Supporting Information

Chiral Phosphoric Acid-Catalyzed Enantioselective aza-Friedel–Crafts Reaction of Naphthols and Electron-Rich Phenols with 2-Aryl-3*H*-indol-3-ones

Tao Ma,[†] Yonghui He,[†] Xiu-Xiu Qiao, Chang-Peng Zou, Xi-Xi Wu, Ganpeng Li* and Xiao-Jing Zhao* [a]

Key Laboratory of Chemistry in Ethnic Medicinal Resources, Key Laboratory of Natural Products Synthetic Biology of Ethnic Medicinal Endophytes, State Ethnic Affairs Commission & Ministry of Education, School of Ethnic Medicine, Yunnan Minzu University, Kunming, 650500, China

E-mail: ganpeng_li@sina.com, zhaoxj@ymu.edu.cn

[†] These authors contributed equally to this work.

Table of Contents

1. General information 2

2. General procedure for the synthesis of products 3

3. Synthesis applications of **3aa** 22

4. Crystal of **3aa** 23

5. References 25

6. Copies of HPLC 27

7. Copies of NMR spectra 46

1. General information

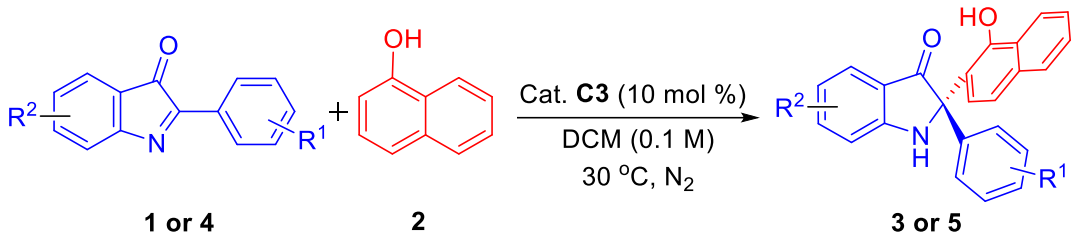
All reactions were performed using oven-dried or flame-dried glassware equipped with a magnetic stir bar before used.

All reagents were purchased from commercial suppliers and used without further purification. All solvents were purified by standard operating method.

Thin-layer chromatography was performed with EMD silica gel 60 GF_{254} plates eluting with solvents indicated, visualized by a 254 nm UV lamp and stained with phosphomolybdic acid (PMA). **^{1}H NMR**, **^{13}C NMR** and **^{19}F NMR** spectra were obtained on Bruker AM-400, Chemical shifts were denoted in ppm (δ), and calibrated by using residual undeuterated solvent $CDCl_3$ (7.26 ppm), tetramethylsilane (0.00 ppm) asinternal reference for ^{1}H NMR and the deuterated solvent $CDCl_3$ (77.00 ppm) tetramethylsilane (0.00 ppm) as internal standard for ^{13}C NMR； solvent d_6-DMSO (2.50 ppm), tetramethylsilane (0.00 ppm) asinternal reference for ^{1}H NMR and the deuterated solvent DMSO-d_6 (39.52 ppm) tetramethylsilane (0.00 ppm) as internal standard for ^{13}C NMR multiplicities are as indicated: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. **High-resolution mass spectral analysis (HRMS) data** was measured on a Bruker impact II (Q-TOF) mass spectrum by means of the ESI technique. **Crystallographic data** were obtained from a Bruker D8 Quest diffractometer. **Optical rotations** were detected on RUDOLPH A21202-J APTV/GW. The **enantiomeric excesses** (ee) of the products were determined by high performance liquid chromatography (HPLC) analysis employing Daicel Chiralpak OD-H, Chiralpak AS-H columns and Chiralpak AD-H columns.

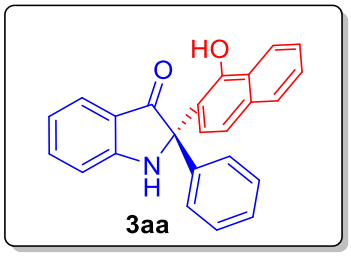
The 2-aryl indoles [1] and 2-aryl substituted 3*H*-indol-3-ones **1** were prepared according to the reported procedures. [2]

2. General procedure for the synthesis of products



1 or 4 **2** **3 or 5**

General procedure for the preparation of **3 or 5:** Unless otherwise noted, reactions were performed: Cat.**C3** (10 mol%), **1** (0.05 mmol), **2** (0.10 mmol) were added to DCM (0.5 mL) under N_2 atmosphere at room temperature. Then stirred for 8-96 h. The resulting yellow mixture was concentrated under vacuum, the crude product was purified by flash column chromatography using petroleum ether/ EtOAc to give the title compound **3 or 5**.



3aa

(S)-2-(1-hydroxynaphthalen-2-yl)-2-phenylindolin-3-one (3aa) According to the general procedure, **3aa** was obtained using 2-phenyl-3*H*-indol-3-one **1a** (10.3 mg, 0.05 mmol) and 1-naphthol **2a** (14.4 mg, 0.1 mmol) in 85% yield (14.9 mg) and 94:6 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

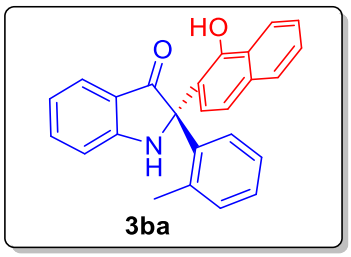
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.12 (s, 1H), 8.19 (d, *J* = 7.6 Hz, 1H), 7.65 – 7.63 (m, 1H), 7.61 – 7.56 (m, 2H), 7.46 – 7.39 (m, 1H), 7.39 – 7.30 (m, 2H), 7.27 (d, *J* = 8.8 Hz, 1H), 7.19 – 7.11 (m, 3H), 7.09 – 7.01 (m, 2H), 6.87 – 6.80 (m, 2H), 5.14 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.0, 160.0, 152.5, 140.5, 138.8, 134.6, 129.1, 128.7, 127.1, 126.8, 126.7, 126.6, 125.7, 125.24, 125.22, 122.9, 120.8, 120.5, 119.4, 117.2, 113.6, 75.77.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{16}NO_2$ $(M-H)^-$: 350.1187, found 350.1184.

Enantiomeric excess is 88% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 23.12 min; major isomer: tr = 29.10 min.

$[\alpha]^{20}D$ = + 437 (c = 1.0, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-2-(o-tolyl)indolin-3-one (3ba) According to the general procedure, **3ba** was obtained using 2-(o-tolyl)-3*H*-indol-3-one **1b** (11.1 mg, 0.05 mmol) and 1-naphthol **2a** (14.4 mg, 0.1 mmol) in 53% yield (9.5 mg) and 64:36 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

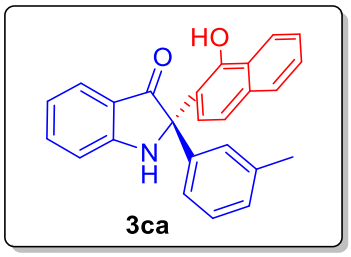
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.17 (s, 1H), 8.30 (s, 1H), 8.21 – 8.08 (m, 1H), 7.87 – 7.76 (m, 1H), 7.62 – 7.52 (m, 2H), 7.51 – 7.44 (m, 2H), 7.41 (d, *J* = 8.7 Hz, 1H), 7.32 (d, *J* = 8.7 Hz, 1H), 7.26 – 7.11 (m, 4H), 7.09 (d, *J* = 8.2 Hz, 1H), 6.83 (t, *J* = 7.4 Hz, 1H), 2.03 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 202.5, 160.1, 151.9, 138.1, 137.4, 137.4, 133.8, 132.3, 127.9, 127.4, 127.3, 126.5, 125.8, 125.4, 125.3, 125.2, 124.6, 122.0, 119.2, 119.0, 118.8, 118.7, 112.8, 75.1, 21.1.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_2$ $(M-H)^-$: 364.1343, found 364.1342.

Enantiomeric excess is 28% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 18.14 min; major isomer: tr = 29.90 min.

$[\alpha]^{20}D$ = + 94 (c = 0.5, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-2-(m-tolyl)indolin-3-one (3ca) According to the general procedure, **3ca** was obtained using 2-(m-tolyl)-3*H*-indol-3-one **1c** (11.1 mg, 0.05 mmol) and 1-naphthol **2a** (14.4 mg, 0.1 mmol) in 87% yield (15.9 mg) and 90:10 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

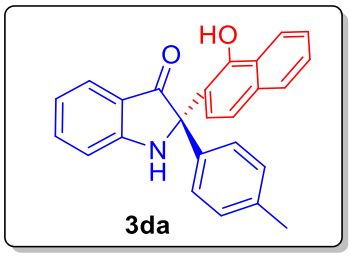
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.00 (s, 1H), 8.23 (s, 1H), 8.20 – 8.18 (m, 1H), 7.83 – 7.81 (m, 1H), 7.50 – 7.42 (m, 4H), 7.38 (d, *J* = 8.7 Hz, 1H), 7.23 (m, 4H), 7.11 (d, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 8.6 Hz, 1H), 6.72 (t, *J* = 7.3 Hz, 1H), 2.26 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 201.3, 160.4, 151.6, 140.2, 137.3, 137.1, 133.8, 128.08, 128.07, 127.5, 127.1, 126.4, 126.2, 125.1, 125.0, 124.5, 124.0, 122.4, 122.0, 118.7, 118.3, 117.3, 111.8, 73.3, 21.21.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_2$ $(M-H)^-$: 364.1343, found 364.1344.

Enantiomeric excess is 80% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 19.71 min; major isomer: tr = 23.94 min.

$[\alpha]^{20}D$ = + 814 (c = 0.25, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-2-(p-tolyl)indolin-3-one (3da) According to the general procedure, **3da** was obtained using 2-(p-tolyl)-3*H*-indol-3-one **1d** (11.1 mg, 0.05 mmol) and 1-naphthol **2a** (14.4 mg, 0.1 mmol) in 86% yield (15.7 mg) and 75:25 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

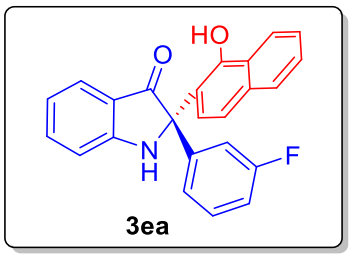
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.26 (s, 1H), 8.34 – 8.31 (m, 1H), 7.78 – 7.76 (m, 1H), 7.73 – 7.70 (m, 2H), 7.59 – 7.55 (m, 1H), 7.50 – 7.43 (m, 2H), 7.40 (d, *J* = 8.7 Hz, 1H), 7.11 – 7.04 (m, 4H), 7.00 – 6.94 (m, 2H), 5.20 (s, 1H), 2.30 (s, 3H).

^{13}C NMR (100MHz, $CDCl_3$) δ 205.2, 160.0, 152.5, 138.7, 138.6, 137.6, 134.6, 129.8, 127.0, 126.7, 126.6, 126.6, 125.6, 125.3, 125.2, 123.0, 120.8, 120.5, 119.3, 117.4, 113.6, 75.6, 21.1.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_2$ $(M-H)^-$: 364.1343, found 364.1344.

Enantiomeric excess is 50% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 27.35 min; major isomer: tr = 33.75 min.

$[\alpha]^{20}D$ = + 497 (c = 0.25, $CHCl_3$).



(S)-2-(3-fluorophenyl)-2-(1-hydroxynaphthalen-2-yl)indolin-3-one (3ea) According to the general procedure, **3ea** was obtained using 2-(3-fluorophenyl)-3*H*-indol-3-one **1e** (11.3 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 90% yield (16.6 mg) and 91:9 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.98 (s, 1H), 8.26 (s, 1H), 8.19 (d, *J* = 7.6 Hz 1H), 7.85 – 7.82 (m, 1H), 7.52 – 7.42 (m, 4H), 7.41 – 7.29 (m, 3H), 7.27 – 7.19 (m, 1H), 7.16 – 7.12 (m, 2H), 7.03 (d, *J* = 8.1 Hz, 1H), 6.74 (t, *J* = 7.4 Hz, 1H).

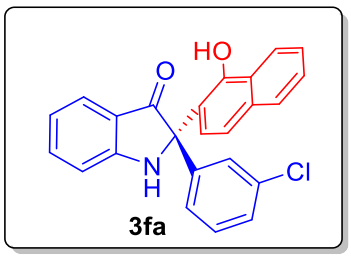
^{13}C NMR (100 MHz, DMSO-d_6) δ 200.4, 162.0 (d, *J* = 241.0 Hz), 160.5, 151.7, 143.5 (d, *J* = 7.0 Hz), 137.4, 133.9, 130.1 (d, *J* = 8.0 Hz), 127.6, 126.3, 126.1, 125.10, 125.05, 124.5, 122.8 (d, *J* = 3.0 Hz), 122.2, 122.0, 118.9, 118.1, 117.5, 114.3 (d, *J* = 21.0 Hz), 113.4 (d, *J* = 23.0 Hz), 111.9, 72.9.

^{19}F NMR (376 MHz, DMSO-d_6) δ -113.3.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}FNO_2$ $(M-H)^-$: 368.1092, found 368.1093.

Enantiomeric excess is 82% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.54 min; major isomer: tr = 11.25 min.

$[\alpha]^{20}D$ = + 421 (c = 0.25, $CHCl_3$).



(S)-2-(3-chlorophenyl)-2-(1-hydroxynaphthalen-2-yl)indolin-3-one (3fa) According to the general procedure, **3fa** was obtained using 2-(3-chlorophenyl)-3*H*-indol-3-one **1f** (12.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 92% yield (17.7 mg) and 93:7 er as a yellow oily

(silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

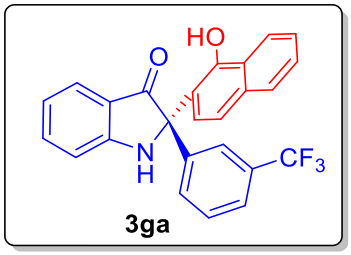
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.31 – 8.29 (m, 1H), 7.79 – 7.77 (m, 1H), 7.73 –7.68 (m, 2H), 7.61 – 7.57 (m, 1H), 7.53 – 7.44 (m, 2H), 7.41 (d, *J* = 8.7 Hz, 1H), 7.30 – 7.28 (m, 1H), 7.21 (t, *J* = 7.9 Hz, 1H), 7.18 (t, *J* = 2.0 Hz, 1H), 7.08 – 7.06 (m, 1H), 7.01 – 6.96 (m, 2H), 5.27 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.3, 159.9, 152.4, 142.4, 139.1, 135.0, 134.7, 130.3, 128.9, 127.1, 126.9, 126.8, 126.7, 125.8, 125.4, 125.0, 124.8, 122.8, 120.9, 120.0, 119.7, 117.0, 113.4, 75.1.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}ClNO_2$ $(M-H)^-$: 384.0797, found 384.0799.

Enantiomeric excess is 88% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.89 min; major isomer: tr = 11.94 min.

$[\alpha]^{20}D$ = + 443 (c = 0.25, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-2-(3-(trifluoromethyl)phenyl)indolin-3-one (3ga) According to the general procedure, **3ga** was obtained using 2-(3-(trifluoromethyl)phenyl)-3*H*-indol-3-one **1g** (13.8 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 91% yield (19.1 mg) and 87:13 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.99 (s, 1H), 8.31 (s, 1H), 8.19 (d, *J* = 8.0 Hz, 1H), 7.85 – 7.83 (m, 1H), 7.80 (s, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.678 –7.66 (m, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.53 – 7.42 (m, 4H), 7.42 – 7.39 (m, 1H), 7.09 (dd, *J* = 17.7, 8.4 Hz, 2H), 6.75 (t, *J* = 7.4 Hz, 1H).

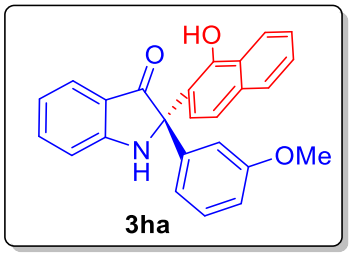
^{13}C NMR (100 MHz, DMSO-d_6) δ 200.3, 160.7, 151.8, 142.3, 137.6, 133.9, 131.0, 129.4, 128.9 (q, *J* = 31.0 Hz), 127.9, 127.7, 126.4, 125.9, 125.2, 125.1, 124.6, 124.3 (q, *J* = 271.0 Hz), 122.6 (q, *J* = 4.0 Hz), 122.3, 122.0, 119.0, 118.0, 117.8, 112.2, 73.0.

^{19}F NMR (376 MHz, DMSO-d_6) δ -60.9.

Enantiomeric excess is 74% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 6.56 min; major isomer: tr = 7.84 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{15}F_3NO_2$ $(M-H)^-$: 418.1060, found 418.1062.

$[\alpha]^{20}D$ = + 150 (c = 0.5, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-2-(3-methoxyphenyl)indolin-3-one (3ha) According to the general procedure, **3ha** was obtained using 2-(3-methoxyphenyl)-3*H*-indol-3-one **1h** (11.7 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 83% yield (15.8 mg) and 78:22 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

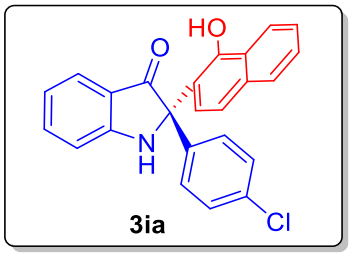
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.98 (s, 1H), 8.23 (s, 1H), 8.19 (d, *J* = 7.8 Hz, 1H), 7.83 – 7.81 (m, 1H), 7.49 – 7.42 (m, 4H), 7.37 (d, *J* = 8.7 Hz, 1H), 7.27 (t, *J* = 8.0 Hz, 1H), 7.14 (d, *J* = 8.6 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 7.06 – 6.99 (m, 2H), 6.90 – 6.88 (m, 1H), 6.72 (t, *J* = 7.4 Hz, 1H), 3.69 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 201.0, 160.4, 159.1, 151.6, 141.7, 137.2, 133.8, 129.2, 127.5, 126.5, 126.2, 125.1, 125.0, 124.4, 122.4, 122.0, 119.2, 118.7, 118.3, 117.3, 113.3, 112.1, 111.7, 73.1, 55.0.

Enantiomeric excess is 56% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 15.69 min; major isomer: tr = 21.18 min

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_3$ $(M-H)^-$: 380.1292, found 380.1293.

$[\alpha]^{20}D$ = + 201 (c = 0.5, $CHCl_3$).



(S)-2-(4-chlorophenyl)-2-(1-hydroxynaphthalen-2-yl)indolin-3-one (3ia) According to the general procedure, **3ia** was obtained using 2-(4-chlorophenyl)-3*H*-indol-3-one **1i** (12.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 87% yield (16.8 mg) and 88:12 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

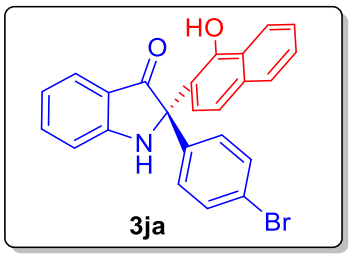
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.28 – 8.26 (m, 1H), 7.75 – 7.73 (m, 1H), 7.68 – 7.65 (m, 2H), 7.57 – 7.53 (m, 1H), 7.48 – 7.41 (m, 2H), 7.38 (d, *J* = 8.8 Hz, 1H), 7.22 – 7.20 (m, 2H), 7.08 – 7.06 (m, 2H), 7.01 – 6.81 (m, 2H), 5.21 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 160.1, 152.5, 139.1, 138.9, 134.8, 134.7, 129.3, 128.2, 127.2, 127.0, 126.7, 125.8, 125.5, 124.8, 122.9, 120.9, 120.0, 119.7, 117.1, 113.4, 75.1.

Enantiomeric excess is 76% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 22.02 min; major isomer: tr = 30.23 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}ClNO_2$ $(M-H)^-$: 384.0797, found 384.0799.

$[\alpha]^{20}D$ = + 184 (c = 0.25, $CHCl_3$).



(S)-2-(4-bromophenyl)-2-(1-hydroxynaphthalen-2-yl)indolin-3-one (3ja) According to the general procedure, **3ja** was obtained using 2-(4-bromophenyl)-3*H*-indol-3-one **1j** (14.3 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 80% yield (17.2 mg) and 92:8 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

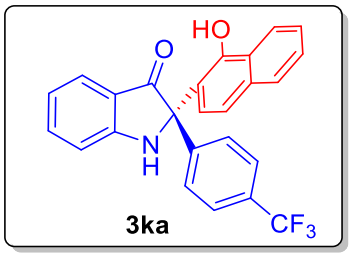
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.97 (s, 1H), 8.26 (s, 1H), 8.21 – 8.19 (m, 1H), 7.84 – 7.82 (m, 1H), 7.56 – 7.54 (m, 2H), 7.51 – 7.44 (m, 4H), 7.43 – 7.38 (m, 3H), 7.17 (d, *J* = 8.6 Hz, 1H), 7.03 (d, *J* = 8.7 Hz, 1H), 6.76 – 6.72 (m, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 200.7, 160.5, 151.7, 140.1, 137.4, 133.9, 131.0, 128.9, 127.6, 126.3, 126.1, 125.1, 125.1, 124.5, 122.2, 122.0, 120.7, 118.9, 118.0, 117.5, 112.0, 73.0.

Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 10.68 min; major isomer: tr = 13.32 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}BrNO_2$ $(M-H)^-$: 428.0292, found 428.0292.

$[\alpha]^{20}D$ = + 86 (c = 0.5, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-2-(4-(trifluoromethyl)phenyl)indolin-3-one (3ga) According to the general procedure, **3ka** was obtained using 2-(4-(trifluoromethyl)phenyl)-3*H*-indol-3-one **1k** (13.8 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 92% yield (19.3 mg) and 92:8 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.97 (s, 1H), 8.32 (s, 1H), 8.20 – 8.18 (m, 1H), 7.86 – 7.84 (m, 1H), 7.72 – 7.70 (m, 2H), 7.66 – 7.63 (m, 2H), 7.53 – 7.44 (m, 4H), 7.42 (d, *J* = 8.8 Hz, 1H), 7.21 – 7.18 (m, 1H), 7.08 – 7.05 (m, 1H), 6.75 (t, *J* = 7.4 Hz, 1H).

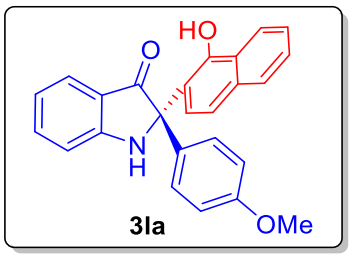
^{13}C NMR (100 MHz, DMSO-d_6) δ 200.1, 160.8, 151.8, 145.7, 137.6, 133.9, 127.7, 127.9 (q, *J* = 31.0 Hz), 127.2, 126.5, 126.3, 125.7, 125.8, 125.1 (q, *J* = 4.0 Hz), 124.5, 122.0, 121.9, 121.5 (q, *J* = 285.0 Hz), 118.9, 117.8, 117.7, 112.1, 73.3.

^{19}F NMR (376 MHz, DMSO-d_6) δ -60.8.

Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 6.36 min; major isomer: tr = 8.40 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{15}F_3NO_2$ $(M-H)^-$: 418.1060, found 418.1063.

$[\alpha]^{20}D$ = + 194 (c = 0.5, $CHCl_3$).



3la

(S)-2-(1-hydroxynaphthalen-2-yl)-2-(4-methoxyphenyl)indolin-3-one (3la) According to the general procedure, **3la** was obtained using 2-(4-methoxyphenyl)-3*H*-indol-3-one **1l** (11.7 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 76% yield (12.1 mg) and 63:37 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

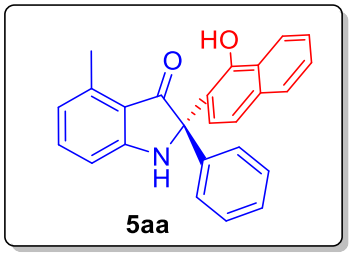
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.25 (s, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.70 – 7.68 (m, 2H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.37 (d, *J* = 8.8 Hz, 1H), 7.09 (d, *J* = 8.7 Hz, 2H), 6.98 (d, *J* = 8.2 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.77 (d, *J* = 8.7 Hz, 2H), 5.59 (s, 1H), 3.73 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.1, 159.1, 158.6, 151.4, 137.6, 133.6, 131.5, 127.1, 126.0, 125.6, 125.5, 124.6, 124.3, 124.1, 121.9, 119.4, 119.2, 118.3, 116.6, 113.3, 112.4, 74.3, 54.2.

Enantiomeric excess is 26% determined by HPLC (Chiralpak AS-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 12.41 min; major isomer: tr = 14.87 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_3$ $(M-H)^-$: 380.1292, found 380.1295.

$[\alpha]^{20}D$ = + 89 (c = 0.5, $CHCl_3$).



5aa

(S)-2-(1-hydroxynaphthalen-2-yl)-4-methyl-2-phenylindolin-3-one (5aa) According to the general procedure, 5**aa** was obtained using 4-methyl-2-phenyl-3*H*-indol-3-one **4a** (11.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 71% yield (13.0 mg) and 93:7 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

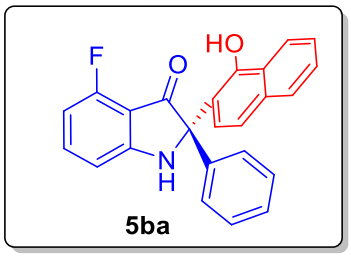
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.39 (s, 1H), 8.34– 88.32 (m, 1H), 7.78– 7.76 (m, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.44 – 7.38 (m, 2H), 7.34 – 7.27 (m, 3H), 7.21– 7.18 (m, 2H), 6.81 (d, *J* = 8.2 Hz, 1H), 6.72 (d, *J* = 7.3 Hz, 1H), 5.13 (s, 1H), 2.62 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.7, 160.6, 152.6, 141.3, 140.9, 138.3, 134.7, 129.1, 128.6, 127.1, 126.8, 126.72, 126.70, 125.24, 125.18, 123.0, 122.2, 119.3, 118.6, 117.6, 110.7, 75.6, 18.4.

Enantiomeric excess is 26% determined by HPLC (Chiralpak AS-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 12.41 min; major isomer: tr = 14.87 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_2$ $(M-H)^-$: 364.1343, found 364.1343.

$[\alpha]^{20}D$ = + 456 (c = 0.25, $CHCl_3$).



5ba

(S)-4-fluoro-2-(1-hydroxynaphthalen-2-yl)-2-phenylindolin-3-one (5ba) According to the general procedure, **5ba** was obtained using 4-fluoro-2-phenyl-3*H*-indol-3-one **4b** (11.3 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 60% yield (11.1 mg) and 93:7 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.67 (s, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 7.79 – 7.77 (m, 1H), 7.70 (d, *J* = 8.7 Hz, 1H), 7.55 – 7.44 (m, 3H), 7.42 (d, *J* = 8.7 Hz, 1H), 7.35 – 7.27 (m, 3H), 7.21 – 7.18 (m, 2H), 6.73 (d, *J* = 8.3 Hz, 1H), 6.53 (t, *J* = 8.6 Hz, 1H), 5.43 (s, 1H).

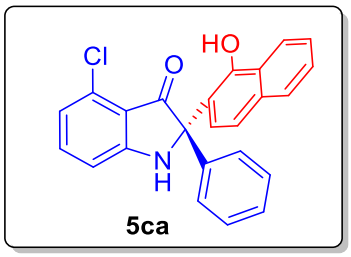
^{13}C NMR (100 MHz, $CDCl_3$) δ 201.6, 160.8 (d, *J* = 5.0 Hz), 159.9 (d, *J* = 263.0 Hz), 152.4, 140.6 (d, *J* = 10.0 Hz), 139.7, 134.8, 129.2, 128.9, 127.1, 126.9, 126.8, 126.7, 125.4, 124.5, 123.0, 119.7, 117.2, 108.70, 108.66, 106.2 (d, *J* = 19.0 Hz), 76.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -110.1.

Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.56 min; major isomer: tr = 10.09 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}FNO_2$ $(M-H)^-$: 368.1092, found 368.1091.

$[\alpha]^{20}D$ = + 395 (c = 0.25, $CHCl_3$).



(S)-4-chloro-2-(1-hydroxynaphthalen-2-yl)-2-phenylindolin-3-one (5ca) According to the general procedure, **5ca** was obtained using 4-chloro-2-phenyl-3*H*-indol-3-one **4c** (12.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 44% yield (8.5 mg) and 94:6 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

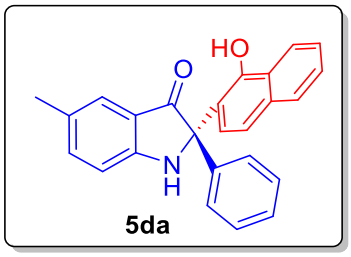
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.01 (s, 1H), 8.57 (s, 1H), 8.20 (d, *J* = 8.3 Hz, 1H), 7.85 – 7.79 (m, 1H), 7.55 – 7.51 (m, 2H), 7.51 – 7.44 (m, 2H), 7.43 – 7.33 (m, 5H), 6.97 (d, *J* = 8.6 Hz, 1H), 6.92 (d, *J* = 8.3 Hz, 1H), 6.66 (d, *J* = 7.6 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 198.2, 161.5, 151.6, 139.4, 137.6, 133.9, 130.8, 128.3, 127.7, 127.6, 126.9, 126.7, 126.3, 125.1, 124.9, 122.6, 122.1, 118.8, 117.6, 114.4, 110.3, 73.5.

Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.62 min; major isomer: tr = 9.72 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}ClNO_2$ $(M-H)^-$: 384.0797, found 384.0799.

$[\alpha]^{20}D$ = + 63 (c = 0.25, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-5-methyl-2-phenylindolin-3-one (5da) According to the general procedure, 5**da** was obtained using 5-methyl-2-phenyl-3*H*-indol-3-one **4d** (11.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 97% yield (17.7 mg) and 91:9 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

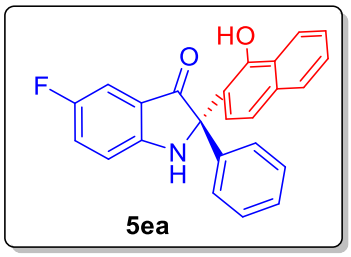
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.39 (s, 1H), 8.21 (d, *J* = 7.7 Hz, 1H), 7.67 – 7.64 (m, 1H), 7.57 (d, *J* = 8.7 Hz, 1H), 7.42 (s, 1H), 7.40 – 7.32 (m, 2H), 7.31 – 7.26 (m, 2H), 7.21 – 7.15 (m, 3H), 7.09 – 7.06 (m, 2H), 6.82 (d, *J* = 8.3 Hz, 1H), 4.97 (s, 1H), 2.23 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 158.2, 152.6, 141.0, 140.2, 134.5, 131.0, 130.0, 128.6, 127.0, 126.74, 126.68, 126.5, 125.7, 125.1, 124.8, 122.9, 121.2, 119.2, 117.1, 113.8, 76.2, 20.6.

Enantiomeric excess is 82% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 21.32 min; major isomer: tr = 28.83 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_2$ $(M-H)^-$: 364.1343, found 364.1343.

$[\alpha]^{20}D$ = + 434 (c = 0.5, $CHCl_3$).



5ea

(S)-5-fluoro-2-(1-hydroxynaphthalen-2-yl)-2-phenylindolin-3-one (5ea) According to the general procedure, **5ea** was obtained using 5-fluoro-2-phenyl-3*H*-indol-3-one **4e** (11.3 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 81% yield (14.9 mg) and 96:4 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.97 (s, 1H), 8.24 – 8.09 (m, 2H), 7.85 – 7.79 (m, 1H), 7.50 – 7.46 (m, 3H), 7.46 – 7.38 (m, 2H), 7.38 – 7.30 (m, 4H), 7.23 (dd, *J* = 7.7, 2.7 Hz, 1H), 7.06 – 7.01 (m, 2H).

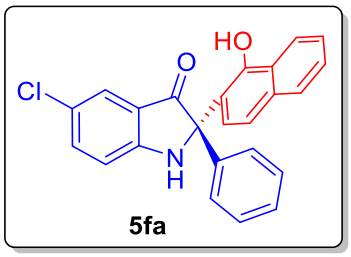
^{13}C NMR (100 MHz, DMSO-d_6) δ 201.0, 157.4, 151.5, 155.0 (d, *J* = 223.0 Hz), 139.8, 133.8, 128.2, 127.6, 127.5, 126.8, 126.4, 126.2, 125.3, 125.05, 125.03, 122.5, 122.0, 118.7, 118.3 (d, *J* = 8.0 Hz), 113.2 (d, *J* = 7.0Hz), 108.9 (d, *J* = 22.0 Hz), 74.3.

^{19}F NMR (376 MHz, DMSO-d_6) δ -127.1.

Enantiomeric excess is 92% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 9.44 min; major isomer: tr = 12.43 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}FNO_2$ $(M-H)^-$: 368.1092, found 368.1094.

$[\alpha]^{20}D$ = + 370 (c = 0.25, $CHCl_3$).



(S)-5-chloro-2-(1-hydroxynaphthalen-2-yl)-2-phenylindolin-3-one (5fa) According to the general procedure, **5fa** was obtained using 5-chloro-2-phenyl-3*H*-indol-3-one **4f** (12.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 82% yield (15.8 mg) and 91:9 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

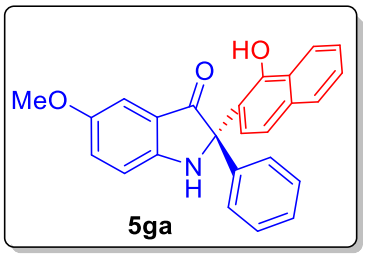
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.96 (s, 1H), 8.42 (s, 1H), 8.18 (d, *J* = 8.0 Hz 1H), 7.82 (d, *J* = 7.3 Hz, 1H), 7.53 – 7.43 (m, 6H), 7.38 – 7.32 (m, 4H), 7.03 – 7.00 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 200.0, 158.7, 151.5, 139.4, 136.7, 133.8, 128.2, 127.6, 126.8, 126.5, 126.5, 126.3, 125.1, 124.9, 123.4, 122.6, 122.0, 120.9, 119.4, 118.8, 113.3, 73.8.

Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 18.91 min; major isomer: tr = 27.68 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}ClNO_2$ $(M-H)^-$: 384.0797, found 384.0798.

$[\alpha]^{20}D$ = + 219 (c = 0.5, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-5-methoxy-2-phenylindolin-3-one (5ga) According to the general procedure, **5ga** was obtained using 5-methoxy-2-phenyl-3H-indol-3-one **4g** (11.9 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 97% yield (18.5 mg) and 94:6 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

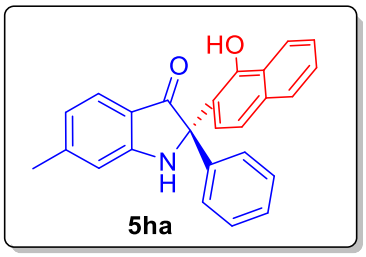
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.11 (s, 1H), 8.18 (d, *J* = 8.2 Hz, 1H), 7.92 (s, 1H), 7.83 – 7.81 (m, 1H), 7.49 – 7.41 (m, 4H), 7.39 – 7.37 (m, 1H), 7.35 – 7.26 (m, 3H), 7.22 – 7.19 (m, 2H), 7.02 (d, *J* = 8.9 Hz, 1H), 6.95 (d, *J* =2.4 Hz,1H), 3.72 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 201.5, 156.6, 152.2, 151.7, 140.6, 133.8, 128.2, 127.9, 127.5, 127.3, 126.7, 126.3, 126.2, 125.2, 125.0, 122.0, 121.9, 118.6, 118.3, 113.8, 104.6, 74.5, 55.5.

Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 13.37 min; major isomer: tr = 17.74 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_3$ $(M-H)^-$: 380.1292, found 380.1294.

$[\alpha]^{20}D$ = + 276 (c = 0.5, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-6-methyl-2-phenylindolin-3-one (5ha) According to the general procedure, 5**ha** was obtained using 6-methyl-2-phenyl-3*H*-indol-3-one **4h** (11.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 90% yield (16.4 mg) and 88:12 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1).

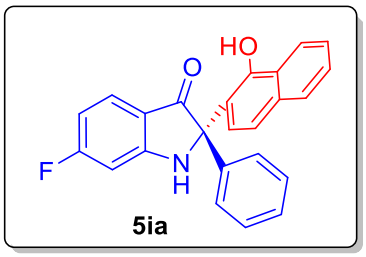
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.05 (s, 1H), 8.24 (s, 1H), 8.18 (d, *J* = 7.9 Hz, 1H), 7.84 – 7.81(m, 1H), 7.50 – 7.40 (m, 4H), 7.37 (t, *J* = 8.6 Hz, 2H), 7.35 – 7.26 (m, 3H), 7.22 (d, *J* = 8.7 Hz, 1H), 6.82 (s, 1H), 6.56 (d, *J* = 8.0 Hz, 1H), 2.31 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 200.8, 161.0, 151.7, 148.7, 140.5, 133.9, 128.2, 127.5, 127.4, 126.7, 126.3, 126.2, 125.3, 125.2, 125.0, 124.3, 122.1, 122.0, 119.3, 118.7, 116.0, 111.7, 73.8.

Enantiomeric excess is 76% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 13.55 min; major isomer: tr = 14.99 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_2$ $(M-H)^-$: 364.1343, found 364.1343.

$[\alpha]^{20}D$ = + 317 (c = 0.5, $CHCl_3$).



(S)-6-fluoro-2-(1-hydroxynaphthalen-2-yl)-2-phenylindolin-3-one (5ia) According to the general procedure, **5ia** was obtained using 6-fluoro-2-phenyl-3*H*-indol-3-one **4i** (11.3 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 94% yield (17.3 mg) and 92:8 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.98 (d, *J* = 8.4 Hz,1H), 8.58 – 8.56 (m, 1H), 8.21 – 8.18 (m, 1H), 7.90 – 7.77 (m, 1H), 7.56 – 7.42 (m, 5H), 7.39 – 7.28 (m, 4H), 7.17 – 7.12 (m, 1H), 6.74 (t, *J* = 8.2 Hz, 1H), 6.55 – 6.50 (m, 1H).

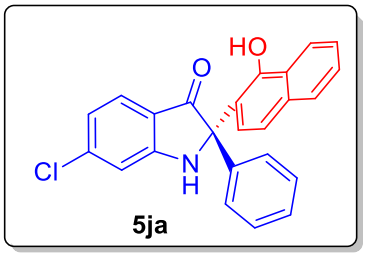
^{13}C NMR (100 MHz, DMSO-d_6) δ 199.2, 168.7 (d, *J* = 250.0 Hz), 161.7 (d, *J* = 15.0 Hz), 151.6, 139.9, 133.9, 128.2, 127.6, 127.5, 127.3, 127.1, 126.6, 126.29, 126.26, 125.1, 122.3, 122.0, 118.8, 115.1, 105.6 (d, *J* = 25.0 Hz), 97.3 (d, *J* = 25.0 Hz), 73.9.

^{19}F NMR (376 MHz, DMSO-d_6) δ -101.2.

Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 22.51 min; major isomer: tr = 28.35 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}FNO_2$ $(M-H)^-$: 368.1092, found 368.1095.

$[\alpha]^{20}D$ = + 257 (c = 0.5, $CHCl_3$).



(S)-6-chloro-2-(1-hydroxynaphthalen-2-yl)-2-phenylindolin-3-one (5ja) According to the general procedure, **5ja** was obtained using 5-chloro-2-phenyl-3*H*-indol-3-one **4j** (12.1 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 84% yield (16.2 mg) and 95:5 er as a yellow oily

(silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

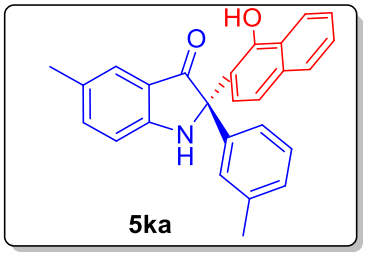
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.97 (s, 1H), 8.51 (s, 1H), 8.18 (d, *J* = 7.9 Hz, 1H), 7.84 – 7.82 (m, 1H), 7.52 – 7.42 (m, 5H), 7.36 (t, *J* = 8.1 Hz, 3H), 7.32 (d, *J* = 6.9 Hz, 1H), 7.06 (d, *J* = 8.7 Hz, 1H), 7.03 (d, *J* = 1.6 Hz, 1H), 6.72 (dd, *J* = 8.2, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 199.7, 160.5, 151.6, 141.9, 139.5, 133.9, 128.3, 127.7, 127.6, 126.7, 126.4, 126.3, 126.1, 125.1, 125.0, 122.5, 122.0, 118.8, 117.4, 117.2, 110.9, 73.6.

Enantiomeric excess is 90% determined by HPLC (Chiralpak OD-H, Hexane/Isopropanol 95/5, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 20.13 min; major isomer: tr = 23.33 min.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{15}ClNO_2$ $(M-H)^-$: 384.0797, found 384.0799.

$[\alpha]^{20}D$ = + 240 (c = 0.5, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-5-methyl-2-(m-tolyl)indolin-3-one (5ka) According to the general procedure, **5ka** was obtained using 5-methyl-2-(m-tolyl)-3*H*-indol-3-one **4k** (11.8 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 75% yield (14.2 mg) and 86:14 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

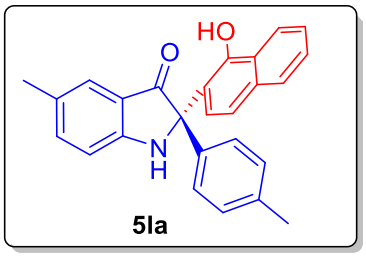
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.09 (s, 1H), 8.28 – 8.13 (m, 1H), 8.07 (s, 1H), 7.89 – 7.73 (m, 1H), 7.49 – 7.42 (m, 2H), 7.39 (d, *J* = 8.7 Hz, 1H), 7.35– 7.32 (m, 1H), 7.30– 7.20 (m, 5H), 7.10 (d, *J* = 6.5 Hz, 1H), 6.98 (d, *J* = 8.3 Hz, 1H), 2.25 (m, 3H), 2.23 (m, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 201.5, 159.1, 151.7, 140.5, 138.9, 137.2, 133.8, 128.10, 128.08, 127.6, 127.1, 126.5, 126.4, 126.2, 125.2, 125.0, 124.0, 123.7, 122.2, 122.1, 118.7, 118.4, 112.1, 73.9, 21.3, 20.1.

Enantiomeric excess is 72% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 18.27 min; major isomer: tr = 24.58 min.

HRMS (ESI) *m/z* calcd. for $C_{26}H_{20}NO_2$ $(M-H)^-$: 378.1500, found 378.1500.

$[\alpha]^{20}D$ = + 179 (c = 0.5, $CHCl_3$).



(S)-2-(1-hydroxynaphthalen-2-yl)-5-methyl-2-(p-tolyl)indolin-3-one (5la) According to the general procedure, **5la** was obtained using 5-methyl-2-(p-tolyl)-3*H*-indol-3-one **4l** (11.8 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 85% yield (16.1 mg) and 78:22 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

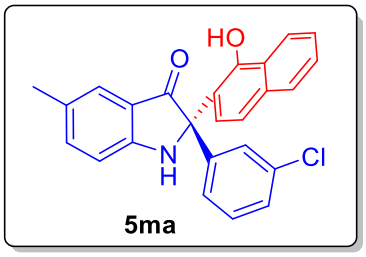
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.06 (s, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 8.03 (s, 1H), 7.83 –7.80 (m, 1H), 7.49 – 7.42 (m, 2H), 7.37 (d, *J* = 8.7 Hz, 1H), 7.35 – 7.27 (m, 4H), 7.22 (d, *J* = 8.6 Hz, 1H), 7.13 (d, *J* = 8.2 Hz, 2H), 6.95 (d, *J* = 8.3 Hz, 1H), 2.27 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 201.7, 159.1, 151.6, 138.8, 137.4, 136.6, 133.8, 128.7, 127.5, 126.7, 126.45, 126.41, 126.2, 125.2, 125.0, 123.7, 122.1, 122.0, 118.6, 118.4, 112.0, 73.7, 20.6, 20.0.

Enantiomeric excess is 56% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 12.08 min; major isomer: tr = 17.56 min.

HRMS (ESI) *m/z* calcd. for $C_{26}H_{20}NO_2$ $(M-H)^-$: 378.1500, found 378.1501.

$[\alpha]^{20}D$ = + 252 (c = 0.5, $CHCl_3$).



(S)-2-(3-chlorophenyl)-2-(1-hydroxynaphthalen-2-yl)-5-methylindolin-3-one (5ma) According to the general procedure, **5ma** was obtained using 2-(3-chlorophenyl)-5-methyl-3*H*-indol-3-one **4m** (12.8 mg, 0.05 mmol) and 1- naphthol **2a** (14.4 mg, 0.1 mmol) in 91% yield (18.2 mg) and 92:8 er

as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

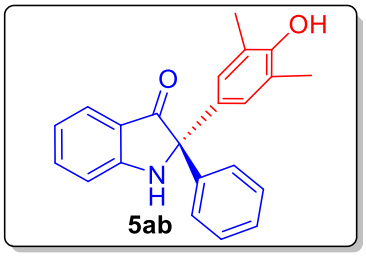
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.27 (s, 1H), 8.30 (d, *J* = 7.9 Hz, 1H), 7.78 – 7.76 (m, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.52 (s, 1H), 7.50 – 7.45 (m, 2H), 7.44 – 7.42 (m, 1H), 7.39 (d, *J* = 8.7 Hz, 1H), 7.30 – 7.27 (m, 1H), 7.21 (t, *J* = 7.9 Hz, 1H), 7.18 (t, *J* = 1.9 Hz, 1H), 7.08 – 7. (m, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 5.09 (s, 1H), 2.34 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.0, 158.2, 152.5, 142.9, 140.5, 135.0, 134.7, 131.0, 130.3, 128.9, 127.1, 126.9, 126.9, 126.6, 125.3, 125.2, 125.1, 125.0, 122.9, 120.7, 119.6, 116.9, 113.7, 75.6, 20.6.

Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 17.97 min; major isomer: tr = 28.27 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{17}ClNO_2$ $(M-H)^-$: 398.0953, found 398.0955.

$[\alpha]^{20}D$ = + 168 (c = 0.5, $CHCl_3$).



5ab

(S)-2-(4-hydroxy-3,5-dimethylphenyl)-2-phenylindolin-3-one (5ab) According to the general procedure, **5ab** was obtained using 2-phenyl-3*H*-indol-3-one **4a** (10.3 mg, 0.05 mmol) and 2,6-dimethylphenol **2b** (12.2 mg, 0.1 mmol) in 68% yield (11.2 mg) and 99:1 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

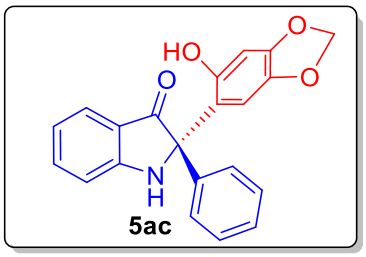
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (s, 1H), 8.28 (s, 1H), 7.50 – 7.46 (m, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.31 – 7.30 (m, 4H), 7.28 – 7.15 (m, 1H), 6.93 (d, *J* = 8.3 Hz, 1H), 6.86 (s, 2H), 6.70 (t, *J* = 7.3 Hz, 1H), 2.10 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 200.3, 160.6, 152.6, 141.3, 137.7, 131.0, 128.2, 127.3, 126.92, 126.89, 124.6, 123.9, 117.5, 117.4, 111.6, 73.5, 16.8.

Enantiomeric excess is 99% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 60/40, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 3.73 min; major isomer: tr = 6.25 min.

HRMS (ESI) *m/z* calcd. for $C_{22}H_{18}NO_2$ $(M-H)^-$: 328.1343, found 328.1344.

$[\alpha]^{20}D$ = + 15 (c = 0.1, CH_3OH).



(S)-2-(6-hydroxybenzo[d][1,3]dioxol-5-yl)-2-phenylindolin-3-one (5ac) According to the general procedure, **5ac** was obtained using 2-phenyl-3*H*-indol-3-one **4a** (10.3 mg, 0.05 mmol) and benzo[d][1,3]dioxol-5-ol **2c** (13.8 mg, 0.1 mmol) in 63% yield (14.3 mg) and 75:25 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

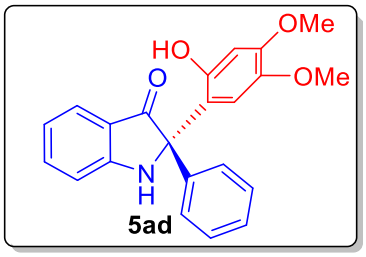
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.56 – 9.43 (m, 1H), 8.00 (s, 1H), 7.47 – 7.43 (m, 1H), 7.42 – 7.36 (m, 3H), 7.31 – 7.27 (m, *J* = 11.2, 4.4 Hz, 2H), 7.26 – 7.22 (m, 1H), 7.06 – 7.00 (m, 1H), 6.67 (t, *J* = 7.4 Hz, 1H), 6.57 – 6.53 (m, 1H), 6.45 – 6.39 (m, 1H), 5.92 (s, 1H), 5.89 (s, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 200.2, 160.5, 151.2, 146.9, 140.2, 139.2, 137.2, 128.0, 127.1, 126.4, 124.3, 118.6, 117.9, 117.1, 111.8, 108.0, 101.0, 98.2, 72.4.

Enantiomeric excess is 50% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 14.90 min; major isomer: tr = 20.10 min.

HRMS (ESI) *m/z* calcd. for $C_{21}H_{14}NO_4$ $(M-H)^-$: 344.0928, found 344.0928.

$[\alpha]^{20}D$ = + 157 (c = 0.5, $CHCl_3$).



(S)-2-(2-hydroxy-4,5-dimethoxyphenyl)-2-phenylindolin-3-one (5ad) According to the general procedure, **5ad** was obtained using 2-phenyl-3*H*-indol-3-one **4a** (10.3 mg, 0.05 mmol) and 3,4-dimethoxyphenol **2d** (15.4 mg, 0.1 mmol) in 83% yield (15.0 mg) and 87:13 er as a yellow oily (silica gel flash chromatography: petroleum ether/EtOAc = 30:1). R_f = 0.50 (petroleum ether/EtOAc = 4:1)

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.34 (d, *J* = 2.8 Hz, 1H), 8.00 (s, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.36 – 7.34 (m, 2H), 7.28 (t, *J* = 7.2 Hz, 2H), 7.25 – 7.18 (m, 1H), 7.02 (d, *J* = 8.3 Hz, 1H), 6.73 (d, *J* = 4.4 Hz, 1H), 6.67 (t, *J* = 7.4 Hz, 1H), 6.45 – 6.44 (m, 1H), 3.69 (s, 3H), 3.55 (s, 3H).

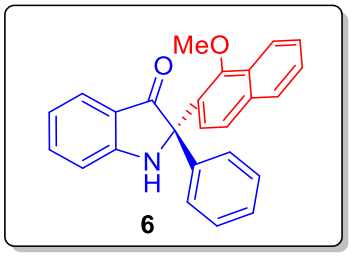
^{13}C NMR (100 MHz, DMSO-d_6) δ 200.2, 160.5, 150.6, 149.3, 140.6, 140.3, 137.2, 127.9, 127.0, 126.3, 124.4, 117.7, 117.5, 117.1, 114.2, 111.8, 101.4, 72.3, 56.8, 55.4.

Enantiomeric excess is 74% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.80 min; major isomer: tr = 11.71 min.

HRMS (ESI) *m/z* calcd. for $C_{22}H_{18}NO_4$ $(M-H)^-$: 360.1241, found 360.1243.

$[\alpha]^{20}D$ = + 298 (c = 0.5, $CHCl_3$).

3. Synthesis applications of 3aa



6

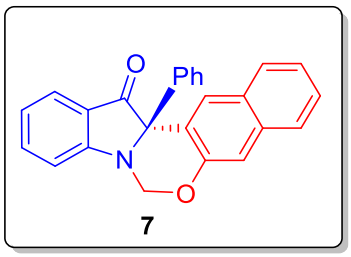
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.94 (m, 1H), 7.90 – 7.84 (m, 1H), 7.82 (d, *J* = 8.7 Hz, 1H), 7.66 – 7.61 (m, 2H), 7.56 – 7.52 (m, 2H), 7.50 – 7.42 (m, 3H), 7.32 – 7.27 (m, 2H), 7.26 – 7.22 (m, 1H), 6.91 (d, *J* = 8.3 Hz, 1H), 6.79 (t, *J* = 7.4 Hz, 1H), 6.53 (s, 1H), 3.27 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 160.1, 155.0, 141.1, 137.5, 134.8, 130.2, 128.3, 128.24, 128.21, 127.5, 126.5, 126.4, 126.0, 125.6, 125.2, 123.7, 122.1, 118.9, 118.7, 111.7, 73.6, 61.8.

Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 70/30, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.28 min; major isomer: tr = 14.36 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{18}NO_2$ $(M-H)^-$: 364.1343, found 364.1342.

$[\alpha]^{20}D$ = + 483 (c = 0.5, $CHCl_3$).



7

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.07 – 8.04 (m, 1H), 7.88 – 7.85 (m, 1H), 7.79 – 7.71 (m, 2H), 7.66 (d, J = 7.7 Hz, 1H), 7.60 – 7.49 (m, 4H), 7.41 – 7.34 (m, 3H), 7.22 – 7.16 (m, 2H), 7.11 – 7.09 (m, 1H), 6.26 (d, J = 11.1 Hz, 1H), 4.99 (d, J = 11.1 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 198.6, 159.4, 148.9, 140.5, 137.8, 133.0, 128.7, 128.4, 127.6, 127.3, 126.2, 125.3, 125.0, 124.0, 122.1, 121.9, 121.5, 120.5, 113.0, 112.3, 71.8, 71.4.

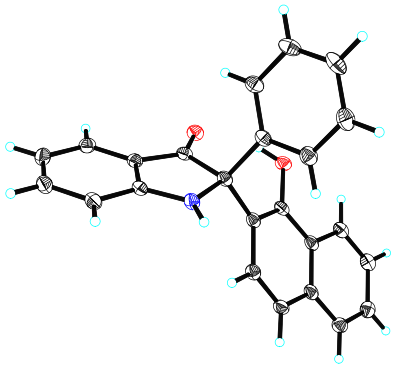
Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 70/30, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 13.24 min; major isomer: tr = 26.40 min.

HRMS (ESI) *m/z* calcd. for $C_{25}H_{17}NNaO_2$ $(M+Na)^+$: 386.1152, found 386.1154.

$[\alpha]^{20}D$ = + 82 (c = 0.5, $CHCl_3$).

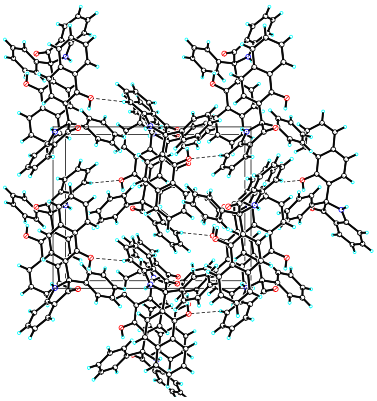
4. Crystal of 3aa

Crystal data for md_zxj372: $C_{24}H_{17}NO_2$, M = 351.38, a = 9.6357(6) Å, b = 12.2218(8) Å, c = 14.9472(10) Å, α = 90°, β = 90°, γ = 90°, V = 1760.3(2) Å^3, T = 150.(2) K, space group $P212121$, Z = 4, μ(Cu Kα) = 0.670 mm^{-1}, 14760 reflections measured, 3343 independent reflections (R_{int} = 0.0484). The final R_1 values were 0.0317 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0836 ($I > 2\sigma(I)$). The final R_1 values were 0.0335 (all data). The final $wR(F^2)$ values were 0.0852 (all data). The goodness of fit on F^2 was 1.067. Flack parameter = -0.12(10).



View of a molecule of **3aa** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of **3aa**.

Hydrogen-bonds are shown as dashed lines.

Table 1. Crystal data and structure refinement for **3aa**.

Identification code	global	
Empirical formula	C24 H17 N O2	
Formula weight	351.38	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.6357(6) Å	α= 90°.
	b = 12.2218(8) Å	β= 90°.
	c = 14.9472(10) Å	γ = 90°.
Volume	1760.3(2) $Å^3$	
Z	4	
Density (calculated)	1.326 Mg/m^3	

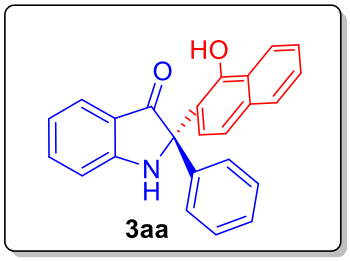
Absorption coefficient	0.670 mm^{-1}	
F(000)	736	
Crystal size	0.420 x 0.190 x 0.150 mm^3	
Theta range for data collection	4.67 to 70.16°.	
Index ranges	-11<=h<=10, -13<=k<=14, -14<=l<=18	
Reflections collected	14760	
Independent reflections	3343 [R(int) = 0.0484]	
Completeness to theta = 70.16°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.91 and 0.57	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3343 / 0 / 245	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0836	
R indices (all data)	R1 = 0.0335, wR2 = 0.0852	
Absolute structure parameter	-0.12(10)	
Largest diff. peak and hole	0.340 and -0.225 $e.Å^{-3}$	

5. Reference

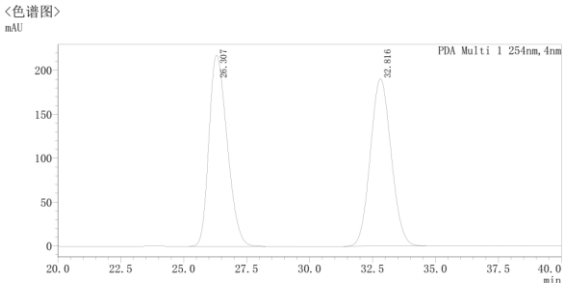
[1]. Lian, X.-L.; Lei, H.; Quan, X.-J.; Ren, Z.-H.; Wang, Y.-Y.; Guan, Z.-H. *Chem. Commun*. **2013**, *49*, 8196.

[2]. (a) Lindsay, A. C.; Leung, I. K. H.; Sperry, J. *Org. Lett.* **2016**, *18*, 5404. (b) Ling, K.-Q. *Synth. Commun.* **1995**, *25*, 3831. (c) Liu, J.-X.; Zhou, Q.-Q.; Deng, J.-G.; Chen, Y.-C. *Org. Biomol. Chem*. **2013**, *11*, 8175. (d) Najahi, E.; Valentin, A.; Fabre, P.-L.; Reybier, K.; Nepveu, F. *Eur. J. Med. Chem*. **2014**, *78*, 269. (e) Huang, J.-R.; Qin, L.; Zhu, Y.-Q.; Song, Q.; Dong, L. *Chem. Commun*. **2015**, *51*, 2844.

6. Copies of HPLC

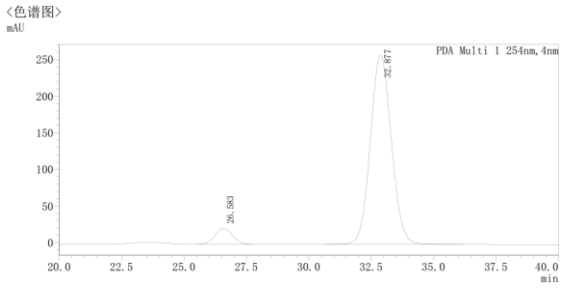


Enantiomeric excess is 88% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 26.58 min; major isomer: tr = 32.88 min.



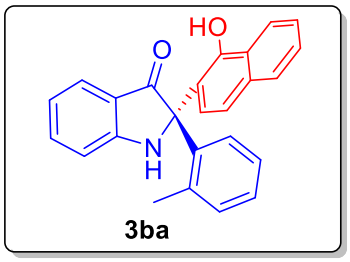
<峰表>
PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	26.307	10984907	217721	49.998
2	32.816	10985892	190686	50.002
总计		21970799	408407	100.000

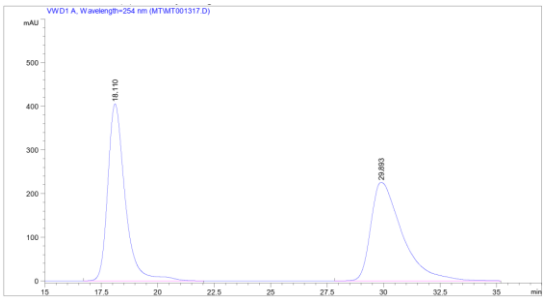


<峰表>
PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	26.583	1033410	21676	6.388
2	32.877	15145171	258363	93.612
总计		16178581	280039	100.000

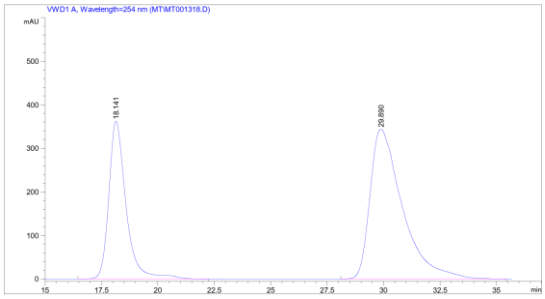


Enantiomeric excess is 28% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 18.14 min; major isomer: tr = 29.90 min.



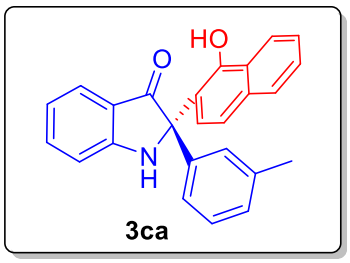
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.110	BB	0.7957	2.15313e4	405.36423	49.8188
2	29.893	BBA	1.4172	2.16879e4	225.27290	50.1812

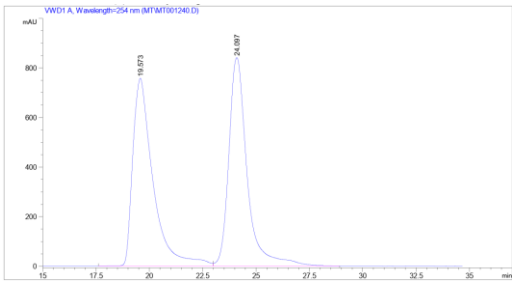


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.141	BB	0.8011	1.91252e4	361.55170	35.8446
2	29.890	BB	1.3554	3.42306e4	343.55420	64.1554

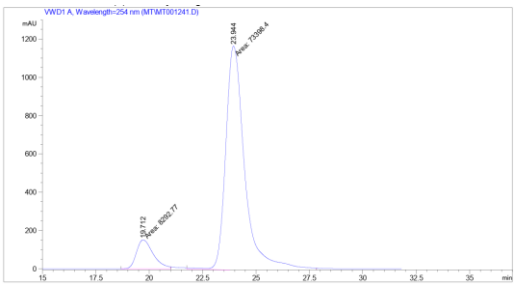


Enantiomeric excess is 80% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 19.71 min; major isomer: tr = 23.94 min.



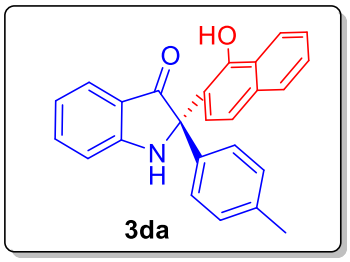
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.573	BV	0.9671	4.98288e4	756.85730	49.9102
2	24.097	VB	0.9000	5.00081e4	839.50391	50.0898

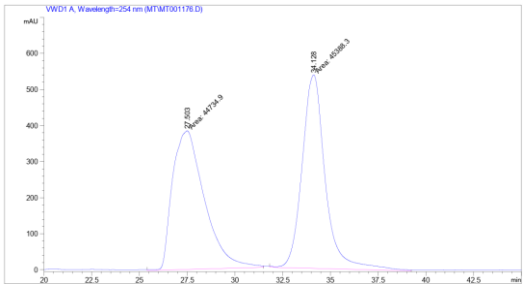


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.712	MM	0.9134	8292.77344	151.31978	10.1514
2	23.944	MM	1.0476	7.33984e4	1167.67822	89.8486

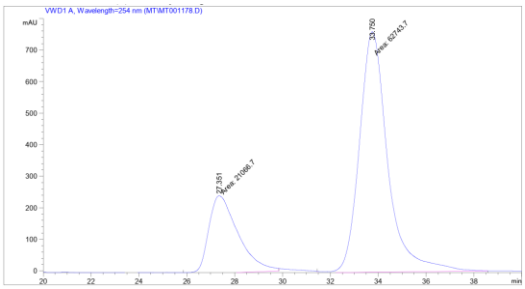


Enantiomeric excess is 50% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 27.35 min; major isomer: tr = 33.75 min.



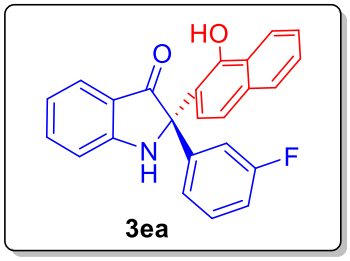
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.503	MM	1.9396	4.47349e4	384.39560	49.6375
2	34.128	MM	1.4077	4.53883e4	537.38129	50.3625

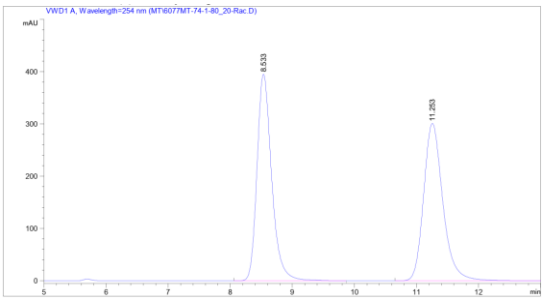


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.351	MM	1.4306	2.10667e4	245.42554	25.1361
2	33.750	MM	1.3727	6.27437e4	761.82507	74.8639

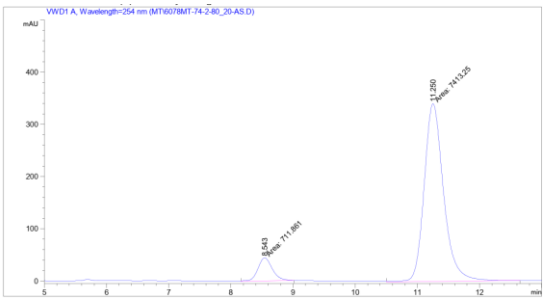


Enantiomeric excess is 82% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.54 min; major isomer: tr = 11.25 min.



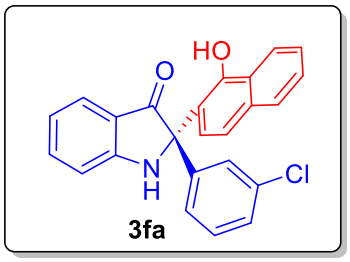
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.533	BB	0.2488	6461.44092	395.14221	49.9621
2	11.253	BB	0.3278	6471.23584	301.03995	50.0379

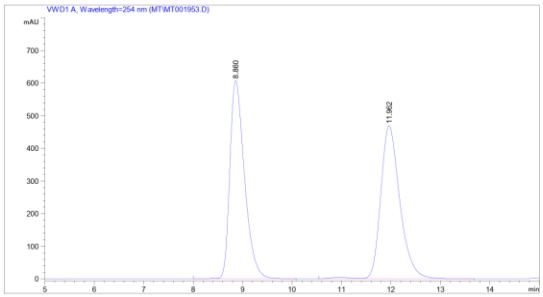


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.543	MM	0.2690	711.86139	44.10577	8.7613
2	11.250	MM	0.3628	7413.24707	340.53333	91.2387

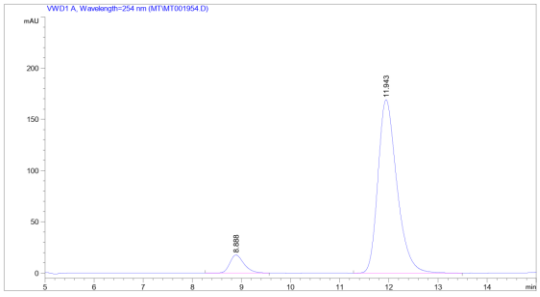


Enantiomeric excess is 88% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.89 min; major isomer: tr = 11.94 min.



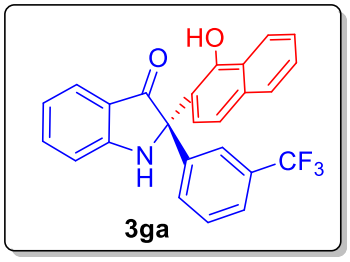
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.860	BB	0.3134	1.24497e4	606.74719	49.7268
2	11.962	VB R	0.4059	1.25865e4	468.28336	50.2732

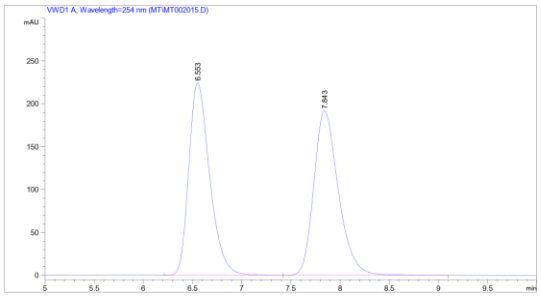


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.888	BB	0.3014	347.89841	17.54316	7.1243
2	11.943	BB	0.4069	4535.38721	169.07838	92.8757

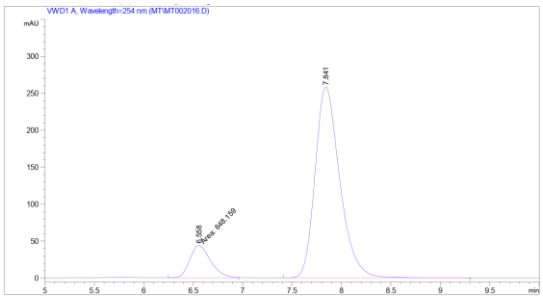


Enantiomeric excess is 74% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 6.56 min; major isomer: tr = 7.84 min.



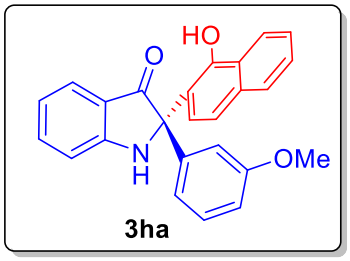
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.553	BB	0.2249	3303.63477	224.25764	49.8251
2	7.843	BB	0.2643	3326.83008	191.85947	50.1749

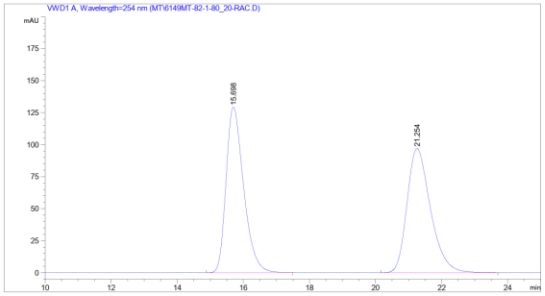


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.558	MM	0.2458	648.15942	43.94016	12.6222
2	7.841	BB	0.2657	4486.92920	258.19019	87.3778

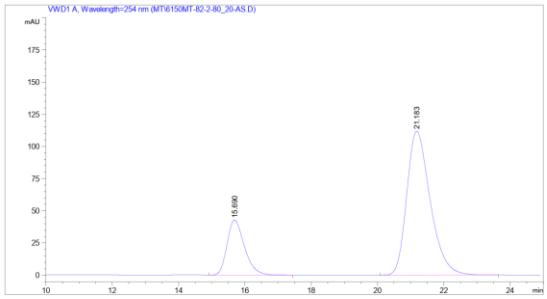


Enantiomeric excess is 56% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 15.69 min; major isomer: tr = 21.18 min



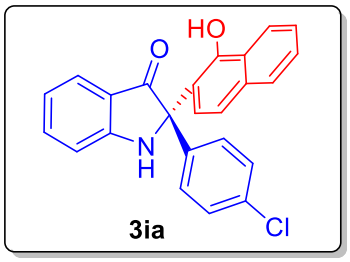
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.698	BB	0.5617	4762.98926	129.33043	49.9424
2	21.254	BB	0.7542	4773.97412	96.83360	50.0576

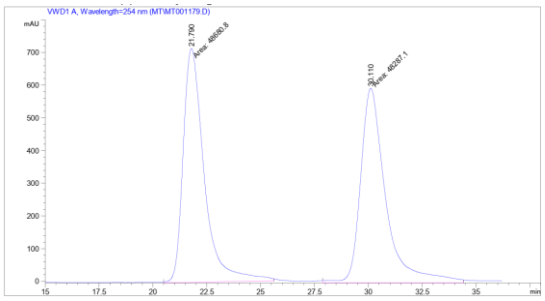


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.690	BB	0.5589	1560.03833	42.73273	22.1160
2	21.183	BB	0.7485	5493.86377	111.76221	77.8840

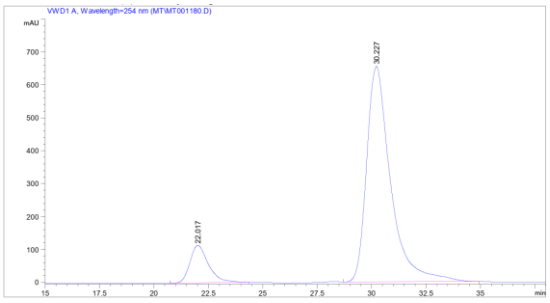


Enantiomeric excess is 76% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 22.02 min; major isomer: tr = 30.23 min.



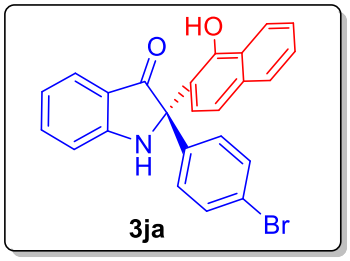
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.790	MM	1.1346	4.86808e4	715.10095	50.2030
2	30.110	MM	1.3530	4.82871e4	594.79370	49.7970

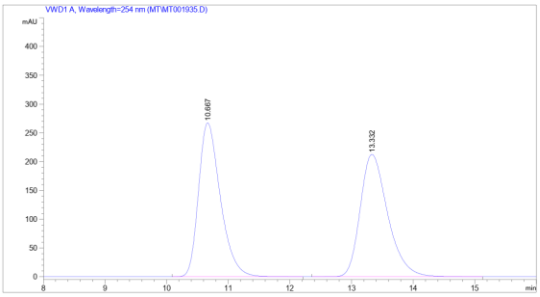


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.017	BB	0.8847	6747.94043	113.98557	11.8538
2	30.227	BB	1.1445	5.01787e4	654.44641	88.1462

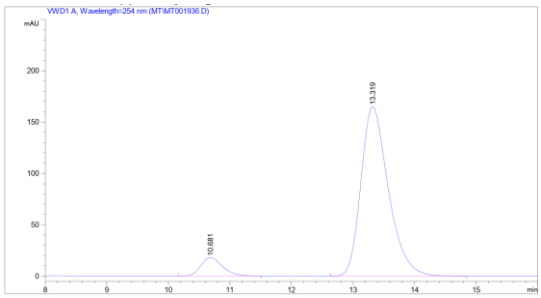


Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 10.68 min; major isomer: tr = 13.32 min.



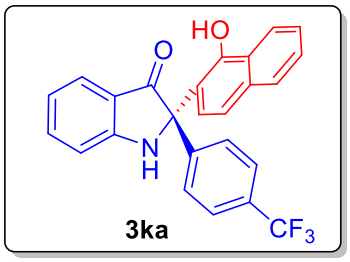
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.667	BB	0.3752	6579.19092	267.24911	49.9437
2	13.332	BB	0.4739	6594.01611	212.58794	50.0563

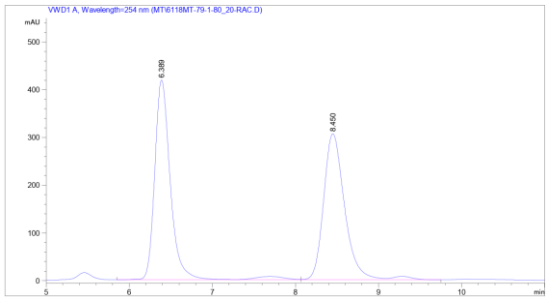


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.681	BB	0.3719	433.04770	17.85584	7.8266
2	13.319	BB	0.4697	5100.00195	164.95390	92.1734

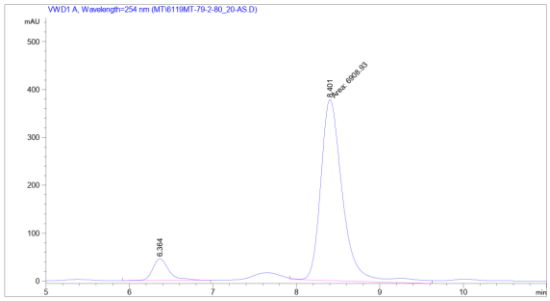


Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 6.36 min; major isomer: tr = 8.40 min.



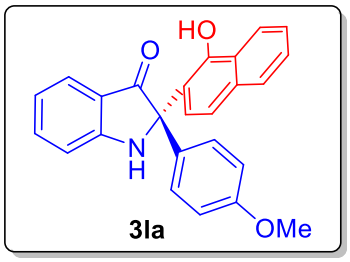
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.389	BV R	0.1954	5569.66846	418.41360	50.5879
2	8.450	VV R	0.2650	5440.21191	306.10239	49.4121

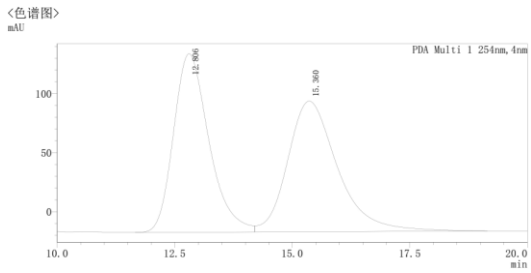


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.364	BB	0.2054	607.48541	45.02724	8.0821
2	8.401	MM	0.3049	6908.92676	377.71390	91.9179



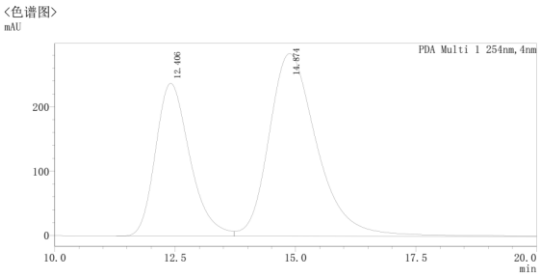
Enantiomeric excess is 26% determined by HPLC (Chiralpak AS-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 12.41 min; major isomer: tr = 14.87 min.



〈峰表〉

PDA Ch1 254nm

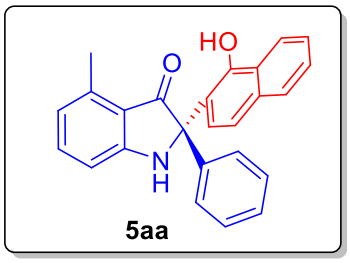
峰号	保留时间	面积	高度	面积%
1	12.806	7908831	151066	49.258
2	15.360	8147007	110497	50.742
总计		16055838	261564	100.000



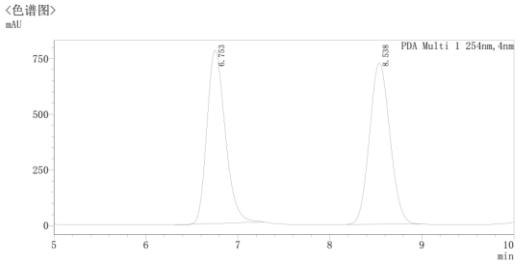
〈峰表〉

PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	12.406	11824734	237517	37.450
2	14.874	19750367	283752	62.550
总计		31575100	521269	100.000



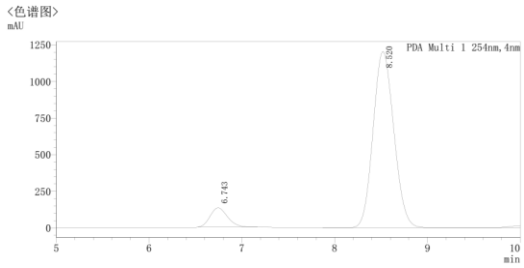
Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 6.74 min; major isomer: tr = 8.52 min.



〈峰表〉

PDA Ch1 254nm

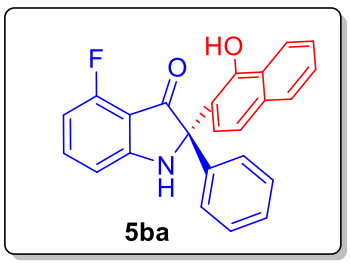
峰号	保留时间	面积	高度	面积%
1	6.753	10768852	777831	49.111
2	8.538	11158687	723578	50.889
总计		21927539	1501409	100.000



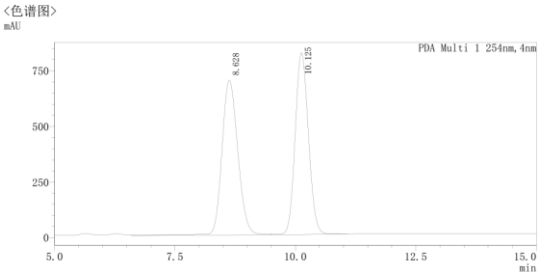
〈峰表〉

PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	6.743	1713465	131527	8.270
2	8.520	19006387	1203458	91.730
总计		20719852	1334985	100.000



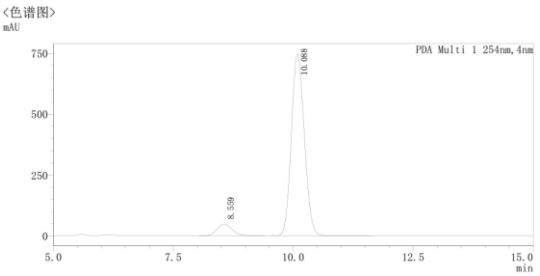
Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.56 min; major isomer: tr = 10.09 min.



〈峰表〉

PDA Ch1 254nm

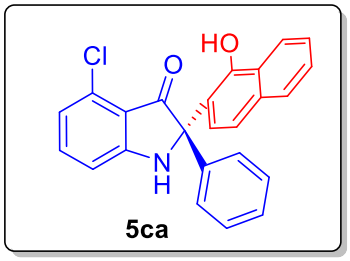
峰号	保留时间	面积	高度	面积%
1	8.628	16179415	696634	50.801
2	10.125	15669405	818276	49.199
总计		31848820	1514910	100.000



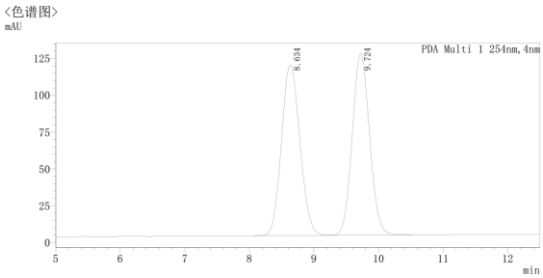
〈峰表〉

PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	8.559	1023737	47920	6.766
2	10.088	14107268	747425	93.234
总计		15131004	795345	100.000



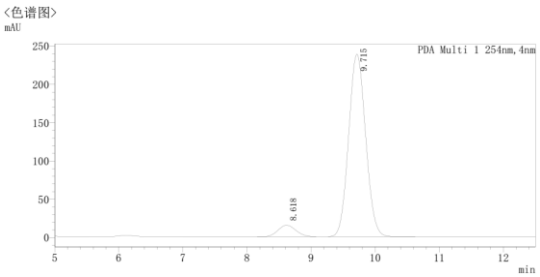
Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.62 min; major isomer: tr = 9.72 min.



〈峰表〉

PDA Ch1 254nm

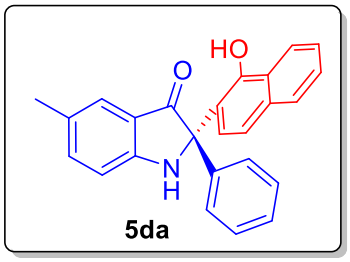
峰号	保留时间	面积	高度	面积%
1	8.634	2304195	115952	50.011
2	9.724	2303136	123447	49.989
总计		4607331	239399	100.000



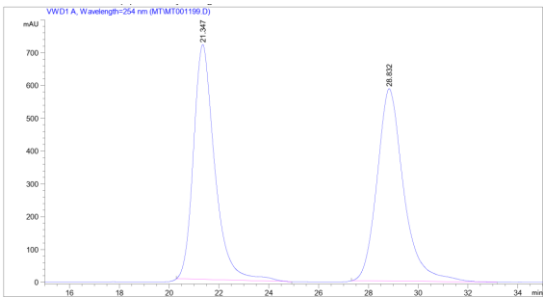
〈峰表〉

PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	8.618	293660	15062	6.257
2	9.715	4399881	238382	93.743
总计		4693541	253444	100.000

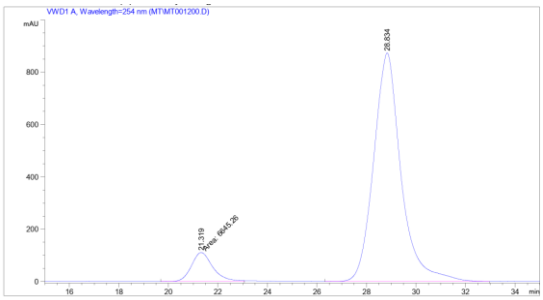


Enantiomeric excess is 82% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 21.32 min; major isomer: tr = 28.83 min.



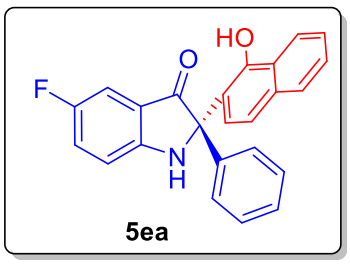
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.347	BB	0.8575	4.24219e4	715.74384	49.3810
2	28.832	BB	1.0608	4.34855e4	586.67297	50.6190

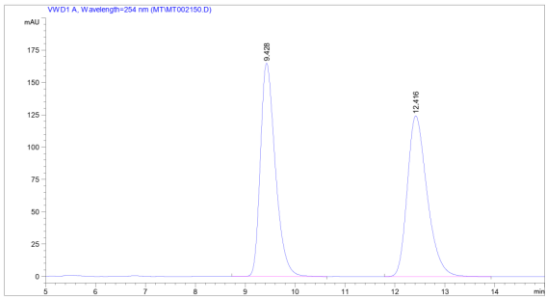


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.319	MM	1.0032	6645.25537	110.39558	9.0251
2	28.834	BB	1.1600	6.69854e4	873.21155	90.9749

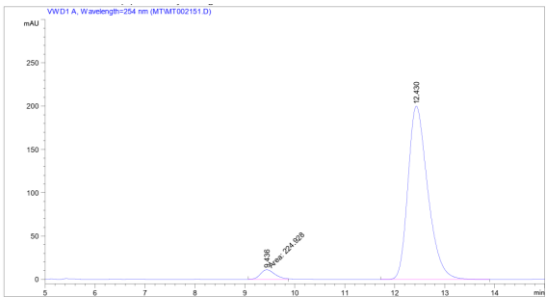


Enantiomeric excess is 92% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 9.44 min; major isomer: tr = 12.43 min.



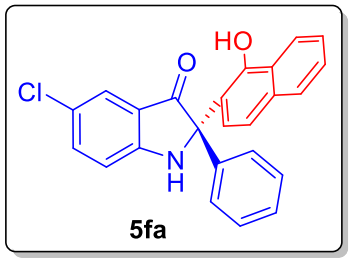
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.428	BB	0.3174	3429.21191	165.03946	49.9940
2	12.416	BB	0.4209	3430.04053	124.32121	50.0060



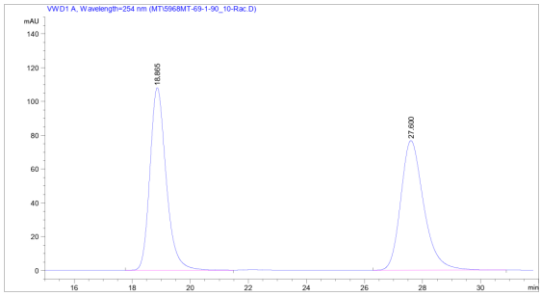
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.436	MM	0.3386	224.92831	11.07024	3.9341
2	12.430	BB	0.4186	5492.41260	199.86919	96.0659



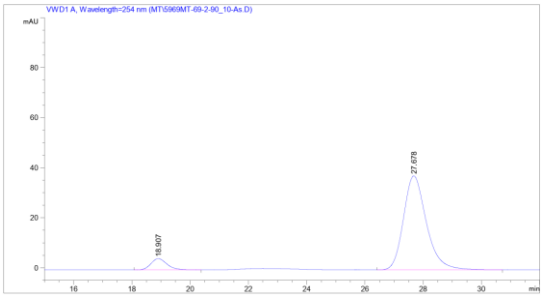
5fa

Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 18.91 min; major isomer: tr = 27.68 min.



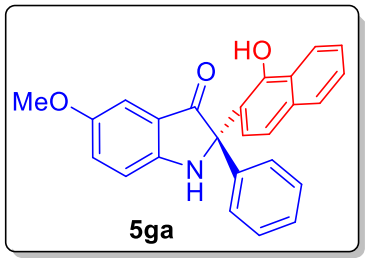
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.865	BB	0.5933	4199.43896	108.08907	49.8663
2	27.600	BB	0.8379	4221.95166	76.73201	50.1337



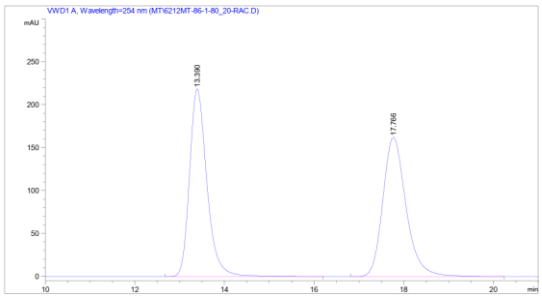
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.907	BB	0.5848	174.11121	4.52654	7.8052
2	27.678	BB	0.8294	2056.59717	37.58110	92.1948



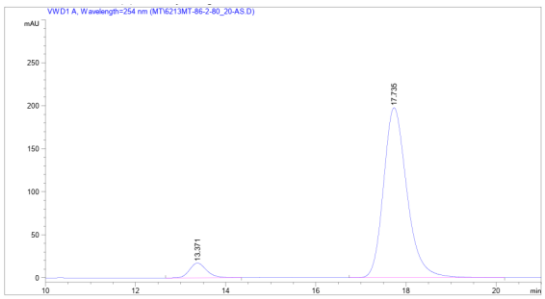
5ga

Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 13.37 min; major isomer: tr = 17.74 min.



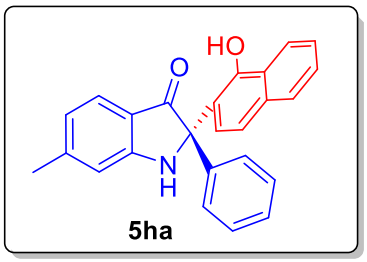
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.390	BB	0.4097	5874.41943	218.48900	50.1829
2	17.766	BB	0.5496	5831.60303	162.12424	49.8171

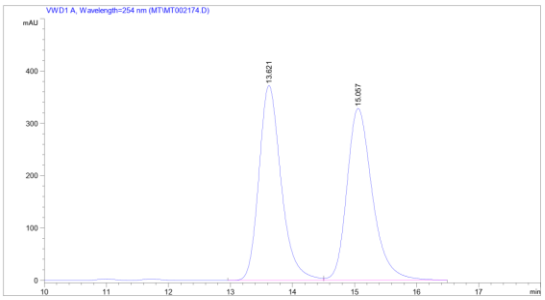


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.371	BB	0.3990	445.66245	17.10506	5.8830
2	17.735	BB	0.5508	7129.74463	197.68385	94.1170

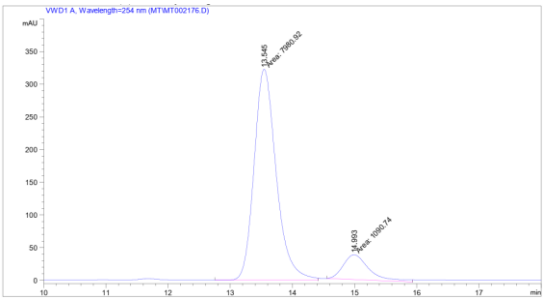


Enantiomeric excess is 76% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 13.55 min; major isomer: tr = 14.99 min.



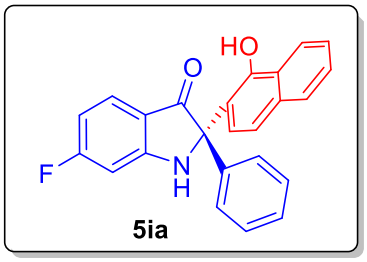
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.621	BV	0.3802	9265.69727	372.45215	49.8030
2	15.057	VBA	0.4357	9339.01758	328.42880	50.1970



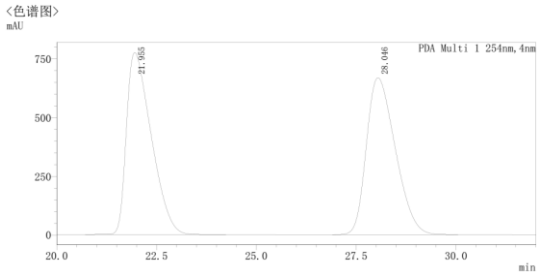
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.545	MM	0.4121	7980.91650	322.79153	87.9764
2	14.993	MM	0.4802	1090.73865	37.85950	12.0236



5ia

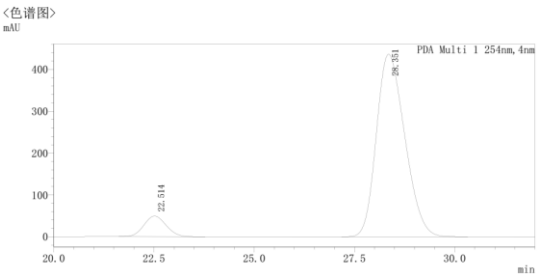
Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 22.51 min; major isomer: tr = 28.35 min.



〈峰表〉

PDA Ch1 254nm

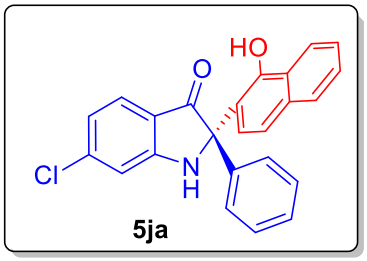
峰号	保留时间	面积	高度	面积%
1	21.955	33379278	774165	49.883
2	28.046	33536295	667132	50.117
总计		66915572	1441297	100.000



〈峰表〉

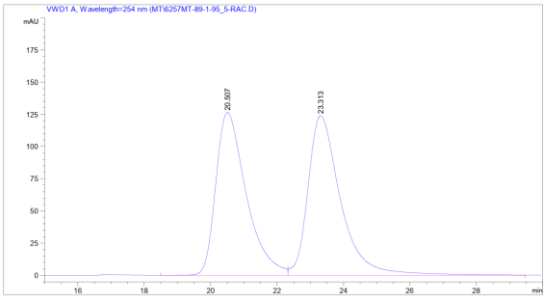
PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	22.514	1897750	49265	8.113
2	28.351	21493355	436391	91.887
总计		23391106	485656	100.000



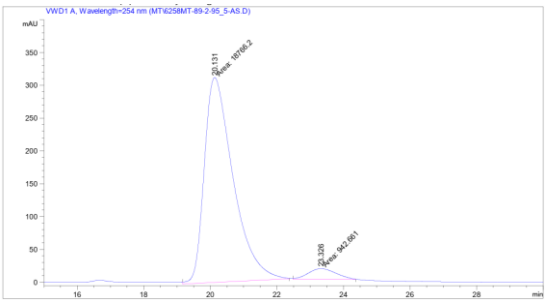
5ja

Enantiomeric excess is 90% determined by HPLC (Chiralpak OD-H, Hexane/Isopropanol 95/5, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 20.13 min; major isomer: tr = 23.33 min.



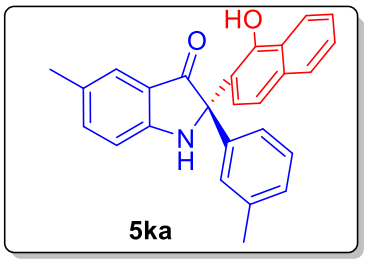
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.507	BV	0.9588	8035.20850	126.37903	48.6392
2	23.313	VB	1.0328	8484.81055	123.76013	51.3608

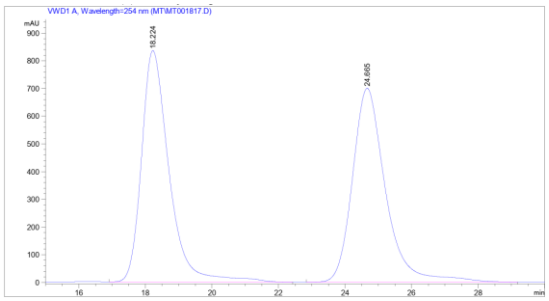


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.131	MM	1.0026	1.87662e4	311.95663	95.2171
2	23.326	MM	0.9658	942.66150	16.26694	4.7829

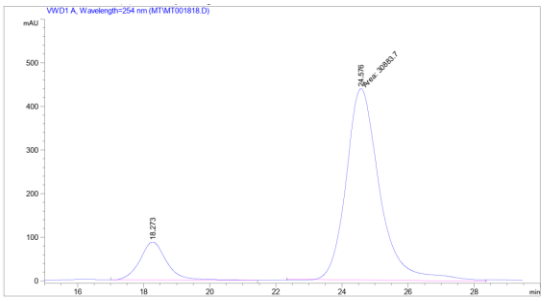


Enantiomeric excess is 72% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 18.27 min; major isomer: tr = 24.58 min.



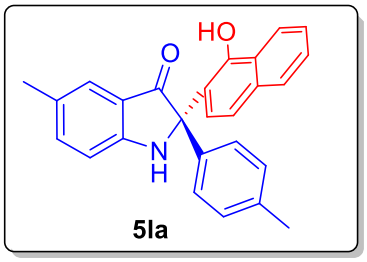
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.224	BB	0.8633	4.79313e4	835.54248	49.8505
2	24.665	BB	1.0449	4.82187e4	699.80945	50.1495



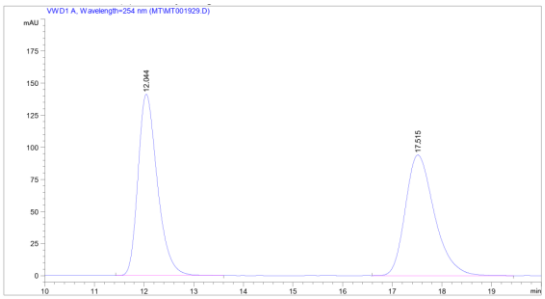
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.273	BB	0.8463	4956.06299	87.17032	13.8284
2	24.576	MM	1.1750	3.08837e4	438.07288	86.1716



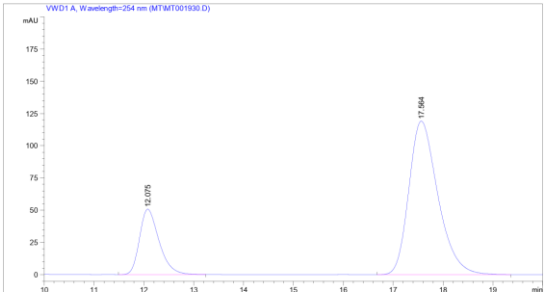
5la

Enantiomeric excess is 56% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 12.08 min; major isomer: tr = 17.56 min.



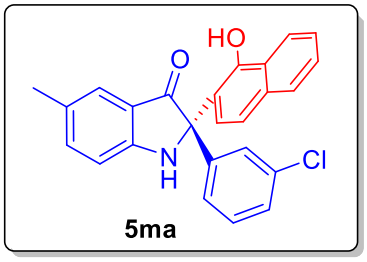
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.044	BB	0.4136	3818.23291	141.16299	50.0251
2	17.515	BB	0.6220	3814.40820	93.87920	49.9749



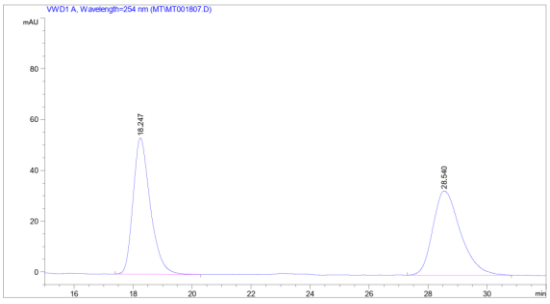
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.075	BB	0.4135	1374.15601	50.65971	22.1748
2	17.564	BB	0.6197	4822.76953	119.03105	77.8252



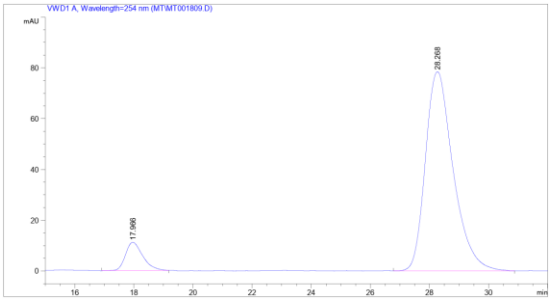
5ma

Enantiomeric excess is 84% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 90/10, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 17.97 min; major isomer: tr = 28.27 min.



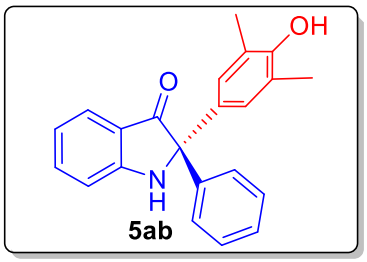
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.247	BB	0.6148	2171.59888	53.58863	50.2724
2	28.540	BB	1.0002	2148.06909	33.14143	49.7276

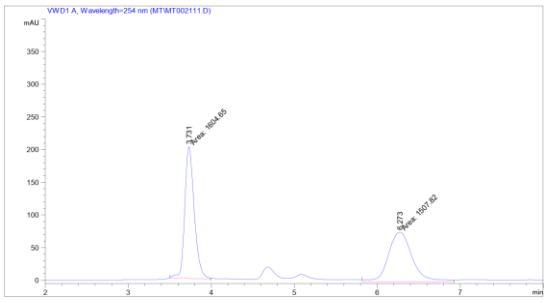


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.966	BB	0.6120	451.02298	11.10104	8.1058
2	28.268	BB	0.9794	5113.16992	78.34838	91.8942

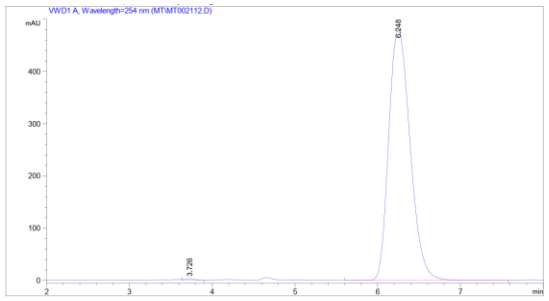


Enantiomeric excess is 99% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 60/40, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 3.73 min; major isomer: tr = 6.25 min.



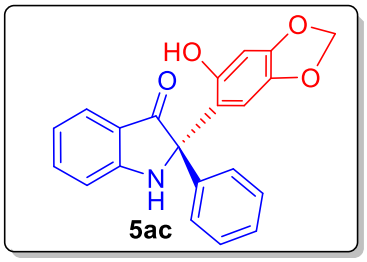
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.731	MM	0.1326	1604.65369	201.69762	51.5556
2	6.273	MM	0.3325	1507.81860	75.57365	48.4444

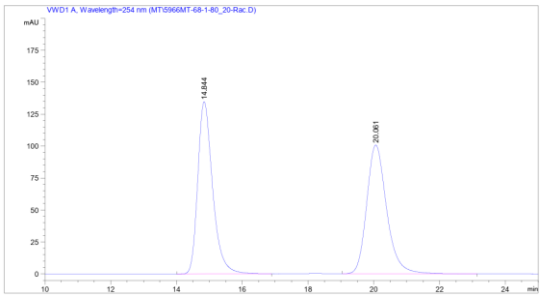


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.726	VB	0.1193	21.89407	2.76678	0.2541
2	6.248	BB	0.2847	8594.51465	478.05939	99.7459

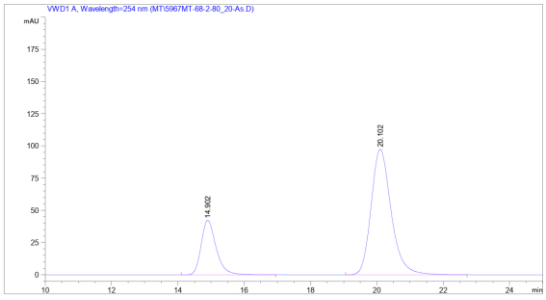


Enantiomeric excess is 50% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 14.90 min; major isomer: tr = 20.10 min.



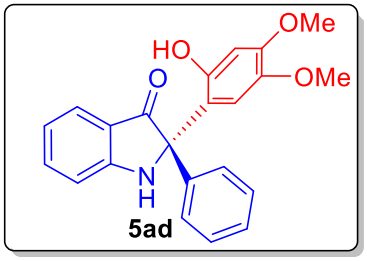
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.844	BB	0.4784	4232.55469	134.78165	49.9878
2	20.061	BB	0.6434	4234.61279	100.74392	50.0122

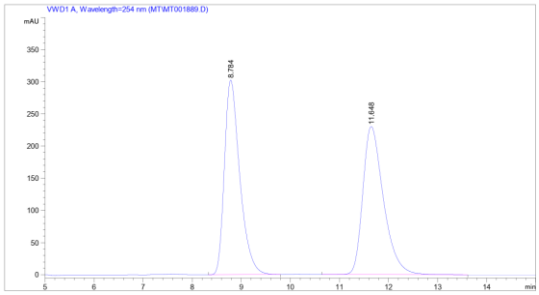


Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.902	BB	0.4776	1329.67017	42.31599	24.5067
2	20.102	BB	0.6423	4096.07373	97.46844	75.4933

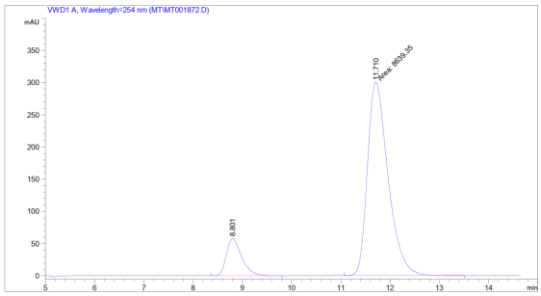


Enantiomeric excess is 74% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 80/20, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.80 min; major isomer: tr = 11.71 min.



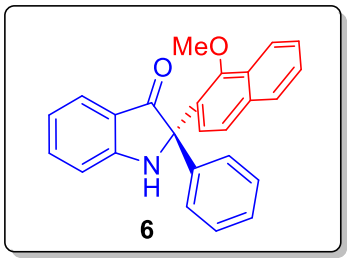
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.784	BB	0.3288	6581.73096	302.53720	49.3853
2	11.648	BB	0.4428	6745.57813	230.25417	50.6147



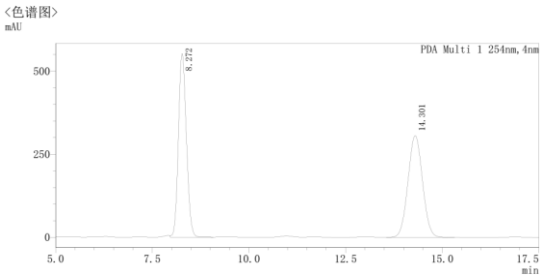
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.801	BB	0.3282	1256.94458	57.92688	12.7012
2	11.710	MM	0.4813	8639.34668	299.17529	87.2988



6

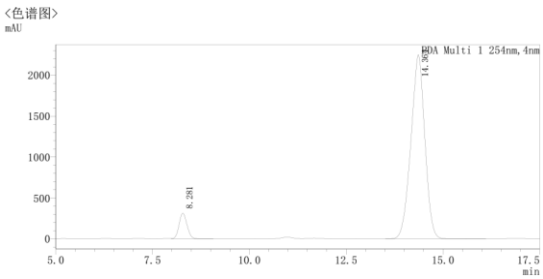
Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 70/30, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 8.28 min; major isomer: tr = 14.36 min.



〈峰表〉

PDA Ch1 254nm

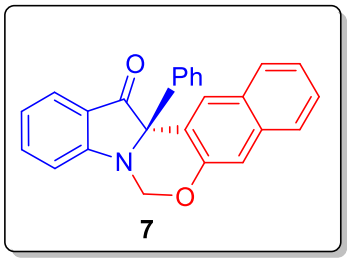
峰号	保留时间	面积	高度	面积%
1	8.272	7943640	551891	49.918
2	14.301	7969732	305828	50.082
总计		15913371	857719	100.000



〈峰表〉

PDA Ch1 254nm

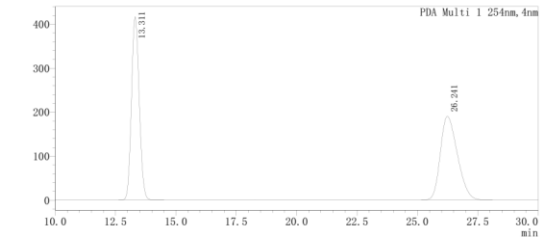
峰号	保留时间	面积	高度	面积%
1	8.281	4491101	312655	7.401
2	14.364	56193511	2249054	92.599
总计		60684612	2561709	100.000



7

Enantiomeric excess is 86% determined by HPLC (Chiralpak AD-H, Hexane/Isopropanol 70/30, flow rate = 1.0 mL/min, 254 nm): minor isomer: tr = 13.24 min; major isomer: tr = 26.40 min.

<色谱图>

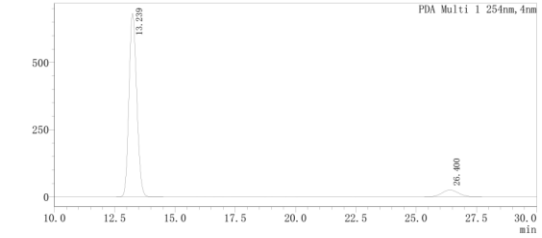


<峰表>

PDA Ch1 254nm

峰号	保留时间	面积	高度	面积%
1	13.311	9280202	416318	49.853
2	26.241	9334997	190057	50.147
总计		18615199	606375	100.000

<色谱图>

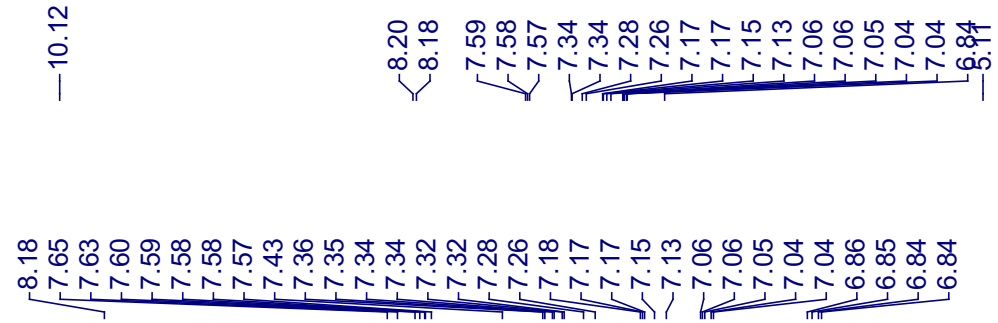


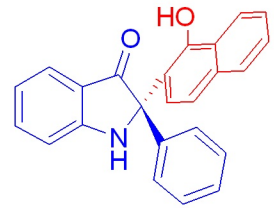
<峰表>

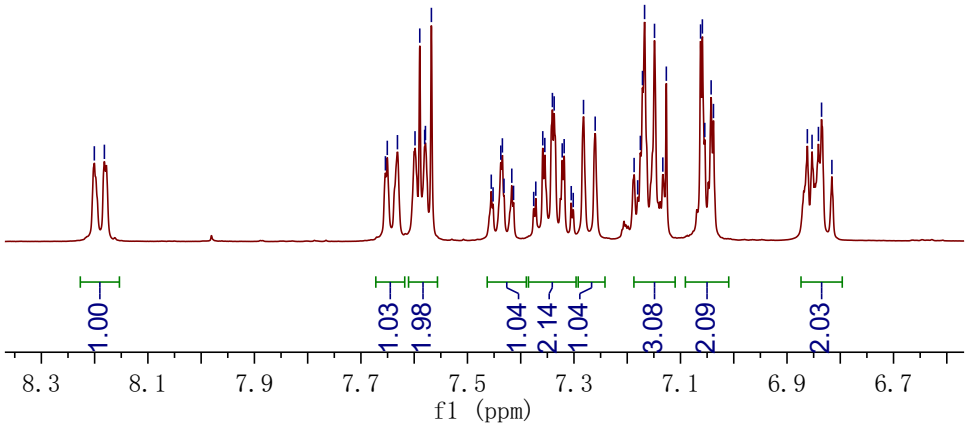
PDA Ch1 254nm

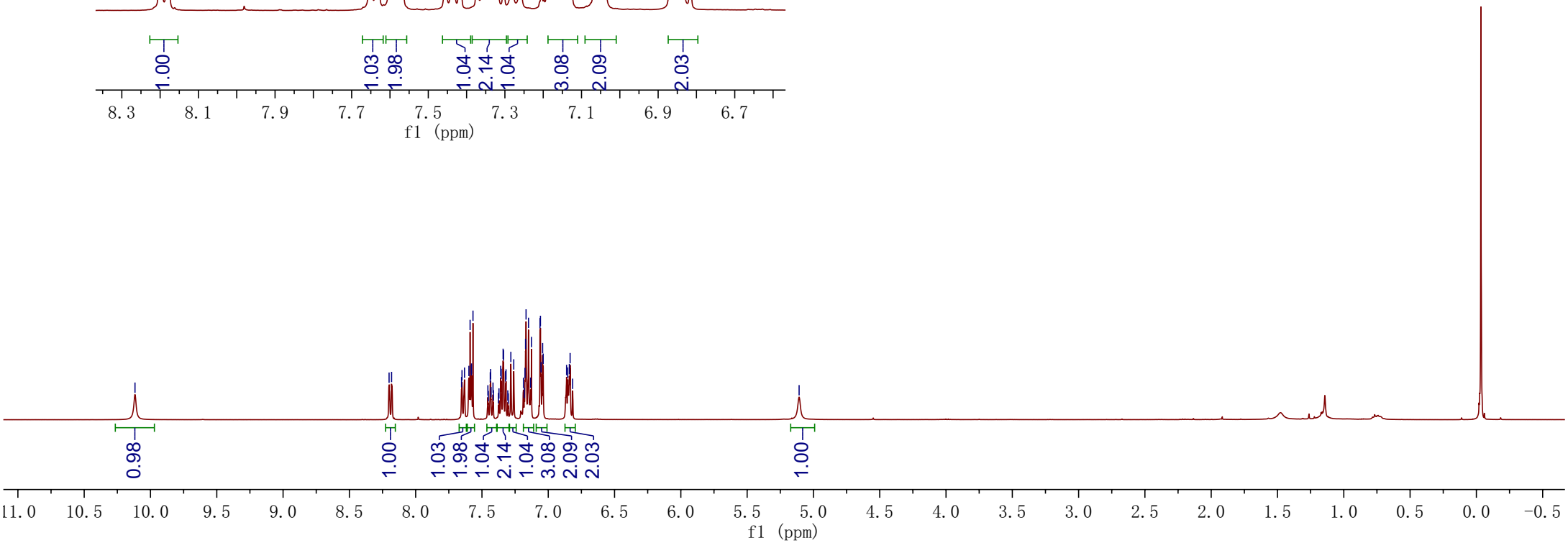
峰号	保留时间	面积	高度	面积%
1	13.239	15271088	681756	92.727
2	26.400	1197774	25210	7.273
总计		16468862	706966	100.000

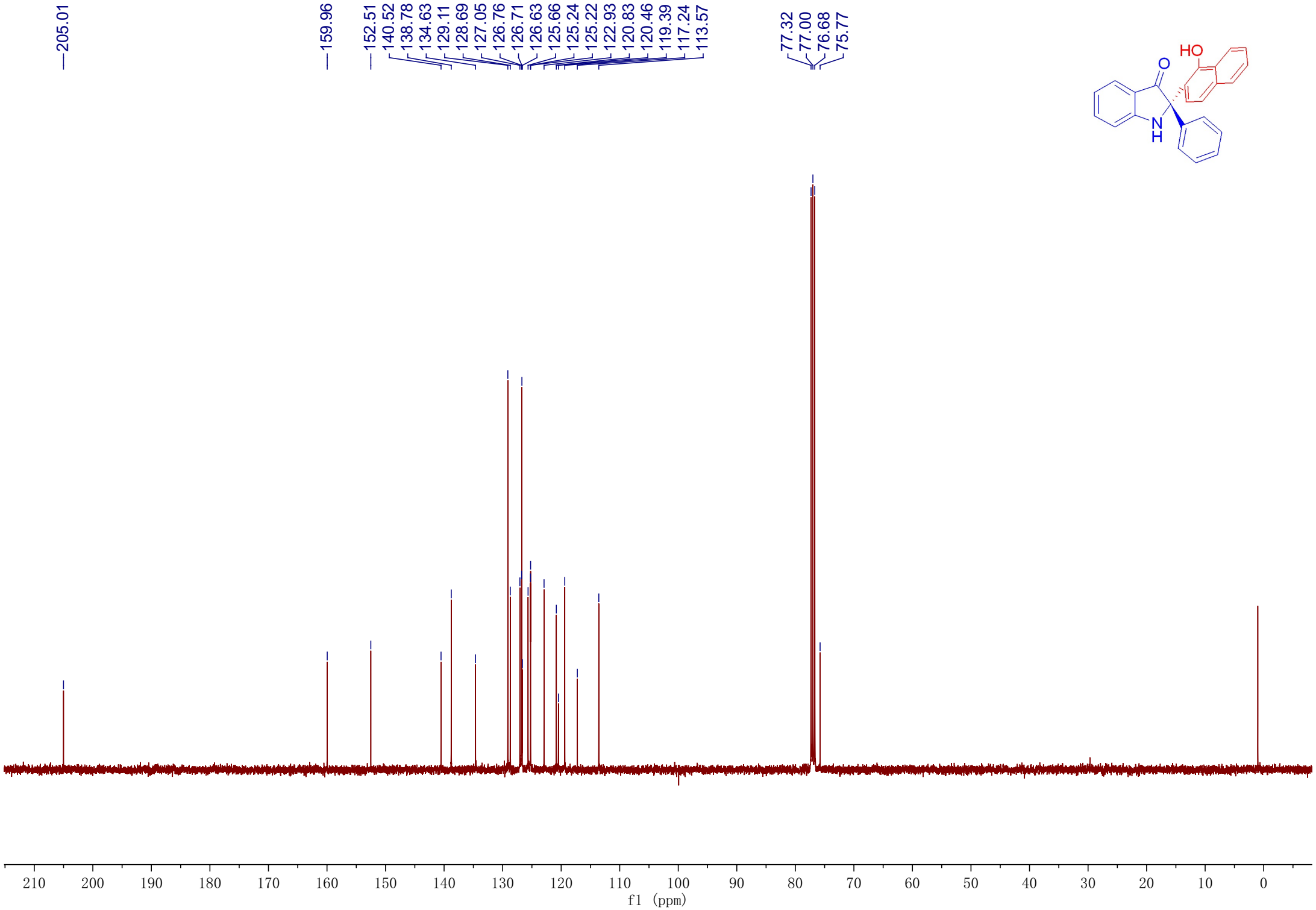
7. Copies of NMR spectra

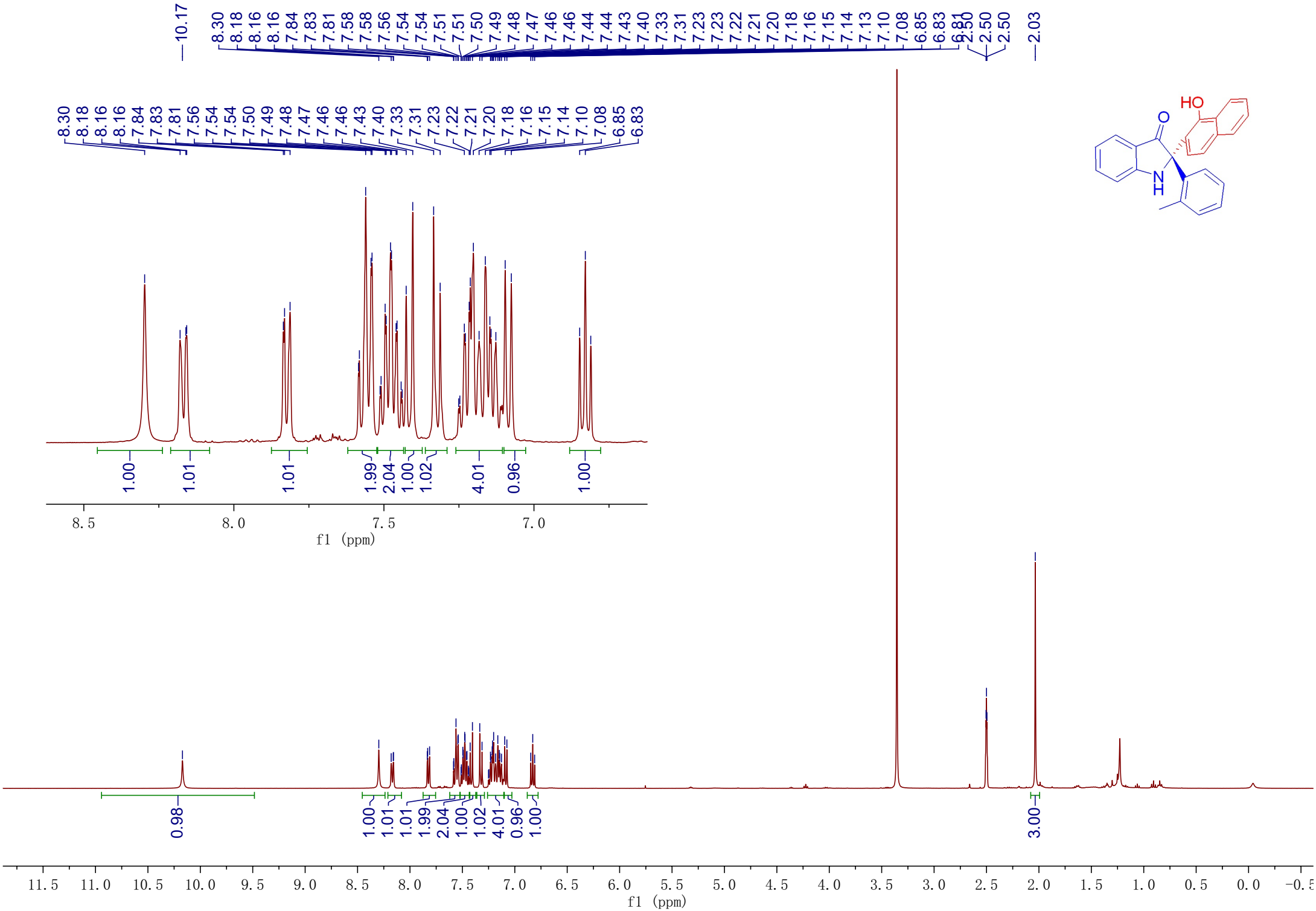

10.12
8.20
8.18
7.59
7.58
7.57
7.34
7.34
7.28
7.26
7.17
7.17
7.15
7.13
7.06
7.06
7.05
7.04
7.04
6.84
6.84
8.18
7.65
7.63
7.60
7.59
7.58
7.58
7.57
7.43
7.36
7.35
7.34
7.34
7.32
7.32
7.28
7.26
7.18
7.17
7.17
7.15
7.13
7.06
7.06
7.05
7.04
7.04
6.86
6.85
6.84
6.84

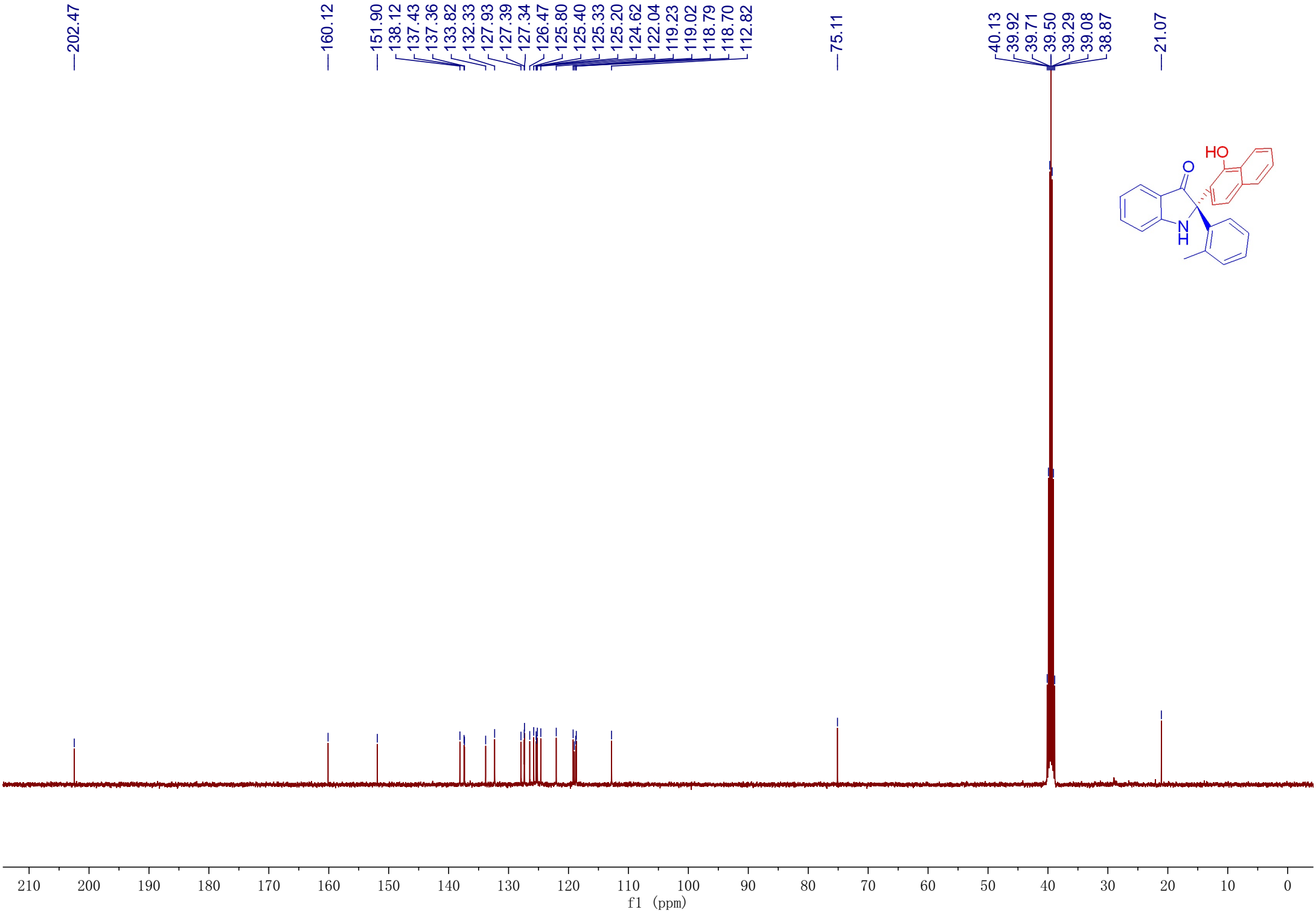

HO
O
N
H

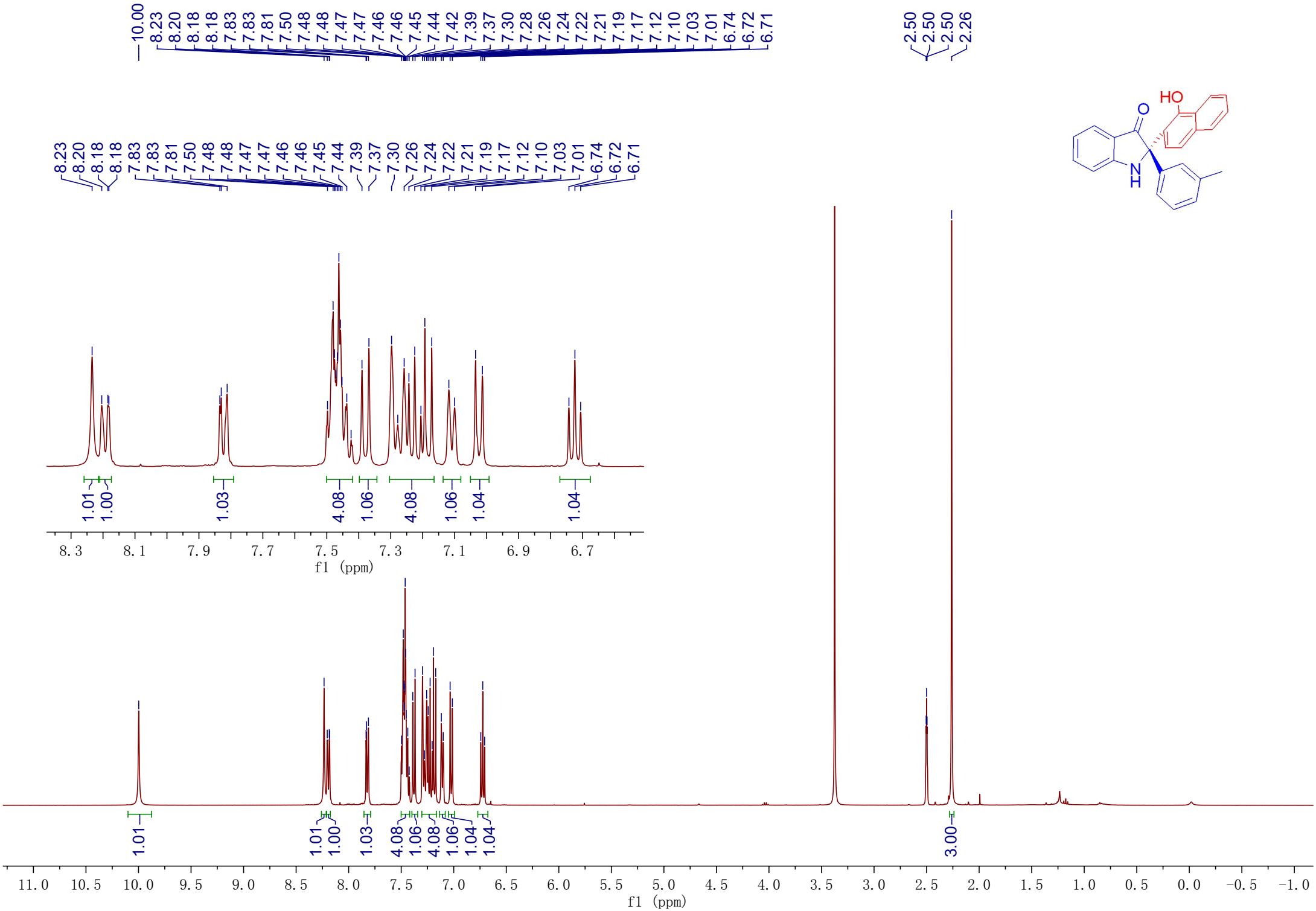

1.00
1.03
1.98
1.04
2.14
1.04
3.08
2.09
2.03
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)

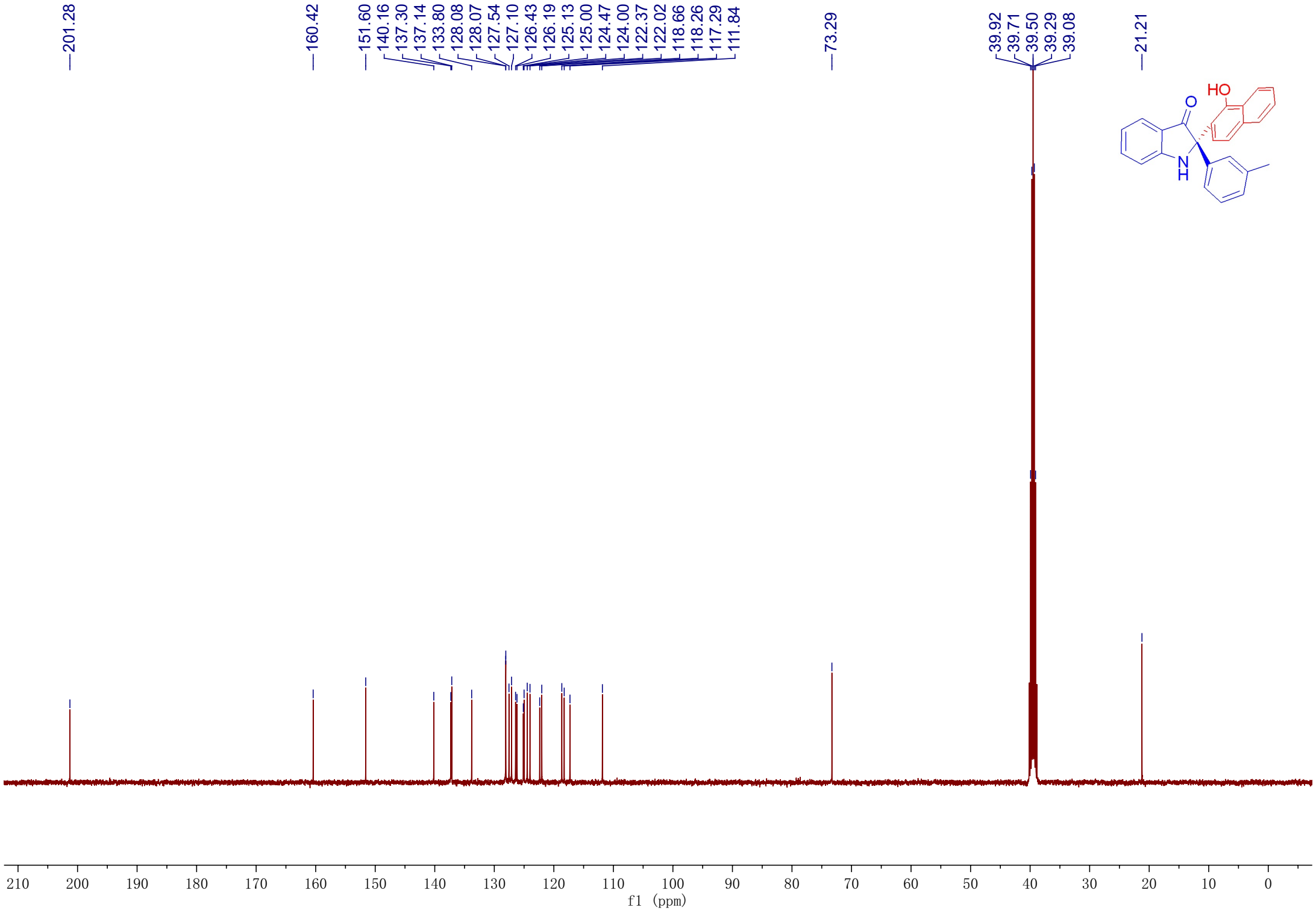

0.98
1.00
1.03
1.98
1.04
2.14
1.04
3.08
2.09
2.03
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

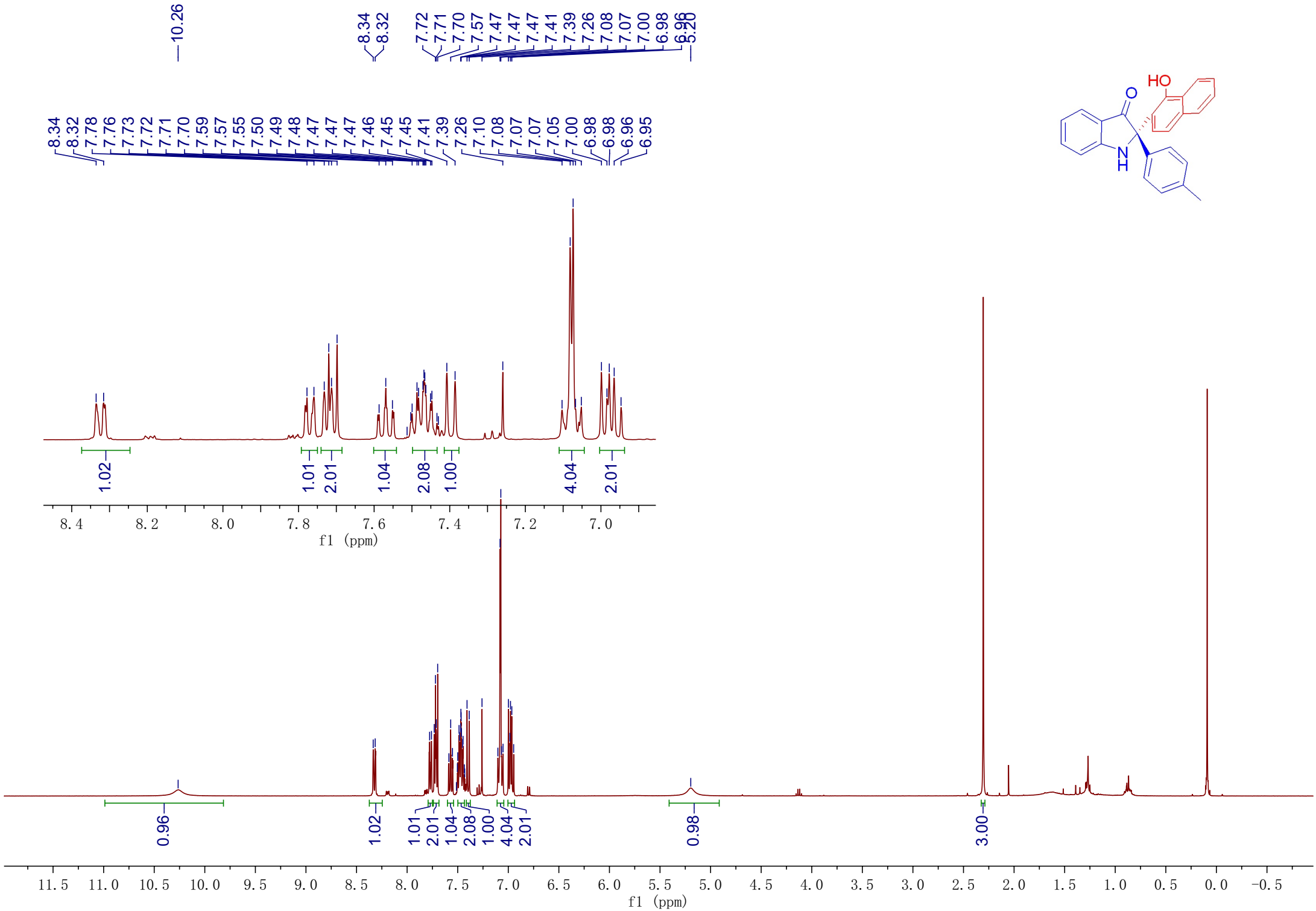

205.01
159.96
152.51
140.52
138.78
134.63
129.11
128.69
127.05
126.76
126.71
126.63
125.66
125.24
125.22
122.93
120.83
120.46
119.39
117.24
113.57
77.32
77.00
76.68
75.77
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

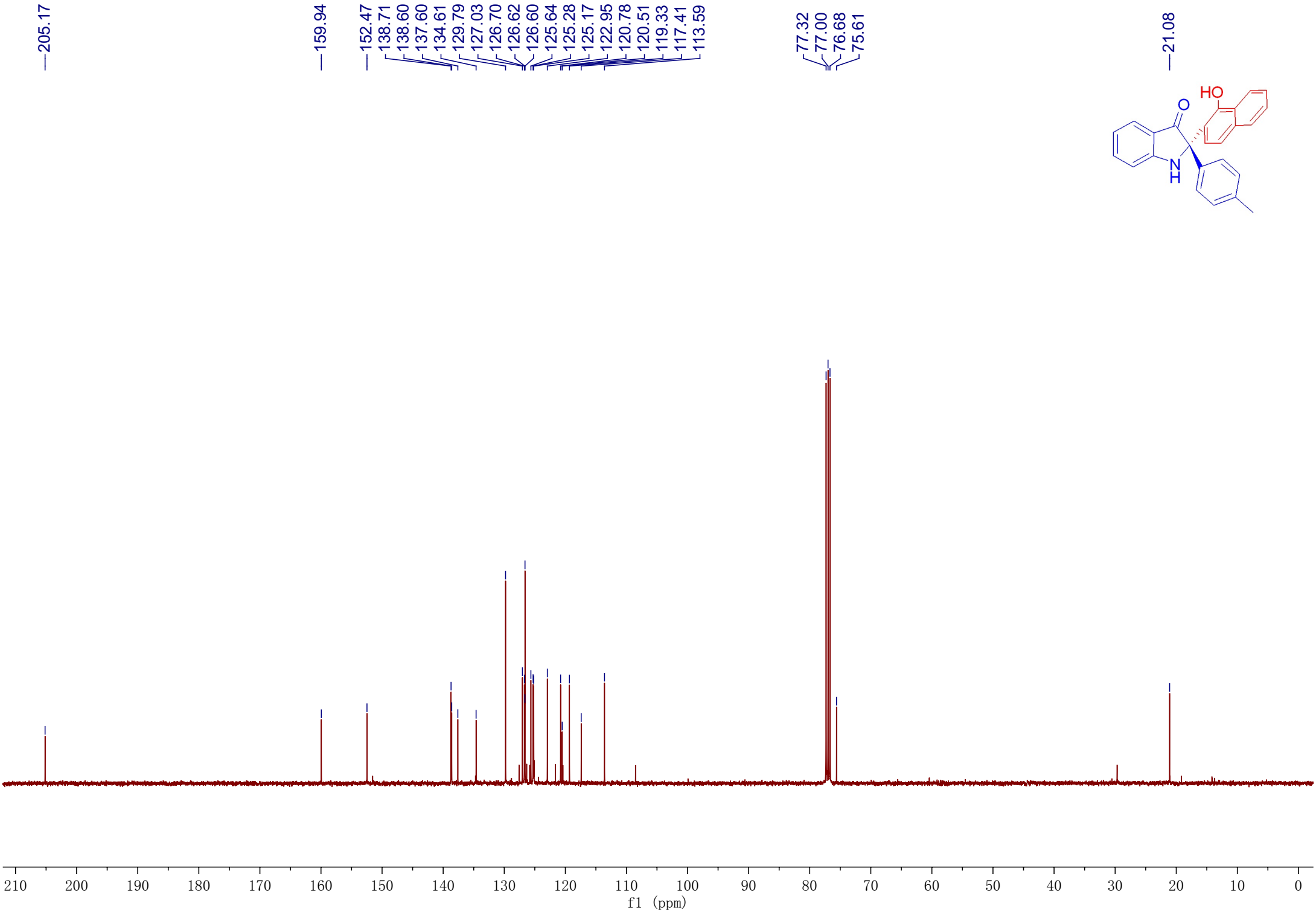

10.17
8.30
8.18
8.16
8.16
7.84
7.83
7.81
7.58
7.58
7.56
7.54
7.54
7.51
7.51
7.50
7.49
7.48
7.47
7.46
7.46
7.44
7.44
7.43
7.40
7.33
7.31
7.23
7.23
7.22
7.21
7.20
7.18
7.16
7.15
7.14
7.13
7.10
7.08
6.85
6.83
6.81
2.50
2.50
2.50
2.03
HO
O
N
H
1.00
1.01
1.01
1.99
2.04
1.00
1.02
4.01
0.96
1.00
8.5
8.0
7.5
7.0
f1 (ppm)
0.98
1.00
1.01
1.01
1.99
2.04
1.00
1.02
4.01
0.96
1.00
3.00
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

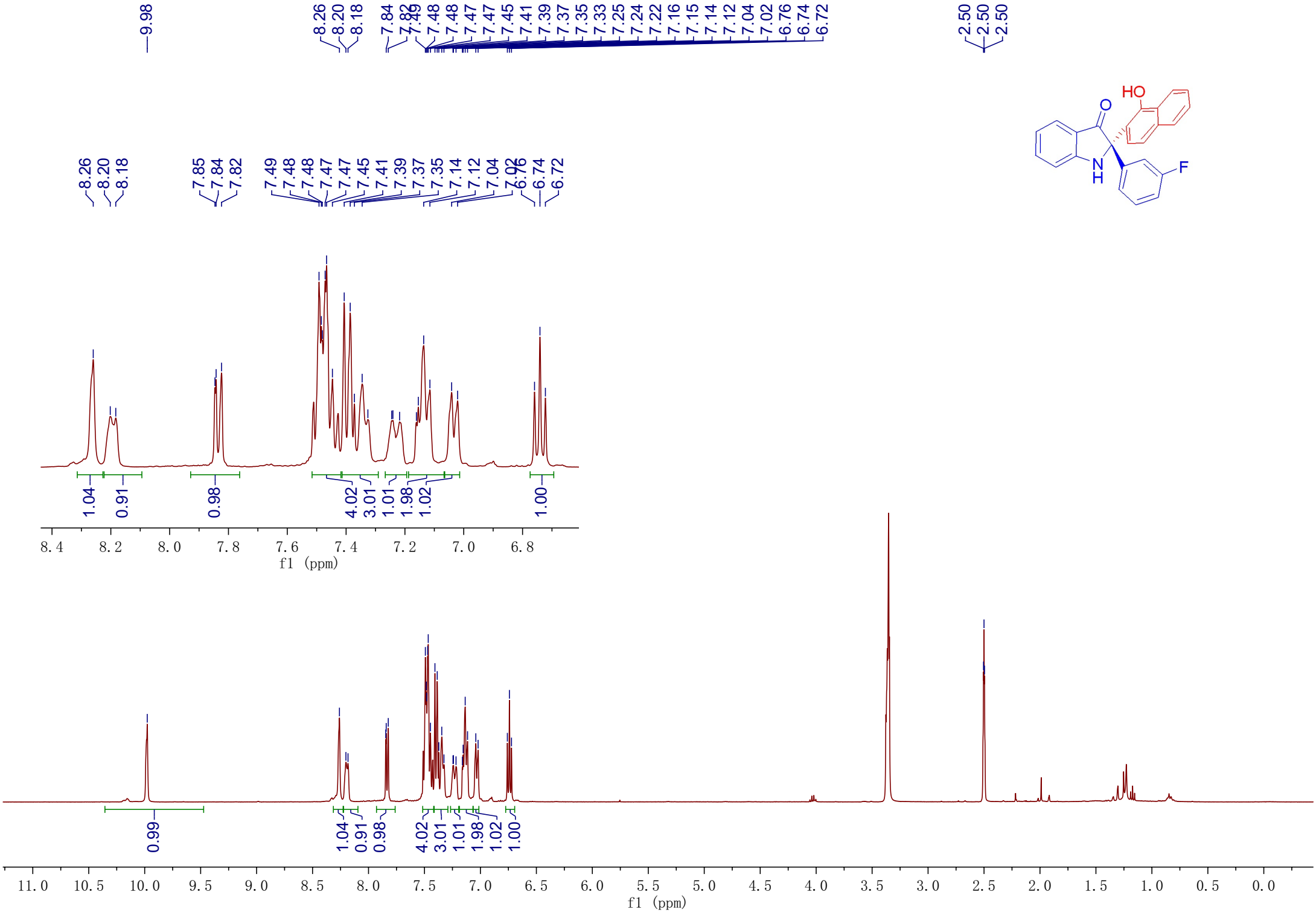

202.47
160.12
151.90
138.12
137.43
137.36
133.82
132.33
127.93
127.39
127.34
126.47
125.80
125.40
125.33
125.20
124.62
122.04
119.23
119.02
118.79
118.70
112.82
75.11
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.07
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

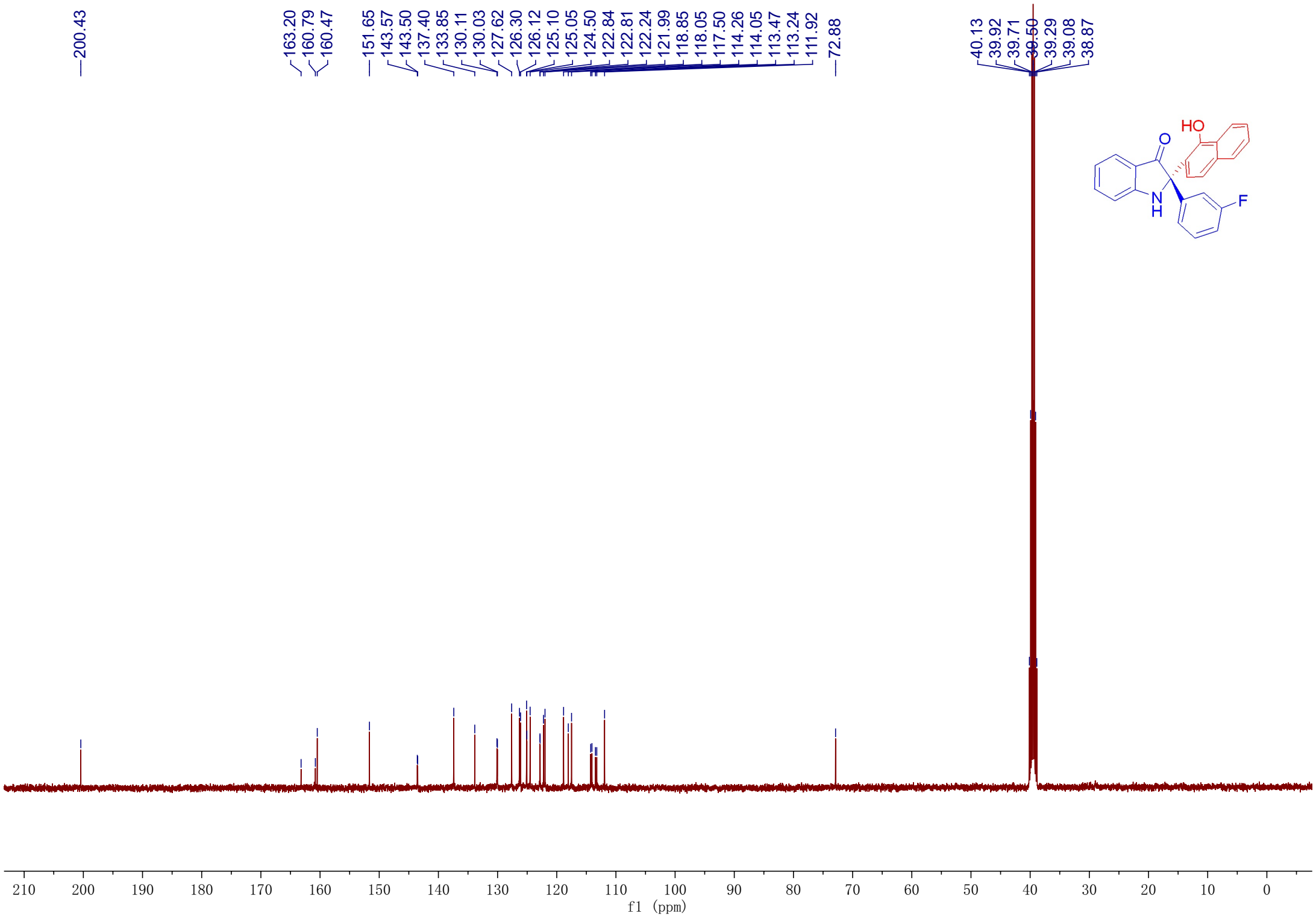

10.00
8.23
8.20
8.18
8.18
7.83
7.83
7.81
7.50
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.42
7.39
7.37
7.30
7.28
7.26
7.24
7.22
7.21
7.19
7.17
7.12
7.10
7.03
7.01
6.74
6.72
6.71
2.50
2.50
2.50
2.26
HO
O
NH
1.01
1.00
1.03
4.08
1.06
4.08
1.06
1.04
1.04
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
1.01
1.01
1.00
1.03
4.08
1.06
4.08
1.06
1.04
1.04
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

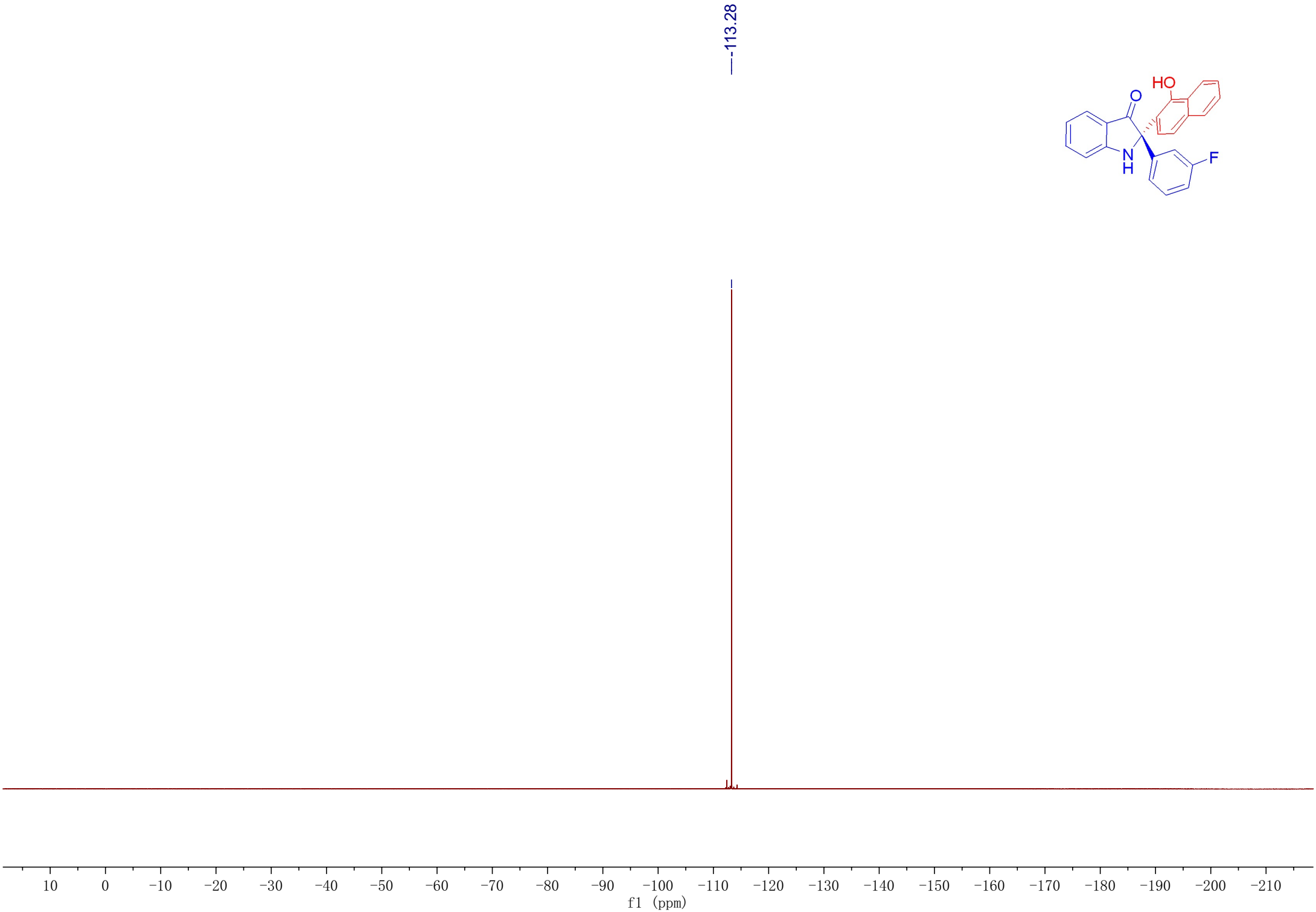

201.28
160.42
151.60
140.16
137.30
137.14
133.80
128.08
128.07
127.54
127.10
126.43
126.19
125.13
125.00
124.47
124.00
122.37
122.02
118.66
118.26
117.29
111.84
73.29
39.92
39.71
39.50
39.29
39.08
21.21
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

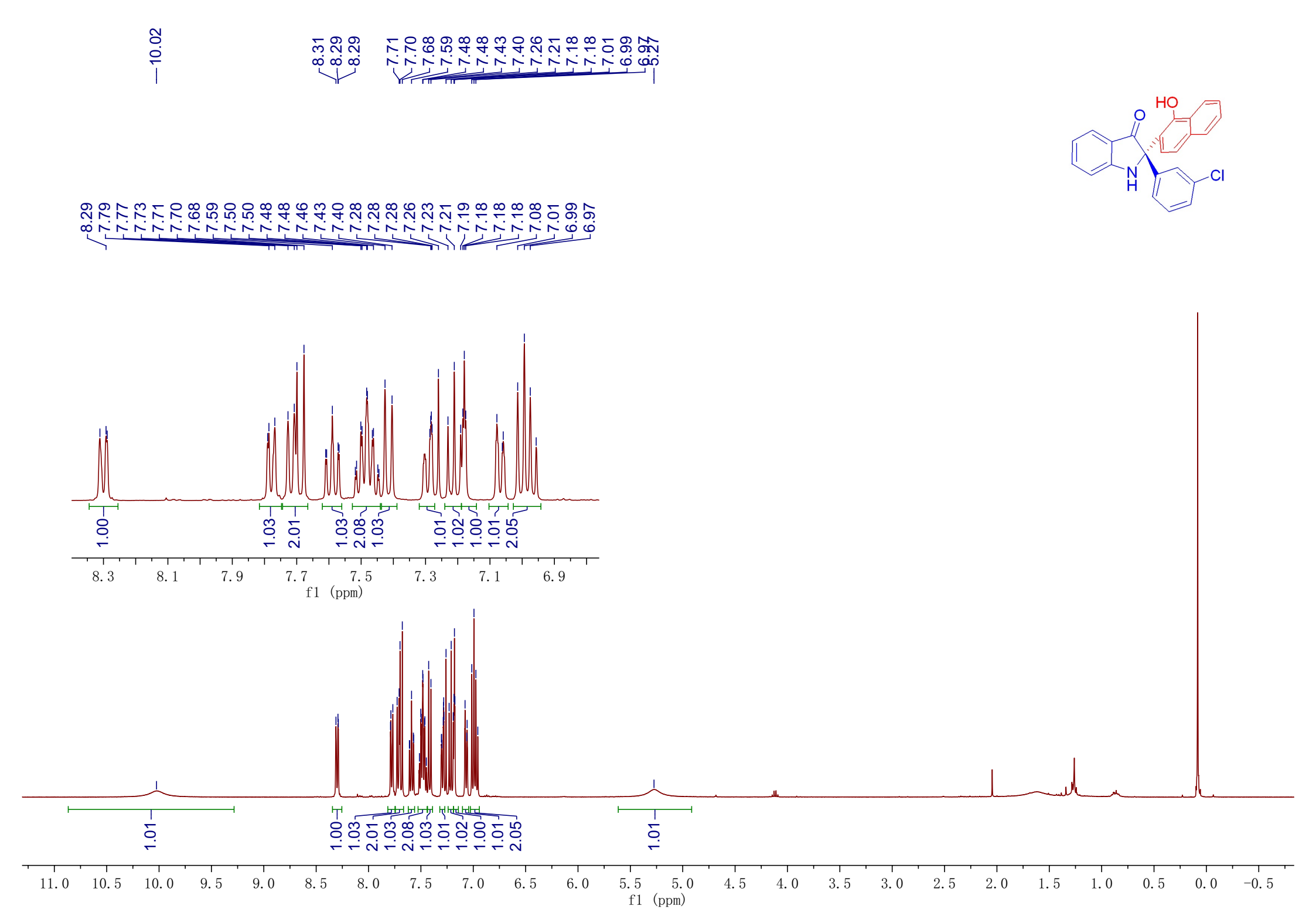

10.26
8.34
8.32
7.72
7.71
7.70
7.57
7.47
7.47
7.47
7.41
7.39
7.26
7.08
7.07
7.00
6.98
6.96
5.20
HO
O
N
H
f1 (ppm)
f1 (ppm)

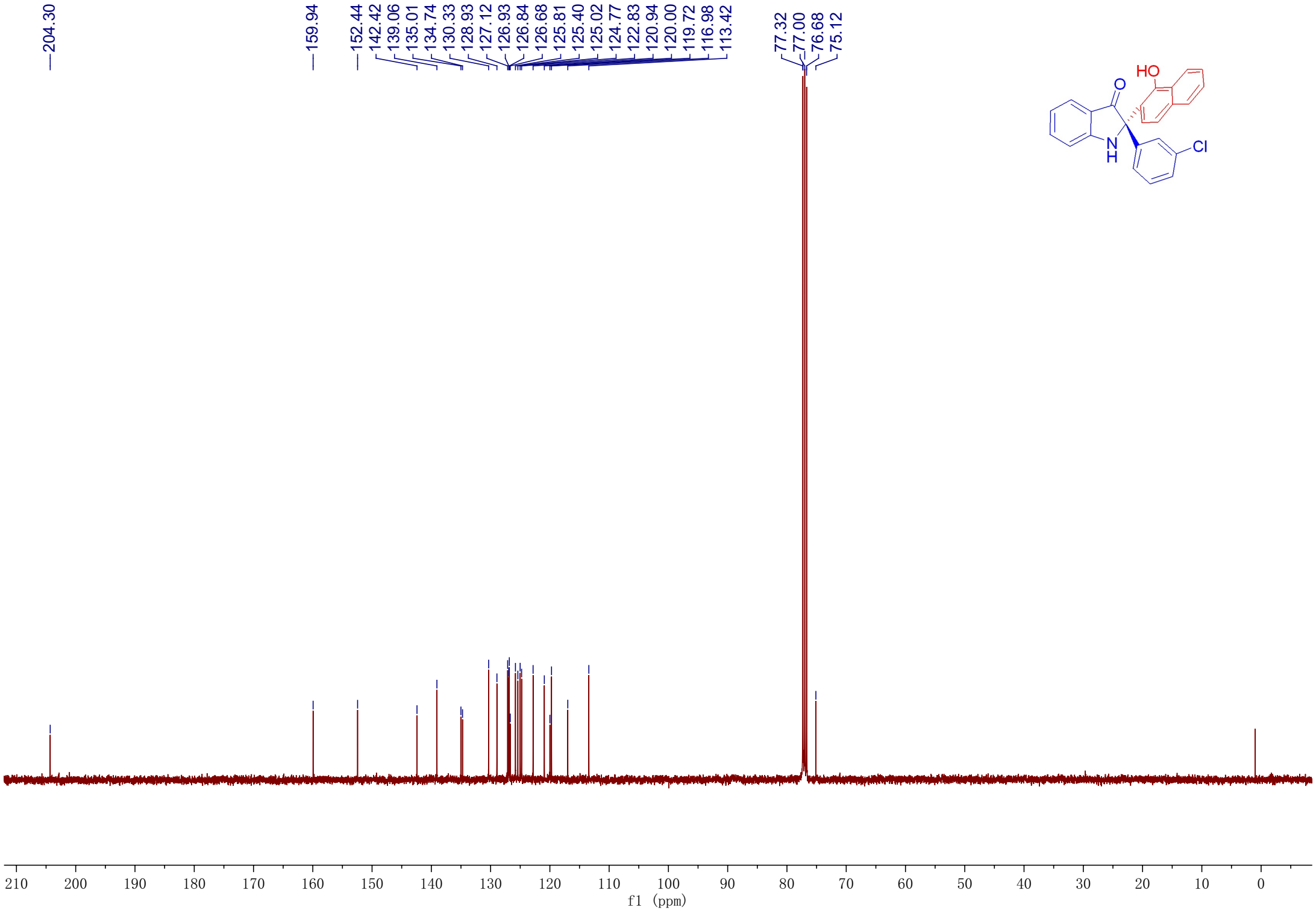

205.17
159.94
152.47
138.71
138.60
137.60
134.61
129.79
127.03
126.70
126.62
126.60
125.64
125.28
125.17
122.95
120.78
120.51
119.33
117.41
113.59
77.32
77.00
76.68
75.61
21.08
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

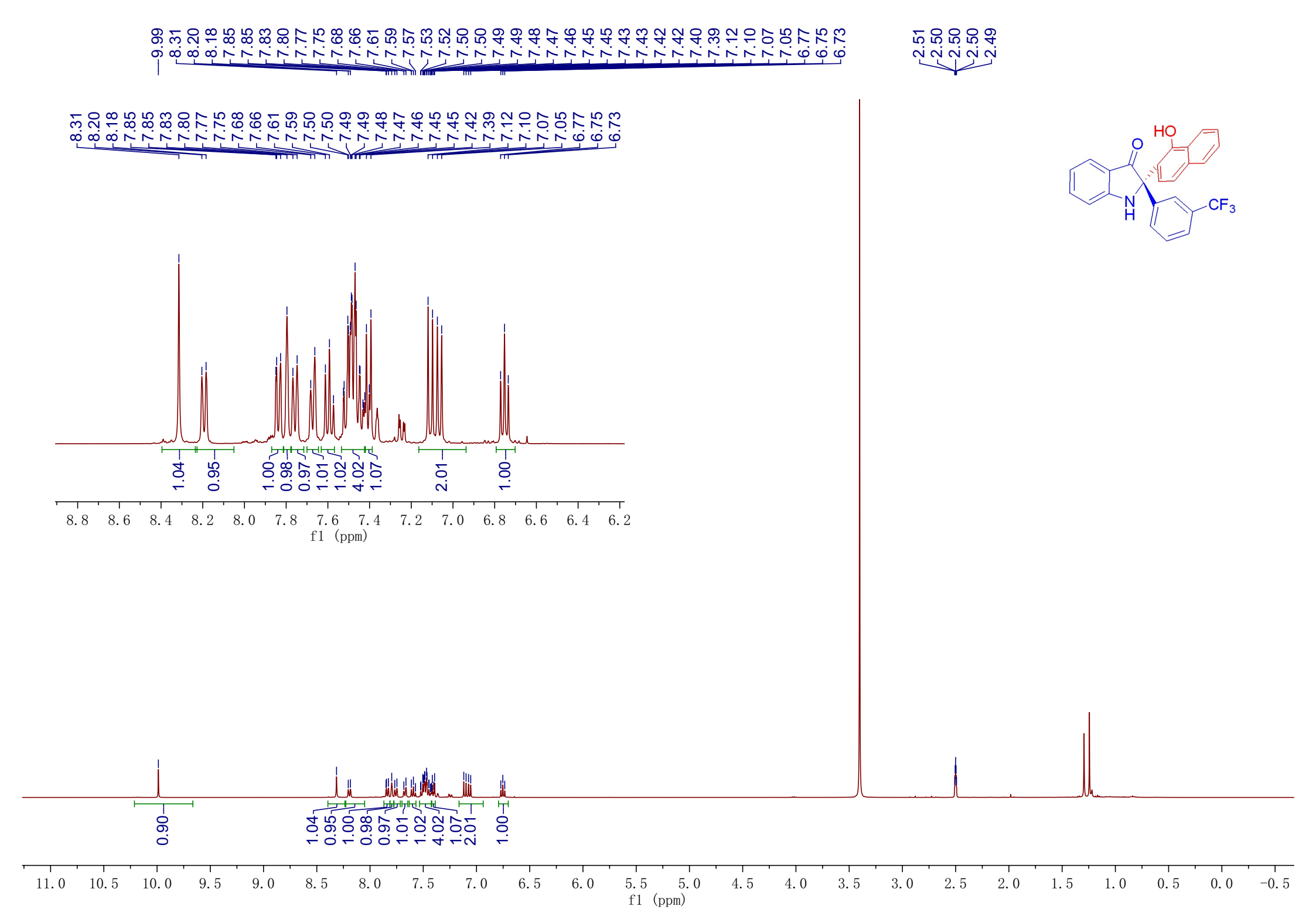

9.98
8.26
8.20
8.18
7.84
7.82
7.49
7.48
7.48
7.47
7.47
7.45
7.41
7.39
7.37
7.35
7.33
7.25
7.24
7.22
7.16
7.15
7.14
7.12
7.04
7.02
6.76
6.74
6.72
2.50
2.50
2.50
HO
O
N
H
F
1.04
0.91
0.98
4.02
3.01
1.01
1.98
1.02
1.00
f1 (ppm)
0.99
f1 (ppm)

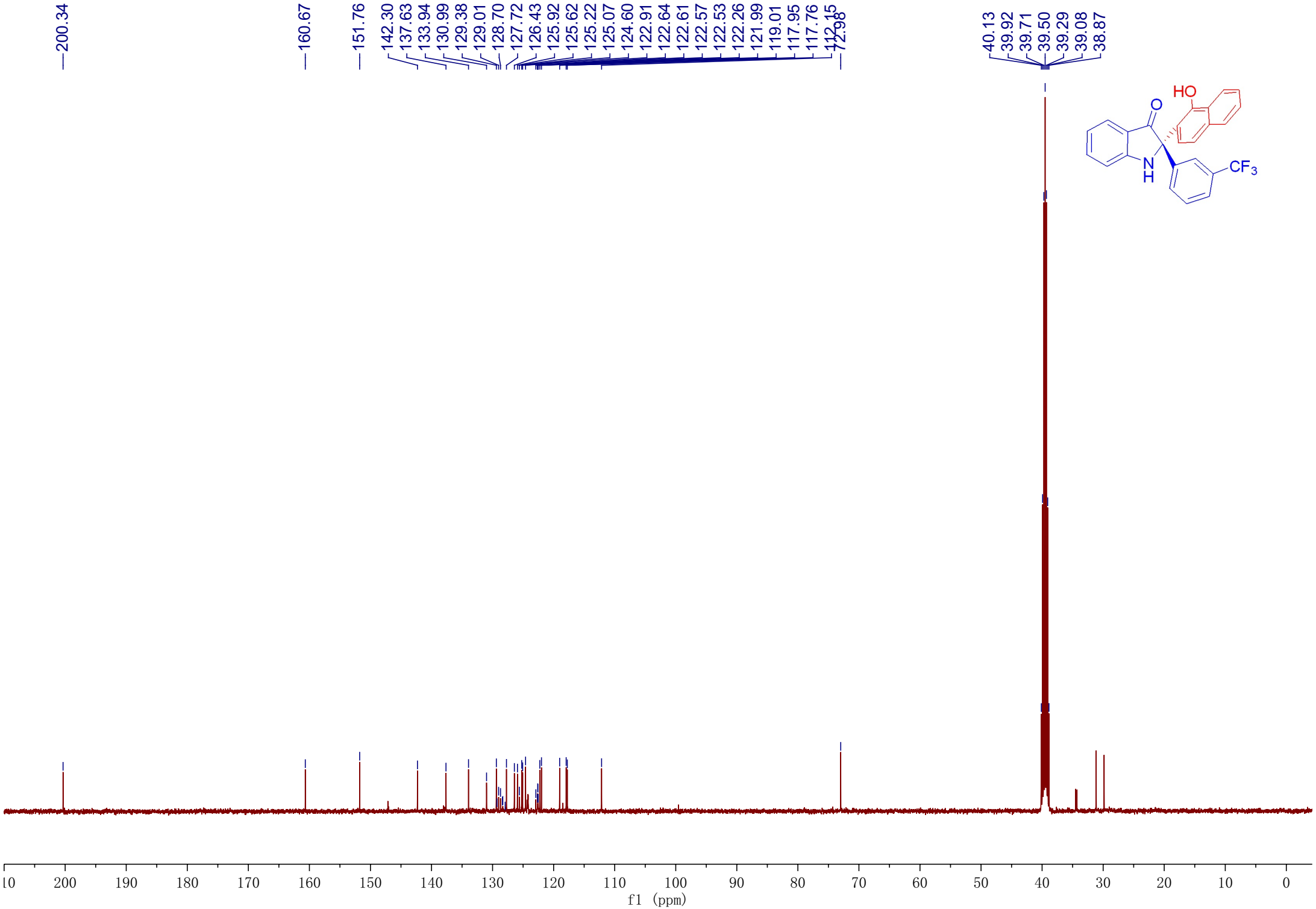

200.43
163.20
160.79
160.47
151.65
143.57
143.50
137.40
133.85
130.11
130.03
127.62
126.30
126.12
125.10
125.05
124.50
122.84
122.81
122.24
121.99
118.85
118.05
117.50
114.26
114.05
113.47
113.24
111.92
72.88
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
N
H
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

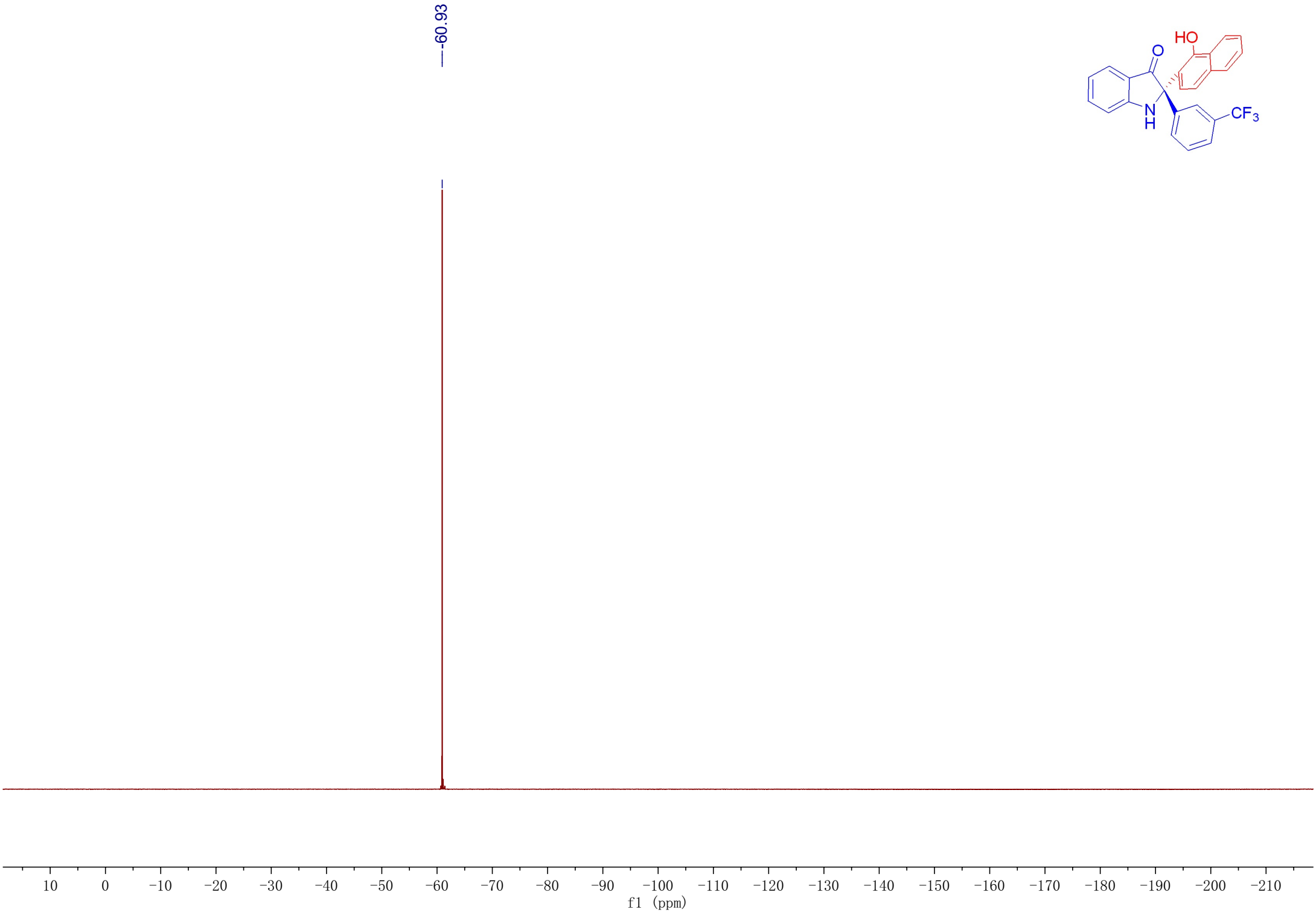

-113.28
HO
O
N
H
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

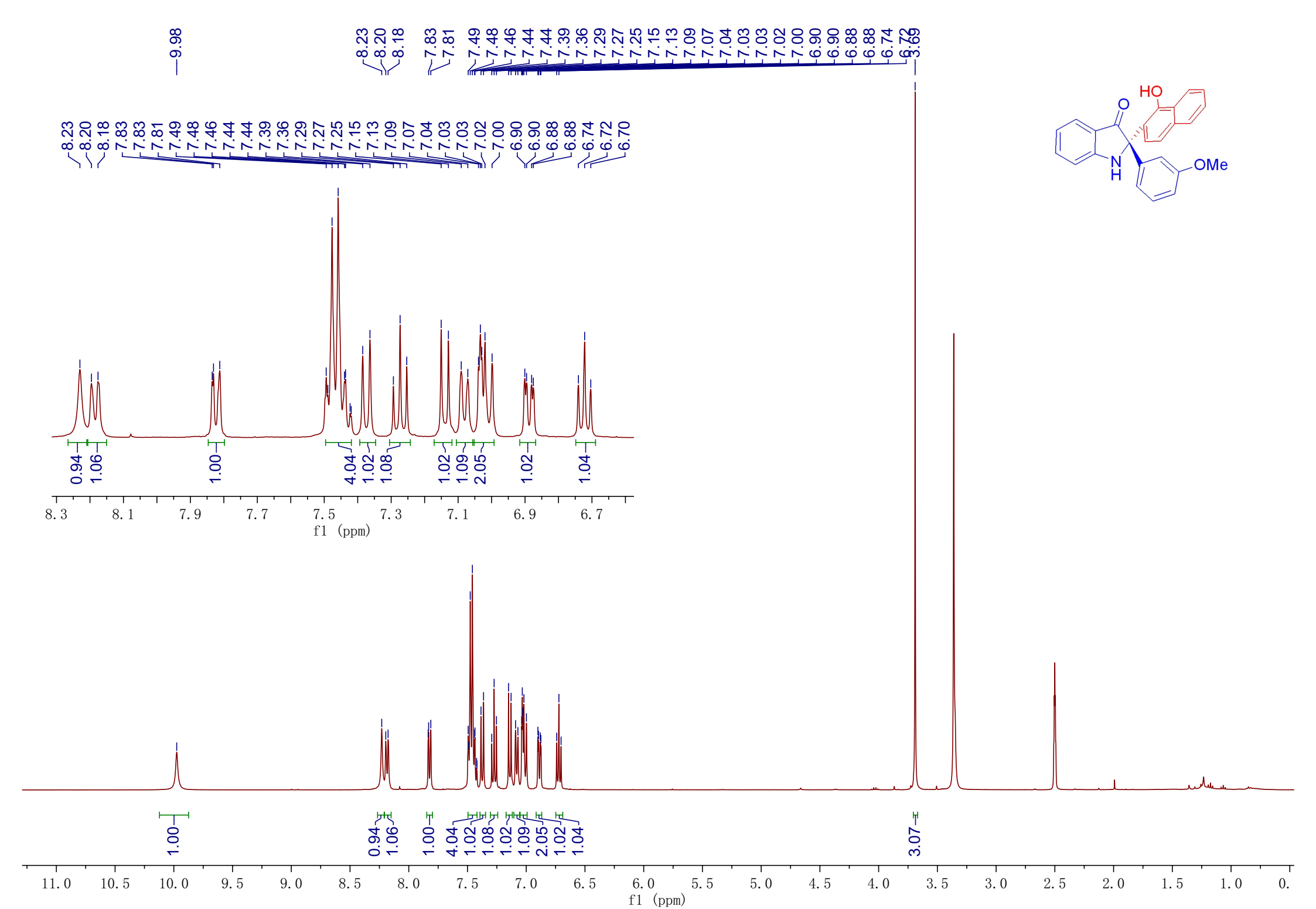

10.02
8.31
8.29
8.29
7.71
7.70
7.68
7.59
7.48
7.48
7.43
7.40
7.26
7.21
7.18
7.18
7.01
6.99
6.97
6.97
8.29
7.79
7.77
7.73
7.71
7.70
7.68
7.59
7.50
7.50
7.48
7.48
7.46
7.43
7.40
7.28
7.28
7.28
7.26
7.23
7.21
7.19
7.18
7.18
7.18
7.08
7.01
6.99
6.97
HO
O
N
H
Cl
1.00
1.03
2.01
1.03
2.08
1.03
1.01
1.02
1.00
1.01
2.05
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
f1 (ppm)
1.01
1.00
1.03
2.01
1.03
2.08
1.03
1.01
1.02
1.00
1.01
2.05
1.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

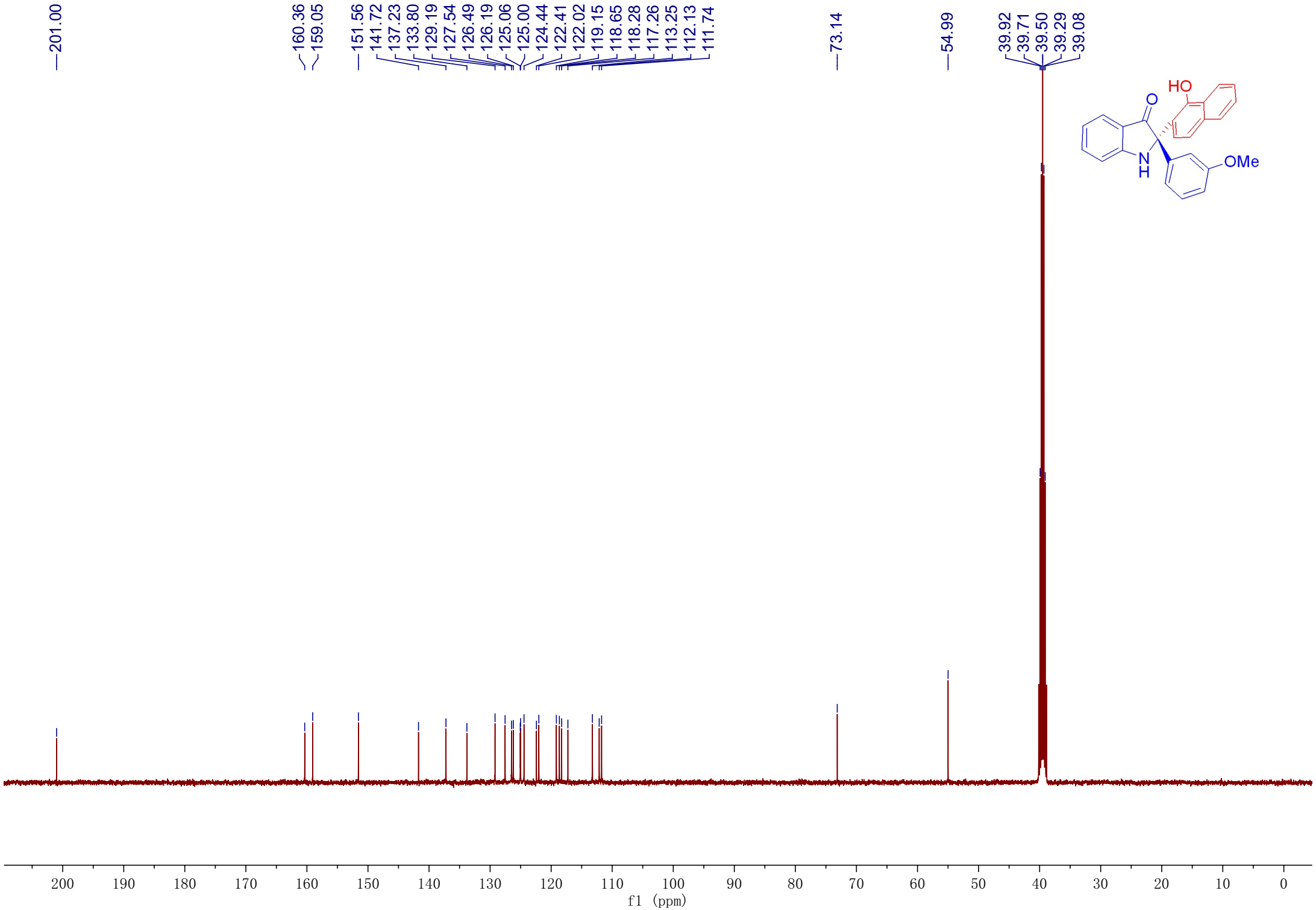

204.30
159.94
152.44
142.42
139.06
135.01
134.74
130.33
128.93
127.12
126.93
126.84
126.68
125.81
125.40
125.02
124.77
122.83
120.94
120.00
119.72
116.98
113.42
77.32
77.00
76.68
75.12
HO
O
N
H
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

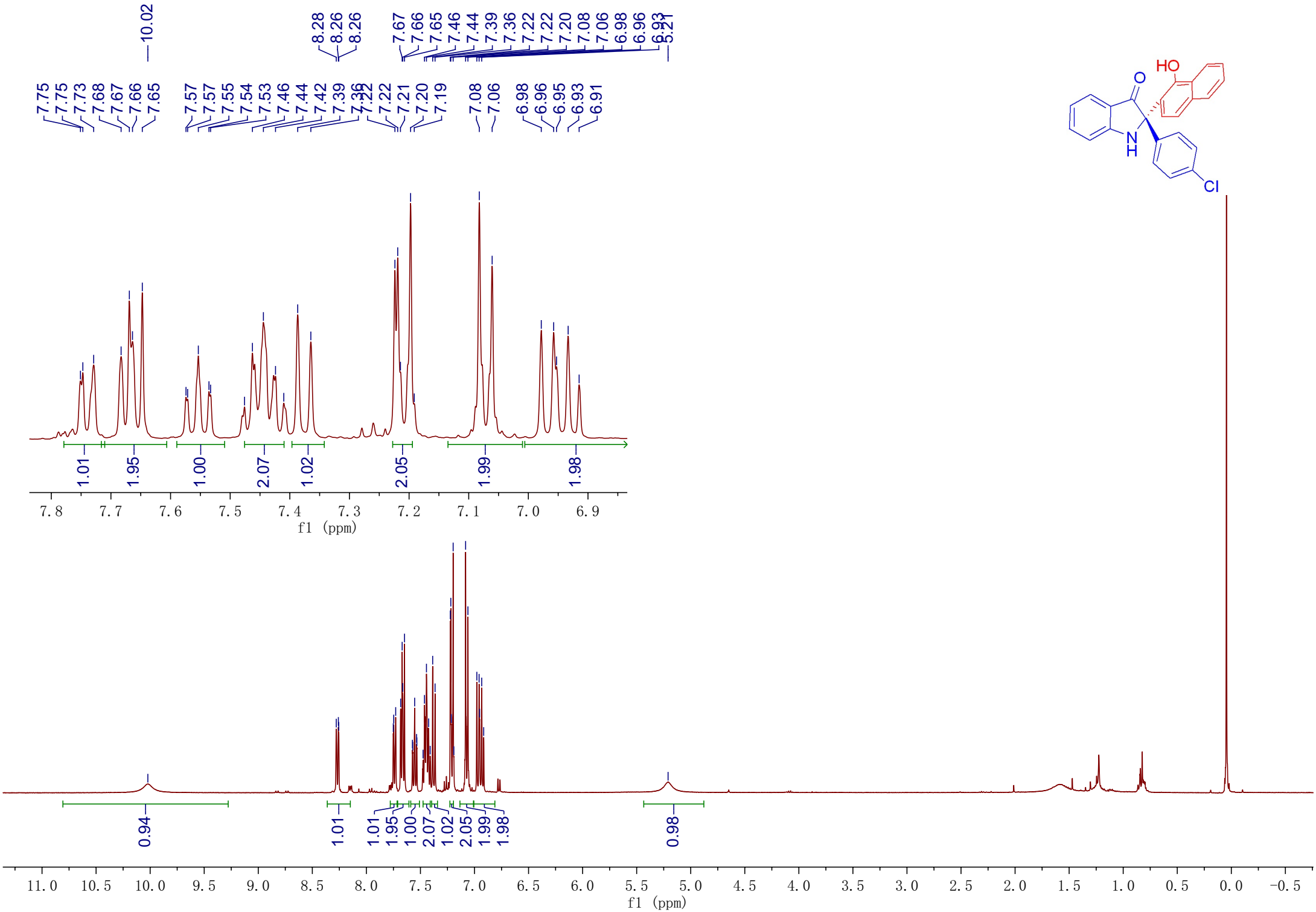

9.99
8.31
8.20
8.18
7.85
7.85
7.83
7.80
7.77
7.75
7.68
7.66
7.61
7.59
7.57
7.53
7.52
7.50
7.50
7.49
7.49
7.48
7.47
7.46
7.45
7.45
7.43
7.43
7.42
7.42
7.40
7.39
7.12
7.10
7.07
7.05
6.77
6.75
6.73
2.51
2.50
2.50
2.50
2.49
HO
O
N
H
CF3
1.04
0.95
1.00
0.98
0.97
1.01
1.02
4.02
1.07
2.01
1.00
f1 (ppm)
0.90
f1 (ppm)

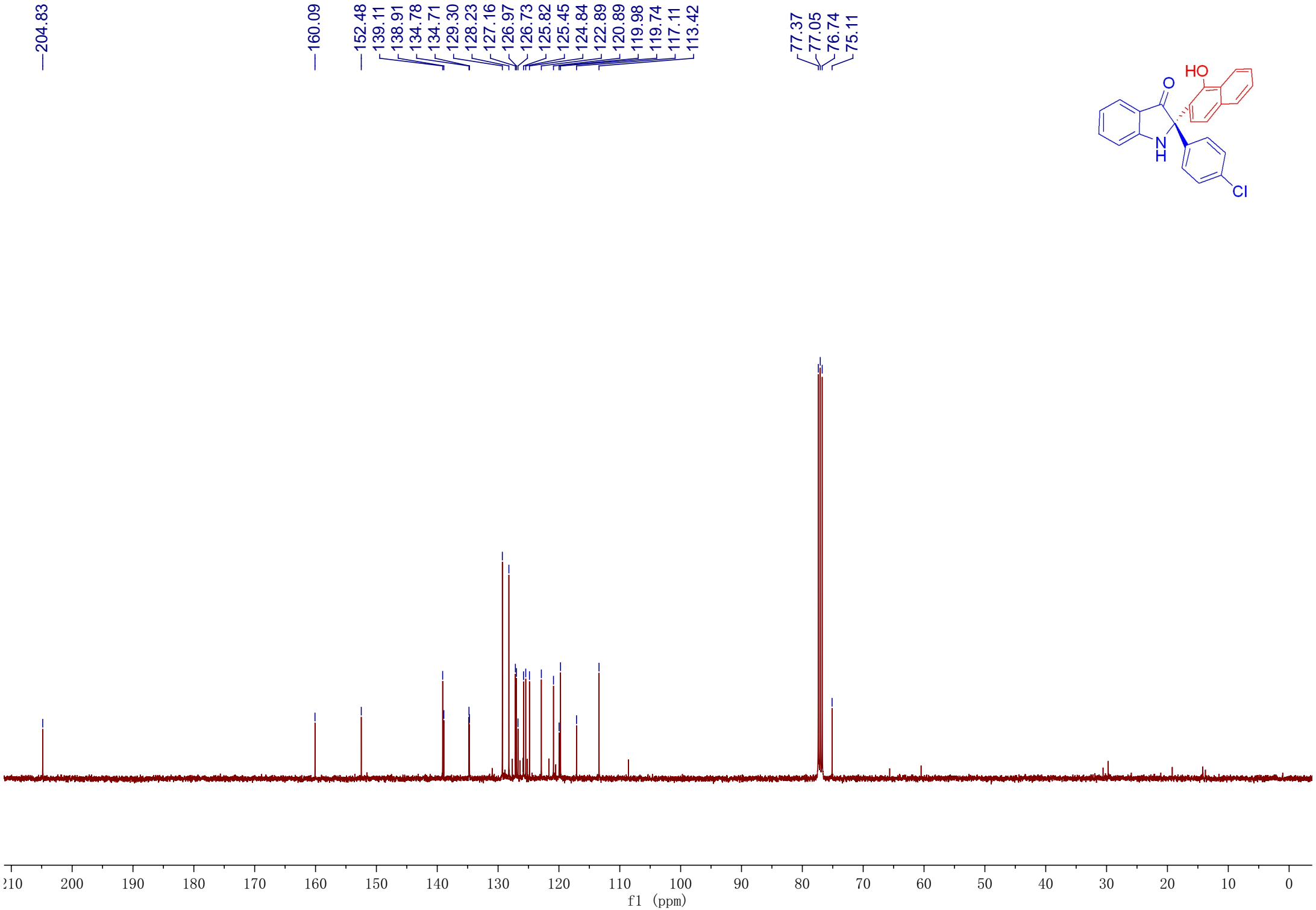

200.34
160.67
151.76
142.30
137.63
133.94
130.99
129.38
129.01
128.70
127.72
126.43
125.92
125.62
125.22
125.07
124.60
122.91
122.64
122.61
122.57
122.53
122.26
121.99
119.01
117.95
117.76
112.15
77.98
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
N
H
CF3
f1 (ppm)

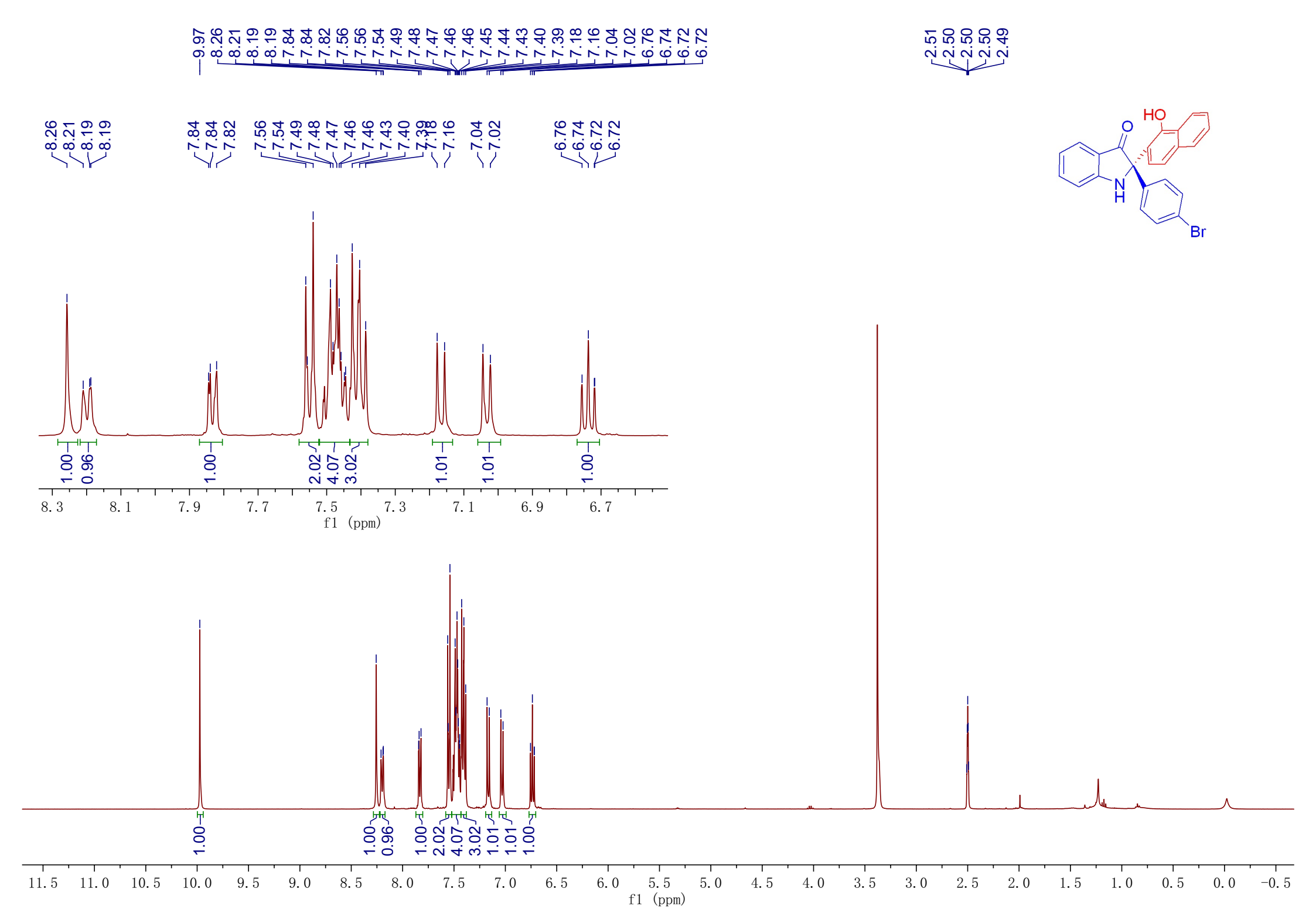

-60.93
HO
O
N
H
CF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

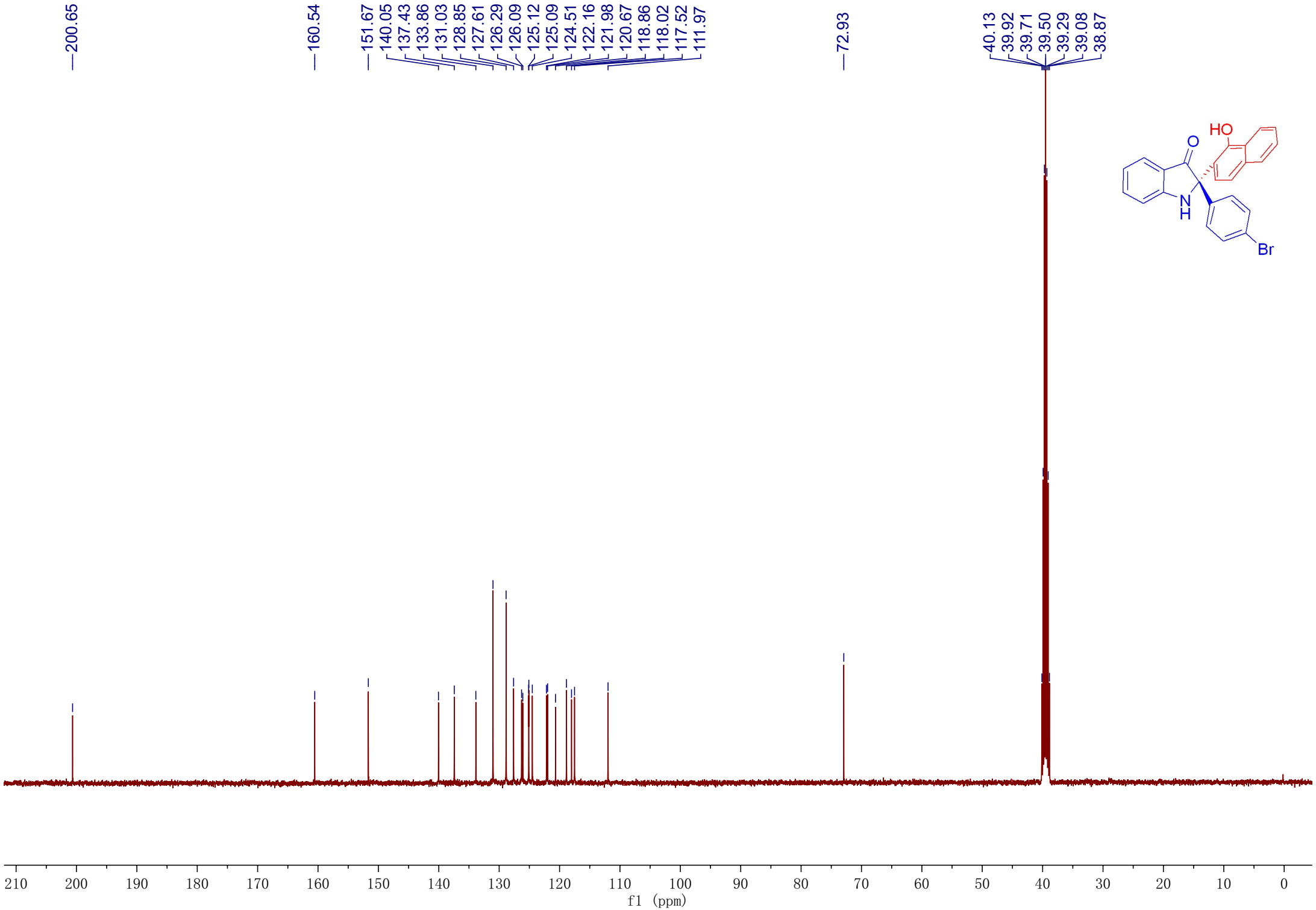

9.98
8.23
8.20
8.18
7.83
7.81
7.49
7.48
7.46
7.44
7.44
7.39
7.36
7.29
7.27
7.25
7.15
7.13
7.09
7.07
7.04
7.03
7.03
7.02
7.00
6.90
6.90
6.88
6.88
6.74
6.72
6.70
3.69
HO
O
N
H
OMe
0.94
1.06
1.00
4.04
1.02
1.08
1.02
1.09
2.05
1.02
1.04
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
1.00
0.94
1.06
1.00
4.04
1.02
1.08
1.02
1.09
2.05
1.02
1.04
3.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.
f1 (ppm)

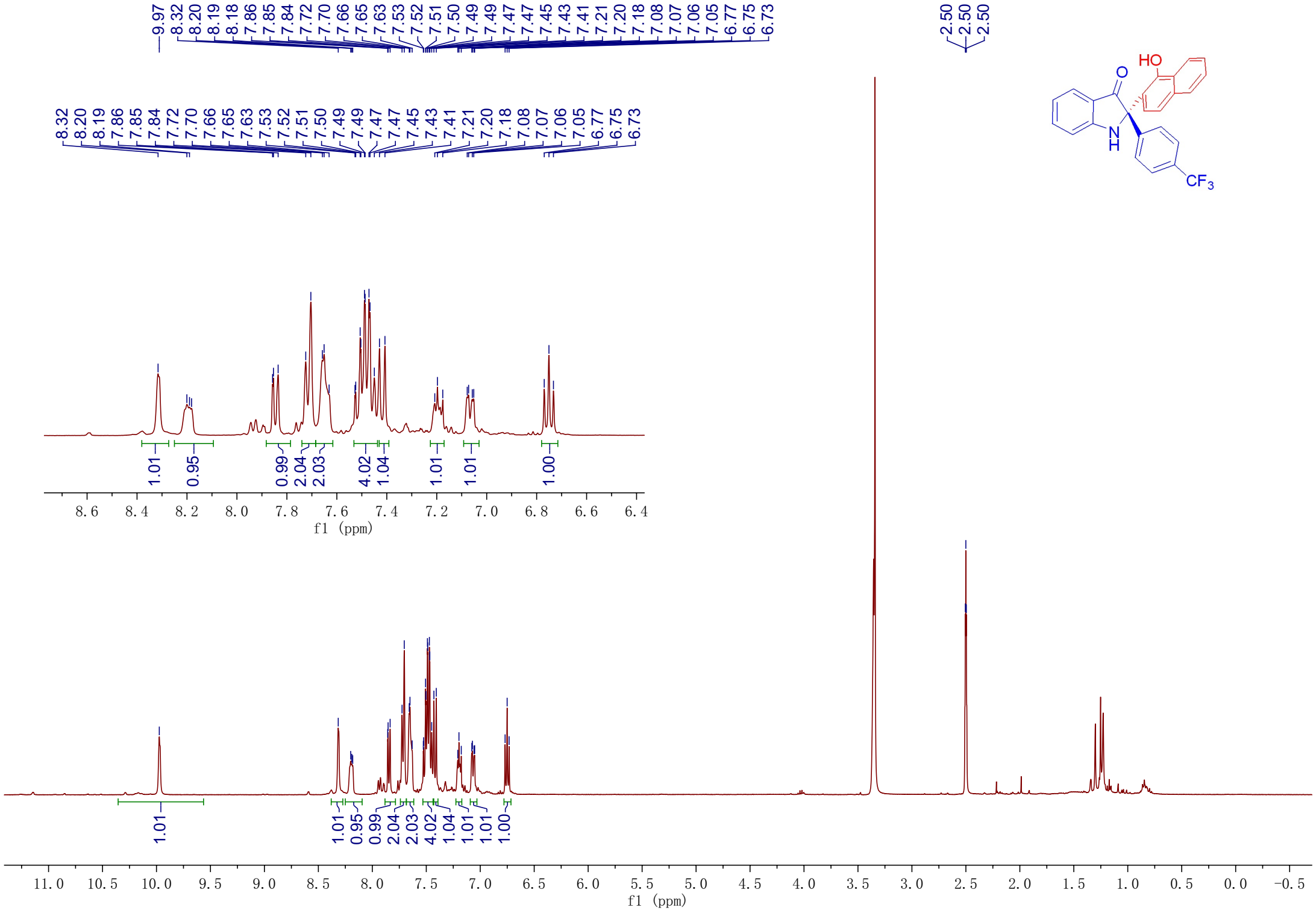

201.00
160.36
159.05
151.56
141.72
137.23
133.80
129.19
127.54
126.49
126.19
125.06
125.00
124.44
122.41
122.02
119.15
118.65
118.28
117.26
113.25
112.13
111.74
73.14
54.99
39.92
39.71
39.50
39.29
39.08
HO
O
N
H
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

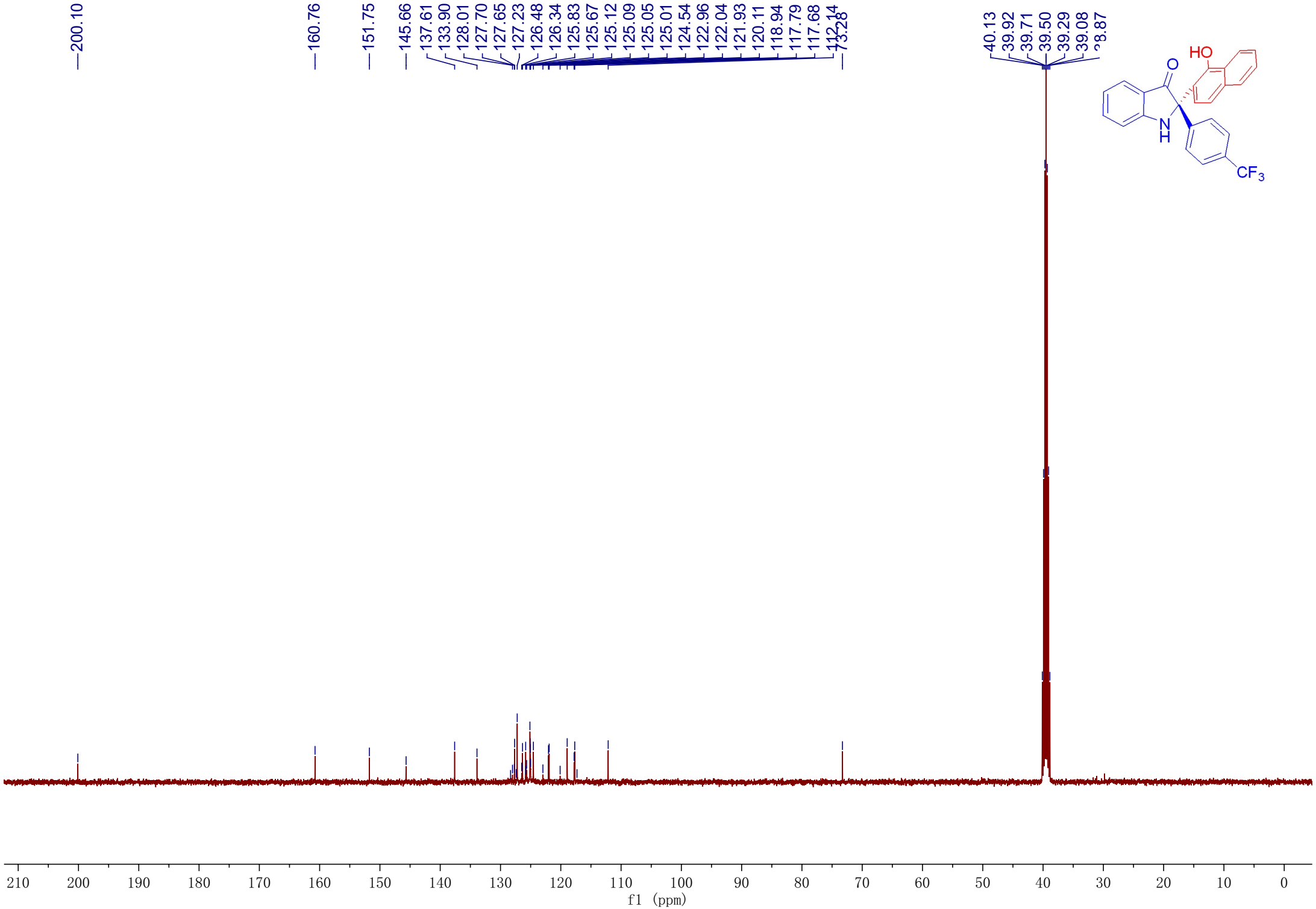

10.02
8.28
8.26
8.26
7.67
7.66
7.65
7.46
7.44
7.39
7.36
7.22
7.22
7.20
7.08
7.06
6.98
6.96
6.93
5.21
7.75
7.75
7.73
7.68
7.67
7.66
7.65
7.57
7.57
7.55
7.54
7.53
7.46
7.44
7.42
7.39
7.36
7.22
7.21
7.20
7.19
7.08
7.06
6.98
6.96
6.95
6.93
6.91
HO
O
N
H
Cl
1.01
1.95
1.00
2.07
1.02
2.05
1.99
1.98
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
0.94
1.01
1.01
1.95
1.00
2.07
1.02
2.05
1.99
1.98
0.98
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

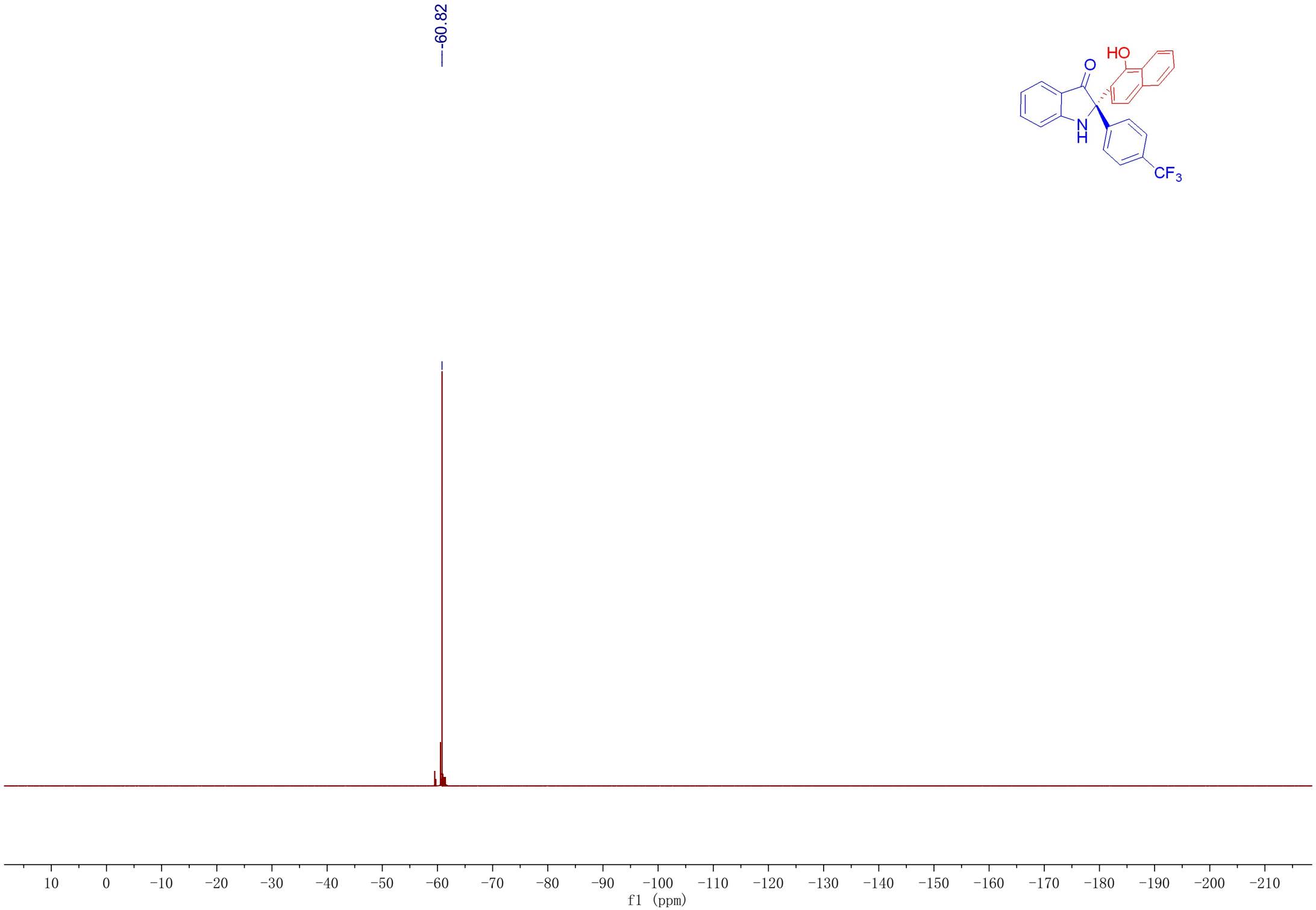

204.83
160.09
152.48
139.11
138.91
134.78
134.71
129.30
128.23
127.16
126.97
126.73
125.82
125.45
124.84
122.89
120.89
119.98
119.74
117.11
113.42
77.37
77.05
76.74
75.11
HO
O
N
H
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

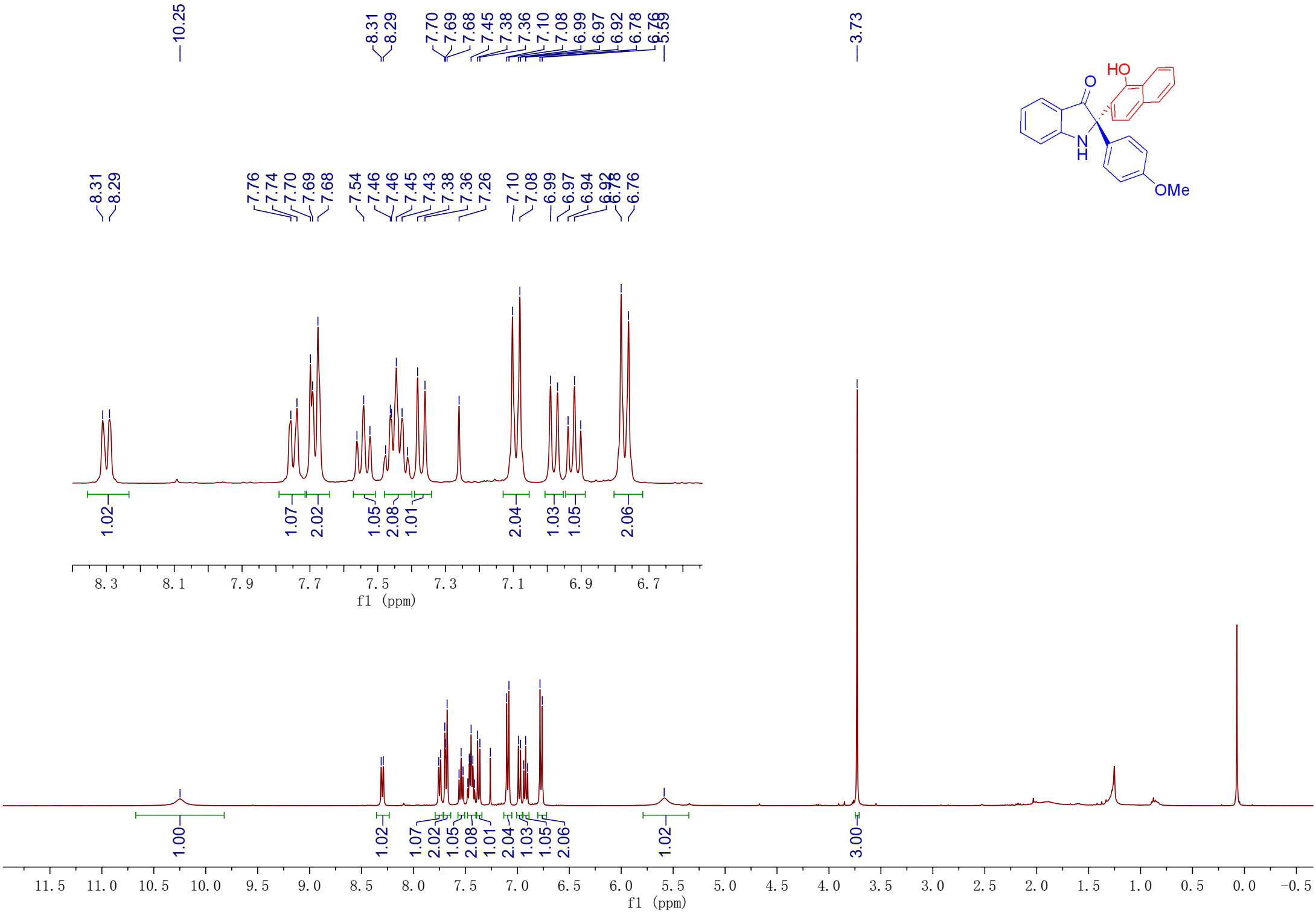

9.97
8.26
8.21
8.19
8.19
7.84
7.84
7.82
7.56
7.56
7.54
7.49
7.48
7.47
7.46
7.46
7.45
7.44
7.43
7.40
7.39
7.18
7.16
7.04
7.02
6.76
6.74
6.72
6.72
2.51
2.50
2.50
2.50
2.49
HO
O
N
H
Br
1.00
0.96
1.00
2.02
4.07
3.02
1.01
1.01
1.00
f1 (ppm)

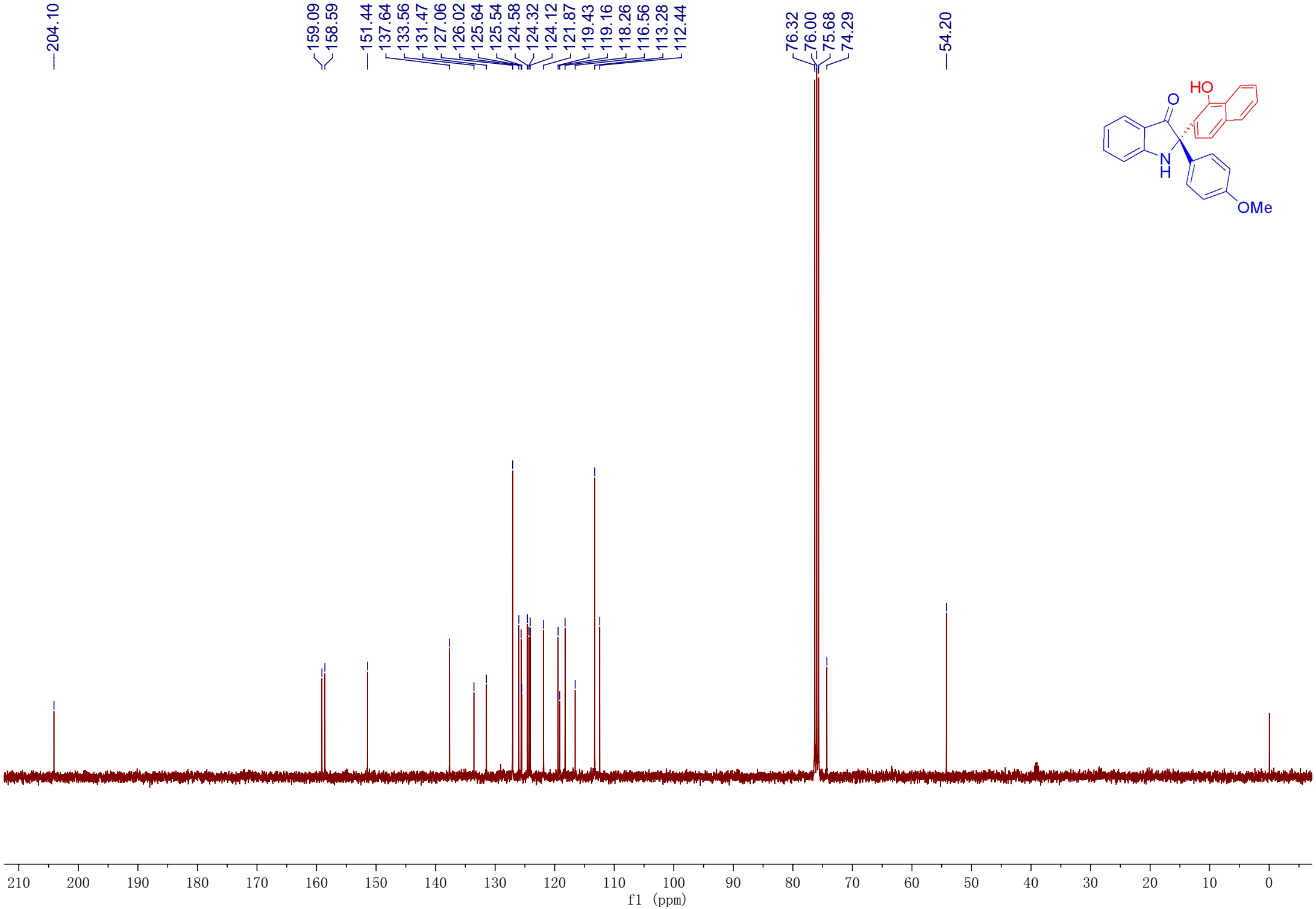

200.65
160.54
151.67
140.05
137.43
133.86
131.03
128.85
127.61
126.29
126.09
125.12
125.09
124.51
122.16
121.98
120.67
118.86
118.02
117.52
111.97
72.93
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
N
H
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

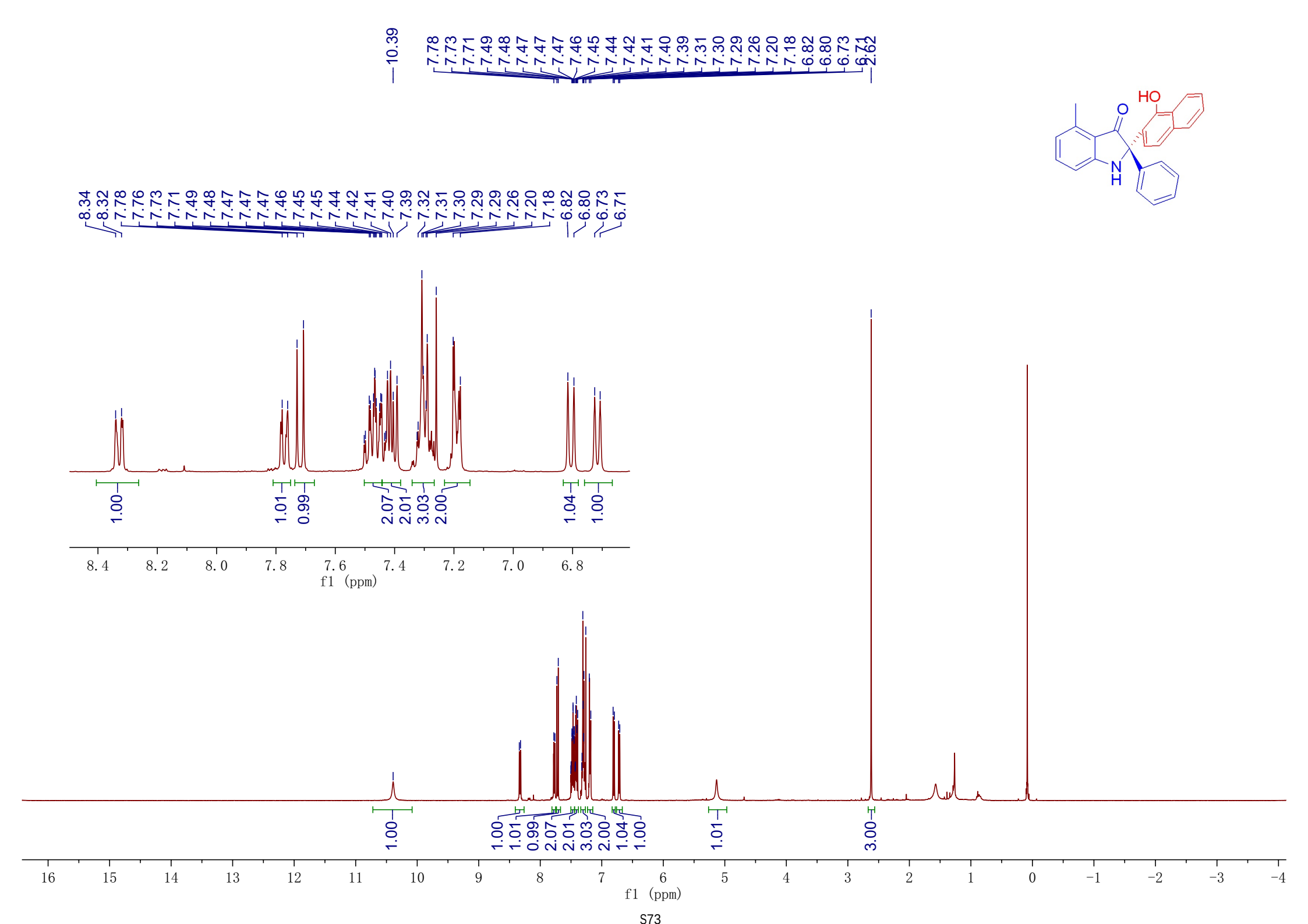

9.97
8.32
8.20
8.19
8.18
8.86
8.85
8.84
8.72
8.70
8.66
8.65
8.63
8.53
8.52
8.51
8.50
8.49
8.49
8.47
8.47
8.45
8.43
8.41
8.21
8.20
8.18
8.08
8.07
8.06
8.05
6.77
6.75
6.73
2.50
2.50
2.50
HO
O
N
H
CF3
1.01
0.95
0.99
2.04
2.03
4.02
1.04
1.01
1.01
1.00
f1 (ppm)

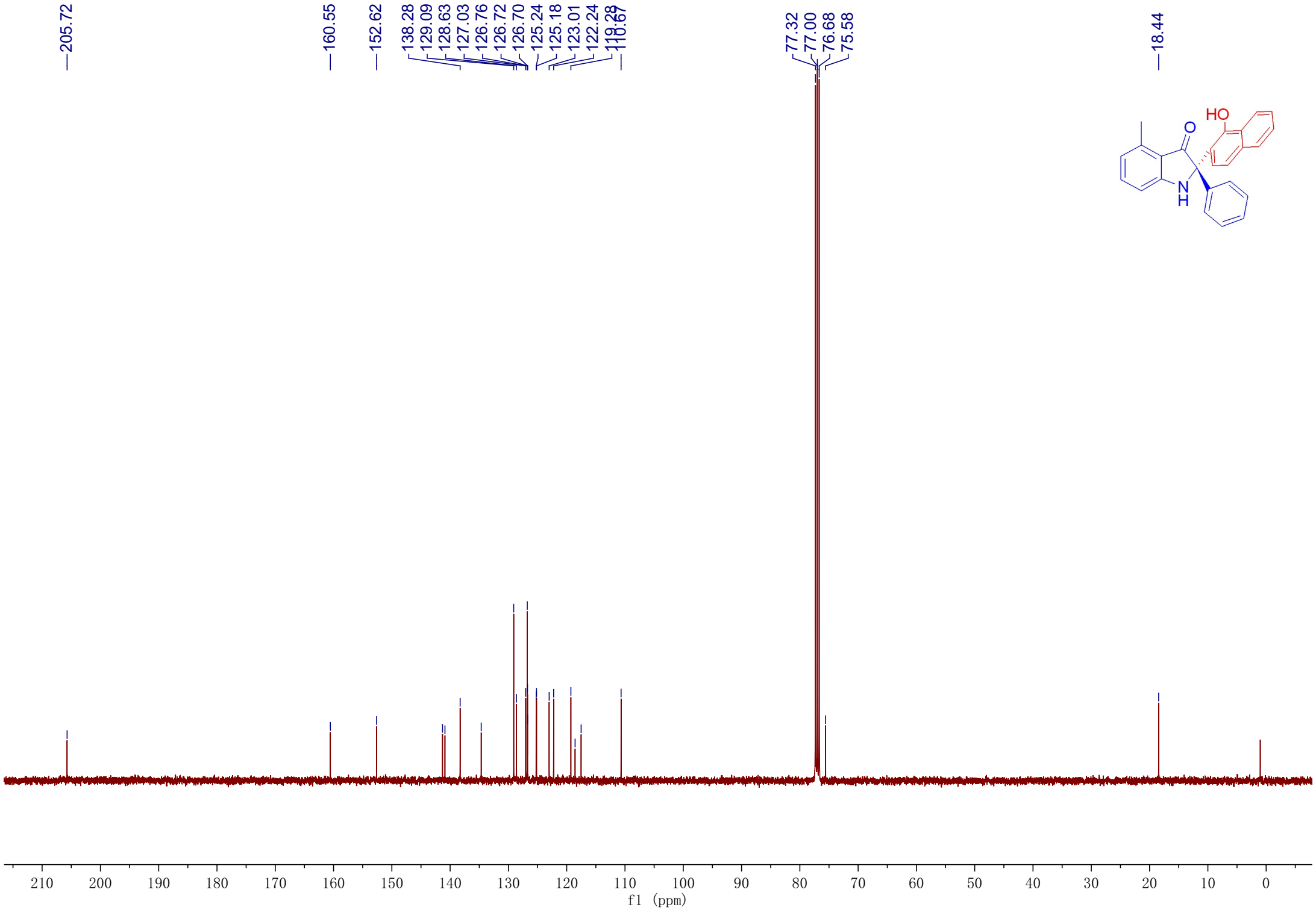

200.10
160.76
151.75
145.66
137.61
133.90
128.01
127.70
127.65
127.23
126.48
126.34
125.83
125.67
125.12
125.09
125.05
125.01
124.54
122.96
122.04
121.93
120.11
118.94
117.79
117.68
112.14
73.28
40.13
39.92
39.71
39.50
39.29
39.08
HO
O
N
H
CF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

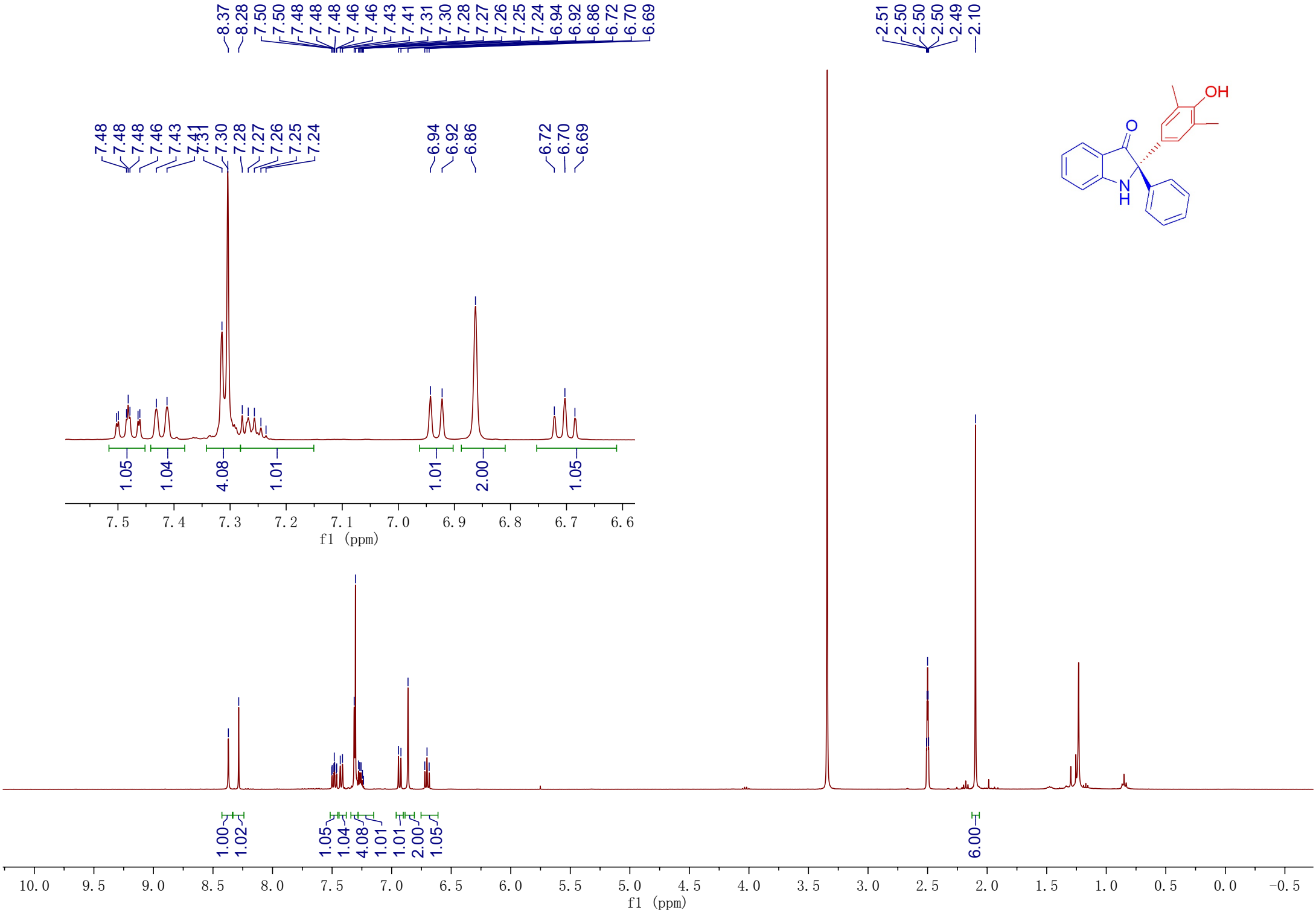

-60.82
HO
O
N
H
CF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

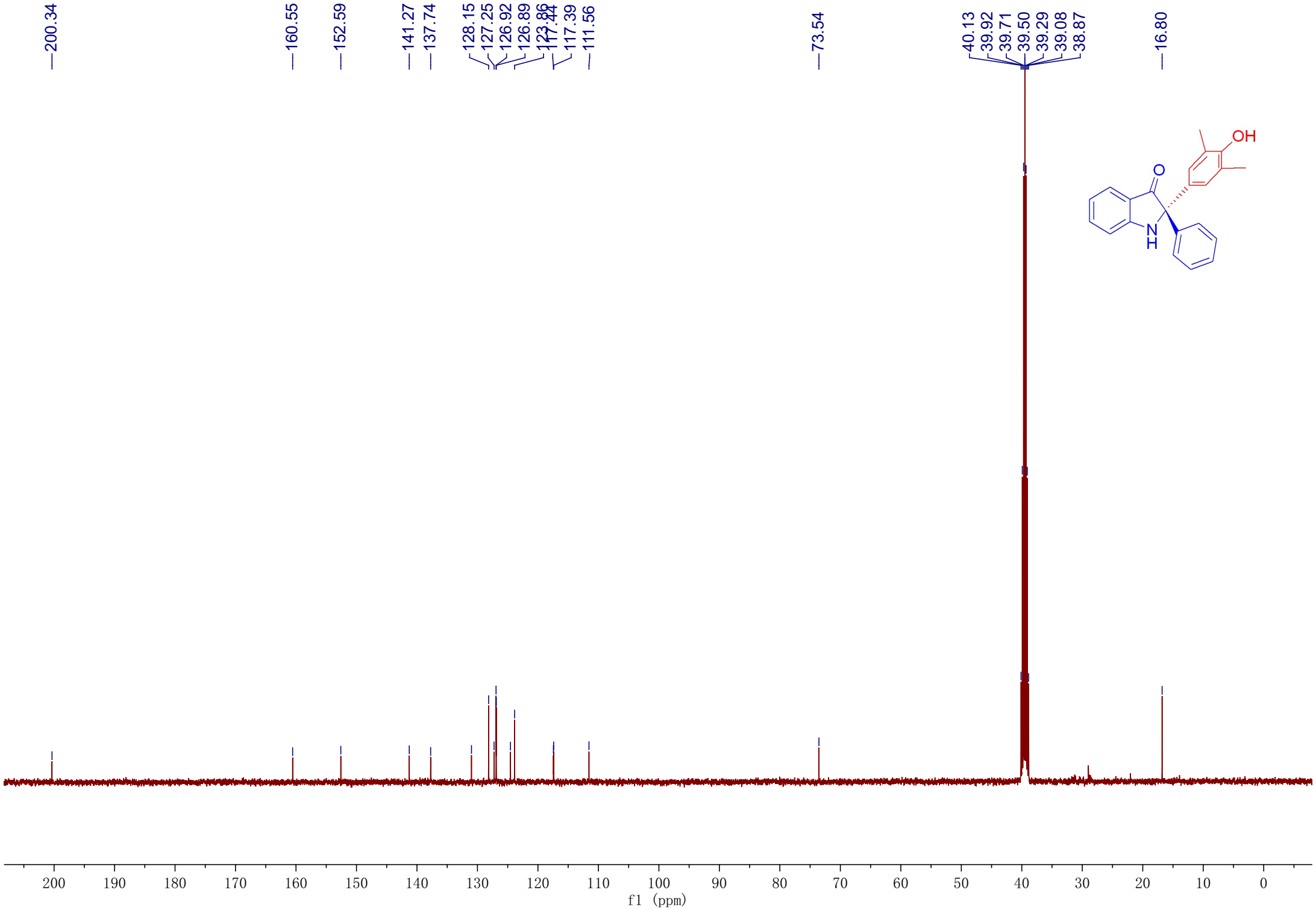

10.25
8.31
8.29
7.70
7.69
7.68
7.45
7.38
7.36
7.10
7.08
6.99
6.97
6.92
6.78
6.76
6.59
3.73
HO
O
N
H
OMe
1.02
1.07
2.02
1.05
2.08
1.01
2.04
1.03
1.05
2.06
f1 (ppm)
1.00
1.02
1.07
2.02
1.05
2.08
1.01
2.04
1.03
1.05
2.06
1.02
3.00
f1 (ppm)

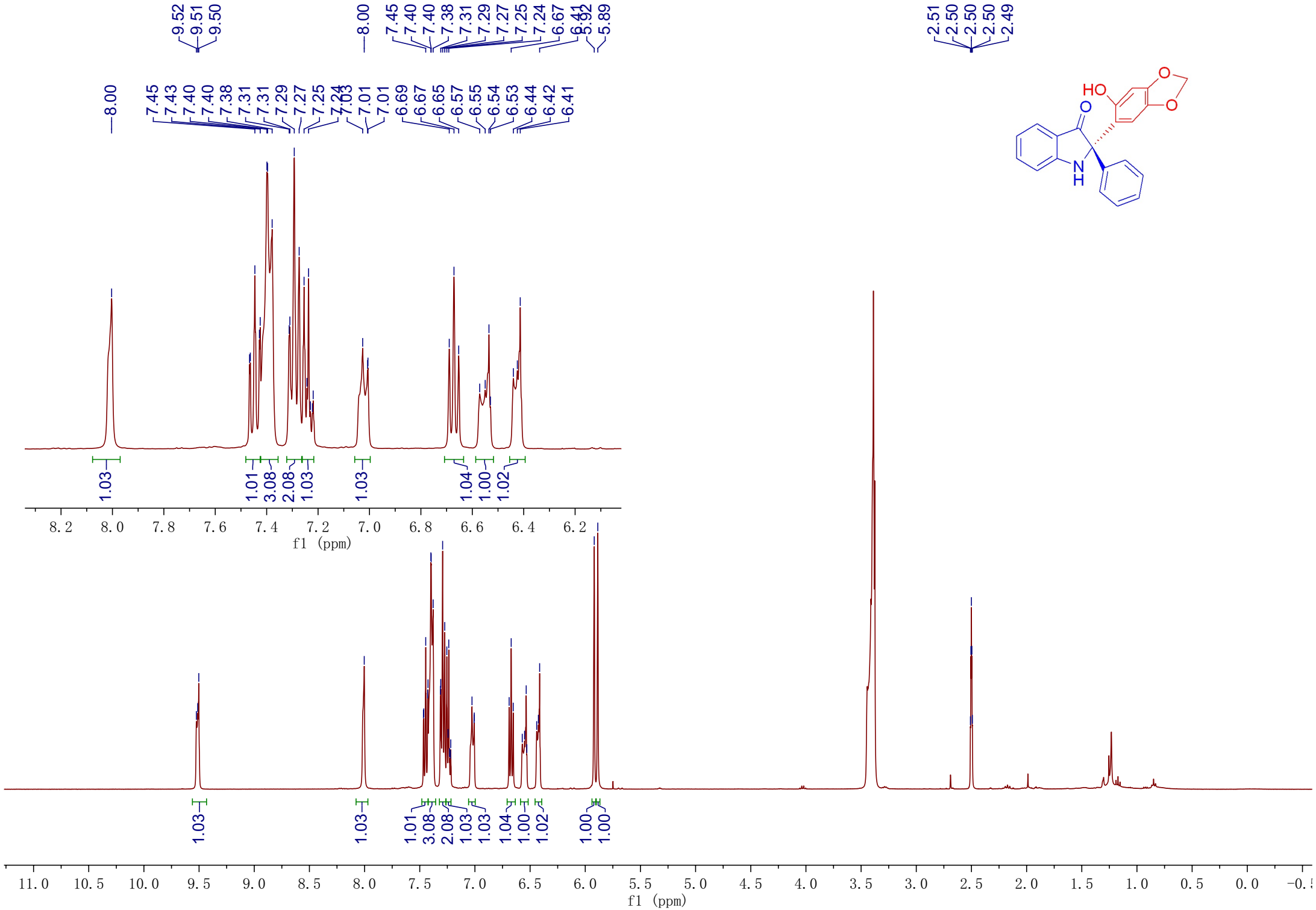

204.10
159.09
158.59
151.44
137.64
133.56
131.47
127.06
126.02
125.64
125.54
124.58
124.32
124.12
121.87
119.43
119.16
118.26
116.56
113.28
112.44
76.32
76.00
75.68
74.29
54.20
HO
O
N
H
OMe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

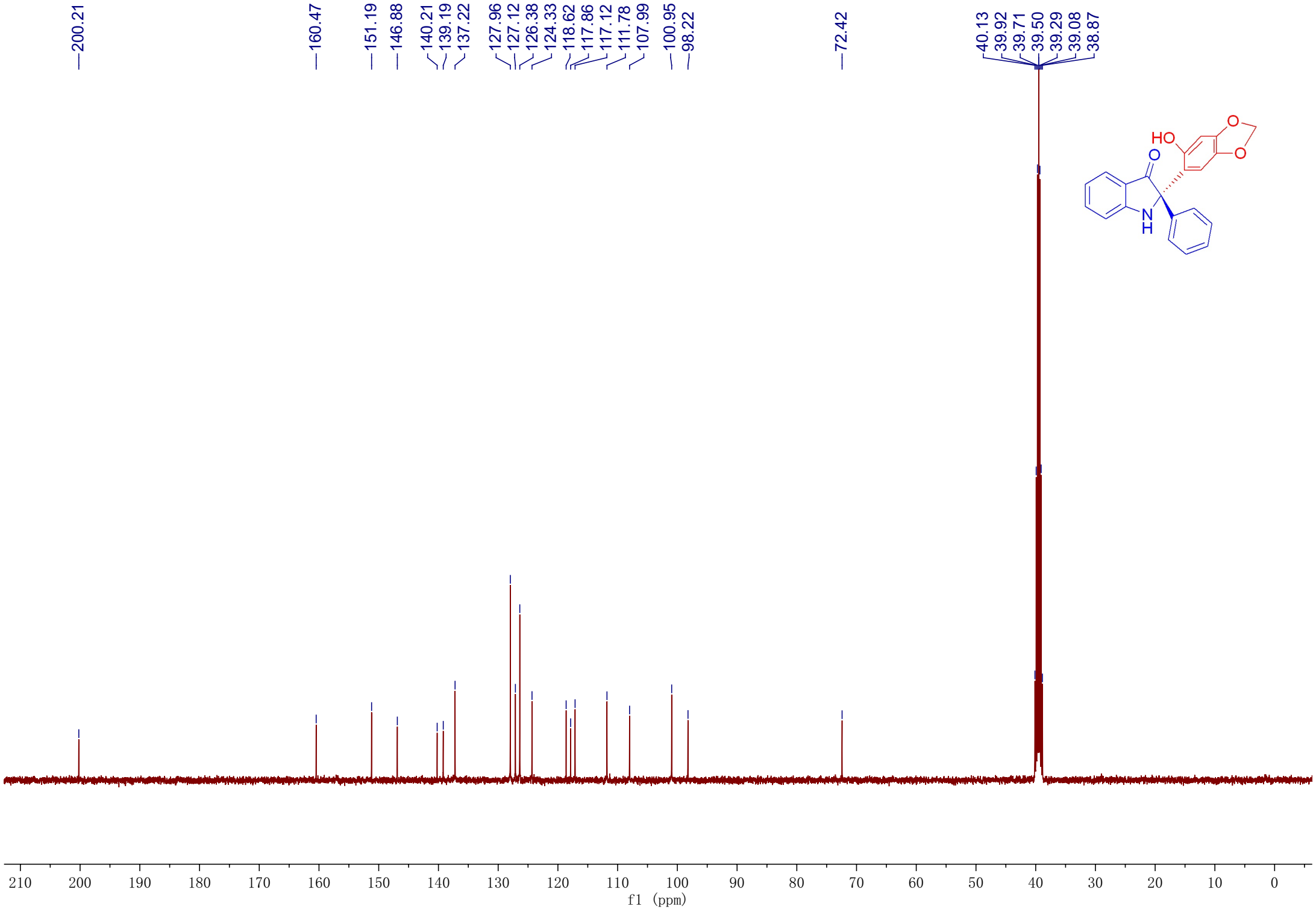

10.39
7.78
7.73
7.71
7.49
7.48
7.47
7.47
7.47
7.46
7.45
7.44
7.42
7.41
7.40
7.39
7.31
7.30
7.29
7.26
7.20
7.18
6.82
6.80
6.73
6.71
2.62
HO
O
N
H
8.34
8.32
7.78
7.76
7.73
7.71
7.49
7.48
7.47
7.47
7.47
7.46
7.45
7.45
7.44
7.42
7.41
7.40
7.39
7.32
7.31
7.30
7.29
7.29
7.26
7.20
7.18
6.82
6.80
6.73
6.71
1.00
1.01
0.99
2.07
2.01
3.03
2.00
1.04
1.00
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
f1 (ppm)
1.00
1.00
1.01
0.99
2.07
2.01
3.03
2.00
1.04
1.00
1.01
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
−4
f1 (ppm)

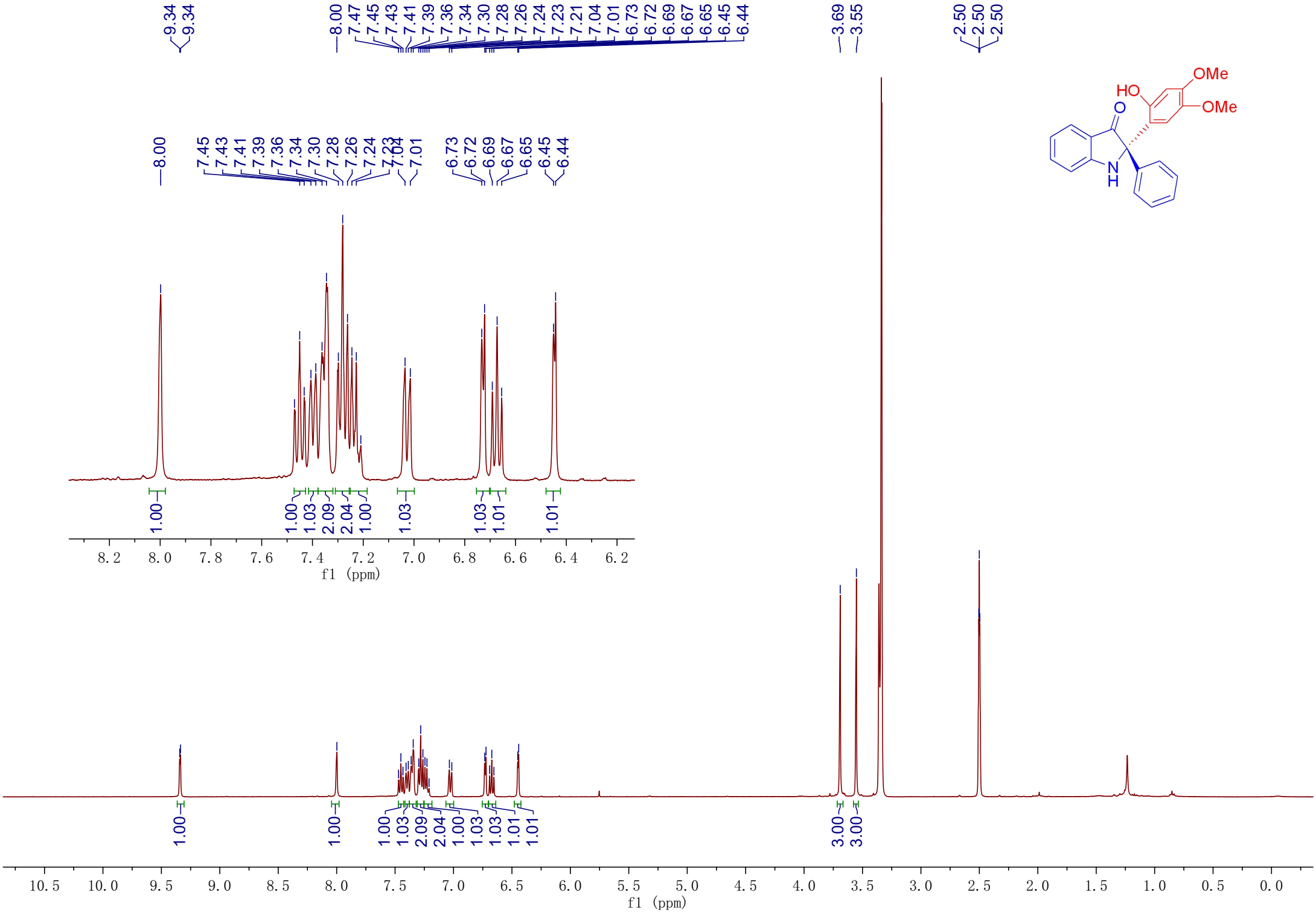

205.72
160.55
152.62
138.28
129.09
128.63
127.03
126.76
126.72
126.70
125.24
125.18
123.01
122.24
119.28
110.67
77.32
77.00
76.68
75.58
18.44
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

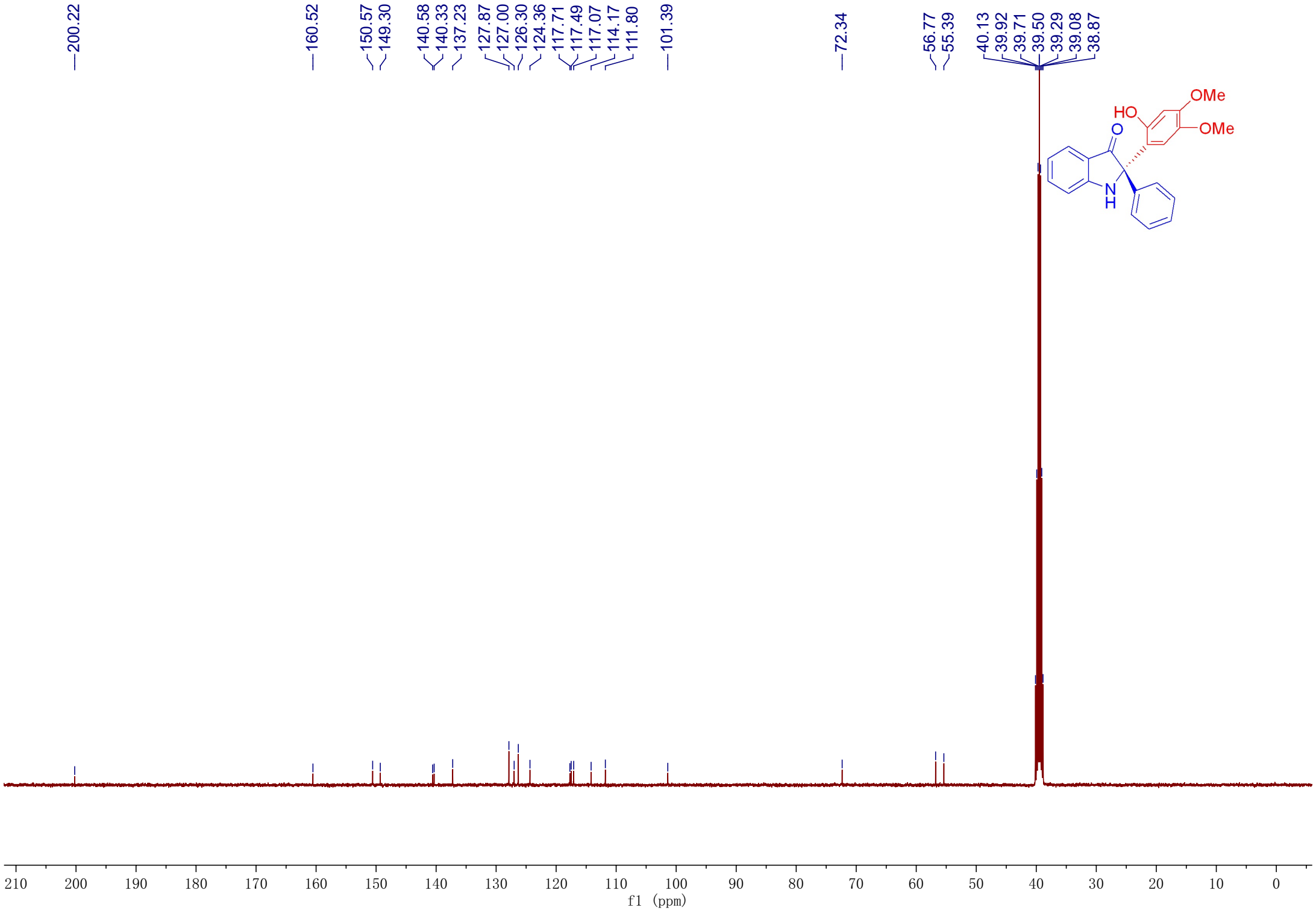

8.37
8.28
7.50
7.50
7.48
7.48
7.48
7.46
7.46
7.43
7.41
7.31
7.30
7.28
7.27
7.26
7.25
7.24
6.94
6.92
6.86
6.72
6.70
6.69
2.51
2.50
2.50
2.50
2.49
2.10
OH
O
N
H
1.05
1.04
4.08
1.01
1.01
2.00
1.05
f1 (ppm)
1.00
1.02
1.05
1.04
4.08
1.01
1.01
2.00
1.05
6.00
f1 (ppm)

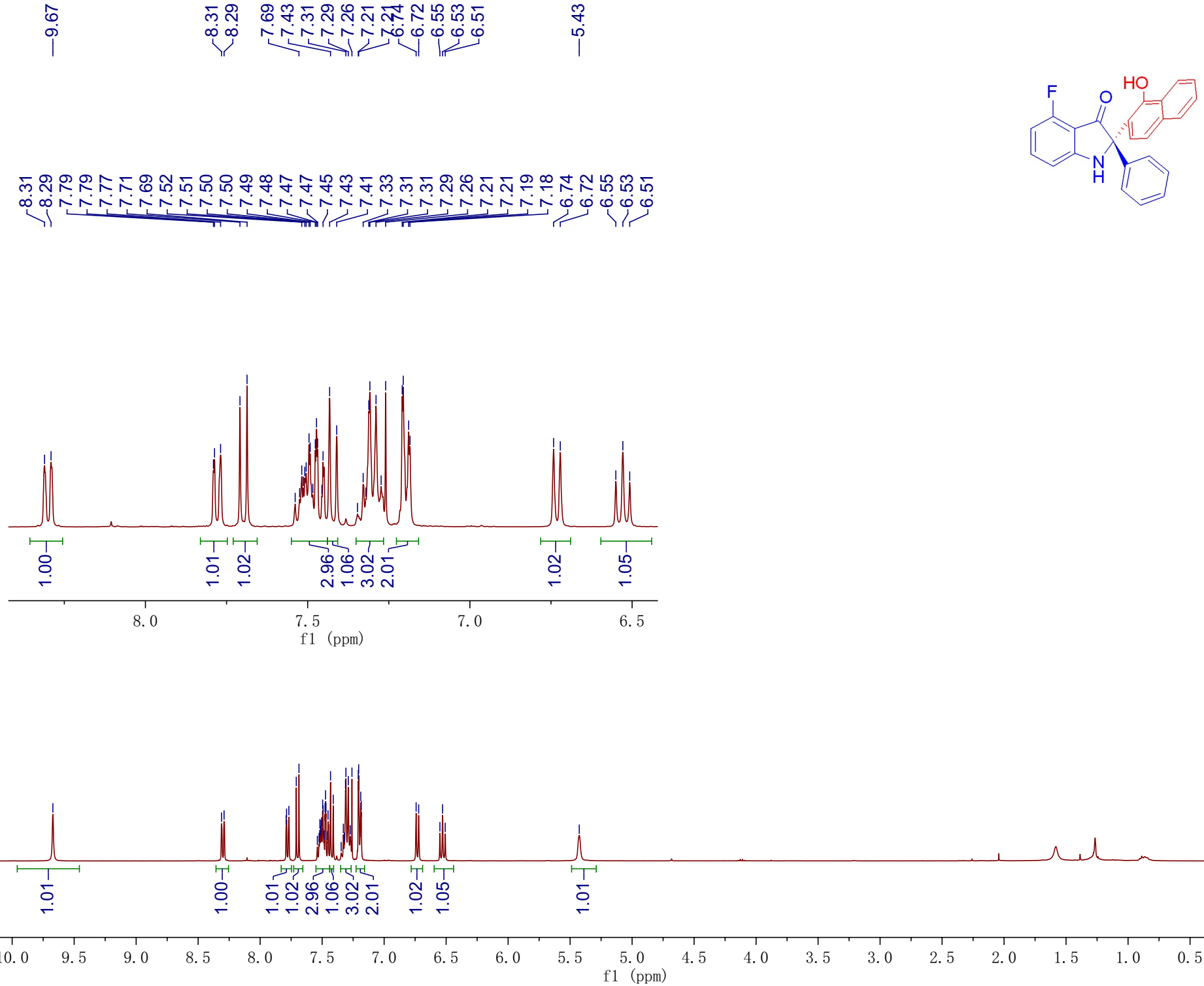

200.34
160.55
152.59
141.27
137.74
128.15
127.25
126.92
126.89
123.86
117.44
117.39
111.56
73.54
40.13
39.92
39.71
39.50
39.29
39.08
38.87
16.80
OH
O
N
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

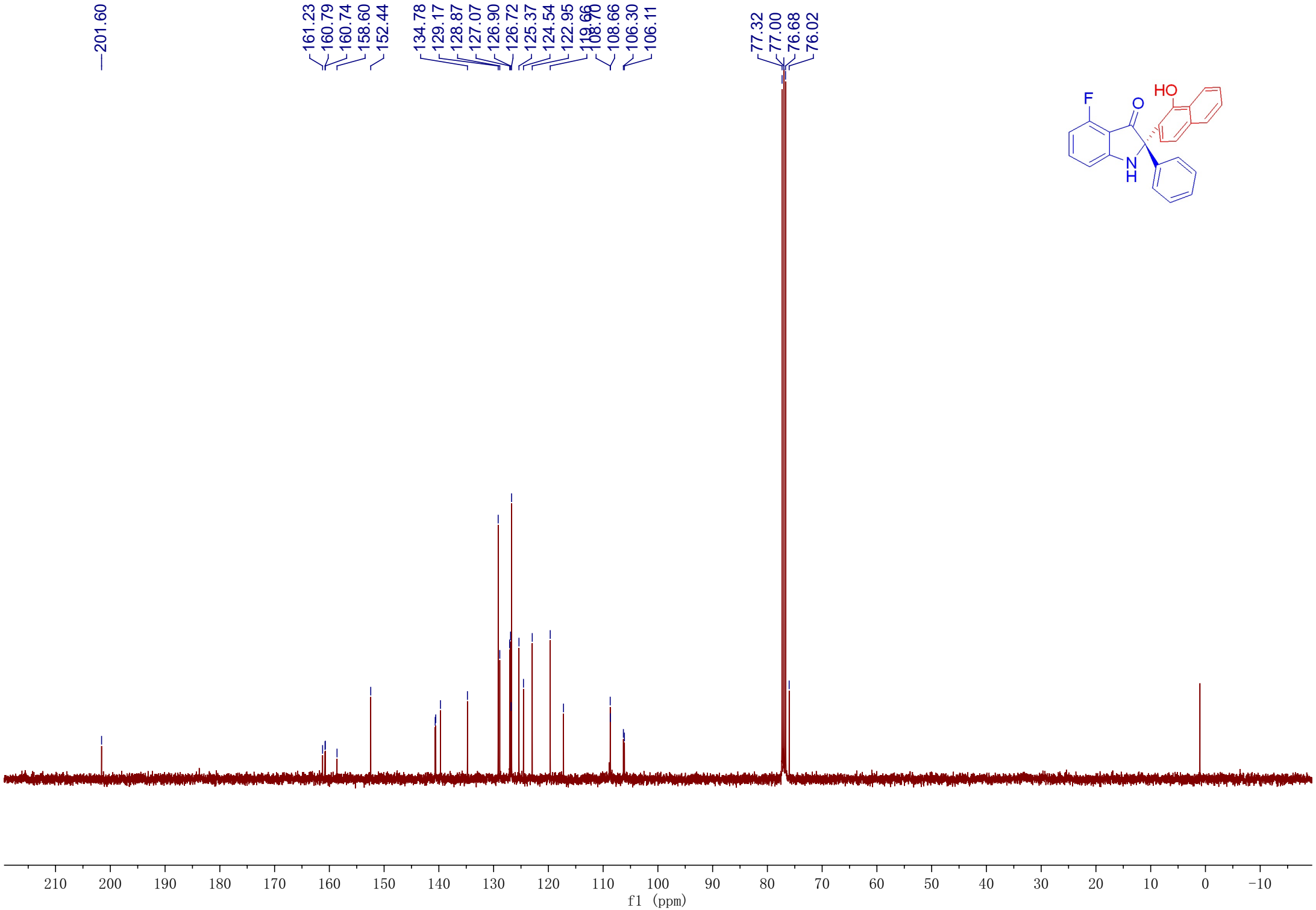

9.52
9.51
9.50
8.00
7.45
7.40
7.40
7.38
7.31
7.29
7.27
7.25
7.24
6.67
6.41
5.92
5.89
2.51
2.50
2.50
2.50
2.49
HO
O
O
O
N
H
1.03
1.01
3.08
2.08
1.03
1.03
1.04
1.00
1.02
f1 (ppm)

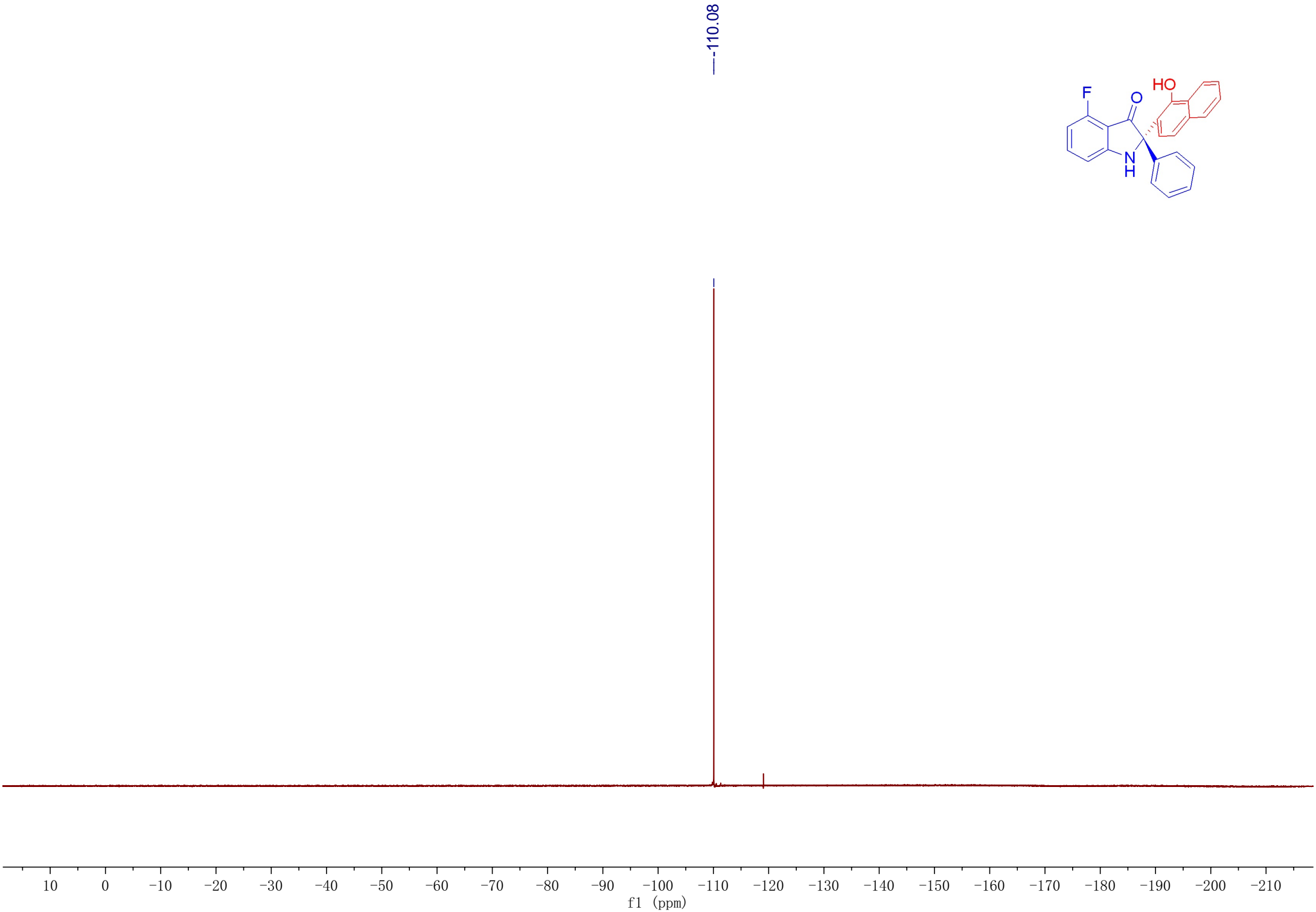

200.21
160.47
151.19
146.88
140.21
139.19
137.22
127.96
127.12
126.38
124.33
118.62
117.86
117.12
111.78
107.99
100.95
98.22
72.42
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
O
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

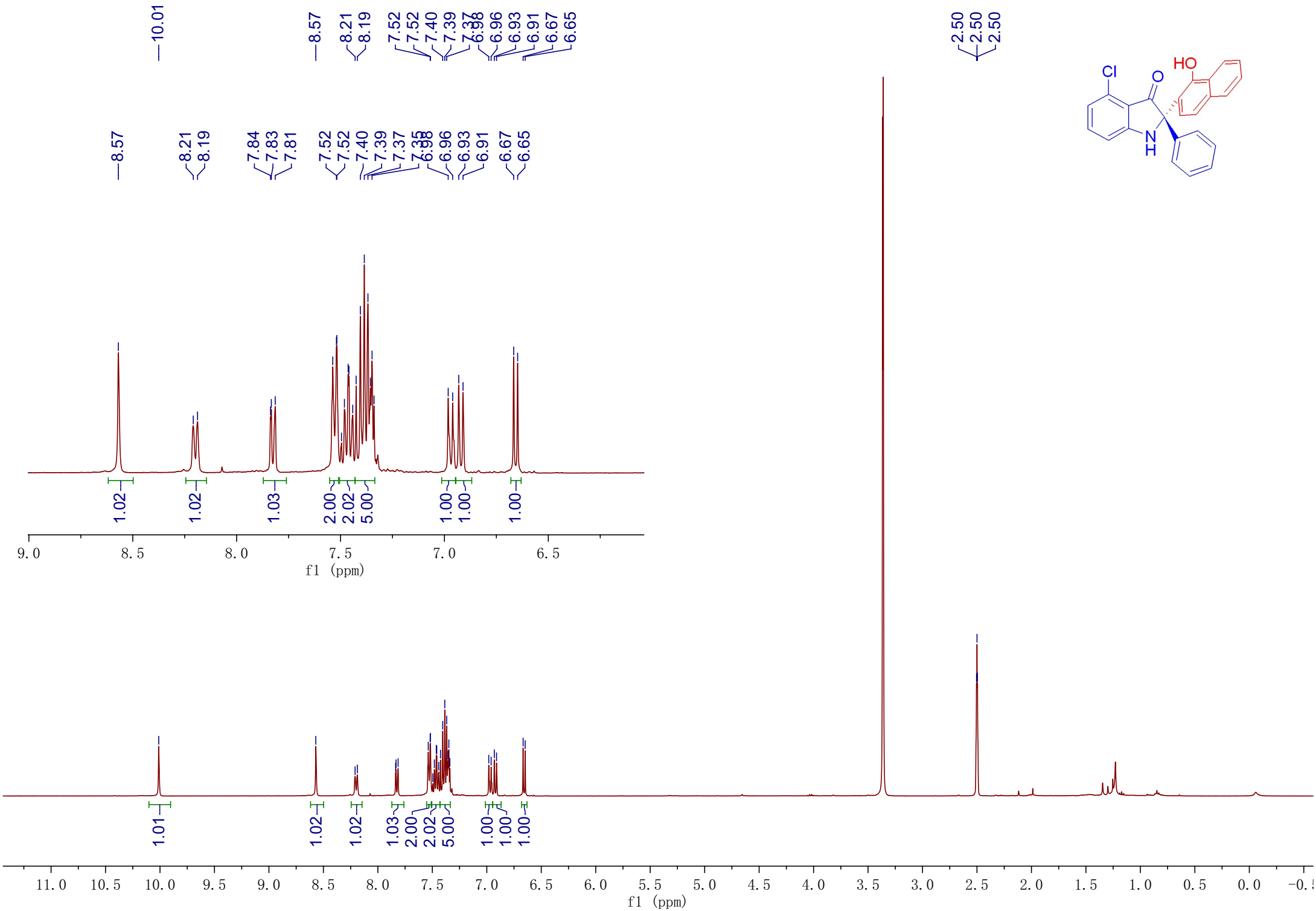

9.34
9.34
8.00
7.47
7.45
7.43
7.41
7.39
7.36
7.34
7.30
7.28
7.26
7.24
7.23
7.21
7.04
7.01
6.73
6.72
6.69
6.67
6.65
6.45
6.44
3.69
3.55
2.50
2.50
2.50
OMe
HO
O
OMe
N
H
1.00
1.00
1.03
2.09
2.04
1.00
1.03
1.03
1.01
1.01
f1 (ppm)
3.00
3.00
f1 (ppm)

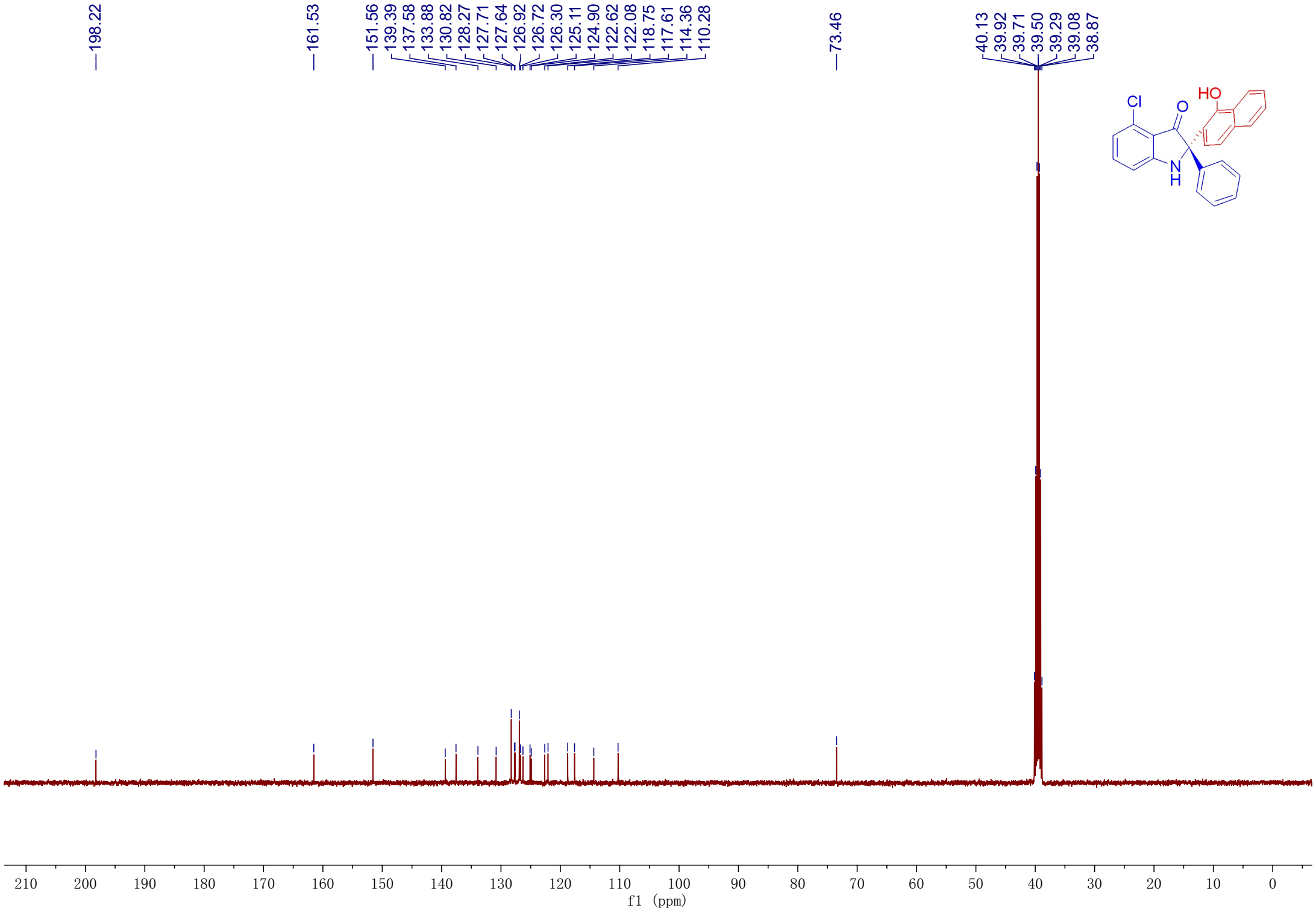

200.22
160.52
150.57
149.30
140.58
140.33
137.23
127.87
127.00
126.30
124.36
117.71
117.49
117.07
114.17
111.80
101.39
72.34
56.77
55.39
40.13
39.92
39.71
39.50
39.29
39.08
38.87
OMe
HO
OMe
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

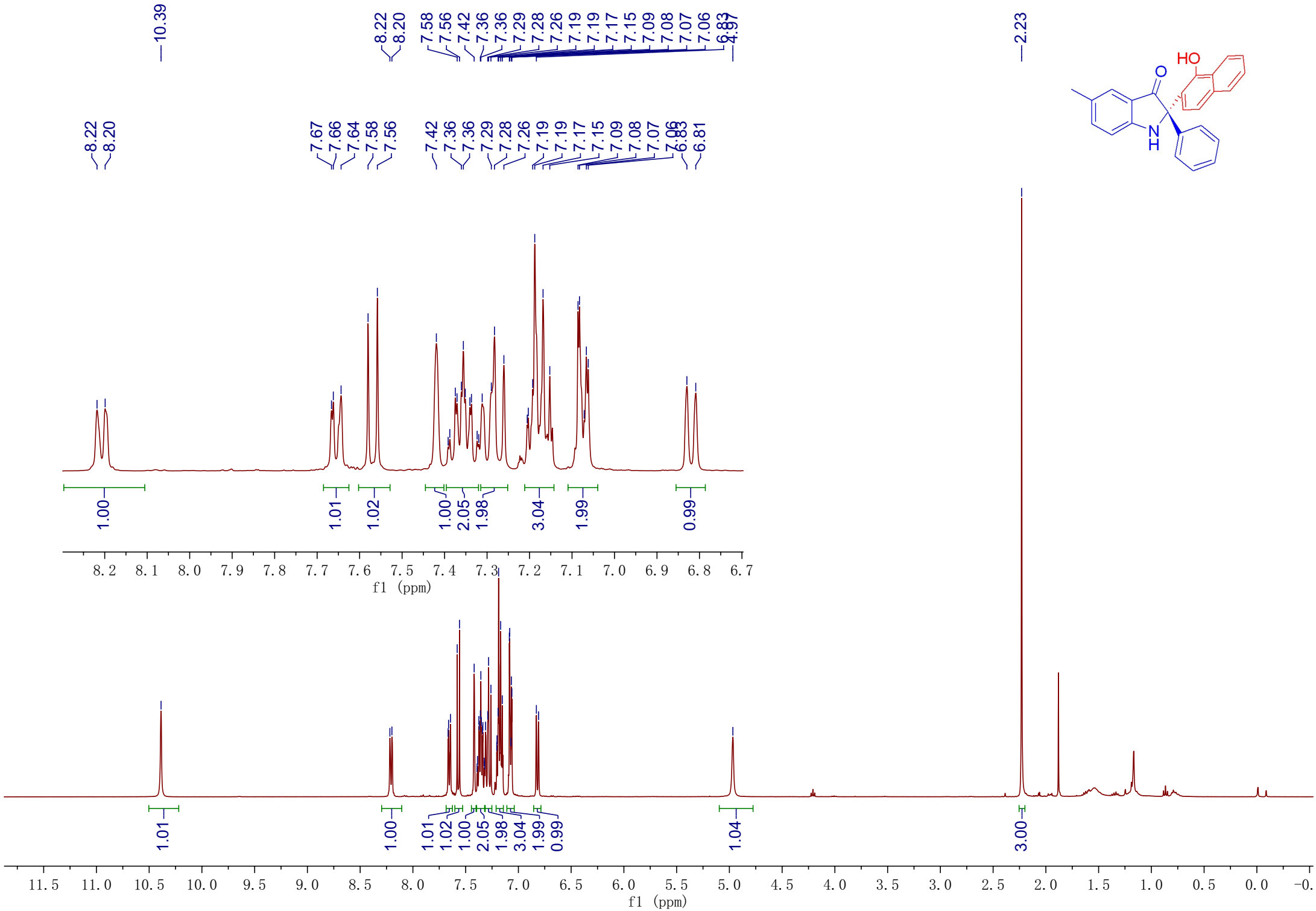

9.67
8.31
8.29
7.69
7.43
7.31
7.29
7.26
7.21
7.21
6.74
6.72
6.55
6.53
6.51
5.43
F
O
HO
N
H
1.00
1.01
1.02
2.96
1.06
3.02
2.01
1.02
1.05
8.0
7.5
7.0
6.5
f1 (ppm)
1.01
1.00
1.01
1.02
2.96
1.06
3.02
2.01
1.02
1.05
1.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

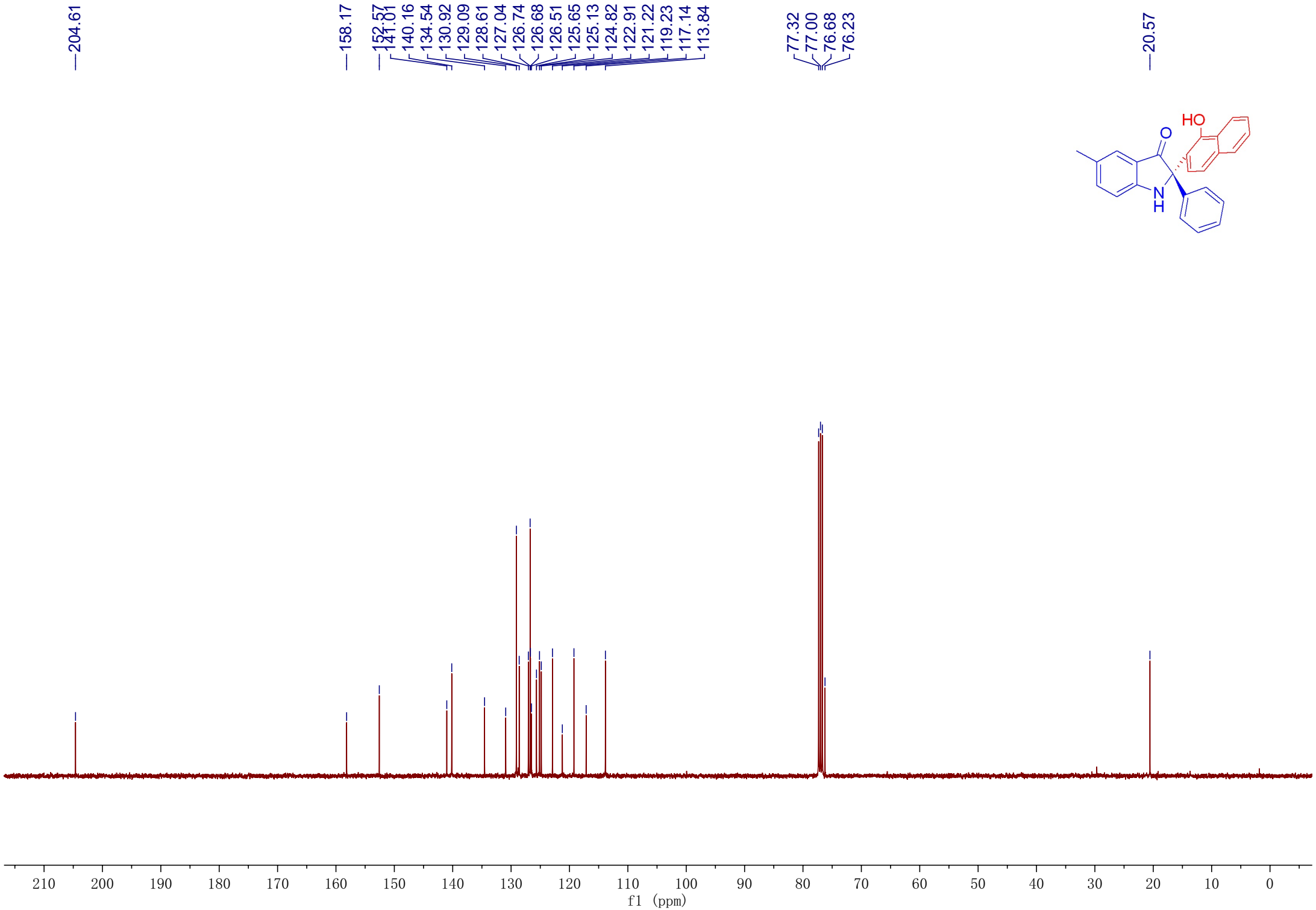

201.60
161.23
160.79
160.74
158.60
152.44
134.78
129.17
128.87
127.07
126.90
126.72
125.37
124.54
122.95
119.66
108.70
108.66
106.30
106.11
77.32
77.00
76.68
76.02
F
O
HO
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

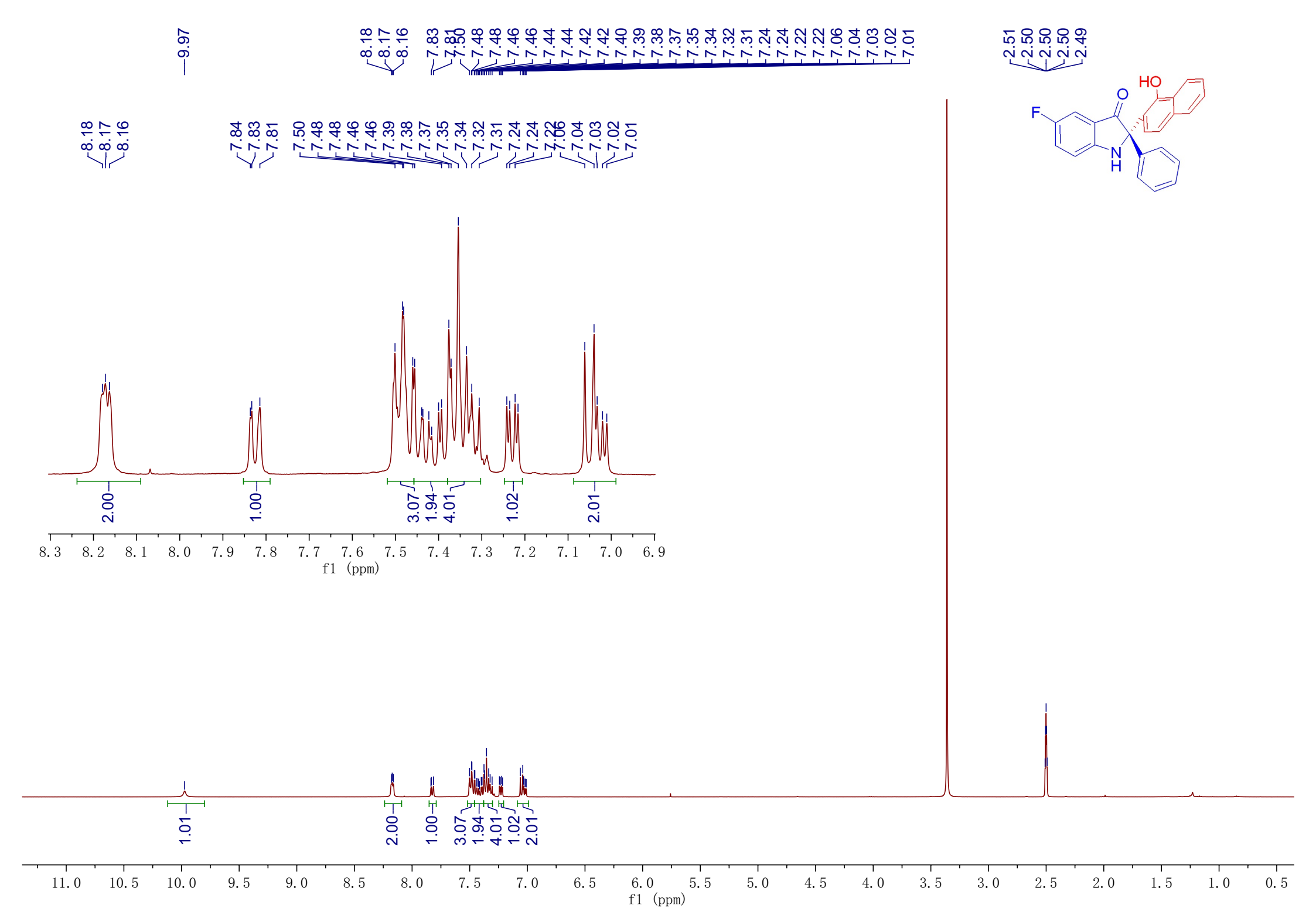

-110.08
F
O
HO
N
H
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

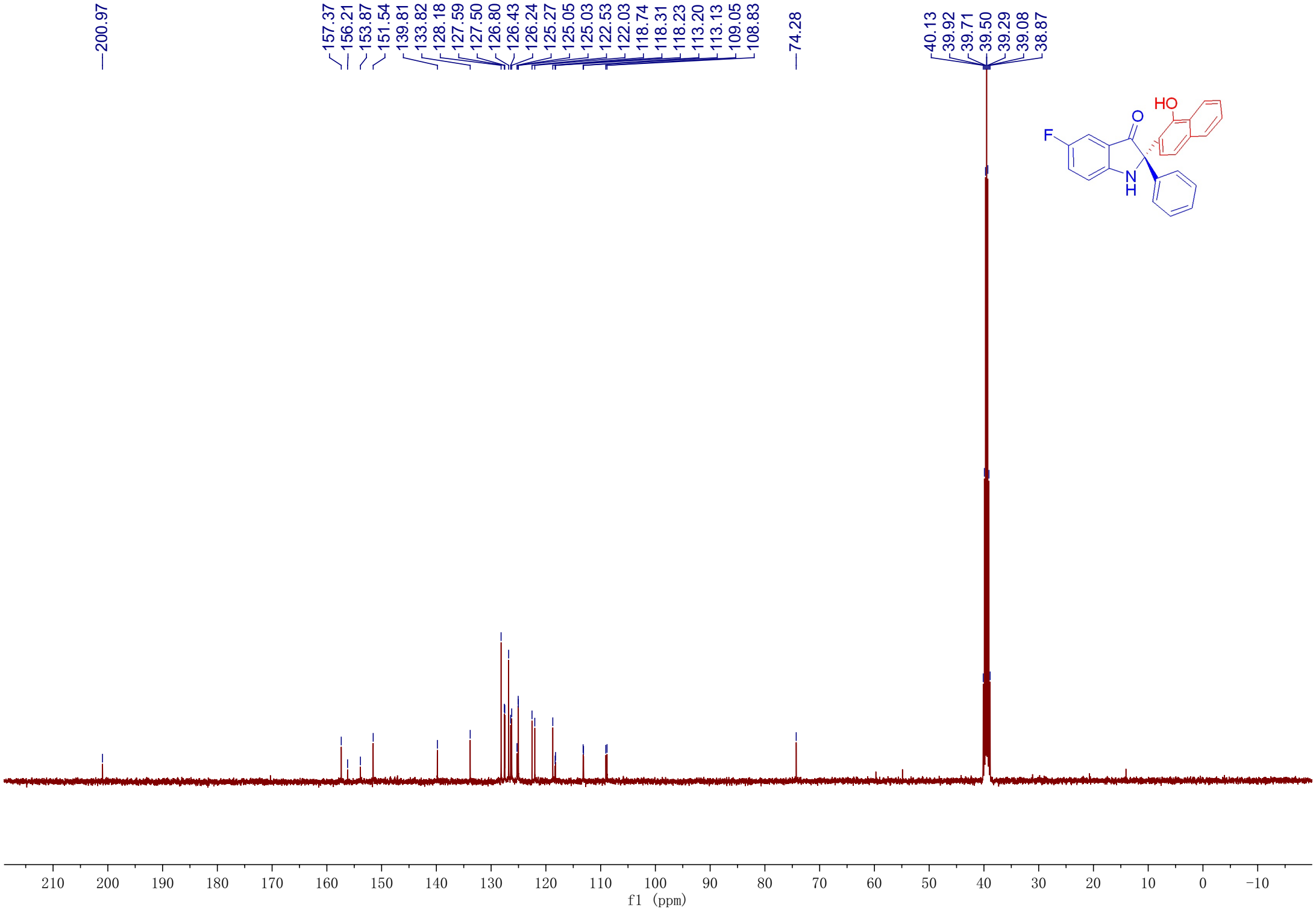

10.01
8.57
8.21
8.19
7.52
7.52
7.40
7.39
7.37
6.98
6.96
6.93
6.91
6.67
6.65
2.50
2.50
2.50
Cl
O
HO
N
H
1.01
1.02
1.02
1.03
2.00
2.02
5.00
1.00
1.00
1.00
f1 (ppm)

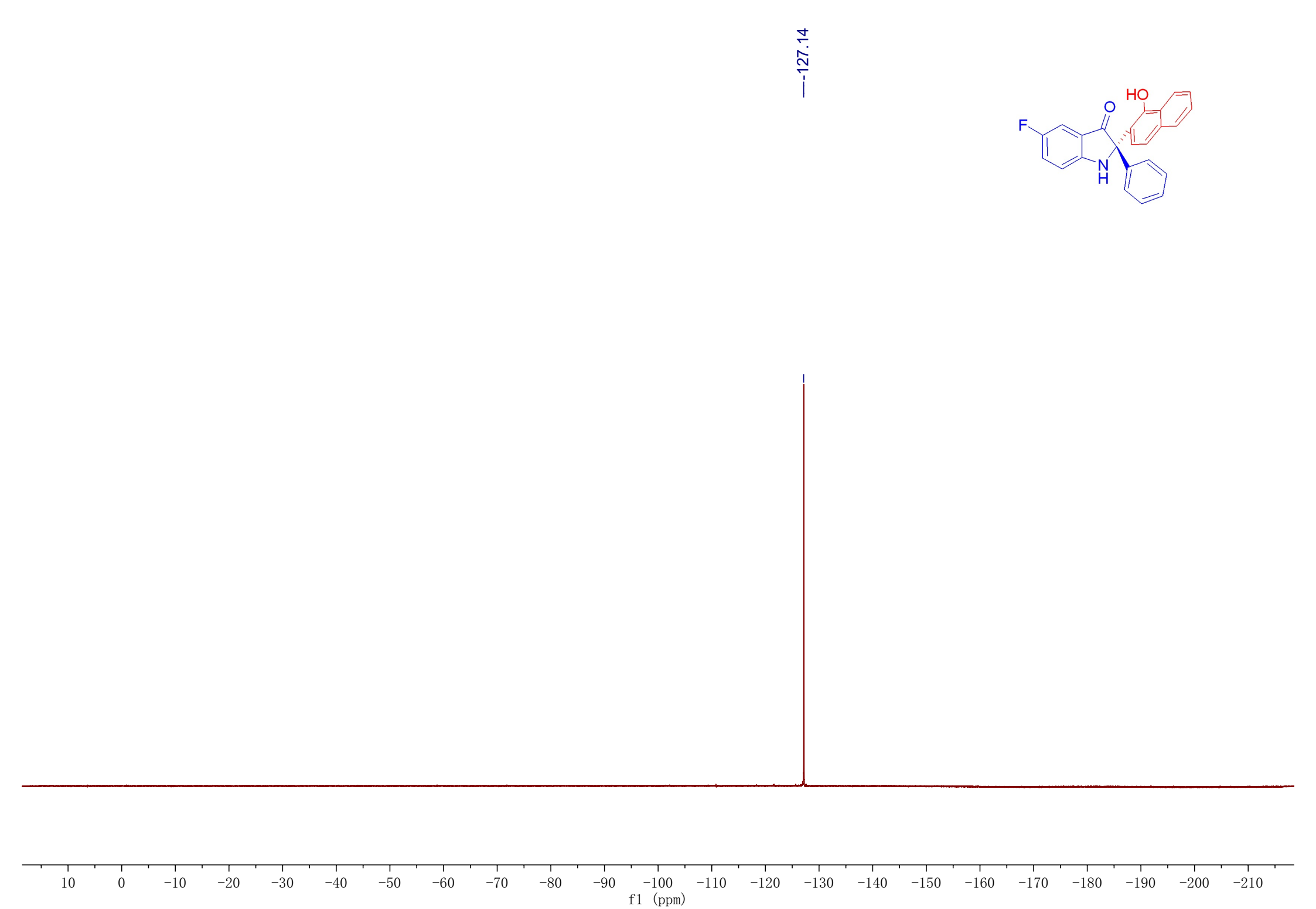

198.22
161.53
151.56
139.39
137.58
133.88
130.82
128.27
127.71
127.64
126.92
126.72
126.30
125.11
124.90
122.62
122.08
118.75
117.61
114.36
110.28
73.46
40.13
39.92
39.71
39.50
39.29
39.08
38.87
Cl
O
HO
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

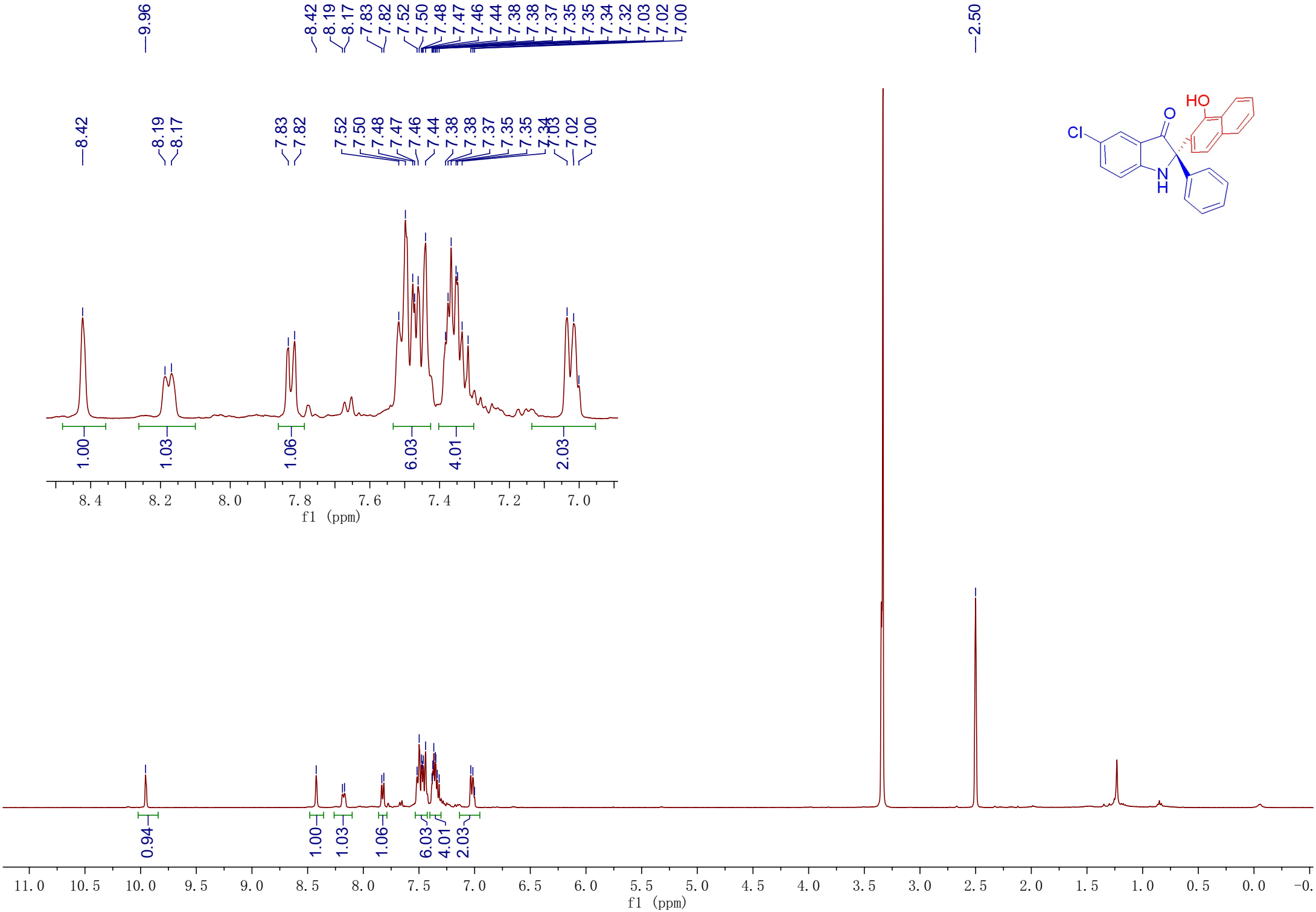

10.39
8.22
8.20
7.58
7.56
7.42
7.36
7.36
7.29
7.28
7.26
7.19
7.19
7.17
7.15
7.09
7.08
7.07
7.06
6.83
4.97
2.23
HO
O
N
H
7.67
7.66
7.64
7.58
7.56
7.42
7.36
7.36
7.29
7.28
7.26
7.19
7.19
7.17
7.15
7.09
7.08
7.07
7.06
6.83
6.81
1.00
1.01
1.02
1.00
2.05
1.98
3.04
1.99
0.99
f1 (ppm)
1.01
1.00
1.01
1.02
1.00
2.05
1.98
3.04
1.99
0.99
1.04
3.00
f1 (ppm)

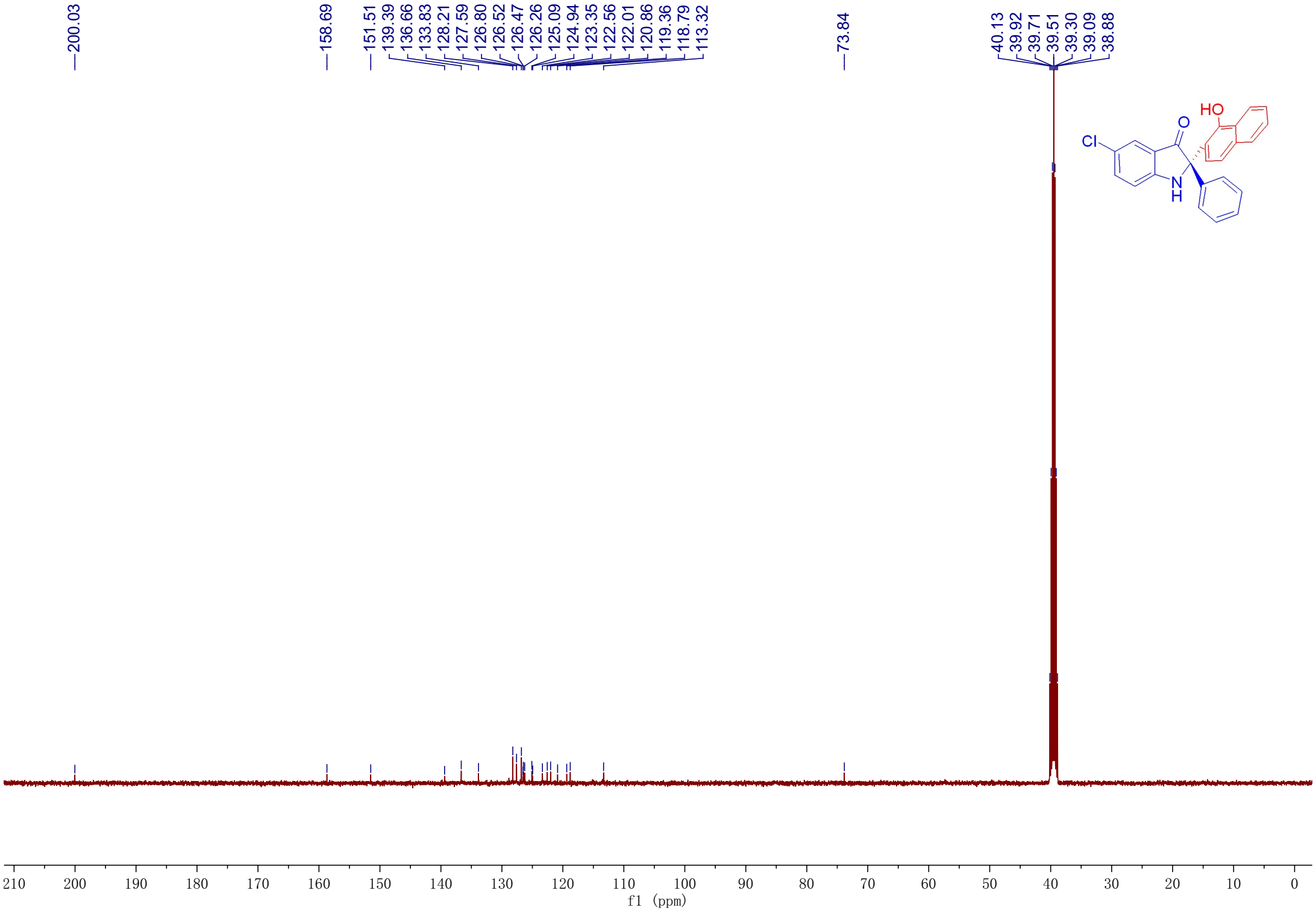

204.61
158.17
152.57
141.01
140.16
134.54
130.92
129.09
128.61
127.04
126.74
126.68
126.51
125.65
125.13
124.82
122.91
121.22
119.23
117.14
113.84
77.32
77.00
76.68
76.23
20.57
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

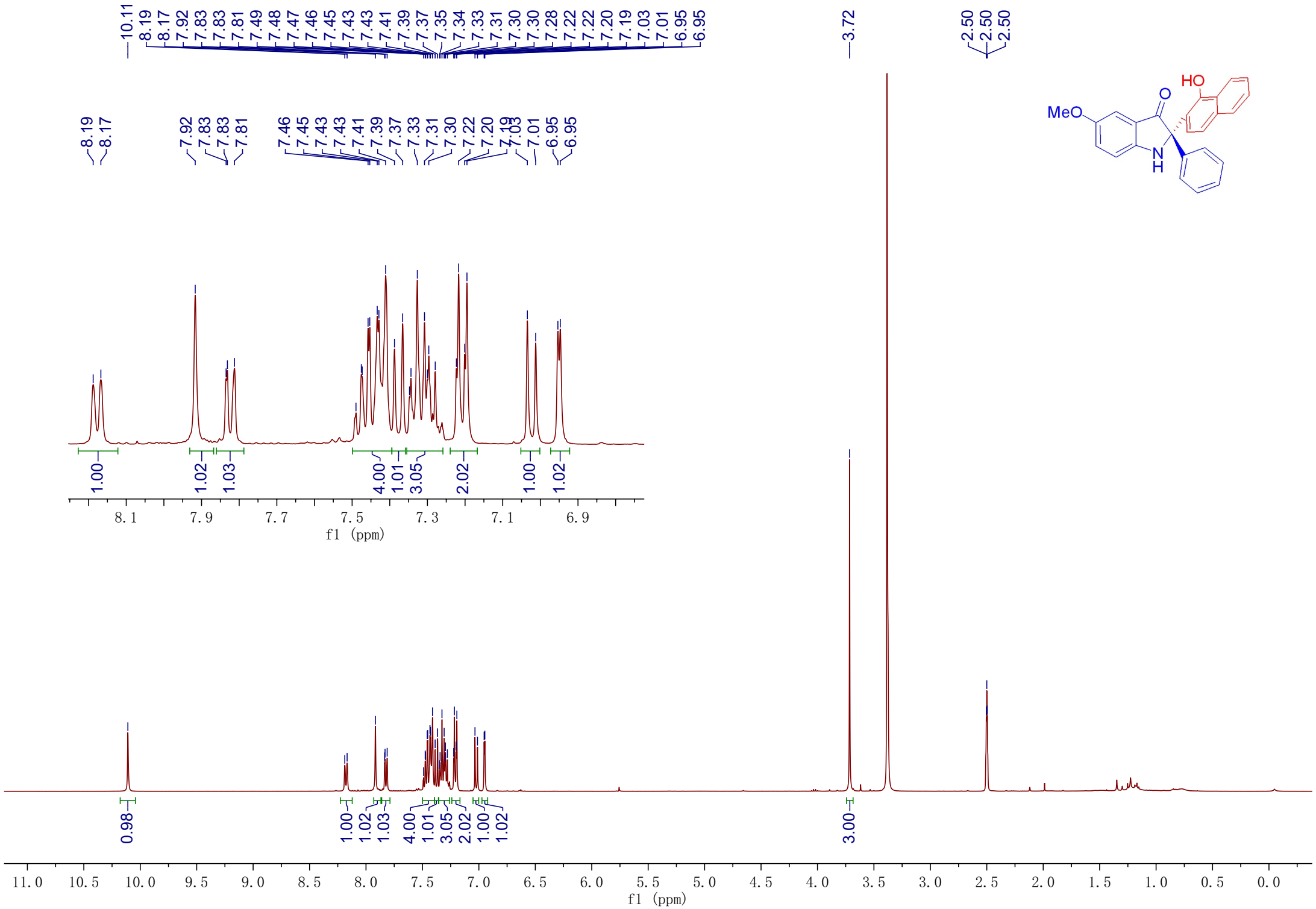

9.97
8.18
8.17
8.16
7.83
7.81
7.50
7.48
7.48
7.46
7.46
7.44
7.44
7.42
7.42
7.40
7.39
7.38
7.37
7.35
7.34
7.32
7.31
7.24
7.24
7.22
7.22
7.06
7.04
7.03
7.02
7.01
2.51
2.50
2.50
2.50
2.49
HO
O
F
N
H
2.00
1.00
3.07
1.94
4.01
1.02
2.01
f1 (ppm)
1.01
2.00
1.00
3.07
1.94
4.01
1.02
2.01
f1 (ppm)

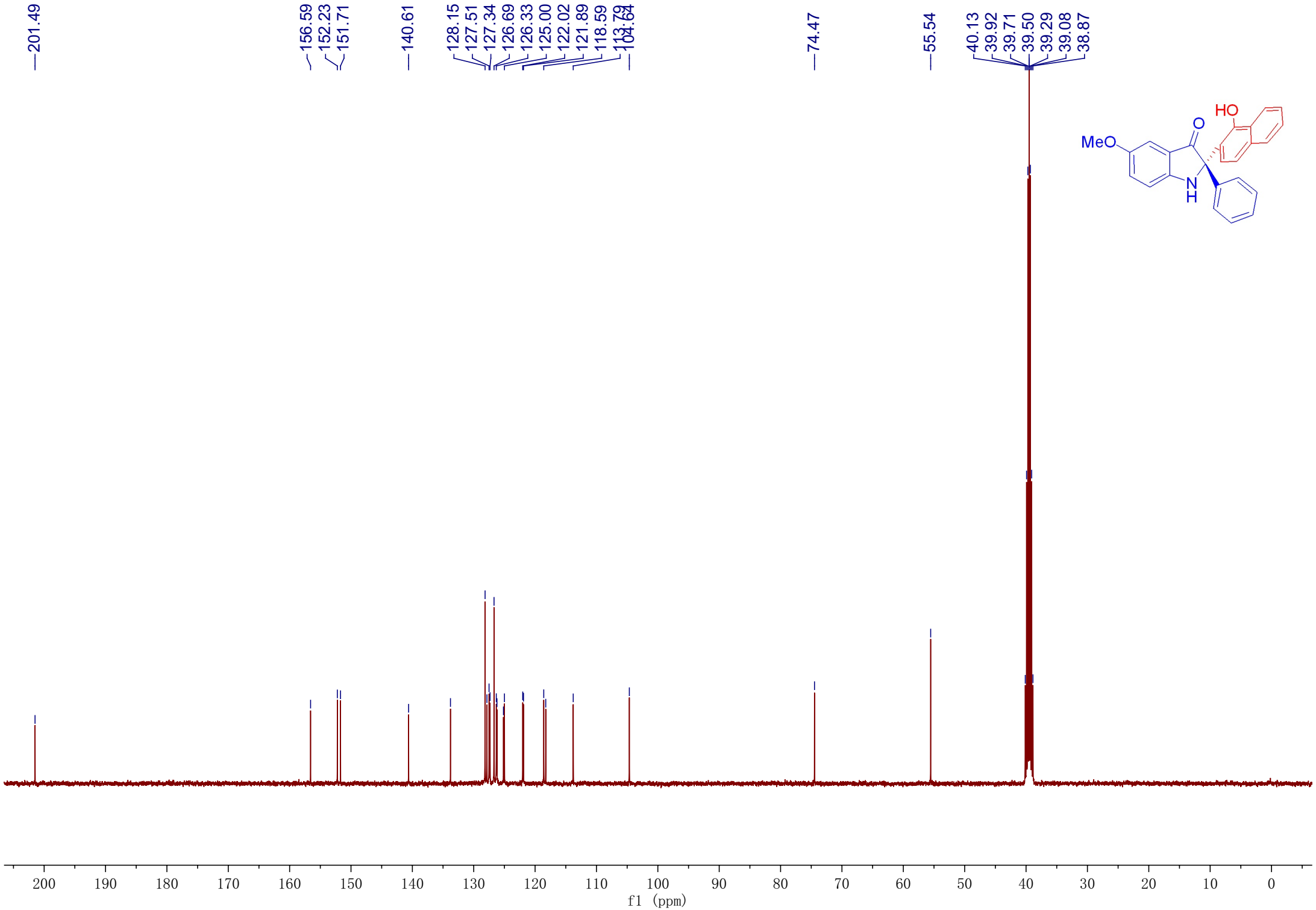

200.97
157.37
156.21
153.87
151.54
139.81
133.82
128.18
127.59
127.50
126.80
126.43
126.24
125.27
125.05
125.03
122.53
122.03
118.74
118.31
118.23
113.20
113.13
109.05
108.83
74.28
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
F
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

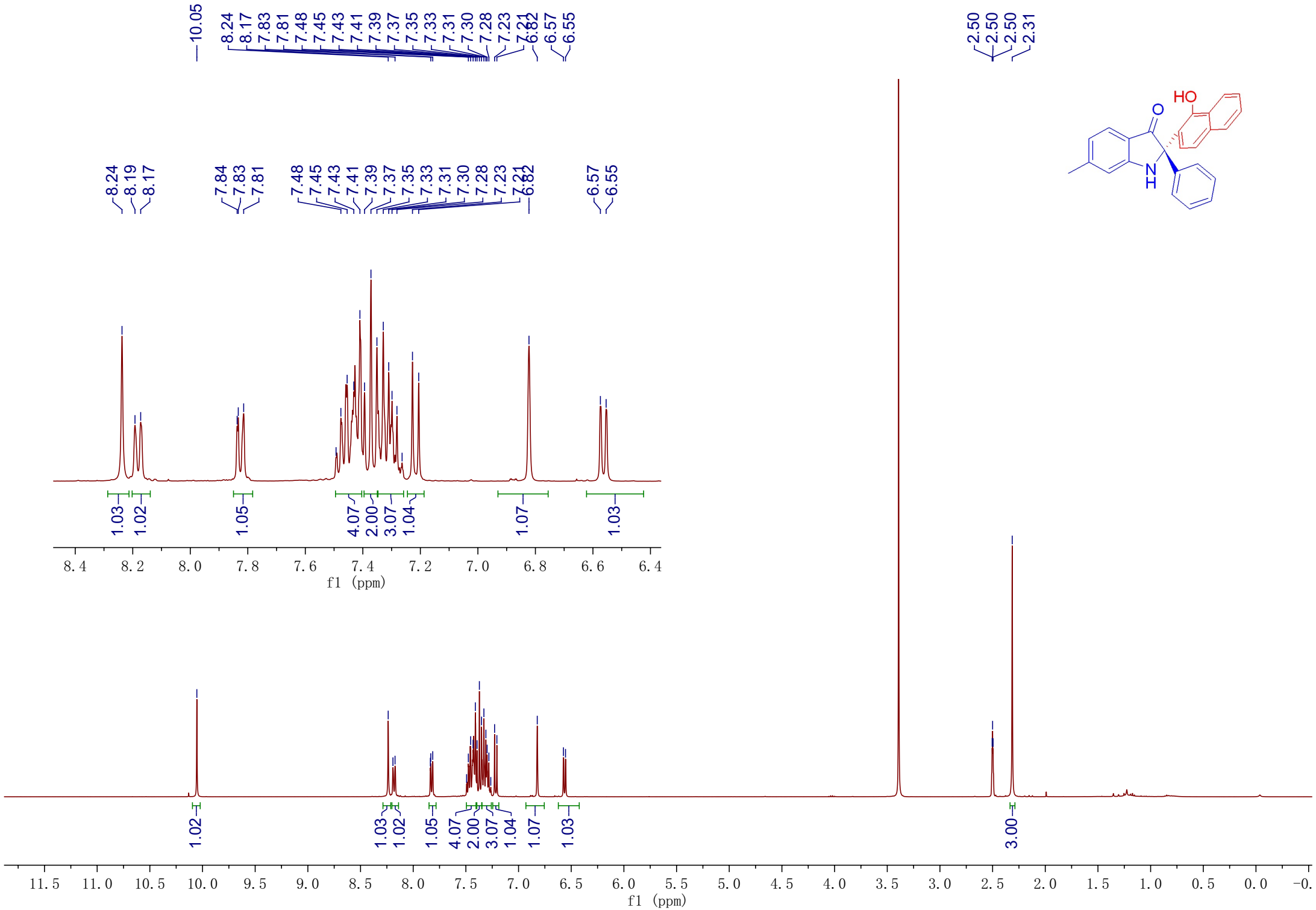

-127.14
HO
O
F
N
H
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

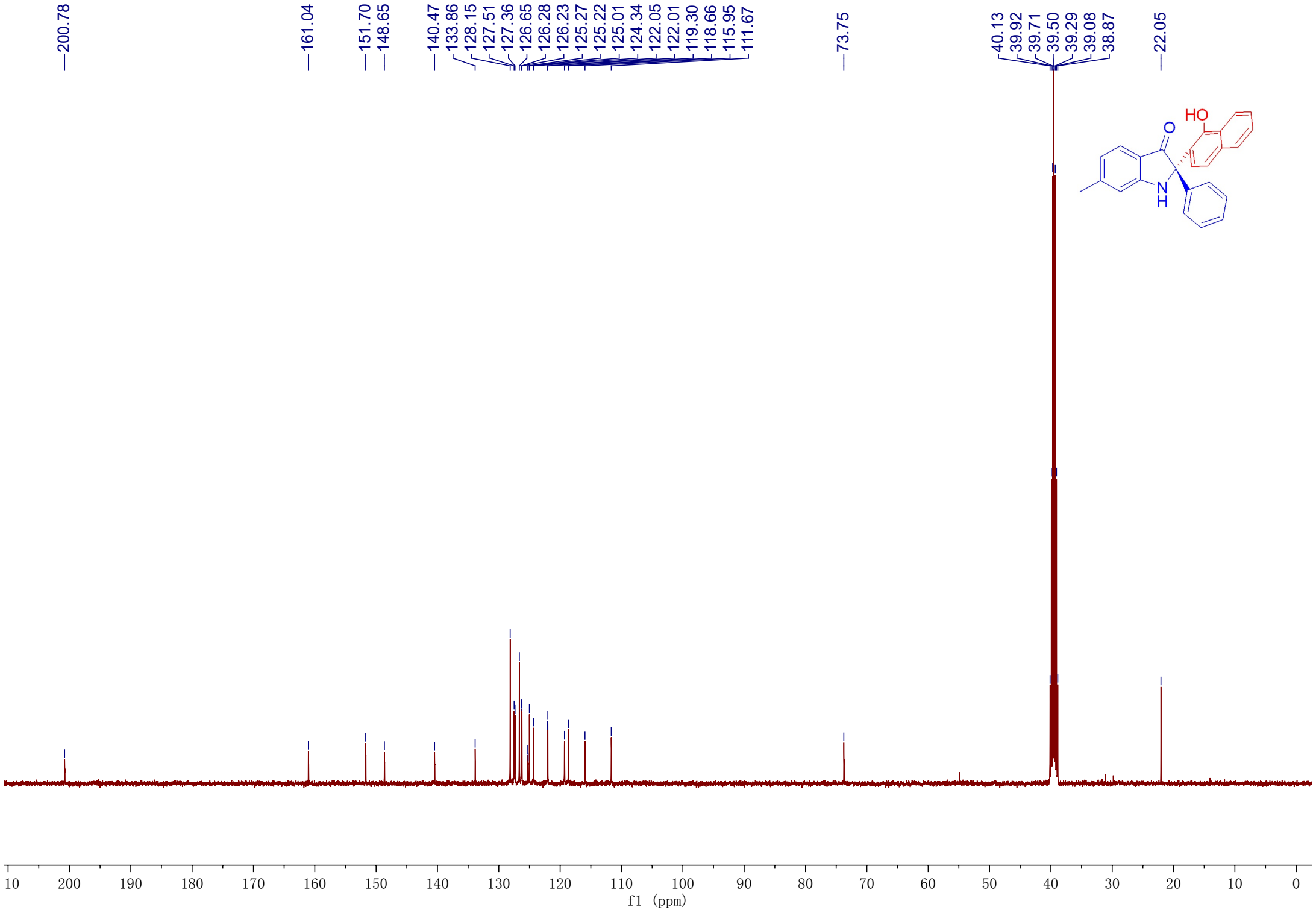

9.96
8.42
8.19
8.17
7.83
7.82
7.52
7.50
7.48
7.47
7.46
7.44
7.38
7.38
7.37
7.35
7.35
7.34
7.32
7.03
7.02
7.00
2.50
HO
O
Cl
N
H
1.00
1.03
1.06
6.03
4.01
2.03
f1 (ppm)
0.94
1.00
1.03
1.06
6.03
4.01
2.03
f1 (ppm)

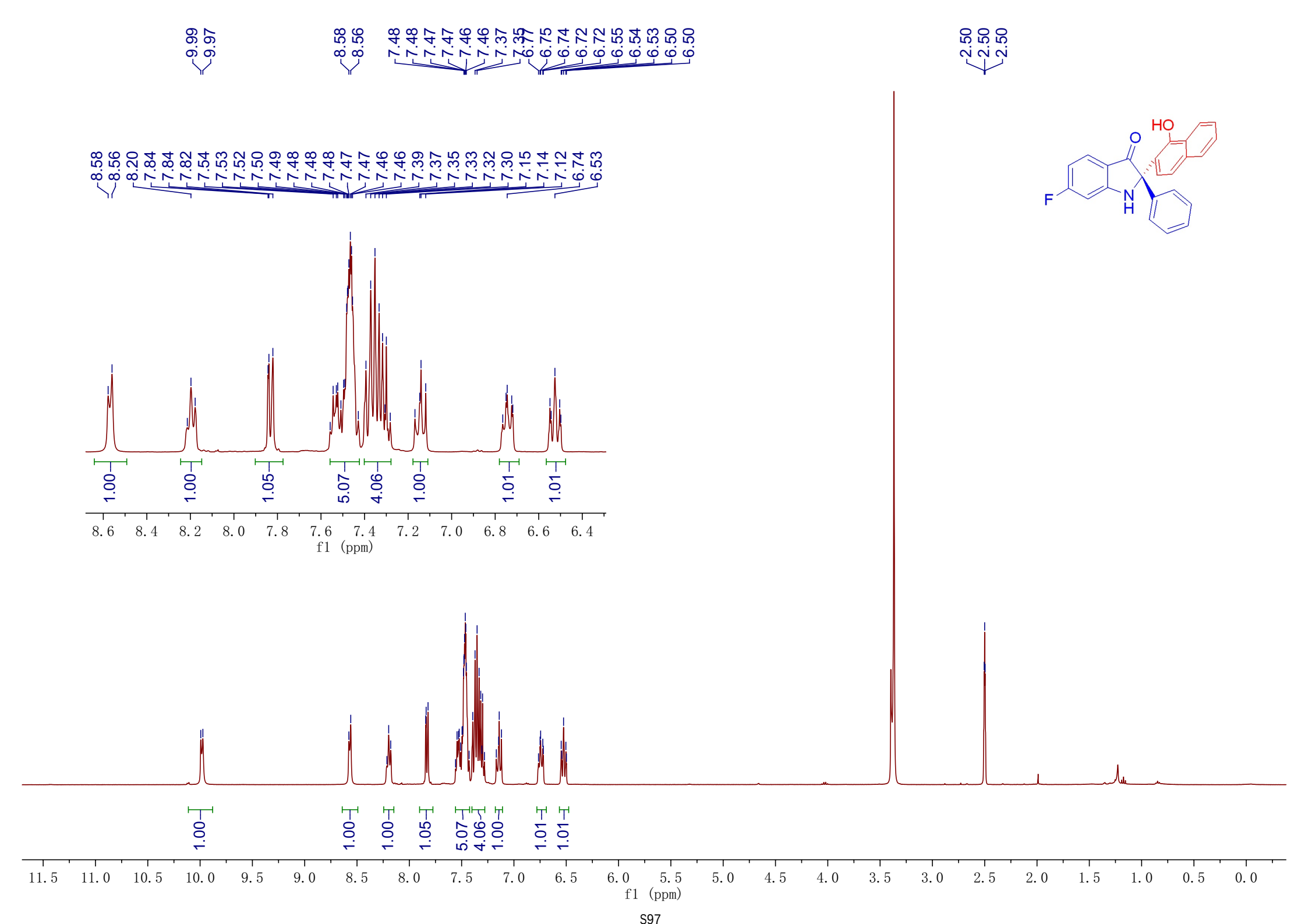

200.03
158.69
151.51
139.39
136.66
133.83
128.21
127.59
126.80
126.52
126.47
126.26
125.09
124.94
123.35
122.56
122.01
120.86
119.36
118.79
113.32
73.84
40.13
39.92
39.71
39.51
39.30
39.09
38.88
HO
O
Cl
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

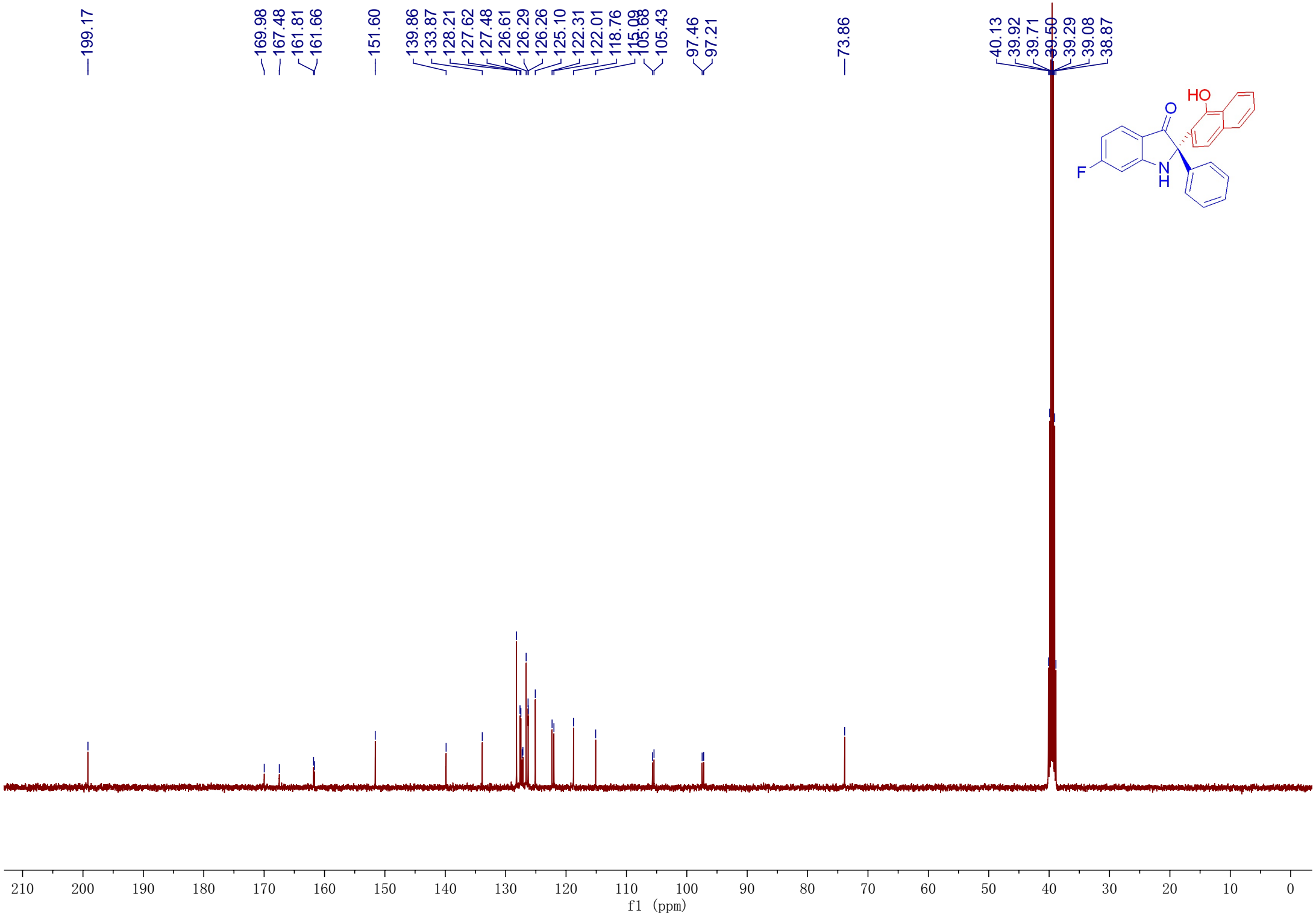

10.11
8.19
8.17
7.92
7.83
7.83
7.81
7.49
7.48
7.47
7.46
7.45
7.43
7.43
7.41
7.39
7.37
7.35
7.34
7.33
7.31
7.30
7.30
7.28
7.22
7.22
7.20
7.19
7.03
7.01
6.95
6.95
3.72
2.50
2.50
2.50
HO
O
MeO
N
H
1.00
1.02
1.03
4.00
1.01
3.05
2.02
1.00
1.02
8.1
7.9
7.7
7.5
7.3
7.1
6.9
f1 (ppm)
0.98
1.00
1.02
1.03
4.00
1.01
3.05
2.02
1.00
1.02
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

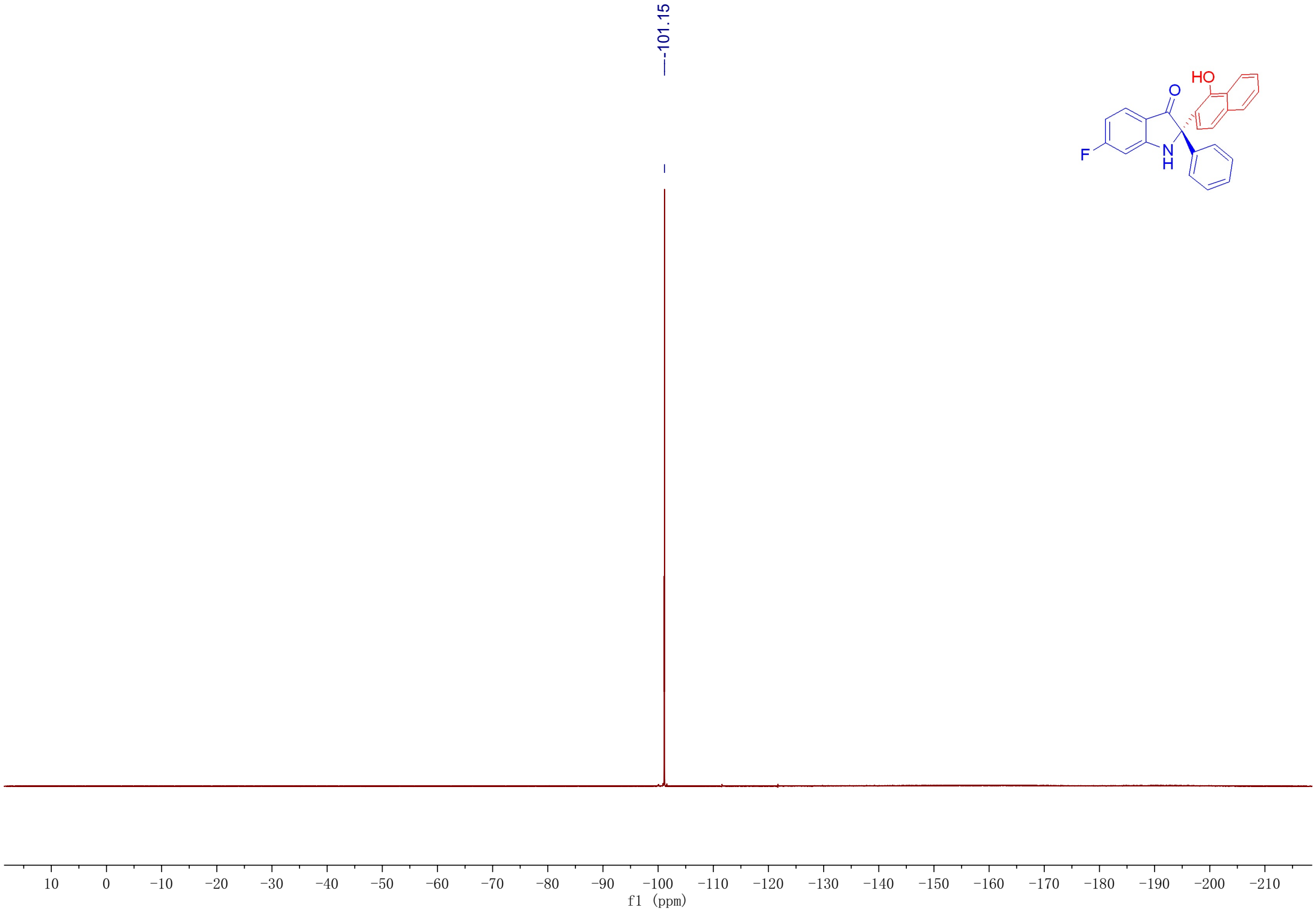

201.49
156.59
152.23
151.71
140.61
128.15
127.51
127.34
126.69
126.33
125.00
122.02
121.89
118.59
113.79
104.64
74.47
55.54
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
MeO
N
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

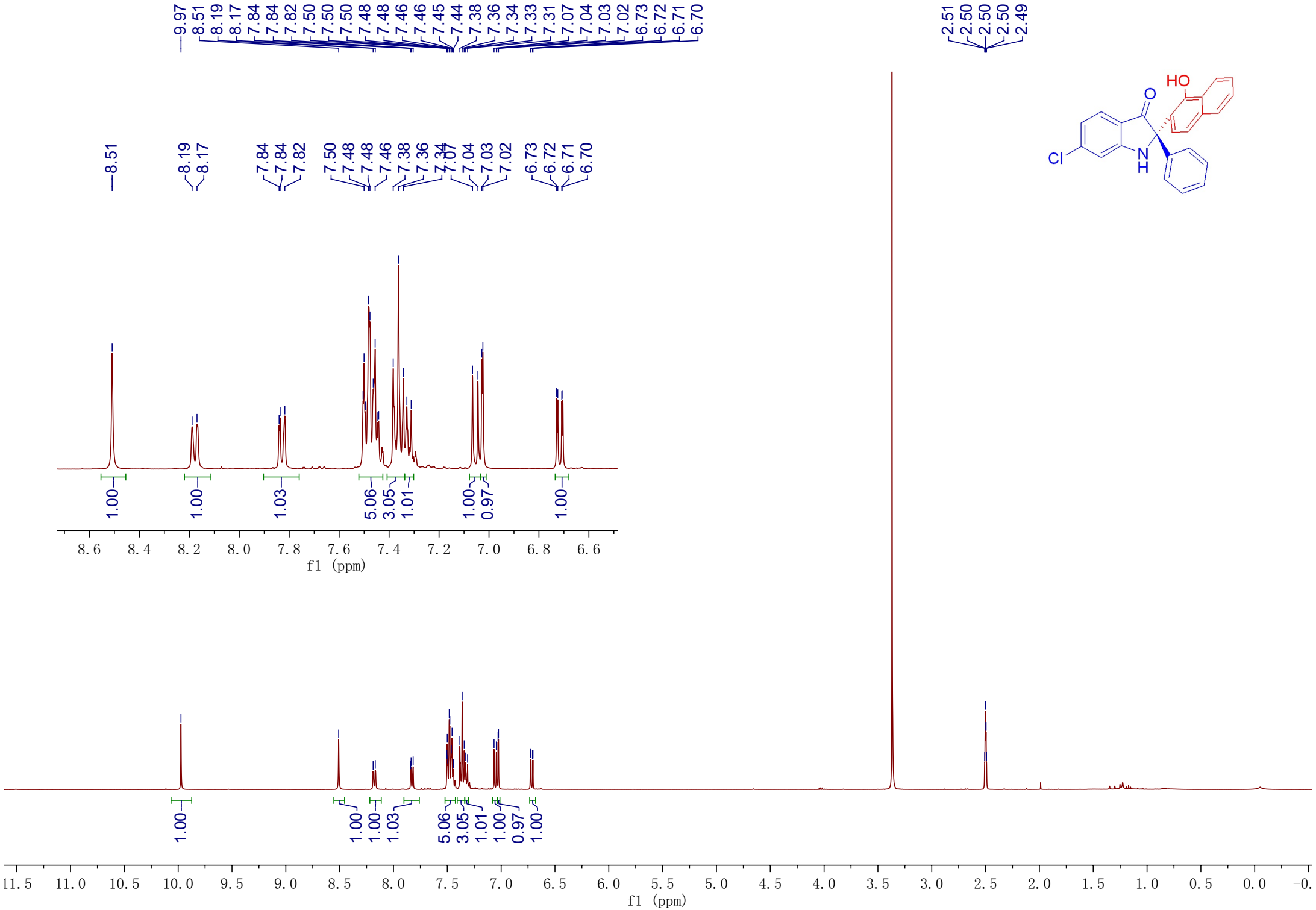

10.05
8.24
8.17
7.83
7.81
7.48
7.45
7.43
7.41
7.39
7.37
7.35
7.33
7.31
7.30
7.28
7.23
7.21
6.82
6.57
6.55
2.50
2.50
2.50
2.31
HO
O
N
H
1.02
1.03
1.02
1.05
4.07
2.00
3.07
1.04
1.07
1.03
3.00
f1 (ppm)

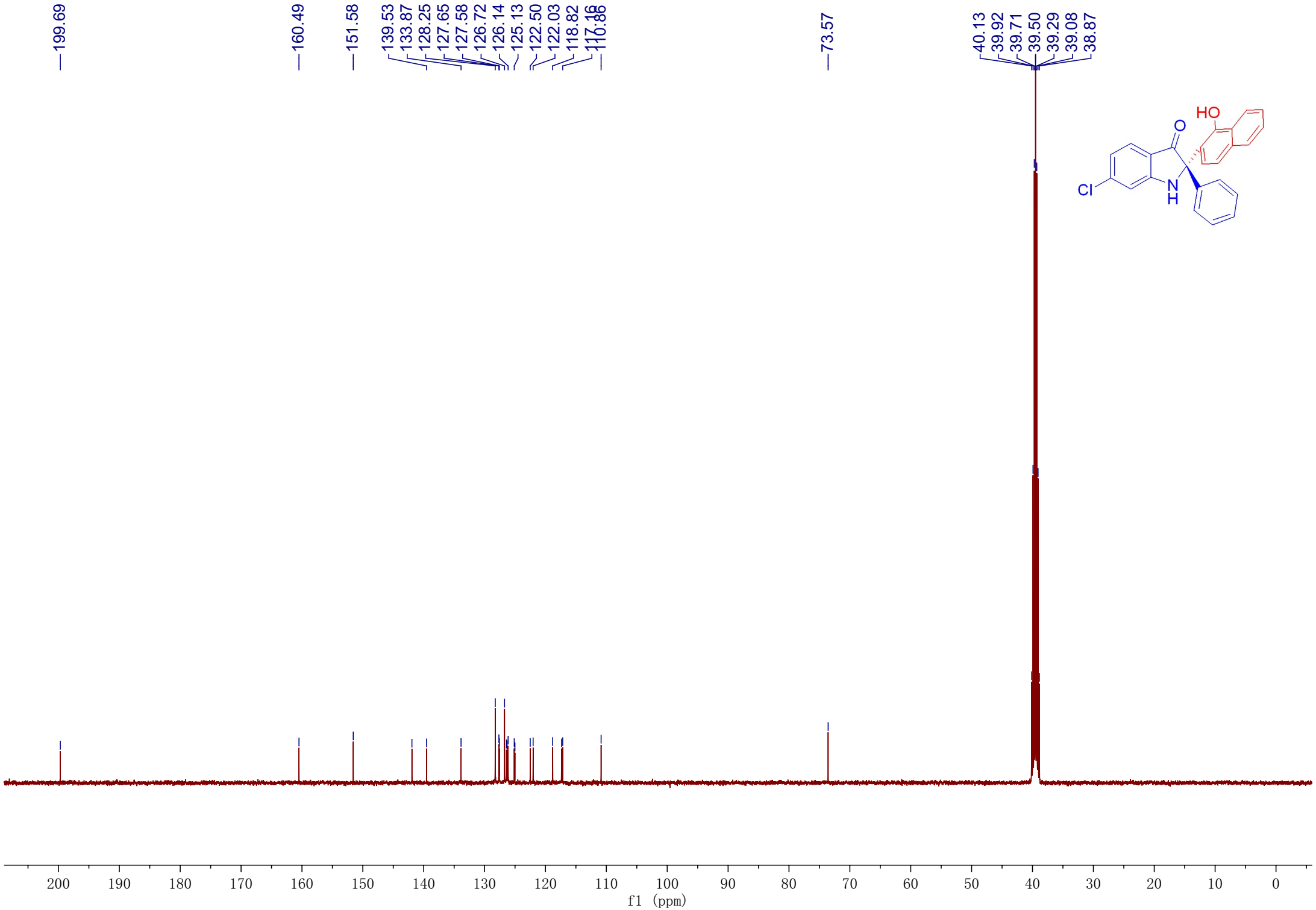

200.78
161.04
151.70
148.65
140.47
133.86
128.15
127.51
127.36
126.65
126.28
126.23
125.27
125.22
125.01
124.34
122.05
122.01
119.30
118.66
115.95
111.67
73.75
40.13
39.92
39.71
39.50
39.29
39.08
38.87
22.05
HO
O
N
H
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

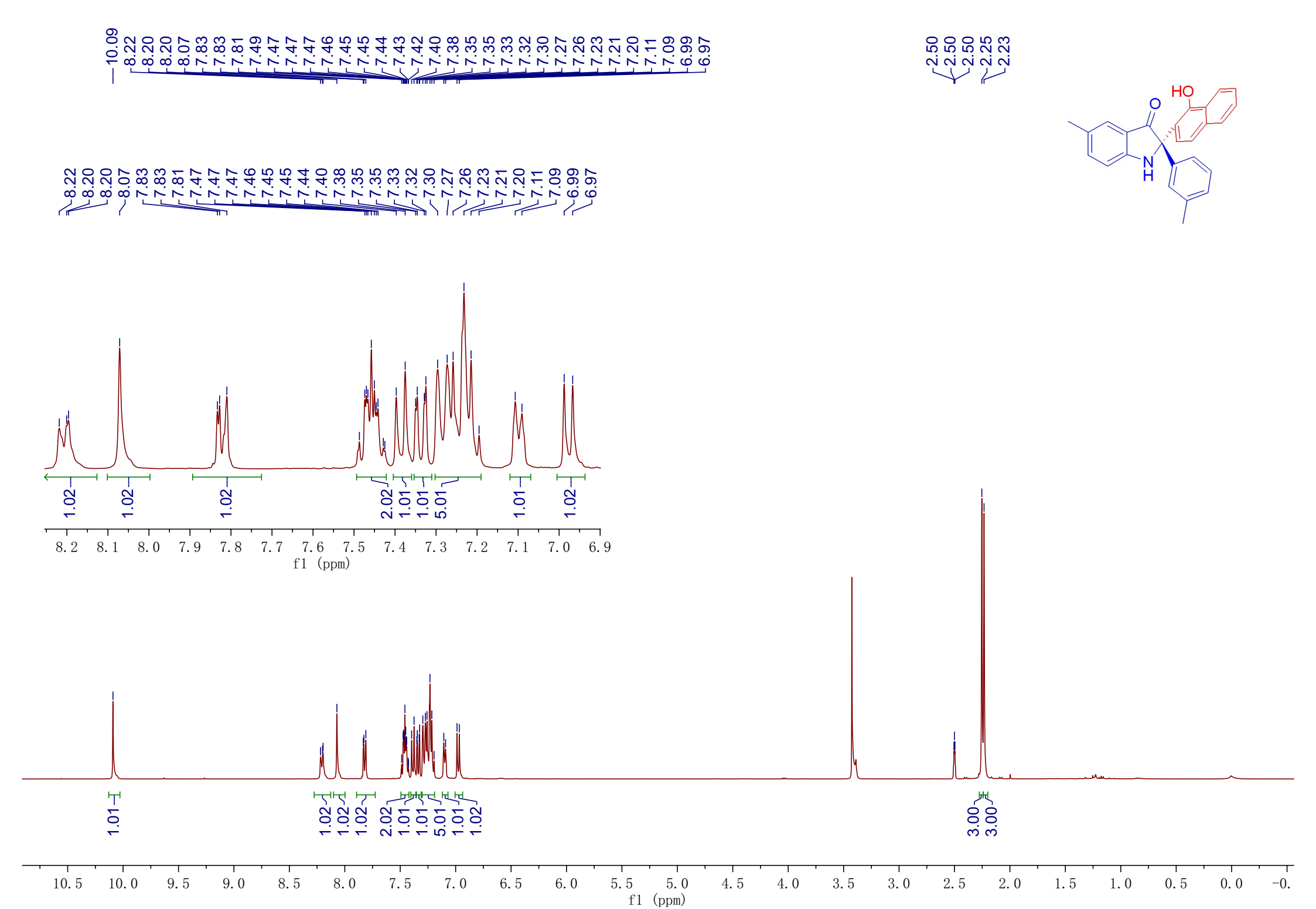

9.99
9.97
8.58
8.56
7.48
7.48
7.47
7.47
7.46
7.46
7.37
7.35
6.77
6.75
6.74
6.72
6.72
6.55
6.54
6.53
6.50
6.50
2.50
2.50
2.50
HO
O
F
N
H
1.00
1.00
1.05
5.07
4.06
1.00
1.01
1.01
f1 (ppm)

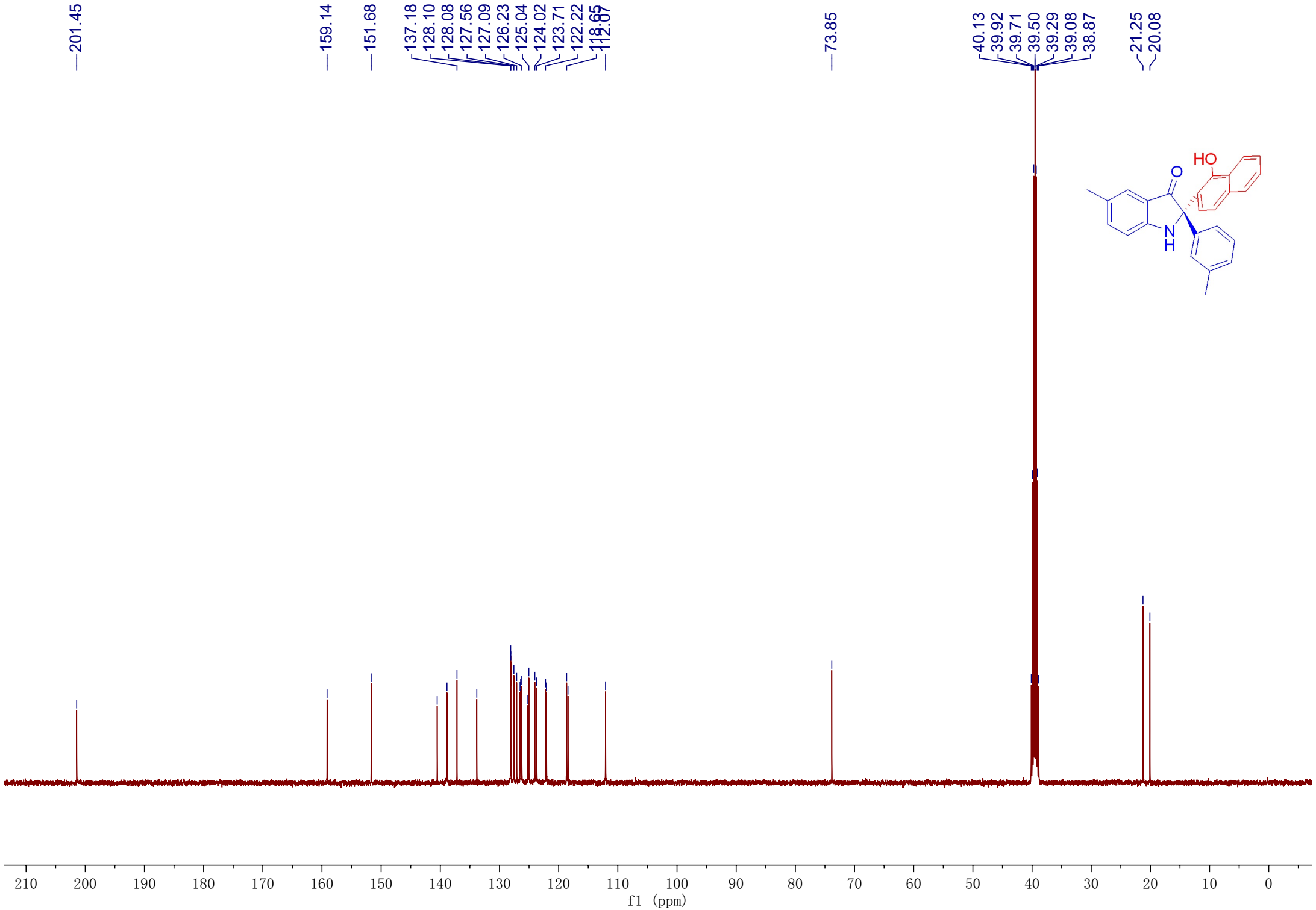

199.17
169.98
167.48
161.81
161.66
151.60
139.86
133.87
128.21
127.62
127.48
126.61
126.29
126.26
125.10
122.31
122.01
118.76
115.09
105.68
105.43
97.46
97.21
73.86
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
F
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-101.15
HO
O
F
N
H
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)

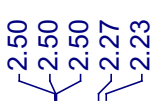

9.97
8.51
8.19
8.17
7.84
7.84
7.82
7.50
7.50
7.50
7.48
7.48
7.46
7.46
7.45
7.44
7.38
7.36
7.34
7.33
7.31
7.07
7.04
7.03
7.02
6.73
6.72
6.71
6.70
2.51
2.50
2.50
2.50
2.49
HO
O
Cl
N
H
1.00
1.00
1.03
5.06
3.05
1.01
1.00
0.97
1.00
f1 (ppm)


199.69
160.49
151.58
139.53
133.87
128.25
127.65
127.58
126.72
126.14
125.13
122.50
122.03
118.82
73.57
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
O
Cl
N
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

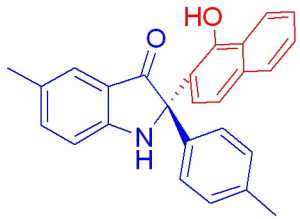

10.09
8.22
8.20
8.20
8.07
7.83
7.83
7.81
7.49
7.47
7.47
7.47
7.46
7.45
7.45
7.44
7.43
7.42
7.40
7.38
7.35
7.35
7.33
7.32
7.30
7.27
7.26
7.23
7.21
7.20
7.11
7.09
6.99
6.97
2.50
2.50
2.50
2.25
2.23
HO
O
N
H
1.02
1.02
1.02
2.02
1.01
1.01
5.01
1.01
1.02
f1 (ppm)
1.01
1.02
1.02
1.02
2.02
1.01
1.01
5.01
1.01
1.02
3.00
3.00
f1 (ppm)

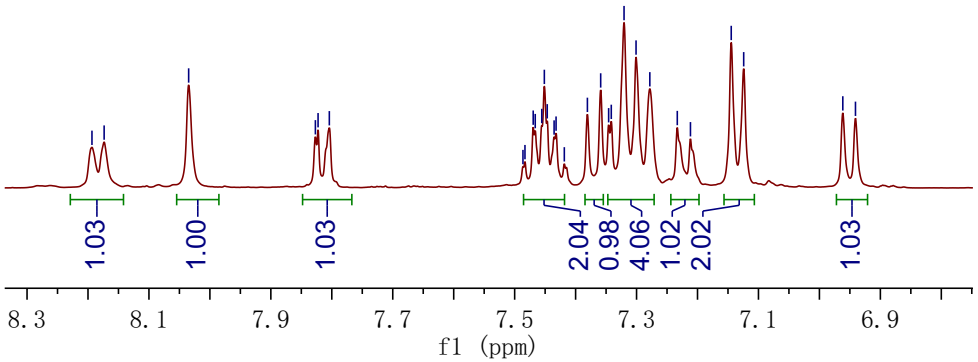

201.45
159.14
151.68
137.18
128.10
128.08
127.56
127.09
126.23
125.04
124.02
123.71
122.22
73.85
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.25
20.08
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

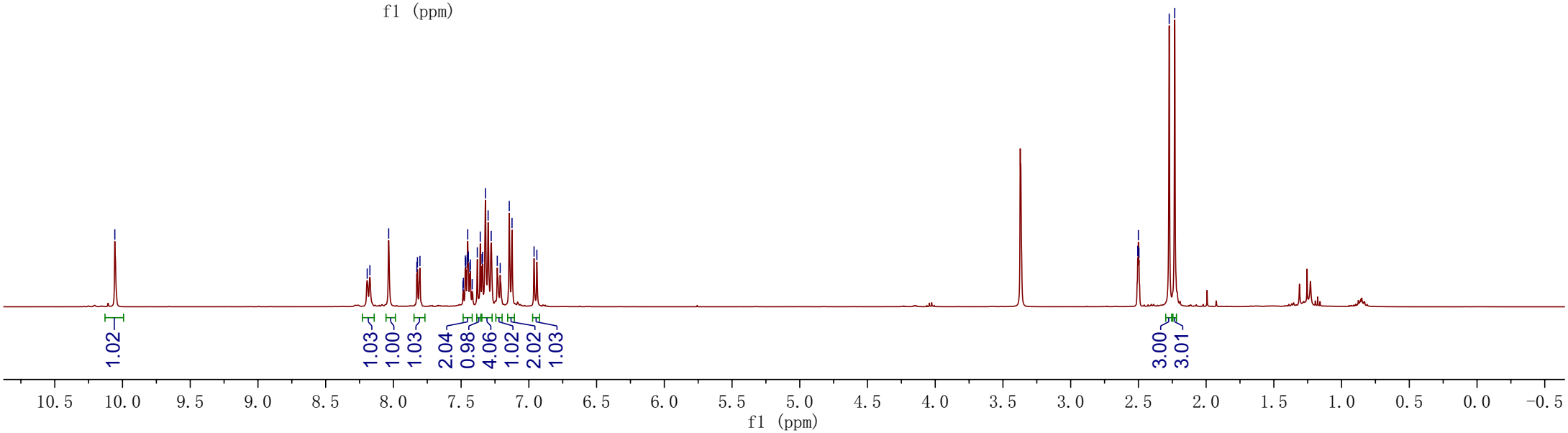

10.06
8.19
8.17
8.03
7.83
7.82
7.80
7.49
7.48
7.47
7.47
7.46
7.45
7.45
7.44
7.43
7.42
7.38
7.36
7.35
7.34
7.32
7.30
7.28
7.23
7.21
7.14
7.12
6.96
6.94

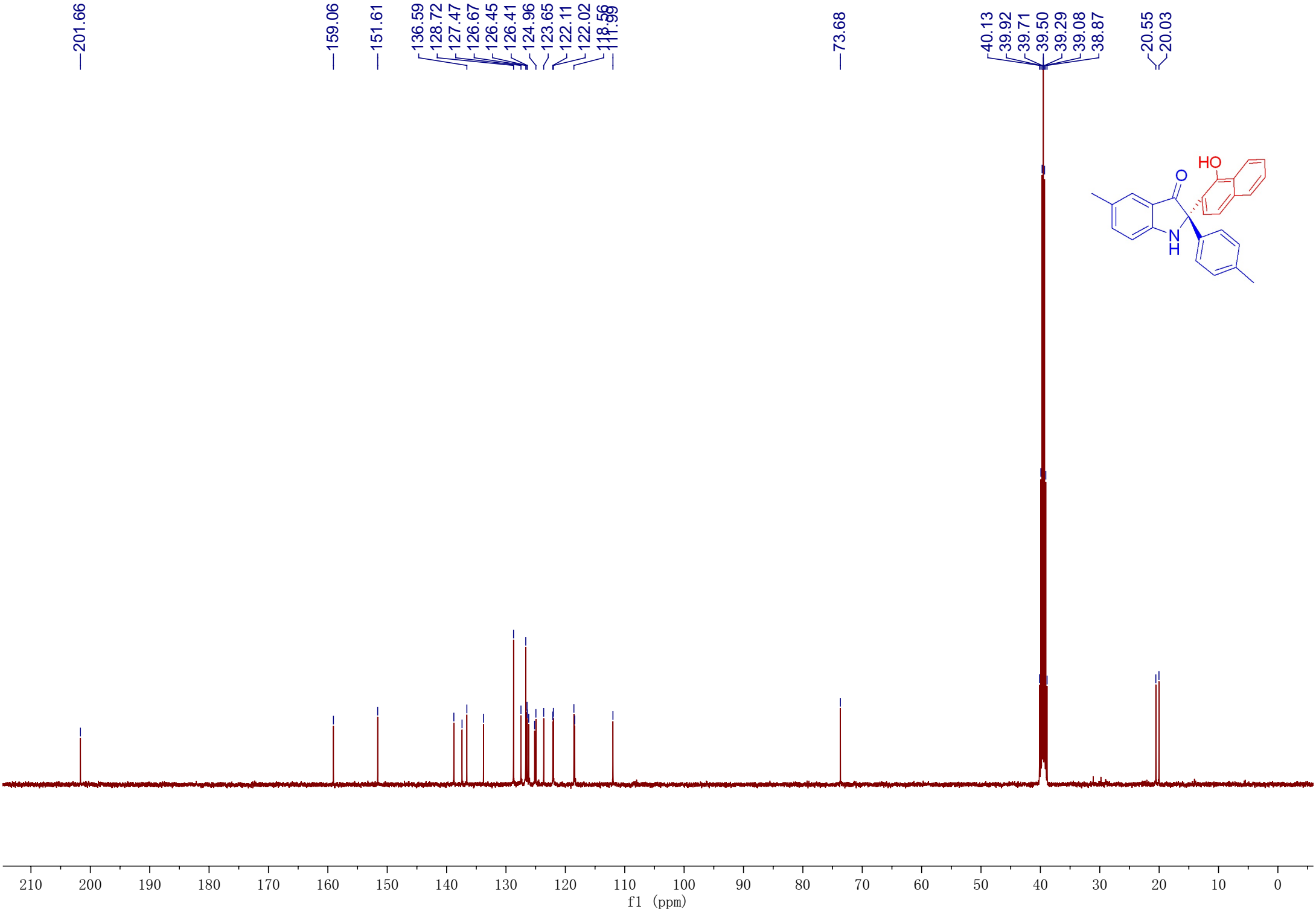

2.50
2.50
2.50
2.27
2.23

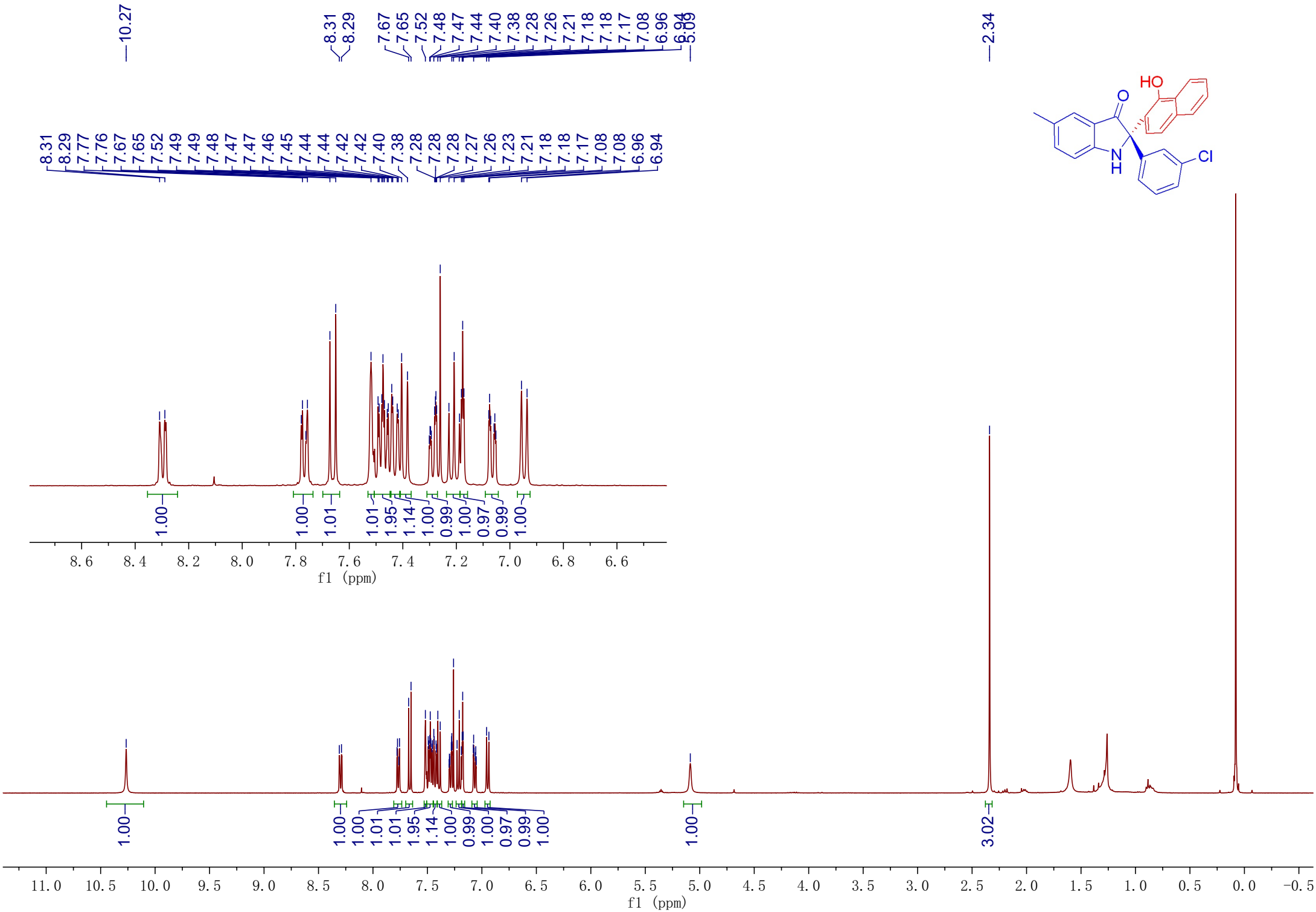

8.19
8.17
8.03
7.83
7.82
7.80
7.47
7.46
7.45
7.45
7.38
7.36
7.35
7.34
7.32
7.30
7.28
7.23
7.14
7.12
6.96
6.94

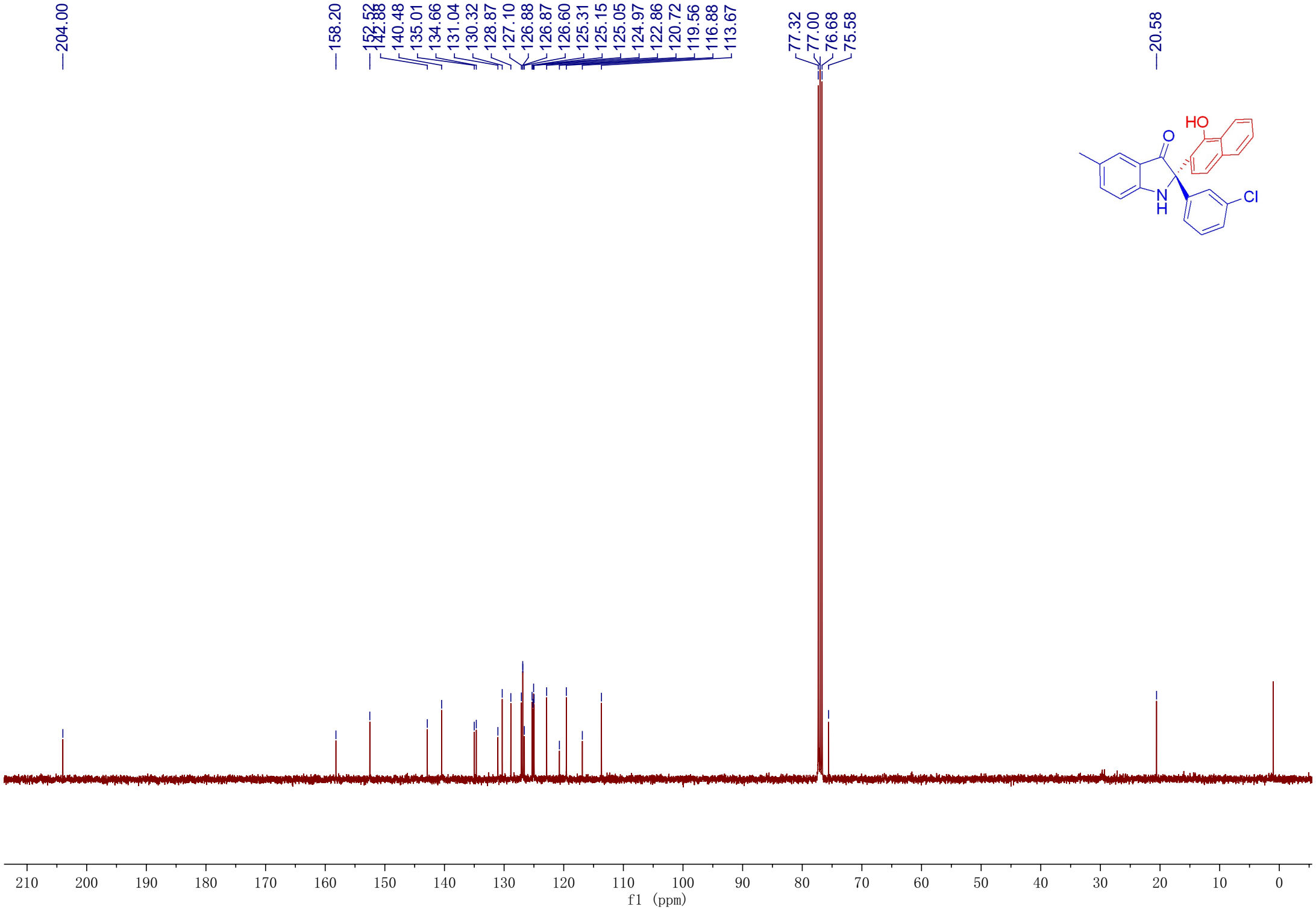

HO
O
N
H

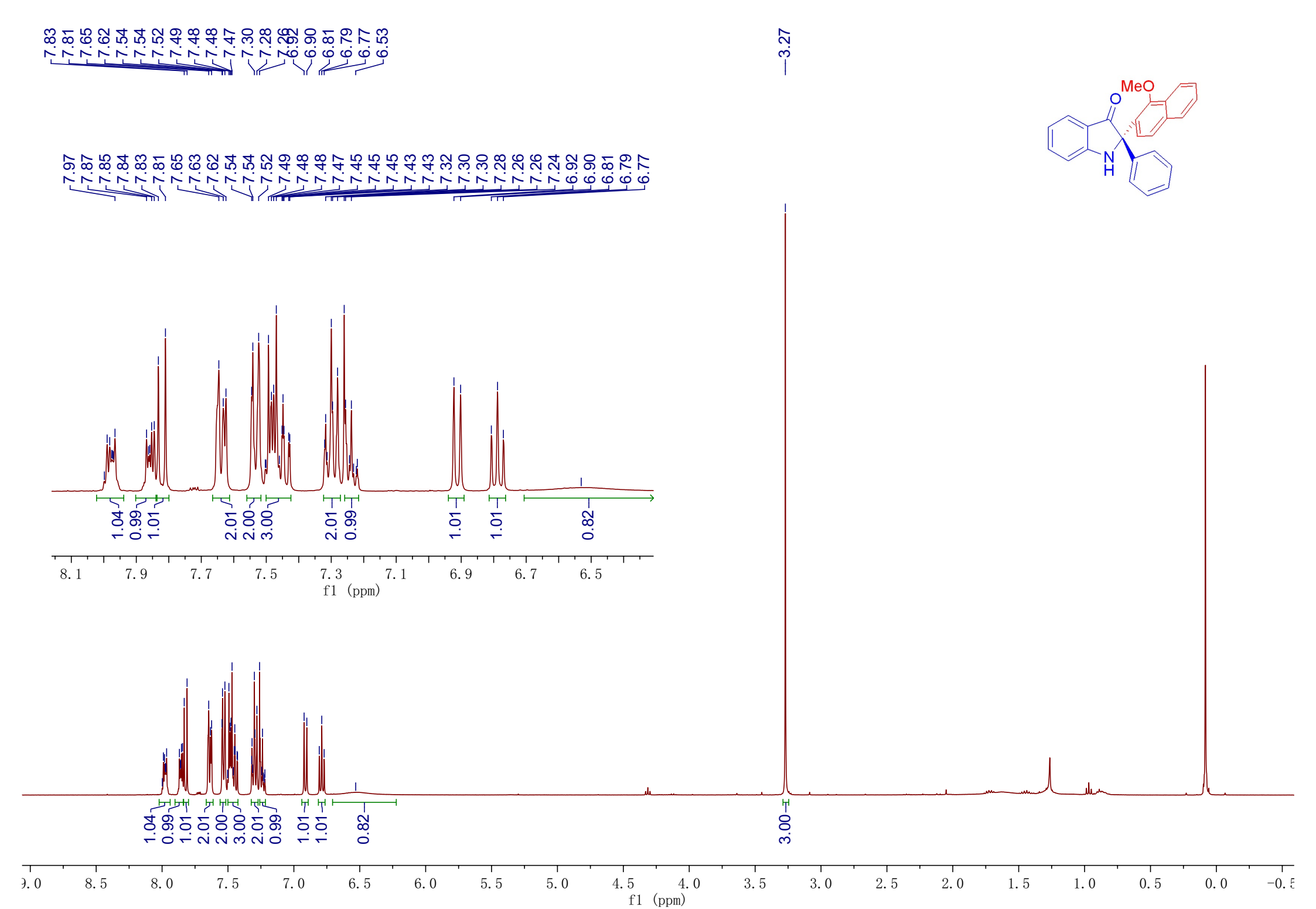

1.03
1.00
1.03
2.04
0.98
4.06
1.02
2.02
1.03
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
f1 (ppm)

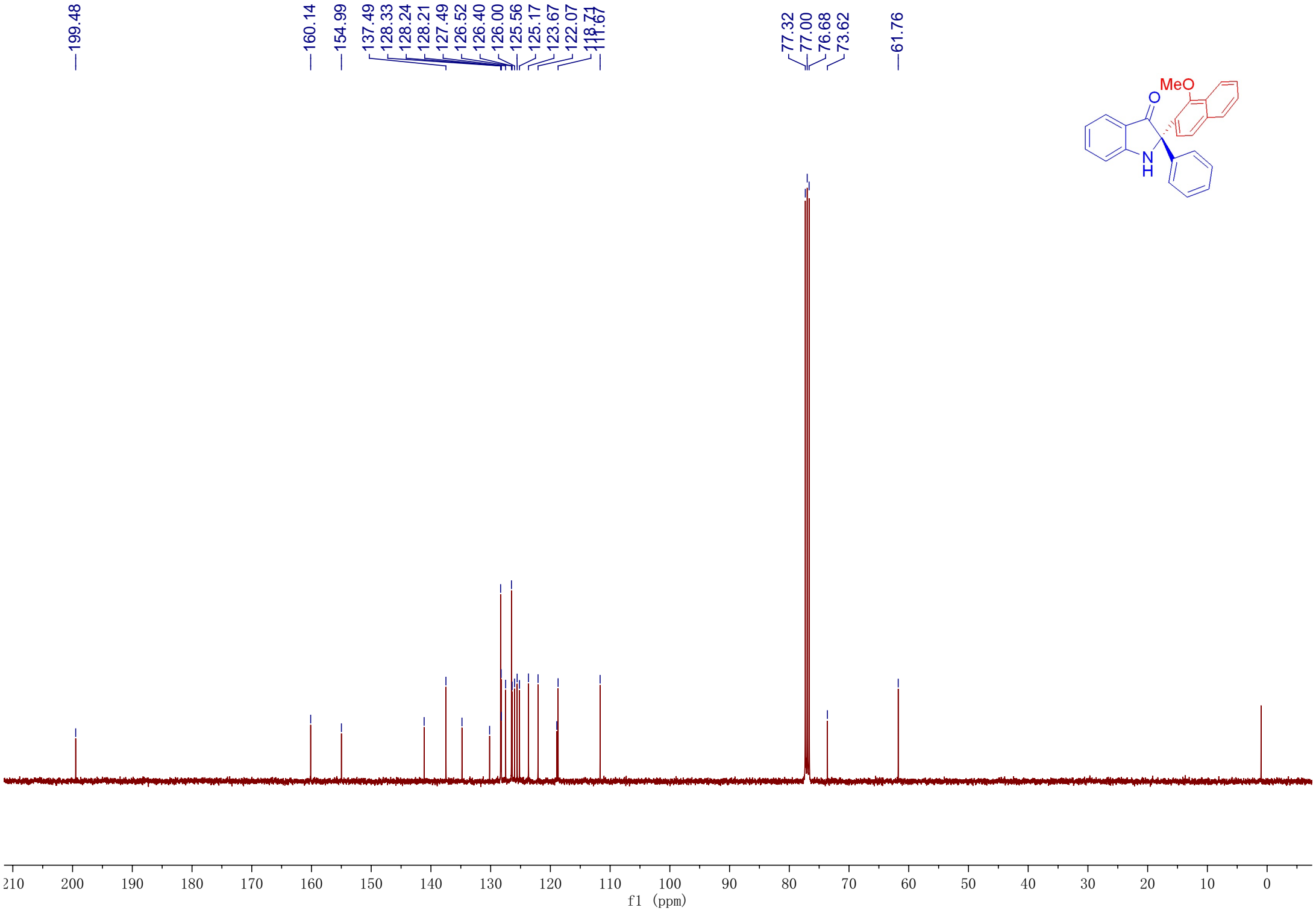

1.02
1.03
1.00
1.03
2.04
0.98
4.06
1.02
2.02
1.03
3.00
3.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

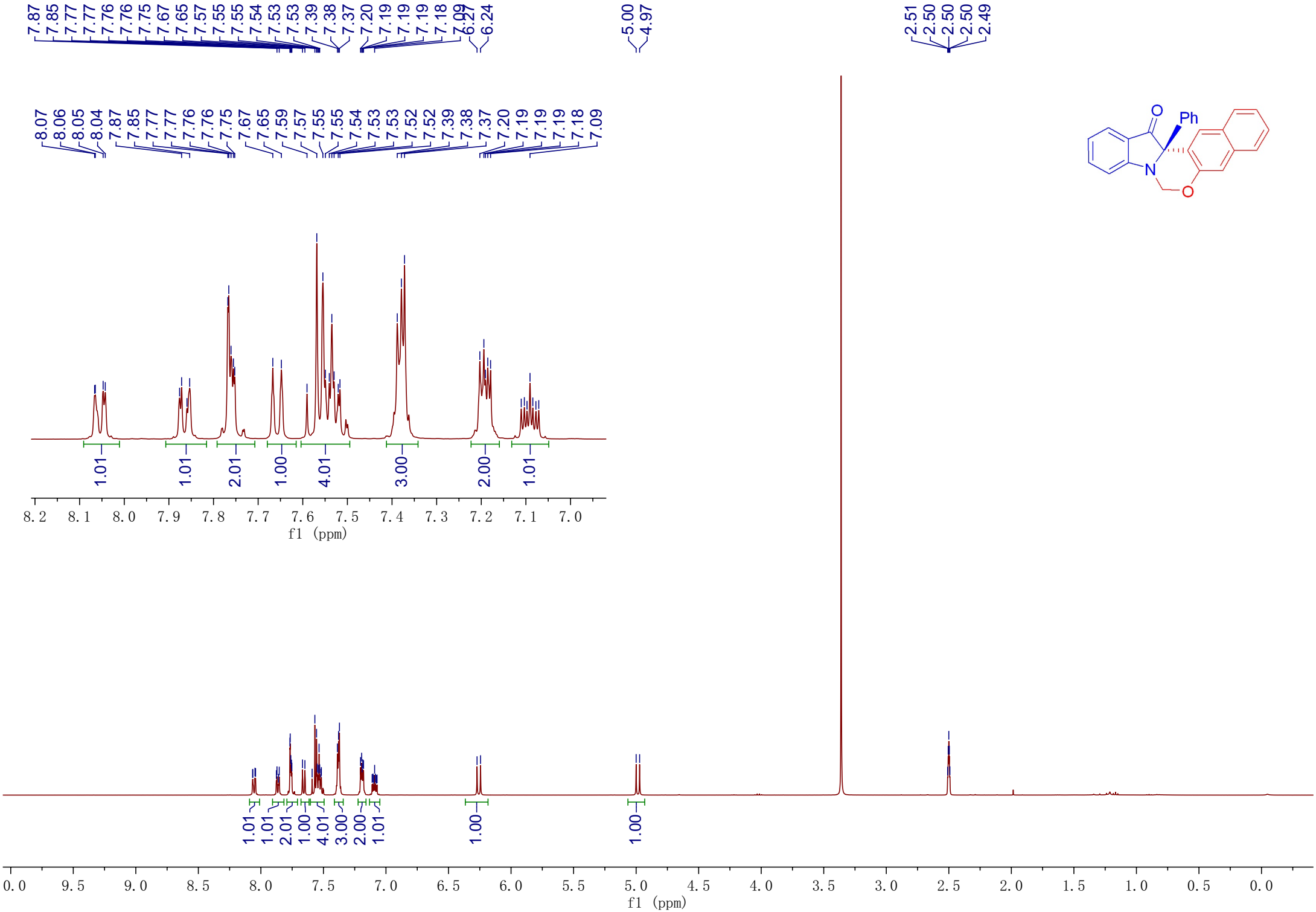

201.66
159.06
151.61
136.59
128.72
127.47
126.67
126.45
126.41
124.96
123.65
122.11
122.02
73.68
40.13
39.92
39.71
39.50
39.29
39.08
38.87
20.55
20.03
HO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

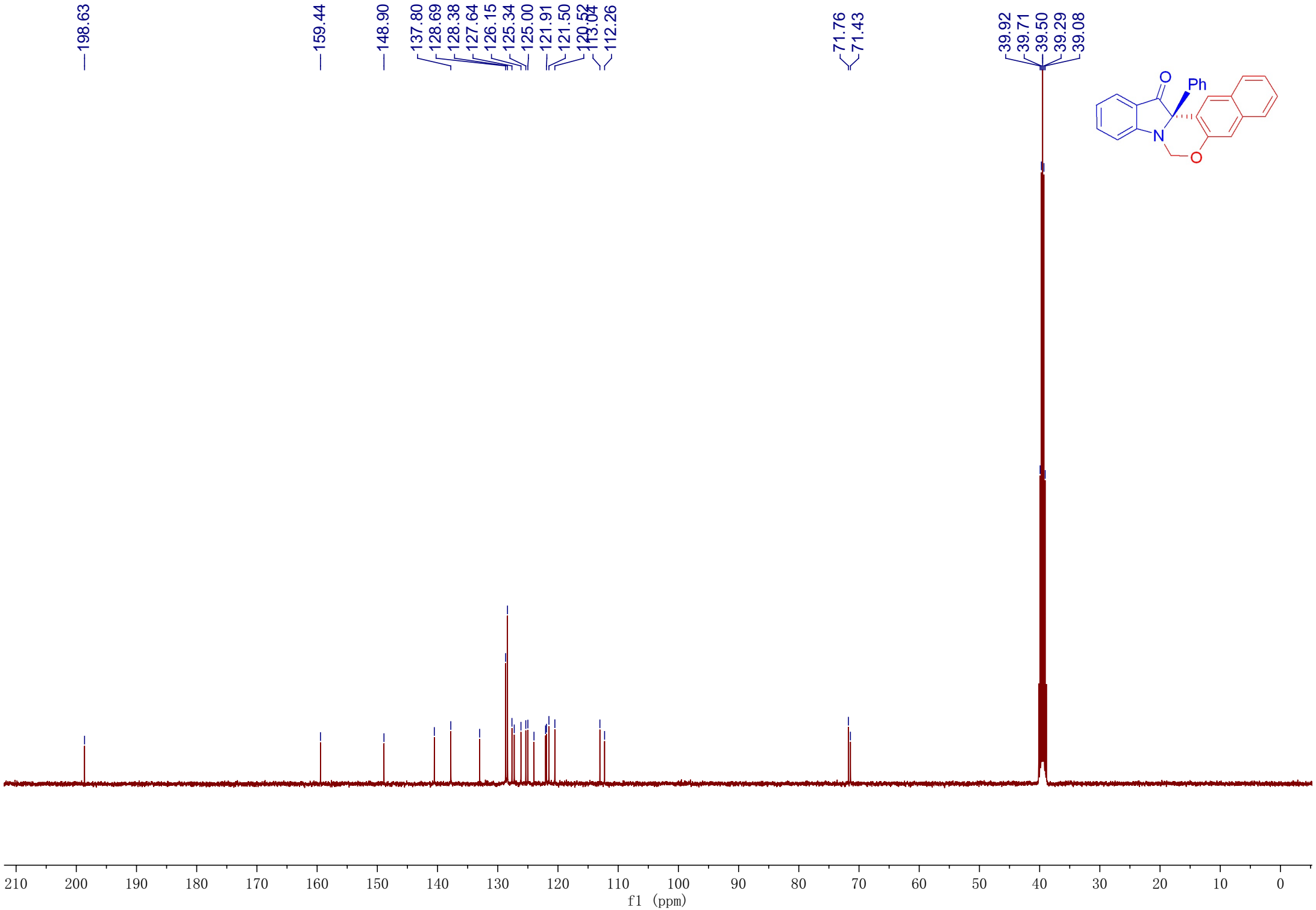

10.27
8.31
8.29
7.67
7.65
7.52
7.48
7.47
7.44
7.40
7.38
7.28
7.26
7.21
7.18
7.18
7.17
7.08
6.96
6.94
5.09
2.34
HO
O
N
H
Cl
f1 (ppm)
f1 (ppm)


204.00
158.20
152.52
142.88
140.48
135.01
134.66
131.04
130.32
128.87
127.10
126.88
126.87
126.60
125.31
125.15
125.05
124.97
122.86
120.72
119.56
116.88
113.67
77.32
77.00
76.68
75.58
20.58
HO
O
N
H
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)


7.83
7.81
7.65
7.62
7.54
7.54
7.52
7.49
7.48
7.48
7.47
7.30
7.28
7.26
6.92
6.90
6.81
6.79
6.77
6.53
3.27
MeO
O
N
H
7.97
7.87
7.85
7.84
7.83
7.81
7.65
7.63
7.62
7.54
7.54
7.52
7.49
7.48
7.48
7.47
7.45
7.45
7.45
7.43
7.43
7.32
7.30
7.30
7.28
7.26
7.26
7.24
6.92
6.90
6.81
6.79
6.77
1.04
0.99
1.01
2.01
2.00
3.00
2.01
0.99
1.01
1.01
0.82
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
6.5
f1 (ppm)
1.04
0.99
1.01
2.01
2.00
3.00
2.01
0.99
1.01
1.01
0.82
3.00
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)


199.48
160.14
154.99
137.49
128.33
128.24
128.21
127.49
126.52
126.40
126.00
125.56
125.17
123.67
122.07
118.71
111.67
77.32
77.00
76.68
73.62
61.76
MeO
O
N
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.87 7.85 7.77 7.77 7.76 7.76 7.75 7.67 7.65 7.57 7.55 7.55 7.54 7.53 7.53 7.39 7.38 7.37 7.20 7.19 7.19 7.19 7.18 7.09 6.27 6.24
5.00 4.97
2.51 2.50 2.50 2.50 2.49
8.07 8.06 8.05 8.04 7.87 7.85 7.77 7.77 7.76 7.76 7.75 7.67 7.65 7.59 7.57 7.55 7.55 7.54 7.53 7.53 7.52 7.52 7.39 7.38 7.37 7.20 7.19 7.19 7.19 7.18 7.09
O
Ph
N
O
1.01 1.01 2.01 1.00 4.01 3.00 2.00 1.01
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
1.01 1.01 2.01 1.00 4.01 3.00 2.00 1.01 1.00 1.00
0.0 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)


198.63
159.44
148.90
137.80
128.69
128.38
127.64
126.15
125.34
125.00
121.91
121.50
120.52
113.04
112.26
71.76
71.43
39.92
39.71
39.50
39.29
39.08
O
Ph
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)