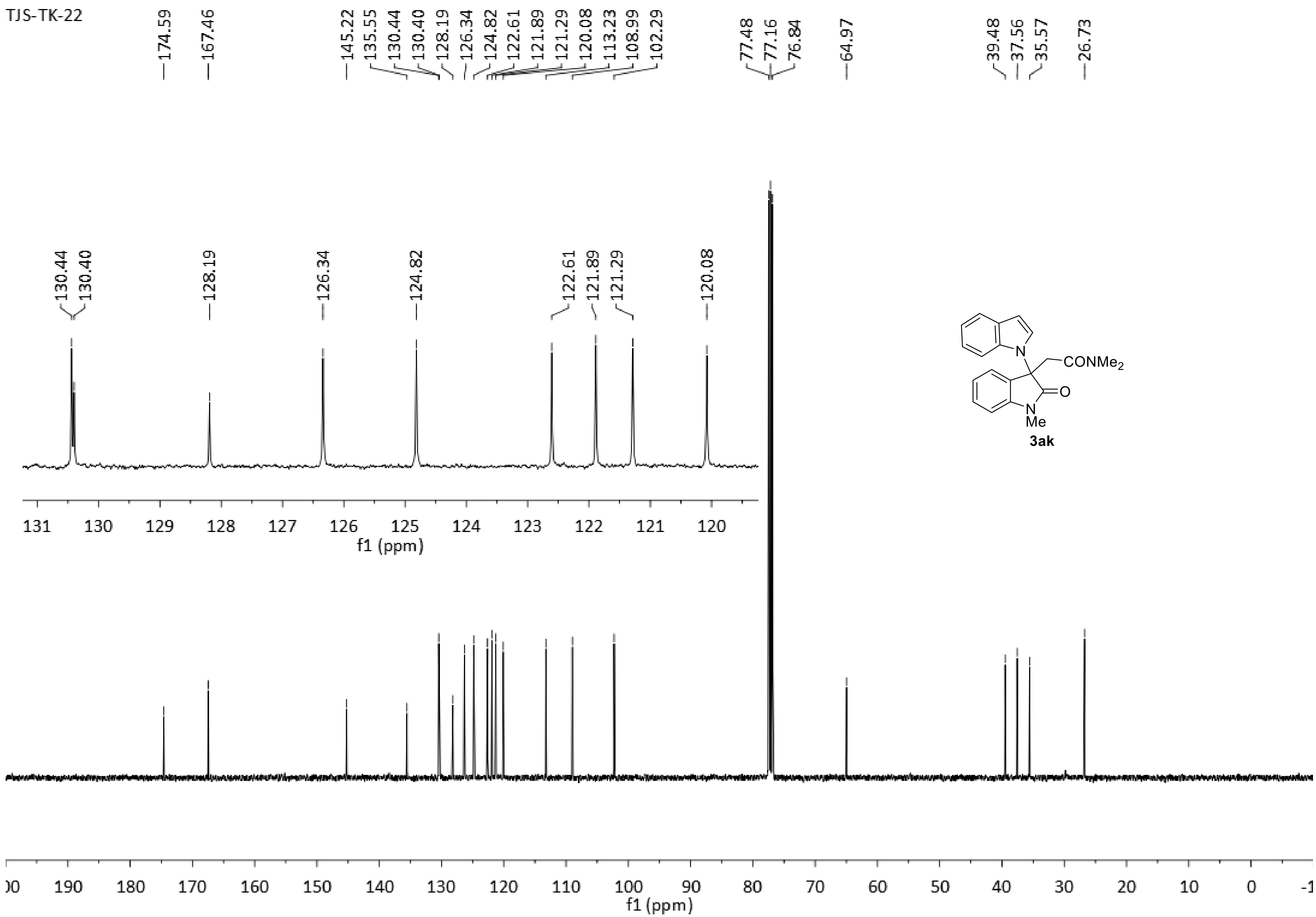

TJS-TK-10-4
8.311 8.299 7.622 7.613 7.593 7.303 7.284 7.260 7.173 7.155 7.076 7.057 7.038 7.018 6.934 6.915 6.895 6.729 6.717 6.663 6.652 6.631 6.525 6.504 3.974 3.946 3.749 3.721 2.946
7.622 7.613 7.593 7.322 7.303 7.284 7.260 7.173 7.155 7.076 7.057 7.038 7.018 6.934 6.915 6.895 6.729 6.717 6.663 6.652 6.631 6.525 6.504
2.00 1.01 1.00 2.02 1.02 2.00 1.99 1.01
f1 (ppm)
N
O
N
Me
N
3ai
1.99 2.00 1.01 1.00 2.02 1.02 2.00 1.99 1.01 2.03 3.00
f1 (ppm)

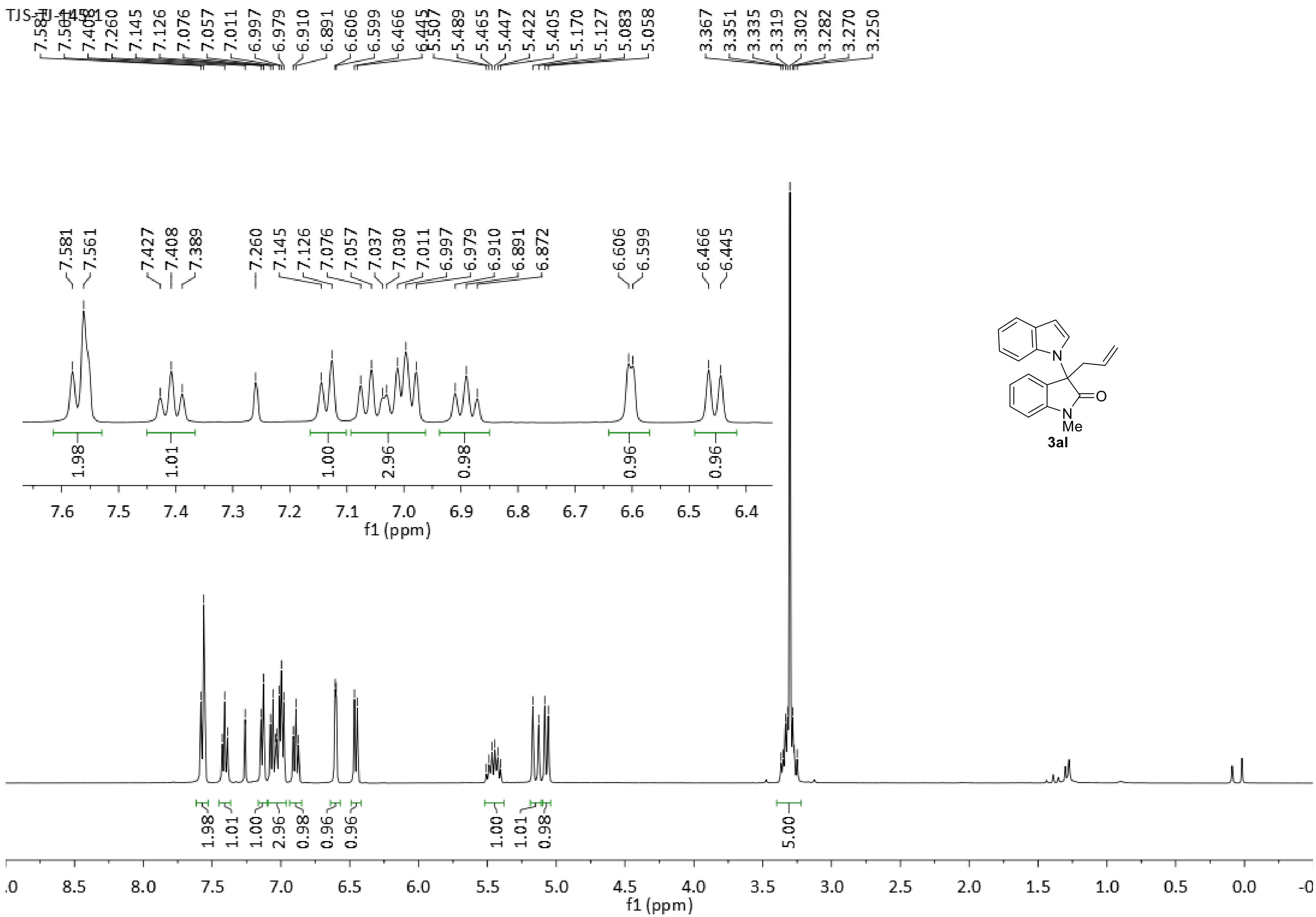

TJS-TK-10-4
173.64
149.18
142.95
141.86
135.68
130.44
129.93
127.51
125.45
125.02
124.29
123.52
122.20
121.31
120.32
111.18
108.76
103.12
77.48
77.16
76.84
67.36
42.77
26.08
142.947
141.858
135.683
130.440
129.928
127.508
125.451
125.023
124.286
123.523
122.201
121.307
120.320
f1 (ppm)
N
O
N
Me
N
3ai
f1 (ppm)


TJS-TJ-149-3-1
CO2Me
N
O
N
Me
3aj
f1 (ppm)
f1 (ppm)

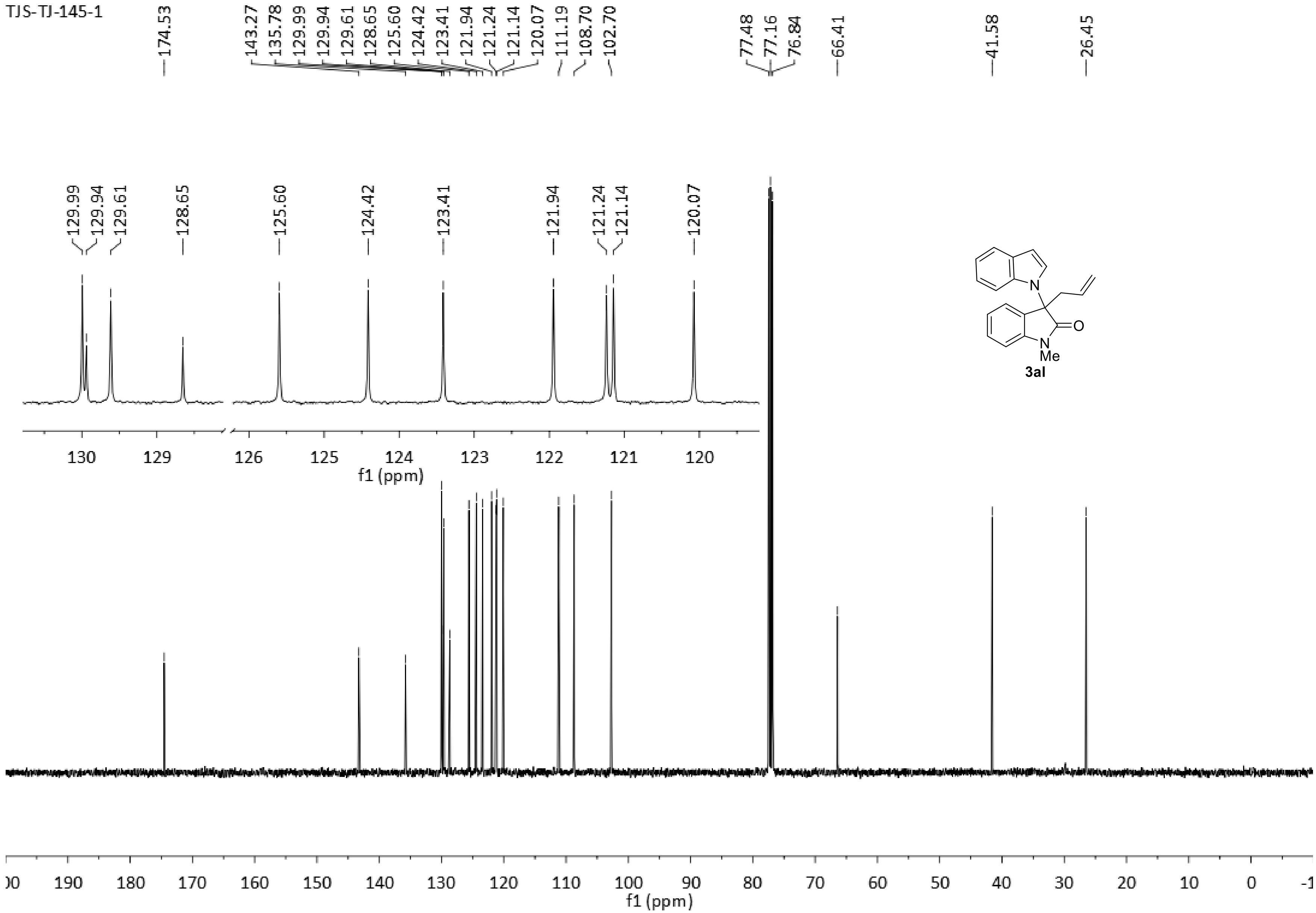

TJS-TJ-149-3-1
173.92
168.58
144.52
135.60
130.82
130.30
127.34
125.85
125.31
123.30
122.11
121.32
120.27
112.18
109.02
102.96
77.48
77.16
76.84
64.05
52.15
41.23
26.77
N
CO2Me
O
N
Me
3aj
f1 (ppm)

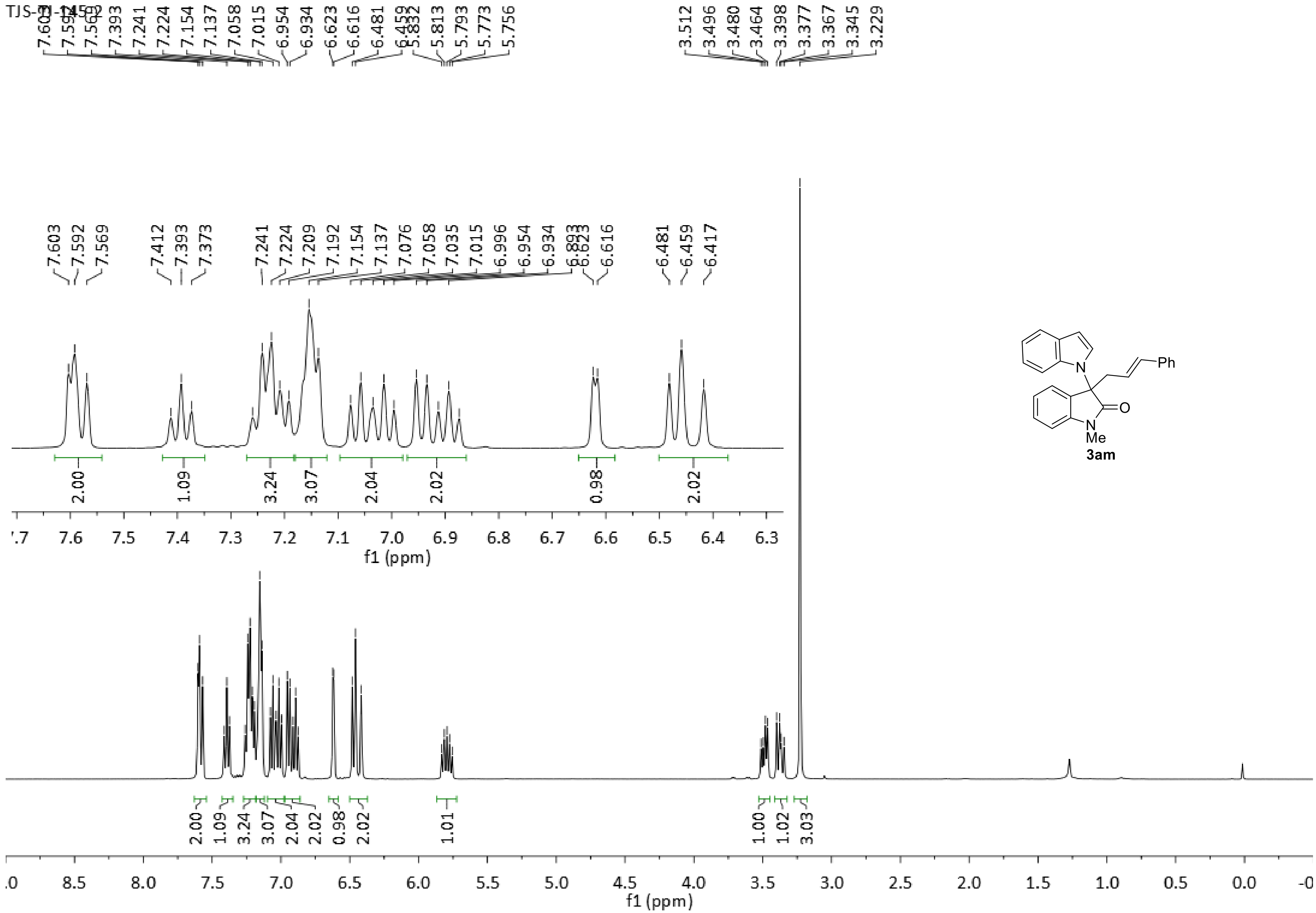

TJS-TK-22
CONMe2
N
O
N
Me
3ak
f1 (ppm)
f1 (ppm)


TJS-TK-22
174.59
167.46
145.22
135.55
130.44
130.40
128.19
126.34
124.82
122.61
121.89
121.29
120.08
113.23
108.99
102.29
77.48
77.16
76.84
64.97
39.48
37.56
35.57
26.73
130.44
130.40
128.19
126.34
124.82
122.61
121.89
121.29
120.08
131 130 129 128 127 126 125 124 123 122 121 120
f1 (ppm)
N
CONMe2
O
N
Me
3ak
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

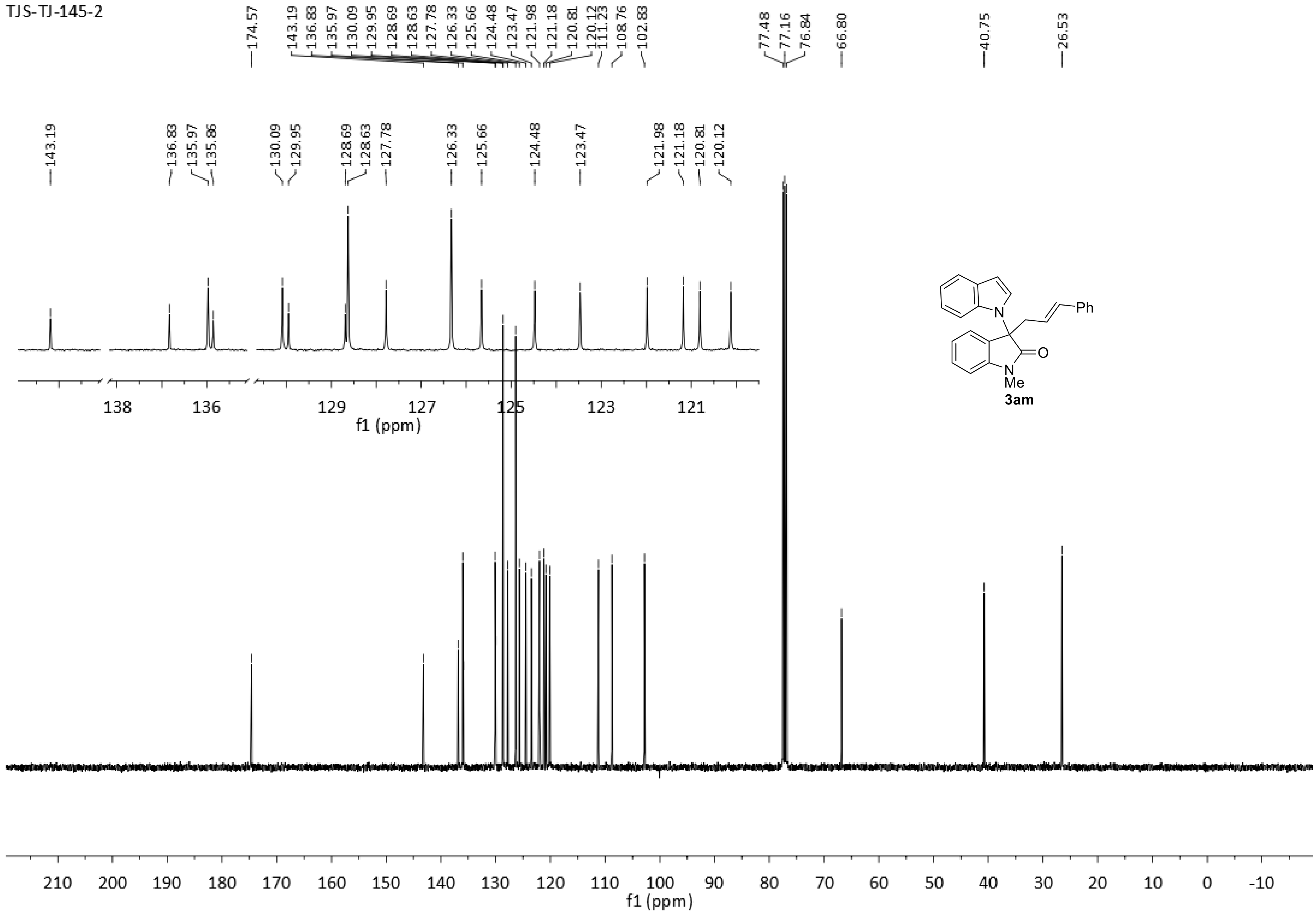

TJS-TJ-14501
7.581
7.561
7.427
7.408
7.389
7.260
7.145
7.126
7.076
7.057
7.037
7.030
7.011
6.997
6.979
6.910
6.891
6.872
6.606
6.599
6.466
6.445
5.507
5.489
5.465
5.447
5.422
5.405
5.170
5.127
5.083
5.058
3.367
3.351
3.335
3.319
3.302
3.282
3.270
3.250
1.98
1.01
1.00
2.96
0.98
0.96
0.96
1.00
1.01
0.98
5.00
f1 (ppm)
N
O
Me

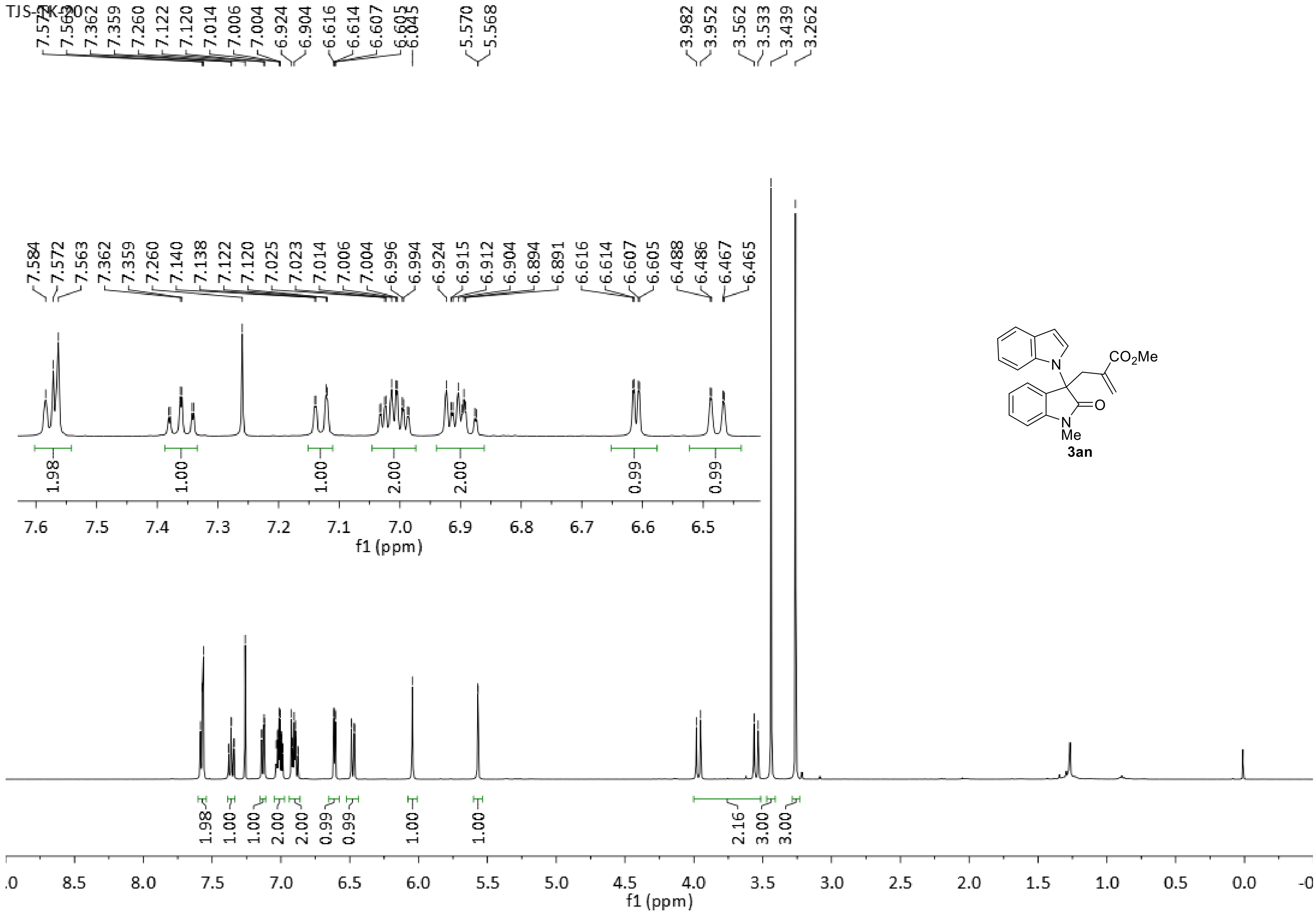
3al


TJS-TJ-145-1
174.53
143.27
135.78
129.99
129.94
129.61
128.65
125.60
124.42
123.41
121.94
121.24
121.14
120.07
111.19
108.70
102.70
77.48
77.16
76.84
66.41
41.58
26.45
N
O
N
Me
3al
f1 (ppm)

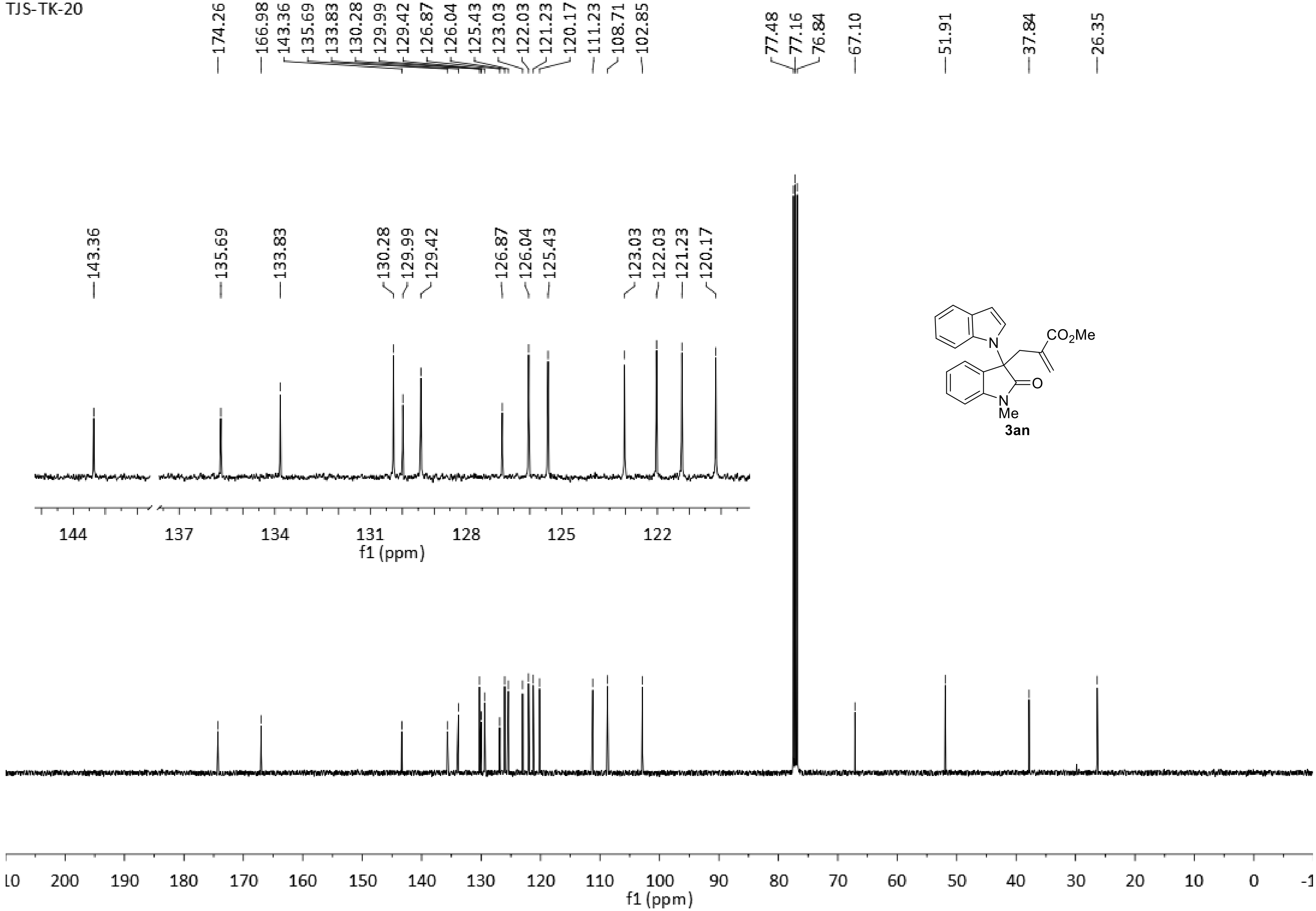


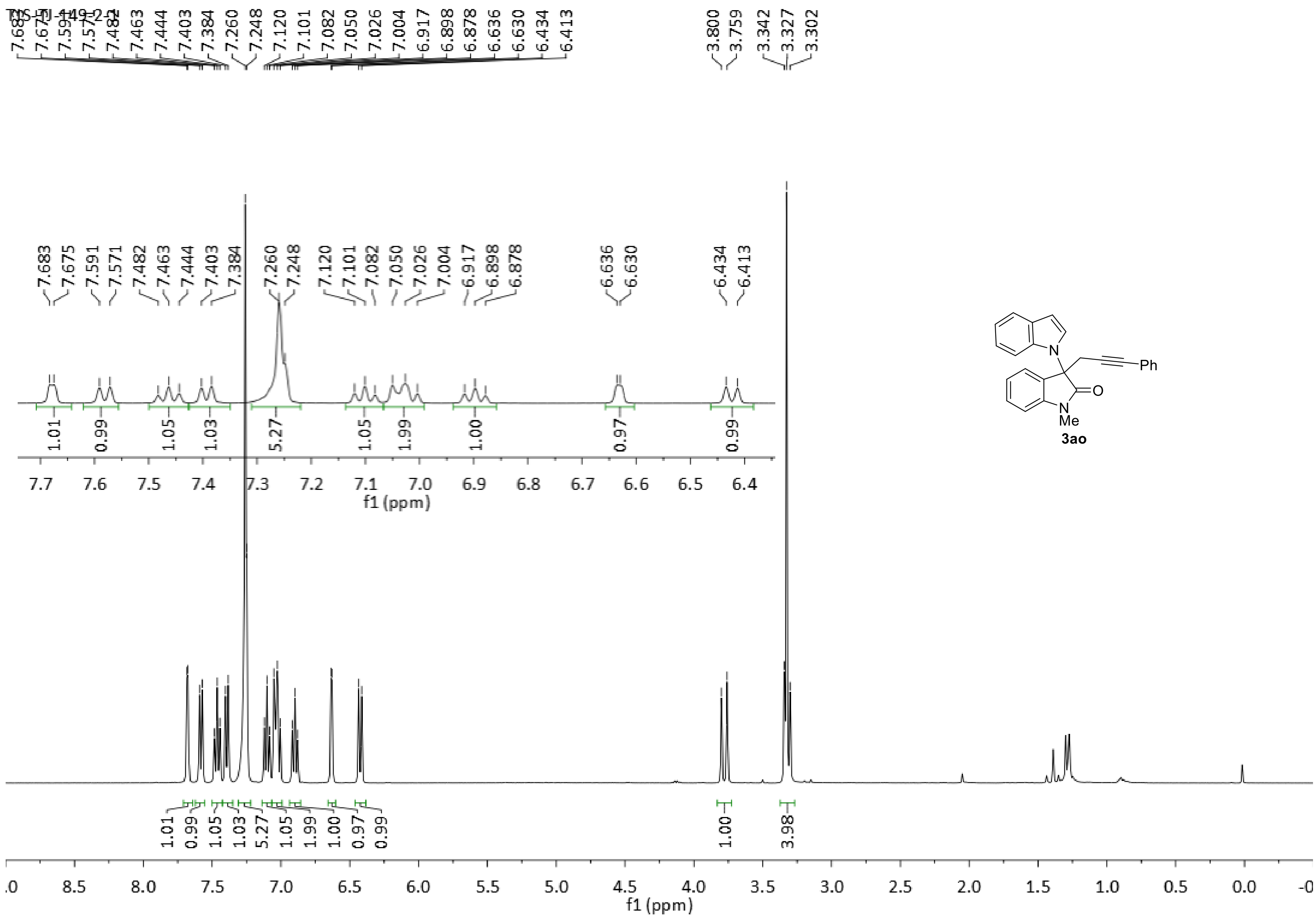
7.603 7.592 7.569 7.412 7.393 7.373 7.241 7.224 7.209 7.192 7.154 7.137 7.076 7.058 7.035 7.015 6.996 6.954 6.934 6.893 6.623 6.616 6.481 6.459 6.417
2.00 1.09 3.24 3.07 2.04 2.02 0.98 2.02
f1 (ppm)
3.512 3.496 3.480 3.464 3.398 3.377 3.367 3.345 3.229
2.00 1.09 3.24 3.07 2.04 2.02 0.98 2.02 1.01 1.00 1.02 3.03
f1 (ppm)
N
Ph
O
N
Me
3am

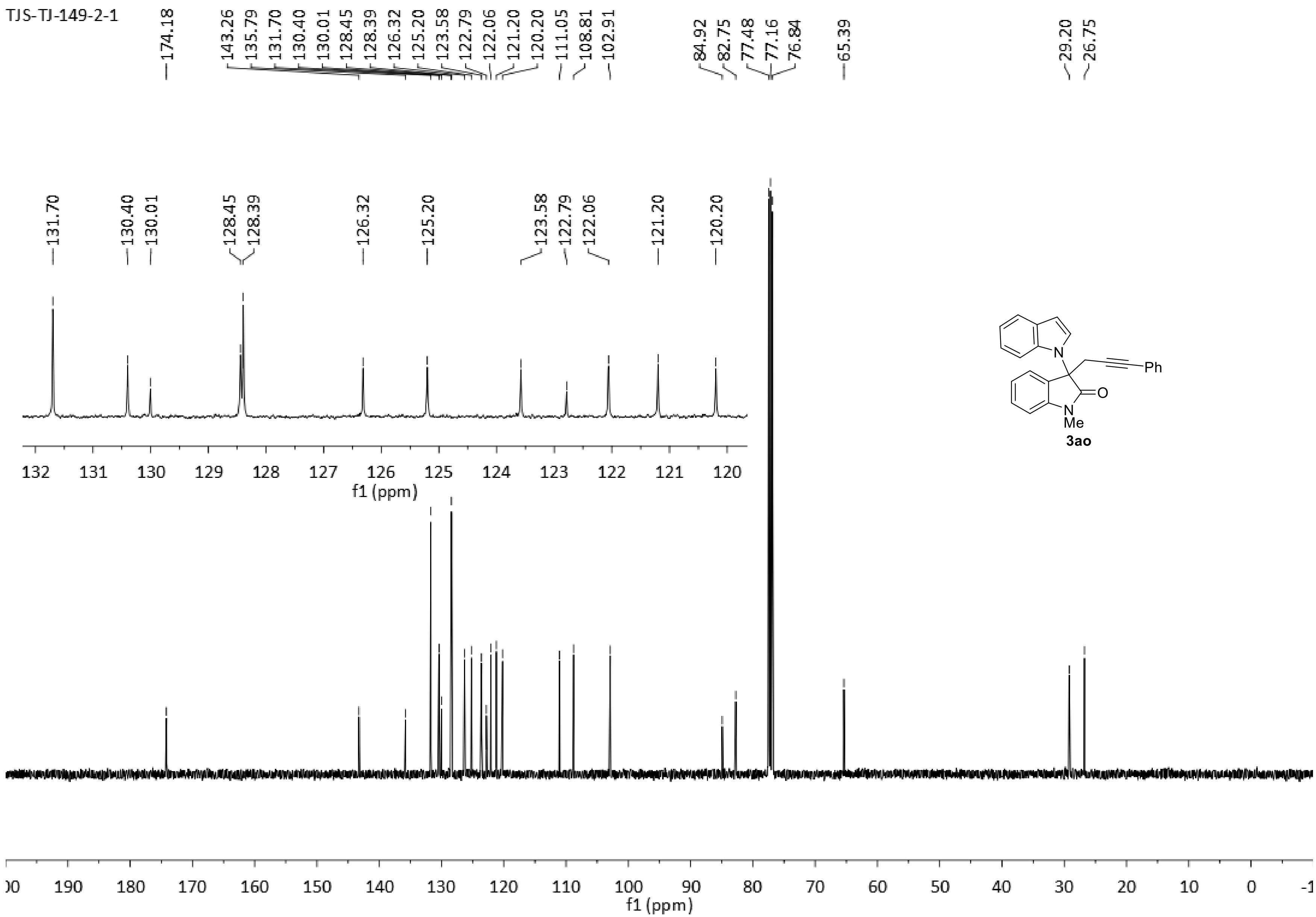

TJS-TJ-145-2
174.57
143.19
136.83
135.97
130.09
129.95
128.69
128.63
127.78
126.33
125.66
124.48
123.47
121.98
121.18
120.81
120.12
111.23
108.76
102.83
77.48
77.16
76.84
66.80
40.75
26.53
143.19
136.83
135.97
135.86
130.09
129.95
128.69
128.63
127.78
126.33
125.66
124.48
123.47
121.98
121.18
120.81
120.12
138
136
129
127
125
123
121
f1 (ppm)
N
Ph
O
N
Me
3am
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

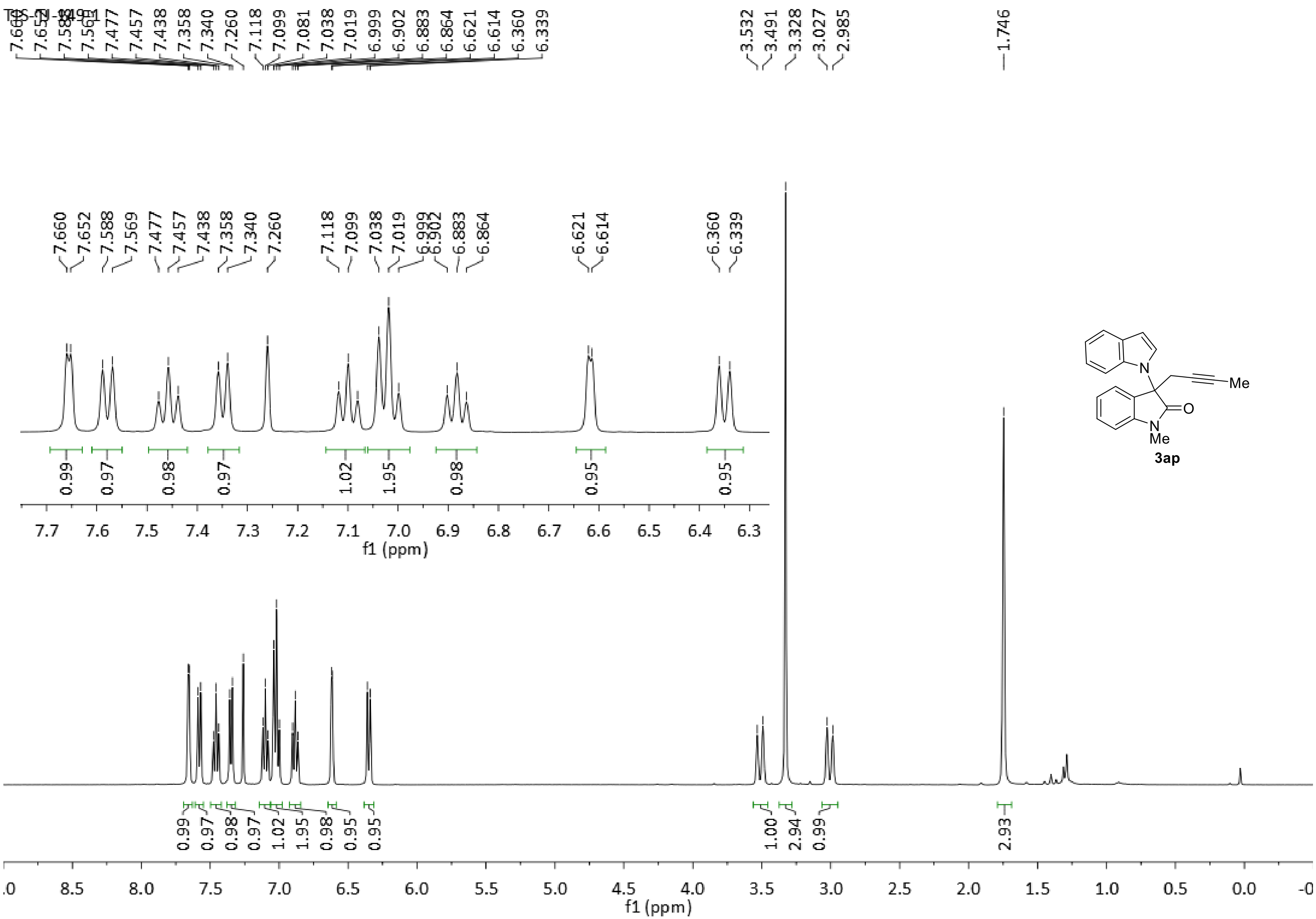

TJS-TK-20
7.572 7.563 7.362 7.359 7.260 7.122 7.120 7.014 7.006 7.004 6.924 6.904 6.616 6.614 6.607 6.605 6.045
5.570 5.568
3.982 3.952 3.562 3.533 3.439 3.262
7.584 7.572 7.563 7.362 7.359 7.260 7.140 7.138 7.122 7.120 7.025 7.023 7.014 7.006 7.004 6.996 6.994 6.924 6.915 6.912 6.904 6.894 6.891 6.616 6.614 6.607 6.605 6.488 6.486 6.467 6.465
1.98 1.00 1.00 2.00 2.00 0.99 0.99
f1 (ppm)
CO2Me
N
O
Me
3an
1.98 1.00 1.00 2.00 2.00 0.99 0.99 1.00 1.00 2.16 3.00 3.00
f1 (ppm)

TJS-TK-20

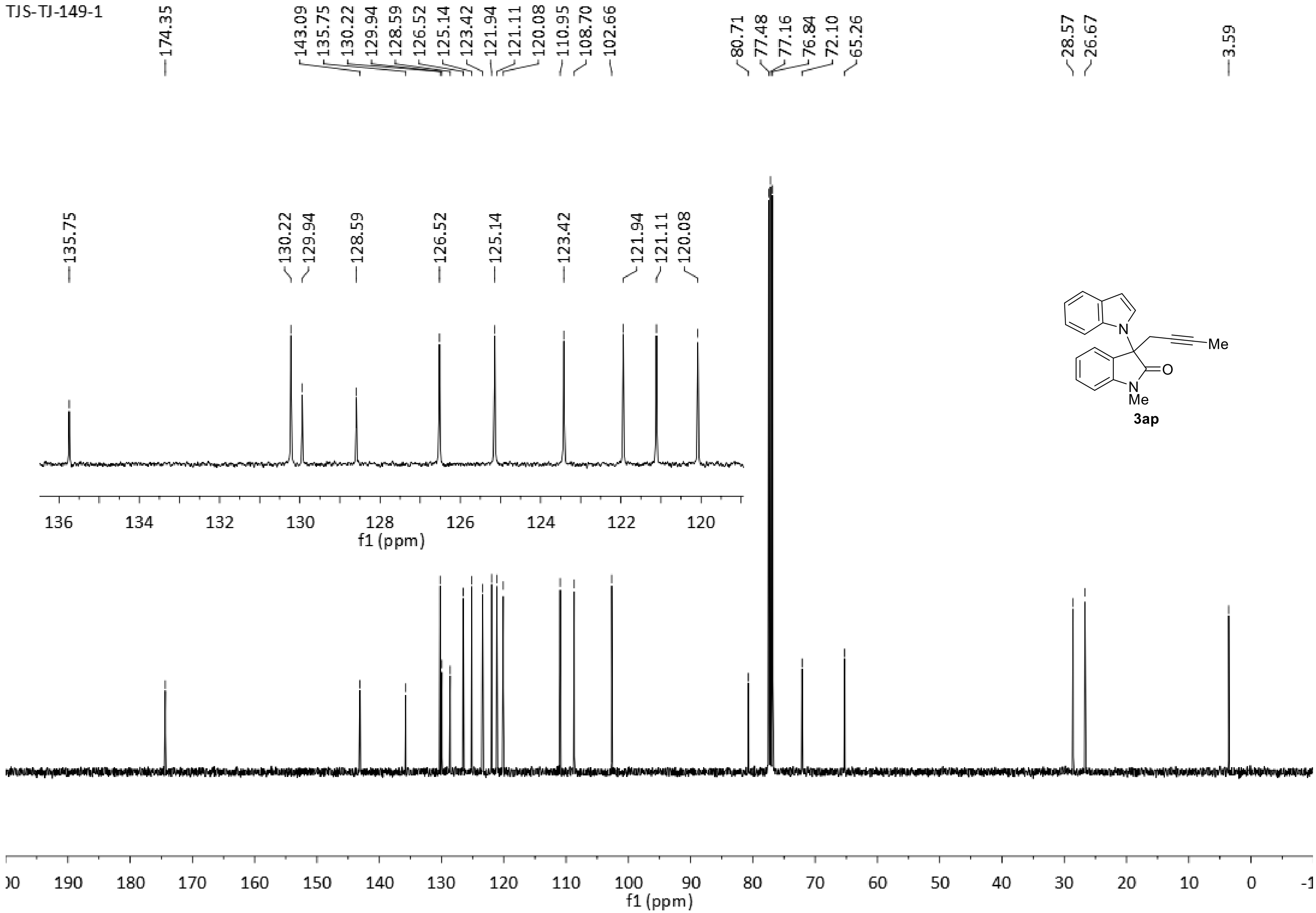

174.26
166.98
143.36
135.69
133.83
130.28
129.99
129.42
126.87
126.04
125.43
123.03
122.03
121.23
120.17
111.23
108.71
102.85
77.48
77.16
76.84
67.10
51.91
37.84
26.35
N
CO2Me
O
N
Me
3an
144
137
134
131
128
125
122
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


f1 (ppm)
N
Ph
O
N
Me
3ao

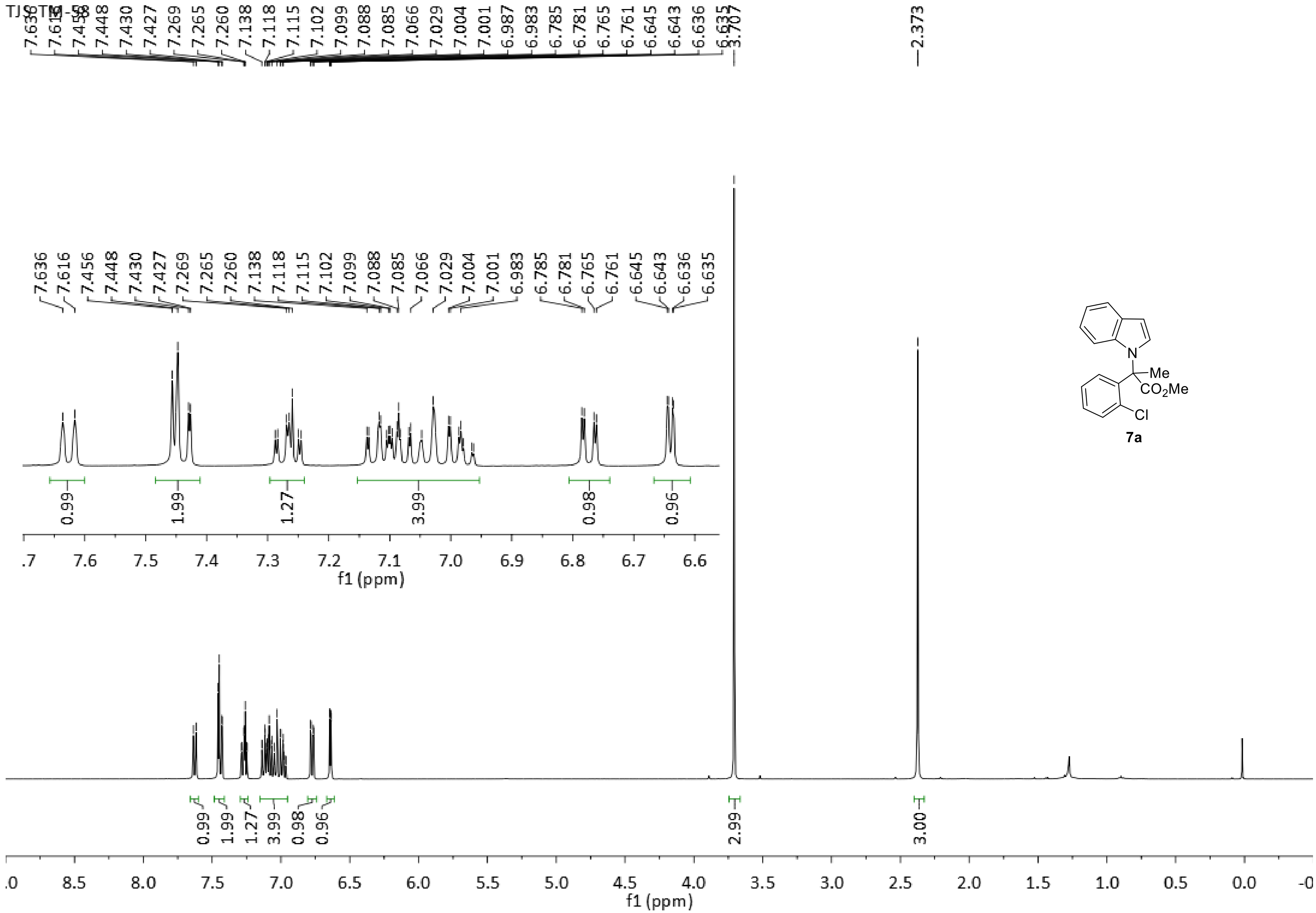

TJS-TJ-149-2-1
174.18
143.26
135.79
131.70
130.40
130.01
128.45
128.39
126.32
125.20
123.58
122.79
122.06
121.20
120.20
111.05
108.81
102.91
84.92
82.75
77.48
77.16
76.84
65.39
29.20
26.75
131.70
130.40
130.01
128.45
128.39
126.32
125.20
123.58
122.79
122.06
121.20
120.20
132 131 130 129 128 127 126 125 124 123 122 121 120
f1 (ppm)
N
Ph
O
N
Me
3ao
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

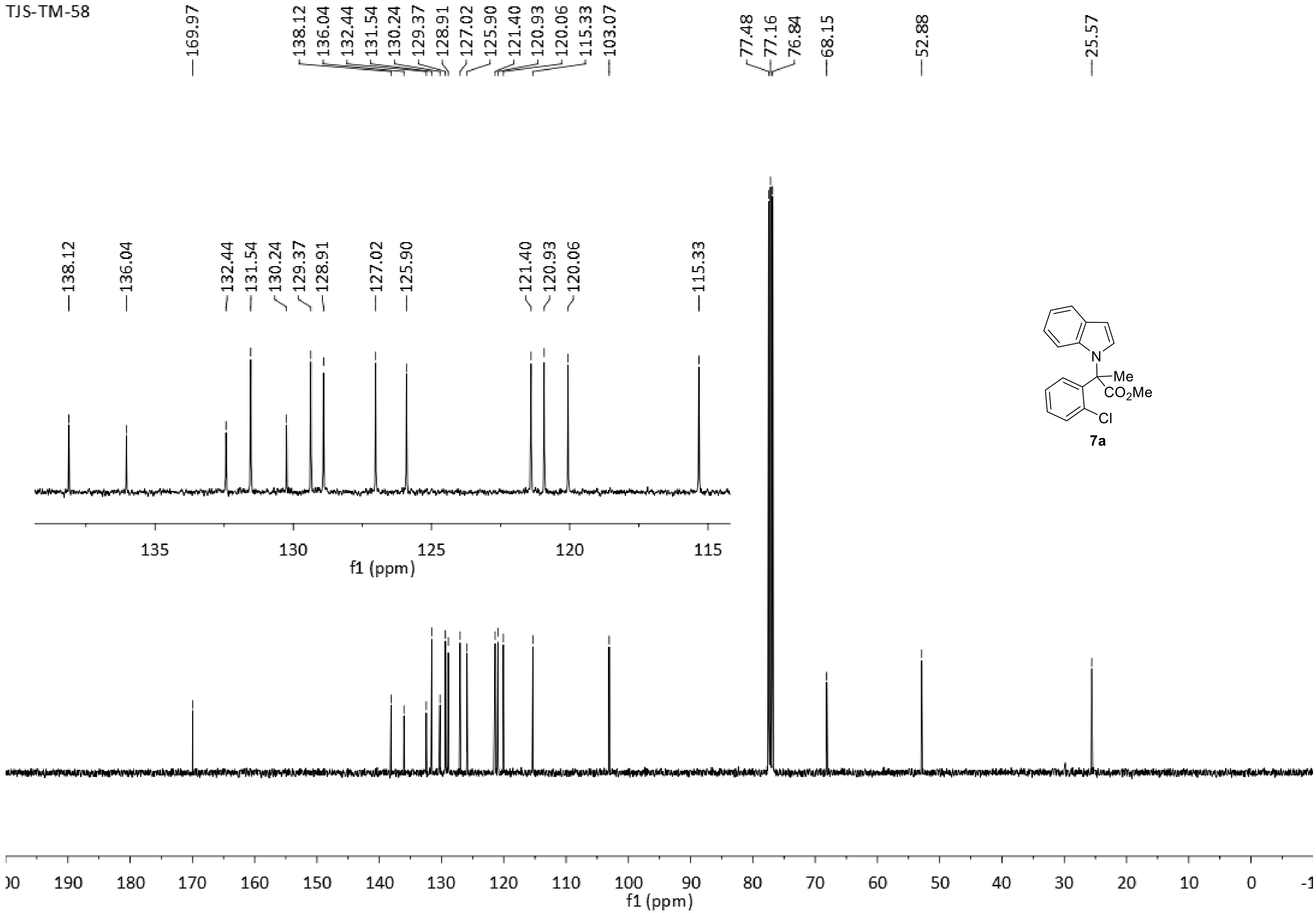

7.660 7.652 7.588 7.569 7.477 7.457 7.438 7.358 7.340 7.260 7.118 7.099 7.081 7.038 7.019 6.999 6.902 6.883 6.864 6.621 6.614 6.360 6.339
3.532 3.491 3.328 3.027 2.985
1.746
0.99 0.97 0.98 0.97 1.02 1.95 0.98 0.95 0.95
1.00 2.94 0.99
2.93
f1 (ppm)
N
Me
O
3ap

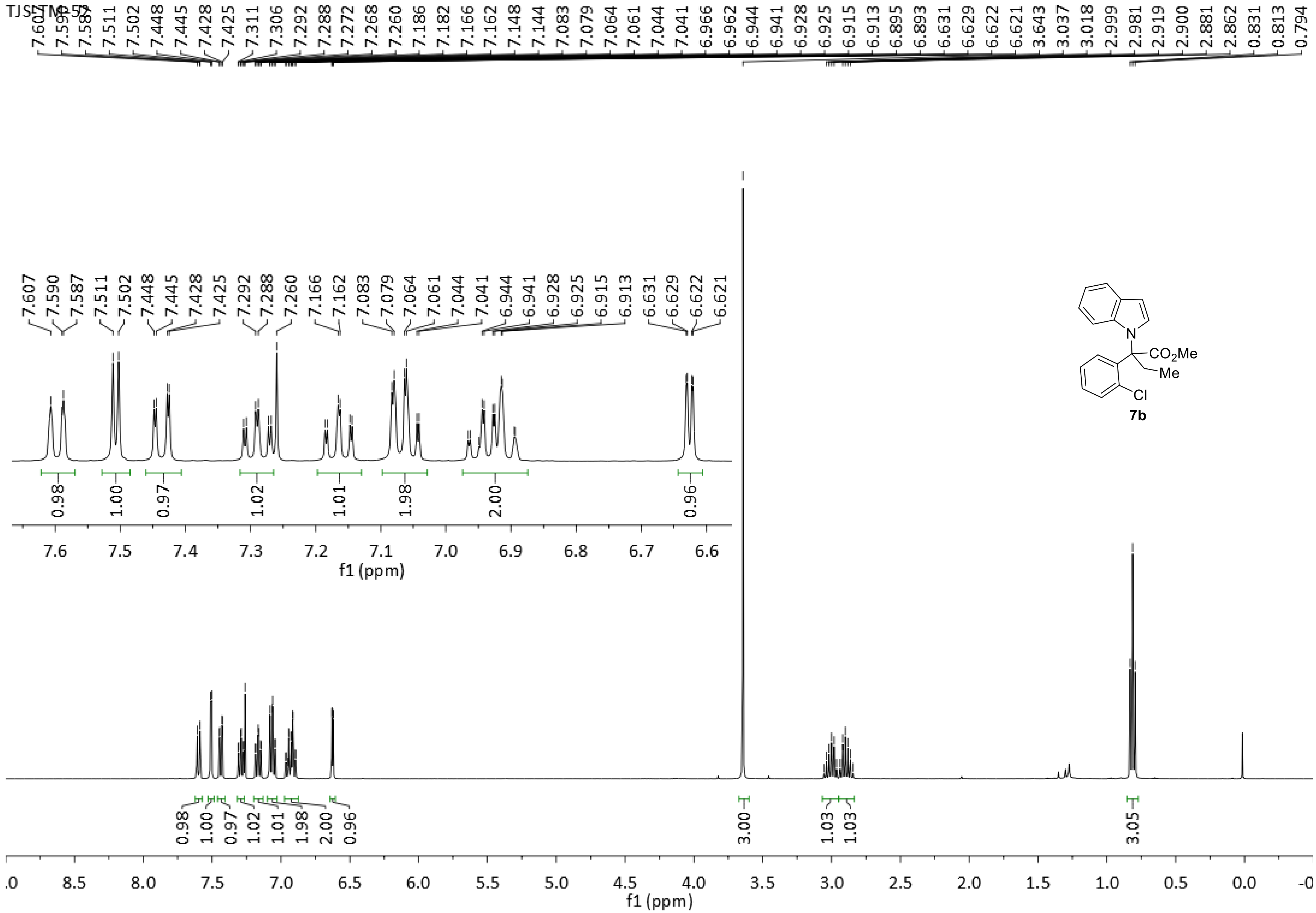
TJS-TJ-149-1

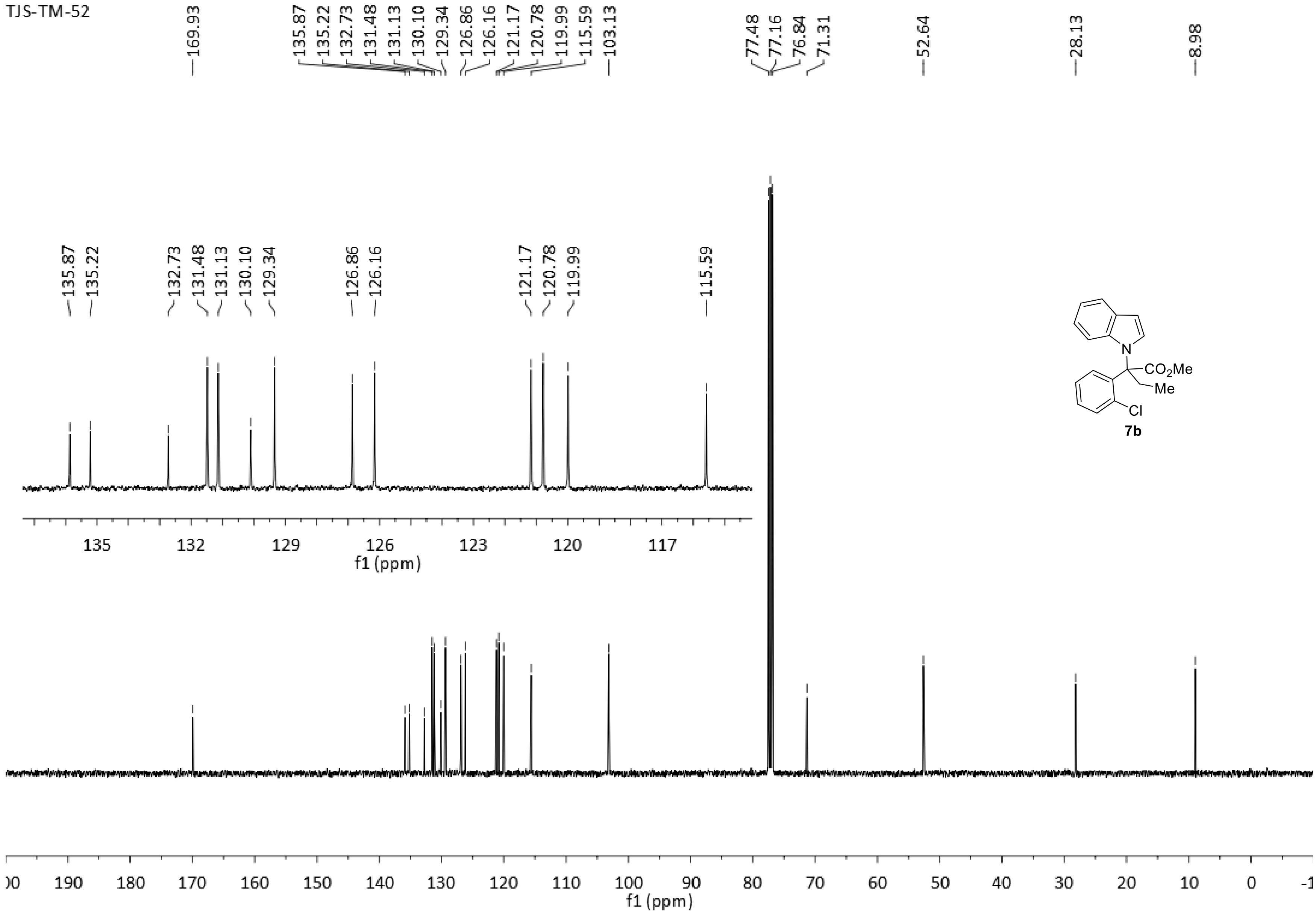


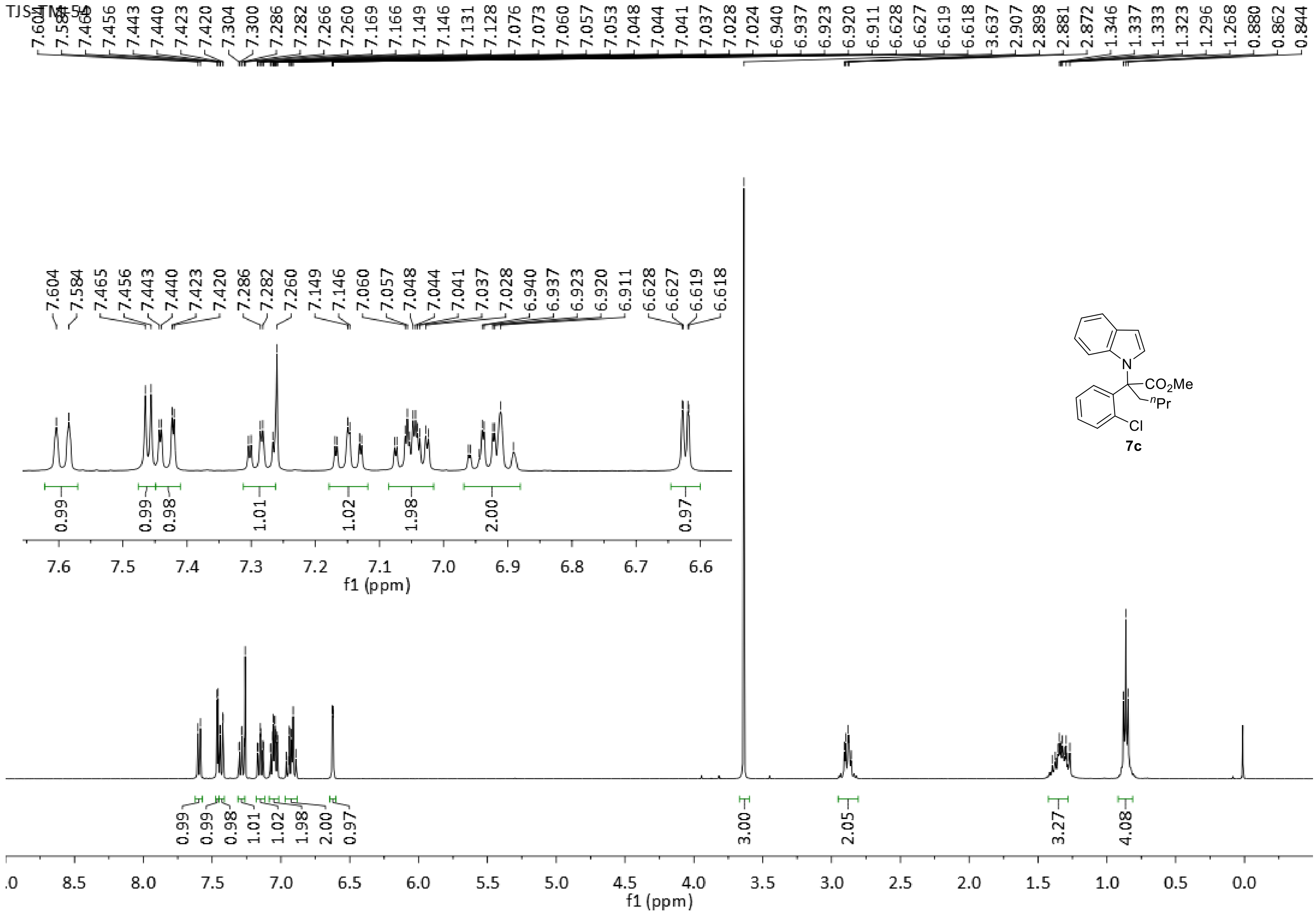
3ap

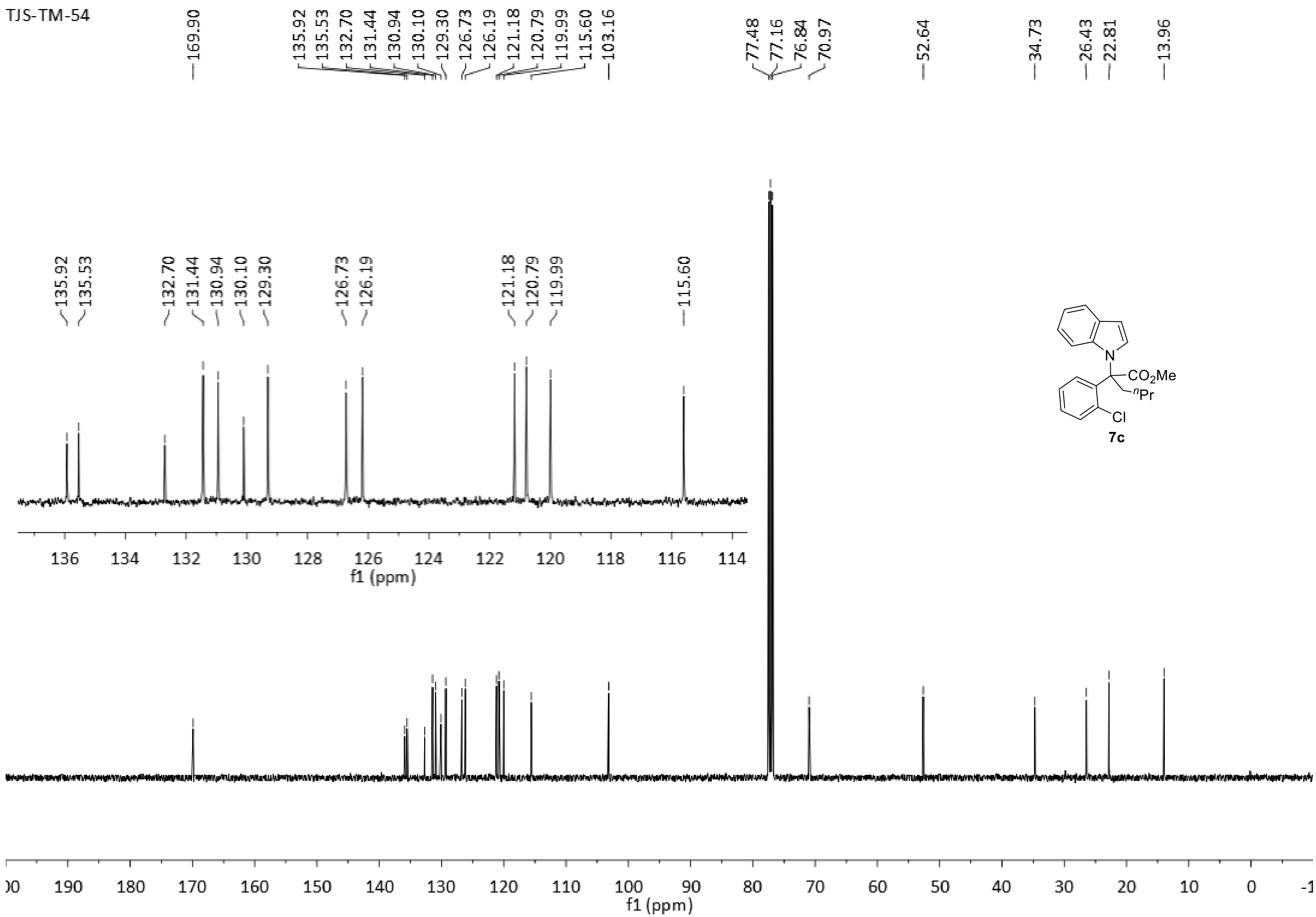

TJS-TM-58
7.636 7.616 7.456 7.448 7.430 7.427 7.269 7.265 7.260 7.138 7.118 7.115 7.102 7.099 7.088 7.085 7.066 7.029 7.004 7.001 6.987 6.983 6.785 6.781 6.765 6.761 6.645 6.643 6.636 6.635 3.707
2.373
7.636 7.616 7.456 7.448 7.430 7.427 7.269 7.265 7.260 7.138 7.118 7.115 7.102 7.099 7.088 7.085 7.066 7.029 7.004 7.001 6.983 6.785 6.781 6.765 6.761 6.645 6.643 6.636 6.635
0.99 1.99 1.27 3.99 0.98 0.96
f1 (ppm)
N
Me
CO_2Me
Cl
7a
0.99 1.99 1.27 3.99 0.98 0.96
2.99
3.00
f1 (ppm)

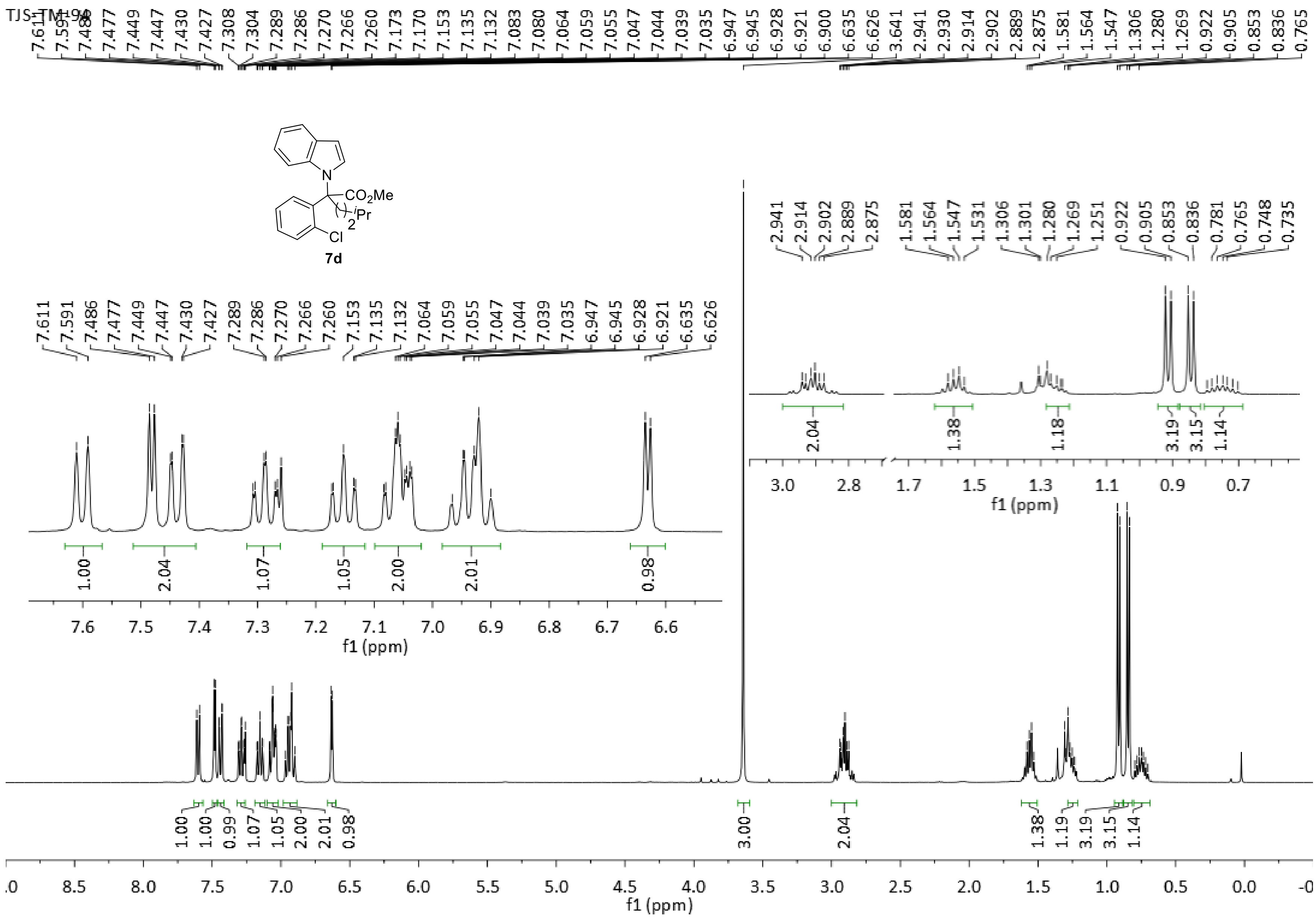

TJS-TM-58
169.97
138.12
136.04
132.44
131.54
130.24
129.37
128.91
127.02
125.90
121.40
120.93
120.06
115.33
103.07
77.48
77.16
76.84
68.15
52.88
25.57
Me
CO2Me
Cl
N
7a
135
130
125
120
115
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

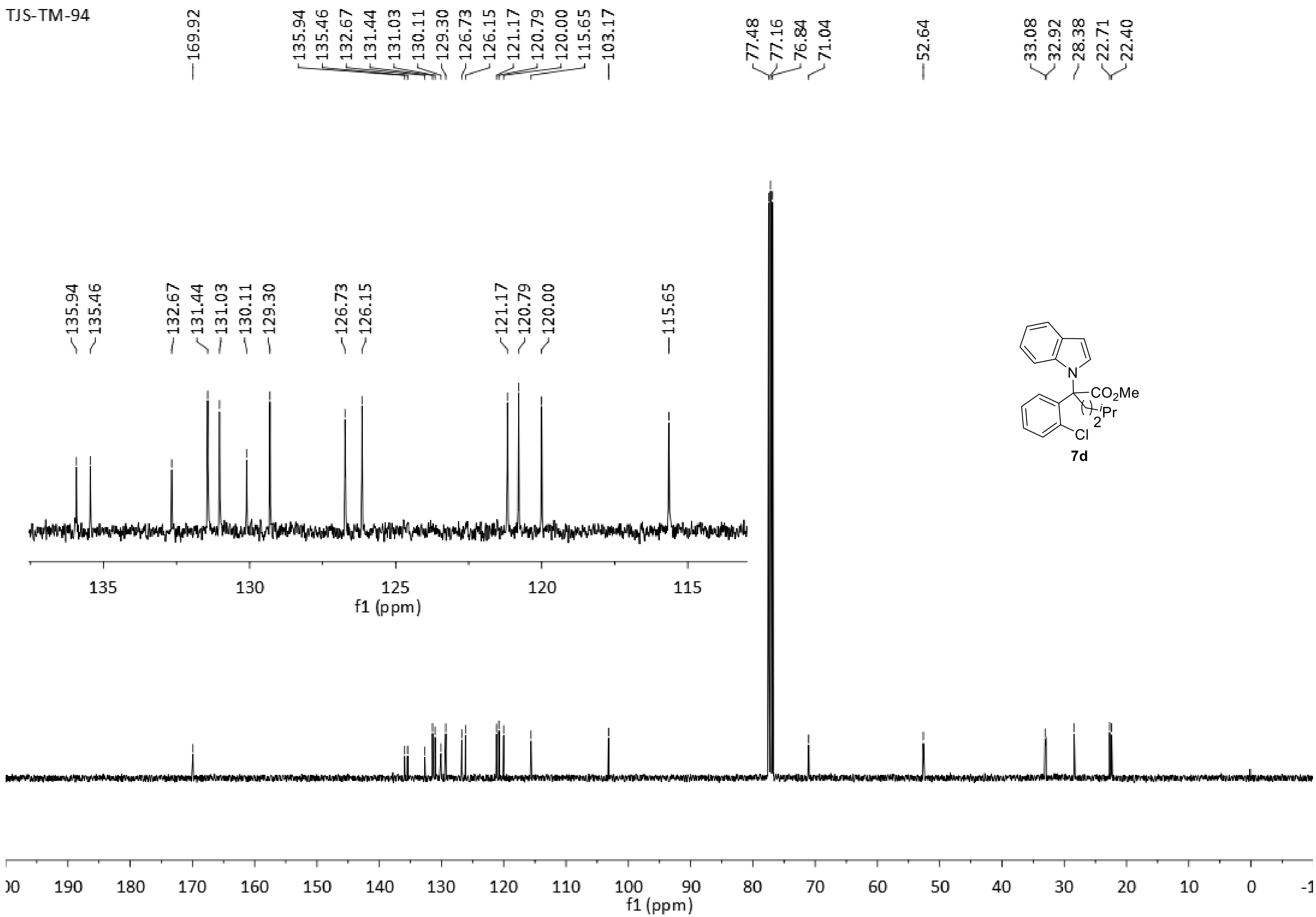

TJS-TM-152
7.607 7.590 7.587 7.511 7.502 7.448 7.445 7.428 7.425 7.311 7.306 7.292 7.288 7.272 7.268 7.260 7.186 7.182 7.166 7.162 7.148 7.144 7.083 7.079 7.064 7.061 7.044 7.041 6.966 6.962 6.944 6.941 6.928 6.925 6.915 6.913 6.895 6.893 6.631 6.629 6.622 6.621 3.643 3.037 3.018 2.999 2.981 2.919 2.900 2.881 2.862 0.831 0.813 0.794
0.98 1.00 0.97 1.02 1.01 1.98 2.00 0.96
f1 (ppm)
0.98 1.00 0.97 1.02 1.01 1.98 2.00 0.96 3.00 1.03 1.03 3.05
f1 (ppm)
N
CO2Me
Me
Cl
7b

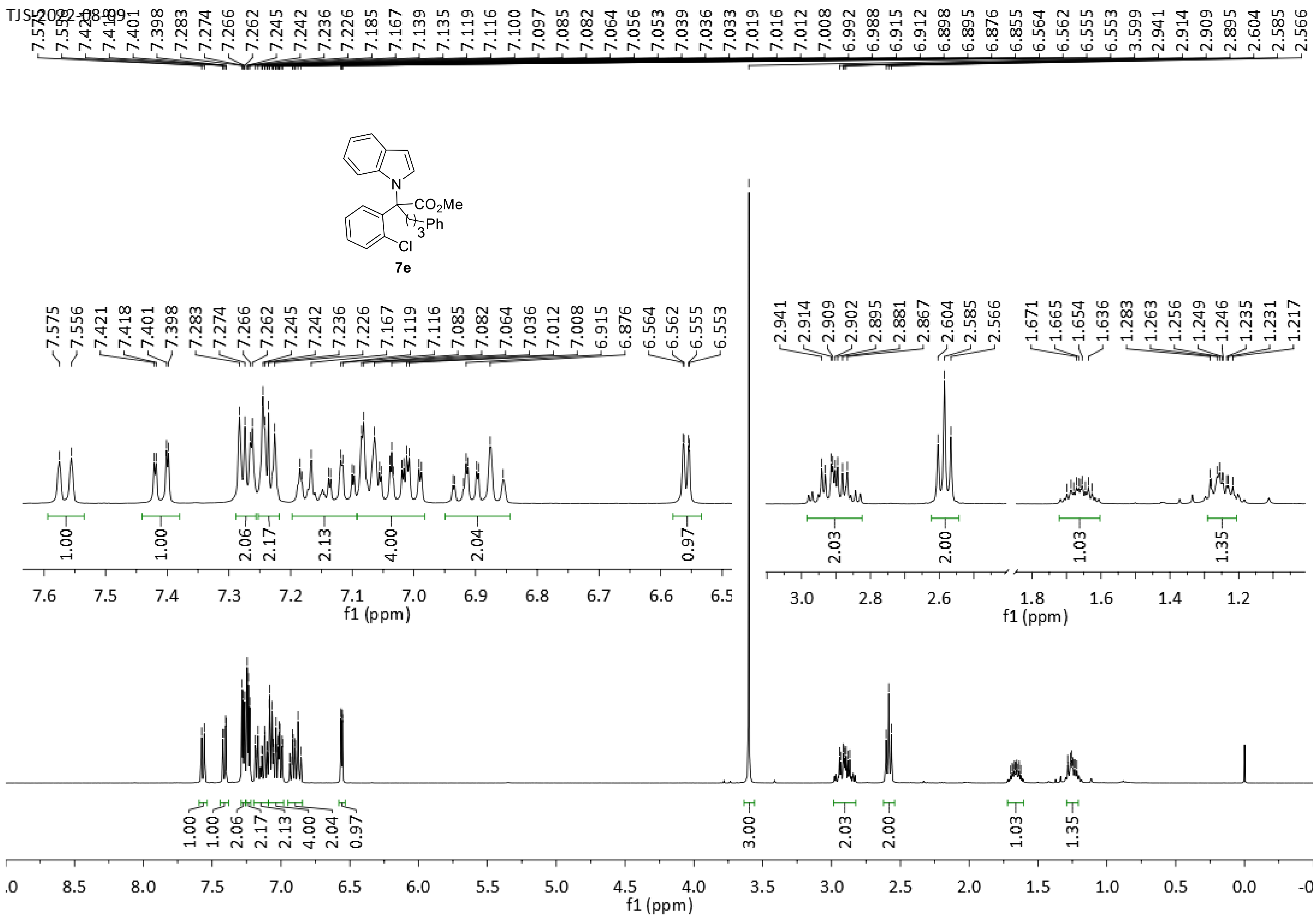

TJS-TM-52
169.93
135.87
135.22
132.73
131.48
131.13
130.10
129.34
126.86
126.16
121.17
120.78
119.99
115.59
103.13
77.48
77.16
76.84
71.31
52.64
28.13
8.98
135 132 129 126 123 120 117
f1 (ppm)
N
CO_2Me
Me
Cl
7b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

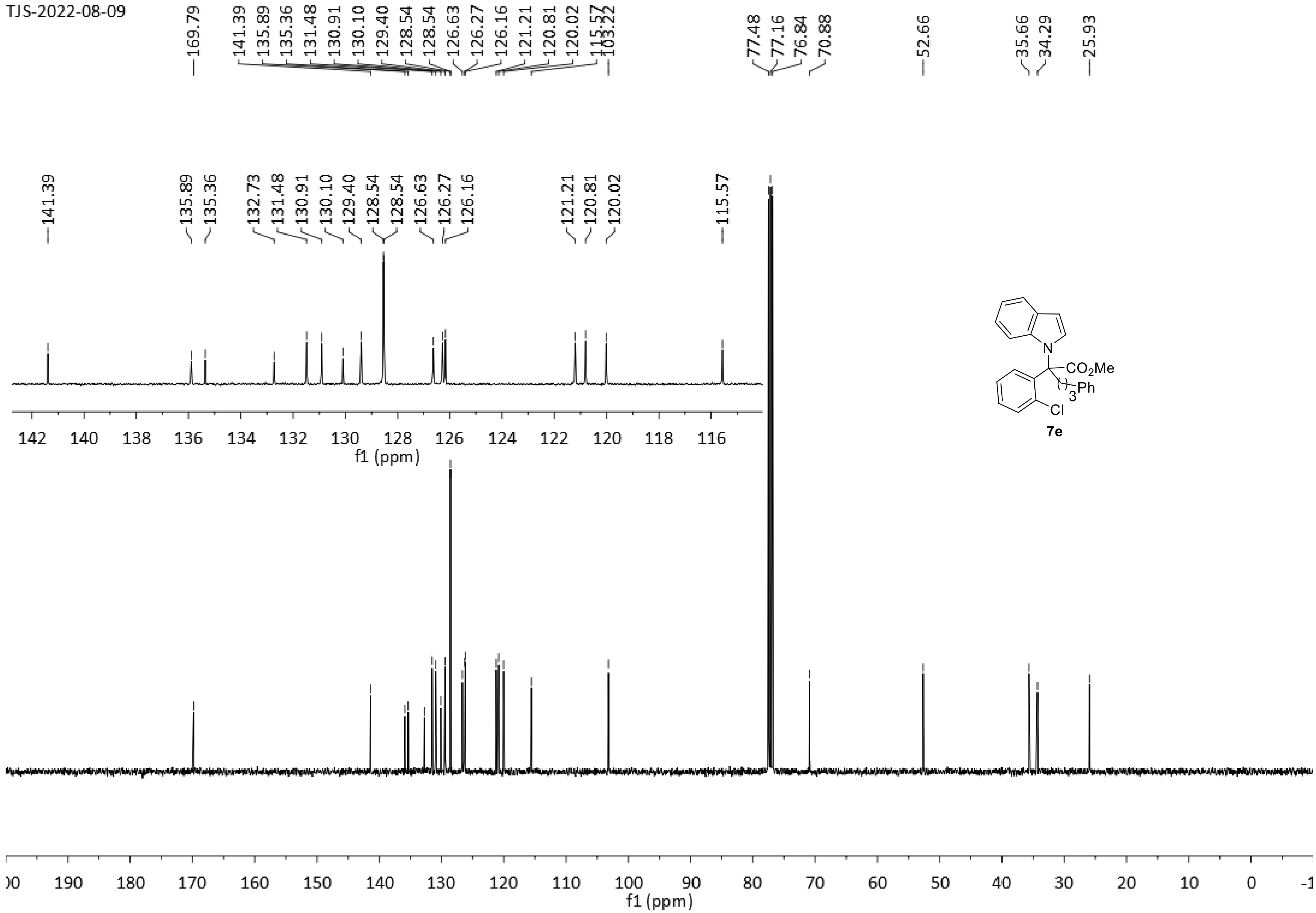

TJS-TM-54
7.604
7.584
7.465
7.456
7.443
7.440
7.423
7.420
7.304
7.300
7.286
7.282
7.266
7.260
7.169
7.166
7.149
7.146
7.131
7.128
7.076
7.073
7.060
7.057
7.053
7.048
7.044
7.041
7.037
7.028
7.024
6.940
6.937
6.923
6.920
6.911
6.628
6.627
6.619
6.618
3.637
2.907
2.898
2.881
2.872
1.346
1.337
1.333
1.323
1.296
1.268
0.880
0.862
0.844
0.99
0.99
0.98
1.01
1.02
1.98
2.00
0.97
f1 (ppm)
N
CO_2Me
^{n}Pr
Cl
7c
3.00
2.05
3.27
4.08
f1 (ppm)


TJS-TM-54
169.90
135.92
135.53
132.70
131.44
130.94
130.10
129.30
126.73
126.19
121.18
120.79
119.99
115.60
103.16
77.48
77.16
76.84
70.97
52.64
34.73
26.43
22.81
13.96
136 134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
N
CO2Me
nPr
Cl
7c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

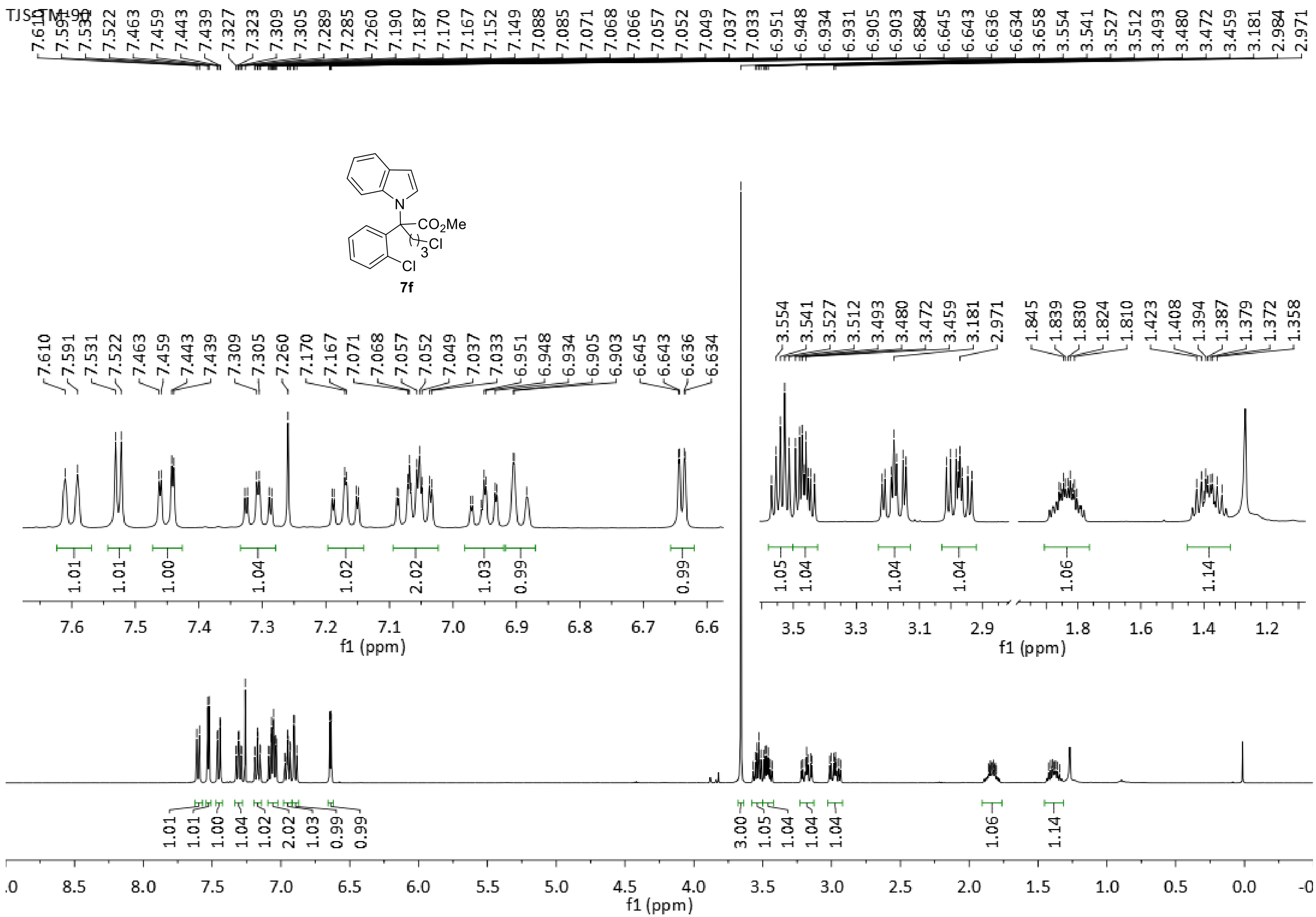

TJS-TM-94
CO2Me
N
iPr
2
Cl
7d
f1 (ppm)

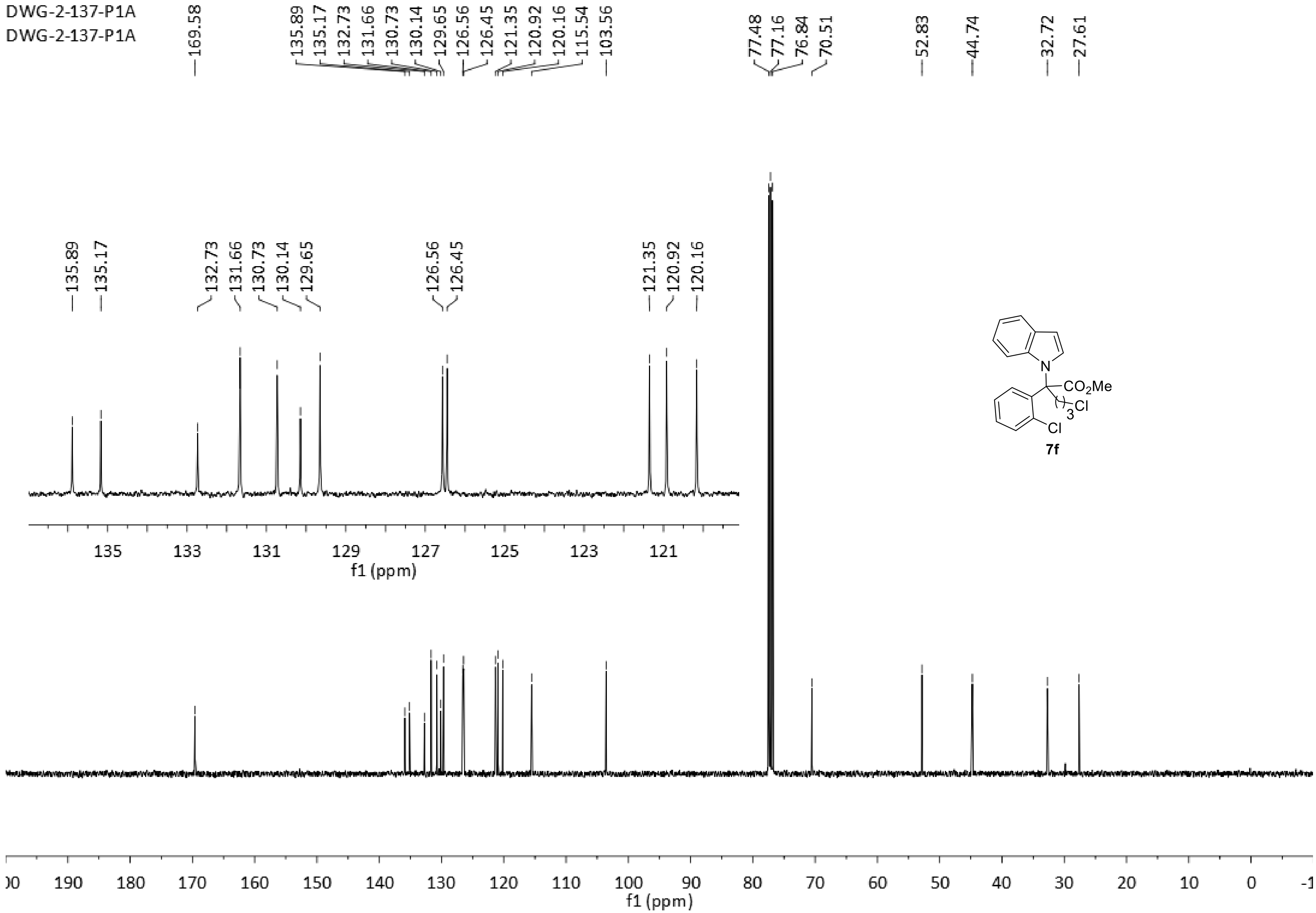

TJS-TM-94
169.92
135.94
135.46
132.67
131.44
131.03
130.11
129.30
126.73
126.15
121.17
120.79
120.00
115.65
103.17
77.48
77.16
76.84
71.04
52.64
33.08
32.92
28.38
22.71
22.40
f1 (ppm)
N
CO2Me
iPr
2
Cl
7d


TJS-2022-08-09
N
CO2Me
Ph
3
Cl
7e
1.00
1.00
2.06
2.17
2.13
4.00
2.04
0.97
3.00
2.03
2.00
1.03
1.35
f1 (ppm)

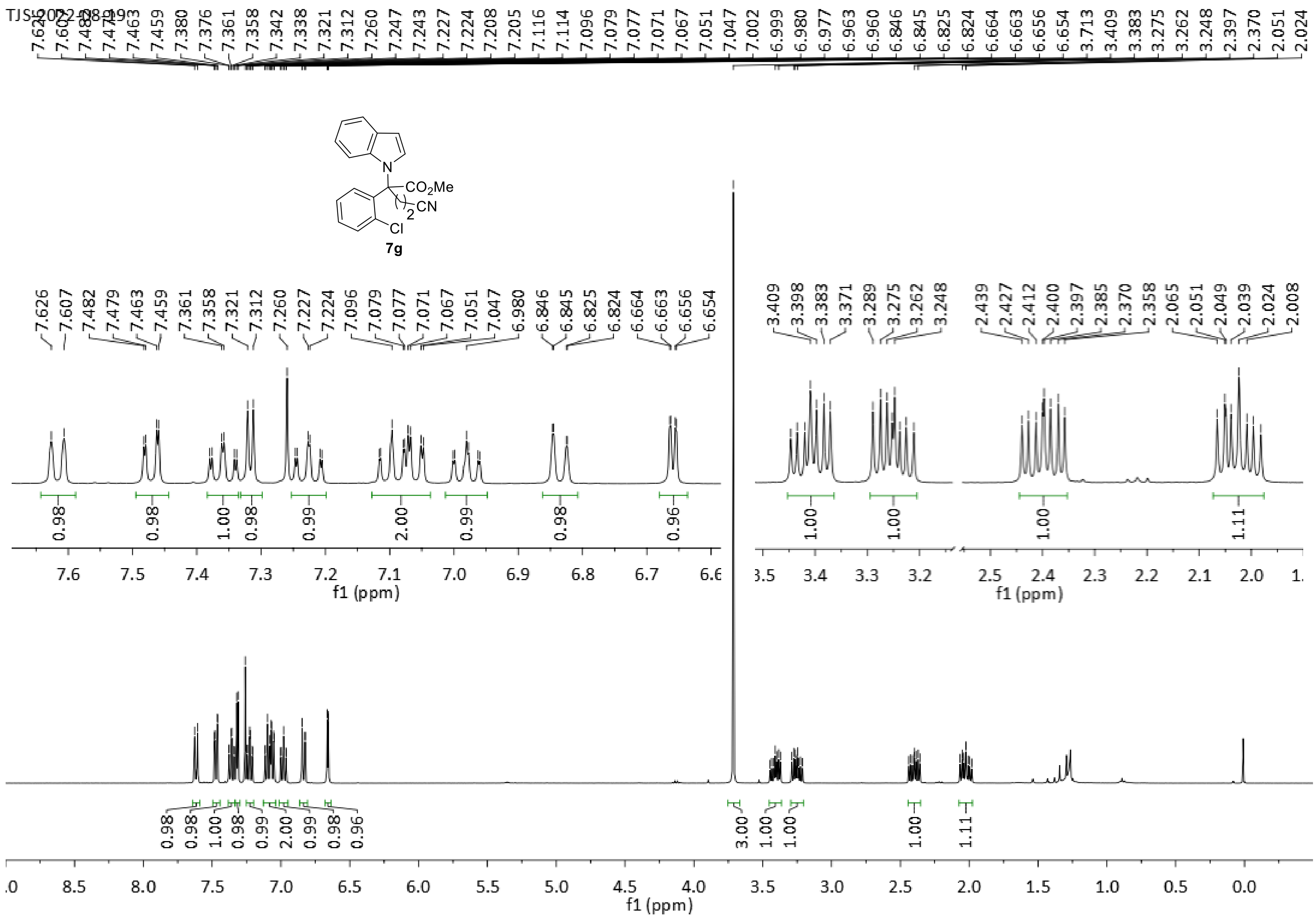

TJS-2022-08-09
169.79
141.39
135.89
135.36
131.48
130.91
130.10
129.40
128.54
128.54
126.63
126.27
126.16
121.21
120.81
120.02
115.57
103.22
77.48
77.16
76.84
70.88
52.66
35.66
34.29
25.93
141.39
135.89
135.36
132.73
131.48
130.91
130.10
129.40
128.54
128.54
126.63
126.27
126.16
121.21
120.81
120.02
115.57
142 140 138 136 134 132 130 128 126 124 122 120 118 116
f1 (ppm)
N
CO_2Me
$)_3Ph$
Cl
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

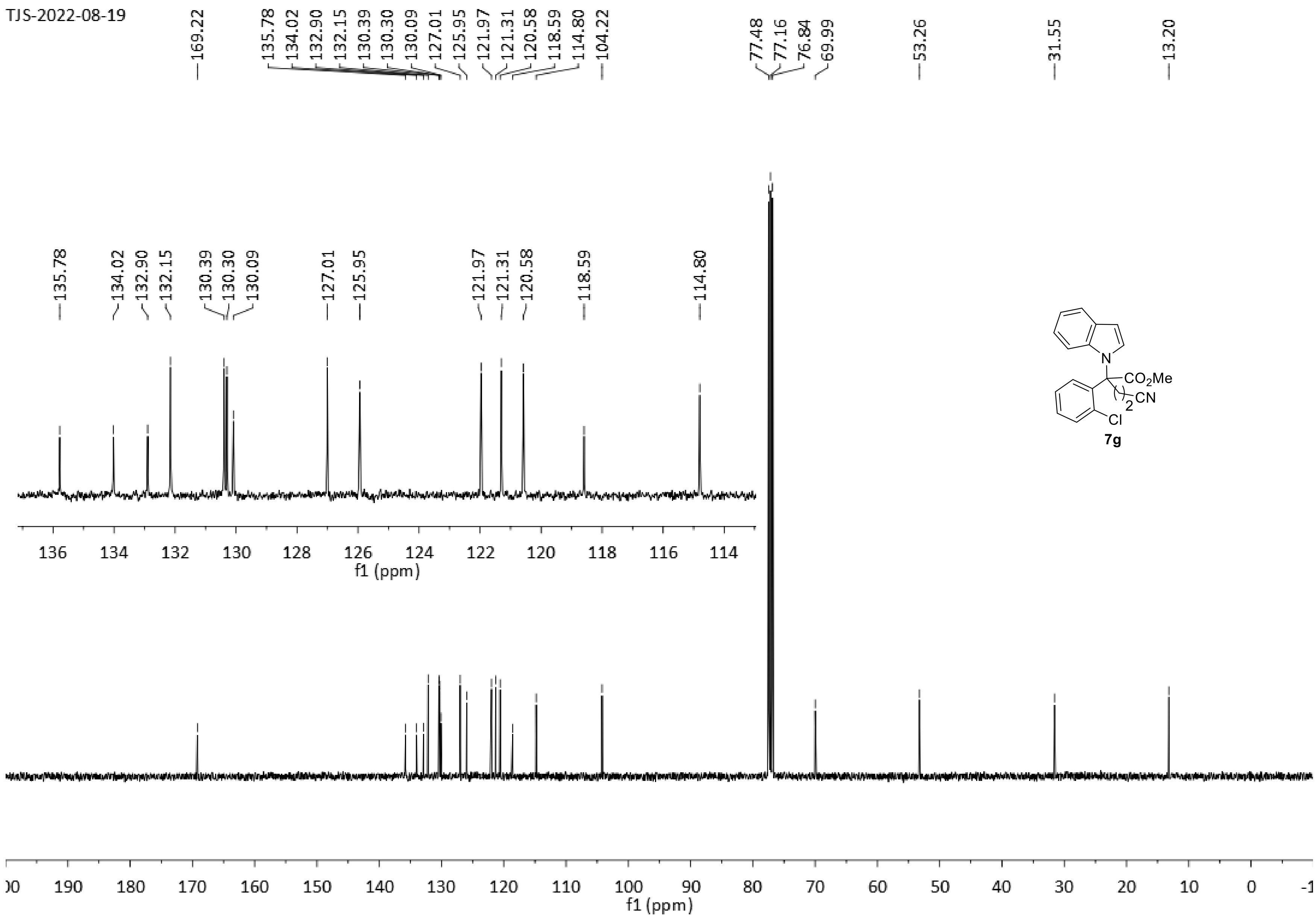
7e

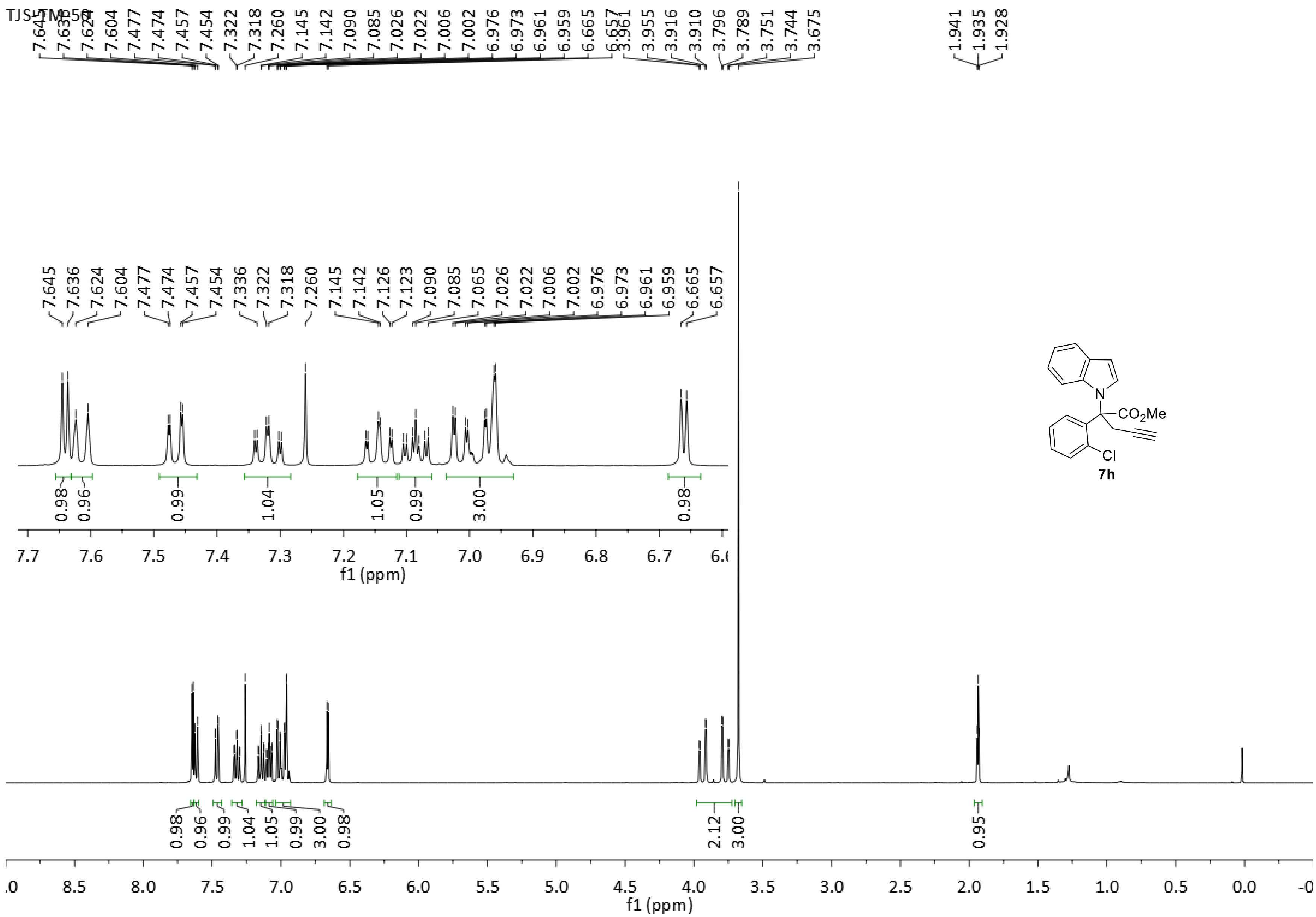

TJS-TM-90
CO2Me
Cl
3
Cl
N
7f
f1 (ppm)
f1 (ppm)
f1 (ppm)

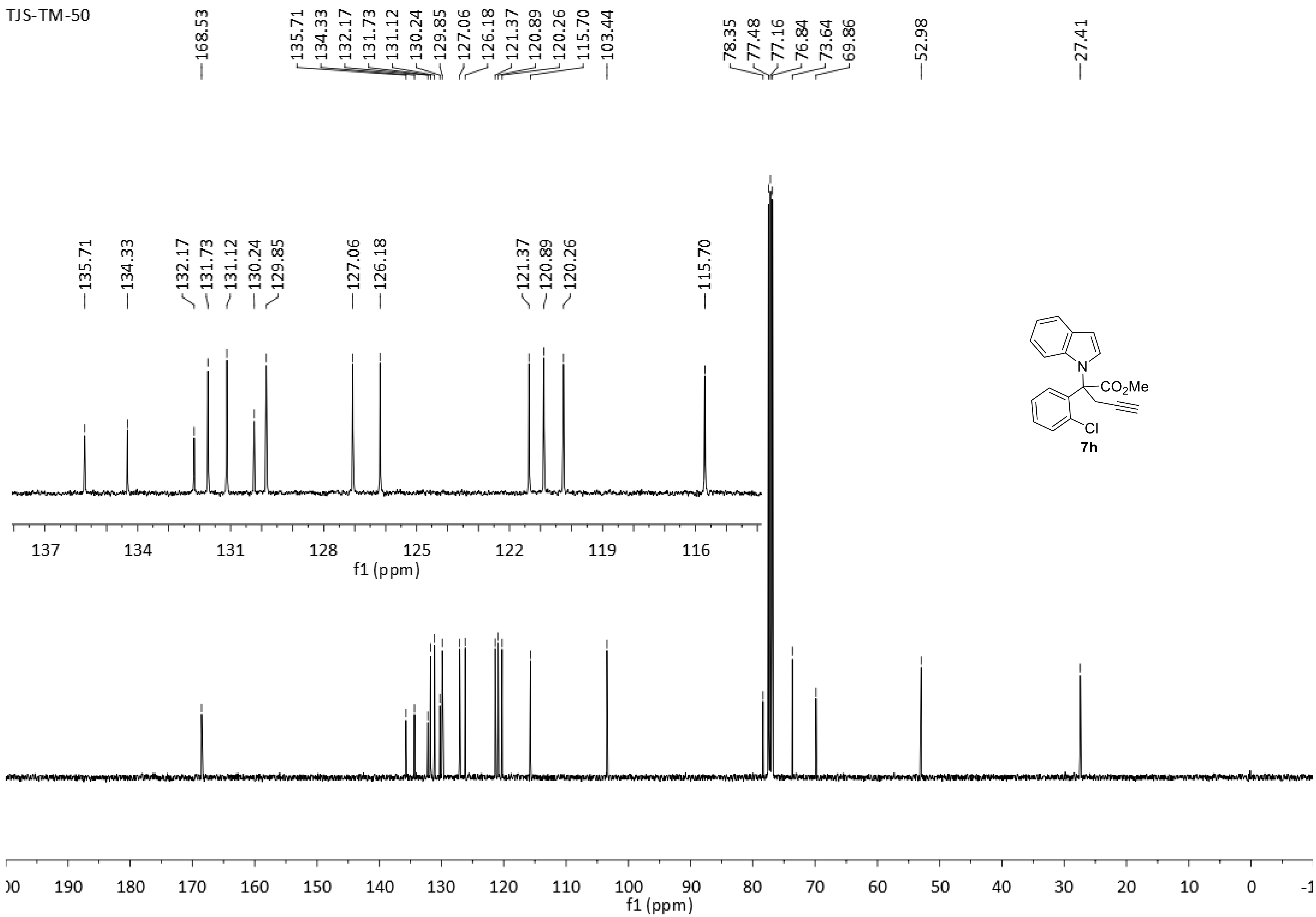


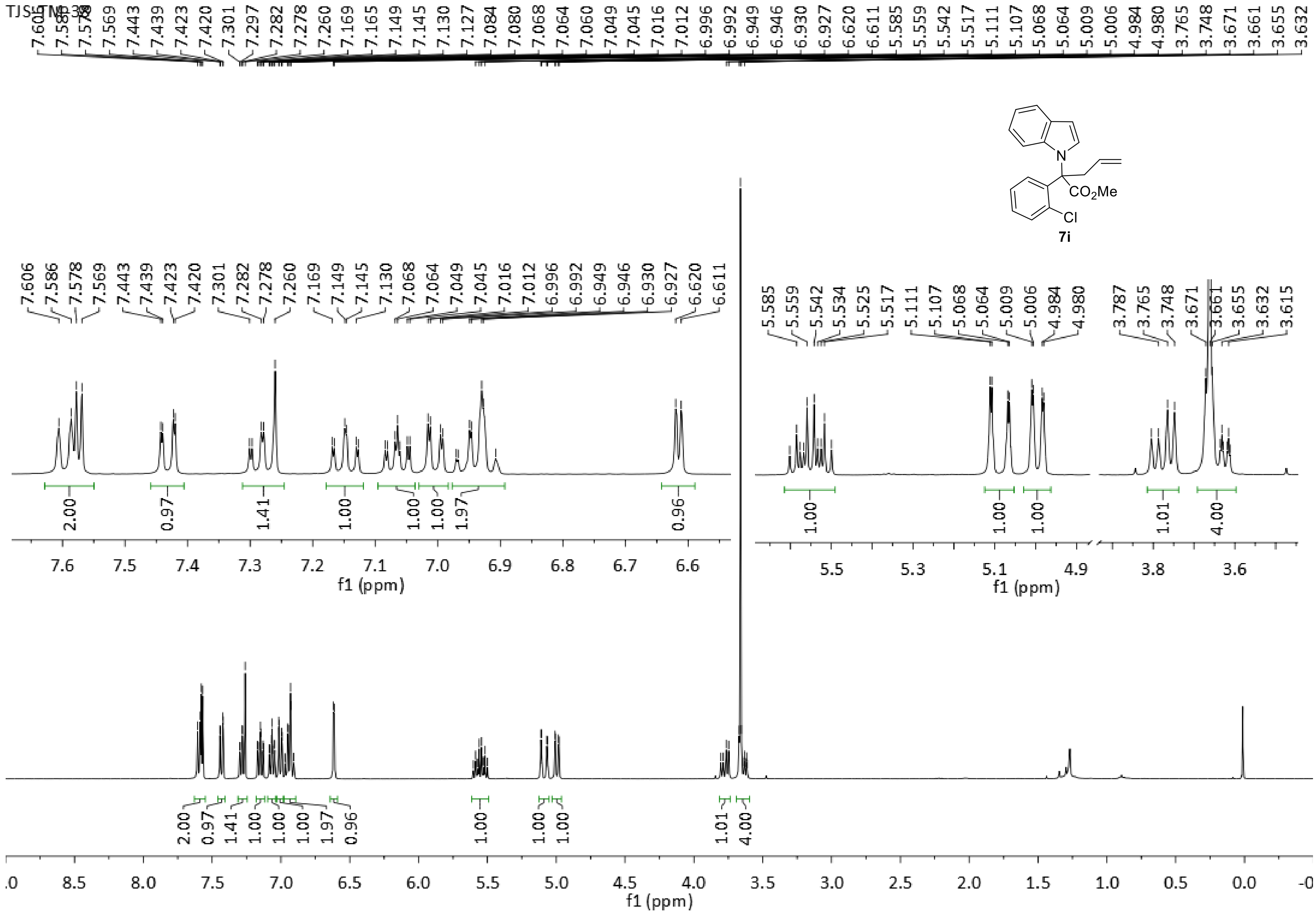
DWG-2-137-P1A
DWG-2-137-P1A
169.58
135.89
135.17
132.73
131.66
130.73
130.14
129.65
126.56
126.45
121.35
120.92
120.16
115.54
103.56
77.48
77.16
76.84
70.51
52.83
44.74
32.72
27.61
N
CO2Me
Cl
3
Cl
7f
135
133
131
129
127
125
123
121
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


TJS-2022-08-19
N
CO2Me
CN
Cl
7g
f1 (ppm)

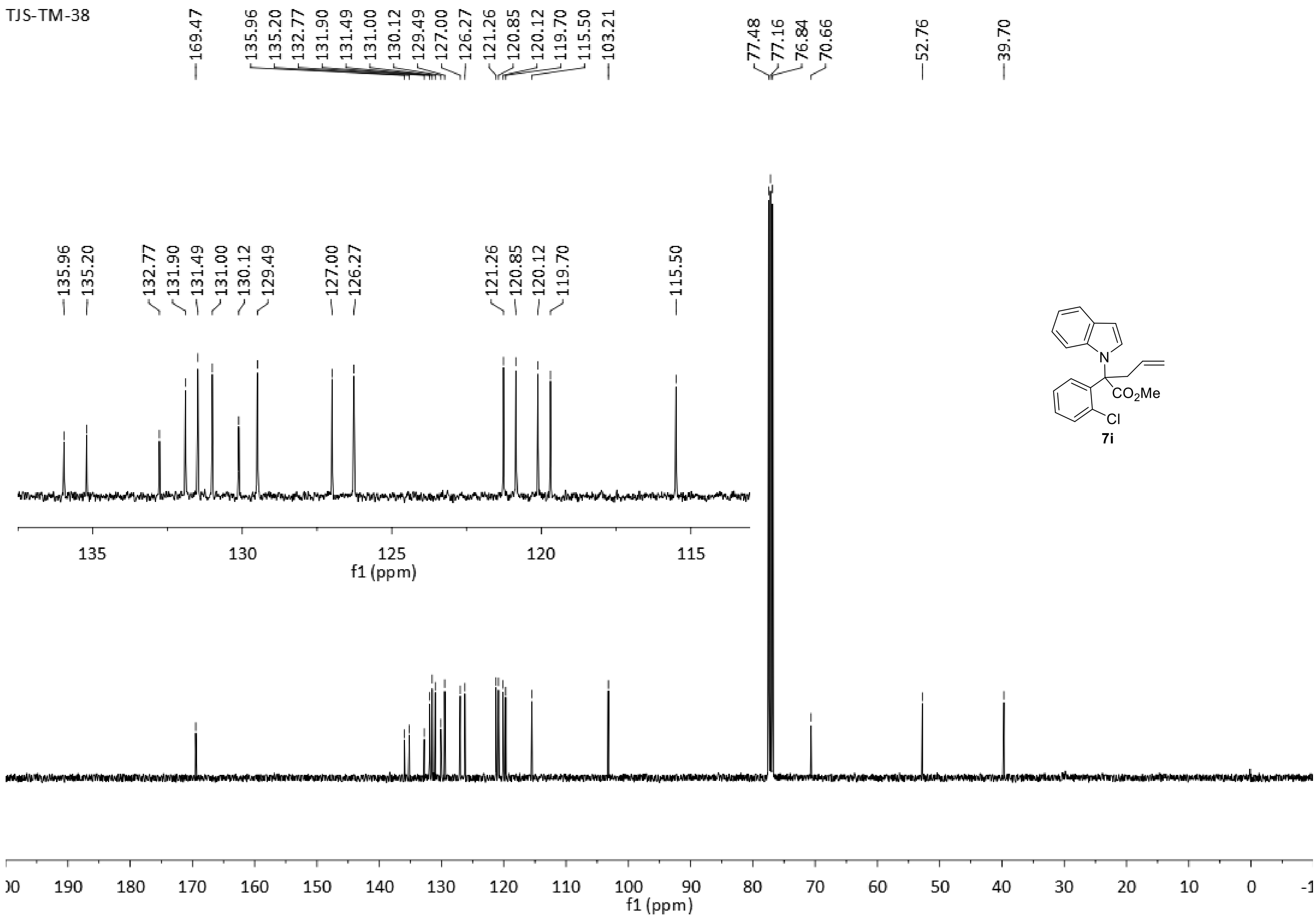

TJS-2022-08-19
169.22
135.78
134.02
132.90
132.15
130.39
130.30
130.09
127.01
125.95
121.97
121.31
120.58
118.59
114.80
104.22
77.48
77.16
76.84
69.99
53.26
31.55
13.20
f1 (ppm)
N
CO2Me
CN
2
Cl
7g

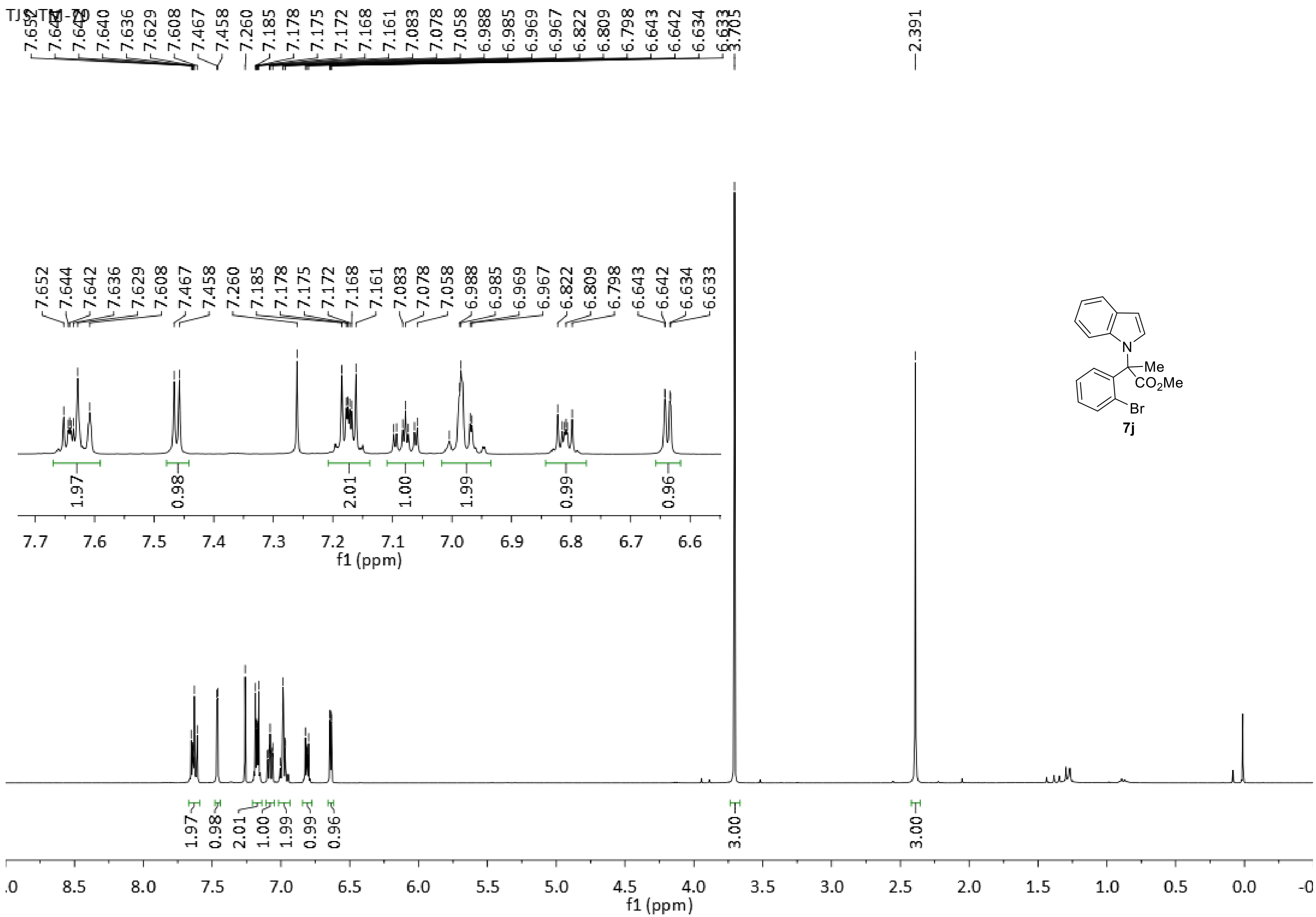

TJS-TM-250
N
CO2Me
Cl
7h
f1 (ppm)
0.98 0.96 0.99 1.04 1.05 0.99 3.00 0.98
2.12 3.00
0.95


TJS-TM-50
168.53
135.71
134.33
132.17
131.73
131.12
130.24
129.85
127.06
126.18
121.37
120.89
120.26
115.70
103.44
78.35
77.48
77.16
76.84
73.64
69.86
52.98
27.41
f1 (ppm)
N
CO_2Me
Cl
7h

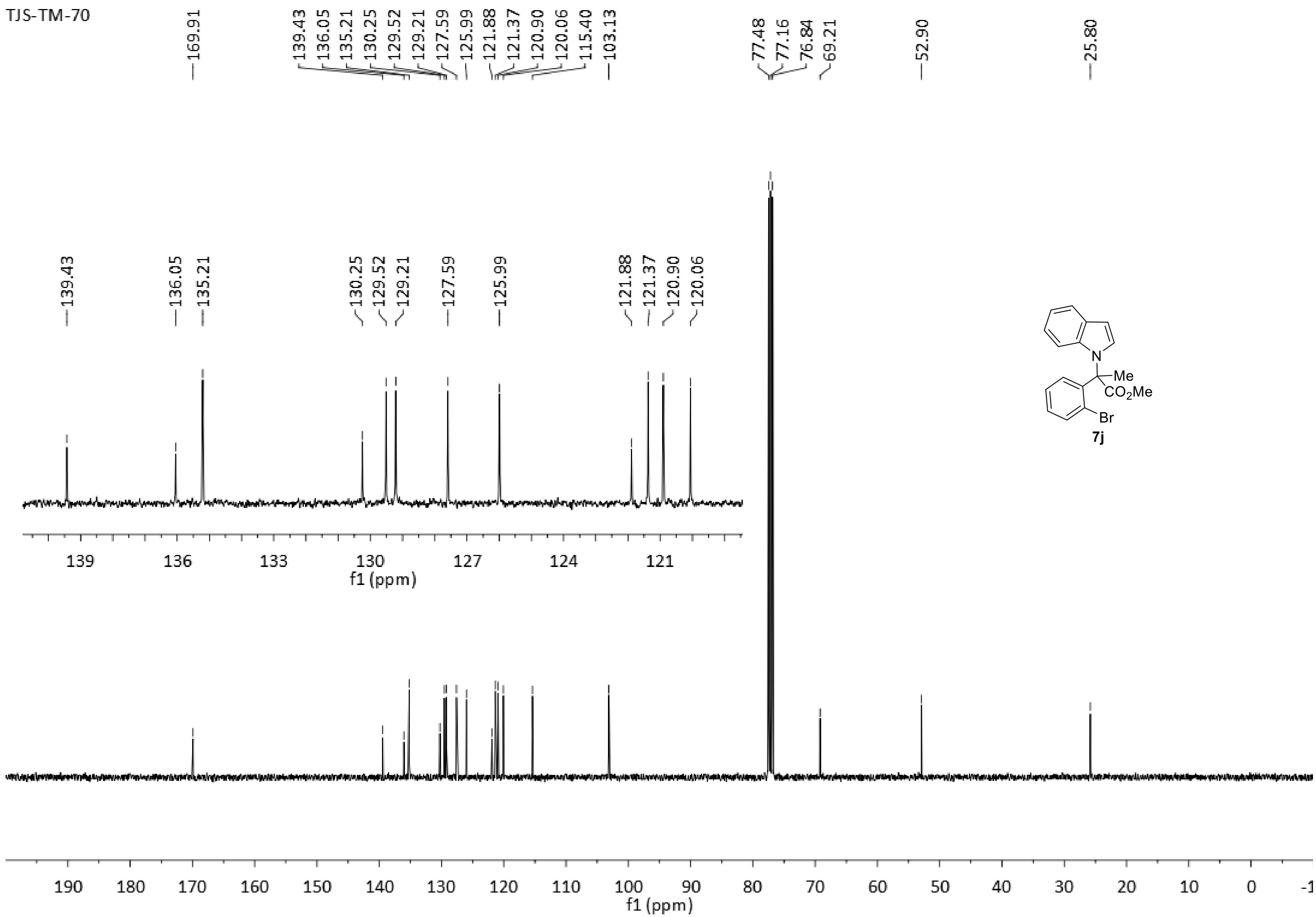


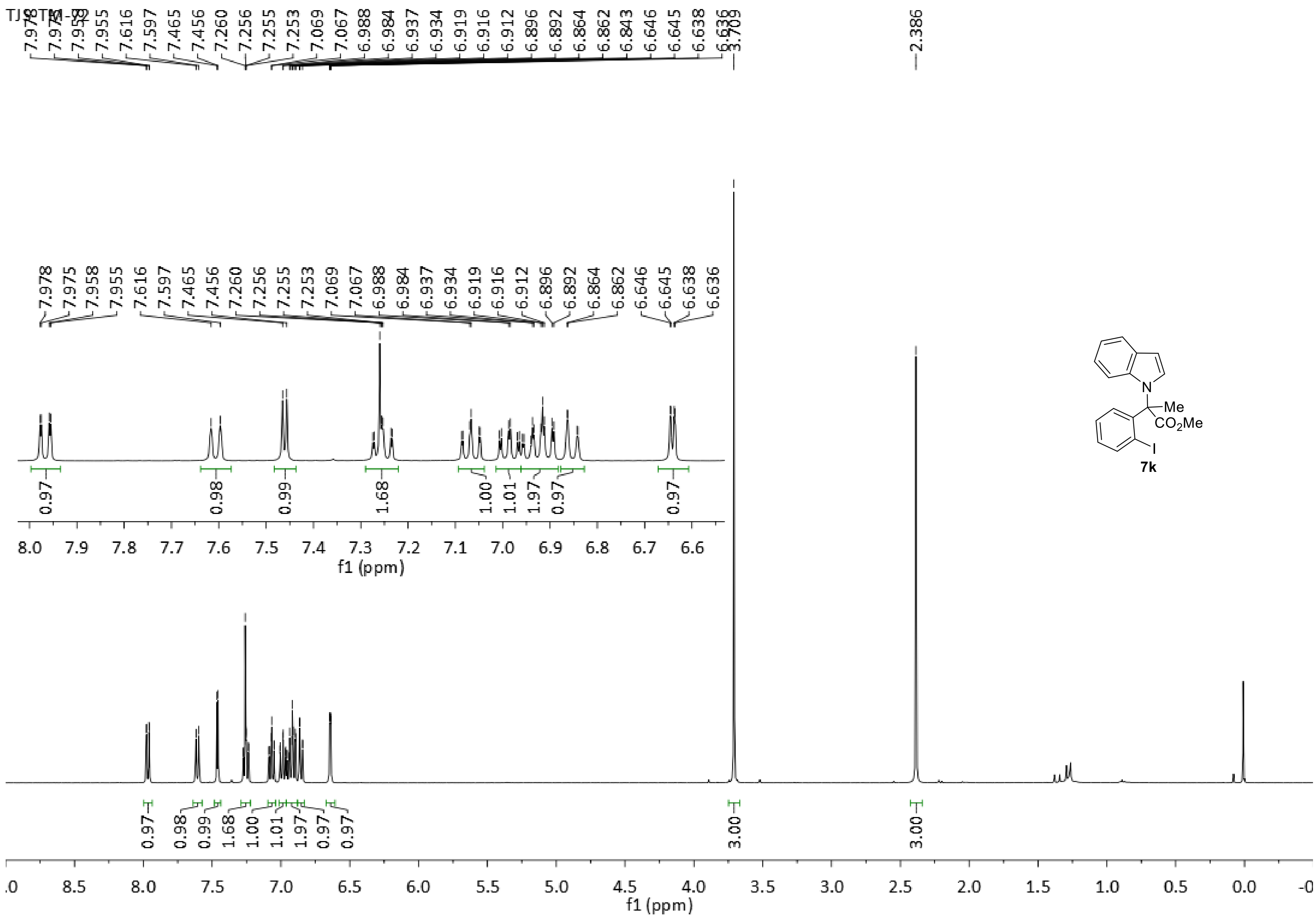
N
CO2Me
Cl
7i
f1 (ppm)


TJS-TM-38
169.47
135.96
135.20
132.77
131.90
131.49
131.00
130.12
129.49
127.00
126.27
121.26
120.85
120.12
119.70
115.50
103.21
77.48
77.16
76.84
70.66
52.76
39.70
N
CO2Me
Cl
7i
f1 (ppm)

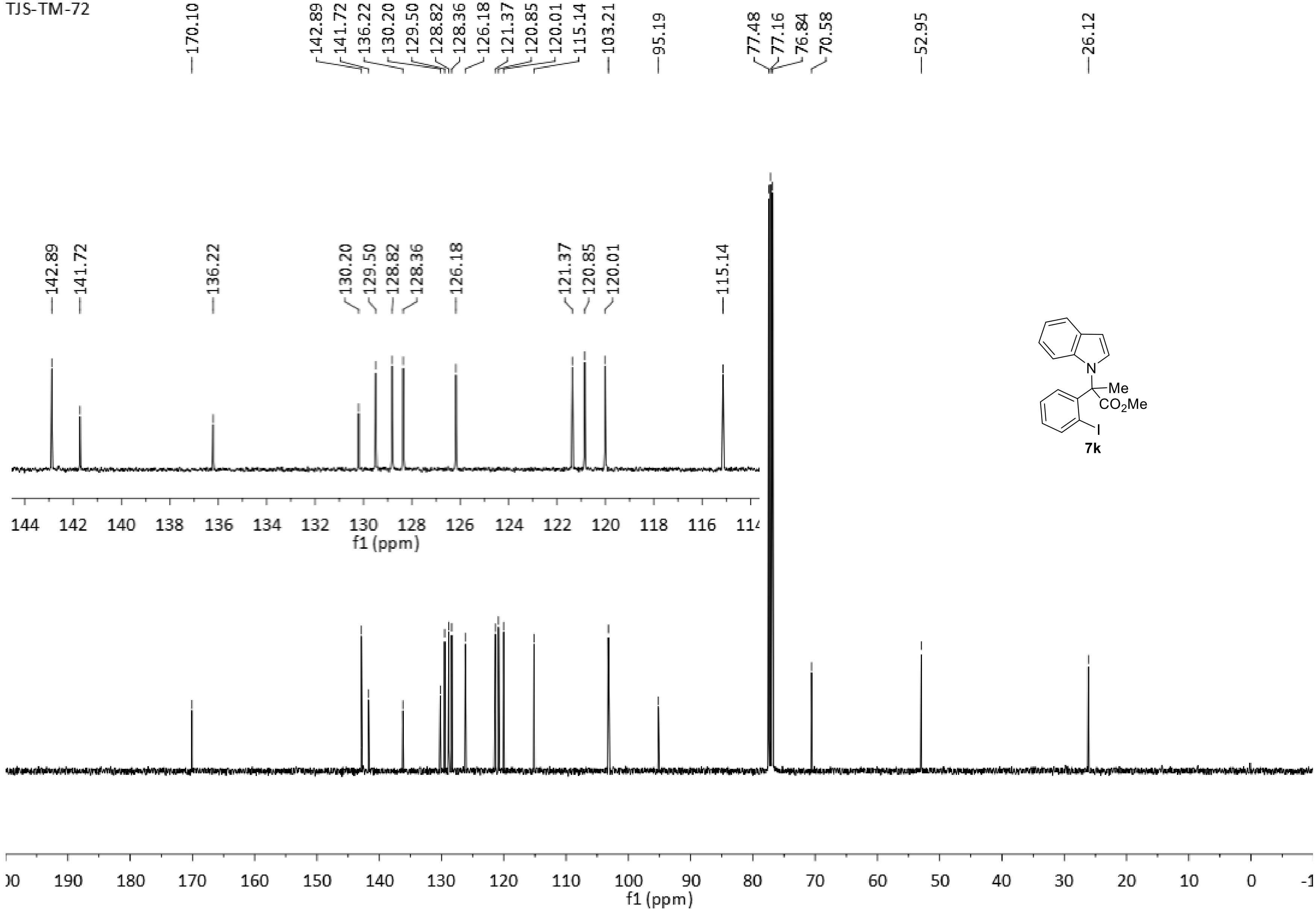


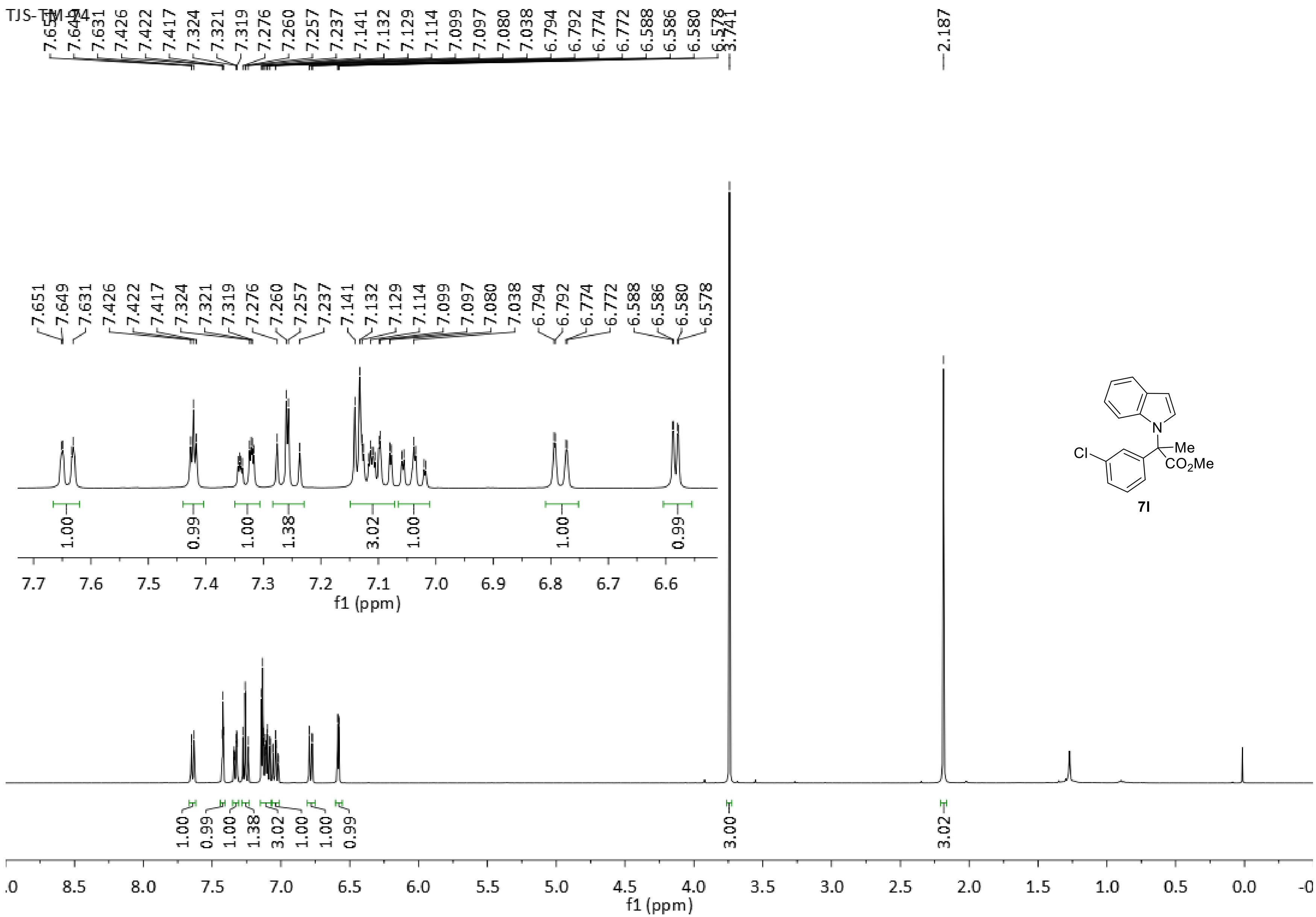
7.652
7.644
7.642
7.636
7.629
7.608
7.467
7.458
7.260
7.185
7.178
7.175
7.172
7.168
7.161
7.083
7.078
7.058
6.988
6.985
6.969
6.967
6.822
6.809
6.798
6.643
6.642
6.634
6.633
3.705
2.391
1.97
0.98
2.01
1.00
1.99
0.99
0.96
3.00
3.00
f1 (ppm)
N
Me
CO_2Me
Br
7j

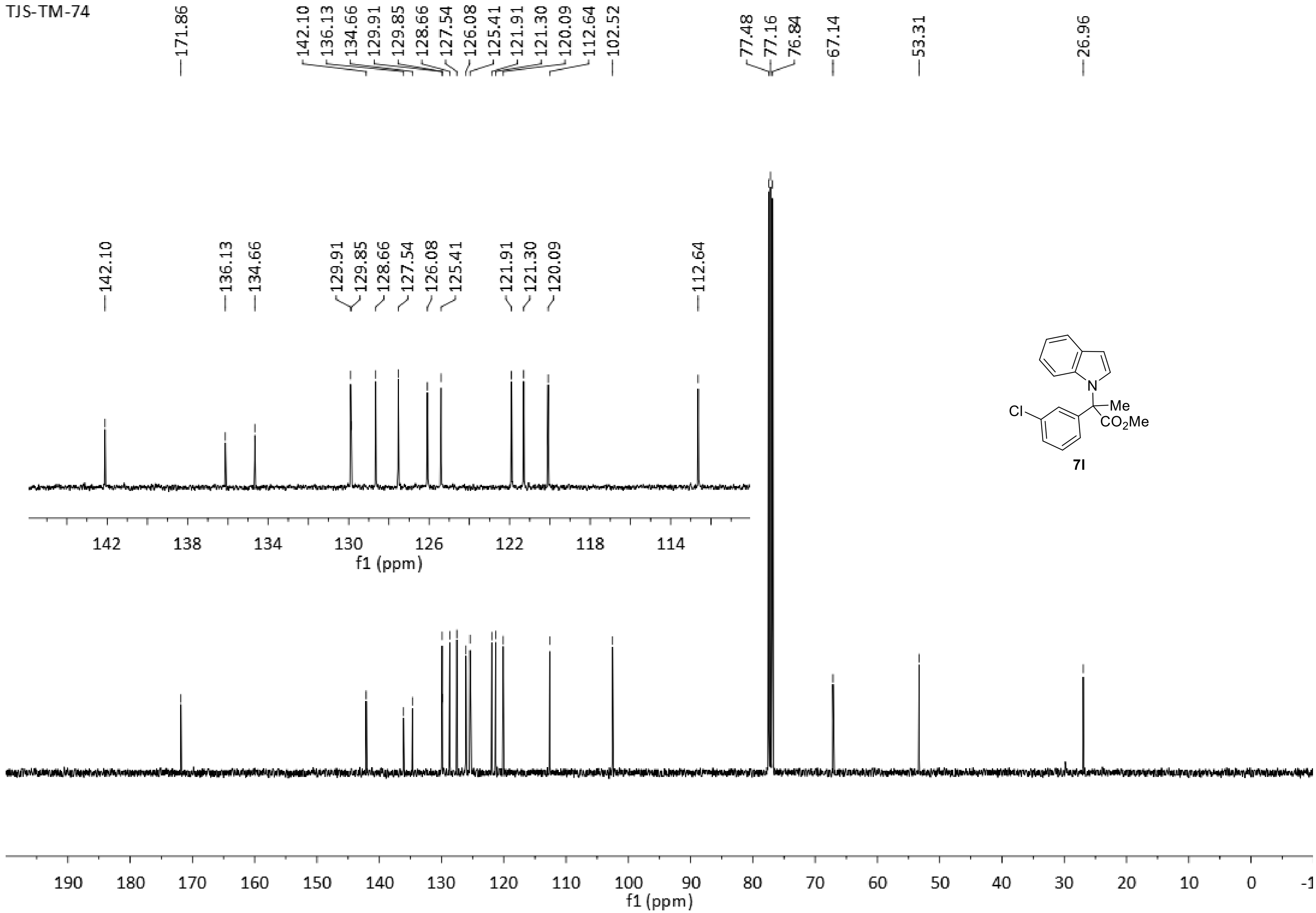

TJS-TM-70
169.91
139.43
136.05
135.21
130.25
129.52
129.21
127.59
125.99
121.88
121.37
120.90
120.06
115.40
103.13
77.48
77.16
76.84
69.21
52.90
25.80
139 136 133 130 127 124 121
f1 (ppm)
Me
CO2Me
N
Br
7j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


7.978
7.975
7.958
7.955
7.616
7.597
7.465
7.456
7.260
7.256
7.255
7.253
7.069
7.067
6.988
6.984
6.937
6.934
6.919
6.916
6.912
6.896
6.892
6.864
6.862
6.843
6.646
6.645
6.638
6.636
3.709
2.386
0.97
0.98
0.99
1.68
1.00
1.01
1.97
0.97
0.97
3.00
3.00
f1 (ppm)
N
Me
CO2Me
I
7k

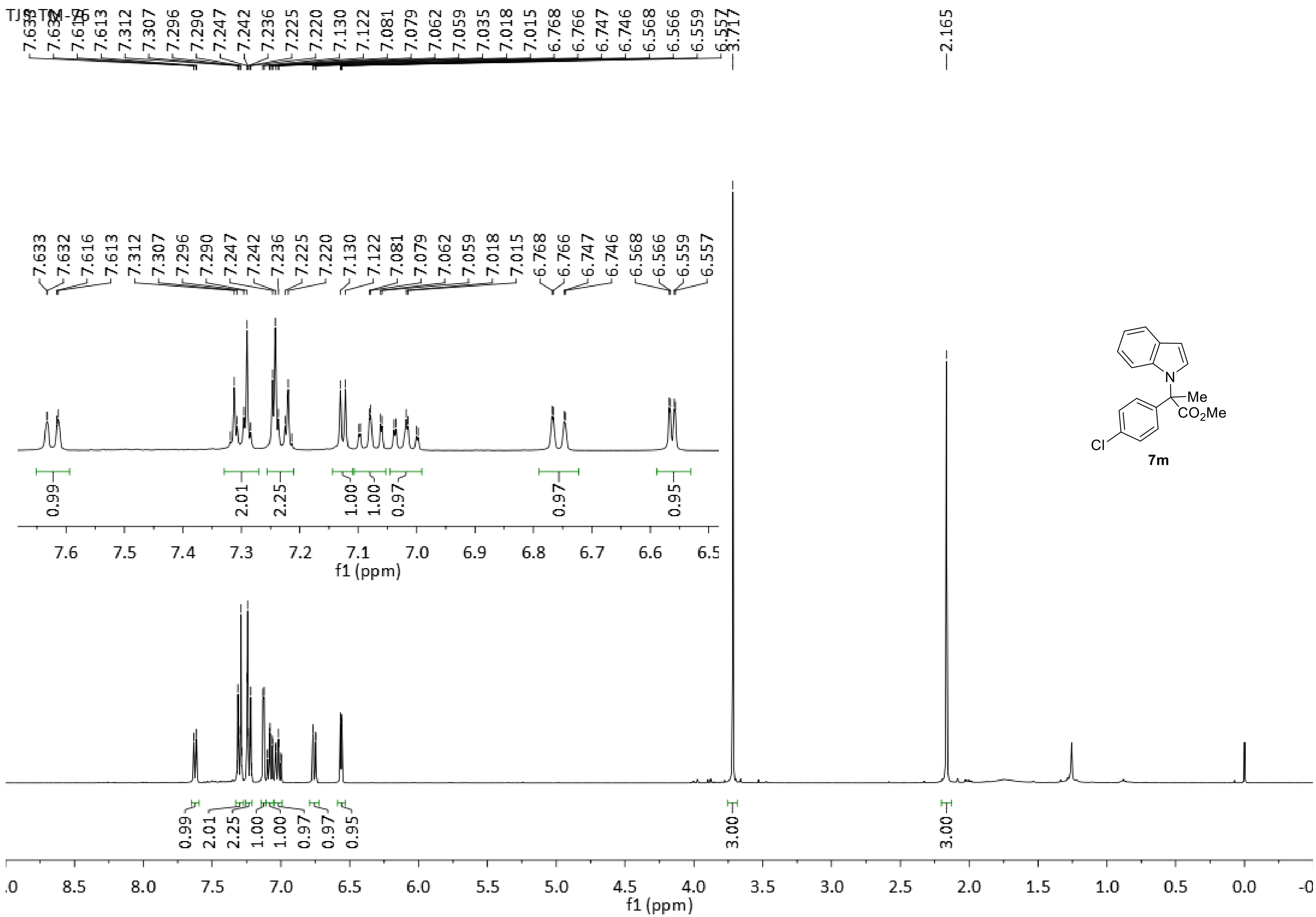
TJS-TM-72

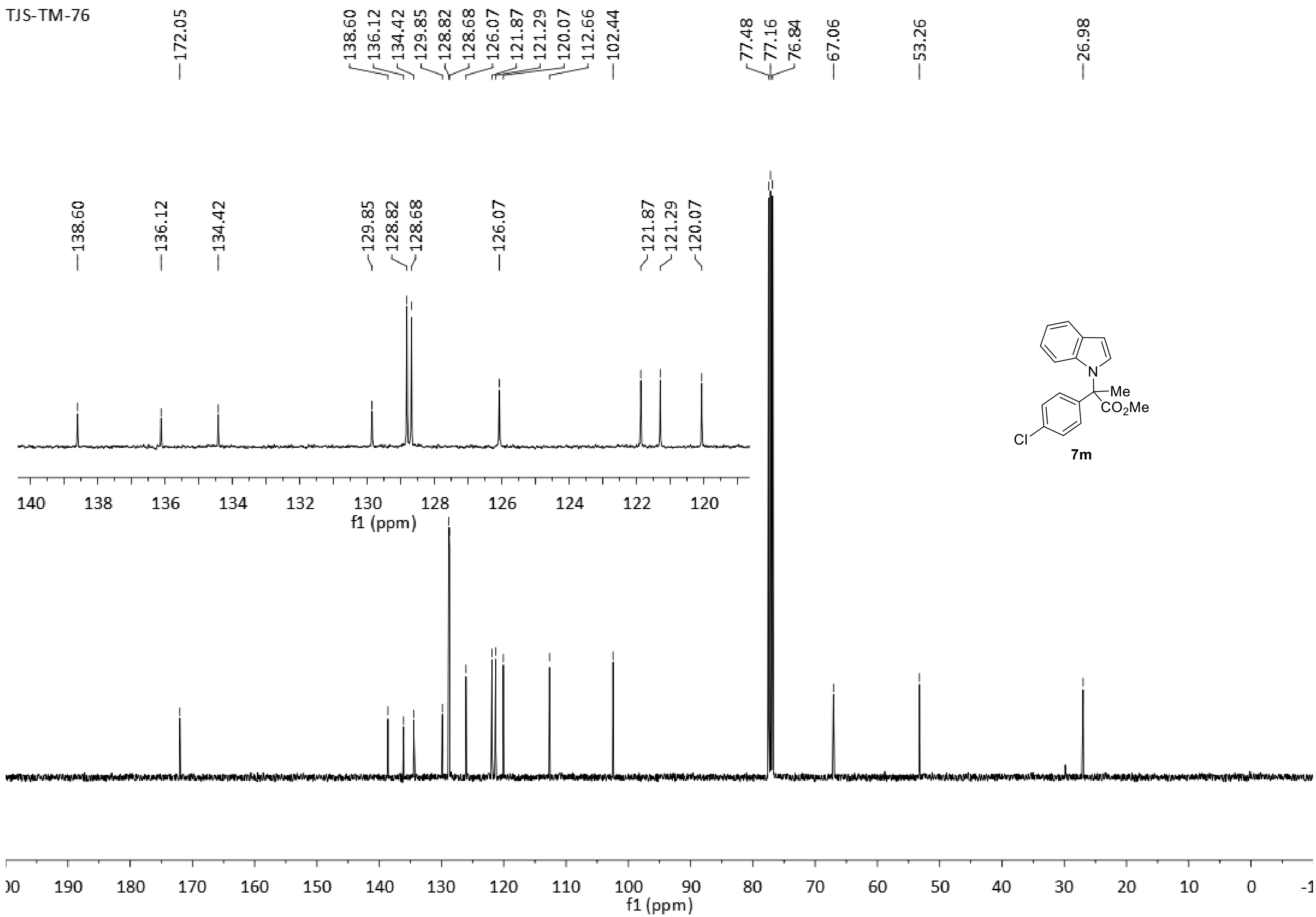

170.10
142.89
141.72
136.22
130.20
129.50
128.82
128.36
126.18
121.37
120.85
120.01
115.14
103.21
95.19
77.48
77.16
76.84
70.58
52.95
26.12
N
Me
CO_2Me
I
7k
f1 (ppm)
f1 (ppm)

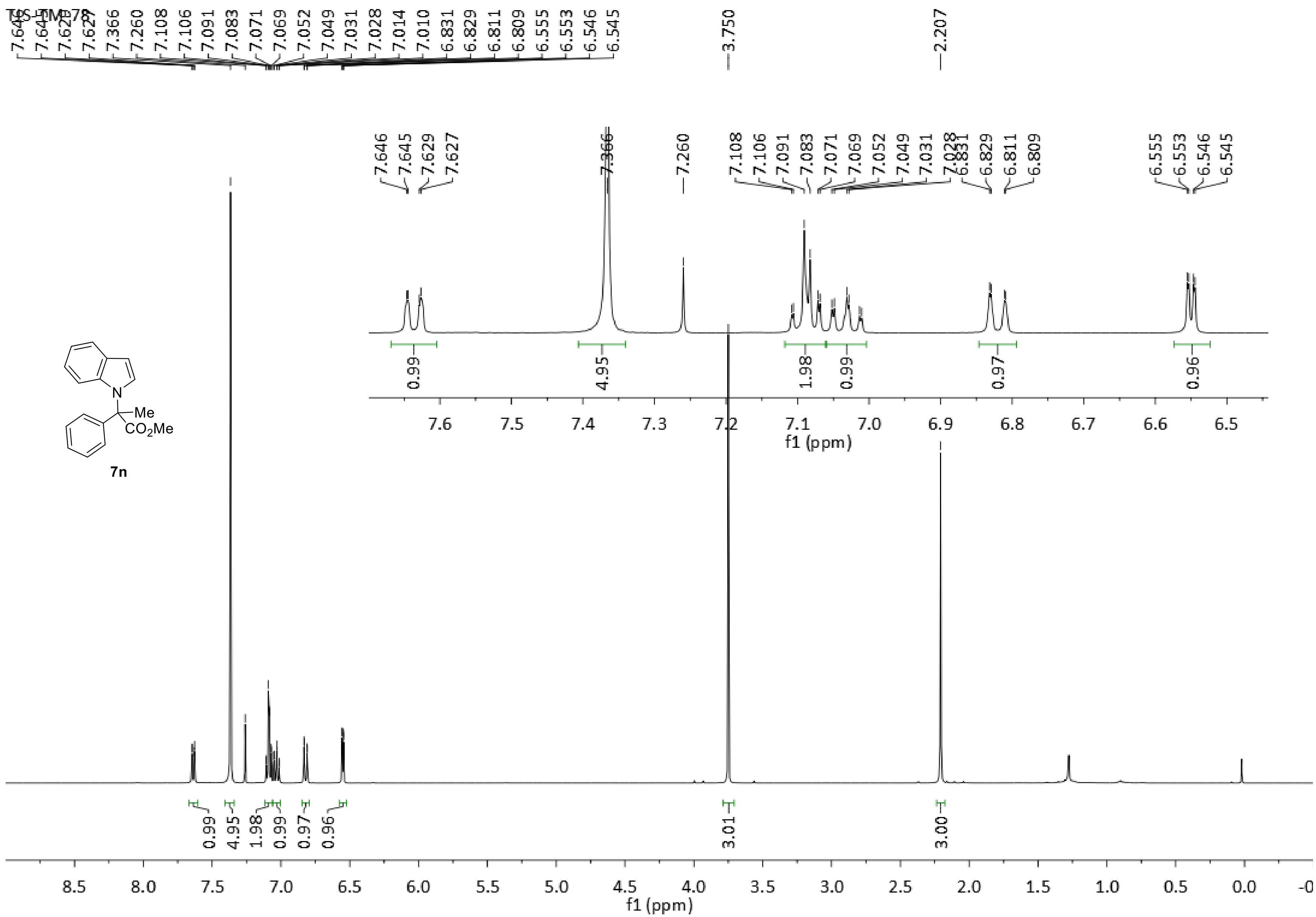

TJS-TM-74
f1 (ppm)
N
Cl
Me
CO2Me
7l


TJS-TM-74
171.86
142.10
136.13
134.66
129.91
129.85
128.66
127.54
126.08
125.41
121.91
121.30
120.09
112.64
102.52
77.48
77.16
76.84
67.14
53.31
26.96
f1 (ppm)
N
Cl
Me
CO_2Me

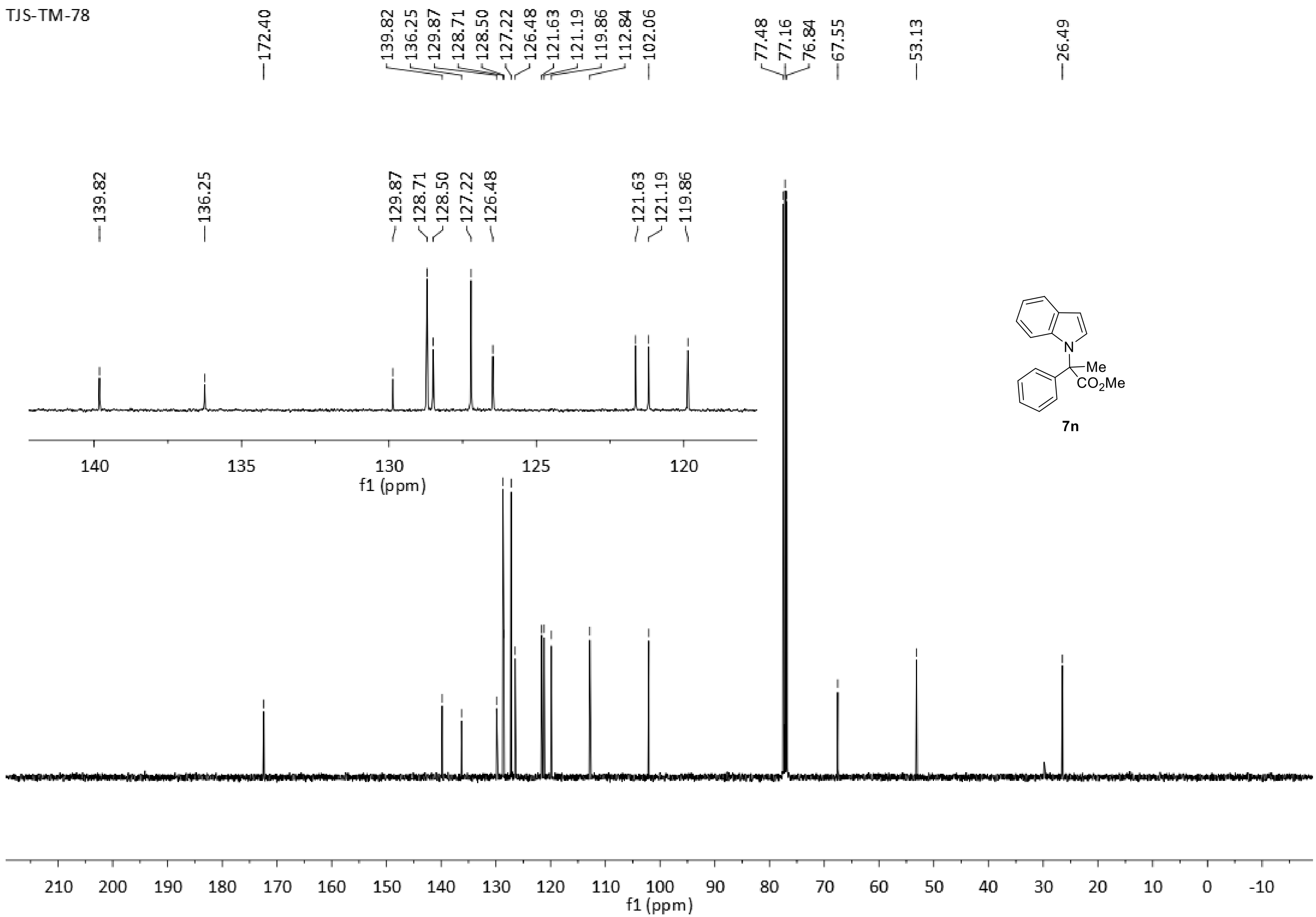
7l

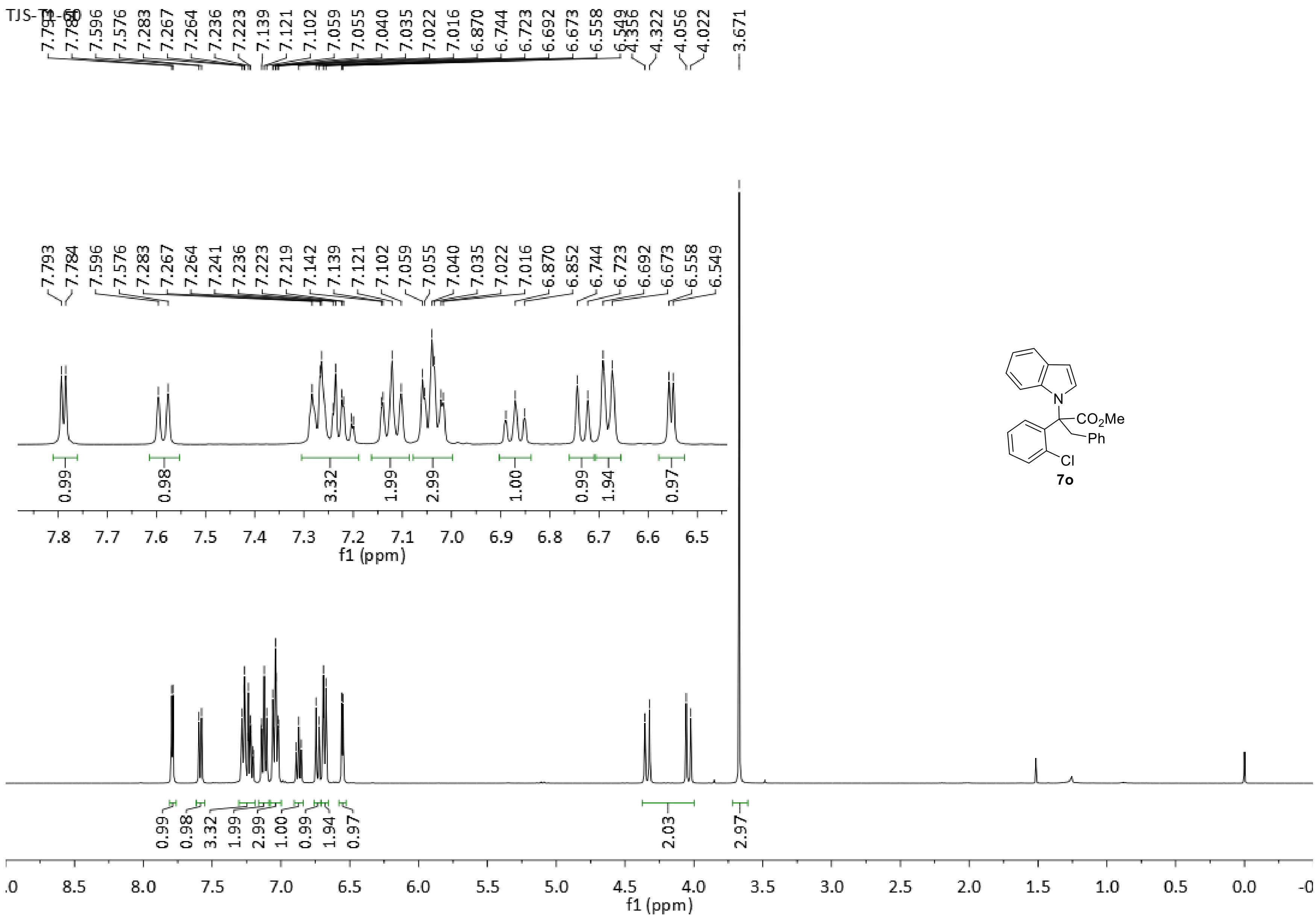

TJS-TM-76
7.633 7.632 7.616 7.613 7.312 7.307 7.296 7.290 7.247 7.242 7.236 7.225 7.220 7.130 7.122 7.081 7.079 7.062 7.059 7.035 7.018 7.015 6.768 6.766 6.747 6.746 6.568 6.566 6.559 6.557 3.717
2.165
0.99 2.01 2.25 1.00 1.00 0.97 0.97 0.95
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
f1 (ppm)
N
Me
CO2Me
Cl
7m
0.99 2.01 2.25 1.00 1.00 0.97 0.97 0.95 3.00 3.00
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
f1 (ppm)

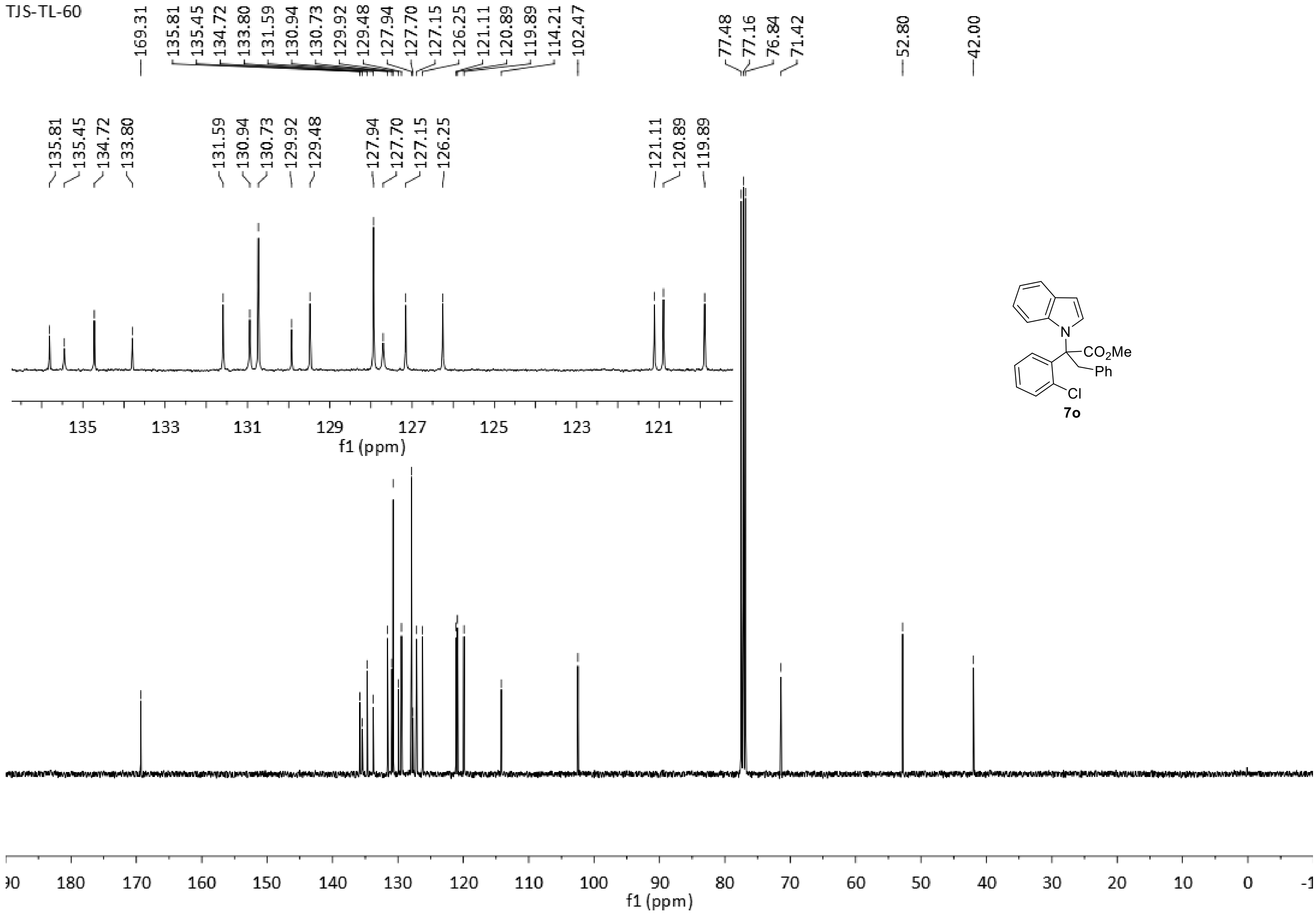

TJS-TM-76
172.05
138.60
136.12
134.42
129.85
128.82
128.68
126.07
121.87
121.29
120.07
112.66
102.44
77.48
77.16
76.84
67.06
53.26
26.98
N
Me
CO_2Me
Cl
7m
140 138 136 134 132 130 128 126 124 122 120
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

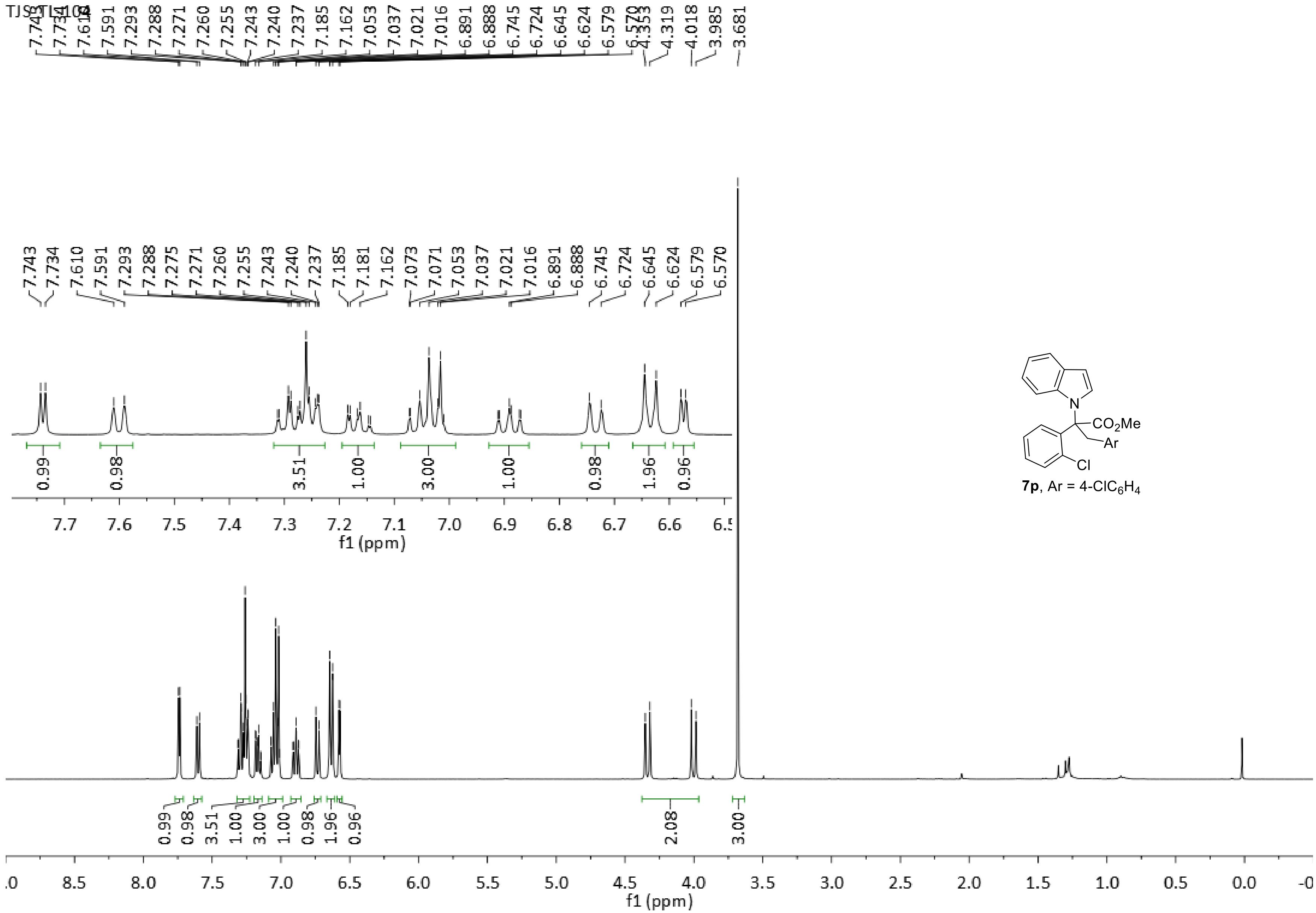


TJS-TM-78
7n
3.750
2.207
0.99
4.95
1.98
0.99
0.97
0.96
3.01
3.00
f1 (ppm)


TJS-TM-78
172.40
139.82
136.25
129.87
128.71
128.50
127.22
126.48
121.63
121.19
119.86
112.84
102.06
77.48
77.16
76.84
67.55
53.13
26.49
Me
CO_2Me
7n
f1 (ppm)

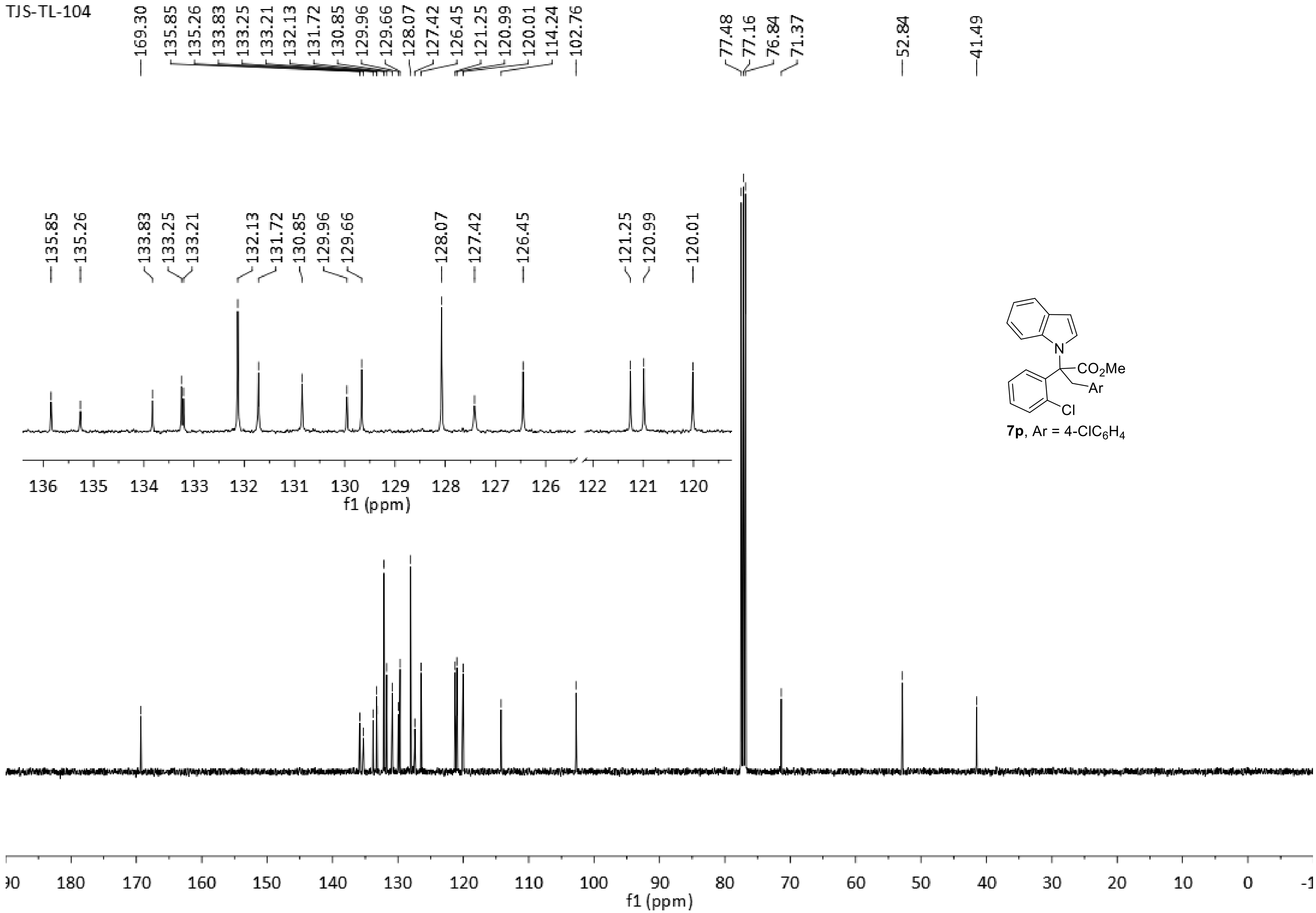

TJS-III-60
CO2Me
Ph
N
Cl
7o
f1 (ppm)


TJS-TL-60
169.31
135.81
135.45
134.72
133.80
131.59
130.94
130.73
129.92
129.48
127.94
127.70
127.15
126.25
121.11
120.89
119.89
114.21
102.47
77.48
77.16
76.84
71.42
52.80
42.00
f1 (ppm)
N
CO_2Me
Ph
Cl
7o

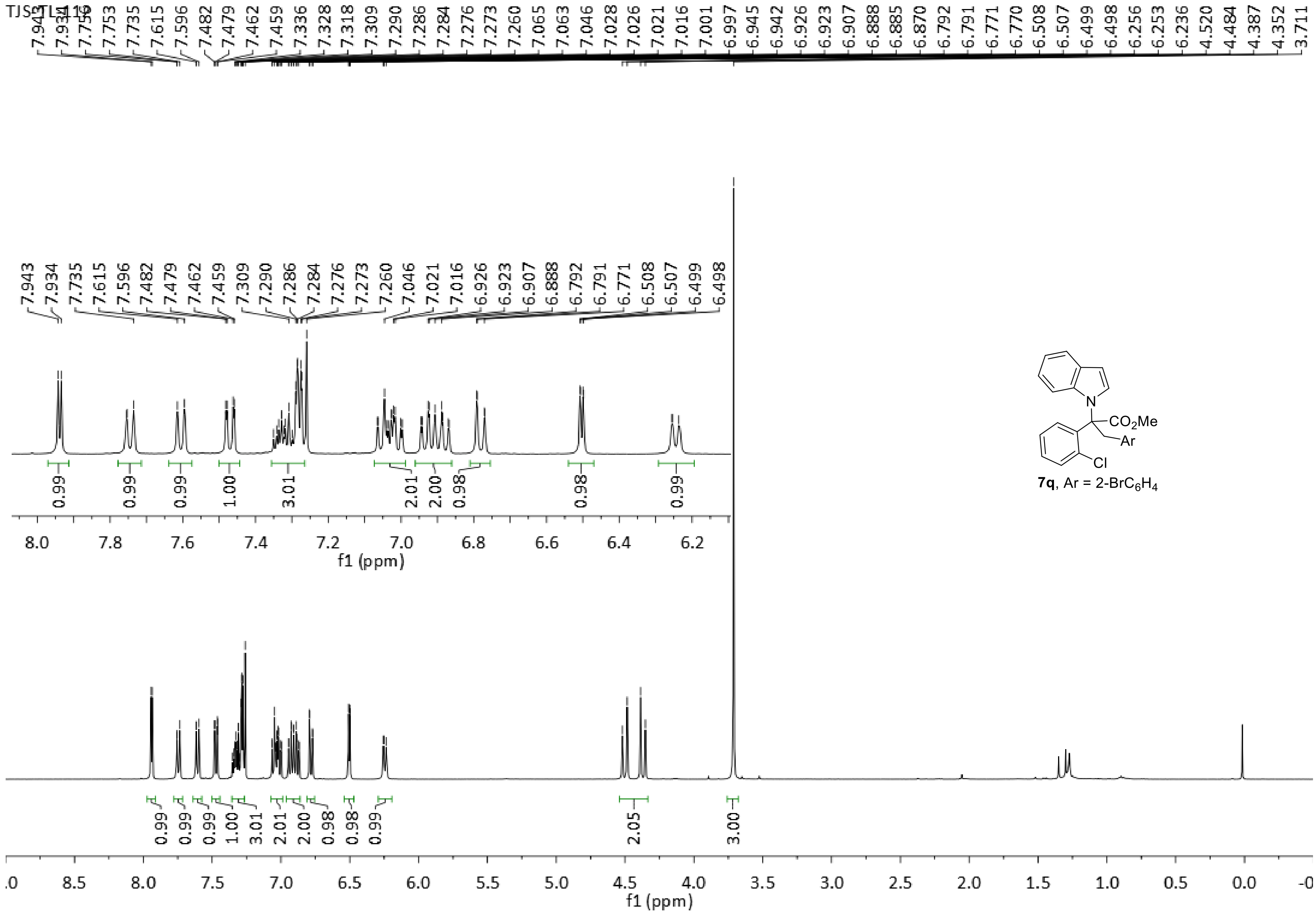


7p, Ar = 4-ClC$_6$H$_4$

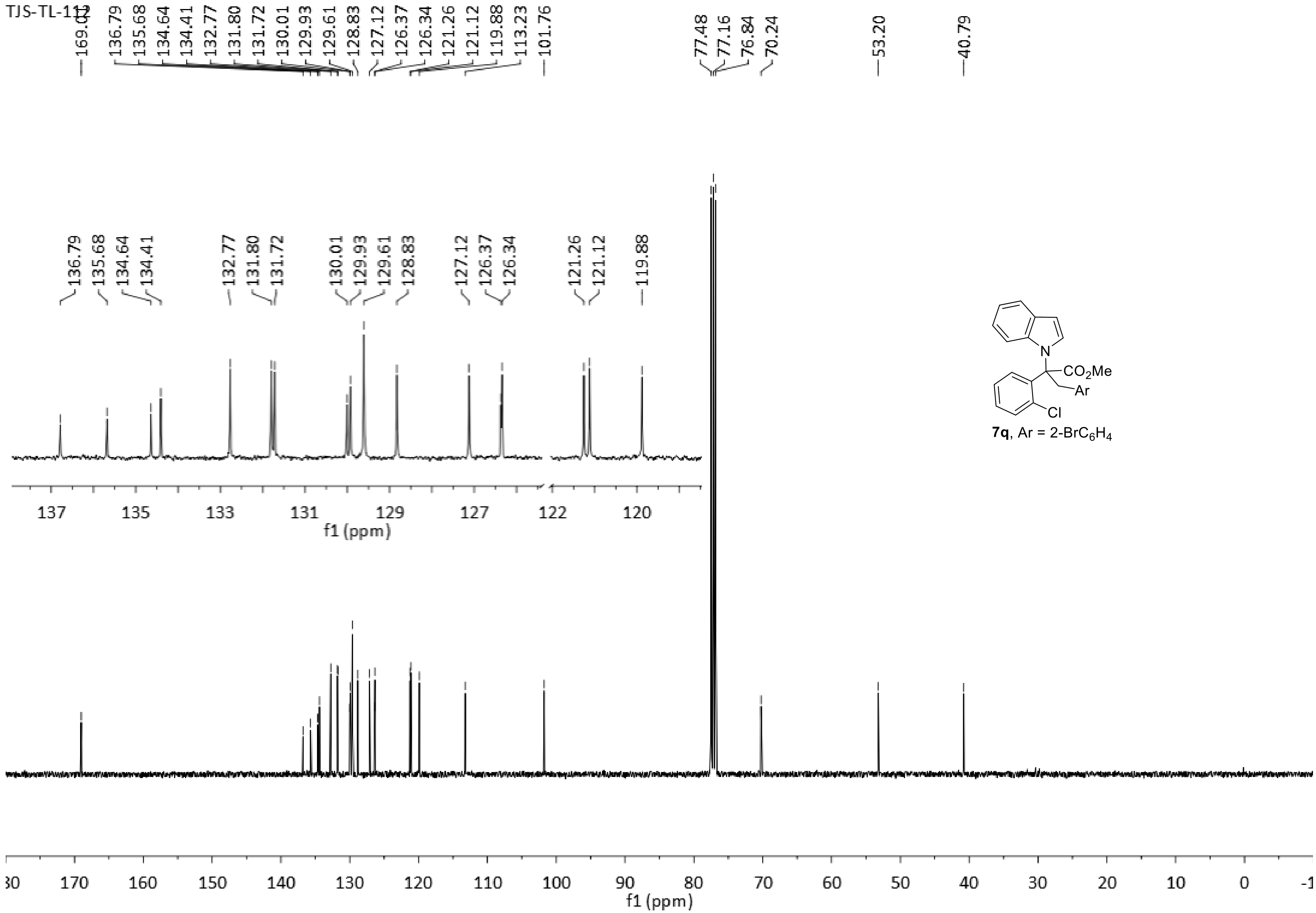
TJS-TL-104



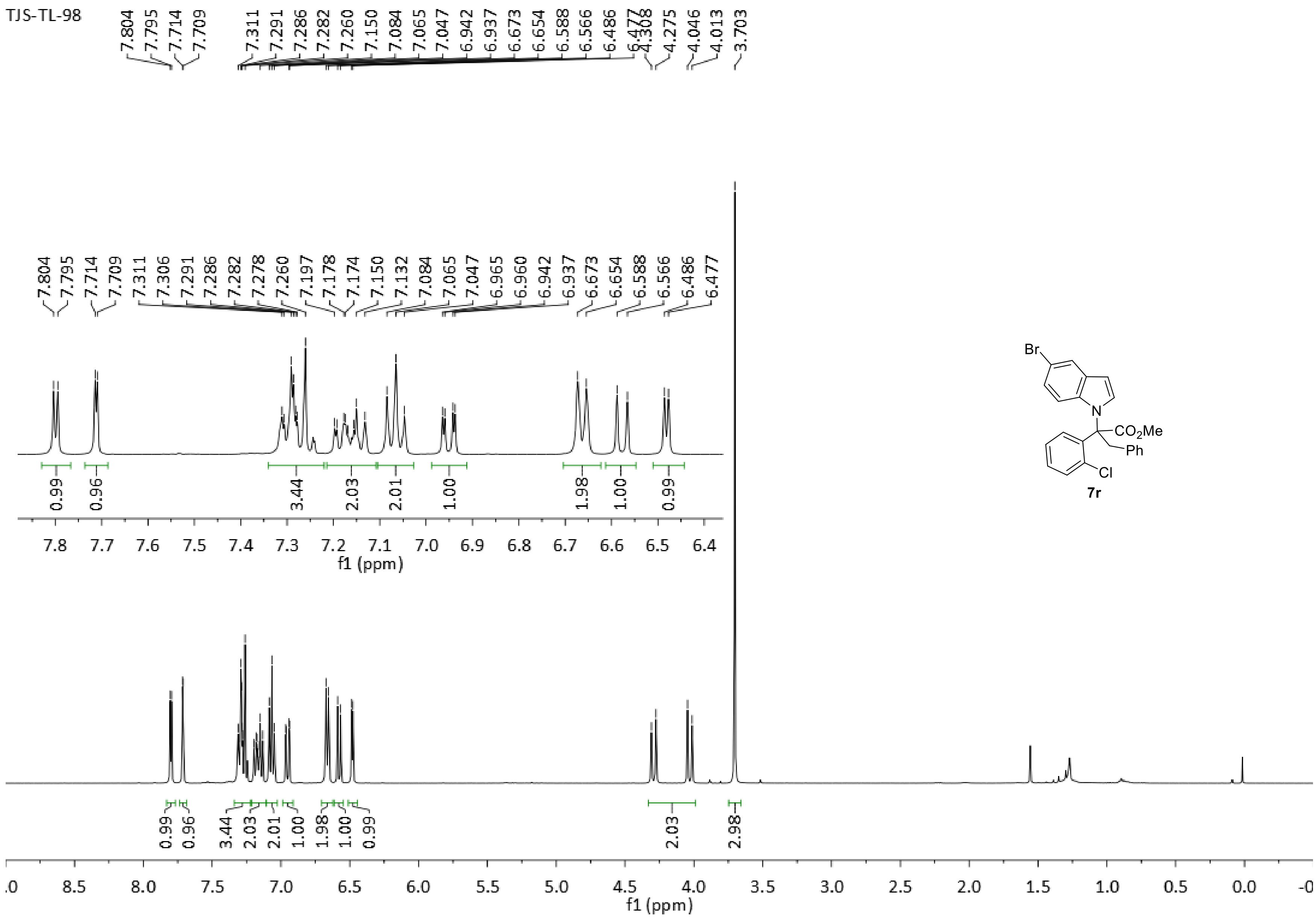
7p, Ar = 4-ClC_6H_4



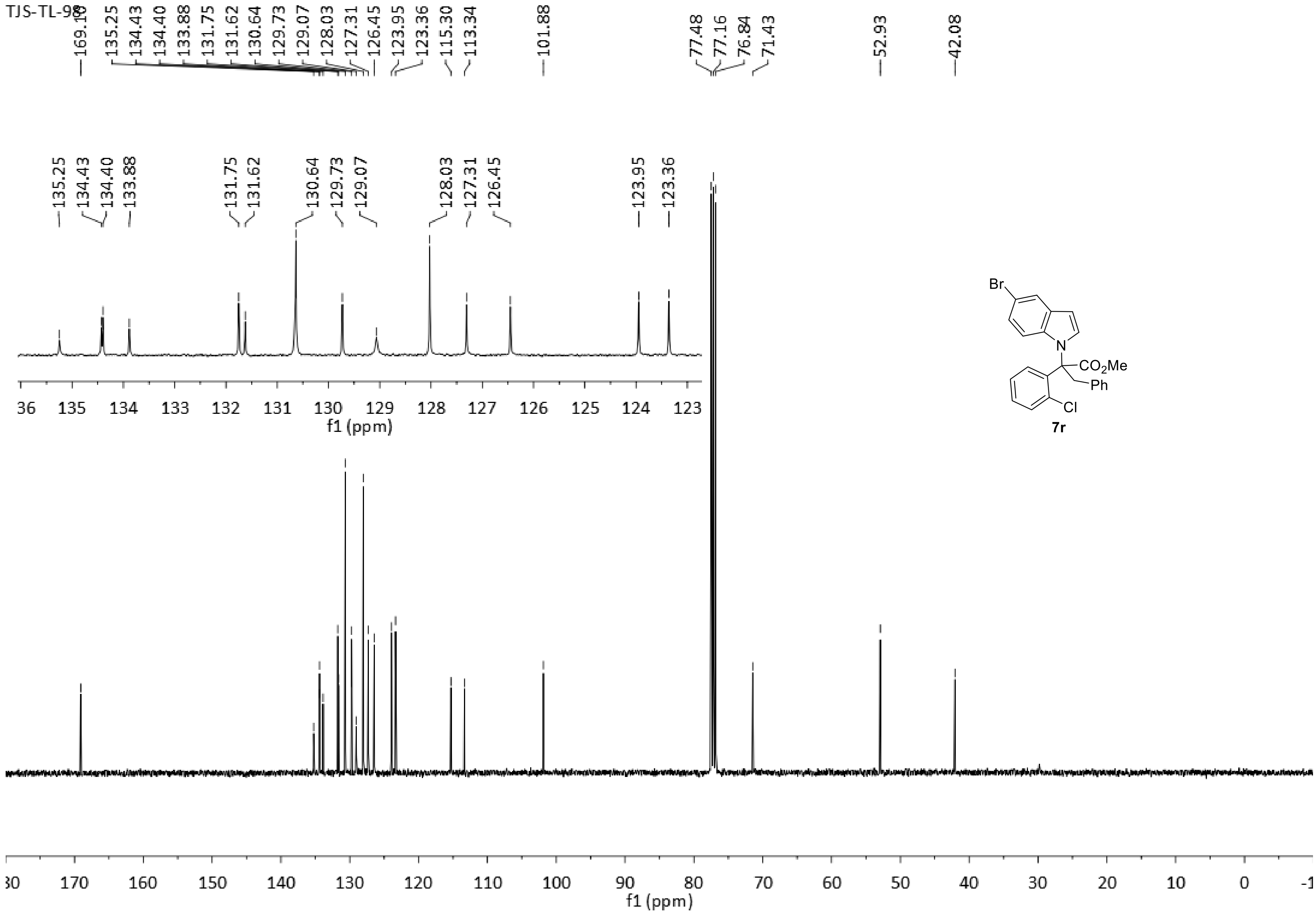
7q, Ar = 2-BrC_6H_4

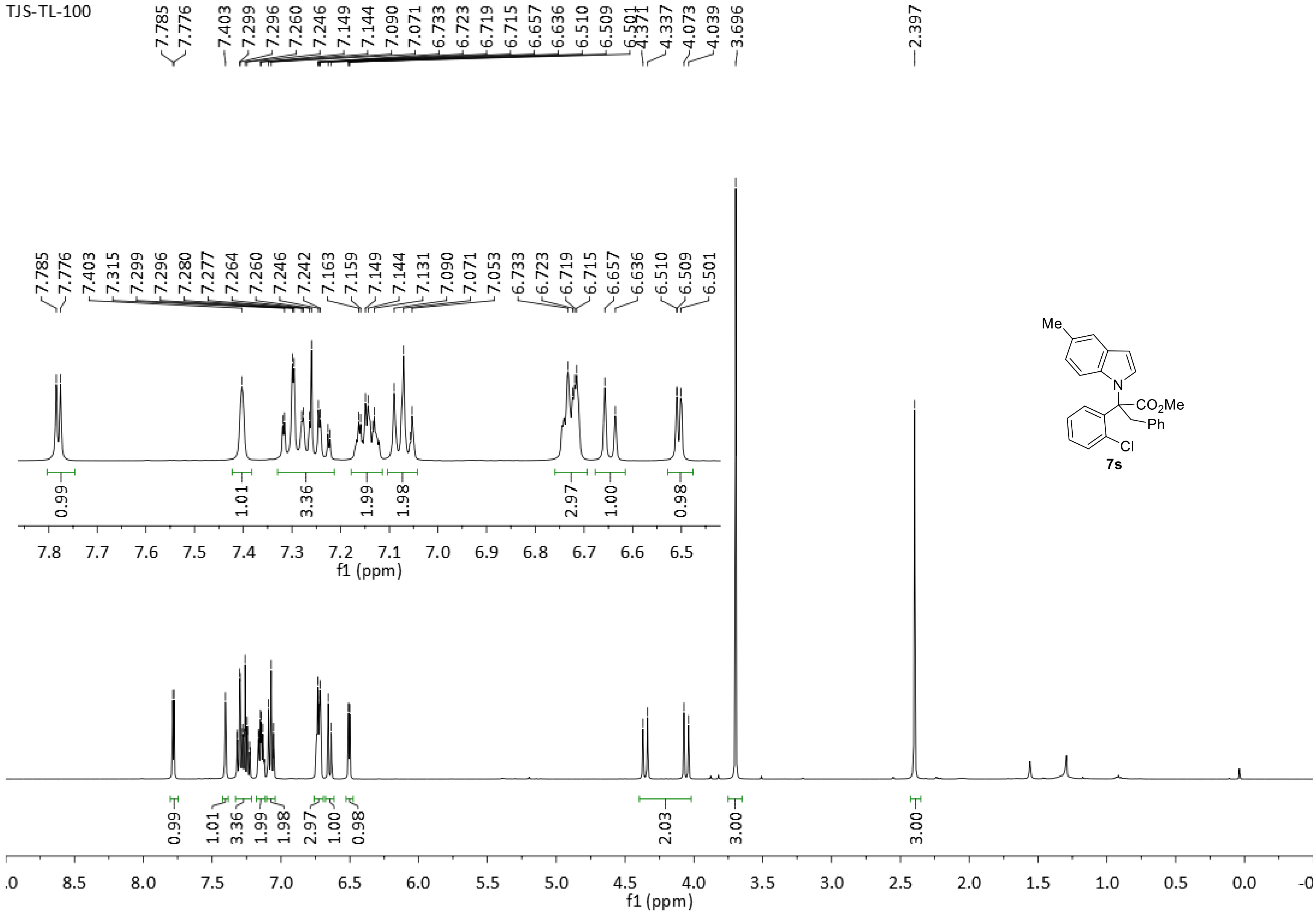


7q, Ar = 2-BrC_6H_4

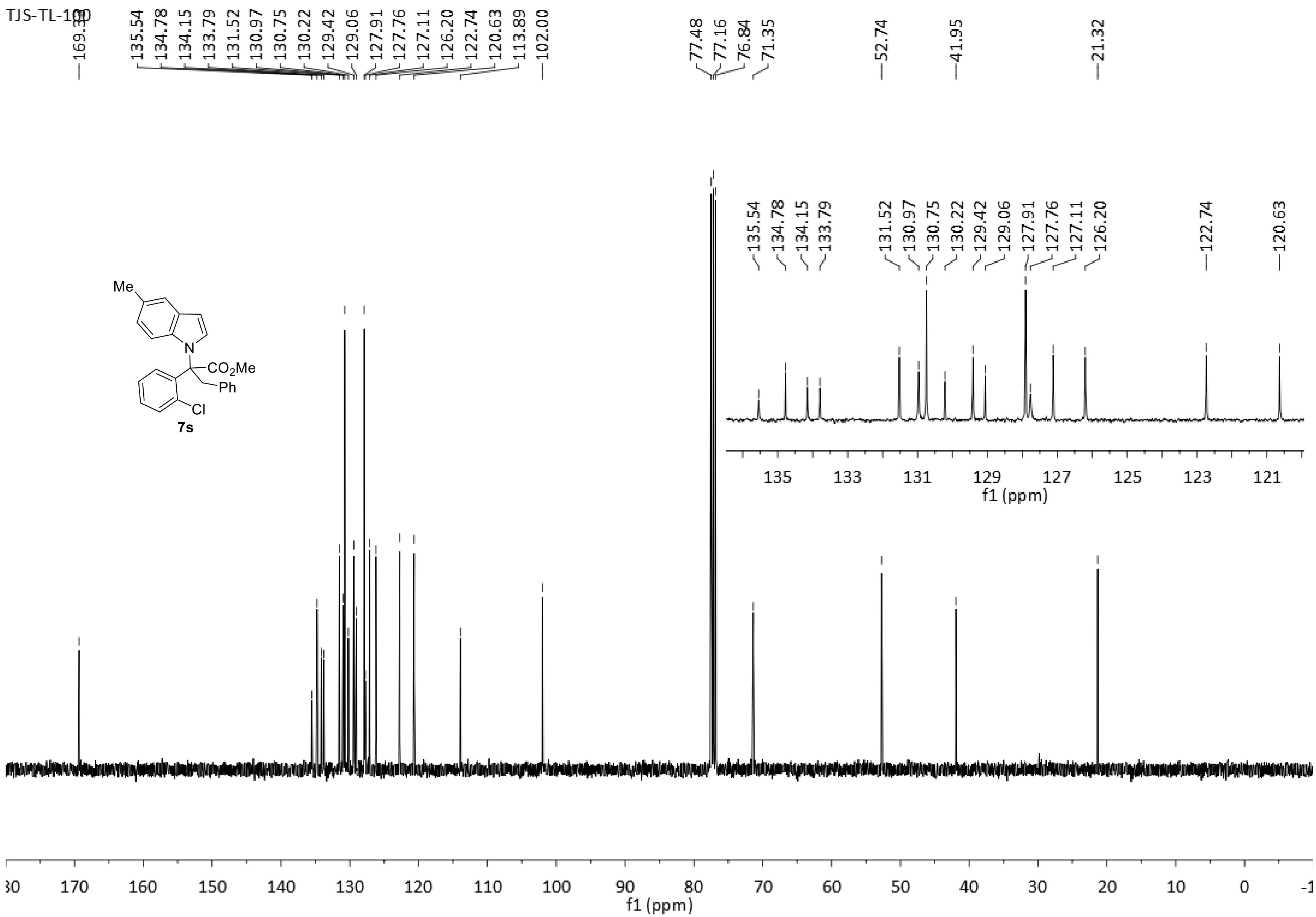


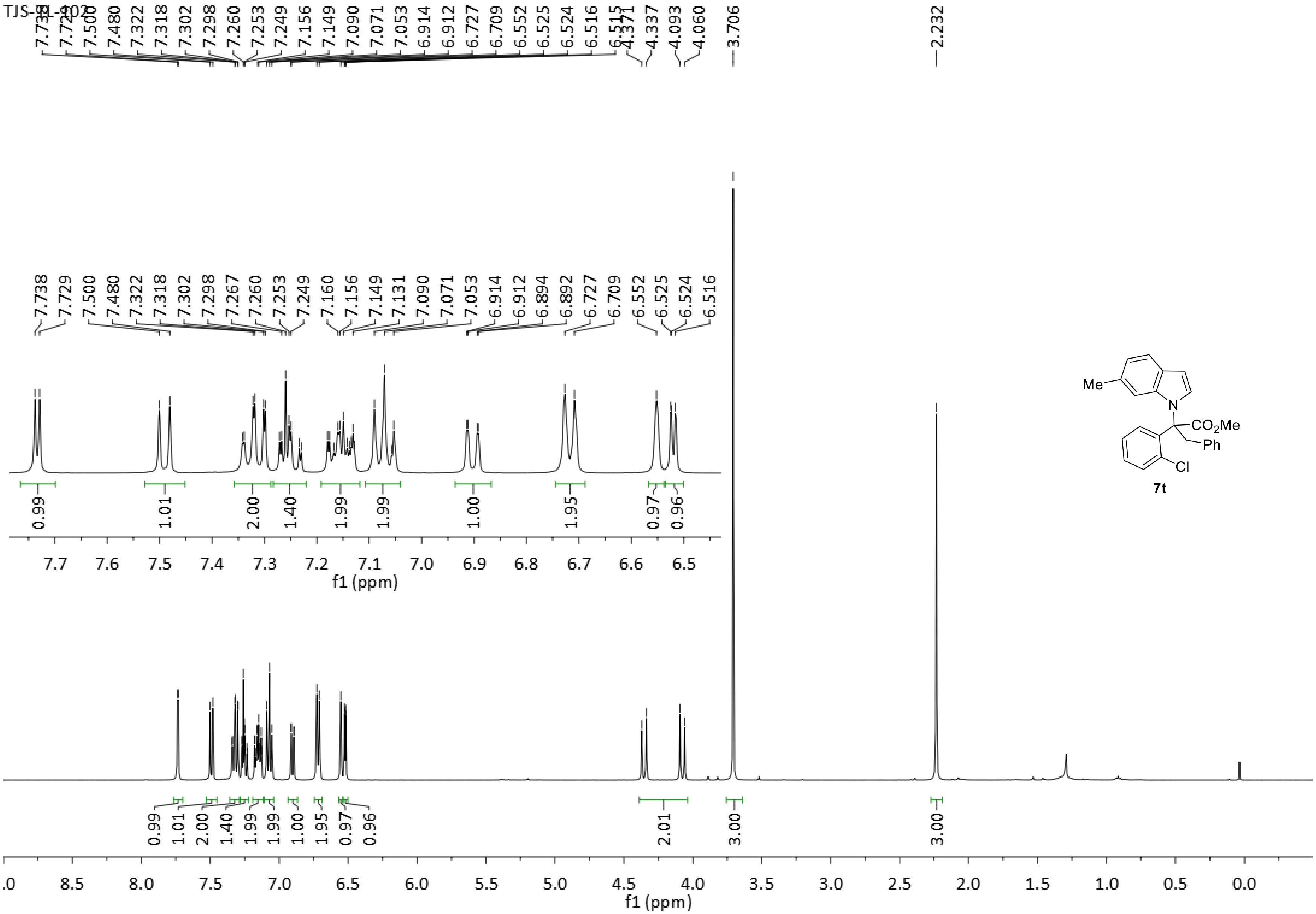
TJS-TL-98
f1 (ppm)
f1 (ppm)
Br
N
CO2Me
Ph
Cl
7r


TJS-TL-98
169.10
135.25
134.43
134.40
133.88
131.75
131.62
130.64
129.73
129.07
128.03
127.31
126.45
123.95
123.36
115.30
113.34
101.88
77.48
77.16
76.84
71.43
52.93
42.08
f1 (ppm)
Br
N
CO2Me
Ph
Cl
7r


TJS-TL-100
7.785
7.776
7.403
7.299
7.296
7.260
7.246
7.149
7.144
7.090
7.071
6.733
6.723
6.719
6.715
6.657
6.636
6.510
6.509
6.501
4.371
4.337
4.073
4.039
3.696
2.397
7.785
7.776
7.403
7.315
7.299
7.296
7.280
7.277
7.264
7.260
7.246
7.242
7.163
7.159
7.149
7.144
7.131
7.090
7.071
7.053
6.733
6.723
6.719
6.715
6.657
6.636
6.510
6.509
6.501
0.99
1.01
3.36
1.99
1.98
2.97
1.00
0.98
f1 (ppm)
0.99
1.01
3.36
1.99
1.98
2.97
1.00
0.98
2.03
3.00
3.00
f1 (ppm)
Me
N
CO2Me
Ph
Cl

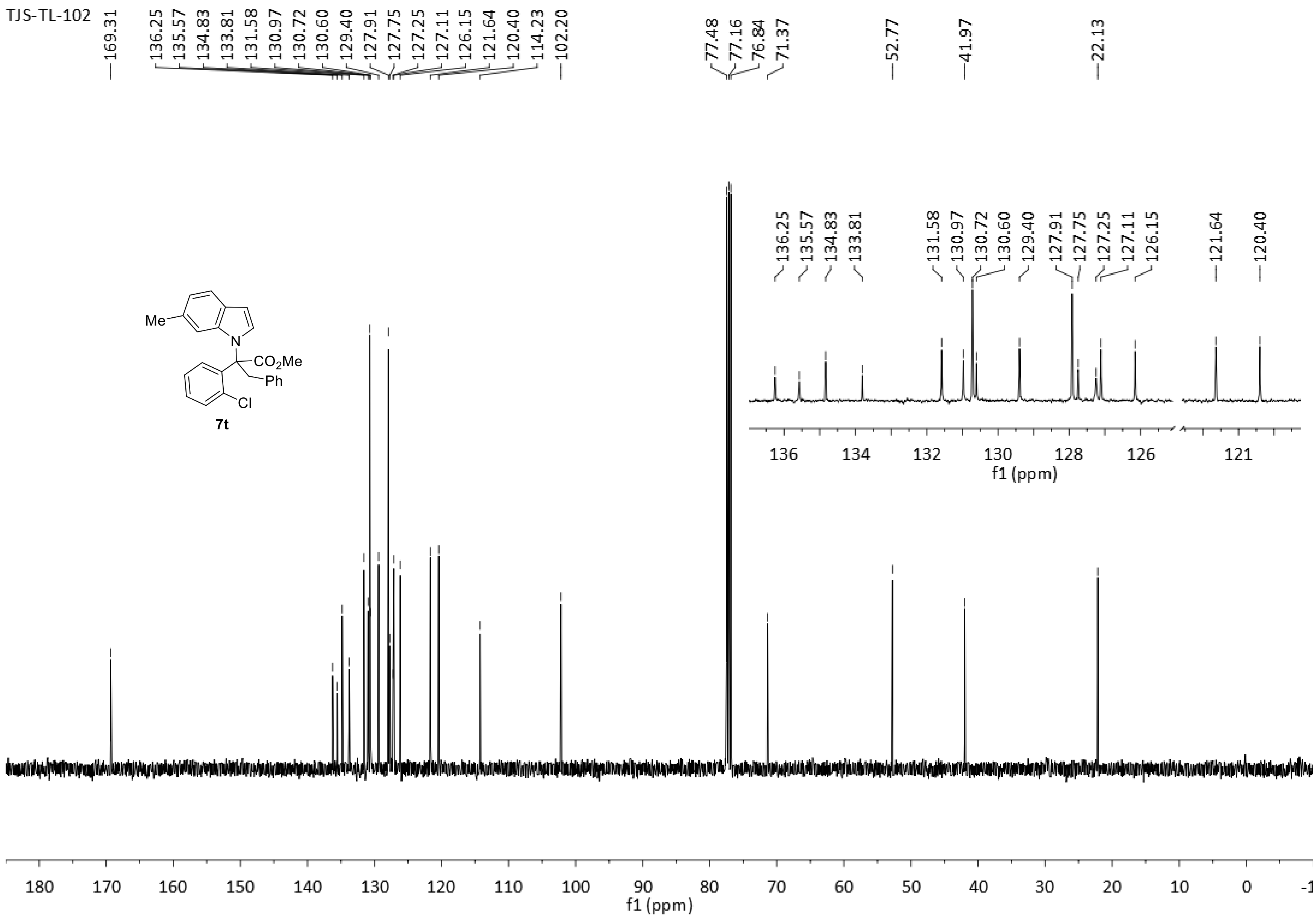
7s

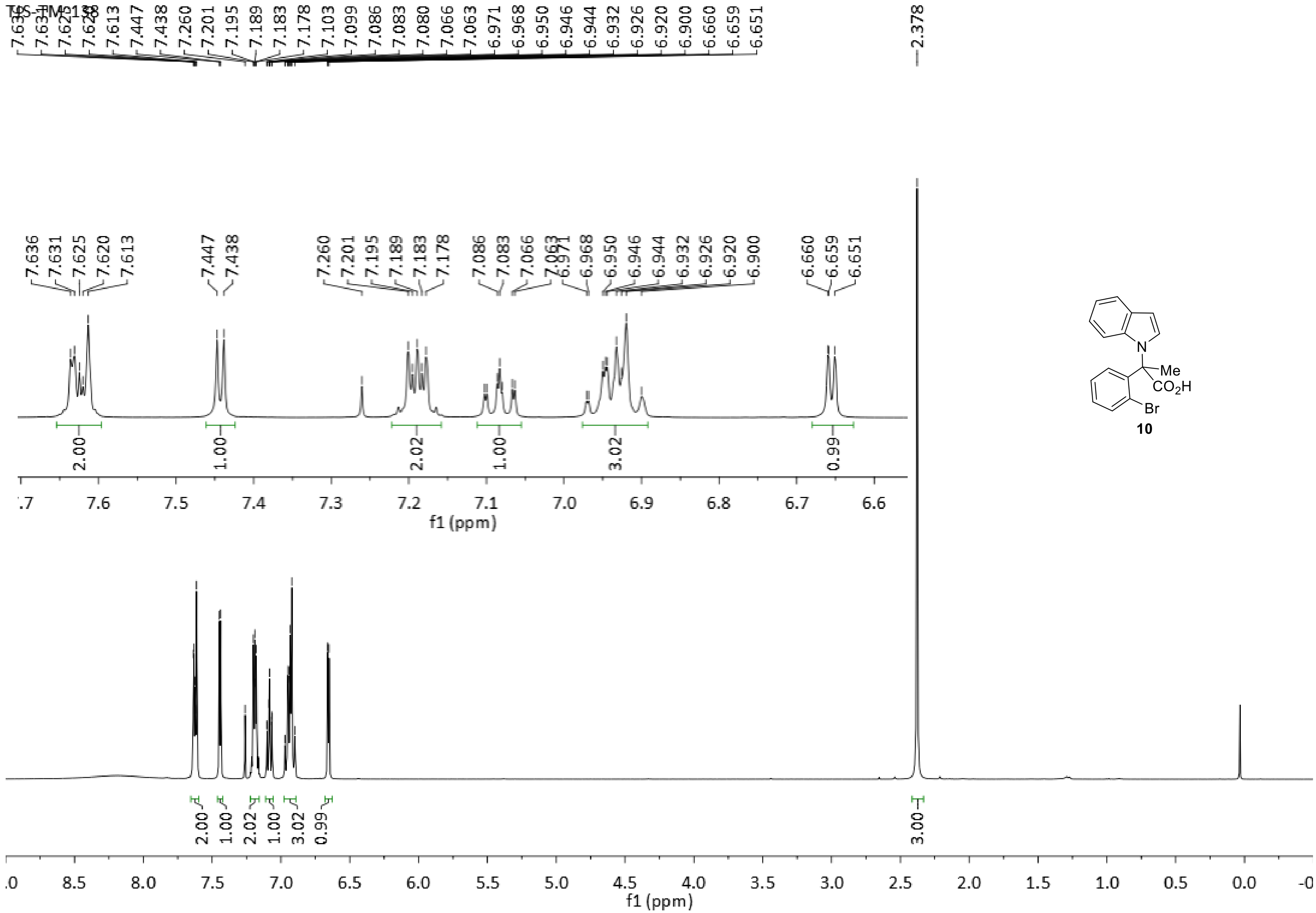

TJS-TL-100
169.30
135.54
134.78
134.15
133.79
131.52
130.97
130.75
130.22
129.42
129.06
127.91
127.76
127.11
126.20
122.74
120.63
113.89
102.00
77.48
77.16
76.84
71.35
52.74
41.95
21.32
Me
N
CO_2Me
Ph
Cl
7s
f1 (ppm)

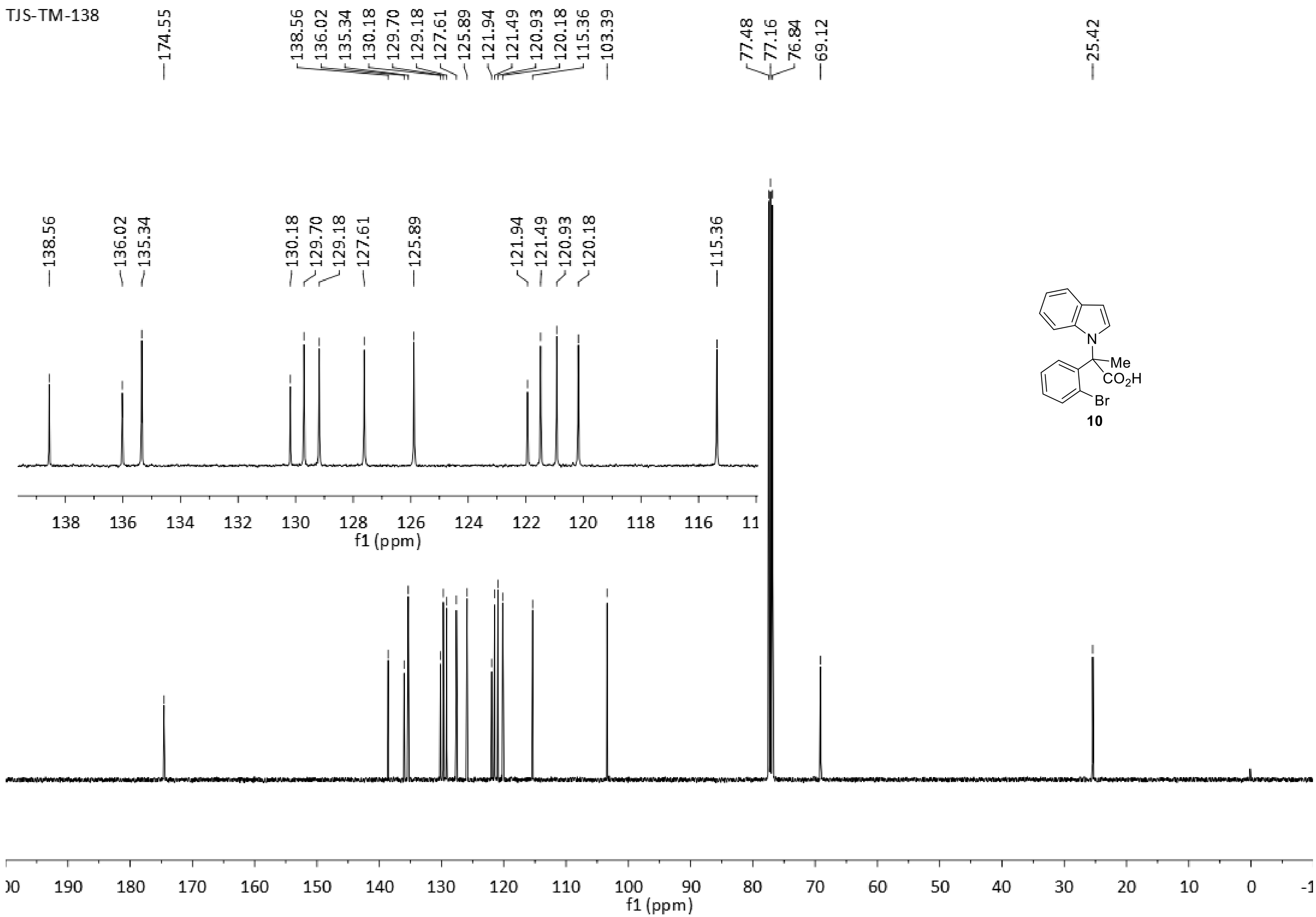


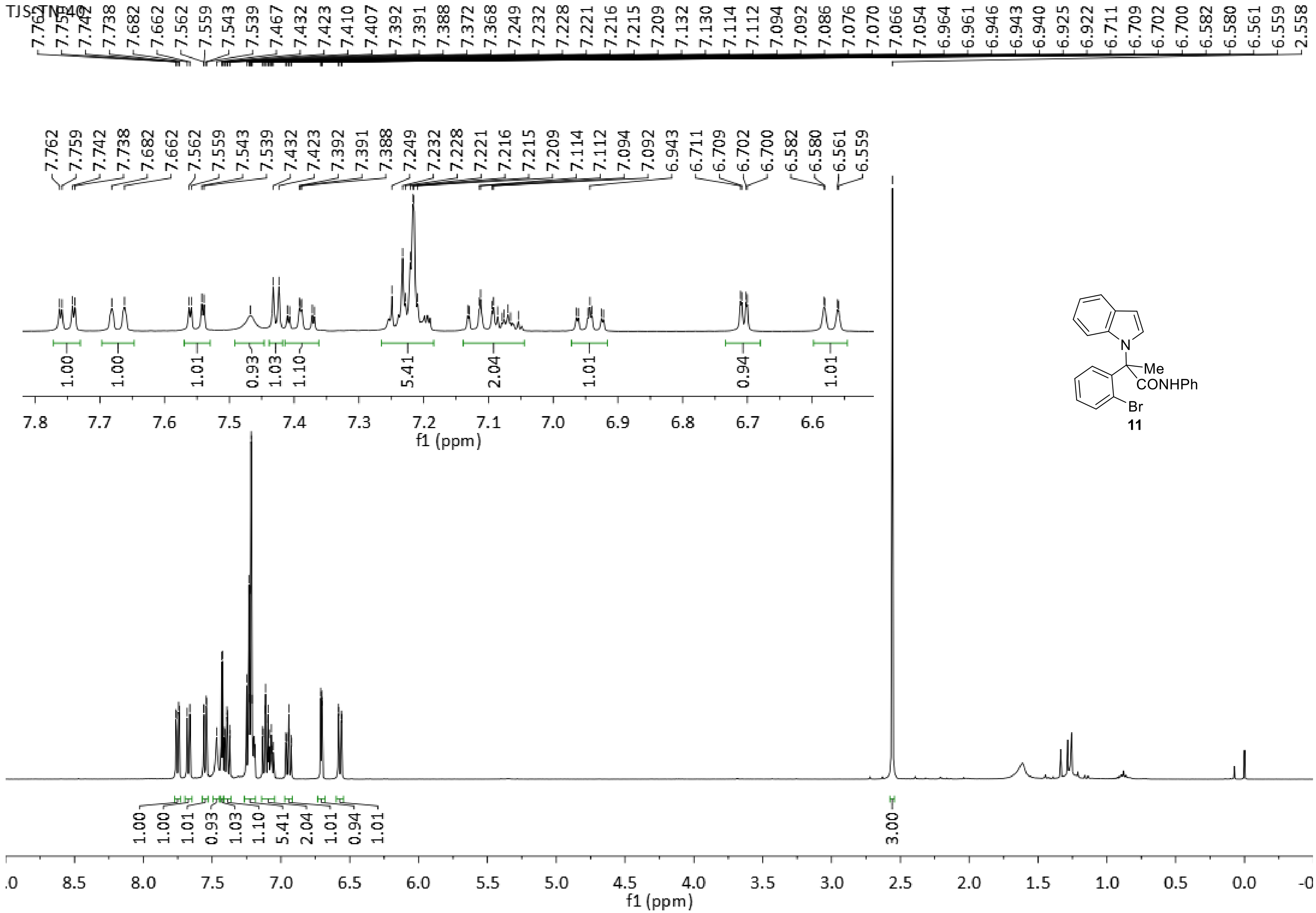
TJS-III-102
7.738
7.729
7.500
7.480
7.322
7.318
7.302
7.298
7.260
7.253
7.249
7.156
7.149
7.090
7.071
7.053
6.914
6.912
6.727
6.709
6.552
6.525
6.524
6.516
6.515
4.371
4.337
4.093
4.060
3.706
2.232
7.738
7.729
7.500
7.480
7.322
7.318
7.302
7.298
7.267
7.260
7.253
7.249
7.160
7.156
7.149
7.131
7.090
7.071
7.053
6.914
6.912
6.894
6.892
6.727
6.709
6.552
6.525
6.524
6.516
0.99
1.01
2.00
1.40
1.99
1.99
1.00
1.95
0.97
0.96
f1 (ppm)
2.01
3.00
3.00
f1 (ppm)
Me
N
CO_2Me
Ph
Cl

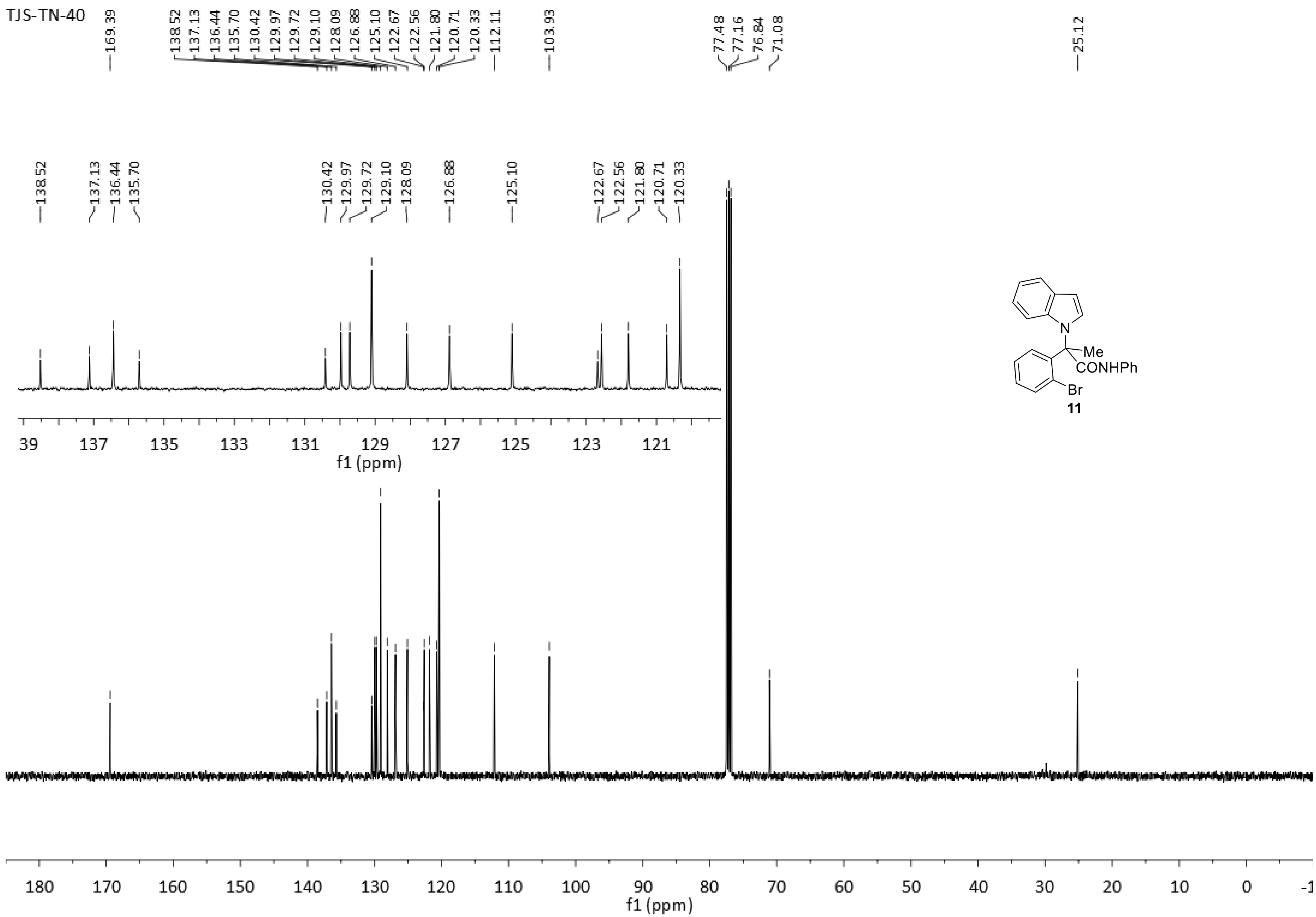
7t

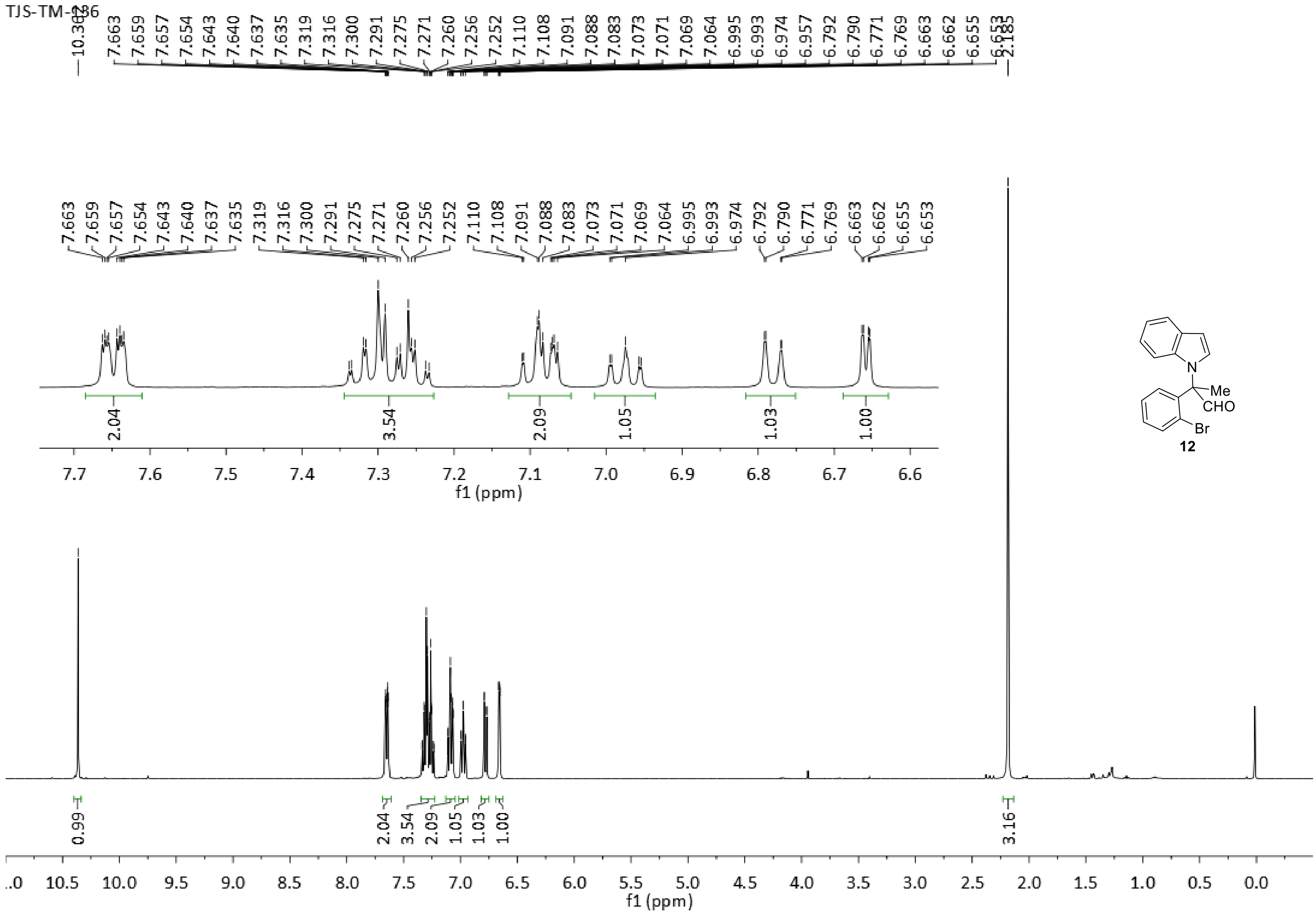

TJS-TL-102
169.31
136.25
135.57
134.83
133.81
131.58
130.97
130.72
130.60
129.40
127.91
127.75
127.25
127.11
126.15
121.64
120.40
114.23
102.20
77.48
77.16
76.84
71.37
52.77
41.97
22.13
Me
N
CO_2Me
Ph
Cl
7t
f1 (ppm)

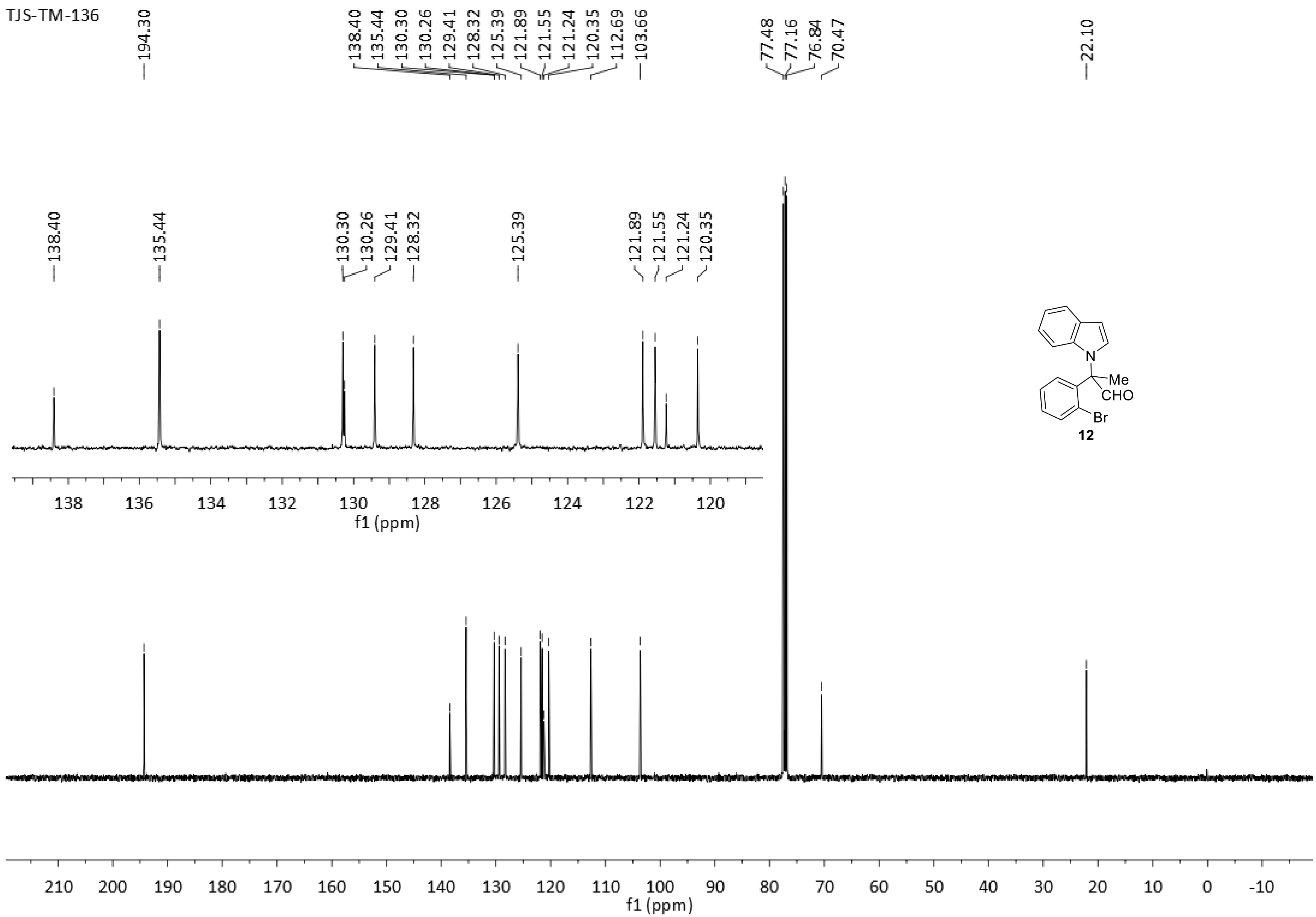

N
Me
CO2H
Br
10
f1 (ppm)
2.378
2.00
1.00
2.02
1.00
3.02
0.99
3.00

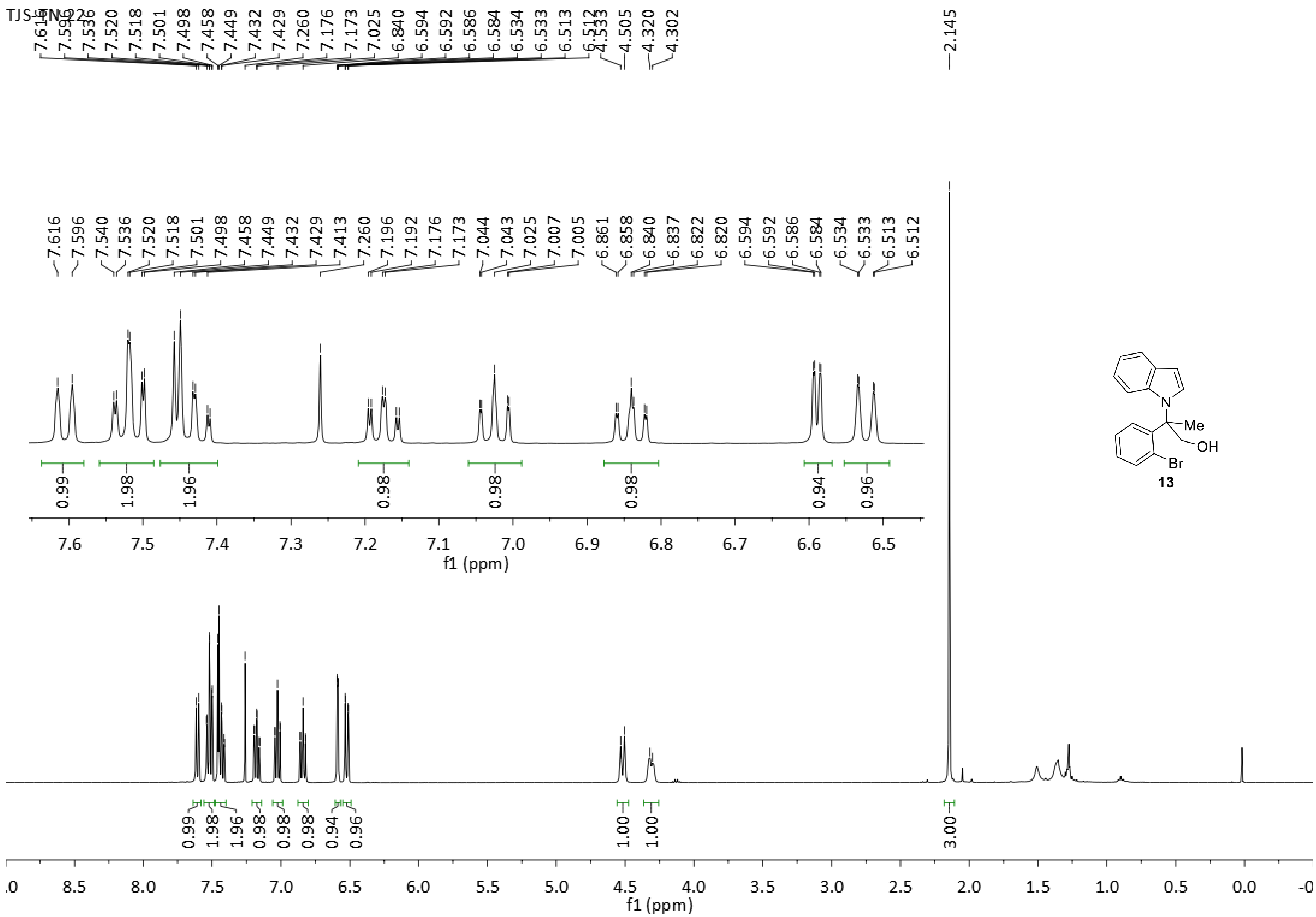

TJS-TM-138
174.55
138.56
136.02
135.34
130.18
129.70
129.18
127.61
125.89
121.94
121.49
120.93
120.18
115.36
103.39
77.48
77.16
76.84
69.12
25.42
138.56
136.02
135.34
130.18
129.70
129.18
127.61
125.89
121.94
121.49
120.93
120.18
115.36
138
136
134
132
130
128
126
124
122
120
118
116
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
N
Me
CO_2H
Br
10

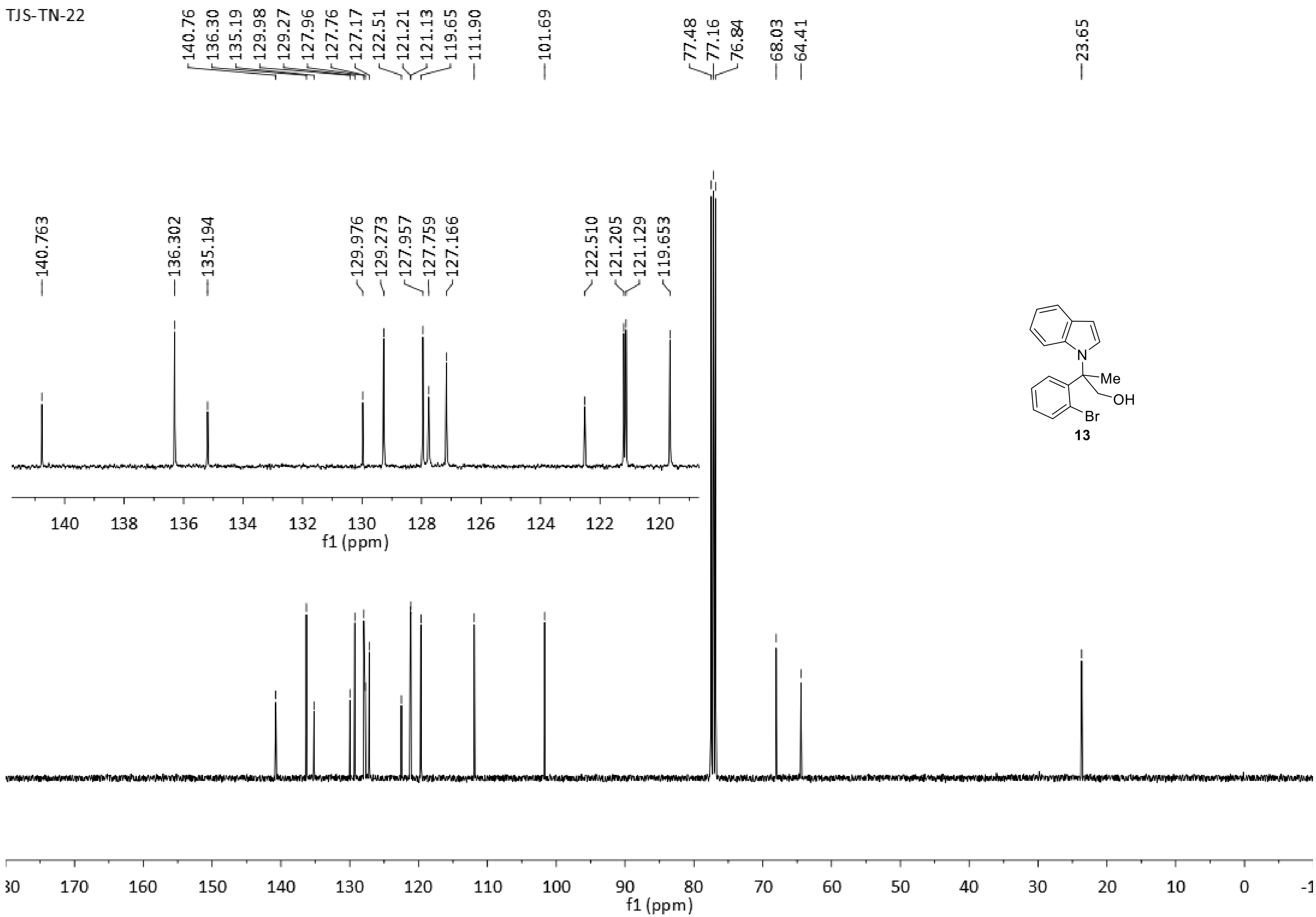

TJS-TN-40
N
Me
CONHPh
Br
11
1.00 1.00 1.01 0.93 1.03 1.10 5.41 2.04 1.01 0.94 1.01
3.00
f1 (ppm)

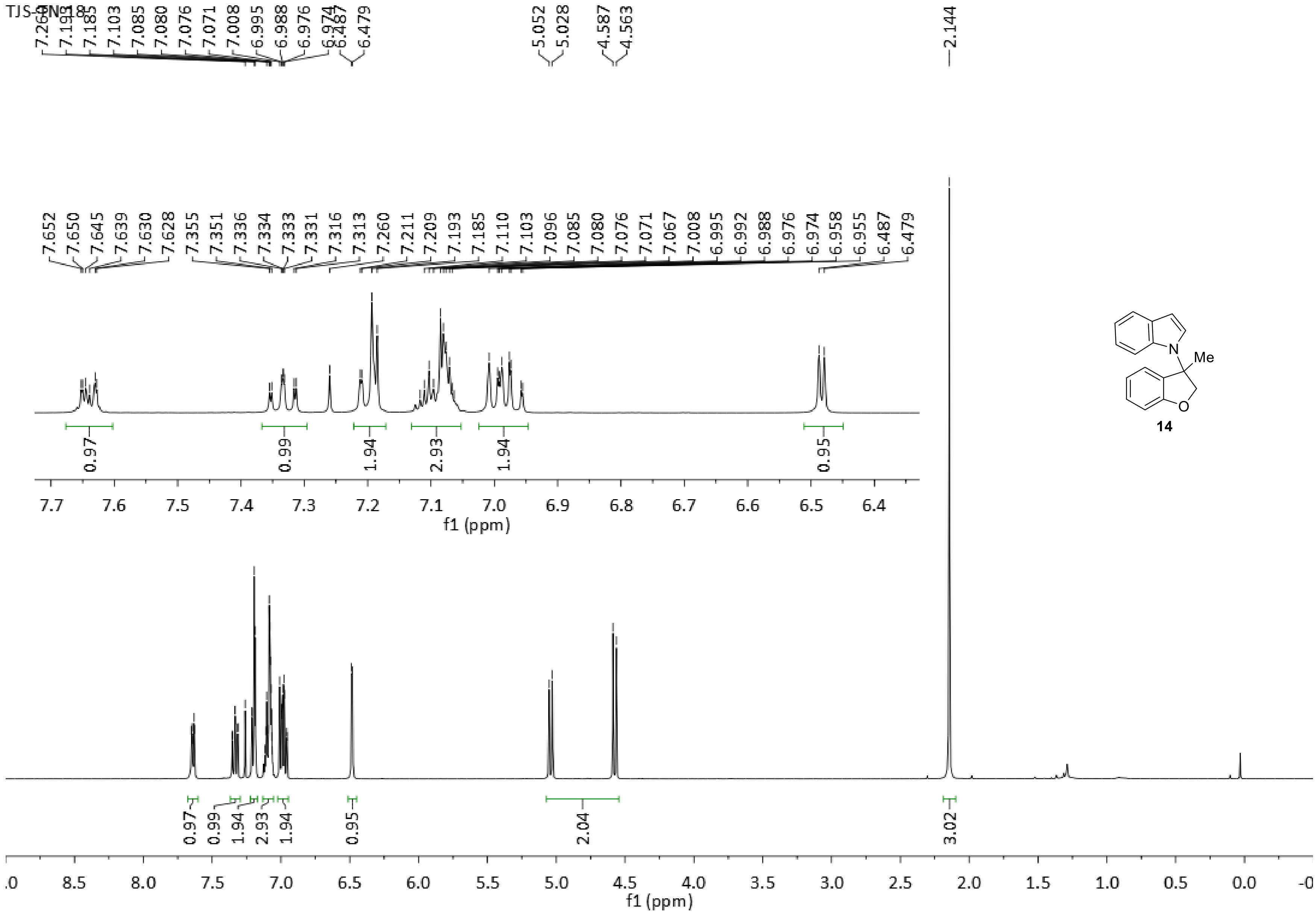

TJS-TN-40
169.39
138.52
137.13
136.44
135.70
130.42
129.97
129.72
129.10
128.09
126.88
125.10
122.67
122.56
121.80
120.71
120.33
112.11
103.93
77.48
77.16
76.84
71.08
25.12
f1 (ppm)
f1 (ppm)
N
Me
CONHPh
Br
11

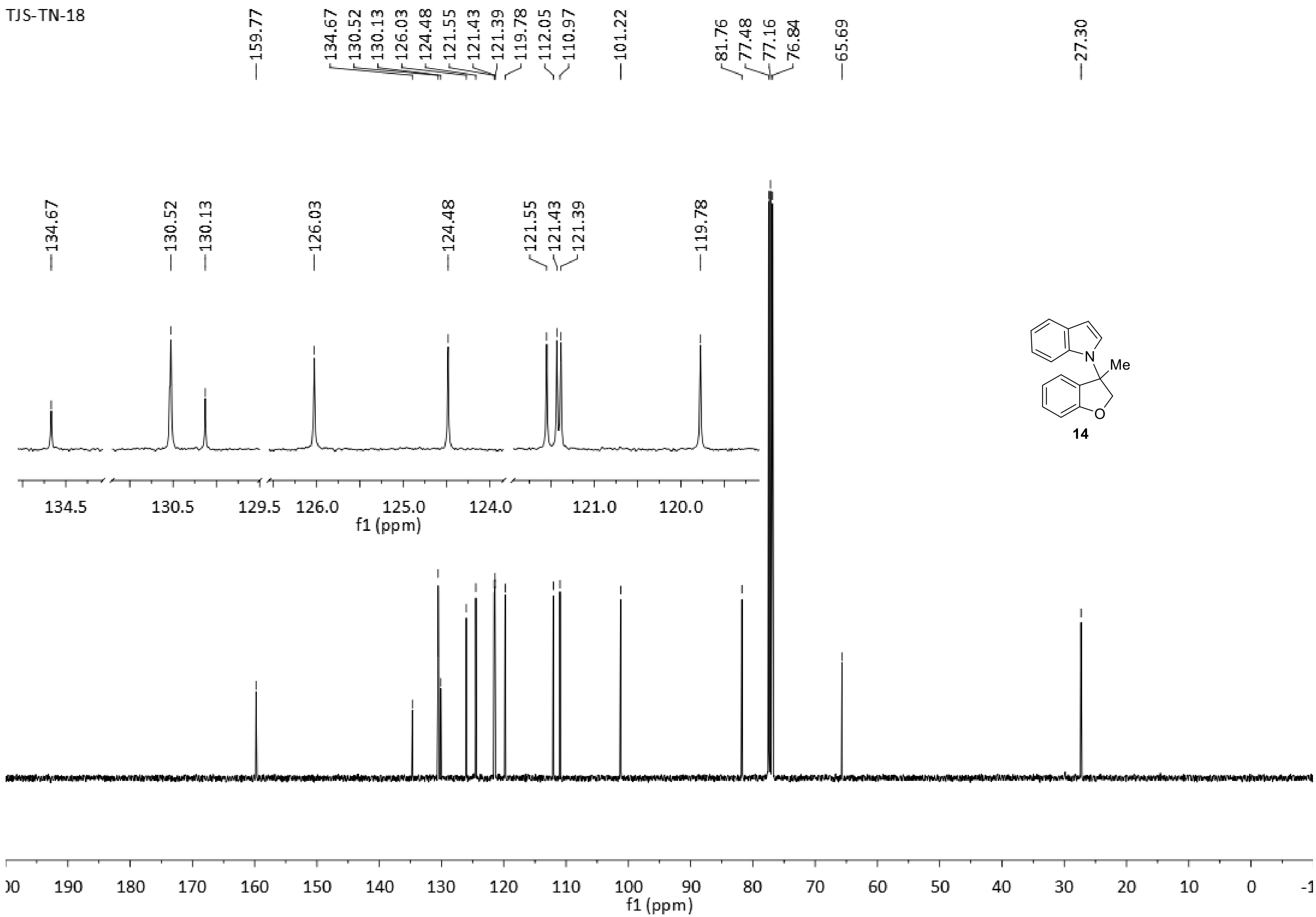

TJS-TM-186
10.363
7.663 7.659 7.657 7.654 7.643 7.640 7.637 7.635 7.319 7.316 7.300 7.291 7.275 7.271 7.260 7.256 7.252 7.110 7.108 7.091 7.088 7.083 7.073 7.071 7.069 7.064 6.995 6.993 6.974 6.957 6.792 6.790 6.771 6.769 6.663 6.662 6.655 6.653
2.185
2.04
3.54
2.09
1.05
1.03
1.00
0.99
3.16
f1 (ppm)
N
Me
CHO
Br
12

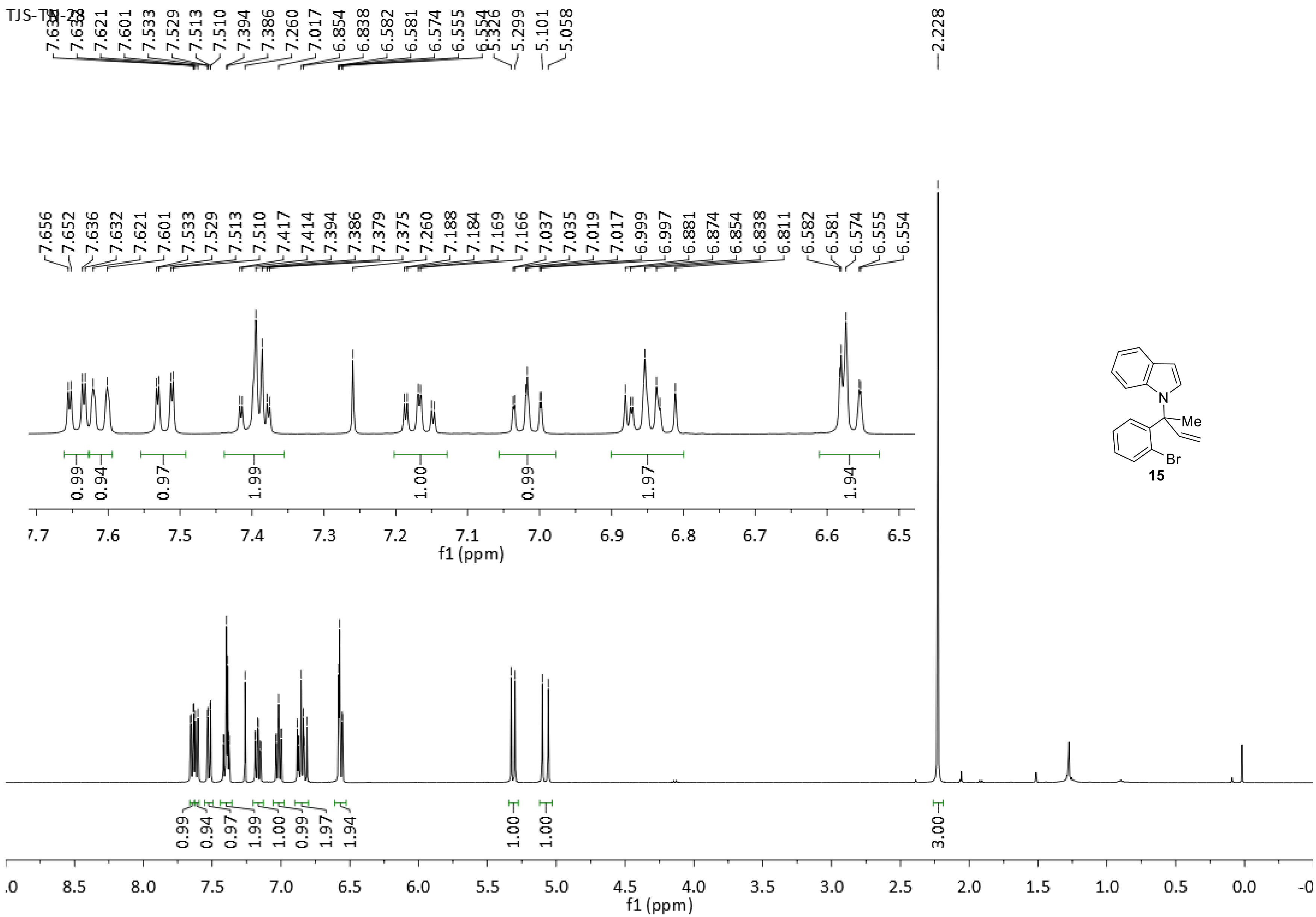

TJS-TM-136
194.30
138.40
135.44
130.30
130.26
129.41
128.32
125.39
121.89
121.55
121.24
120.35
112.69
103.66
77.48
77.16
76.84
70.47
22.10
f1 (ppm)
Me
CHO
N
Br
12

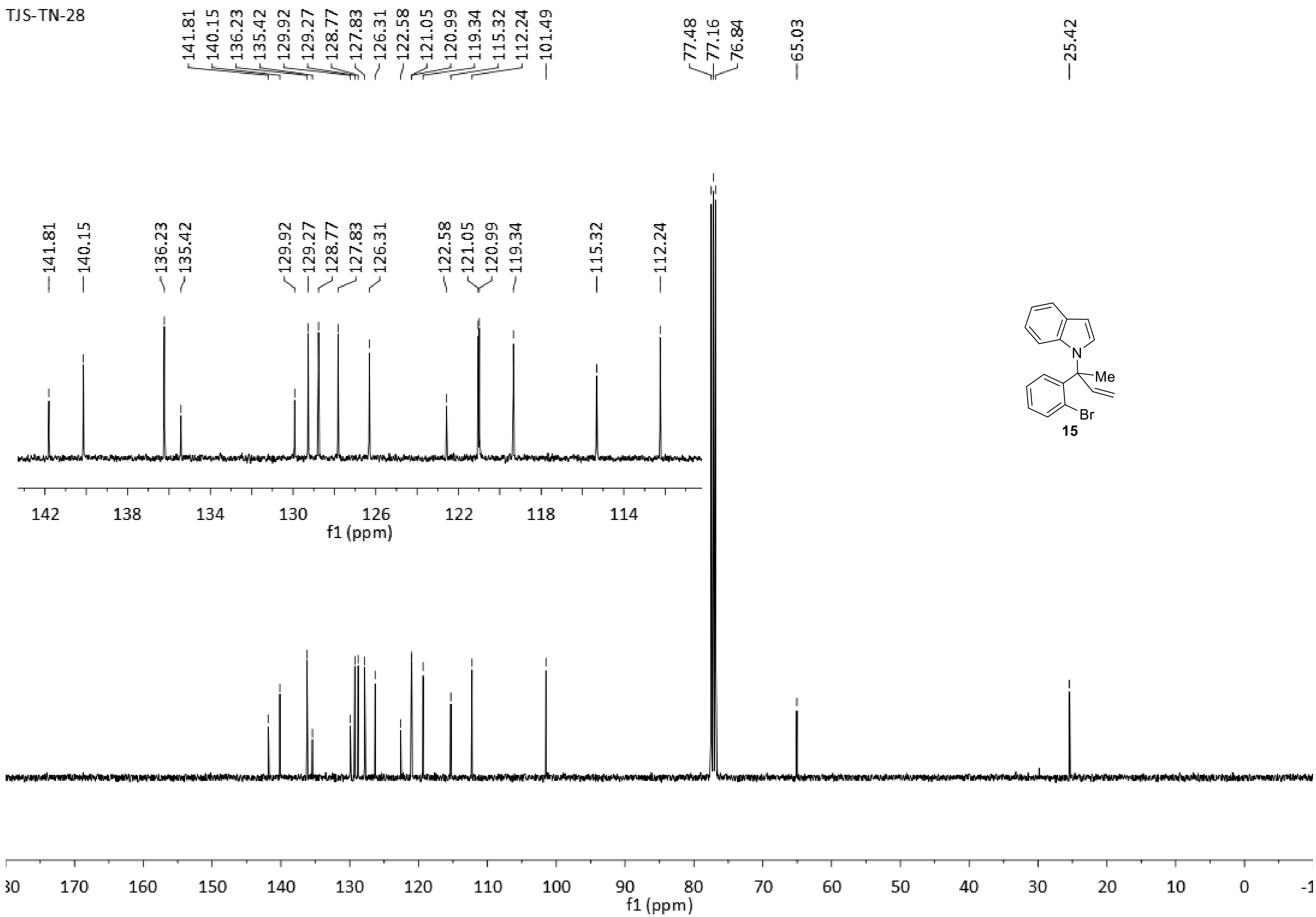

TJS-TN-22
2.145
0.99
1.98
1.96
0.98
0.98
0.98
0.94
0.96
1.00
1.00
3.00
f1 (ppm)
N
Me
OH
Br
13

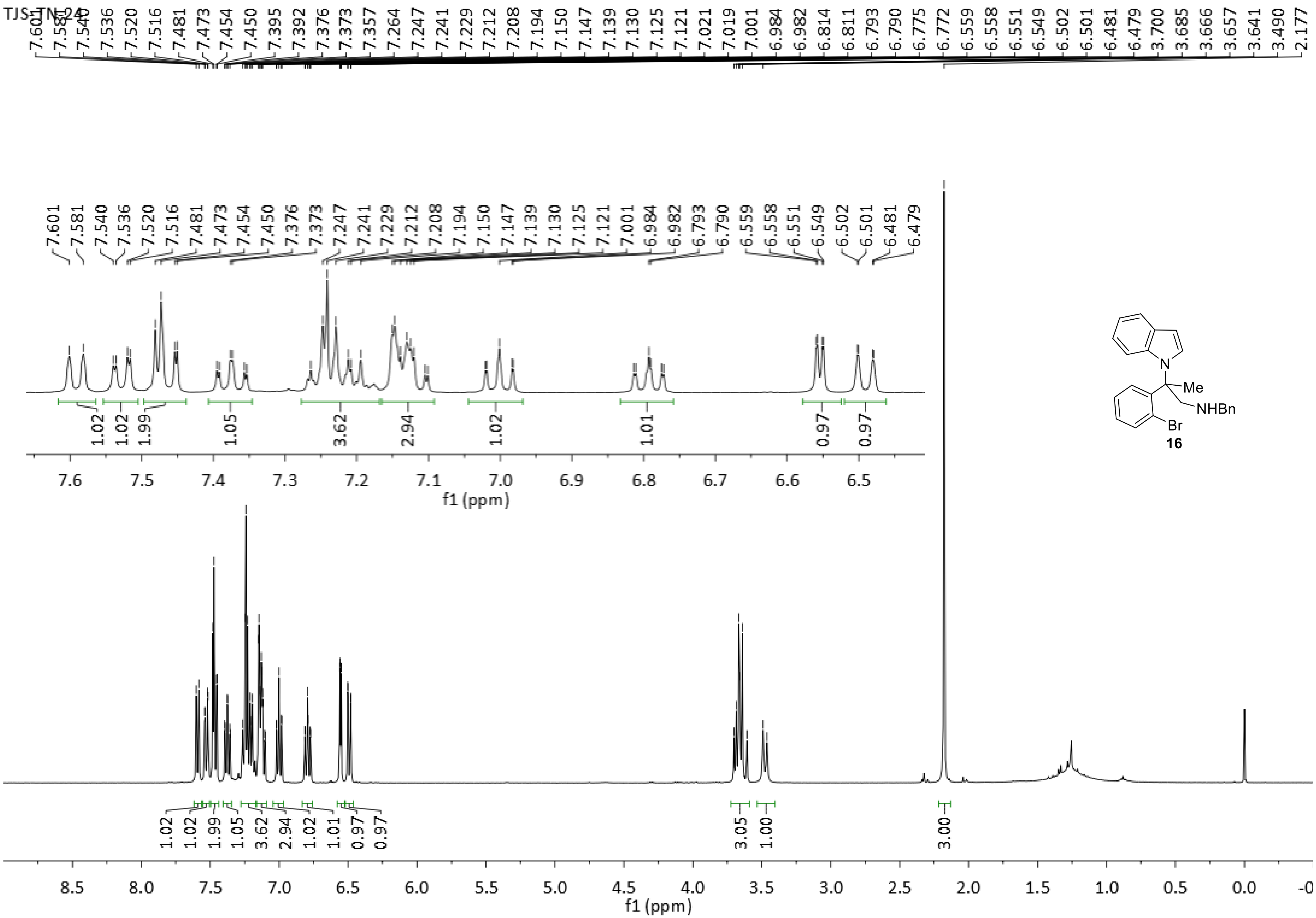

TJS-TN-22
140.76
136.30
135.19
129.98
129.27
127.96
127.76
127.17
122.51
121.21
121.13
119.65
111.90
101.69
77.48
77.16
76.84
68.03
64.41
23.65
140.763
136.302
135.194
129.976
129.273
127.957
127.759
127.166
122.510
121.205
121.129
119.653
f1 (ppm)
N
Me
OH
Br
13
f1 (ppm)


7.652 7.650 7.645 7.639 7.630 7.628 7.355 7.351 7.336 7.334 7.333 7.331 7.316 7.313 7.260 7.211 7.209 7.193 7.185 7.110 7.103 7.096 7.085 7.080 7.076 7.071 7.067 7.008 6.995 6.992 6.988 6.976 6.974 6.958 6.955 6.487 6.479
0.97
0.99
1.94
2.93
1.94
0.95
f1 (ppm)
5.052 5.028 4.587 4.563
2.144
2.04
3.02
f1 (ppm)
N
Me
O
14

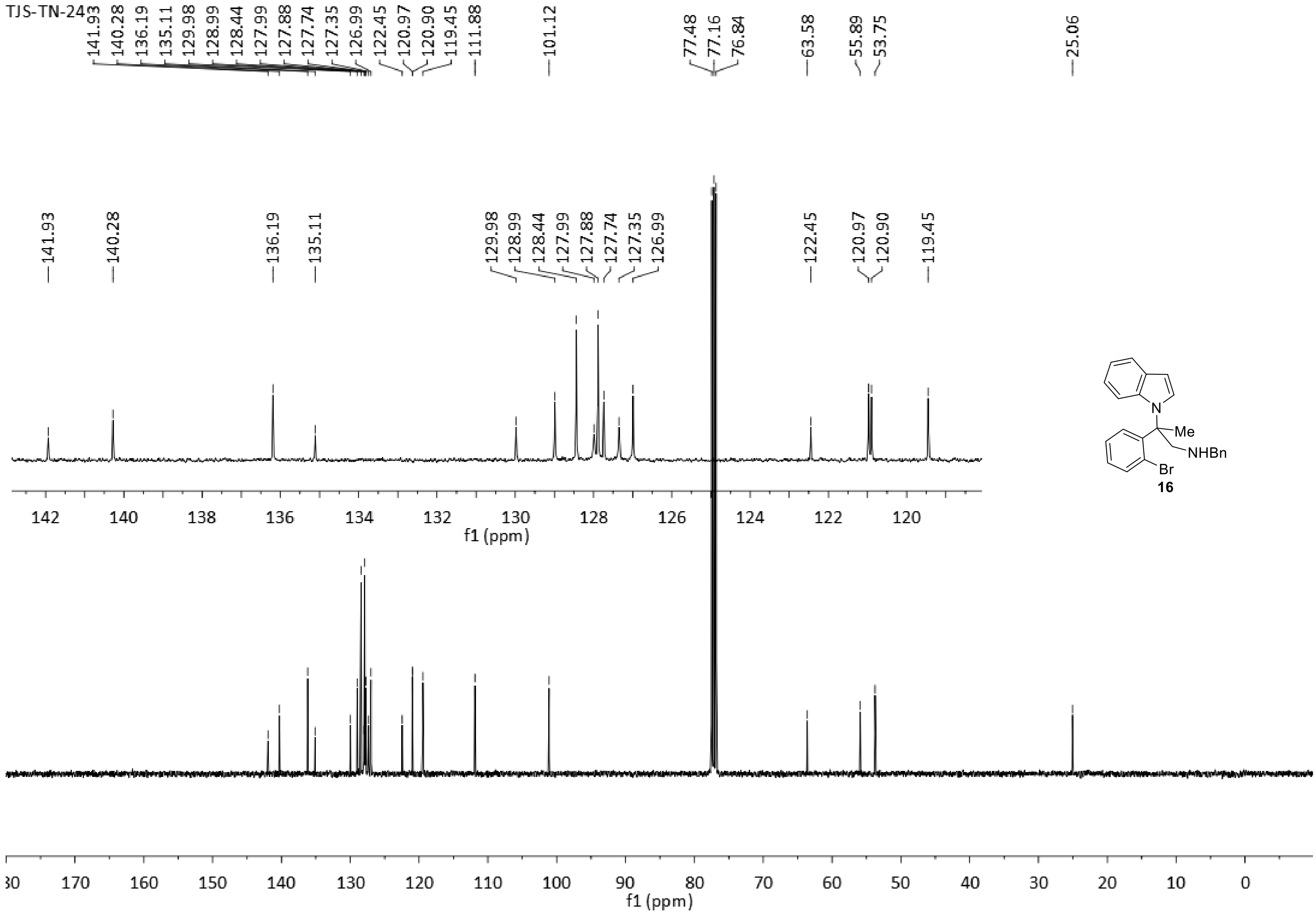

TJS-TN-18
159.77
134.67
130.52
130.13
126.03
124.48
121.55
121.43
121.39
119.78
112.05
110.97
101.22
81.76
77.48
77.16
76.84
65.69
27.30
Me
N
O
14
f1 (ppm)

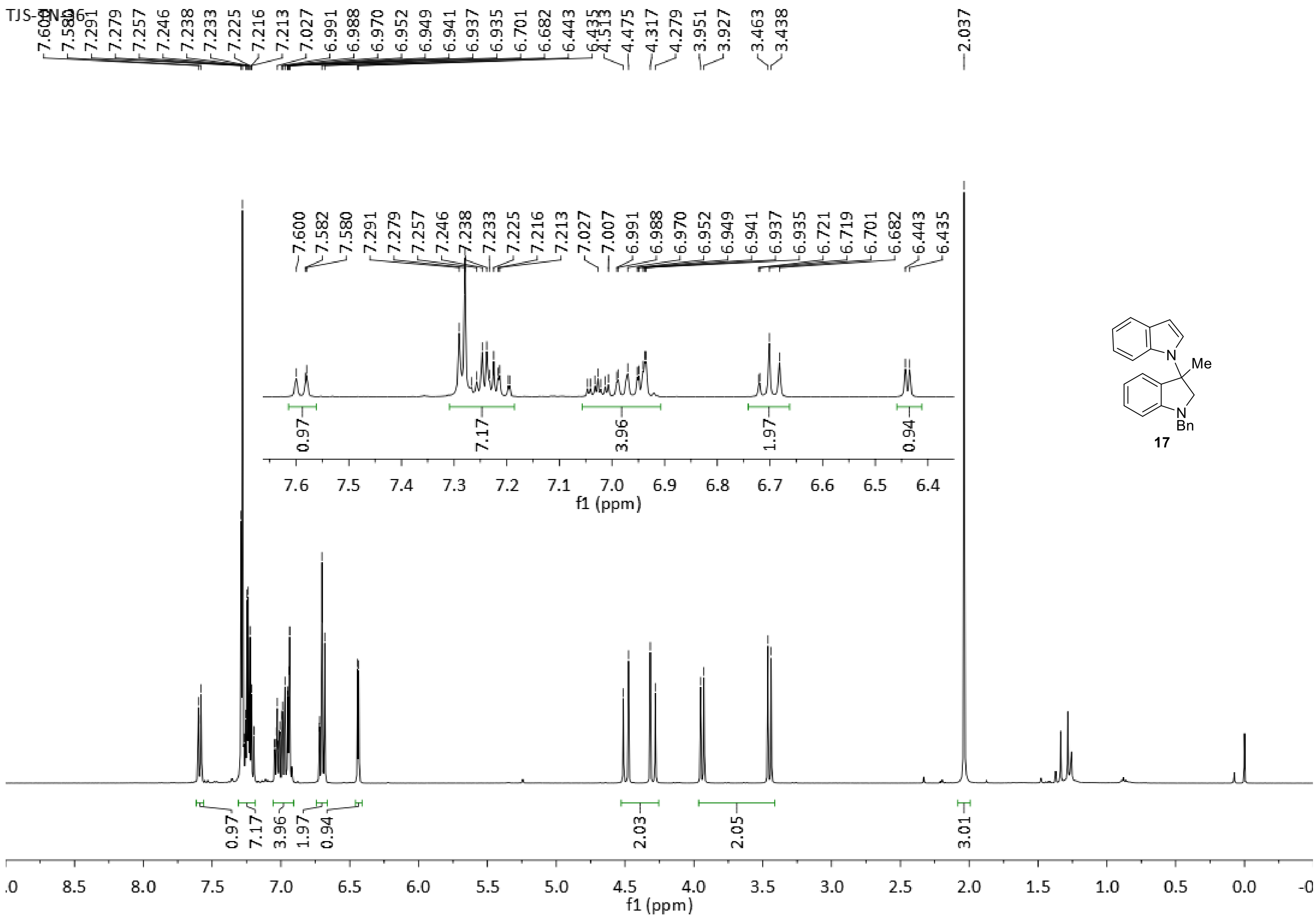

TJS-TN-28
f1 (ppm)
Me
Br
15

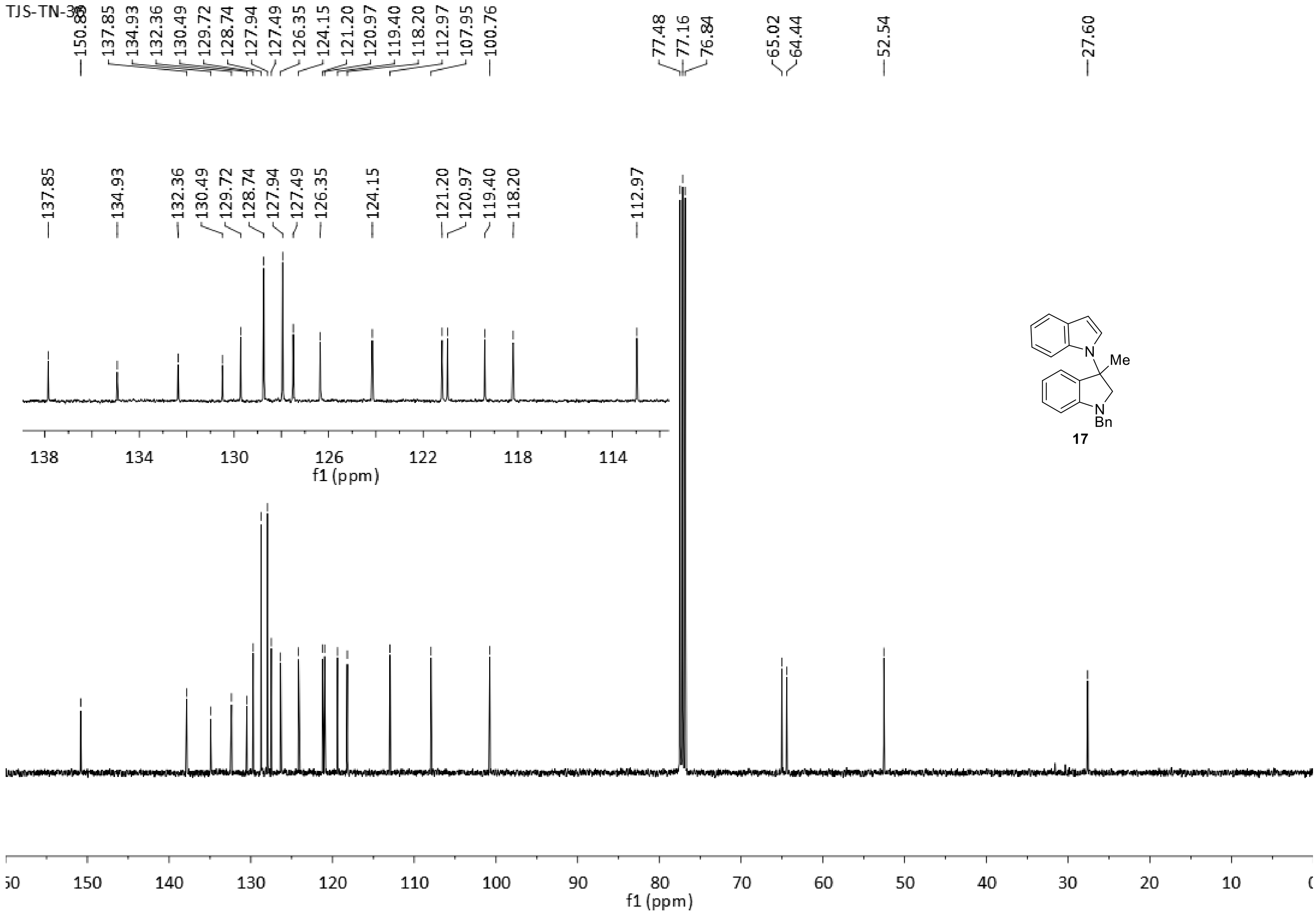

TJS-TN-28
141.81
140.15
136.23
135.42
129.92
129.27
128.77
127.83
126.31
122.58
121.05
120.99
119.34
115.32
112.24
101.49
77.48
77.16
76.84
65.03
25.42
142 138 134 130 126 122 118 114
f1 (ppm)
N
Me
Br
15
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



TJS-TN-24
7.601 7.581 7.540 7.536 7.520 7.516 7.481 7.473 7.454 7.450 7.395 7.392 7.376 7.373 7.357 7.264 7.247 7.241 7.229 7.212 7.208 7.194 7.150 7.147 7.139 7.130 7.125 7.121 7.021 7.019 7.001 6.984 6.982 6.814 6.811 6.793 6.790 6.775 6.772 6.559 6.558 6.551 6.549 6.502 6.501 6.481 6.479 3.700 3.685 3.666 3.657 3.641 3.490 2.177
1.02 1.02 1.99 1.05 3.62 2.94 1.02 1.01 0.97 0.97
3.05 1.00 3.00
f1 (ppm)
N
Me
NHBn
Br
16


TJS-TN-24
141.93
140.28
136.19
135.11
129.98
128.99
128.44
127.99
127.88
127.74
127.35
126.99
122.45
120.97
120.90
119.45
111.88
101.12
77.48
77.16
76.84
63.58
55.89
53.75
25.06
f1 (ppm)
f1 (ppm)
N
Me
NHBn
Br
16


TJS-3N-36
7.600
7.582
7.580
7.291
7.279
7.257
7.246
7.238
7.233
7.225
7.216
7.213
7.027
7.007
6.991
6.988
6.970
6.952
6.949
6.941
6.937
6.935
6.721
6.719
6.701
6.682
6.443
6.435
4.513
4.475
4.317
4.279
3.951
3.927
3.463
3.438
2.037
0.97
7.17
3.96
1.97
0.94
2.03
2.05
3.01
f1 (ppm)
Me
N
Bn
17


TJS-TN-36
150.86
137.85
134.93
132.36
130.49
129.72
128.74
127.94
127.49
126.35
124.15
121.20
120.97
119.40
118.20
112.97
107.95
100.76
77.48
77.16
76.84
65.02
64.44
52.54
27.60
138
134
130
126
122
118
114
f1 (ppm)
N
Me
N
Bn
17
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)