# Supporting Information

for

# Facile synthesis of Carbo- and Heterocycles via Fe(III)-Catalyzed Alkene Hydrofunctionalization

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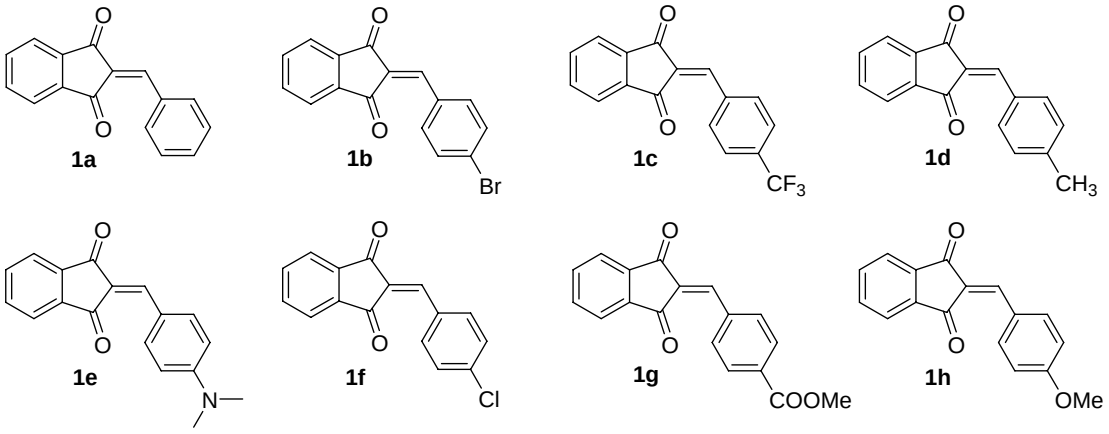
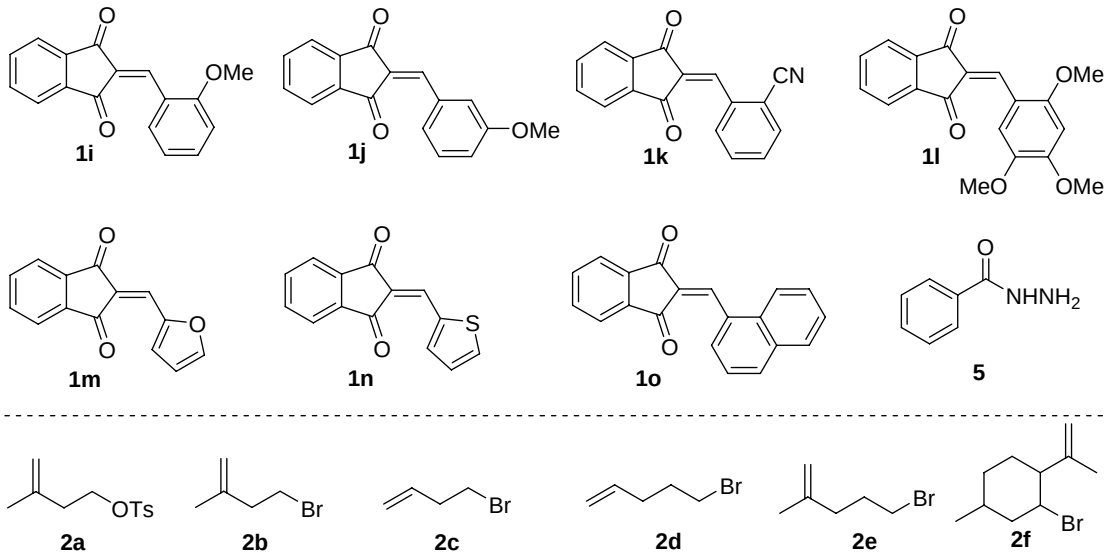
## 1. General Information:

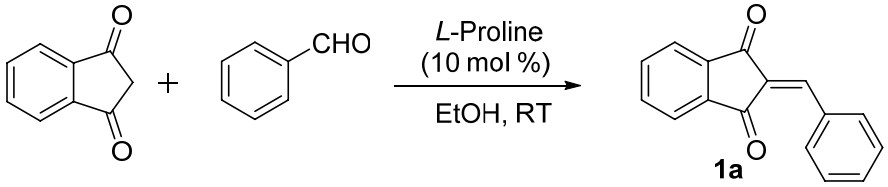
Infrared spectra were obtained on a FTIR spectrometer. $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded on BRUKER AVANCE III 600 or BRUKER AVANCE III 400 spectrometer. $CDCl_3$ was used as solvent. Chemical shifts were referenced relative to residual solvent. The following abbreviations are used to describe peak patterns where appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = double doublet, td = triple doublet. Coupling constants (*J*) are reported in Hertz (Hz). HRMS were performed on Agilent Technologies 6224 TOF LC/MS (ESI). Melting points were measured with micro melting point apparatus.

$Fe(acac)_3$, $PhSiH_3$, EtOH, THF, NaOAc were commercial available, and the 1,3-diones (**1a-1o**) and benzoyl hydrazine were prepared easily. The olefins bearing an (pseudo)halide tether (**2a-2f**) were commercially available or prepared according the literature.



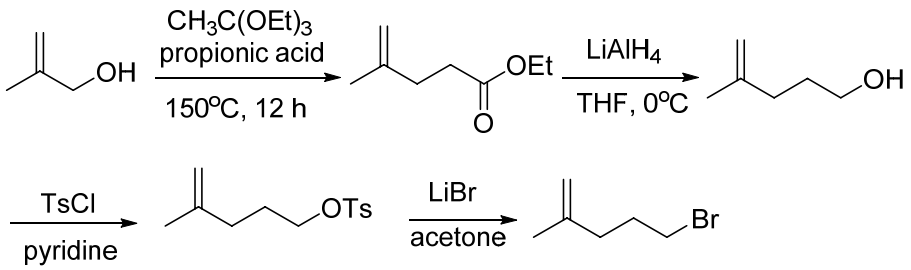



## 2. Typical Procedure for Synthesis of 1a:




To a 50 mL flask containing 1*H*-indene-1,3(2H)-dione (1.46 g, 10 mmol), 20 mL EtOH and benzaldehyde (1.27 g, 12 mmol), *L*-Proline (318 mg, 3 mmol) was added. After the completion of the reaction as indicated by Thin Layer Chromatography (TLC), ethyl acetate was added to the crude reaction mixture. The reaction mixture in ethyl acetate was added to water for the removal of the catalyst. The organic layer was separated, dried over anhydrous $Na_2SO_4$ and evaporated under a vacuum. The crude products were purified by flash column chromatography on silica gel using ethyl acetate/Petroleum ether (v/v, 1:10) as eluent to get 2-benzylidene-1*H*-indene-1,3(2*H*)-dione **1a** (1.68 g, 72% yield).

## 3. Typical Procedure for Synthesis of 2e:



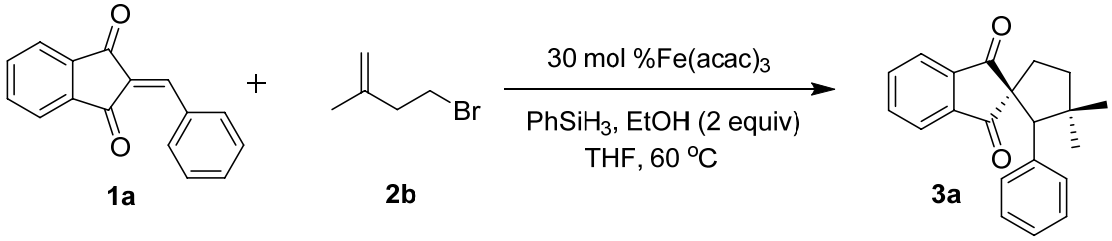

The solution of 2-methallyl alcohol (3.6 g, 50 mmol), propionic acid (3 mL) in triethyl orthoacetate 20 mL was refluxed for 12 hours. The reaction mixture was diluted with ether (200 mL) extracted with 10% HCl solution (200 mL), saturated $NaHCO_3$ and brine. The combined organic layer was dried over $MgSO_4$ and concentrated in vacuo afforded the ester in quantitative yield (7.0 g).

To the suspension of $LiAlH_4$ (1.14 g, 30 mmol) in THF (50 mL), was added the solution of ester (2.84 g, 20 mmol) in THF (10 mL) at 0 °C under Ar. The reaction was carried out for 20 minutes and then worked up with water (24 mL) followed by 2M NaOH (8 mL). The reaction mixture was filtered through celite. The filtrate was extracted with brine and dried over $MgSO_4$ to obtain alcohol (1.64 g, 82%).

To the solution of alcohol (1.64 g, 16.4 mmol) in pyridine (30 mL) was added *p*-toluenesulfonylchloride (3.11 g, 16.4 mmol) at 0 °C. The reaction was stirred for overnight and then extracted with 6M HCl solution, brine solution and dried over $MgSO_4$. The crude product was purified by column chromatography to obtain 4-methylpent-4-en-1-yl 4-methylbenzenesulfonate in high yield (3.66 g, 88%).

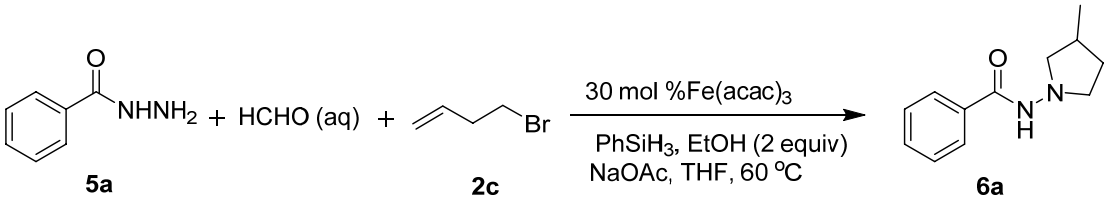
The suspension of 4-methylpent-4-en-1-yl 4-methylbenzenesulfonate (3.66 g, 14.4 mmol) and Lithium bromide (2.47 g, 28.8 mmol) in acetone (60 mL) was refluxed for 8 hours. After extraction with pentane and water, the combined organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo to give crude product which was purified by flash column chromatography on silica gel using Petroleum ether as eluent to get **2e** (1.68 g, 72% yield).

**4. Typical Procedure for Synthesis of 3a:**




A Schlenk tube containing $Fe(acac)_3$ (21.3 mg, 30 mol %) and 2-benzylidene-1*H*-indene-1,3(2*H*)-dione **1a** (46.8 mg, 0.2 mmol) were evacuated and purged with Argon three times. Afterwards, 4-bromo-2-methylbut-1-ene **2b** (64.8 mg, 0.4 mmol), $PhSiH_3$ (21.6 mg, 0.2 mmol), EtOH (18.4 mg, 0.4 mmol) and 2 ml THF was added via syringe. The solution was kept at 60 °C for 6 h. Then the solution was diluted with ethyl acetate and transferred to a round bottom flask. Silica gel was added to the flask and volatiles were evaporated under vacuum. The purification was performed by flash column chromatography on silica gel using ethyl acetate/petroleum ether (v/v, 1:10) as eluent to give **3a** as a white solid (49.8 mg, 82% yield).

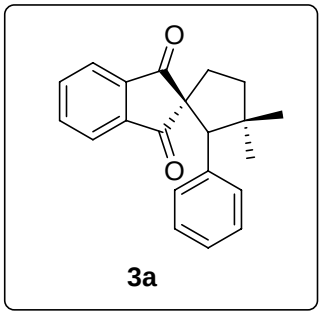
## 5. Typical Procedure for Synthesis of 6a:




A Schlenk tube containing $Fe(acac)_3$ (21.3 mg, 30 mol %), benzoyl hydrazone **5** (46.8 mg, 0.2 mmol) and NaOAc (27.2 mg, 0.2 mmol) were evacuated and purged with Argon three times. Afterwards, 4-bromobut-1-ene **2c** (54 mg, 0.4 mmol), $PhSiH_3$ (21.6 mg, 0.2 mmol), EtOH (18.4 mg, 0.4 mmol) and 2 ml THF was added via syringe. The solution was kept at 60 °C for 6 h. Then the solution was diluted with ethyl acetate and transferred to a round bottom flask. Silica gel was added to the flask and volatiles were evaporated under vacuum. The purification was performed by HPLC using MeOH/$H_2O$ (v/v, 70:30) as eluent to give **6a** as a pale yellow solid (20.8 mg, 51% yield).

## 6. Characterization of 3, 4 and 6:

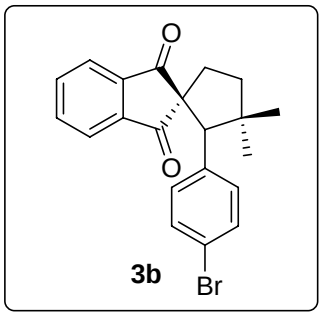
### 3,3-Dimethyl-2-phenylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3a)




White solid; m.p. 128-129 °C; $R_f$ = 0.50 (EtOAc/Petroleum ether 1:10); $^1H$ NMR ($CDCl_3$, 600MHz), δ: 7.81-7.76 (m, 2H), 7.67-7.63 (m, 2H), 7.07-7.03 (m, 5H), 3.31 (s, 1H), 2.43-2.29 (m, 1H), 2.11-2.07 (m, 1H), 1.99-1.97

(m, 2H), 1.27 (s, 3H), 1.01 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 205.23, 204.28, 142.90, 141.51, 136.42, 135.60, 135.23, 130.70, 127.92, 127.09, 123.16, 122.98, 67.20, 66.39, 45.06, 42.28, 32.11, 28.85, 23.45; IR (KBr) *v*: 2956, 2870, 1736, 1690, 1589, 1442, 1361, 1269, 1138, 813, 763, 702 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{21}H_{21}O_2$ ($M+H^+$): 305.1541; Found: 305.1544.

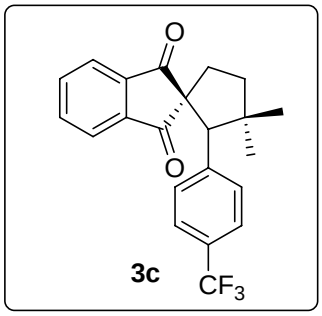
**2-(4-Bromophenyl)-3,3-dimethylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3b)**




Pale yellow solid; m.p. 129-130 ºC; $R_f$ = 0.68 (EtOAc/Petroleum ether 1:20); $^1$H NMR ($CDCl_3$, 600MHz), δ: 7.83-7.80 (m, 2H), 7.72-7.69 (m, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.4 Hz, 2H), 3.29 (s, 1H), 2.32-2.27 (m, 1H), 2.09-2.05 (m, 1H), 1.98-1.95 (m, 2H), 1.25 (s, 3H), 1.00 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.95, 204.08, 142.68, 141.43, 135.86, 135.55, 135.53, 132.41, 131.10, 123.30, 123.12, 121.37, 66.06, 66.01, 45.04, 42.16, 32.60, 28.76, 23.36; IR (KBr) *v*: 2961, 2931, 2844, 1736, 1690, 1583, 1477, 1254, 1153, 1072, 1006, 788 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{21}H_{20}BrO_2$ ($M+H^+$): 383.0646; Found: 383.0648.

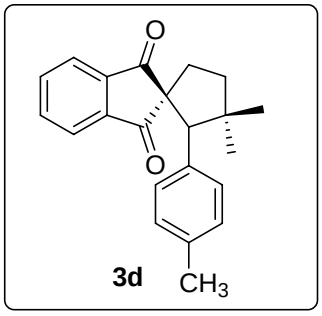
**3,3-Dimethyl-2-(4-(trifluoromethyl)phenyl)spiro[cyclopentane-1,2'-**

**indene]-1',3'-dione (3c)**




Pale yellow solid; m.p. 93-94 °C; $R_f$ = 0.60 (EtOAc/Petroleum ether 1:30); $^1$H NMR ($CDCl_3$, 600MHz), δ: 7.84-7.81 (m, 2H), 7.71-7.69 (m, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 3.41 (s, 1H), 2.34-2.29 (m, 1H), 2.12-2.08 (m, 1H), 2.01-1.98 (m, 2H), 1.27 (s, 3H), 1.03 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.68, 203.92, 142.57, 141.68 (q, *J* = 268.5 Hz), 141.36, 135.92, 135.64, 131.05, 129.33 (q, *J* = 31.5 Hz), 124.86 (q, *J* = 4.5 Hz), 123.34, 123.20, 66.05, 66.00, 45.26, 42.21, 32.98, 28.80, 23.48; $^{19}$F NMR (CDCl3, 376Hz), δ: -62.67; IR (KBr) *v*: 2951, 2931, 2860, 2363, 1746, 1690, 1538, 1477, 1330, 1280, 1097, 1016, 844, 808 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{20}F_3O_2$ ($M+H^+$): 373.1415; Found: 373.1405.

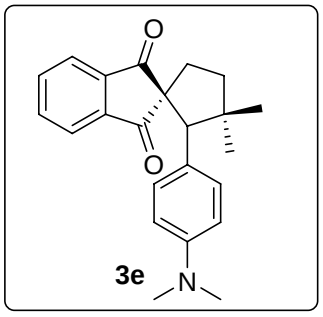
**3,3-Dimethyl-2-(*p*-tolyl)spiro[cyclopentane-1,2'-indene]-1',3'-dione (3d)**




Pale yellow solid; m.p. 117-118 °C; $R_f$ = 0.60 (EtOAc/Petroleum ether

1:20); $^{1}$H NMR ($CDCl_3$, 600MHz), δ: 7.81-7.78 (m, 2H), 7.66-7.64 (m, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 3.29 (s, 1H), 2.32-2.27 (m, 1H), 2.15 (s, 3H), 2.09-2.05 (m, 1H), 1.98-1.95 (m, 2H), 1.25 (s, 3H), 1.00 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 205.37, 204.38, 142.93, 141.55, 136.59, 135.36, 135.20, 133.26, 130.59, 128.63, 123.18, 122.98, 66.81, 66.31, 44.96, 42.21, 32.23, 28.84, 23.43, 20.99; IR (KBr) *v*: 2956, 2936, 2870, 1736, 1695, 1578, 1518, 1467, 1356, 1259, 1148, 910, 742 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{23}O_2$ ($M+H^+$): 319.1698; Found: 319.1706.

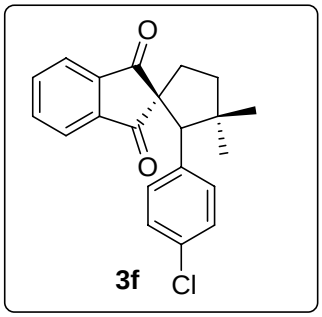
**2-(4-(Dimethylamino)phenyl)-3,3-dimethylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3e)**




Yellow solid; m.p. 93-94 °C; $R_f$ = 0.60 (EtOAc/Petroleum ether 1:5); $^{1}$H NMR ($CDCl_3$, 400MHz), δ: 7.80-7.77 (m, 2H), 7.66-7.63 (m, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 6.42 (d, *J* = 8.8 Hz, 2H), 3.24 (s, 1H), 2.80 (s, 6H), 2.32-2.25 (m, 1H), 2.08-2.02 (m, 1H), 1.96-1.92 (m, 2H), 1.25 (s, 3H), 0.98 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 205.81, 204.61, 149.43, 143.06, 141.68, 135.48, 135.07, 131.46, 124.02, 123.15, 122.91, 111.93, 66.72, 66.44, 44.99, 42.16, 40.48, 32.02, 28.81, 23.38; IR (KBr) *v*: 2946, 2911,

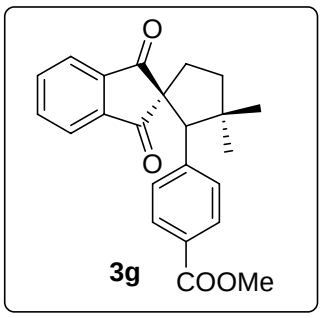
1746, 1700, 1624, 1518, 1356, 1259, 1107, 956, 819 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{23}H_{26}NO_2$ ($M+H^+$): 348.1963; Found: 348.1970.

**2-(4-Chlorophenyl)-3,3-dimethylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3f)**



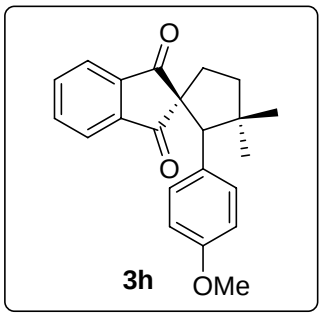

Pale yellow solid; m.p. 119-120 $^oC$; $R_f$ = 0.57 (EtOAc/Petroleum ether 1:20); $^1H$ NMR ($CDCl_3$, 400MHz), δ: 7.83-7.80 (m, 2H), 7.71-7.69 (m, 2H), 7.06-7.00 (m, 4H), 3.30 (s, 1H), 2.34-2.26 (m, 1H), 2.11-2.05 (m, 1H), 1.99-1.95 (m, 2H), 1.25 (s, 3H), 1.00 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 150MHz), δ: 204.96, 204.08, 142.69, 141.44, 135.83, 135.51, 134.99, 133.11, 132.03, 128.13, 123.27, 123.09, 66.08, 66.06, 45.06, 42.16, 32.50, 28.75, 23.34; IR (KBr) *v*: 2946, 2921, 2855, 1736, 1695, 1573, 1492,1366, 1265, 1158, 1011, 813, 778 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{21}H_{20}ClO_2$ ($M+H^+$): 339.1151; Found: 339.1140.

**Methyl 4-(3,3-dimethyl-1',3'-dioxo-1',3'-dihydrospiro[cyclopentane-1,2'-inden]-2-yl)benzoate (3g)**




Pale yellow oil; $R_f$ = 0.22 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.81-7.77 (m, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.67-7.65 (m, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 3.81 (s, 3H), 3.38 (s, 1H), 2.36-2.28 (m, 1H), 2.12-2.06 (m, 1H), 2.01-1.97 (m, 2H), 1.27 (s, 3H), 1.01 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.76, 203.93, 166.99, 142.64, 141.98, 141.32, 135.83, 135.50, 130.70, 129.15, 128.96, 123.26, 123.08, 66.63, 66.13, 52.09, 45.33, 42.28, 32.48, 28.83, 23.45; IR (film) *v*: 2946, 2921, 1715, 1700, 1619, 1604, 1442, 1269, 1178, 1108, 1026, 763 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{23}H_{23}O_4$($M+H^+$): 363.1596; Found: 363.1592.

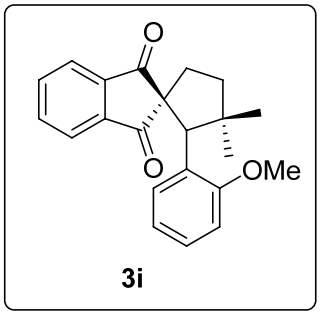
**2-(4-Methoxyphenyl)-3,3-dimethylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3h)**




Pale yellow solid; m.p. 100-101 $^o$C; $R_f$ = 0.40 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.81-7.77 (m, 2H), 7.67-7.65 (m, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.59 (d, *J* = 8.8 Hz, 2H), 3.65 (s, 3H), 3.27

(s, 1H), 2.33-2.22 (m, 1H), 2.09-2.03 (m, 1H), 1.97-1.94 (m, 2H), 1.25 (s, 3H), 0.99 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 205.49, 204.42, 158.58, 142.94, 141.59, 135.60, 135.22, 131.76, 128.38, 123.17, 122.95, 113.26, 66.54, 66.39, 55.12, 44.95, 42.17, 31.98, 28.78, 23.35; IR (KBr) *v*: 2941, 2880, 1740, 1705, 1599, 1508, 1482, 1437, 1350, 1168, 1047, 910, 829 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{23}O_3$ ($M+H^+$): 335.1647; Found: 335.1660.

**2-(2-Methoxyphenyl)-3,3-dimethylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3i)**

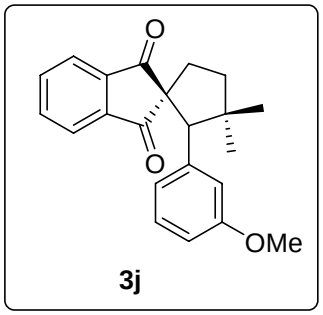



**3i**

Pale yellow solid; m.p. 69-70 °C; $R_f$ = 0.36 (EtOAc/Petroleum ether 1:20); $^1$H NMR ($CDCl_3$, 600MHz), δ: 7.83 (d, $J$ = 7.2 Hz, 1H), 7.65-7.63 (m, 2H), 7.61-7.59 (m, 1H), 7.31 (dd, $J_1$ = 7.8 Hz, $J_2$ = 1.2 Hz, 1H), 6.97 (td, $J_1$ = 7.8 Hz, $J_2$ = 1.2 Hz, 1H), 6.73 (td, $J_1$ = 7.2 Hz, $J_2$ = 1.2 Hz, 1H), 6.50 (d, $J$ = 8.4 Hz, 1H), 4.10 (s, 1H), 3.48 (s, 3H), 2.34-2.29 (m, 1H), 2.11-2.01 (m, 2H), 1.92-1.88 (m, 1H), 1.37 (s, 3H), 1.05 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.67, 204.19, 157.95, 142.59, 141.77, 135.11, 134.85, 130.63, 127.67, 125.33, 122.85, 122.53, 119.92, 110.27, 66.12, 55.52, 55.28, 45.11, 43.39, 31.49, 28.46, 24.00; IR (KBr) *v*: 2951, 2860, 1746,

1695, 1599, 1510, 1471, 1269, 1244, 1107, 1037, 910, 768, 657 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{23}O_3$ ($M+H^+$): 335.1647; Found: 335.1649.

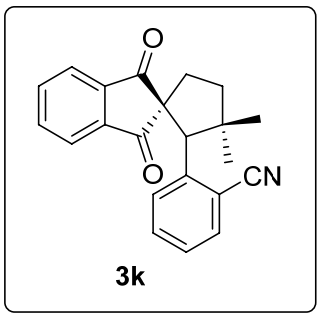
**2-(3-Methoxyphenyl)-3,3-dimethylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3j)**




**3j**

Pale yellow solid; m.p. 106-107 $^oC$; $R_f$ = 0.36 (EtOAc/Petroleum ether 1:20); $^1H$ NMR ($CDCl_3$, 600MHz), δ: 7.82-7.78 (m, 2H), 7.68-7.64 (m, 2H), 6.96 (t, $J$ = 7.8 Hz, 1H), 6.65-6.62 (m, 2H), 6.58 (dd, $J_1$ = 8.4 Hz, $J_2$ = 0.6 Hz, 1H), 3.67 (s, 3H), 3.29 (s, 1H), 2.33-2.28 (m, 1H), 2.10-2.06 (m, 1H), 1.99-1.96 (m, 2H), 1.28 (s, 3H), 1.03 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 150MHz), δ: 205.18, 204.33, 159.00, 142.94, 141.50, 137.98, 135.63, 135.24, 128.80, 123.19, 123.15, 123.04, 116.12, 112.84, 67.14, 66.28, 55.15, 45.07, 42.28, 32.17, 28.90, 23.51; IR (KBr) *v*: 2961, 2931, 2860, 1730, 1690, 1583, 1472, 1447, 1350, 1290, 1168, 1037, 793 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{23}O_3$ ($M+H^+$): 335.1647; Found: 335.1655.

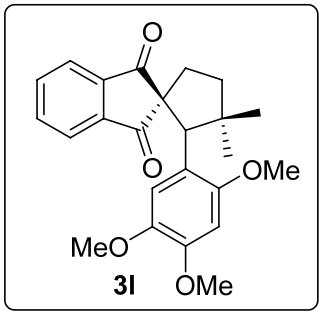
**2-(3,3-Dimethyl-1',3'-dioxo-1',3'-dihydrospiro[cyclopentane-1,2'-inden]-2-yl)benzonitrile (3k)**




**3k**

Pale yellow solid; m.p. 113-114 °C; $R_f$ = 0.48 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.85-7.81 (m, 2H), 7.74-7.69 (m, 2H), 7.38-7.36 (m, 3H), 7.20 (td, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 3.36 (s, 1H), 2.34-2.27 (m, 1H), 2.12-2.06 (m, 1H), 2.01-1.97 (m, 2H), 1.27 (s, 3H), 1.02 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.36, 203.61, 142.44, 141.30, 138.25, 136.00, 135.74, 135.19, 134.18, 130.98, 128.83, 123.37, 123.29, 118.80, 112.22, 65.86, 65.55, 45.20, 42.07, 33.04, 28.76, 23.45; IR (KBr) *v*: 2946, 2925, 2870, 2217, 1746, 1695, 1589, 1477, 1371, 1259, 1132, 925, 788, 732 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{20}NO_2$ ($M+H^+$): 330.1494; Found: 330.1480.

**3,3-Dimethyl-2-(2,4,5-trimethoxyphenyl)spiro[cyclopentane-1,2'-indene]-1',3'-dione (3l)**

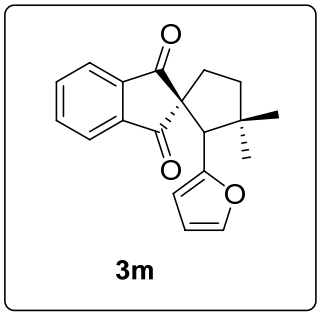



**3l**

Yellow solid; m.p. 122-123 °C; $R_f$ = 0.24 (EtOAc/Petroleum ether 1:8); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.83-7.81 (m, 1H), 7.70-7.67 (m, 1H), 7.66-

7.62 (m, 2H), 6.86 (s, 1H), 6.20 (s, 1H), 4.06 (s, 1H), 3.77 (s, 3H), 3.72 (s, 3H), 3.52 (s, 3H), 2.35-2.28 (m, 1H), 2.11-1.98 (m, 2H), 1.94-1.88 (m, 1H), 1.32 (s, 3H), 1.01 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 205.00, 204.93, 152.75, 147.94, 142.82, 142.18, 141.72, 135.33, 135.01, 122.84, 122.68, 116.57, 114.52, 97.64, 66.15, 57.16, 56.31, 55.83, 55.80, 45.17, 42.79, 31.35, 28.43, 23.79; IR (KBr) *v*: 2936, 2855, 1730, 1705, 1599, 1512, 1462, 1325, 1275, 1203, 1047, 905, 783 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{24}H_{27}O_5$ ($M+H^+$): 395.1858; Found: 395.1851.

**2-(Furan-2-yl)-3,3-dimethylspiro[cyclopentane-1,2'-indene]-1',3'-dione (3m)**

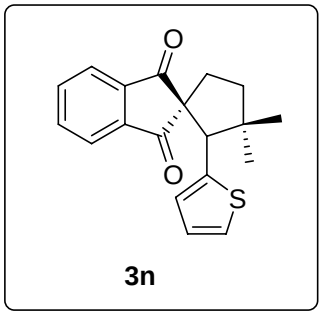



**3m**

Pale yellow solid; m.p. 49-50 $^{o}$C; $R_f$ = 0.48 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.90-7.84 (m, 2H), 7.76-7.72 (m, 2H), 7.03 (d, $J$ = 1.6 Hz, 1H), 6.05 (dd, $J_1$ = 3.2 Hz, $J_2$ = 1.6 Hz, 1H), 5.93 (d, $J$ = 3.2 Hz, 1H), 3.49 (s, 1H), 2.28-2.21 (m, 1H), 2.09-2.02 (m, 1H), 1.97-1.92 (m, 2H), 1.23 (s, 3H), 1.14 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.58, 202.58, 151.11, 142.75, 141.58, 141.35, 135.68, 135.18, 123.21, 123.17, 110.07, 108.75, 64.71, 59.09, 44.58, 42.17, 32.07, 28.92, 23.34; IR (KBr) *v*: 2941, 2865, 2359, 1736, 1700, 1593, 1497, 1437, 1340, 1265, 1234,

1143, 1011, 793, 753 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{19}H_{19}O_3$ ($M+H^+$): 295.1334; Found: 295.1330.

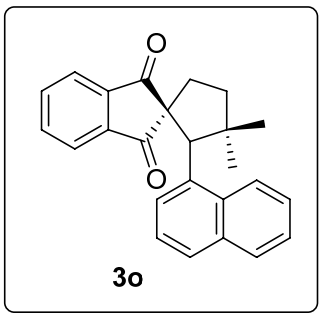
**3,3-Dimethyl-2-(thiophen-2-yl)spiro[cyclopentane-1,2'-indene]-1',3'-dione (3n)**




**3n**

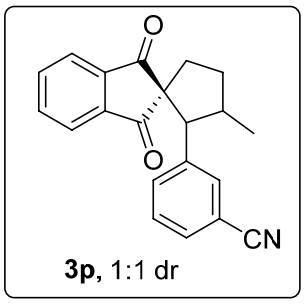
Pale yellow solid; m.p. 70-71 $^oC$; $R_f$ = 0.60 (EtOAc/Petroleum ether 1:10); $^1H$ NMR ($CDCl_3$, 400MHz), δ: 7.87-7.84 (m, 1H), 7.82-7.78 (m, 1H), 7.72-7.68 (m, 2H), 6.93 (d, *J* = 5.2 Hz, 1H), 6.73 (t, *J* = 3.6 Hz, 1H), 6.70 (d, *J* = 3.2 Hz, 1H), 3.65 (s, 1H), 2.32-2.24 (m, 1H), 2.09-2.03 (m, 1H), 1.98-1.94 (m, 2H), 1.32 (s, 3H), 1.08 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 150MHz), δ: 204.88, 203.50, 142.90, 141.67, 137.81, 135.70, 135.30, 127.83, 126.72, 124.29, 123.29, 123.09, 66.21, 61.13, 44.94, 42.05, 32.02, 28.65, 23.23; IR (KBr) *v*: 2966, 2921, 2860, 2359, 1736, 1705, 1583, 1350, 1265, 1128, 1077, 854, 727 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{19}H_{19}O_2S$ ($M+H^+$): 311.1106; Found: 311.1113.

**3,3-Dimethyl-2-(naphthalen-1-yl)spiro[cyclopentane-1,2'-indene]-1',3'-dione (3o)**




Yellow solid; m.p. 126-127 °C; $R_f$ = 0.48 (EtOAc/Petroleum ether 1:20); $^1$H NMR ($CDCl_3$, 400MHz), δ: 8.12 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 2H), 7.57-7.48 (m, 4H), 7.44 (td, $J_1$ = 7.8 Hz, $J_2$ = 1.2 Hz, 1H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.26 (t, *J* = 8.4 Hz, 1H), 4.56 (s, 1H), 2.47-2.38 (m, 1H), 2.23-2.14 (m, 2H), 2.12-2.04 (m, 1H), 1.39 (s, 3H), 1.00 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 205.29, 204.52, 142.88, 141.30, 135.49, 135.08, 133.88, 133.46, 132.52, 128.84, 128.32, 127.51, 126.28, 125.20, 124.63, 123.38, 122.96, 66.65, 57.58, 45.96, 42.75, 32.41, 28.95, 23.91; IR (KBr) *v*: 2941, 2865, 1730, 1700, 1583, 1457, 1386, 1254, 788, 732 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{25}H_{22}O_2Na$ ($M+Na^+$): 377.1518; Found: 377.1511.

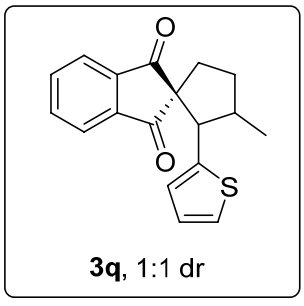
**3-(3-Methyl-1',3'-dioxo-1',3'-dihydrospiro[cyclopentane-1,2'-inden]-2-yl)benzonitrile (3p)**




Pale yellow oil; $R_f$ = 0.32 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$,

400MHz), δ: 7.94 and 7.88 (m, 1H), 7.80-7.71 (m, 2H), 7.69-7.64 (m, 1H), 7.43 (m, 0.5H), 7.35-7.30 (m, 1.5H), 7.28-7.24 (m, 1.5H), 7.19-7.15 (m, 0.5H), 3.58 (d, *J* = 8.0 Hz, 0.5H), 3.19 (d, *J* = 12.4 Hz, 0.5H), 3.02-2.95 and 2.88-2.81 (m, 1H), 2.36-2.28 (m, 1H), 2.23-1.96 (m, 2H), 1.77-1.67 (m, 1H), 0.96 (d, *J* = 6.0 Hz, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 203.99 and 203.40, 203.30 and 202.12, 142.21 and 141.88, 141.83 and 141.11, 139.05 and 138.72, 135.96 and 135.89, 135.74 and 135.70, 134.76 and 133.70, 133.19 and 132.22, 130.91 and 130.76, 129.07 and 128.79, 123.50 and 123.35, 123.04 and 123.02, 118.85 and 118.64, 112.35 and 112.16, 65.75 and 65.41, 61.87 and 59.32, 39.37 and 38.62, 34.20 and 33.51, 32.54 and 32.08, 17.34 and 16.67; IR (film) *v*: 2971, 2960, 2219, 1766, 1699, 1549, 1508, 1491, 1369, 1294, 1127, 1007, 890, 810, 703 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{21}H_{18}NO_2$ ($M+H^+$): 316.1337; Found: 316.1336.

**3-Methyl-2-(thiophen-2-yl)spiro[cyclopentane-1,2'-indene]-1',3'-dione (3q)**

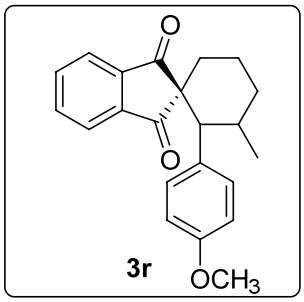



**3q**, 1:1 dr

Yellow soild; m.p. 113-114 °C; $R_f$ = 0.44 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.92-7.87 (m, 1H), 7.83-7.65 (m, 3H), 7.01 and 6.91 (d, *J* = 5.2 Hz, 1H), 6.78 and 6.66 (t, *J* = 4.0 Hz, 1H), 6.69 and

6.62 (d, $J$ = 4.4 Hz, 1H), 3.96 (d, $J$ = 7.6 Hz, 0.5H), 3.42 (d, $J$ = 12.0 Hz, 0.5H), 2.91-2.82 and 2.77-2.70 (m, 1H), 2.32-2.21 and 2.19-2.05 (m, 3H), 2.01-1.96 and 1.74-1.64 (m, 1H), 1.12-1.04 (d, $J$ = 6.8 Hz, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.32 and 204.02, 203.79 and 202.41, 142.69 and 142.36, 142.29 and 141.59, 139.96 and 139.11, 135.72 and 135.63, 135.35 and 135.34, 127.39 and 126.65, 126.59 and 126.05, 124.33 and 124.18, 123.30, 123.06 and 122.93, 66.08 and 65.86, 58.06 and 54.84, 41.26 and 39.69, 34.17 and 33.52, 32.04 and 31.43, 17.92 and 16.62; IR (KBr) $v$: 2927, 2941, 2840, 2348, 1736, 1707, 1593, 1349, 1263, 1127, 1086, 864, 725 cm$^{-1}$; HRMS (ESI) ($m/z$): calcd for $C_{18}H_{17}O_2S$ ($M+H^+$): 297.0949; Found: 297.0932.

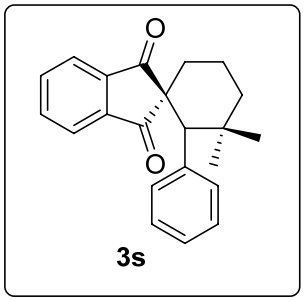
**2-(4-Methoxyphenyl)-3-methylspiro[cyclohexane-1,2'-indene]-1',3'-dione (3r)**




Pale yellow soild; m.p. 91-92 ºC; $R_f$ = 0.39 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.77-7.76 (m, 1H), 7.69-7.67 (m, 1H), 7.64-7.60 (m, 2H), 6.89 (d, $J$ = 7.2 Hz, 2H), 6.51 (d, $J$ = 7.6 Hz, 2H), 3.59 (s, 3H), 2.75 (d, $J$ = 11.6 Hz, 1H), 2.71-2.64 (m, 1H), 2.20-2.09 (m, 1H), 2.04-2.00 (m, 1H), 1.88-1.81 (m, 1H), 1.73-1.68 (m, 2H), 1.31-1.20 (m, 1H),

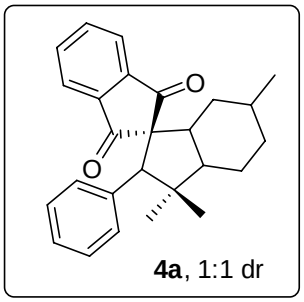
0.67 (d, $J$ = 6.4 Hz, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.47, 204.43, 158.06, 141.77, 140.83, 135.43, 135.21, 131.97, 122.95, 122.82, 59.03, 55.08, 53.62, 35.09, 32.29, 31.08, 21.32, 20.70; IR (KBr) $v$: 2941, 2865, 1740, 1700, 1599, 1518, 1467, 1269, 1183, 1031, 813 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{22}O_3Na$ (M+Na$^+$): 357.1467; Found: 357.1472.

**3,3-Dimethyl-2-phenylspiro[cyclohexane-1,2'-indene]-1',3'-dione (3s)**



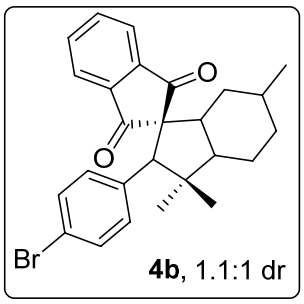

Pale yellow solid; m.p. 96-97 $^o$C; $R_f$ = 0.64 (EtOAc/Petroleum ether 1:10); $^1$H NMR ($CDCl_3$, 600MHz), δ: 7.90 (d, $J$ = 7.8 Hz, 1H), 7.69 (td, $J_1$ = 6.9 Hz, $J_2$ = 1.8 Hz, 1H), 7.61-7.59 (m, 2H), 6.96-6.94 (m, 5H), 3.07 (s, 1H), 2.35-2.27 (m, 1H), 1.80-1.73 (m, 2H), 1.67-1.64 (m, 1H), 1.59-1.58 (m, 1H), 1.57-1.52 (m, 1H), 1.35 (s, 3H), 0.78 (s, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 204.95, 204.34, 142.17, 140.65, 138.18, 135.58, 135.15, 127.60, 126.60, 123.05, 123.04, 58.94, 57.79, 42.13, 34.44, 33.00, 32.75, 22.50, 18.62; IR (KBr) $v$: 2951, 2855, 1736, 1730, 1690, 1518, 1356, 1259, 1153, 819, 738 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{22}H_{23}O_2$ (M+H$^+$): 319.1698; Found: 319.1686.

**3,3,6-trimethyl-2-phenyl-2,3,3a,4,5,6,7,7a-octahydro-1,2'-spirobi[indene]-1',3'-dione (4a)**



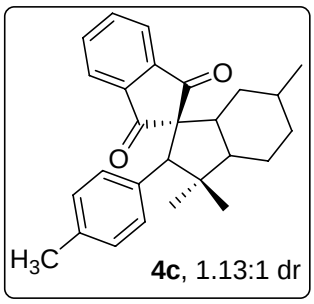

Pale yellow solid; m.p. 121-122 $^{o}$C; $R_f$ = 0.68 (EtOAc/Petroleum ether 1:30); $^{1}$H NMR ($CDCl_3$, 400MHz), δ: 7.94-7.92 and 7.86-7.84 (m, 1H), 7.80-7.76 (m, 1H), 7.75-7.69 (m, 1H), 7.68-7.65 (m, 1H), 7.18-7.15 (m, 1H), 7.12-7.06 (m, 4H), 3.45 and 3.43 (s, 1H), 2.53-2.25 (m, 1H), 2.16-1.77 (m, 3H), 1.33 (m, 1H), 1.28-1.22 (m, 2H), 1.08 and 0.94 (d, 6H), 1.02-0.94 (m, 2H), 0.81 (d, 1.5H), 0.76 (d, 1.5H); $^{13}$C NMR ($CDCl_3$, 100MHz), δ: 204.37 and 204.32, 203.89 and 203.77, 143.15 and 142.85, 142.32 and 142.05, 137.56, 136.69, 135.70, 135.40, 135.32, 131.58 and 130.66, 127.93 and 127.74, 126.95 and 126.81, 123.02 and 122.87, 122.85 and 122.81, 68.95 and 67.40, 66.64 and 65.29, 55.06 and 52.90, 52.70 and 52.09, 45.42 and 42.24, 36.04 and 35.17, 34.98 and 34.78, 33.42 and 32.87, 27.28 and 27.18, 27.01 and 22.27, 26.66 and 26.41, 22.31 and 18.12; IR (KBr) *v*: 2960, 2939, 1790, 1720, 1580, 1507, 1481, 1366, 1210, 1125, 997, 896, 820, 763 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{26}H_{29}O_2$ (M+H$^+$): 373.2167; Found: 373.2166.

**2-(4-bromophenyl)-3,3,6-trimethyl-2,3,3a,4,5,6,7,7a-octahydro-1,2'-spirobi[indene]-1',3'-dione (4b)**




Pale yellow oil; $R_f$ = 0.45 (EtOAc/Petroleum ether 1:40); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.94-7.35 and 7.87-7.85 (m, 1H), 7.82-7.79 (m, 1H), 7.77-7.74 (m, 1H), 7.72-7.67 (m, 1H), 7.24-7.22 (m, 1H), 7.21-7.18 (m, 1H), 7.07-7.04 (m, 1H), 6.98-6.96 (m, 1H), 3.40 and 3.39 (s, 1H), 2.48-2.06 (m, 2H), 1.80-1.71 (m, 2H), 1.62-1.55 (m, 1H), 1.25-1.20 (m, 2H), 1.05 and 0.92 (d, 6H), 0.98-0.93 (m, 2H), 0.79 (d, 1.36H), 0.75 (d, 1.5H); $^{13}$C NMR ($CDCl_3$, 100MHz), δ: 204.20 and 204.05, 203.57 and 203.56, 143.01 and 142.72, 142.28 and 141.99, 136.63 and 135.90, 135.76 and 135.62, 135.57, 133.30, 132.40 and 131.10, 130.91, 123.15 and 122.98, 122.94 and 122.89, 121.28 and 121.05, 68.96 and 67.20, 65.56 and 64.37, 54.97 and 52.98, 52.71 and 52.40, 45.41 and 42.24, 35.99 and 35.17, 34.92 and 34.71, 33.38 and 32.85, 27.21 and 22.24, 27.11 and 27.04, 26.60 and 26.37, 22.28 and 18.06; IR (film) *v*: 2928, 2912, 2870, 1786, 1726, 1540, 1508, 1309, 1169, 1002, 918, 743, 769, 703 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{26}H_{28}BrO_2$ ($M+H^+$): 451.1272; Found: 451.1281.

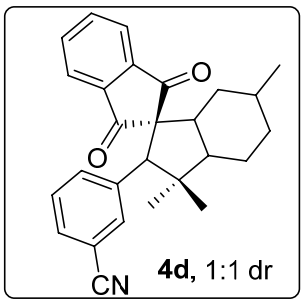
**3,3,6-trimethyl-2-(p-tolyl)-2,3,3a,4,5,6,7,7a-octahydro-1,2'-spirobi[indene]-1',3'-dione (4c)**



**4c**, 1.13:1 dr

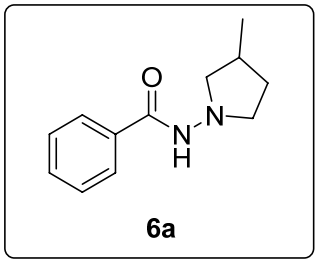
Pale yellow solid; m.p. 155-156 °C; $R_f$ = 0.35 (EtOAc/Petroleum ether 1:50); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.94-7.92 and 7.86-7.83 (m, 1H), 7.80-7.76 (m, 1H), 7.75-7.70 (m, 1H), 7.68-7.65 (m, 1H), 7.05 and 6.98 (d, *J* = 8.4 Hz, 2H), 6.90 and 6.87 (d, *J* = 8.0 Hz, 2H), 2.51-2.44 and 2.30-2.23 (m, 1H), 2.18 and 2.16 (s, 3H), 2.14-2.08 and 1.59-1.56 (m, 1H), 1.81-1.71 (m, 2H), 1.37-1.33 (m, 2H), 1.28-1.21(m, 2H), 1.10 and 0.93 (d, 6H), 1.01-0.97 (m, 1H), 0.80 (d, 1.4H), 0.76 (d, 1.58H); $^{13}$C NMR ($CDCl_3$, 100MHz), δ: 204.48 and 204.46, 204.01 and 203.87, 143.21 and 142.91, 142.39 and 142.12, 136.46 and 136.31, 135.67 and 135.37, 135.29, 134.45 and 133.57, 131.48, 130.56, 128.66, 128.48, 123.06 and 122.87, 122.85 and 122.83, 69.01 and 67.42, 66.27 and 64.93, 55.03 and 52.90, 52.69 and 52.16, 45.34 and 42.14, 36.06 and 35.20, 35.02 and 34.80, 33.44 and 32.89, 27.30 and 18.11, 27.20 and 26.99, 26.66 and 26.44, 22.33 and 22.29, 21.04 and 21.00; IR (film) *v*: 2973, 2910, 1787, 1716, 1593, 1578, 1481, 1366, 1284, 1107, 973, 921, 856, 723 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{27}H_{31}O_2$ ($M+H^+$): 387.2324; Found: 387.2327.

**3-(3,3,6-trimethyl-1',3'-dioxo-1',2,3,3a,3',4,5,6,7,7a-decahydro-1,2'-spirobi[inden]-2-yl)benzonitrile (4d)**




Brown oil; $R_f$ = 0.3 (EtOAc/Petroleum ether 1:30); $^1$H NMR ($CDCl_3$, 400MHz), δ: 7.96-7.94 and 7.89-7.87 (m, 1H), 7.83-7.58 (m, 2H), 7.75-7.69 (m, 1H), 7.49-7.47 (m, 1H), 7.40-7.36 (m, 2H), 7.26-7.18 (m, 1H), 3.46 (s, 1H), 2.49-2.42 and 2.28-2.21 (m, 1H), 2.14-2.04 and 1.60-1.56 (m, 1H), 1.82-1.72 (m, 2H), 1.33-1.30 (m, 1H), 1.25-1.20 (m, 2H), 1.08 and 0.94 (d, 6H), 0.98-0.89 (m, 2H), 0.80 (d, 1.5H), 0.75 (d, 1.5H); $^{13}$C NMR ($CDCl_3$, 100MHz), δ: 203.78 and 203.56, 203.12 and 203.09, 142.82 and 142.56, 142.17 and 141.91, 139.32 and 138.45, 136.16 and 136.09, 135.78 and 135.74, 134.74 and 135.24, 135.07 and 134.09, 130.86 and 130.77, 128.87 and 128.63, 123.23 and 123.15, 123.13 and 122.95, 118.99 and 118.95, 112.21 and 112.01, 69.00 and 67.13, 65.02 and 64.03, 54.84 and 53.17, 52.81 and 52.71, 45.59 and 42.47, 35.93 and 35.16, 34.83 and 34.63, 33.32 and 32.82, 27.14 and 27.05, 26.59 and 26.31, 22.23 and 22.20, 27.09 and 18.17; IR (film) *v*: 2947, 2919, 2902,2308, 1792, 1738, 1674, 1532, 1481, 1343, 1286, 1109, 923, 847, 810, 703 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{27}H_{28}NO_2$ ($M+H^+$): 398.2120; Found: 398.2138.

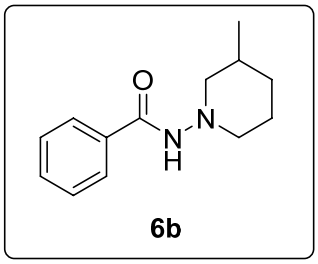
**_N_-(3-methylpyrrolidin-1-yl)benzamide (6a)**




**6a**

Pale yellow solid; m.p. 125-126 $^{o}$C; $R_f$ = 0.20 (EtOAc/Petroleum ether 1:3); $^{1}$H NMR ($CDCl_3$, 600MHz), δ: 7.72 (d, 2H), 7.49 (t, 1H), 7.42 (t, 2H), 6.83 (s, 1H), 3.31-3.28 (m, 1H), 3.23-3.20 (m, 1H), 2.98-2.94 (m, 1H), 2.57-2.54 (m, 1H), 2.42-2.38 (m, 1H), 2.13-2.10 (m, 1H), 1.52-1.48 (m, 1H), 1.09 (d, *J* = 6.6 Hz, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ: 166.29, 134.04, 131.67, 128.74, 127.12, 63.34, 55.82, 31.61, 30.97, 19.94; IR (KBr) *v*: 2981, 2846, 1776, 1605, 1593, 1518, 1447, 1340, 1254, 1234, 1041, 860, 732 cm$^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{12}H_{17}N_2O$ ($M+H^+$): 205.1341; Found: 205.1344.

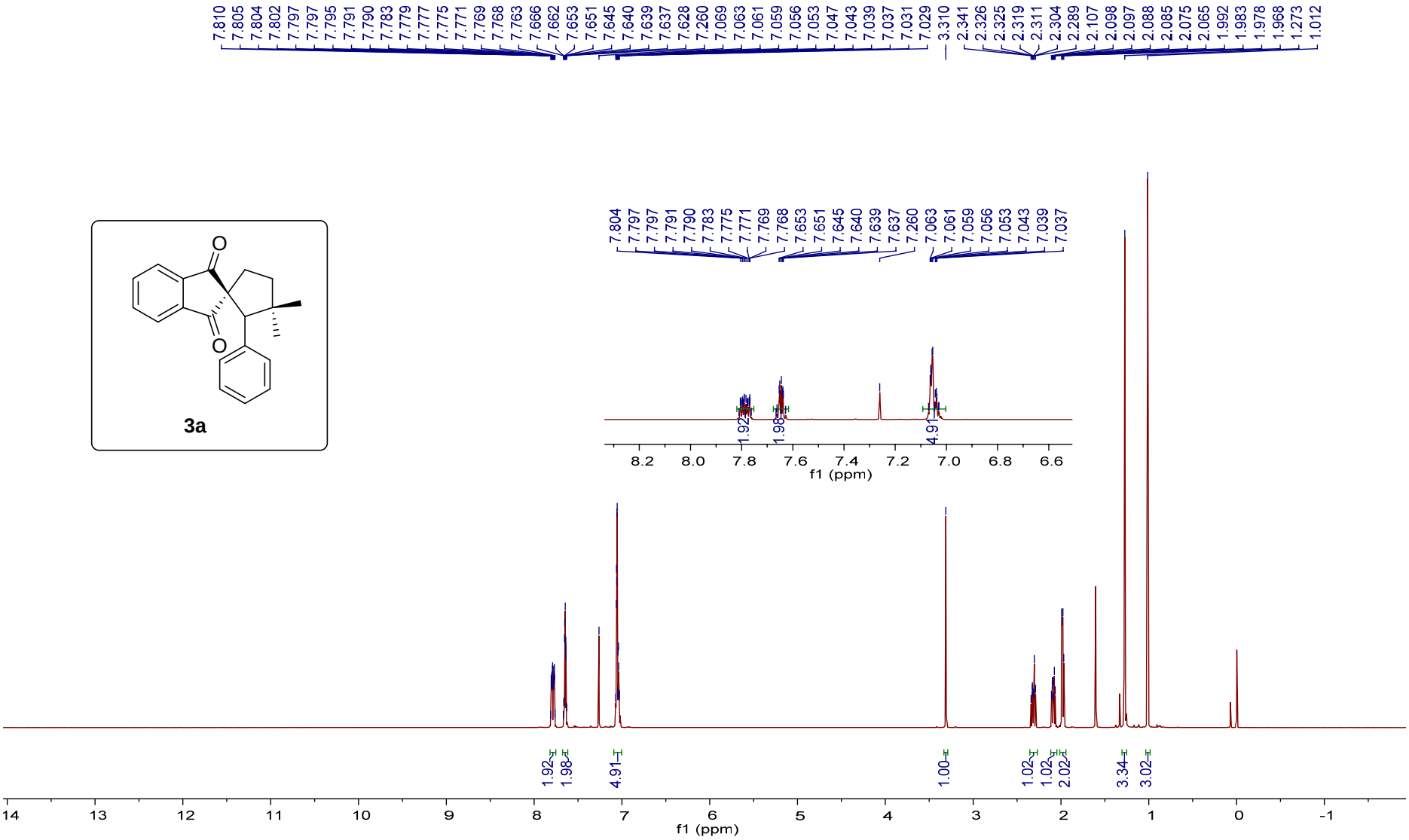
***N*-(3-methylpiperidin-1-yl)benzamide (6b)**




**6b**

White solid; m.p. 161-162 $^{o}$C; $R_f$ = 0.27 (EtOAc/Petroleum ether 1:3); $^{1}$H NMR ($CDCl_3$, 600MHz), δ: 7.72 (d, 2H), 7.49 (t, 1H), 7.41 (t, 2H), 6.77 (s, 1H), 3.24-3.20 (m, 2H), 2.43-2.39 (m, 1H), 2.13-2.10 (m, 1H), 1.97-1.93 (m, 1H), 1.84-1.78 (m, 1H), 1.72-1.71 (m, 3H), 0.90 (d, *J* = 6.6 Hz, 3H); $^{13}$C NMR ($CDCl_3$, 150MHz), δ:165.51, 134.20, 131.64, 128.72, 127.13,

64.40, 56.59, 32.11, 31.05, 24.88, 19.50; IR (KBr) *v*: 2983, 2849, 1786, 1601, 1598, 1518, 1447, 1347, 1254, 1134, 1041, 860, 739 $cm^{-1}$; HRMS (ESI) (*m/z*): calcd for $C_{13}H_{19}N_2O$ ($M+H^+$): 219.1497; Found: 219.1504.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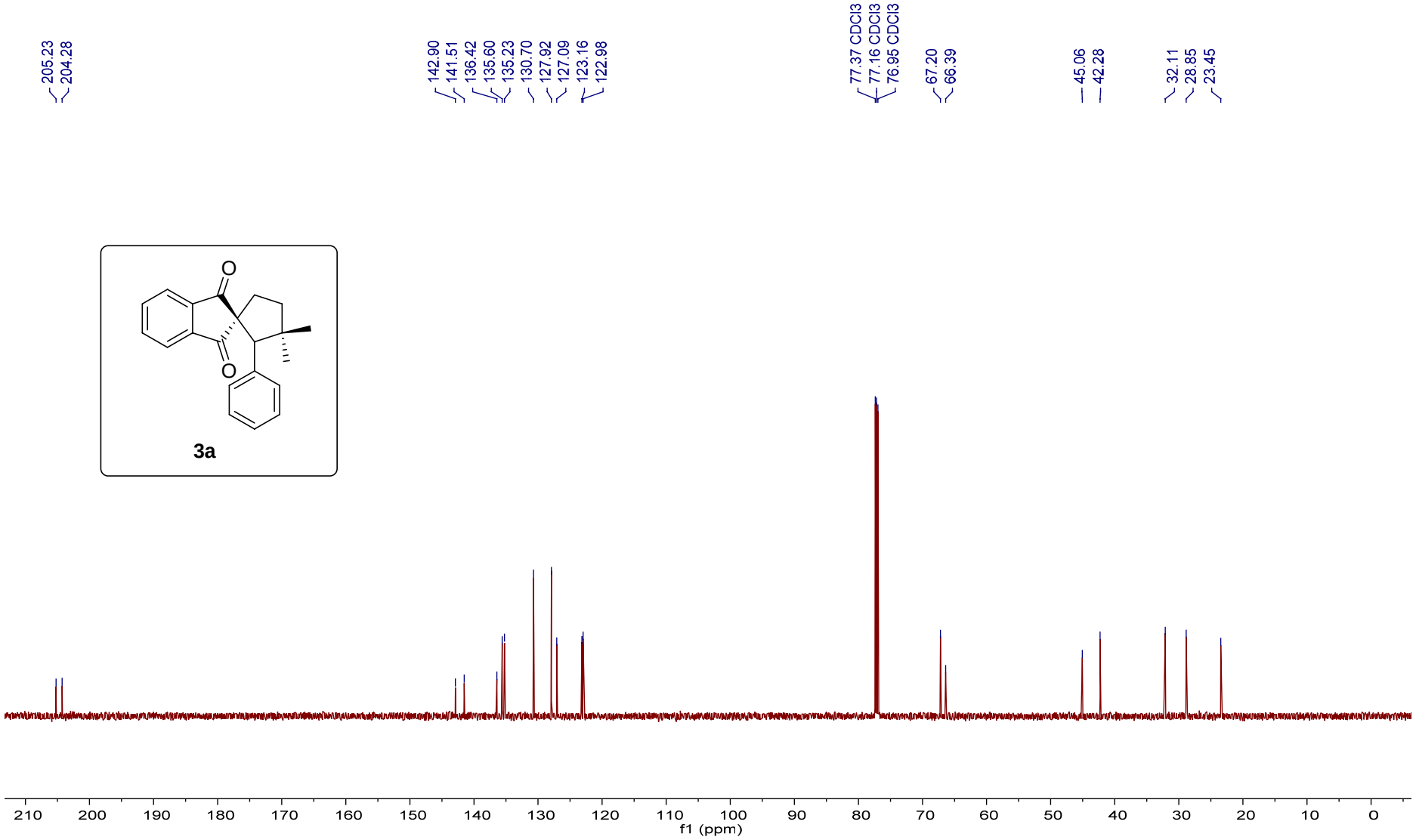
7.805
7.804
7.802
7.797
7.797
7.795
7.791
7.790
7.783
7.779
7.777
7.775
7.771
7.769
7.768
7.763
7.666
7.662
7.653
7.651
7.645
7.640
7.639
7.637
7.628
7.260
7.069
7.063
7.061
7.059
7.056
7.053
7.047
7.043
7.039
7.037
7.031
7.029
3.310
2.341
2.326
2.325
2.319
2.311
2.304
2.289
2.107
2.098
2.097
2.088
2.085
2.075
2.065
1.992
1.983
1.978
1.968
1.273
1.012
O
O
3a
7.804
7.797
7.797
7.791
7.790
7.783
7.775
7.771
7.769
7.768
7.653
7.651
7.645
7.640
7.639
7.637
7.260
7.063
7.061
7.059
7.056
7.053
7.043
7.039
7.037
1.92
1.98
4.91
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
f1 (ppm)
1.92
1.98
4.91
1.00
1.02
1.02
2.02
3.34
3.02
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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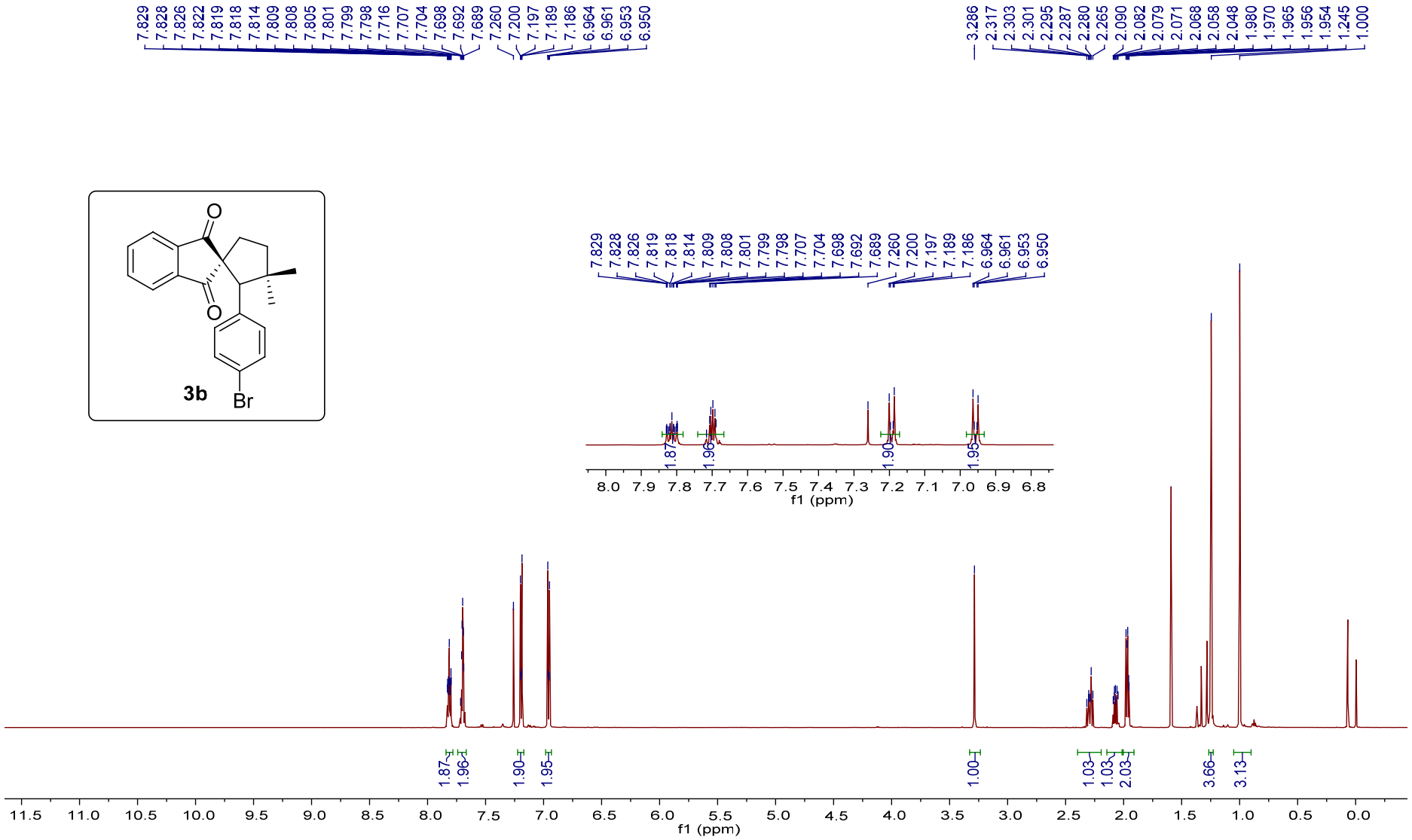
142.90
141.51
136.42
135.60
135.23
130.70
127.92
127.09
123.16
122.98
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
67.20
66.39
45.06
42.28
32.11
28.85
23.45
O
O
3a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.822
7.819
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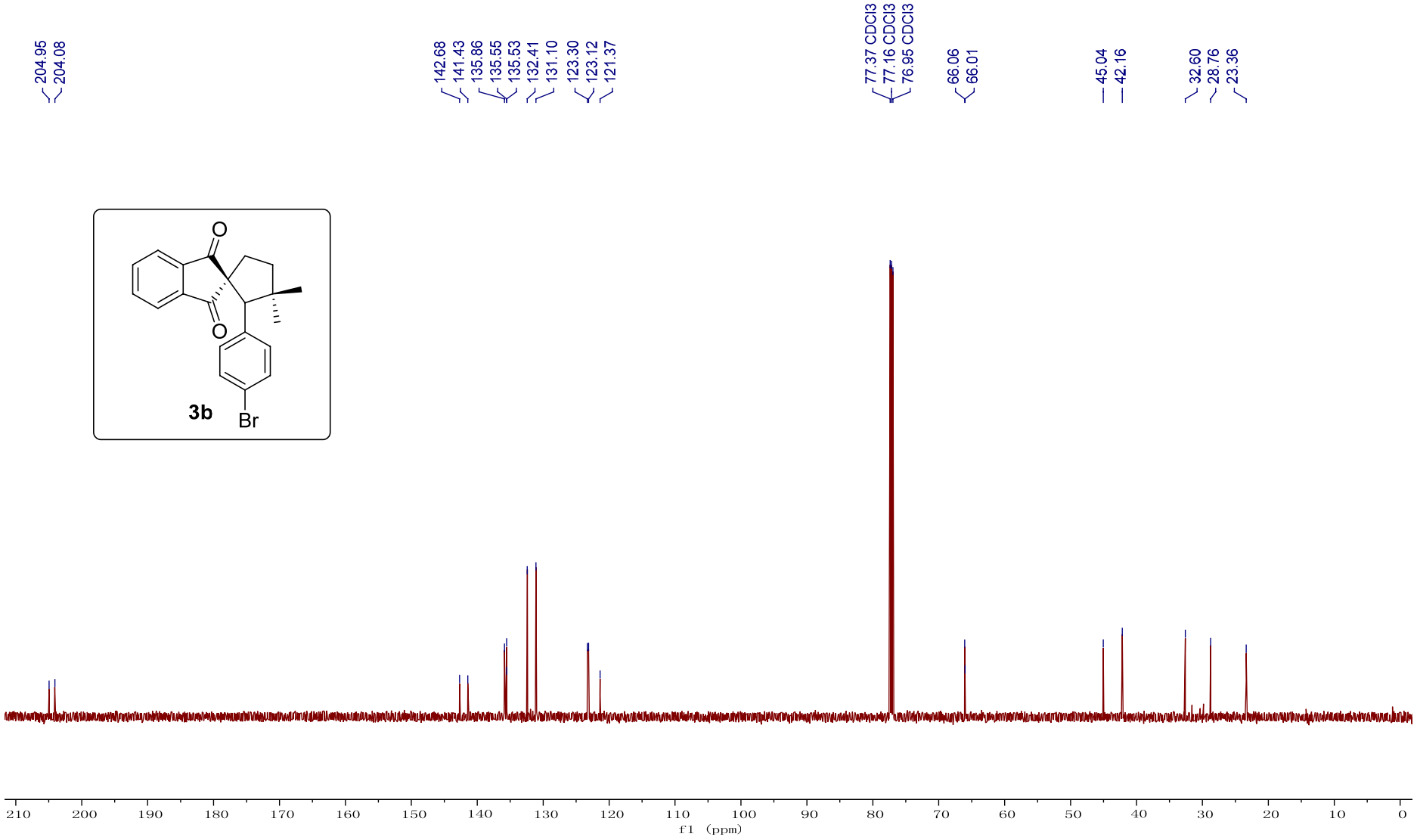
7.814
7.809
7.808
7.805
7.801
7.799
7.798
7.716
7.707
7.704
7.698
7.692
7.689
7.260
7.200
7.197
7.189
7.186
6.964
6.961
6.953
6.950
3.286
2.317
2.303
2.301
2.295
2.287
2.280
2.265
2.090
2.082
2.079
2.071
2.068
2.058
2.048
1.980
1.970
1.965
1.956
1.954
1.245
1.000
O
O
3b
Br
1.87
1.96
1.90
1.95
1.00
1.03
1.03
2.03
3.66
3.13
f1 (ppm)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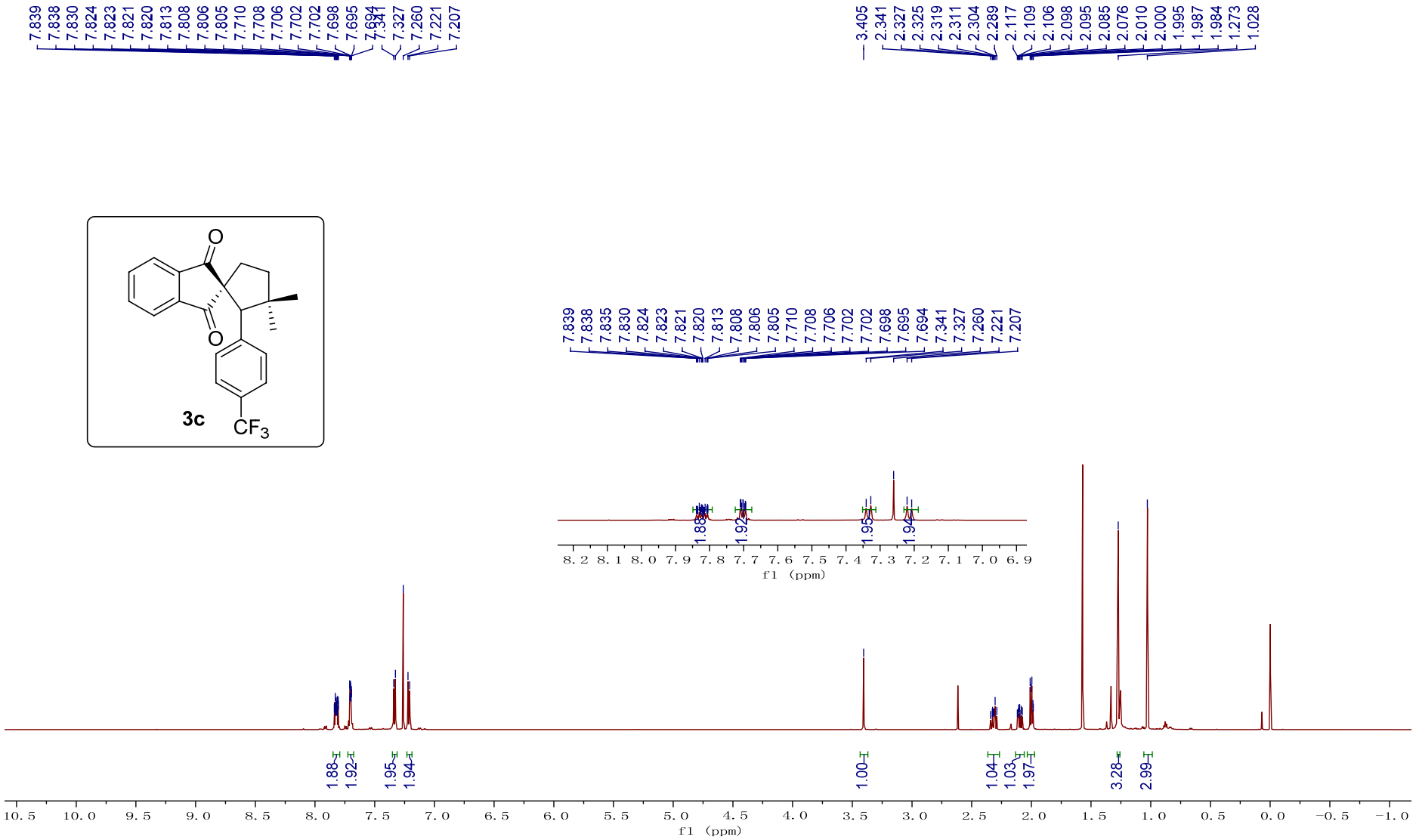
204.08
142.68
141.43
135.86
135.55
135.53
132.41
131.10
123.30
123.12
121.37
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.06
66.01
45.04
42.16
32.60
28.76
23.36
O
O
3b
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.830
7.824
7.823
7.821
7.820
7.813
7.808
7.806
7.805
7.710
7.708
7.706
7.702
7.702
7.698
7.695
7.694
7.341
7.327
7.260
7.221
7.207
3.405
2.341
2.327
2.325
2.319
2.311
2.304
2.289
2.117
2.109
2.106
2.098
2.095
2.085
2.076
2.010
2.000
1.995
1.987
1.984
1.273
1.028
O
O
3c
CF3
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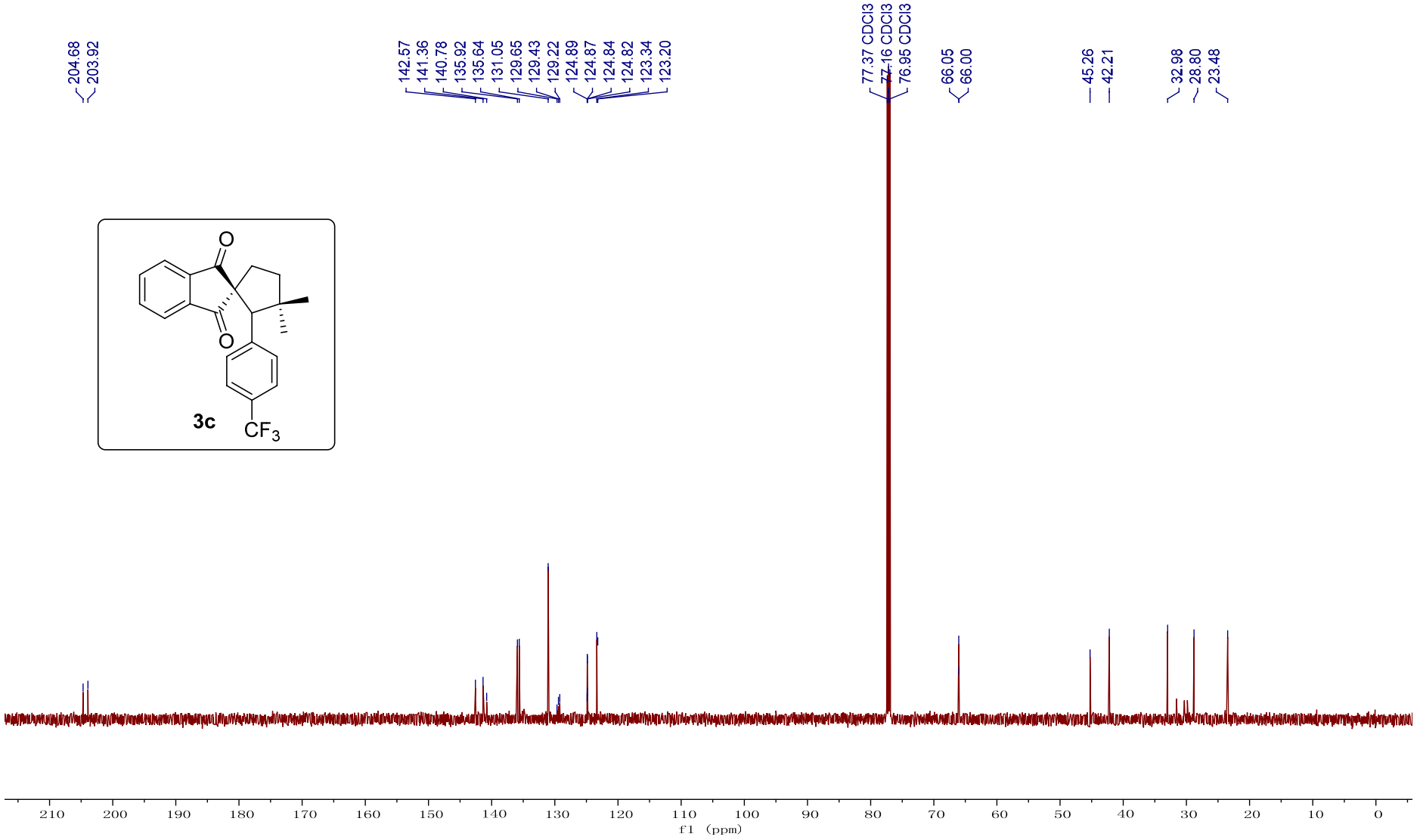
1.95
1.94
1.00
1.04
1.03
1.97
3.28
2.99
f1 (ppm)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142.57
141.36
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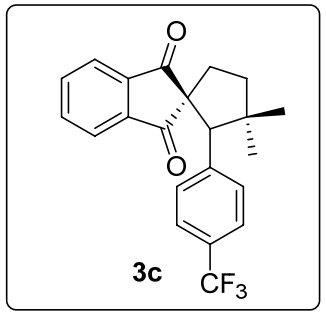
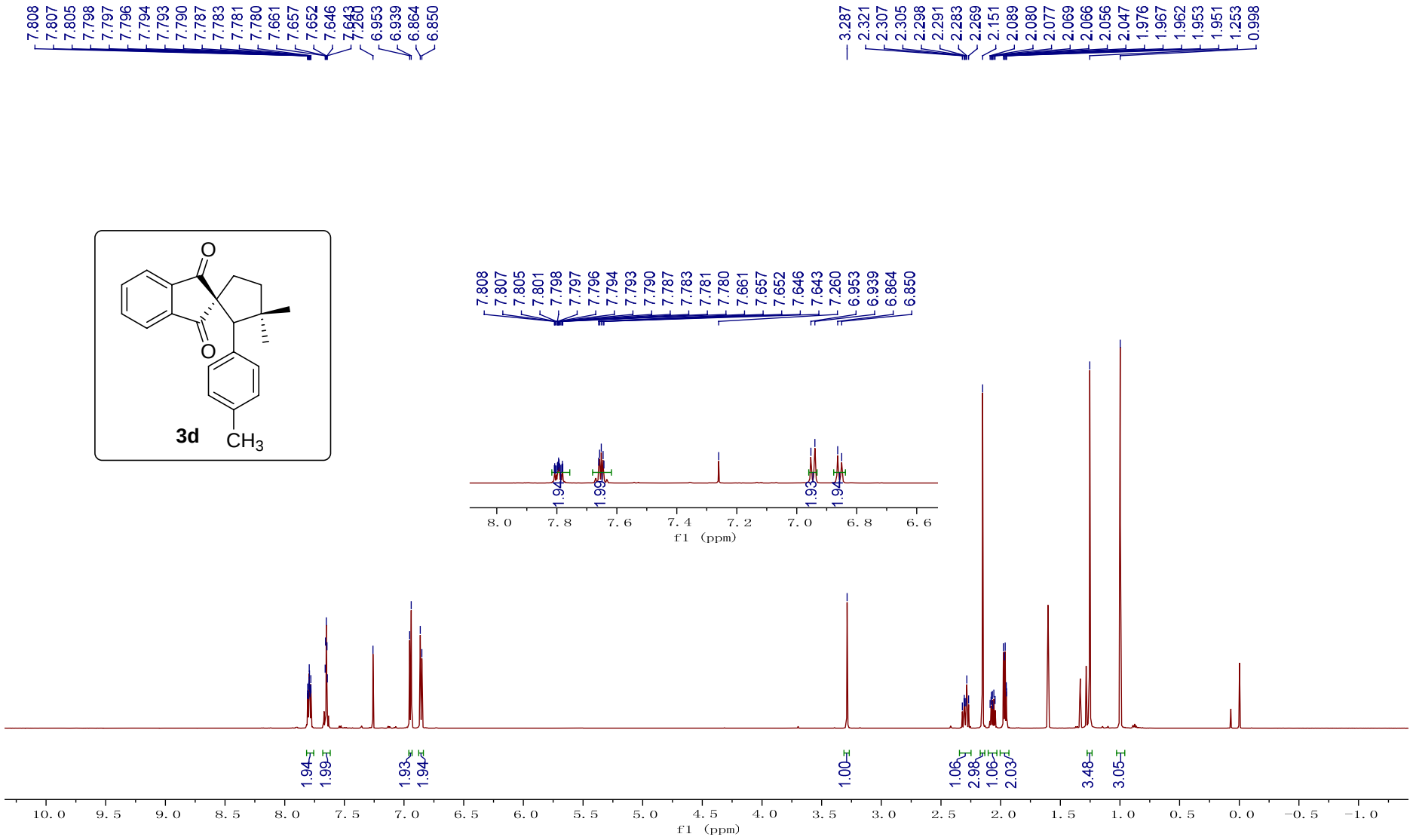
135.92
135.64
131.05
129.65
129.43
129.22
124.89
124.87
124.84
124.82
123.34
123.20
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.05
66.00
45.26
42.21
32.98
28.80
23.48
O
O
3c
CF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
O
3c
CF3


-62.67
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)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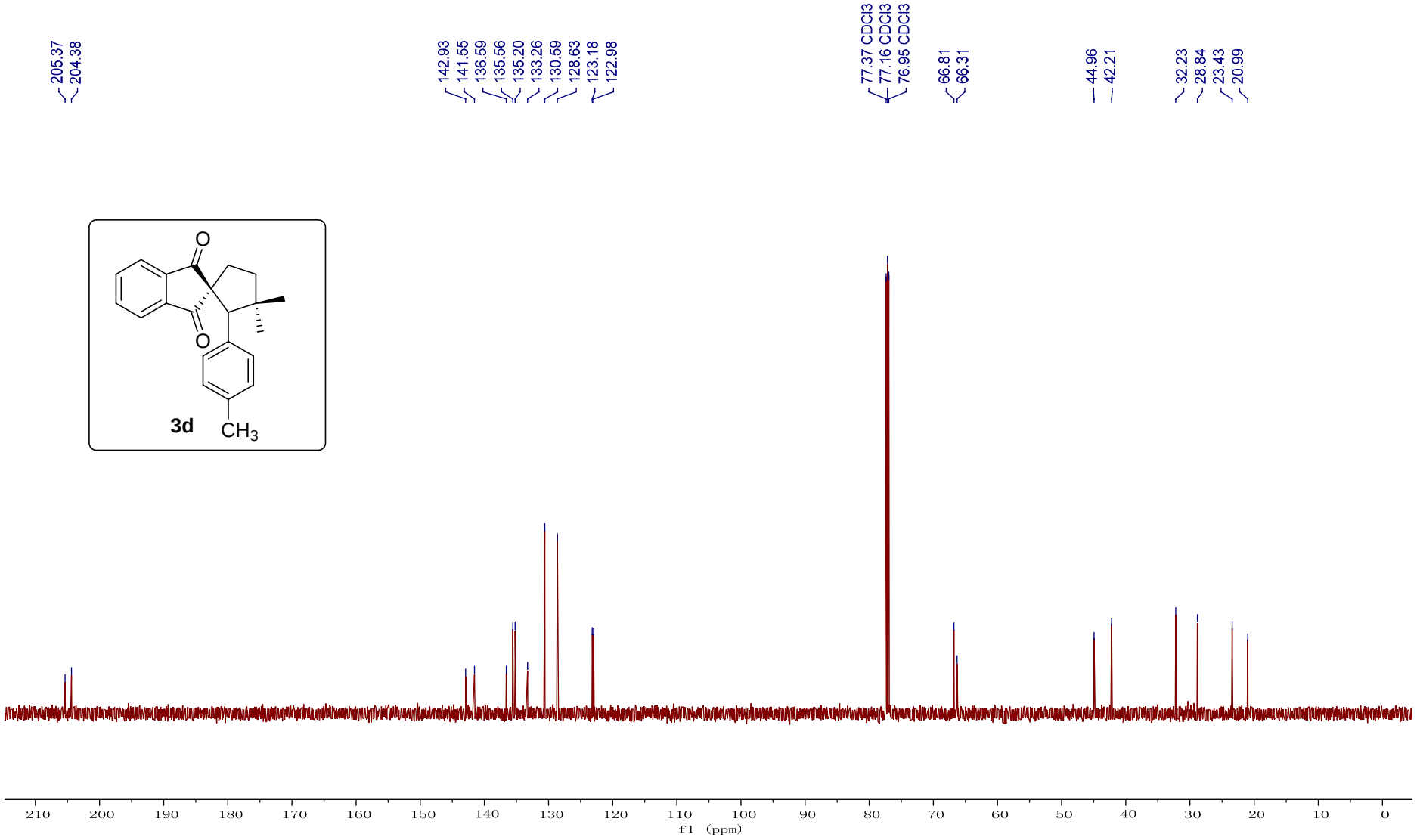
7.797
7.796
7.794
7.793
7.790
7.787
7.783
7.781
7.780
7.661
7.657
7.652
7.646
7.643
7.260
6.953
6.939
6.864
6.850
3.287
2.321
2.307
2.305
2.298
2.291
2.283
2.269
2.151
2.089
2.080
2.077
2.069
2.066
2.056
2.047
1.976
1.967
1.962
1.953
1.951
1.253
0.998
O
O
3d
CH3
1.94
1.99
1.93
1.94
1.00
1.06
2.98
1.06
2.03
3.48
3.05
f1 (ppm)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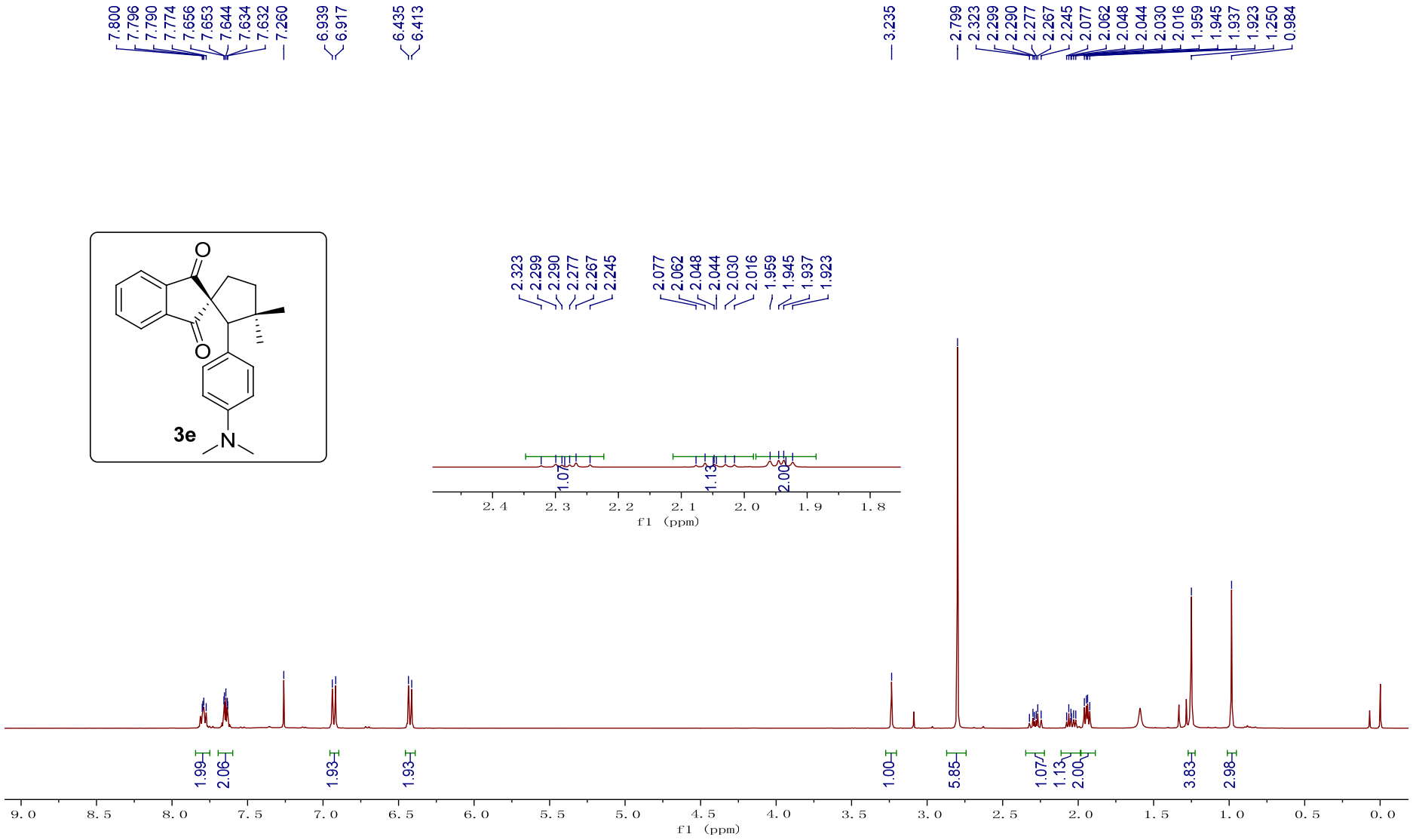
141.55
136.59
135.56
135.20
133.26
130.59
128.63
123.18
122.98
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.81
66.31
44.96
42.21
32.23
28.84
23.43
20.99
O
O
3d
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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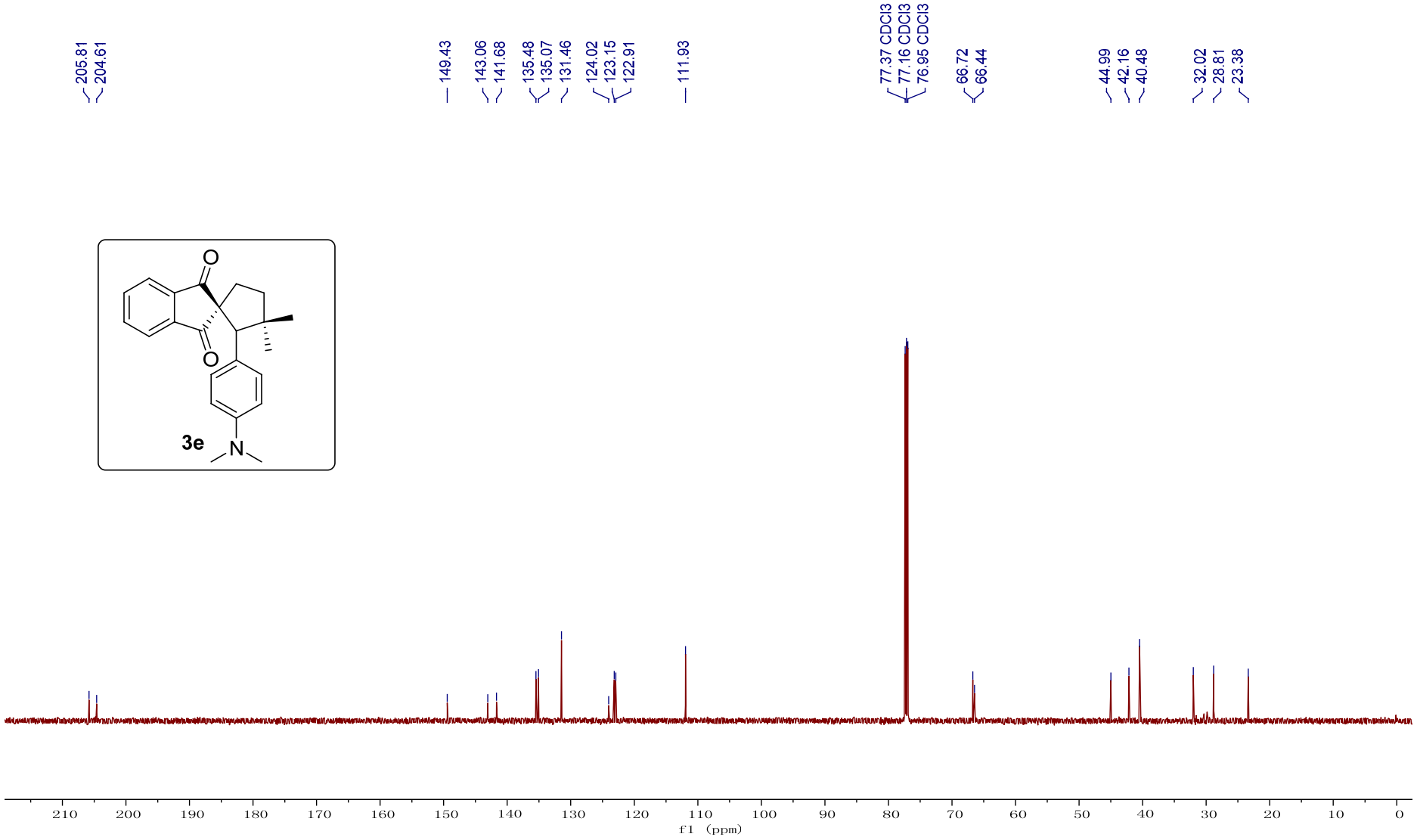
7.644
7.634
7.632
7.260
6.939
6.917
6.435
6.413
3.235
2.799
2.323
2.299
2.290
2.277
2.267
2.245
2.077
2.062
2.048
2.044
2.030
2.016
1.959
1.945
1.937
1.923
1.250
0.984
3e
O
O
N
1.07
1.13
2.00
f1 (ppm)
1.99
2.06
1.93
1.93
1.00
5.85
1.07
1.13
2.00
3.83
2.98
f1 (ppm)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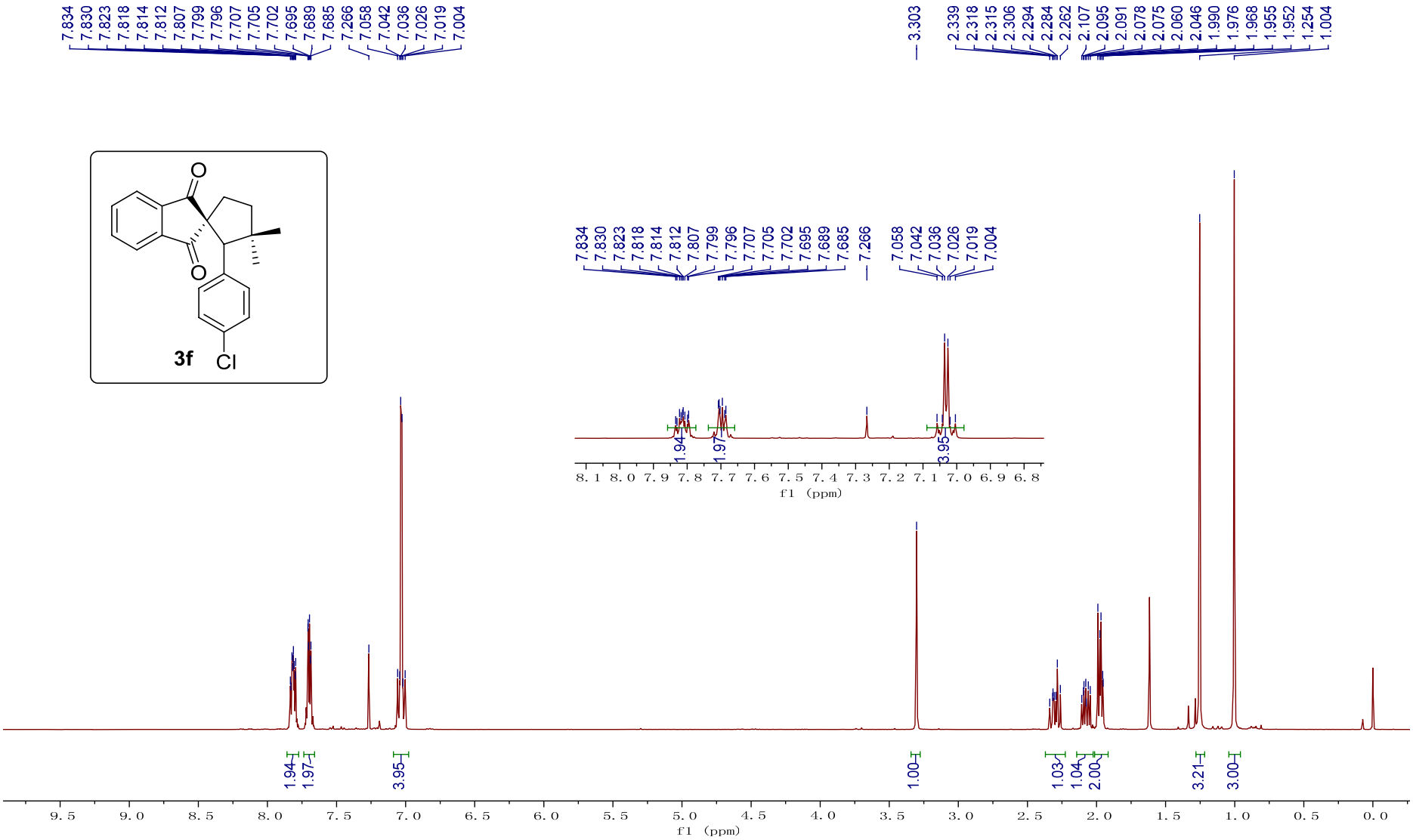
143.06
141.68
135.48
135.07
131.46
124.02
123.15
122.91
111.93
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.72
66.44
44.99
42.16
40.48
32.02
28.81
23.38
O
O
3e
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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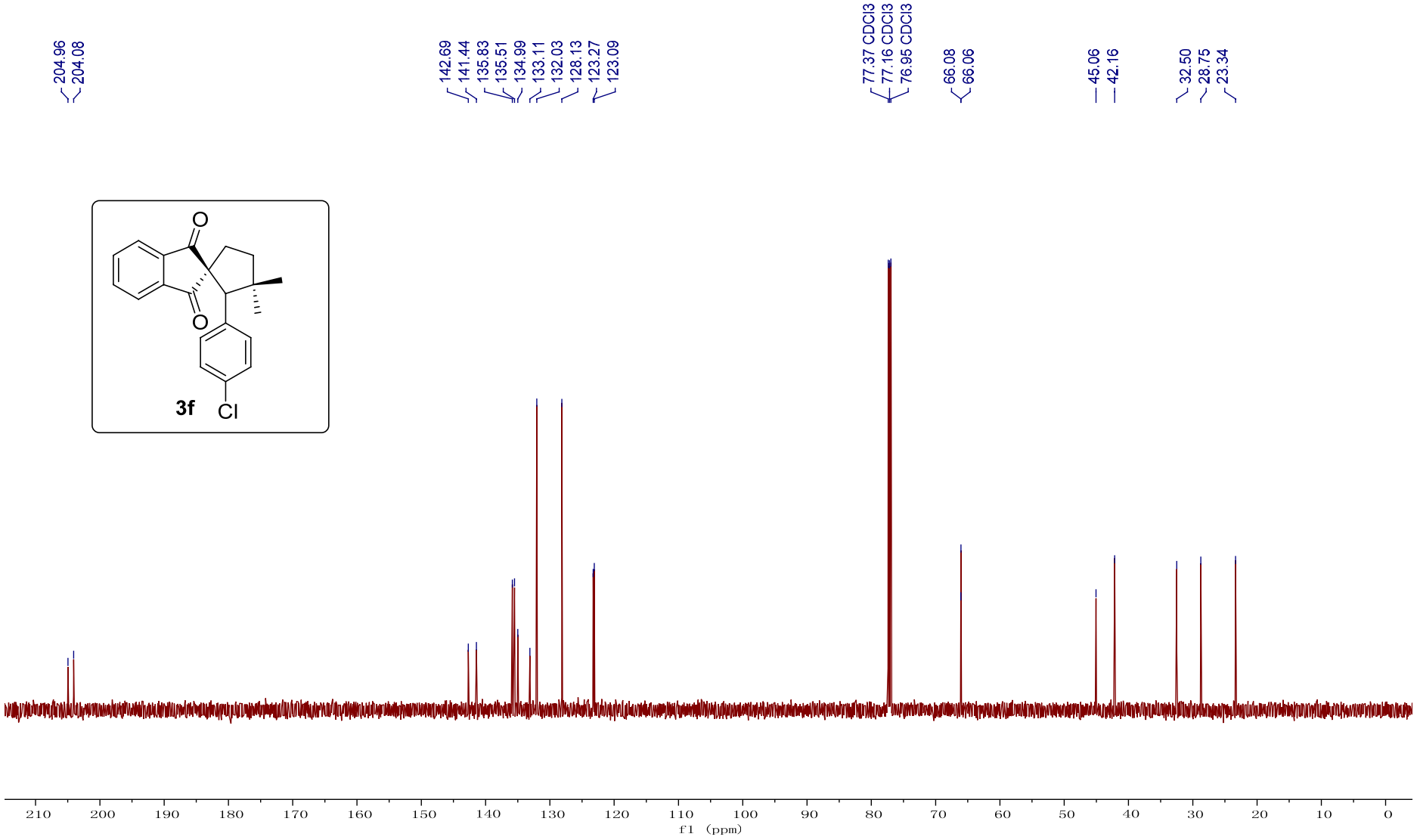
7.814
7.812
7.807
7.799
7.796
7.707
7.705
7.702
7.695
7.689
7.685
7.266
7.058
7.042
7.036
7.026
7.019
7.004
3.303
2.339
2.318
2.315
2.306
2.294
2.284
2.262
2.107
2.095
2.091
2.078
2.075
2.060
2.046
1.990
1.976
1.968
1.955
1.952
1.254
1.004
O
O
3f
Cl
1.94
1.97
3.95
f1 (ppm)
1.00
1.03
1.04
2.00
3.21
3.00
f1 (ppm)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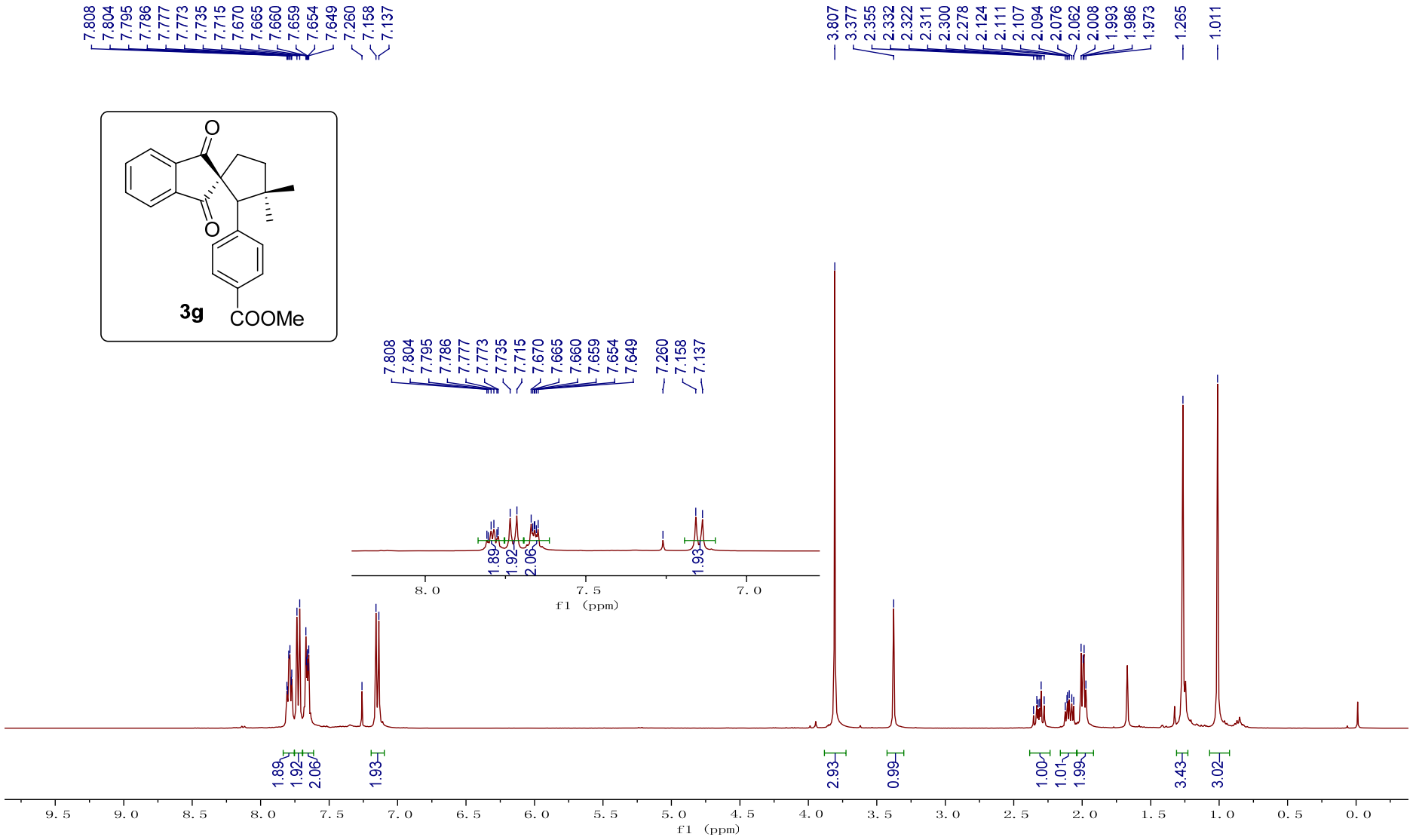
141.44
135.83
135.51
134.99
133.11
132.03
128.13
123.27
123.09
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.08
66.06
45.06
42.16
32.50
28.75
23.34
O
O
3f
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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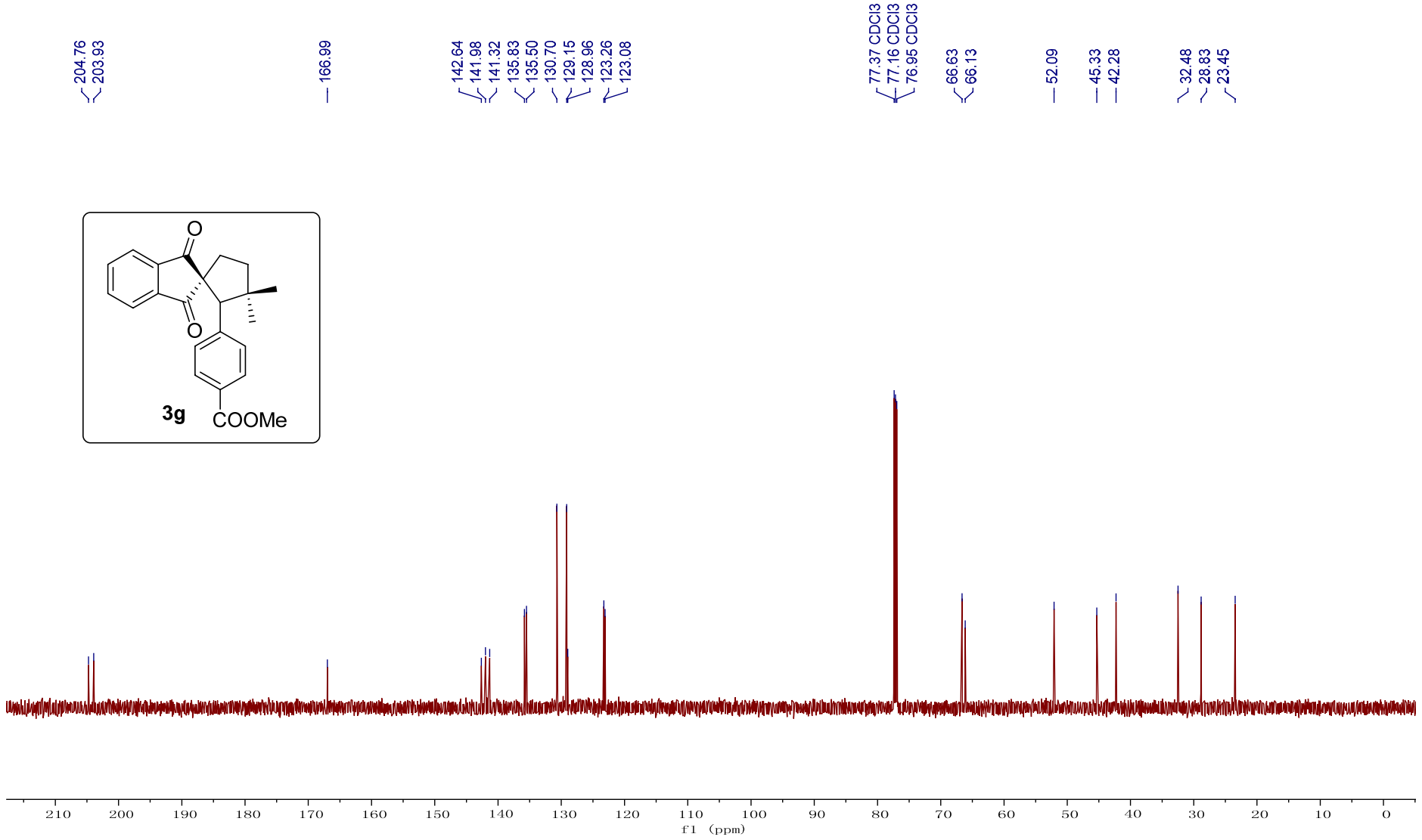
7.804
7.795
7.786
7.777
7.773
7.735
7.715
7.670
7.665
7.660
7.659
7.654
7.649
7.260
7.158
7.137
3.807
3.377
2.355
2.332
2.322
2.311
2.300
2.278
2.124
2.111
2.107
2.094
2.076
2.062
2.008
1.993
1.986
1.973
1.265
1.011
3g
COOMe
1.89
1.92
2.06
1.93
2.93
0.99
1.00
1.01
1.99
3.43
3.02
f1 (ppm)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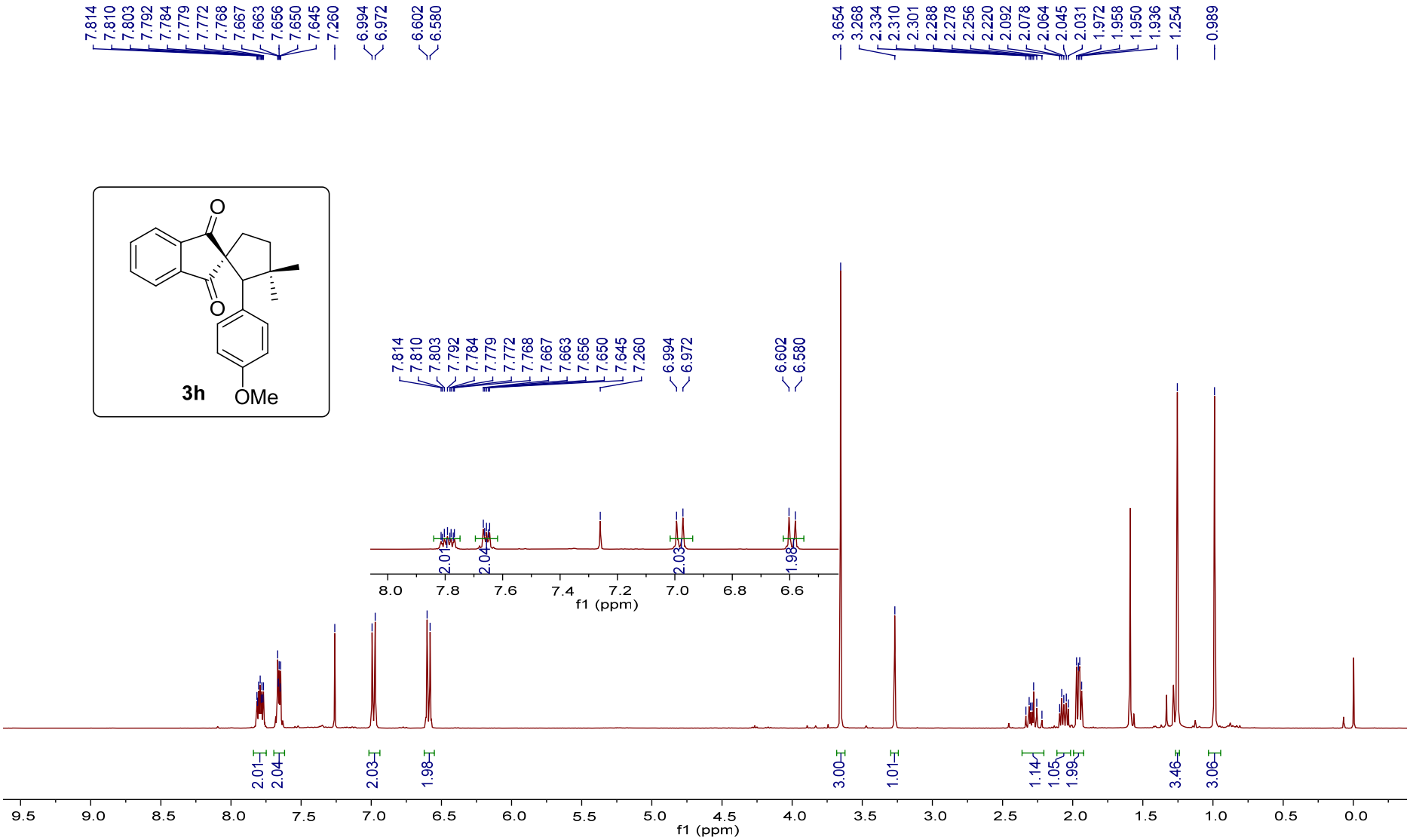
141.32
135.83
135.50
130.70
129.15
128.96
123.26
123.08
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.63
66.13
52.09
45.33
42.28
32.48
28.83
23.45
O
O
3g
COOMe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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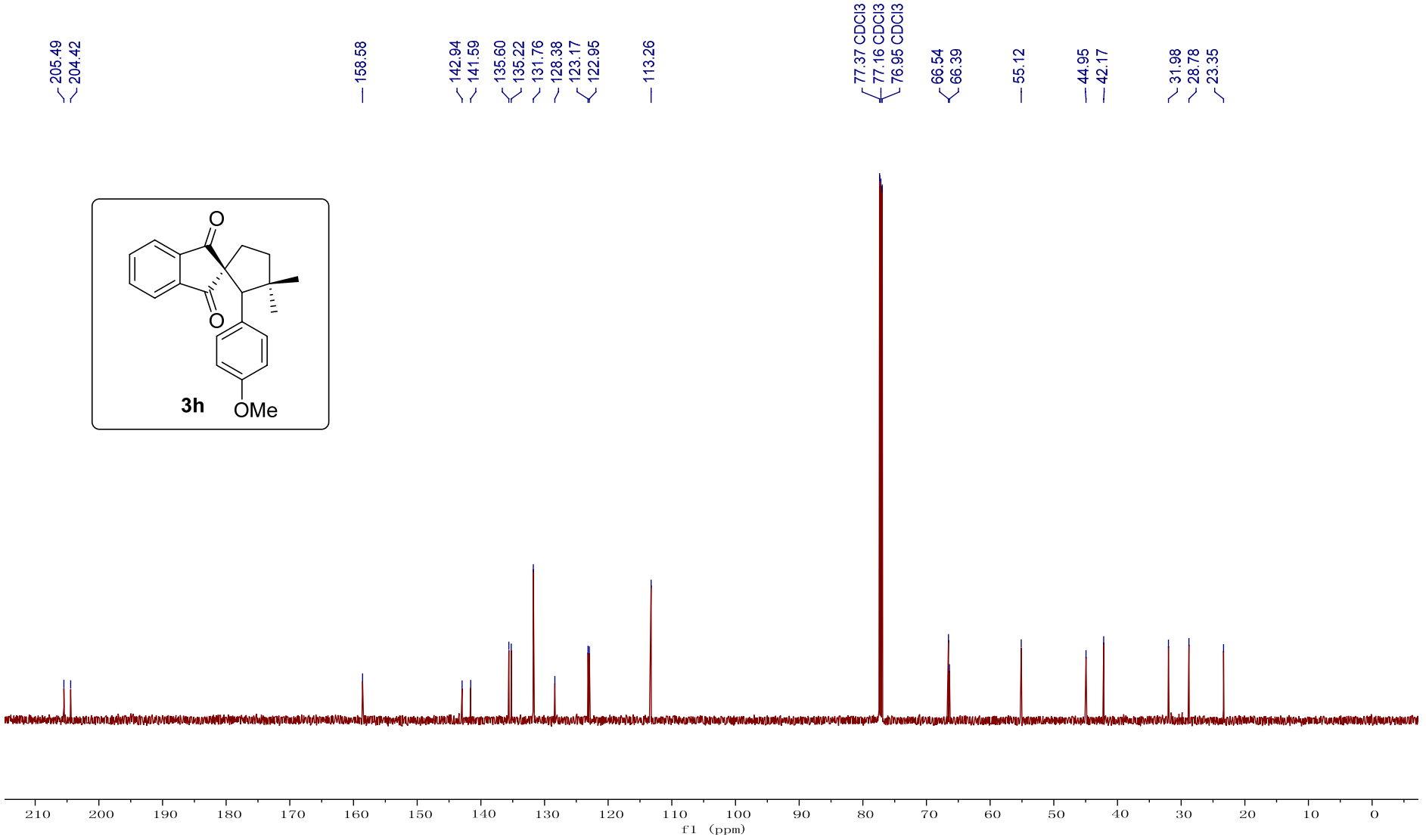
7.810
7.803
7.792
7.784
7.779
7.772
7.768
7.667
7.663
7.656
7.650
7.645
7.260
6.994
6.972
6.602
6.580
3.654
3.268
2.334
2.310
2.301
2.288
2.278
2.256
2.220
2.092
2.078
2.064
2.045
2.031
1.972
1.958
1.950
1.936
1.254
0.989
3h
OMe
f1 (ppm)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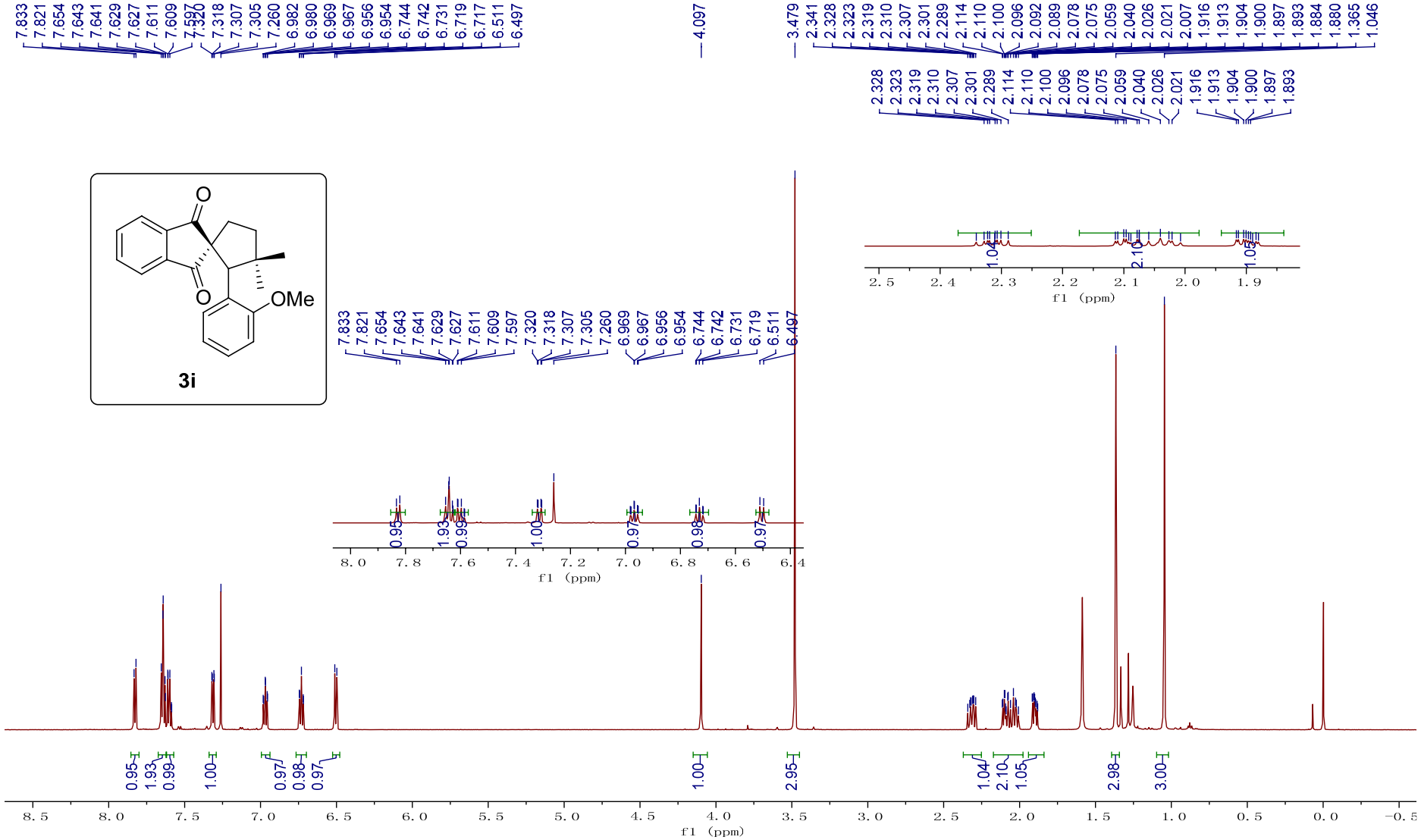
135.22
131.76
128.38
123.17
122.95
113.26
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.54
66.39
55.12
44.95
42.17
31.98
28.78
23.35
O
O
3h
OMe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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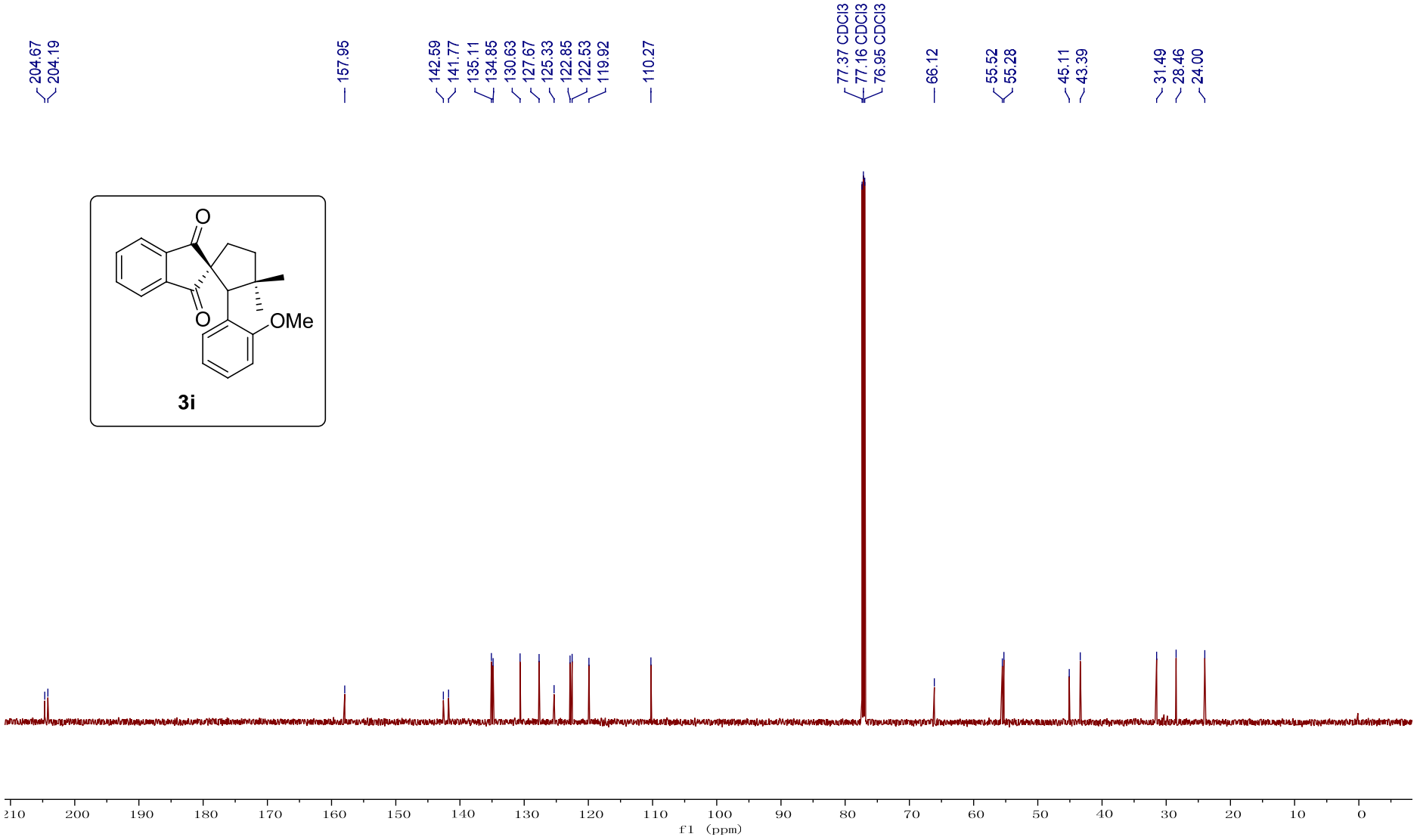
7.611
7.609
7.597
7.320
7.318
7.307
7.305
7.260
6.982
6.980
6.969
6.967
6.956
6.954
6.744
6.742
6.731
6.719
6.717
6.511
6.497
4.097
3.479
2.341
2.328
2.323
2.319
2.310
2.307
2.301
2.289
2.114
2.110
2.100
2.096
2.092
2.089
2.078
2.075
2.059
2.040
2.026
2.021
2.007
1.916
1.913
1.904
1.900
1.897
1.893
1.884
1.880
1.365
1.046
O
O
OMe
3i
0.95
1.93
0.99
1.00
0.97
0.98
0.97
1.00
2.95
1.04
2.10
1.05
2.98
3.00
f1 (ppm)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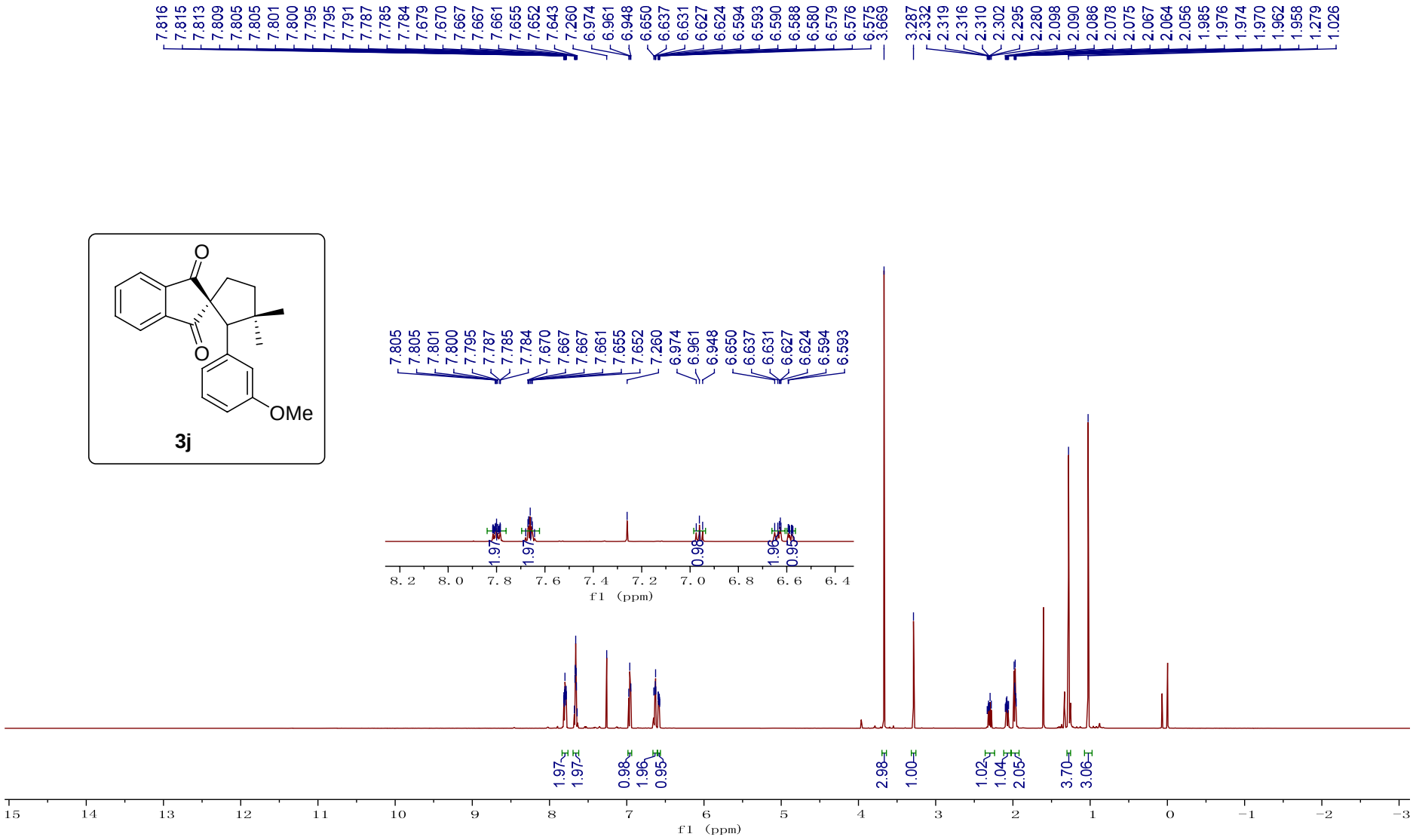
134.85
130.63
127.67
125.33
122.85
122.53
119.92
110.27
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.12
55.52
55.28
45.11
43.39
31.49
28.46
24.00
O
O
OMe
3i
f1 (ppm)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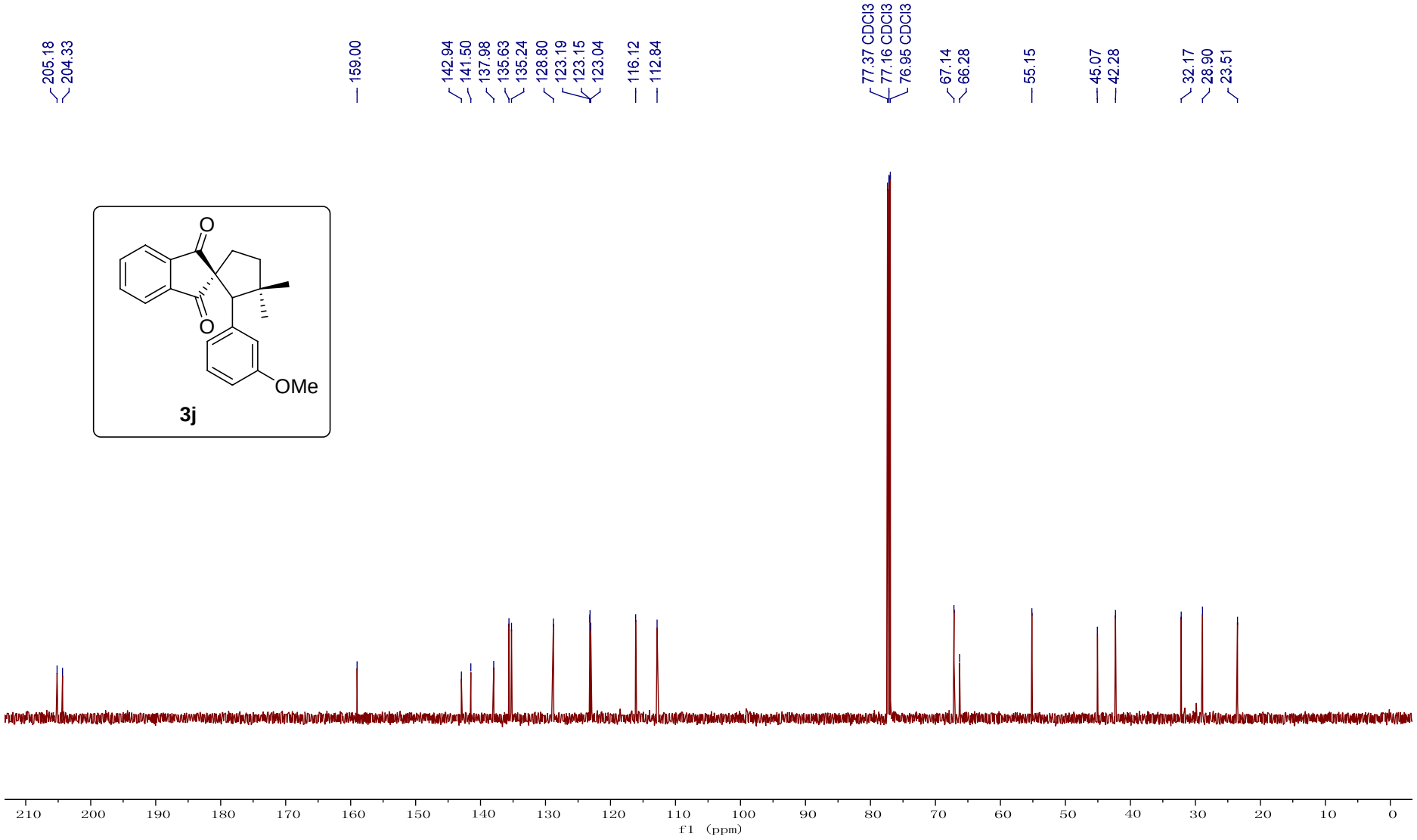
O
O
OMe
3j
7.805 7.805 7.801 7.800 7.795 7.787 7.785 7.784 7.670 7.667 7.667 7.661 7.655 7.652 7.260 6.974 6.961 6.948 6.650 6.637 6.631 6.627 6.624 6.594 6.593
1.97 1.97 0.98 1.96 0.95
8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4
f1 (ppm)
1.97 1.97 0.98 1.96 0.95 2.98 1.00 1.02 1.04 2.05 3.70 3.06
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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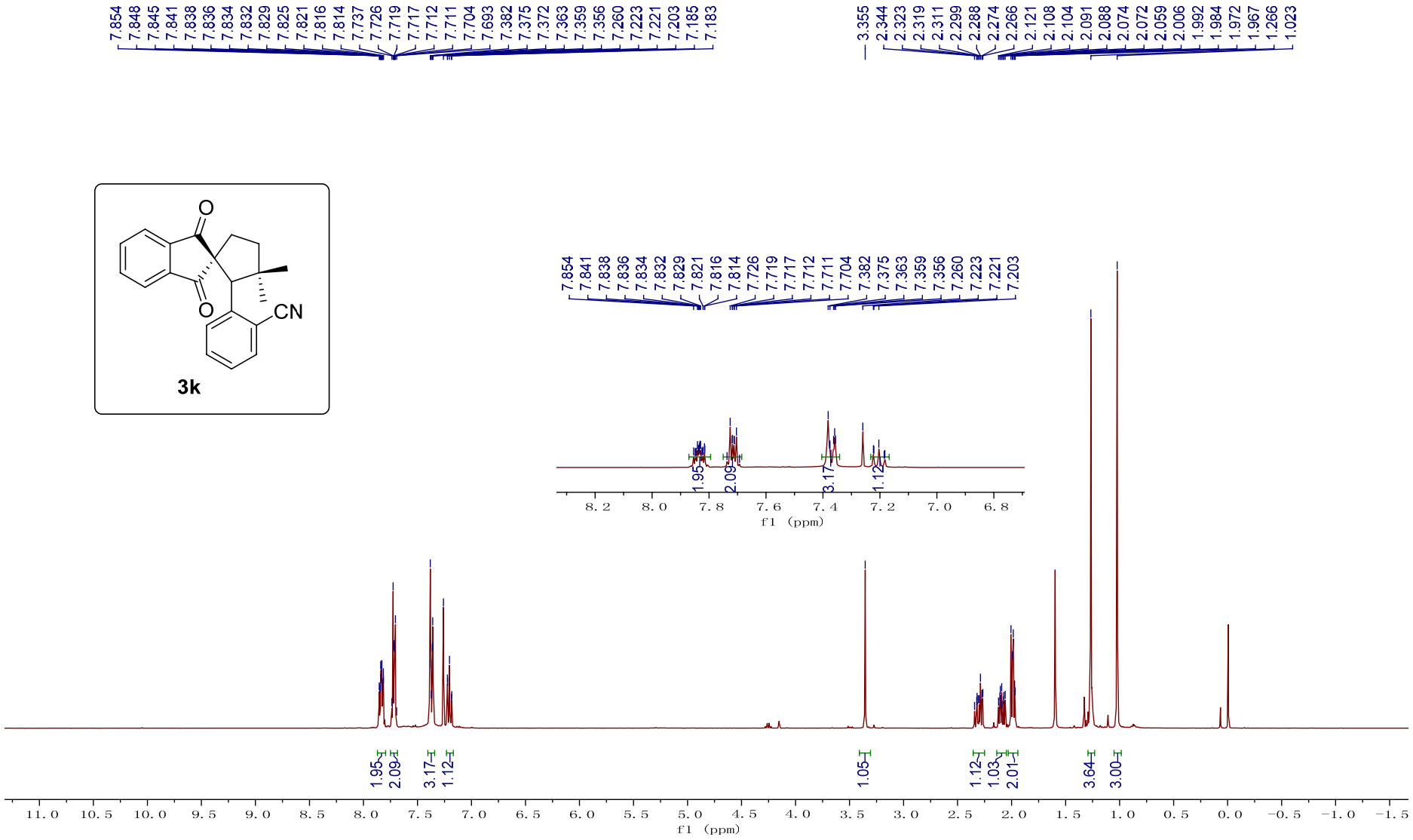
141.50
137.98
135.63
135.24
128.80
123.19
123.15
123.04
116.12
112.84
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
67.14
66.28
55.15
45.07
42.28
32.17
28.90
23.51
O
O
OMe
3j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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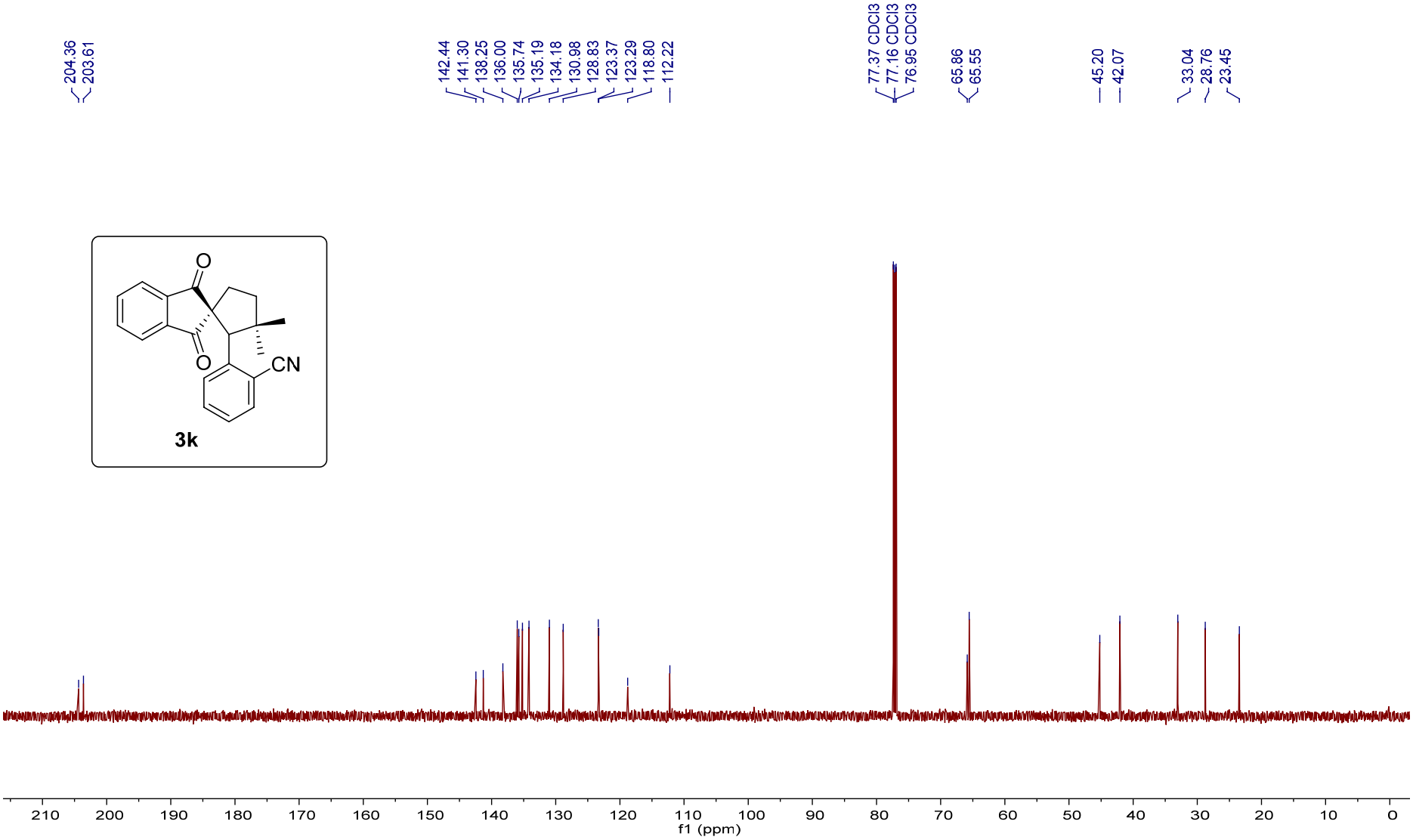
7.829
7.825
7.821
7.816
7.814
7.737
7.726
7.719
7.717
7.712
7.711
7.704
7.693
7.382
7.375
7.372
7.363
7.359
7.356
7.260
7.223
7.221
7.203
7.185
7.183
3.355
2.344
2.323
2.319
2.311
2.299
2.288
2.274
2.266
2.121
2.108
2.104
2.091
2.088
2.074
2.072
2.059
2.006
1.992
1.984
1.972
1.967
1.266
1.023
O
O
CN
3k
1.95
2.09
3.17
1.12
1.05
1.12
1.03
2.01
3.64
3.00
f1 (ppm)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136.00
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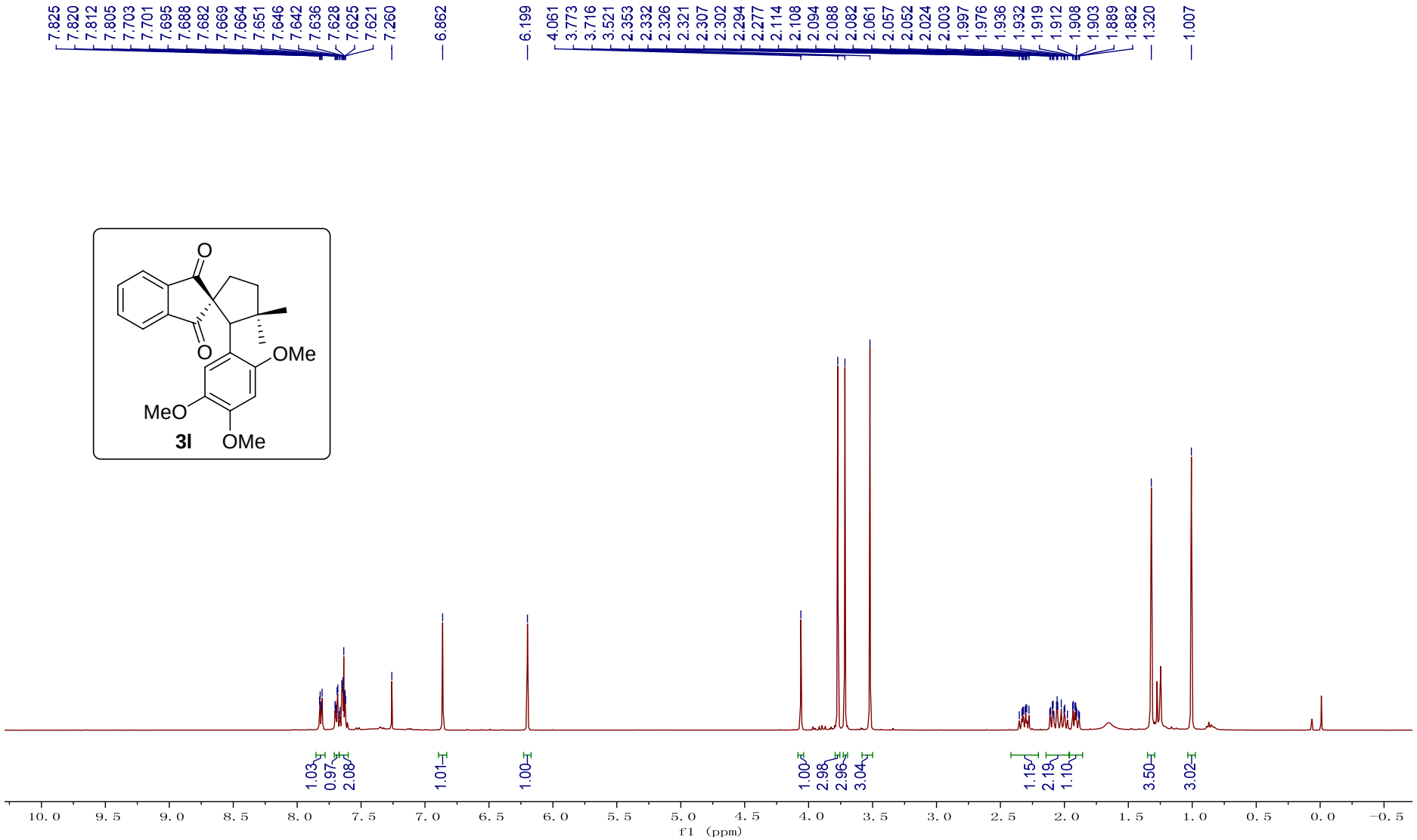
135.19
134.18
130.98
128.83
123.37
123.29
118.80
112.22
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
65.86
65.55
45.20
42.07
33.04
28.76
23.45
O
O
CN
3k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.805
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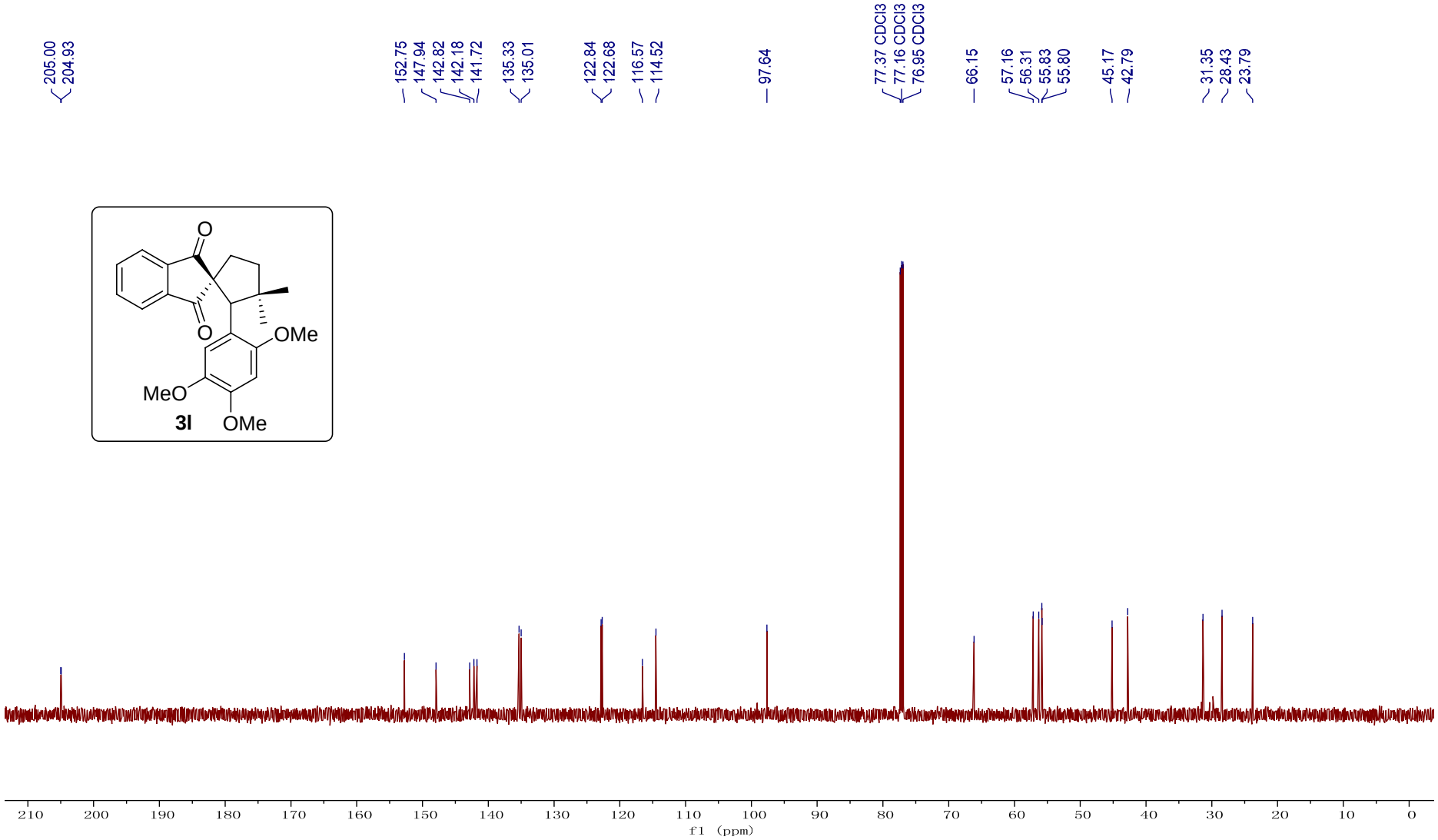
7.682
7.669
7.664
7.651
7.646
7.642
7.636
7.628
7.625
7.621
7.260
6.862
6.199
4.061
3.773
3.716
3.521
2.353
2.332
2.326
2.321
2.307
2.302
2.294
2.277
2.114
2.108
2.094
2.088
2.082
2.061
2.057
2.052
2.024
2.003
1.997
1.976
1.936
1.932
1.919
1.912
1.908
1.903
1.889
1.882
1.320
1.007
O
O
OMe
MeO
OMe
3l
1.03
0.97
2.08
1.01
1.00
1.00
2.98
2.96
3.04
1.15
2.19
1.10
3.50
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)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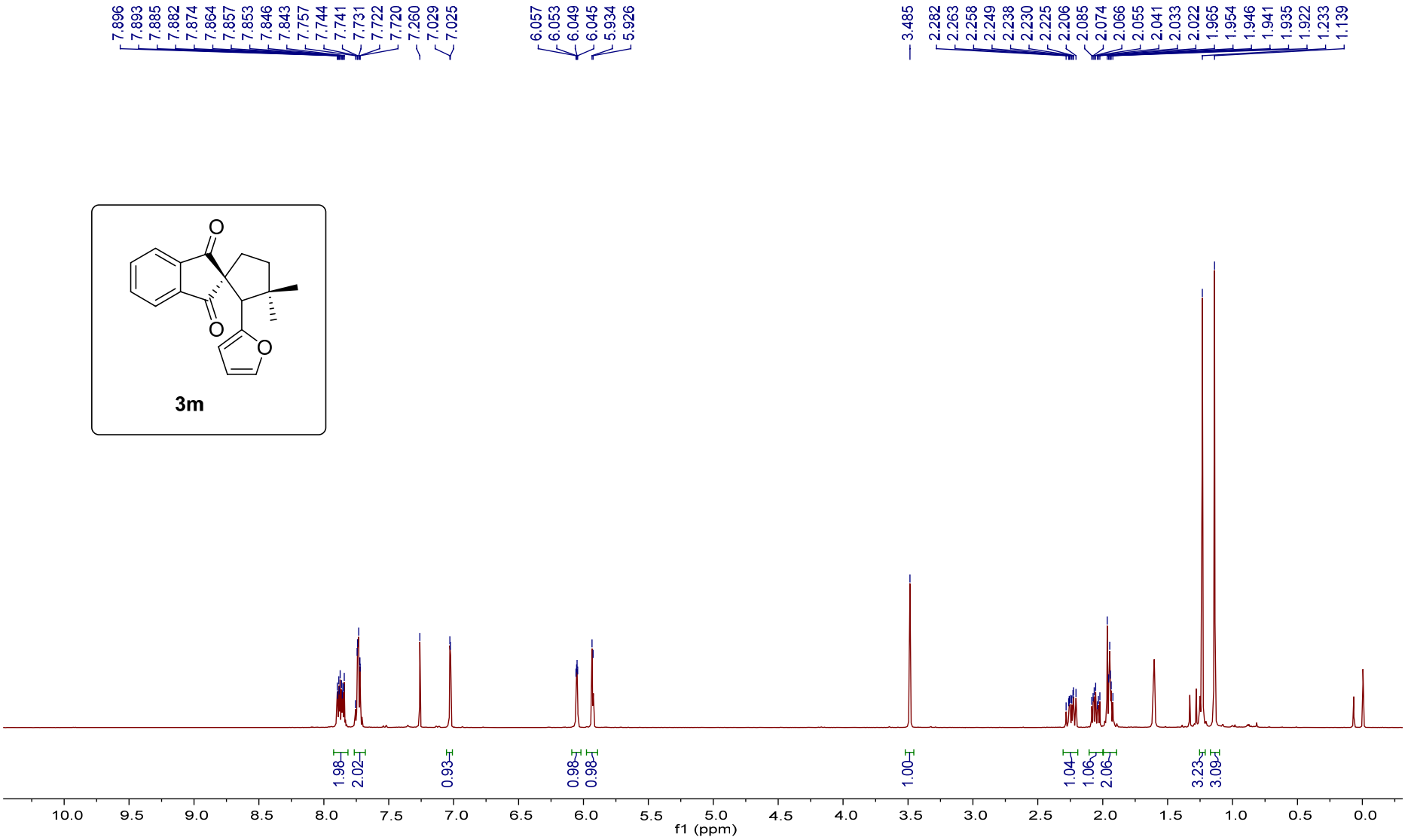
152.75
147.94
142.82
142.18
141.72
135.33
135.01
122.84
122.68
116.57
114.52
97.64
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.15
57.16
56.31
55.83
55.80
45.17
42.79
31.35
28.43
23.79
O
O
OMe
MeO
OMe
3l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.882
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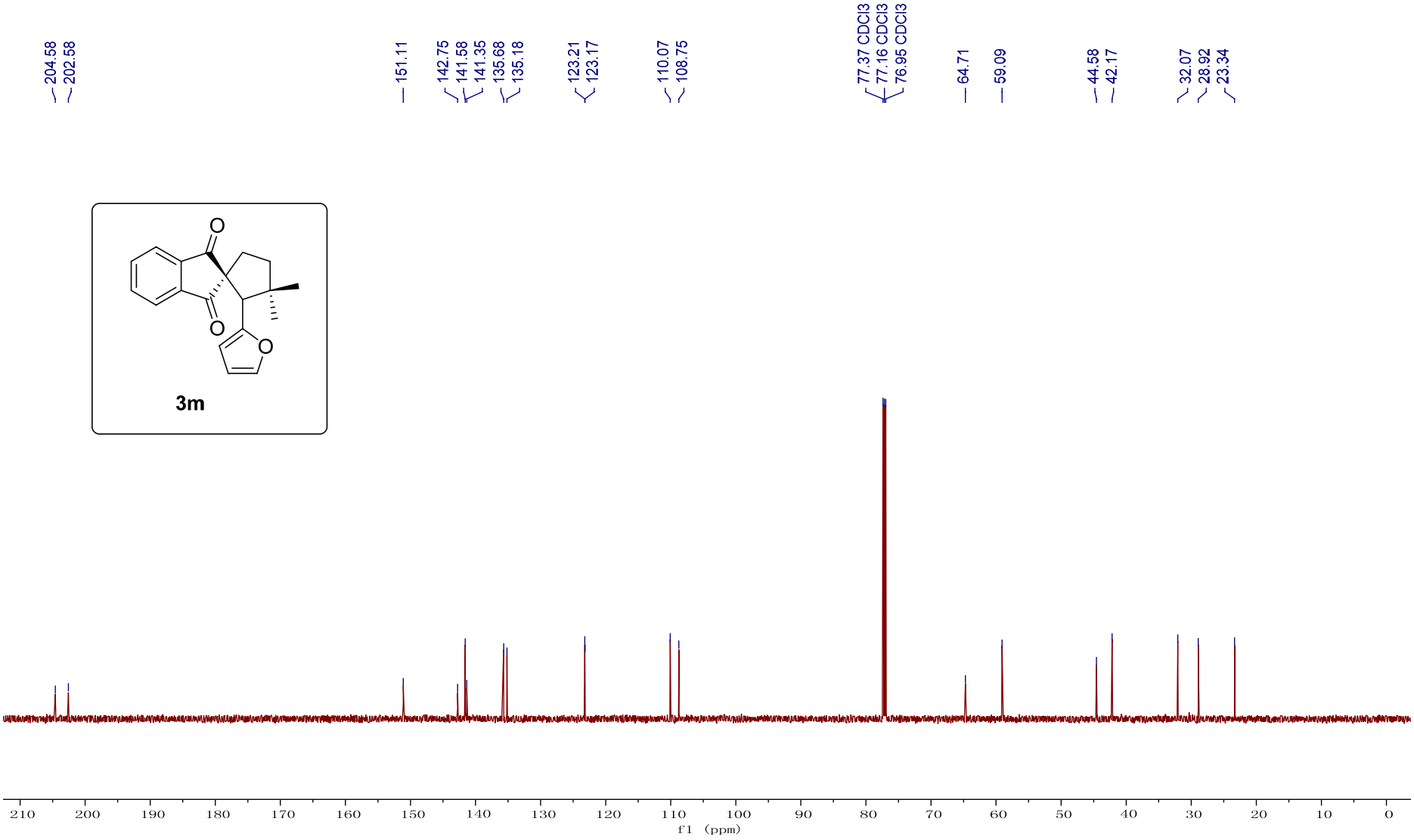
7.853
7.846
7.843
7.757
7.744
7.741
7.731
7.722
7.720
7.260
7.029
7.025
6.057
6.053
6.049
6.045
5.934
5.926
3.485
2.282
2.263
2.258
2.249
2.238
2.230
2.225
2.206
2.085
2.074
2.066
2.055
2.041
2.033
2.022
1.965
1.954
1.946
1.941
1.935
1.922
1.233
1.139
O
O
O
3m
1.98
2.02
0.93
0.98
0.98
1.00
1.04
1.06
2.06
3.23
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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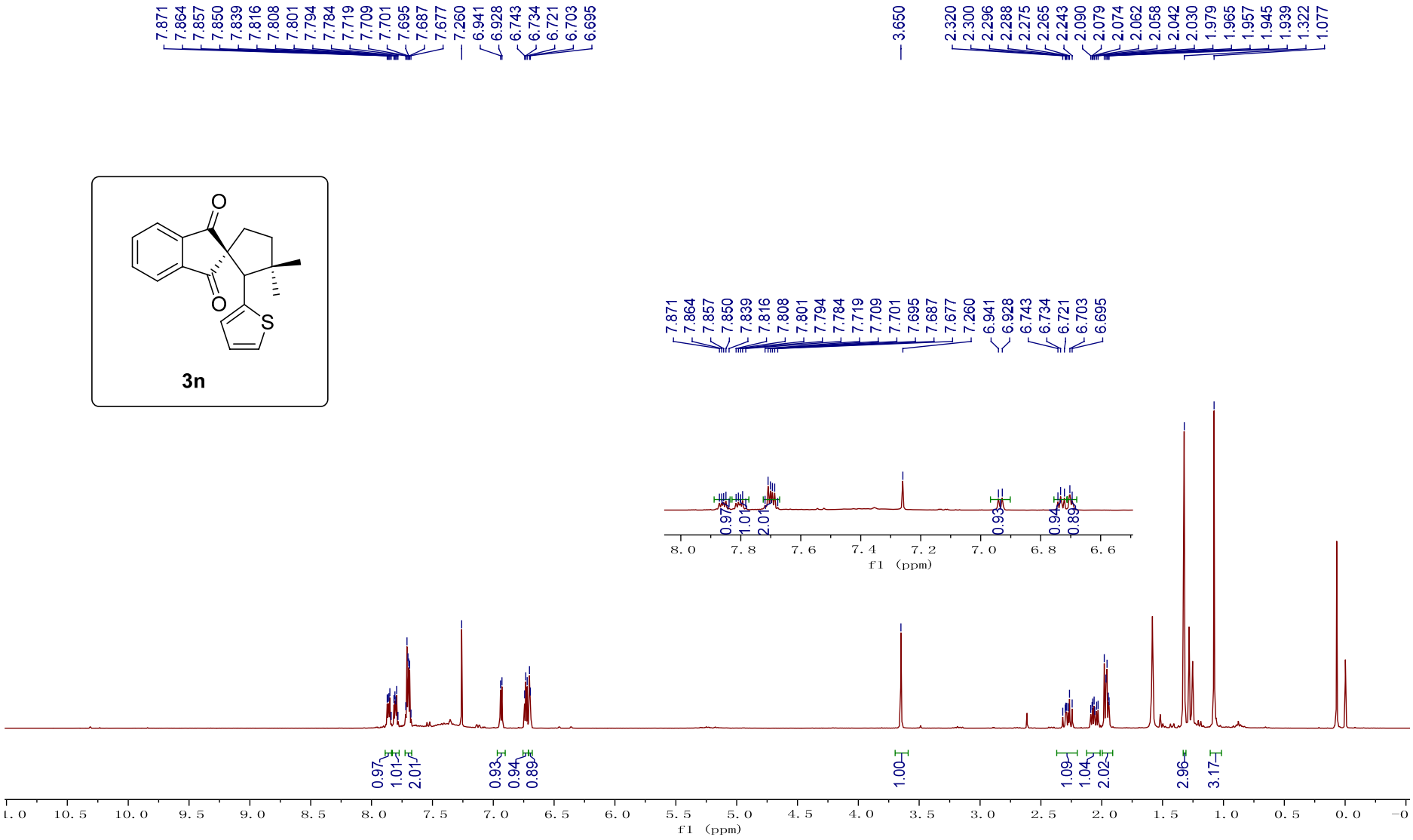
141.35
135.68
135.18
123.21
123.17
110.07
108.75
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
64.71
59.09
44.58
42.17
32.07
28.92
23.34
O
O
O
3m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.857
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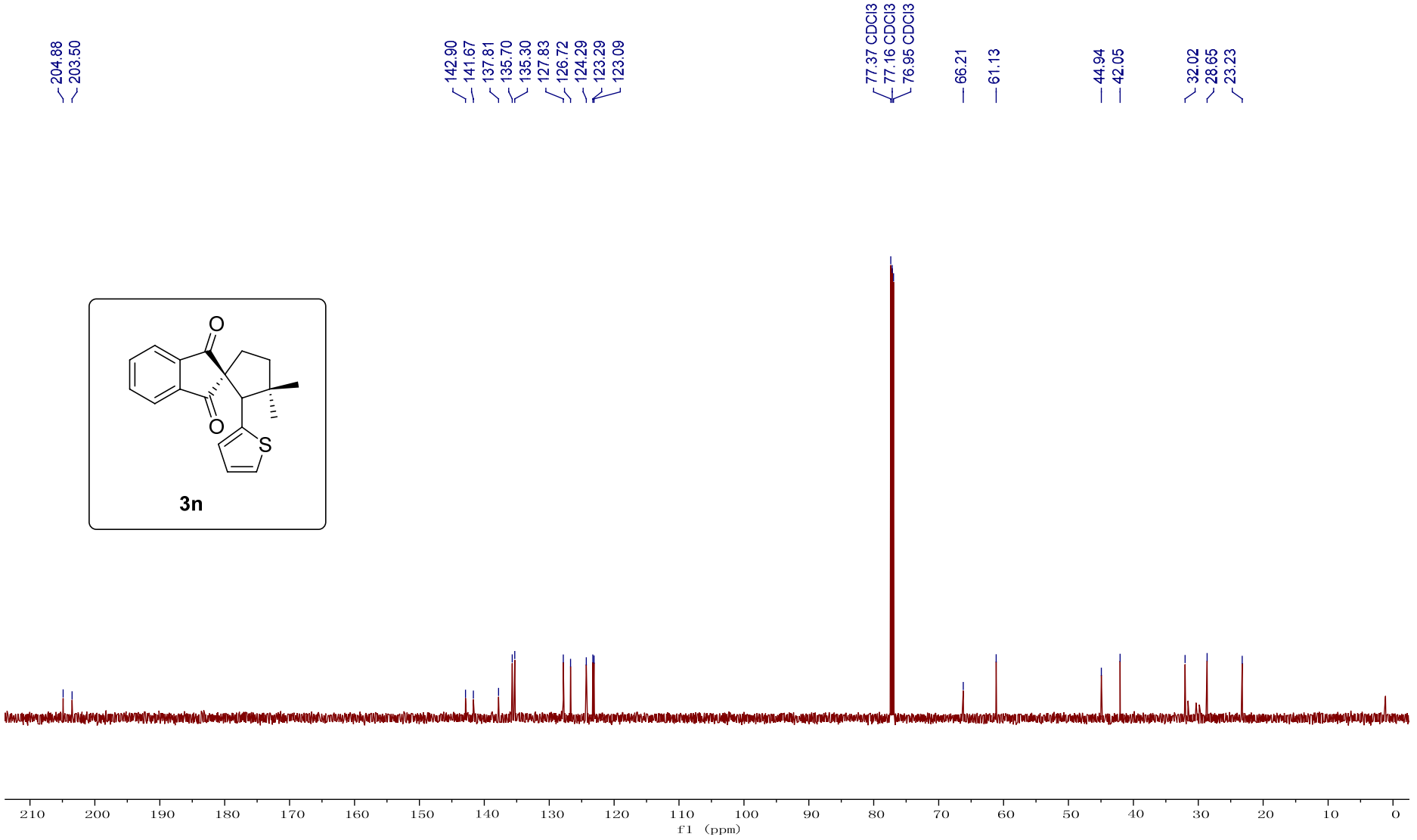
7.801
7.794
7.784
7.719
7.709
7.701
7.695
7.687
7.677
7.260
6.941
6.928
6.743
6.734
6.721
6.703
6.695
3.650
2.320
2.300
2.296
2.288
2.275
2.265
2.243
2.090
2.079
2.074
2.062
2.058
2.042
2.030
1.979
1.965
1.957
1.945
1.939
1.322
1.077
O
O
S
3n
0.97
1.01
2.01
0.93
0.94
0.89
1.00
1.09
1.04
2.02
2.96
3.17
f1 (ppm)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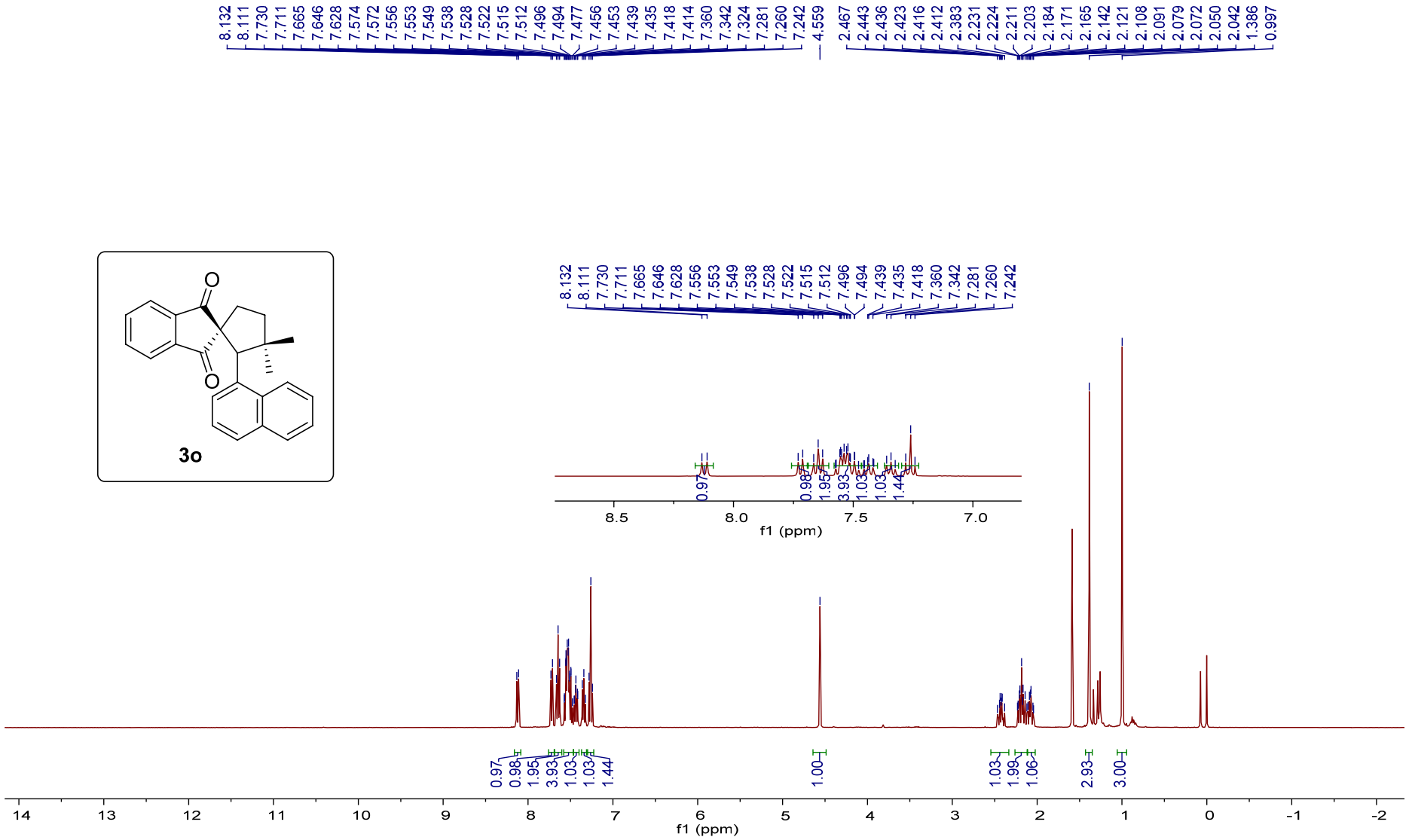
127.83
126.72
124.29
123.29
123.09
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.21
61.13
44.94
42.05
32.02
28.65
23.23
O
O
S
3n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.132
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7.665
7.646
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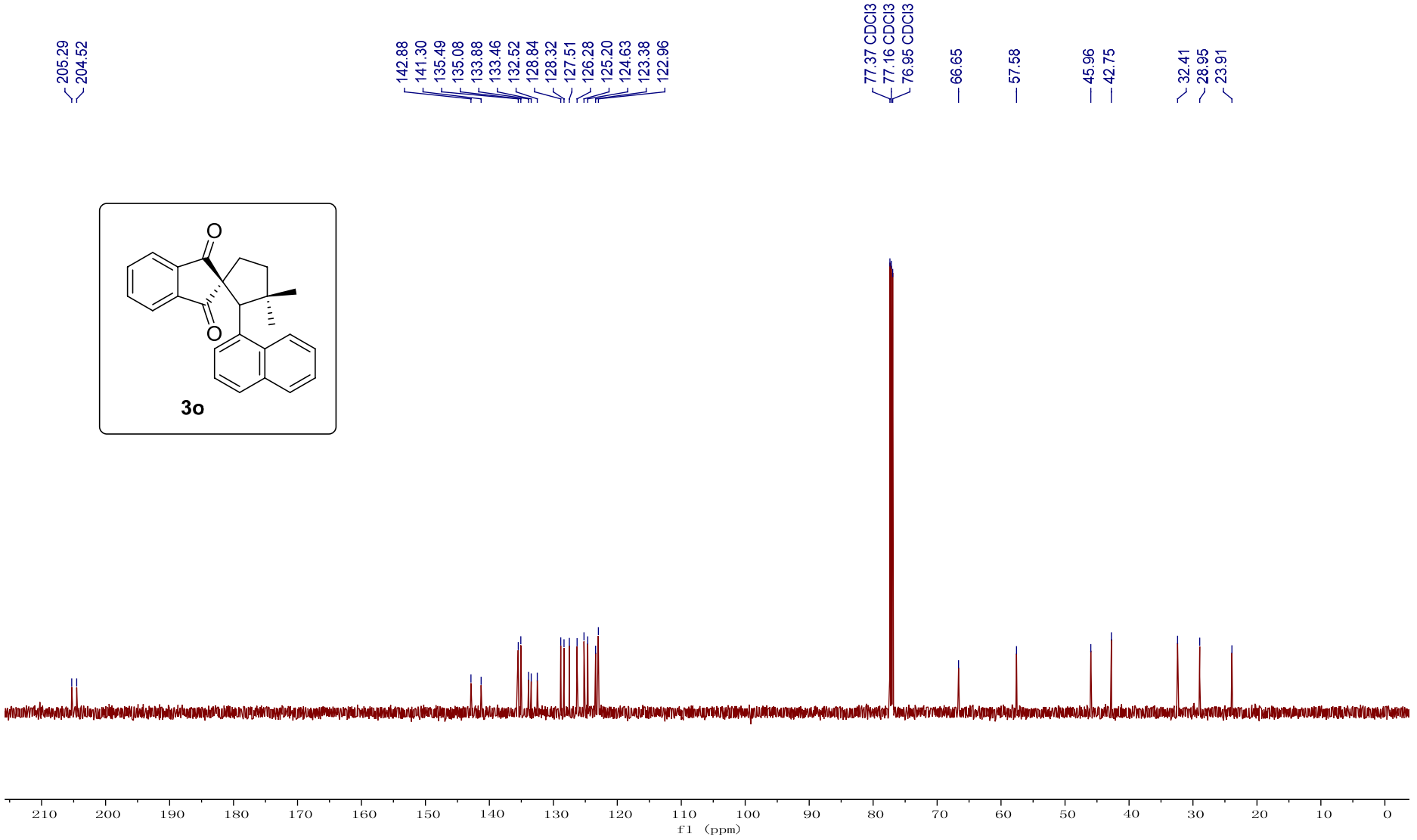
7.574
7.572
7.556
7.553
7.549
7.538
7.528
7.522
7.515
7.512
7.496
7.494
7.477
7.456
7.453
7.439
7.435
7.418
7.414
7.360
7.342
7.324
7.281
7.260
7.242
4.559
2.467
2.443
2.436
2.423
2.416
2.412
2.383
2.231
2.224
2.211
2.203
2.184
2.171
2.165
2.142
2.121
2.108
2.091
2.079
2.072
2.050
2.042
1.386
0.997
3o
f1 (ppm)
0.97
0.98
1.95
3.93
1.03
1.03
1.44
1.00
1.03
1.99
1.06
2.93
3.00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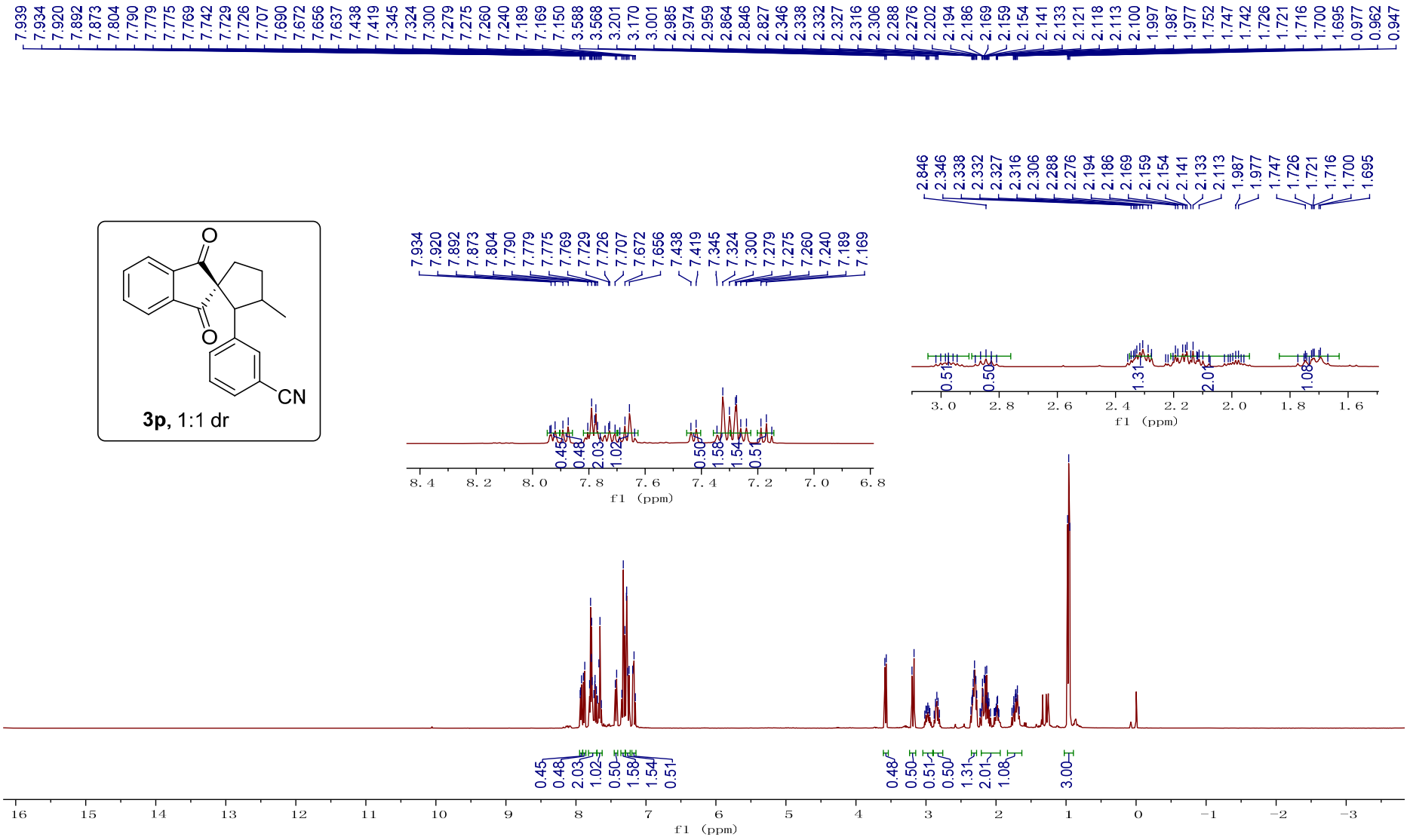
135.08
133.88
133.46
132.52
128.84
128.32
127.51
126.28
125.20
124.63
123.38
122.96
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.65
57.58
45.96
42.75
32.41
28.95
23.91
O
O
3o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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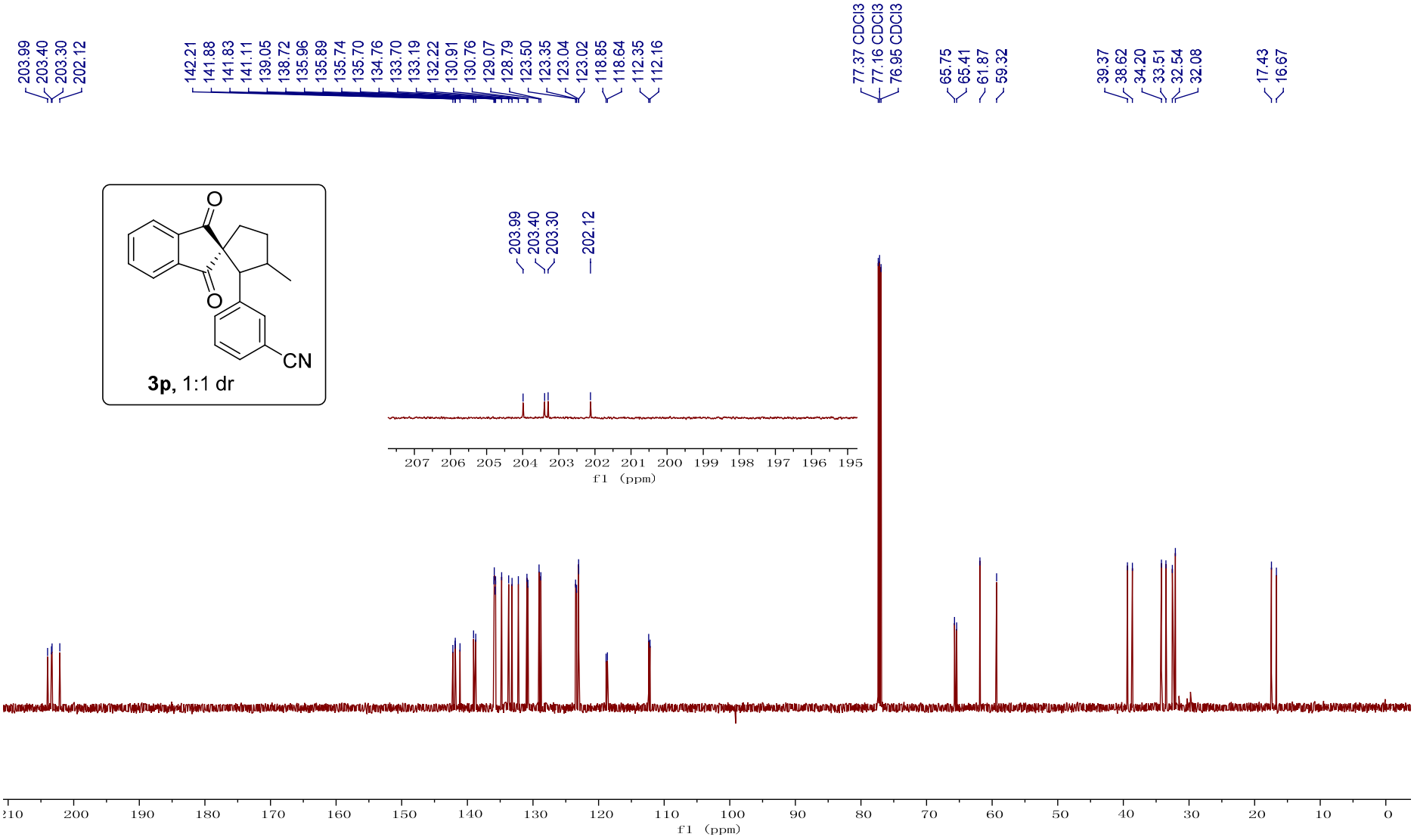
7.779
7.775
7.769
7.742
7.729
7.726
7.707
7.690
7.672
7.656
7.637
7.438
7.419
7.345
7.324
7.300
7.279
7.275
7.260
7.240
7.189
7.169
7.150
3.588
3.568
3.201
3.170
3.001
2.985
2.974
2.959
2.864
2.846
2.827
2.346
2.338
2.332
2.327
2.316
2.306
2.288
2.276
2.202
2.194
2.186
2.169
2.159
2.154
2.141
2.133
2.121
2.118
2.113
2.100
1.997
1.987
1.977
1.752
1.747
1.742
1.726
1.721
1.716
1.700
1.695
0.977
0.962
0.947
O
O
CN
3p, 1:1 dr
0.45
0.48
2.03
1.02
0.50
1.58
1.54
0.51
0.48
0.50
0.51
0.50
1.31
2.01
1.08
3.00
f1 (ppm)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202.12
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141.11
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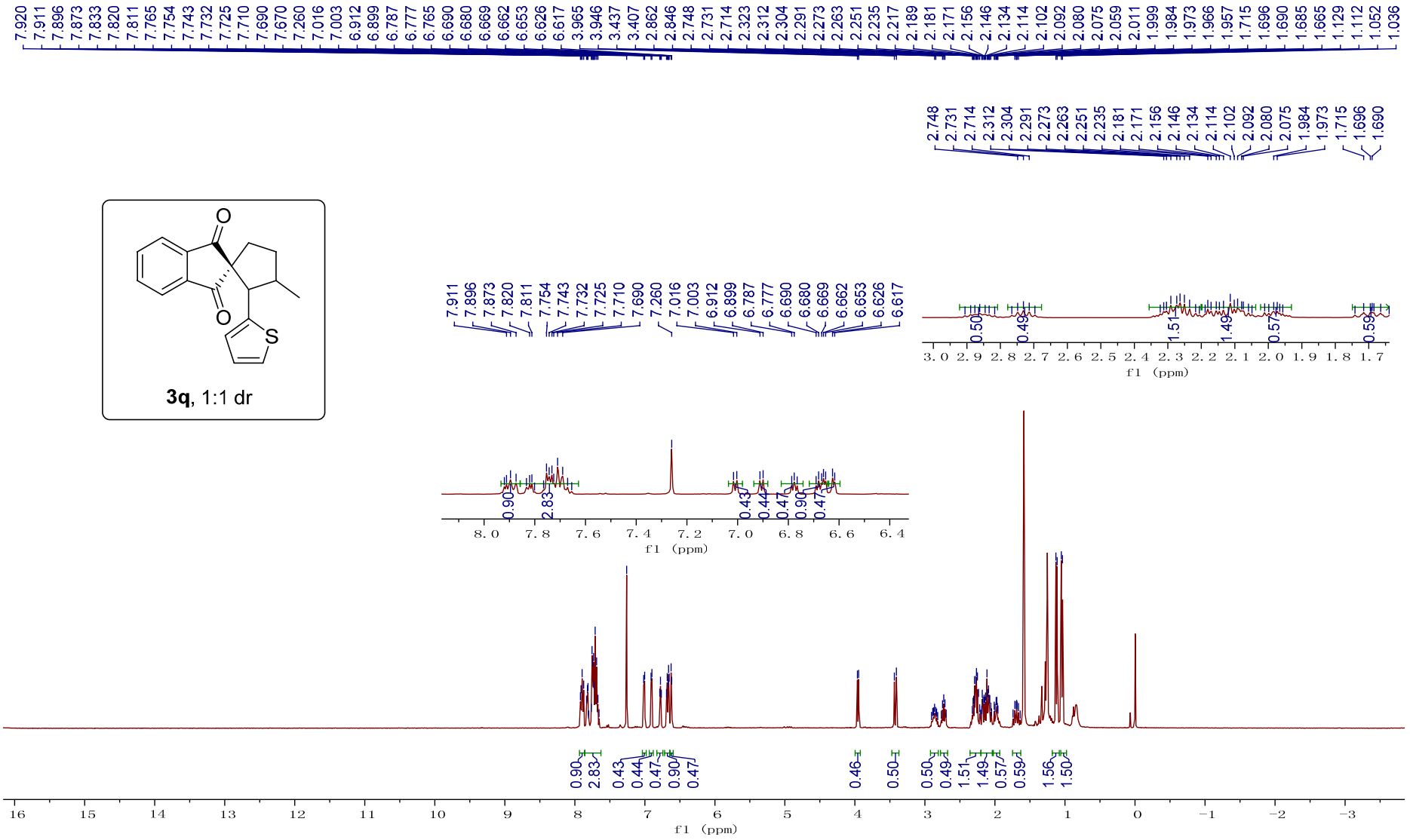
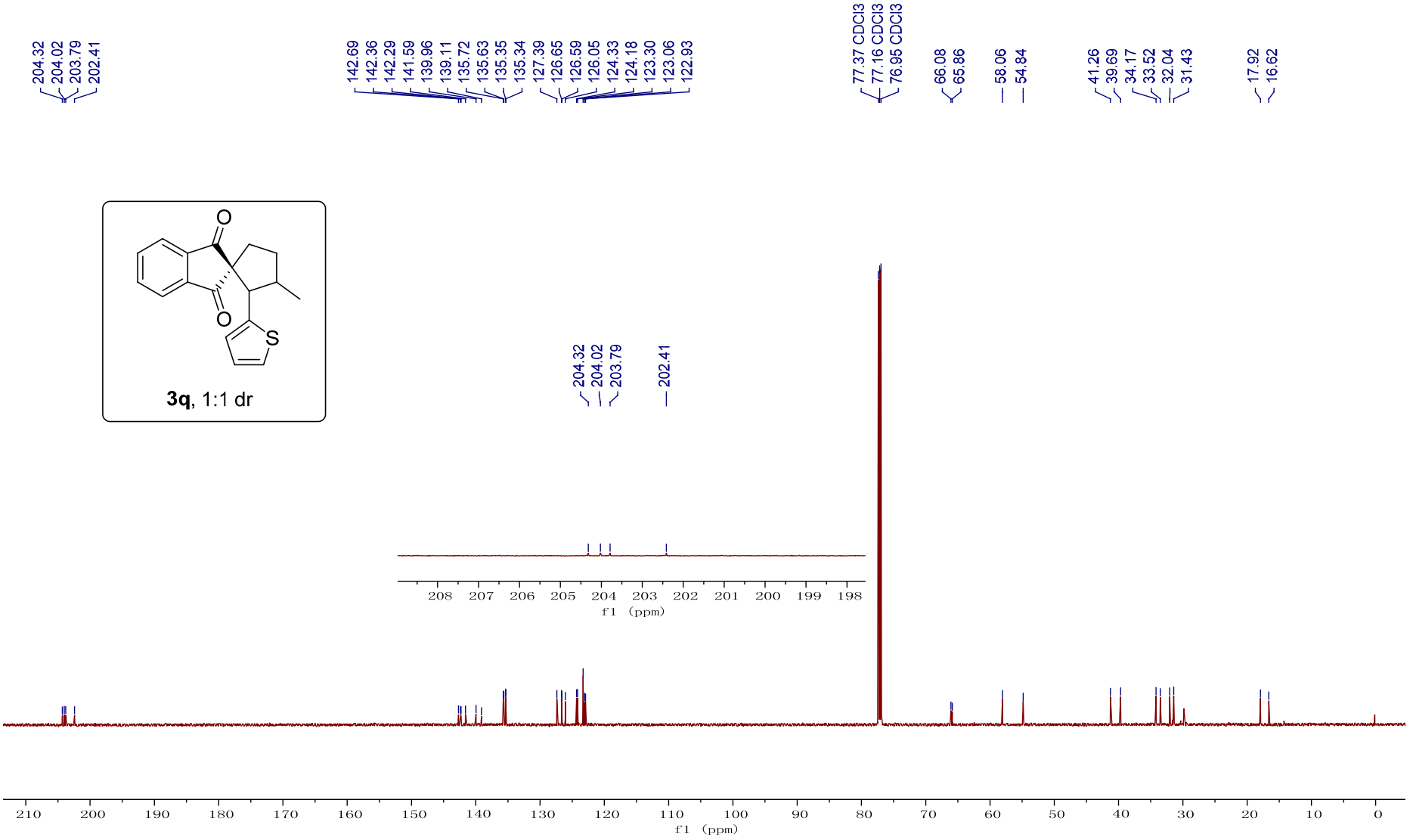
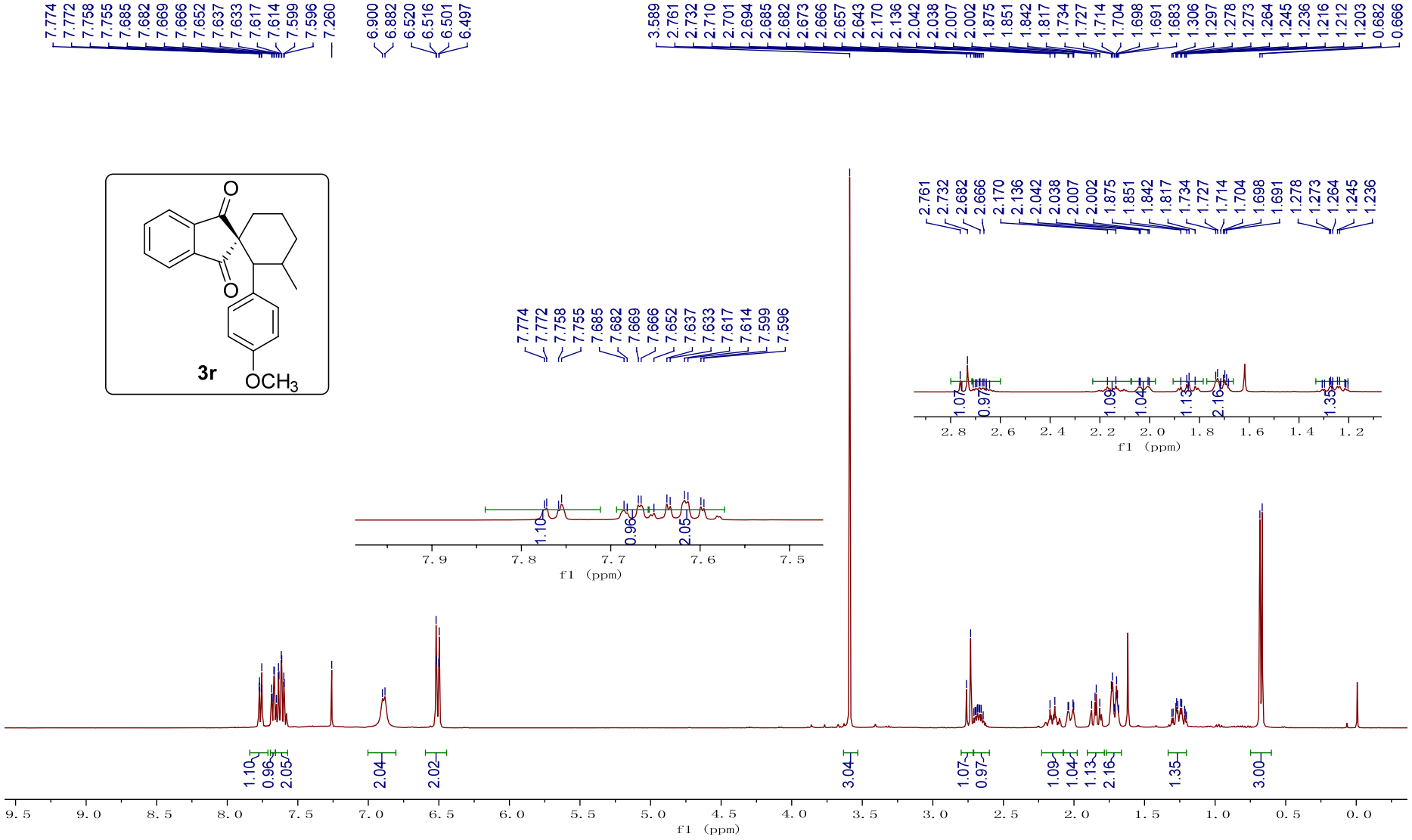
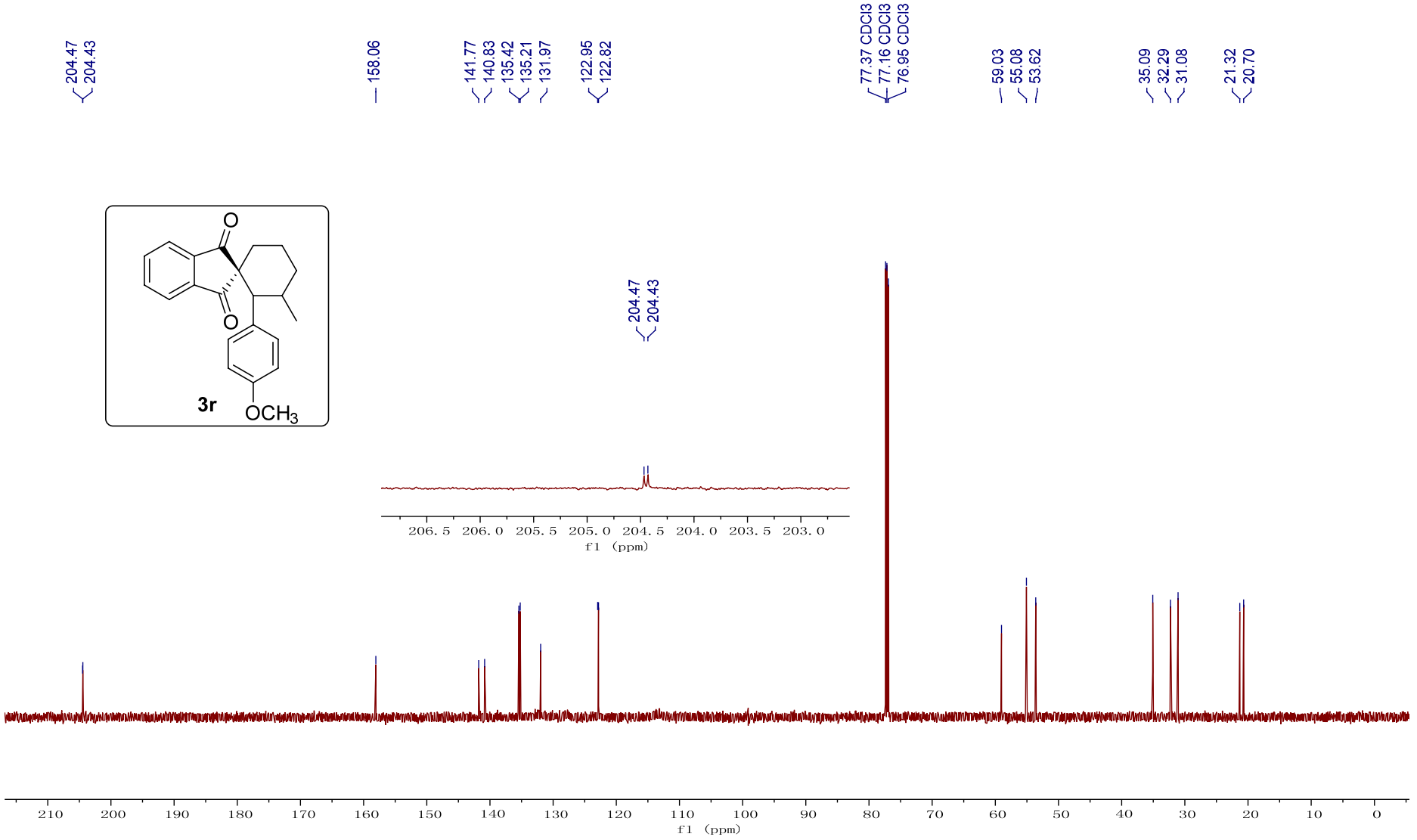
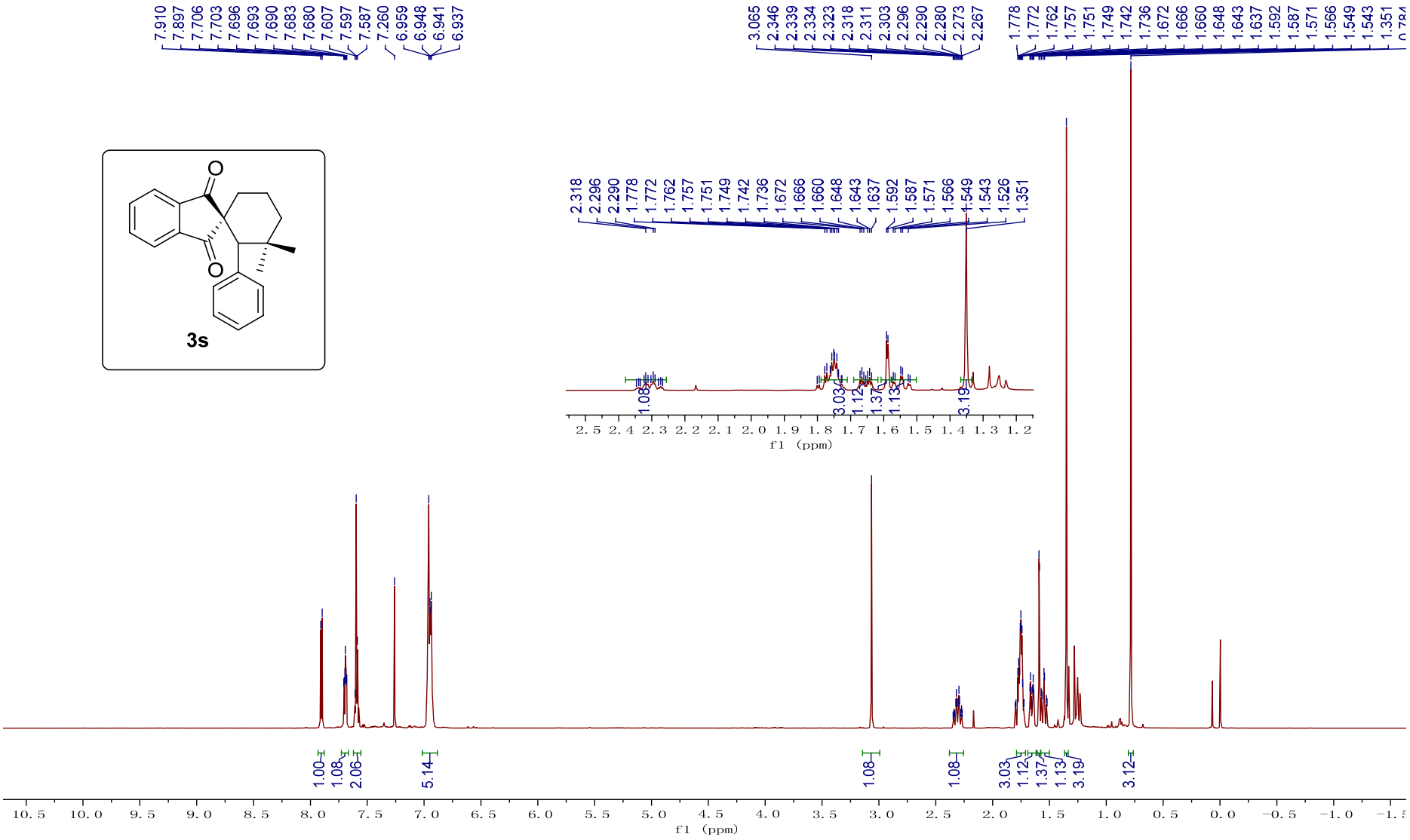
138.72
135.96
135.89
135.74
135.70
134.76
133.70
133.19
132.22
130.91
130.76
129.07
128.79
123.50
123.35
123.04
123.02
118.85
118.64
112.35
112.16
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
65.75
65.41
61.87
59.32
39.37
38.62
34.20
33.51
32.54
32.08
17.43
16.67
O
O
CN
3p, 1:1 dr
f1 (ppm)
f1 (ppm)

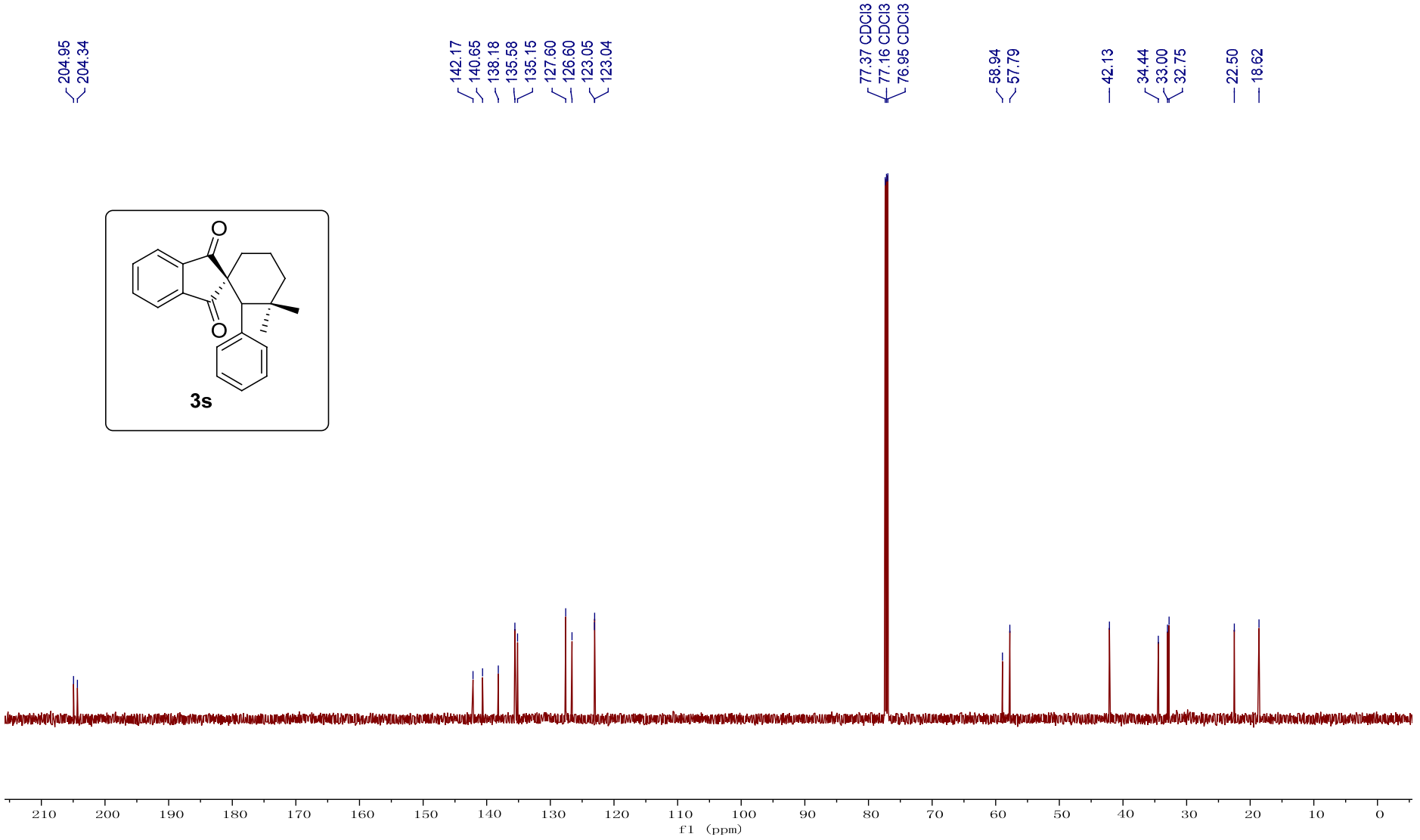

7.920 7.911 7.896 7.873 7.833 7.820 7.811 7.765 7.754 7.743 7.732 7.725 7.710 7.690 7.670 7.260 7.016 7.003 6.912 6.899 6.787 6.777 6.765 6.690 6.680 6.669 6.662 6.653 6.626 6.617 3.965 3.946 3.437 3.407 2.862 2.846 2.748 2.731 2.714 2.323 2.312 2.304 2.291 2.273 2.263 2.251 2.235 2.217 2.189 2.181 2.171 2.156 2.146 2.134 2.114 2.102 2.092 2.080 2.075 2.059 2.011 1.999 1.984 1.973 1.966 1.957 1.715 1.696 1.690 1.685 1.665 1.129 1.112 1.052 1.036
O
O
S
3q, 1:1 dr
f1 (ppm)
0.90 2.83 0.43 0.44 0.47 0.90 0.47 0.46 0.50 0.50 0.49 1.51 1.49 0.57 0.59 1.56 1.50

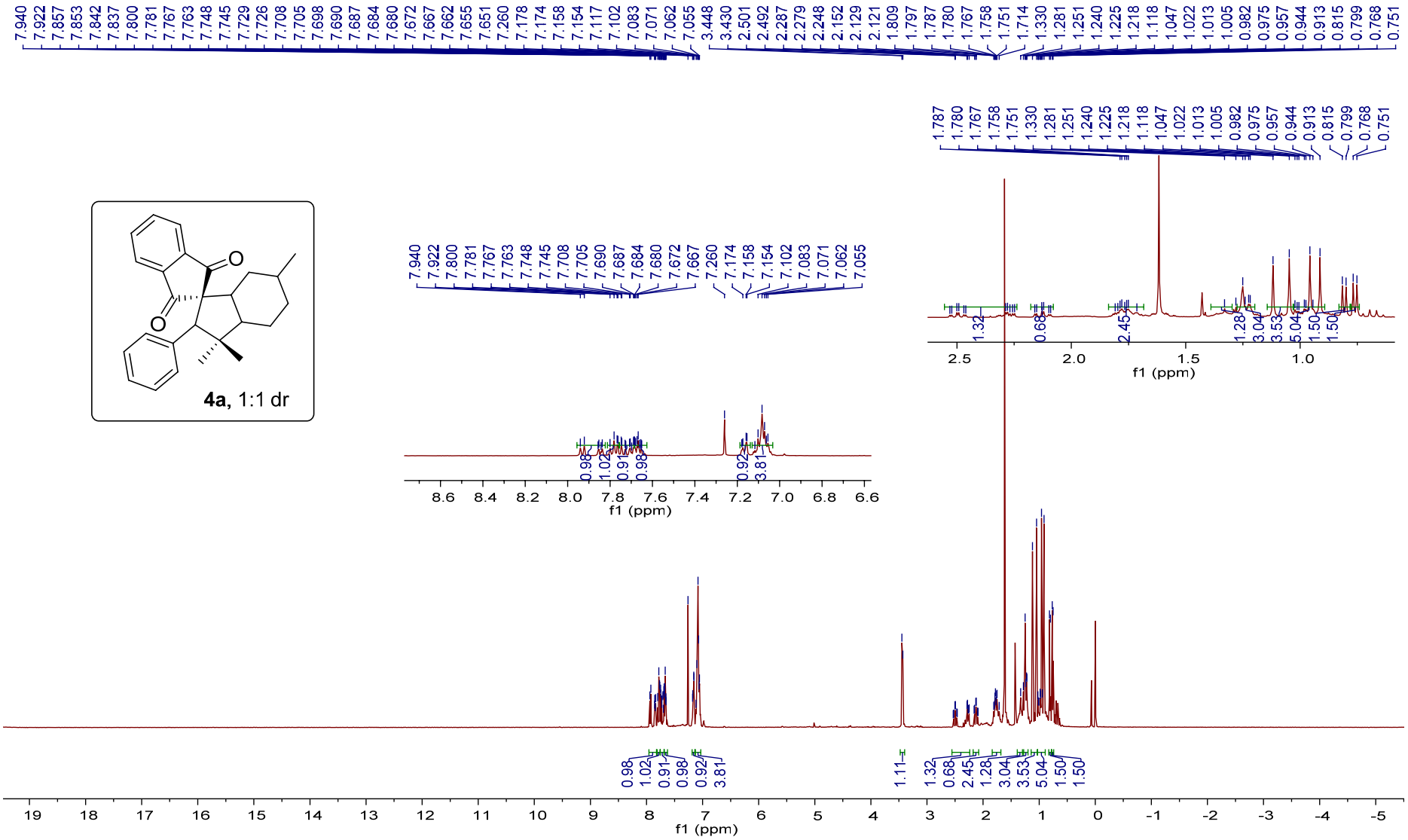

204.32
204.02
203.79
202.41
142.69
142.36
142.29
141.59
139.96
139.11
135.72
135.63
135.35
135.34
127.39
126.65
126.59
126.05
124.33
124.18
123.30
123.06
122.93
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
66.08
65.86
58.06
54.84
41.26
39.69
34.17
33.52
32.04
31.43
17.92
16.62
O
O
S
3q, 1:1 dr
204.32
204.02
203.79
202.41
208 207 206 205 204 203 202 201 200 199 198
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

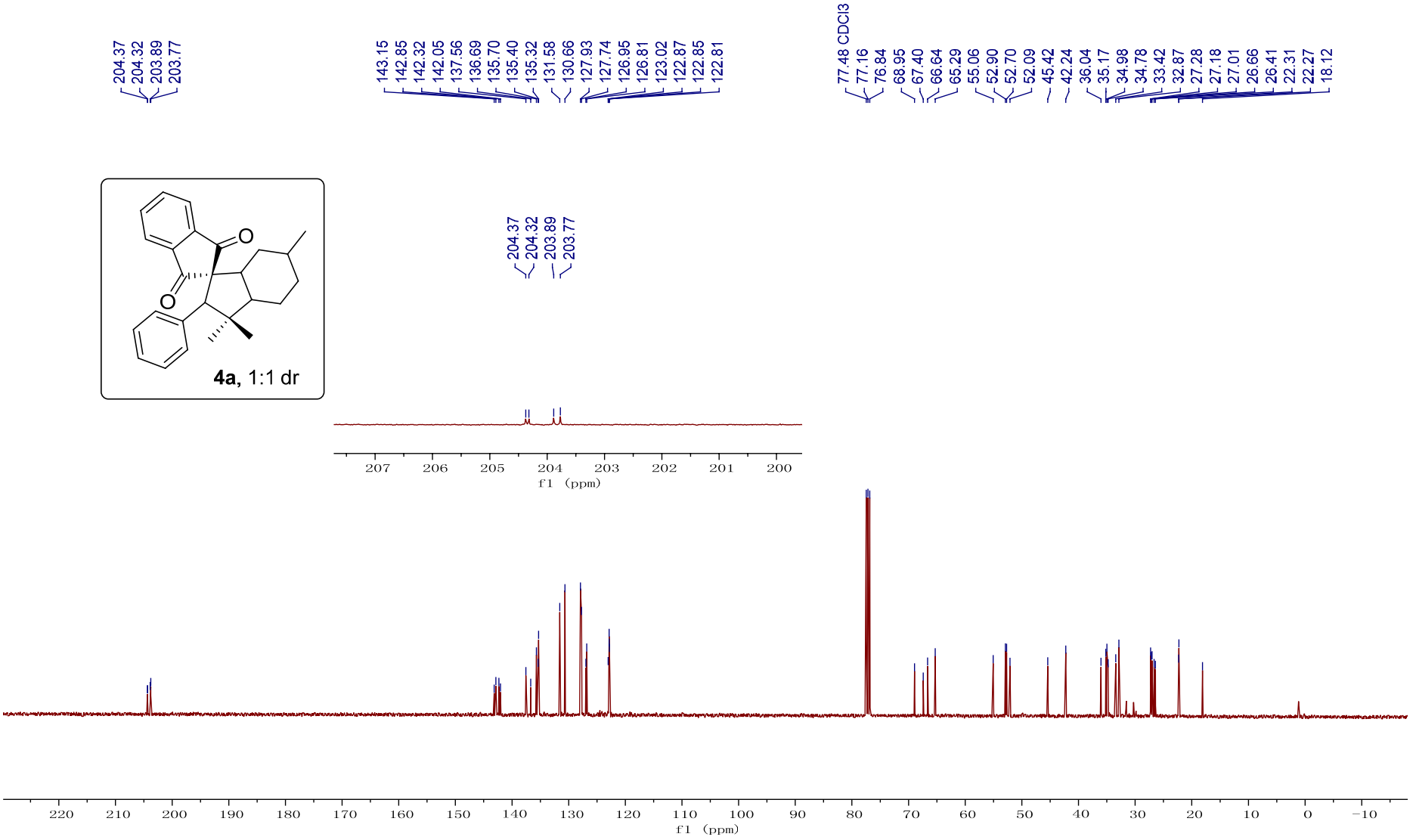

7.774
7.772
7.758
7.755
7.685
7.682
7.669
7.666
7.652
7.637
7.633
7.617
7.614
7.599
7.596
7.260
6.900
6.882
6.520
6.516
6.501
6.497
3.589
2.761
2.732
2.710
2.701
2.694
2.685
2.682
2.673
2.666
2.657
2.643
2.170
2.136
2.042
2.038
2.007
2.002
1.875
1.851
1.842
1.817
1.734
1.727
1.714
1.704
1.698
1.691
1.683
1.306
1.297
1.278
1.273
1.264
1.245
1.236
1.216
1.212
1.203
0.682
0.666
O
O
3r
OCH3
f1 (ppm)
1.10
0.96
2.05
2.04
2.02
3.04
1.07
0.97
1.09
1.04
1.13
2.16
1.35
3.00

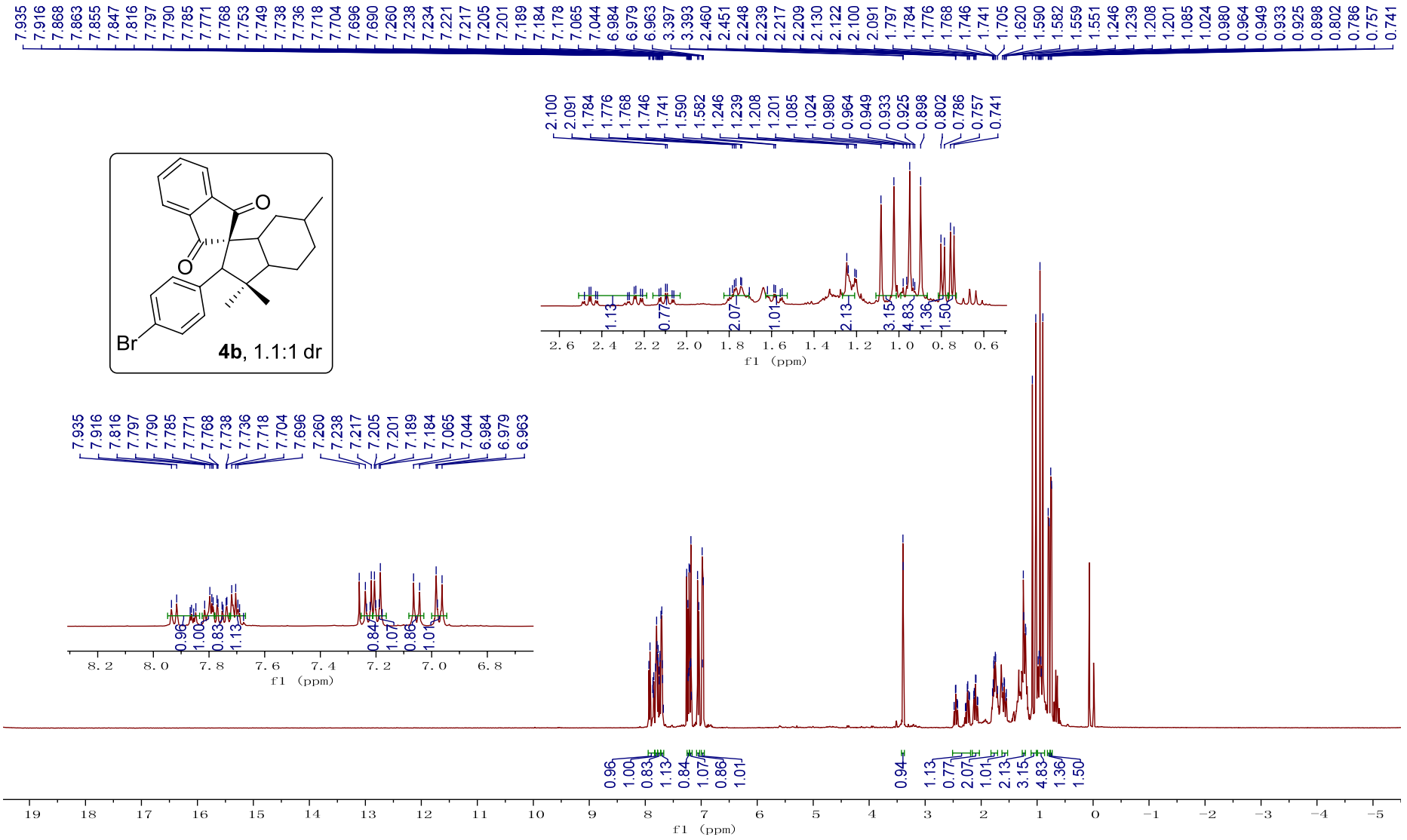

204.47
204.43
158.06
141.77
140.83
135.42
135.21
131.97
122.95
122.82
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
59.03
55.08
53.62
35.09
32.29
31.08
21.32
20.70
O
O
3r
OCH3
206.5 206.0 205.5 205.0 204.5 204.0 203.5 203.0
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

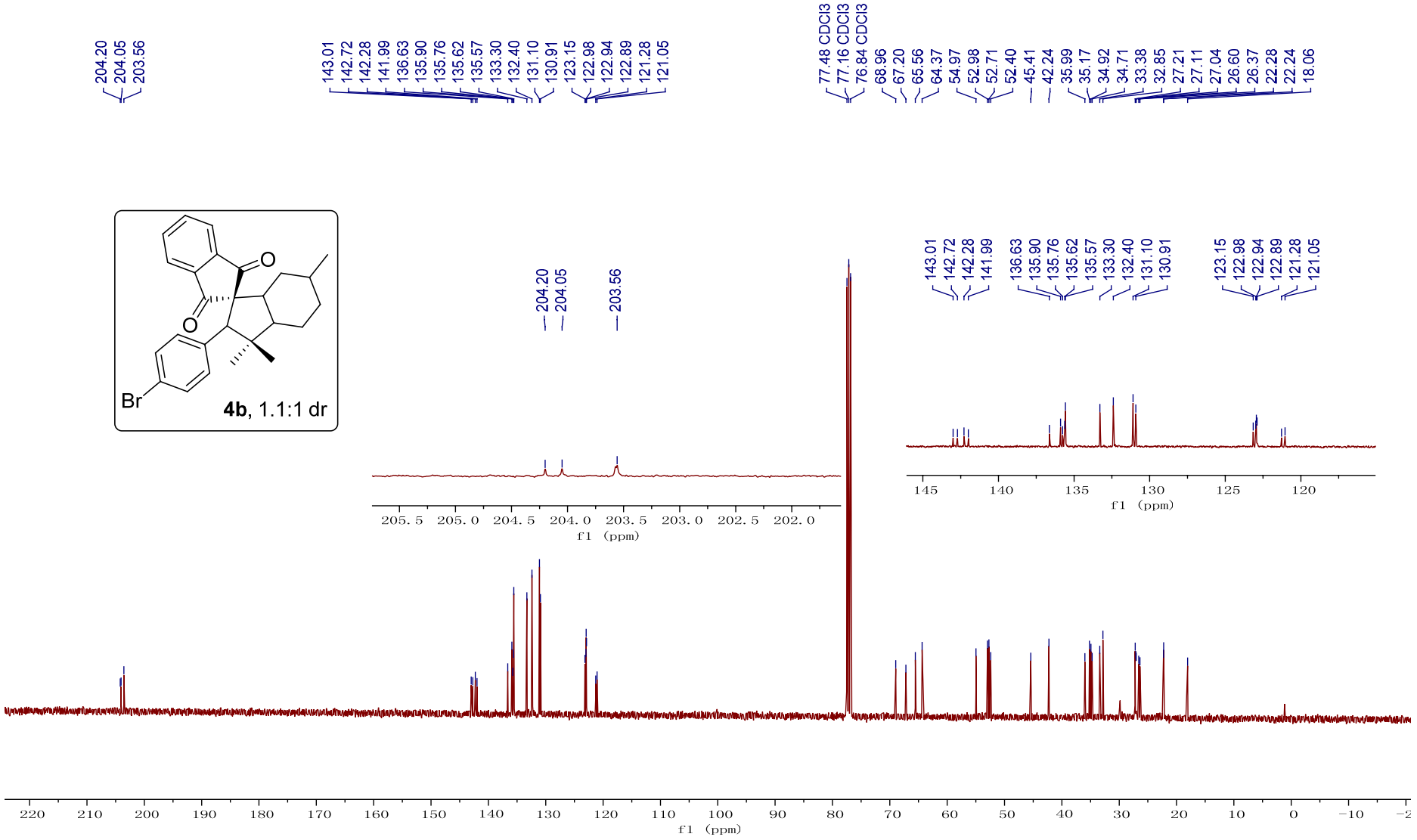

3s
f1 (ppm)

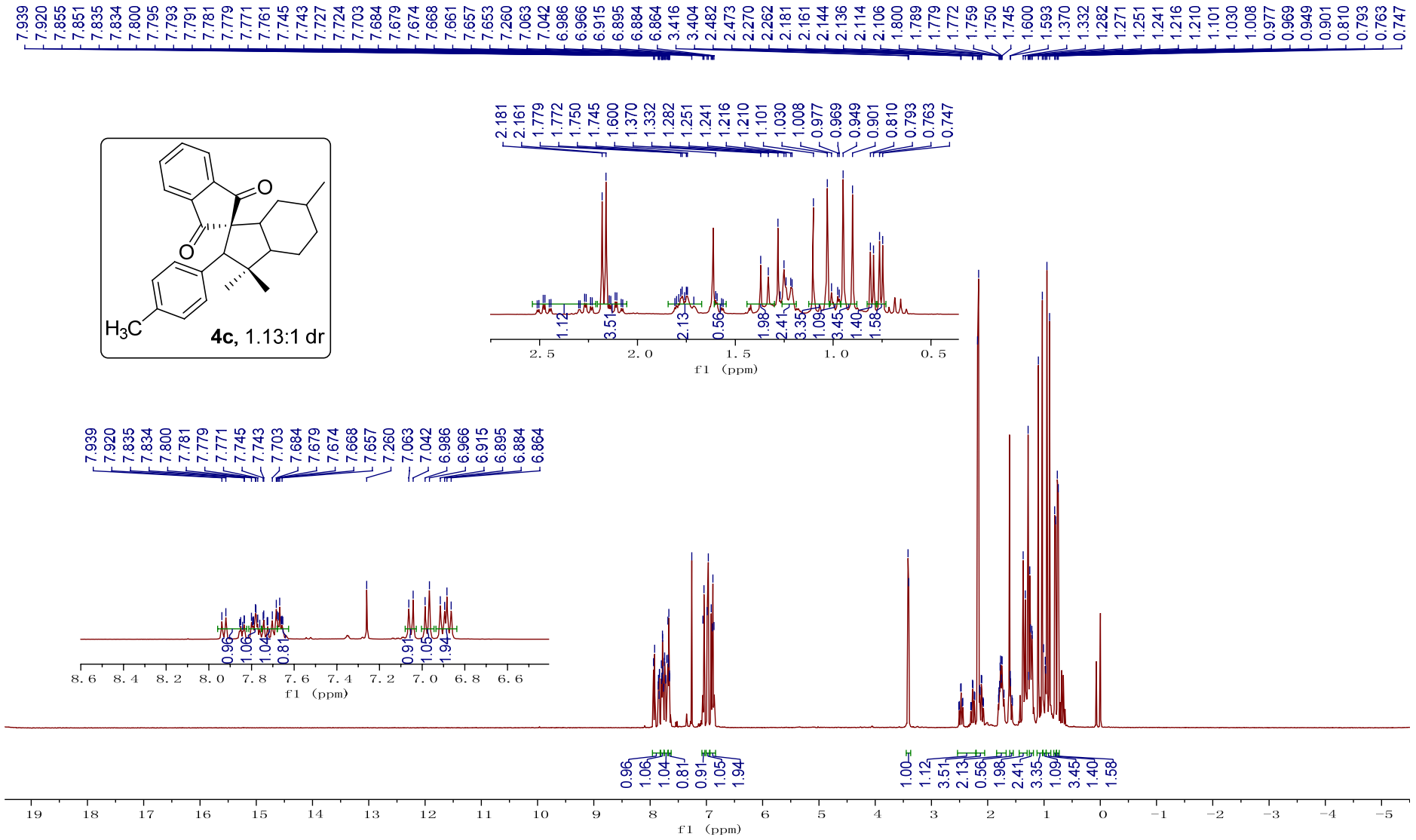

204.95
204.34
142.17
140.65
138.18
135.58
135.15
127.60
126.60
123.05
123.04
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
58.94
57.79
42.13
34.44
33.00
32.75
22.50
18.62
O
O
3s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

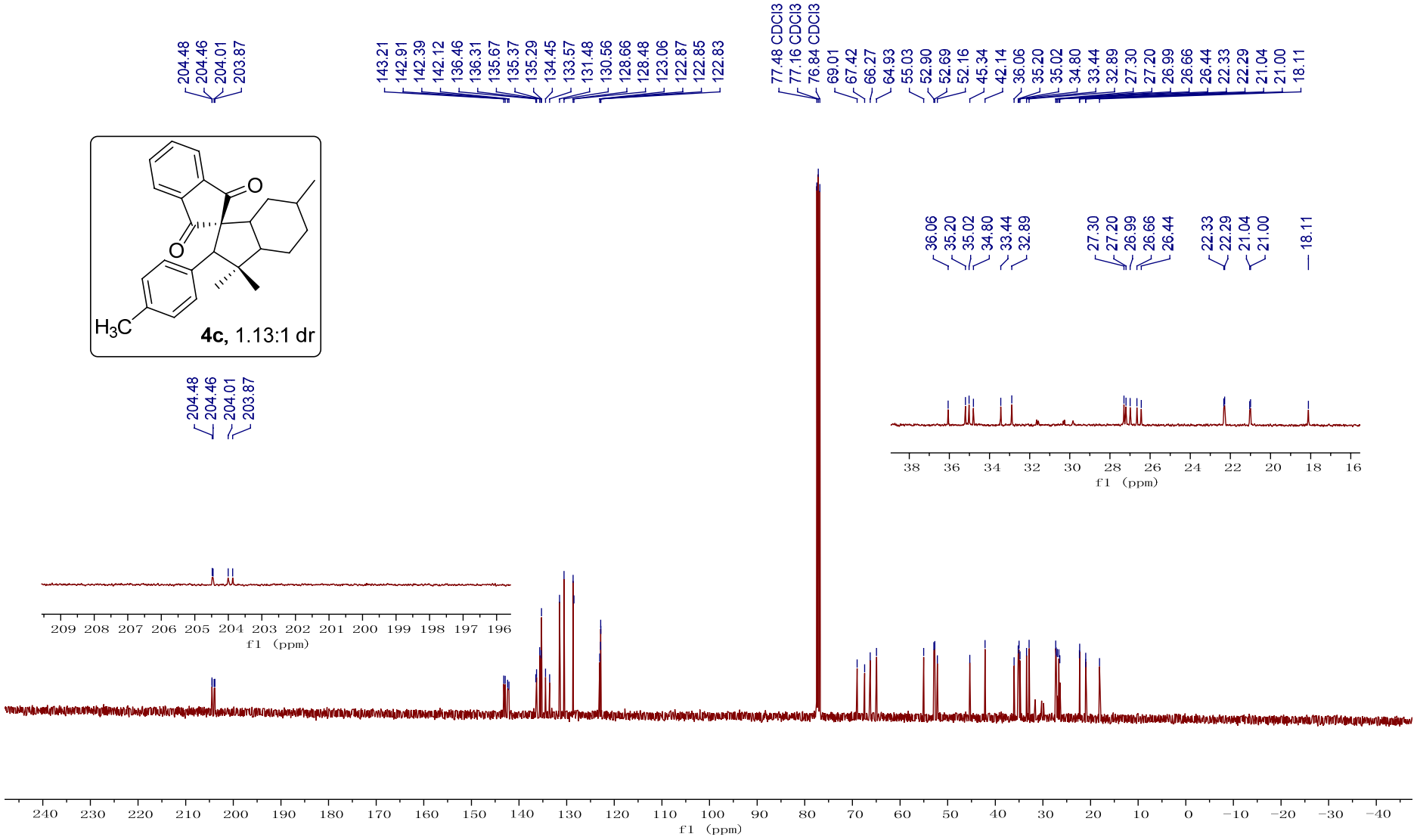

4a, 1:1 dr
f1 (ppm)

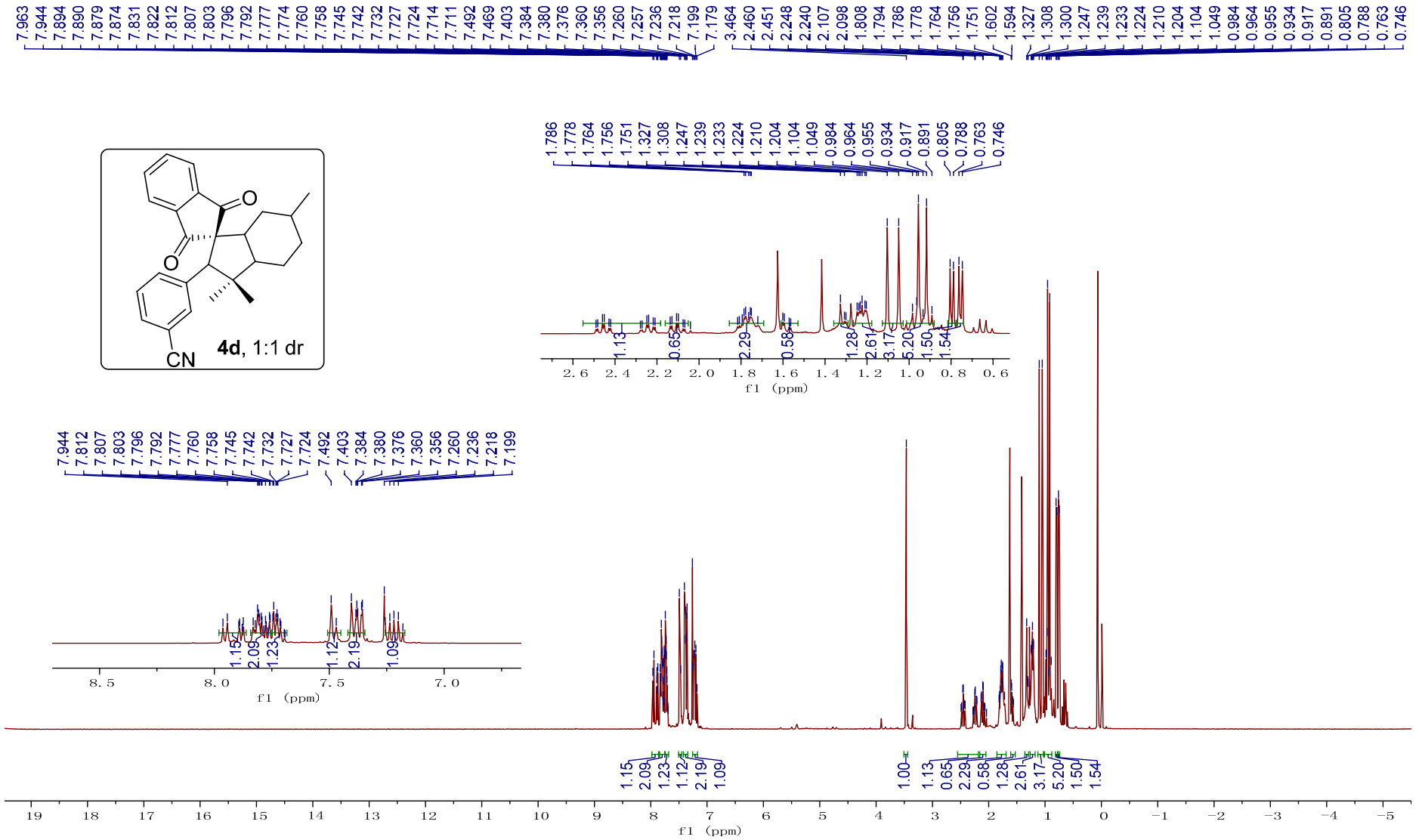

204.37
204.32
203.89
203.77
143.15
142.85
142.32
142.05
137.56
136.69
135.70
135.40
135.32
131.58
130.66
127.93
127.74
126.95
126.81
123.02
122.87
122.85
122.81
77.48 CDCl3
77.16
76.84
68.95
67.40
66.64
65.29
55.06
52.90
52.70
52.09
45.42
42.24
36.04
35.17
34.98
34.78
33.42
32.87
27.28
27.18
27.01
26.66
26.41
22.31
22.27
18.12
O
O
4a, 1:1 dr
204.37
204.32
203.89
203.77
207
206
205
204
203
202
201
200
f1 (ppm)
220
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)

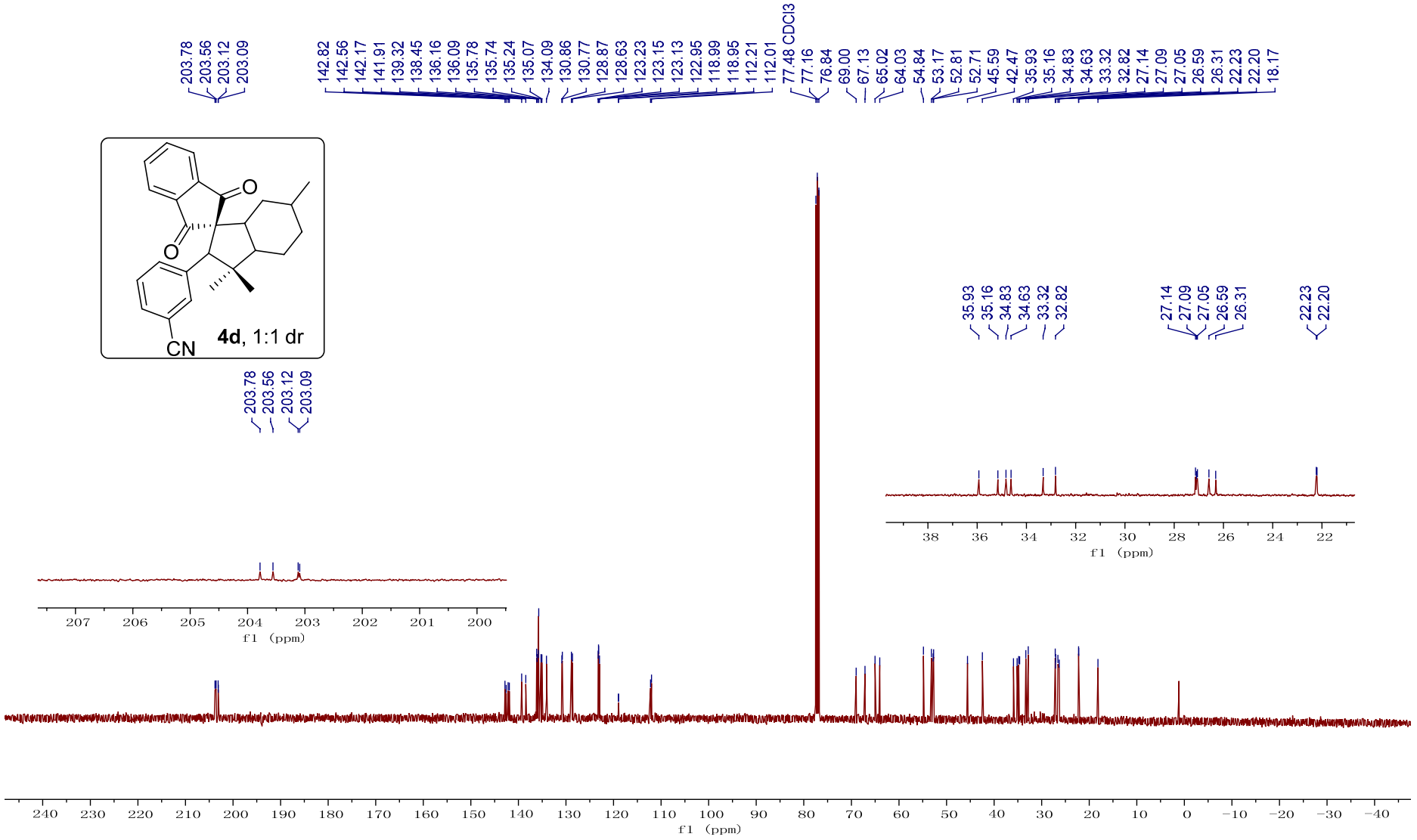

Br
4b, 1.1:1 dr
f1 (ppm)

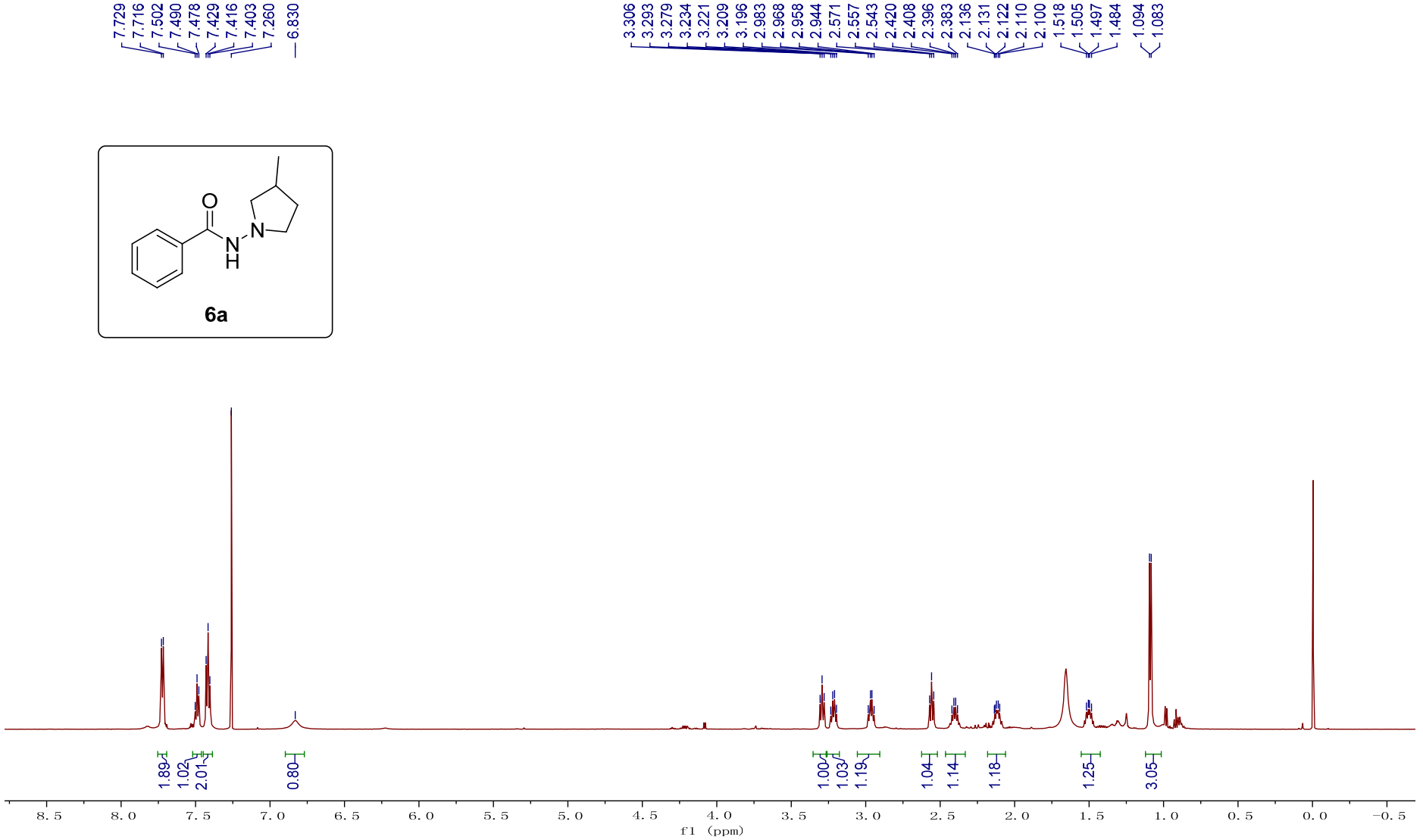

204.20
204.05
203.56
143.01
142.72
142.28
141.99
136.63
135.90
135.76
135.62
135.57
133.30
132.40
131.10
130.91
123.15
122.98
122.94
122.89
121.28
121.05
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
68.96
67.20
65.56
64.37
54.97
52.98
52.71
52.40
45.41
42.24
35.99
35.17
34.92
34.71
33.38
32.85
27.21
27.11
27.04
26.60
26.37
22.28
22.24
18.06
O
O
Br
4b, 1.1:1 dr
f1 (ppm)

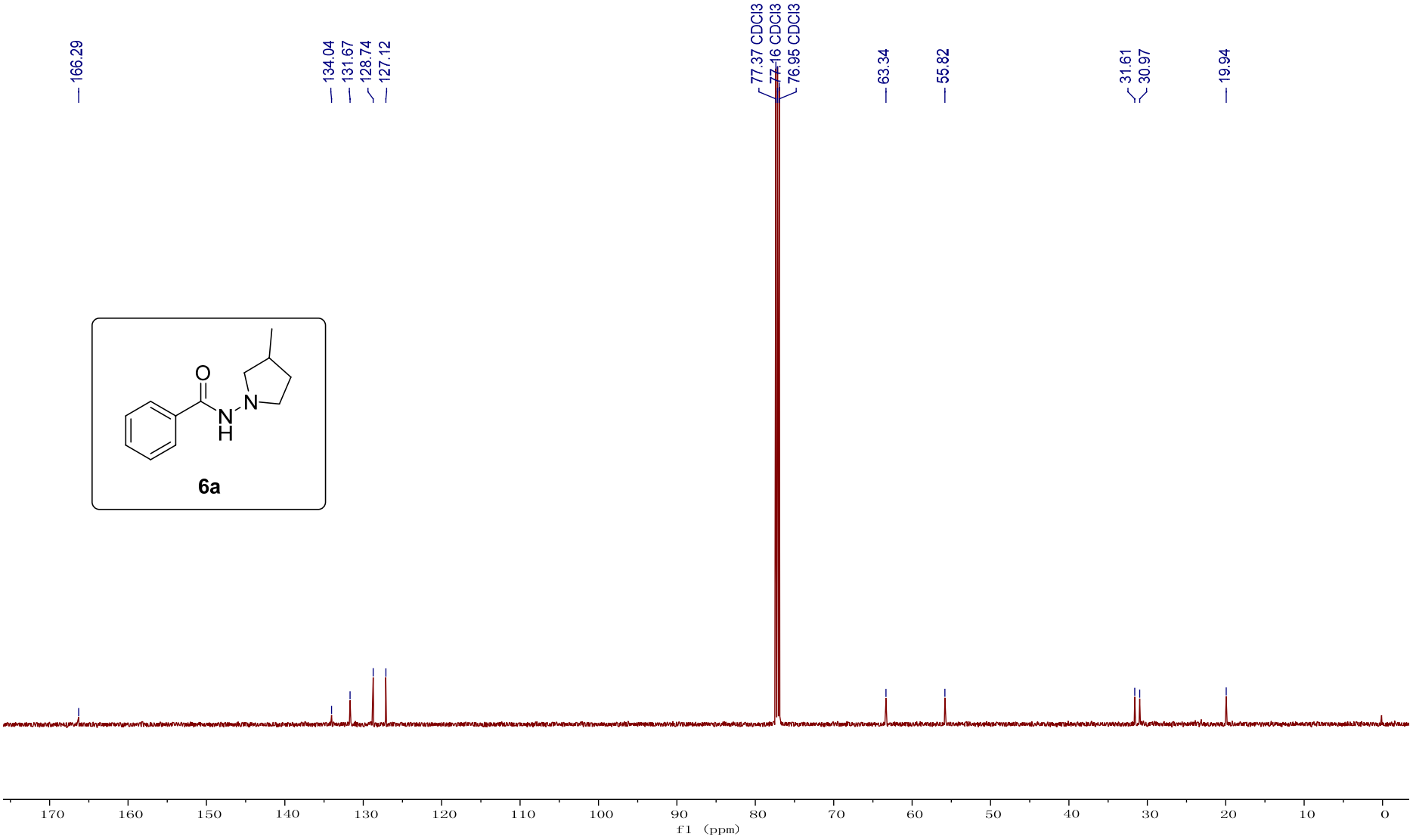

4c, 1.13:1 dr
f1 (ppm)

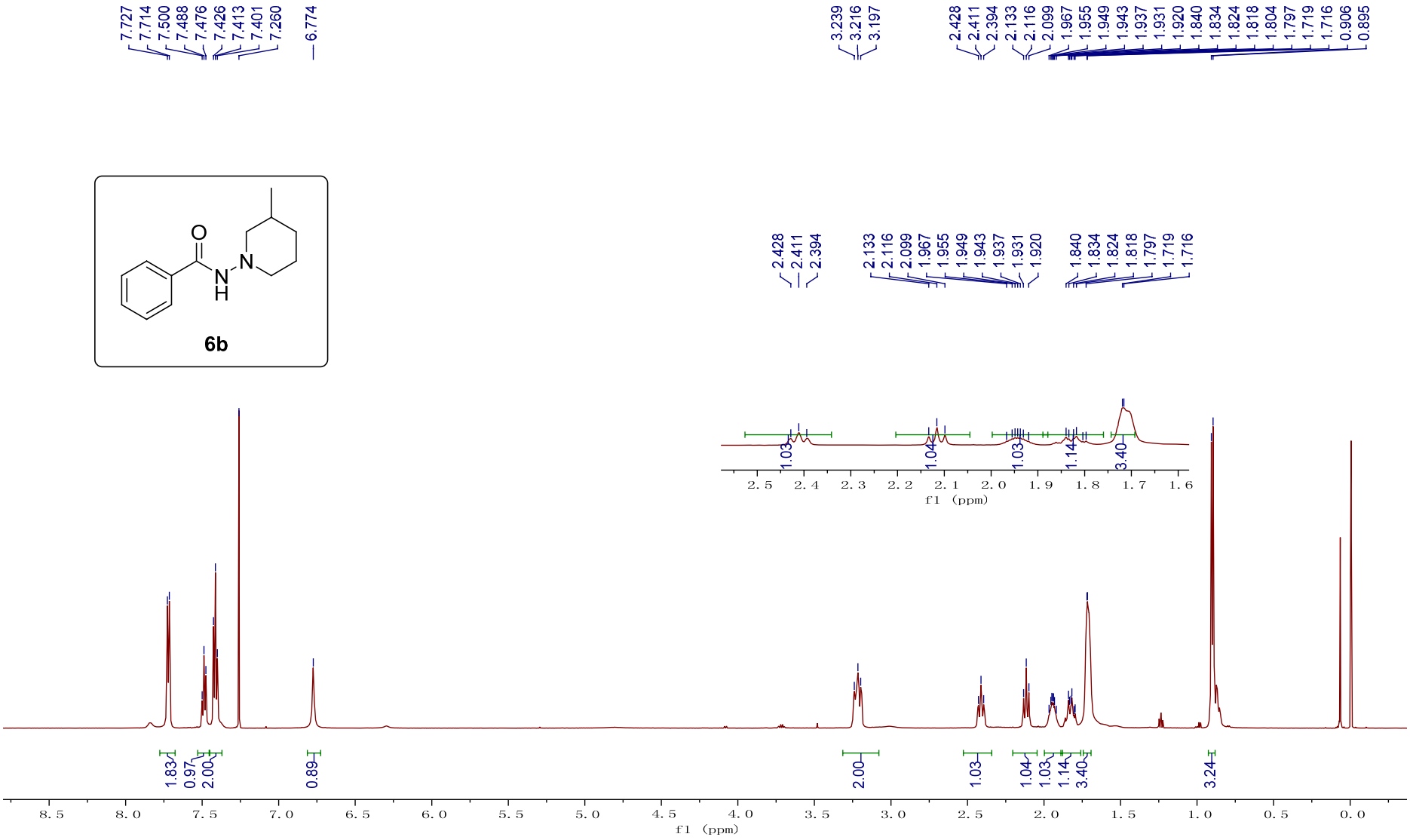

204.48
204.46
204.01
203.87
143.21
142.91
142.39
142.12
136.46
136.31
135.67
135.37
135.29
134.45
133.57
131.48
130.56
128.66
128.48
123.06
122.87
122.85
122.83
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
69.01
67.42
66.27
64.93
55.03
52.90
52.69
52.16
45.34
42.14
36.06
35.20
35.02
34.80
33.44
32.89
27.30
27.20
26.99
26.66
26.44
22.33
22.29
21.04
21.00
18.11
O
O
H3C
4c, 1.13:1 dr
f1 (ppm)
f1 (ppm)
f1 (ppm)


4d, 1:1 dr
CN
O
O
f1 (ppm)


203.78
203.56
203.12
203.09
142.82
142.56
142.17
141.91
139.32
138.45
136.16
136.09
135.78
135.74
135.24
135.07
134.09
130.86
130.77
128.87
128.63
123.23
123.15
123.13
122.95
118.99
118.95
112.21
112.01
77.48 CDCl3
77.16
76.84
69.00
67.13
65.02
64.03
54.84
53.17
52.81
52.71
45.59
42.47
35.93
35.16
34.83
34.63
33.32
32.82
27.14
27.09
27.05
26.59
26.31
22.23
22.20
18.17
O
O
CN
4d, 1:1 dr
f1 (ppm)


7.729
7.716
7.502
7.490
7.478
7.429
7.416
7.403
7.260
6.830
3.306
3.293
3.279
3.234
3.221
3.209
3.196
2.983
2.968
2.958
2.944
2.571
2.557
2.543
2.420
2.408
2.396
2.383
2.136
2.131
2.122
2.110
2.100
1.518
1.505
1.497
1.484
1.094
1.083
O
N
N
H
6a
1.89
1.02
2.01
0.80
1.00
1.03
1.19
1.04
1.14
1.18
1.25
3.05
f1 (ppm)


166.29
134.04
131.67
128.74
127.12
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
63.34
55.82
31.61
30.97
19.94
O
N
N
H
6a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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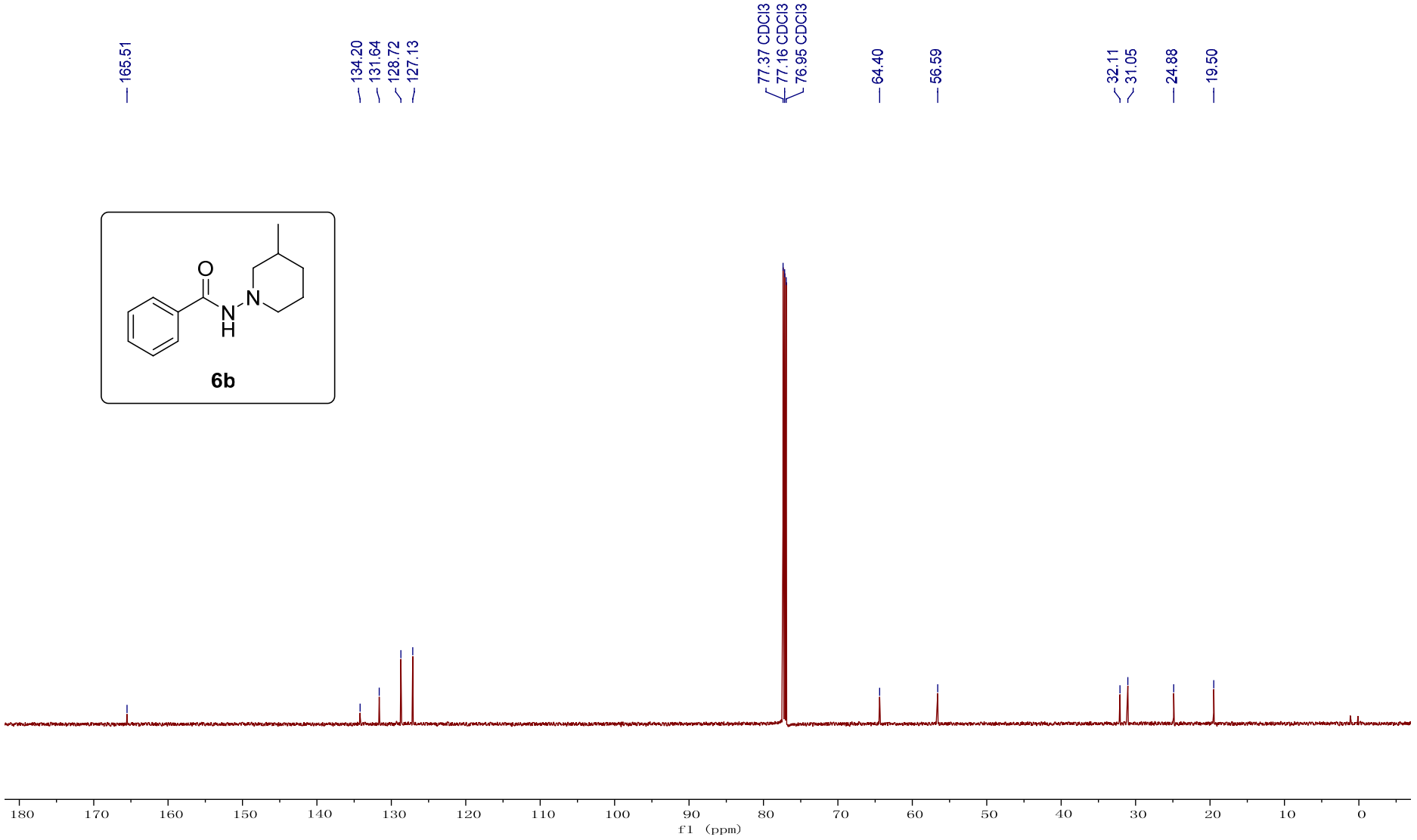
7.714
7.500
7.488
7.476
7.426
7.413
7.401
7.260
6.774
3.239
3.216
3.197
2.428
2.411
2.394
2.133
2.116
2.099
1.967
1.955
1.949
1.943
1.937
1.931
1.920
1.840
1.834
1.824
1.818
1.804
1.797
1.719
1.716
0.906
0.895
O
N
N
H
6b
1.03
1.04
1.03
1.14
3.40
f1 (ppm)
1.83
0.97
2.00
0.89
2.00
1.03
1.04
1.03
1.14
3.40
3.24
f1 (ppm)


165.51
134.20
131.64
128.72
127.13
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
64.40
56.59
32.11
31.05
24.88
19.50
O
N
N
H
6b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)