Supporting Information

Completely regioselective insertion of unsymmetrical alkynes into electron-deficient alkenes for the synthesis of new pentacyclic indoles

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Context

Experimental

General Information.

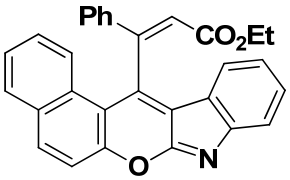
^{1}H NMR (^{13}C NMR) spectra were measured on a Bruker DPX 400 MHz spectrometer in $CDCl_3$ (DMSO-d_6) with chemical shift (δ) given in ppm relative to TMS as internal standard [(s = singlet, d = doublet, t = triplet, brs = broad singlet, m = multiplet), coupling constant (Hz)]. HRMS (ESI) was determined by using microTOF-QII HRMS/MS instrument (BRUKER). X-Ray crystallographic analysis was performed with a Siemens SMART CCD and a Siemens P4 diffractometer.

General procedure for the synthesis of compounds 3

Example for the synthesis of **3a**.

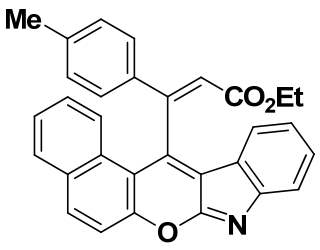
Under the air conditions, 1-(phenylethynyl)naphthalen-2-ol (**1a**, 0.22 mmol, 53.7 mg), (*E*)-ethyl 2-(2-oxoindolin-3-ylidene)acetate (**2a**, 0.2 mmol, 43.4 mg) and $Yb(OTf)_3$ (10 mol %, 12.4 mg) were added in a 25-mL reaction vial, Then, DCE (2.0 mL) was added into this reaction system. The reaction vial was sealed and heated at 100 ^{o}C for 12 h until TLC (petroleum ether: ethyl acetate= 2:1) revealed that conversion of the starting material **2a** was completed. Then the reaction mixture was concentrated in vacuum, and the resulting residue was purified by column chromatography on silica gel (eluent, petroleum ether/ ethyl acetate = 9:1) to afford the desired product **3a** as orange solid.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3a)



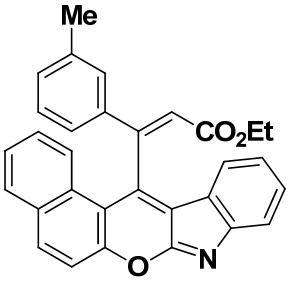
Orange solid, 77.6 mg, 88%; mp 259-260 ^{o}C; ^{1}H NMR (400 MHz, DMSO; δ, ppm) 8.80 (d, J = 8.4 Hz, 1H), 8.42 (d, J = 8.8 Hz, 1H), 8.17-8.13 (m, 1H), 8.11 (d, J = 9.2 Hz, 1H), 7.86-7.81 (m, 2H), 7.70 (d, J = 7.6 Hz, 1H), 7.62-7.53 (m, 3H), 7.48-7.41 (m, 2H), 7.40-7.35 (m, 3H), 7.14-7.10 (m, 1H), 3.80-3.71 (m, 2H), 0.77 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO; δ, ppm) 165.0, 163.0, 153.0, 152.1, 151.4, 144.9, 134.9, 134.4, 131.6, 131.3, 130.1, 130.0, 129.9, 129.9, 128.6, 128.2, 126.3, 124.9, 123.4, 123.0, 122.5, 121.1, 119.3, 119.2, 118.9, 113.8, 60.5, 13.9. IR (KBr, v, cm^{-1}) 2967, 1712, 1622, 1546, 1516, 1180, 818. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{22}NO_3$ 444.1600; Found 444.1602.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(p-tolyl)acrylate (3b)



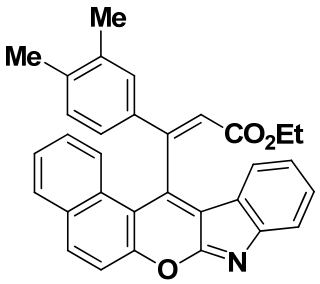
Orange solid, 81 mg, 89%; mp 227-228 ºC; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.85 (d, J = 8.4 Hz, 1H), 8.14 (d, J = 8.8 Hz, 1H), 7.95-7.91 (m, 2H), 7.75-7.70 (m, 2H), 7.55-7.43 (m, 5H), 7.15-7.08 (m, 3H), 7.05 (s, 1H), 3.82-3.74 (m, 2H), 2.30 (s, 3H), 0.80 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.9, 163.1, 152.6, 152.0, 151.8, 144.8, 141.8, 134.0, 131.5, 131.3, 130.4, 130.3, 129.6, 128.0, 127.6, 125.8, 125.1, 123.3, 123.2, 122.2, 121.4, 119.2, 118.7, 118.0, 114.1, 60.6, 21.5, 13.6. IR (KBr, v, cm^{-1}) 2978, 1702, 1622, 1555, 1516, 1178, 840. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1756; Found 458.1748.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(m-tolyl)acrylate (3c)



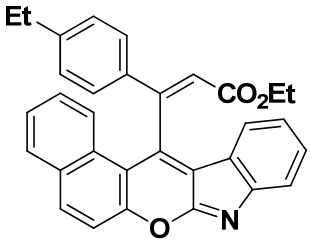
Orange solid, 78.5 mg, 86%; mp 239-240 ºC; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.84 (d, J = 8.4 Hz, 1H), 8.13 (d, J = 8.8 Hz, 1H), 7.95-7.90 (m, 2H), 7.74-7.71 (m, 2H), 7.53-7.42 (m, 5H), 7.24-7.17 (m, 2H), 7.13-7.08 (m, 2H), 3.82-3.74 (m, 2H), 2.27 (s, 3H), 0.80 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.7 163.1, 152.8, 151.9, 151.9, 144.4, 139.3, 134.3, 133.9, 132.1, 131.3, 130.2, 129.5, 129.4, 127.9, 127.9, 125.7, 125.0, 124.9, 123.3, 123.1, 122.2, 121.5, 119.2, 118.8, 118.6, 114.1, 60.6, 21.6, 13.6. IR (KBr, v, cm^{-1}) 2981, 1719, 1625, 1546, 1515, 1180, 812. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1756; Found 458.1754.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(3,4-dimethylphenyl)acrylate (3d)



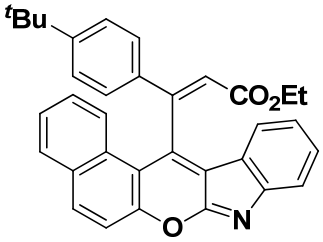
Orange solid, 86 mg, 91%; mp 214-215 ºC; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.85 (d, J = 8.4 Hz, 1H), 8.13 (d, J = 9.2 Hz, 1H), 7.96-7.90 (m, 2H), 7.75-7.70 (m, 2H), 7.52-7.43 (m, 4H), 7.36-7.34 (m, 1H), 7.12-7.05 (m, 3H), 3.81-3.73 (m, 2H), 2.20 (s, 3H), 2.17 (s, 3H), 0.79 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.9, 163.1, 152.6, 151.9, 151.9, 144.8, 140.6, 137.9, 133.9, 131.8, 131.2, 130.8, 130.3, 129.5, 129.4, 128.4, 127.9, 125.7, 125.3, 125.1, 123.3, 123.2, 122.1, 121.4, 119.1, 118.6, 117.6, 114.2, 60.5, 20.1, 19.8, 13.6. IR (KBr, v, cm^{-1}) 2974, 1705, 1623, 1555, 1510, 1189, 814. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{32}H_{26}NO_3$ 472.1913; Found 472.1906.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(4-ethylphenyl)acrylate (3e)



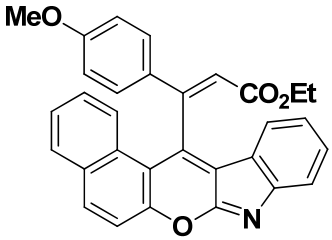
Orange solid, 85 mg, 90%; mp 186-187 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.86 (d, J = 8.4 Hz, 1H), 8.14 (d, J = 8.8 Hz, 1H), 7.95-7.91 (m, 2H), 7.76-7.70 (m 2H), 7.56 (d, J = 8.4 Hz, 2H), 7.53-7.44 (m, 3H), 7.15 (d, J = 8.4 Hz, 2H), 7.13-7.09 (m, 1H), 7.06 (s, 1H), 3.82-3.74 (m, 2H), 2.60 (q, J = 7.6 Hz, 2H), 1.17 (t, J = 7.6 Hz, 3H), 0.80 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.9, 163.1, 152.7, 152.0, 151.9, 147.8, 144.8, 134.0, 131.8, 131.3, 130.3, 129.6, 129.5, 129.1, 128.0, 127.6, 125.8, 125.1, 123.3, 123.2, 122.2, 121.4, 119.2, 118.7, 118.0, 114.1, 60.6, 28.7, 15.0, 13.6. IR (KBr, v, cm^{-1}) 2957, 1705, 1623, 1554, 1515, 1175, 834. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{32}H_{26}NO_3$ 472.1913; Found 472.1916.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(4-(tert-butyl)phenyl)acrylate (3f)



Orange solid, 88 mg, 88%; mp 238-239 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.91-8.86 (m, 1H), 8.14 (d, J = 8.8 Hz, 1H), 7.96-7.91 (m, 2H), 7.77 (d, J = 7.2 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.58-7.54 (m, 2H), 7.53-7.44 (m, 3H), 7.35-7.31 (m, 2H), 7.13-7.09 (m, 1H), 7.06 (s, 1H), 3.83-3.75 (m, 2H), 1.24 (s, 9H), 0.79 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.9, 163.1, 154.6, 152.7, 151.9, 151.9, 144.7, 133.9, 131.4, 131.2, 130.3, 129.5, 129.5, 128.0, 127.4, 126.5, 125.7, 125.1, 123.3, 123.2, 122.1, 121.3, 119.2, 118.6 118.1, 114.1, 60.6, 34.9, 31.1, 13.6. IR (KBr, v, cm^{-1}) 2962, 1172, 1623, 1560, 1513, 1180, 820. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{34}H_{30}NO_3$ 500.2226; Found 500.2245.

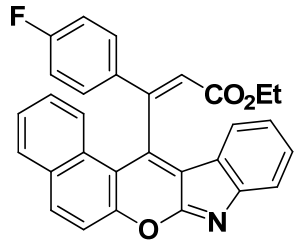
(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(4-methoxyphenyl)acrylate (3g)



Orange solid, 61 mg, 64%; mp 229-230 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.85 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 7.6 Hz, 2H), 7.75 (d, J = 6.8 Hz, 2H), 7.60-7.45 (m, 5H), 7.14-7.11 (m, 1H), 6.98 (s, 1H), 6.83 (d, J = 8.8 Hz, 2H), 3.83-3.70 (m, 5H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.9, 162.0, 152.0, 151.3, 134.4, 131.3, 129.6, 129.2, 128.1, 126.3, 126.0, 125.0, 123.1, 122.5, 118.8, 118.5, 116.4,

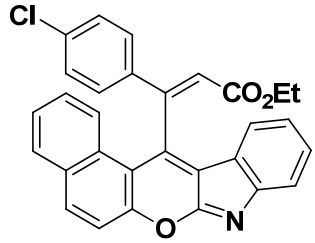
115.1, 114.3, 60.5, 55.4, 13.6. IR (KBr, *v*, cm^{-1}) 2979, 1705, 1595, 1548, 1513, 1166, 830. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_4$ 474.1705; Found 474.1729.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(4-fluorophenyl)acrylate (3h)



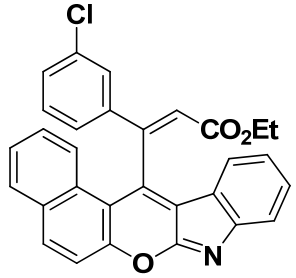
Orange solid, 72.2 mg, 78%; mp 250-251 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.80 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 9.2 Hz, 1H), 7.97-7.92 (m, 2H), 7.75-7.72 (m, 2H), 7.67-7.61 (m, 2H), 7.55-7.46 (m, 3H), 7.15-7.11 (m, 1H), 7.04-7.00 (m, 3H), 3.83-3.77 (m, 2H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 163.4 ($^1J_{CF}$ = 234.3 Hz), 160.1, 157.7, 152.4, 151.3, 147.1, 135.1, 133.8, 131.4, 131.3, 130.1, 129.7, 128.3, 127.5, 126.1, 124.9, 123.2, 123.1, 120.5 ($^4J_{CF}$ = 4.1 Hz), 119.5 ($^3J_{CF}$ = 8.6 Hz), 119.1, 118.5, 116.8 ($^2J_{CF}$ = 24.2 Hz), 114.0, 109.7, 109.5, 60.8, 13.7. IR (KBr, *v*, cm^{-1}) 2976, 1715, 1599, 1546, 1511, 1176, 817. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}FNO_3$ 462.1505; Found 462.1518.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(4-chlorophenyl)acrylate (3i)



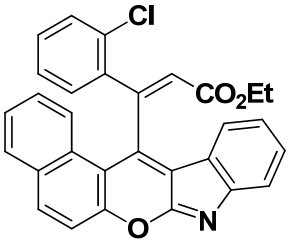
Orange red solid, 79.6 mg, 83%; mp 212-213 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.78 (d, J = 8.4 Hz, 1H), 8.15 (d, J = 8.8 Hz, 1H), 7.98-7.91 (m, 2H), 7.74-7.70 (m, 2H), 7.59-7.45 (m, 5H), 7.34-7.28 (m, 2H), 7.14-7.10 (m, 1H), 7.08 (s, 1H), 3.85-3.76 (m, 2H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.5, 163.0, 152.6, 152.1, 150.6, 143.8, 137.4, 134.3, 132.9, 131.3, 130.1, 129.9, 129.9, 129.8, 128.8, 128.1, 125.9, 124.7, 123.0, 122.9, 122.4, 121.5, 119.6, 119.4, 118.7, 113.8, 60.9, 13.6. IR (KBr, *v*, cm^{-1}) 2977, 1702, 1623, 1556, 1516, 1179, 816. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_3$ 478.1210; Found 478.1227.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(3-chlorophenyl)acrylate (3j)



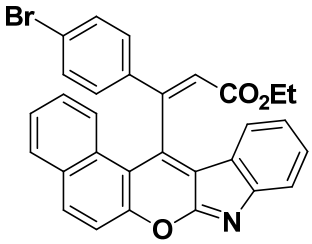
Orange solid, 76 mg, 80%; mp 247-248 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.76 (d, J = 8.4 Hz, 1H), 8.18-7.86 (m, 3H), 7.72 (d, J = 9.6 Hz, 3H), 7.55-.47 (m, 3H), 7.42 (d, J = 6.8 Hz, 1H), 7.36-7.34 (m, 1H), 7.26-7.14 (m, 2H), 7.11 (s, 1H), 3.79 (s, 2H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.4, 163.0, 152.1, 150.3 135.8, 134.3, 131.4, 131.3, 130.9, 130.1, 129.8, 128.2, 127.2, 126.0, 124.7, 122.9, 122.4, 120.4, 119.5, 118.7, 113.8, 60.9, 13.6. IR (KBr, v, cm^{-1}) 2982, 1721, 1605, 1547, 1515, 1181, 814. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_3$ 478.1210; Found 478.1219.

(E)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(2-chlorophenyl)acrylate (3k)



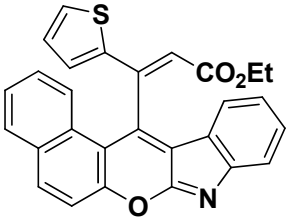
Orange solid, 44 mg, 46%; mp 241-242 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 9.06 (d, J = 8.8 Hz, 1H), 8.09 (d, J = 7.6 Hz, 1H), 8.01-7.74 (m, 4H), 7.66-7.62 (m, 1H), 7.59-7.50 (m, 3H), 7.44 (s, 1H), 7.20-7.15 (m, 2H), 7.02 (d, J = 7.6 Hz, 1H), 6.95-6.91 (m, 1H), 3.92-3.80 (m, 2H), 0.83 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 165.1, 162.9, 152.3, 146.6, 134.1, 133.5, 132.4, 131.0, 130.9, 130.0, 129.4, 128.0, 127.6, 126.6, 126.0, 125.5, 123.1, 122.5, 119.4, 118.4, 113.5, 60.9, 13.7. IR (KBr, v, cm^{-1}) 2977, 1723, 1620, 1554, 1513, 1179, 811. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_3$ 478.1210; Found 478.1225.

(Z)-Ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(4-bromophenyl)acrylate (3l)



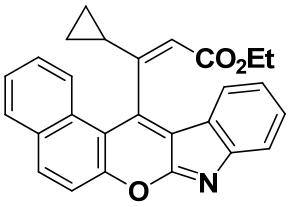
Orange solid, 76 mg, 73%; mp 230-231 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.77 (d, J = 8.4 Hz, 1H), 8.15 (d, J = 8.8 Hz, 1H), 7.97-7.89 (m, 2H), 7.73-7.70 (m, 2H), 7.54-7.44 (m, 7H), 7.14-7.08 (m, 2H), 3.84-3,76 (m, 2H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.5, 163.1, 152.0, 145.9, 139.3, 134.1, 131.2, 131.0, 130.0, 129.6, 129.0, 128.1, 125.8, 124.8, 123.1, 122.4, 119.3, 118.6, 116.5, 113.6, 60.7, 13.6. IR (KBr, v, cm^{-1}) 2977, 1703, 1623, 1556, 1516, 1180, 816. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}BrNO_3$ 522.0705; Found 522.0720.

(E)-ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-(thiophen-2-yl)acrylate (3m)



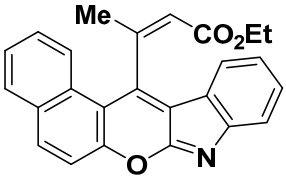
Orange solid, 68 mg, 76%; mp 230-231 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.89-8.83 (m, 1H), 8.13 (s, 1H), 7.94 (d, J = 6.8 Hz, 2H), 7.80-7.72 (m, 2H), 7.55-7.43 (m, 4H), 7.16-7.13 (m, 1H), 6.99 (s, 1H), 6.92 (s, 1H), 6.87 (s, 1H), 3.77 (q, J = 7.2 Hz, 2H), 0.80 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.5, 163.1, 152.0, 145.9, 139.3, 134.1, 131.2, 131.0, 129.9, 129.6, 129.0, 128.1, 125.8, 124.8, 123.1, 122.4, 119.3, 118.6, 116.5, 113.6, 60.7, 13.6. IR (KBr, v, cm^{-1}) 2981, 1706, 1620, 1544, 1511, 1172, 815. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{20}NO_3S$ 450.1164; Found 450.1154.

(Z)-ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-cyclopropylacrylate (3n)



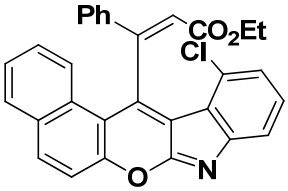
Orange solid, 24 mg, 29%; mp 200-201 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 9.11 (d, J = 8.8 Hz, 1H), 8.19-7.94 (m, 3H), 7.87 (d, J = 8.0 Hz, 1H), 7.79-7.64 (m, 2H), 7.62-7.59 (m, 1H), 7.57-7.50 (m, 1H), 7.33-7.26 (m, 1H), 6.58 (s, 1H), 3.75-3.70 (m, 2H), 2.29-2.24 (m, 1H), 1.33-1.19 (m, 2H), 1.03-0.91 (m, 2H), 0.76 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.3, 162.5, 157.9, 151.7, 134.1, 131.3, 129.6, 128.0, 125.9, 125.9, 125.2, 123.1, 123.1, 122.4, 119.1, 118.6, 113.7, 60.3, 18.5, 13.6, 9.6, 9.3. IR (KBr, v, cm^{-1}) 2984, 1704, 1619, 1554, 1515, 1185, 814. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{27}H_{22}NO_3$ 408.1600; Found 408.1595.

(Z)-ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)but-2-enoate (3o)



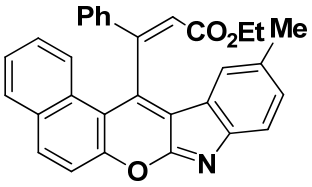
Orange solid, 39 mg, 51%; mp 175-176 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.80 (d, J = 8.8 Hz, 1H), 8.17 (d, J = 8.8 Hz, 1H), 8.02 (d, J = 7.2 Hz, 1H), 7.95 (d, J = 7.6 Hz, 1H), 7.89 (d, J = 8.8 Hz, 1H), 7.80-7.69 (m, 2H), 7.65-7.61 (m, 1H), 7.58-7.54 (m, 1H), 7.30-7.27 (m, 1H), 6.39 (d, J = 1.2 Hz, 1H), 4.44-4.35 (m, 2H), 2.80 (d, J = 1.2 Hz, 3H), 1.39 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 165.9, 165.8, 152.8, 152.4, 134.6, 131.4, 130.0, 129.8, 129.8, 128.4, 126.1, 125.0, 123.0, 122.7, 121.5, 119.3, 118.5, 112.1, 60.8, 19.1, 14.3. IR (KBr, v, cm^{-1}) 3052, 1711, 1622, 1559, 1510, 1187, 807. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{25}H_{19}NO_3Na$ 404.1263; Found 404.1267.

(Z)-Ethyl 3-(12-chlorobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3p)



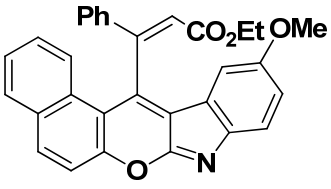
Orange solid, 74.4 mg, 81%; mp 189-190 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.96 (d, J = 8.8 Hz, 1H), 8.12 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 7.6 Hz, 2H), 7.66-7.59 (m, 3H), 7.49-7.31 (m, 6H), 7.16 (d, J = 7.6 Hz, 1H), 7.09 (s, 1H), 3.78 (q, J = 7.2 Hz, 2H), 0.83 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm) 164.8, 162.3, 152.3, 151.9, 137.4, 135.3, 131.5, 130.6, 130.0, 129.8, 129.4, 129.2, 127.8, 127.5, 126.0, 125.7, 125.3, 121.5, 118.2, 118.0, 113.5, 60.5, 13.6. IR (KBr, *v*, cm^{-1}) 2980, 1714, 1601, 1552, 1517, 1174, 821. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_3$ 478.1210; Found 478.1215.

(Z)-ethyl 3-(11-methylbenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3q)



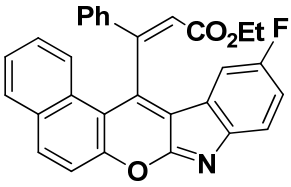
Orange solid, 77.6 mg, 88%; mp 261-262 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.84 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.95-7.91 (m, 2H), 7.65-7.61 (m, 3H), 7.54-7.44 (m, 3H), 7.39-7.27 (m, 4H), 7.10 (s, 1H), 3.80 (q, *J* = 7.2 Hz, 2H), 2.35 (s, 3H), 0.79 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm) 164.7, 162.2, 151.9, 151.7, 144.8, 134.4, 134.1, 131.8, 131.3, 131.1, 130.7, 130.2, 129.6, 129.5 127.9, 127.6, 125.8, 125.0, 123.4, 122.9, 121.2, 119.2, 118.6, 114.1, 60.7, 21.7, 13.6. IR (KBr, *v*, cm^{-1}) 2989, 1715, 1621, 1547, 1510, 1176, 816. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1756; Found 458.1767.

(Z)-ethyl 3-(11-methoxybenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3r)



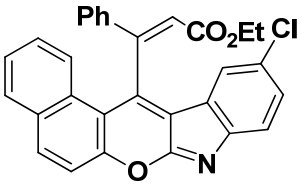
Red-brown solid, 75.5 mg, 80%; mp 252-253 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.82 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 7.95-7.93 (m, 1H), 7.90 (d, *J* = 9.2 Hz, 1H), 7.68-7.64 (m, 2H), 7.61 (d, *J* = 8.8 Hz, 1H), 7.52-7.43 (m, 2H), 7.40-7.32 (m, 3H), 7.28 (d, *J* = 2.4 Hz, 1H), 7.09 (s, 1H), 7.06-7.03 (m, 1H), 3.83-3.76 (m, 2H), 3.74 (s, 3H), 0.81 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm) 164.6, 162.1, 155.4, 152.0, 151.6, 146.4, 144.5, 134.4, 134.0, 131.2, 131.2, 130.2, 129.6, 127.9, 127.6, 125.7, 124.9, 123.7, 121.6, 119.4, 119.0, 118.6, 115.9, 113.8, 108.7, 60.7, 55.9, 13.6. IR (KBr, *v*, cm^{-1}) 2977, 1712, 1622, 1555, 1491, 1198, 816. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_4$ 474.1705; Found 474.1711.

(Z)-ethyl 3-(11-fluorobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3s)



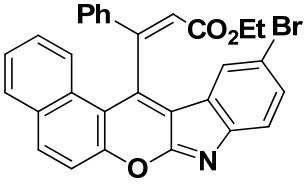
Orange red solid, 84 mg, 91%; mp 285-286 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.83 (d, J = 8.4 Hz, 1H), 8.20 (d, J = 9.2 Hz, 1H), 7.98-7.94 (m, 2H), 7.69-7.66 (m, 1H), 7.65-7.60 (m, 2H), 7.56-7.47 (m, 2H), 7.44-7.34 (m, 4H), 7.22-7.17 (m, 1H), 7.11 (s, 1H), 3.83 (q, J = 7.2 Hz, 2H), 0.87 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.5, 164.3 ($^{1}J_{CF}$ = 252.0 Hz), 162.7, 152.0, 150.6, 134.3, 131.3, 130.4 ($^{6}J_{CF}$ = 4.1 Hz), 130.1, 129.7 ($^{4}J_{CF}$ = 10.6 Hz), 129.6 ($^{5}J_{CF}$ = 8.7 Hz), 128.1, 125.9, 124.7, 122.9, 122.4, 121.2, 119.1 ($^{2}J_{CF}$ = 19.6 Hz), 119.0, 118.6, 116.8 ($^{3}J_{CF}$ = 21.9 Hz), 113.9, 60.8, 13.6. IR (KBr, v, cm^{-1}) 2981, 1711, 1623, 1557, 1513, 1177, 820. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}FNO_3$ 462.1505; Found 462.1521.

(Z)-ethyl 3-(11-chlorobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3t)



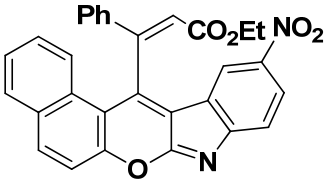
Orange solid, 88 mg, 92%; mp 261-262 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.83 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 8.8 Hz, 1H), 7.97-7.91 (m, 2H), 7.68-7.61 (m, 4H), 7.55-7.47 (m, 2H), 7.44-7.34 (m, 4H), 7.12 (s, 1H), 3.83 (q, J = 7.2 Hz, 2H), 0.87 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.6, 162.8, 152.3, 151.4, 134.9, 134.0, 131.4, 131.3, 130.1, 129.7, 129.5, 128.2, 127.5, 126.0, 124.9, 124.1, 122.7, 120.3, 120.0, 119.2, 118.5, 114.0, 60.8, 13.7. IR (KBr, v, cm^{-1}) 2985, 1711, 1616, 1542, 1510, 1179, 823. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_3$ 478.1210; Found 478.1220.

(Z)-ethyl 3-(11-bromobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3u)



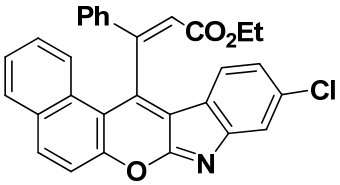
Orange solid, 80 mg, 77%; mp 282-283 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.83 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 9.2 Hz, 1H), 7.97-7.86 (m, 2H), 7.82 (s, 1H), 7.64-7.46 (m, 6H), 7.43-7.33 (m, 3H), 7.11 (s, 1H), 3.83 (q, J = 7.2 Hz, 2H), 0.87 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.6, 163.0, 152.3, 151.4, 146.2, 134.7, 134.1, 132.2, 131.3, 131.3, 130.1, 129.7, 128.2, 127.6, 126.0, 125.6, 124.9, 124.8, 120.6, 119.2, 118.5, 115.0, 113.9, 60.8, 13.7. IR (KBr, v, cm^{-1}) 2985, 1711, 1616, 1542, 1519, 1181, 817. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}BrNO_3$ 522.0705; Found 522.0718.

(Z)-ethyl 3-(11-nitrobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3v)



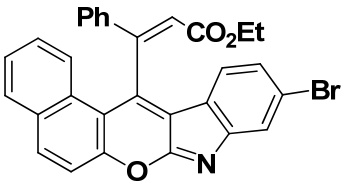
Orange yellow solid, 84 mg, 86%; mp 240-241 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.88 (d, *J* = 8.4 Hz, 1H), 8.65 (d, *J* = 2.4 Hz, 1H), 8.38-8.36 (m, 1H), 8.24 (d, *J* = 9.2 Hz, 1H), 8.02-.93 (m, 2H), 7.79 (d, *J* = 6.8 Hz, 1H), 7.69-7.65 (m, 2H), 7.60-7.52 (m, 2H), 7.44-7.35 (m, 3H), 7.20 (s, 1H), 3.82 (q, *J* = 7.2 Hz, 2H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm) 165.9, 164.6, 152.8, 151.3, 142.9, 135.7, 134.0, 131.7, 131.5, 130.1, 129.9, 129.9, 128.7, 127.7, 126.5, 125.0, 125.0, 123.0, 120.1, 119.2, 119.0, 118.5, 114.4, 60.9, 13.8. IR (KBr, *v*, cm^{-1}) 2983, 1712, 1627, 1538, 1509, 1174, 817. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}N_2O_5$ 489.1450; Found 489.1458.

(Z)-ethyl 3-(10-chlorobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3w)



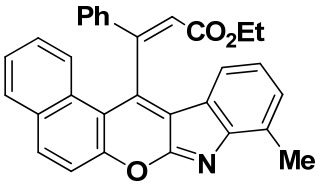
Orange yellow solid, 90 mg, 94%; mp 263-264 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.83 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 2H), 7.78-7.57 (m, 4H), 7.54-7.46 (m, 2H), 7.42-7.31 (m, 3H), 7.08 (d, *J* = 8.8 Hz, 2H), 3.84-3.76 (m, 2H), 0.84 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm) 164.6, 163.7, 152.1, 151.5, 135.3, 134.5, 134.0, 131.3, 131.3, 130.1, 129.6, 128.1, 127.5, 126.0, 124.9, 123.5, 122.5, 119.6, 119.1, 118.5, 114.1, 60.8, 13.6. IR (KBr, *v*, cm^{-1}) 2976, 1716, 1616, 1550, 1517, 1176, 819. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_3$ 478.1210; Found 478.1227.

(Z)-ethyl 3-(10-bromobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3x)



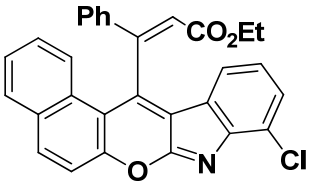
Orange yellow solid, 97 mg, 88%; mp 270-271 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.83 (d, *J* = 8.8 Hz, 1H), 8.15 (d, *J* = 9.2 Hz, 1H), 8.03-7.72 (m, 3H), 7.64-7.57 (m, 3H), 7.54-7.45 (m, 2H), 7.41-7.31 (m, 3H), 7.24-7.22 (m, 1H), 7.09 (s, 1H), 3.84-3.76 (m, 2H), 0.84 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm) 164.6, 163.7, 152.2, 151.6, 134.4, 134.0, 131.3, 131.3, 130.1, 129.6, 128.1, 127.5, 126.0, 125.2, 124.9, 123.8, 123.5, 122.5, 122.0, 120.7, 119.1, 118.5, 114.1, 60.8, 13.6. IR (KBr, *v*, cm^{-1}) 2976, 1716, 1615, 1548, 1516, 1175, 1175, 819. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}BrNO_3$ 522.0705; Found 522.0721.

(Z)-ethyl 3-(9-methylbenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3y)



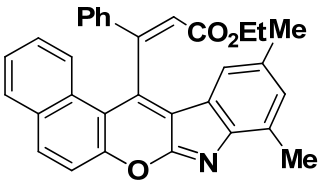
Orange red solid, 78 mg, 85%; mp 237-238 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.85 (d, J = 8.4 Hz, 1H), 8.12 (d, J = 9.2 Hz, 1H), 7.95-7.89 (m, 2H), 7.67-7.63 (m, 2H), 7.60 (d, J = 7.6 Hz, 1H), 7.52-7.44 (m, 2H), 7.39-7.28 (m, 4H), 7.09 (s, 1H), 7.04-7.00 (m, 1H), 3.82-3.76 (m, 2H), 2.67 (s, 3H), 0.80 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.7, 162.4, 151.9 151.8, 144.3, 134.4, 133.9, 131.3, 131.0, 130.7, 130.2, 129.5, 129.5, 128.5, 127.8, 127.6, 125.7, 124.9, 122.7, 122.1, 121.8, 120.7, 119.1, 118.6, 60.6, 17.1, 13.6. IR (KBr, v, cm^{-1}) 2982, 1705, 1624, 1557, 1516, 1178, 814. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1756; Found 458.1750.

(Z)-ethyl 3-(9-chlorobenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3z)



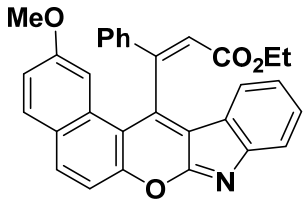
Orange red solid, 92 mg, 96%; mp 270-271 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.84 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 8.8 Hz, 1H), 7.97-7.89 (m, 2H), 7.68-7.61 (m, 3H), 7.54-7.45 (m, 3H), 7.40-7.31 (m, 3H), 7.10 (s, 1H), 7.05-7.01 (m, 1H), 3.83-3.78 (m, 2H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.6, 163.3, 152.4, 151.5, 149.5, 146.3, 134.7, 134.1, 131.3, 131.3, 130.2, 129.7, 129.7, 129.5, 128.2, 127.6, 126.0, 125.0, 124.8, 124.1, 122.8, 121.4, 119.2, 118.7, 114.0, 60.8, 13.7. IR (KBr, v, cm^{-1}) 2980, 1704, 1617, 1544, 1507, 1171, 815. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_3$ 478.1210; Found 478.1232.

(Z)-ethyl 3-(9,11-dimethylbenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3aa)



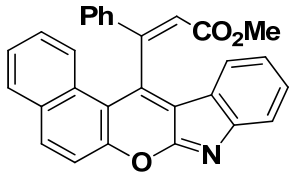
Red-brown solid, 73 mg, 77%; mp 214-215 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.84 (d, J = 8.4 Hz, 1H), 8.10 (d, J = 9.2 Hz, 1H), 7.94-7.86 (m, 2H), 7.67-7.63 (m, 2H), 7.51-7.42 (m, 2H), 7.39-7.30 (m, 4H), 7.12 (s, 1H), 7.09 (s, 1H), 3.79 (q, J = 7.2 Hz, 2H), 2.63 (s, 3H), 2.31 (s, 3H), 0.78 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.8, 162.1, 151.9, 151.9, 149.1, 143.8, 134.7, 133.7, 131.9, 131.5, 131.3, 131.03, 130.3, 129.6, 129.5, 128.1, 127.8, 127.7, 125.6, 125.0, 122.9, 121.9, 121.1, 119.2, 118.7, 114.0, 60.7, 21.7, 17.1, 13.6. IR (KBr, v, cm^{-1}) 2979, 1716, 1616, 1559, 1515, 1194, 810. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{32}H_{26}NO_3$ 472.1913; Found 472.1887.

(Z)-ethyl 3-(2-methoxybenzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3bb)



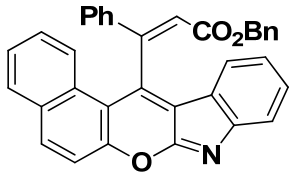
Orange solid, 75.5 mg, 80%; mp 219-220 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.14 (d, J = 2.0 Hz, 1H), 8.05 (d, J = 5.2 Hz, 1H), 7.90-7.61 (m, 6H), 7.46 -7.33(m, 4H), 7.17-7.06 (m, 3H), 3.79-3.74 (m, 2H), 3.56 (s, 3H), 0.79 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.6, 163.1, 159.2, 152.6, 151.6, 133.6, 131.7, 131.4, 130.9, 129.7, 129.4, 127.3, 126.3, 122.9, 122.1, 121.2, 119.2, 118.1, 117.5, 116.0, 113.5, 105.7, 60.7, 55.0, 13.5. IR (KBr, v, cm^{-1}) 3049, 1720, 1622, 1540, 1518, 1179, 828. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{31}H_{23}NO_4Na$ 496.1525; Found 496.1533.

(Z)-methyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3cc)



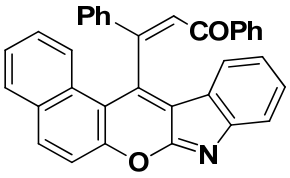
Orange yellow solid, 70.6 mg, 82%; mp 295-296 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.83 (d, J = 8.4 Hz, 1H), 8.14 (d, J = 9.2 Hz, 1H), 7.95-7.92 (m, 2H), 7.74-7.71 (m, 2H), 7.66-7.62 (m, 2H), 7.53-7.44 (m, 3H), 7.40-7.31 (m, 3H), 7.13-7.07 (m, 2H), 3.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 165.0, 163.0, 152.5, 152.0, 144.3, 134.2, 134.0, 131.3, 131.2, 130.2, 129.6, 129.6, 127.9, 127.6, 125.7, 124.9, 123.2, 122.9, 122.2, 121.3, 119.2, 118.7, 118.5, 113.9, 51.8. IR (KBr, v, cm^{-1}) 2949, 1711, 1619, 1543, 1510, 1168, 815. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{29}H_{20}NO_3$ 430.1443; Found 430.1466.

(Z)-benzyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenylacrylate (3dd)



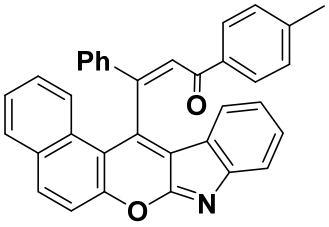
Orange red solid, 84.6 mg, 84%; mp 120-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.85 (d, J = 8.4 Hz, 1H), 8.09 (d, J = 9.2 Hz, 1H), 7.95-7.92 (m, 1H), 7.81 (d, J = 9.2 Hz, 1H), 7.77-7.72 (m, 2H), 7.64-7.61 (m, 2H), 7.53-7.44 (m, 3H), 7.38-7.30 (m, 3H), 7.23-7.19 (m, 1H), 7.15 (s, 1H), 7.13-7.08 (m, 3H), 6.81-6.74 (m, 2H), 4.76 (q, J = 12.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 164.6, 162.9, 152.6, 152.2, 151.9, 144.0, 134.7, 134.3, 133.9, 131.2, 131.2, 130.1, 129.6, 129.5, 128.4, 128.2, 127.9, 127.8, 127.6, 125.7, 124.9, 123.1, 123.0, 122.3, 121.4, 119.2, 118.9, 118.6, 113.8, 66.7. IR (KBr, v, cm^{-1}) 2968, 1718, 1622, 1548, 1515, 1159, 817. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{35}H_{24}NO_3$ 506.1756; Found 506.1773.

(Z)-3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-1,3-diphenylprop-2-en-1-one (3ee)



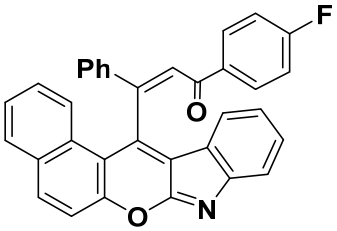
Orange yellow solid, 52 mg, 55%; mp 168-169 ºC; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.94 (d, J = 8.4 Hz, 1H), 8.22-8.11 (m, 2H), 7.98-7.83 (m, 5H), 7.72-7.69 (m, 3H), 7.52-7.45 (m, 3H), 7.42-7.33 (m, 6H), 7.05 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 188.4, 152.1, 152.0, 137.3, 134.7, 134.2, 133.3, 131.3, 130.4, 129.6, 129.6, 129.4, 128.7, 128.4, 128.0, 127.8, 125.8, 124.8, 123.1, 122.8, 122.6, 122.1, 119.1, 118.7, 114.5. IR (KBr, v, cm^{-1}) 3051, 1653, 1619, 1551, 1512, 1212, 818. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{34}H_{22}NO_2$ 476.1651; Found 476.1664.

(Z)-3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-phenyl-1-(p-tolyl)prop-2-en-1-one (3ff)



Orange solid, 51 mg, 52%; mp 167-168 ºC; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.97 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 10.4 Hz, 2H), 7.96-7.92 (m, 2H), 7.85 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 8.4 Hz, 2H), 7.73-7.68 (m, 3H), 7.52-7.44 (m, 2H), 7.42-7.34 (m, 4H), 7.19 (d, J = 8.4 Hz, 2H), 7.06 (t, J = 7.6 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 187.9, 162.4, 152.0, 151.6, 144.4, 134.8, 134.7, 134.4, 131.4, 131.2, 130.4, 129.6, 129.6, 129.4, 128.6, 128.0, 127.8, 125.9, 124.9, 123.0, 122.8, 122.6, 122.3, 120.0, 118.8, 118.6, 114.7, 21.7. IR (KBr, v, cm^{-1}) 3051, 1648, 1606, 1553, 1512, 1199, 818. HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{35}H_{23}NO_2Na$ 512.1626; Found 512.1636.

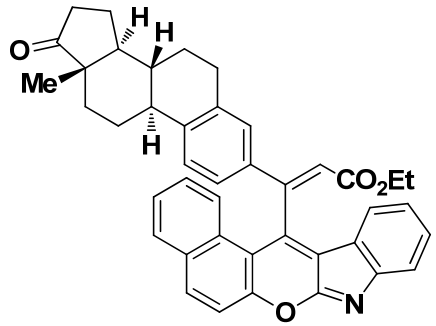
(Z)-3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-1-(4-fluorophenyl)-3-phenylprop-2-en-1-one (3gg)



Orange solid, 43.2 mg, 44%; mp 191-192 ºC; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.93 (d, J = 8.4 Hz, 1H), 8.18 (d, J = 8.8 Hz, 1H), 8.14 (s, 1H), 7.96 (d, J = 8.8 Hz, 2H), 7.92-7.89 (m, 2H), 7.83 (d, J = 7.6 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 7.2 Hz, 2H), 7.54-7.45 (m, 2H), 7.44-7.35 (m, 4H), 7.09-7.03 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm) 186.8, 167.1, 163.3 ($^{1}J_{CF}$ = 252.6 Hz), 152.2, 152.1, 134.7, 134.4, 133.6 ($^{4}J_{CF}$ = 2.9 Hz), 131.50, 131.4, 131.1, 131.0, 130.2, 129.7, 129.7, 129.6, 128.2, 127.8, 126.1, 124.8, 122.5 ($^{3}J_{CF}$ = 7.3 Hz), 122.4, 119.8, 118.8, 118.6, 115.9 ($^{2}J_{CF}$ = 21.8 Hz), 114.7. IR (KBr, v, cm^{-1}) 3051, 1648, 1570, 1551, 1511, 1212, 842. HRMS

(ESI) m/z: $[M+Na]^+$ Calcd for $C_{34}H_{20}FNO_2Na$ 516.1376; Found 516.1382.

(Z)-ethyl 3-(benzo[5,6]chromeno[2,3-b]indol-13-yl)-3-((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl)acrylate (3hh)



Orange yellow solid, 100 mg, 81%; mp 213-214 ºC; ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm) 8.86 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.95-7.91 (m, 2H), 7.77-7.70 (m, 2H), 7.54-7.41 (m, 4H), 7.30 (d, *J* = 19.2 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.13-7.09 (m, 1H), 7.05 (d, *J* = 0.8 Hz, 1H), 3.80-3.75 (m, 2H), 2.78-2.73 (m, 2H), 2.51-2.44 (m, 1H), 2.28-1.89 (m, 6H), 1.65-1.37 (m, 6H), 0.86 (s, 3H), 0.81-0.77 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm) 220.7, 164.9, 163.1, 152.7, 152.0, 151.9, 144.8, 143.5, 137.9, 134.0, 131.9, 131.3, 130.3, 129.6, 129.5, 128.0, 126.6, 125.7, 125.2, 125.1, 125.0, 123.3, 123.3, 122.2, 121.4, 119.2, 118.7, 118.1, 114.2, 60.6, 50.5, 48.0, 44.6, 37.7 35.9, 31.6, 29.5, 26.3, 25.5, 21.6, 13.9, 13.7. IR (KBr, *v*, cm^{-1}) 2930, 1735, 1716, 1623, 1158, 1516, 1184, 817. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{42}H_{38}NO_4$ 620.2801; Found 620.2824.

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Computational details.

All calculations were carried out by using Gaussian 09 program[1]. The geometries of the substances were optimized using DFT with the B3LYP functional[2, 3]. The 6-31G(d) basis set was used for the atoms, except that Sc atom was treated by SDD effective core potential basis set. Frequency was analyzed to confirm the optimized structure was a minimum or a transition state, and to obtain Gibbs free energy of each species. To illuminate the influence of the solvent (1,2-dichloroethane, DCE) on the reaction, the SMD model single-point energy calculations were carried out based on the gas-phase geometries by using SMD-M06 functional. The free energy of each species in solution was deemed as the sum of the gas-phase free energy and the free energy of solvation.

References

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4. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B.* 2009, 113, 6378-6396.
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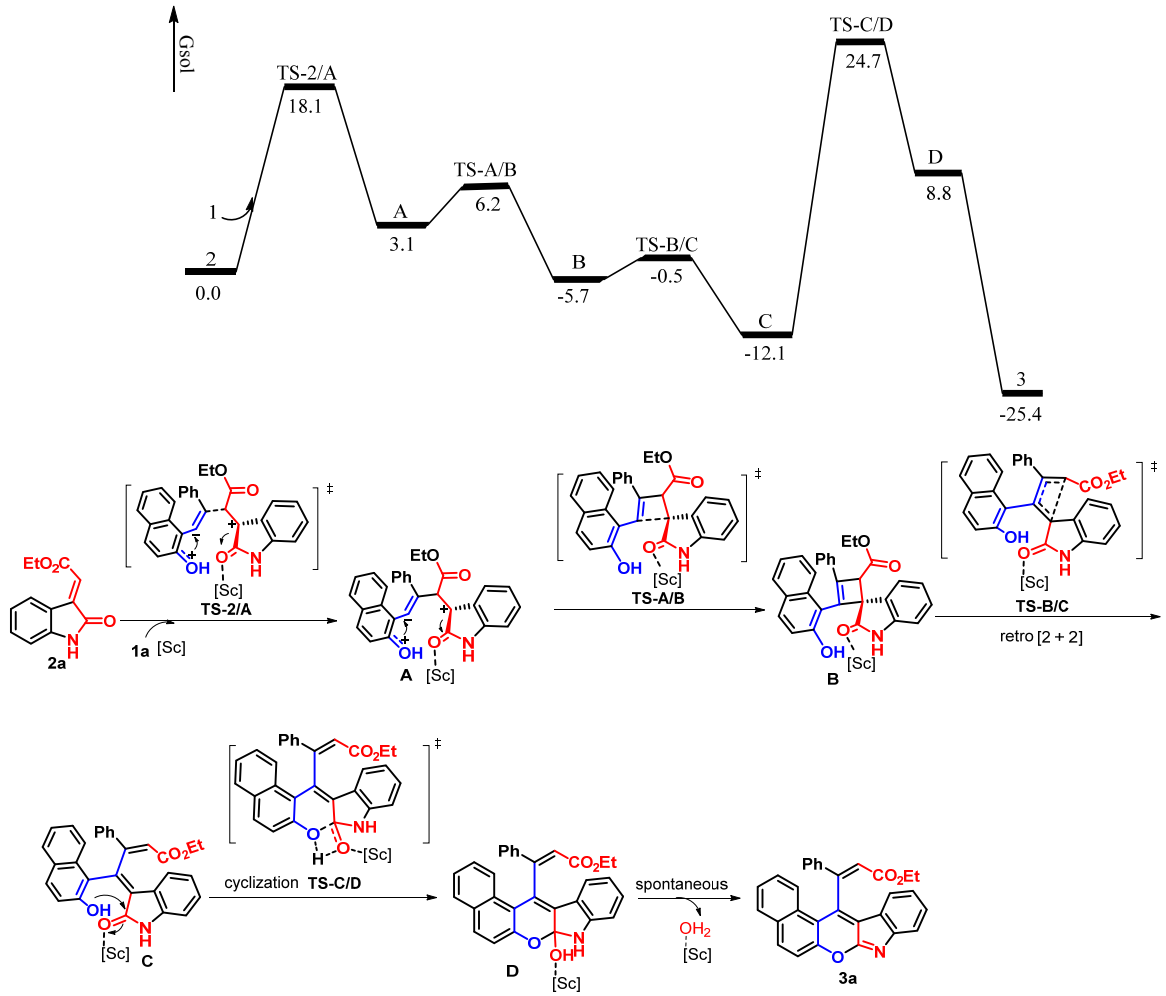

Figure S1. Gibbs free energy profiles of the proposed mechanism

Table S1. Electronic energies (E_{elec}), Zero-point energies(ZPE), Gibbs free energies (G_{gas}), and solvent free energies ($\triangle G_{sol}$) of all stationary points. The E_{elec}, ZPE, G_{gas}, energies are in a. u. and G_{sol} are in kcal/mol.

Species	E_{elec}	ZPE	G_{gas}	$\triangle G_{sol}$
2+1+[Sc]	-3482.285349	0.516102	-3481.862805	-52.05
TS-2/A	-3482.251451	0.515269	-3481.830263	-54.36
A	-3482.2734343	0.517419	-3481.850329	-56.79
TS-A/B	-3482.267604	0.516483	-3481.845323	-56.84
B	-3482.2933893	0.518888	-3481.86558	-56
TS-B/C	-3482.2931376	0.51736	-3481.86307	-52.35
C	-3482.3067709	0.518154	-3481.878724	-54.18
TS-C/D	-3482.2507968	0.517077	-3481.821019	-53.53
D	-3482.2793241	0.51823	-3481.849293	-51.72
TS-D/3	-3482.2781825	0.516927	-3481.848736	-52.75
3	-3482.3249983	0.517402	-3481.900924	-53.49

Table S2. Calculated Cartesian coordinates of all stationary points

2+1+[Sc]

C	3.66841700	0.27974100	3.07685200
C	3.95422400	1.38641000	2.26735800
C	5.26685200	1.61550600	1.77956300
C	5.49641900	2.41463000	6.15656200
C	2.35736000	0.04215000	3.55555000
C	2.88692900	2.29043500	1.95181300
C	1.55820700	2.03616200	2.42824200
C	1.32531400	0.89298400	3.23739600
C	0.50777600	2.91356000	2.05500300
H	-0.49537100	2.69895900	2.41475200
C	0.72940200	4.01194700	1.24696300
C	2.03265900	4.27964500	0.78233400
C	3.09982000	3.45540500	1.14588400
H	2.17161300	-0.83310200	4.17457800
H	0.32101400	0.69321000	3.59916200
H	-0.09165800	4.66233300	0.96466600
H	2.21395600	5.12625900	0.12690700
H	4.06657100	3.57254600	0.65405600
C	4.61109400	3.50709700	5.65383400
C	5.33099600	2.43606700	7.61833500
C	4.41711200	3.46761100	7.91347300
C	4.02766200	3.80058700	9.19880500
C	4.59228200	3.05729300	10.24378000
C	5.50596200	2.03157000	9.98425700
C	5.88274400	1.71053200	8.67564300

H	3.32179500	4.60219700	9.39212300
H	4.31488400	3.28660300	11.26786600
H	5.93138300	1.47265700	10.81172000
H	6.58474700	0.91034400	8.48461800
C	6.38673900	1.82914100	1.34649300
C	7.69787900	2.05648300	0.83561400
C	7.88113800	2.79580600	-0.35132100
C	8.82159800	1.53621200	1.51104700
C	9.16311900	3.00442900	-0.85120700
H	7.01830200	3.19862500	-0.87188000
C	10.09798000	1.75254800	0.99882100
H	8.68258500	0.98240500	2.43360900
C	10.27274200	2.48248900	-0.18027500
H	9.29652000	3.57331500	-1.76664700
H	10.96023400	1.35016800	1.52265000
H	11.27143900	2.64556600	-0.57527500
C	6.22116300	1.70766200	5.26033600
H	6.15658500	1.99736400	4.21473900
C	7.19896400	0.60420900	5.47569900
O	8.17648200	0.49085800	4.76481000
O	6.88156500	-0.23287800	6.47323100
C	7.79923200	-1.35344300	6.67058300
H	8.77349500	-0.94822600	6.95875800
H	7.91973600	-1.86438100	5.71140000
C	7.20750100	-2.25458300	7.73565800
H	7.86872500	-3.11340300	7.89044700
H	7.10232000	-1.73208100	8.69181900
H	6.22431800	-2.63026600	7.43524900
O	4.42820900	3.83916300	4.43971600
N	4.00471500	4.07346400	6.70044500
H	3.34555100	4.85014800	6.63218800
O	4.69633200	-0.54745700	3.39386600
H	4.35999500	-1.31369100	3.88632600
C	1.83585700	8.33372900	4.12144000
S	2.52486300	6.67077400	4.65457000
O	2.01271400	5.66242700	3.63390900
O	2.15573800	6.43529400	6.04750300
O	4.01735500	6.71672600	4.36384700
F	2.13321800	8.51481200	2.83954700
F	0.52327300	8.31358400	4.29462000
F	2.39744300	9.27281500	4.86603500
S	5.72085800	6.30510800	1.15193300
C	6.48318100	7.93132700	1.70241600
F	6.11584800	8.86653900	0.83832100
F	6.04464900	8.23132500	2.92093700
F	7.79952400	7.78740700	1.70946700

O	6.24299100	5.97563900	-0.15724800
O	4.20801600	6.48993900	1.28095400
Sc	3.99123100	5.09752500	2.92423100
O	6.00094200	5.31901200	2.29496600

TS-2/A

C	3.03170500	-0.19032300	4.12120400
C	3.38626600	0.81392700	3.18304600
C	4.71594200	0.98447200	2.84647200
C	5.20252600	2.70286700	5.32027400
C	1.69302400	-0.34138500	4.54025400
C	2.34494000	1.65753400	2.61544300
C	0.99865200	1.48335200	3.05860500
C	0.71426900	0.47598900	4.02260100
C	-0.02716700	2.30451000	2.52503700
H	-1.04753100	2.15933800	2.87000600
C	0.26326000	3.26242900	1.57558000
C	1.59215400	3.42217300	1.12738600
C	2.61373000	2.63689400	1.63574400
H	1.44261800	-1.10888500	5.26817400
H	-0.31424600	0.34621300	4.34970800
H	-0.52645600	3.88251900	1.16294100
H	1.81961800	4.15982900	0.36388900
H	3.62505200	2.75463600	1.26019700
C	4.26604400	3.77312000	5.30674700
C	4.84037600	1.88601600	6.47540500
C	3.73370700	2.51431600	7.09922900
C	3.11133300	2.01165600	8.23644800
C	3.61666100	0.82390400	8.76734300
C	4.70214900	0.17091400	8.16274400
C	5.31819500	0.68614000	7.02107700
H	2.26905800	2.52123700	8.69514400
H	3.16377500	0.40421200	9.66035900
H	5.07841800	-0.74955700	8.60020100
H	6.15088400	0.17260500	6.55921200
C	5.91620100	1.30922000	2.72013200
C	7.14255300	1.13240700	1.95997100
C	7.79818100	2.22811200	1.37363800
C	7.67464900	-0.16116000	1.80186200
C	8.95820600	2.02765700	0.62698000
H	7.39629700	3.22977100	1.49239300
C	8.83643900	-0.34993700	1.05700000
H	7.16687900	-1.00436300	2.25940600
C	9.47997600	0.74232200	0.46780900
H	9.45570100	2.87836000	0.17098400
H	9.23729400	-1.35164700	0.93179500

H	10.38486100	0.59123200	-0.11337500
C	6.22332600	2.62535600	4.34196500
H	6.26160000	3.48818900	3.68410700
C	7.63302300	2.21738600	4.69793400
O	8.52330200	3.03763600	4.62652900
O	7.78181400	0.95298800	5.09430600
C	9.14762700	0.55534000	5.42957100
H	9.49593100	1.18885100	6.24982700
H	9.77545300	0.75093400	4.55635500
C	9.12136200	-0.91324500	5.80119700
H	10.13729300	-1.24552900	6.03879900
H	8.49312700	-1.09119300	6.68005000
H	8.74691200	-1.52162000	4.97207800
O	4.18687300	4.78027500	4.47489300
N	3.41875700	3.65947400	6.35829400
H	2.70104900	4.33668400	6.57995500
O	4.01478500	-0.97077400	4.59443700
H	3.67763800	-1.54566400	5.30211200
C	4.57310900	10.21439400	4.16856500
S	4.52962000	8.58822700	5.10568300
O	3.32299700	7.84147900	4.52648100
O	4.55007000	8.84621200	6.52697100
O	5.69818700	7.78341100	4.50692300
F	4.46052600	9.94305500	2.86634000
F	3.55730100	10.95845300	4.57131100
F	5.72715700	10.81130300	4.41428600
S	4.86580500	6.04601200	0.79844800
C	5.55820500	7.55946600	-0.06912100
F	4.66806300	7.98518000	-0.95006900
F	5.78289000	8.49580900	0.85348900
F	6.68959600	7.21966200	-0.66407500
O	4.65289000	4.99236500	-0.17139200
O	3.63846800	6.56706000	1.55820000
Sc	4.49786600	6.38730100	3.49443600
O	5.85007800	5.77615800	1.93998400

A

C	3.37703100	-1.08796300	3.13616600
C	3.66783700	0.18427500	2.51743300
C	4.85303600	0.78148100	2.75770800
C	4.95639400	2.66508200	4.97934100
C	2.11204200	-1.67820800	2.99921600
C	2.63714000	0.81814500	1.67844700
C	1.36853600	0.17756000	1.55671300
C	1.14725700	-1.05275600	2.23295400
C	0.35106100	0.76937900	0.76800200

H	-0.61010700	0.26944800	0.68597300
C	0.58317900	1.96382000	0.11347100
C	1.83844300	2.58921800	0.23248200
C	2.85076100	2.02657700	1.00170600
H	1.90058500	-2.62699400	3.48477100
H	0.17375100	-1.52663600	2.13196200
H	-0.19509100	2.41752700	-0.49159000
H	2.03192200	3.52572000	-0.28122500
H	3.81064200	2.52684400	1.06684600
C	4.21019200	3.80669300	5.21305200
C	4.51224800	1.68870500	5.94672800
C	3.47063500	2.29569200	6.70538900
C	2.80215700	1.62846100	7.73197000
C	3.19591700	0.32295900	8.01557400
C	4.23570300	-0.29276700	7.29366300
C	4.89891900	0.37438000	6.26743500
H	2.01143600	2.11230000	8.29848800
H	2.70283600	-0.21983600	8.81653600
H	4.54077500	-1.30125300	7.56124700
H	5.71761600	-0.09884100	5.73698600
C	5.95873100	1.44722400	2.92341300
C	7.10864800	1.17907600	2.00666000
C	7.85458200	2.24418900	1.47552300
C	7.44083300	-0.14112900	1.66190500
C	8.91688400	1.98296700	0.61060700
H	7.60926900	3.27164300	1.72581400
C	8.50240600	-0.39229800	0.79462800
H	6.88292100	-0.96395500	2.09914700
C	9.24173700	0.66847900	0.26660600
H	9.49164600	2.81052200	0.20547100
H	8.75801300	-1.41643600	0.53898800
H	10.07197700	0.47198200	-0.40526700
C	6.05340400	2.59121300	3.95706600
H	6.01258400	3.50870200	3.36044800
C	7.42094100	2.65459300	4.65556600
O	7.99894200	3.70556500	4.83515600
O	7.84084900	1.45921400	5.07945600
C	9.09469400	1.44557100	5.82391800
H	8.98195100	2.10081300	6.69206100
H	9.87511200	1.86339400	5.18168600
C	9.37657600	0.00922100	6.21580000
H	10.31885100	-0.03998900	6.77146200
H	8.58122000	-0.38636300	6.85548800
H	9.46666600	-0.62886100	5.33083400
O	4.27037200	4.99233600	4.61723200
N	3.30676700	3.58686600	6.22826300

H	2.68914100	4.29408400	6.59903700
O	4.36007700	-1.65904000	3.82300900
H	4.05188600	-2.46721500	4.27049800
C	5.73067800	10.26957000	4.33916400
S	5.46962800	8.70036600	5.32897800
O	4.10338500	8.19056300	4.86085700
O	5.64568600	8.98598700	6.73423800
O	6.42080800	7.68842100	4.67386300
F	5.54182900	9.97941500	3.04715800
F	4.84921600	11.17389100	4.73451900
F	6.96734700	10.69946000	4.53185300
S	4.79463800	6.12879300	1.03070400
C	5.53509400	7.48544500	-0.02862700
F	4.58029300	8.00039400	-0.78786700
F	6.03792600	8.41824300	0.77889000
F	6.49587000	6.95892400	-0.77398000
O	4.29090800	5.08255900	0.15879700
O	3.79009200	6.84111500	1.93227500
Sc	4.89218400	6.53990900	3.75621300
O	5.90953200	5.75141900	2.00451000

TS-A/B

C	3.27797200	-0.63746000	3.44821400
C	3.59856900	0.63730600	2.89324500
C	4.85118600	1.16885200	3.10236900
C	5.22456300	2.49380800	4.92864300
C	1.98070600	-1.17290500	3.32462700
C	2.56519900	1.36708700	2.16260300
C	1.25966600	0.80073600	2.05795700
C	1.00606800	-0.46469500	2.65714300
C	0.24456800	1.49695400	1.35495500
H	-0.74425900	1.05202200	1.28380100
C	0.51095000	2.71537400	0.76384100
C	1.80531700	3.26696100	0.85654100
C	2.81229300	2.60773500	1.54407400
H	1.75771900	-2.14636900	3.75412300
H	0.00809700	-0.88747400	2.57336500
H	-0.26701600	3.24357300	0.22177400
H	2.02447100	4.21686400	0.37738000
H	3.80599900	3.03931300	1.59264600
C	4.32106600	3.57488000	4.90071600
C	4.82354800	1.67897300	6.06809200
C	3.65073600	2.26372300	6.60762800
C	2.97153300	1.73269100	7.70115300
C	3.50020300	0.58023900	8.28072300
C	4.66431300	-0.01799000	7.76800200

C	5.32772100	0.51368500	6.66451800
H	2.07544600	2.20280600	8.09559300
H	3.00701100	0.14436100	9.14416100
H	5.05705800	-0.91045000	8.24659500
H	6.21629500	0.03561300	6.26819900
C	6.14261900	1.44282600	3.00826800
C	7.05128600	0.93980400	1.95794500
C	8.17751300	1.69485800	1.58990400
C	6.80400300	-0.28230200	1.31011600
C	9.02970600	1.24061200	0.58459600
H	8.38752500	2.64226500	2.07821700
C	7.65865700	-0.73209200	0.30746500
H	5.95594900	-0.88905100	1.61326600
C	8.77214600	0.02894900	-0.05976100
H	9.89490600	1.83452100	0.30531200
H	7.46210300	-1.68124000	-0.18255500
H	9.43925500	-0.32451700	-0.84046600
C	6.49401600	2.45036600	4.08176100
H	6.63260800	3.43634600	3.62291100
C	7.76313900	2.24175500	4.91545800
O	8.31412200	3.16220800	5.47683900
O	8.16200500	0.96421200	4.95588900
C	9.37232300	0.69805400	5.72552300
H	9.18094500	0.97279900	6.76692300
H	10.16567700	1.34770900	5.34610700
C	9.70349400	-0.77178300	5.56274000
H	10.61770700	-1.00351900	6.11917400
H	8.89904500	-1.40584200	5.94971100
H	9.86798700	-1.02224800	4.51025000
O	4.32458600	4.63210200	4.12028800
N	3.36835100	3.40964300	5.85886700
H	2.60620900	4.05500100	6.01630400
O	4.26252900	-1.30753900	4.06099700
H	3.92704900	-2.14047700	4.43413300
C	3.53286800	10.02334500	3.63889300
S	3.43533300	8.38509800	4.54794900
O	2.79713900	7.42475100	3.53674100
O	2.76405500	8.57494200	5.81386700
O	4.88688400	7.88217400	4.57437500
F	4.12580100	9.80742300	2.46219200
F	2.30388700	10.47662900	3.45464100
F	4.24696400	10.86761200	4.36351000
S	5.85906400	5.92035100	0.82895100
C	6.21859700	7.50302800	-0.11095600
F	5.58238800	7.45961900	-1.27056800
F	5.77580300	8.52631100	0.62130700

F	7.52526600	7.59842300	-0.29086100
O	6.35284700	4.78810600	0.07542600
O	4.35301300	5.97933600	1.11536900
Sc	4.57272000	6.28316200	3.22405500
O	6.45304000	6.16184600	2.22041600

B

C	2.62368400	0.49250700	3.64485100
C	3.45922100	1.36019800	2.94688800
C	4.81863200	1.64910700	3.44140300
C	5.24721000	2.49485700	4.66991000
C	1.29833800	0.23570600	3.21582600
C	2.96049000	1.98842400	1.74980500
C	1.61548300	1.72680800	1.32371800
C	0.80850500	0.84363700	2.08749200
C	1.11653700	2.34536800	0.14613900
H	0.09379400	2.13459700	-0.15626300
C	1.90789600	3.18490700	-0.60363200
C	3.23973200	3.43523300	-0.19718200
C	3.75011900	2.86070400	0.94903100
H	0.67740200	-0.45222400	3.78616300
H	-0.20897100	0.64491700	1.76168700
H	1.52106600	3.64705900	-1.50664100
H	3.86979100	4.08079900	-0.80156200
H	4.77932100	3.05043400	1.23222500
C	4.75246400	3.92178000	4.71006600
C	4.97306400	2.04528200	6.08874600
C	4.38166300	3.09840200	6.79332300
C	4.00649100	3.02370300	8.12546200
C	4.25373100	1.80880100	8.77417200
C	4.84301500	0.73732400	8.09395400
C	5.20309700	0.84208400	6.74459800
H	3.55103700	3.86111700	8.64489800
H	3.98323900	1.70079900	9.81977200
H	5.02087500	-0.19466300	8.62174100
H	5.64193100	0.00300400	6.21734500
C	6.08805000	1.46626900	2.99664200
C	6.71303800	0.78475900	1.87111200
C	8.08178800	0.97713800	1.60751000
C	5.97424800	-0.07034500	1.03015200
C	8.69314900	0.34317700	0.52800900
H	8.67125000	1.62678300	2.24869400
C	6.59021400	-0.70724900	-0.04285900
H	4.92058500	-0.23831200	1.22690200
C	7.94938700	-0.50124500	-0.29920600
H	9.74959300	0.50494100	0.33447800

H	6.01022700	-1.36680900	-0.68183600
H	8.42638000	-0.99912800	-1.13848000
C	6.71568900	2.35573300	4.05515500
H	7.06857100	3.31806100	3.66652100
C	7.77390200	1.88746800	5.04391000
O	8.32890900	2.65746400	5.79821600
O	7.99640300	0.56955000	4.98102500
C	9.01653400	0.04657600	5.88187200
H	8.69128400	0.23263600	6.90987800
H	9.93922600	0.60946000	5.71537500
C	9.17722300	-1.42988500	5.57970000
H	9.94465100	-1.85582600	6.23447800
H	8.24216600	-1.97371600	5.74838000
H	9.48465900	-1.58582600	4.54117300
O	4.79887400	4.75956200	3.73586200
N	4.25907900	4.20696900	5.90659400
H	3.87334200	5.11633600	6.14937600
O	3.12386700	-0.12461000	4.75374600
H	2.44019500	-0.69227500	5.14361700
C	4.13259600	9.87009100	5.25411000
S	4.84033900	8.13683400	5.44215200
O	3.69183800	7.19721400	5.04298000
O	5.40248400	7.96960600	6.76253600
O	5.78415700	7.97806100	4.23467400
F	3.55120400	9.94441000	4.05772900
F	3.24411700	10.05723600	6.21347600
F	5.12485000	10.73650700	5.34304500
S	4.06627200	7.39538900	0.60892300
C	4.37744100	9.23618500	0.38206900
F	3.22802400	9.82333200	0.09914200
F	4.87192500	9.71139300	1.52778500
F	5.24966600	9.39415700	-0.59631400
O	3.59765200	6.82928900	-0.63245200
O	3.13728300	7.32073300	1.83946900
Sc	4.60306100	6.63036400	3.16252500
O	5.37603200	6.85891800	1.20892200

TS-B/C

C	3.06488600	2.17606100	1.86166200
C	4.09428400	1.39062600	2.35786700
C	4.93841500	1.90105100	3.45443200
C	4.38238900	2.29996900	4.73619100
C	2.23850500	1.76915500	0.79530900
C	4.30946500	0.09785300	1.76195900
C	3.46983700	-0.32607500	0.67910700
C	2.44213900	0.53735600	0.21941600

C	3.67723500	-1.60265100	0.09255000
H	3.03543100	-1.90982900	-0.72876800
C	4.66891200	-2.43661300	0.55636200
C	5.48737200	-2.02590500	1.63429900
C	5.31371500	-0.79249700	2.22689100
H	1.45678800	2.42973700	0.42709200
H	1.80972800	0.21572800	-0.60308400
H	4.82191200	-3.41068700	0.10198200
H	6.26273500	-2.69219000	2.00123500
H	5.94192500	-0.50094400	3.06127900
C	4.44668100	3.68554400	5.19572900
C	3.60861800	1.59743200	5.72852300
C	3.38419500	2.49923800	6.79930700
C	2.75550400	2.11637200	7.97546100
C	2.32557800	0.78860300	8.05988000
C	2.53800000	-0.12595700	7.01290300
C	3.19525800	0.26145700	5.84879100
H	2.60056200	2.81078500	8.79488100
H	1.81863800	0.45672800	8.96072700
H	2.18689200	-1.14736300	7.11923900
H	3.37319600	-0.44445300	5.04373600
C	6.28677600	2.20135400	3.47944200
C	7.27093400	2.30868100	2.39679000
C	8.63537100	2.13379200	2.70286400
C	6.90632000	2.58859800	1.06498300
C	9.60807400	2.25005400	1.71292900
H	8.92906300	1.87857700	3.71770000
C	7.88059800	2.69740200	0.07783600
H	5.86499000	2.74311100	0.80850700
C	9.23202200	2.53199700	0.39811600
H	10.65510300	2.11088800	1.96454400
H	7.58792700	2.92041100	-0.94391400
H	9.98816400	2.61946200	-0.37657000
C	6.64667400	2.52820200	4.85146400
H	7.24361400	3.42180900	5.03818900
C	6.69094200	1.59057300	6.00678200
O	6.78879500	1.98691200	7.15242900
O	6.64794500	0.29596700	5.64215200
C	6.74831900	-0.66813800	6.73131400
H	5.87755900	-0.54357500	7.38108900
H	7.64178600	-0.43099700	7.31530400
C	6.81444100	-2.05034000	6.11316600
H	6.88441600	-2.80247500	6.90587300
H	5.91904600	-2.26147300	5.51909300
H	7.69325000	-2.15154000	5.46850100
O	4.71664400	4.73147900	4.48914100

N	3.90101900	3.75347400	6.43095500
H	3.78118700	4.62073700	6.93962500
O	2.83200700	3.46242500	2.40252400
H	1.97712200	3.79237900	2.05929300
C	4.70472600	7.68447400	-0.13738800
S	5.52995600	6.68409200	1.21962200
O	4.89966300	7.20677900	2.51923800
O	6.96344200	6.78959700	1.07363100
O	4.88984700	5.29624400	1.11809600
F	5.02525000	8.95825400	0.02367700
F	5.13358000	7.23348100	-1.30686000
F	3.38418200	7.52475100	-0.04052900
S	1.17661600	6.49691400	3.34540400
C	1.00133300	8.31571200	2.91502100
F	0.58227500	8.95707000	3.99394700
F	2.18900600	8.77935100	2.53222900
F	0.12480300	8.42647400	1.92854900
O	-0.10004600	5.99276300	3.80492700
O	2.36109500	6.41924400	4.30405100
Sc	3.75236900	5.48970500	2.92991000
O	1.76459500	5.85243800	2.08039600

C

C	2.65682200	2.31411100	3.80786100
C	3.98996800	2.80100500	3.87934500
C	4.80893600	2.40669700	5.06905600
C	4.45382900	2.69716900	6.37142100
C	1.94554400	2.27911000	2.58163300
C	4.62750900	3.22392800	2.63051400
C	3.90008000	3.12885300	1.39723200
C	2.56081300	2.64974500	1.41526300
C	4.50897600	3.52873500	0.18379700
H	3.93463200	3.45297200	-0.73522900
C	5.80097700	4.01197300	0.16758100
C	6.51574400	4.12486000	1.37706700
C	5.94445200	3.74946900	2.58041300
H	0.92465200	1.91423900	2.60052500
H	2.01237100	2.59590800	0.47941600
H	6.26283000	4.31352200	-0.76727300
H	7.52922100	4.51508100	1.37083000
H	6.51390900	3.86904300	3.49227300
C	3.52362300	3.79483400	6.73585400
C	4.86027500	2.10445800	7.66821000
C	4.18129300	2.81486100	8.67962600
C	4.26897200	2.51070600	10.02819200
C	5.07668000	1.42483200	10.38175800

C	5.74790700	0.68532300	9.40228000
C	5.64943100	1.01216200	8.04663000
H	3.73156800	3.08328900	10.77769200
H	5.17723000	1.15436000	11.42800600
H	6.36522100	-0.15697500	9.69789800
H	6.19638600	0.43067100	7.31466100
C	5.99566500	1.53631800	4.80489200
C	5.81504900	0.36156600	3.90917000
C	6.72043500	0.10169500	2.86632700
C	4.72878200	-0.51009400	4.09623000
C	6.55030800	-1.01118900	2.04433600
H	7.54639700	0.78375800	2.68786600
C	4.56313400	-1.62504700	3.27581800
H	4.02007000	-0.33076900	4.90107300
C	5.47432600	-1.87845300	2.24802600
H	7.25528200	-1.19688200	1.23919200
H	3.72579300	-2.29655800	3.44150100
H	5.34387200	-2.74505600	1.60657700
C	7.17750700	1.91529000	5.33790300
H	7.24613200	2.84929600	5.89101000
C	8.49172600	1.22167500	5.16391400
O	9.46272000	1.78403700	4.70312400
O	8.46173900	-0.04045800	5.61129200
C	9.70028900	-0.79864100	5.47826500
H	10.49945800	-0.24127500	5.97491600
H	9.94436600	-0.86236100	4.41359000
C	9.46896000	-2.16188500	6.09816400
H	10.37947200	-2.76331000	6.00776400
H	9.22177600	-2.07463300	7.16098000
H	8.65545400	-2.69094700	5.59213500
O	2.94057400	4.63065000	5.97846000
N	3.40680600	3.82677800	8.06877100
H	2.85561400	4.52737000	8.55168500
O	1.97956800	1.80522100	4.85369500
H	2.55760000	1.73514100	5.63453800
C	5.41872100	8.54382400	3.53368000
S	4.88625000	7.40447400	4.92581700
O	3.35858900	7.40113300	4.86130600
O	5.51577200	7.82839000	6.15703500
O	5.21261300	5.99891300	4.40531200
F	4.84228200	8.12688200	2.40586800
F	5.02698100	9.77439200	3.82219800
F	6.73760400	8.48119500	3.42230600
S	1.05997400	5.90335600	2.42381800
C	0.54985800	7.70842900	2.30558800
F	-0.73471000	7.79189500	2.61488800

F	1.27740000	8.42926400	3.15189800
F	0.76179000	8.10956700	1.05991500
O	0.20693100	5.13823700	1.53925400
O	1.03736500	5.56023300	3.91448200
Sc	3.16637400	5.41422400	4.12922200
O	2.56810700	5.89028200	2.13525100

TS-C/D

C	2.35883300	2.09086800	3.29810800
C	3.73133500	2.50137800	2.95930600
C	4.56956500	2.91792200	4.09331900
C	3.98402400	3.65187500	5.10349500
C	1.74433000	1.05278600	2.50847000
C	4.29472300	2.05666000	1.68625500
C	3.55059700	1.16031900	0.85620600
C	2.30811800	0.62832300	1.34447200
C	4.03707900	0.82813300	-0.42129700
H	3.46567600	0.13620000	-1.03402300
C	5.21206000	1.38574500	-0.91099600
C	5.93404600	2.28345800	-0.11721600
C	5.49022100	2.61562700	1.16397800
H	0.77959600	0.68687700	2.84308000
H	1.78722900	-0.10122200	0.72990300
H	5.56478300	1.12853000	-1.90451600
H	6.85616600	2.72077700	-0.48831000
H	6.10772500	3.25973600	1.78131900
C	2.68182300	4.25745900	4.88504100
C	4.21578100	3.75636900	6.55248900
C	3.06725300	4.36348900	7.10501800
C	2.88564800	4.56545300	8.46333900
C	3.91802300	4.14485400	9.30838800
C	5.06763800	3.53613000	8.79115800
C	5.22939400	3.33204500	7.41829700
H	1.98631100	5.02827700	8.85772500
H	3.82104200	4.29297100	10.37924000
H	5.85343200	3.21820100	9.46902500
H	6.13156300	2.86549700	7.04041500
C	5.95378200	2.38430000	4.26258600
C	6.13840100	0.91097000	4.17163800
C	7.22154900	0.35230100	3.47160800
C	5.21817700	0.04947200	4.79414500
C	7.38736700	-1.03056900	3.41156900
H	7.92541300	1.00109800	2.95840900
C	5.38998300	-1.33288700	4.73771300
H	4.38020400	0.46342900	5.34954100
C	6.47467700	-1.87673900	4.04590700

H	8.22700500	-1.44742700	2.86278300
H	4.67923400	-1.98479700	5.23737600
H	6.60620800	-2.95381200	3.99863400
C	6.94438900	3.27851700	4.46977200
H	6.72753700	4.34226300	4.41270300
C	8.39311000	2.96725900	4.66969000
O	9.25795300	3.39946200	3.93587300
O	8.60634400	2.21108900	5.75581800
C	9.99285700	1.85725800	6.02987900
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H	10.37321200	1.28911100	5.17555000
C	10.01195000	1.04965900	7.31216800
H	11.04125500	0.75808900	7.54572900
H	9.62409100	1.63518200	8.15184300
H	9.41059900	0.14066500	7.21258800
O	2.36430400	4.91798700	3.71247900
N	2.18885700	4.70319300	6.04497800
H	1.34976500	5.26002400	6.14233400
O	1.70272400	2.61939000	4.25269800
H	1.42517400	4.76341000	3.47304200
C	0.98204600	5.87490600	-1.02095000
S	1.64026100	4.28403300	-0.26206900
O	3.16755800	4.38000900	-0.35000000
O	1.00213400	3.17049300	-0.92955600
O	1.41993700	4.42338900	1.24896600
F	1.56295400	6.91762400	-0.44215800
F	1.25909300	5.84959500	-2.31549500
F	-0.32742800	5.90478700	-0.81840600
S	4.84703900	6.97314700	2.14139300
C	5.73893000	7.55176400	0.59611700
F	7.02947500	7.66596000	0.86580300
F	5.54755300	6.63619500	-0.35870000
F	5.22842200	8.71397700	0.22226900
O	5.10142300	7.89978100	3.22174000
O	5.34284400	5.52632200	2.32048700
Sc	3.53630600	4.57036400	1.73088100
O	3.40978100	6.74409200	1.69912100

D

C	2.11615100	2.18636700	4.13538700
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C	3.71353800	2.80290900	6.32883200
C	1.29634600	1.70727700	3.09661300
C	3.86023200	2.84991100	2.54950100
C	2.99796200	2.39587300	1.48847600

C	1.74950500	1.78659100	1.80270900
C	3.38682300	2.59108400	0.14173200
H	2.72612500	2.24093900	-0.64598500
C	4.56811300	3.23445100	-0.16890200
C	5.40131200	3.70554100	0.86396400
C	5.06459000	3.51602500	2.19388400
H	0.31349800	1.32002200	3.34157400
H	1.12116400	1.43792000	0.98862500
H	4.85020100	3.38687300	-1.20586100
H	6.32373400	4.22369100	0.61985300
H	5.72990100	3.88207700	2.96492100
C	2.22397900	3.02980000	6.27937400
C	4.04580100	2.60950600	7.73337100
C	2.83171000	2.66292800	8.45834700
C	2.77680100	2.46120100	9.82882500
C	3.97994900	2.19213000	10.49039000
C	5.19518300	2.13821100	9.79507100
C	5.24182800	2.34767500	8.41753300
H	1.83739100	2.50983600	10.37077700
H	3.96755300	2.02785000	11.56359000
H	6.11346500	1.93233000	10.33542600
H	6.18625600	2.29900400	7.88809500
C	5.80154500	2.43874300	5.01077100
C	6.20809100	1.14694200	4.39396700
C	7.31806700	1.06537600	3.53441200
C	5.47532200	-0.02311100	4.66015400
C	7.69315200	-0.15475300	2.97462600
H	7.87830200	1.96260900	3.28873800
C	5.85519500	-1.24317000	4.10280100
H	4.62121100	0.01675500	5.33089700
C	6.96498000	-1.31265900	3.25793900
H	8.55050800	-0.19915300	2.30911500
H	5.28695400	-2.14021000	4.33158600
H	7.25834700	-2.26227800	2.82001700
C	6.65110100	3.37637300	5.47897500
H	6.26067100	4.33568400	5.80821400
C	8.14348600	3.29232200	5.50614900
O	8.85214200	4.08214300	4.91614400
O	8.58405900	2.29047300	6.28151500
C	10.02922400	2.13088200	6.36473600
H	10.46442600	3.08308800	6.68089800
H	10.40384400	1.90600700	5.36129600
C	10.30860300	1.00982200	7.34577700
H	11.38947300	0.85293200	7.42447400
H	9.92557000	1.25398100	8.34177700
H	9.84797200	0.07391700	7.01452100

O	1.95097700	4.40113600	5.69110400
N	1.74252400	2.96352700	7.59537900
H	0.83706200	2.53290100	7.74675800
O	1.58290900	2.15791700	5.39548700
H	1.66107900	4.99233100	6.41060500
C	4.59704200	8.58668800	3.90444400
S	4.12405000	7.15404100	5.02600600
O	2.61185600	6.98060300	4.85536900
O	4.62121200	7.41284200	6.35991300
O	4.65089000	5.90389000	4.30729500
F	3.99332100	9.67664000	4.35166800
F	5.91256300	8.72239700	3.94634200
F	4.19823600	8.30951200	2.66640800
S	1.06451200	5.67888400	1.70057100
C	0.30451100	7.39766100	1.73321100
F	-1.01106400	7.26783500	1.66346100
F	0.64965400	8.00365800	2.86584900
F	0.76903900	8.07049800	0.69109500
O	0.59371100	4.99138200	0.51741300
O	0.73228400	5.06091900	3.06324100
Sc	2.73764000	5.11037100	3.81145100
O	2.57406400	5.90389300	1.83998000

TS-D/3

C	2.09002500	2.35745800	4.05044400
C	3.44720000	2.72734900	3.88776100
C	4.31959400	2.66803600	5.08931000
C	3.69590800	2.70546700	6.30150200
C	1.23661300	2.01979800	2.98156700
C	3.91440300	2.90438700	2.51412900
C	3.04465700	2.53007700	1.42954800
C	1.72673800	2.07053000	1.69950400
C	3.48839800	2.66693800	0.09130900
H	2.81711000	2.37346900	-0.71069200
C	4.73503800	3.18293200	-0.18981500
C	5.57371600	3.59239600	0.86676800
C	5.17904800	3.45737900	2.18518800
H	0.21483500	1.72999200	3.20050900
H	1.08284900	1.80796800	0.86571500
H	5.06487100	3.28986900	-1.21845900
H	6.54543900	4.02434700	0.64684100
H	5.83964200	3.79822500	2.96920500
C	2.21716800	2.89910200	6.28440700
C	4.04731900	2.48817100	7.70239800
C	2.83704200	2.48942100	8.43666500
C	2.79023100	2.27657400	9.80498600

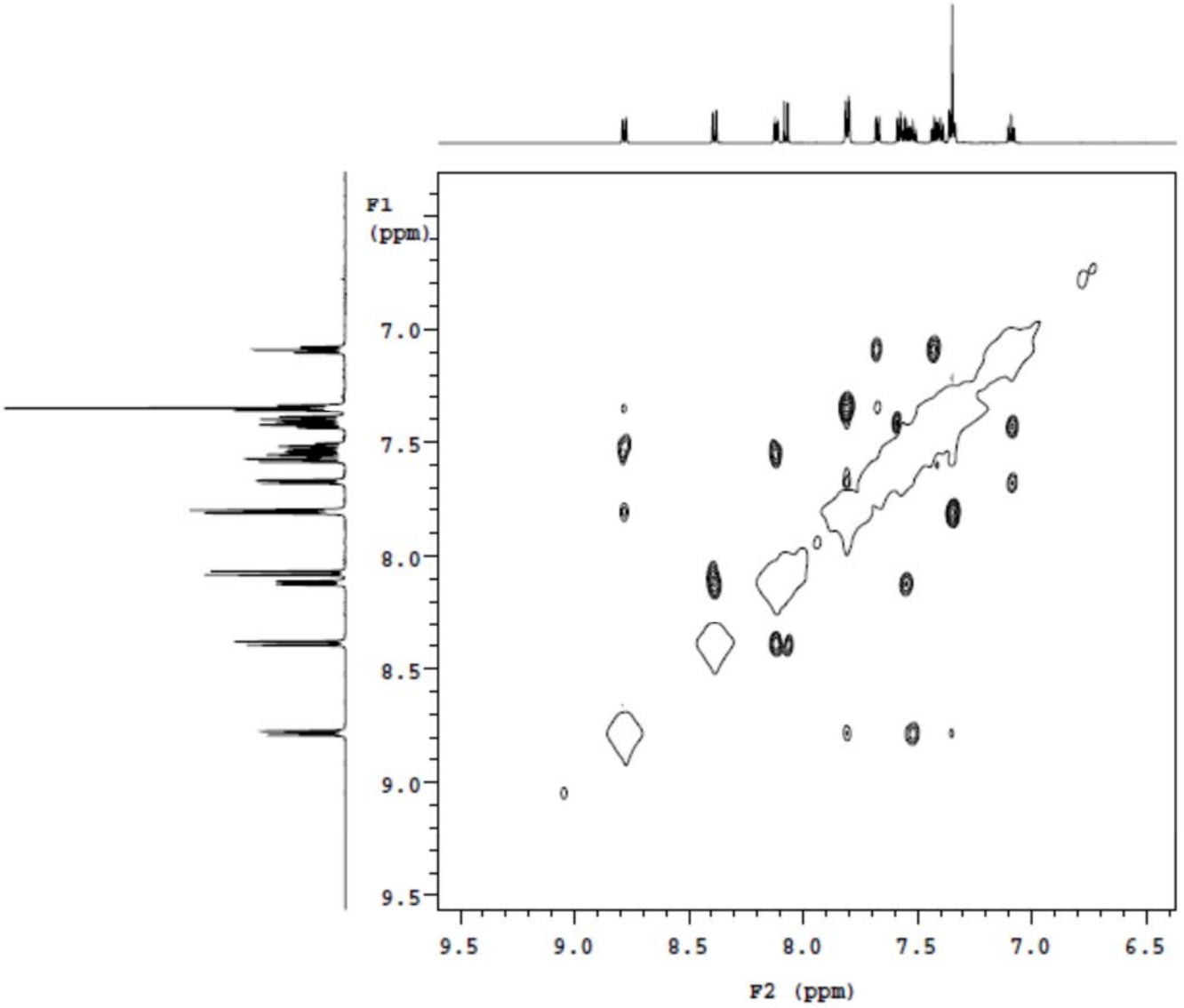
C	4.00486500	2.04220600	10.45943900
C	5.21655700	2.03452200	9.75739900
C	5.25243300	2.25955100	8.38090200
H	1.85112200	2.28554300	10.34958000
H	4.00273400	1.86682100	11.53086000
H	6.14362500	1.85221300	10.29121200
H	6.19724800	2.24737000	7.85061200
C	5.79359300	2.42433600	5.00417400
C	6.22777400	1.13283200	4.40681200
C	7.37007300	1.05290400	3.58991900
C	5.49061800	-0.03992300	4.64820200
C	7.77193000	-0.16733600	3.05009000
H	7.93394500	1.95139300	3.35856500
C	5.89674100	-1.26005300	4.10987100
H	4.61095200	-0.00292000	5.28481800
C	7.03879100	-1.32776600	3.30935300
H	8.65366200	-0.20967000	2.41710600
H	5.32301500	-2.15841400	4.31875100
H	7.35278800	-2.27741100	2.88607700
C	6.61682800	3.37971300	5.48139300
H	6.20254700	4.33299600	5.79986000
C	8.11048800	3.32647200	5.52933900
O	8.81229100	4.10993100	4.92329700
O	8.55871900	2.35883500	6.34312300
C	10.00547400	2.23045800	6.45315600
H	10.41739900	3.20134300	6.74240000
H	10.39934000	1.97843700	5.46368500
C	10.29110800	1.14964000	7.47661200
H	11.37344800	1.01715300	7.57686300
H	9.88814200	1.42053400	8.45776100
H	9.85411400	0.19375300	7.17140800
O	1.97961300	4.48422600	5.79988000
N	1.74543300	2.74145500	7.56578800
H	0.80132200	2.42272500	7.74240200
O	1.53541300	2.23638400	5.30426400
H	1.74398400	5.00368500	6.58863600
C	4.64105100	8.50732600	3.56051400
S	4.20204500	7.20992400	4.84631200
O	2.66781800	7.17272300	4.85955200
O	4.87752700	7.51531600	6.08798800
O	4.52447300	5.87222600	4.17074500
F	4.19264900	9.67909200	3.98075700
F	5.95654600	8.52428000	3.42099800
F	4.05802800	8.17231200	2.41065900
S	0.61918500	5.75584100	1.98952900
C	0.25019900	7.57709400	1.71466400

F	-1.04832000	7.76648700	1.88544100
F	0.94175700	8.29421600	2.59779100
F	0.61579900	7.89163000	0.48096300
O	-0.17110700	4.97891700	1.05891100
O	0.40332500	5.51983500	3.48506300
Sc	2.48627600	5.26516800	3.95467400
O	2.14706900	5.64282800	1.88770500

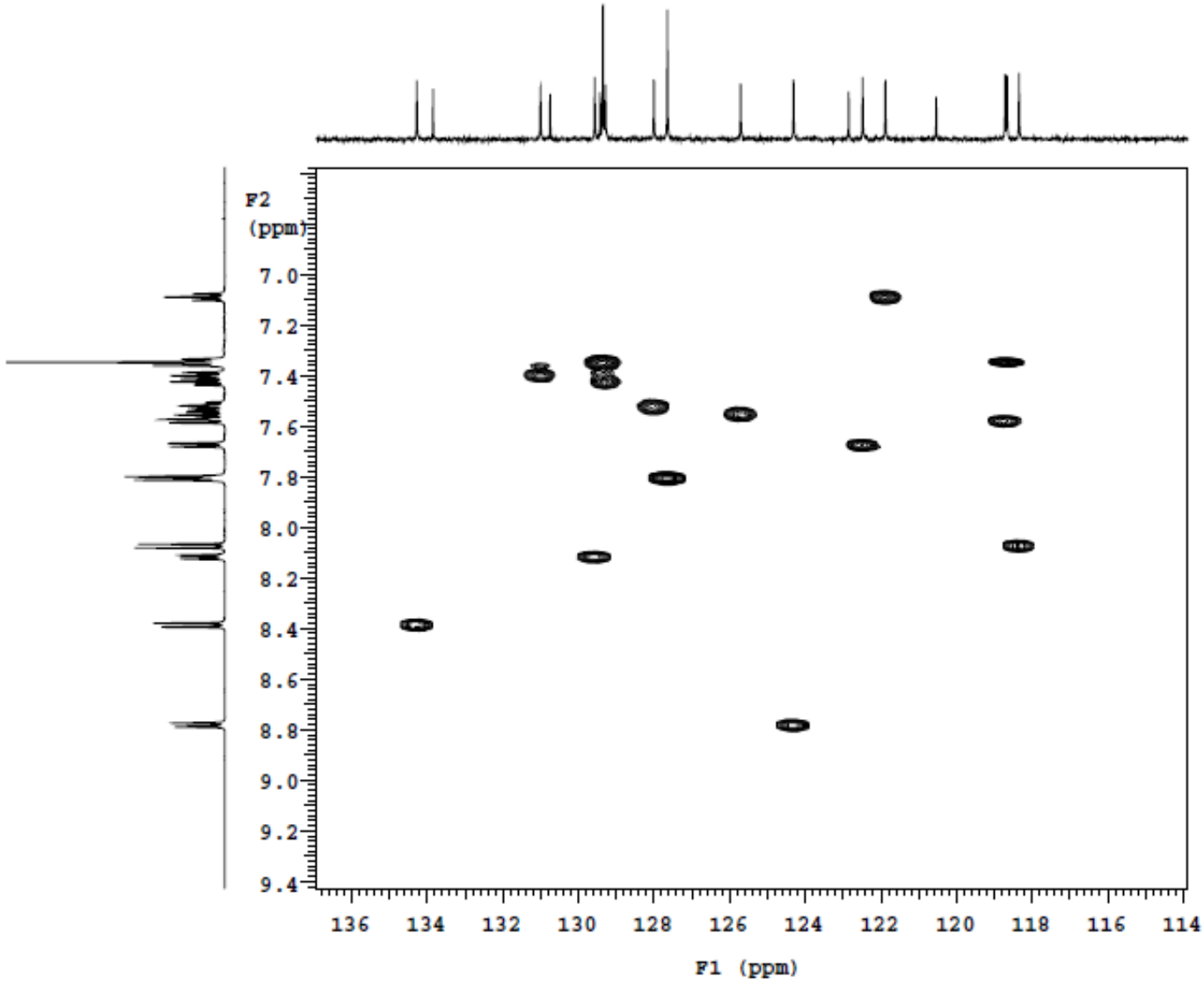
3

C	3.16431500	3.78993900	3.45000100
C	4.49332800	3.30480800	3.40221700
C	5.11630200	2.90981600	4.65025900
C	4.41446000	3.10923100	5.83586200
C	2.38476700	4.11427800	2.32851200
C	5.10112000	3.24622500	2.07181600
C	4.28814800	3.54373700	0.92432700
C	2.93895300	3.96324000	1.08578300
C	4.83433200	3.46146600	-0.38049100
H	4.18845500	3.68177900	-1.22594400
C	6.15706900	3.12968200	-0.57591700
C	6.97394000	2.89041000	0.54397200
C	6.46317800	2.94719300	1.82908400
H	1.36884900	4.46356500	2.47926900
H	2.35164800	4.18716300	0.19992300
H	6.57010000	3.07328000	-1.57814600
H	8.02732800	2.66606300	0.40543600
H	7.14187500	2.79315900	2.65107600
C	3.10595600	3.65593300	5.76182200
C	4.62917900	2.86947900	7.26452100
C	3.45300400	3.31273400	7.92243600
C	3.28654800	3.25512000	9.29970400
C	4.34049800	2.72202400	10.04394600
C	5.51011200	2.26562800	9.41868700
C	5.67088500	2.33422100	8.03518700
H	2.37763000	3.60712800	9.77746000
H	4.24925400	2.65979300	11.12386000
H	6.31010400	1.85145700	10.02414700
H	6.58533200	1.97852700	7.57618800
C	6.45369200	2.24083700	4.77264700
C	6.50992700	0.79468600	4.42402200
C	7.64982100	0.23855600	3.81403000
C	5.41364300	-0.04573000	4.68773500
C	7.69802600	-1.11824700	3.50294600
H	8.49423800	0.87208200	3.56042300
C	5.46620500	-1.40390900	4.37831200
H	4.52165800	0.35614900	5.15856500

C	6.60825300	-1.94521600	3.78598900
H	8.58444700	-1.52774400	3.02727200
H	4.61370100	-2.03895800	4.60092100
H	6.64679700	-3.00214400	3.53938100
C	7.48163500	2.98936400	5.21712600
H	7.34664000	4.05960200	5.35787300
C	8.88327700	2.52342800	5.45905900
O	9.83542200	2.96989200	4.85474600
O	8.94987900	1.60551400	6.43593400
C	10.27762700	1.08985100	6.74275400
H	10.94123400	1.93757100	6.93382000
H	10.64854900	0.56384100	5.85755400
C	10.14615600	0.17236600	7.94177500
H	11.12702400	-0.24506500	8.19211600
H	9.77494500	0.71789900	8.81533600
H	9.46347400	-0.65668600	7.73059500
O	-0.00551100	5.02436500	6.93804100
N	2.53656100	3.78390300	6.95712200
H	1.59584200	4.18185700	7.11000200
O	2.49133700	3.96232000	4.64014600
H	-0.73004400	4.51043500	7.32731600
C	2.19000400	9.60066900	5.02682800
S	1.98987500	8.26585000	6.32674700
O	0.51719600	8.36414500	6.74152600
O	2.99790100	8.43883000	7.34833800
O	2.00558000	6.96100400	5.52266500
F	1.99818100	10.78141100	5.59004300
F	3.40939000	9.51268300	4.51630000
F	1.27889800	9.38987900	4.07267200
S	-2.03769600	6.41128000	3.88712800
C	-2.25346300	8.02060100	2.94950600
F	-3.49922800	8.43569200	3.09844600
F	-1.40334000	8.91355100	3.46334700
F	-1.97410100	7.80857800	1.67205200
O	-2.97004800	5.42937600	3.38227500
O	-2.14973300	6.82580500	5.35834600
Sc	-0.08767800	6.55041300	5.80915200
O	-0.53845300	6.10284300	3.76312900

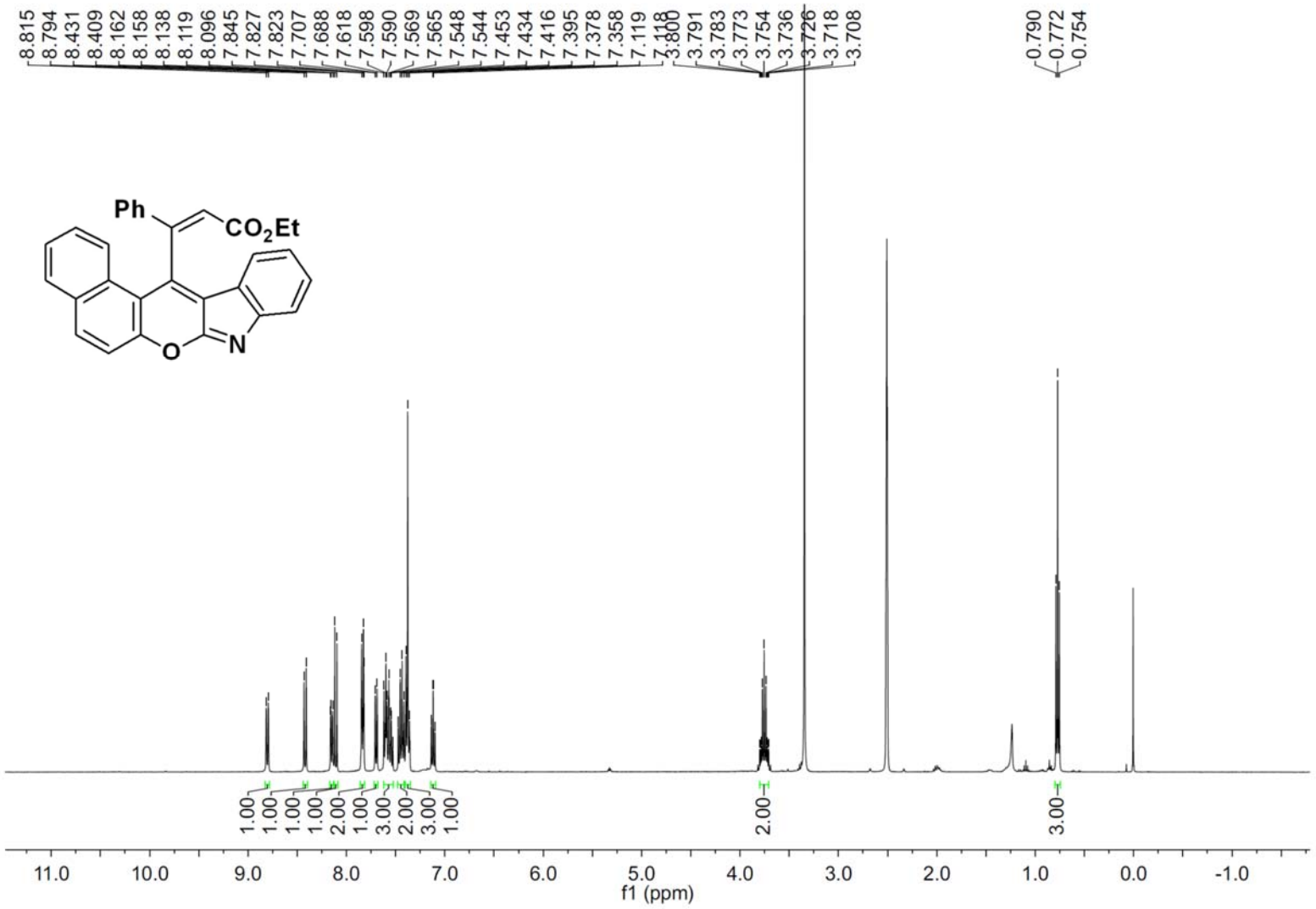


^{1}H-^{1}H NOESY Spectrum of Compound 3a

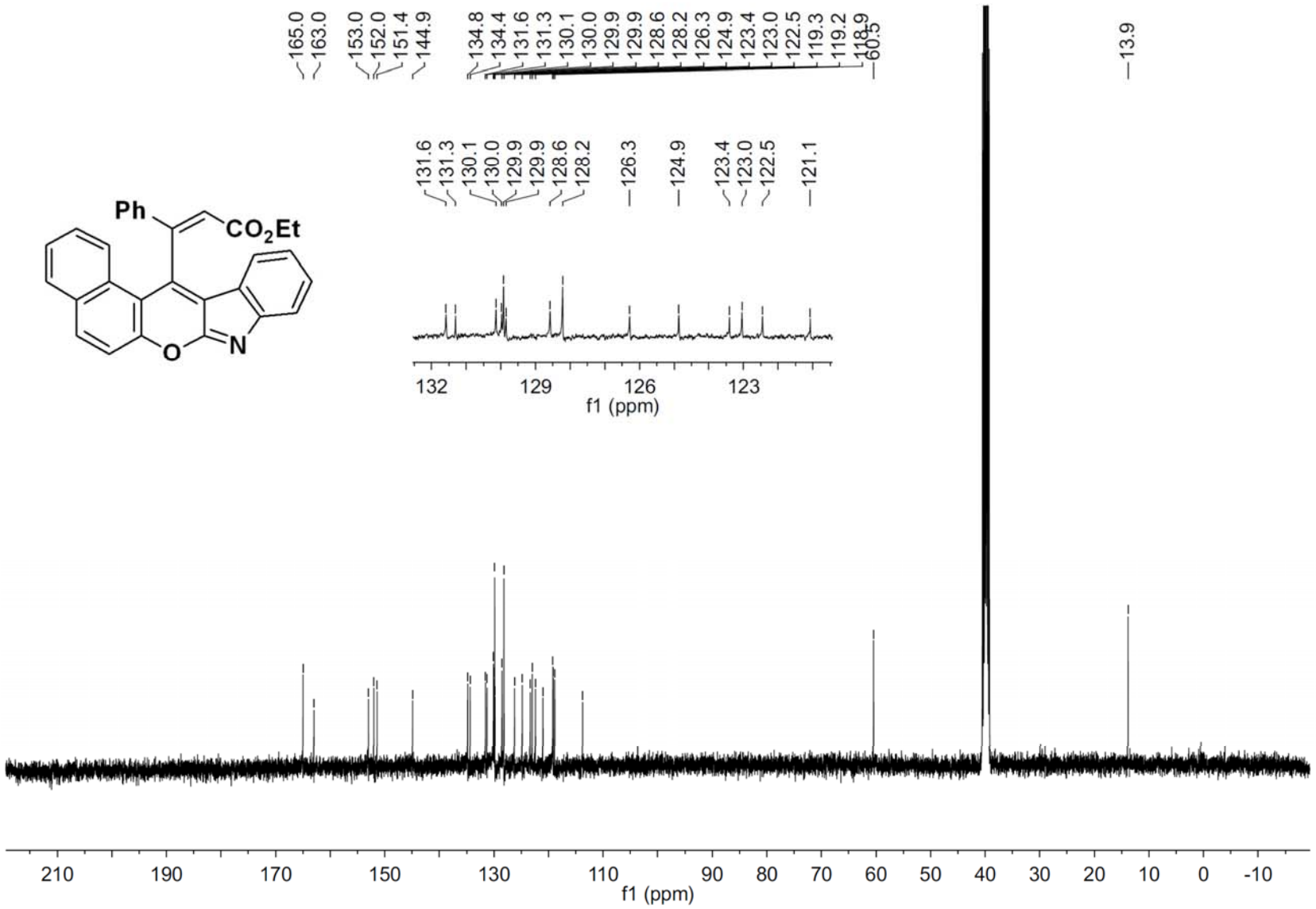


HSQC Spectrum of Compound 3a

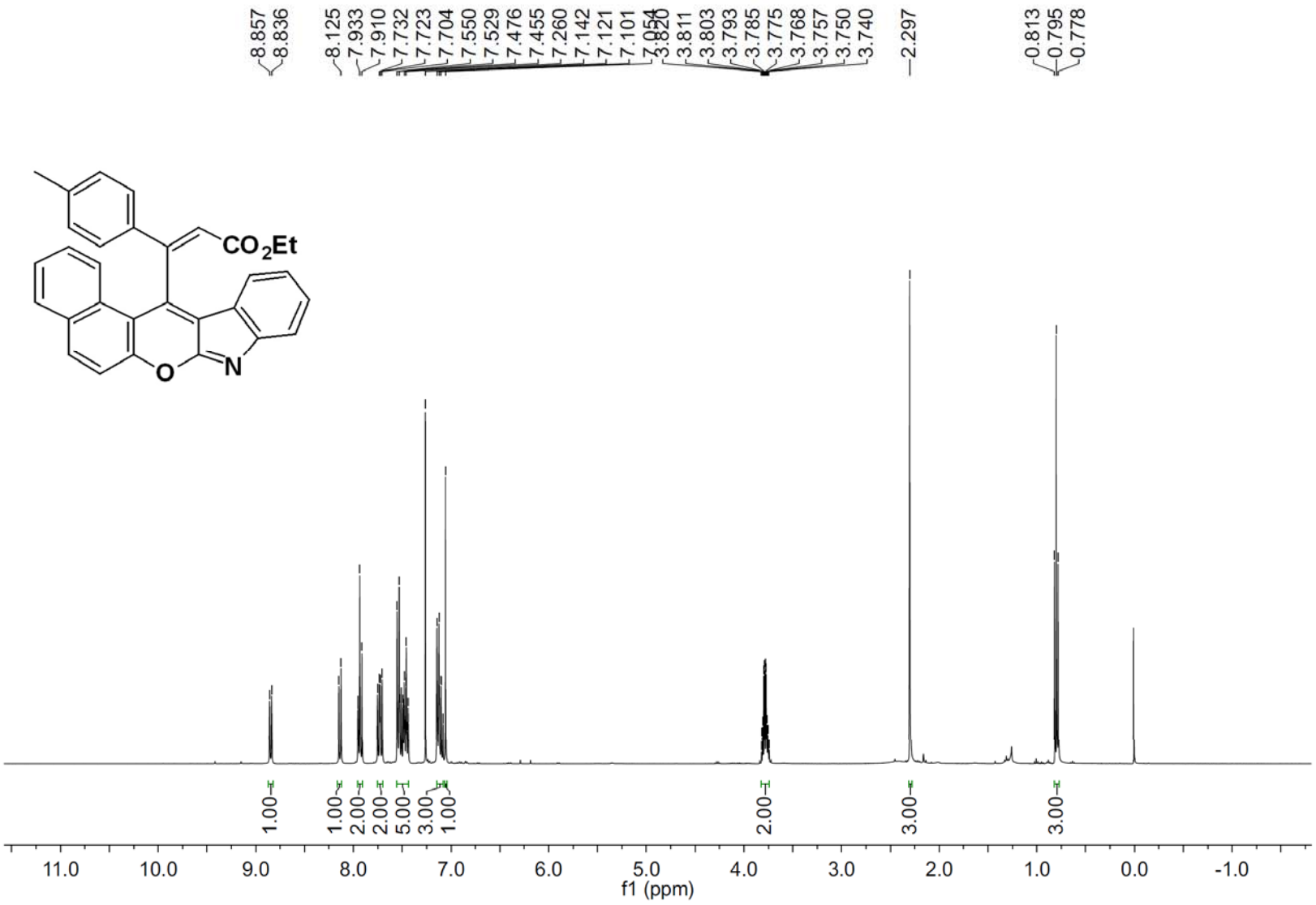
Copies of ^{1}H NMR and ^{13}C NMR Spectrum of Compound 3



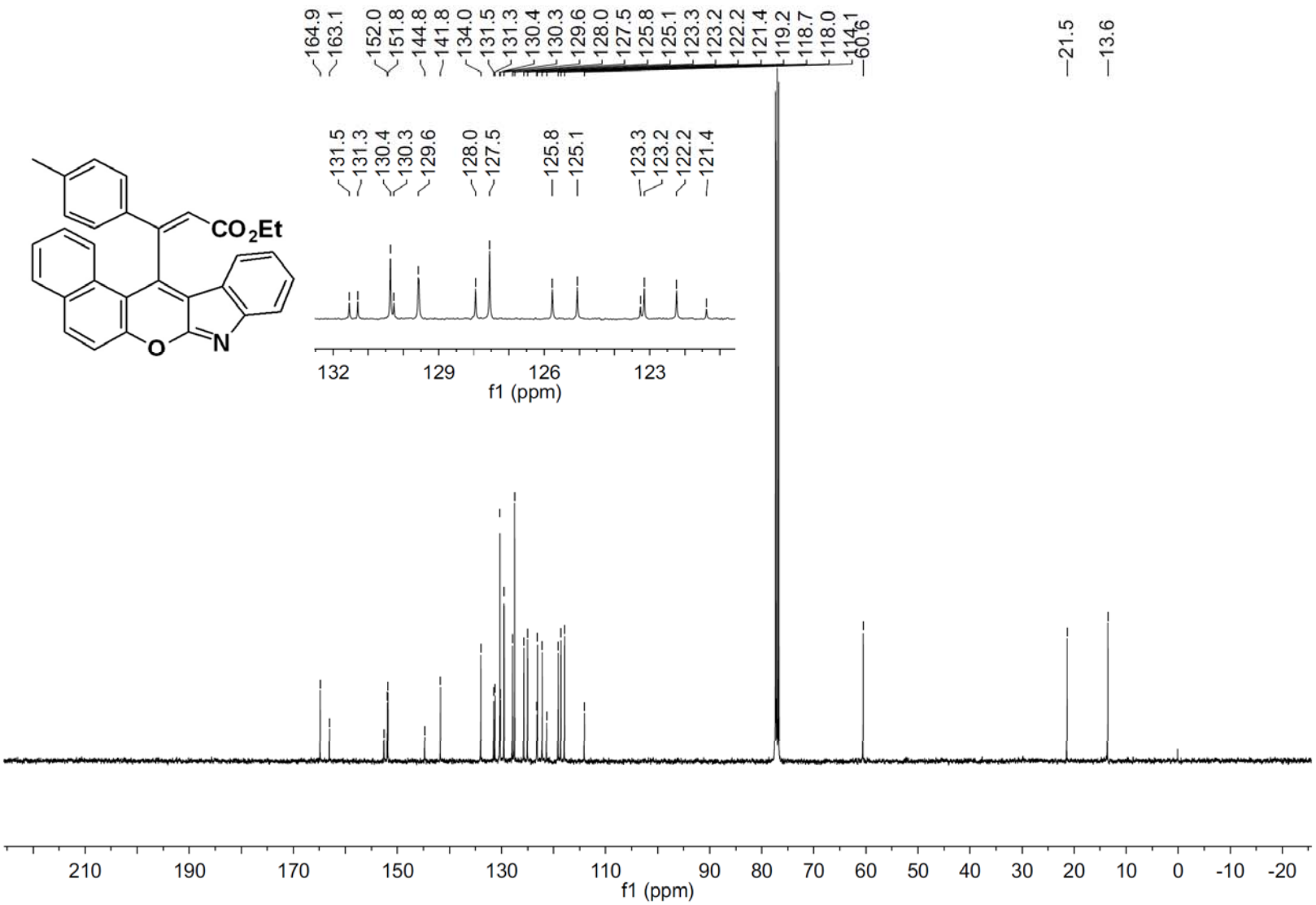
^{1}H NMR Spectrum of Compound 3a



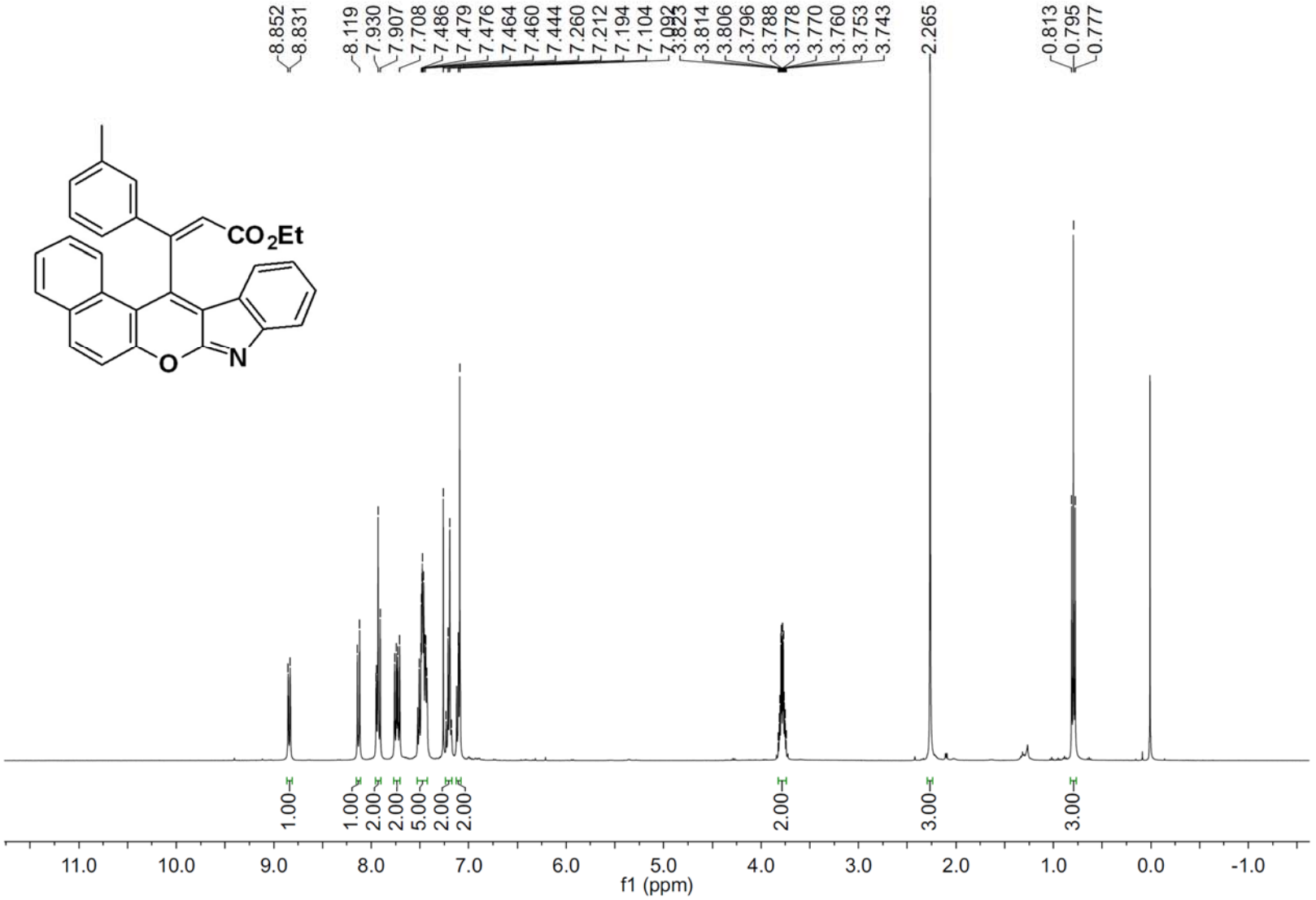
^{13}C NMR Spectrum of Compound 3a



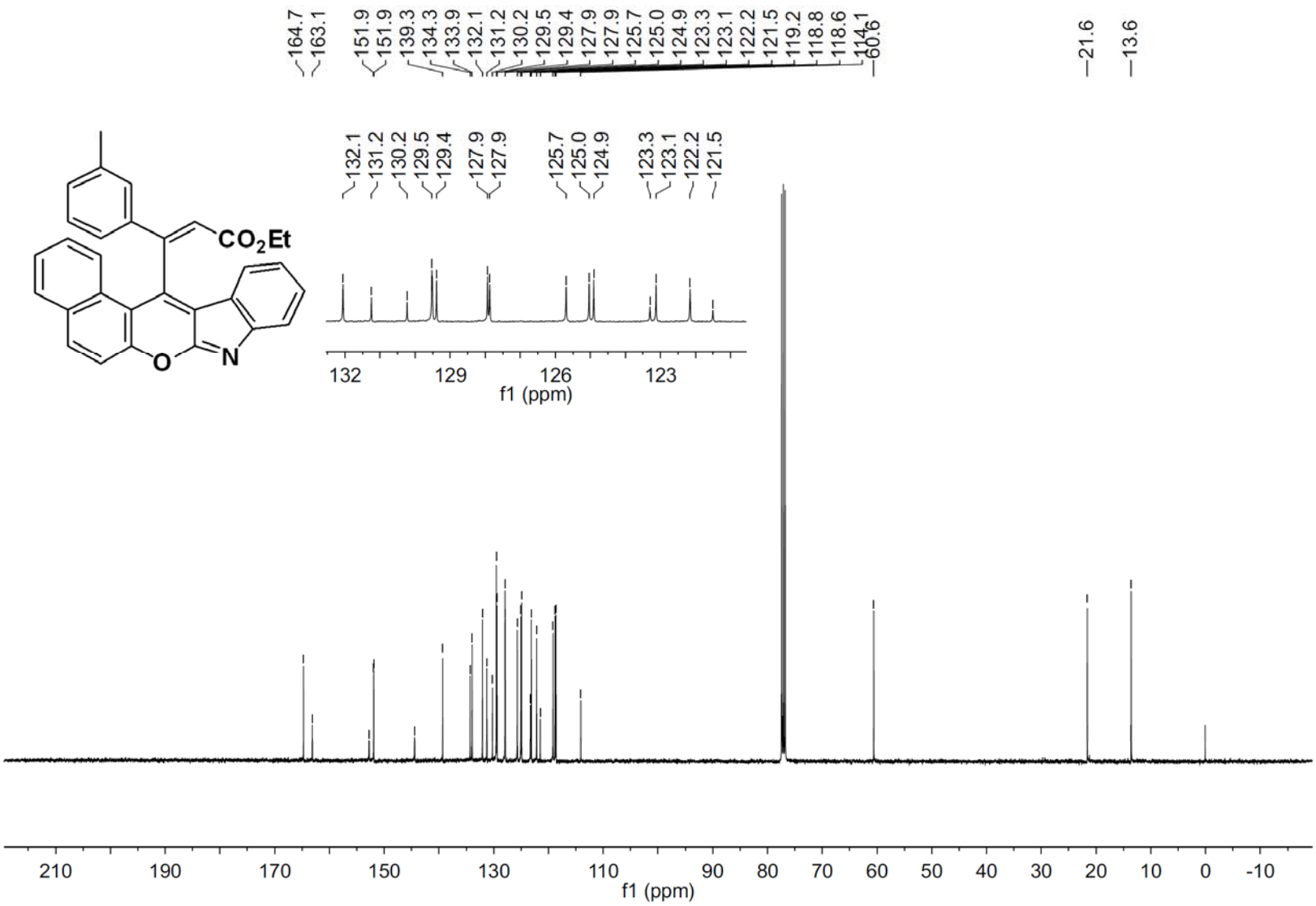
^{1}H NMR Spectrum of Compound 3b



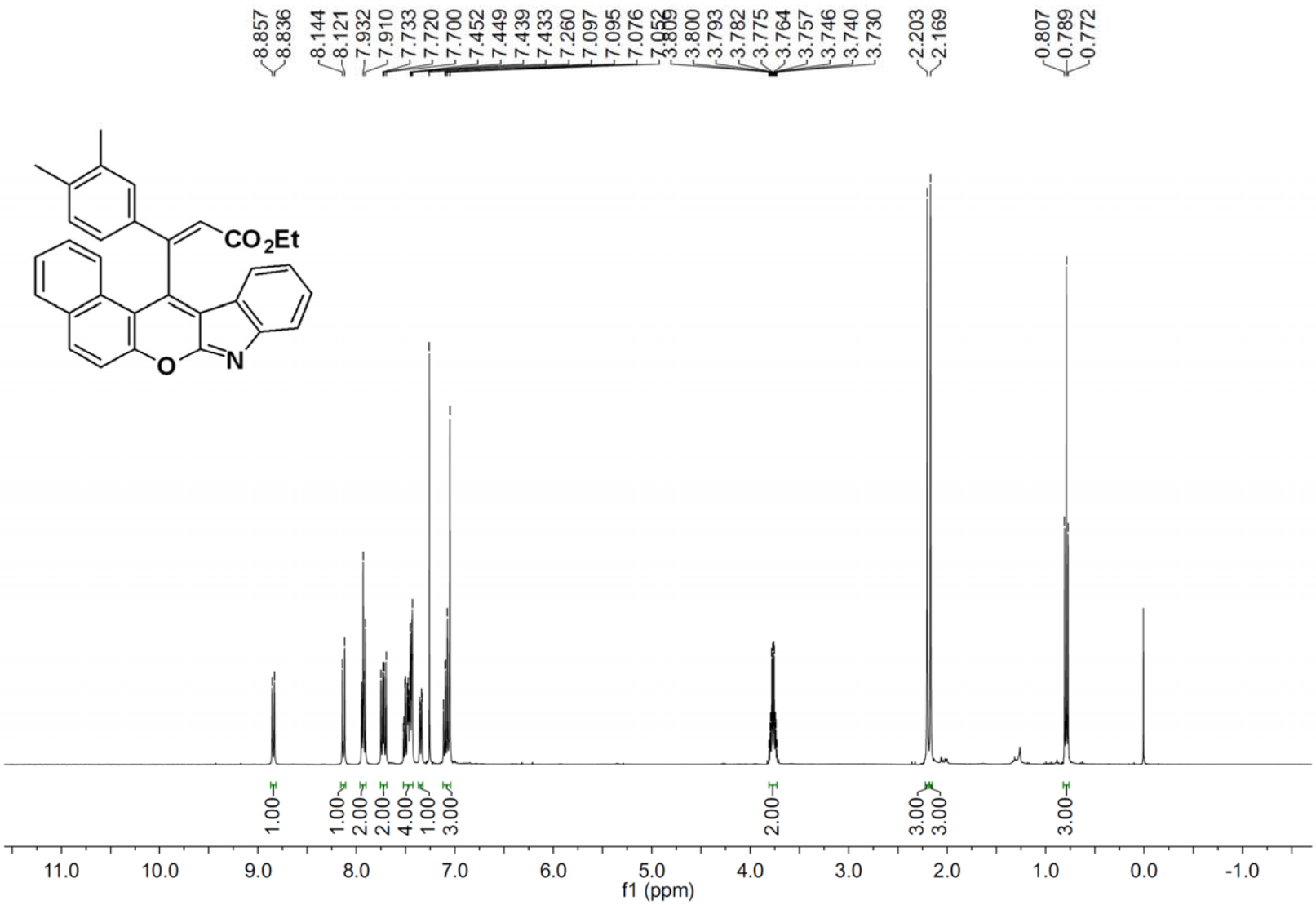
^{13}C NMR Spectrum of Compound 3b



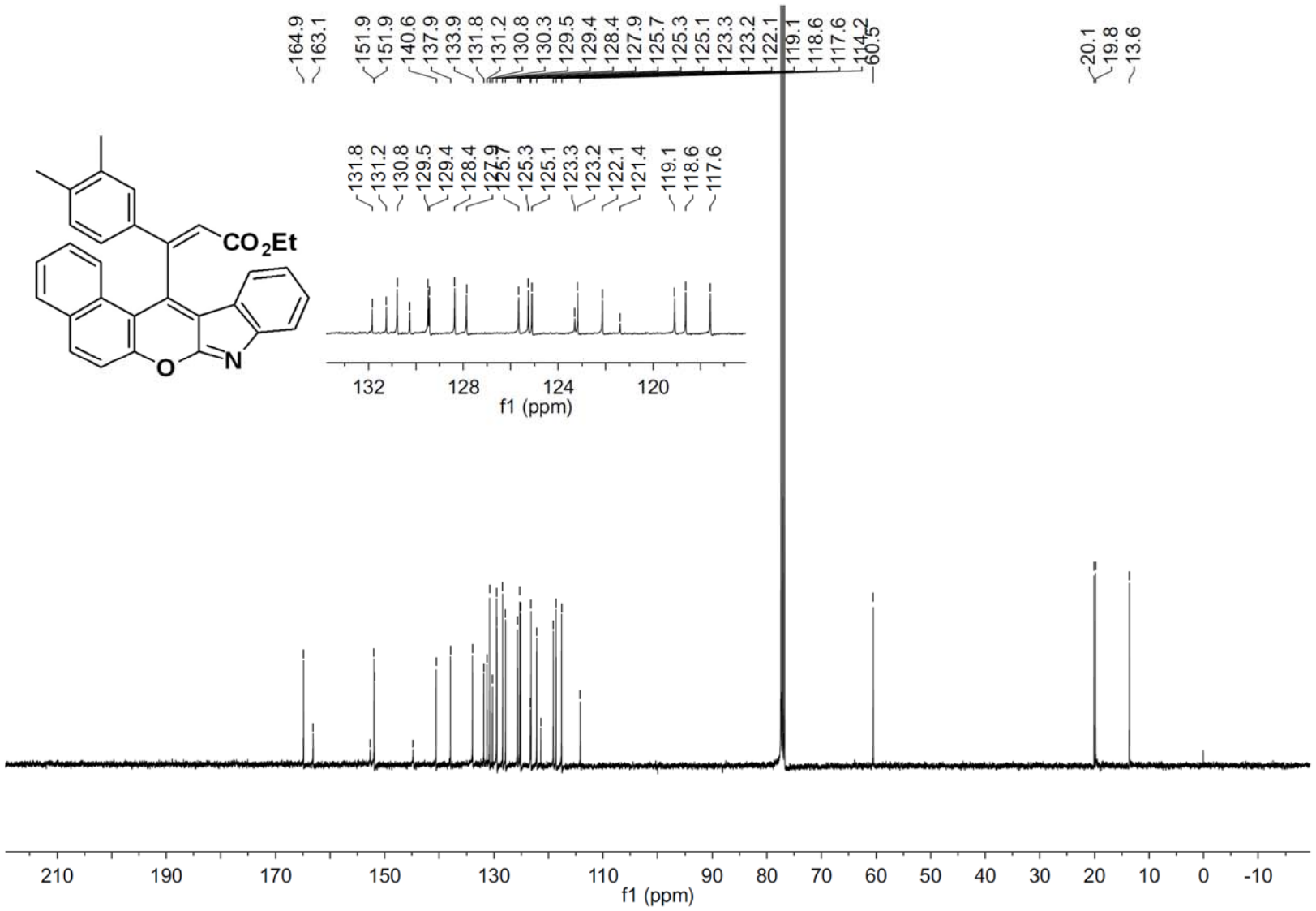
^{1}H NMR Spectrum of Compound 3c



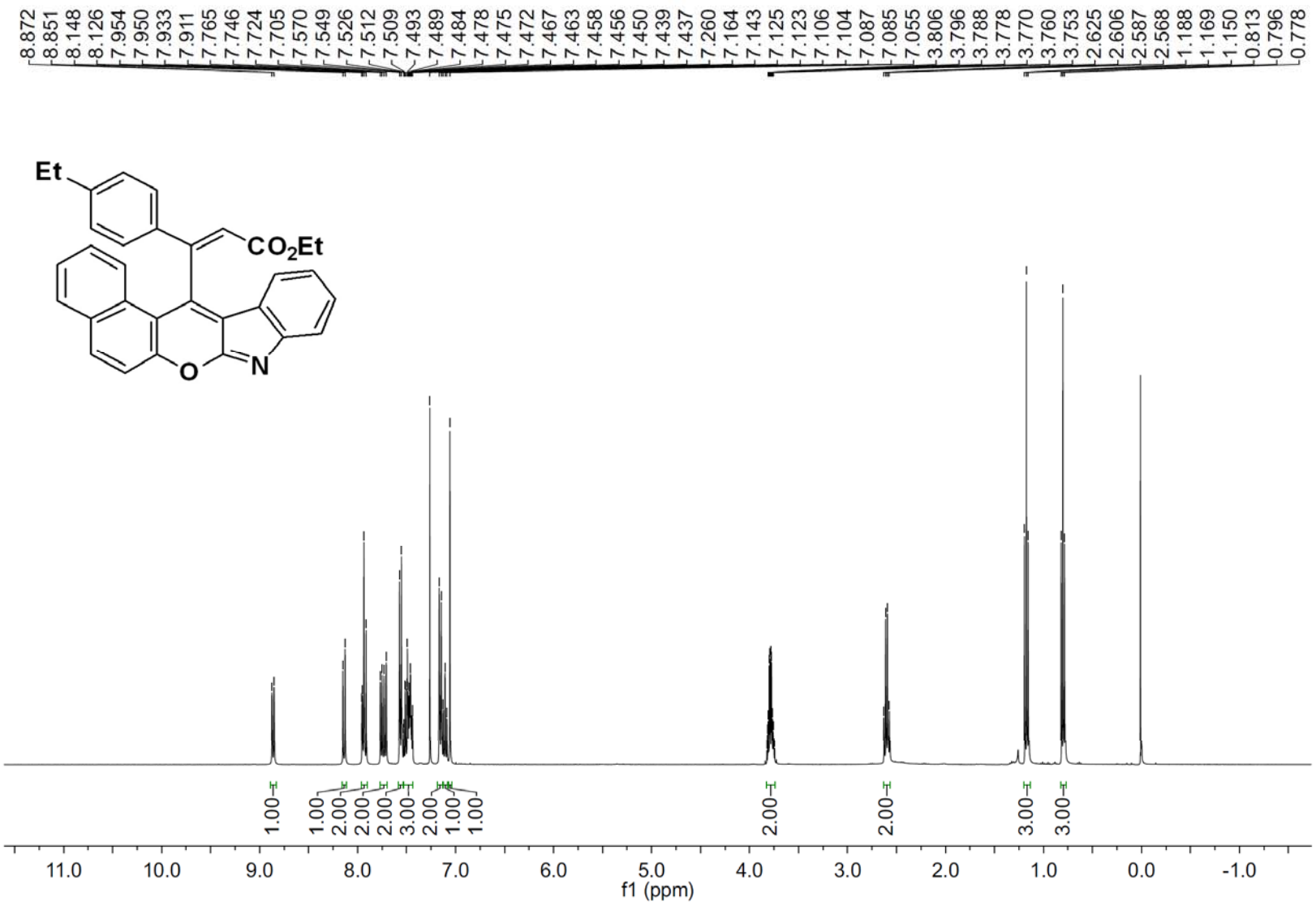
^{13}C NMR Spectrum of Compound 3c



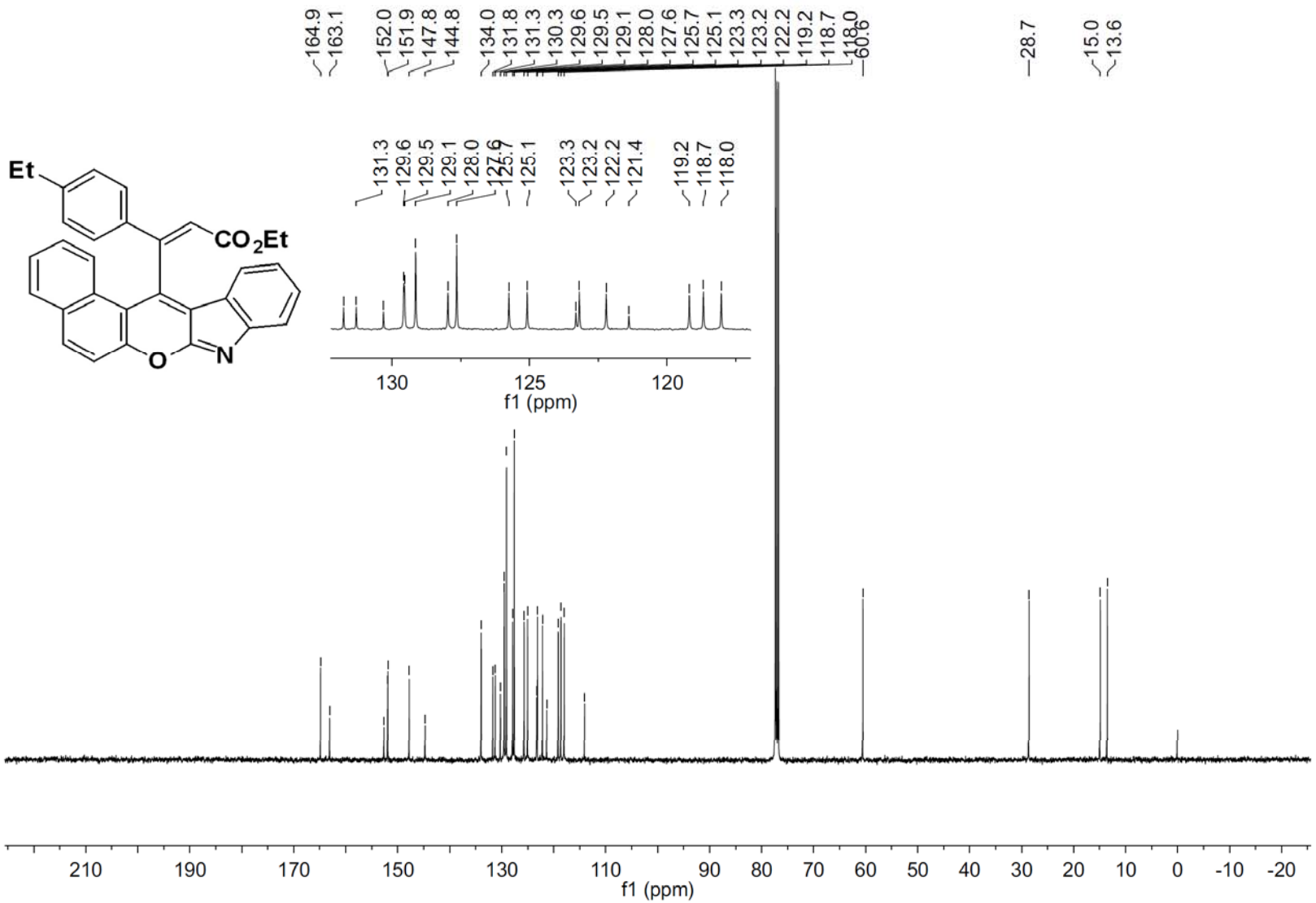
^{1}H NMR Spectrum of Compound 3d



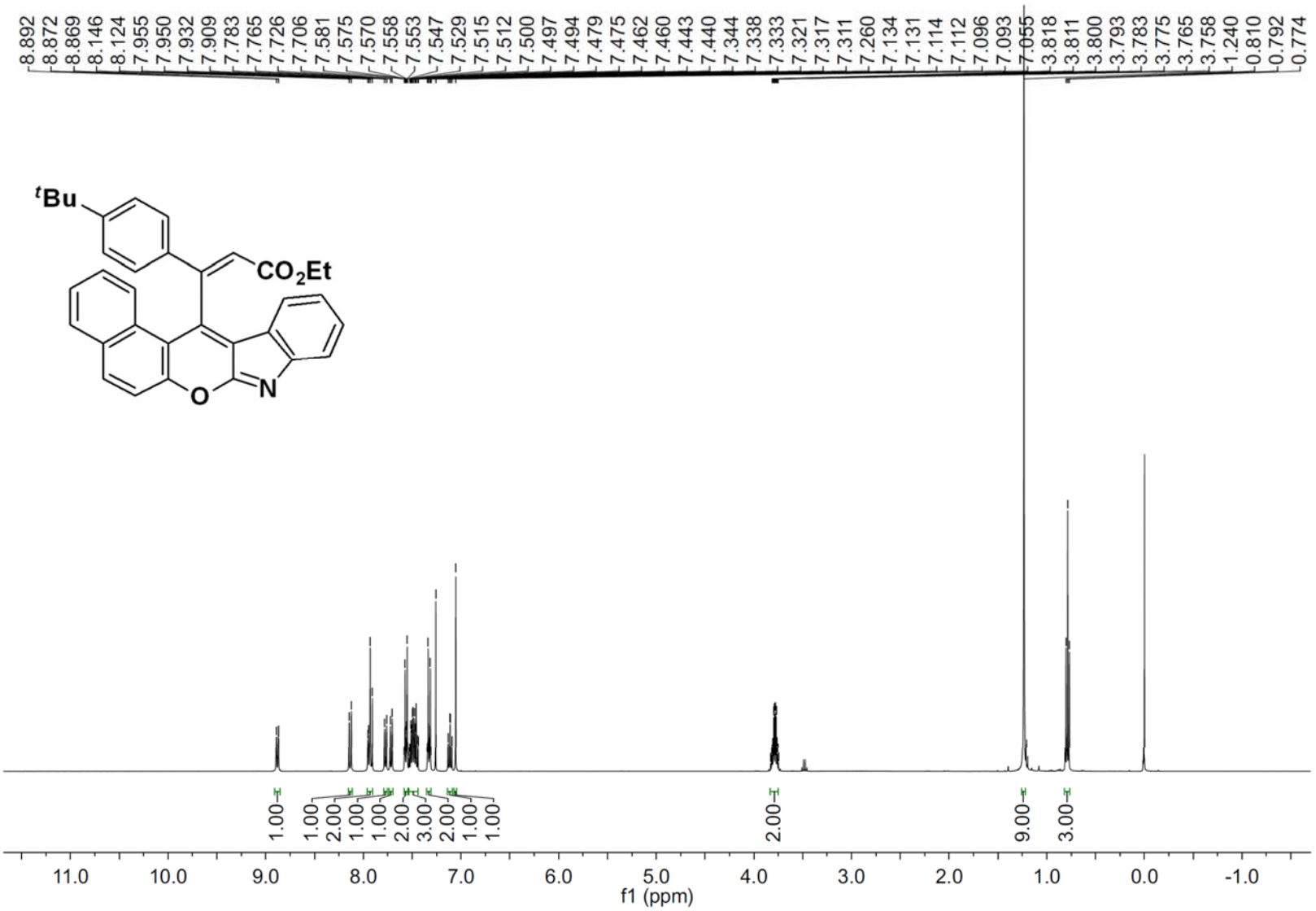
^{13}C NMR Spectrum of Compound 3d



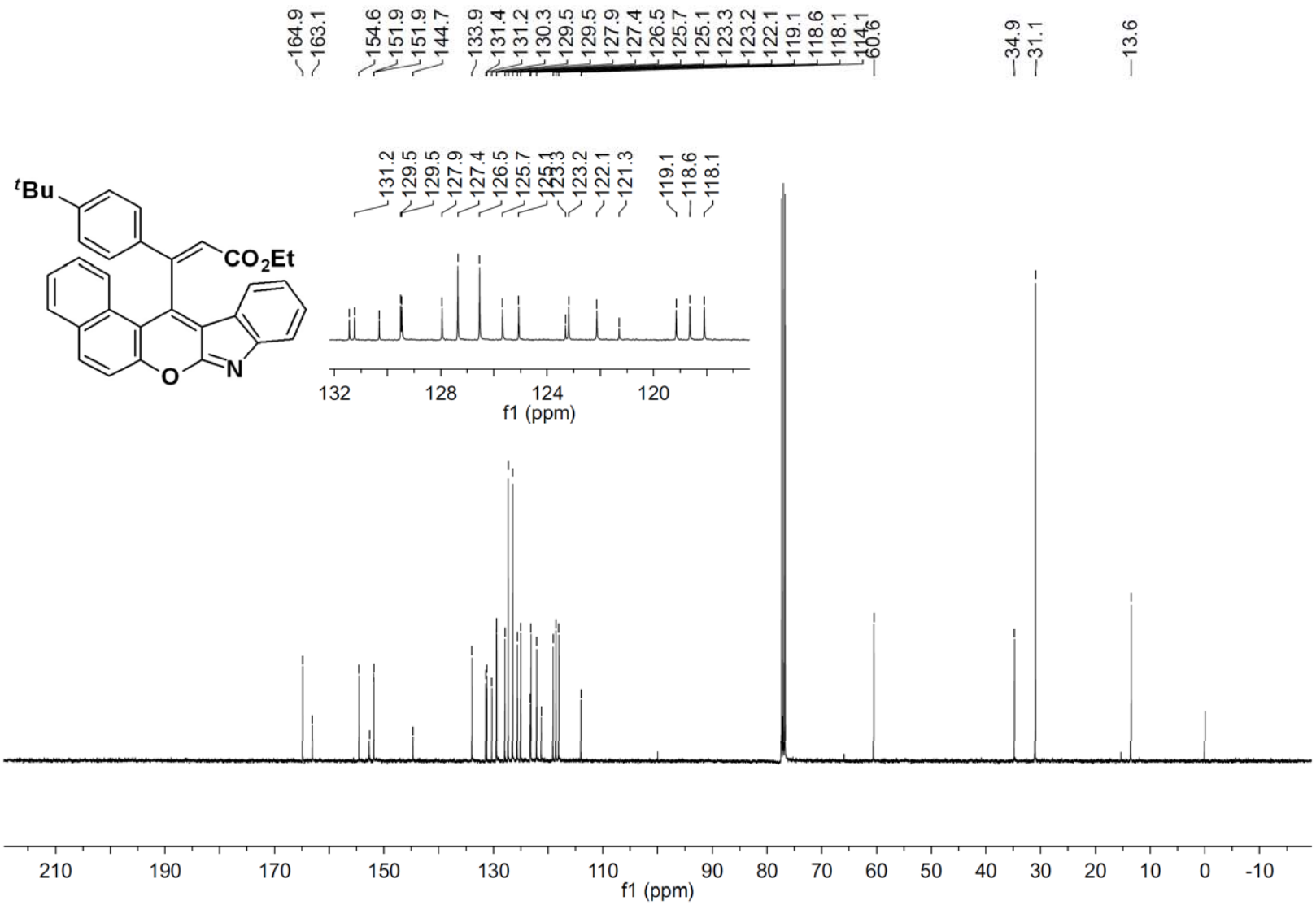
^{1}H NMR Spectrum of Compound 3e



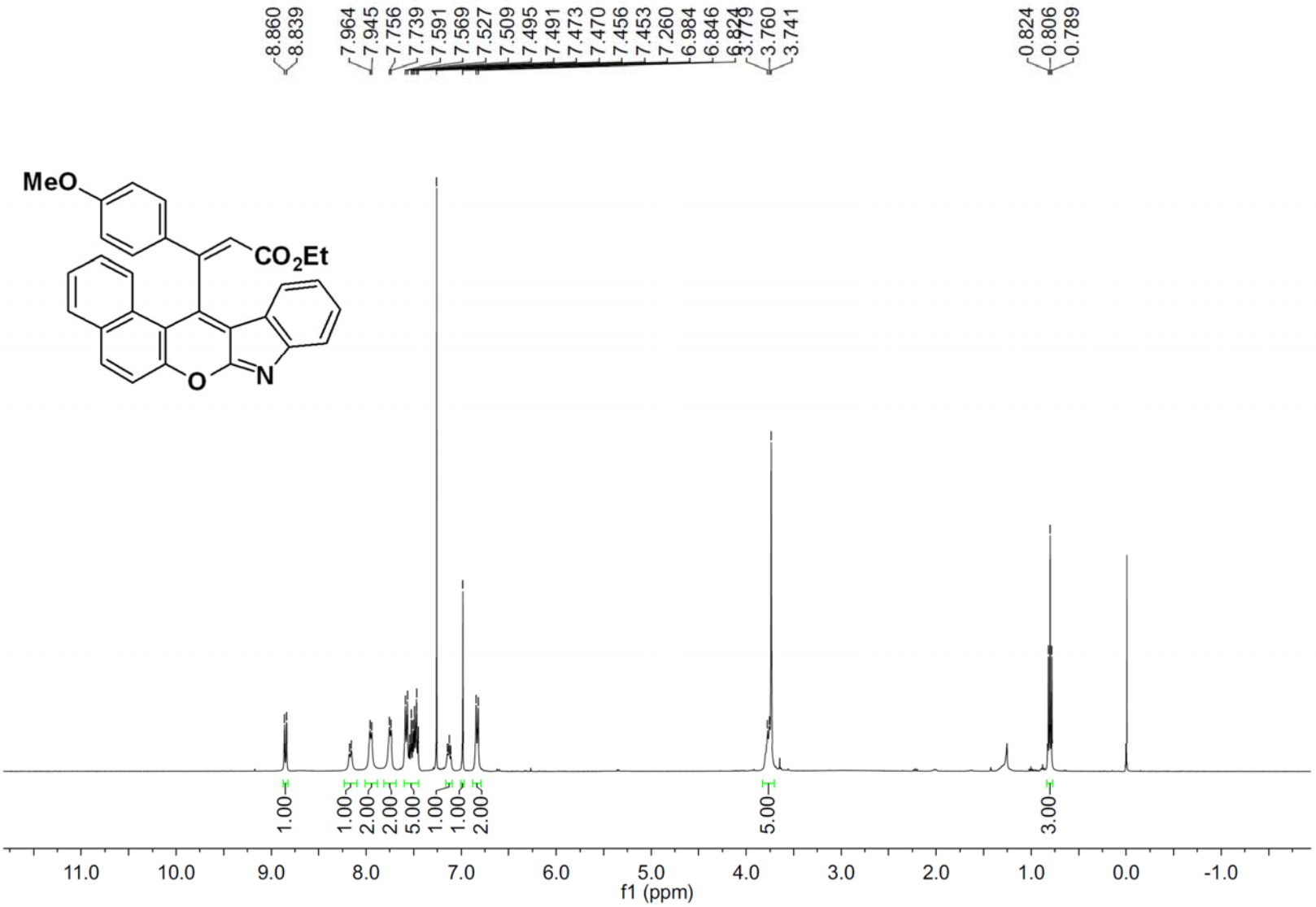
^{13}C NMR Spectrum of Compound 3e



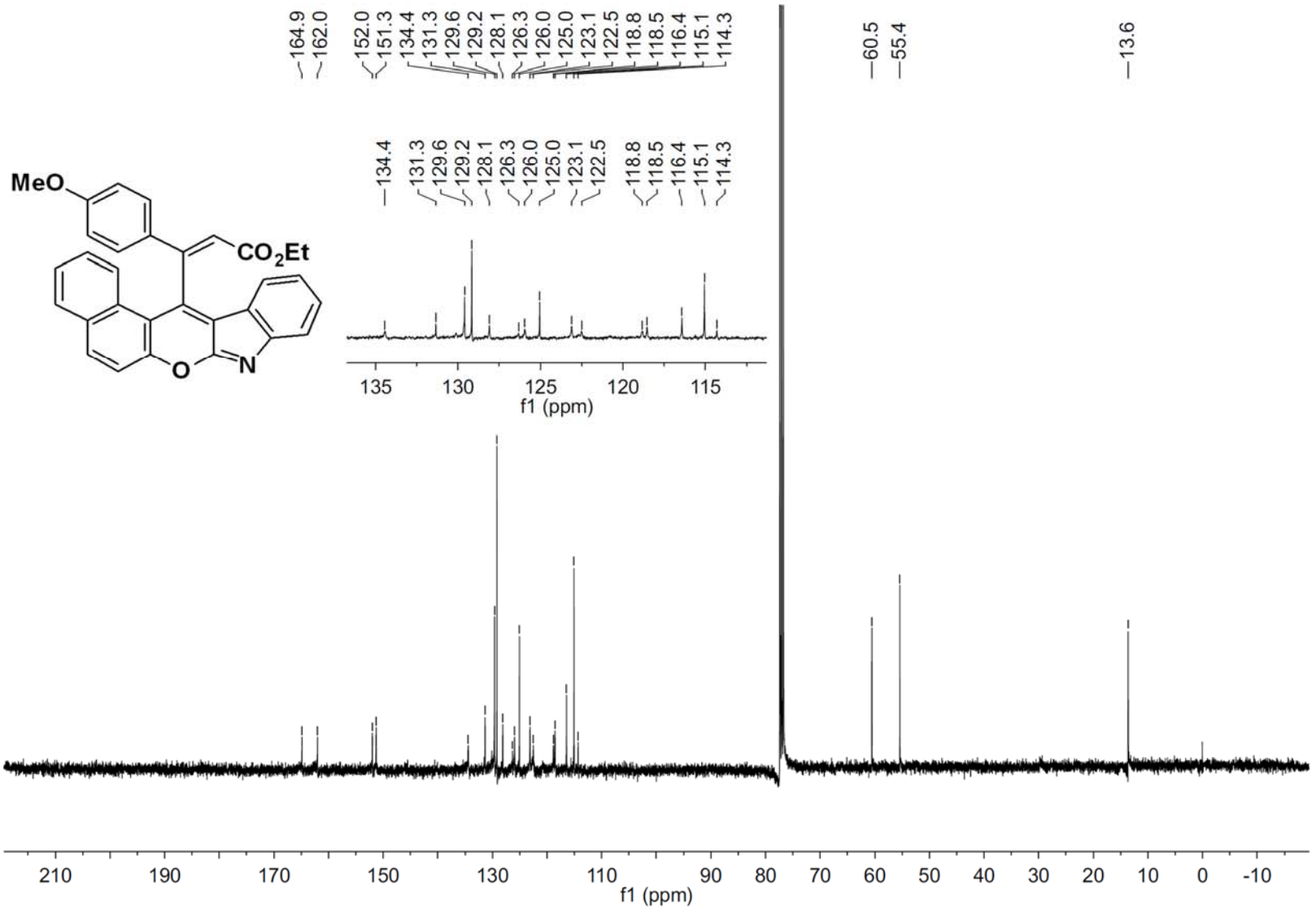
^{1}H NMR Spectrum of Compound 3f



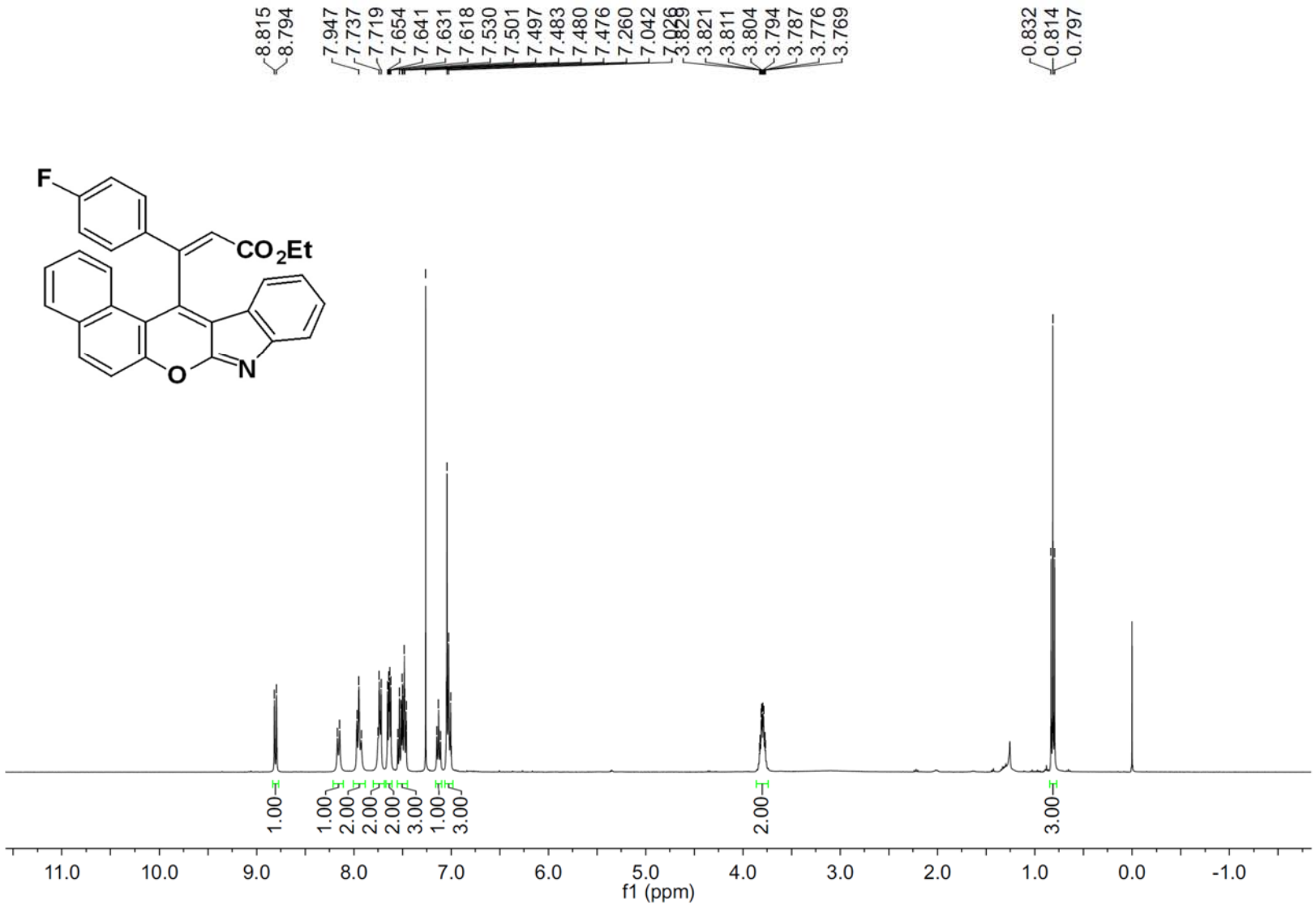
^{13}C NMR Spectrum of Compound 3f



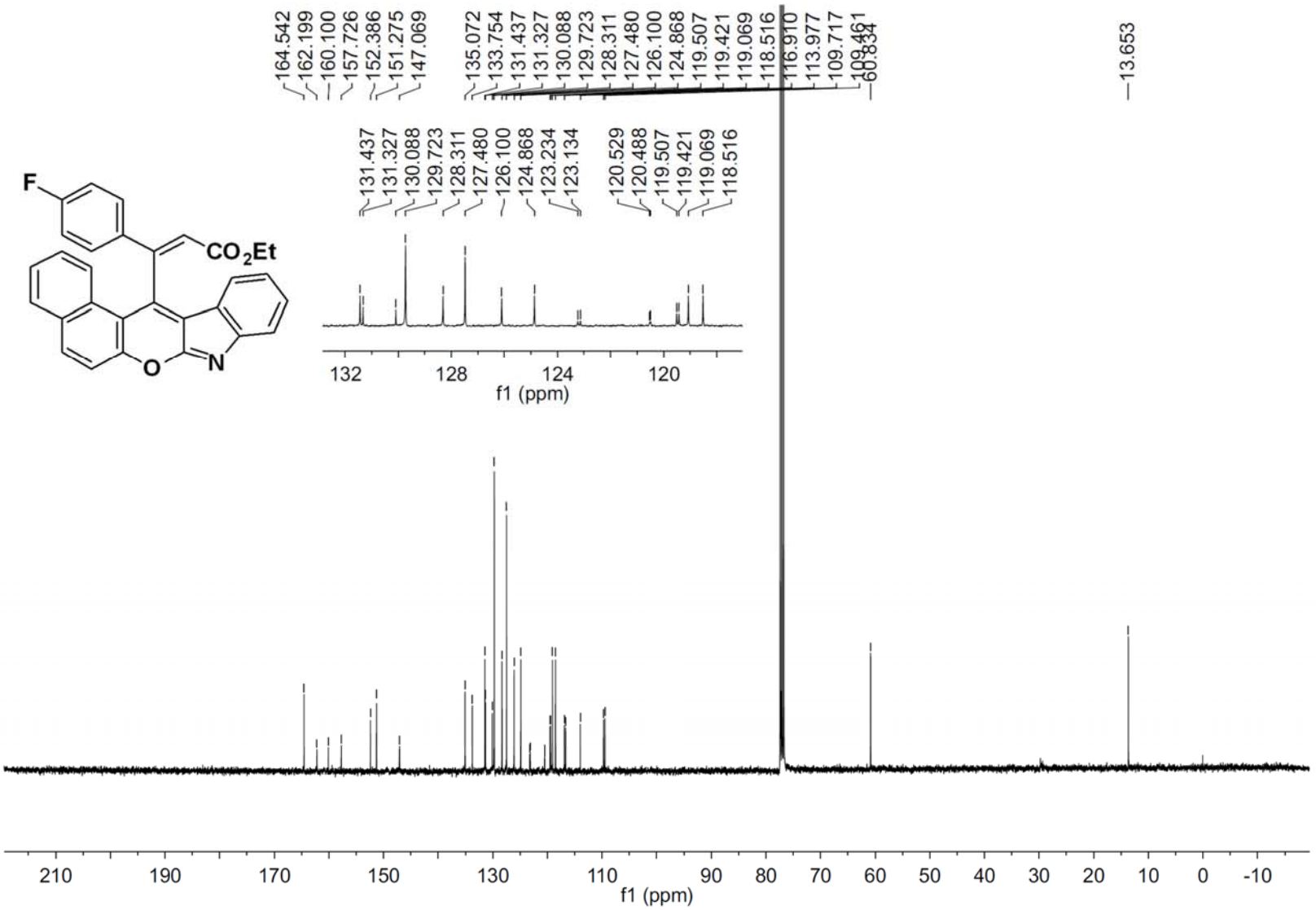
^{1}H NMR Spectrum of Compound 3g



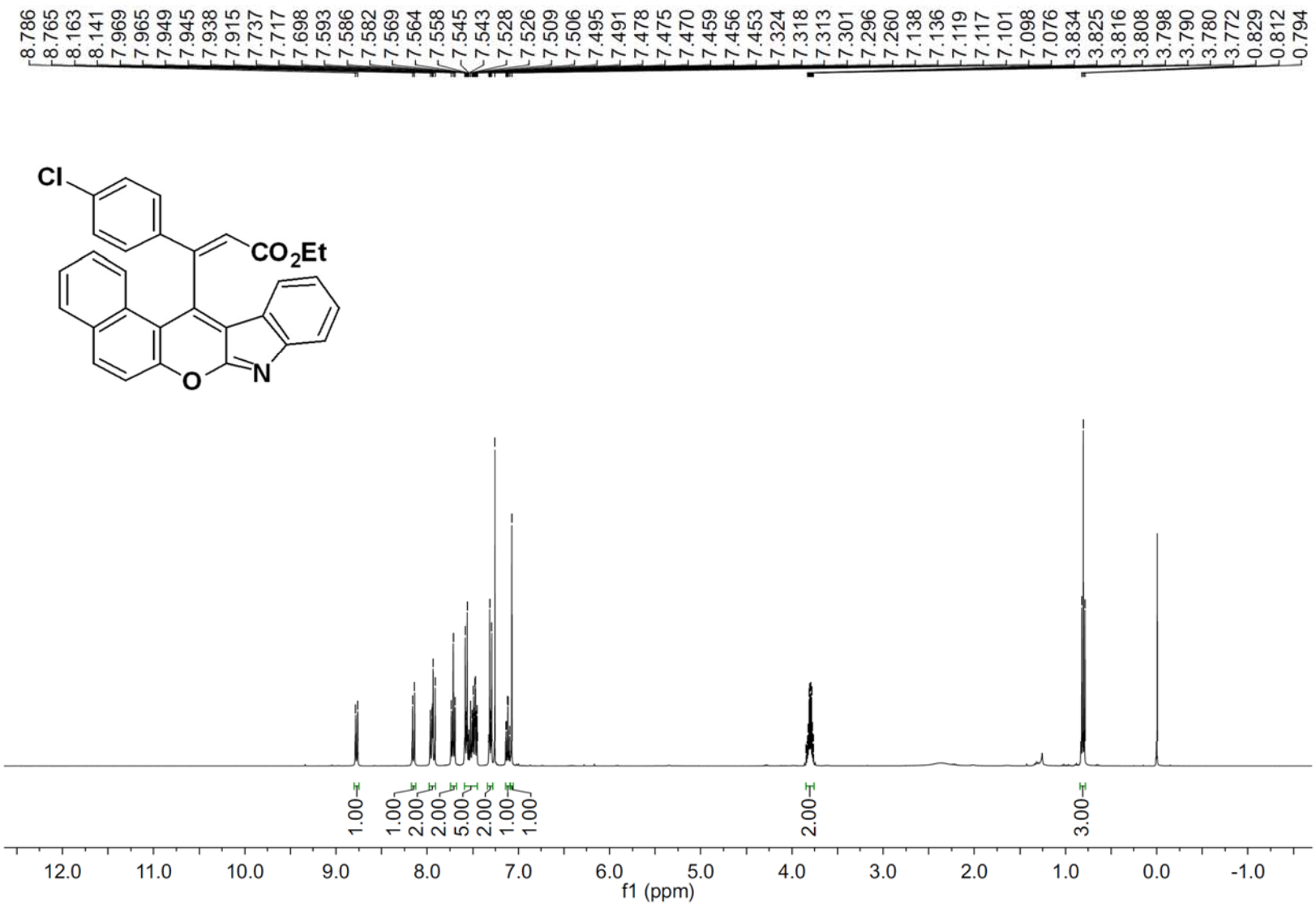
^{13}C NMR Spectrum of Compound 3g



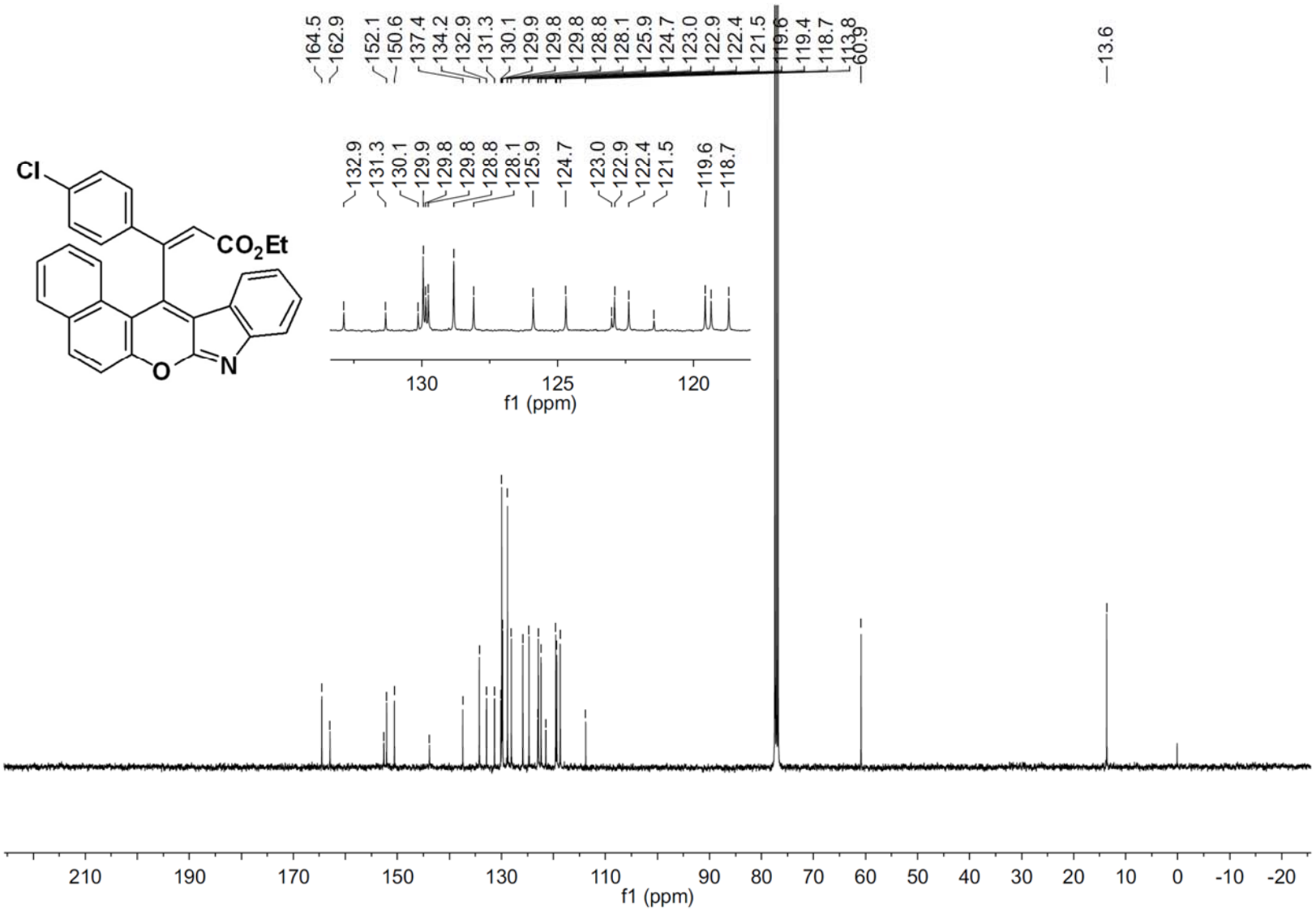
^{1}H NMR Spectrum of Compound 3h



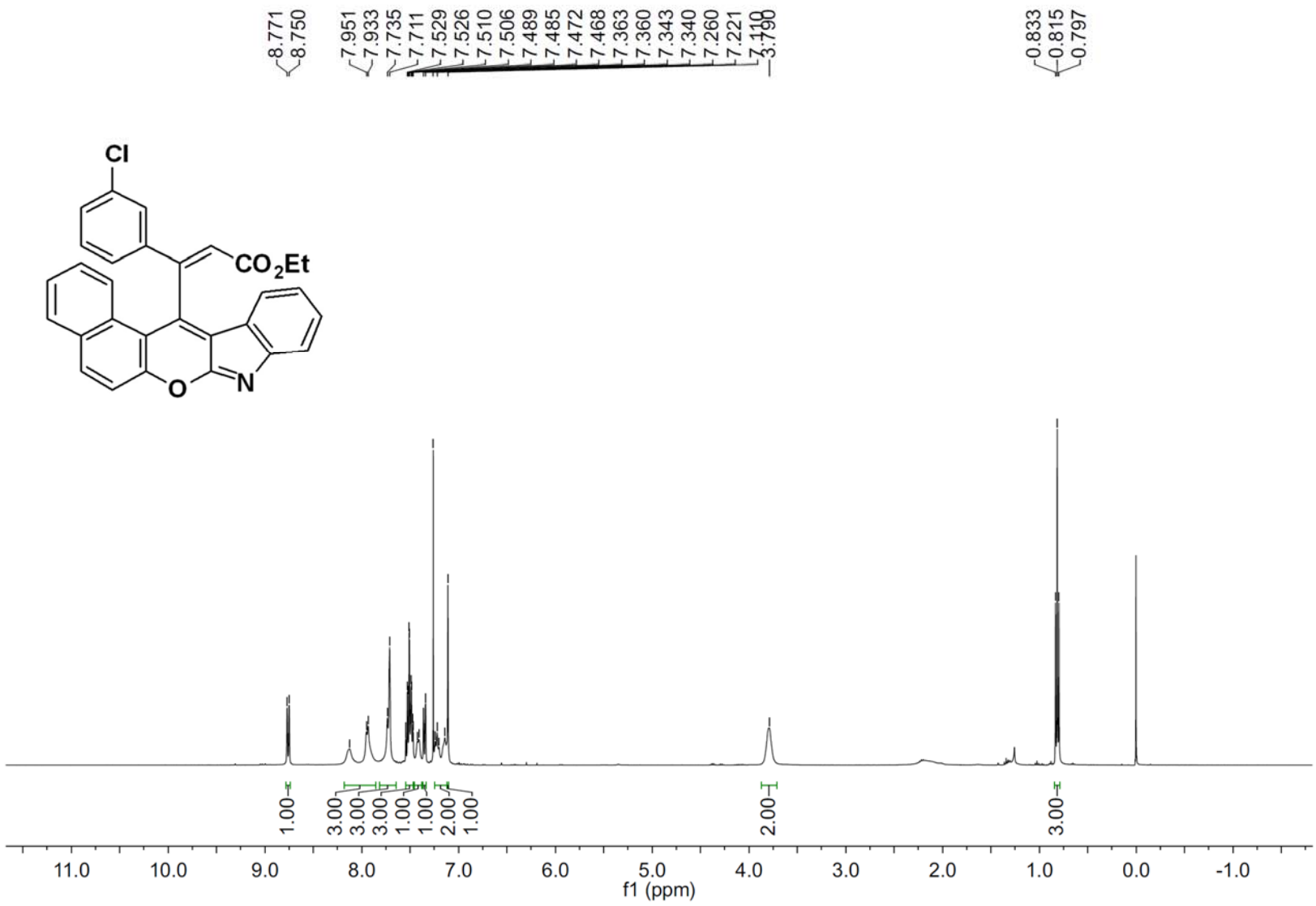
^{13}C NMR Spectrum of Compound 3h



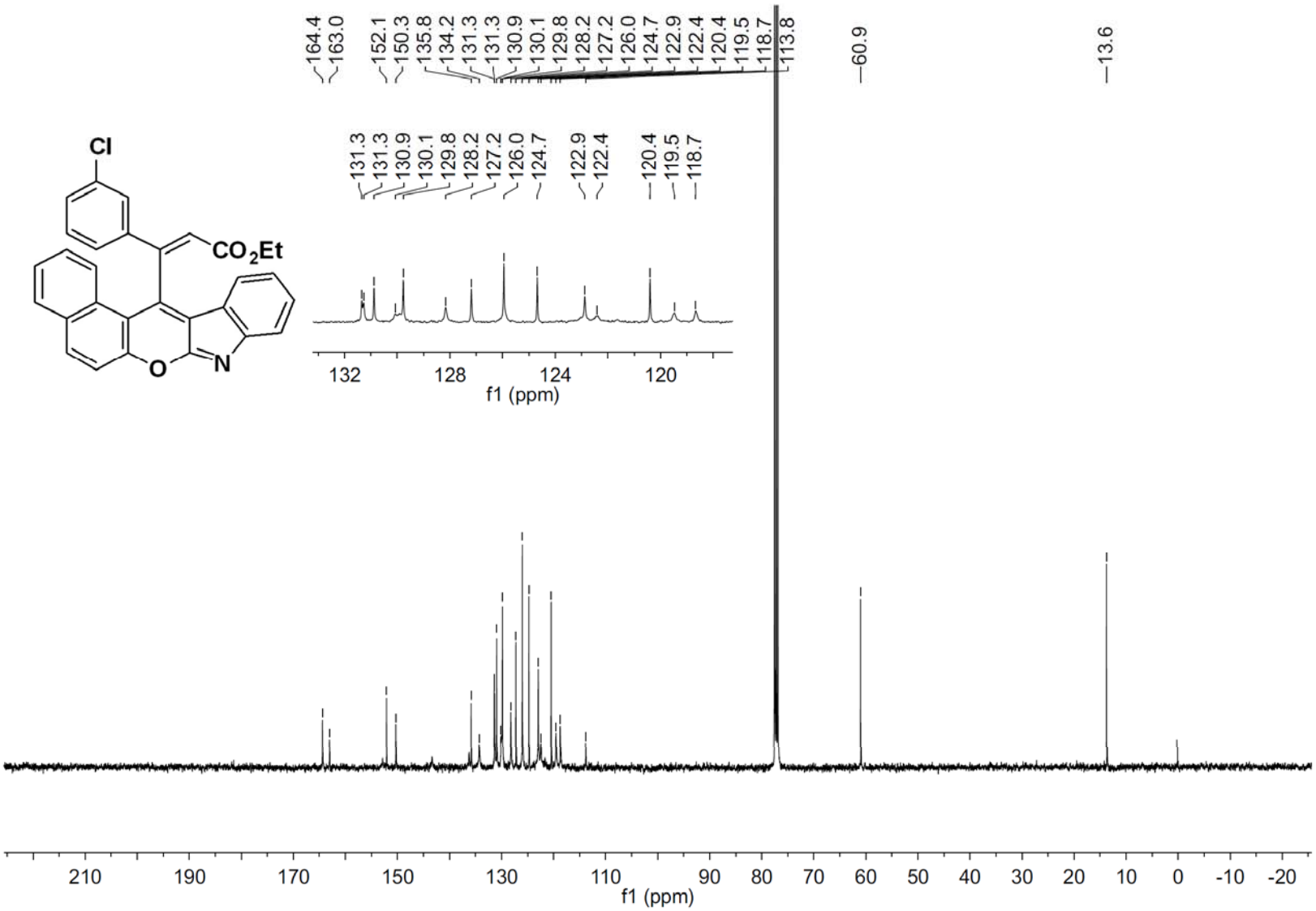
^{1}H NMR Spectrum of Compound 3i



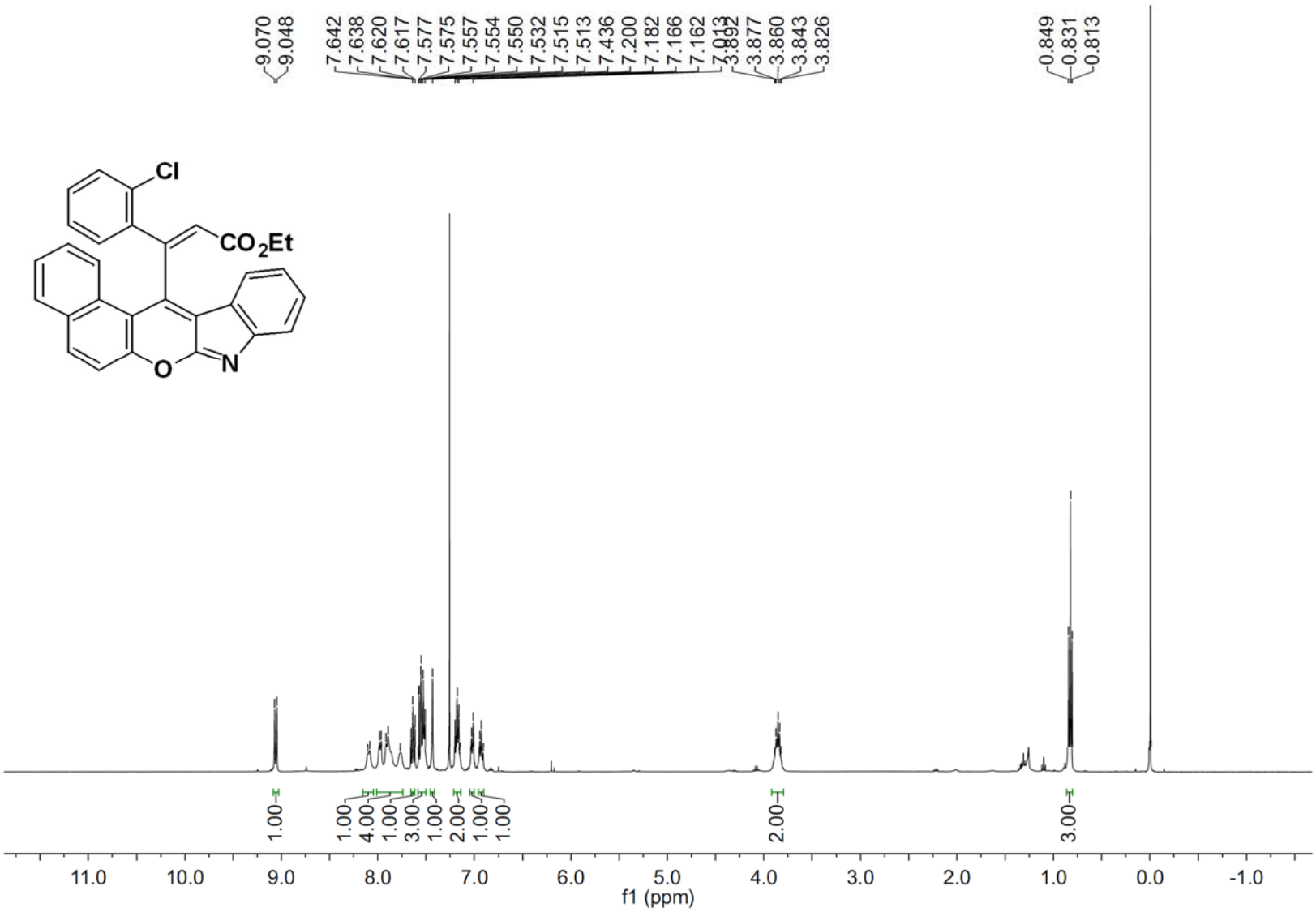
^{13}C NMR Spectrum of Compound 3i



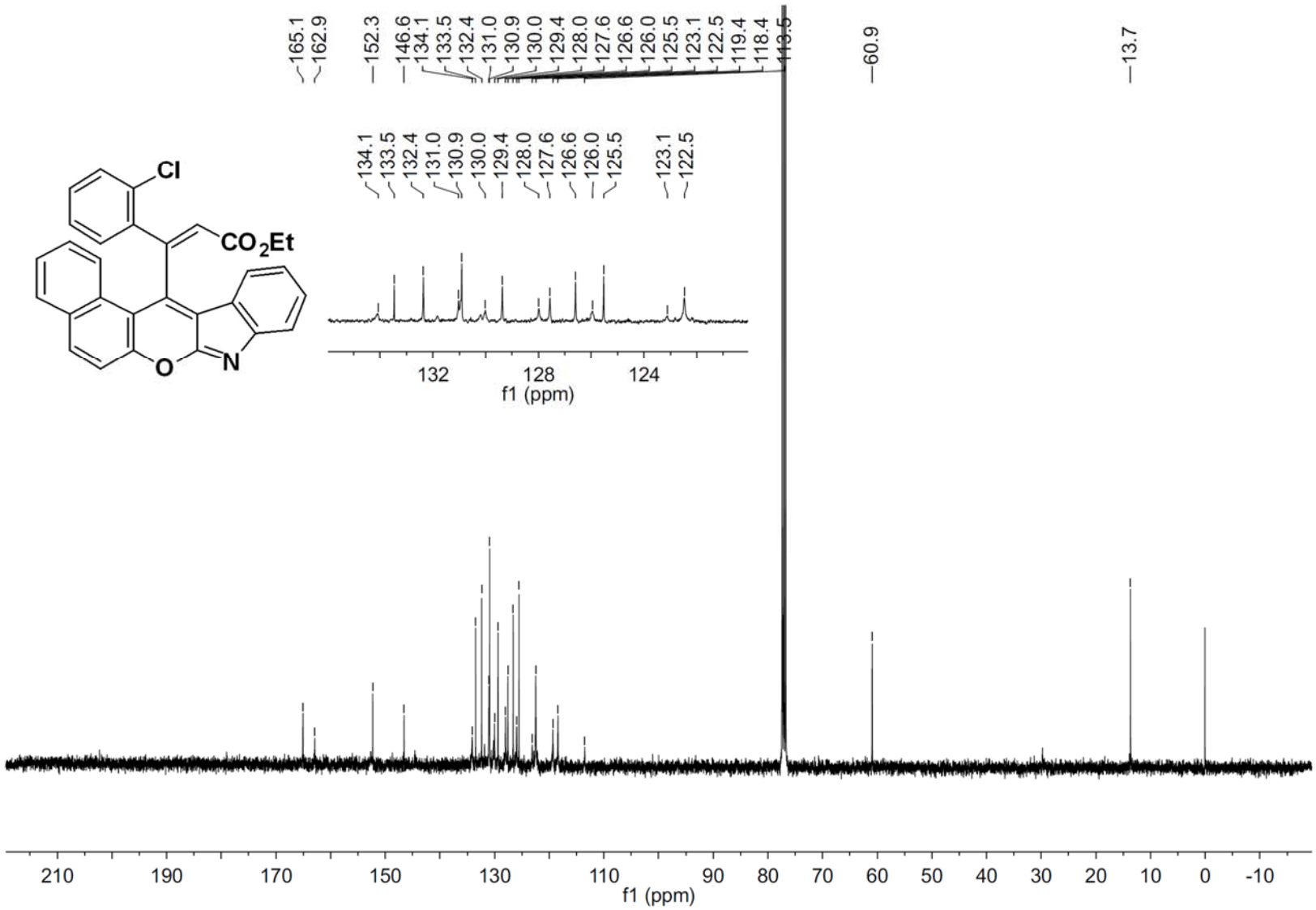
^{1}H NMR Spectrum of Compound 3j



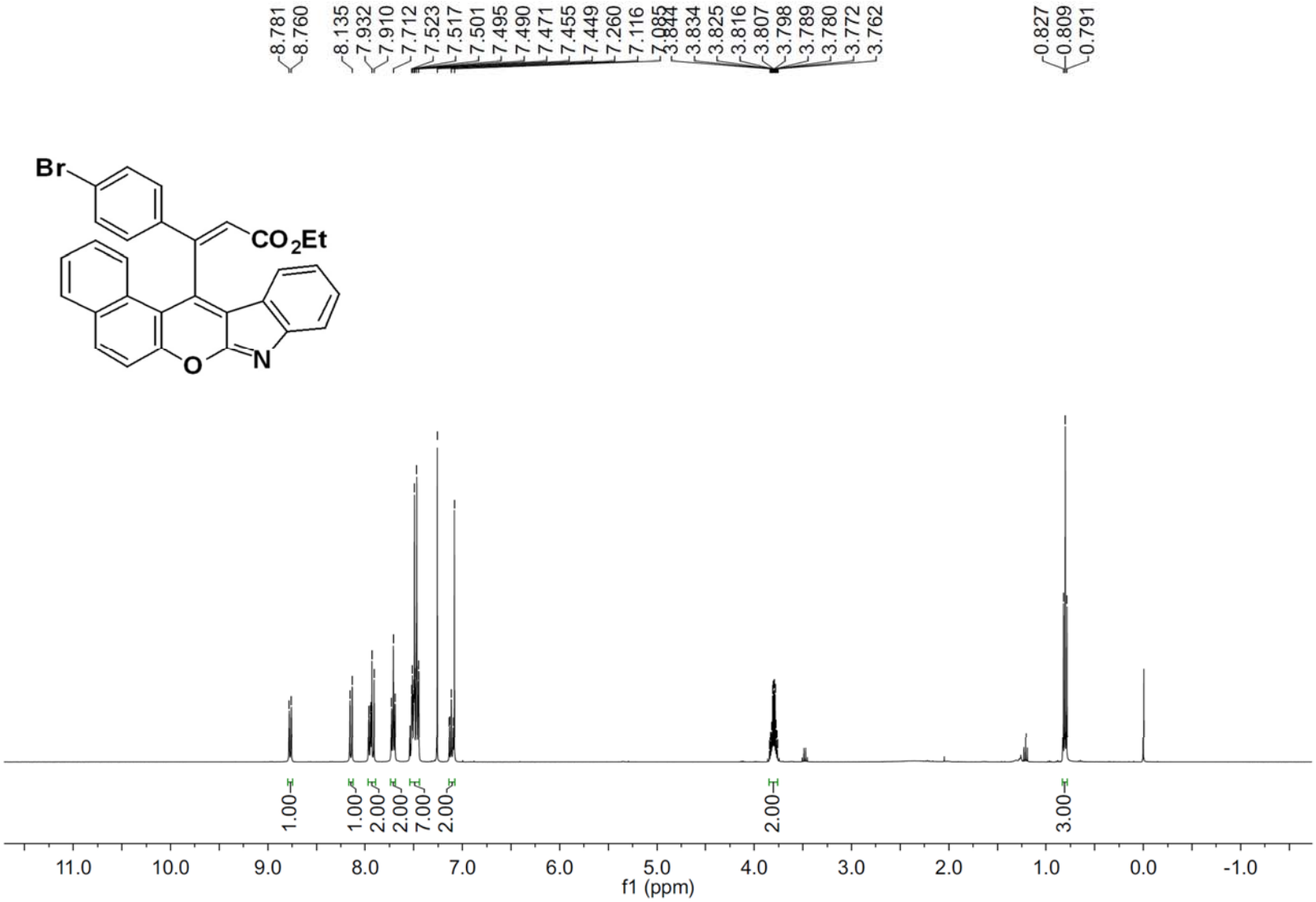
^{13}C NMR Spectrum of Compound 3j



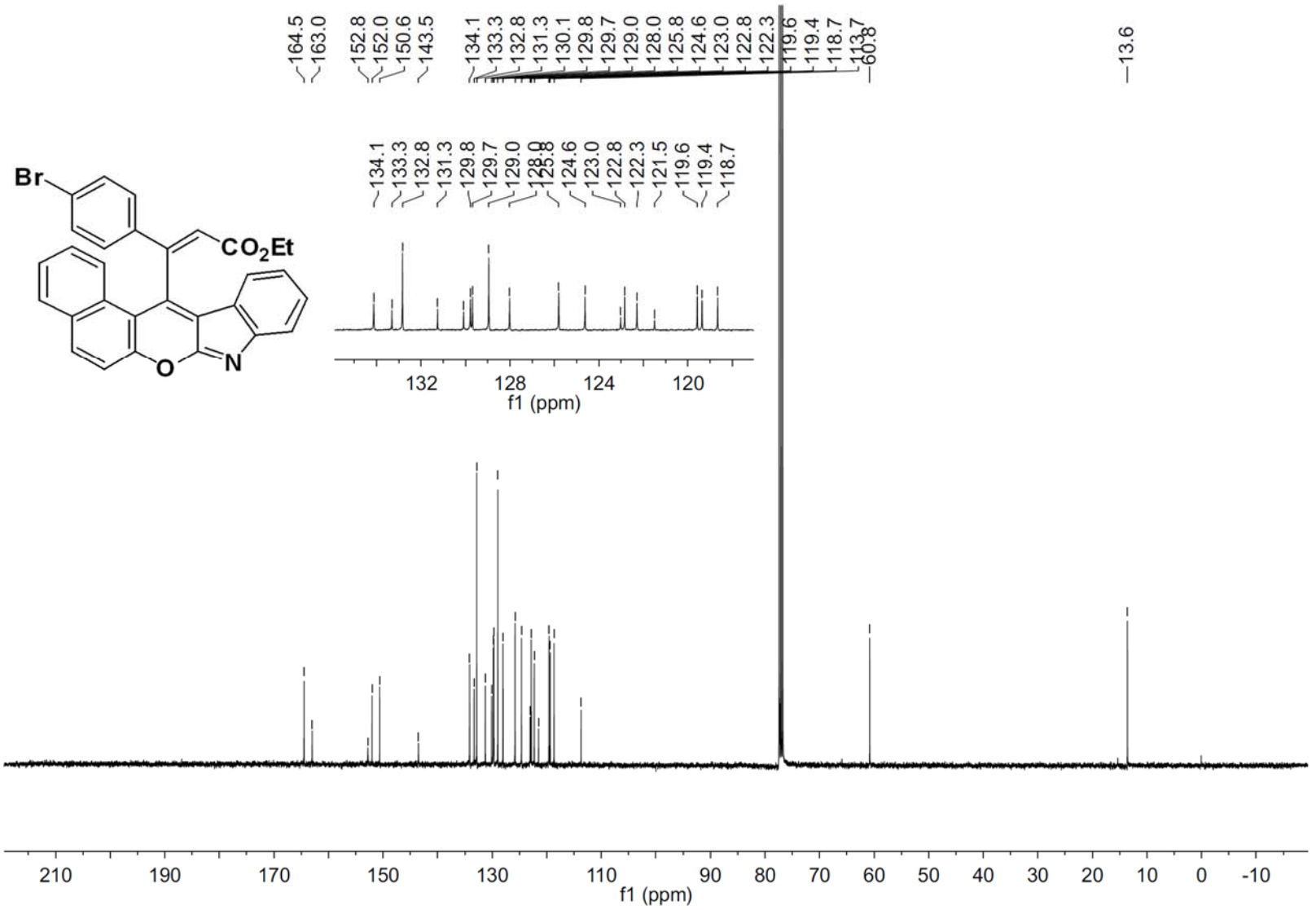
^{1}H NMR Spectrum of Compound 3k



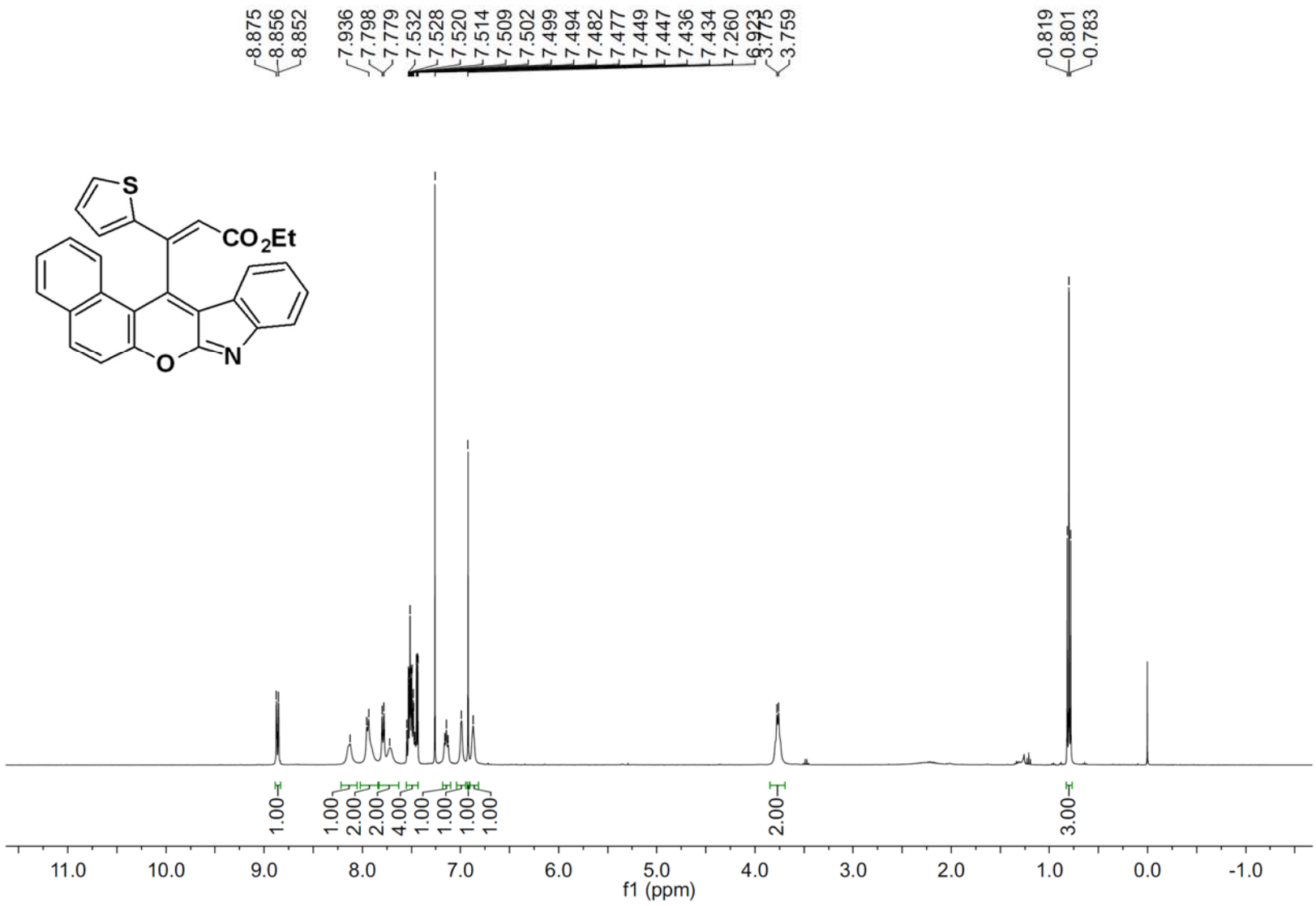
^{13}C NMR Spectrum of Compound 3k



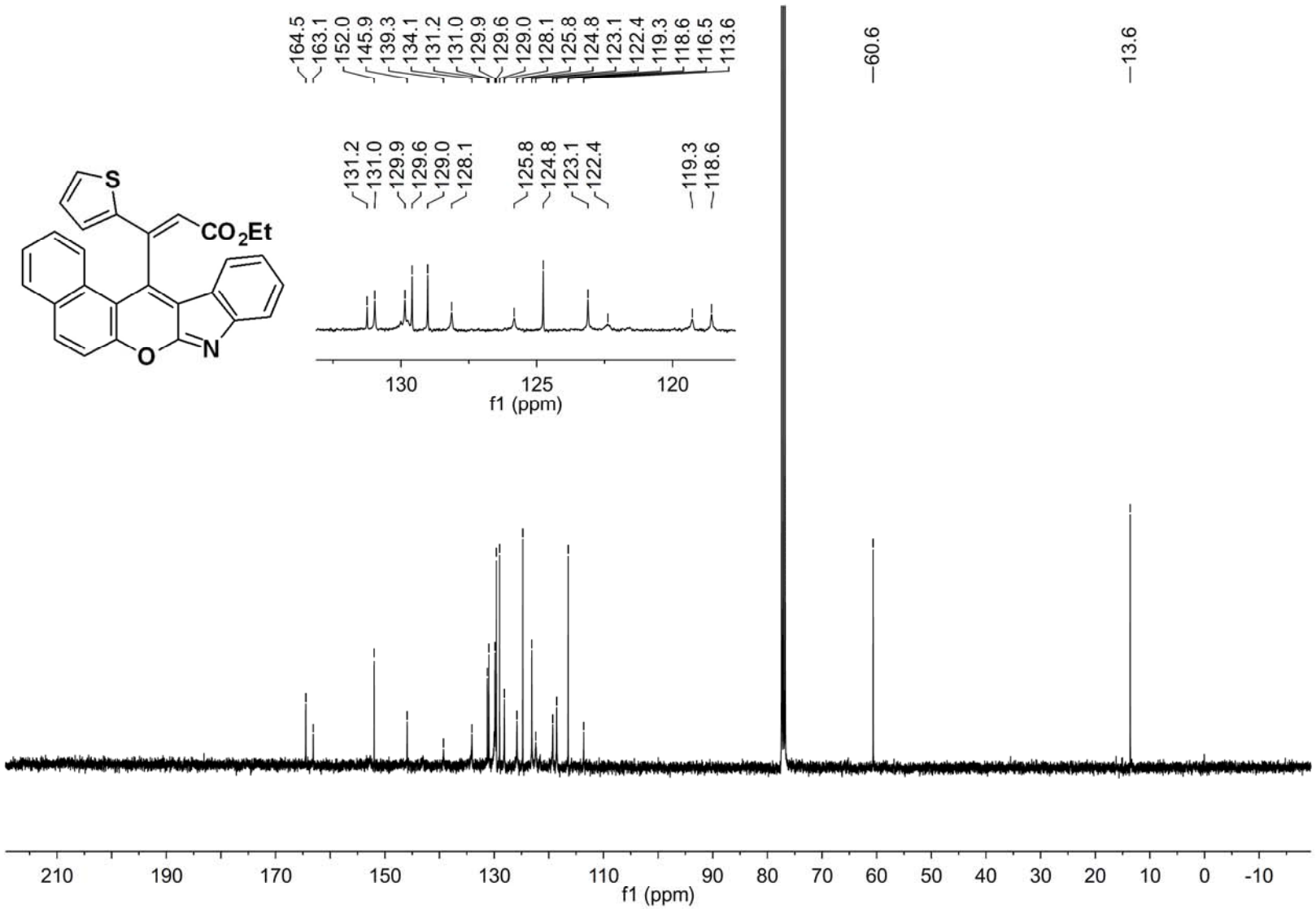
^{1}H NMR Spectrum of Compound 3l



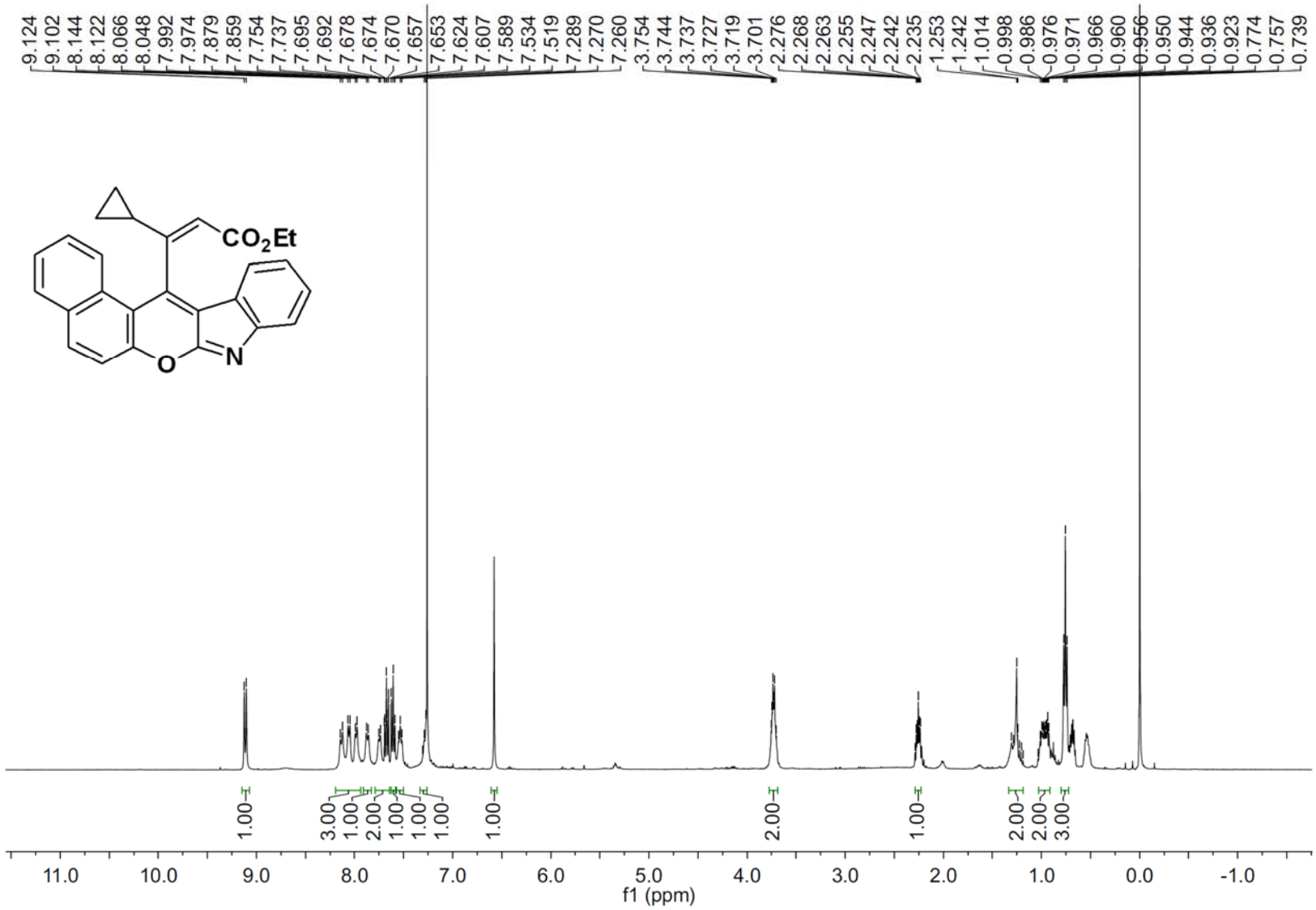
^{13}C NMR Spectrum of Compound 3l



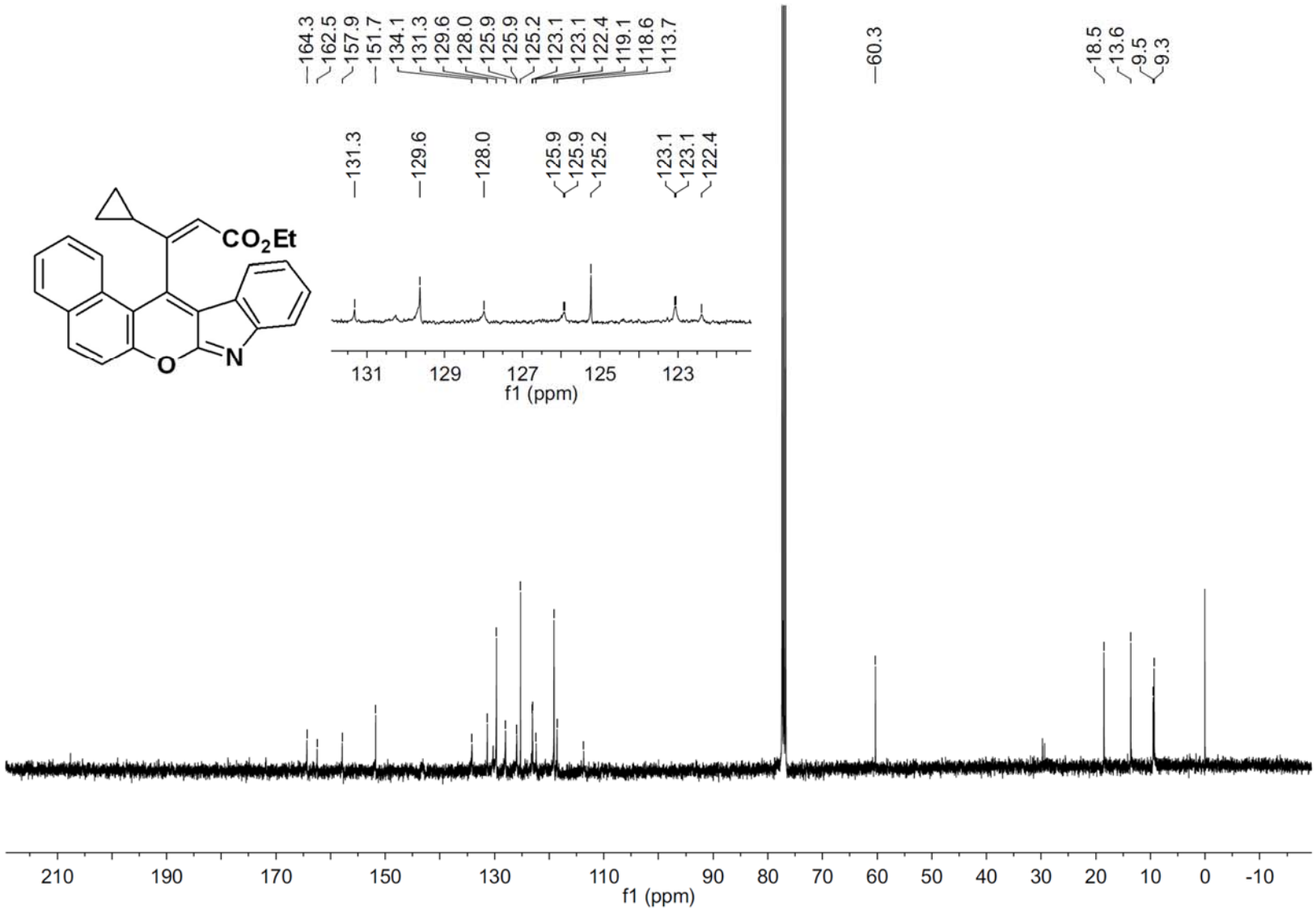
^{1}H NMR Spectrum of Compound 3m



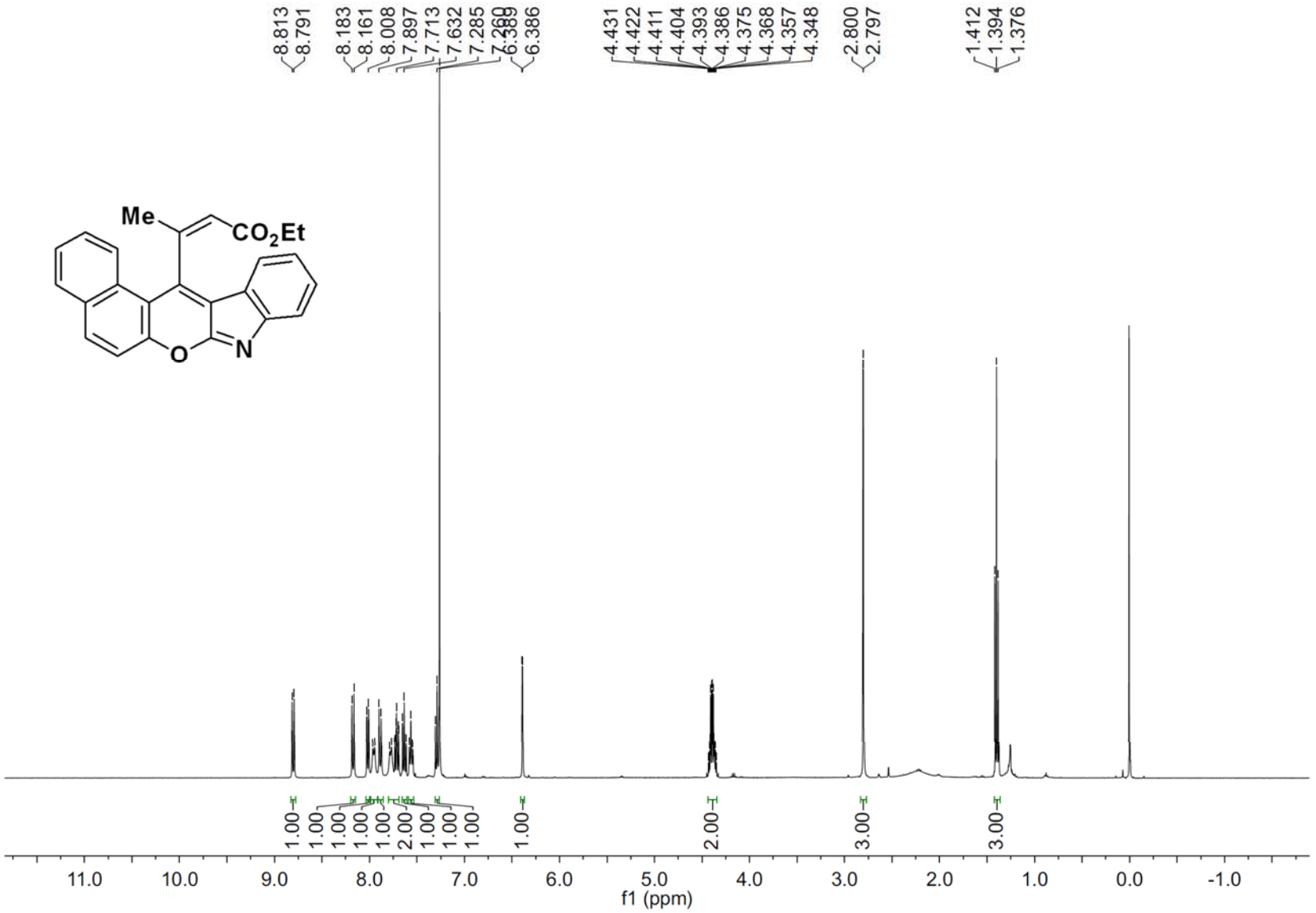
^{13}C NMR Spectrum of Compound 3m



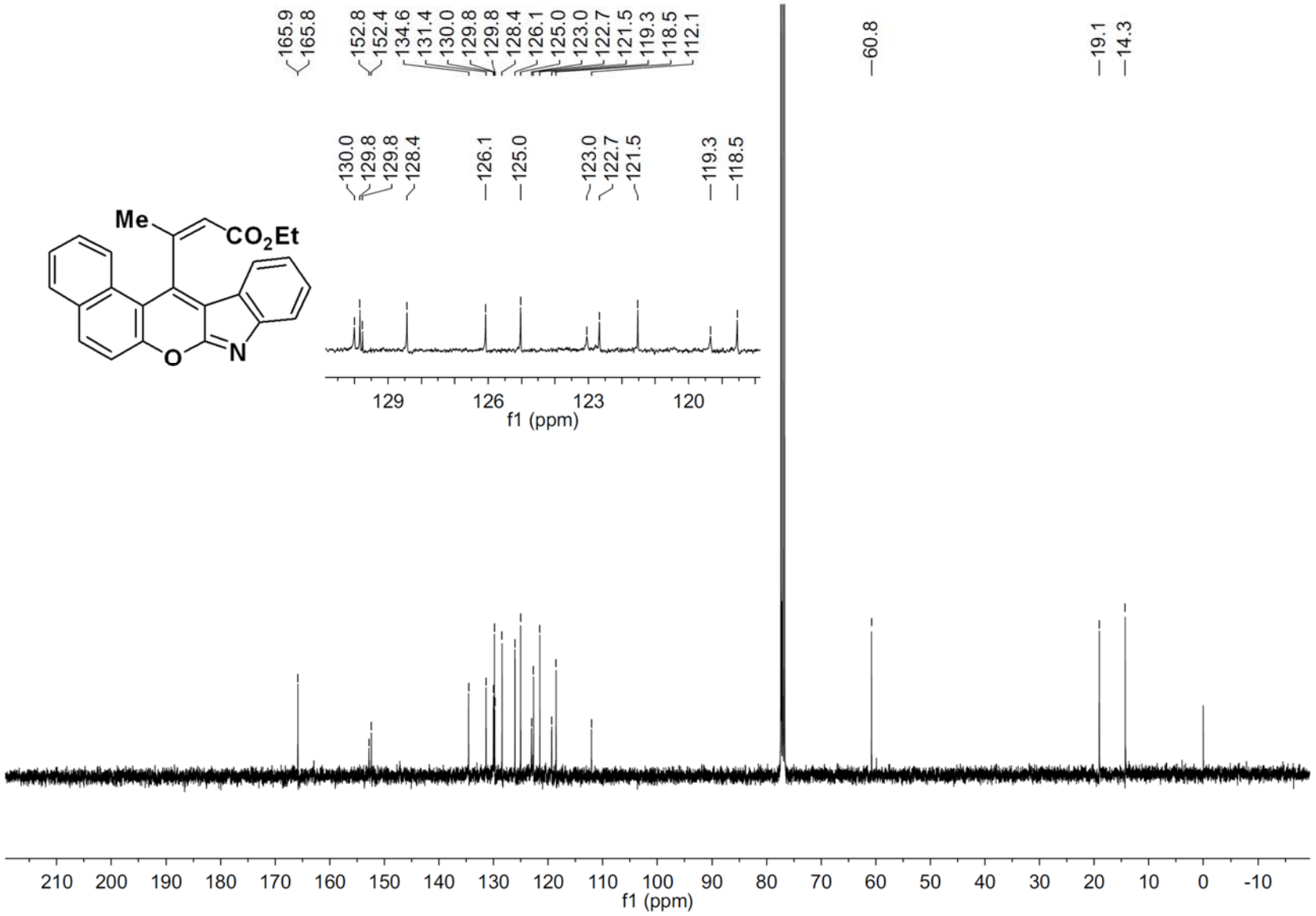
^{1}H NMR Spectrum of Compound 3n



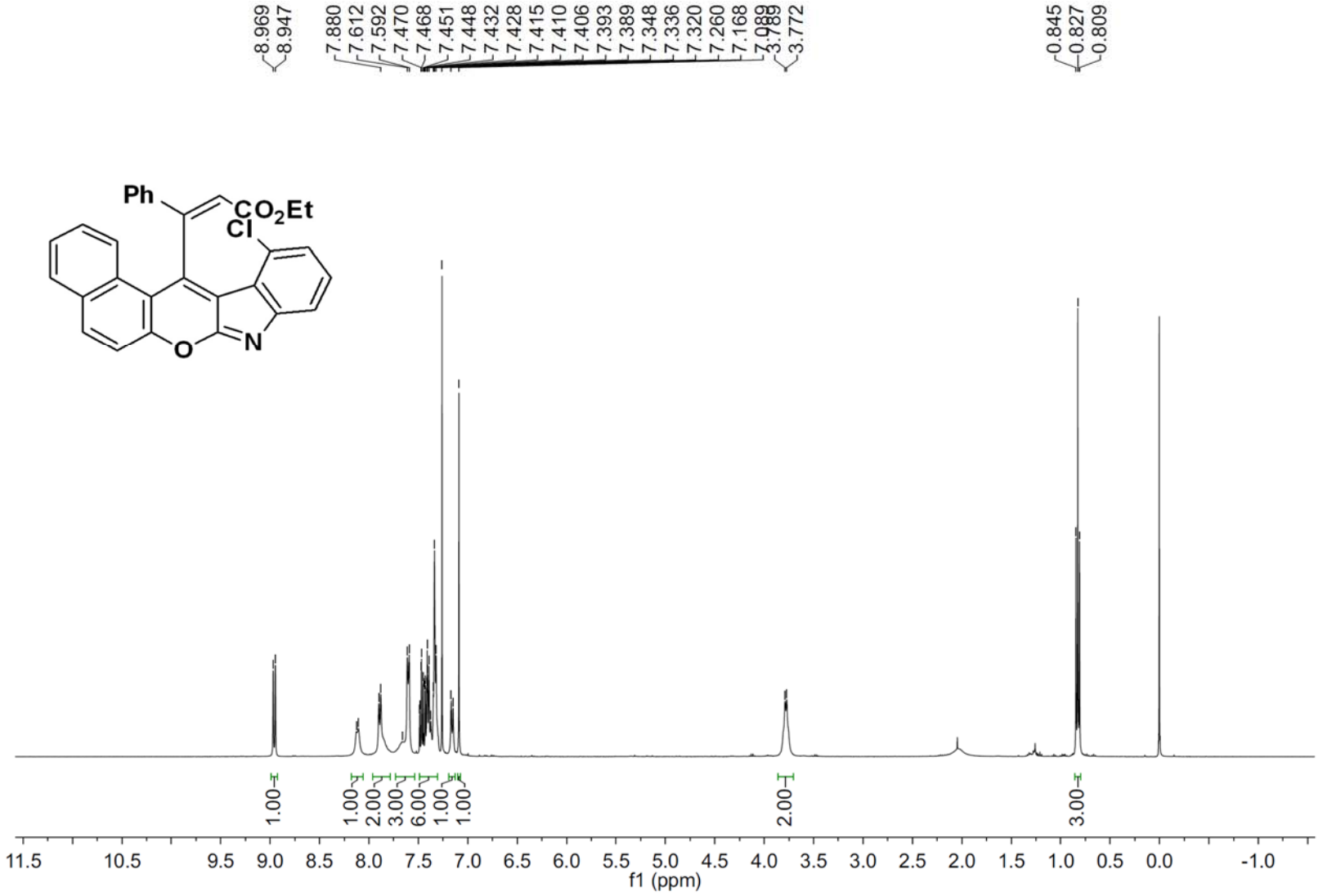
^{13}C NMR Spectrum of Compound 3n



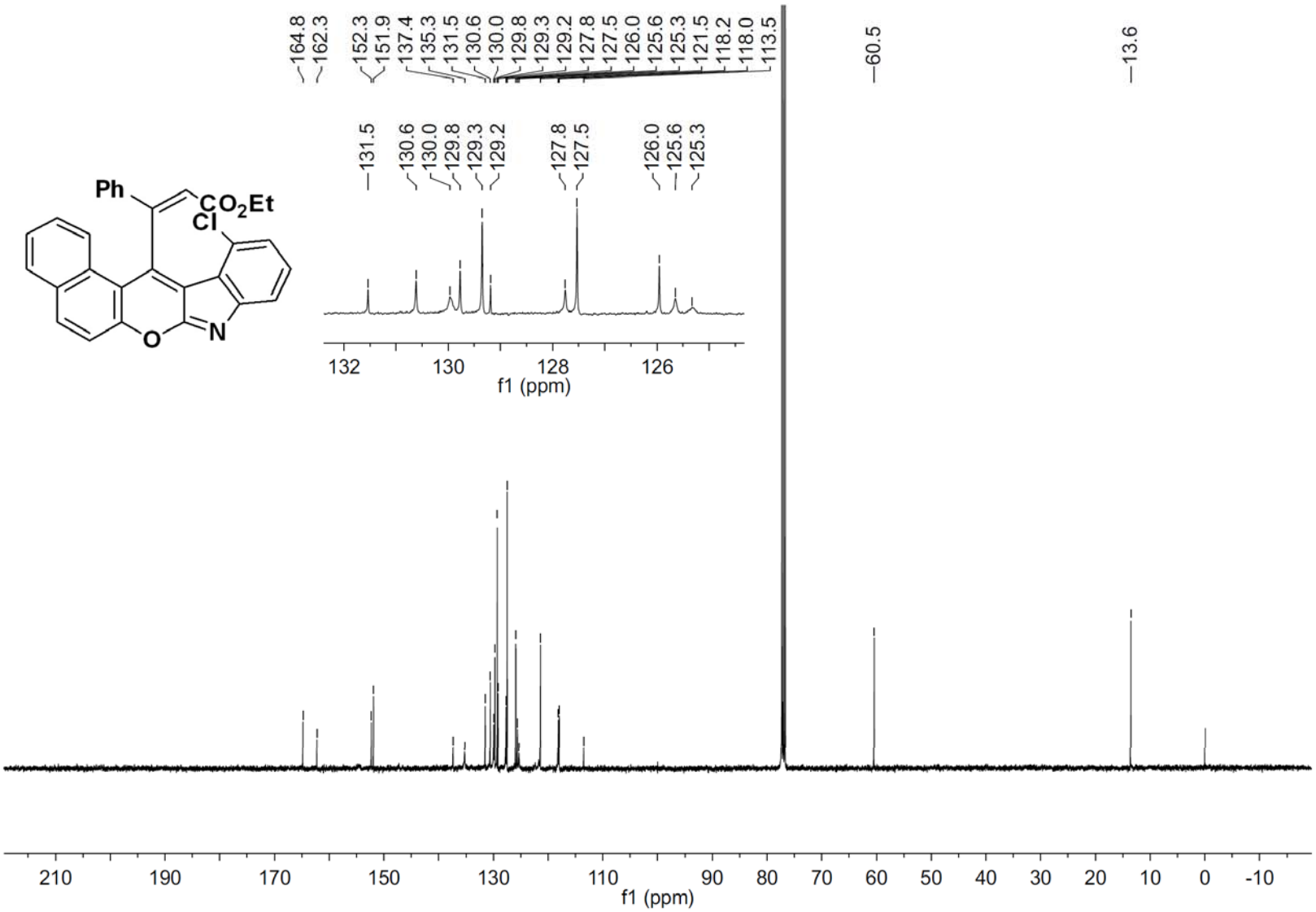
^{1}H NMR Spectrum of Compound 3o



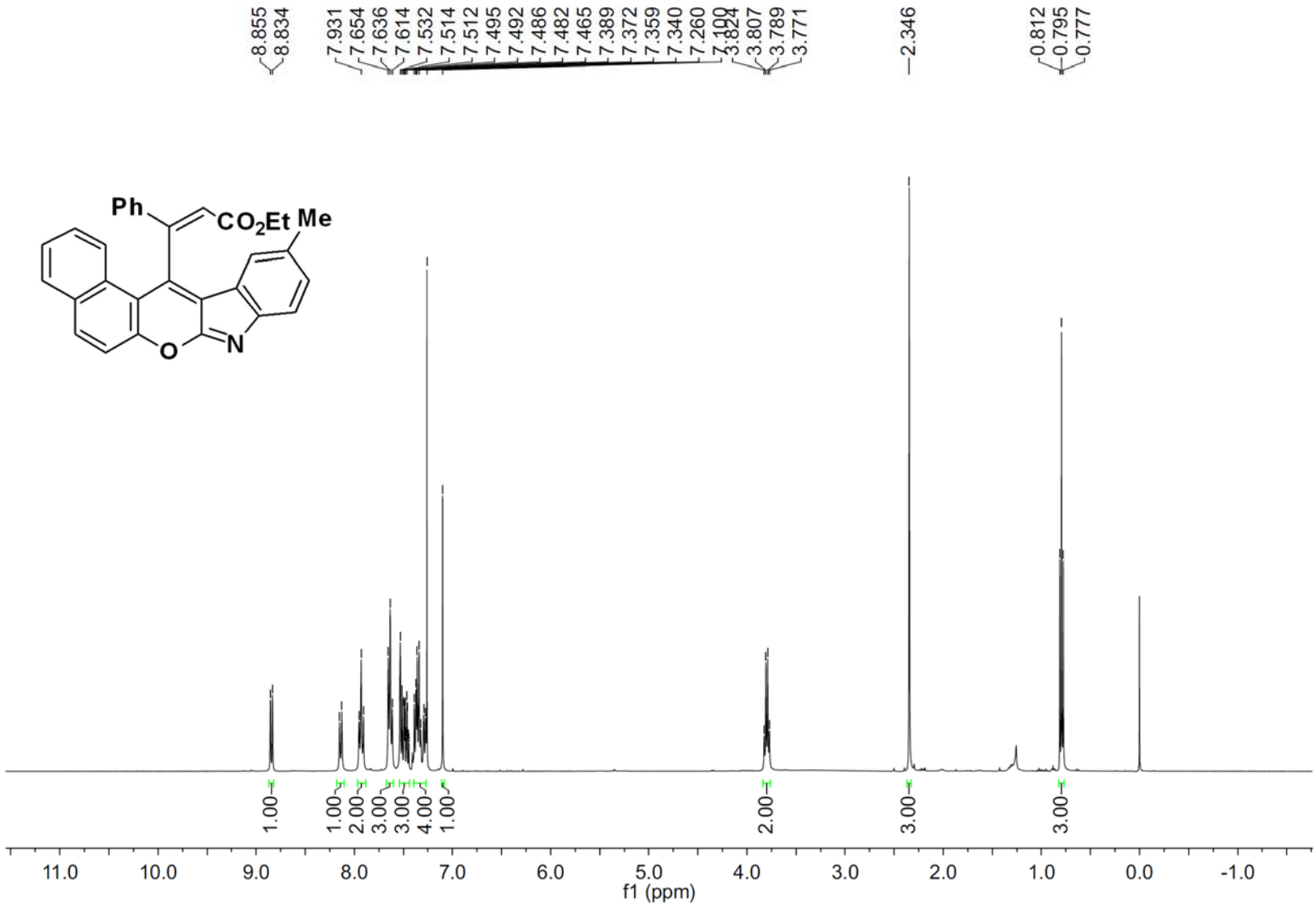
^{13}C NMR Spectrum of Compound 3o



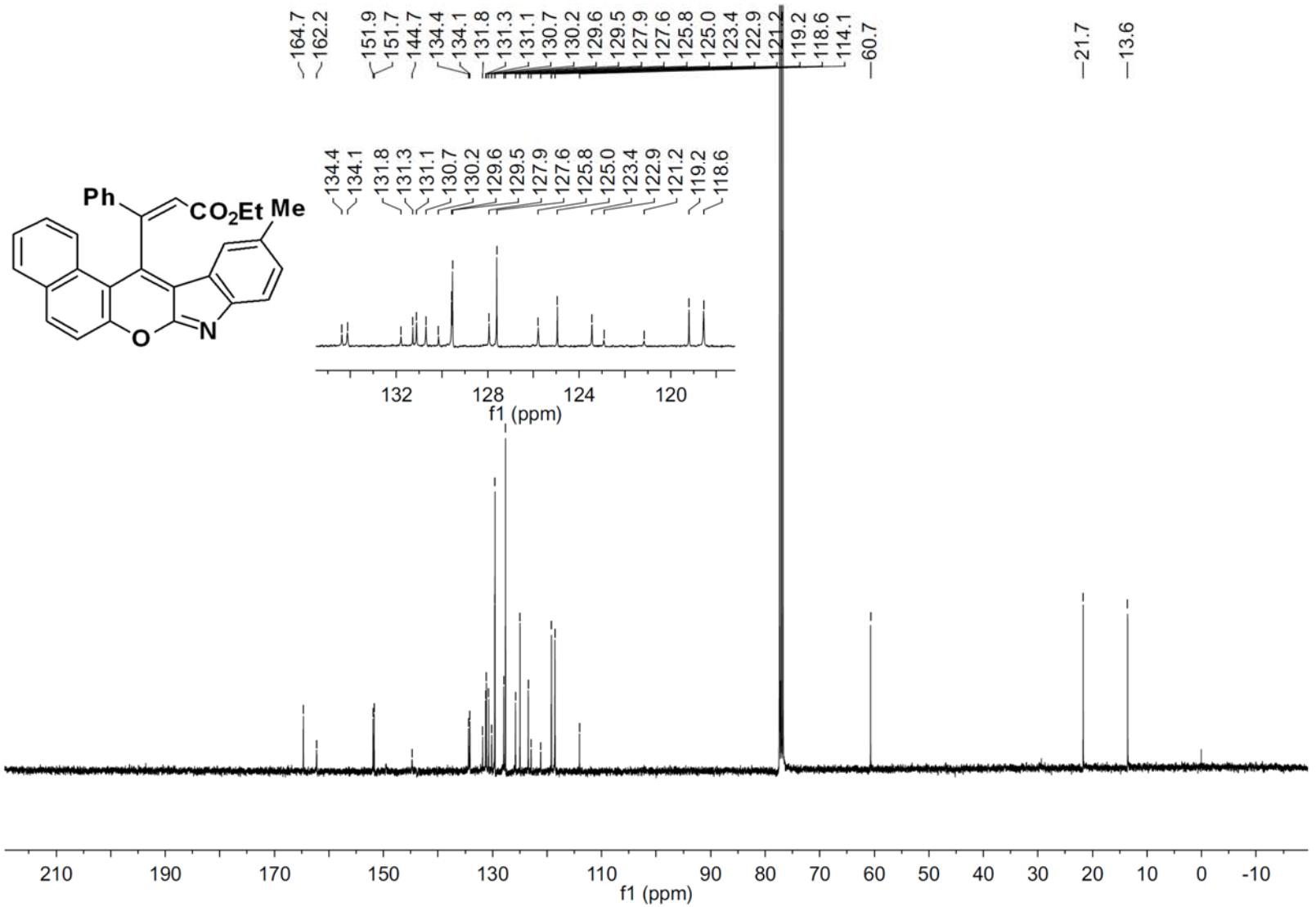
^{1}H NMR Spectrum of Compound 3p



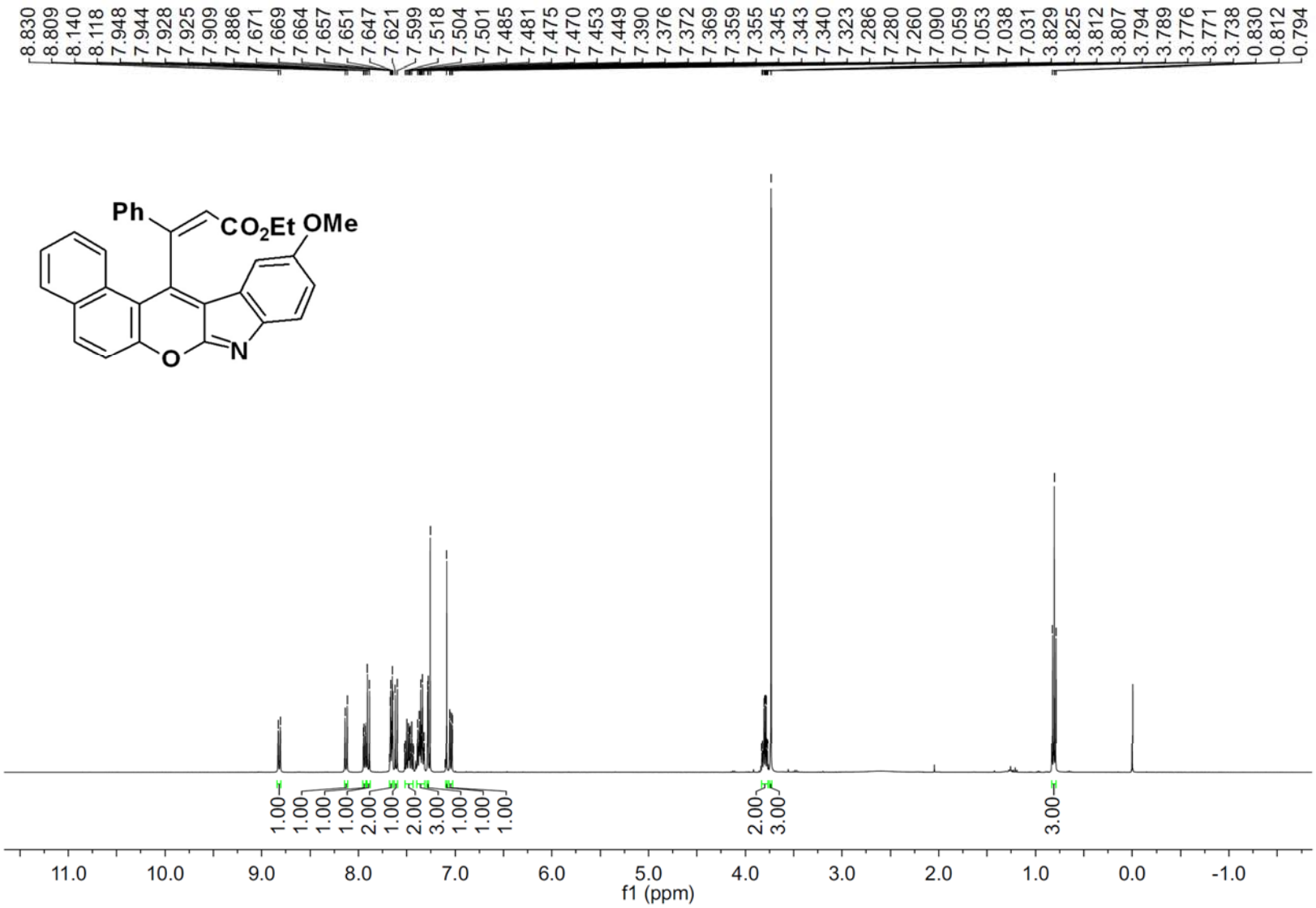
^{13}C NMR Spectrum of Compound 3p



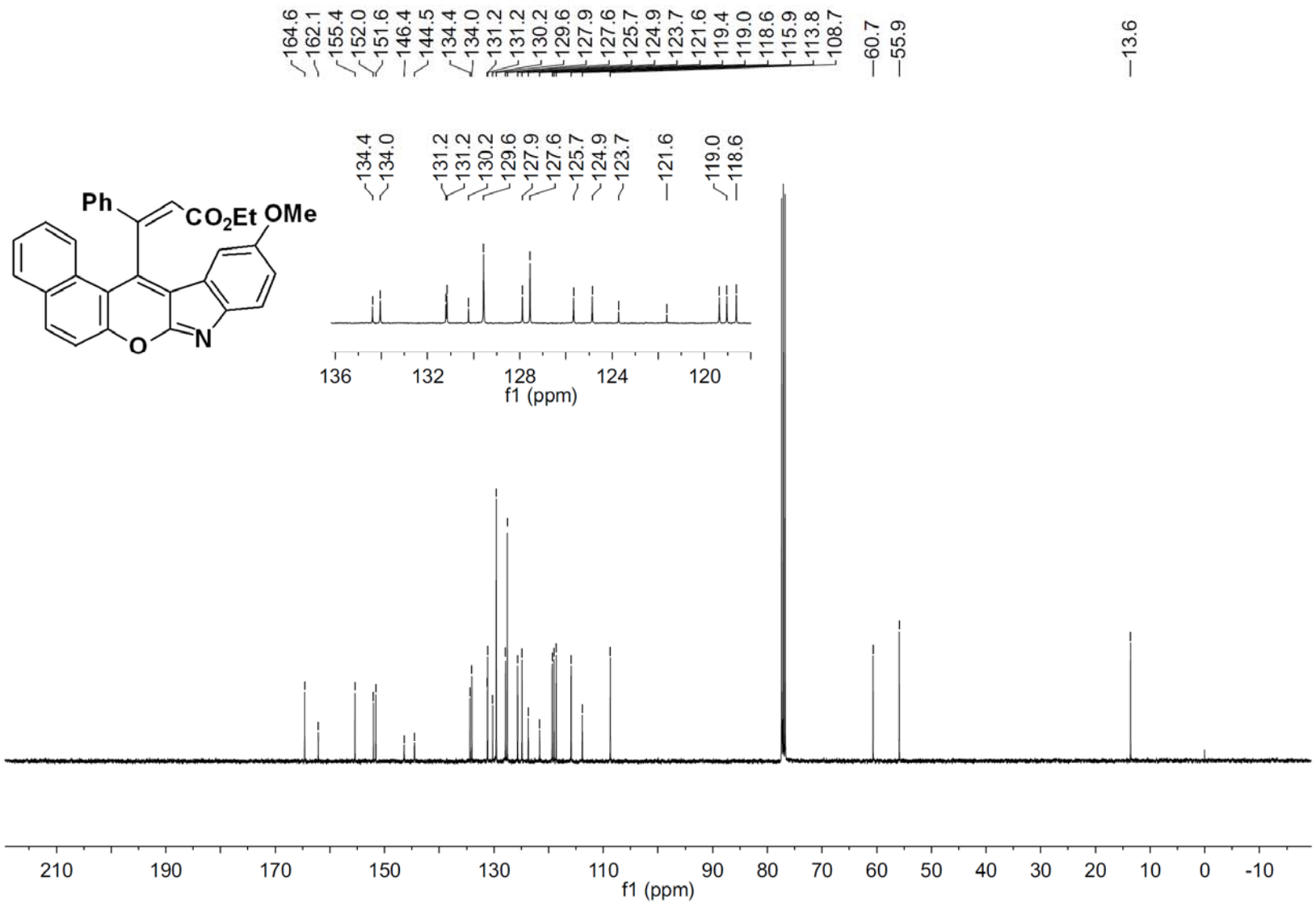
^{1}H NMR Spectrum of Compound 3q



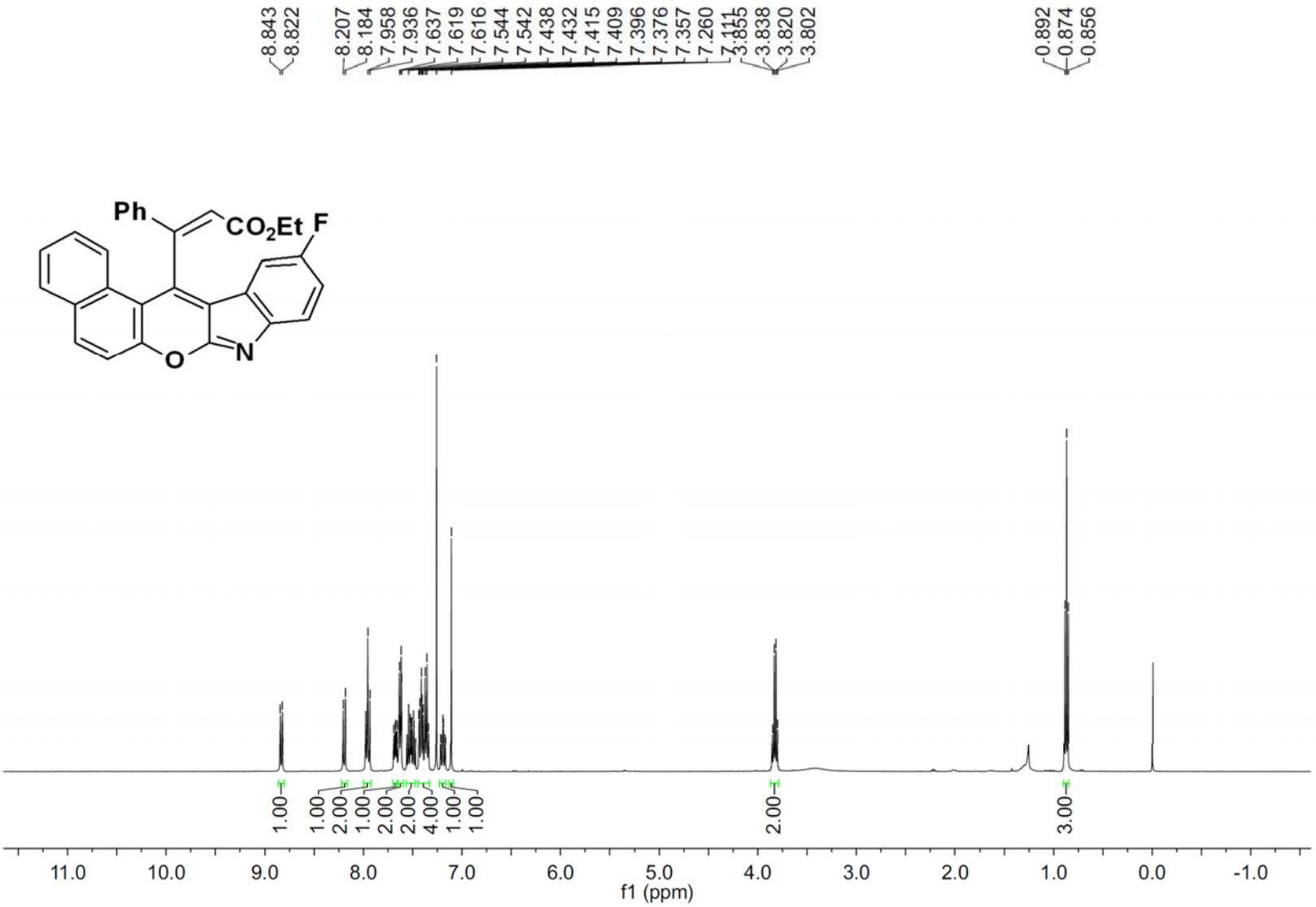
^{13}C NMR Spectrum of Compound 3q



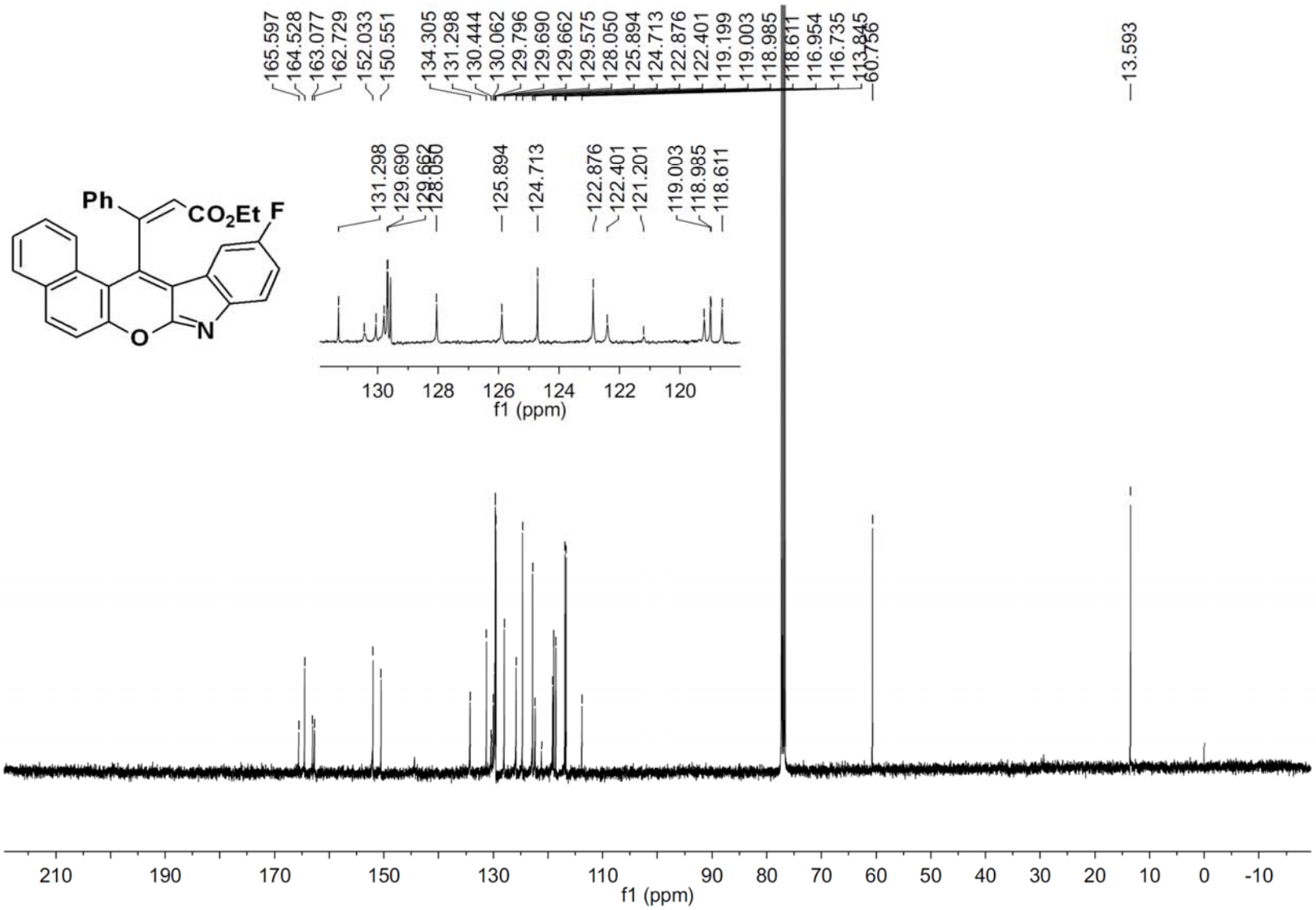
^{1}H NMR Spectrum of Compound 3r



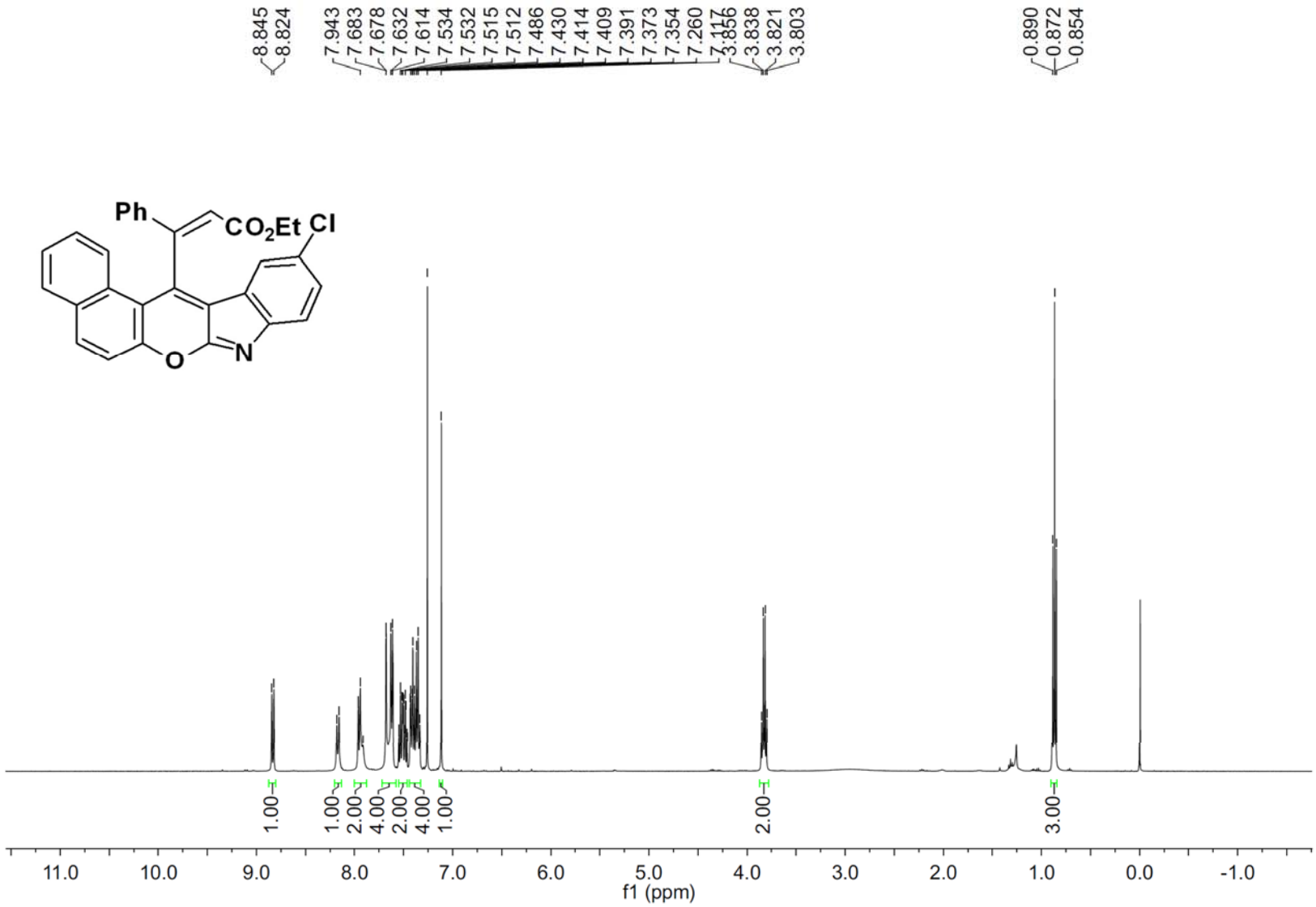
^{13}C NMR Spectrum of Compound 3r



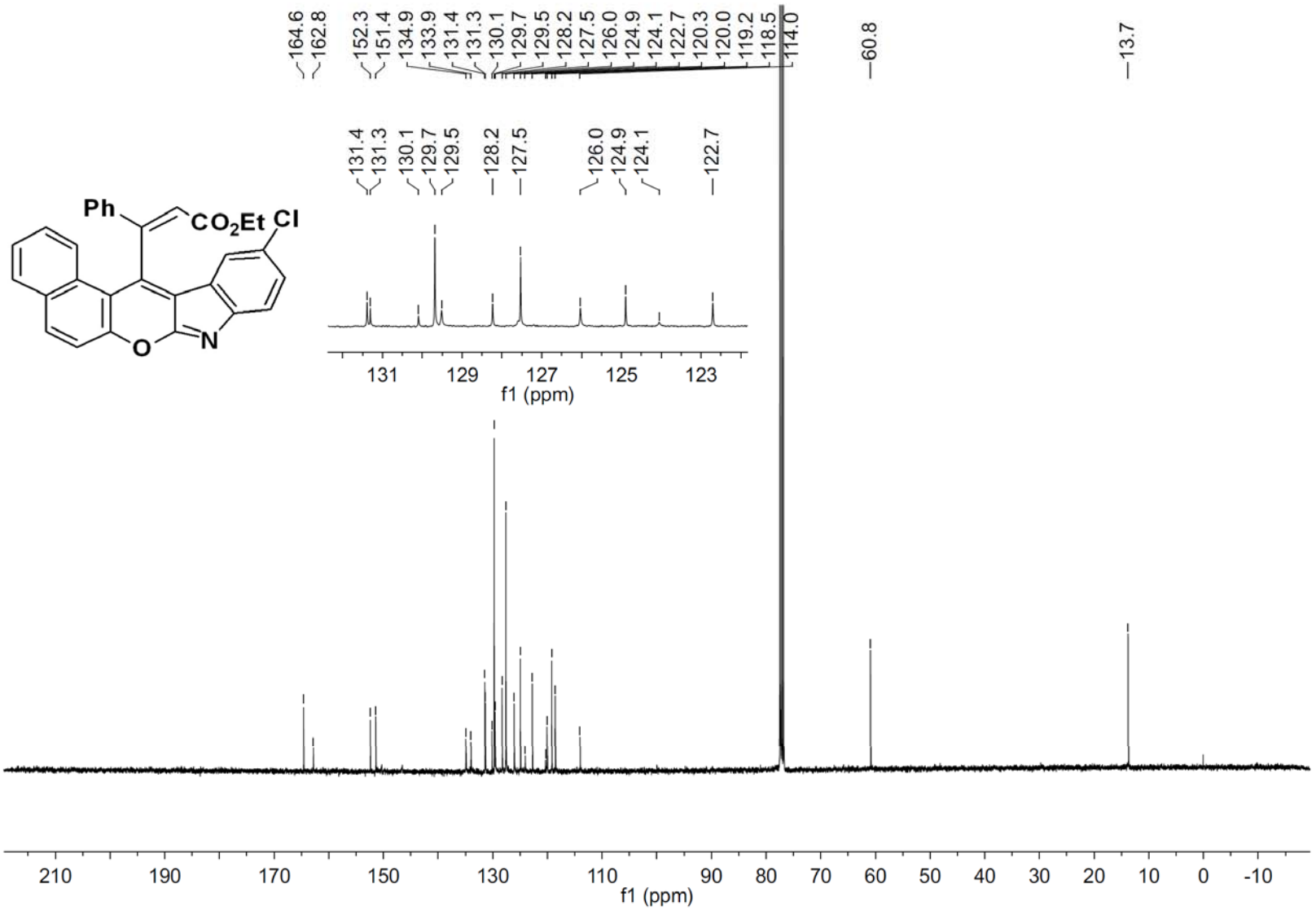
^{1}H NMR Spectrum of Compound 3s



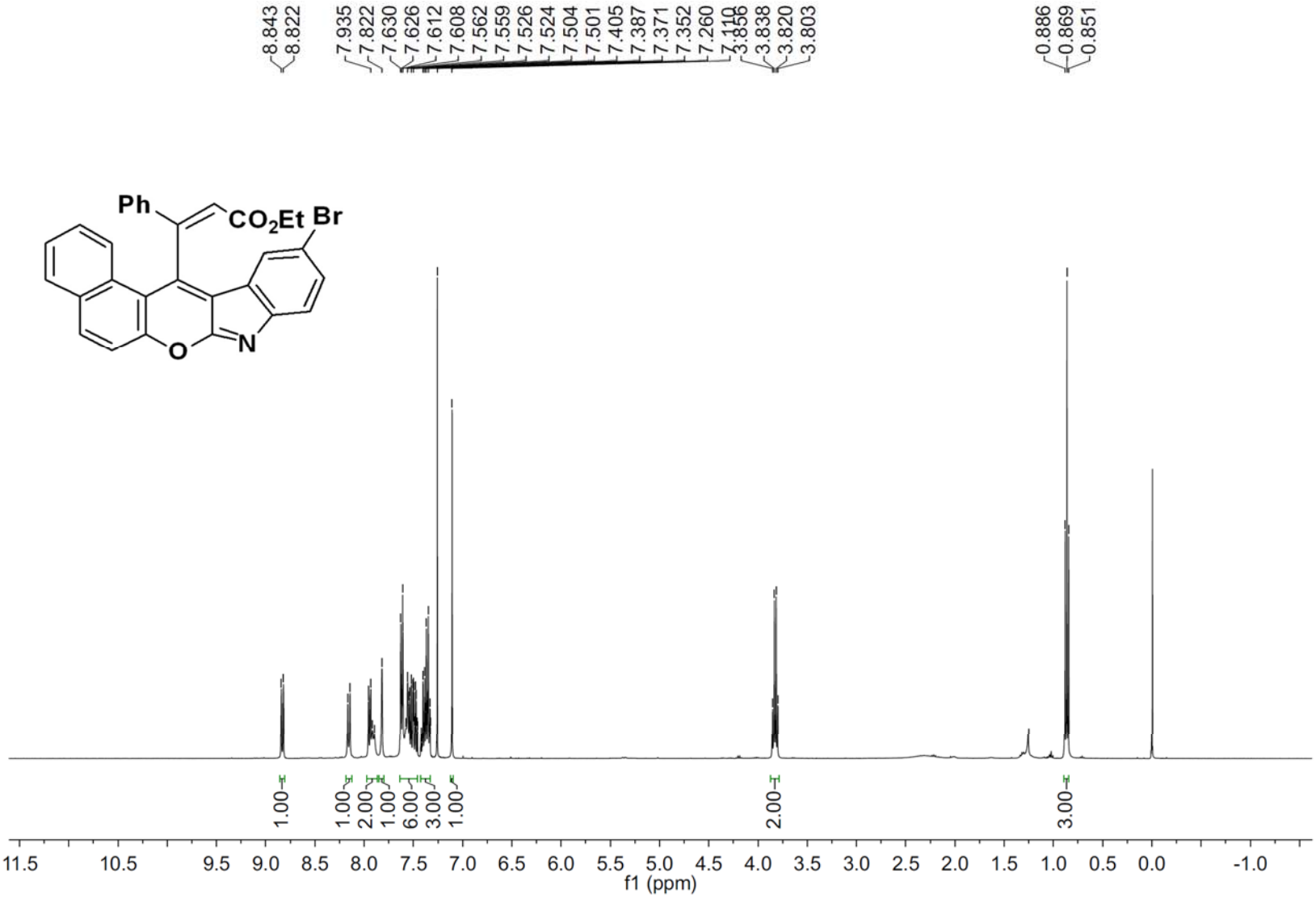
^{13}C NMR Spectrum of Compound 3s



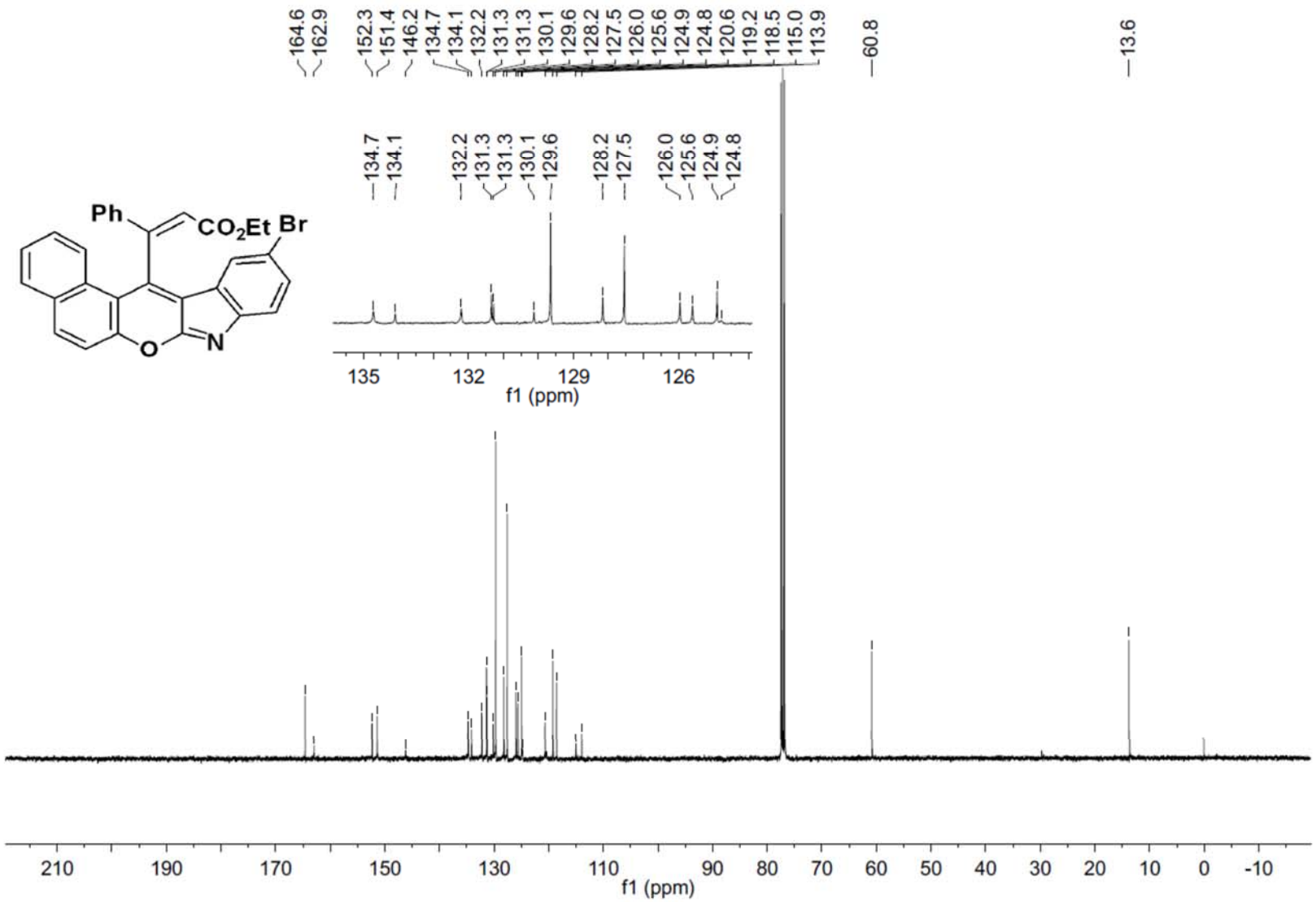
^{1}H NMR Spectrum of Compound 3t



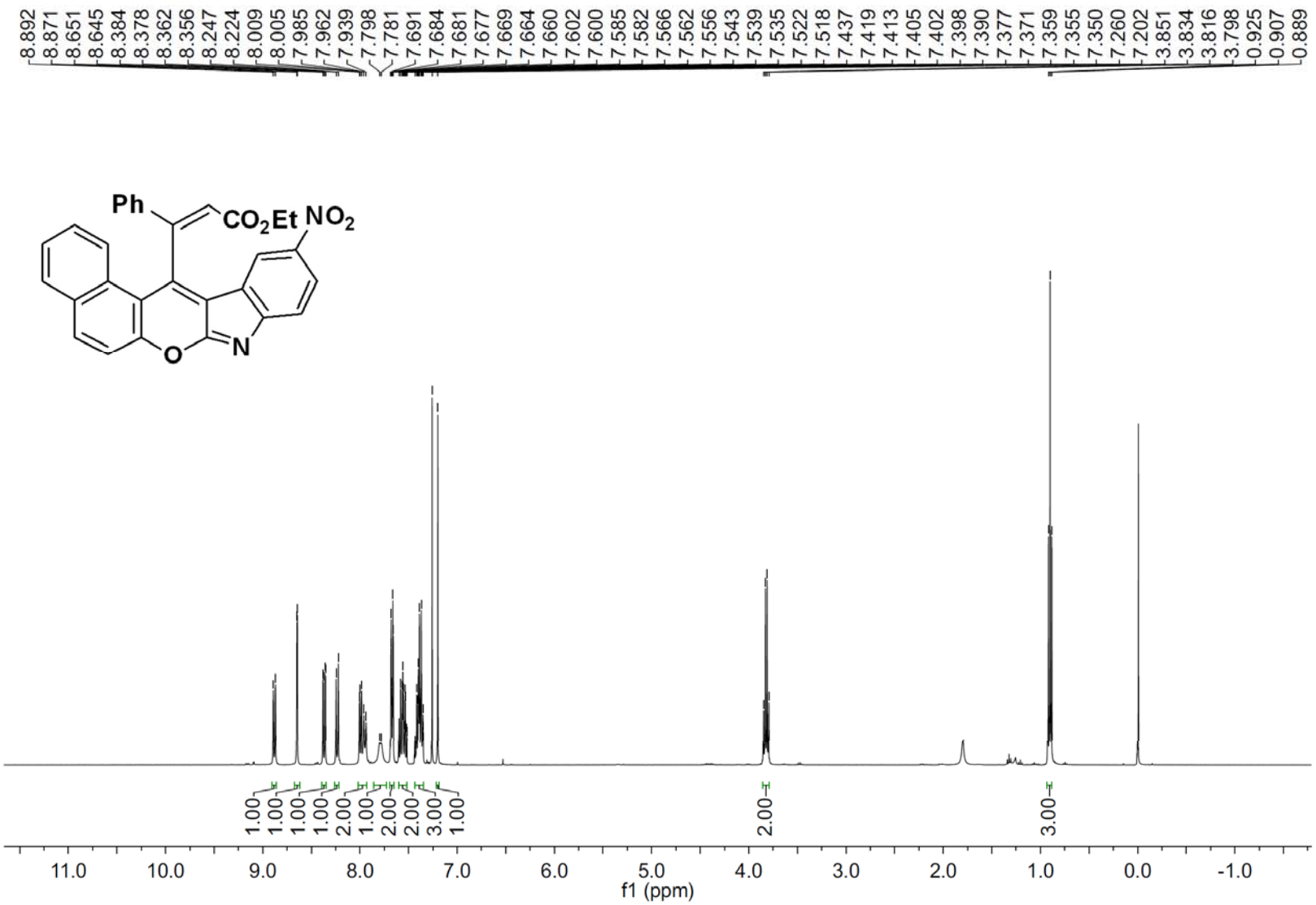
^{13}C NMR Spectrum of Compound 3t



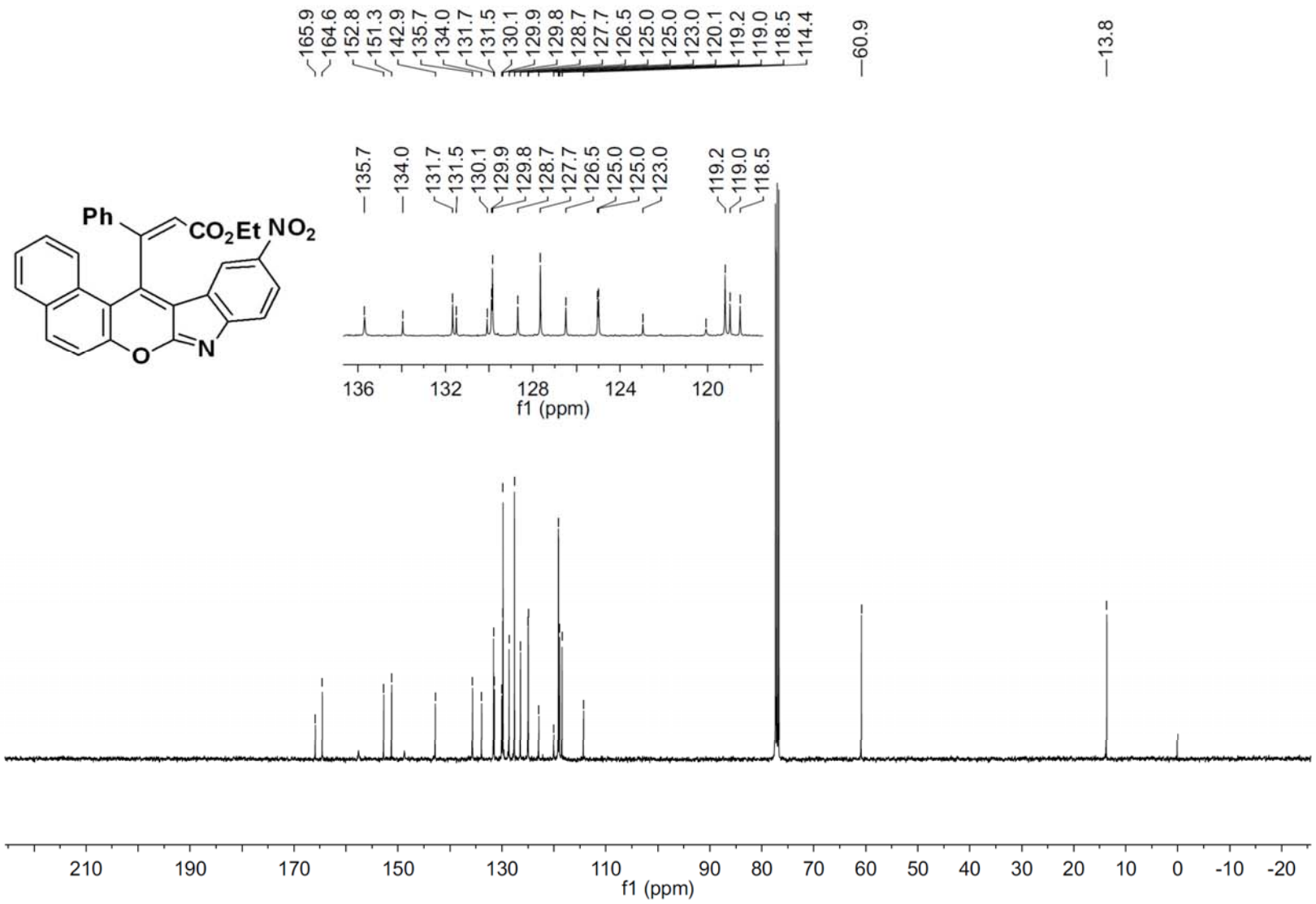
^{1}H NMR Spectrum of Compound 3u



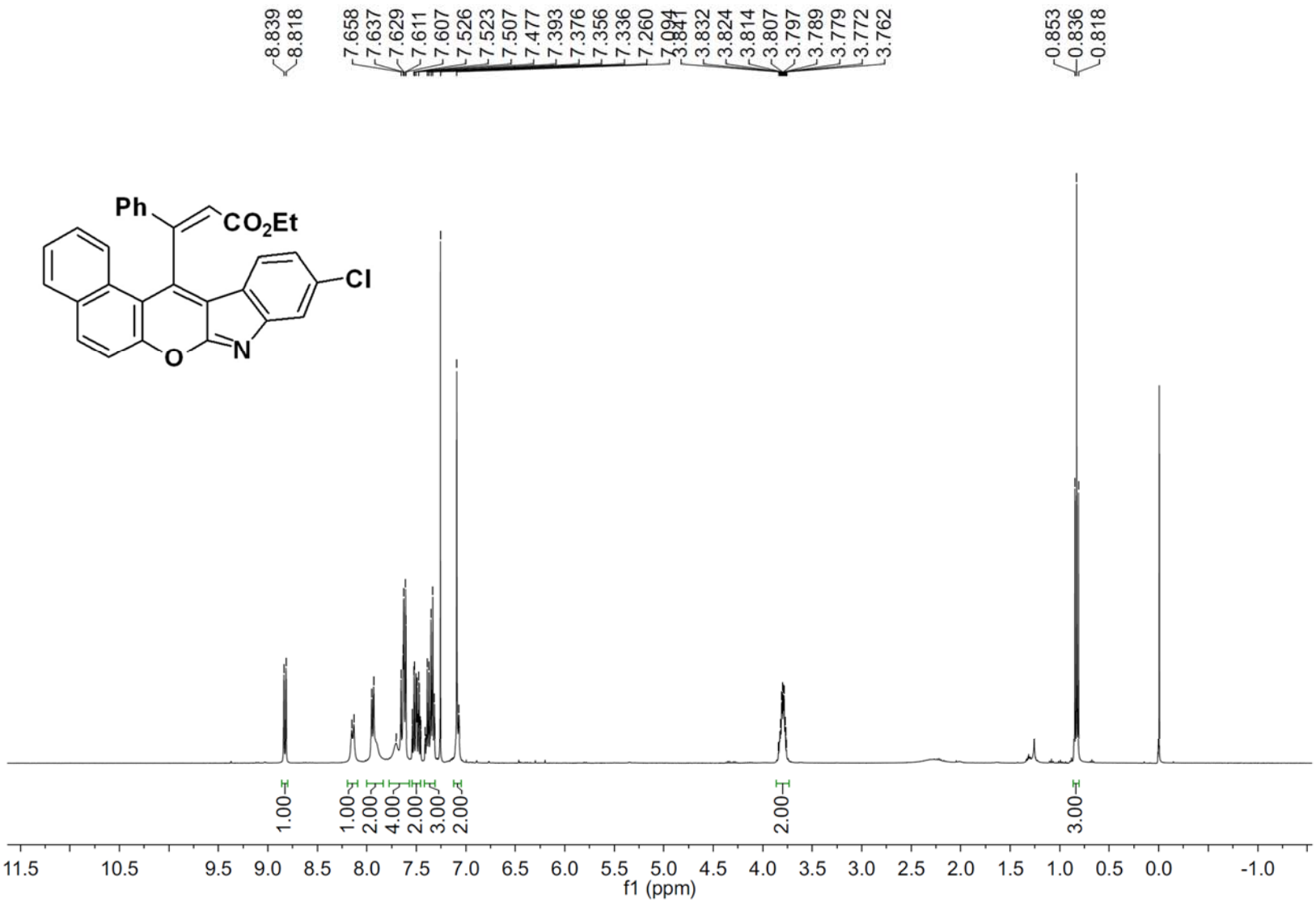
^{13}C NMR Spectrum of Compound 3u



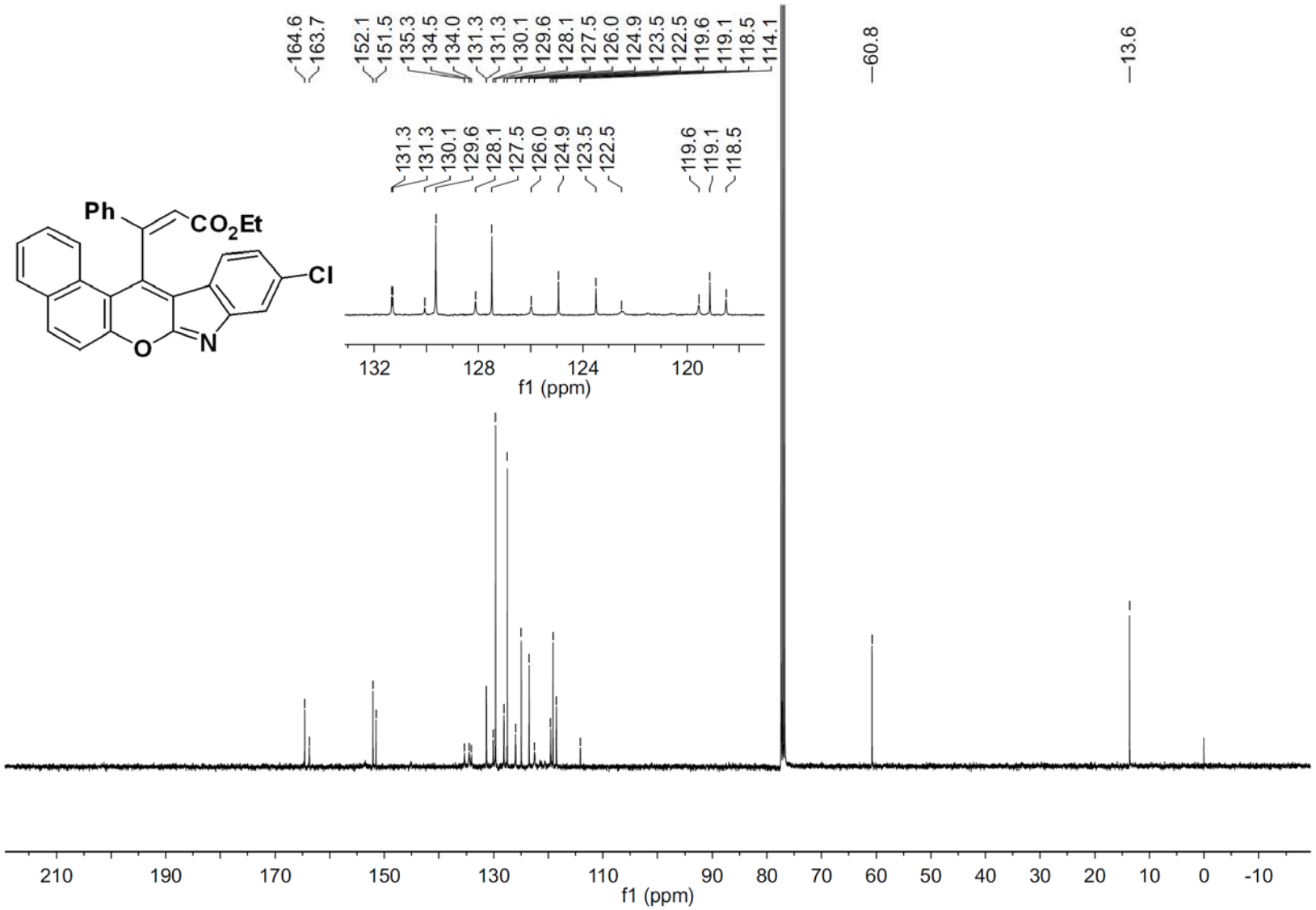
^{1}H NMR Spectrum of Compound 3v



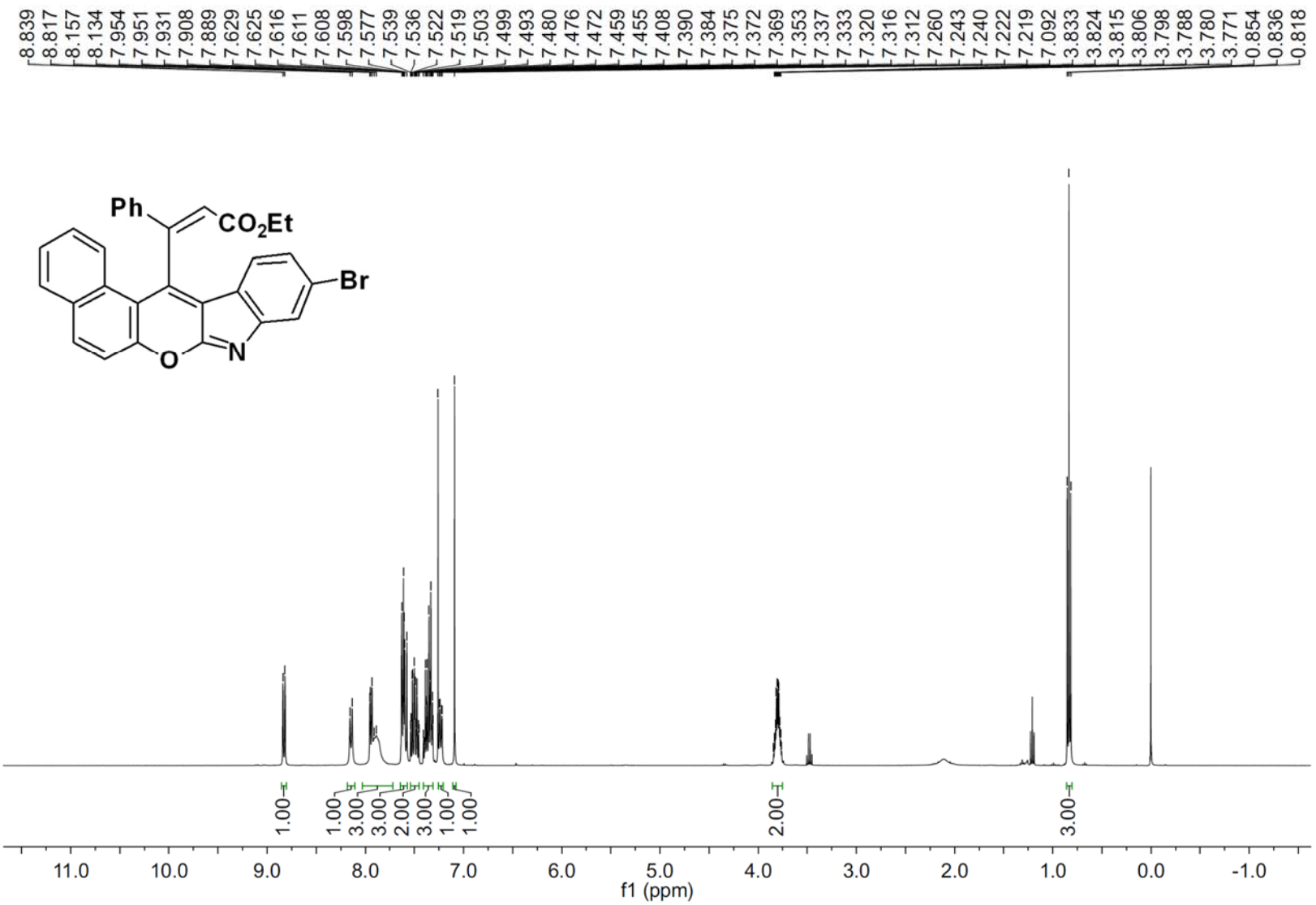
^{13}C NMR Spectrum of Compound 3v



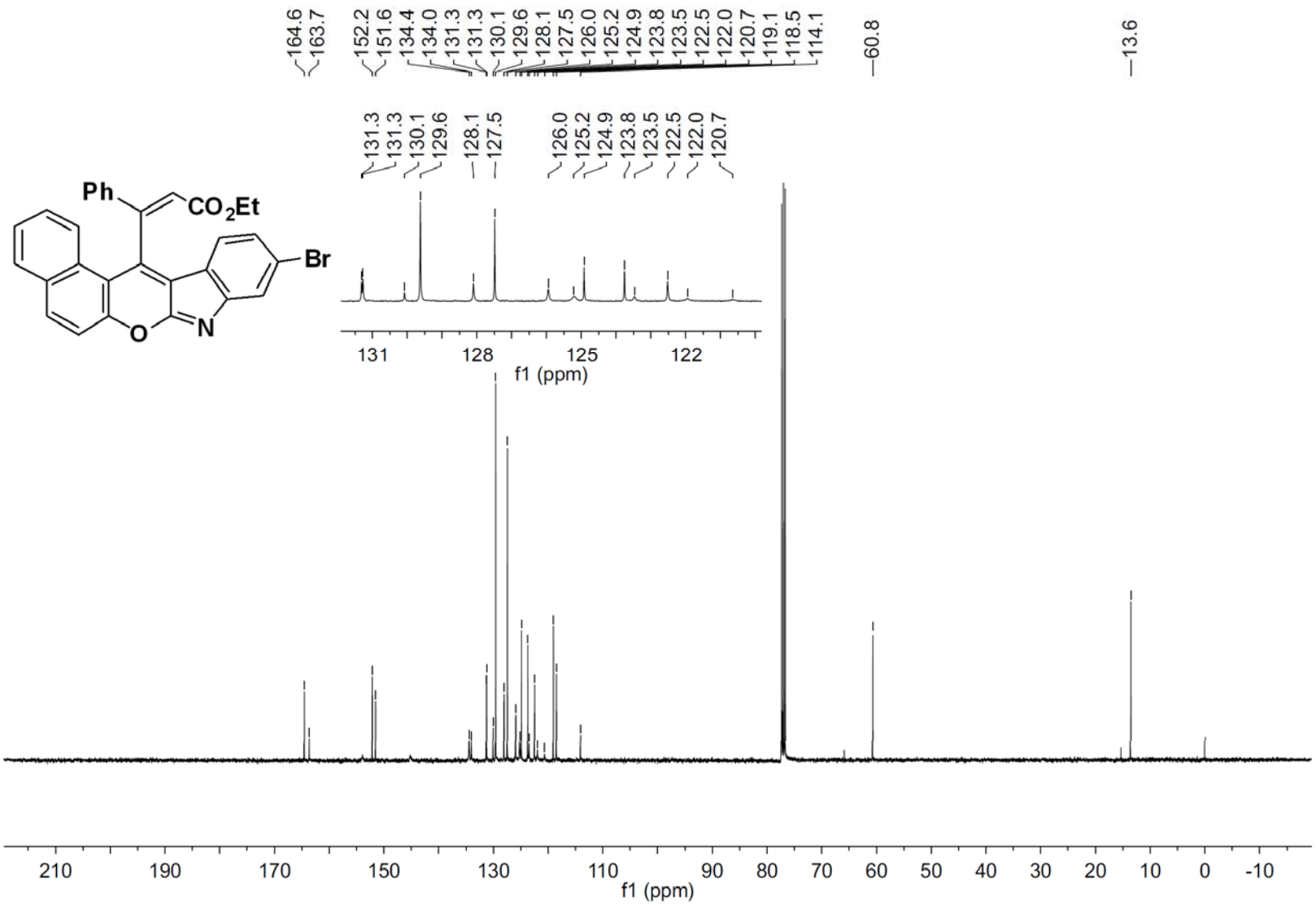
^{1}H NMR Spectrum of Compound 3w



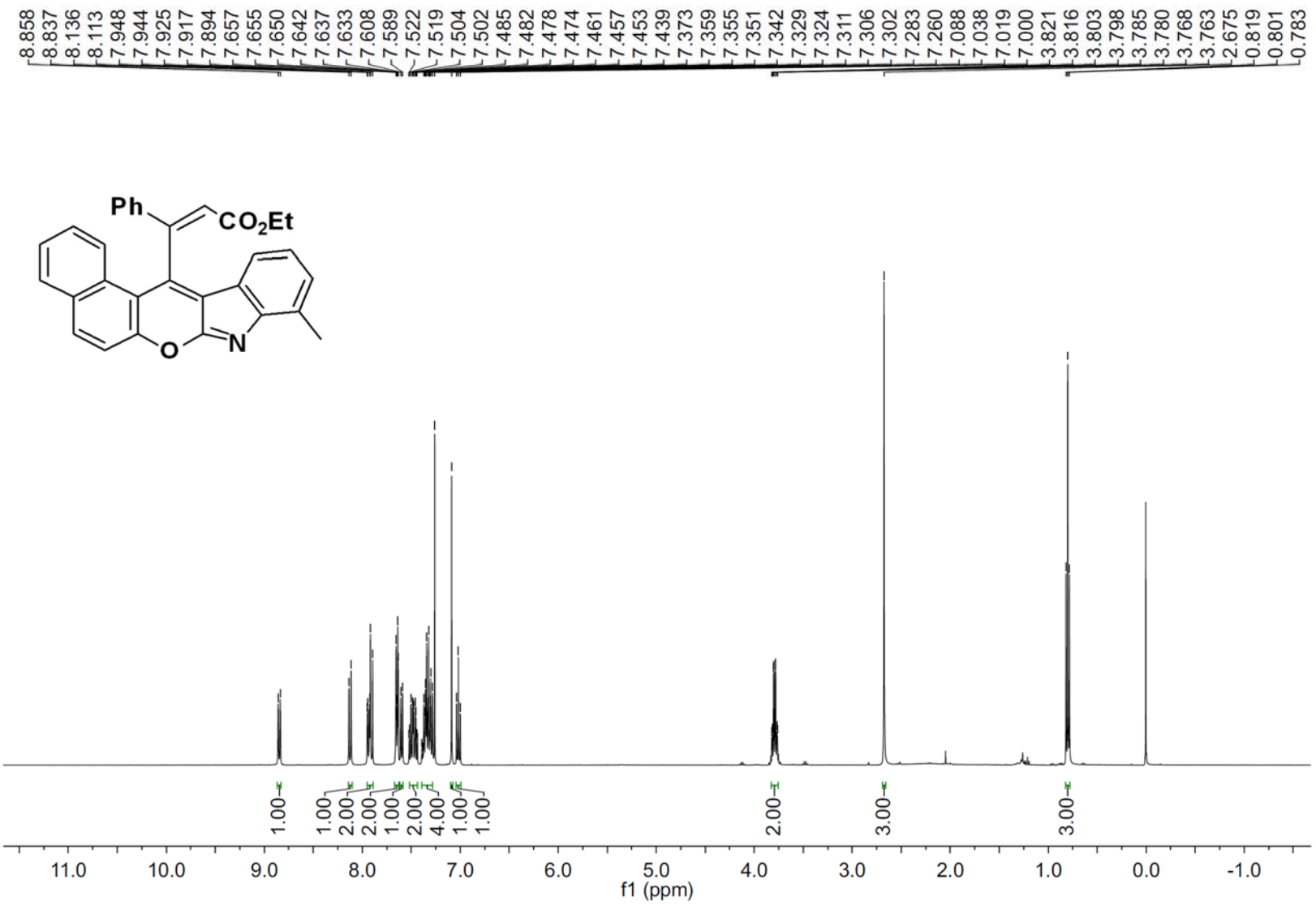
^{13}C NMR Spectrum of Compound 3w



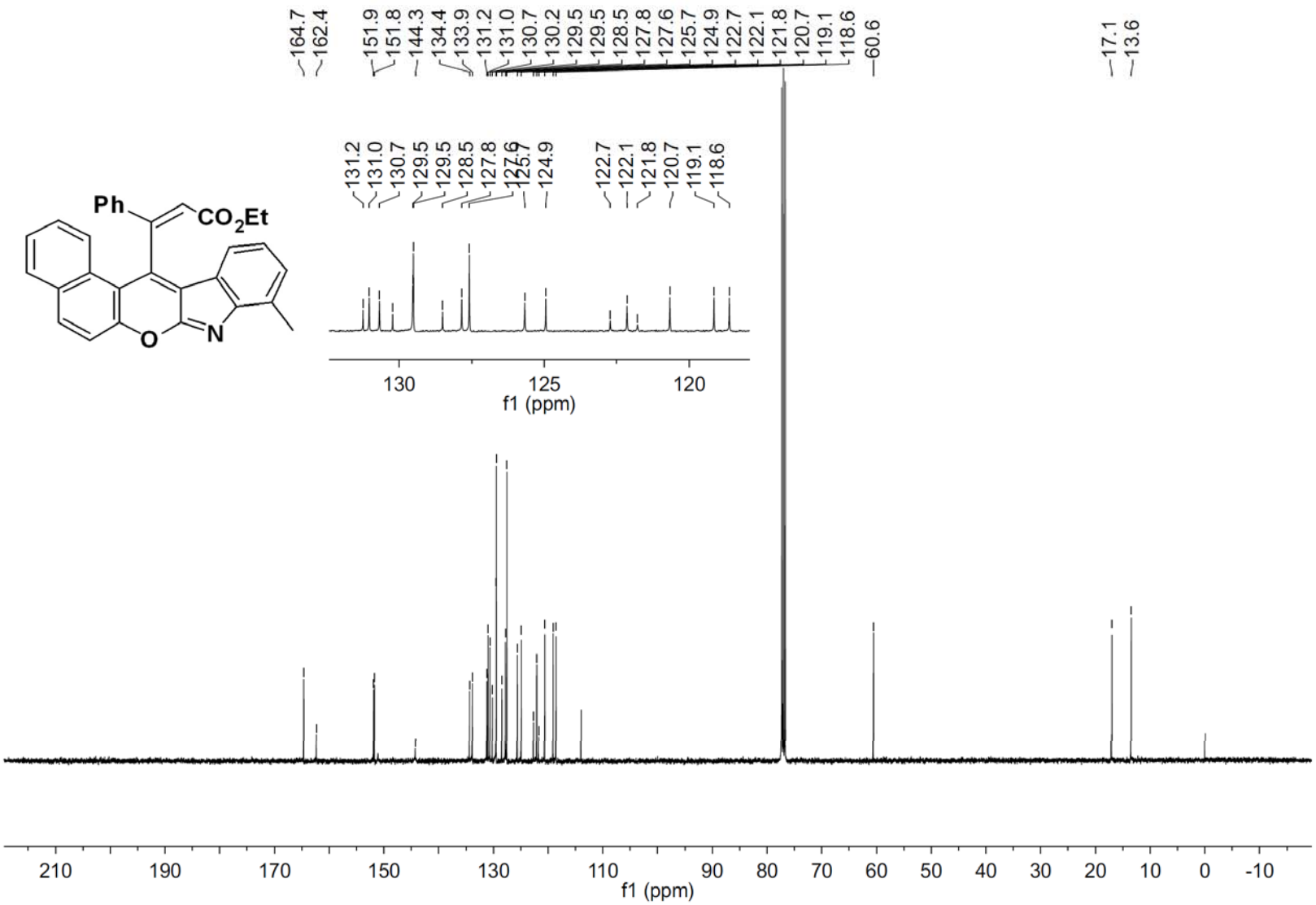
^{1}H NMR Spectrum of Compound 3x



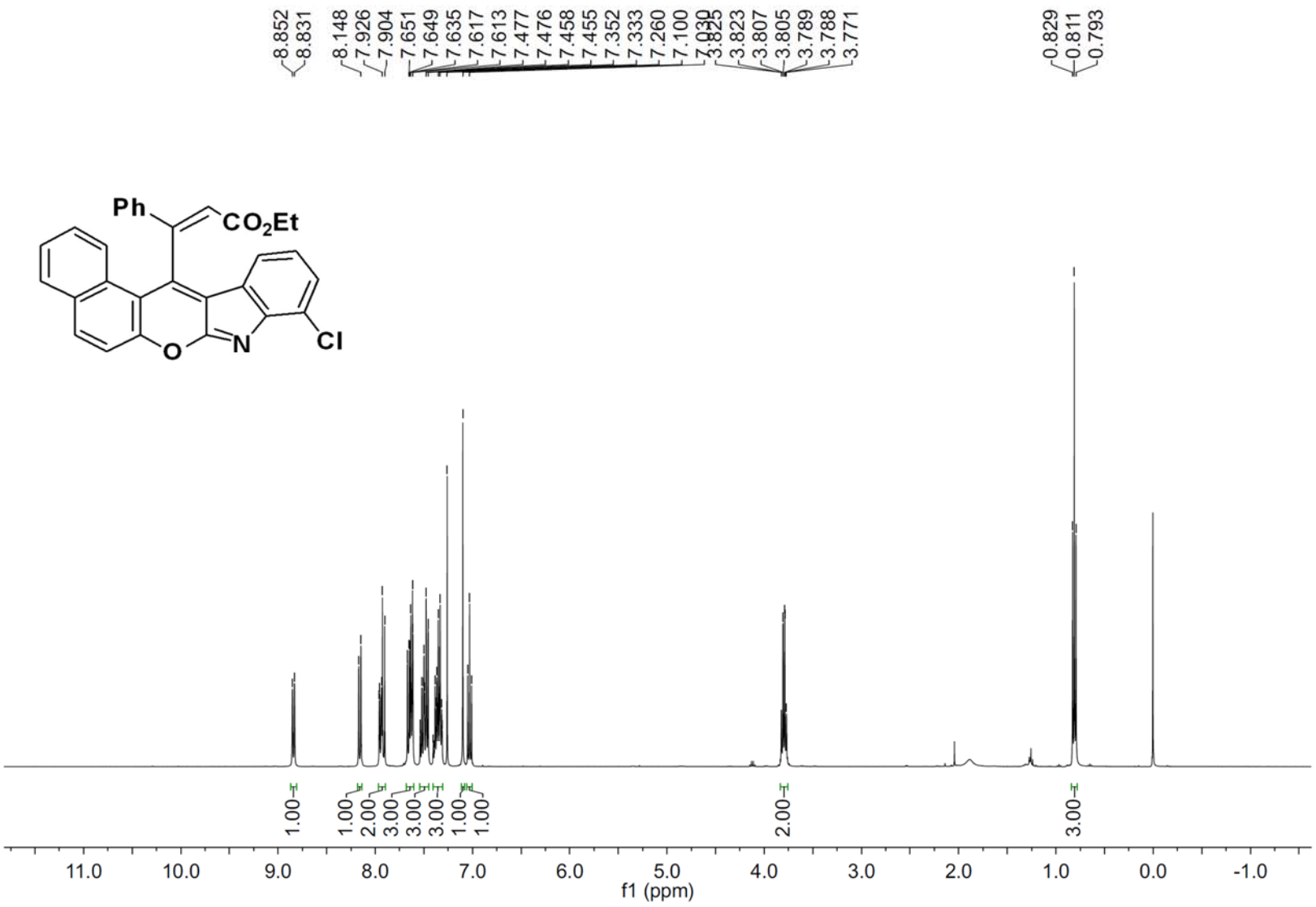
^{13}C NMR Spectrum of Compound 3x



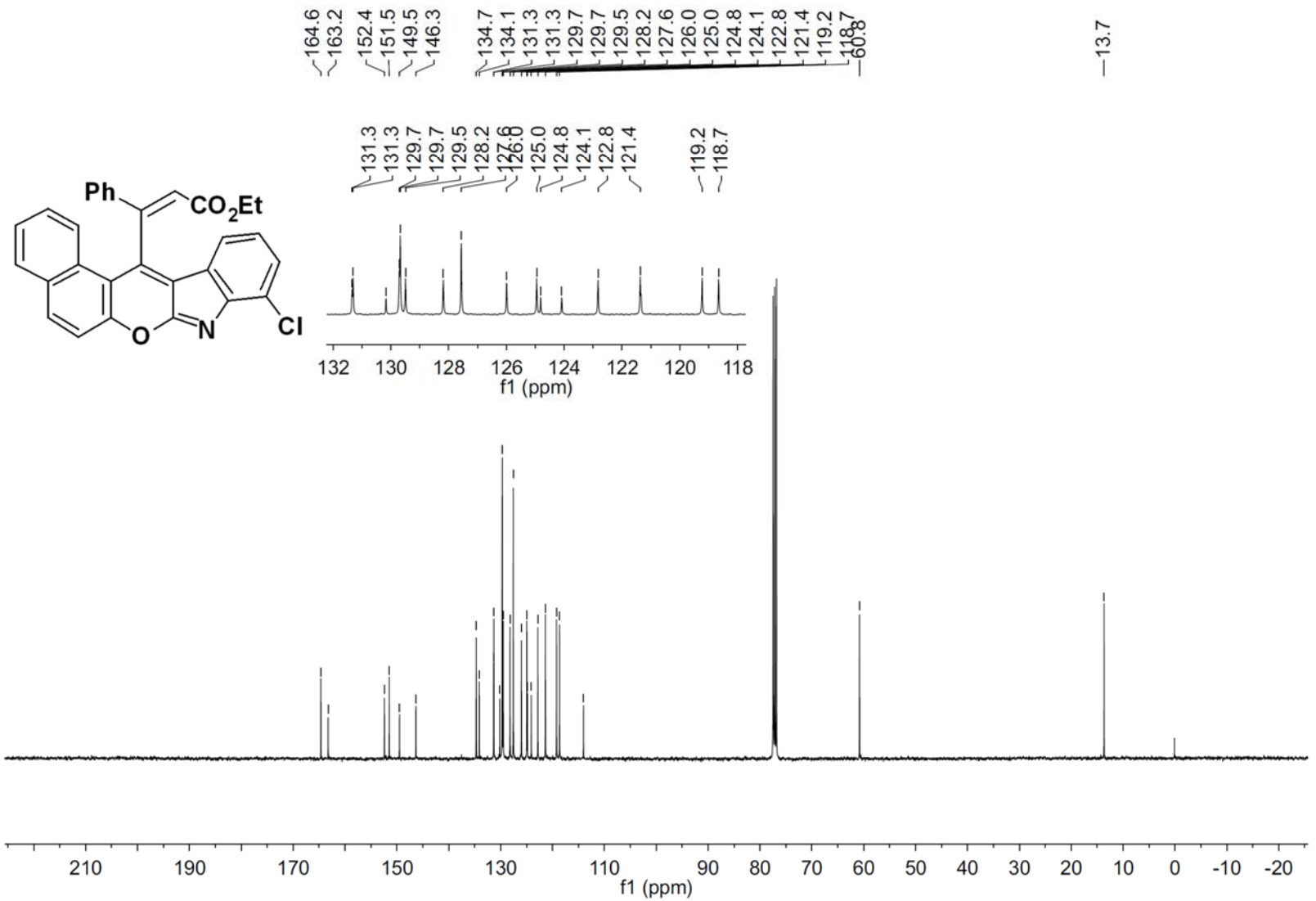
^{1}H NMR Spectrum of Compound 3y



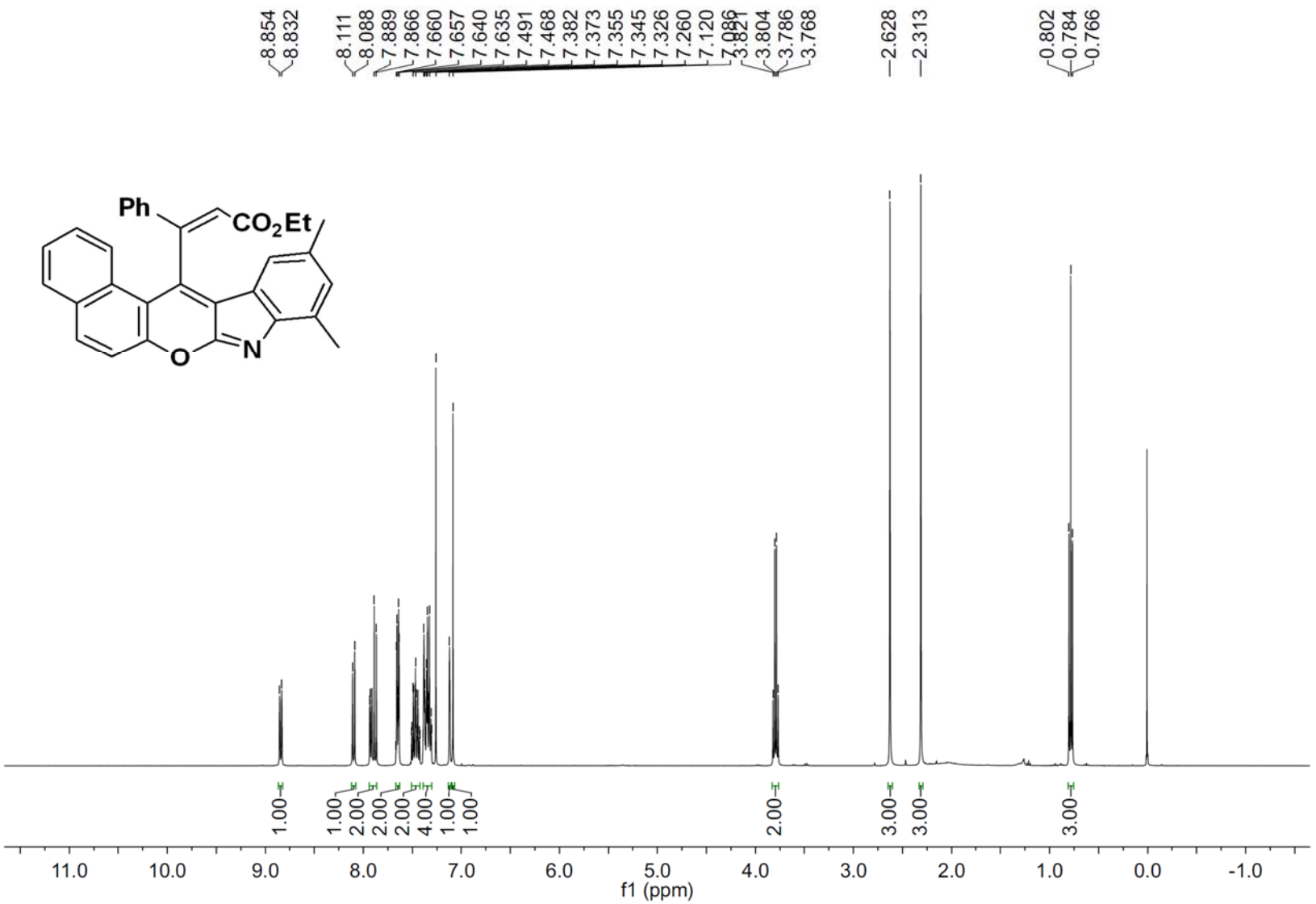
^{13}C NMR Spectrum of Compound 3y



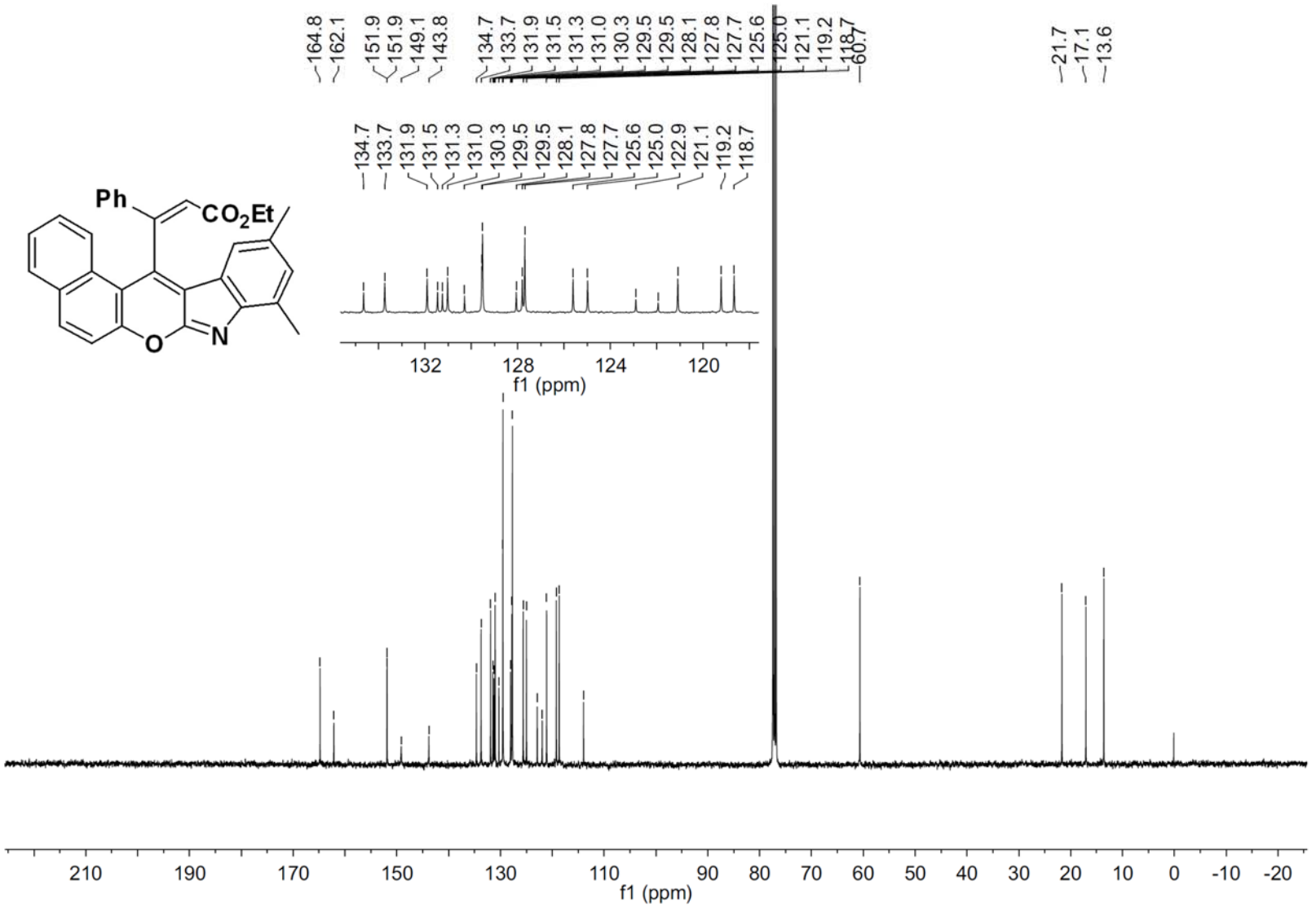
^{1}H NMR Spectrum of Compound 3z



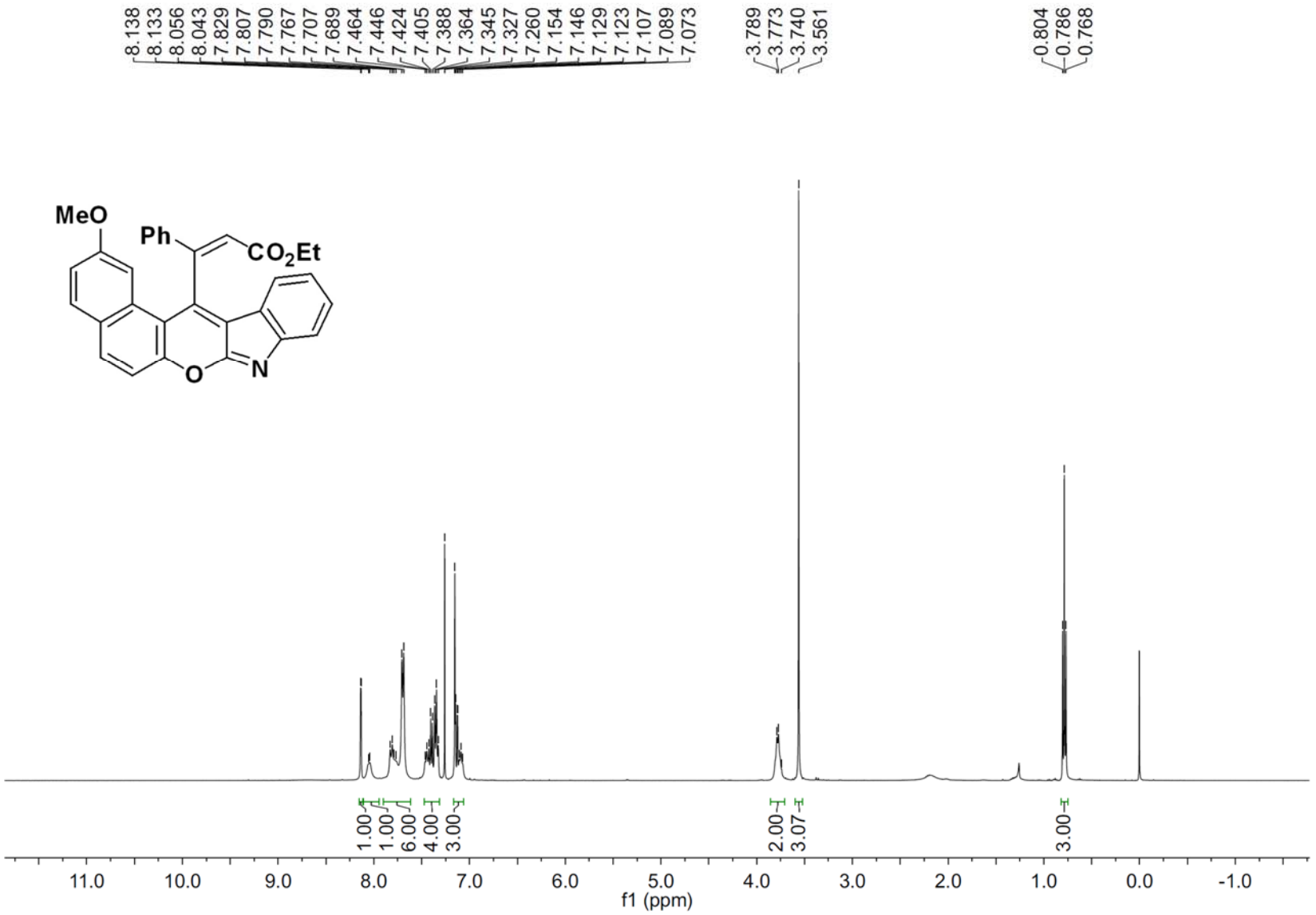
^{13}C NMR Spectrum of Compound 3z



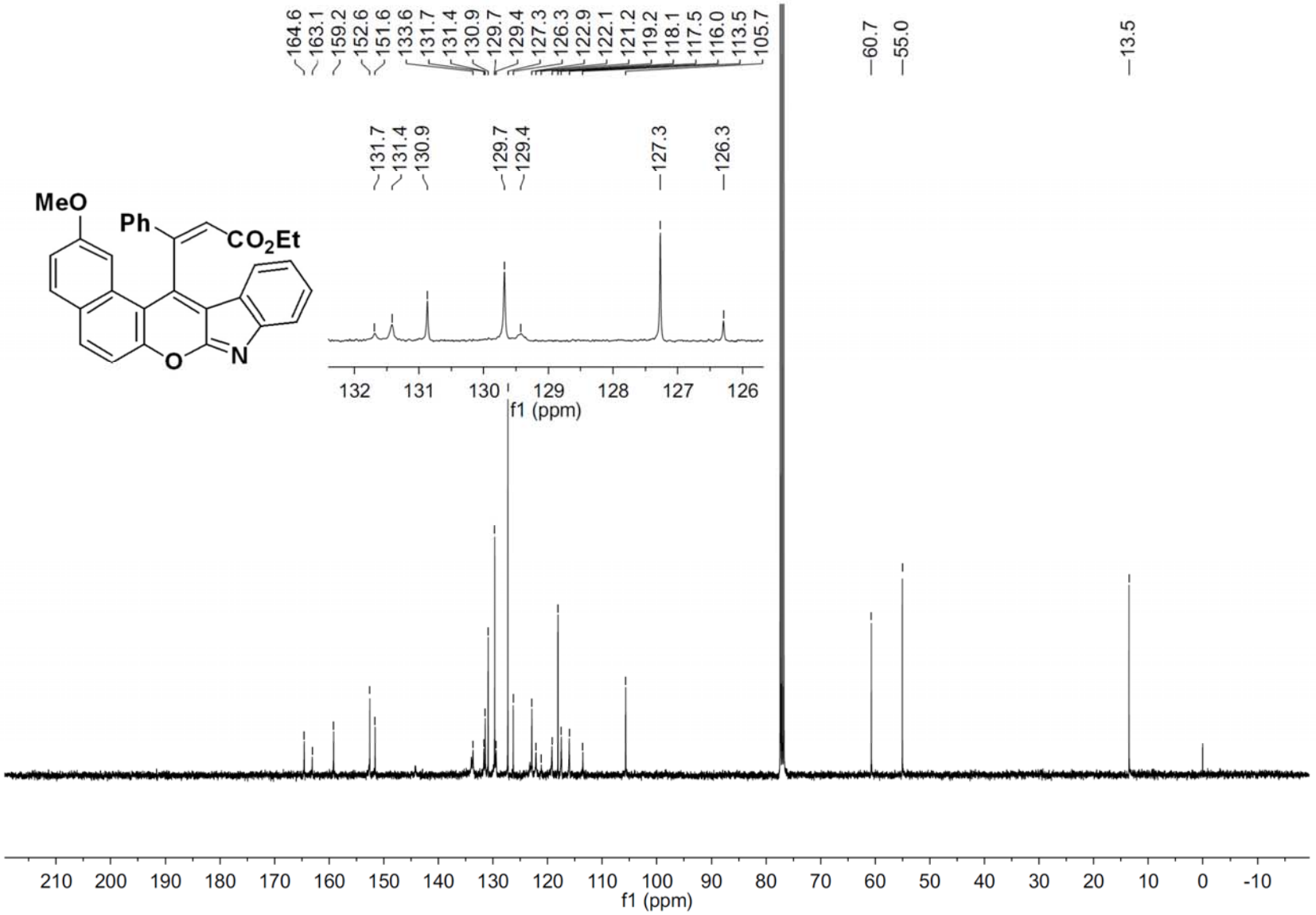
^{1}H NMR Spectrum of Compound 3aa



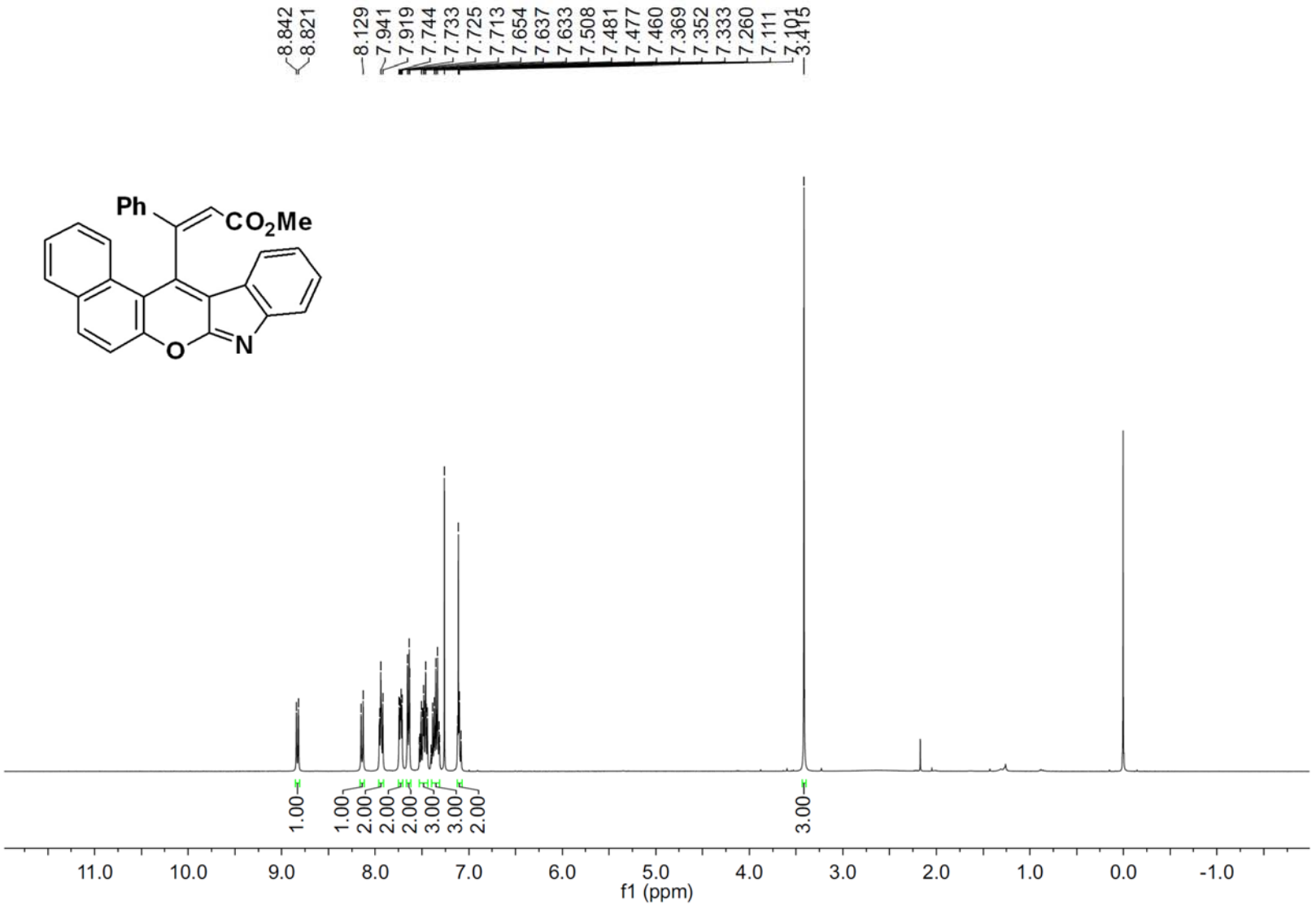
^{13}C NMR Spectrum of Compound 3aa



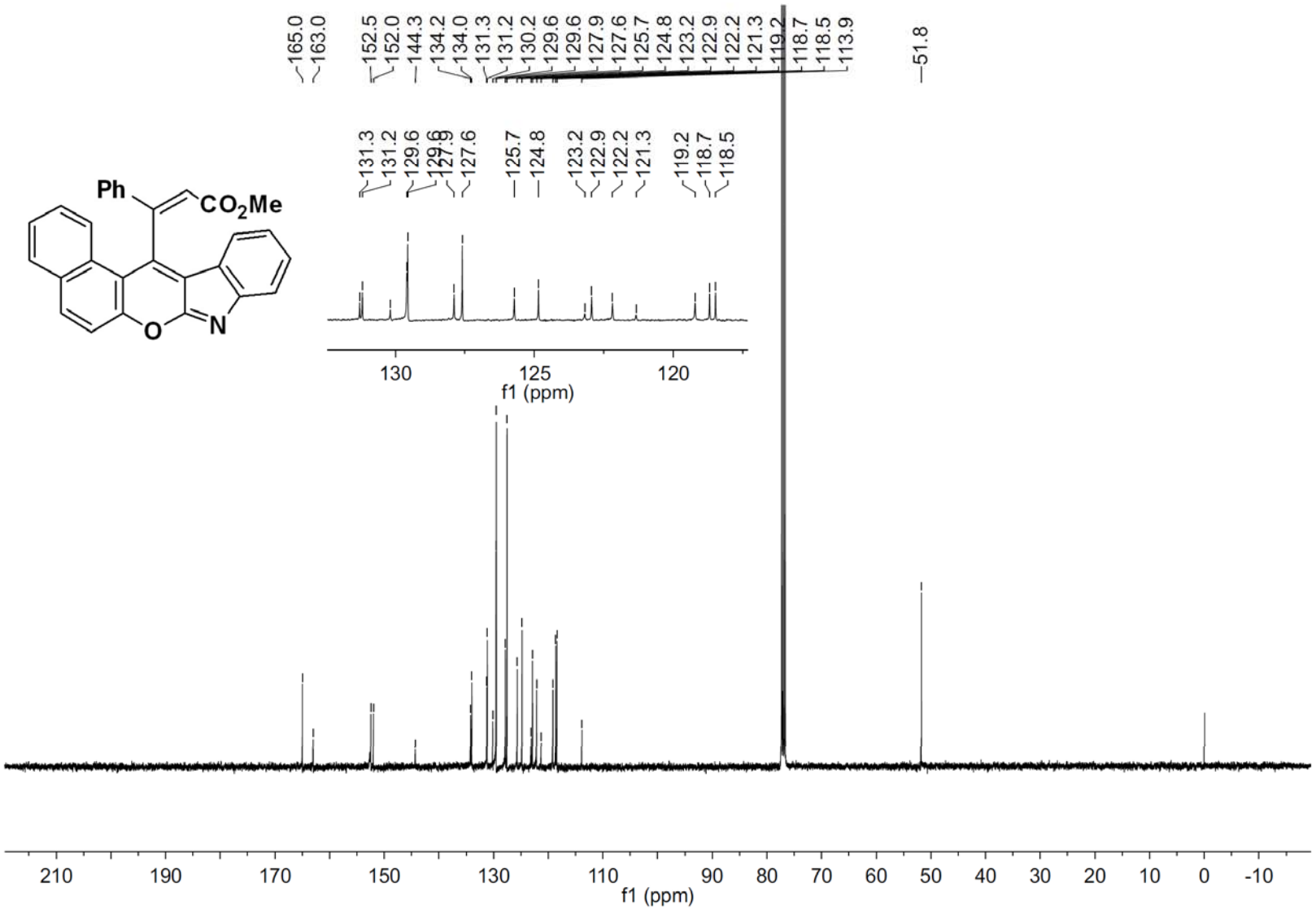
^{1}H NMR Spectrum of Compound 3bb



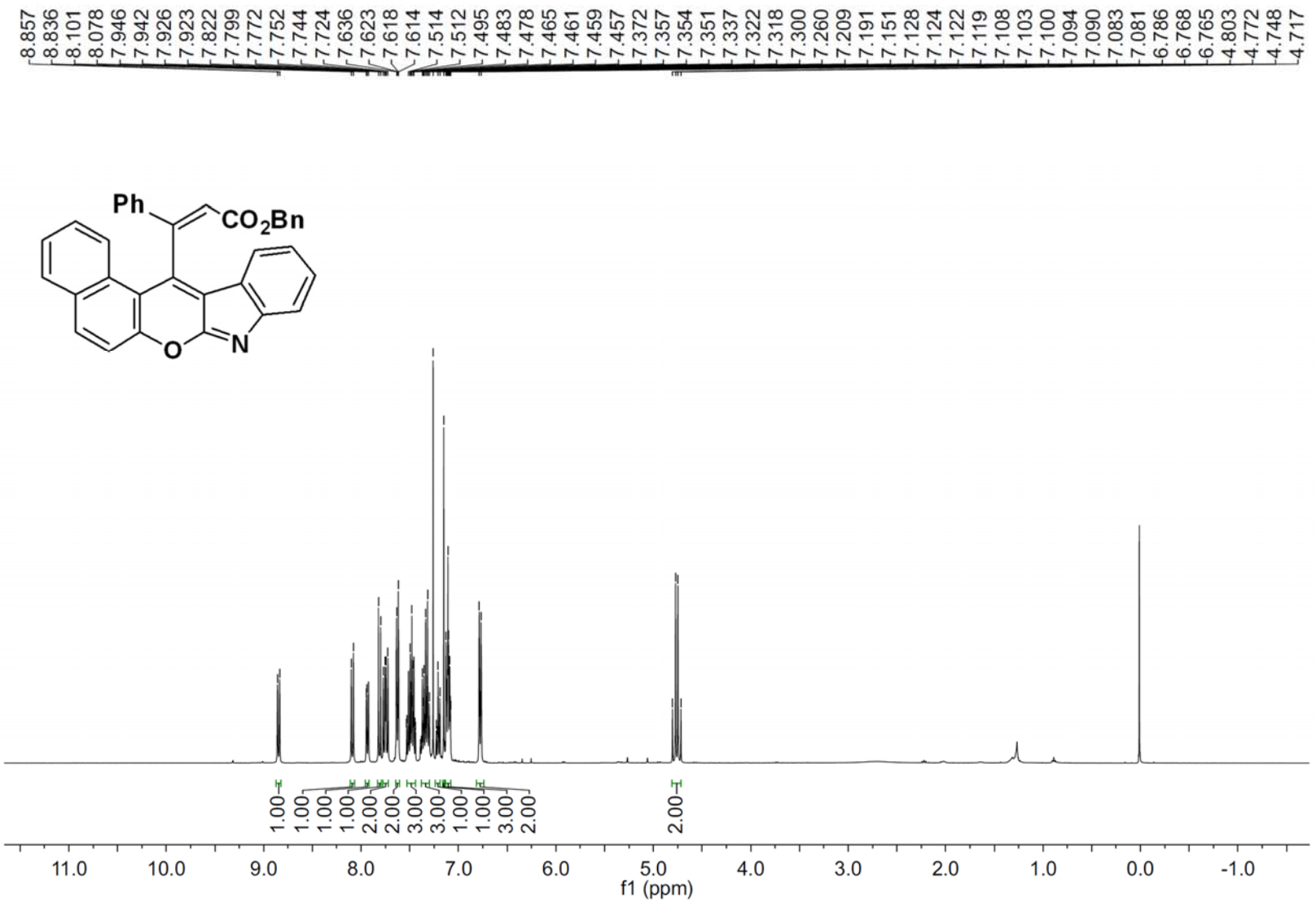
^{13}C NMR Spectrum of Compound 3bb



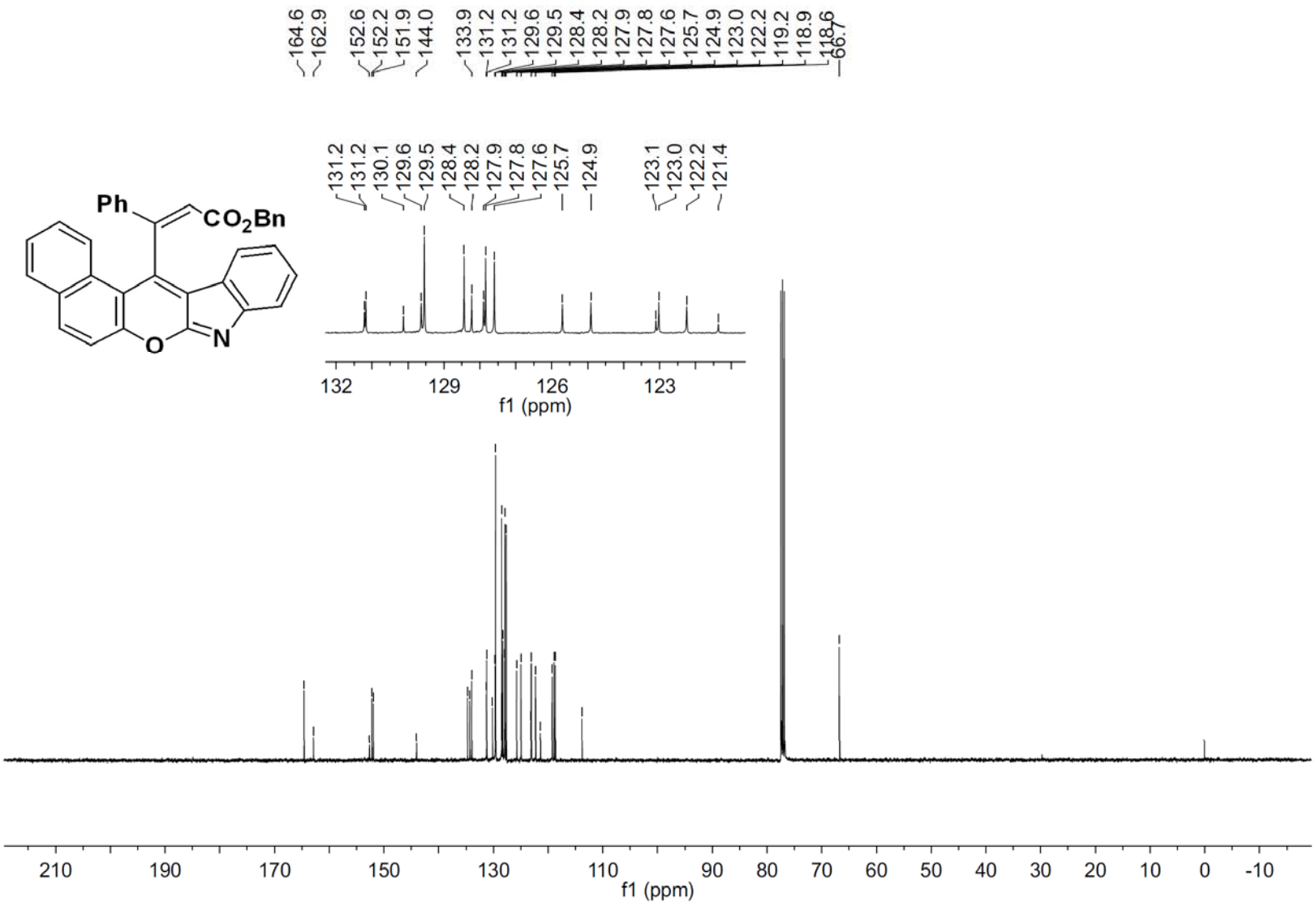
^{1}H NMR Spectrum of Compound 3cc



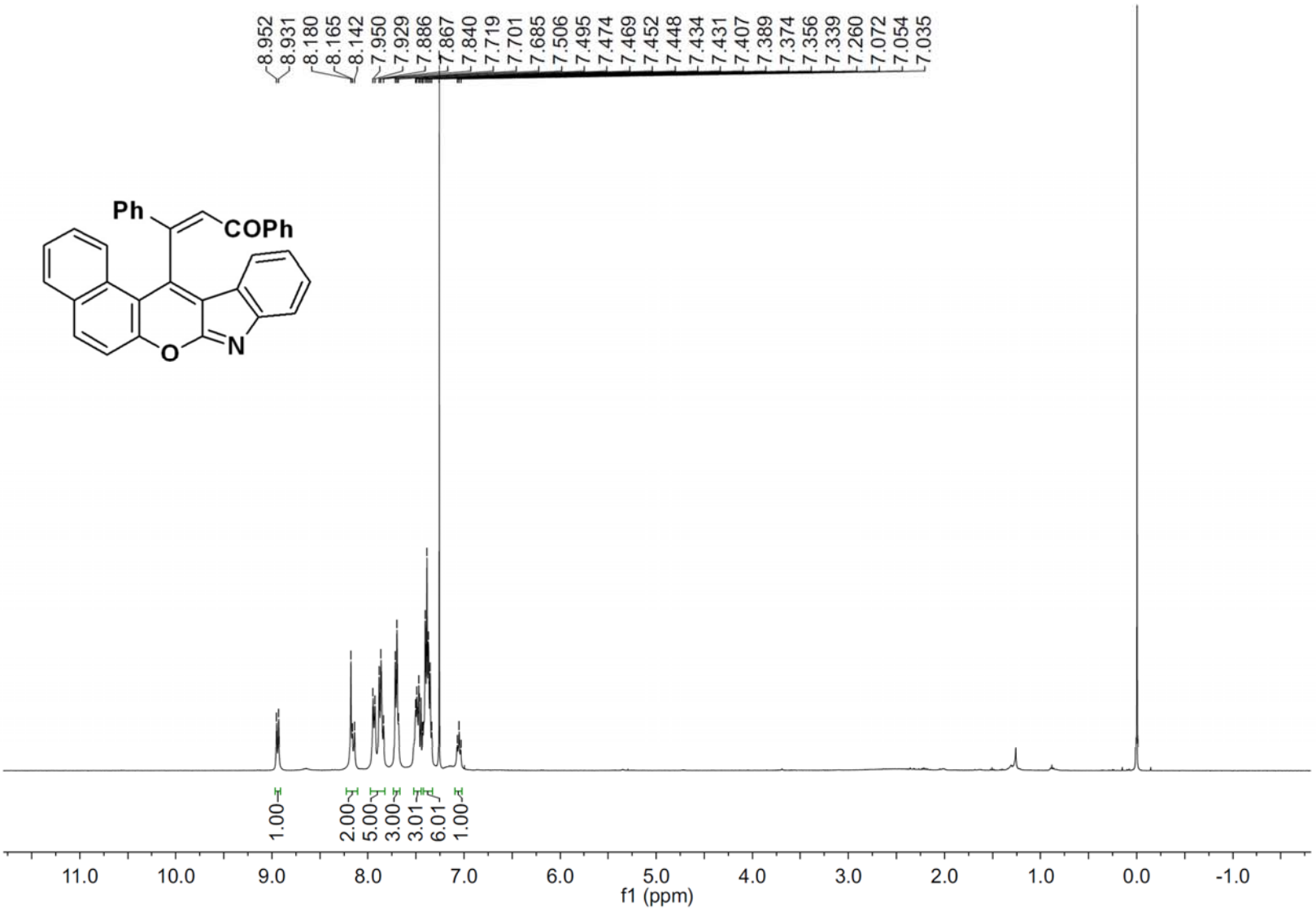
^{13}C NMR Spectrum of Compound 3cc



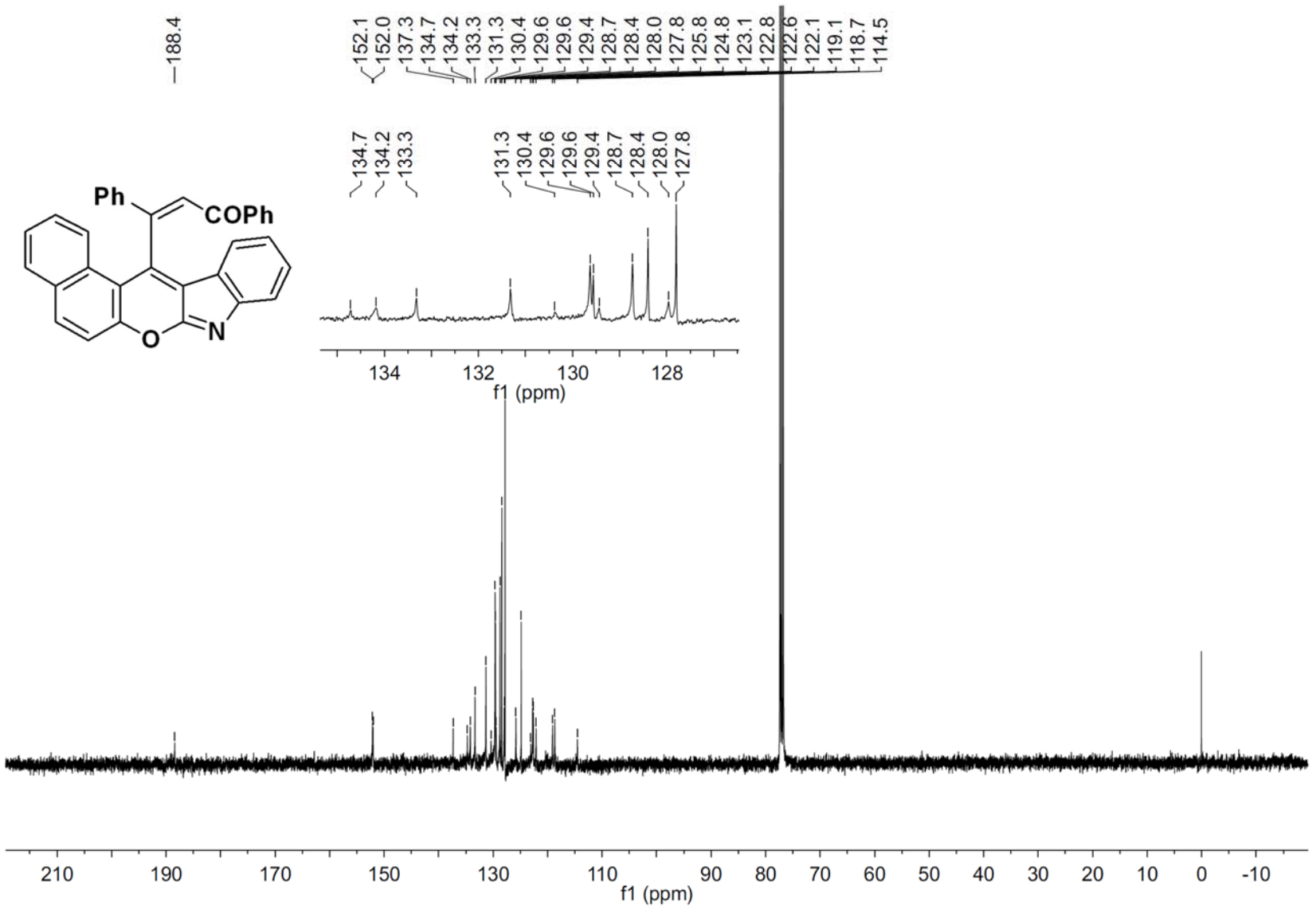
^{1}H NMR Spectrum of Compound 3dd



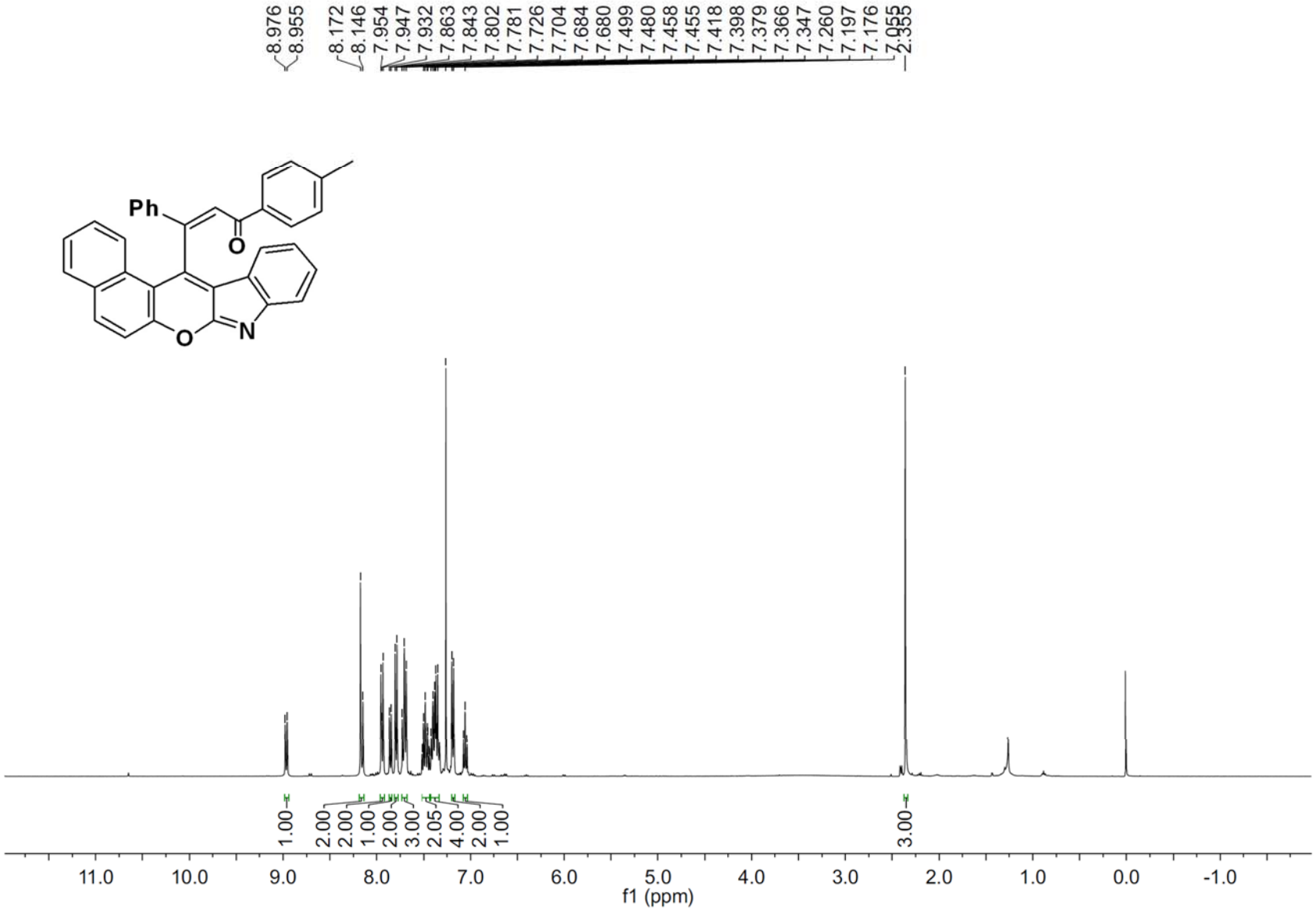
^{13}C NMR Spectrum of Compound 3dd



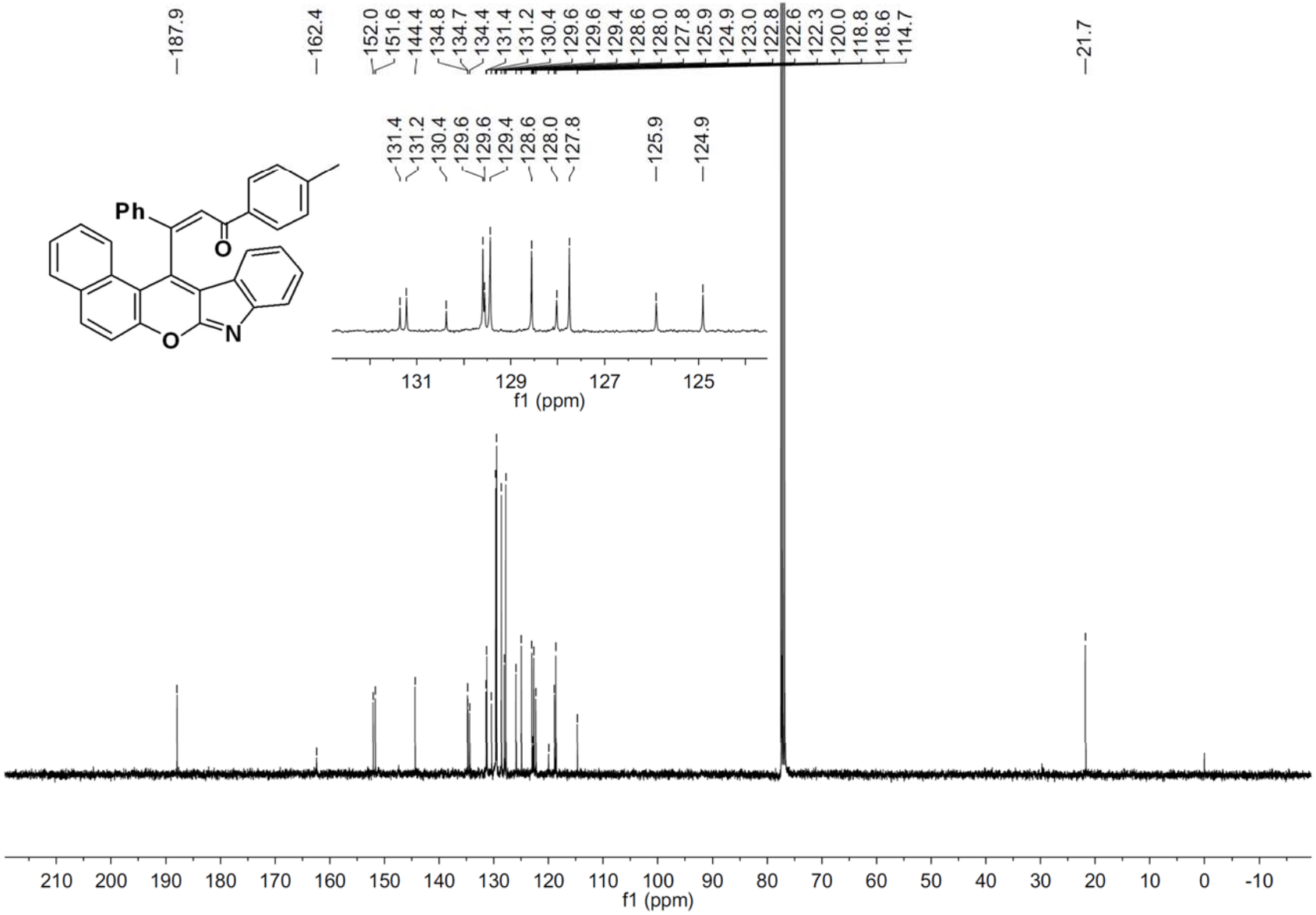
^{1}H NMR Spectrum of Compound 3ee



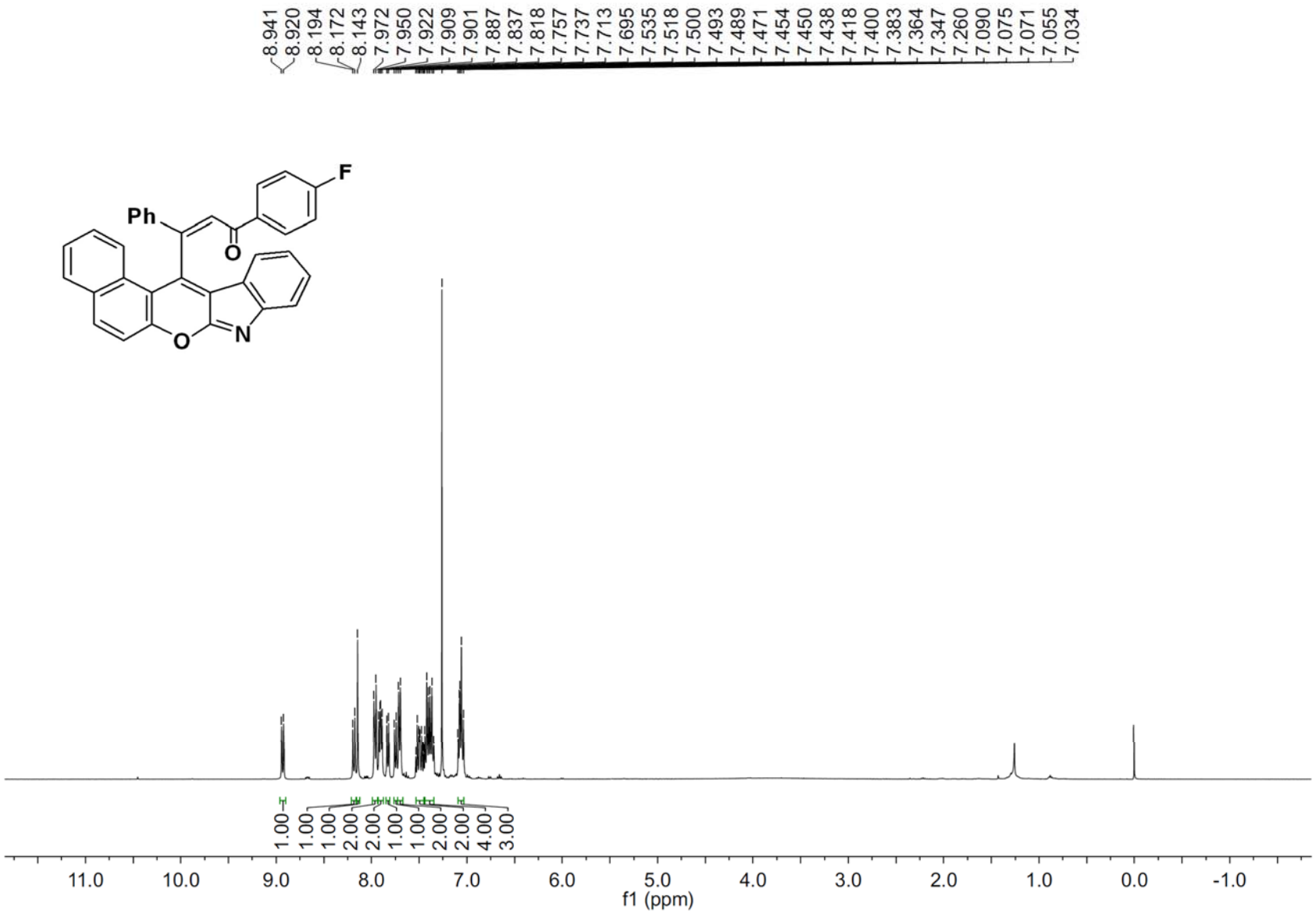
^{13}C NMR Spectrum of Compound 3ee



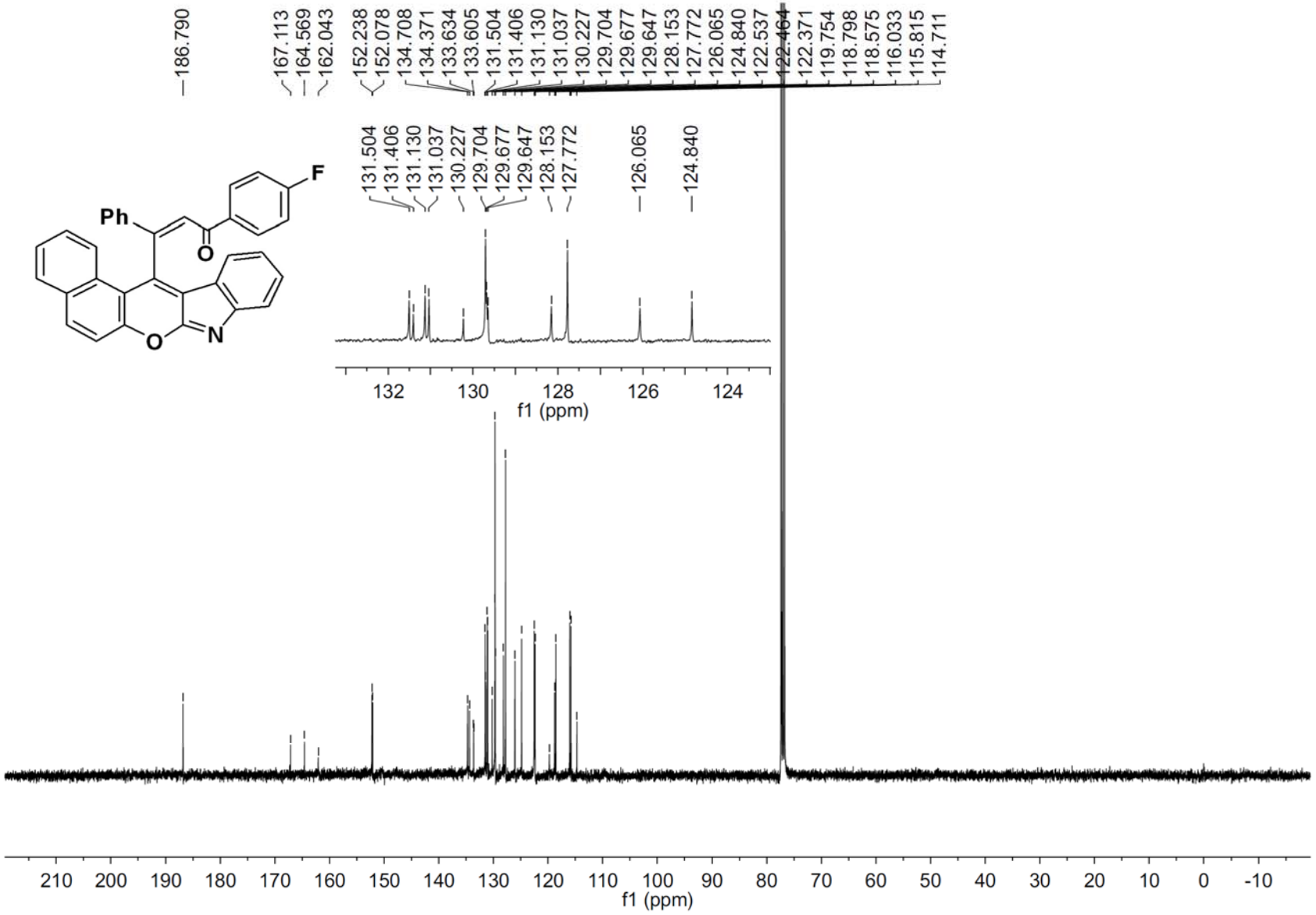
^{1}H NMR Spectrum of Compound 3ff



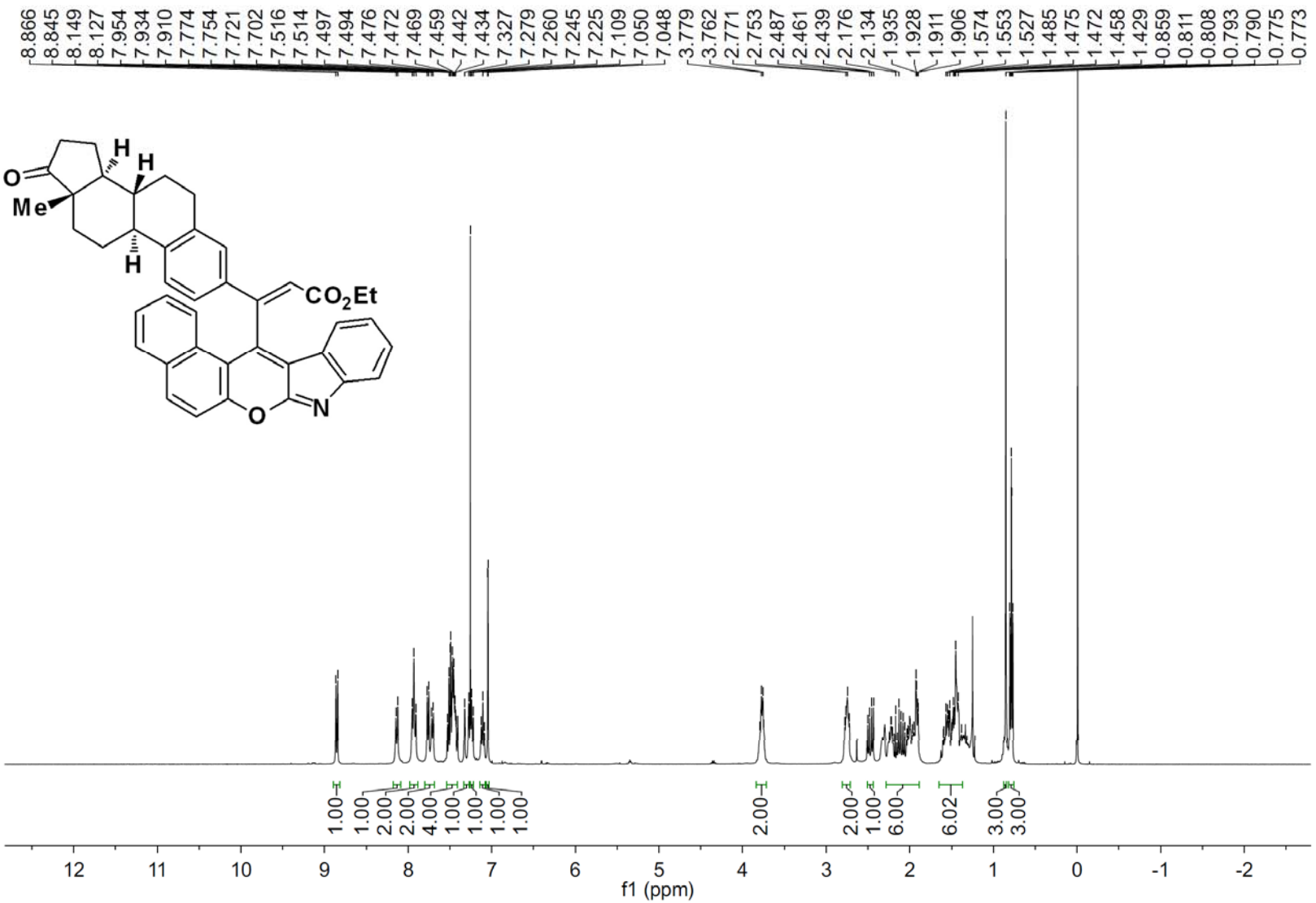
^{13}C NMR Spectrum of Compound 3ff



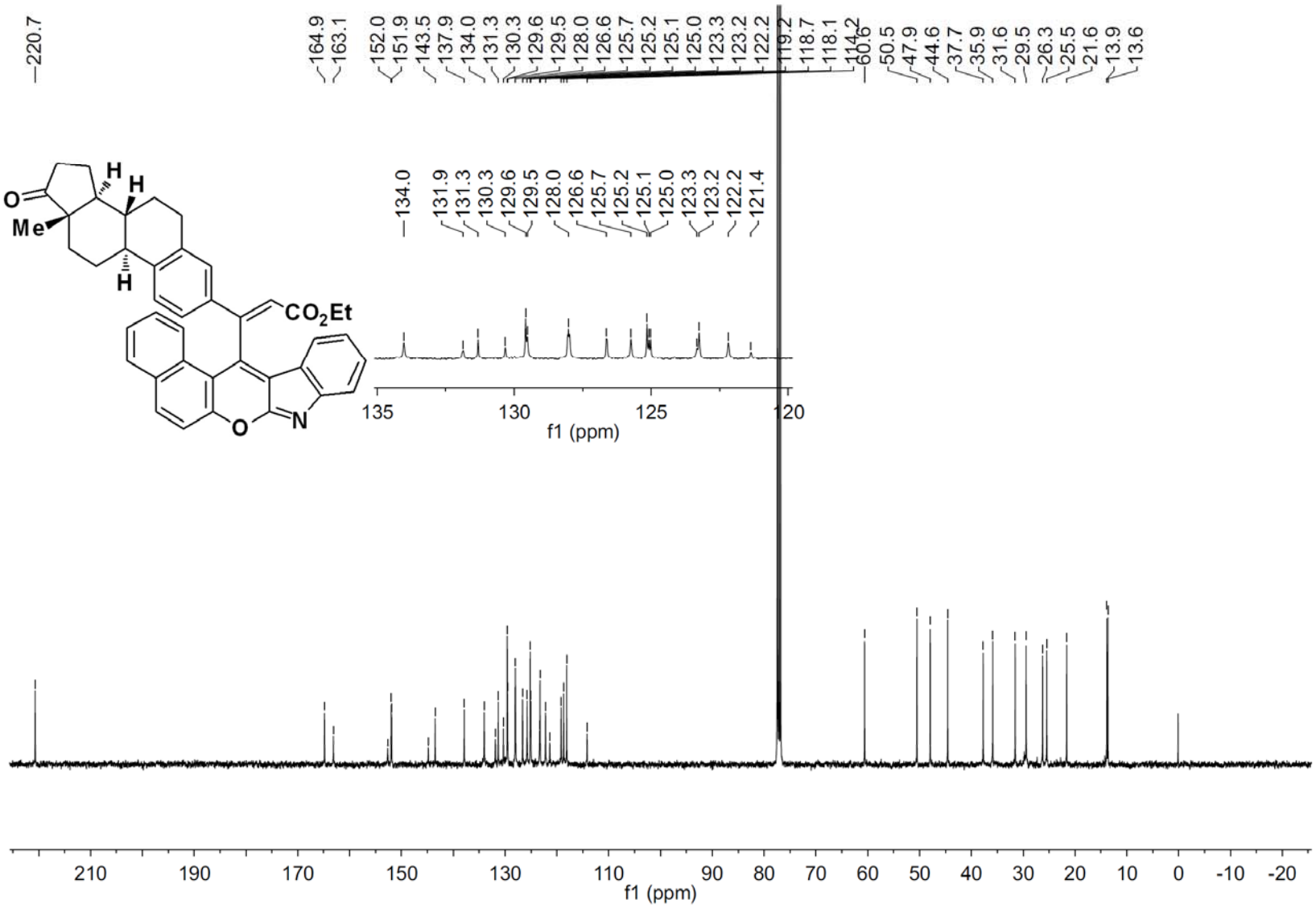
^{1}H NMR Spectrum of Compound 3gg



^{13}C NMR Spectrum of Compound 3gg



^{1}H NMR Spectrum of Compound 3hh



^{13}C NMR Spectrum of Compound 3hh