Electronic Supporting Information

Synthesis of 2-arylchromeno[2,3,4,5-lmna]phenanthridines through a sequential multicomponent assembly, oxygenation and 6πe electrocyclization reactions

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General information and methods

Melting points were determined on a melting point apparatus, Büchi B-540, and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on 400, 500, and 600 MHz and 100, 125, and 150 MHz NMR spectrometers. TMS was used as an internal reference; chemical shifts (δ scale) are reported in parts per million(ppm). ^{1}H NMR spectra are reported in the order of multiplicity, coupling constant (J value) in Hertz (Hz), and number of protons; signals were characterized as *s* (singlet), *d* (doublet), *t* (triplet), *m* (multiplet), and *bs* (broad). IR spectra were recorded on an IR spectrophotometer. HRMS spectra were recorded using ESI and UHPLC-QTOF mode. The crystal structure was determined using a single-crystal XRD diffractometer. X-ray crystal structures were determined with a diffractometer. The UV-Visible absorption spectra were recorded using quartz cuvettes with a 10-mm path length and wavelengths ranging from 300 nm to 500 nm on a Agilent Cary Series spectrometer. For all spectra, baseline correction was utilized. The emission spectra were acquired on a Fluoromax Plus spectrophotometer using standard 10 mm path quartz cuvettes. All the experiments were carried out at room temperature.

Crystal refinement data

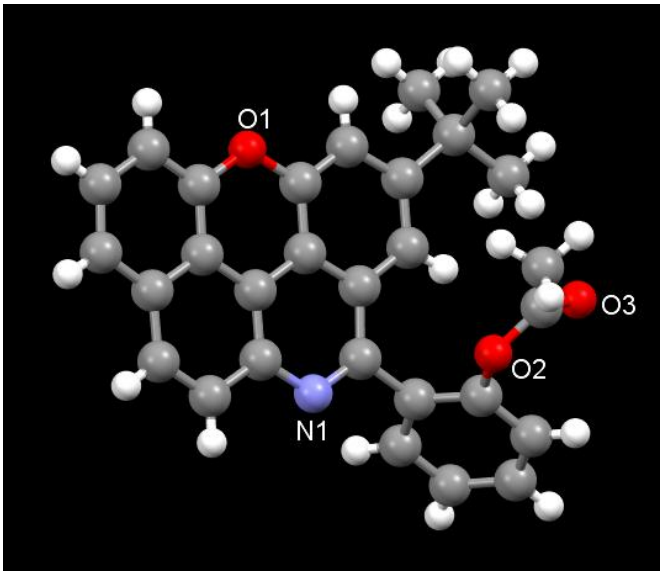


Figure S1. ORTEP Diagrams of compound **5aa** (CCDC No. **2362310**)

Table S1. Crystal data and structure refinement for compound **5aa**

Entry	Identification Code	Compound 5aa
01	Empirical formula	C_{29} H_{25} N O_4
02	Formula weight	451.50
03	Temperature	297 K
04	Wavelength	0.71073
05	Radiation type	Mo Kα
06	Radiation system	Fine-focus sealed tube
07	Crystal system	Triclinic
08	Space group	P-1
09	Cell length	a=7.165(3) b=11.129(4) c=16.227(7)
10	Cell angle	α=102.949(11) β=100.339(11) γ=106.162(11)
11	Cell volume	1170.1(8)
12	Density	1.281
13	Completeness to theta	98.2
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F2
16	Index ranges	-8<=h<=8, -13<=k<=13, -19<=l<=19
17	Reflection number	23631
18	Theta range	2.828-25.043
19	Cell formula units Z	2
20	CCDC no	2362310

Complete crystallographic data of compound **5aa** (CCDC no. **2362310**) for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk).

Experimental Section

General Experimental Procedure for the Synthesis of 2-(4-(*tert*-butyl)chromeno[2,3,4,5-*Imna*]phenanthridin-2-yl)phenol (5a). A reaction mixture containing the 2-naphthylamine **1** (35.75 mg, 0.25 mmol), salicylaldehyde (**2a**, 30.53 mg, 0.25 mmol), 4-*tert*-butylcyclohexanone (**3a**, 38.56 mg, 0.25 mmol), CSA (17.42 mg, 30 mol%) in DMSO (1 mL) was stirred at 80 °C (3-5 hr) 120 °C for 12 hr (TLC Monitored). Then, the reaction mixture was extracted with DCM (3×5 ml). The organic layer was washed with brine solution, dried over anhydrous Na_2SO_4, filtrated, and evaporated under reduced pressure. The desired product **5a** was purified by column chromatography. Same procedure was followed for the preparation of substrate **5b-5r.**

General Experimental Procedure of 5aa and mention its characterization data in the last

The characterization data for the compounds **5a-r**

2-(4-(tert-butyl)chromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenol (5a)

Dark yellow solid, (63 mg, 65%), mp 177-178 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.10 (s, 1H), 8.10 (d, *J* = 1.0 Hz, 1H), 7.93 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.87 (d, *J* = 9.0 Hz, 1H), 7.83 (d, *J* = 9.0 Hz, 1H), 7.49 (d, *J* = 4.5 Hz, 1H), 7.48 (d, *J* = 5.9 Hz, 1H), 7.43 (d, *J* = 1.1 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.22 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.10 (dd, *J* = 6.2, 2.3 Hz, 1H), 7.06 – 7.02 (m, 1H), 1.42 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.9, 157.6, 153.3, 152.7, 151.9, 134.9, 132.5, 131.3, 130.1, 128.9, 127.9, 126.6, 124.8, 122.4, 121.6, 120.7, 118.8, 118.8, 118.4, 116.8, 115.6, 112.5, 110.0, 35.8, 31.4; IR (neat)ν_{max}: 2960, 1618, 1263, 1251, 734 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{21}NO_2$ 392.1545 (M + H$^+$); Found 392.1548.

2-(4-(tert-butyl)chromeno[2,3,4,5-lmna]phenanthridin-2-yl)-4-chlorophenol (5b)

Yellow solid, (72 mg, 68%), mp 211-212 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.78 (s, 1H), 8.08 (d, *J* = 1.5 Hz, 1H), 7.95 (d, *J* = 2.5 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.54 – 7.48 (m, 2H), 7.45 (t, *J* = 1.9 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.15 (d, *J* = 8.8 Hz, 1H), 7.13 – 7.09 (m, 1H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6, 156.1, 153.7, 152.7, 152.0, 134.7, 132.6, 131.0, 129.7, 129.25, 128.1, 126.5, 124.6, 123.6, 122.5, 122.4, 120.8, 119.8, 118.7, 116.3, 116.0, 112.7, 110.2, 35.9, 31.4; IR (neat) ν_{max}: 2963, 1621, 1276, 1261, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{20}ClNO_2$ 426.1255 (M + H$^+$); Found 426.1258.

4-bromo-2-(4-(tert-butyl)chromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenol (5c)

Dark Yellow solid, (78 mg, 67%), mp 189-190 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.27 (s, 1H), 8.11 (d, *J* = 2.5 Hz, 1H), 8.09 (d, *J* = 1.5 Hz, 1H), 7.86 (d, *J* = 2.9 Hz, 2H), 7.53 – 7.50 (m, 2H), 7.50 – 7.47 (m, 1H), 7.46 (d, *J* = 1.5 Hz, 1H), 7.14 – 7.09 (m, 2H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 156.0, 153.7, 152.7, 152.1, 134.7, 133.8, 132.7, 132.6, 129.2, 128.2, 126.5, 124.6, 123.0, 122.4, 120.8, 120.2, 118.7,

116.4, 116.0, 112.7, 110.6, 110.2, 35.9, 31.4; IR (neat) ν_{max}: 2957, 1621, 1275, 1260, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{20}BrNO_2$ 470.0750 ($M + H^+$); Found 470.0751.

2-(4-(tert-butyl)chromeno[2,3,4,5-lmna]phenanthridin-2-yl)-4-methoxyphenol (5d)

Yellow solid, (73 mg, 70%), mp 150-151 °C; ^1H NMR (600 MHz, $CDCl_3$) δ 11.37 (s, 1H), 8.13 (s, 1H), 7.87 – 7.81 (m, 2H), 7.50 (d, *J* = 6.7 Hz, 2H), 7.46 (d, *J* = 3.1 Hz, 1H), 7.44 (d, *J* = 1.4 Hz, 1H), 7.15 (d, *J* = 8.9 Hz, 1H), 7.10 (dd, *J* = 6.5, 2.1 Hz, 1H), 7.02 (dd, *J* = 8.9, 3.0 Hz, 1H), 3.85 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 153.3, 152.7, 152.2, 152.0, 151.6, 135.0, 132.5, 129.0, 128.0, 126.6, 124.8, 122.4, 121.8, 120.7, 119.1, 118.7, 118.2, 116.7, 115.6, 114.5, 112.5, 110.0, 56.1, 35.8, 31.5; IR (neat)ν_{max}: 2962, 1618, 1275, 1260, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{28}H_{23}NO_3$ 422.1751 ($M + H^+$); Found 422.1764.

4-(tert-butyl)-2-phenylchromeno[2,3,4,5-lmna]phenanthridine (5e)

Yellow solid, (55 mg, 59%), mp 203-204 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 9.0 Hz, 1H), 7.84 (d, *J* = 9.2 Hz, 2H), 7.82 (s, 1H), 7.71 (s, 1H), 7.58 (t, *J* = 7.3 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 1H), 7.49 (d, *J* = 4.3 Hz, 2H), 7.40 (s, 1H), 7.09 (q, *J* = 4.4 Hz, 1H), 1.37 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 153.0, 152.9, 151.9, 139.8, 137.2, 132.4, 129.5, 129.0, 128.7, 128.6, 128.1, 127.4, 125.4, 121.5, 120.6, 119.1, 116.2, 115.5, 111.7, 109.7, 35.7, 31.4; IR (neat) ν_{max}: 2962, 1618, 1262, 1248, 822 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{21}NO$ 376.1696 ($M + H^+$); Found 376.1700.

4-(tert-butyl)-2-(4-fluorophenyl)chromeno[2,3,4,5-lmna]phenanthridine (5f)

Light yellow solid, (63 mg, 64%), mp 143-144 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 9.0 Hz, 1H), 7.86 – 7.79 (m, 3H), 7.65 (d, *J* = 1.5 Hz, 1H), 7.51 – 7.47 (m, 2H), 7.40 (d, *J* = 1.5 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.10 (t, *J* = 4.3 Hz, 1H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.3, 162.4, 158.4, 153.1, 152.8, 151.9, 137.1, 132.4, 131.4, 131.3, 128.7, 128.0, 127.5, 125.3, 121.5, 120.6, 119.0, 115.8, 115.8, 115.6, 115.5, 111.8, 109.8, 35.7, 31.4; ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.6; IR (neat) ν_{max}: 2963, 1618, 1275, 1261, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{20}FNO$ 394.1602 ($M + H^+$); Found 394.1603.

4-(tert-butyl)-2-(4-chlorophenyl)chromeno[2,3,4,5-lmna]phenanthridine (5g)

Light yellow solid, (63 mg, 62%), mp 151-152 °C; ^1H NMR (600 MHz, $CDCl_3$) δ 8.00 (d, *J* = 9.0 Hz, 1H), 7.85 (d, *J* = 9.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.65 (d, *J* = 1.3 Hz, 1H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.41 (s, 1H), 7.11 (m, *J* = 4.3 Hz, 1H), 1.38 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.2, 153.2, 152.9, 152.0, 138.2, 137.2, 135.1, 132.5, 130.9, 128.9, 128.8, 128.0, 127.6, 125.2, 121.5, 120.6, 119.0, 115.7, 115.7, 111.9, 109.8, 35.8, 31.4; IR (neat) ν_{max}: 2924, 1619, 1261, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{20}ClNO$ 410.1306 ($M + H^+$); Found 410.1307.

4-(tert-butyl)-2-(p-tolyl)chromeno[2,3,4,5-lmna]phenan-thridine (5h)

Light yellow solid, (55 mg, 57%), mp 153-154 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, *J* = 9.0 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 7.76 – 7.71 (m, 3H), 7.49 – 7.45 (m, 2H), 7.40 – 7.36 (m, 3H), 7.08 (dd, *J* = 5.0,

3.7 Hz, 1H), 2.49 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 152.8, 151.9, 138.9, 137.2, 136.9, 132.4, 129.4, 129.3, 128.5, 128.1, 127.3, 125.4, 121.4, 120.5, 119.1, 116.3, 115.3, 111.6, 109.6, 35.7, 31.4, 21.5; IR (neat) ν_{max}: 2964, 1619, 1262, 749 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{28}H_{23}NO$ 390.1852 ($M + H^+$); Found 390.1853.

4-(tert-butyl)-2-(4-nitrophenyl)chromeno[2,3,4,5-lmna]phenanthridine (5i)

Red solid, (63 mg, 60%), mp 123-124 °C; 1H NMR (400 MHz, CDCl3) δ 8.45 (d, J = 8.7 Hz, 2H), 8.02 (d, J = 8.7 Hz, 2H), 7.99 (d, J = 9.0 Hz, 1H), 7.86 (d, J = 9.1 Hz, 1H), 7.59 (d, J = 1.5 Hz, 1H), 7.54 – 7.51 (m, 2H), 7.44 (d, J = 1.5 Hz, 1H), 7.13 (dd, J = 6.3, 2.4 Hz, 1H), 1.38 (s, 9H); 13C NMR (125 MHz, CDCl3) δ 156.8, 153.7, 152.9, 152.1, 148.2, 146.1, 137.1, 132.7, 130.6, 129.2, 127.9, 127.9, 124.9, 124.0, 121.7, 120.8, 118.8, 116.1, 115.0, 112.2, 110.1, 35.8, 31.4; IR (neat) νmax: 2924, 1619, 1346, 1260, 800 cm-1; HRMS (ESI-QTOF) Calcd for C27H20N2O3 421.1547 (M + H+); Found 421.1547.

4-(tert-butyl)-2-(3-methoxyphenyl)chromeno[2,3,4,5-lmna]phenanthridine (5j)

Dark yellow solid, (60 mg, 60%), mp 138-139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 9.0 Hz, 1H), 7.84 (d, *J* = 9.1 Hz, 1H), 7.74 (d, *J* = 1.5 Hz, 1H), 7.51 – 7.46 (m, 3H), 7.40 (s, 1H), 7.40 – 7.38 (m, 1H), 7.36 (dd, *J* = 2.6, 1.5 Hz, 1H), 7.12 – 7.05 (m, 2H), 3.91 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 159.4, 153.0, 152.9, 151.9, 141.0, 137.1, 132.5, 129.6, 128.6, 128.1, 127.4, 125.3, 121.9, 121.5, 120.6, 119.1, 116.2, 115.6, 115.3, 114.5, 111.7, 109.7, 55.5, 35.7, 31.4; IR (neat) ν_{max}: 2958, 1618, 1275, 1261, 749 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{28}H_{23}NO_2$ 406.1802 ($M + H^+$); Found 406.1802.

2-(chromeno[2,3,4,5-imna]phenanthridine-2-yl)phenol (5k)

Yellow solid, (36 mg, 44%), mp 254-255 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.88 (s, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.93 – 7.90 (m, 1H), 7.90 – 7.84 (m, 2H), 7.58 (t, *J* = 8.2 Hz, 1H), 7.51 (d, *J* = 3.3 Hz, 1H), 7.50 (s, 1H), 7.41 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.21 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.11 (dd, *J* = 5.9, 2.8 Hz, 1H), 7.03 (td, *J* = 7.5, 1.3 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.7, 157.5, 152.4, 152.2, 135.2, 132.4, 131.4, 130.3, 129.2, 129.0, 128.4, 126.6, 125.1, 124.3, 121.6, 120.9, 120.8, 119.0, 118.8, 118.4, 115.6, 114.0, 110.1; IR (neat) ν_{max}: 2975, 1275, 1260, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{23}H_{13}NO_2$ 336.1019 ($M + H^+$); Found 336.1019.

2-(4-methylchromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenol (5l)

Light Yellow solid, (45 mg, 52%), mp 267-268 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.96 (s, 1H), 7.92 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.89 – 7.86 (m, 2H), 7.83 (d, *J* = 9.0 Hz, 1H), 7.50 (d, *J* = 4.4 Hz, 1H), 7.48 (d, *J* = 5.8 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.17 (s, 1H), 7.10 (dd, *J* = 6.2, 2.5 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 2.55 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.7, 157.0, 152.5, 152.0, 140.0, 134.8, 132.5, 131.3, 130.2, 128.9, 127.9, 126.6, 125.2, 122.4, 121.7, 120.7, 120.4, 118.9, 118.7, 118.3, 115.8, 115.5, 110.0, 22.7; IR (neat) ν_{max}: 2928, 1624, 1275, 1260, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{24}H_{15}NO_2$ 350.1176 ($M + H^+$); Found 350.1176.

4-bromo-2-(4-methylchromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenol (5m)

Brown solid, (57 mg, 54%), mp 171-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.00 (s, 1H), 8.04 (d, *J* = 2.4 Hz, 1H), 7.85 (d, *J* = 1.9 Hz, 2H), 7.82 (s, 1H), 7.52 – 7.49 (m, 2H), 7.49 – 7.46 (m, 1H), 7.20 (s, 1H), 7.12 (dd, *J* = 6.8, 1.9 Hz, 1H), 7.09 (d, *J* = 8.8 Hz, 1H), 2.58 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 155.4, 152.5, 152.0, 140.4, 134.6, 133.8, 132.5, 132.4, 129.2, 128.0, 126.4, 124.9, 123.3, 122.3, 120.8, 120.2, 119.7, 118.5, 116.0, 115.7, 110.7, 110.2, 22.8; IR (neat)ν_{max}: 2924, 1620, 1276, 1261, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{24}H_{14}BrNO_2$ 428.0281 (M + H$^+$); Found 428.0281.

2-(5-methylchromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenol (5n)

Yellow solid, (47 mg, 54%), mp 181-182 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.5 Hz, 1H), 7.90 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.89 – 7.82 (m, 2H), 7.53 – 7.46 (m, 2H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.20 (d, *J* = 8.3 Hz, 1H), 7.13 (dd, *J* = 6.6, 2.0 Hz, 1H), 7.02 (t, *J* = 7.5 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.8, 157.5, 152.6, 149.3, 135.1, 132.4, 131.7, 131.3, 130.3, 128.9, 128.1, 126.6, 124.2, 124.0, 123.5, 121.6, 120.6, 120.4, 118.9, 118.8, 118.3, 115.7, 110.0, 15.6; IR (neat) ν_{max}: 2962, 1275, 1260, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{24}H_{15}NO_2$ 350.1176 (M + H$^+$); Found 350.1188.

2-(4-ethylchromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenol (5o)

Dark Yellow solid, (46 mg, 51%), mp 136-137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.69 (s, 1H), 9.03 (dd, *J* = 8.5, 6.2 Hz, 2H), 8.38 (d, *J* = 1.9 Hz, 1H), 8.04 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.99 (t, *J* = 8.6 Hz, 2H), 7.83 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.74 (m, *J* = 3.1, 1.5 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.43 (ddd, *J* = 8.7, 7.2, 1.7 Hz, 1H), 7.08 – 7.03 (m, 1H), 2.89 (q, *J* = 7.6 Hz, 2H), 1.36 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 158.2, 143.3, 140.1, 133.5, 133.0, 132.0, 131.6, 131.3, 131.2, 129.8, 129.2, 128.9, 127.6, 127.3, 126.9, 126.8, 126.6, 125.63, 120.7, 120.6, 118.8, 118.4, 29.1, 15.6; IR (neat) ν_{max}: 2965, 1614, 1276, 1259, 751 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{25}H_{17}NO_2$ 364.1332 (M + H$^+$); Found 364.1334.

2-(4-isopropylchromeno[2,3,4,5-lmna]phenanthridin-2-yl) phenol (5p)

Yellow solid, (46 mg, 49%), mp 144-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.06 (s, 1H), 7.93 (dd, J = 7.7, 1.5 Hz, 2H), 7.90 – 7.82 (m, 2H), 7.50 (d, J = 3.4 Hz, 1H), 7.49 (s, 1H), 7.44 – 7.39 (m, 1H), 7.26 (s, 1H), 7.21 (dd, J = 8.3, 1.3 Hz, 1H), 7.10 (dd, J = 5.9, 2.8 Hz, 1H), 7.05 (td, J = 7.6, 1.3 Hz, 1H), 3.09 (q, J = 6.9 Hz, 1H), 1.35 (d, J = 6.9 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.8, 157.3, 152.6, 152.2, 151.0, 134.8, 132.5, 131.3, 130.1, 129.0, 127.9, 126.6, 125.2, 122.8, 121.7, 120.7, 118.9, 118.7, 118.4, 118.1, 115.8, 113.0, 110.0, 24.1; IR (neat) ν_{max}: 3006, 1276, 1263, 751 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{26}H_{19}NO_2$ 378.1489 (M + H$^+$); Found 378.1489.

2-(4-phenylchromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenol (5q)

Dark Yellow solid, (51 mg, 50%), mp 227-228 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.92 (s, 1H), 8.23 (s, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.82 (q, *J* = 9.0 Hz, 2H), 7.63 (d, *J* = 7.5 Hz, 2H), 7.53 – 7.48 (m, 3H), 7.47 (d, *J* = 2.7 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.08 (d, *J* = 7.0 Hz, 1H), 7.03 (t, *J* = 7.5

Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.8, 157.6, 152.4, 152.4, 142.6, 140.3, 135.1, 132.4, 131.4, 130.2, 129.2, 129.0, 128.3, 128.3, 127.5, 126.5, 125.2, 123.2, 121.6, 120.8, 119.2, 119.1, 118.6, 118.4, 115.4, 113.3, 110.2; IR (neat) ν_{max}: 2925, 1615, 1275, 1251, 757 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{29}H_{17}NO_2$ 412.1332 (M + H$^+$); Found 412.1333.

3-(tert-butyl)-5-(thiophen-2-yl)-3,4-dihydrobenzo[a]phenanthridin-1(2H)-one (5r)

Yellow solid, (56 mg, 59%), mp 238-239 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.4 Hz, 1H), 7.94 (s, 2H), 7.88 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.58 (ddd, *J* = 8.0, 7.0, 1.2 Hz, 1H), 7.54 (d, *J* = 4.4 Hz, 2H), 7.49 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.21 (t, *J* = 4.4 Hz, 1H), 3.52 (ddd, *J* = 16.2, 3.7, 2.0 Hz, 1H), 3.17 (ddd, *J* = 16.4, 5.6, 2.0 Hz, 1H), 2.84 (dt, *J* = 16.3, 12.9 Hz, 2H), 2.21 (m, *J* = 12.4, 5.6, 3.6 Hz, 1H), 1.07 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 203.5, 151.5, 147.7, 143.4, 140.3, 134.0, 133.3, 131.5, 128.7, 128.7, 128.6, 128.4, 127.8, 127.8, 127.6, 125.7, 121.3, 46.2, 42.2, 32.9, 29.7, 27.3.; IR (neat) ν_{max}: 2959, 1689, 1545, 831 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{25}H_{23}NOS$ 386.1573 (M + H$^+$); Found 386.1574.

General Experimental Procedure for the Synthesis of 2-(8-bromo-4-(*tert*-butyl)chromeno[2,3,4,5-*lmna*]phenanthridin-2-yl)phenol derivatives (7a). A reaction mixture containing the 6-bromo-2-naphthylamine **6** (55.52 mg, 0.25 mmol), Benzaldehyde (26.53 mg, 0.25 mmol), 4-*tert*-butylcyclohexanone (**3a**, 38.56 mg, 0.25 mmol), CSA (17.42 mg, 30 mol%) in DMSO (1 mL) was stirred at 80 °C (3-5 hr) 120 °C for 12 hr (TLC Monitored). Then resulting was extracted with DCM (3×5 ml). The organic layer was washed with brine solution, dried over anhydrous Na_2SO_4, filtrated, and evaporated under reduced pressure. The desired product (**7a**) was purified by column chromatography. Same procedure was followed for the preparation of substrate **7b-7d.**

The characterization data for the compounds **7a-d**.

8-bromo-4-(tert-butyl)-2-phenylchromeno[2,3,4,5-lmna] phenanthridine (7a)

Light Yellow solid, (63 mg, 56%), mp 212-213 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 9.0 Hz, 1H), 7.81 (d, *J* = 7.7 Hz, 2H), 7.77 – 7.73 (m, 2H), 7.65 (s, 1H), 7.58 (t, *J* = 7.4 Hz, 2H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.43 (s, 1H), 7.24 (d, *J* = 1.5 Hz, 1H), 1.37 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 153.3, 153.2, 151.4, 139.5, 137.1, 133.1, 129.4, 129.3, 129.1, 128.7, 126.3, 125.4, 123.0, 122.0, 121.0, 117.9, 116.7, 115.4, 113.3, 112.1, 35.8, 31.4; IR (neat)ν_{max}: 2958, 1616, 1275, 1261, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{20}BrNO$ 454.0801 (M + H$^+$); Found 454.0801.

8-bromo-4-(tert-butyl)-2-(p-tolyl)chromeno[2,3,4,5-lmna] phenanthridine (7b)

Brown solid, (60 mg, 52%), mp 213-214 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 9.1 Hz, 1H), 7.80 (s, 1H), 7.72 (t, *J* = 8.4 Hz, 3H), 7.61 (s, 1H), 7.47 – 7.34 (m, 3H), 7.20 (s, 1H), 2.49 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 153.5, 153.1, 151.4, 139.6, 136.2, 135.7, 133.0, 130.3, 129.5, 128.5, 126.5, 125.2, 123.0, 122.1, 121.0, 117.6, 117.1, 115.4, 113.4, 112.5, 35.8, 31.4, 21.6; IR (neat) ν_{max}: 2963,

1586, 1276, 1261, 750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{28}H_{22}BrNO$ 468.0958 ($M + H^+$); Found 468.0960.

8-bromo-2-(4-bromophenyl)-4-(tert-butyl)chromeno[2,3,4,5-lmna]phenanthridine (7c)

Yellow solid, (70 mg, 53%), mp 219-220 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 9.0 Hz, 1H), 7.73 (s, 1H), 7.71 (d, *J* = 3.6 Hz, 4H), 7.69 – 7.68 (m, 1H), 7.64 – 7.62 (m, 1H), 7.43 – 7.41 (m, 1H), 7.23 – 7.19 (m, 1H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 153.5, 153.2, 151.5, 138.4, 137.0, 133.1, 131.9, 131.1, 129.2, 126.4, 125.1, 123.5, 123.1, 122.2, 121.0, 117.7, 116.2, 115.4, 113.4, 112.2, 35.8, 31.4; IR (neat) ν_{max}: 2986,1275,750 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{27}H_{19}Br_2NO$ 531.9906 ($M + H^+$); Found 531.9909.

***8-bromo-4-(tert-butyl)-2-(3-methoxyphenyl)chromeno[2,3,4,5-lmna]phenanthridine* (7d)**

Dark Yellow solid, (66 mg, 53%), mp 164-165 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 9.1 Hz, 1H), 7.77 (s, 1H), 7.66 (d, *J* = 9.0 Hz, 1H), 7.57 (s, 1H), 7.48 (t, *J* = 7.9 Hz, 1H), 7.41 – 7.33 (m, 3H), 7.15 (s, 1H), 7.09 (d, *J* = 7.0 Hz, 1H), 3.91 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.9, 159.6, 153.2, 153.1, 151.3, 140.7, 136.9, 132.9, 129.6, 129.1, 126.2, 125.2, 122.9, 121.9, 121.9, 120.8, 117.7, 116.7, 115.4, 115.2, 114.5, 113.2, 112.0, 55.5, 35.8, 31.4; IR (neat) ν_{max}: 2959, 1586, 1285, 835 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{28}H_{22}BrNO_2$ 484.0907 ($M + H^+$); Found 484.0907.

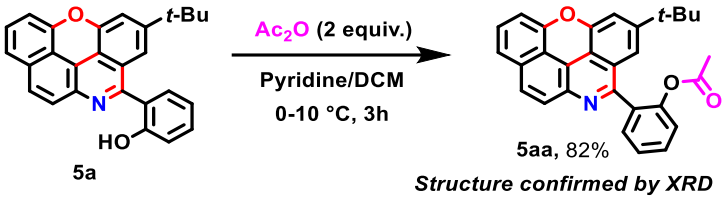
General Procedure for the Synthesis of 4-(*tert*-butyl)-2-phenyl-8-(*p*-tolyl)chromeno[2,3,4,5-*lmna*]phenanthridine (9a). An oven-dried 25 mL two-necked round-bottom flask equipped with a magnetic stir bar was charged with compound **7a** (45.4 mg, 0.1 mmol), the *p*-tolylboronic acid (20.39 mg, 1.5 equiv.), $Pd(PPh_3)_4$ (11.55 mg, 10 mol%), and anhydrous K_2CO_3 (55.2 mg, 4 equiv.). The round-bottom flask was sealed with a rubber septum and adapter. It was then evacuated and backfilled with nitrogen three times. Following this, THF (5.0 mL) and water (1.0 mL) were added through the septum using a syringe. The resulting mixture was stirred under reflux conditions for 24 h. The reaction mixture was allowed to cool to room temperature, then diluted with 5 mL of dichloromethane. It was filtered through filter paper and washed with water. The organic layer was dried over anhydrous sodium sulfate and purified by column chromatography on silica gel using pure hexane, yielding compound **9a**.

4-(tert-butyl)-2-phenyl-8-(p-tolyl)chromeno[2,3,4,5-lmna] phenanthridine (9a)

Orange solid, (29 mg, 62%), mp 273-274 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 9.0 Hz, 1H), 7.86 (d, *J* = 9.1 Hz, 1H), 7.83 (d, *J* = 7.1 Hz, 2H), 7.73 (s, 1H), 7.68 (s, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 1H), 7.42 (s, 1H), 7.34 (s, 1H), 7.32 (d, *J* = 7.9 Hz, 2H), 2.44 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.4, 153.1, 153.0, 151.9, 142.0, 139.7, 138.1, 137.8, 137.1, 132.5, 129.8, 129.5, 129.0, 128.7, 128.4, 127.6, 127.4, 125.4, 121.3, 118.6, 117.9, 116.3, 115.4, 111.8, 109.0, 35.7, 31.4, 21.3; IR (neat) ν_{max}: 2925, 2854, 1263, 732 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{28}H_{22}BrNO_2$ 466.2165 ($M + H^+$); Found 466.2164.

General experimental procedure for the synthesis of 2-(4-(*tert*-butyl)chromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenyl acetate (5aa)

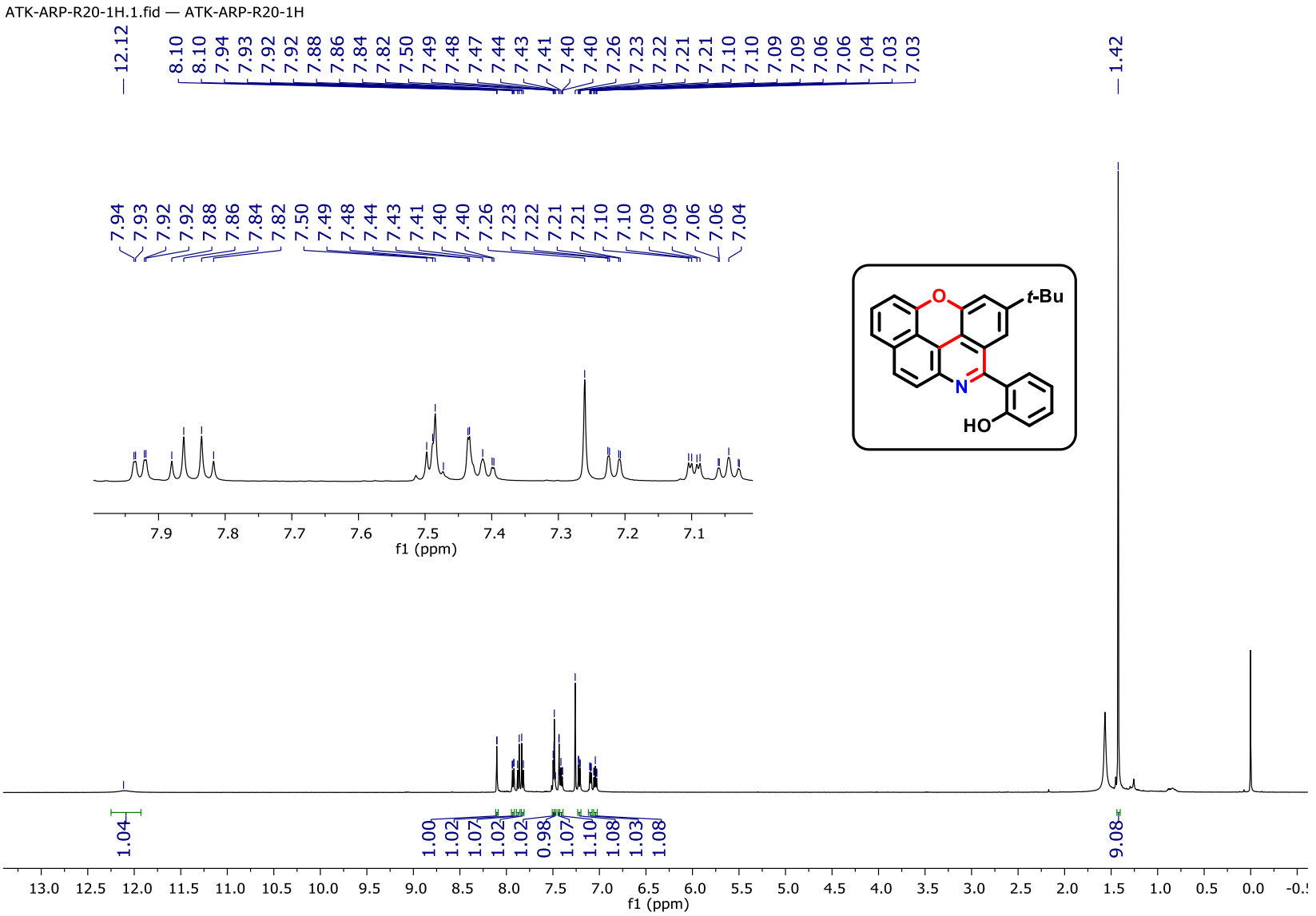
Acetic anhydride (5 mg, 0.2 mmol) was added dropwise to a flask containing 2-(4-(*tert*-butyl)chromeno[2,3,4,5-*Imna*]phen-anthridin-2-yl)phenol (**5a**) (39 mg, 0.1 mmol) in pyridine/DCM (0.5 ml/0.5 ml) at 0-10 ºC for 3 h. After the completion of the reaction (monitored by TLC), the ensuing solution was concentrated to dryness under reduced pressure. Crude product thus obtained was purified by column chromatography (SiO_2; ethyl acetate/ hexane) to afford 2-(4-(*tert*-butyl)chromeno[2,3,4,5-*lmna*]phenanthridin-2-yl)phenyl acetate (**5aa**) in quantitative yield.



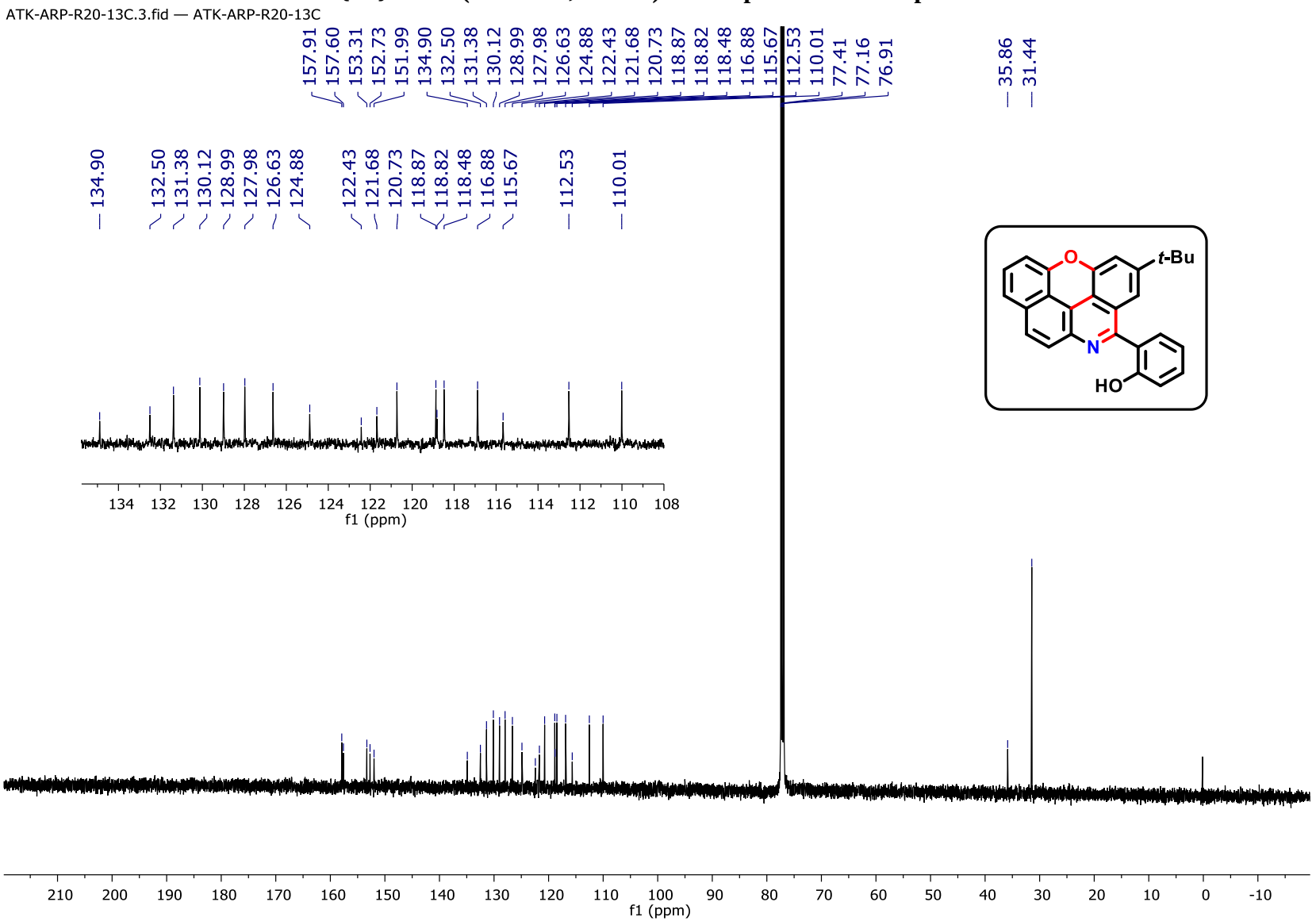
2-(4-(tert-butyl)chromeno[2,3,4,5-lmna]phenanthridin-2-yl)phenyl acetate (5aa)

Yellow solid, (mg, 82%), mp 138-139 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.0 Hz, 1H), 7.85 (d, *J* = 9.0 Hz, 1H), 7.68 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.56 (td, *J* = 7.8, 1.7 Hz, 1H), 7.51 (d, *J* = 4.9 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 1.5 Hz, 1H), 7.38 – 7.34 (m, 2H), 7.12 (t, *J* = 4.4 Hz, 1H), 1.80 (s, 3H), 1.34 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.9, 156.4, 153.2, 152.9, 151.7, 148.6, 137.0, 132.5, 131.9, 131.2, 130.0, 128.8, 128.0, 127.5, 126.2, 125.7, 123.4, 121.0, 120.6, 119.0, 115.8, 115.8, 111.8, 109.8, 35.7, 31.3, 20.8; IR (neat)ν_{max}: 2924, 1767, 1369, 1263, 735 cm^{-1}; HRMS (ESI-QTOF) Calcd for $C_{29}H_{23}NO_3$ 434.1751 ($M + H^+$); Found 434.1751.

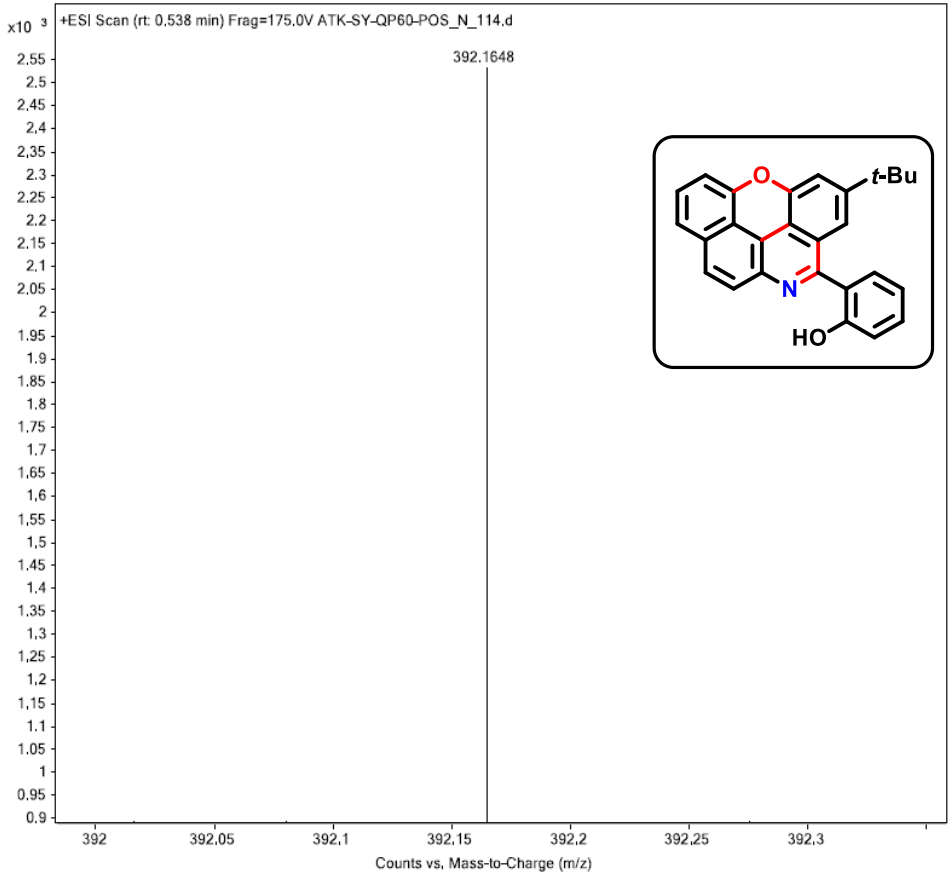
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 5a



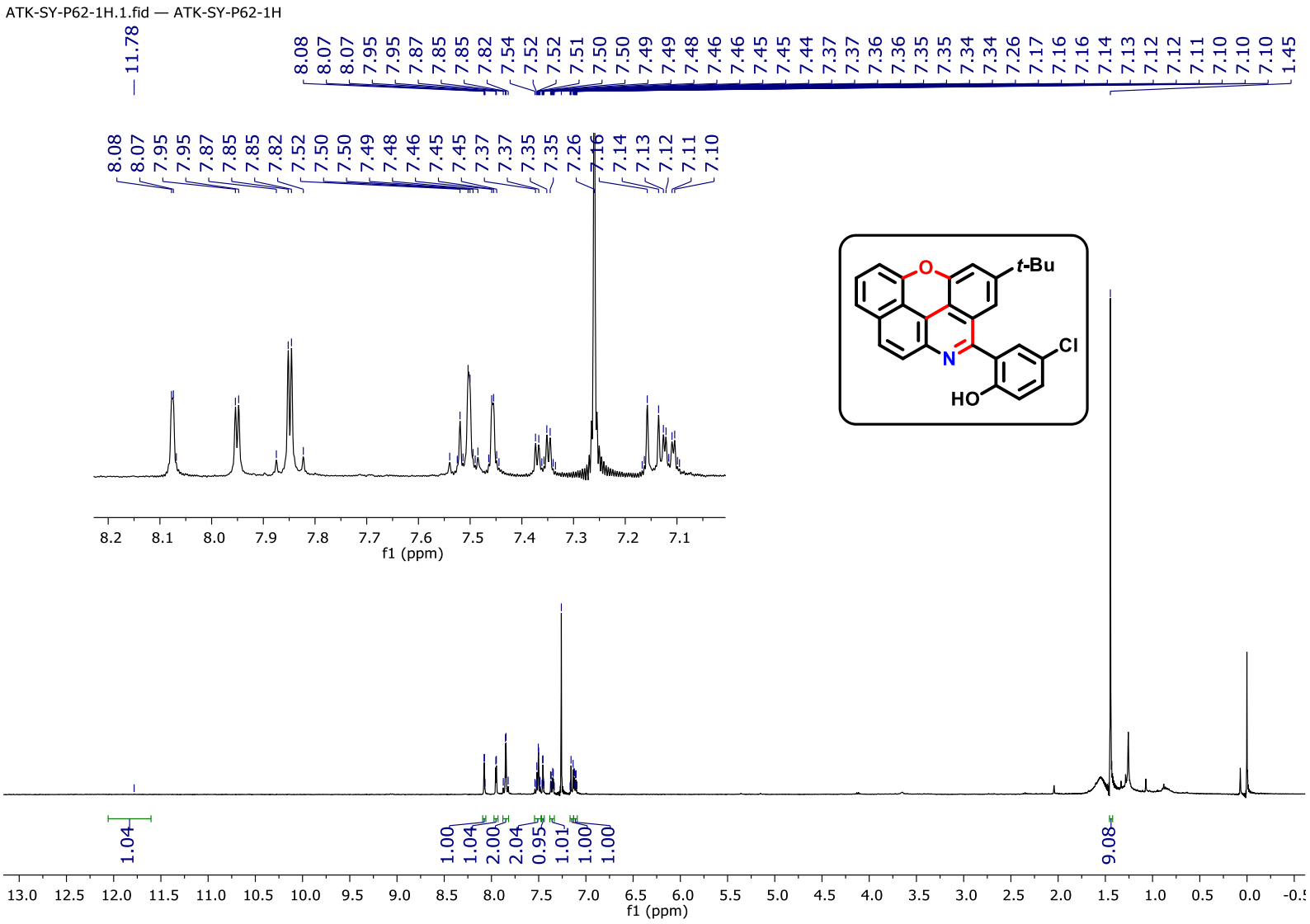
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5a



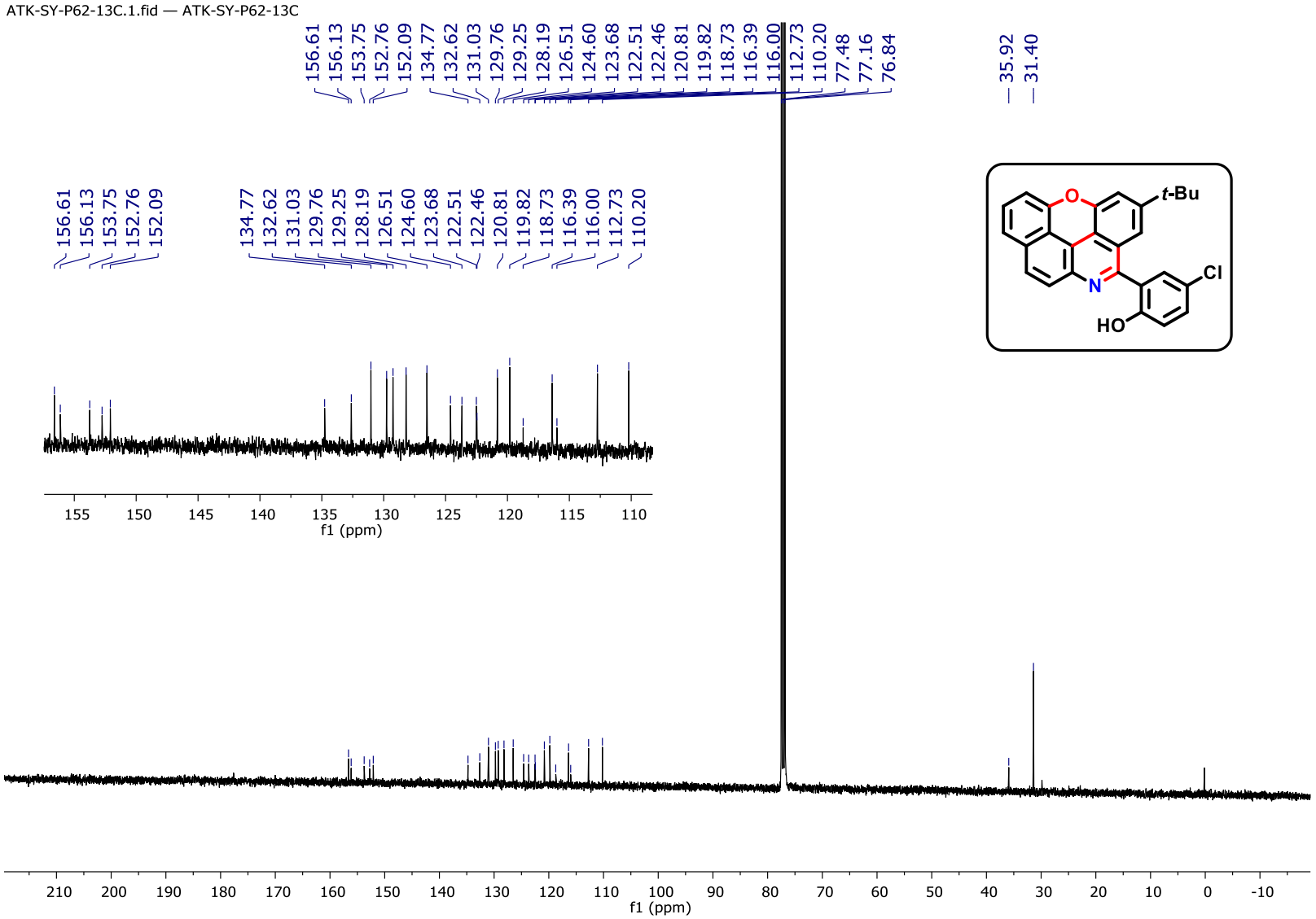
HRMS spectrum of compound 5a



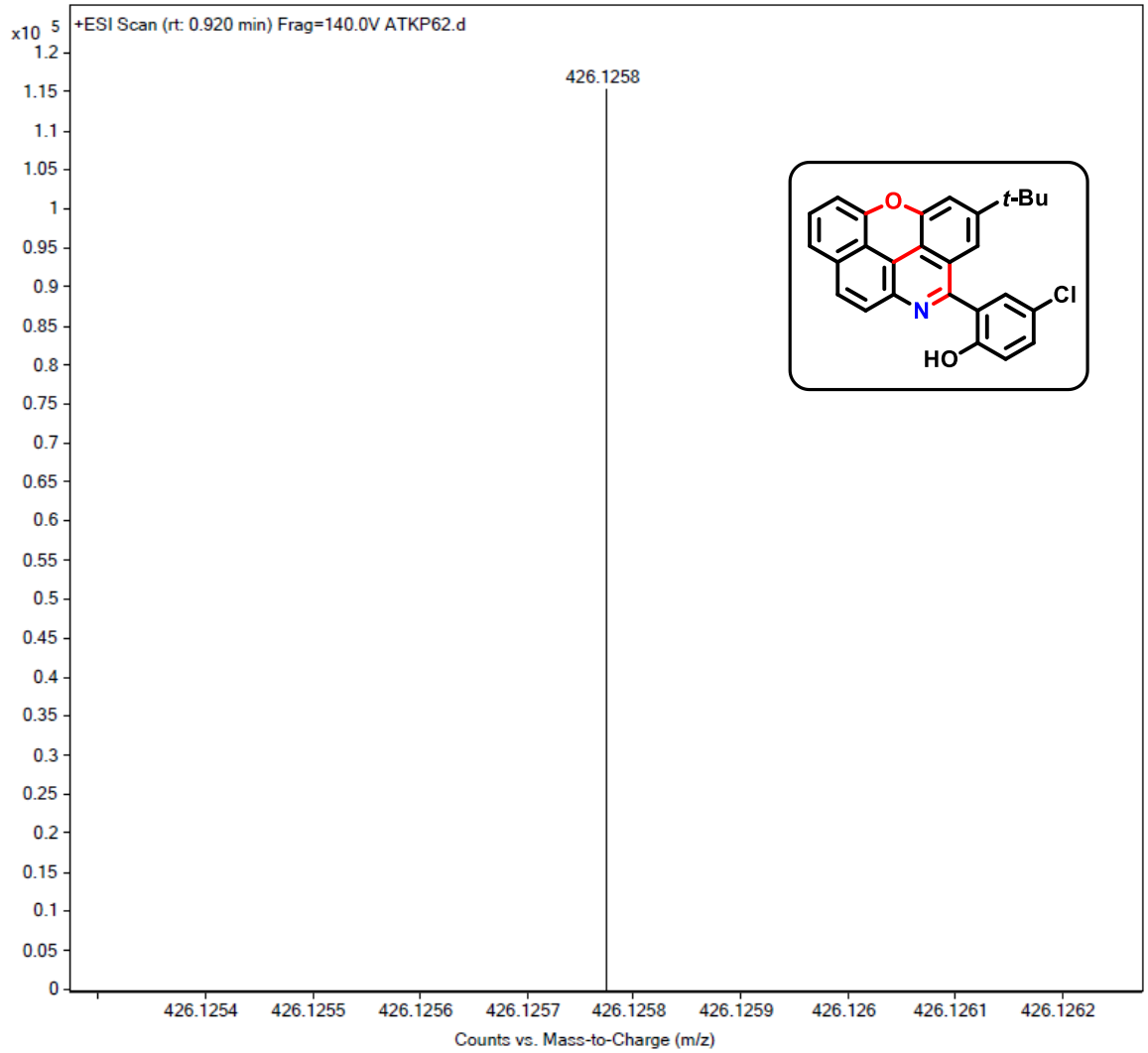
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5b



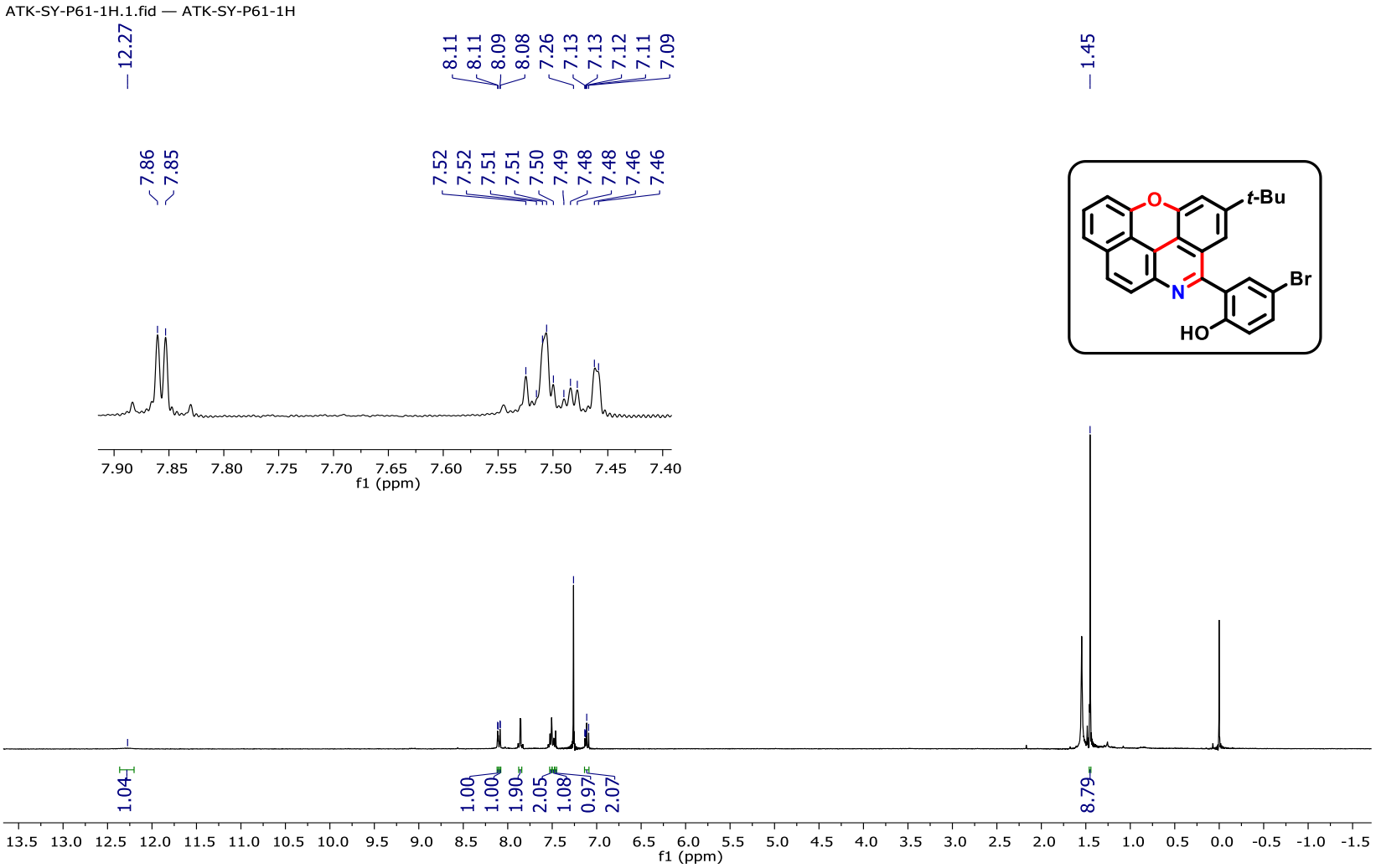
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) NMR spectrum of compound 5b



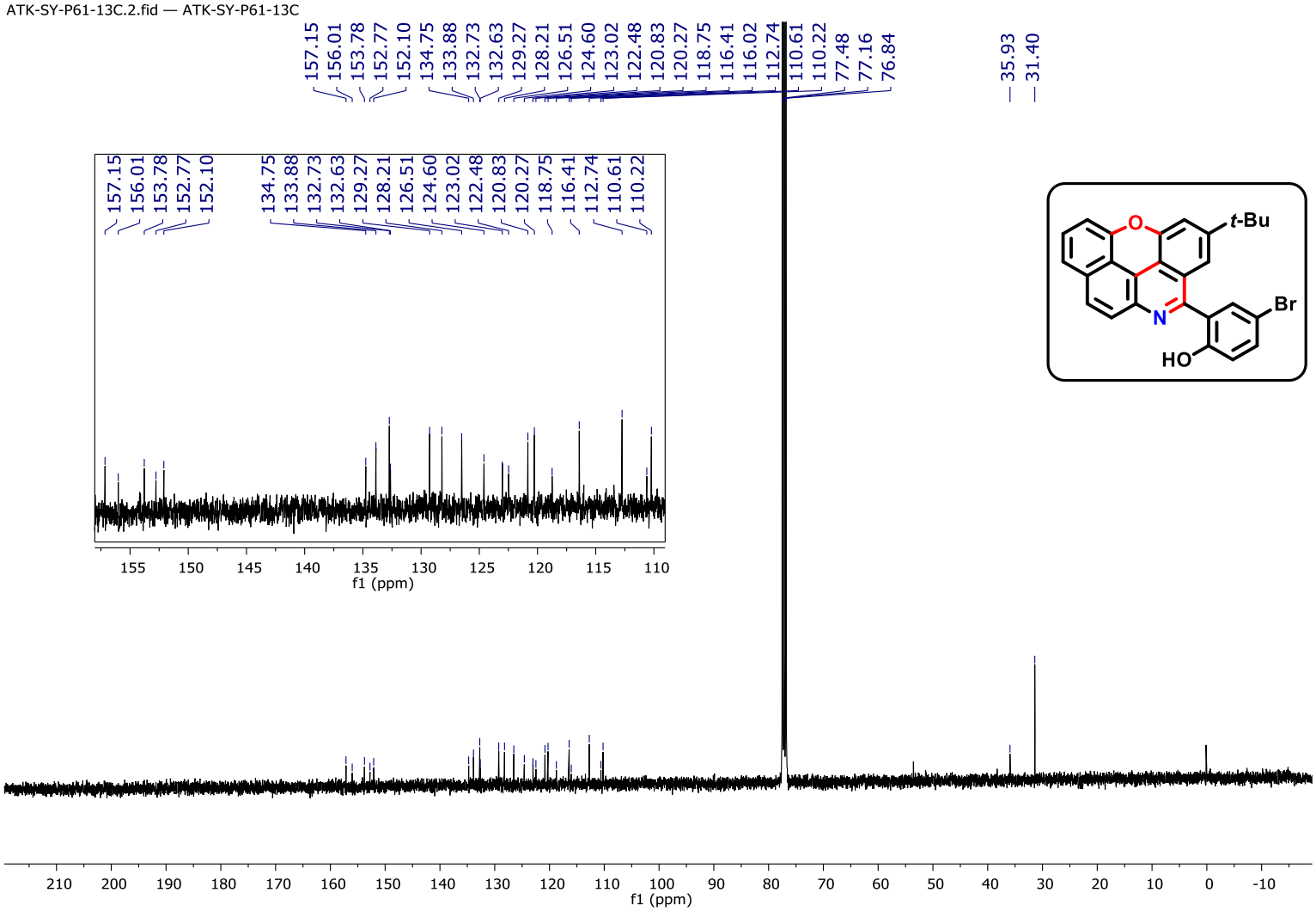
HRMS spectrum of compound 5b



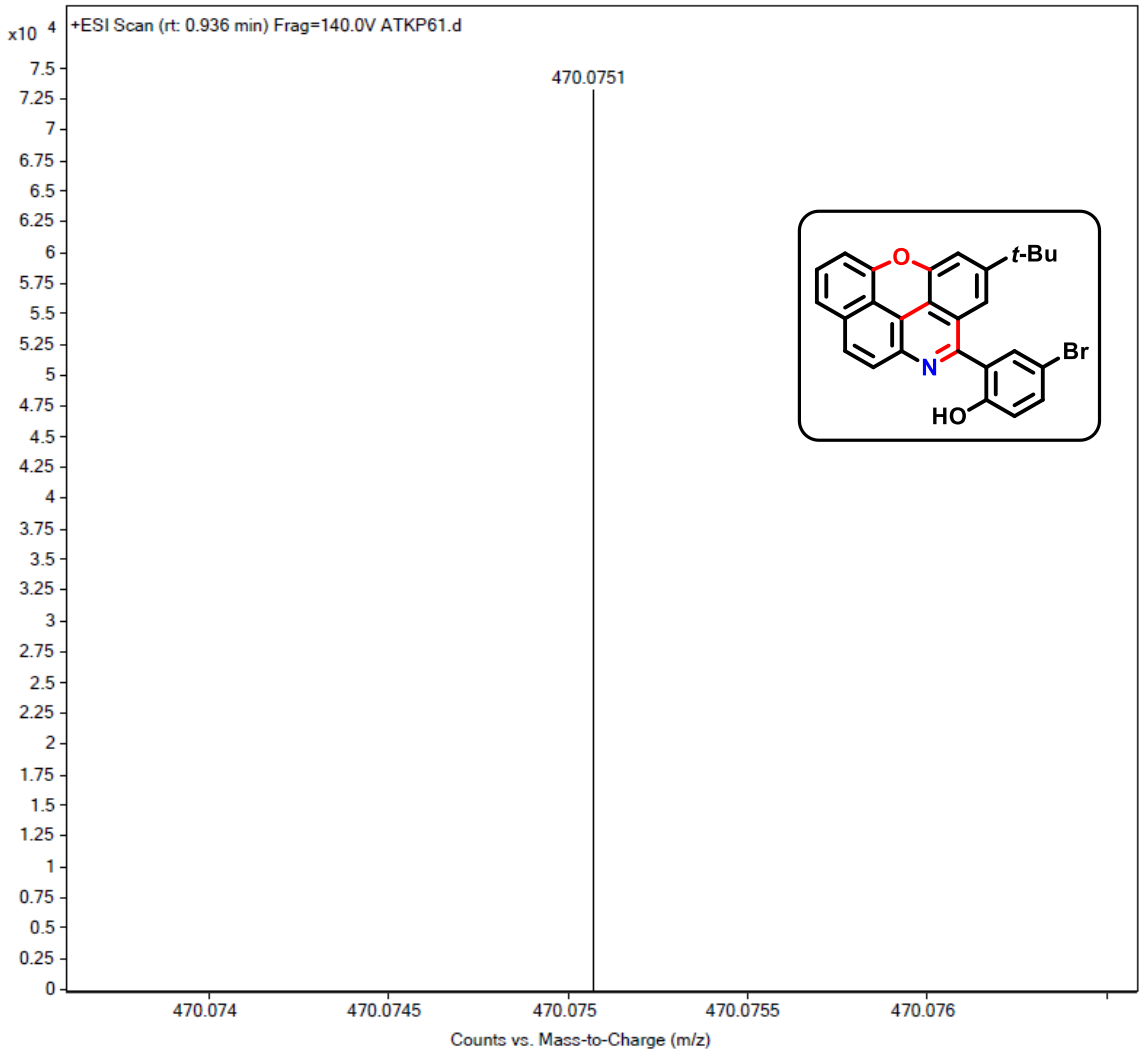
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5c



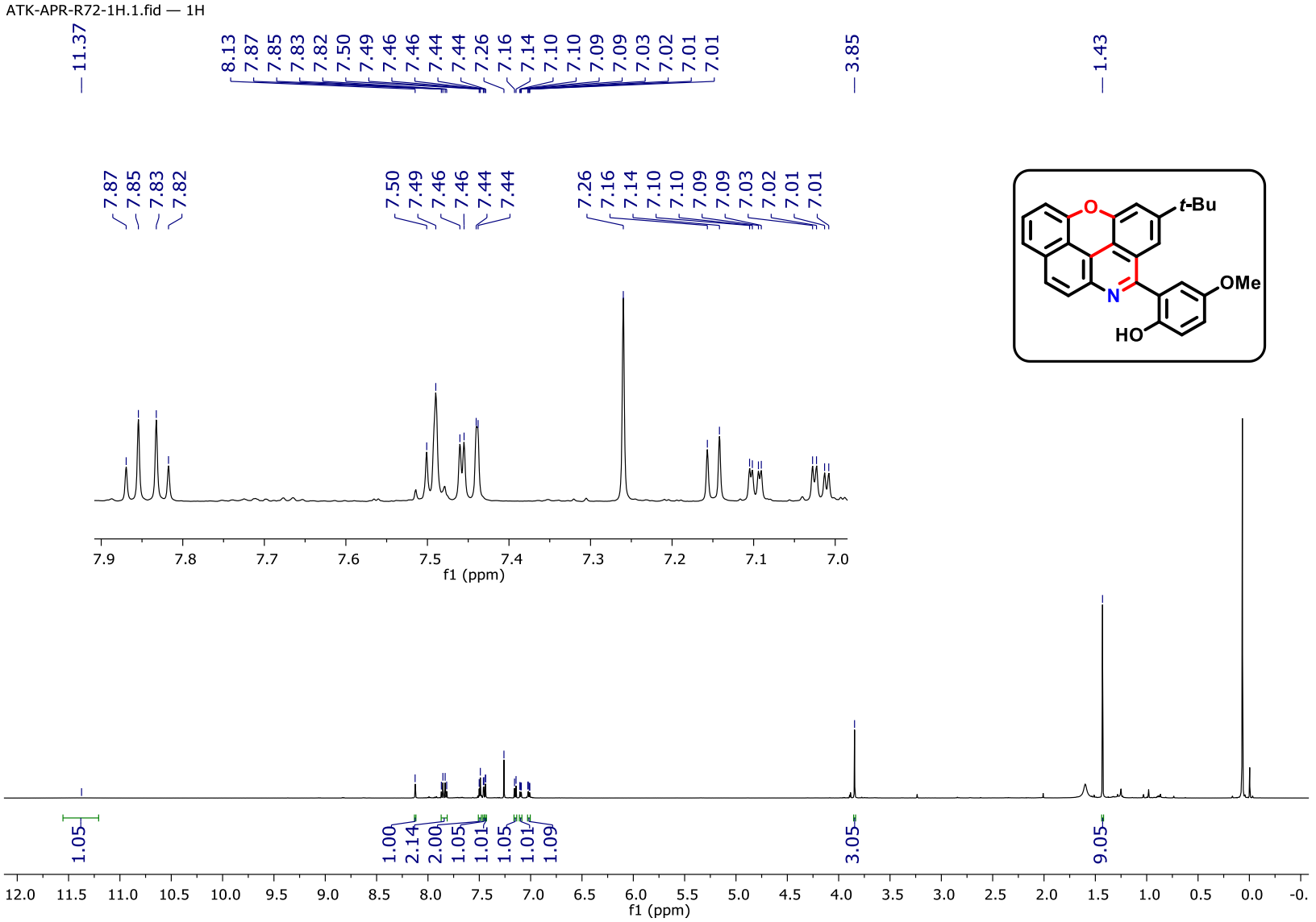
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) NMR spectrum of compound 5c



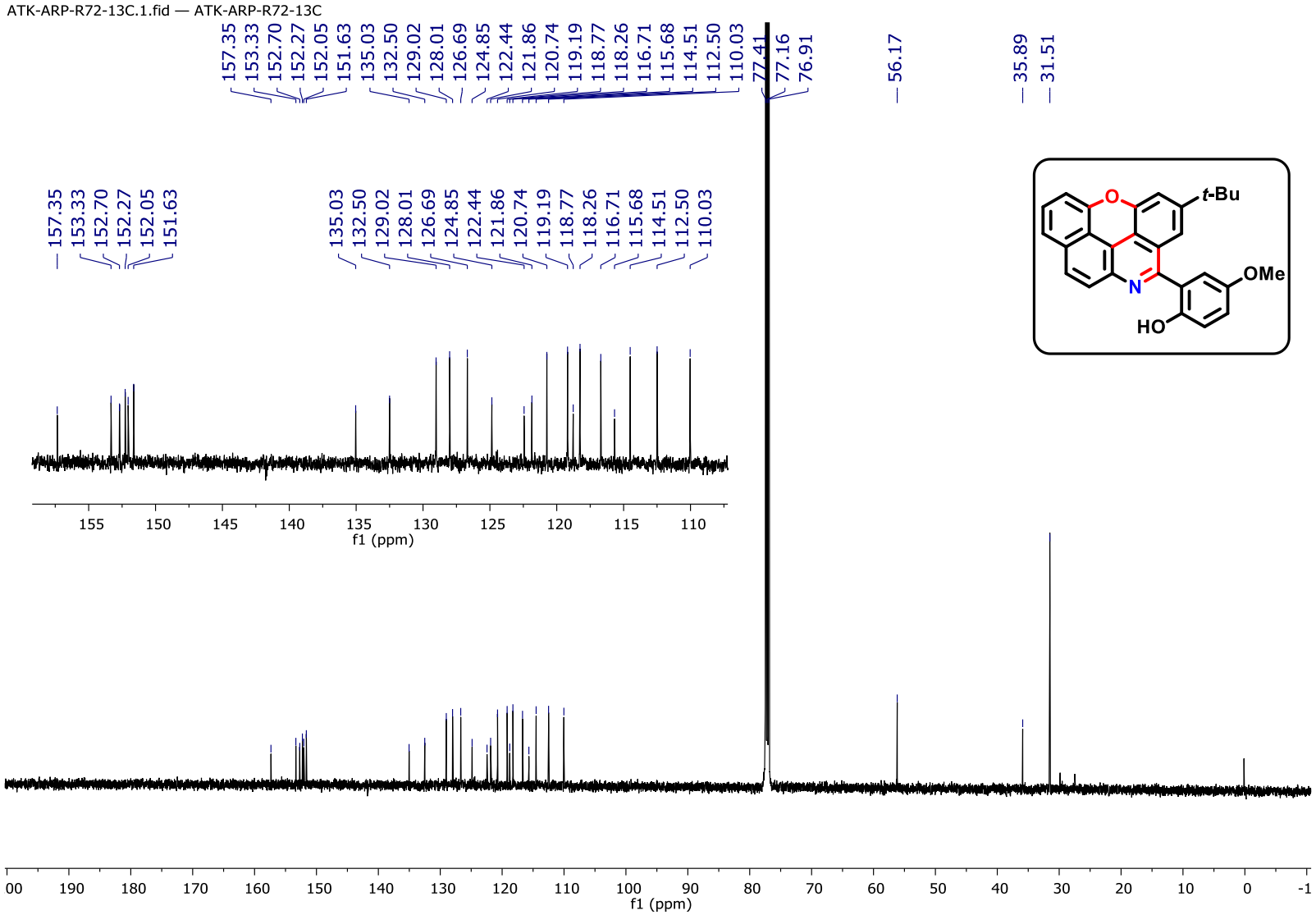
HRMS spectrum of compound 5c



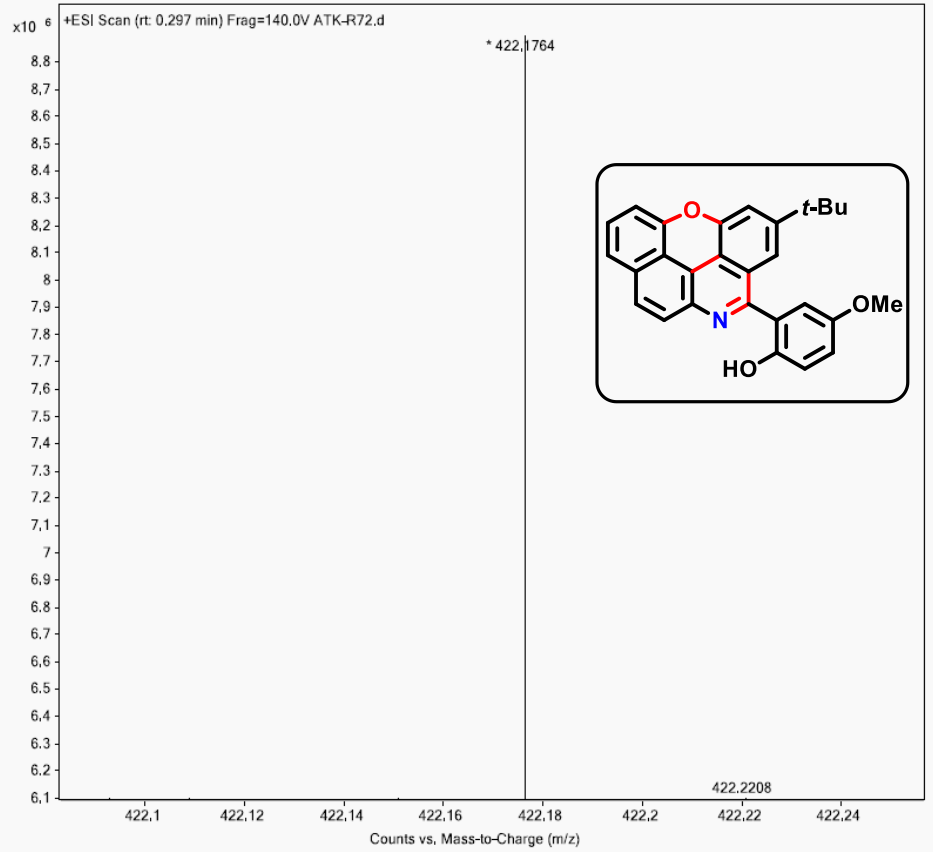
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 5d



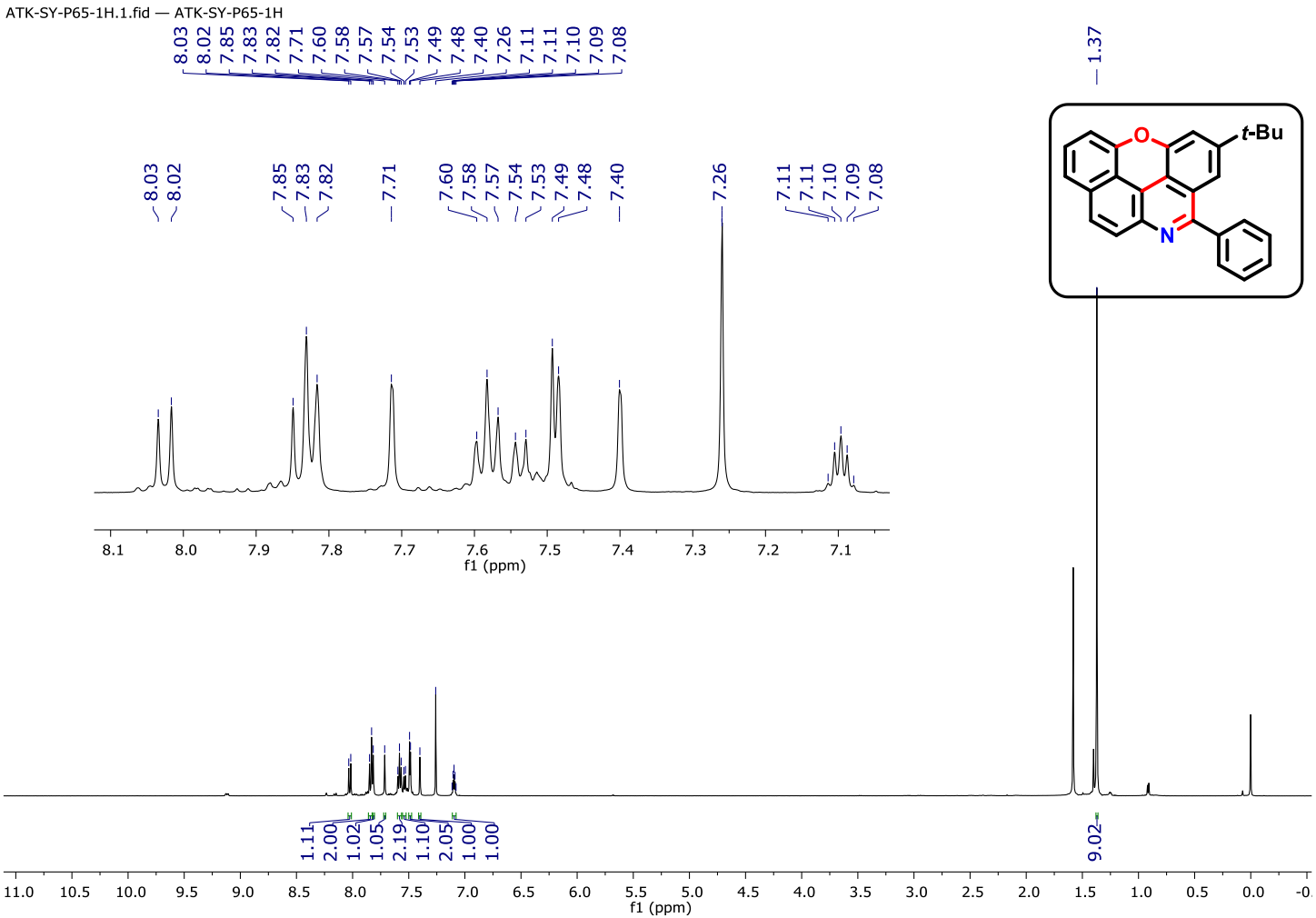
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5d



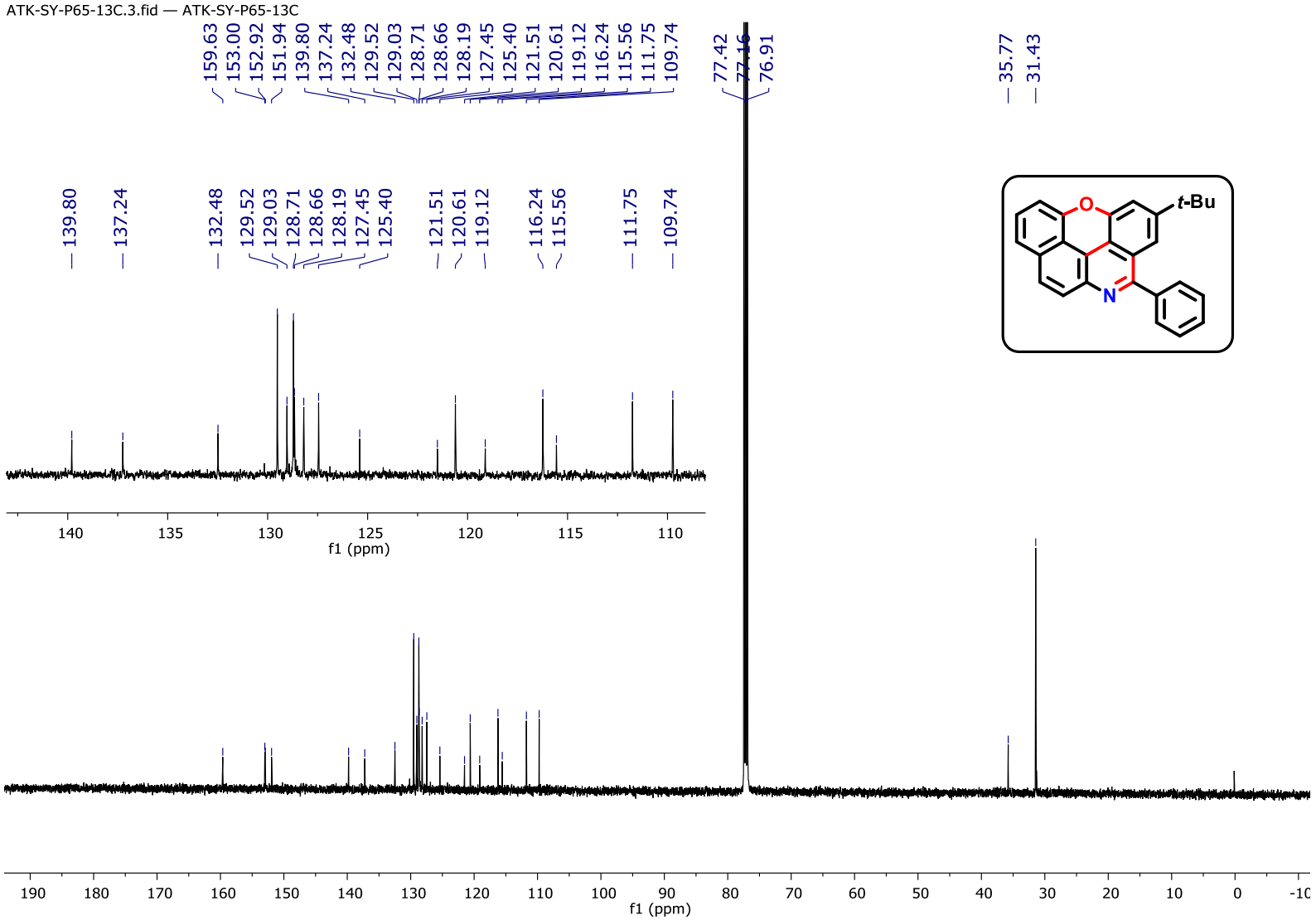
HRMS spectrum of compound 5d



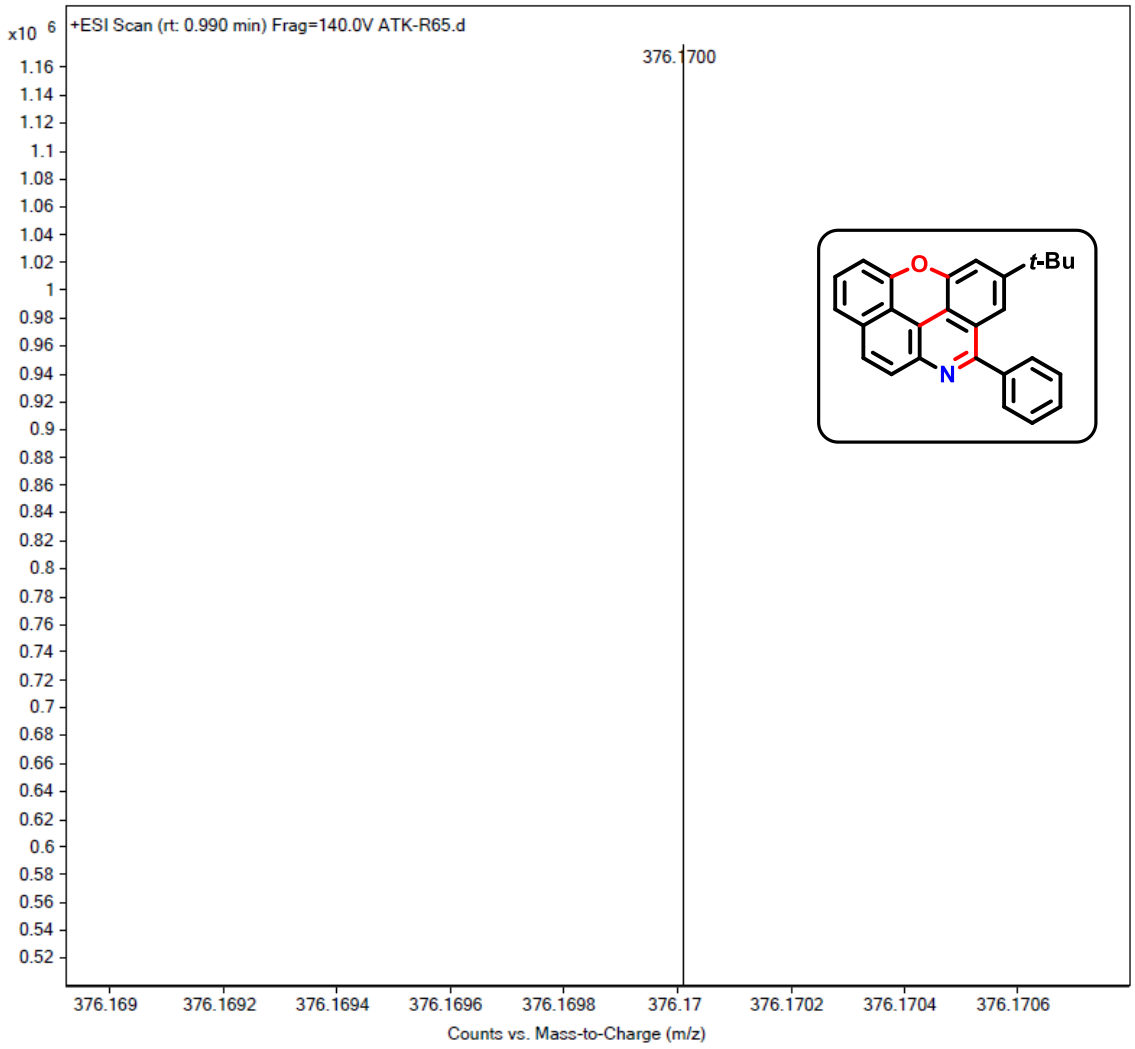
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 5e



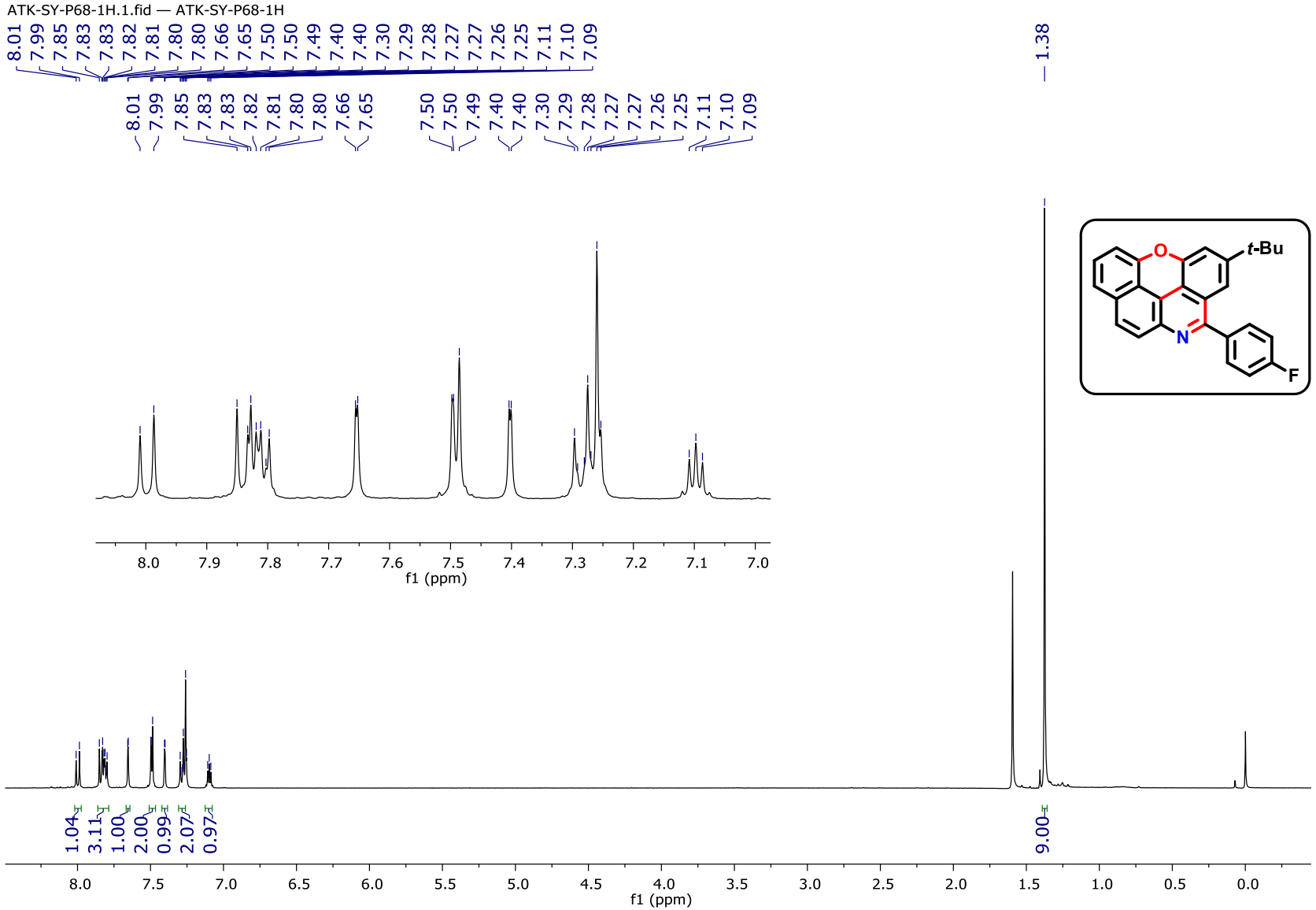
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5e



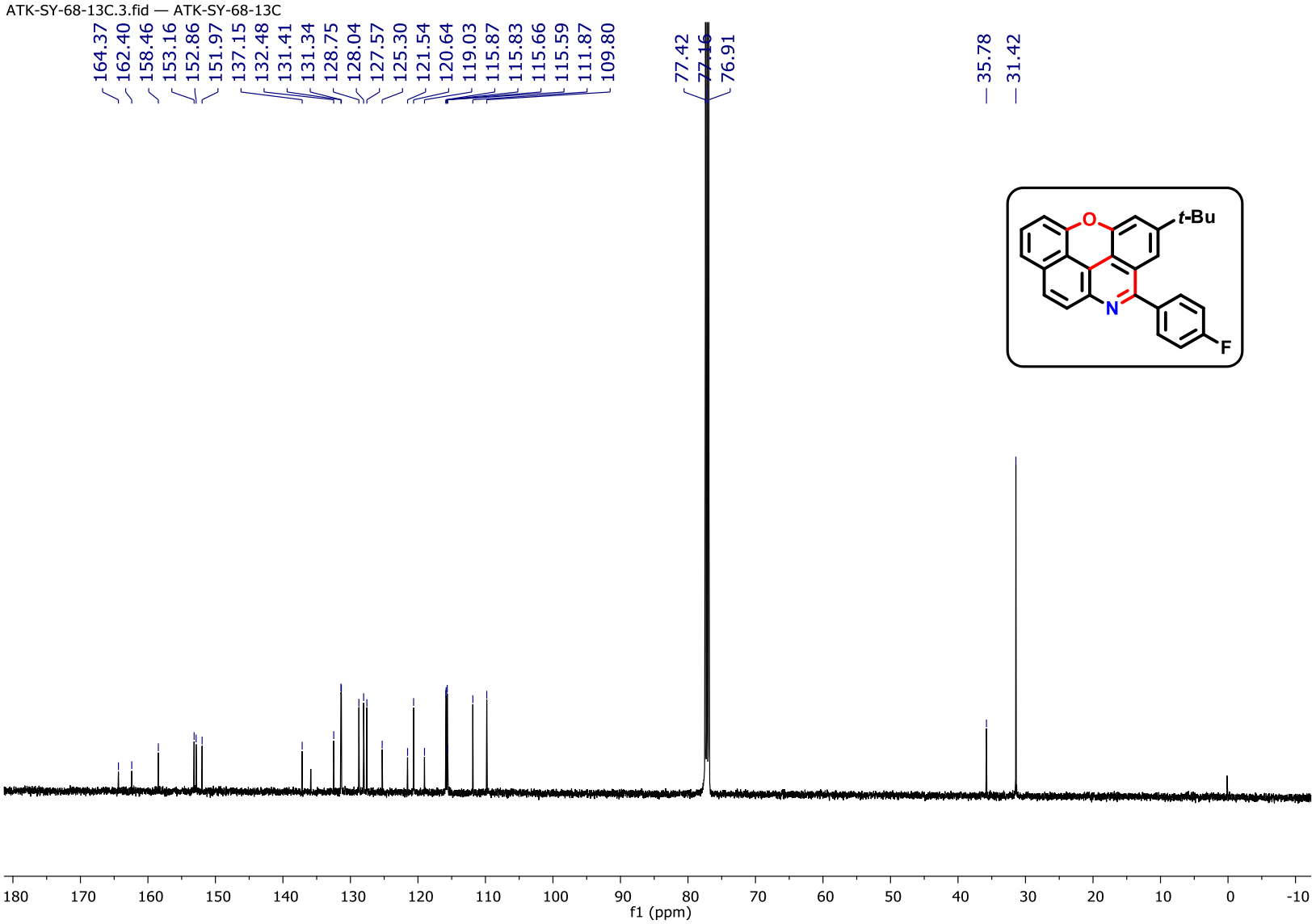
HRMS spectrum of compound 5e



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5f

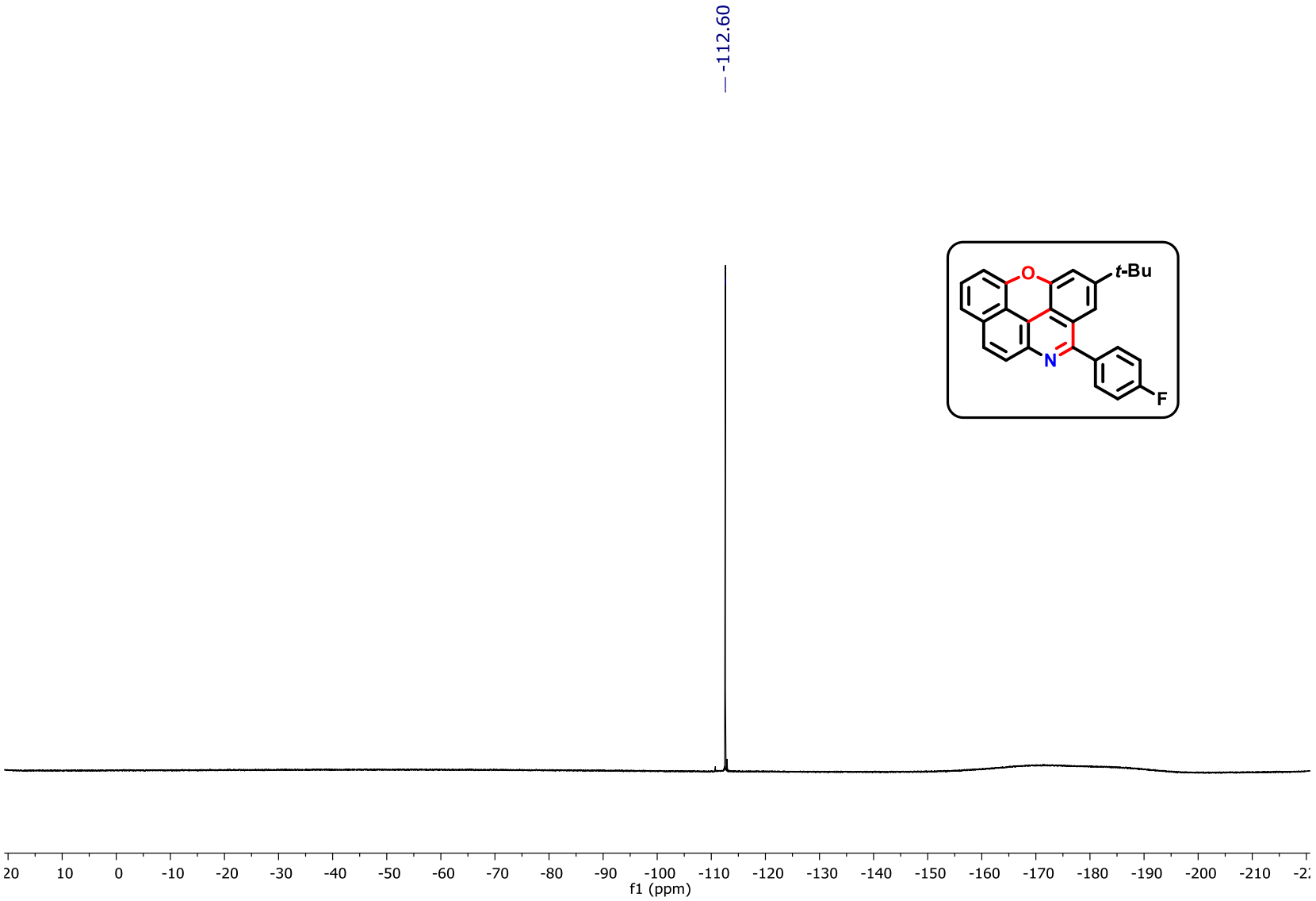


^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5f



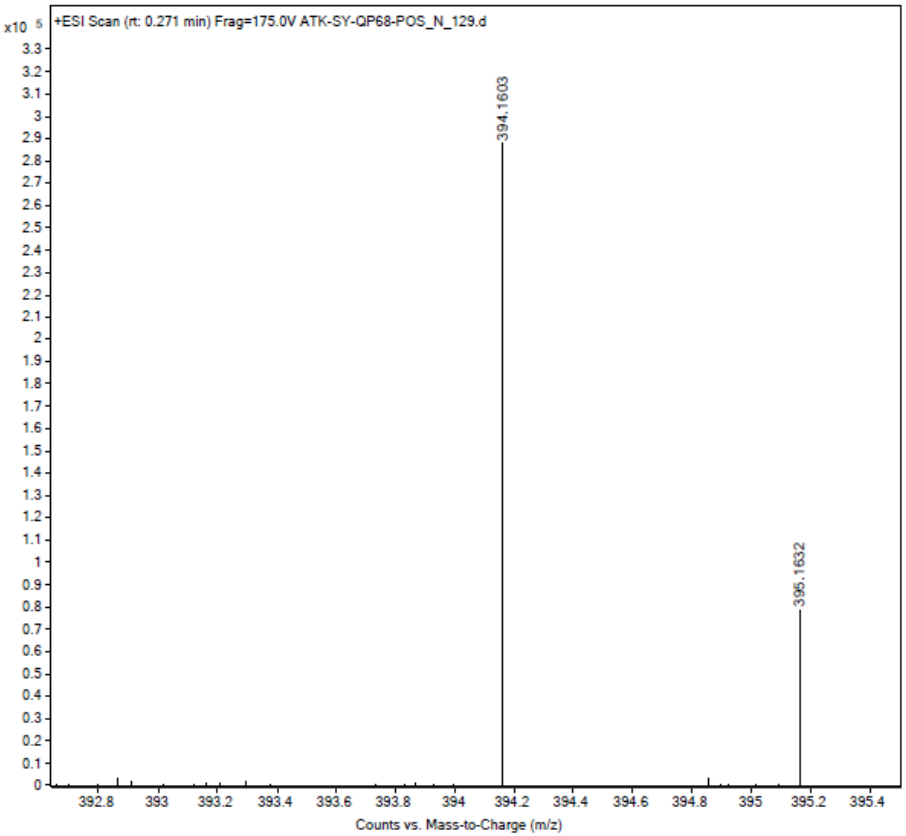
^{19}F {^{1}H} NMR (500 MHz, $CDCl_3$) NMR spectrum of compound 5f

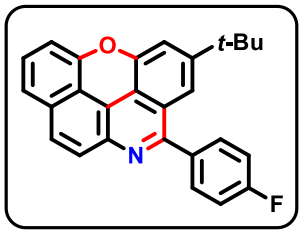
ATK-SY-P68-19F.1.fid — ATK-SY-P68-19F



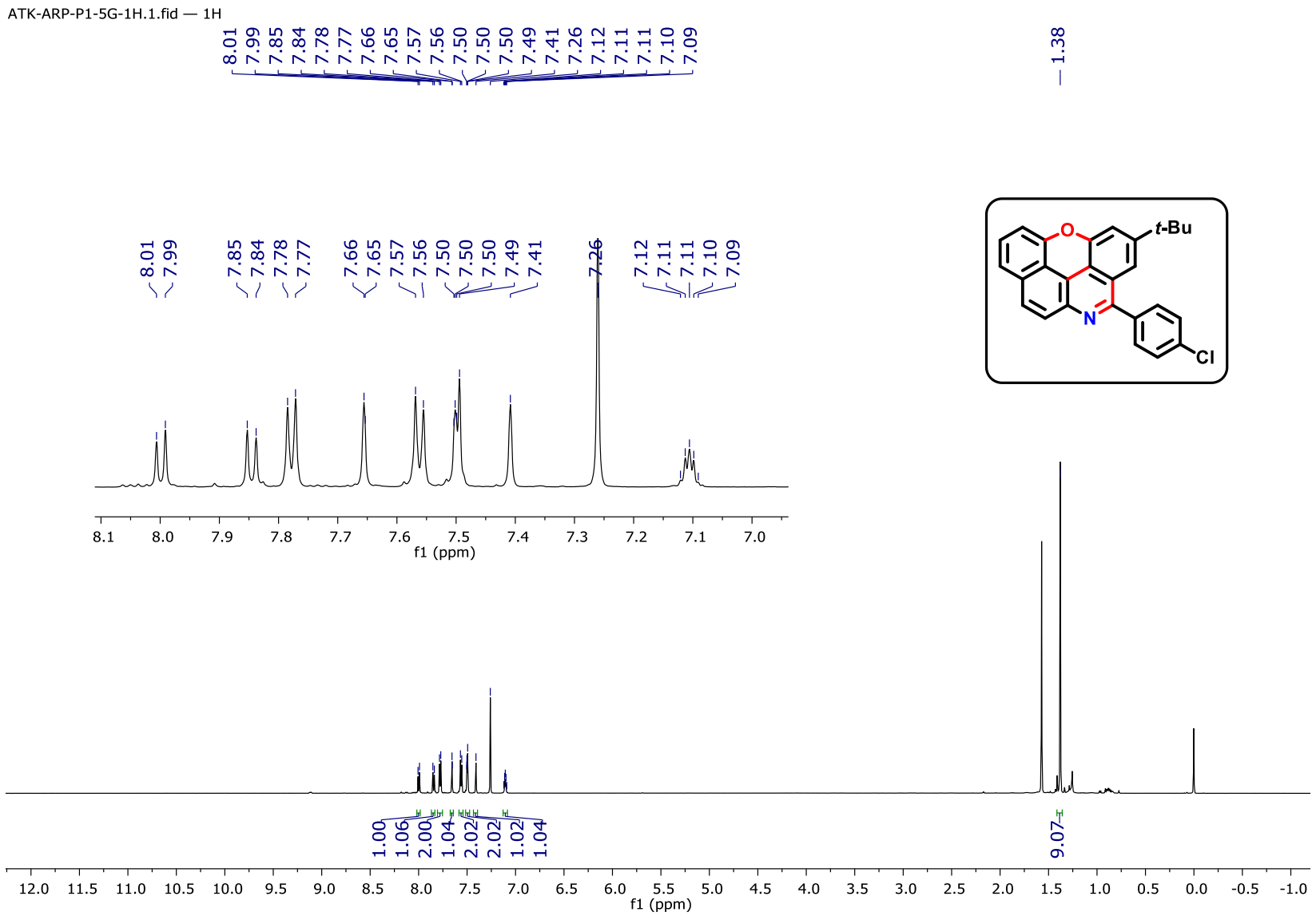
HRMS spectrum of compound 5f

Sample Name	ATK-SY-QP68-POS_N	**Position**	P2-B7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-QP68-POS_N_129.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	27-Jan-23 10:35:52 PM (UTC+05:30)

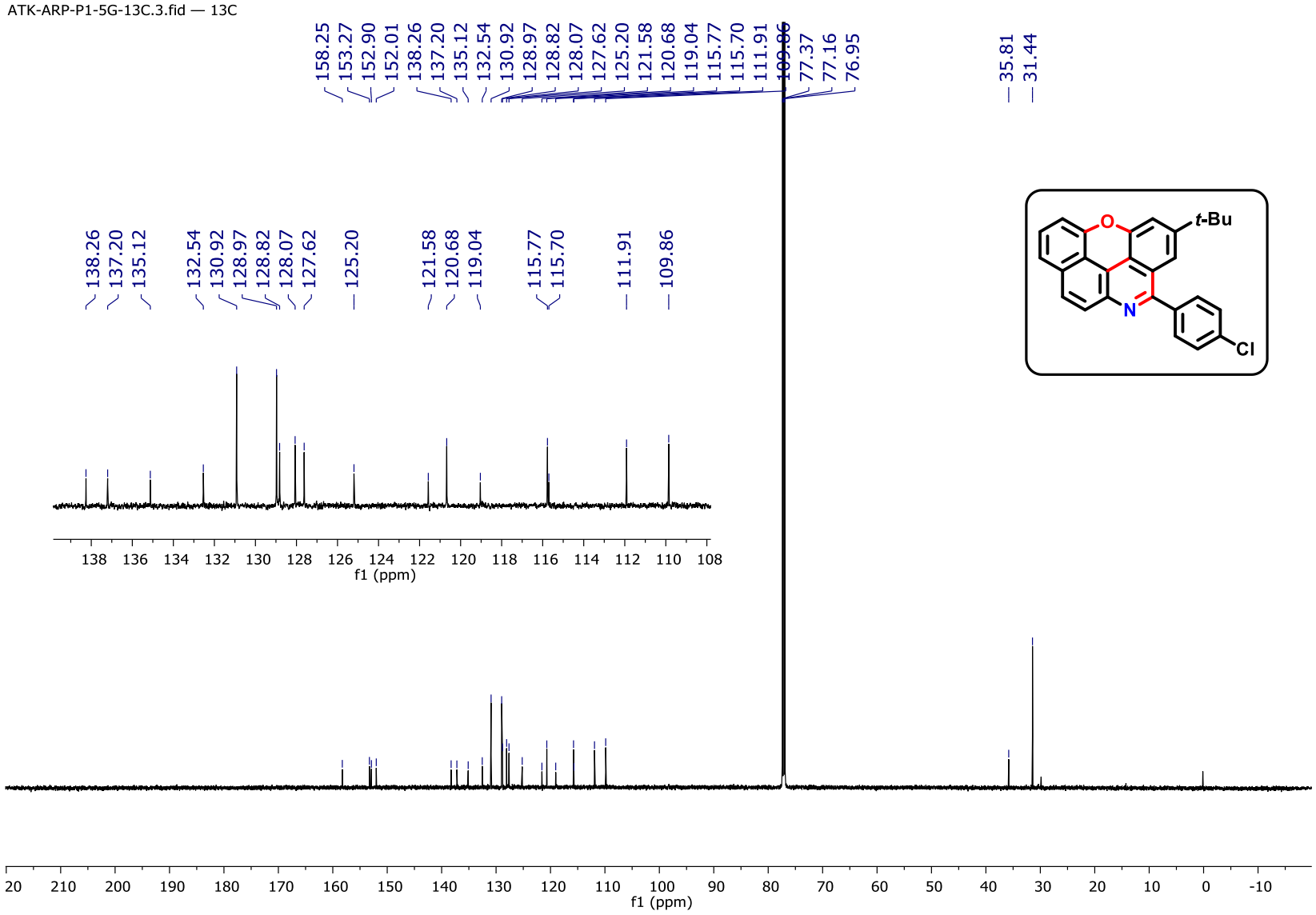




^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5g

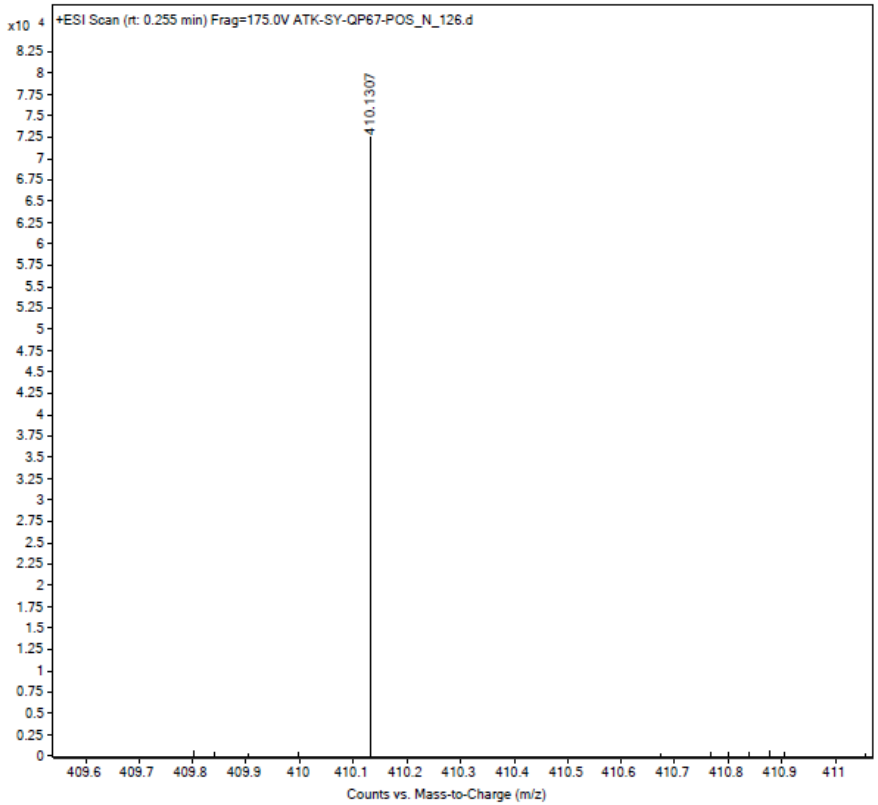


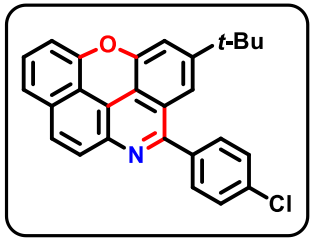
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5g



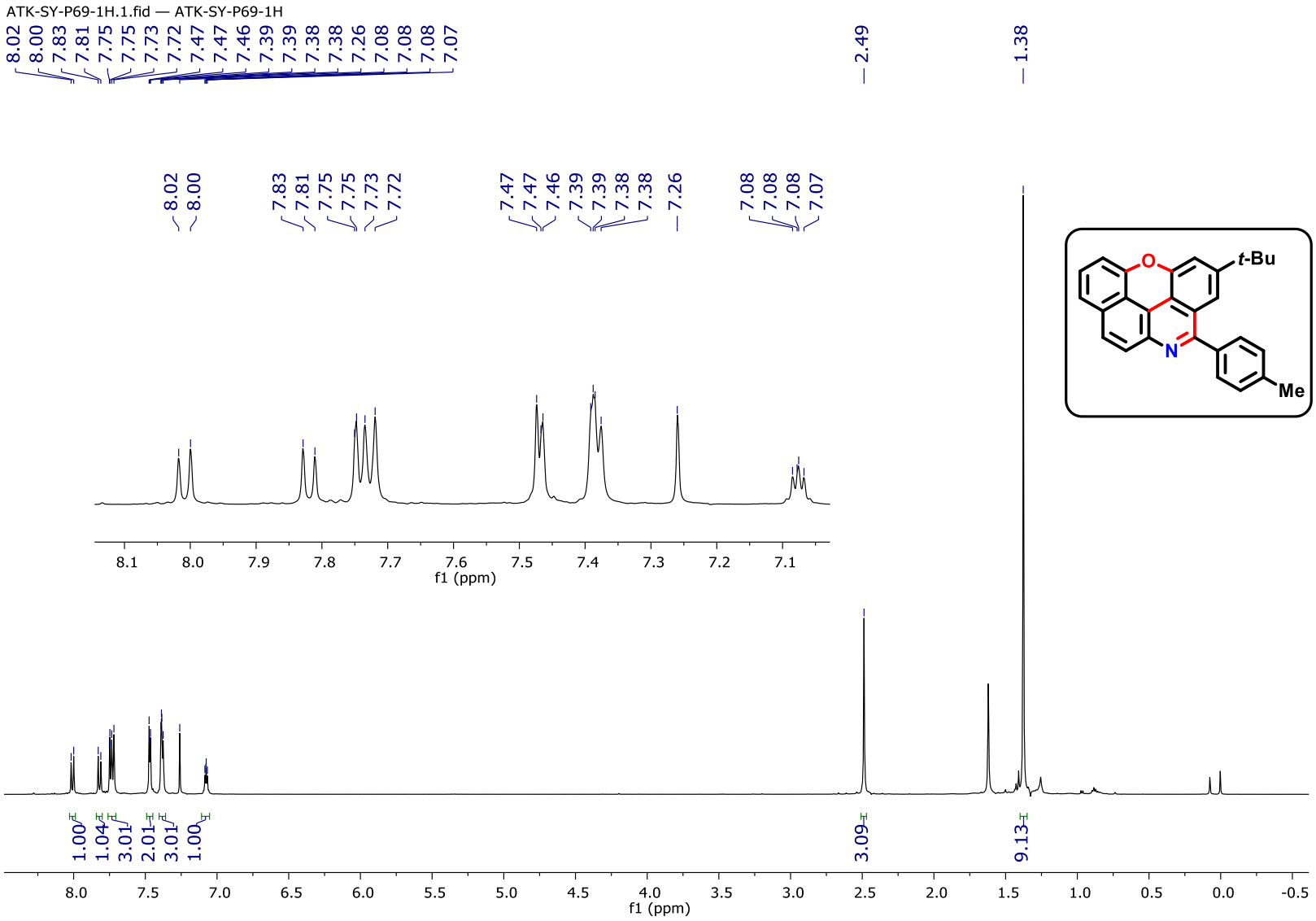
HRMS spectrum of compound 5g

Sample Name	ATK-SY-QP67-POS_N	**Position**	P2-B6	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-QP67-POS_N_126.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	27-Jan-23 10:30:29 PM (UTC+05:30)

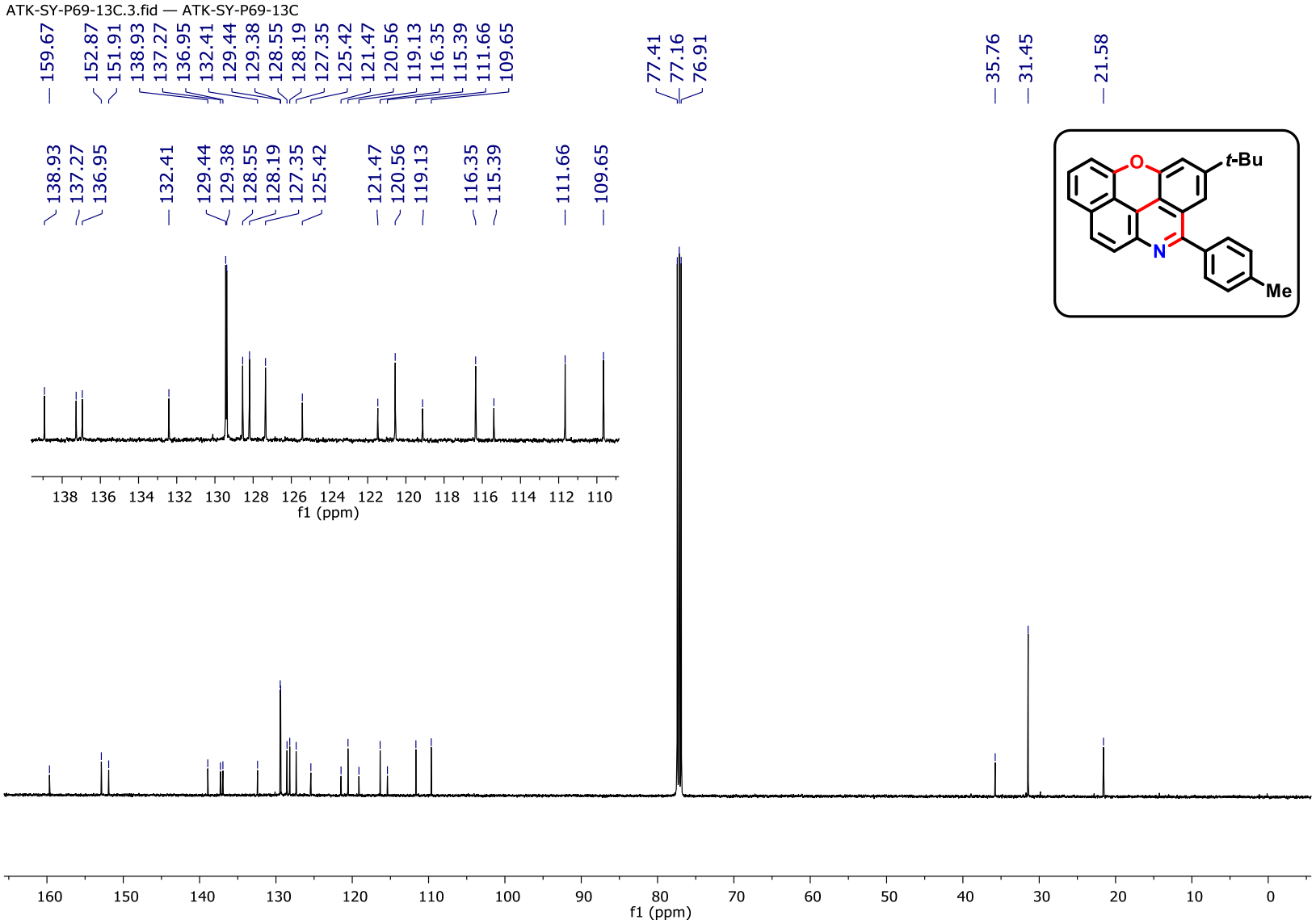




^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 5h

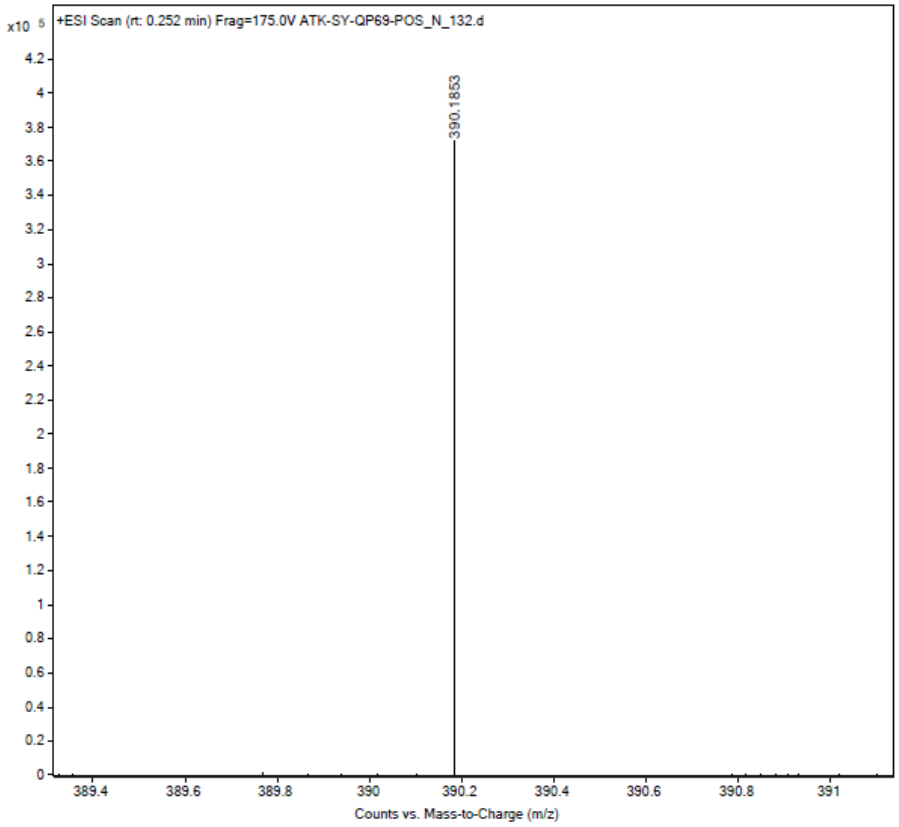


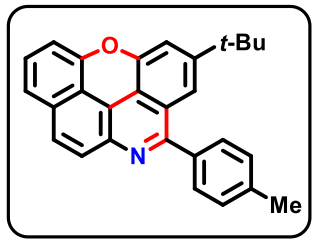
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5h



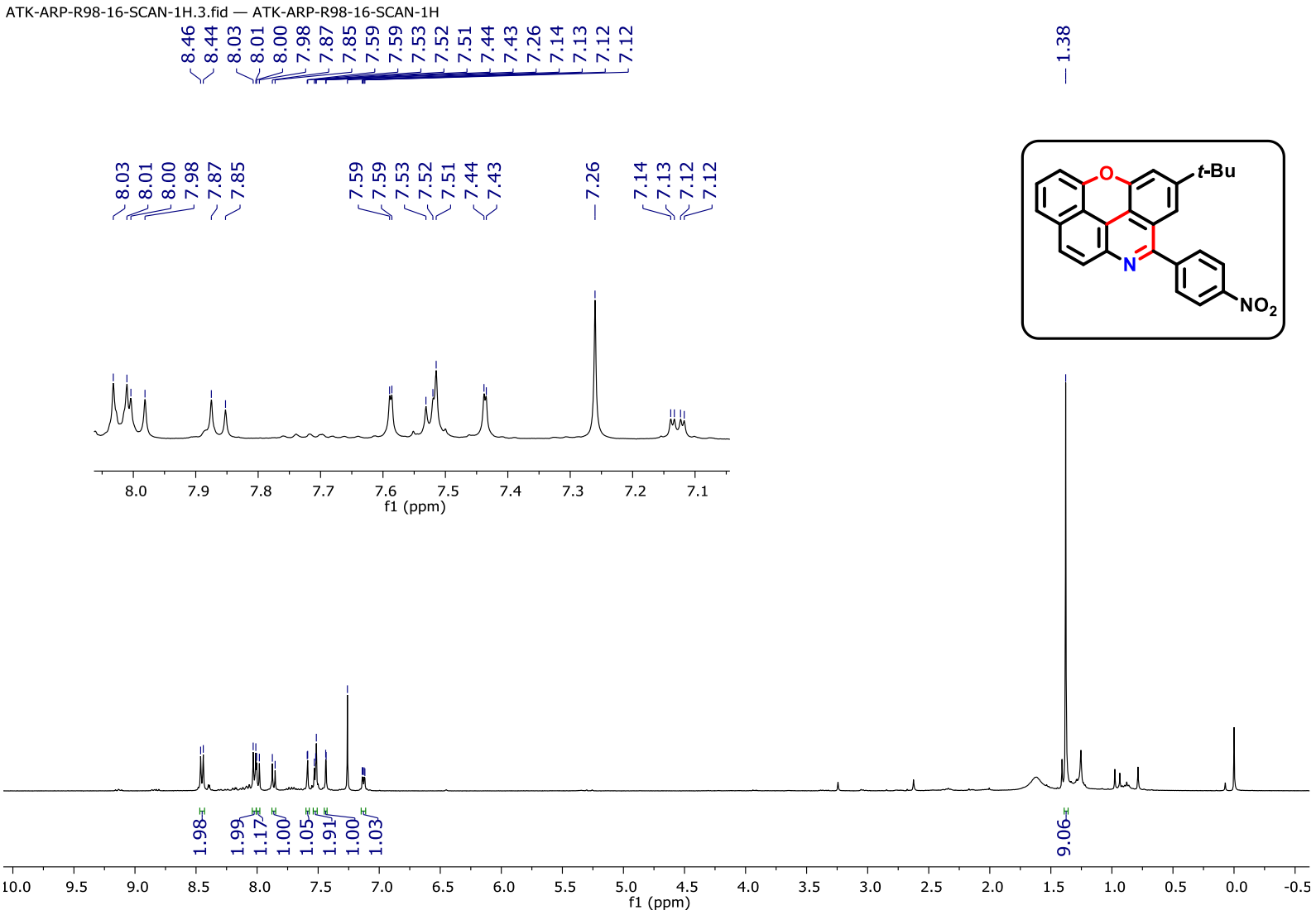
HRMS spectrum of compound 5h

Sample Name	ATK-SY-QP69-POS_N	**Position**	P2-B8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-QP69-POS_N_132.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	27-Jan-23 10:41:17 PM (UTC+05:30)

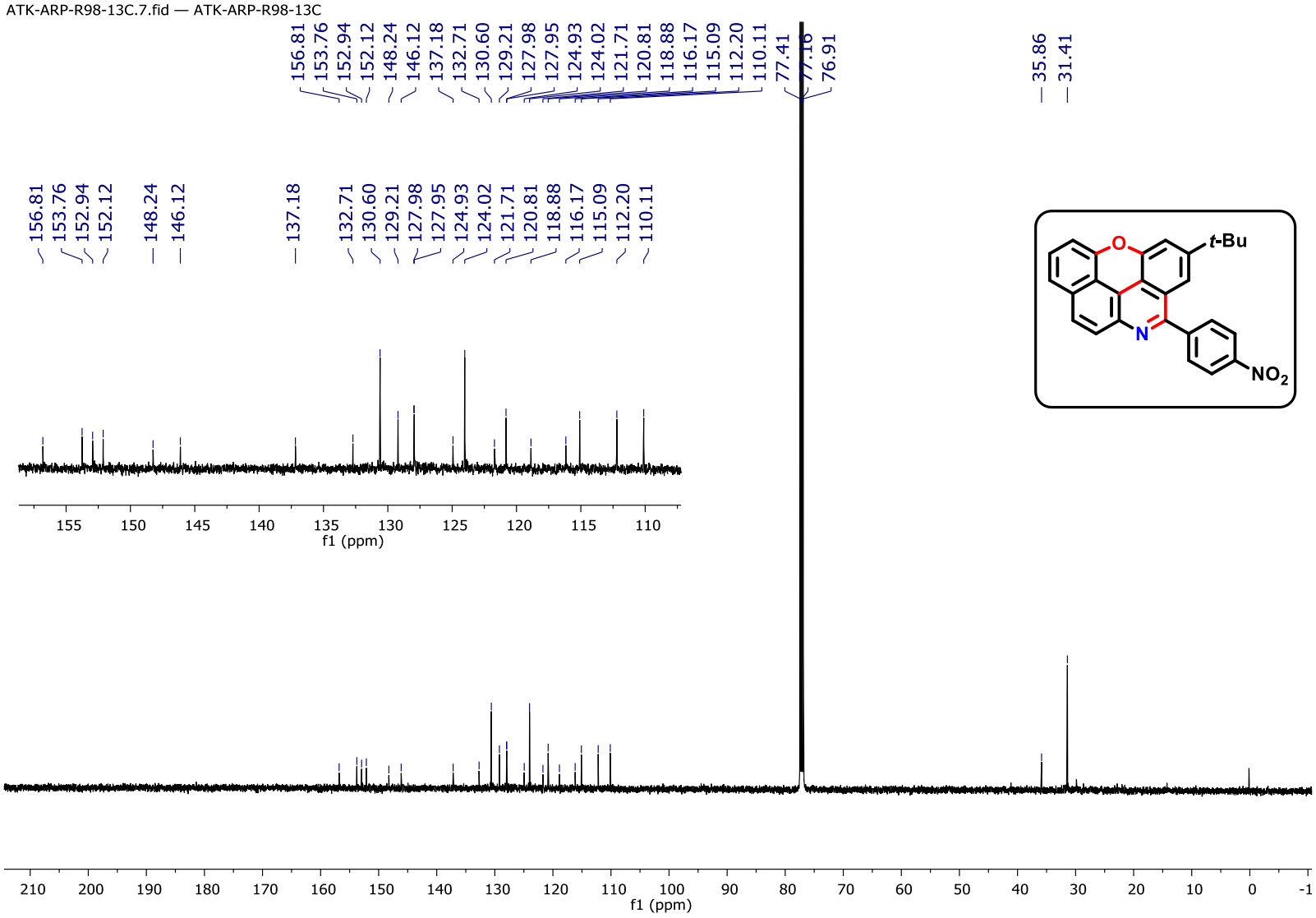




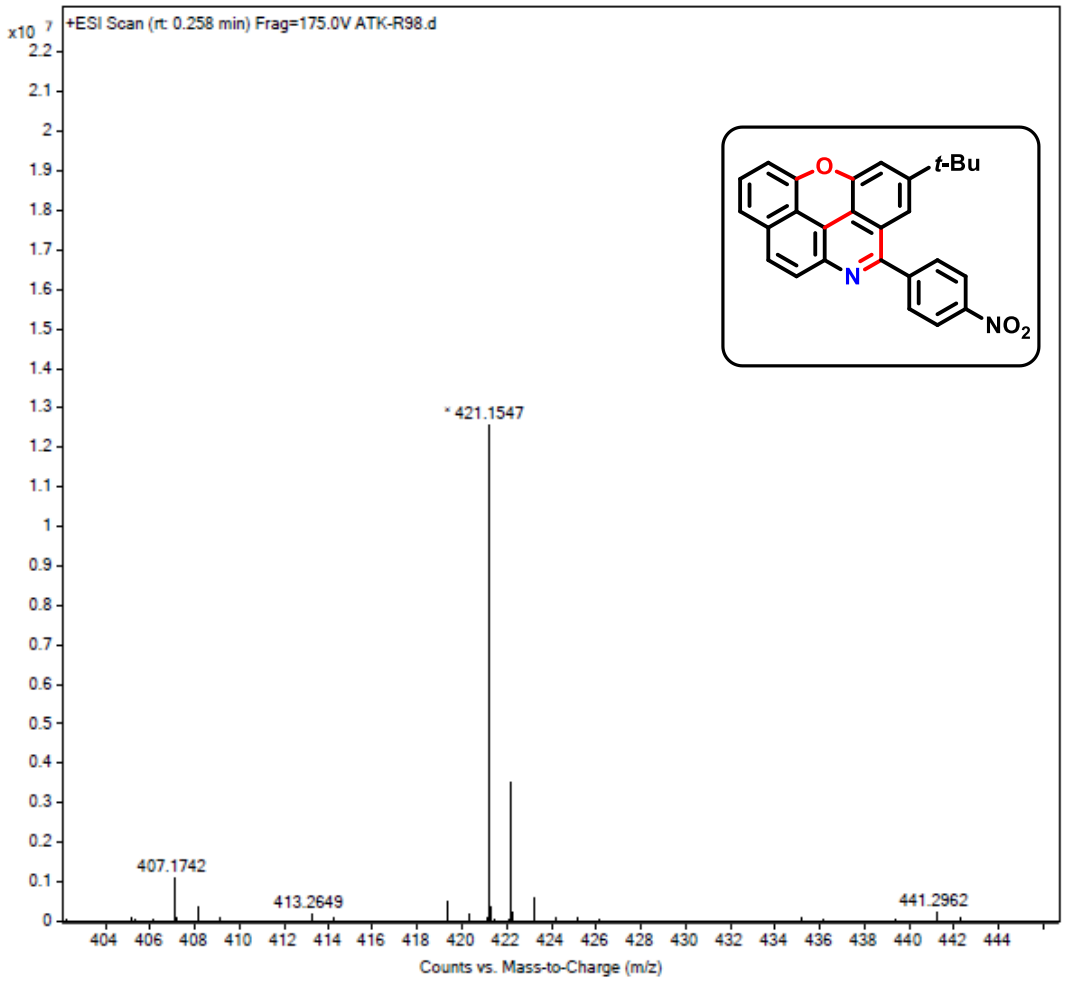
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5i



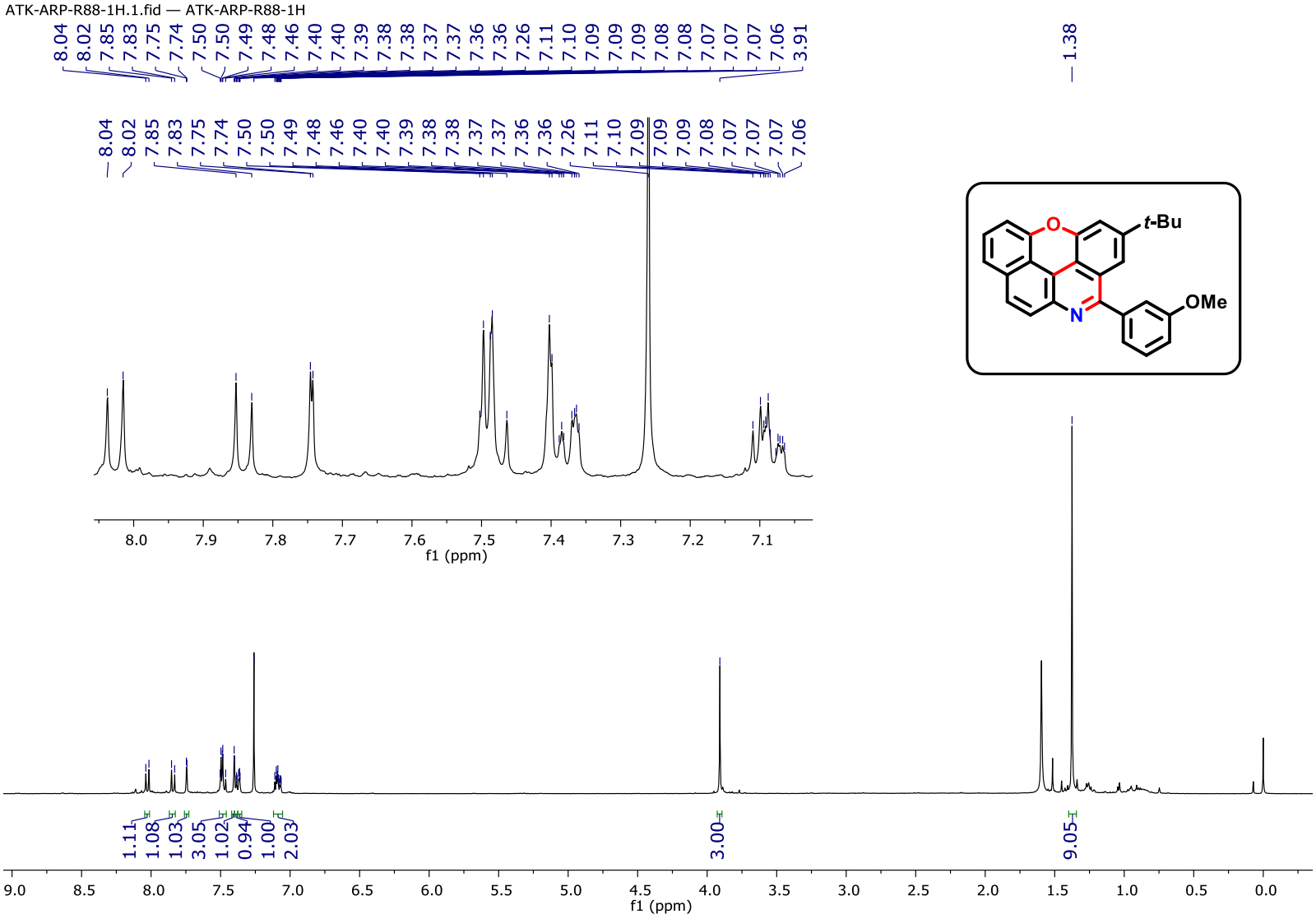
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5i



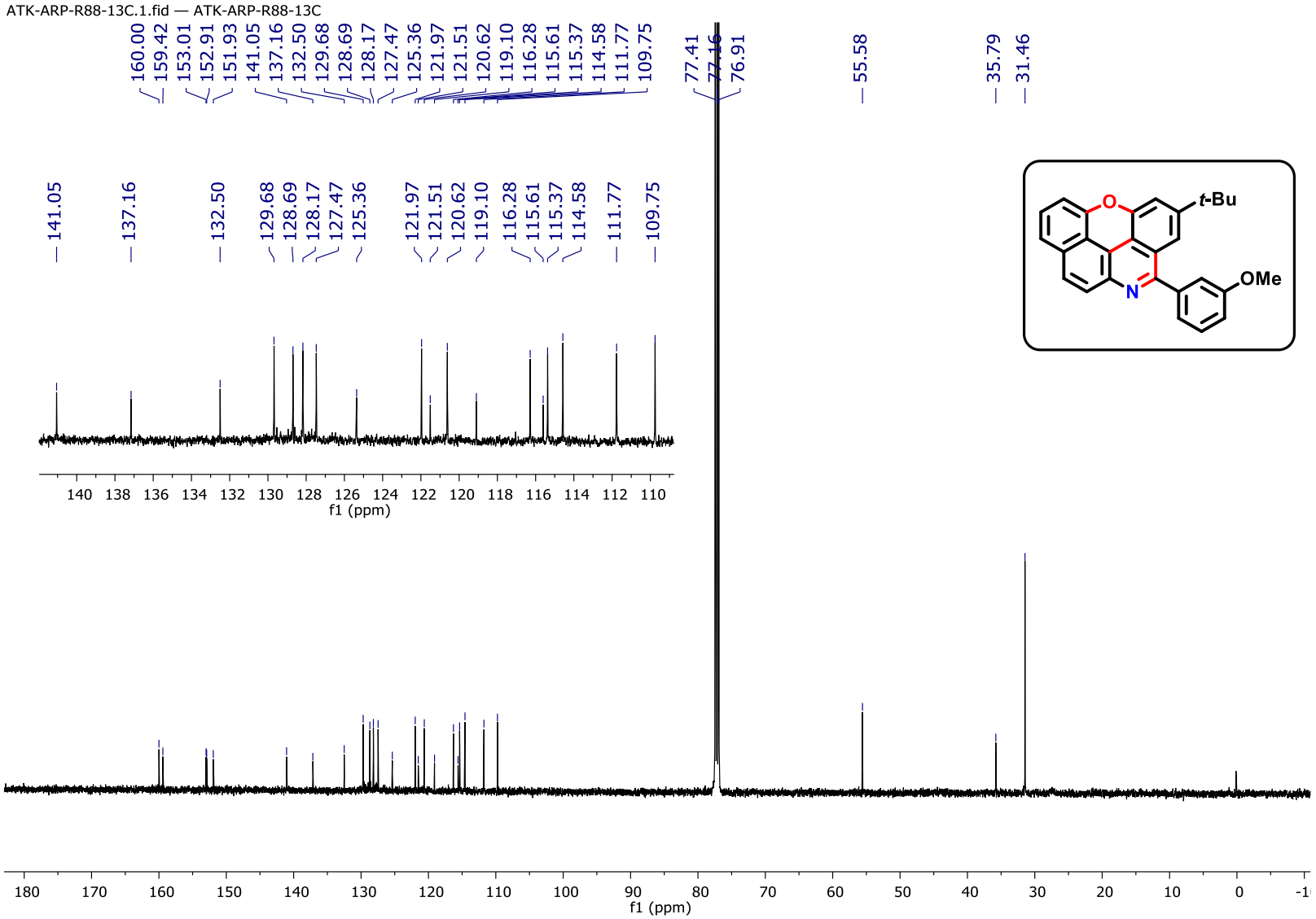
HRMS spectrum of compound 5i



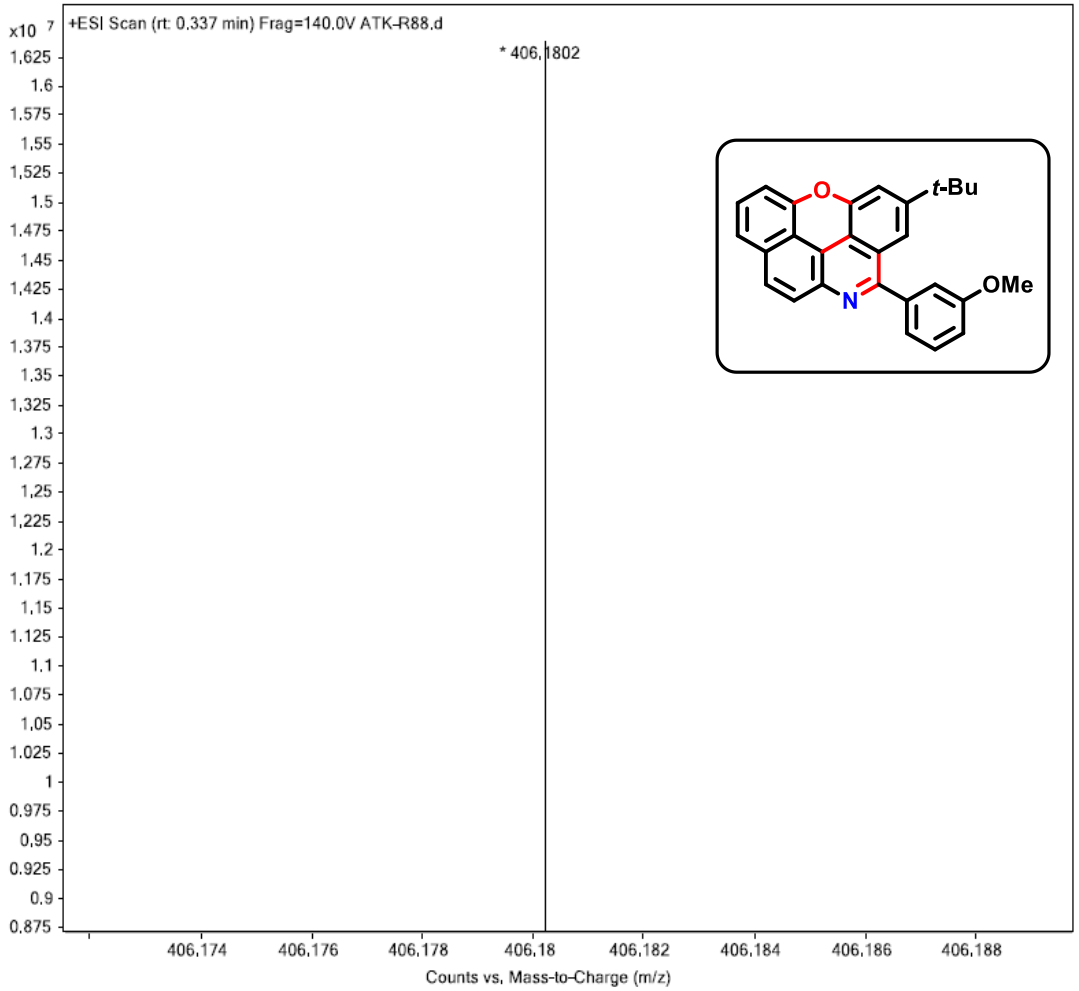
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5j



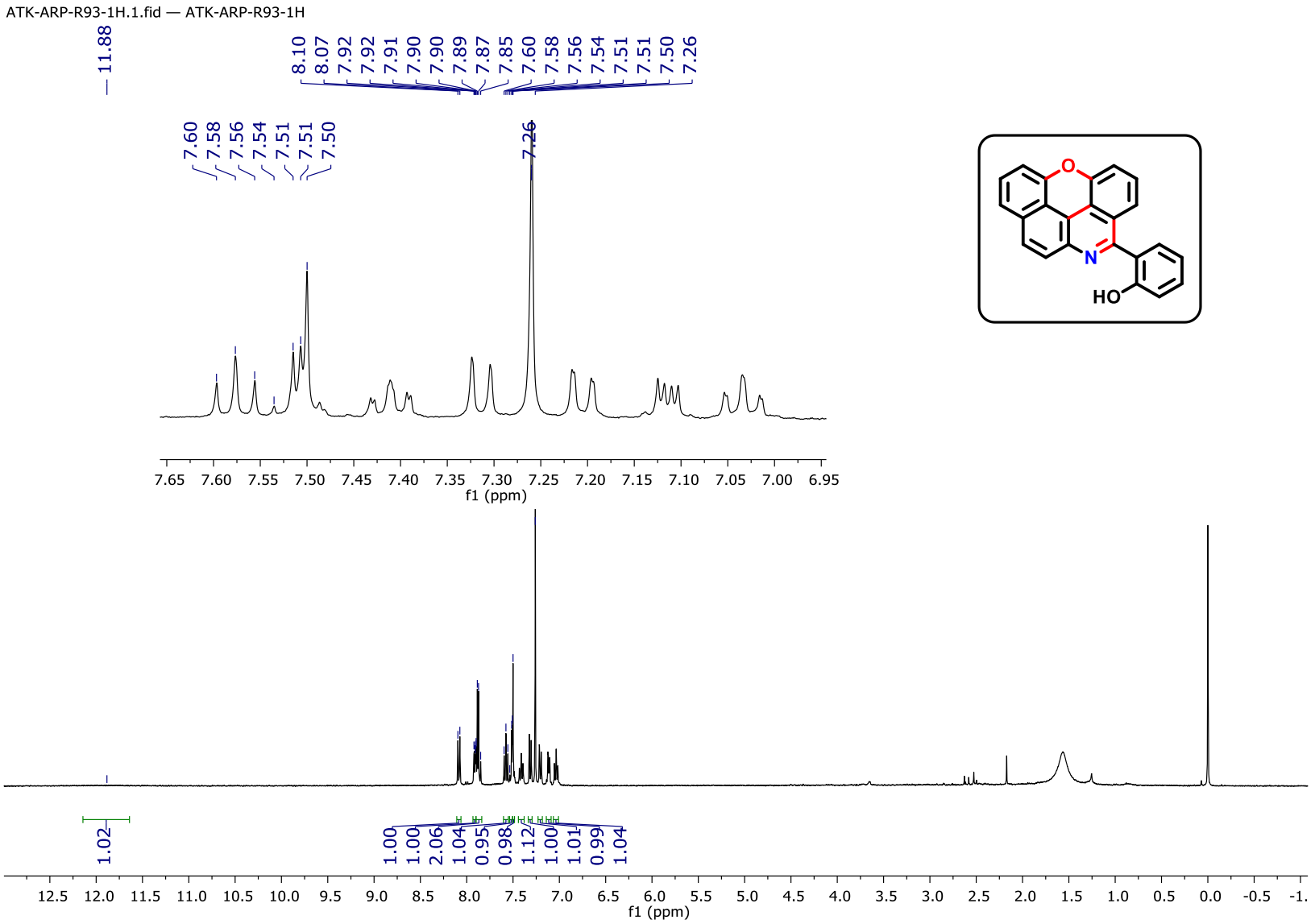
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5j



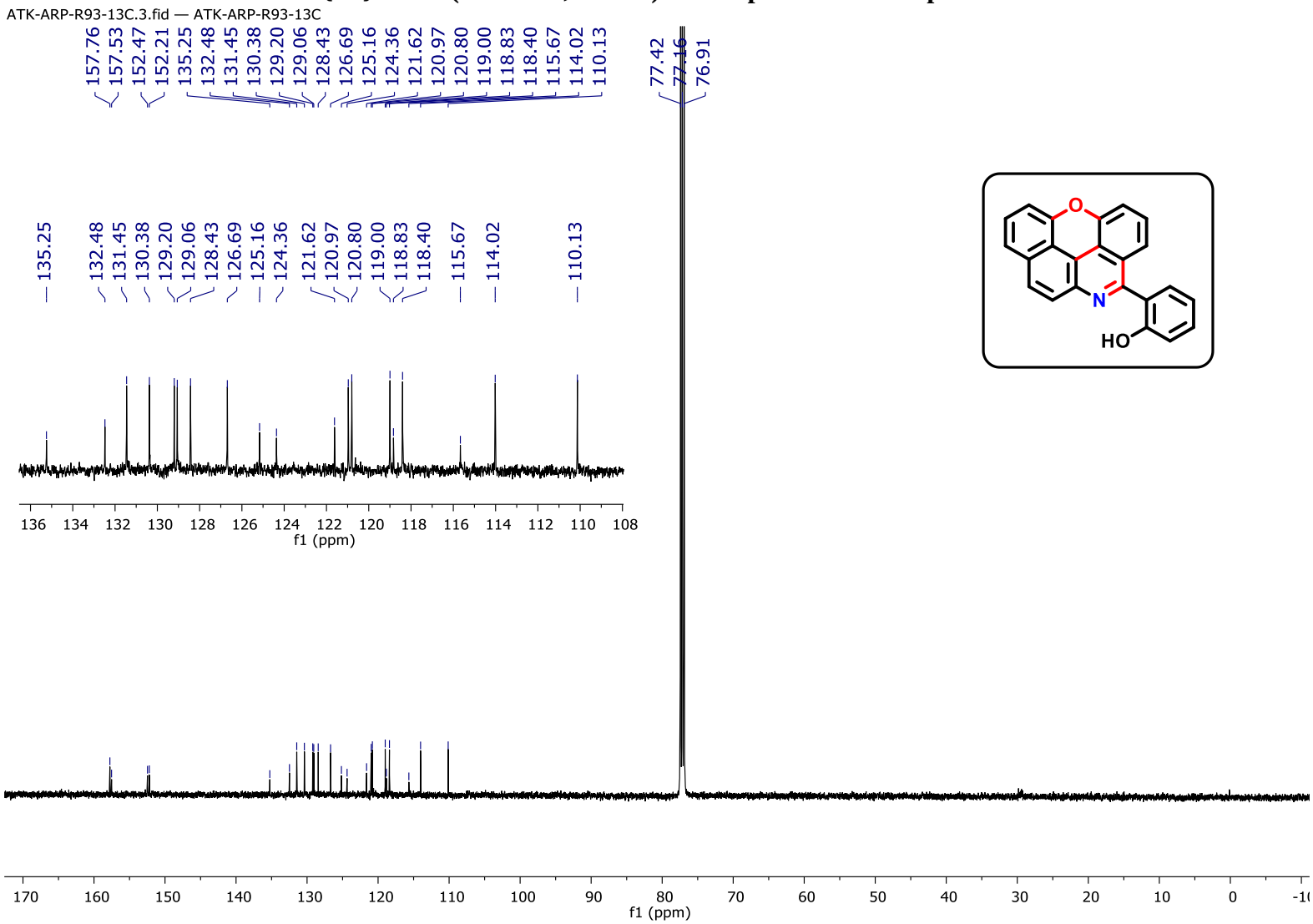
HRMS spectrum of compound 5j



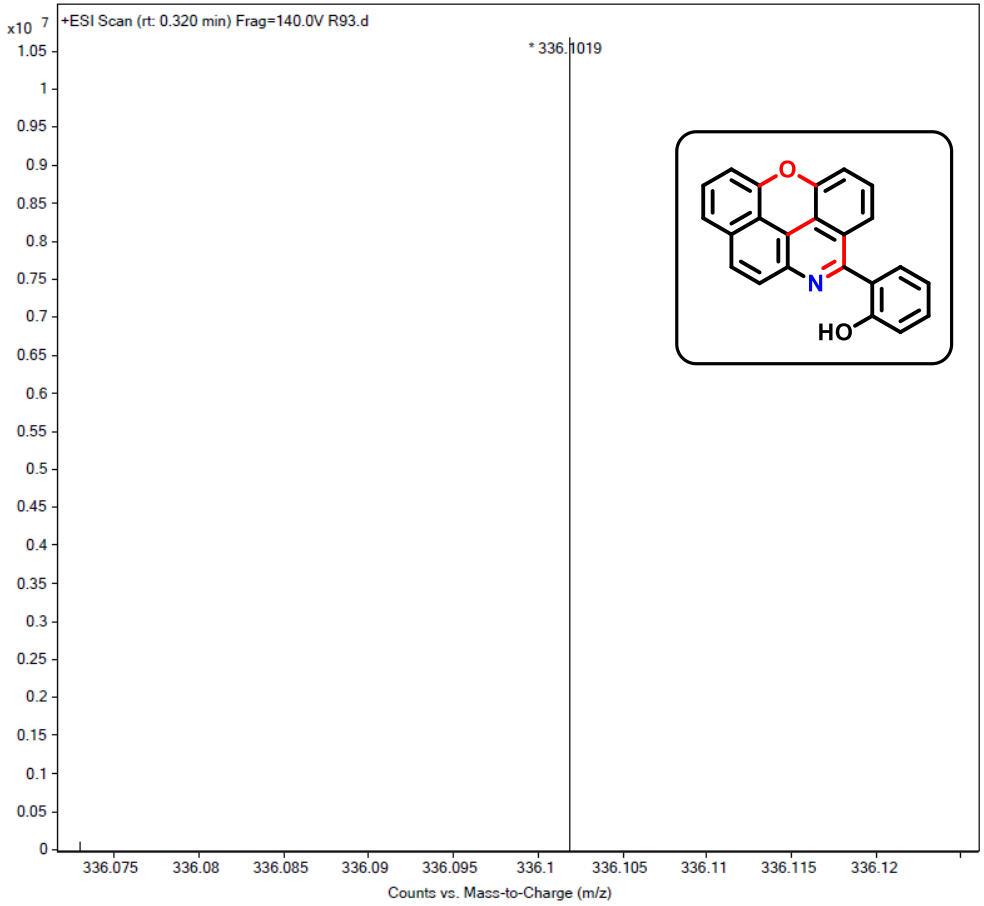
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5k



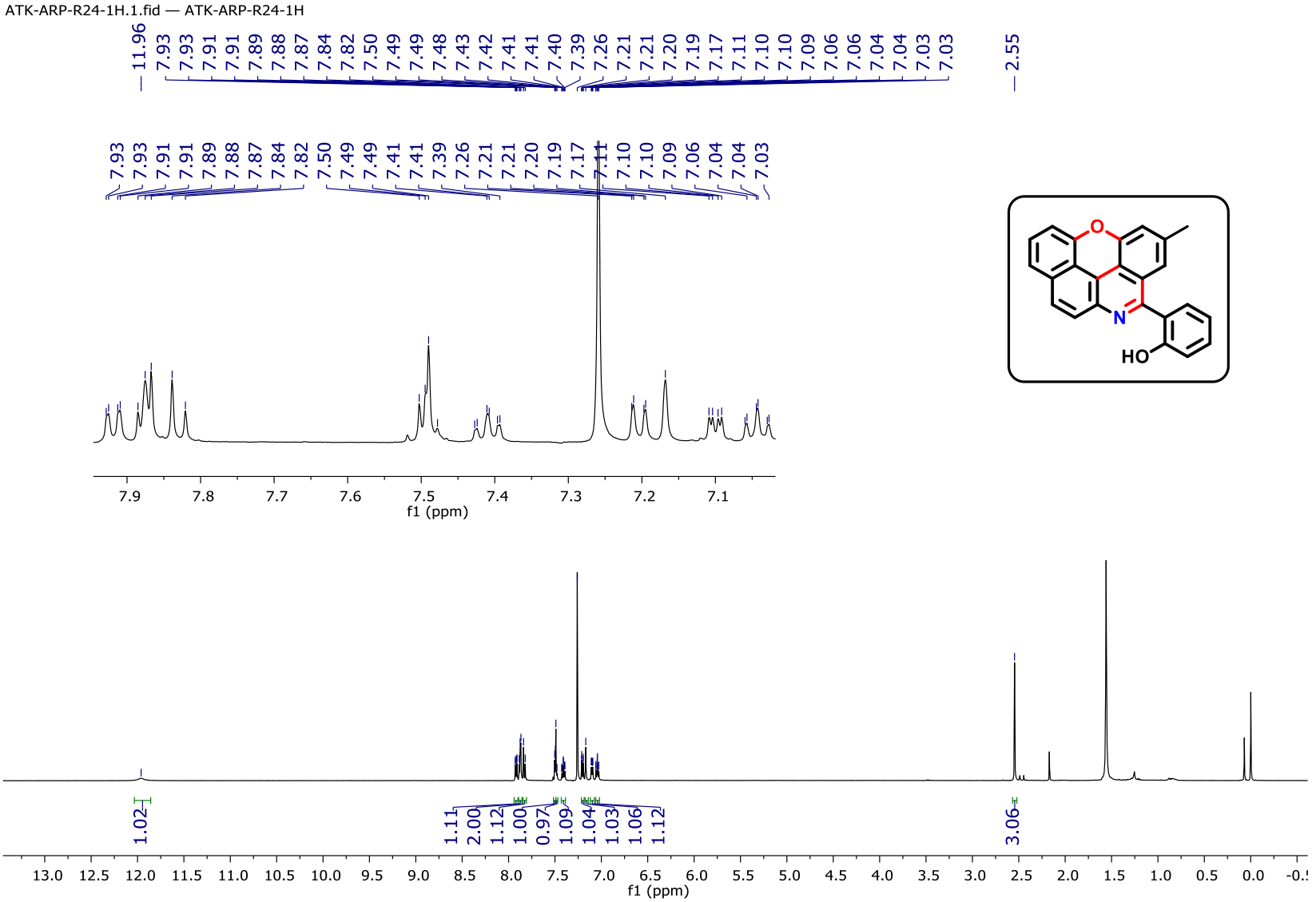
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5k



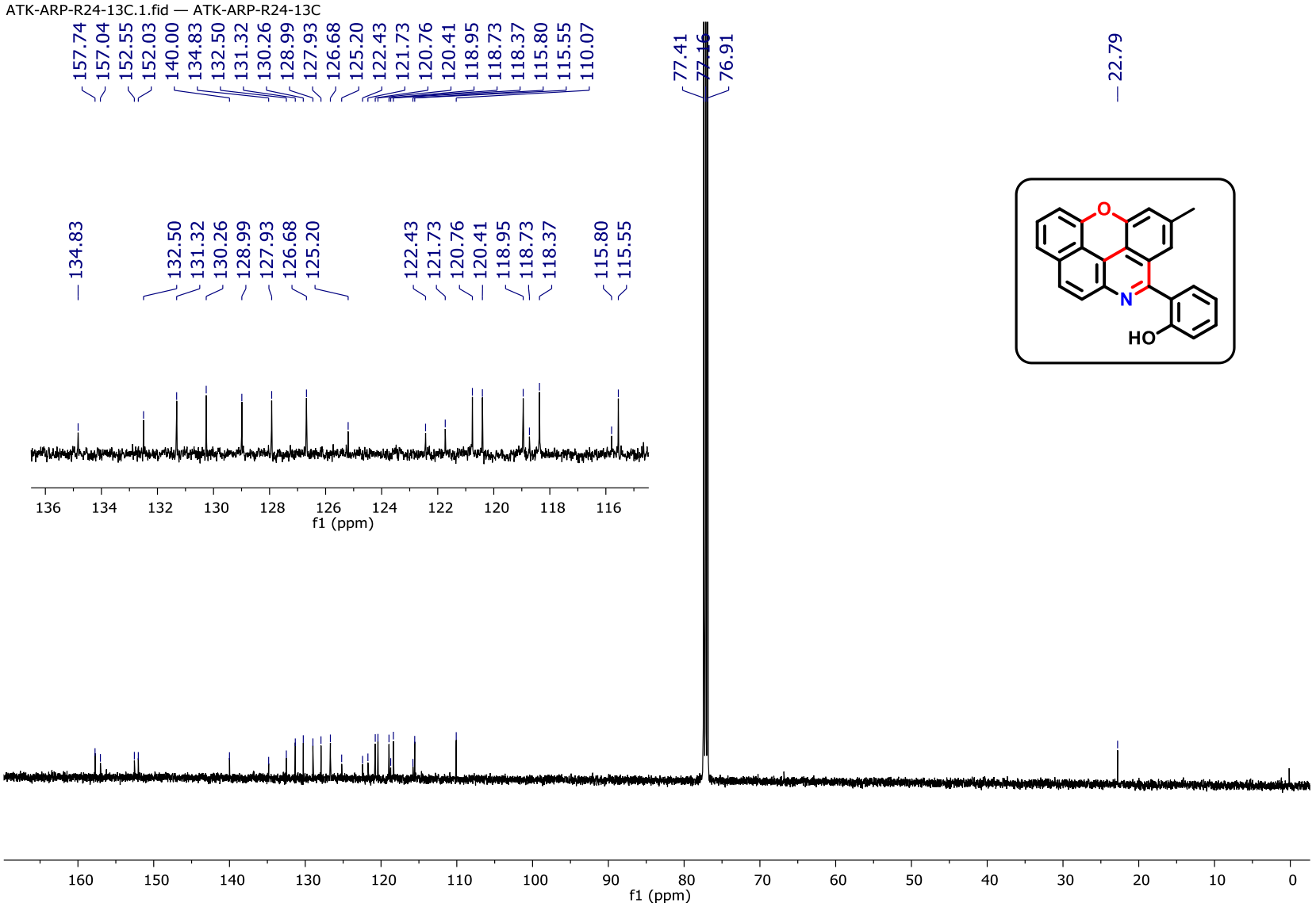
HRMS spectrum of compound 5k



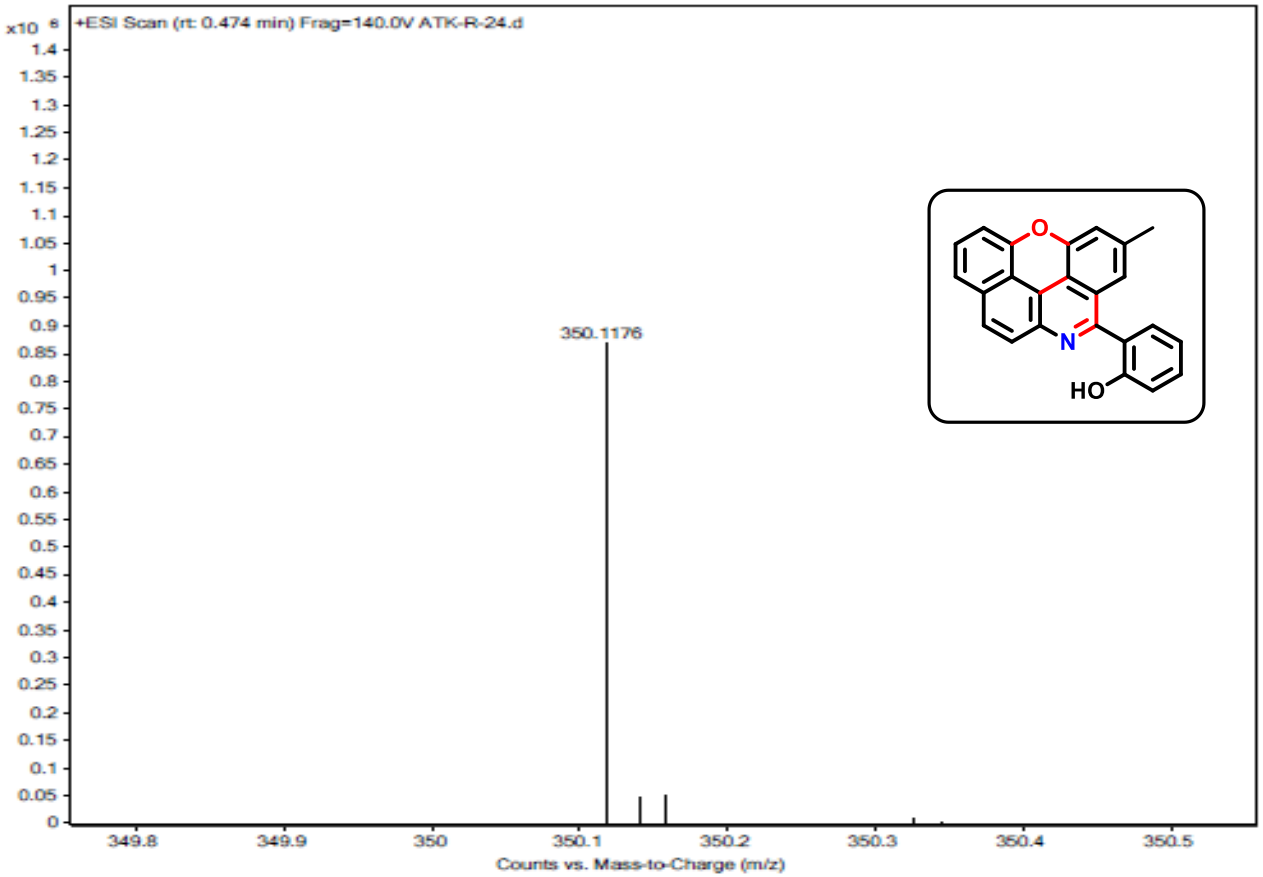
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 5l



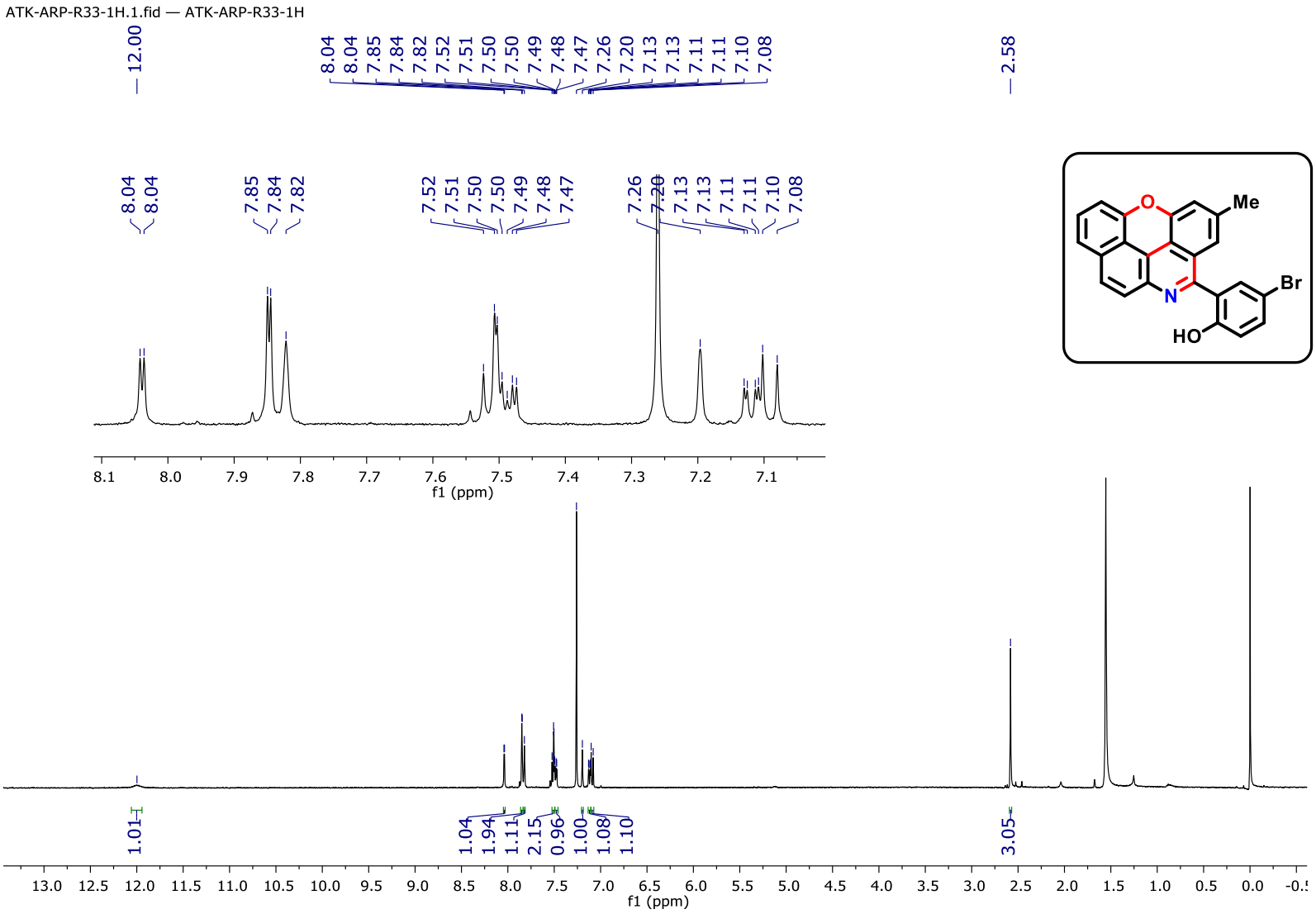
^{13}C {^{1}H } NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5l



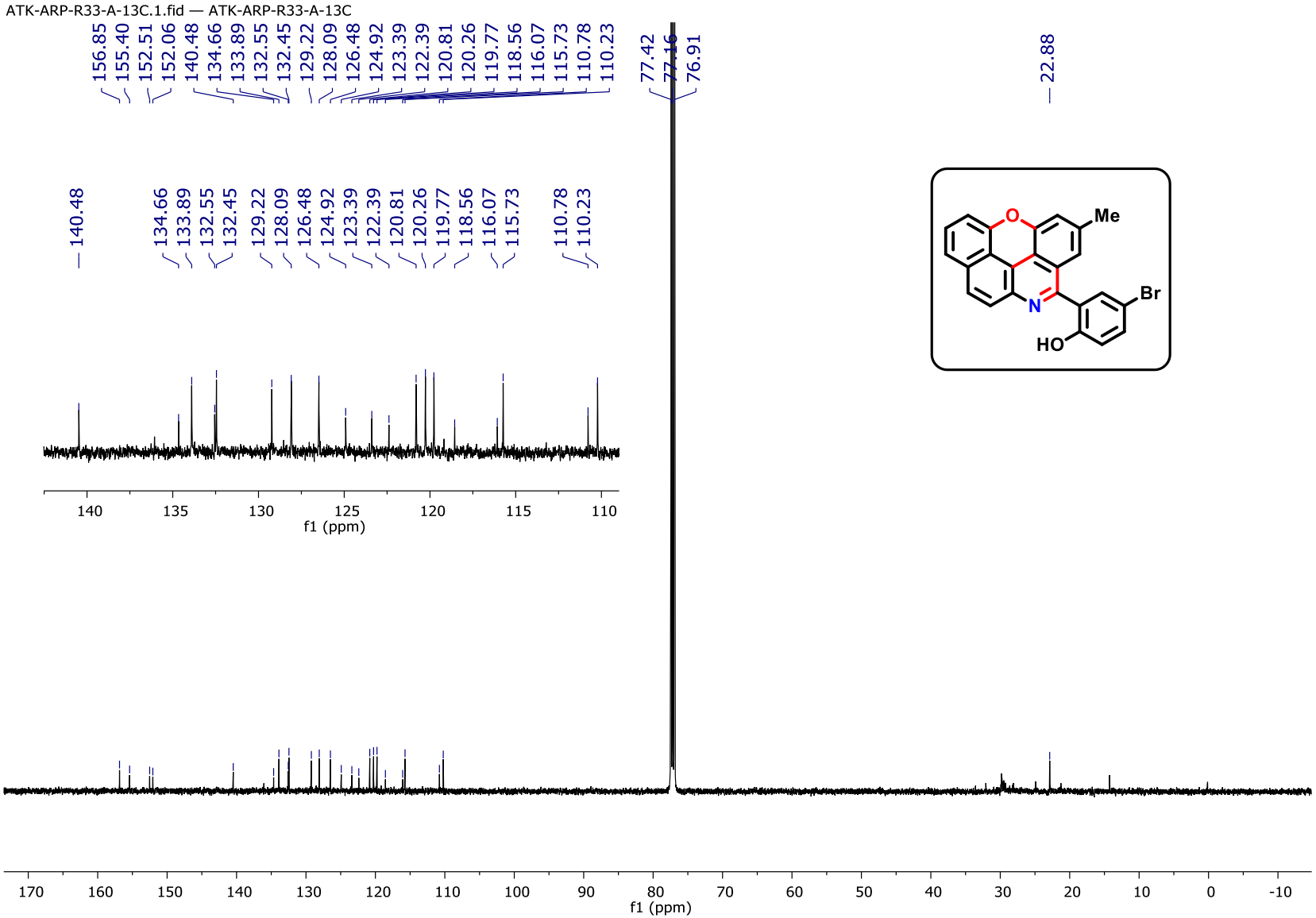
HRMS spectrum of compound 5l



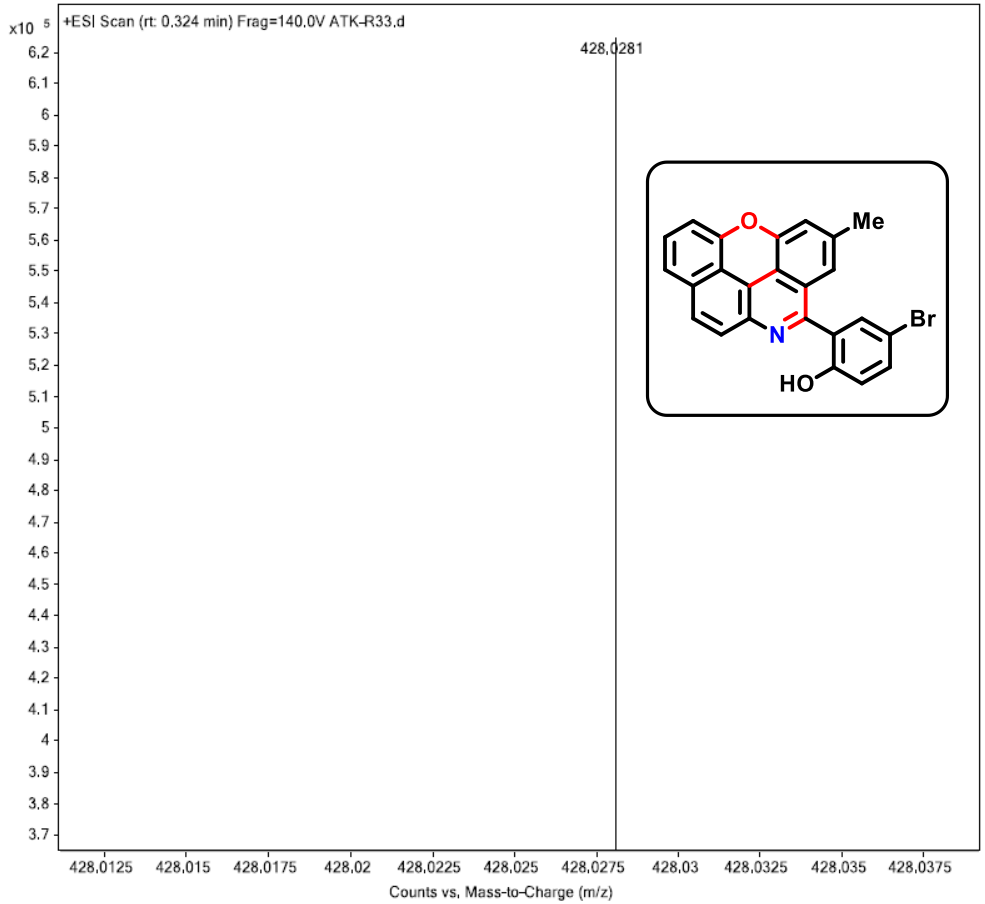
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5m



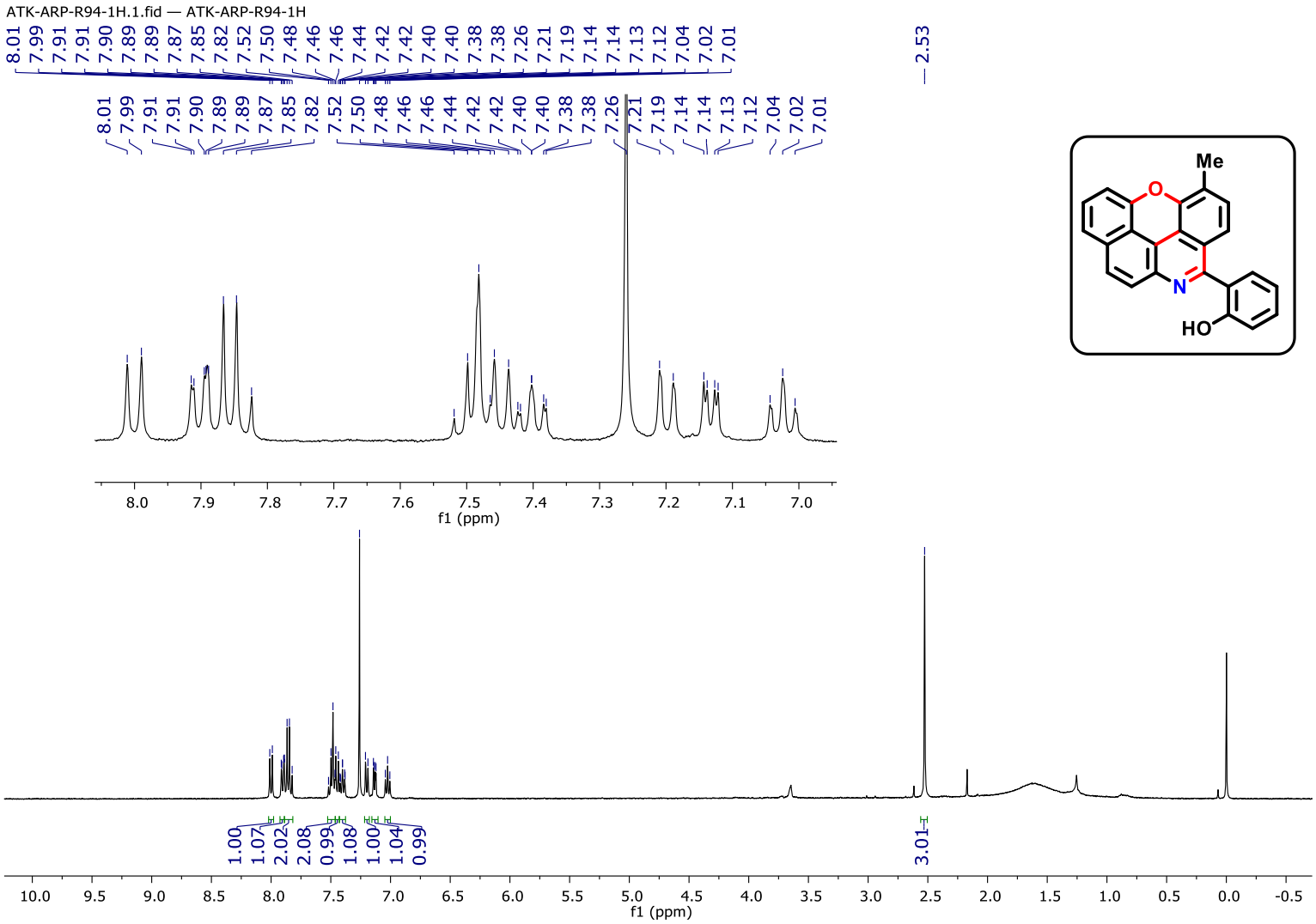
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5m



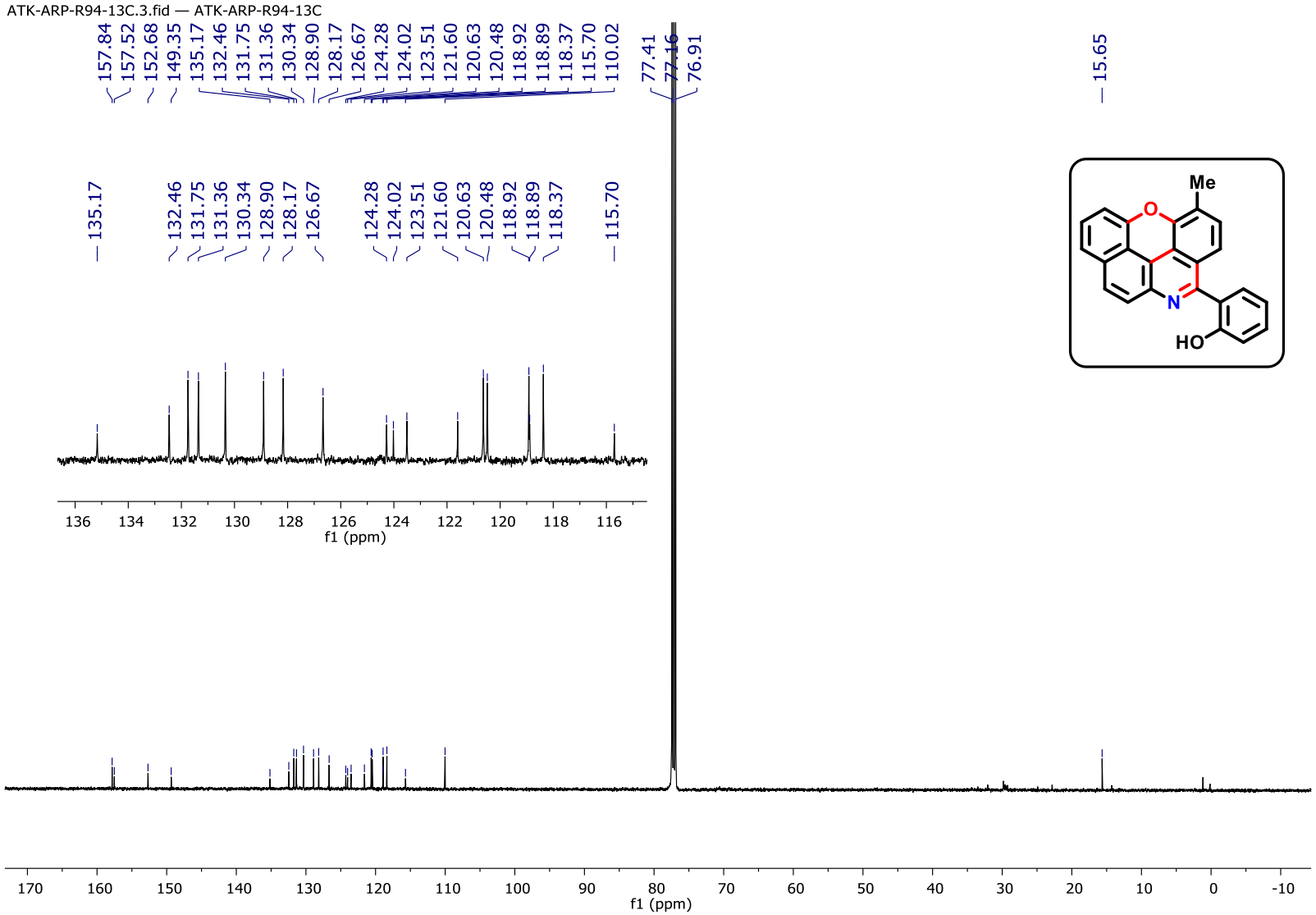
HRMS spectrum of compound 5m



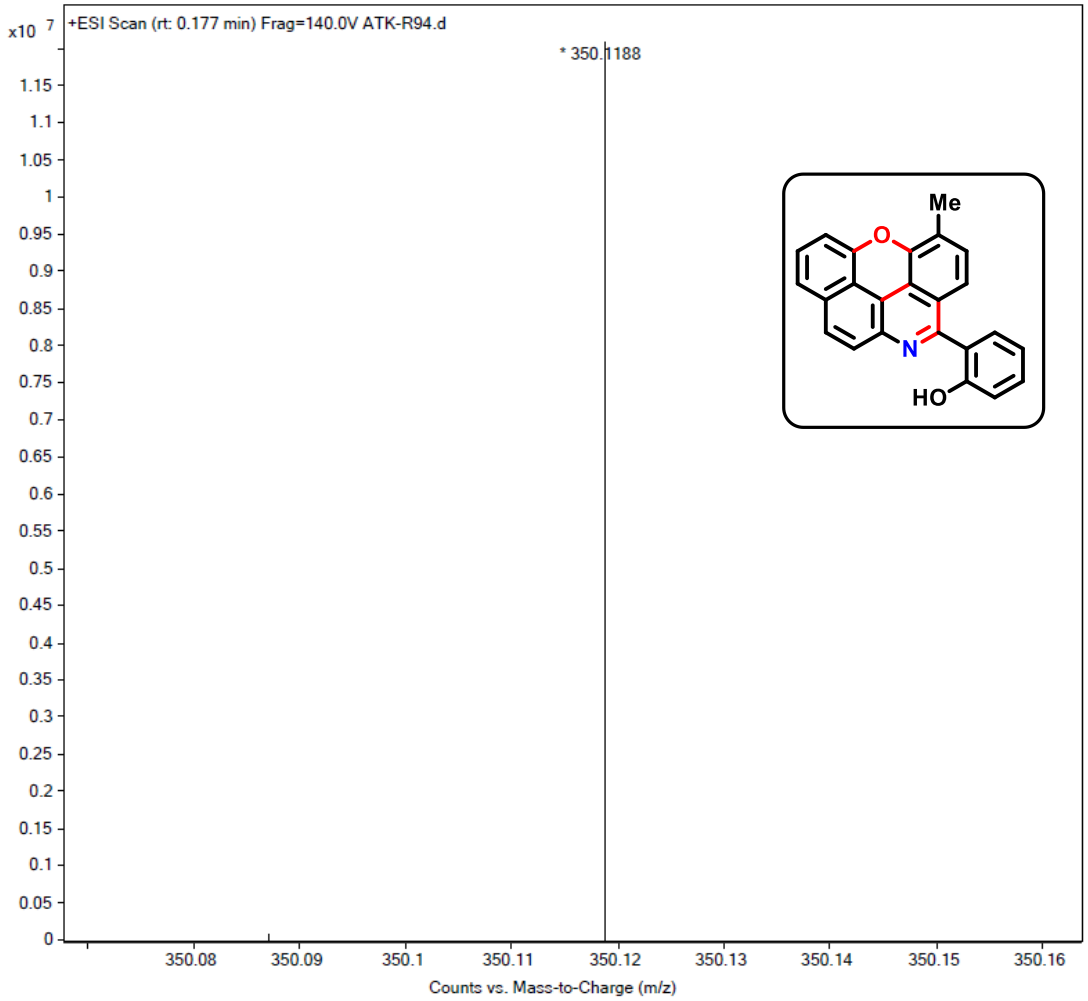
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5n



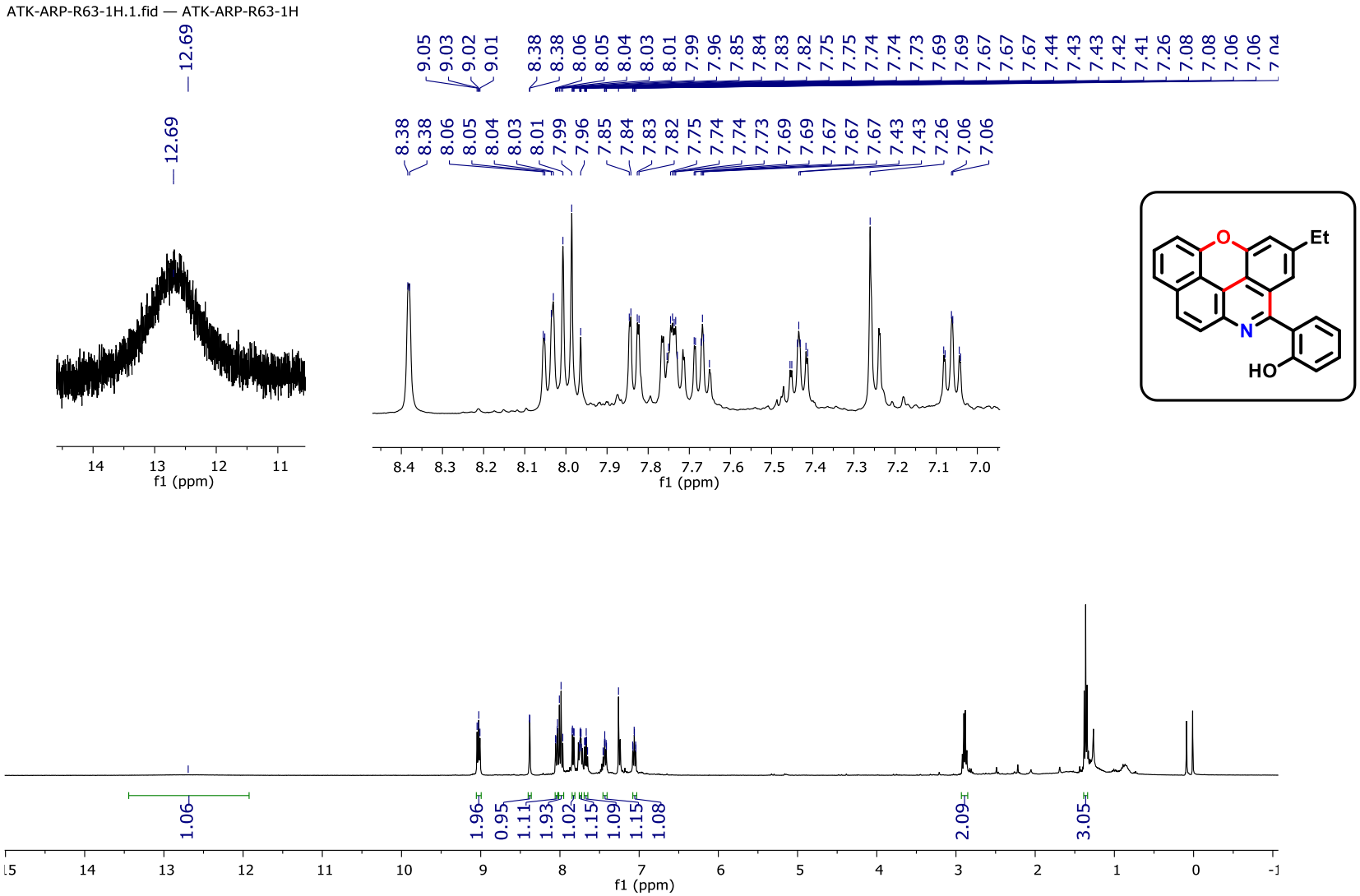
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5n



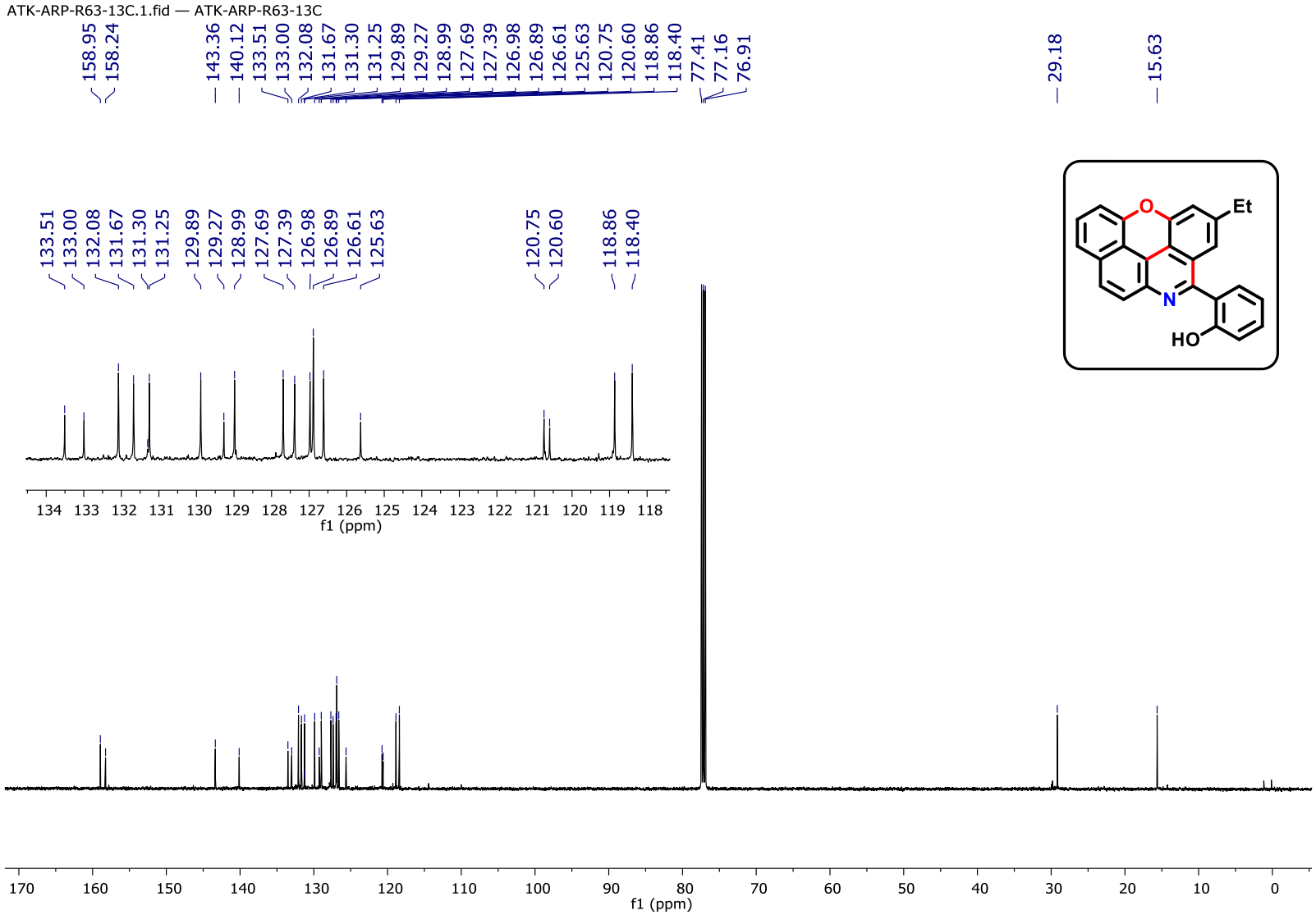
HRMS spectrum of compound 5n



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5o

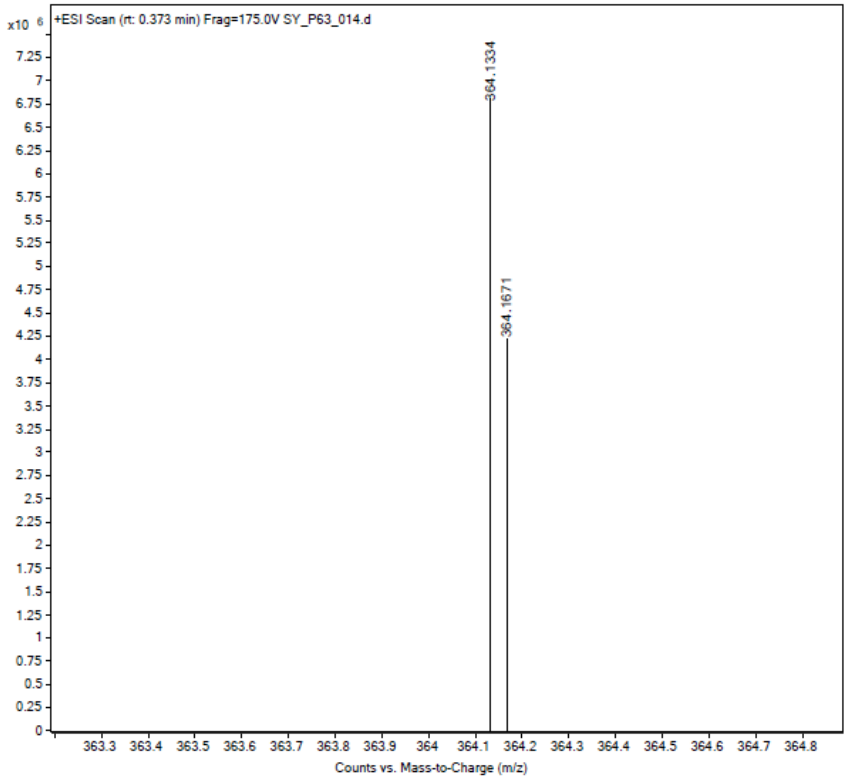


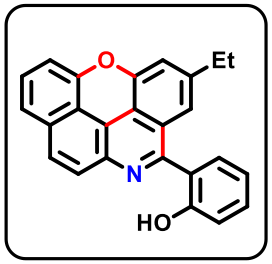
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5o



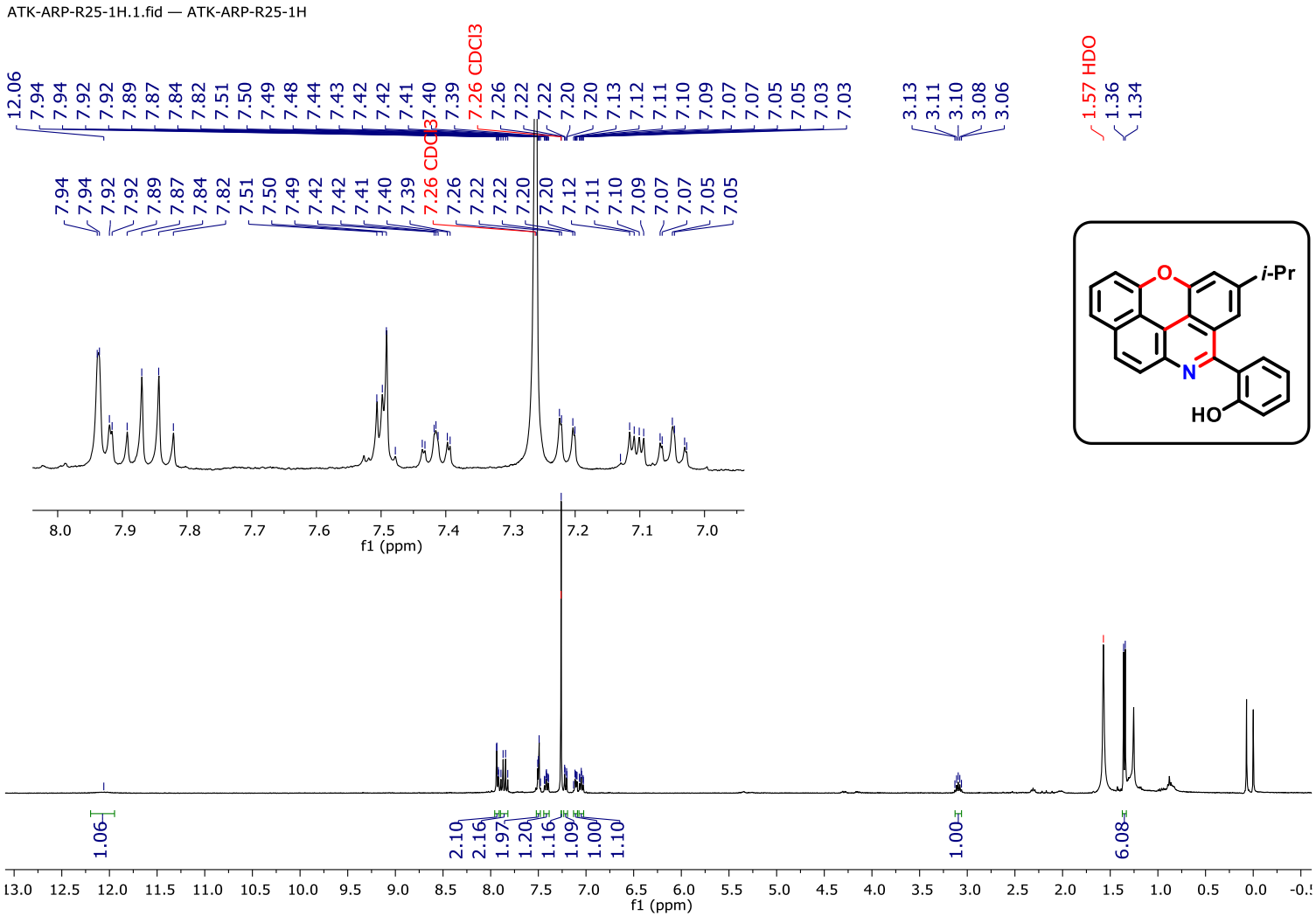
HRMS spectrum of compound 5o

Sample Name	SY_P63	**Position**	P1-B5	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY_P63_014.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	28-Aug-22 12:32:00 AM (UTC+05:30)

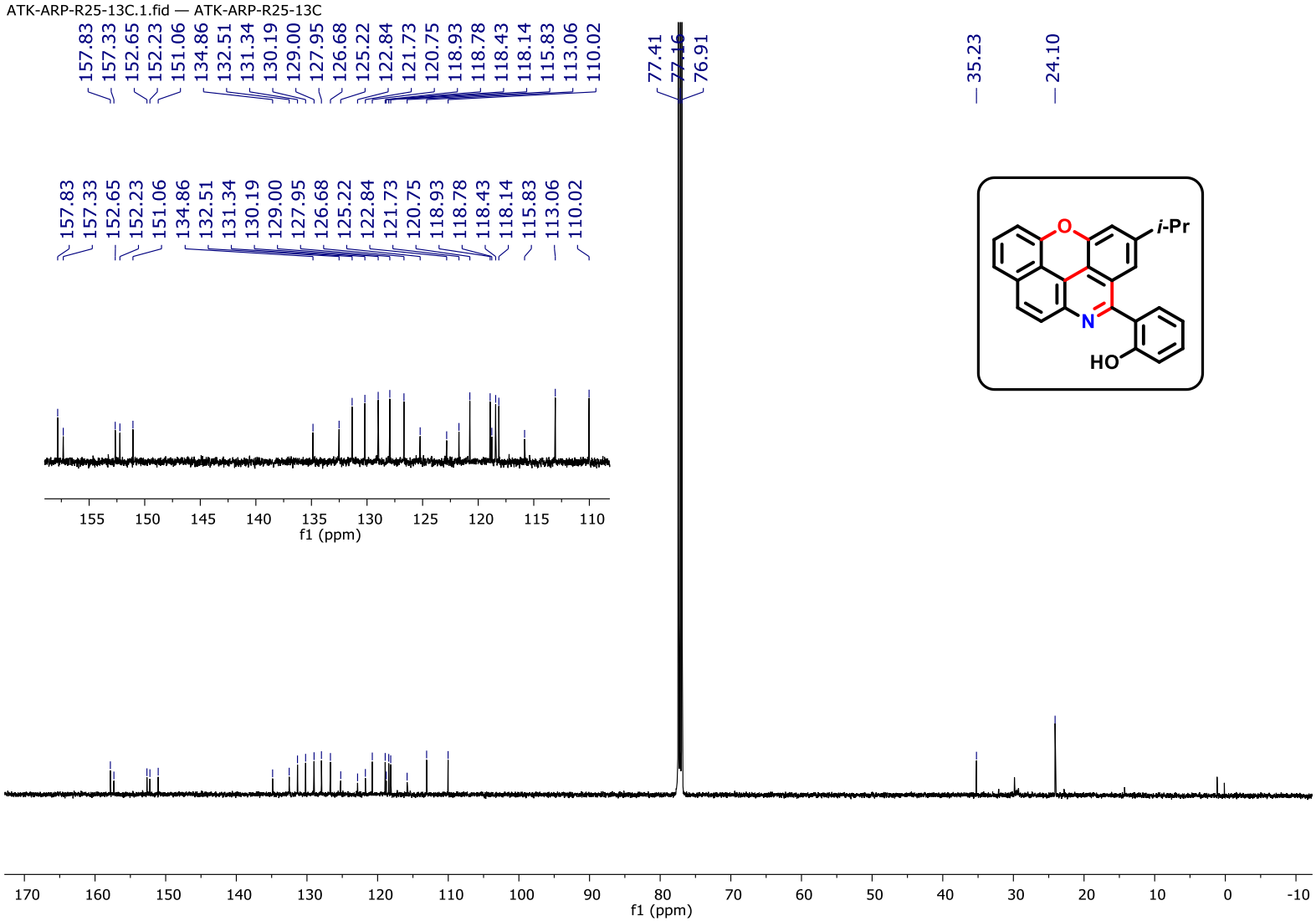




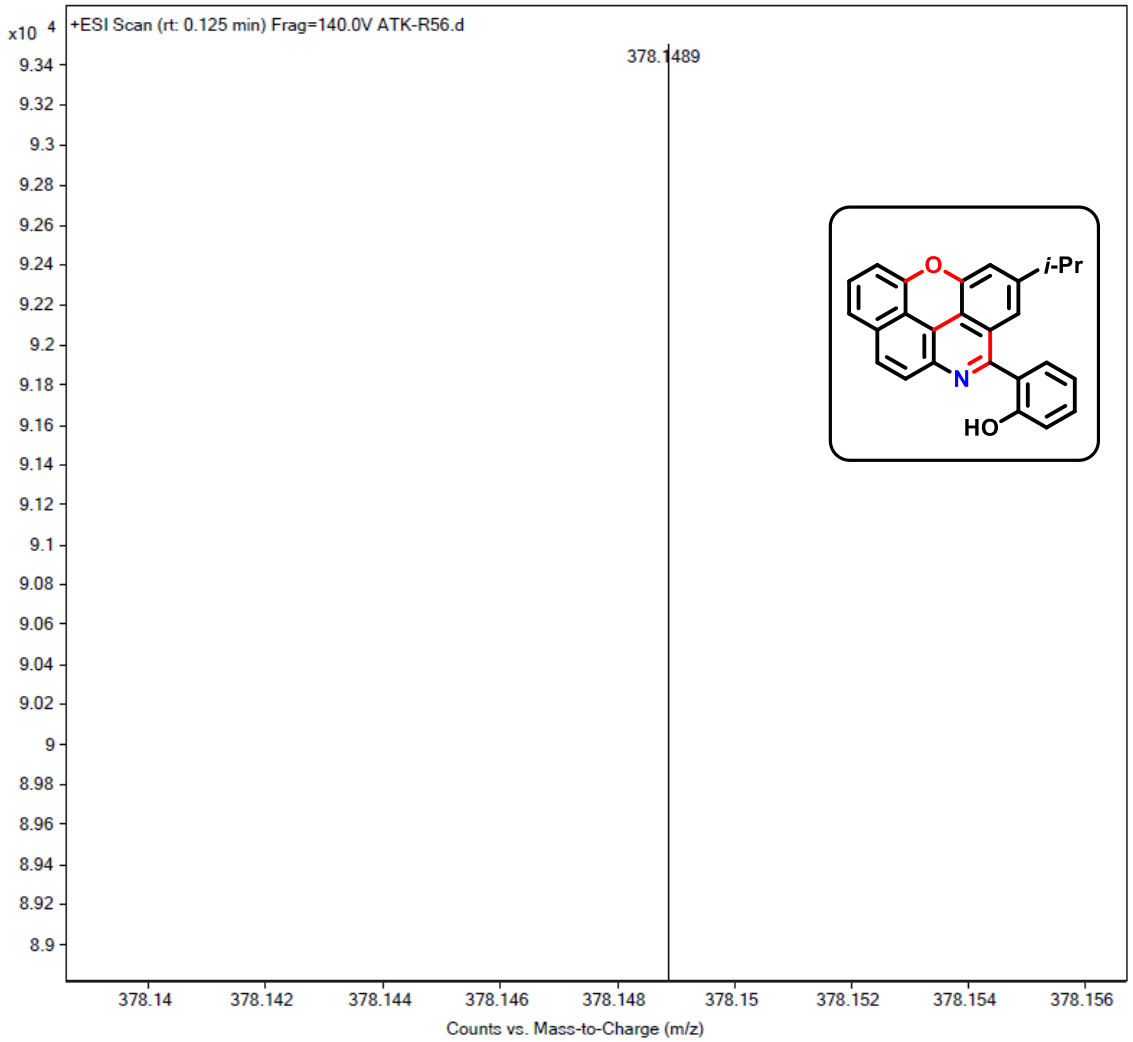
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5p



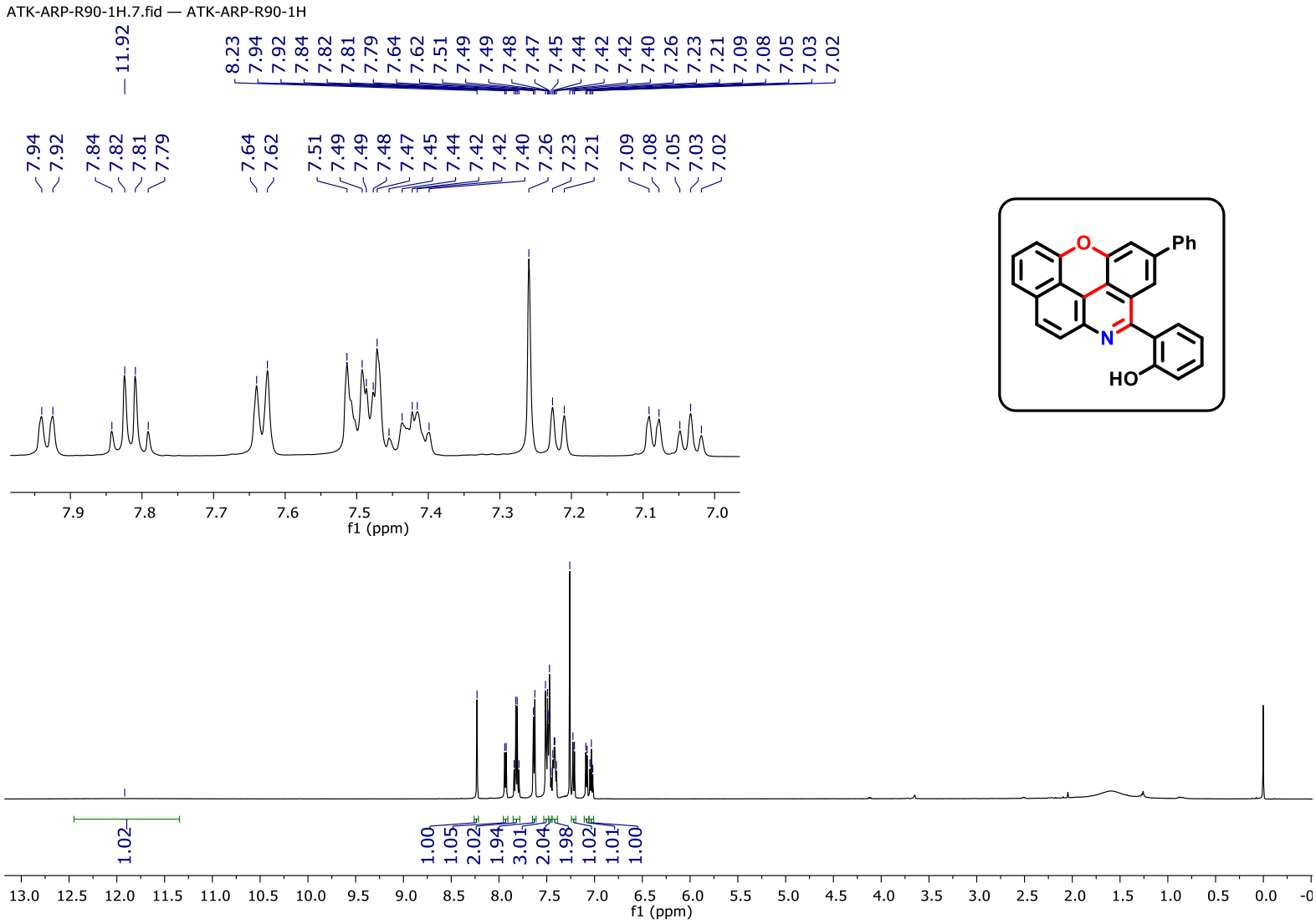
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5p



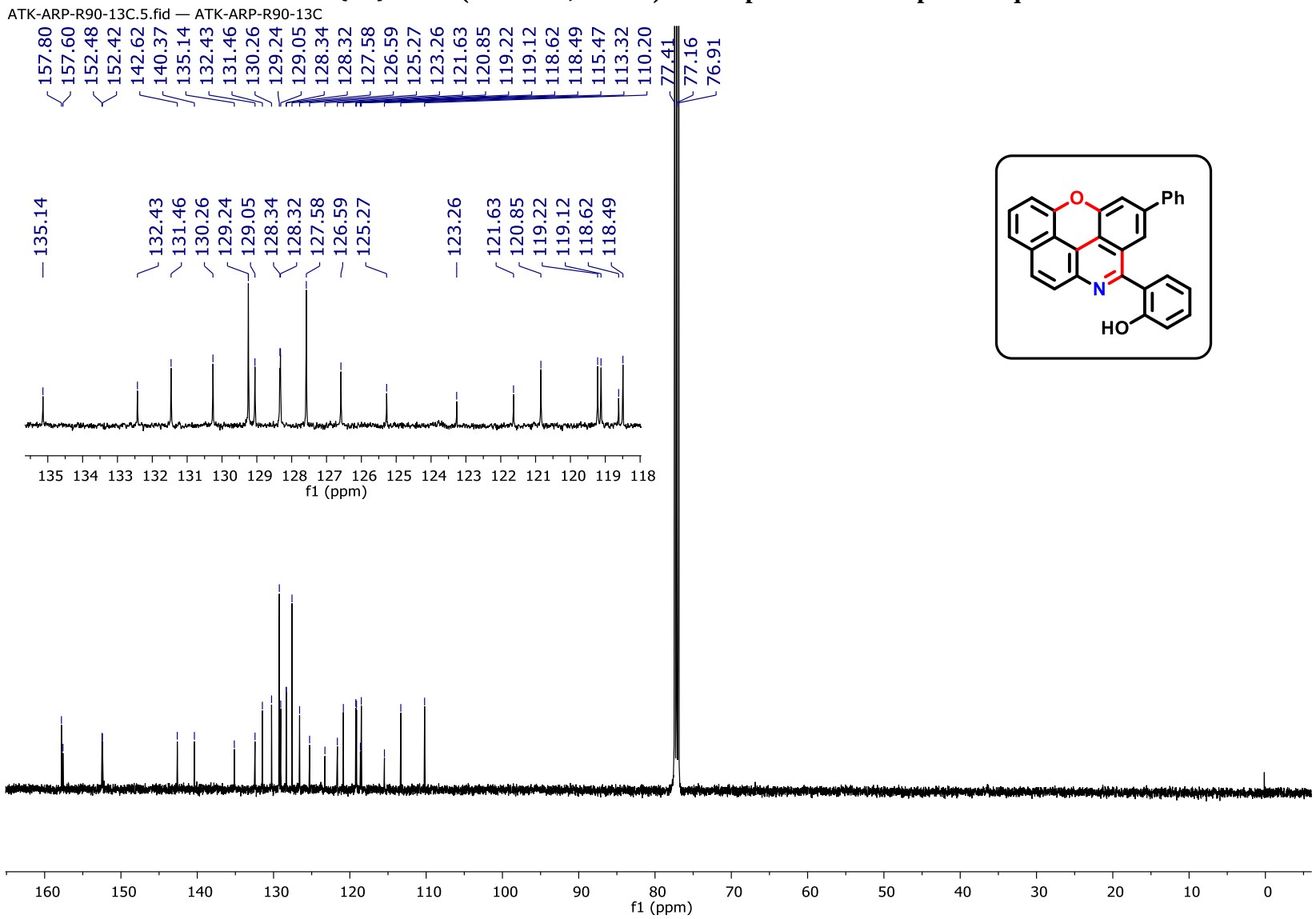
HRMS spectrum of compound 5p



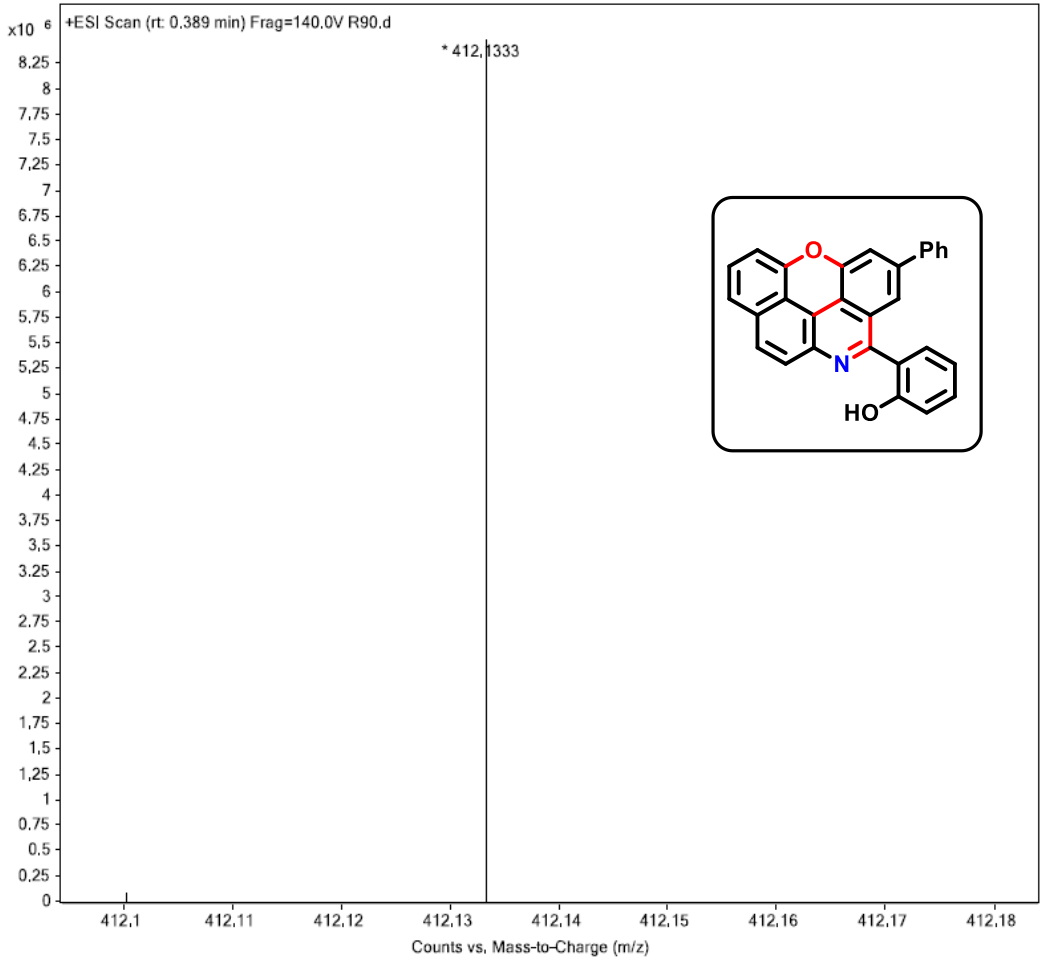
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 5q



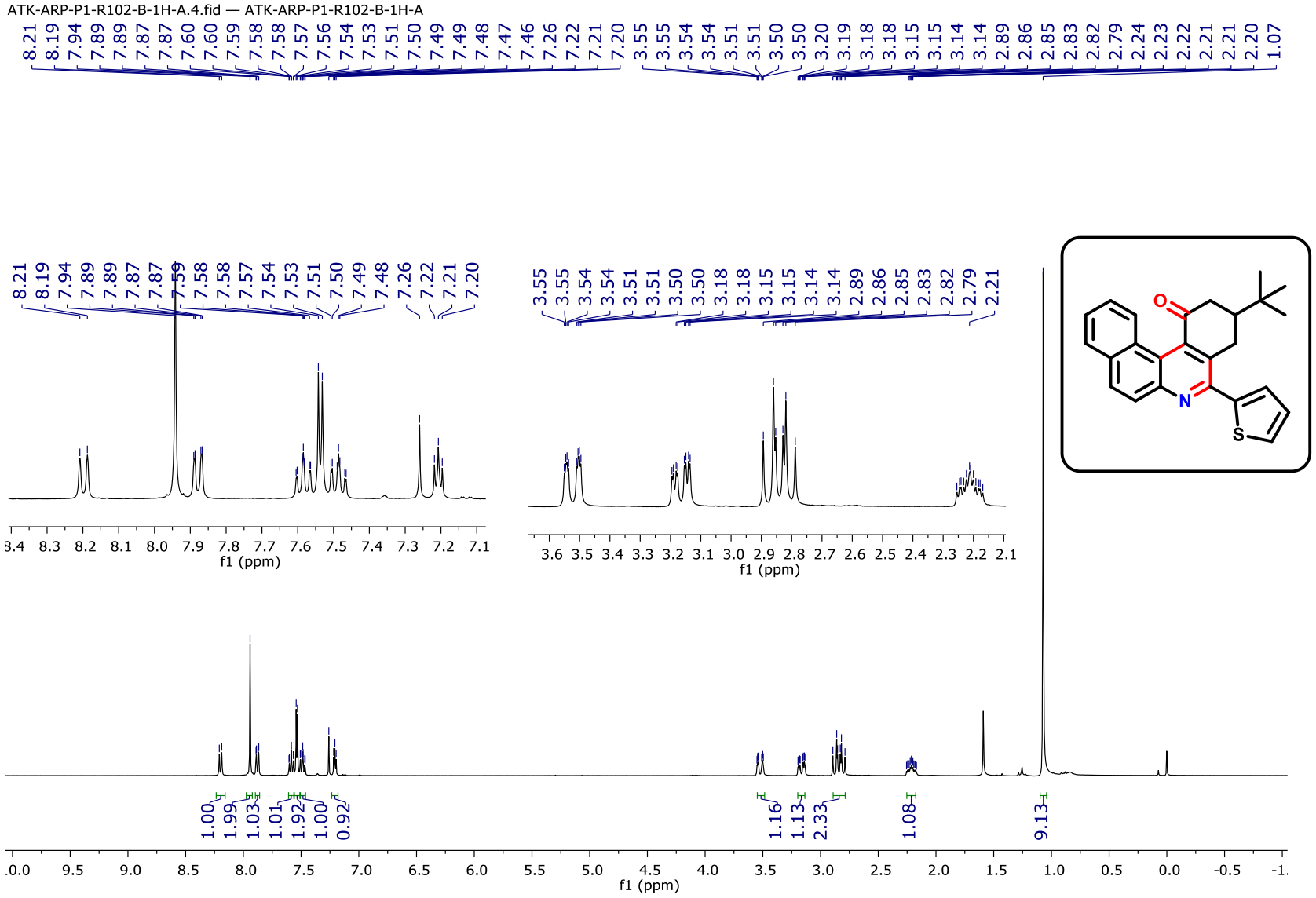
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5q



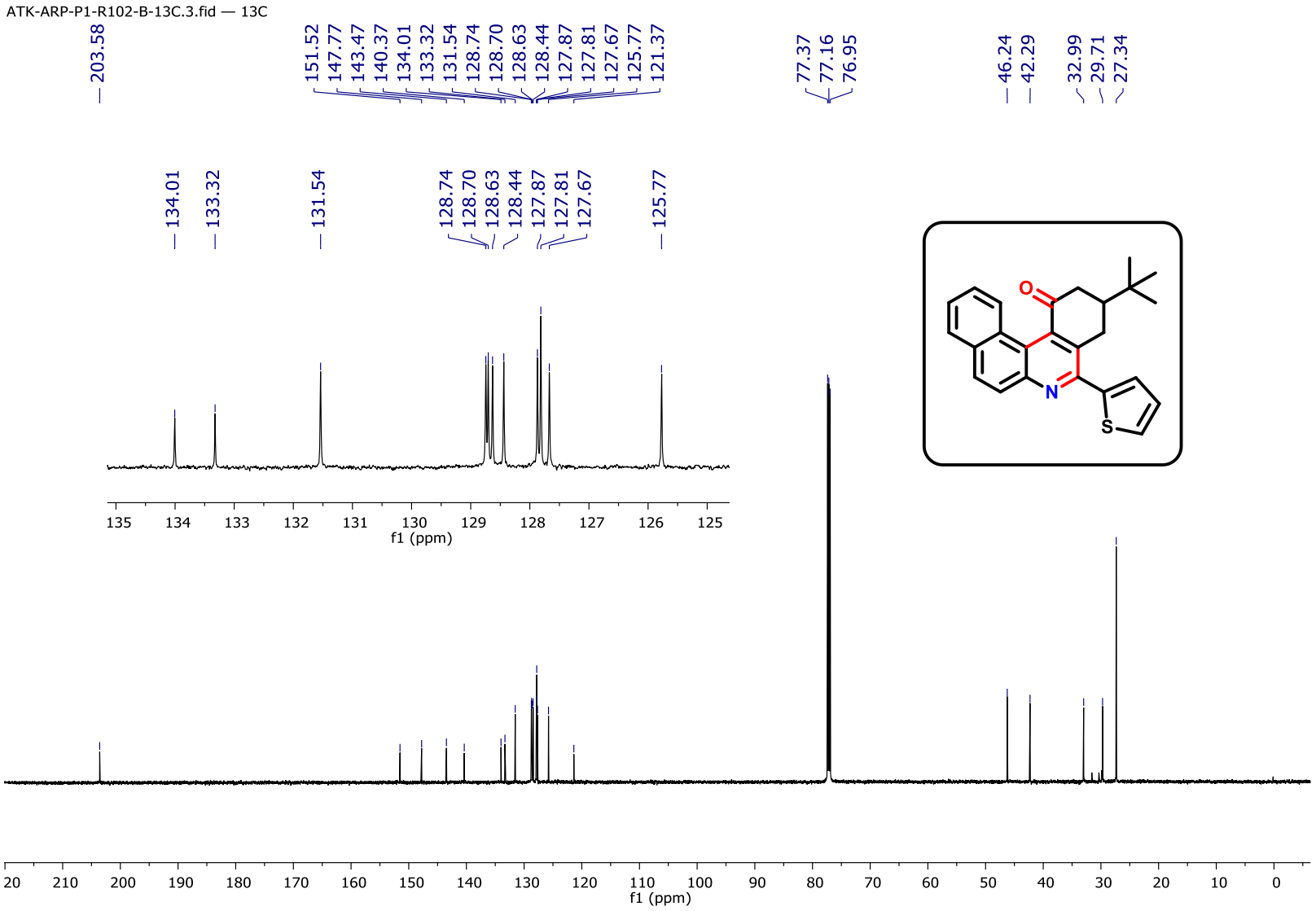
HRMS spectrum of compound 5q



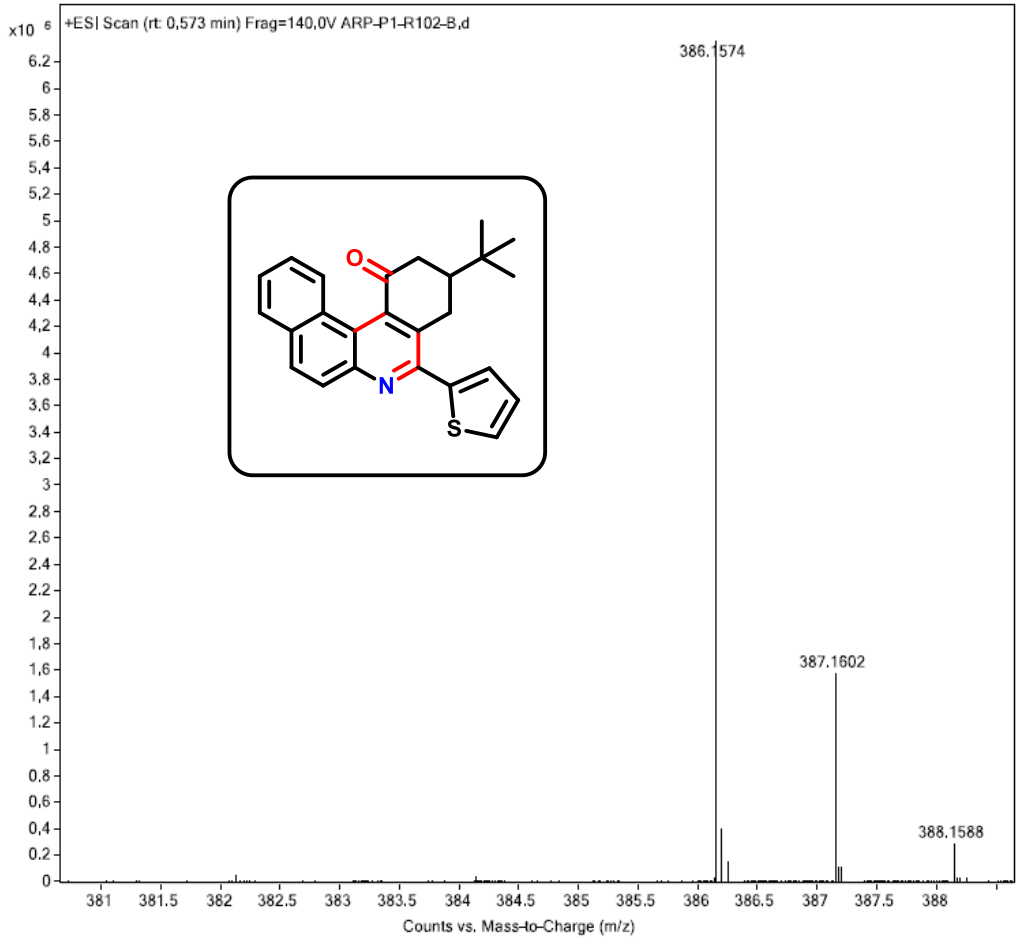
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5r



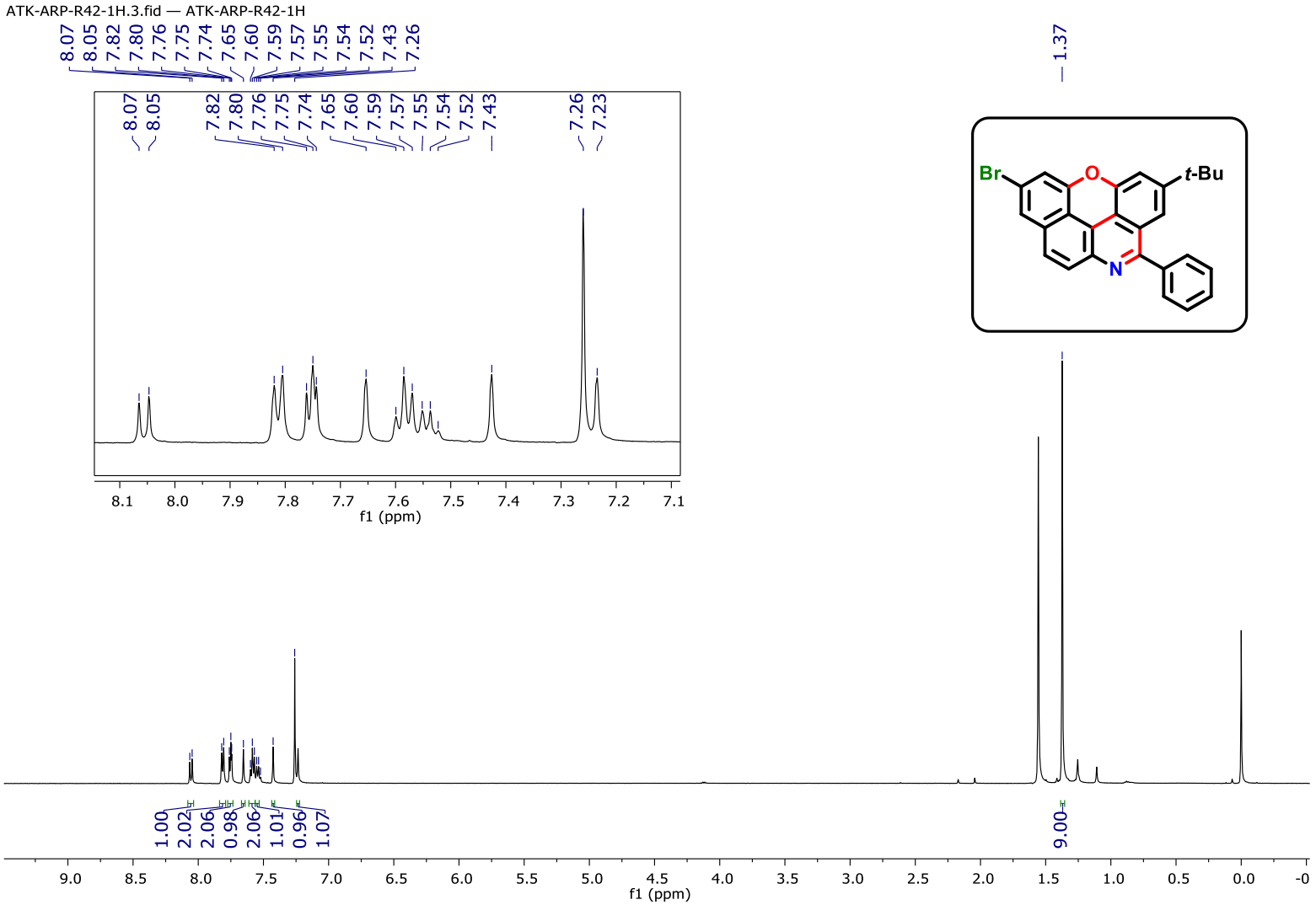
^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) NMR spectrum of compound 5r



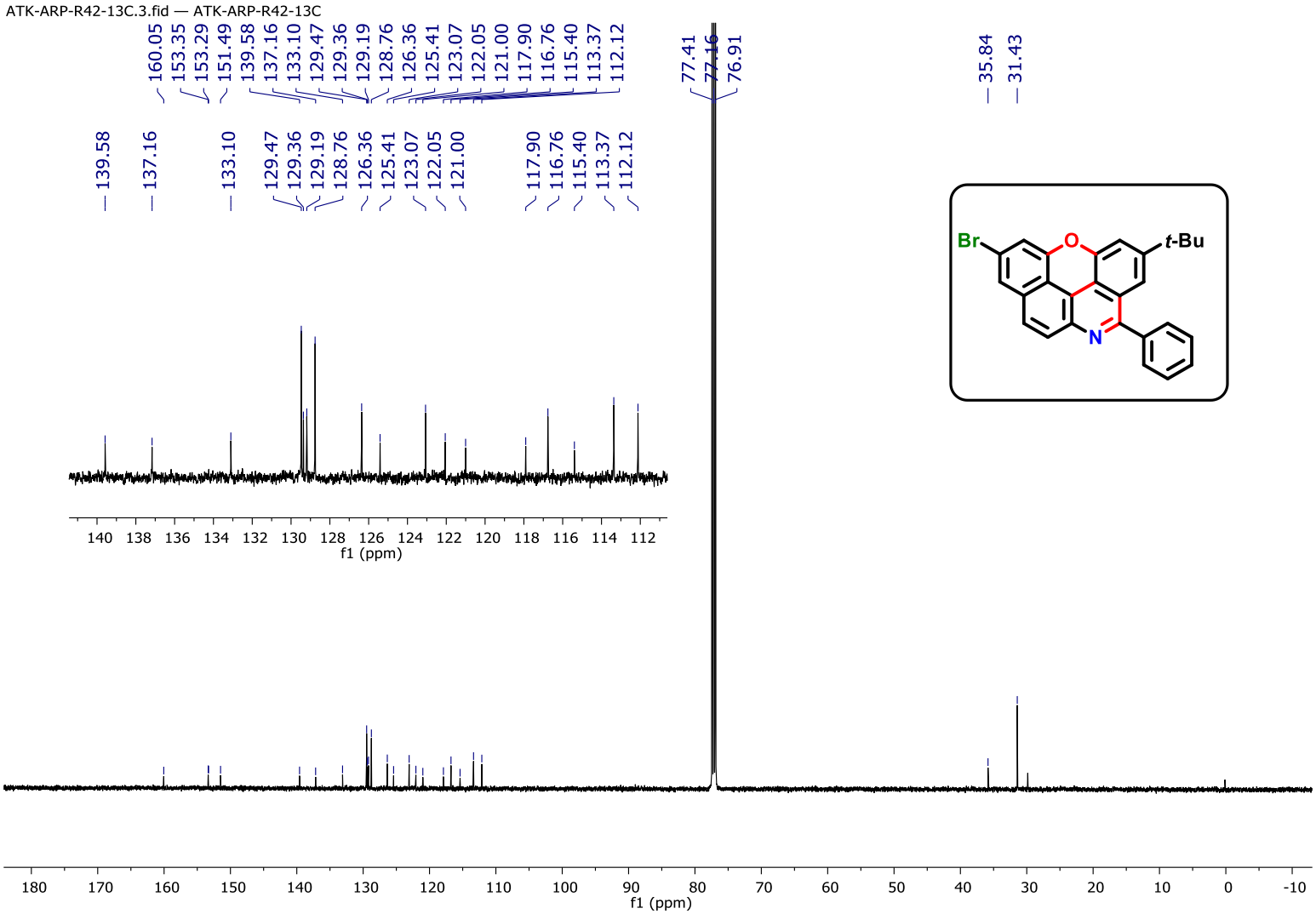
HRMS spectrum of compound 5r



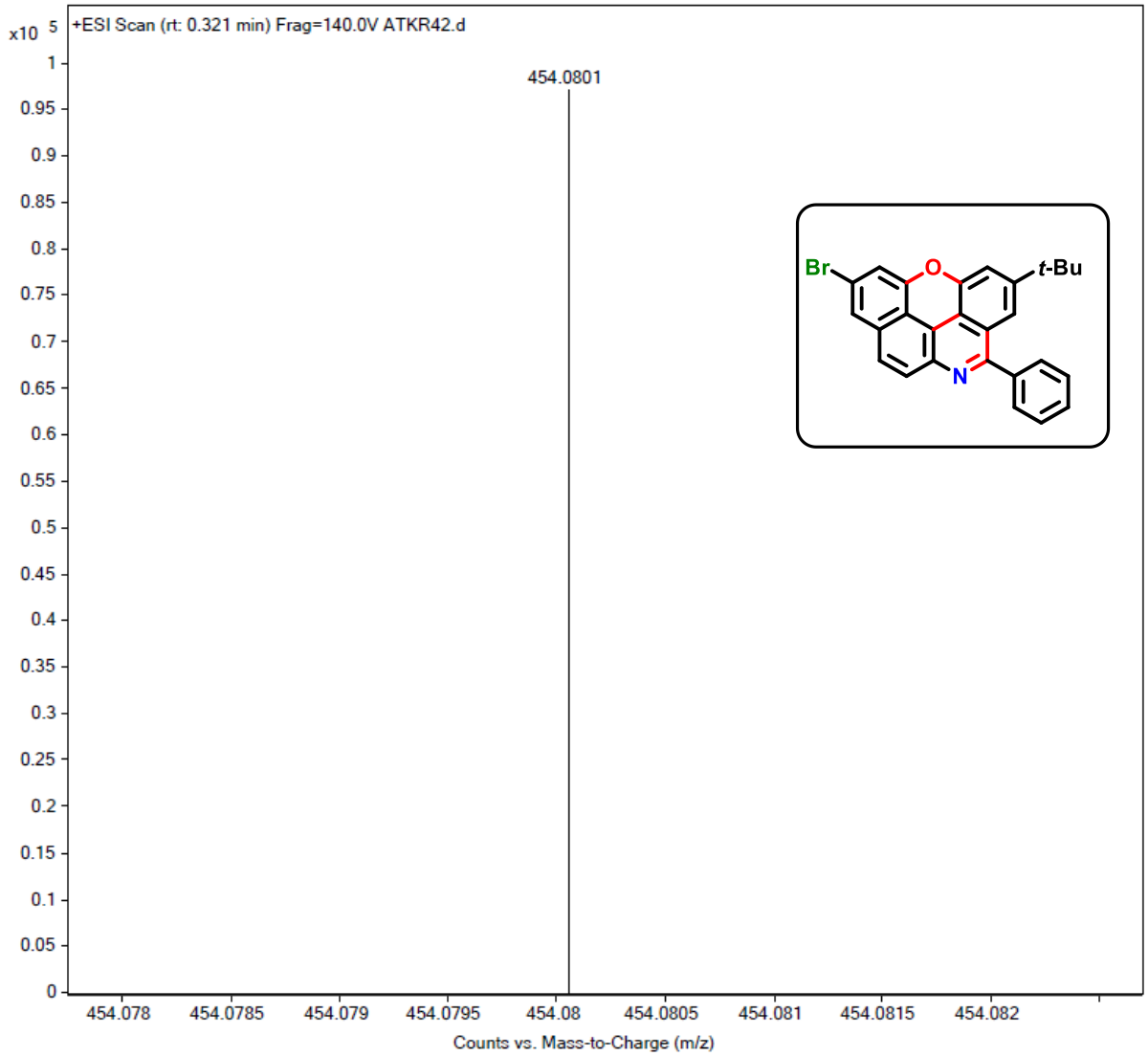
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 7a



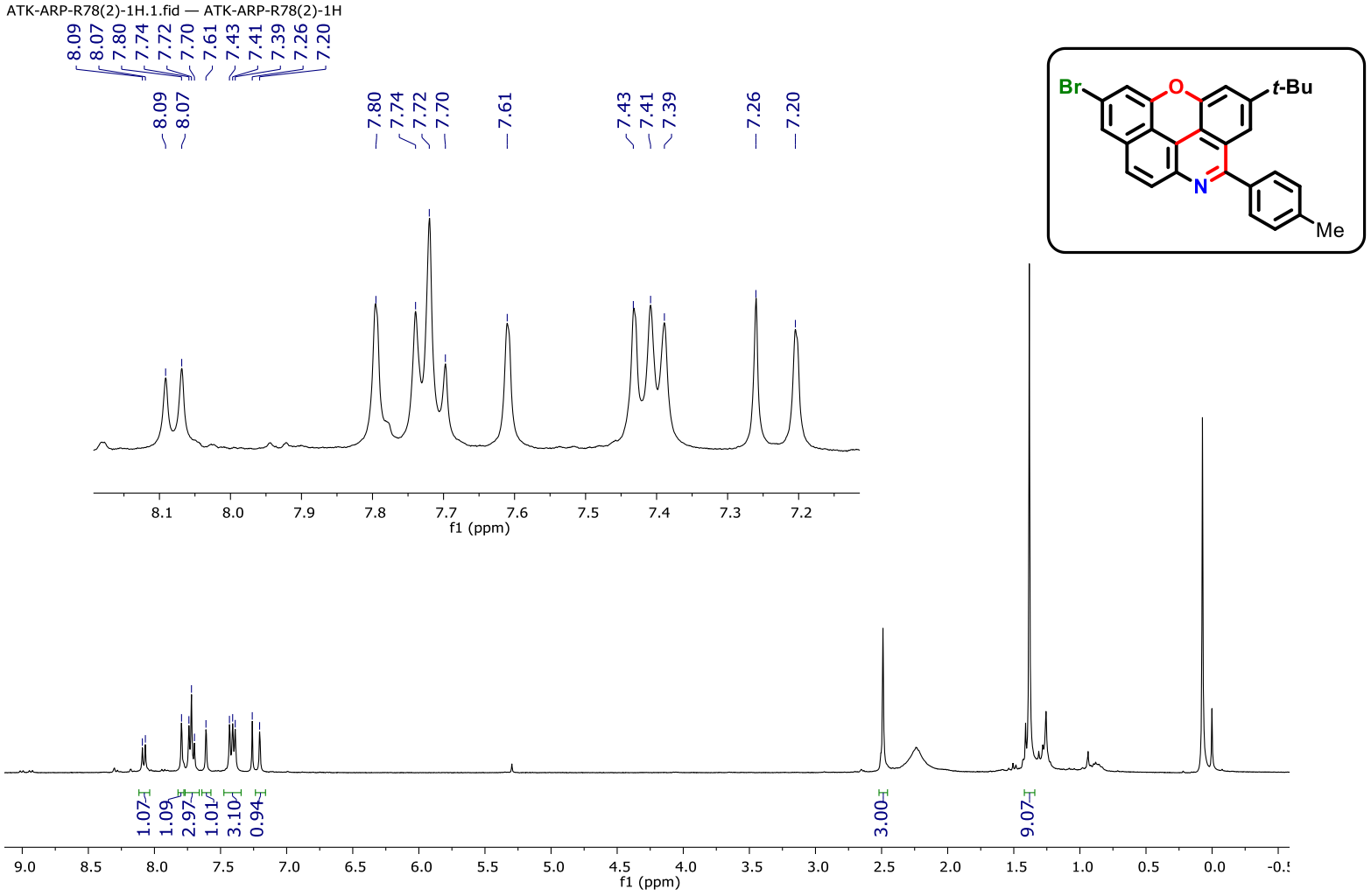
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 7a



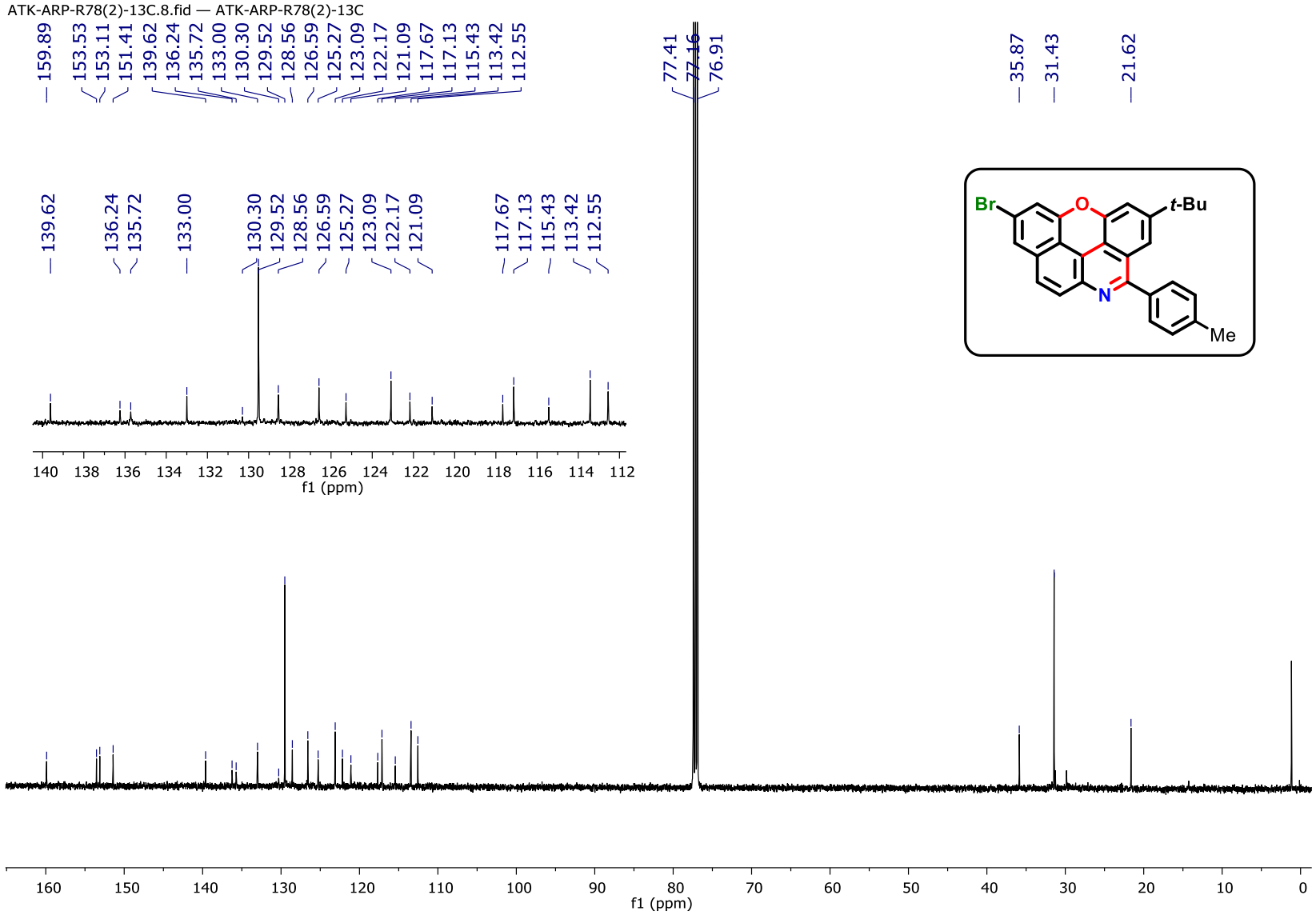
HRMS spectrum of compound 7a



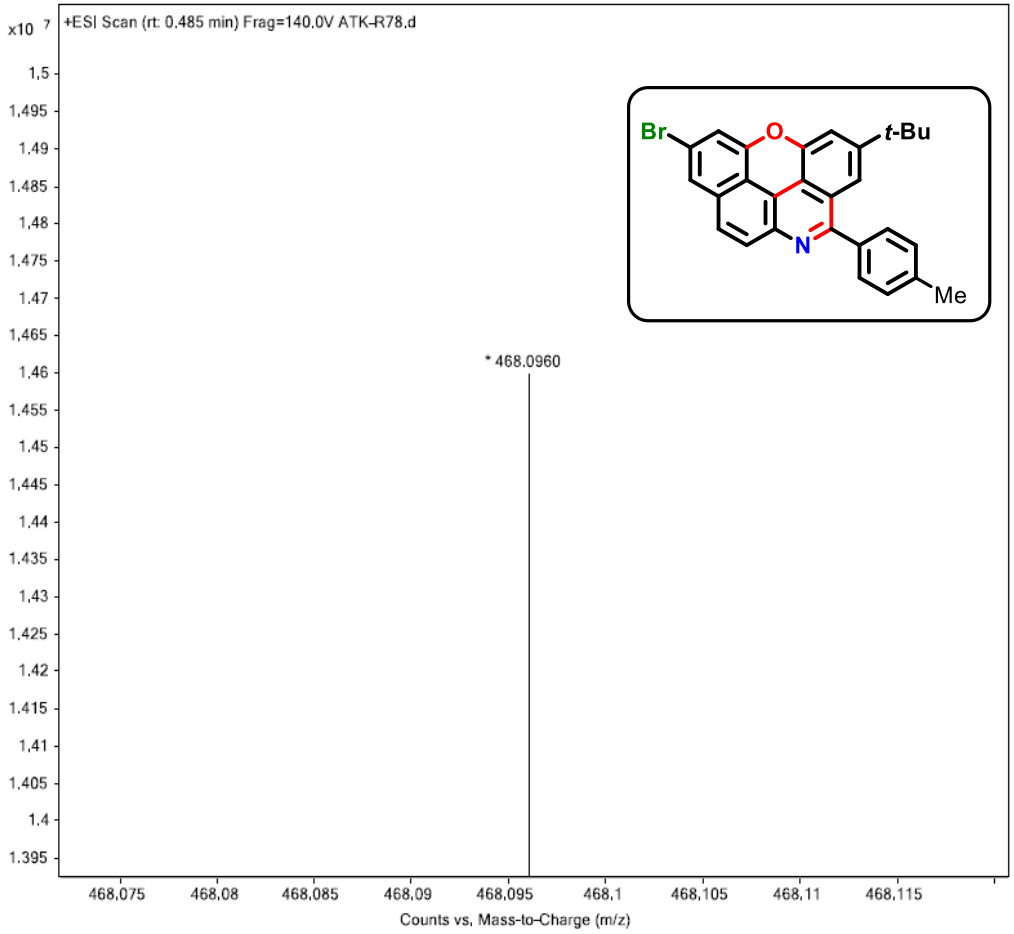
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 7b



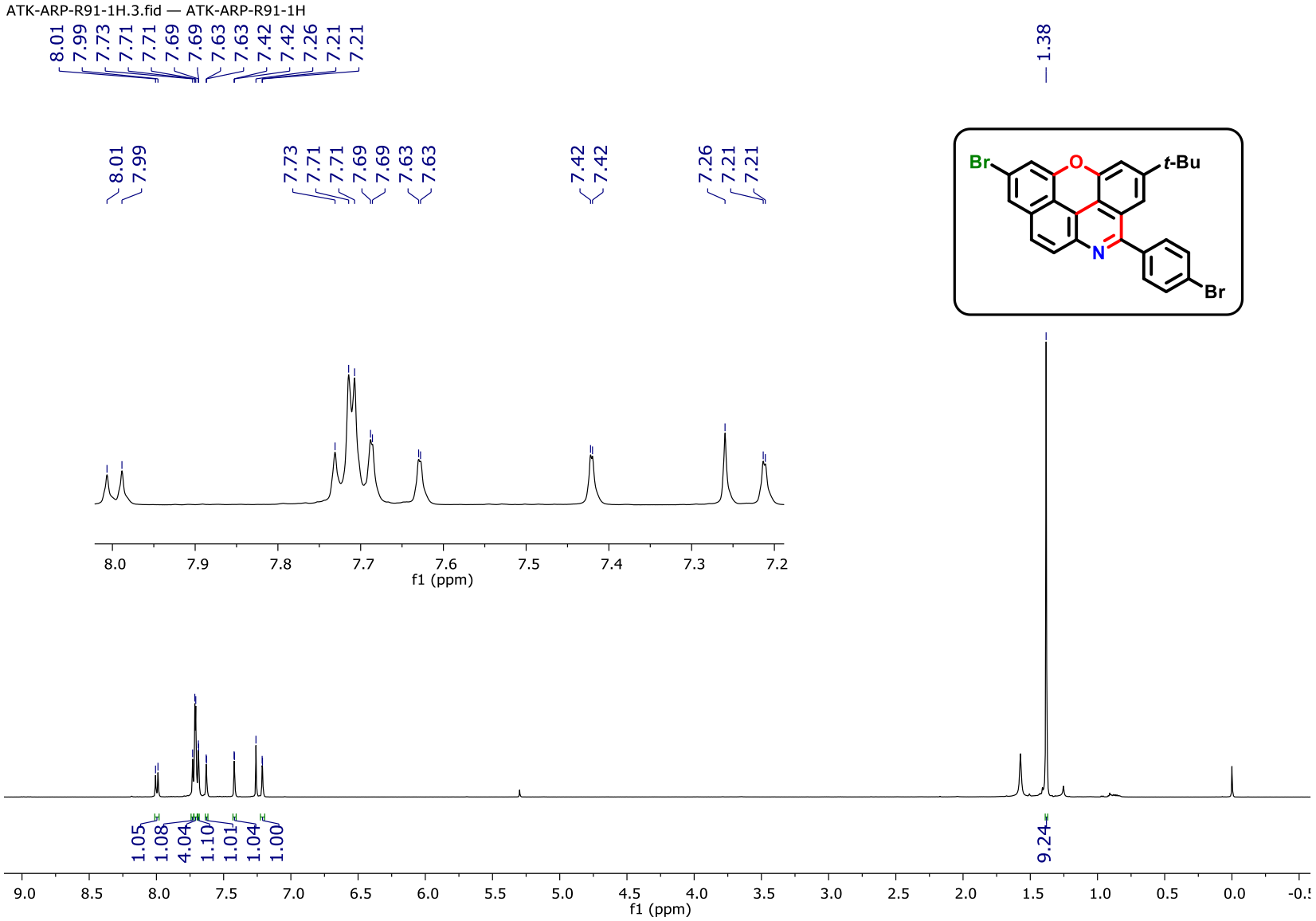
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 7b



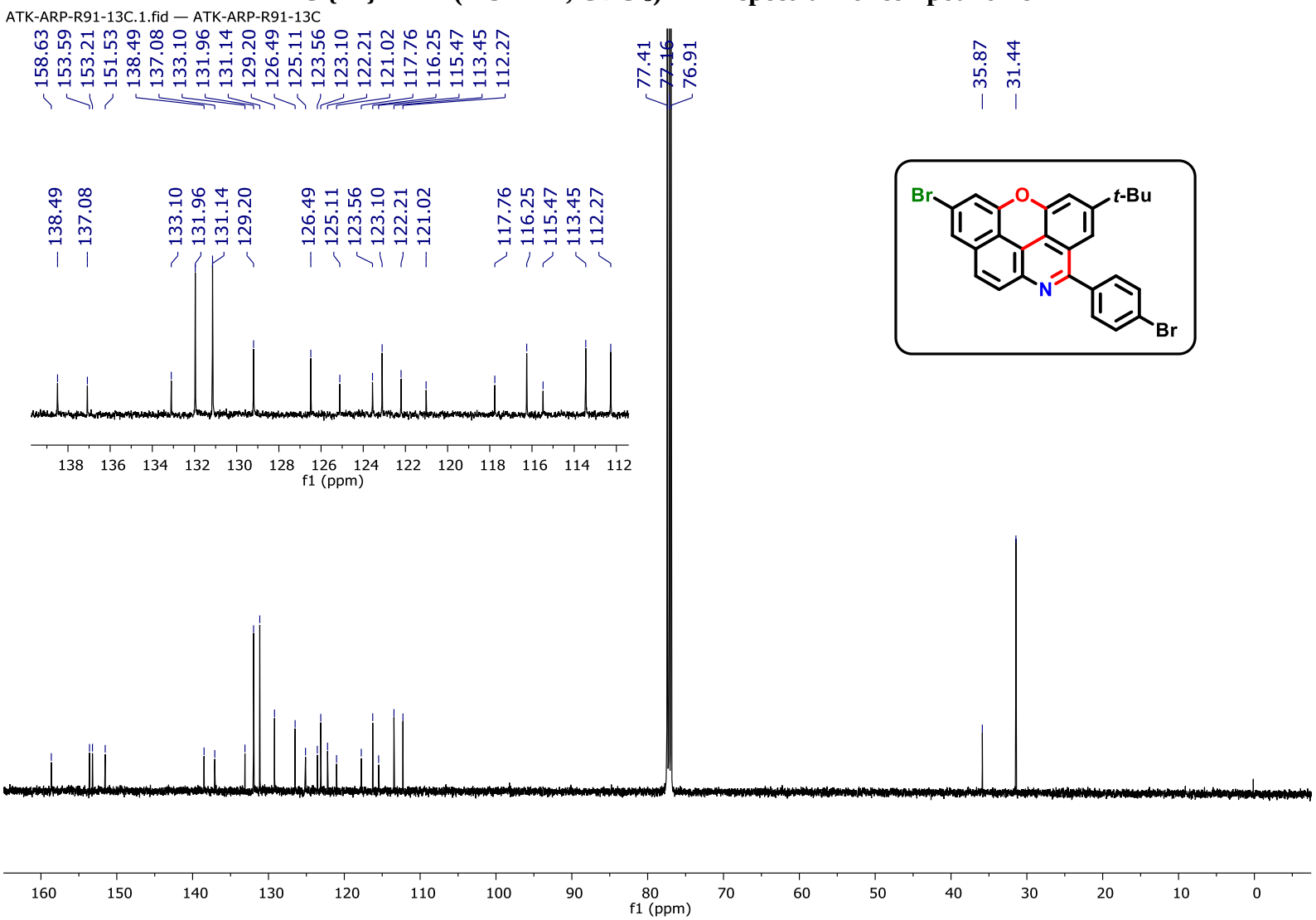
HRMS spectrum of compound 7b



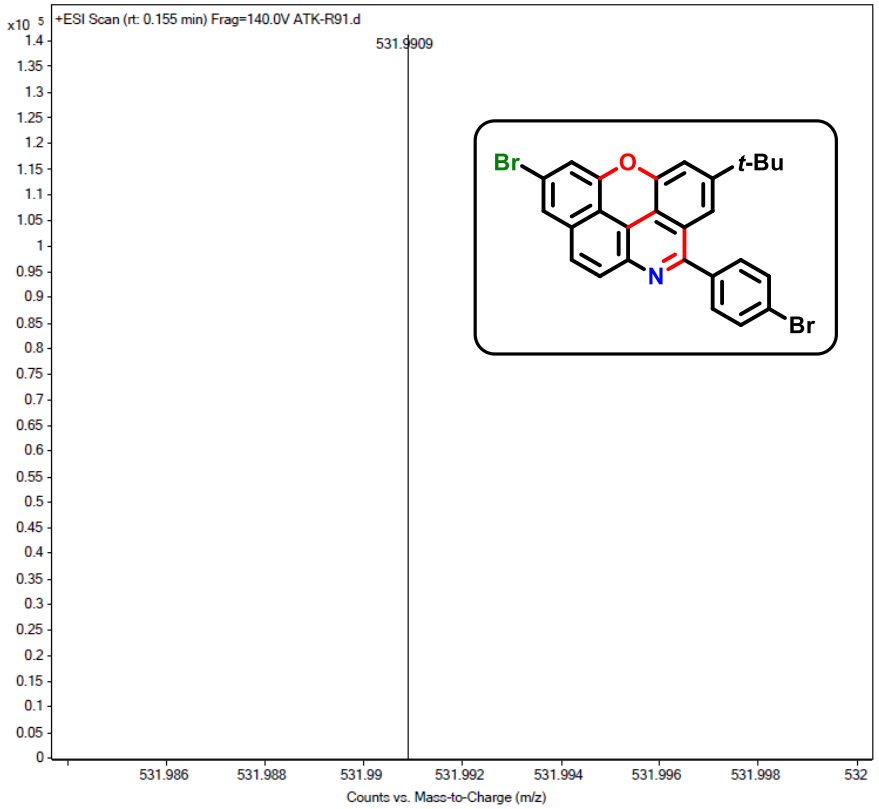
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 7c



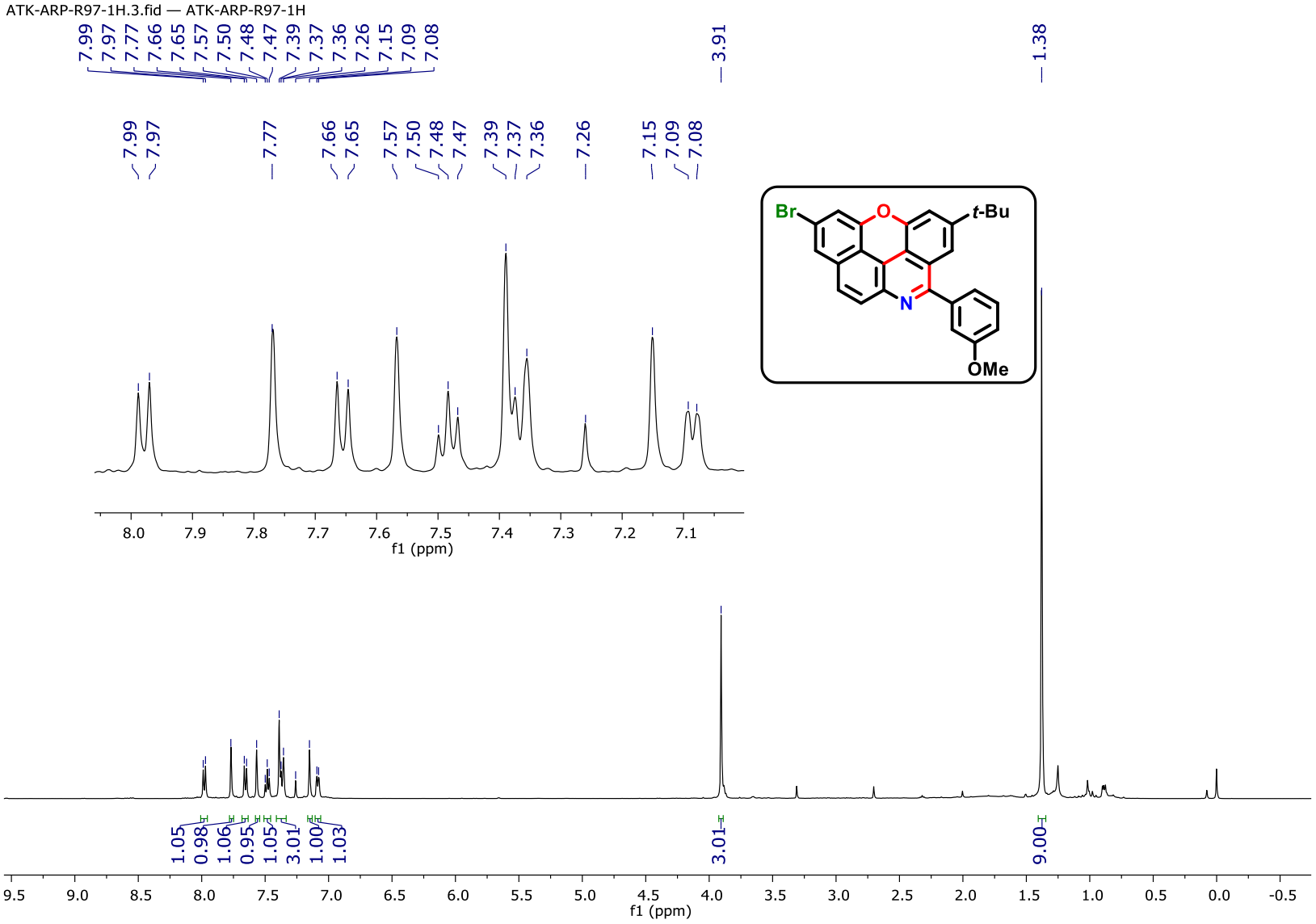
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 7c



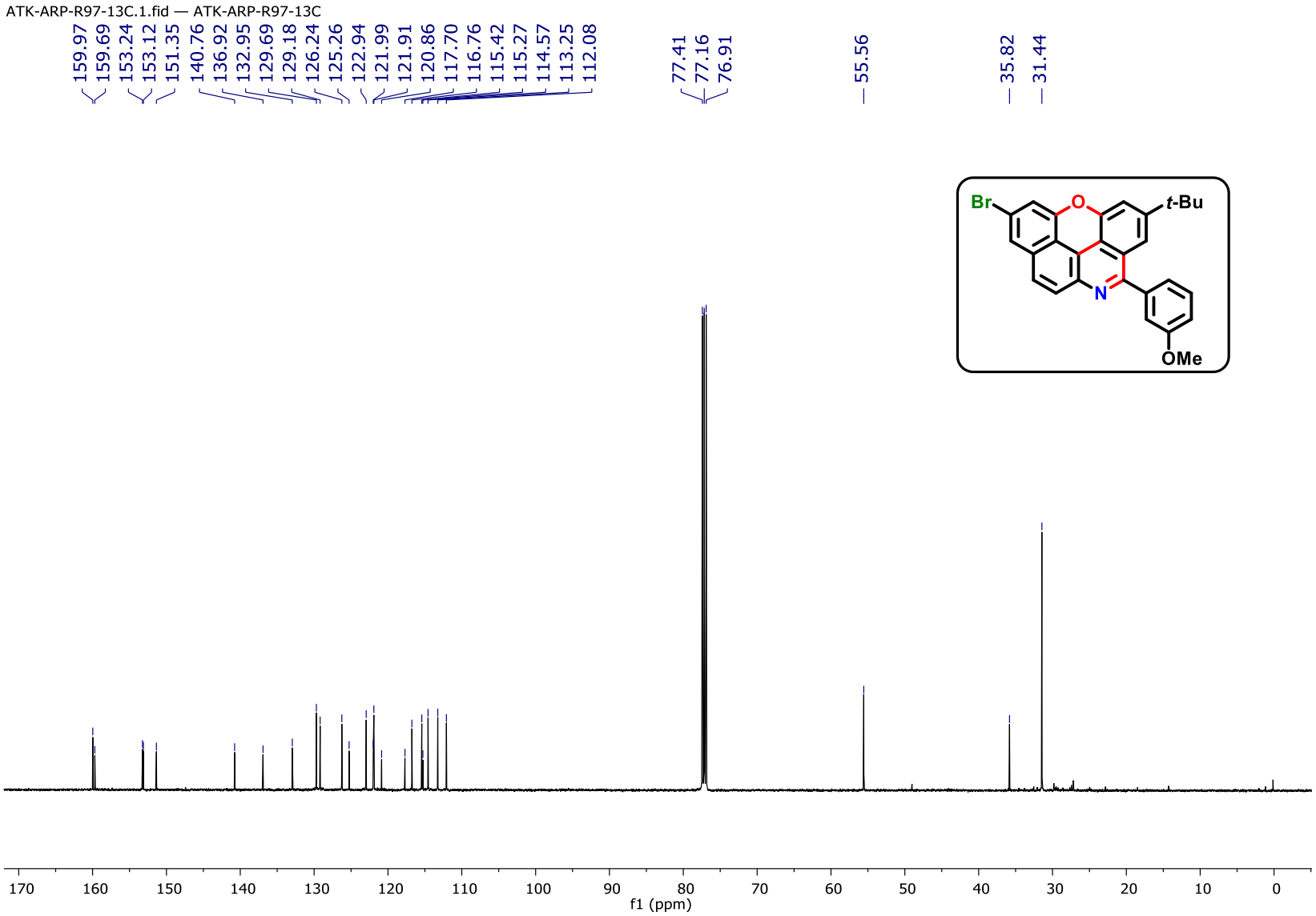
HRMS spectrum of compound 7c



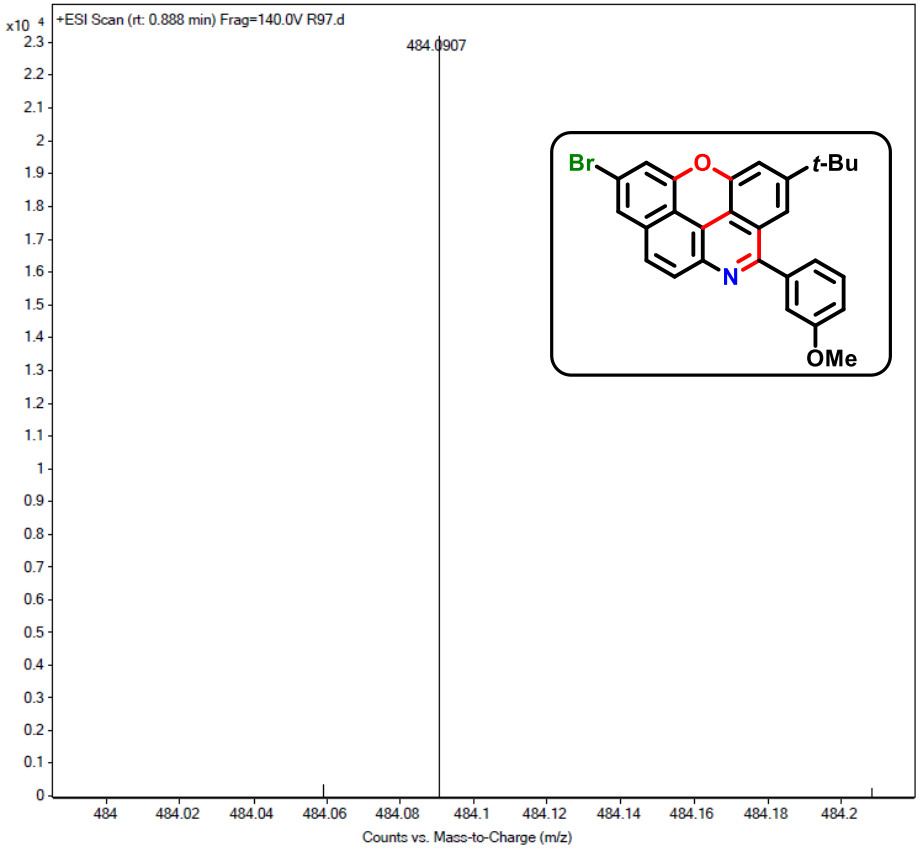
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 7d



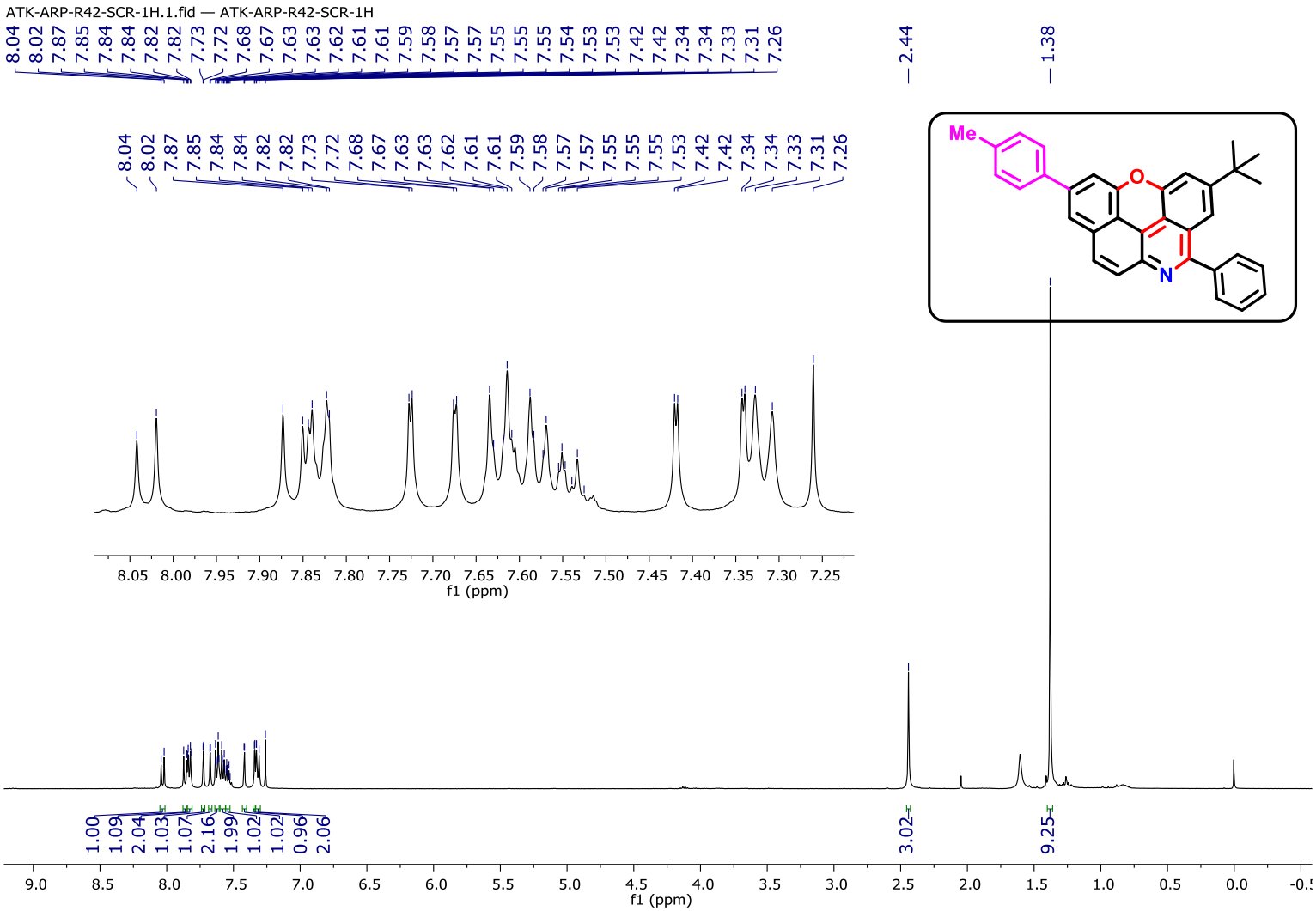
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 7d



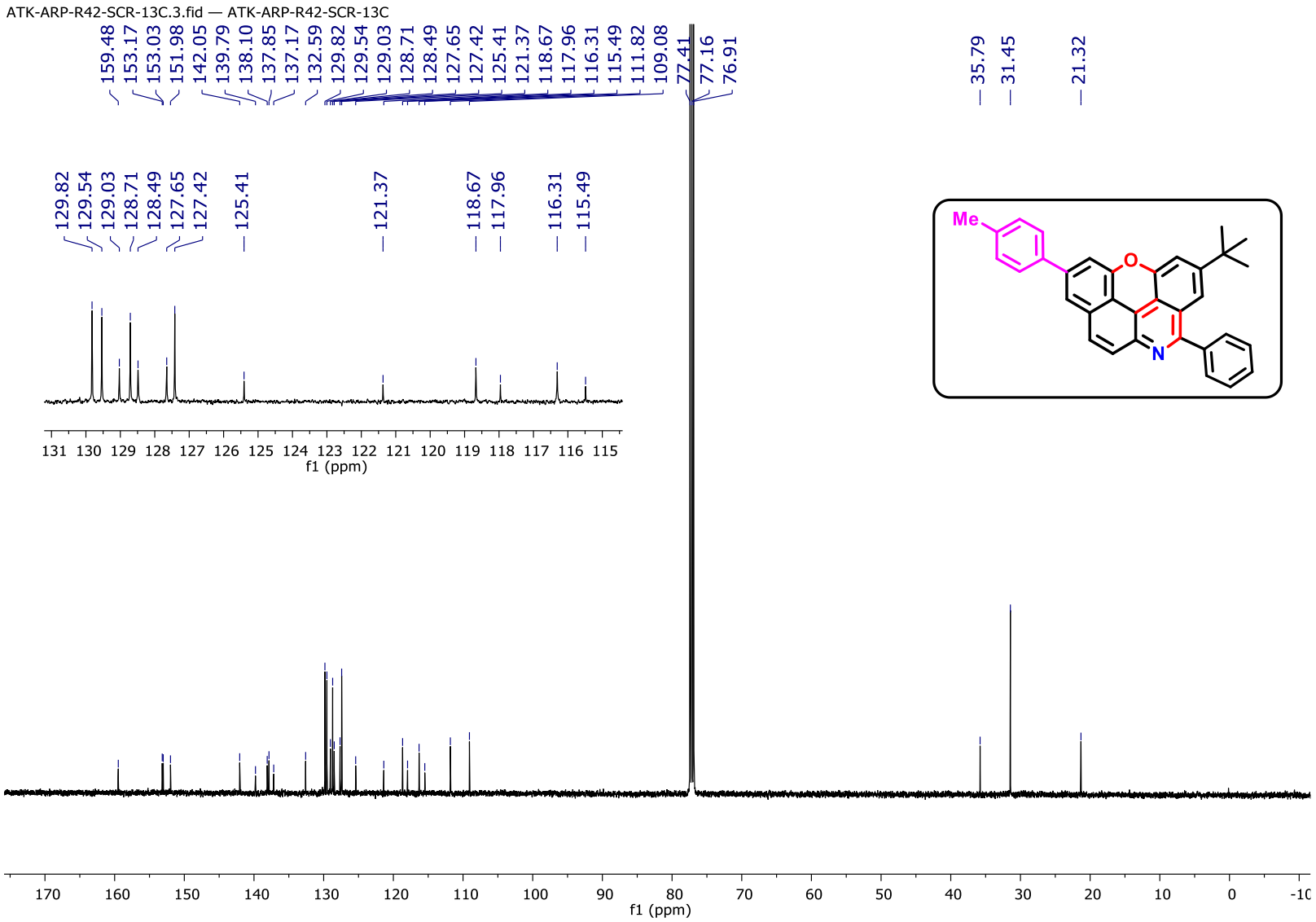
HRMS spectrum of compound 7d



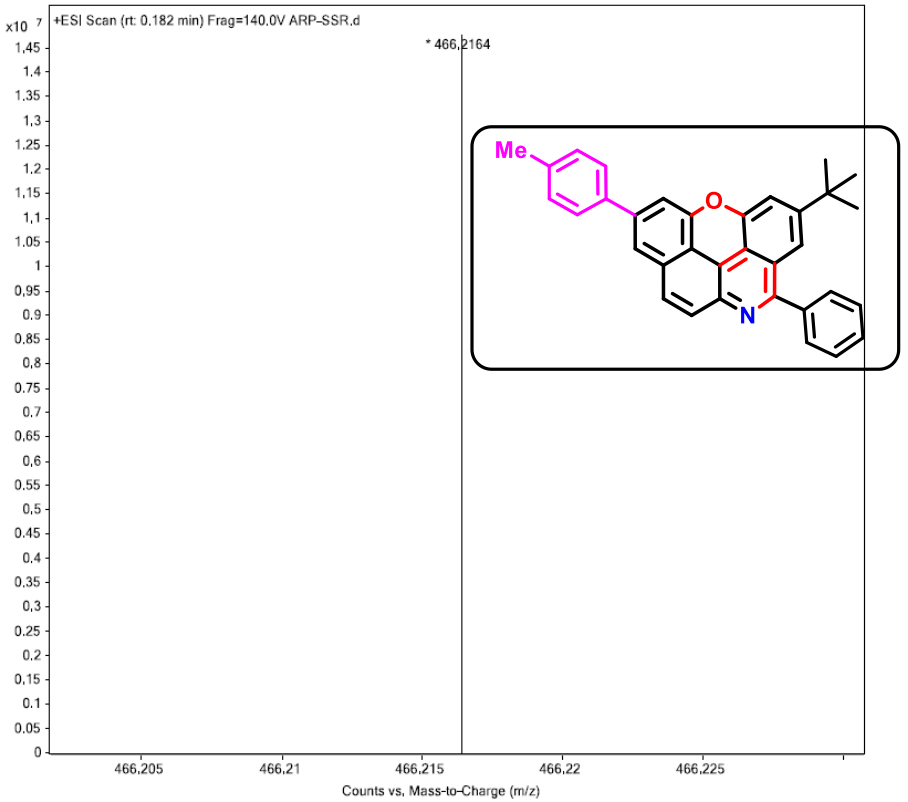
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 9a



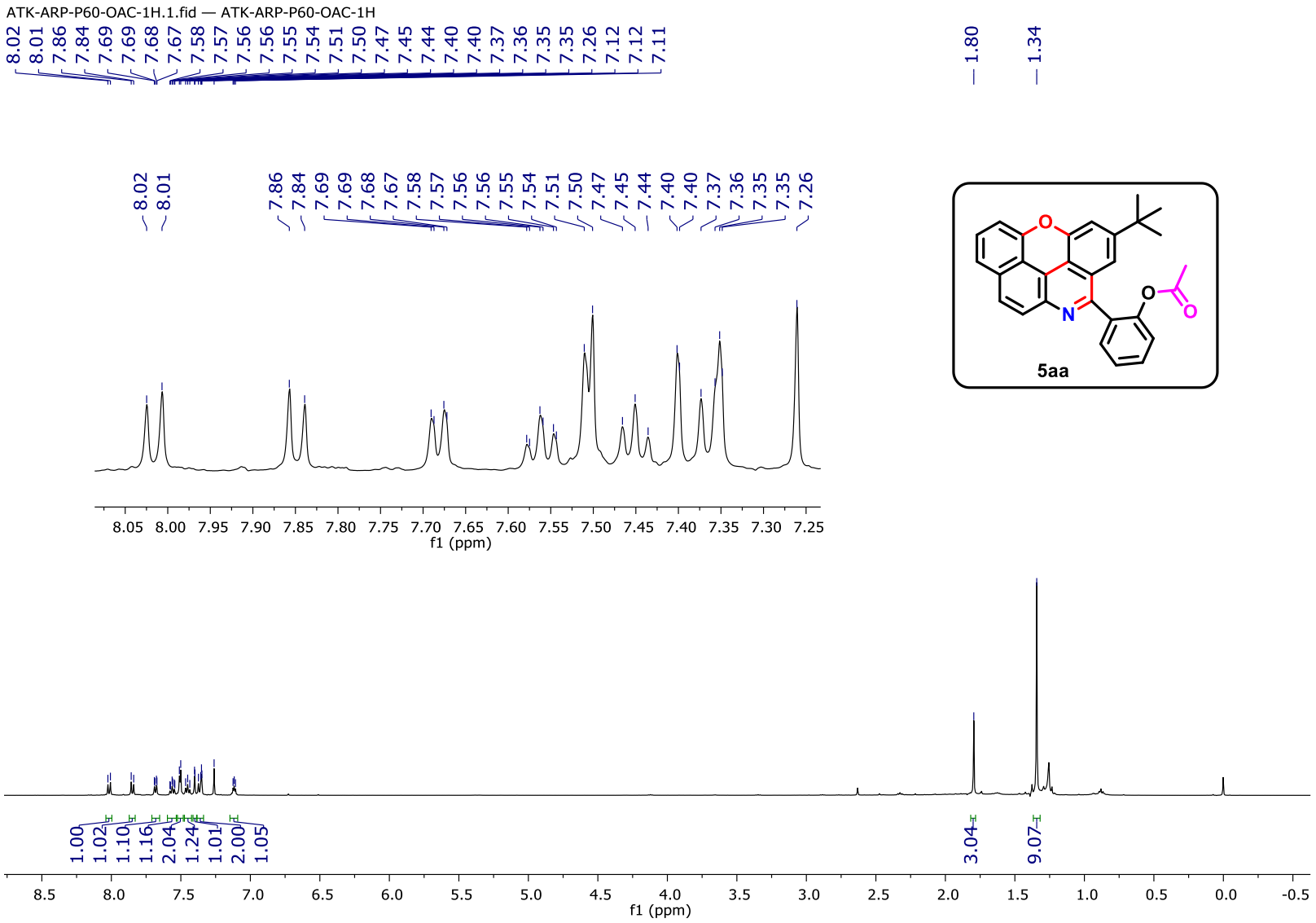
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 9a



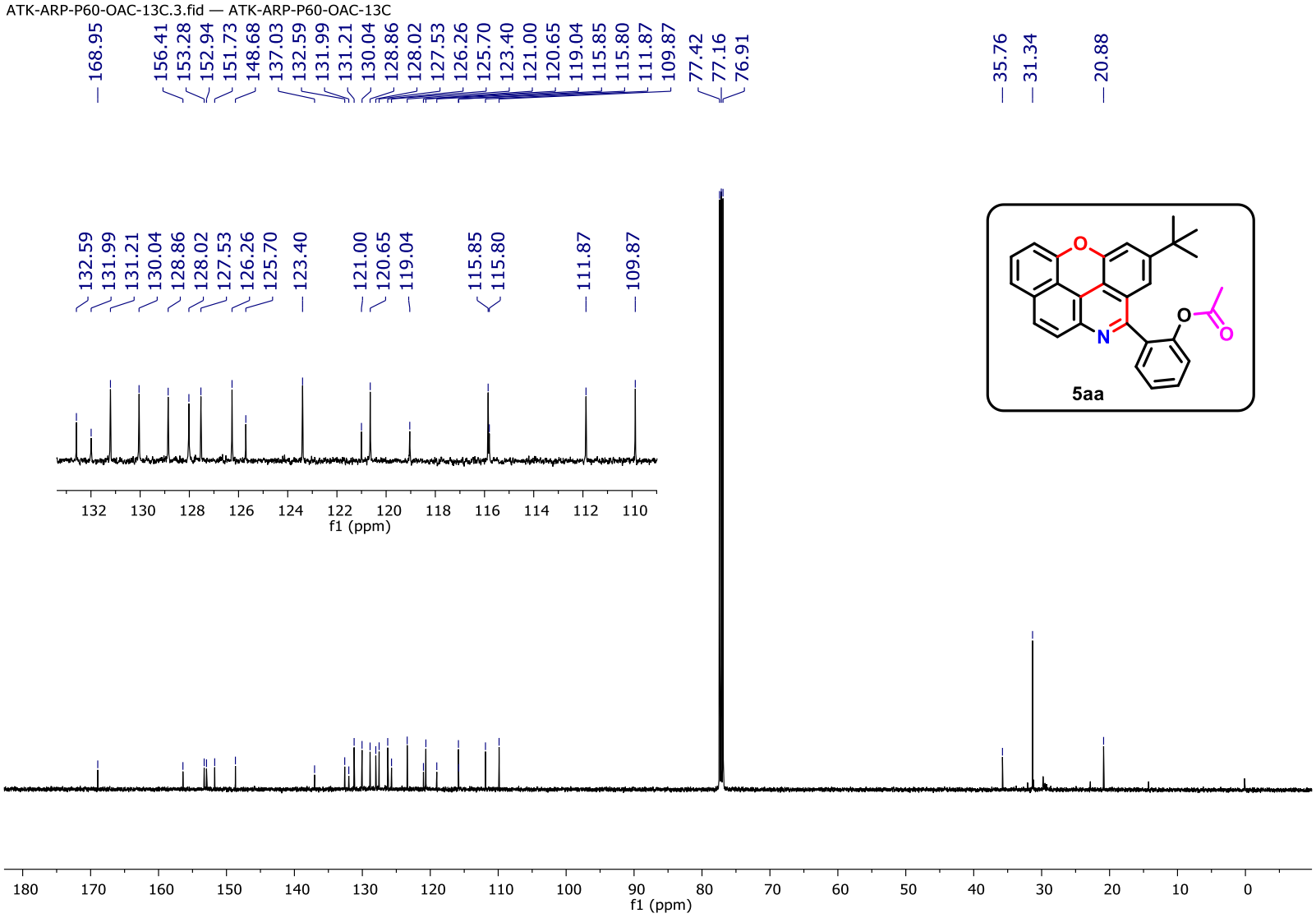
HRMS spectrum of compound 9a



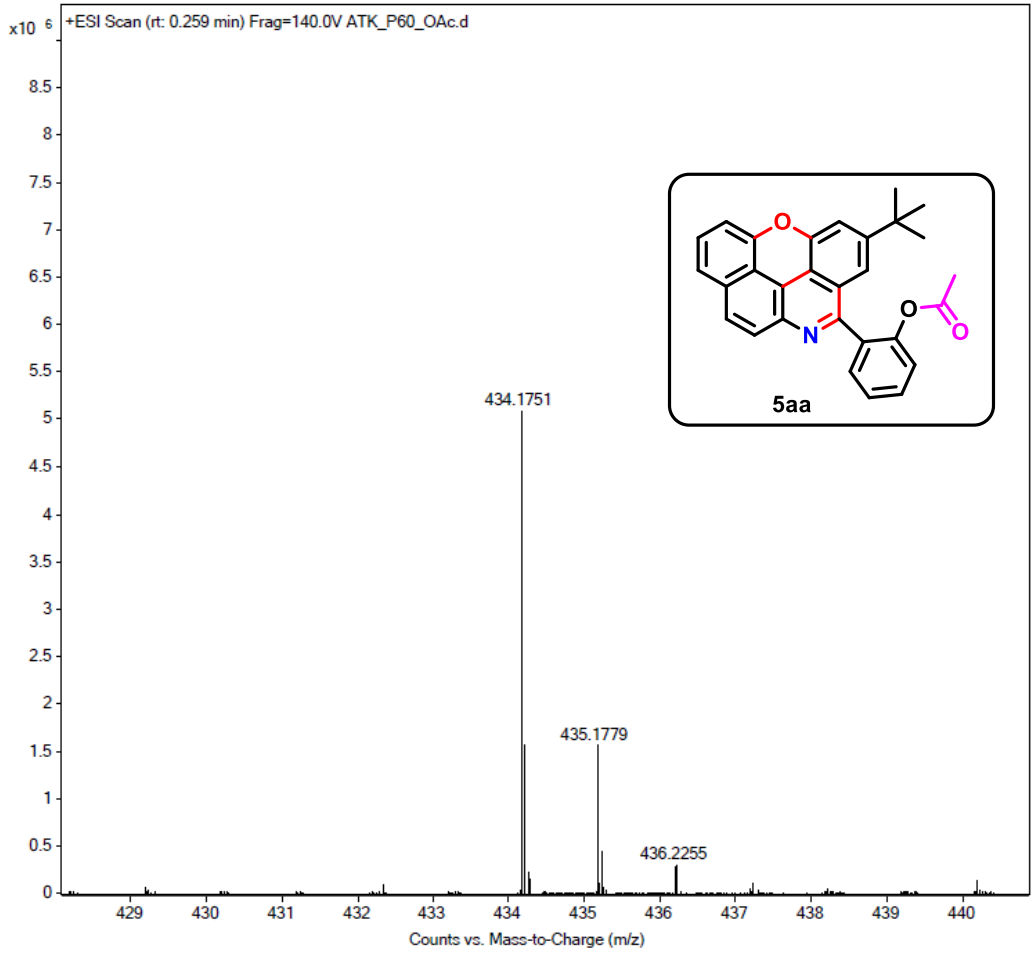
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound 5aa



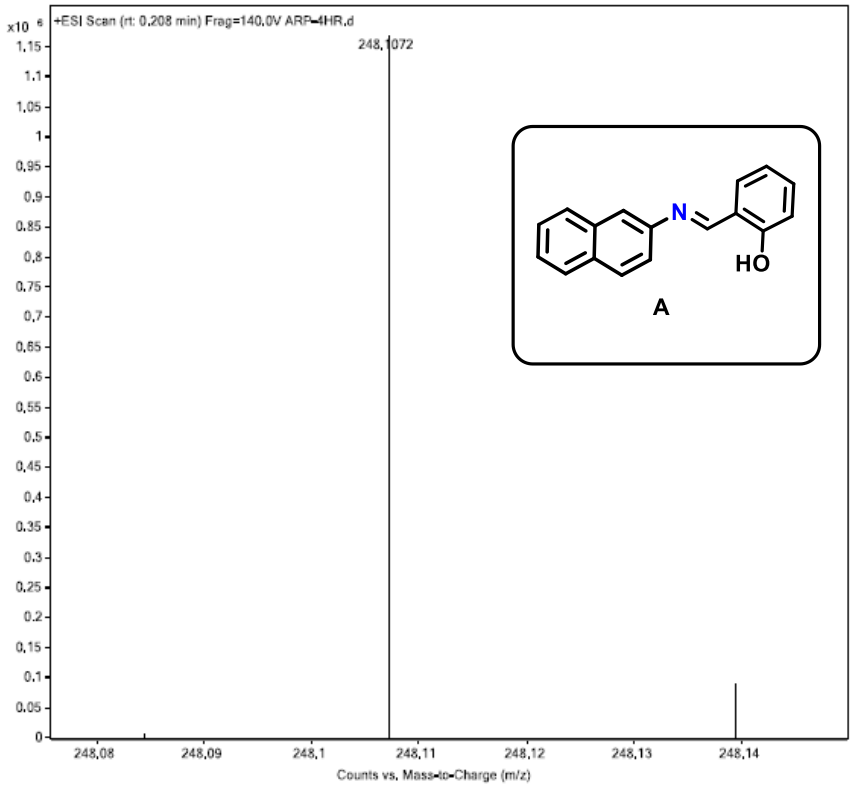
^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) NMR spectrum of compound 5aa



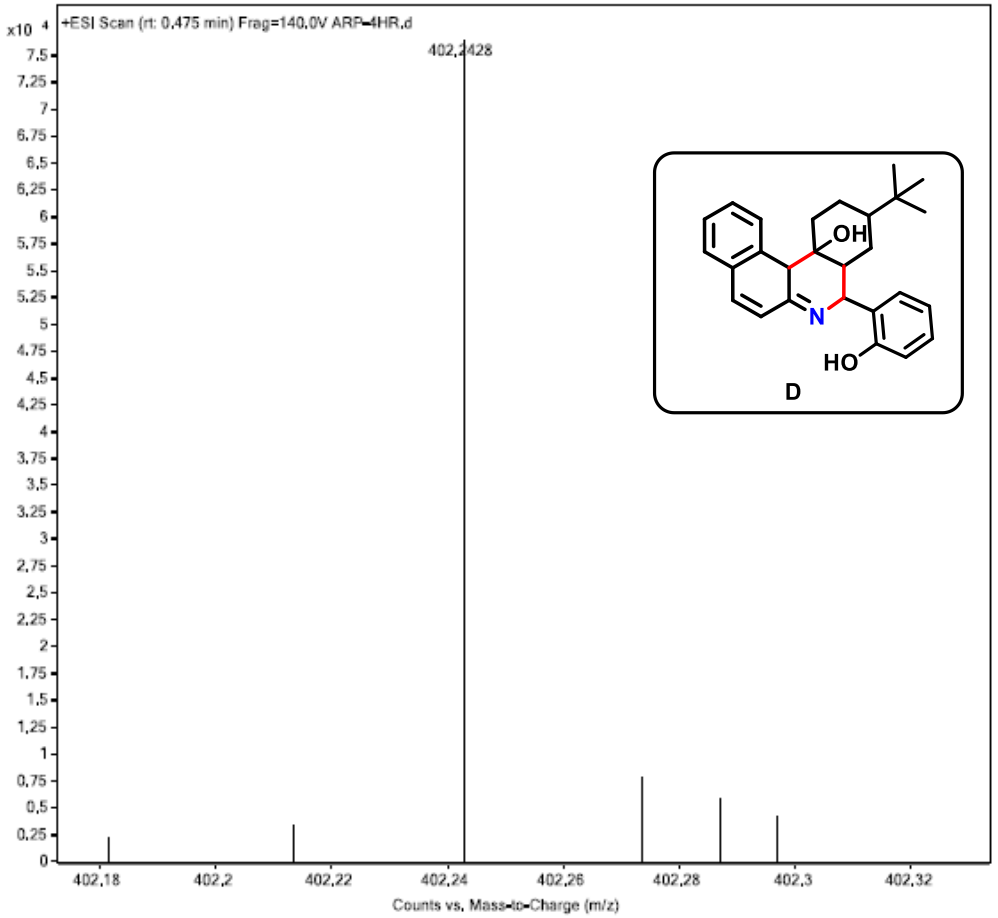
HRMS spectrum of compound 5aa



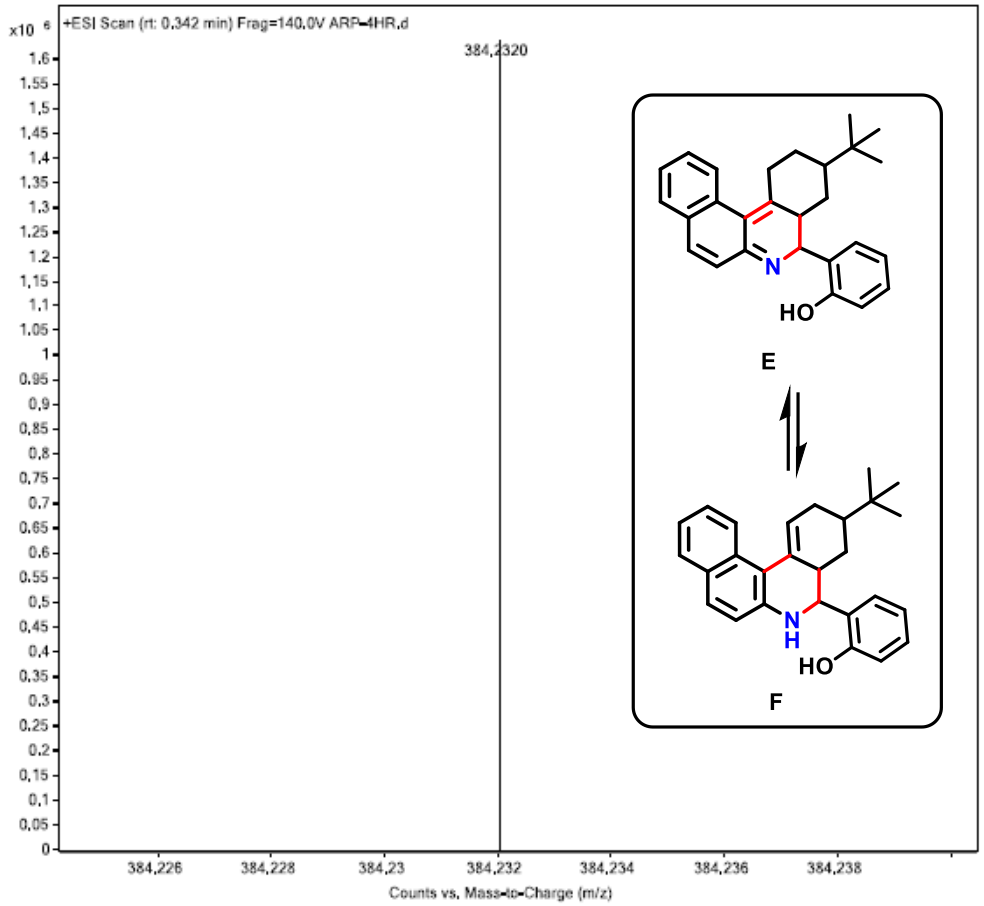
HRMS spectrum of intermediate A of compound 5a



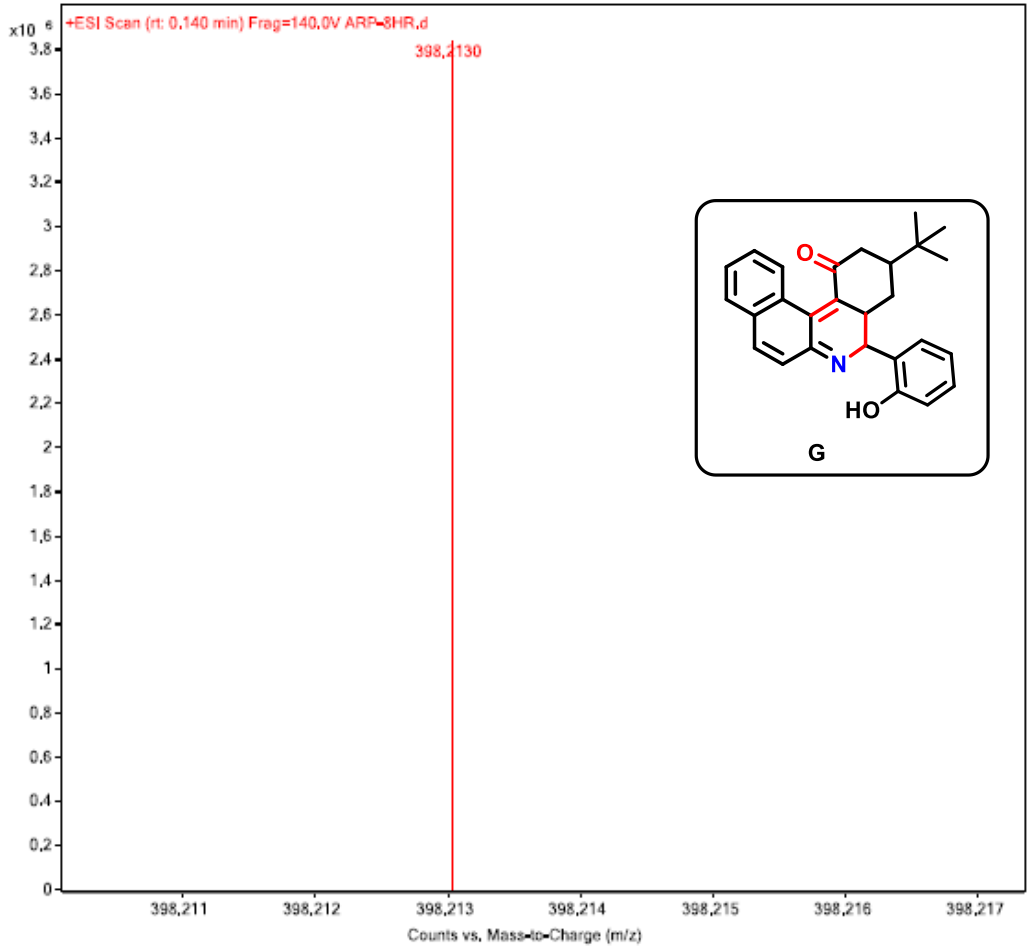
HRMS spectrum of intermediate C and D of compound 5a



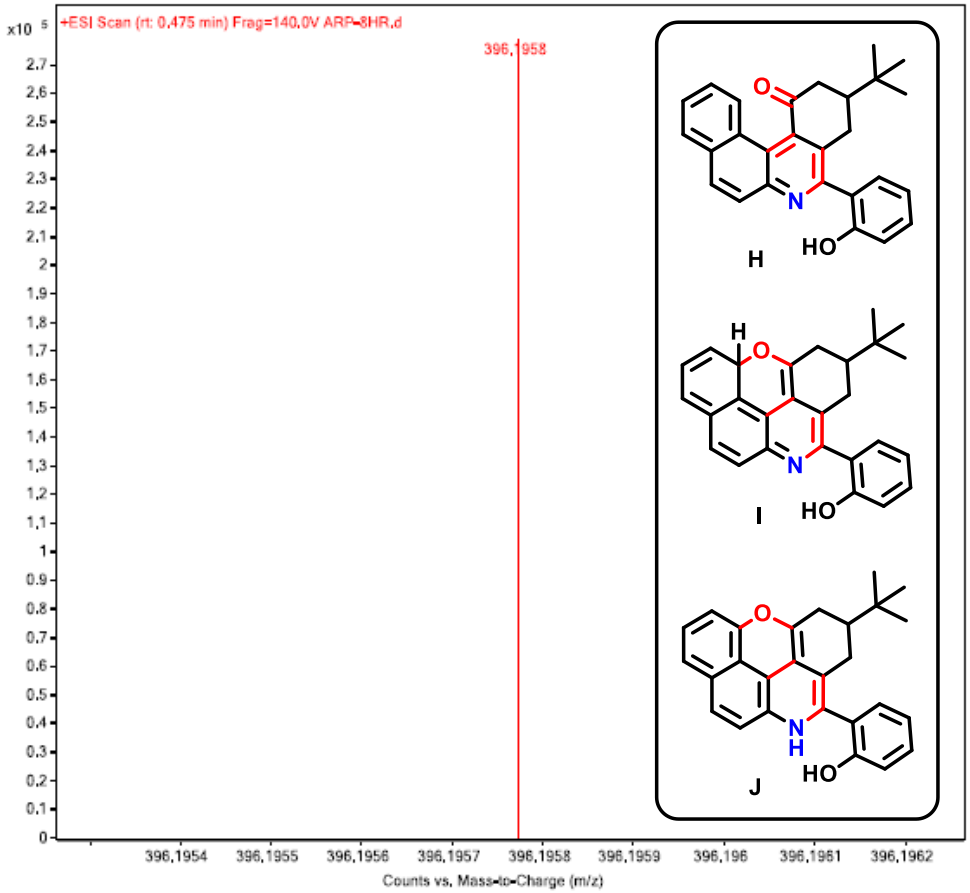
HRMS spectrum of intermediate E and F of compound 5a



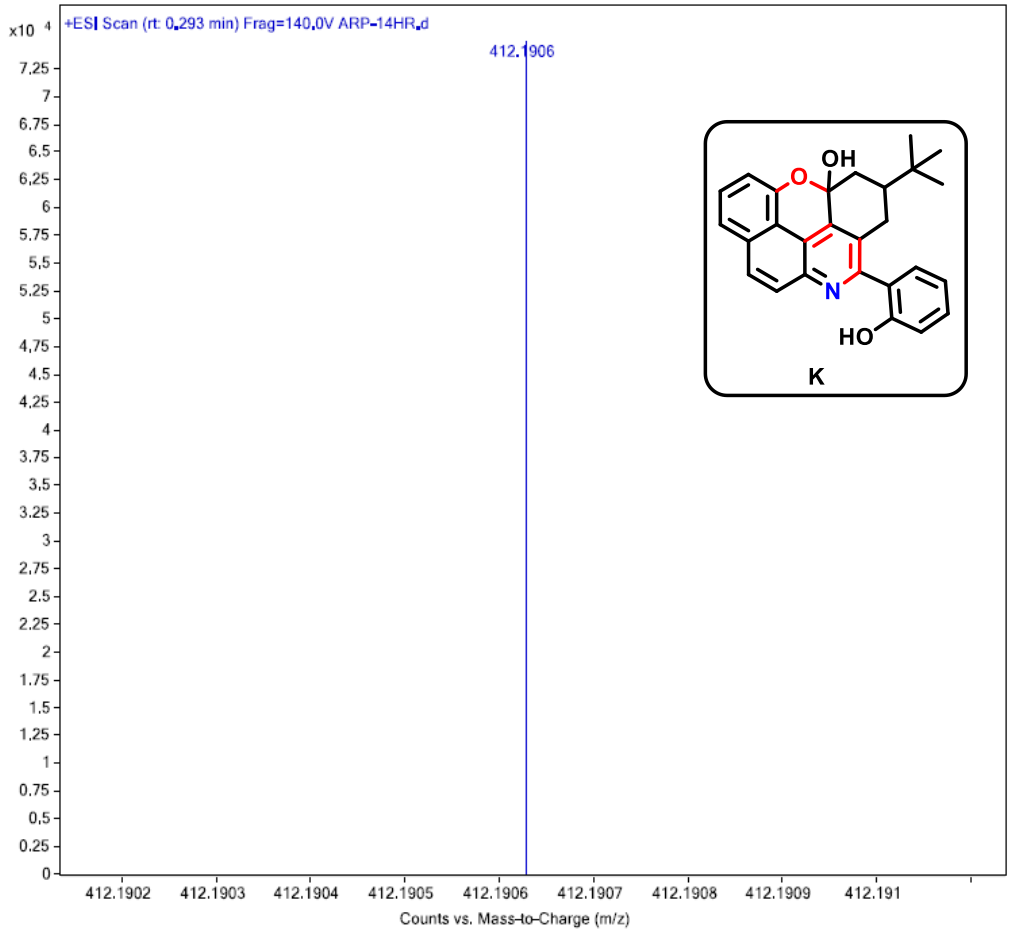
HRMS spectrum of intermediate G of compound 5a



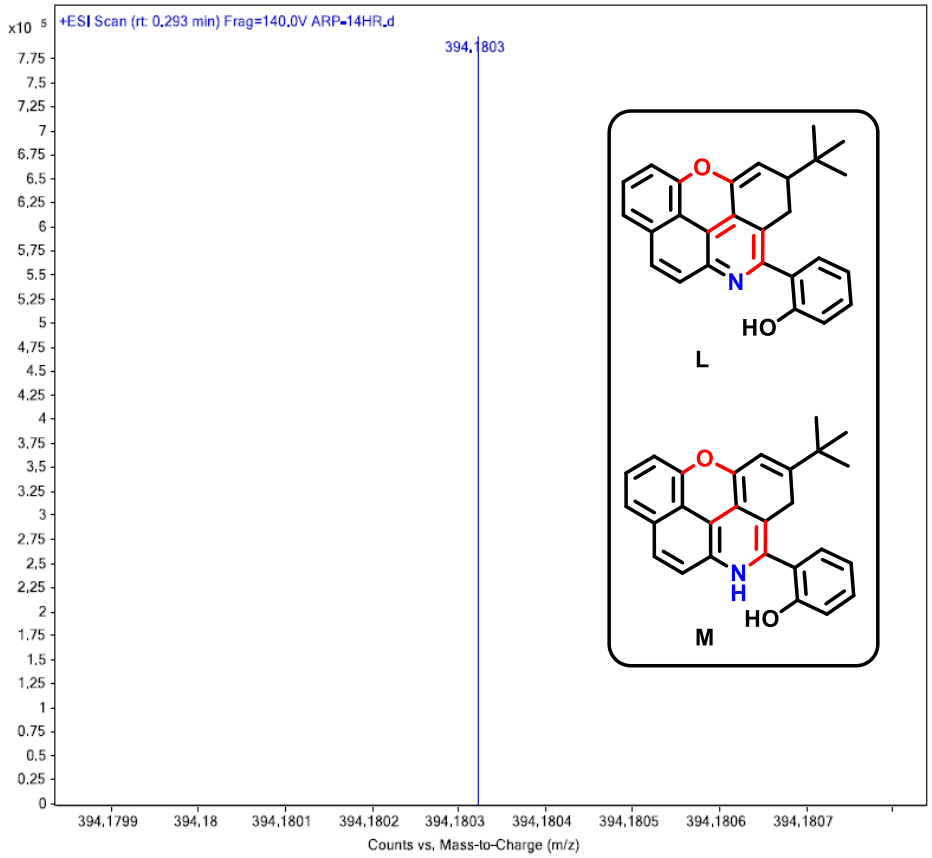
HRMS spectrum of intermediate H, I and J of compound 5a



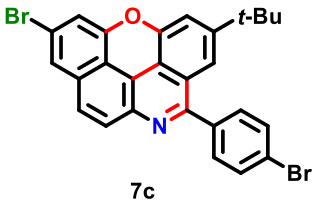
HRMS spectrum of intermediate K of compound 5a



HRMS spectrum of intermediate L and M of compound 5a



Result of Photophysical Experiments of Compound 7c:



7c

M.W. 533.26 g/mol

Compound 7c

To assess the photophysical property, we first recorded the absorption spectra of compound **7c** in two different solvents viz. DMSO and DCM. Compound **7c** exhibited absorption maxima at 420 nm (λ_{max}) and a weaker absorption peak at 397 nm (Figure 1). We then performed emission measurements of the same compound in DMSO and DCM. When the compound was excited at 420 nm (λ_{ex}), it displayed a strong emission at 458 nm and 450 nm in DMSO and DCM, respectively (Figure 2). A similar observation was visualized when the compound was excited at 397 nm (Figure 3). The results confirm that compound 1 is fluorescent in nature and emits in the blue region.

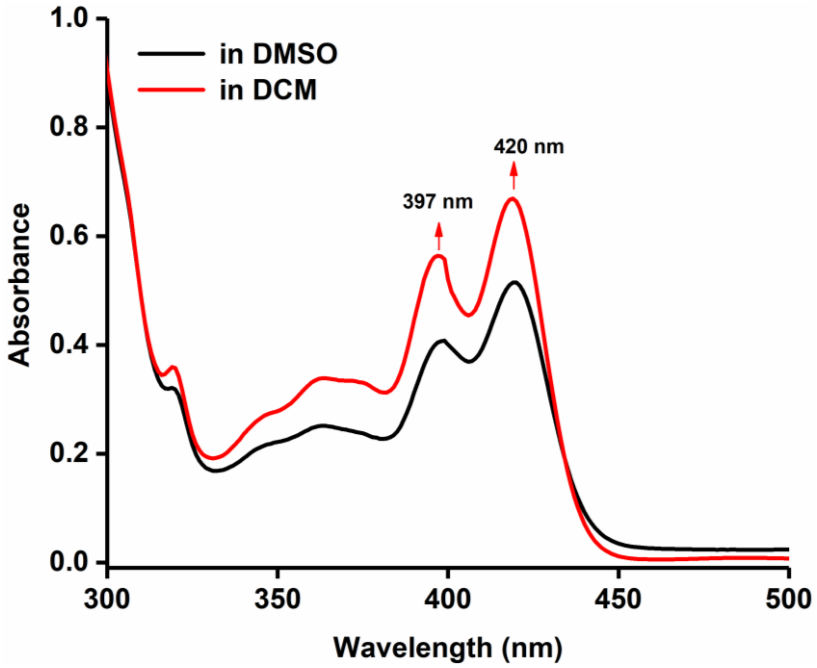


Figure S2: Absorption spectra of compound **7c** in DMSO and DCM. The concentration of the compound was kept at 50 μM.

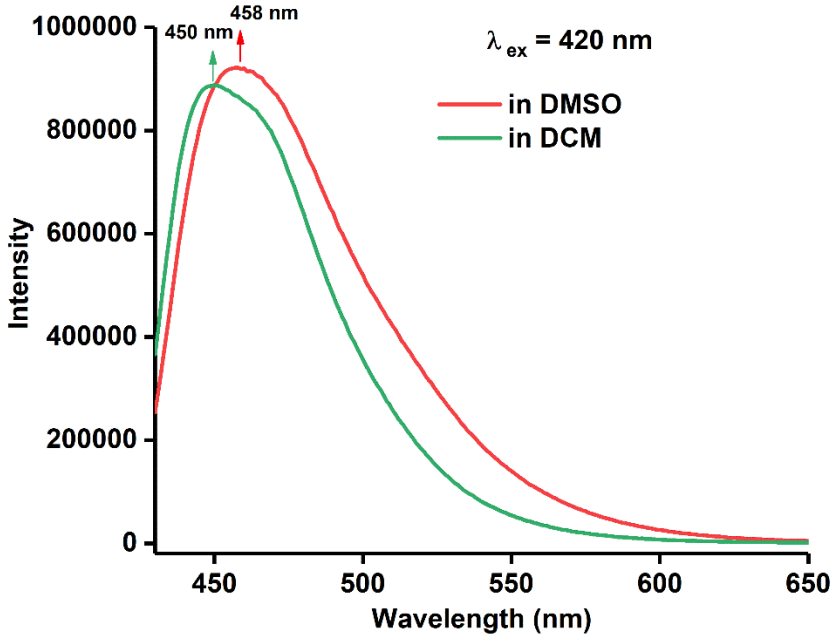


Figure S3: Emission spectra of compound **7c** in DMSO and DCM. The concentration of the compound was 50 μM. λ_{ex}= 420 nm.

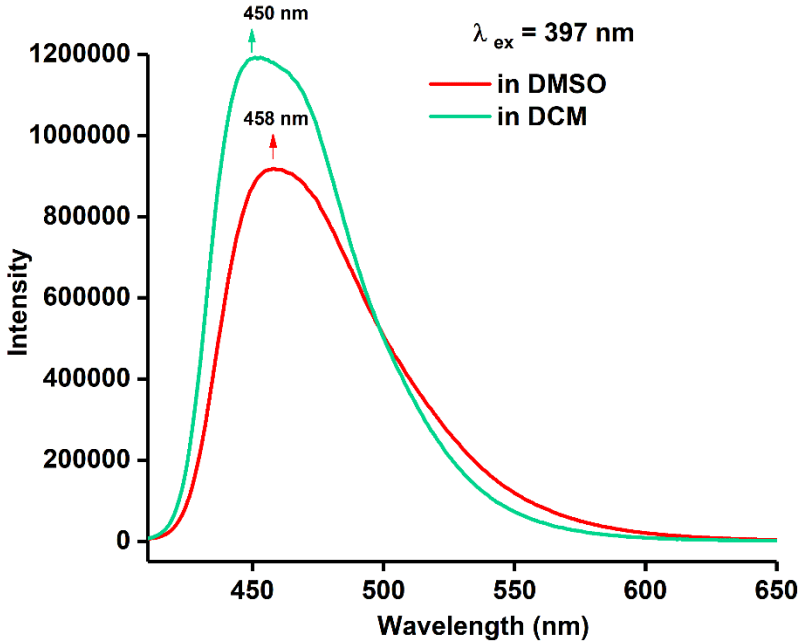


Figure S4: Emission spectra of compound **7c** in DMSO and DCM. The concentration of the compound was 50 μM. λ_{ex}= 397 nm.