Supporting information

Synthesis of fused oxazole containing coumarin derivatives via oxidative cross coupling reaction using a combination of $CuCl_2$ and TBHP

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Experimental General: Melting points were determined on a Büchi melting point apparatus. IR spectra were recorded on Perkin-Elmer 281 IR spectrophotometer. ^{1}H NMR spectra were recorded on Brucker 600 MHz and Varian 400 MHz spectrometer with TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). ^{1}H NMR Spectra are reported in the order: multiplicity, coupling constant (J value) in hertz (Hz) and no. of protons,signals were characterized as s (singlet), d (doublet), t (triplet), m (multiplet), and dd (doublet of double). HRMS spectra were recorded using WATERS MS system, Q-TOF premier and data analyzed using Mass Lynx 4.1. The X-ray crystal structures were determined with a Siemen P-4 diffractometer. Complete crystallographic data of **2a** (CCDC 1405370) 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).

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å) at 298 K. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. The structure was solved by direct methods implemented in SHELX-97 program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. Compound **2a** empirical formula $C_{16}H_9NO_3$, pale yellow crystal, formula wt 263.24, Monoclinic, P2(1)/n, a = 7.1596(4) Å, b = 13.3572(7) Å, c = 13.0999(6)Å, V = 1239.47(11)Å^3, Z = 4, F (0 0 0) = 544, GOF(S) = 0.976. Final indices R_{obs} = 0.0501, wR_{obs} = 0.1013 with I >2r(I); R_{all} = 0.1039, wR_{all} = 0.1238 for all data.

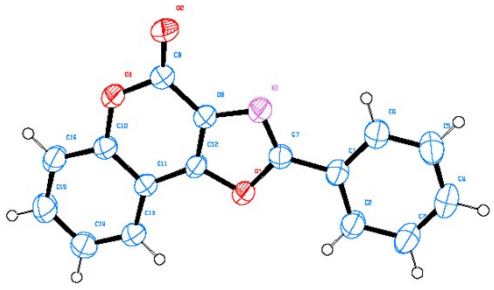
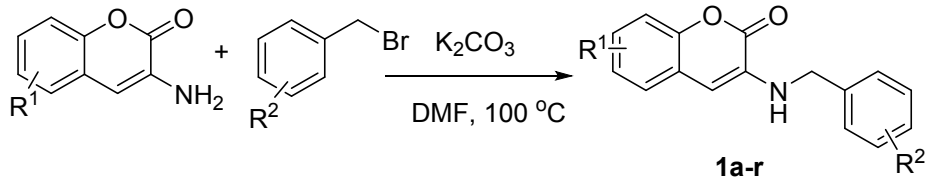


Figure 1. Ortep diagram of **2a** (CCDC number 1405370)

General procedure for the synthesis of various derivatives of 3-(benzylamino)-2H-chromen-2-one (1a-u):



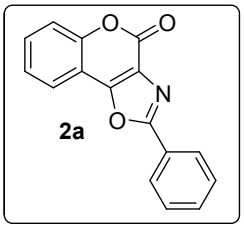
1a-r

Into a 25 mL round bottom flask was taken a mixture of 3-aminocomarin (1 mmol), benzyl bromide (1 mmol) and K_2CO_3 (1.2 mmol) in 3 mL of DMF. The reaction mixture was heated at 100 ^oC for 2-8 h and after completion of the reaction, the reaction mixture was worked-up with ethyl acetate. The crude product obtained after evaporation of the solvent in rotary evaporator was treated with ethanol to remove impurities. Finally a solid pure product (**1a-u**) was obtained in 75-85 %.

General procedure for the synthesis of various derivatives of 2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (2a-u):

Into a 10 mL round bottom flask 0.3 mmol of **1** was taken and then 3 mL of DCM was added into it. Then after adding 20 mol % of $CuCl_2$ and 3 equivalent of TBHP, the reaction mixture was stirred at room temperature 18-24 h. The progress of the reaction was checked by TLC. After completion of the reaction, the reaction mixture was worked up with DCM and the crude product obtained after rotary evaporator was purified with column chromatography eluting with hexane and ethylacetate mixture (9:1). The pure product obtained after column chromatography was characterized by H^1 NMR, ^{13}C NMR and HRMS.

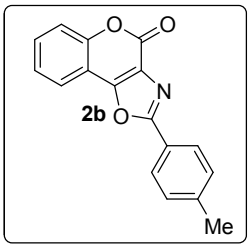
2-phenyl-4H-chromeno[3,4-d]oxazol-4-one(**2a**). Pale yellow solid; Yield = 72% (57 mg); MP = 188-190 ^0C; IR(KBr) ν_{max} = 2958.00, 2923.26, 1756.03, 1606.03, 1261.51, 1156.54, 1103.31, 1064.16 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.2 Hz, 2 H), 7.94 (d, *J* = 7.6 Hz, 1 H), 7.52 (m, 5 H), 7.44 (t, *J* = 7.6 Hz, 1 H) ppm.^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 156.4, 155.5, 153.2, 132.3, 131.9,



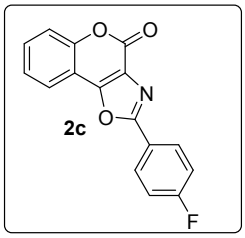
2a

129.3, 127.7, 126.1, 125.9, 125.2, 121.7, 117.9, 111.7 ppm. HRMS [ESI+] m/z: calcd for $C_{16}H_9NO_3$ $[M+H]^+$ = 264.0655(found 264.0655).

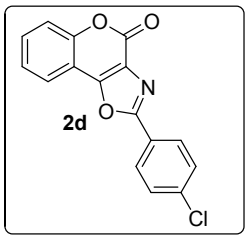
2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (**2b**). Pale yellow solid; Yield = 68% (56 mg); MP = 246 ^{0}C; IR(KBr) ν_{max} = 3062.59, 2920.20, 1756.65, 1639.88, 1261.33, 1155.35, 1101.03, 1065.66 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8 Hz, 2 H), 7.92 (d, *J* = 7.6 Hz, 1 H), 7.60 (t, *J* = 7.6 Hz, 1 H), 7.50 (d, *J* = 8 Hz, 1 H), 7.42 (t, *J* = 4.8 Hz, 1 H), 7.34 (d, *J* = 8 Hz, 2 H), 2.44 (s, 3 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 156.4, 155.2, 153.1, 143.0, 131.7, 130.1, 127.6, 126.1, 125.1, 123.2, 121.6, 117.9, 111.8, 21.9. HRMS [ESI+] m/z: calcd for $C_{17}H_{11}NO_3$ $[M+H]^+$ = 278.0812 (found 278.0813)



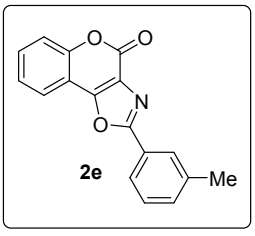
2-(4-fluorophenyl)-4H-chromeno[3,4-d]oxazol-4-one (**2c**). Pale yellow solid; Yield = 64% (54 mg); MP = 233 ^{0}C; IR(KBr) ν_{max} = 2924.10, 2853.13, 1737.29, 1634.64, 1229.50, 1097.64, 1068.25, 1027.01 cm^{-1}; H^1 NMR (600 MHz, $CDCl_3$) δ 8.27 (t, *J* = 7.8 Hz, 2 H), 7.93 (d, *J* = 7.8 Hz, 1 H), 7.62 (t, *J* = 7.8 Hz, 1 H), 7.53 (d, *J* = 8.4 Hz, 1 H), 7.44 (t, *J* = 7.8 Hz, 1 H), 7.25 (t, *J* = 8.4 Hz, 2 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 164.0, 162.7, 156.3, 155.5, 153.2, 132.0, 130.0, 129.95, 125.2, 122.3, 121.6, 118.0, 116.8, 116.6, 111.7 ppm; HRMS [ESI+] m/z: calcd for $C_{16}H_8FNO_3$ $[M+H]^+$ = 282.0561 (found 282.0567)



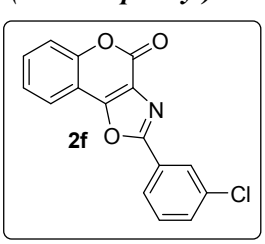
2-(4-chlorophenyl)-4H-chromeno[3,4-d]oxazol-4-one (**2d**). Pale yellow solid; Yield = 60% (54 mg); MP = 226-229 ^{0}C; IR(KBr) ν_{max} = 2963.49, 2925.09, 2845.34, 1760.06, 1604.80, 1261.57, 1093.47, 1020.06 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.4 Hz, 2 H), 7.92 (d, *J* = 8 Hz, 1 H), 7.61 (t, *J* = 7.6 Hz, 1 H), 7.51 (t, *J* = 7.6 Hz, 3 H), 7.43 (t, *J* = 7.6 Hz, 1 H) ppm.^{13}C NMR (100 MHz, $CDCl_3$:CD_2Cl_2 = 5:1)) δ 162.5, 156.1, 155.6, 153.2, 138.5, 132.0, 129.7, 128.8, 125.5, 125.2, 124.4, 121.6, 117.8, 111.5 ppm; [HRMS [ESI+] m/z: calcd for $C_{16}H_8ClNO_3$ $[M+H]^+$ = 298.0265 (found 298.0278)



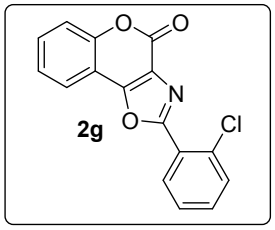
2-(m-tolyl)-4H-chromeno[3,4-d]oxazol-4-one(**2e**). Pale yellow solid; Yield = 62% (52 mg); MP = 188 ^{0}C; IR(KBr) ν_{max} = 2956.72, 2918.40, 1753.81, 1639.30, 1102.98, 1060.65, 1031.94 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1 H), 8.04 (d, *J* = 6.8 Hz, 1 H), 7.93 (d, *J* = 7.6 Hz, 1 H), 7.60 (t, *J* = 7.2 Hz, 1 H), 7.50 (d, *J* = 8.4 Hz, 1 H), 7.42 (t, *J* = 7.6 Hz, 2 H), 7.37 (d, *J* = 7.2 Hz, 1 H), 2.45 (s, 3 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 155.4, 153.2, 139.2, 133.1, 131.8, 129.2, 128.2, 125.8, 125.1, 124.8, 121.6, 117.9, 111.8, 21.5 ppm; [HRMS [ESI+] m/z: calcd for $C_{17}H_{11}NO_3$ $[M+H]^+$ = 278.0812 (found 278.0817)



2-(3-chlorophenyl)-4H-chromeno[3,4-d]oxazol-4-one (**2f**). Pale yellow solid; Yield = 56% (50 mg); MP = 232-234 ^{0}C; IR(KBr) ν_{max} = 2923.34, 2852.57, 1755.61, 1638.29, 1286.06, 1096.19, 1052.92, 1029.17 cm^{-1}; H^1 NMR (600 MHz, $CDCl_3$) δ 8.26 (t, *J* = 1.8 Hz, 1 H), 8.16 (d, *J* = 7.8 Hz, 1 H),7.95 (dd, *J* = 7.8, 1.8 Hz, 1 H) 7.64 (m, 1 H), 7.55 (d, *J* = 7.5 Hz, 1 H), 7.53 (d, *J* = 8.4 Hz, 1 H), 7.50 (t, *J* = 8.4 Hz, 1 H), 7.45 (t, *J* = 7.2 Hz, 1 H) ppm.^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 156.2, 155.7, 153.3, 135.5, 132.3, 132.2, 130.7 , 127.6, 127.5, 126.1, 125.7, 125.3, 121.7, 118.0, 111.6 ppm; HRMS [ESI+] m/z: calcd for $C_{16}H_8ClNO_3$ $[M+H]^+$ = 298.0265 (found 298.0271).

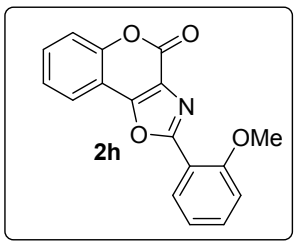


***2-(2-chlorophenyl)-4H-chromeno[3,4-d]oxazol-4-one*(2g)**. Pale yellow solid; Yield = 55% (49 mg);



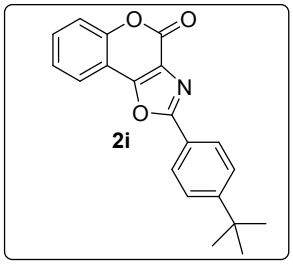
MP = 171-173 ^{0}C; IR(KBr) ν_{max} = 2924.13, 2852.45, 1757.06, 1641.27, 1167.90, 1068.50, 1034.42; H^1 NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1 H), 7.95 (d, *J* = 7.6 Hz, 1 H), 7.63 (t, *J* = 8.8 Hz, 1 H), 7.59 (d, *J* = 8.4 Hz, 1 H), 7.53 (d, *J* = 8 Hz, 1 H), 7.49 (dd, *J* = 7.6, 1.6 Hz, 1 H), 7.46 (d, *J* = 3.6 Hz, 1 H), 7.45 (d, *J* = 3.2 Hz, 1 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 161.6, 156.2, 155.8, 153.4, 133.6, 132.8, 132.2, 131.8, 127.4, 125.8, 125.2, 125.0, 121.9, 118.0, 111.7 ppm. HRMS [APCI+] m/z: calcd for $C_{16}H_8ClNO_3$ $[M+H]^+$ = 298.0265 (found 298.0268).

***2-(2-methoxyphenyl)-4H-chromeno[3,4-d]oxazol-4-one* (2h).** pale yellow solid; Yield = 65 % (57



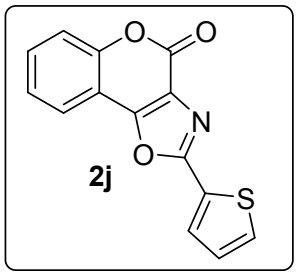
mg); MP = 168-170 ^{o}C; IR 2956.26, 2924.46, 2853.39, 1751.49, 1652.71, 1265.42, 1161.69, 1069.43, 1021.09 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.2 Hz, 1 H), 7.93 (d, *J* = 8 Hz, 1 H), 7.59 (m, 1 H), 7.52 (t, *J* = 8.4 Hz, 2 H), 7.42 (t, *J* = 7.6 Hz, 1 H), 7.11 (m, 2 H), 4.02 (s, 3 H) ppm; 13 C NMR (150 MHz, $CDCl_3$) δ 162.4, 158.6, 156.4, 155.2, 153.2, 138.5, 133.6, 131.7, 131.4, 125.0, 121.7, 121.0, 117.8, 115.0, 112.3, 111.9, 56.2 ppm. HRMS [ESI+] m/z: calcd for $C_{17}H_{11}NO_4$ $[M+H]^+$ = 294.0761 (found 294.0778).

***2-(4-(tert-butyl)phenyl)-4H-chromeno[3,4-d]oxazol-4-on*e(2i)**.pale yellow solid; Yield = 67 % (64



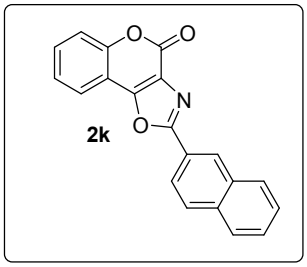
mg); MP =207-209 ^{o}C; IR 3066.92, 2949.93, 1753.50, 1684.67, 1285.19, 1167.19, 1063.56, 1041.90 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.4 Hz, 2 H), 7.94 (d, *J* = 7.6 Hz, 1 H), 7.61 (t, *J* = 7.4 Hz, 1 H), 7.56 (d, *J* = 8.4 Hz, 2 H), 7.51 (d, *J* = 8.8 Hz, 1 H), 7.43 (t, *J* = 7.2 Hz, 1 H), 1.38 (s, 9 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 156.6, 156.1, 155.3, 153.1, 131.8, 127.5, 126.3, 126.1, 125.1, 123.1, 121.6, 117.9, 111.8, 35.4, 31.3 ppm; HRMS [APCI+] m/z: calcd for $C_{19}H_{17}NO_3$ $[M+H]^+$ = 320.1281 (320.1280)

***2-(thiophen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one* (2j)** Pale yellow solid; Yield = 68 % (55 mg); MP



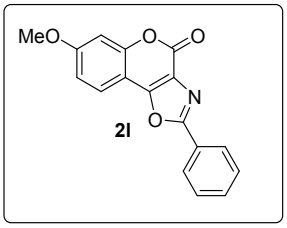
= 170-172 ^{o}C; IR 3095.65, 2924.28, 2853.43, 1752.86, 1634.11, 1210.78, 1101.71, 1068.24, 1032.66 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 3.2 Hz, 1 H), 7.90 (dd, *J* = 7.6, 1.2 Hz, 1 H), 7.60 (m, 2 H), 7.50 (d, *J* = 8 Hz, 1 H), 7.42 (t, *J* = 7.6 Hz, 1 H), 7.21 (t, *J* = 4.8 Hz, 1 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 156.2, 155.0, 153.1, 131.9, 131.3, 130.8, 128.6, 128.0, 126.0, 125.2, 121.6, 117.9, 111.5 ppm; HRMS [ESI+] m/z: calcd for $C_{14}H_7NO_3S$ $[M+H]^+$ = 270.0219 (found 270.0240).

***2-(naphthalen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one* (2k**). Pale yellow solid; Yield = 80% (75 mg);



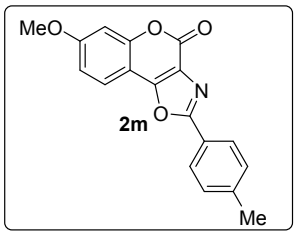
MP = 245^{0}C; IR(KBr) ν_{max} = 2925.03, 2852.61, 1755.81, 1605.26, 1101.74, 1067.46, 1029.24 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1 H), 8.30 (d, *J* = 8.8 Hz, 1 H), 7.99 (d, *J* = 8 Hz, 3 H), 7.90 (d, *J* = 8.8 Hz, 1 H), 7.61 (m, 3 H), 7.53 (d, *J* = 8 Hz, 1 H), 7.46 (t, *J* = 7.6 Hz, 1 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 156.4, 155.5, 153.2, 135.1, 133.0, 131.9, 129.3, 129.2, 128.4, 128.36, 128.2, 127.4, 126.6, 125.2, 123.7, 123.2, 121.7, 118.0, 111.8 ppm; HRMS [ESI+] m/z: calcd for $C_{20}H_{11}NO_3$ $[M+H]^+$ = 314.0812 (found 314.0816)

7-methoxy-2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (**2l**). Pale yellow solid; Yield = 54% (47 mg);

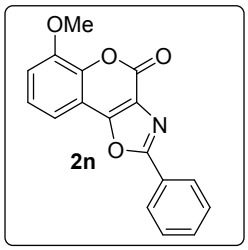


MP = 209 ^{0}C; IR(KBr) ν_{max} = 2924.88, 2852.86, 1748.58, 1638.71, 1151.36, 1117.36, 1061.23, 1029.99 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 6.4 Hz, 2 H), 7.81 (d, *J* = 8.4 Hz, 1 H), 7.54 (m, 3 H), 7.00 (d, *J* = 8.8 Hz, 2 H), 3.91(s, 3 H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 162.3, 156.3, 155.7, 154.8, 131.7, 129.0, 127.2, 125.8, 123.4, 122.3, 113.3, 104.6, 101.6, 55.8 HRMS [ESI+] m/z: calcd for $C_{17}H_{11}NO_4$ $[M+H]^+$ = 294.0761 (found 294.0774)

7-methoxy-2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (**2m**). Pale yellow solid; Yield = 58% (53 mg); MP = 220 ^{0}C; IR(KBr) ν_{max} = 2923.23, 2854.65, 1767.39, 1638.09, 1270.71, 1103.27, 1059.04, 1023.23cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 6.4 Hz, 2 H), 7.79 (d, *J* = 8.4 Hz, 1 H), 7.32 (d, *J* = 6.4 Hz, 2 H), 6.98 (s, 2 H) 3.83 (s, 3 H), 2.36 (s, 3 H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.9, 156.7, 155.9, 155.0, 142.7, 130.0, 127.5, 123.7, 123.4, 122.5, 113.6, 105.0, 101.9, 56.1, 21.9 ppm; HRMS [ESI+] m/z: calcd for $C_{18}H_{13}NO_4$ $[M+H]^+$ = 308.0917 (found 308.0931)

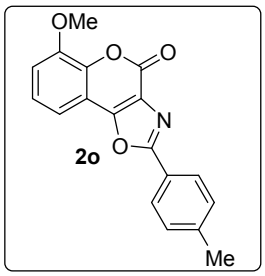


6-methoxy-2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (**2n**). Pale yellow solid; Yield = 66% (58 mg);

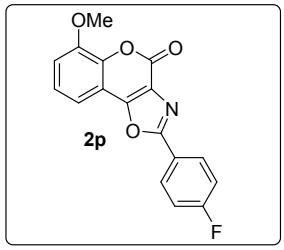


MP = 220 ^{0}C; IR(KBr) ν_{max} = 3063.33, 2997.68, 2928.07, 2844.55, 1759.97, 1640.76, 1277.78, 1075.41, 1043.28, 1002.19 cm^{-1}. H^1 NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 6 Hz, 2 H), 7.56 (m, 3 H), 7.50 (d, *J* = 8 Hz, 1 H), 7.36 (t, *J* = 7.6 Hz, 1 H), 7.14 (d, *J* = 8.4 Hz, 1 H), 4.00(s, 3 H) ppm.^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 155.8, 155.6, 148.2, 132.3, 129.3, 129.0, 127.7, 126.2, 126.0, 125.4, 113.9, 112.9, 112.5, 56.6 ppm; HRMS [ESI+] m/z: calcd for $C_{17}H_{11}NO_4$ $[M+H]^+$ = 294.0761 (found 294.0766)

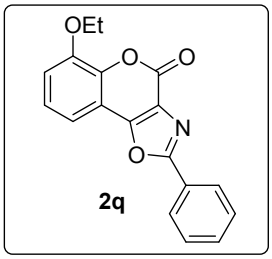
6-methoxy-2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (**2o**). Pale yellow solid; Yield = 66% (61 mg); MP = 238 ^{0}C; IR(KBr) ν_{max} = 2923.41, 2850.78, 1753.51, 1610.64, 1275.99, 1081.42, 1048.66, 996.21cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.2 Hz, 2 H), 7.62 (d, *J* = 8 Hz, 1 H), 7.33 (t, *J*= 8 Hz, 3 H), 7.11 (d, *J* = 7.6 Hz, 1 H), 3.99 (s, 3 H), 2.43 (s, 3 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 155.9, 155.3, 148.1, 143.0, 142.9, 130.0, 127.6, 126.2, 125.3, 123.2, 113.7, 112.9, 112.5, 56.6, 21.9 ppm; HRMS [ESI+] m/z: calcd for $C_{18}H_{13}NO_4$ $[M+H]^+$ = 308.0917 (found 308.0923)



2-(4-fluorophenyl)-6-methoxy-4H-chromeno[3,4-d]oxazol-4-one (**2p**). Pale yellow solid; Yield = 56 % (52 mg); MP = 248 ^{0}C; IR(KBr) ν_{max} = 2923.84, 2852.00, 1751.45, 1637.57, 1277.09, 1100.90, 1081.26, 1046.33cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.26 (dd *J* = 7.6, 5.2 Hz, 2 H), 7.49 (d, *J* = 8 Hz, 1 H), 7.36 (t, *J* = 8 Hz, 1 H), 7.23 (d, *J* = 8.4 Hz, 2 H), 7.15 (d, *J* = 8 Hz, 1 H), 4.01 (s, 3 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 164.0, 162.7, 155.8, 155.7, 148.2, 143.0, 130.0, 129.95, 126.2, 125.4, 122.3, 116.8, 116.6, 113.9, 112.9, 112.4, 56.6 ppm; HRMS [ESI+] m/z: calcd for $C_{17}H_{16}NO_4$ $[M+H]^+$ = 312.0667 (found 312.0682)



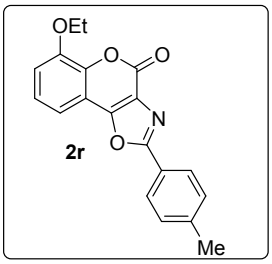
6-ethoxy-2-phenyl-4H-chromeno[3,4-d]oxazol-4-one(**2q**). Pale yellow solid; Yield = 64 % (59 mg);



MP = 218 ^{0}C; IR(KBr) ν_{max} = .2967.46, 2920.28, 2845.34, 1752.51, 1603.25, 1276.85, 1081.11, 1045.09, 1017.41 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 6.4 Hz, 2 H), 7.55 (m, 3 H), 7.49 (d, *J* = 7.6 Hz, 1 H), 7.34 (t, *J* = 8.4 Hz, 1 H), 7.14 (d, *J* = 8 Hz, 1 H), 4.22 (q, *J* = 6.4 Hz, 2 H), 1.54 (t, *J*

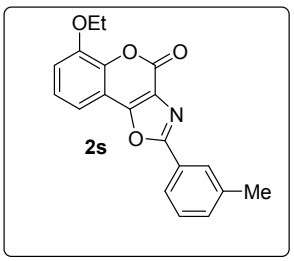
= 6.8 Hz, 3 H) ppm; ^{13}C NMR; (100 MHz, $CDCl_3$) δ 163.6, 156.1, 155.7, 147.6, 143.2, 132.3, 129.3, 127.7, 126.0, 125.4, 115.1, 112.9, 112.6, 65.4, 15.0 ppm. HRMS [ESI+] m/z: calcd for $C_{18}H_{13}NO_4$ $[M+H]^+$ = 308.0917 (found 308.0917).

6-ethoxy-2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (**2r**). Pale yellow solid; Yield = 58% (56 mg);



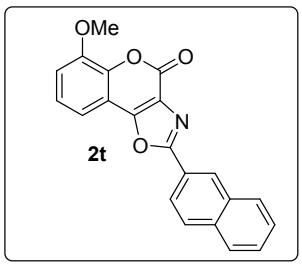
MP = 195-197 ^{0}C; IR(KBr) ν_{max} = 2959.14, 2923.05, 2844.49, 1752.97,1637.36, 1276.51, 1262.41, 1081.73, 1102.88, 1017.50 cm^{-1}. H^1 NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8 Hz, 2 H), 7.39 (d, *J* = 8 Hz, 1 H), 7.23 (m, 3 H), 7.04 (d, *J* = 7.6 Hz, 1 H), 4.14 (q, *J* = 6.4, 2 H), 2.37 (s, 3 H), 1.45 (t, *J* = 7.2, 3 H) ppm.^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 156.1, 155.4, 147.5, 143.1, 142.9, 130.0, 127.6, 126.1, 125.3, 123.2, 115.0, 112.8, 112.6, 65.4, 21.9, 15.0 ppm; HRMS [ESI+] m/z: calcd for $C_{19}H_{15}NO_4$ $[M+H]^+$ = 322.1074 (found 322.1077)

6-ethoxy-2-(m-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (**2s**) Pale yellow solid; Yield = 59% (57 mg);



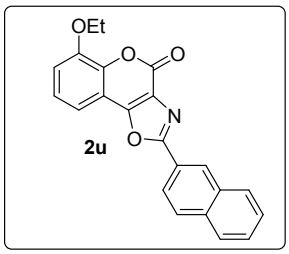
MP = 189 ^{0}C; IR(KBr) ν_{max} = 2924.09, 2852.21, 1747.07, 1640.50, 1278.12, 1104.94, 1047.03, 1019.35 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1 H), 8.03 (d, *J* = 7.2 Hz, 1 H), 7.48 (d, *J* = 8 Hz, 1 H), 7.40 (t, *J* = 8 Hz, 1 H), 7.36 (t, *J* = 5.6 Hz, 1 H), 7.31 (d, *J* = 8 Hz, 1 H) , 7.12 (d, *J* = 7.6 Hz, 1 H), 4.21 (q, *J* = 6.8 Hz, 2 H), 2.45 (s, 3 H), 1.52 (t, *J* = 7.2 Hz, 3 H) ppm.^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 156.0, 155.6, 147.5, 143.1, 139.2, 133.1, 129.2, 128.2, 126.1, 125.8, 125.3, 124.8, 115.0, 112.8, 112.5, 65.4, 21.5, 15.0 ppm; HRMS [ESI+] m/z: calcd for $C_{19}H_{15}NO_4$ $[M+H]^+$ = 322.1074 (found 322.1079)

6-methoxy-2-(naphthalen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one (**2t**). Pale yellow solid; Yield = 7



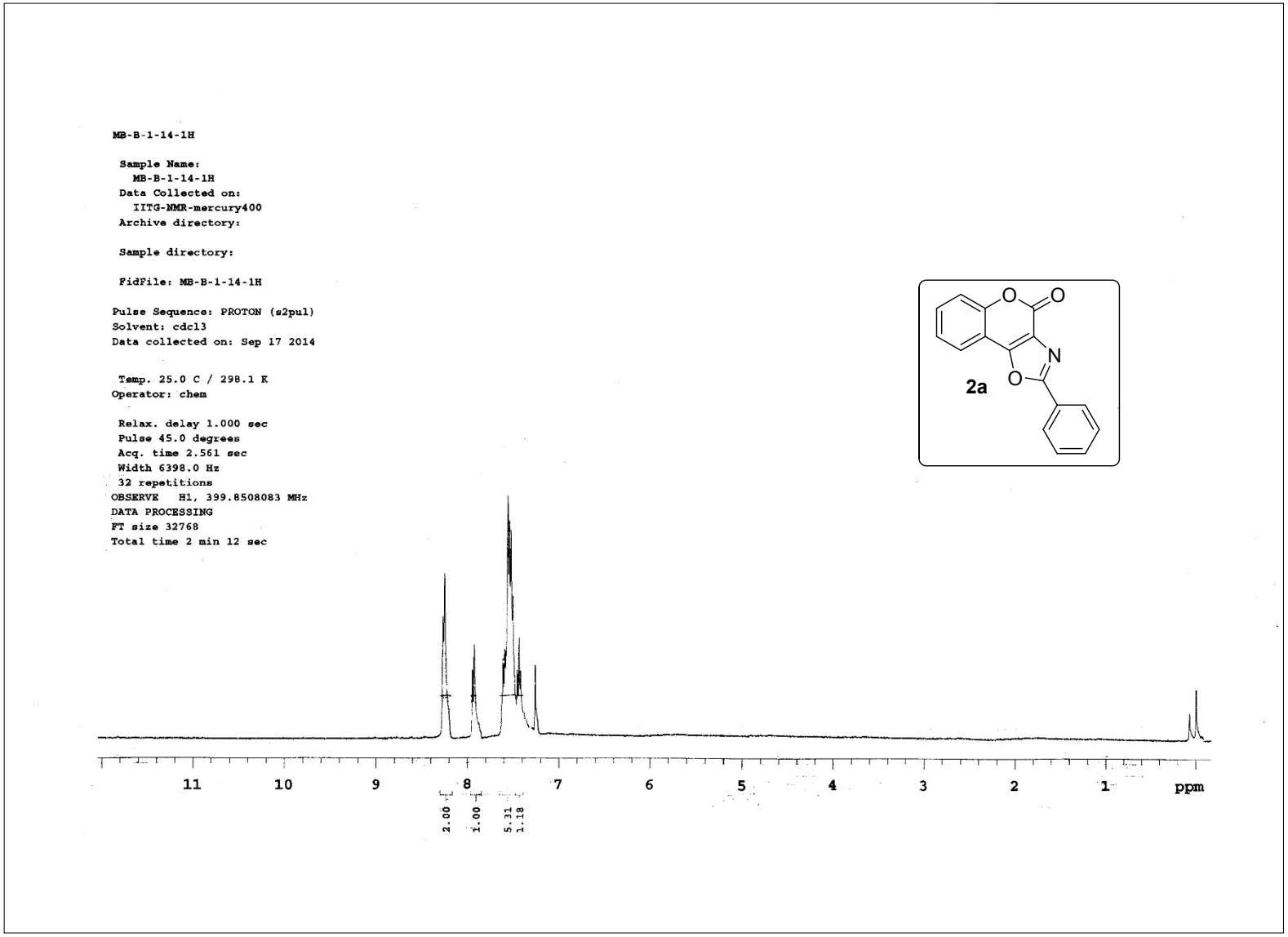
8% (80 mg); MP = 270 ^{0}C IR(KBr) ν_{max} = 2924.69, 2852.94, 1759.34, 1603.15, 1603.15, 1273.60, 1111.62, 1048.71 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 1 H), 8.29 (d, *J* = 8.4 Hz, 1 H), 7.99 (d, *J* = 8 Hz, 2 H), 7.90 (d, *J* = 8.4, 1 H), 7.59 (t, *J* = 3.6 Hz, 2 H), 7.56 (d, *J* = 8 Hz, 1 H), 7.38 (t, *J* = 8 Hz, 1 H), 7.15 (d, *J* = 8 Hz, 1 H), 4.01 (s, 3 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$), δ 163.8, 155.8, 155.7, 148.2, 135.1, 133.1, 129.3, 129.2, 128.4, 128.36, 128.2, 127.4, 126.4, 125.4, 123.8, 123.2, 113.9, 113.0, 112.5, 56.6 ppm; HRMS [ESI+] m/z: calcd for $C_{21}H_{13}NO_4$ $[M+H]^+$ = 344.0917 (found 344.0923)

6-ethoxy-2-(naphthalen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one (**2u**). Pale yellow solid; Yield = 81%

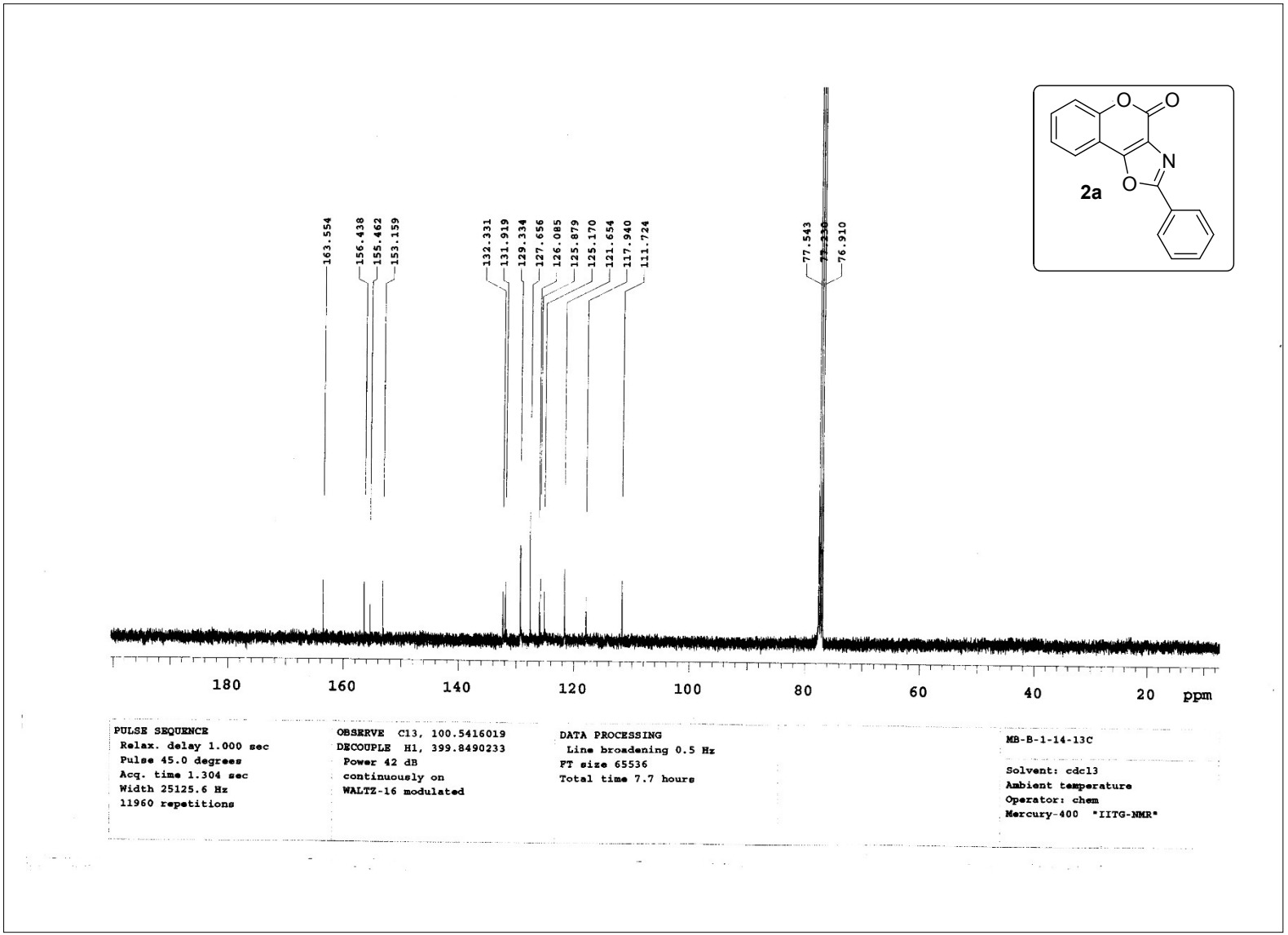


(87 mg); MP = 221^{0}C; IR(KBr) ν_{max} = 2924.43, 2852.64, 1760.02, 1605.56, 1272.39, 2080.36, 1051.17, 1013.12 cm^{-1}; H^1 NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 1 H), 8.29 (d, *J* = 8.4 Hz, 1 H), 7.98 (d, *J* = 8.4 Hz, 2 H), 7.89 (d, *J* = 8.4 Hz, 1 H), 7.59 (t, *J* = 4 Hz, 2 H), 7.54 (d, *J* = 7.6 Hz, 1 H), 7.35 (t, *J* = 7.6 Hz, 1 H), 7.17 (d, *J* = 8 Hz, 1 H), 4.23 (q, *J* = 7.2 Hz, 2 H), 1.54 (t, *J* = 7.2 Hz, 3 H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 156.1, 155.8, 147.6, 135.1, 133.1, 129.3, 129.2, 128.4, 128.3,128.2, 127.4, 126.3, 125.4, 123.7, 123.2, 115.2, 112.9, 112.6, 65.4, 15.0 ppm; HRMS [ESI+] m/z: calcd for $C_{22}H_{15}NO_4$ $[M+H]^+$ = 358.1074 (found 358.1096).

H^1 NMR spectra of **2a**



^{13}C NMR spectra of **2a**



HRMS spectra of **2a**

Sample Name	MB-B-1-14	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-10	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
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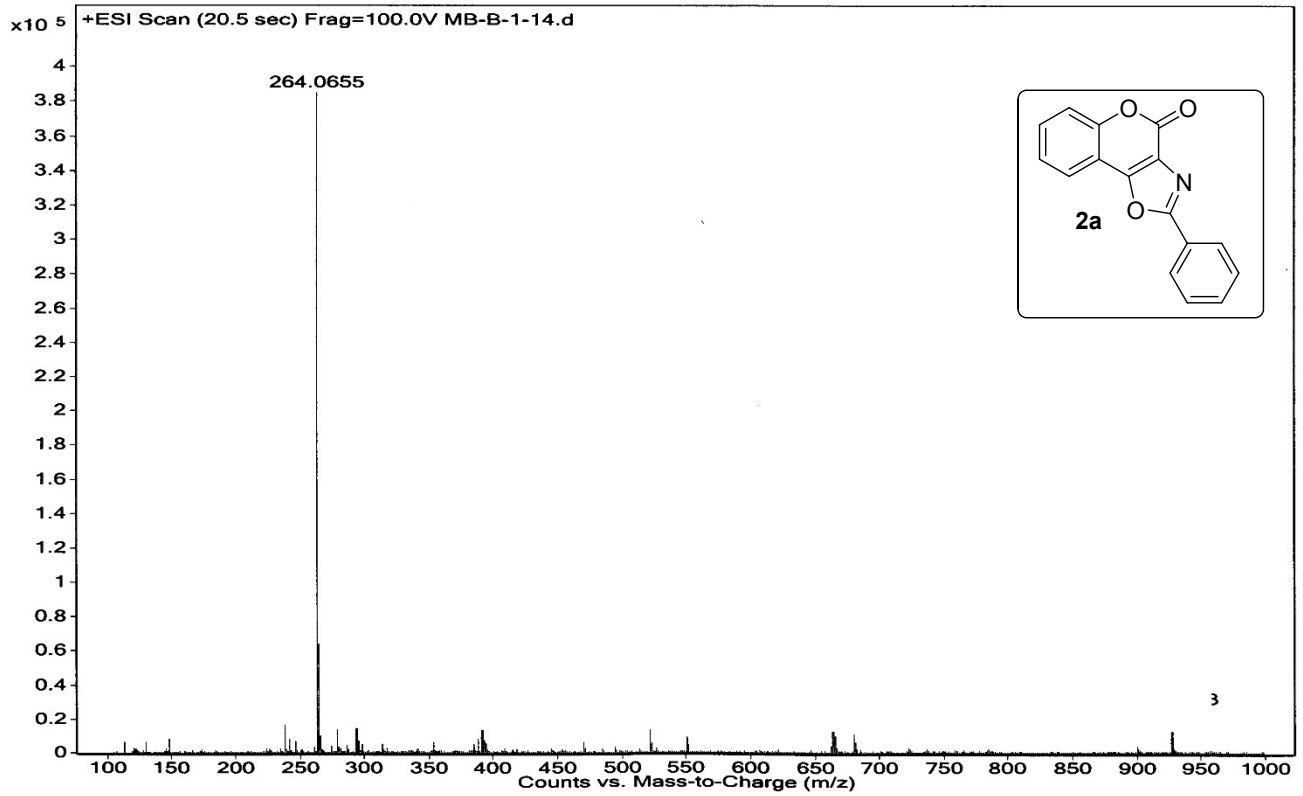
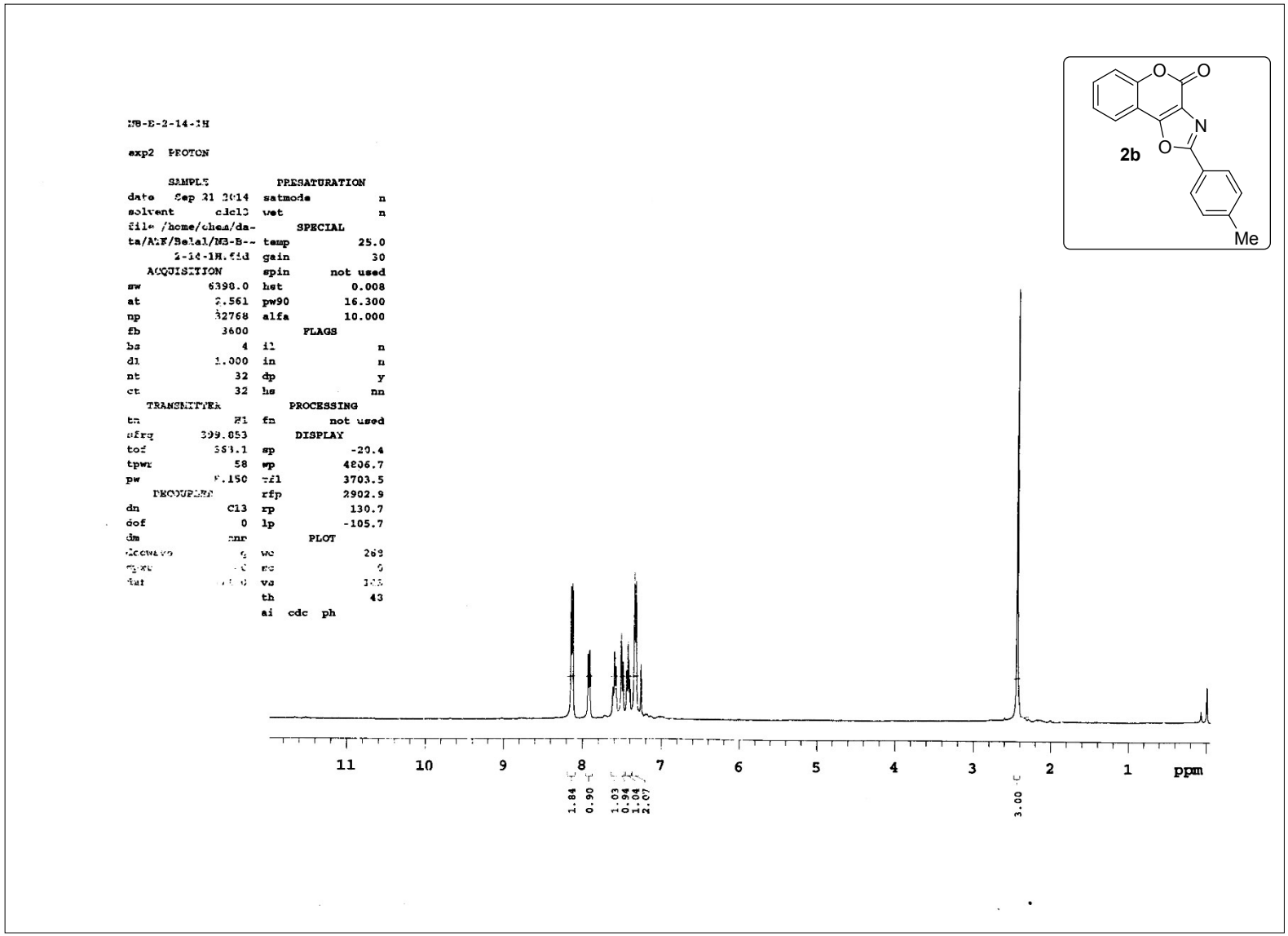
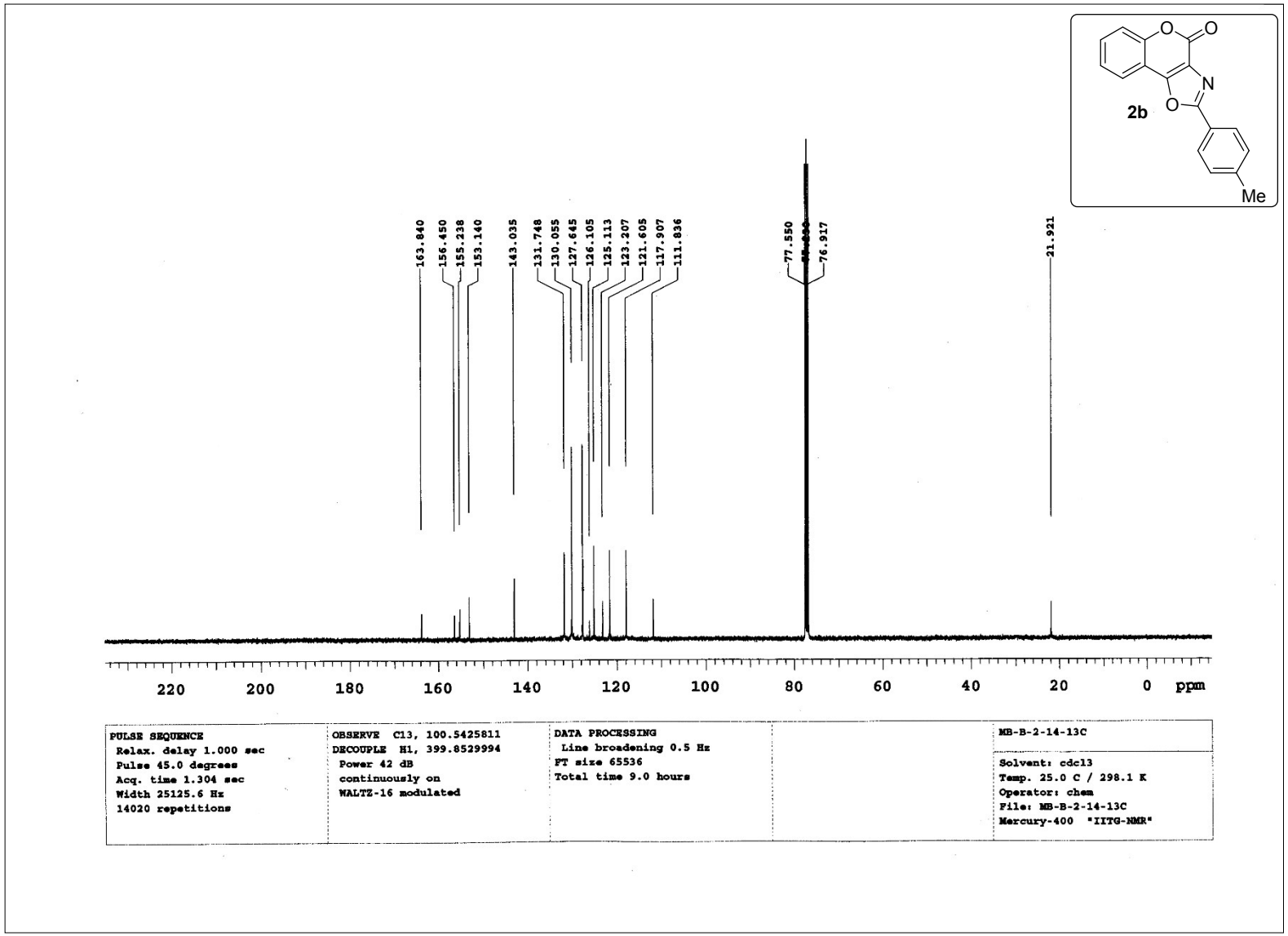


H[1] NMR spectra of **2b**



^{13}C NMR spectra of **2b**



HRMS spectra of **2b**

Sample Name	MB-B-2-14	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-10	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
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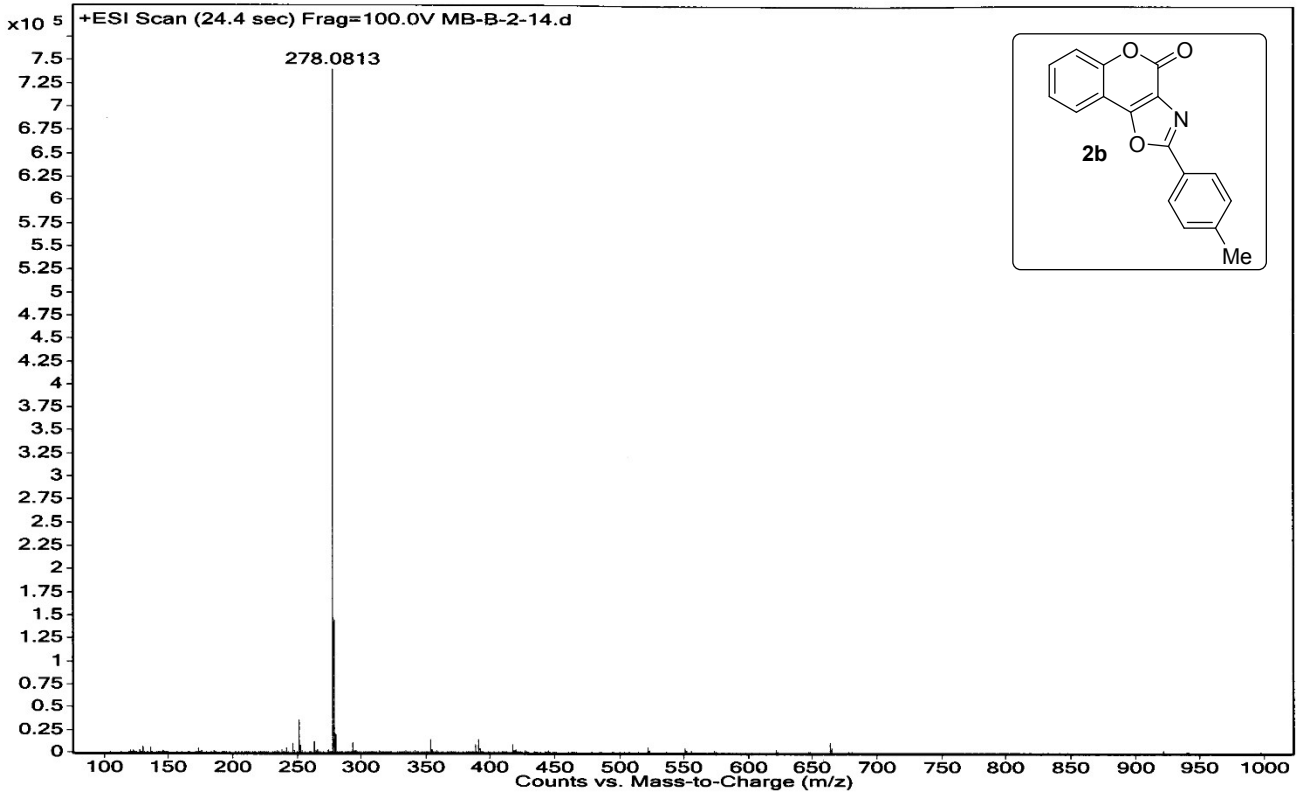
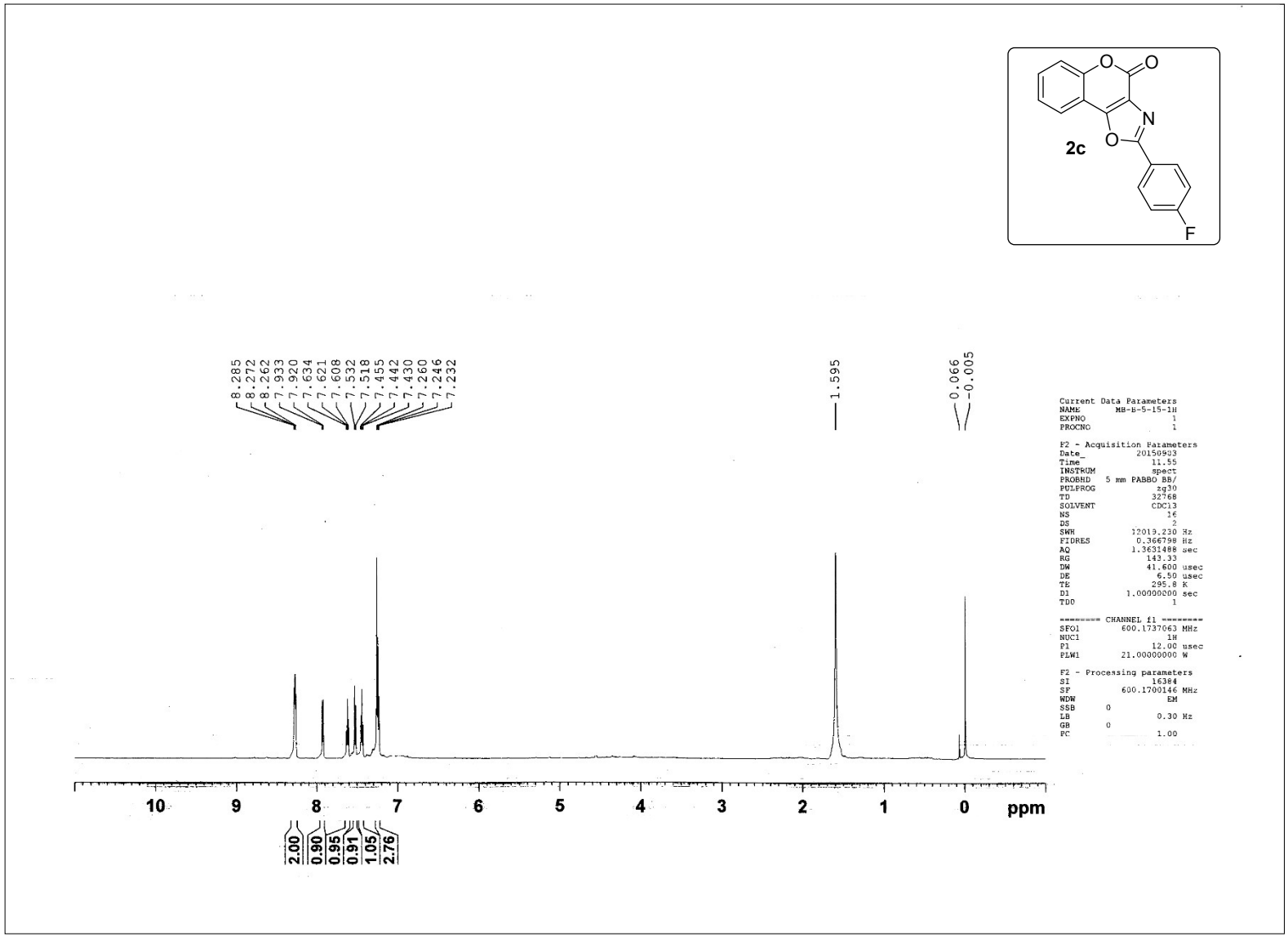
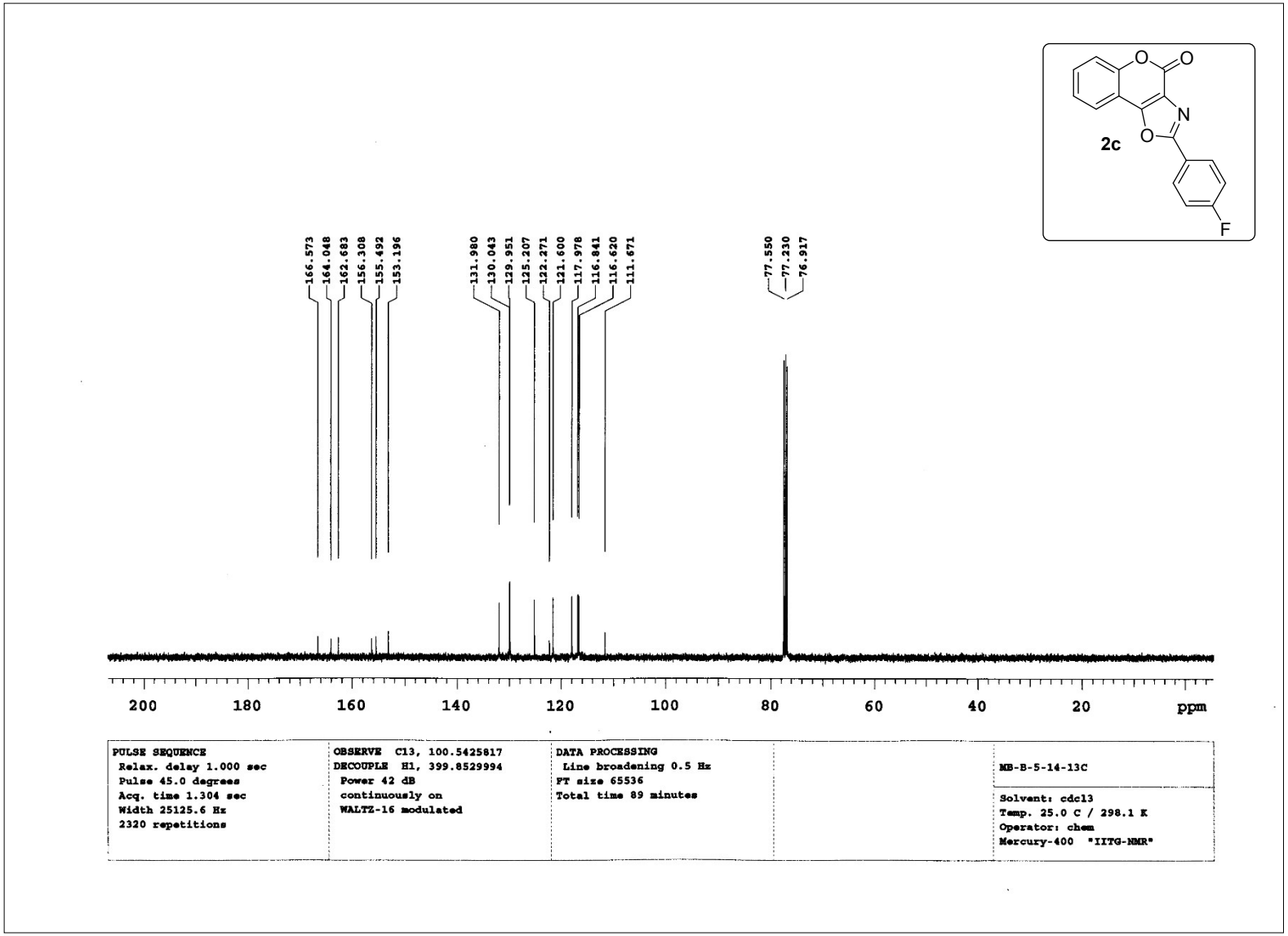


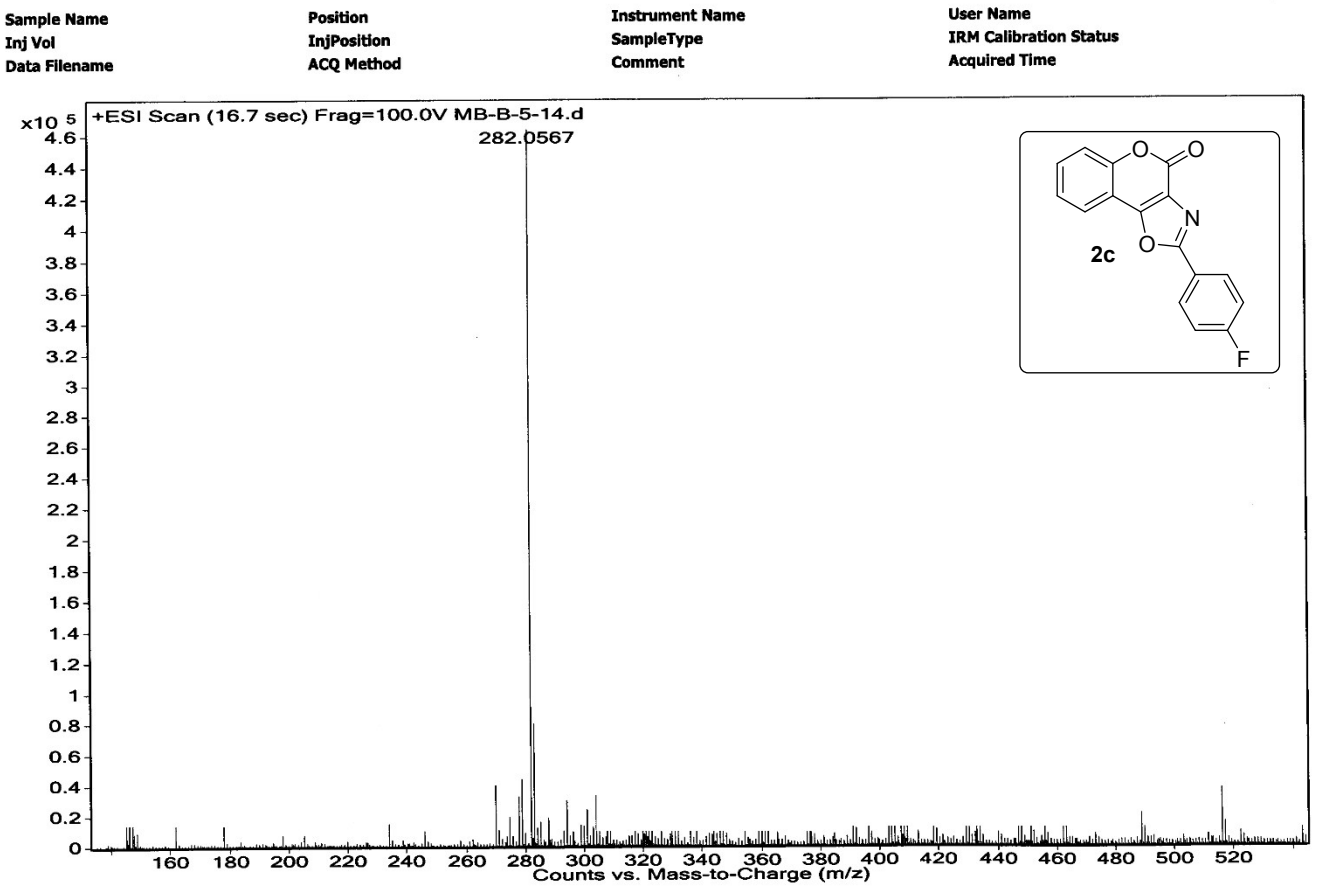
H[1] NMR spectra of **2c**



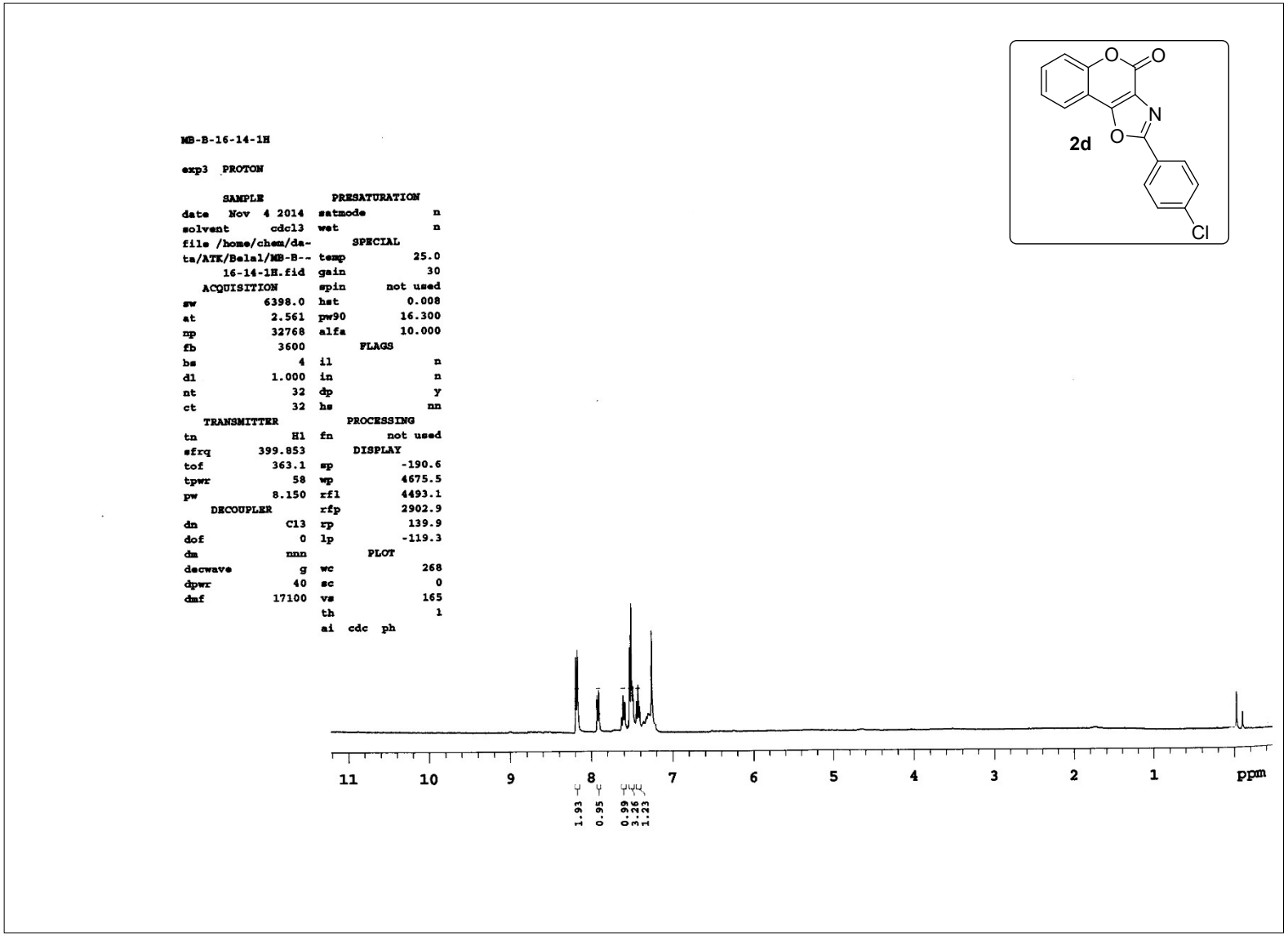
^{13}C NMR spectra of **2c**



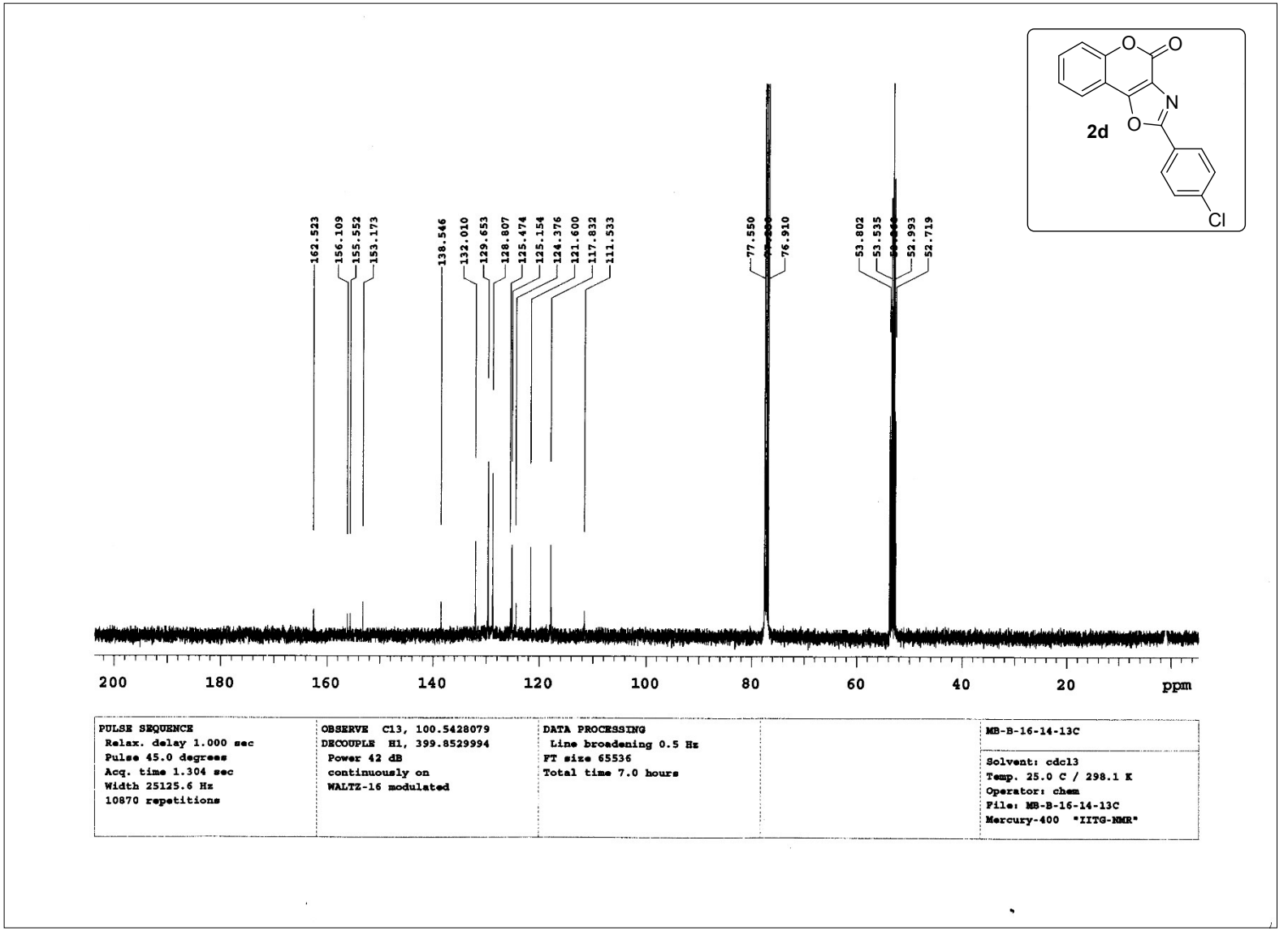
HRMS spectra of **2c**



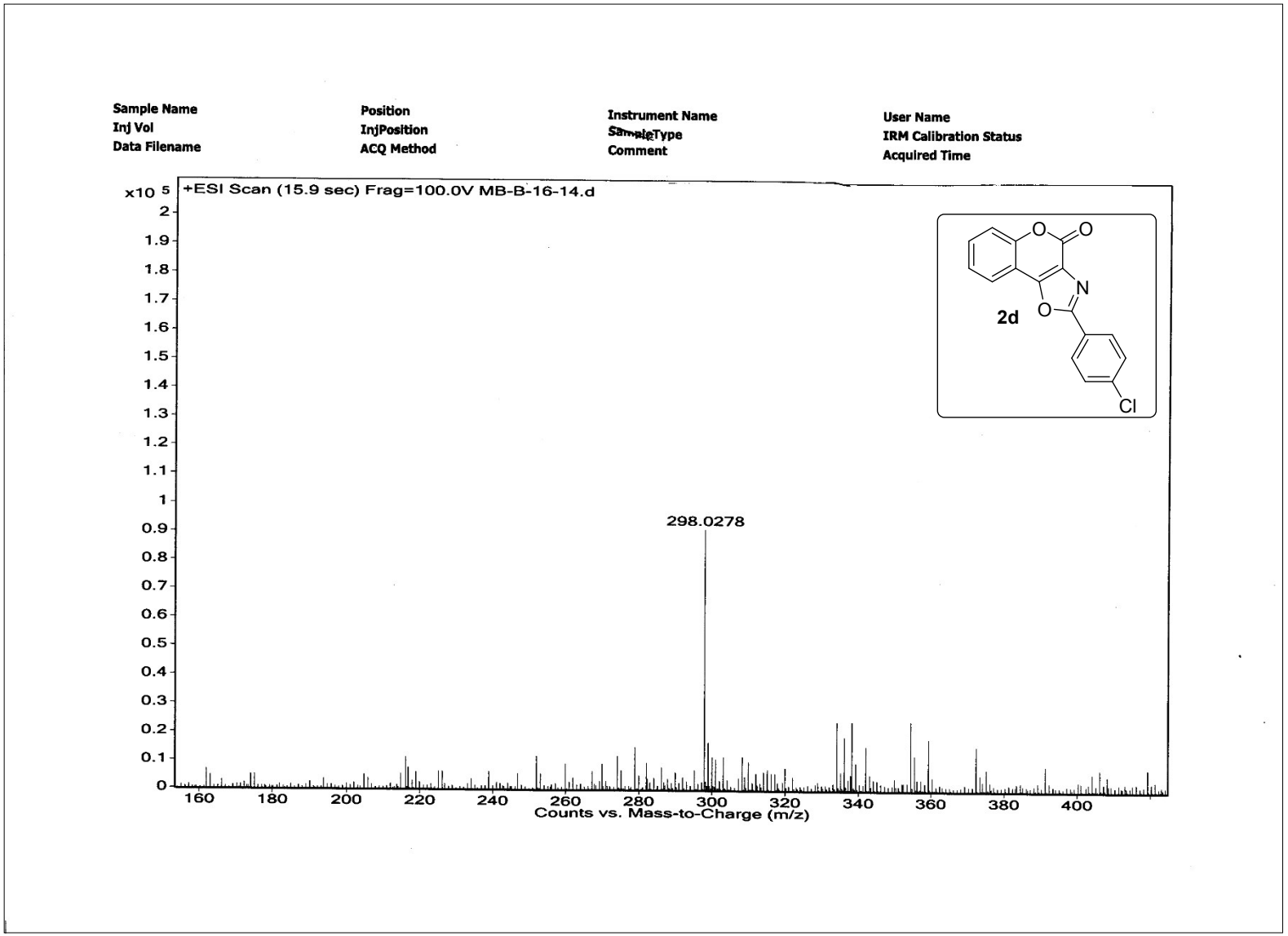
H[1] NMR spectra of **2d**



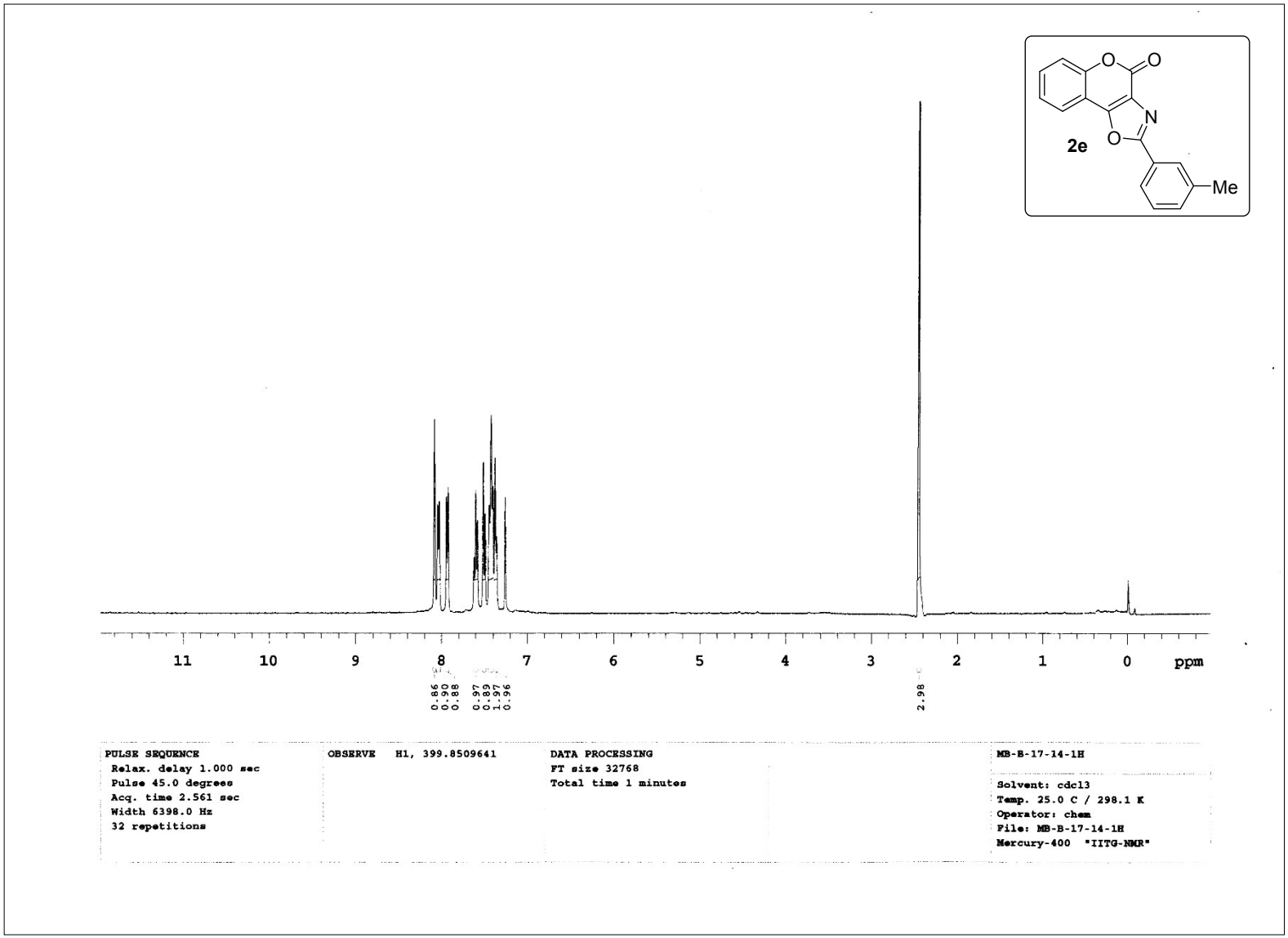
^{13}C NMR spectra of **2d**



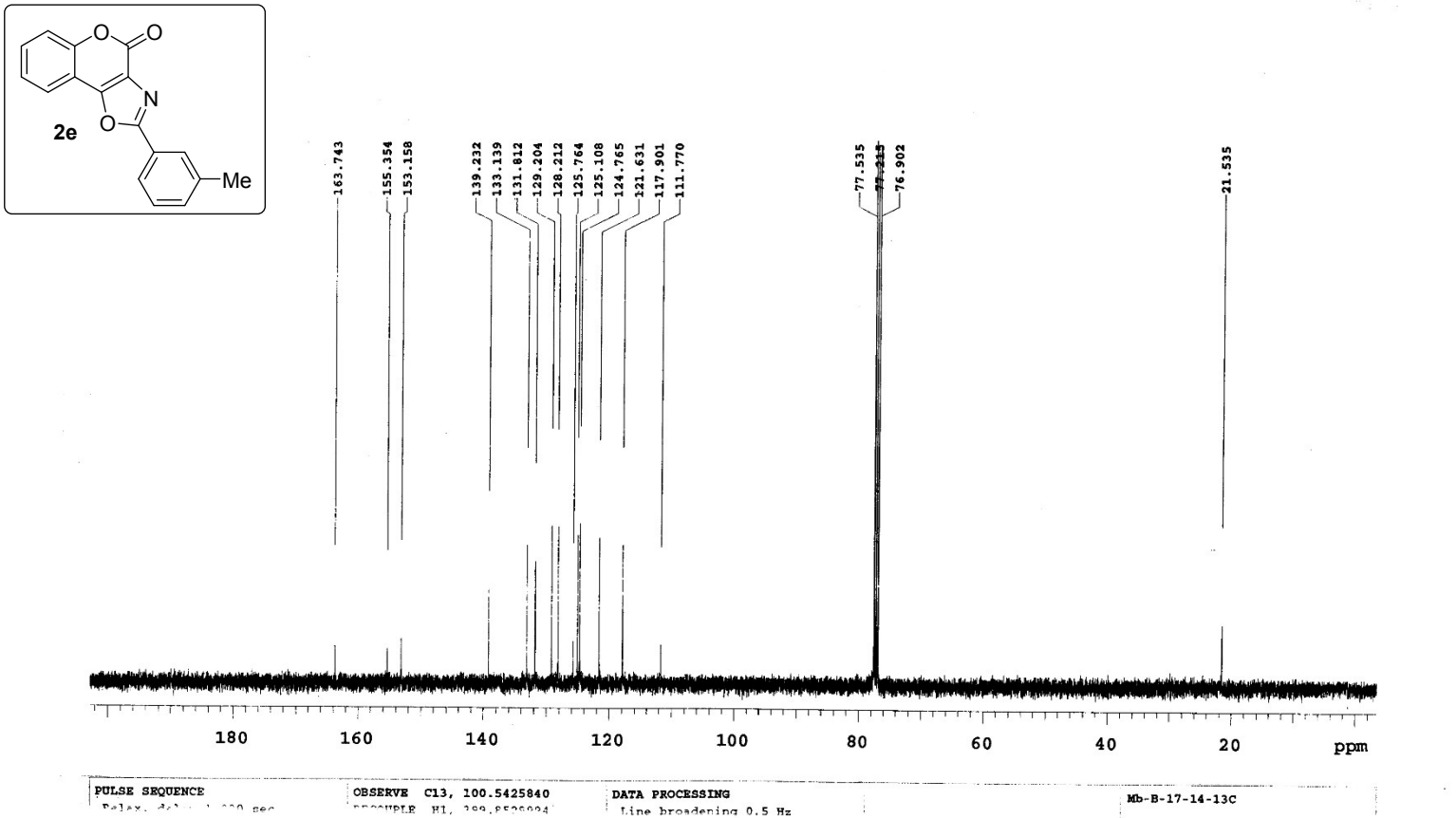
HRMS spectra of **2d**



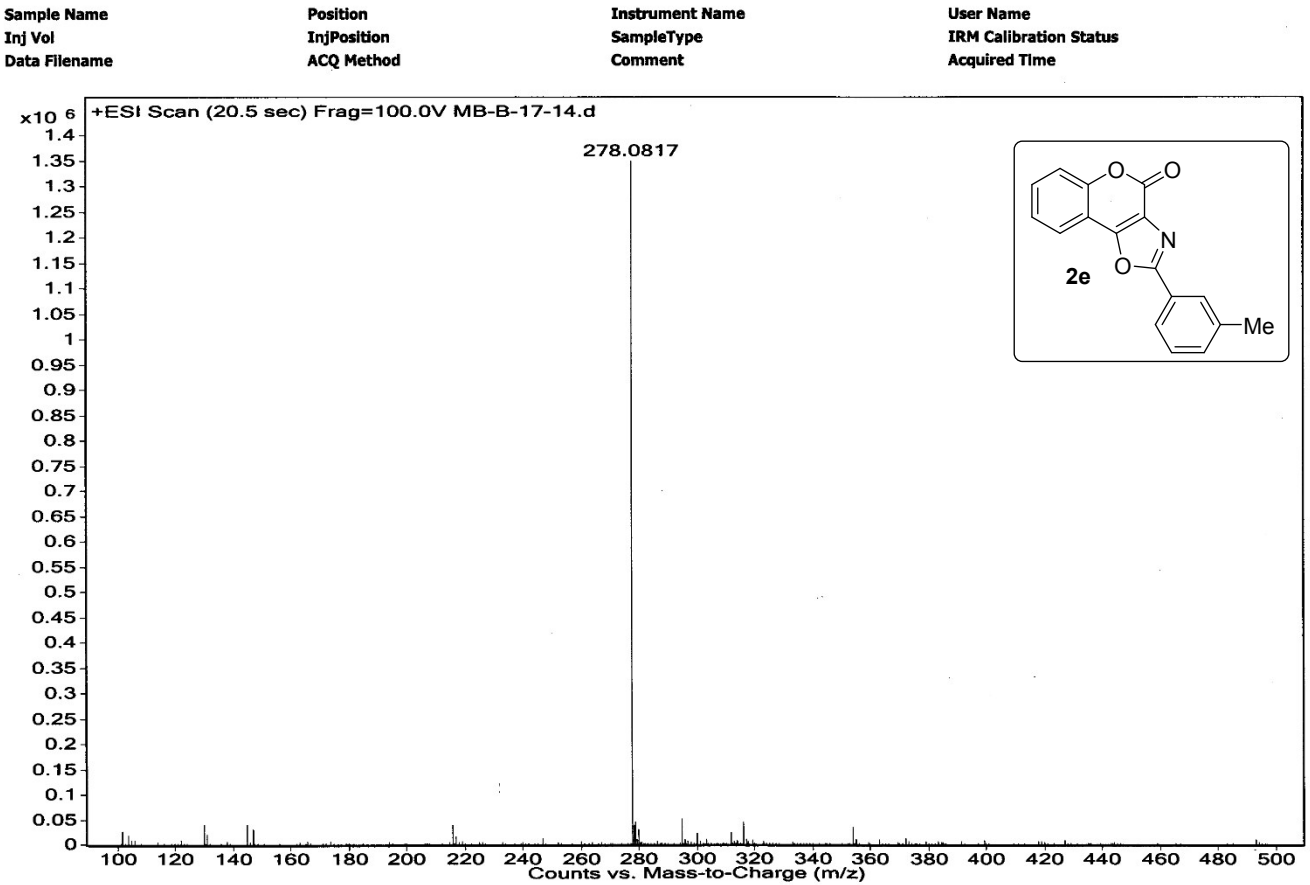
H[1] NMR spectra of **2e**



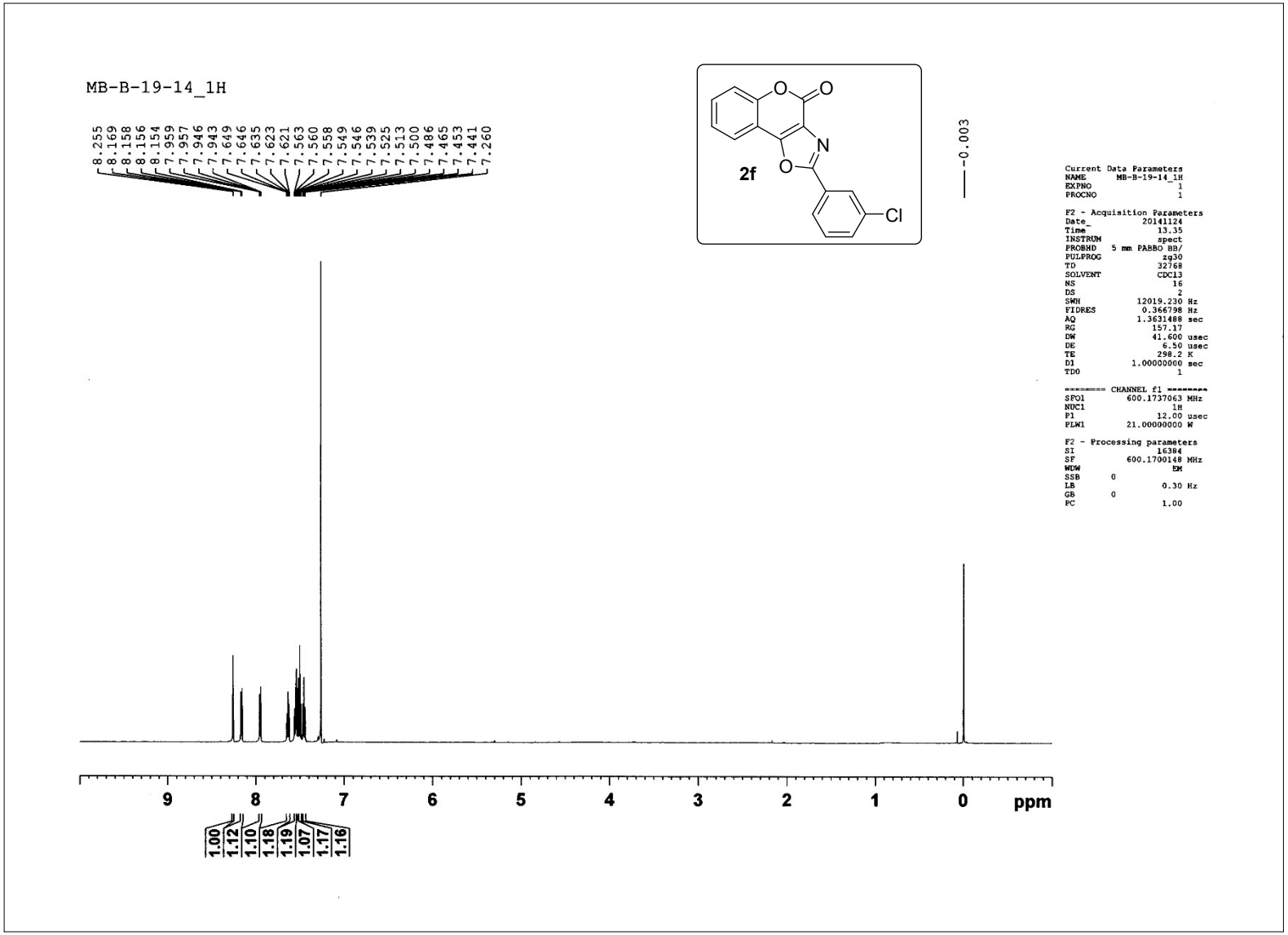
13C NMR spectra of **2e**



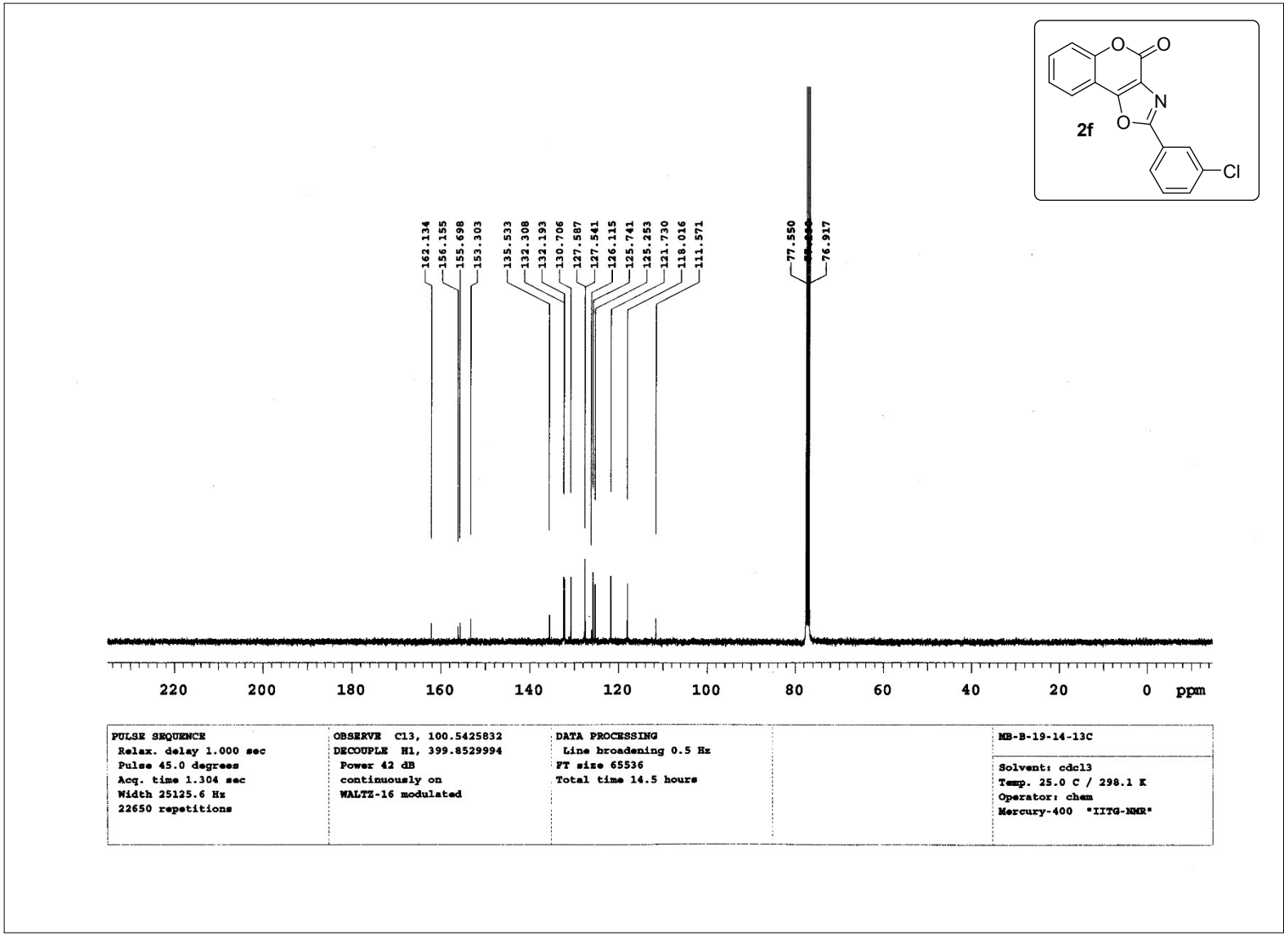
HRMS spectra of **2e**



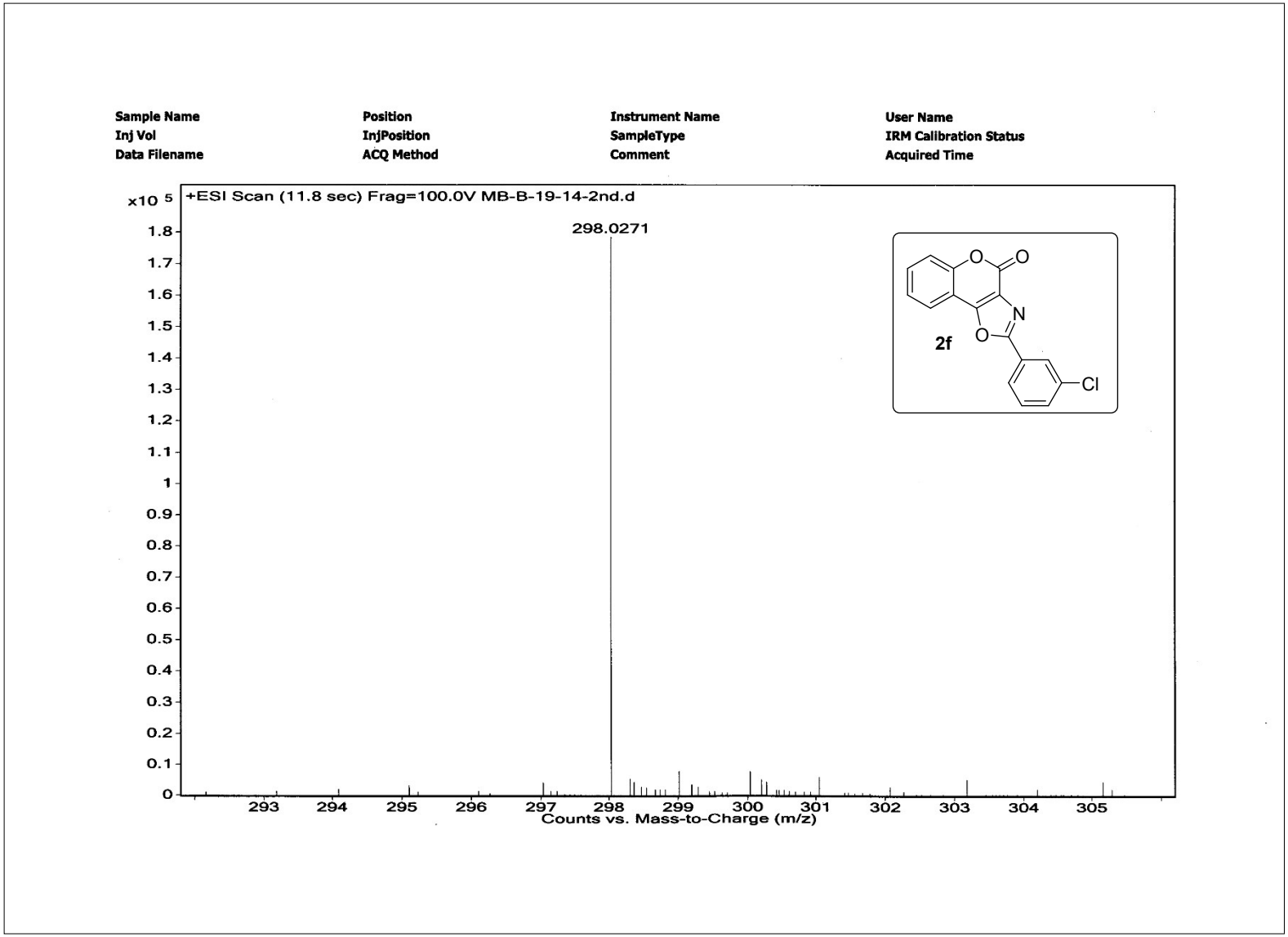
H[1] NMR spectra of **2f**



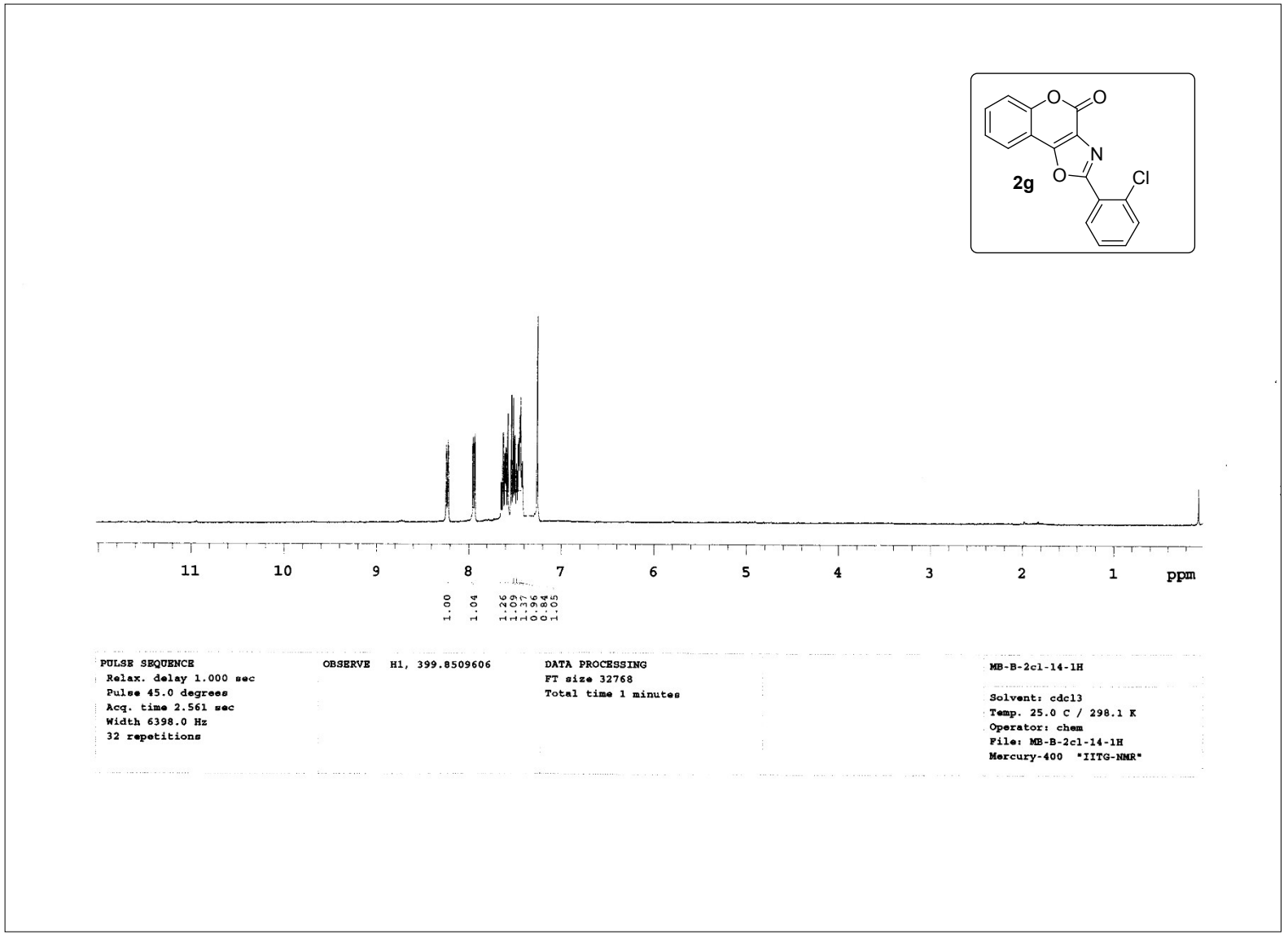
^{13}C NMR spectra of **2f**



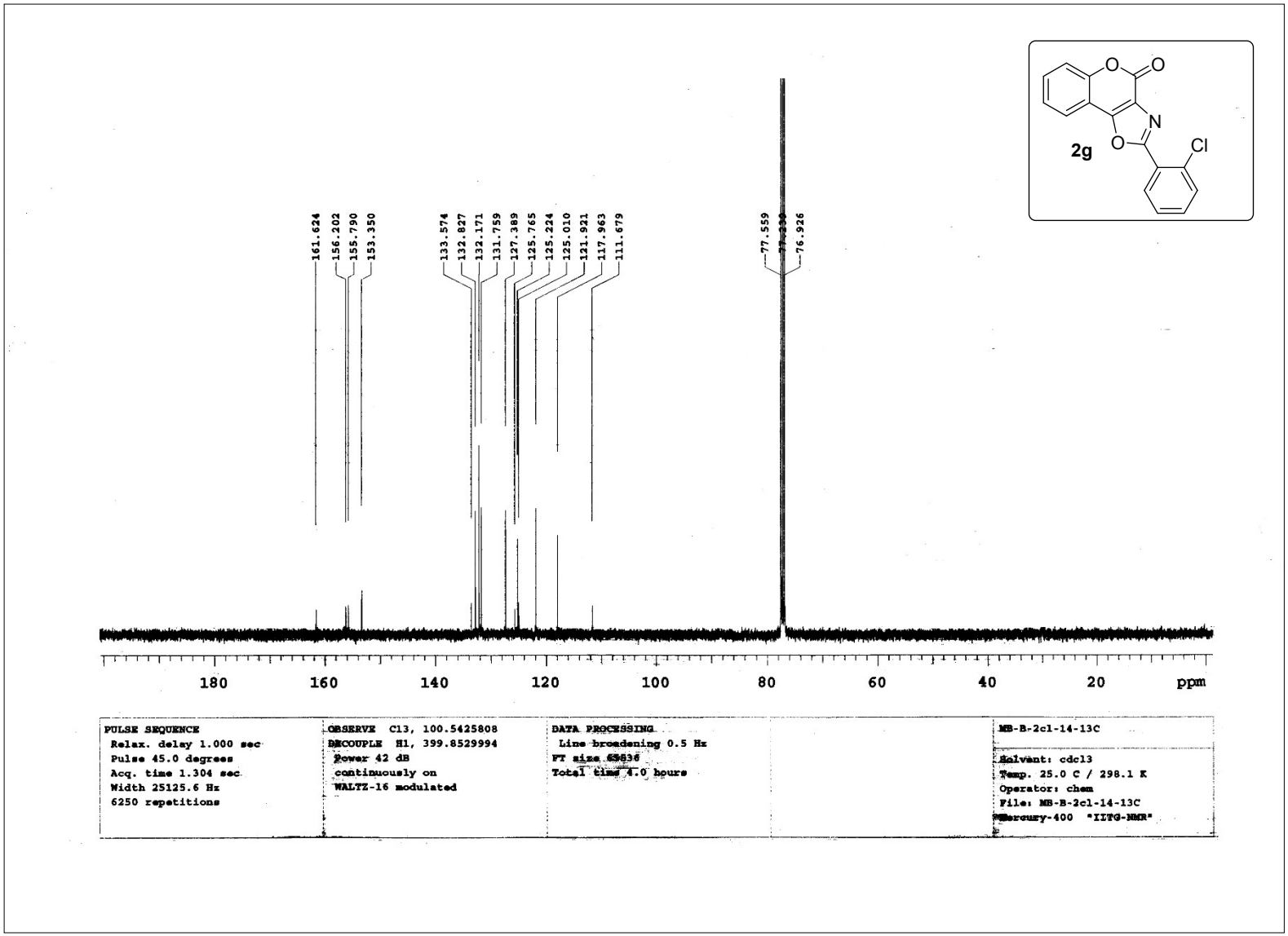
HRMS spectra of **2f**



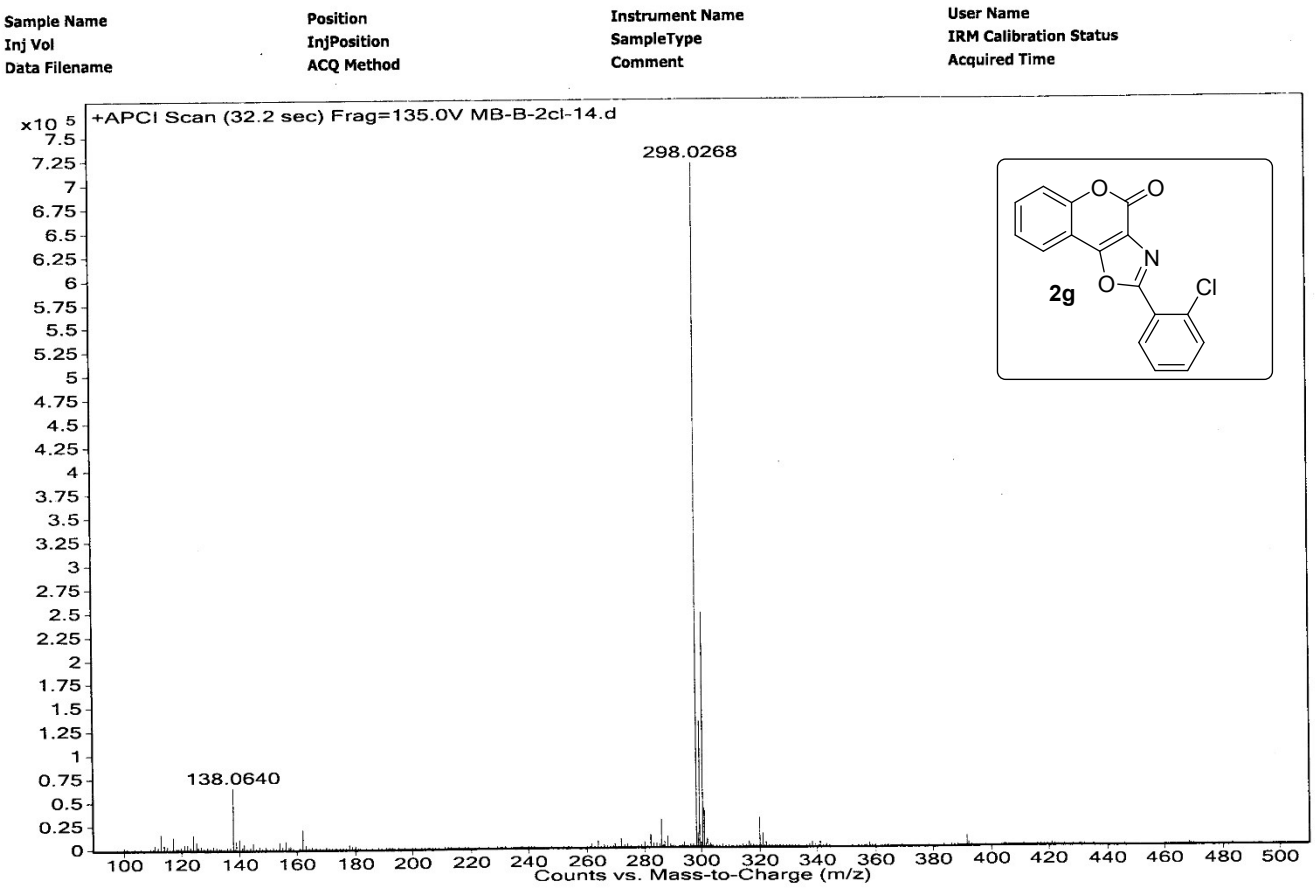
H[1] NMR spectra of **2g**



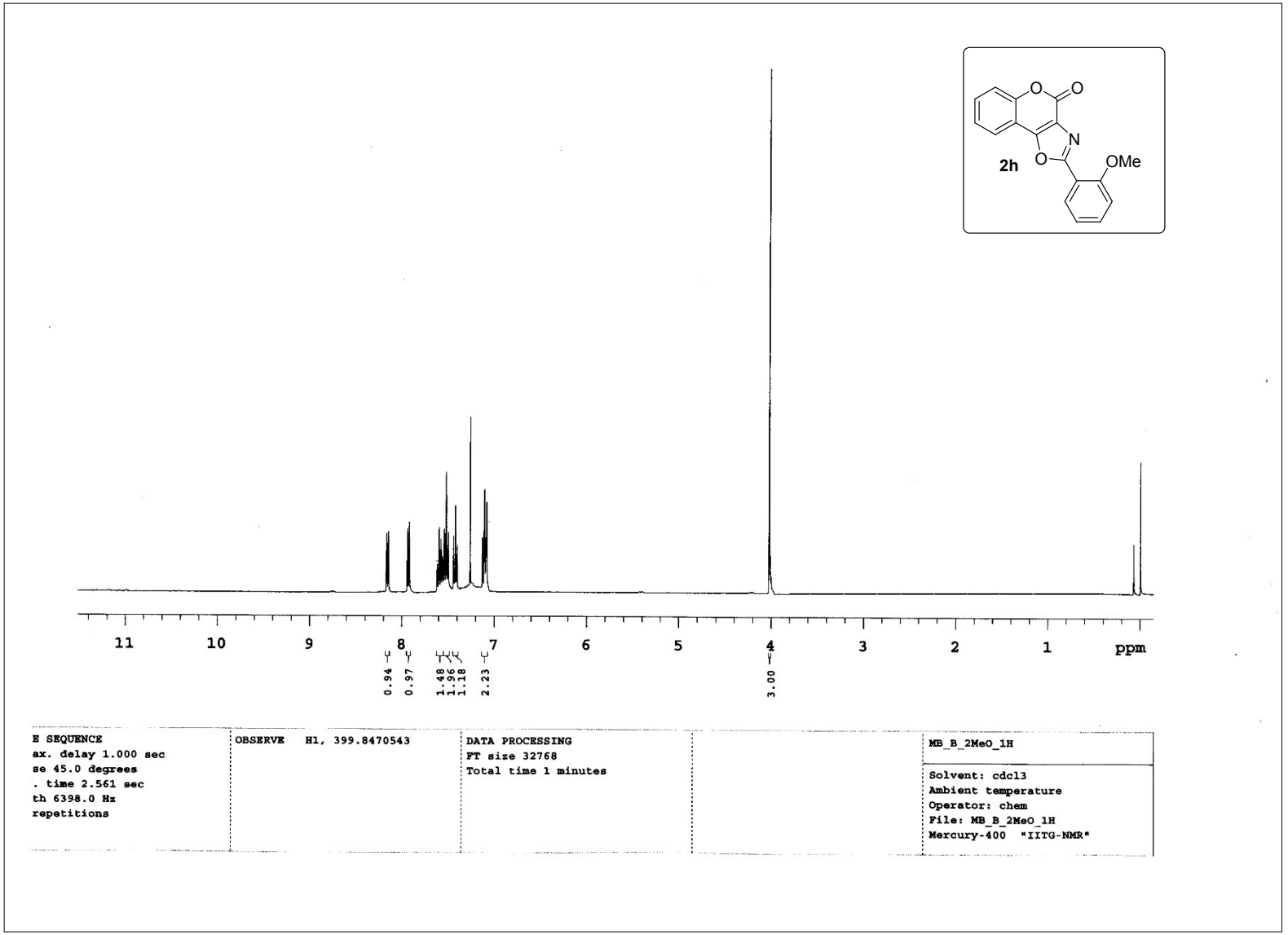
^{13}C NMR spectra of **2g**



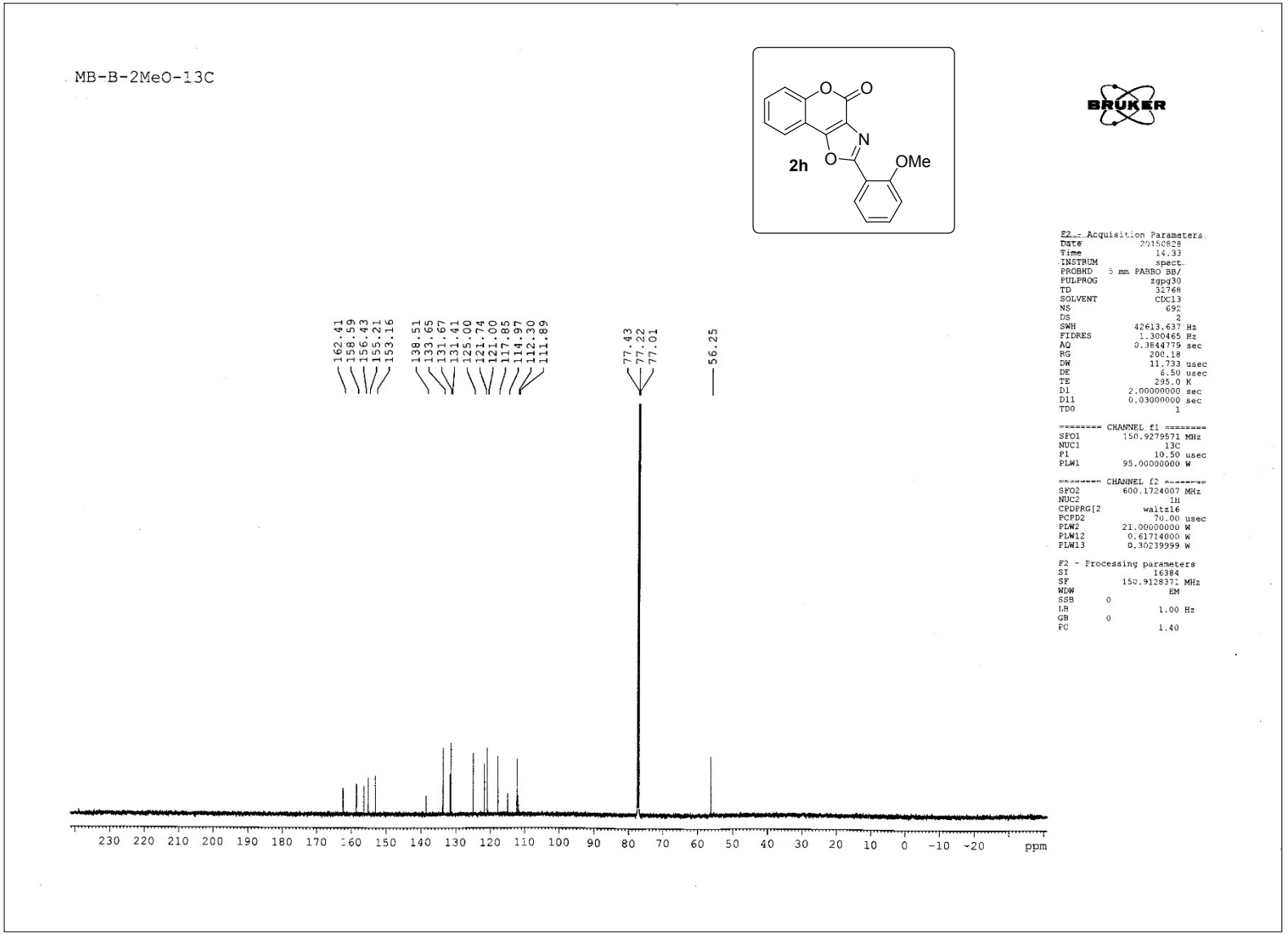
HRMS spectra of **2g**



H[1] NMR spectra of **2h**

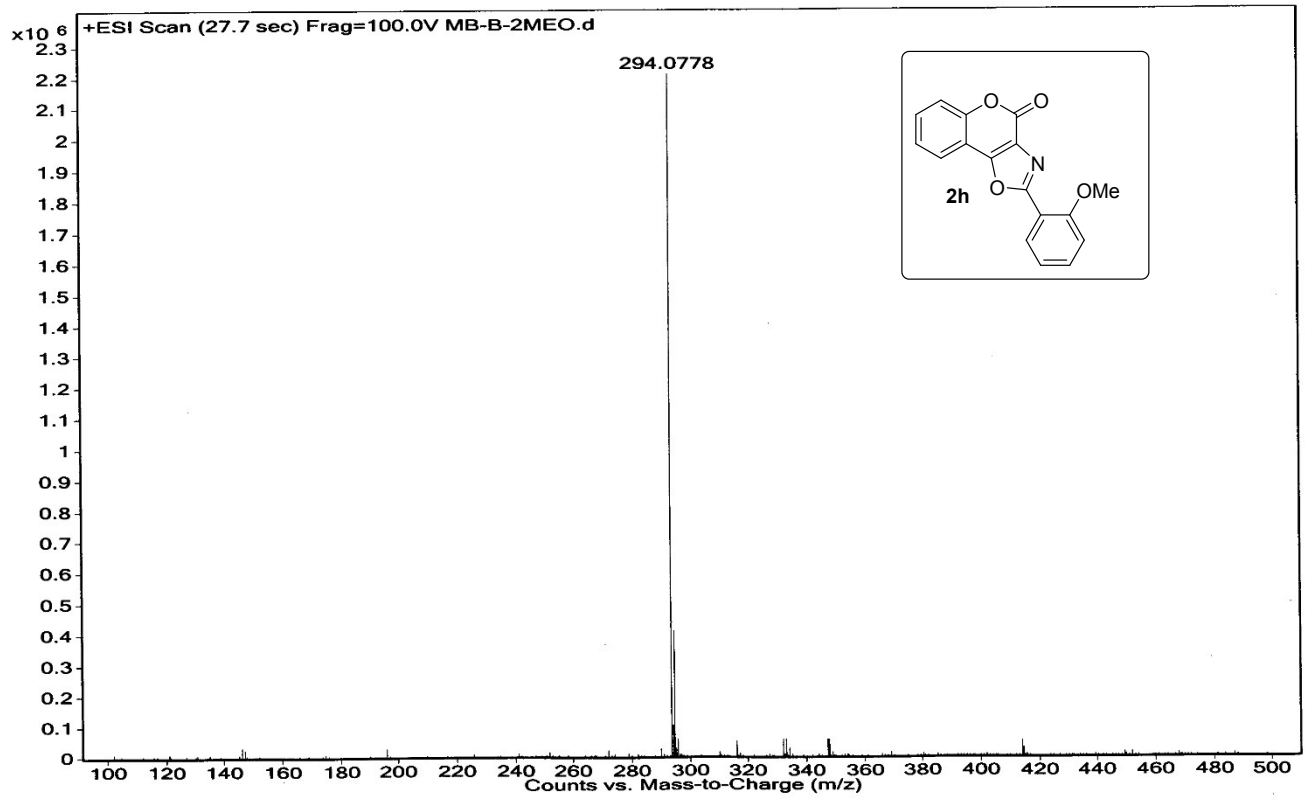


^{13}C NMR spectra of **2h**

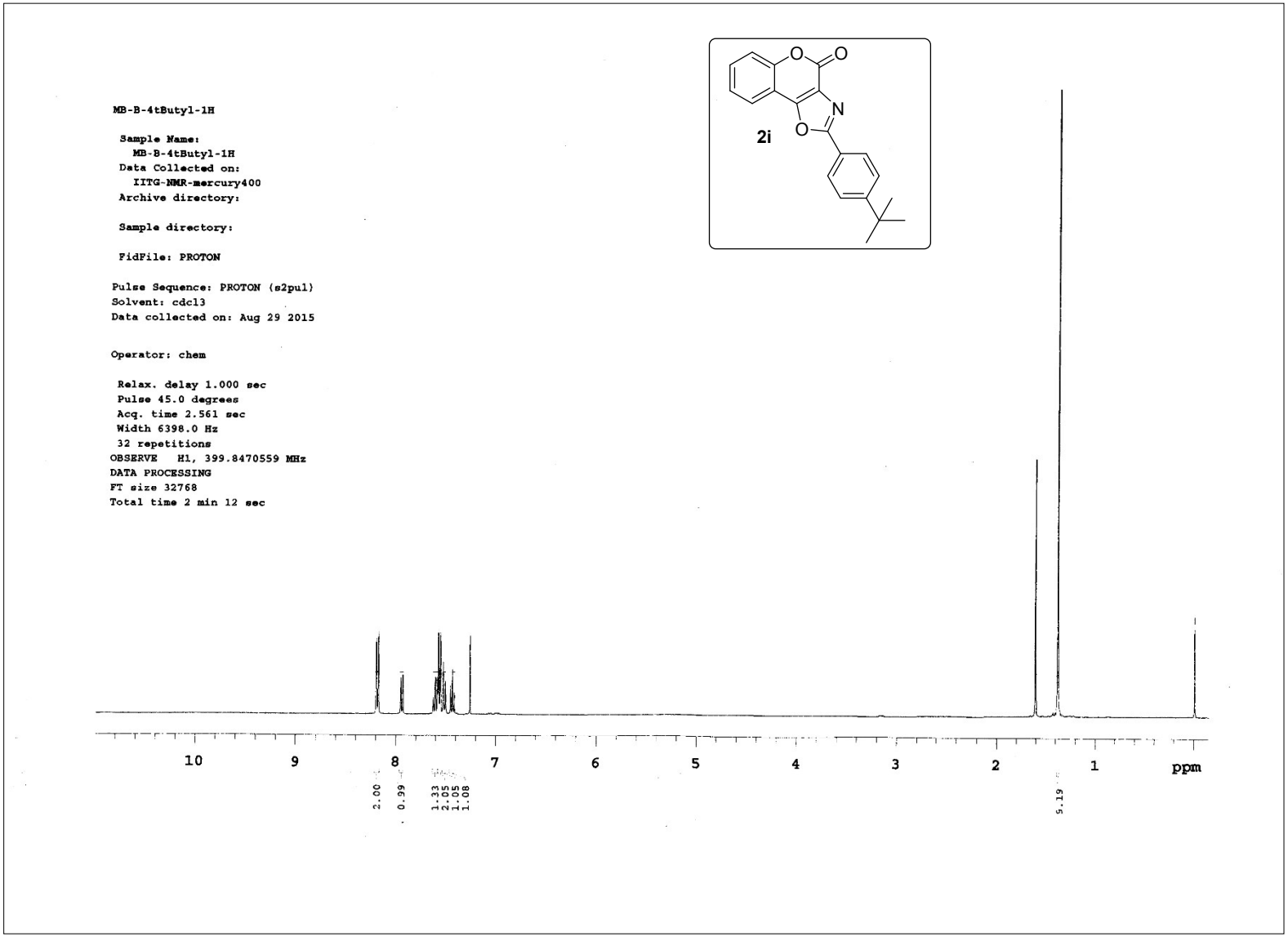


HRMS spectra of **2h**

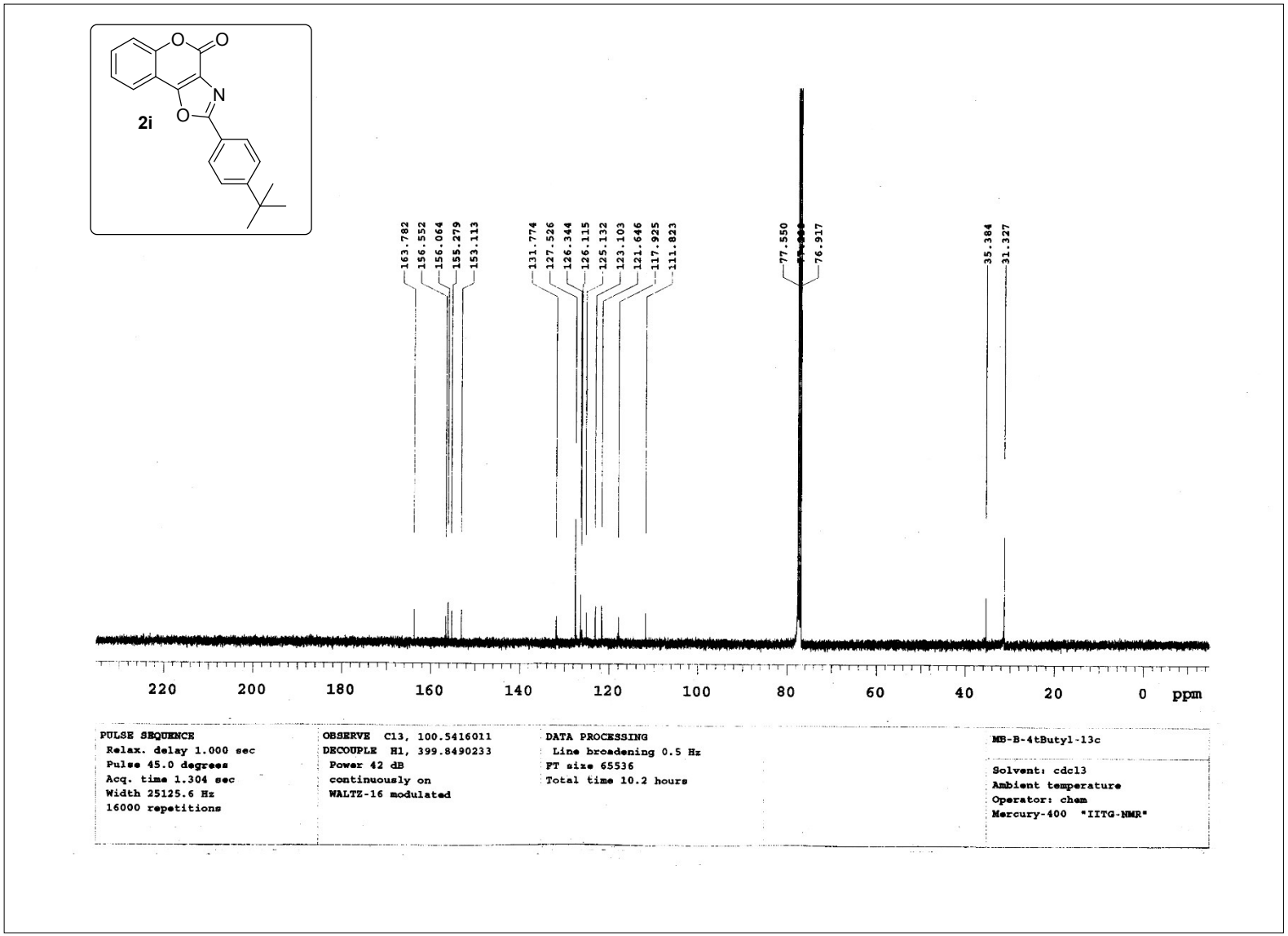
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	MB-B-2MEO.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



H^1 NMR spectra of **2i**

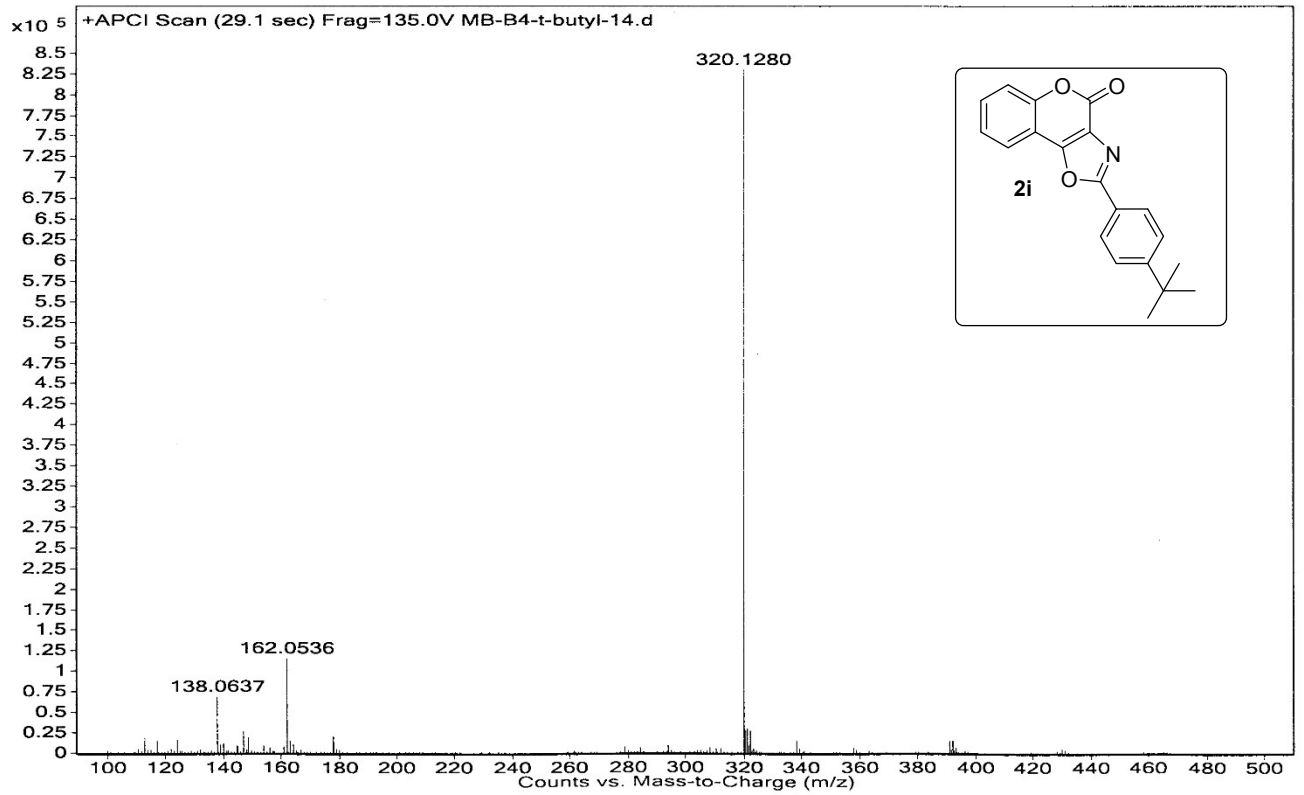


^{13}C NMR spectra of **2i**

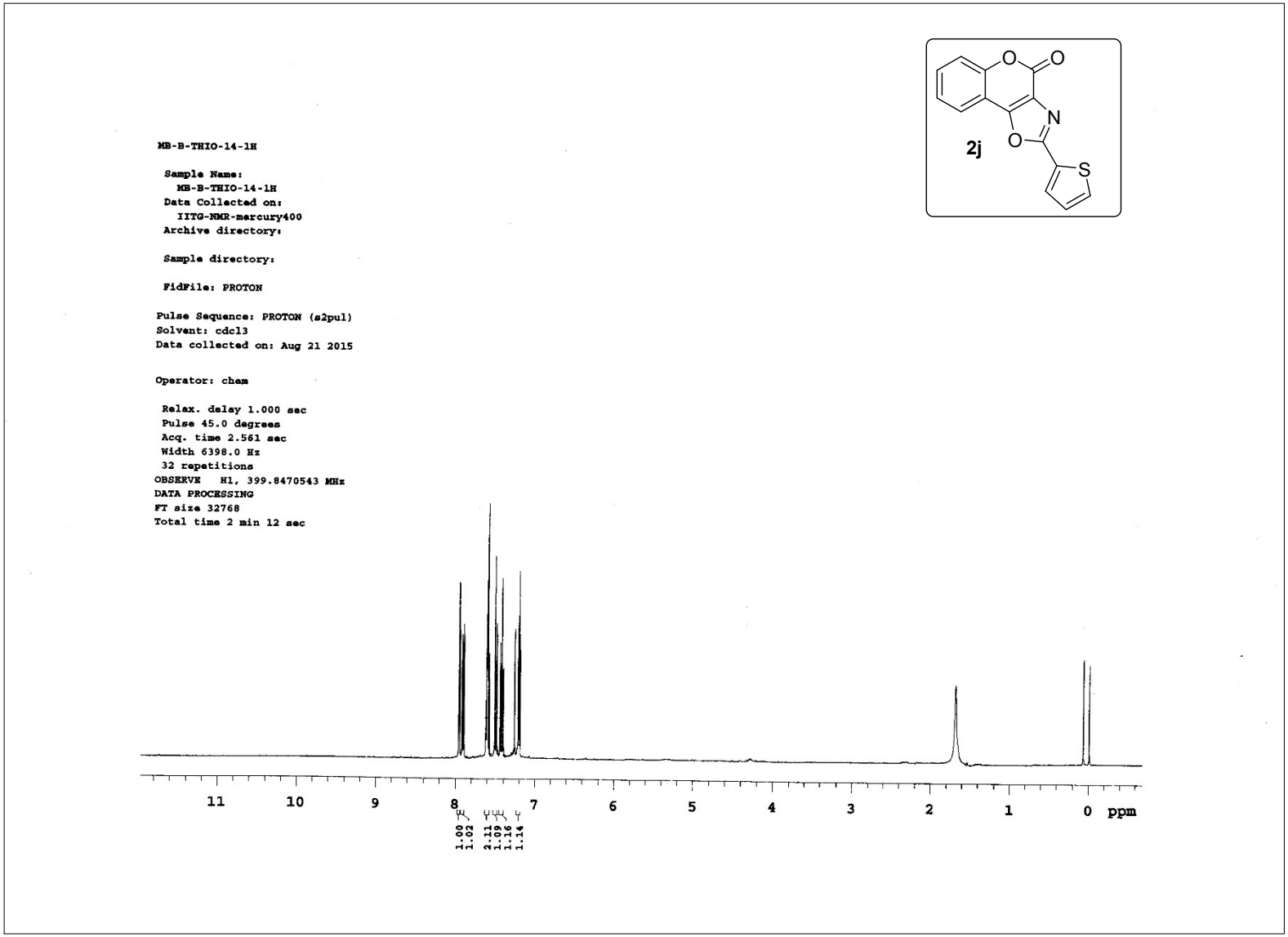


HRMS spectra of **2i**

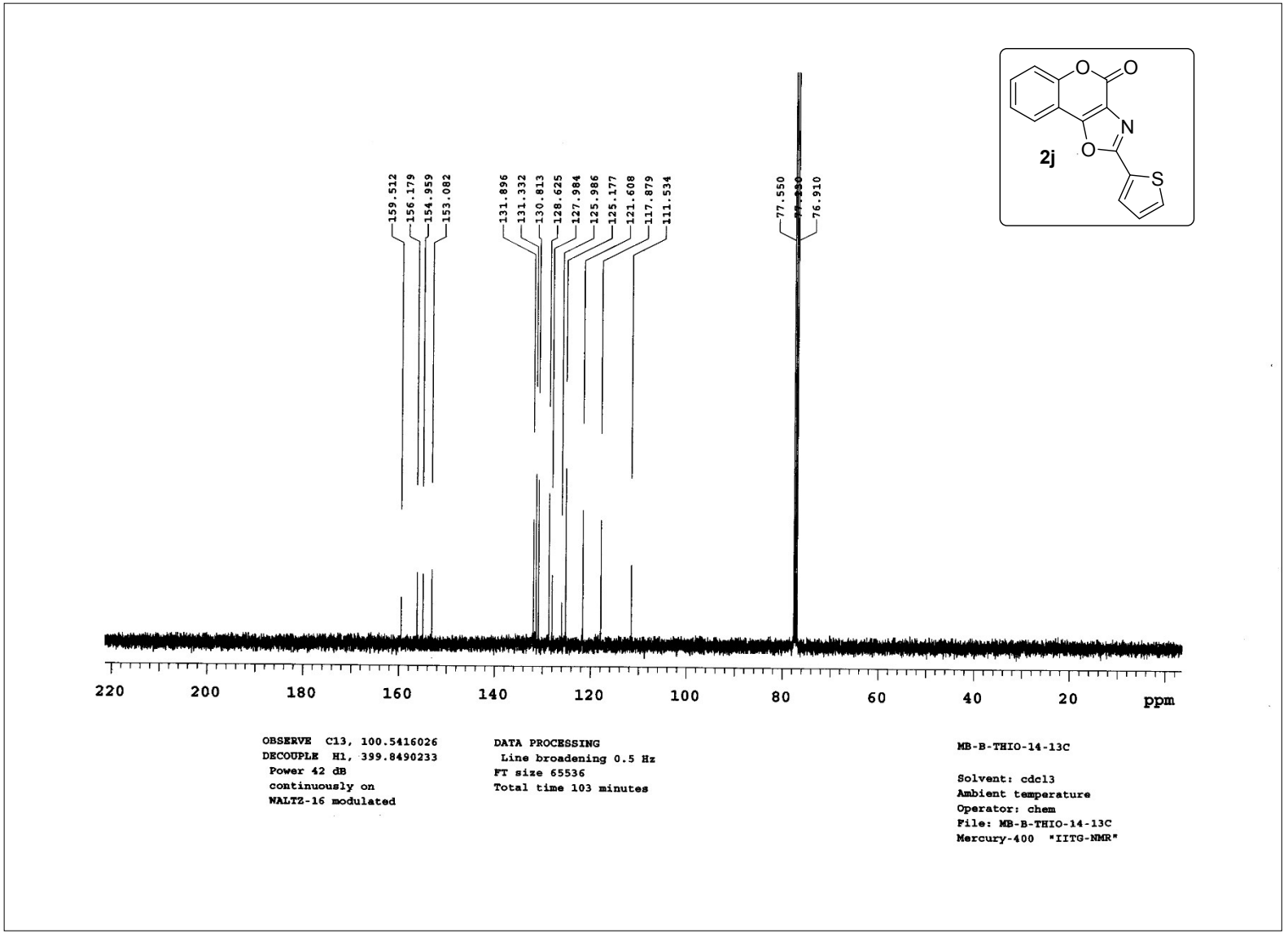
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



H^1 NMR spectra of **2j**



^{13}C NMR spectra of **2j**



HRMS spectra of **2j**

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
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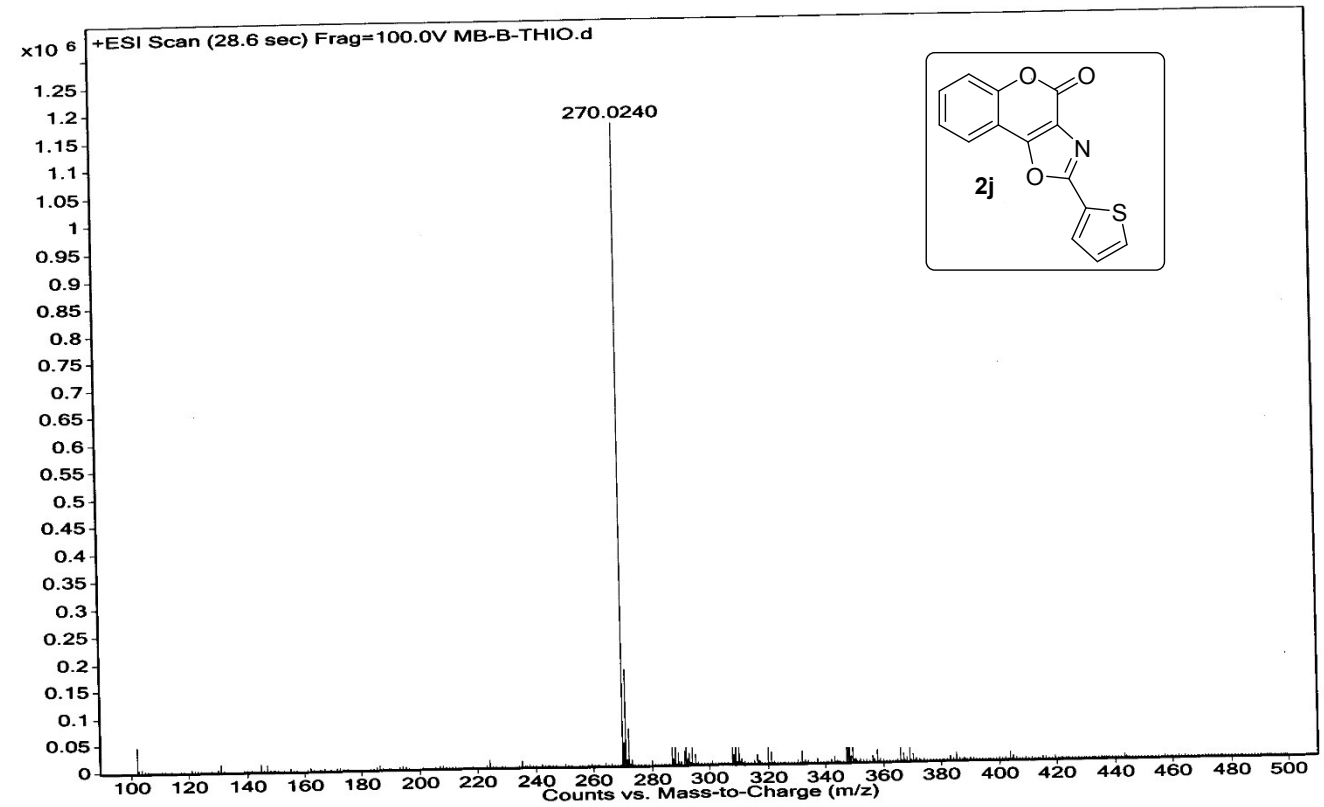
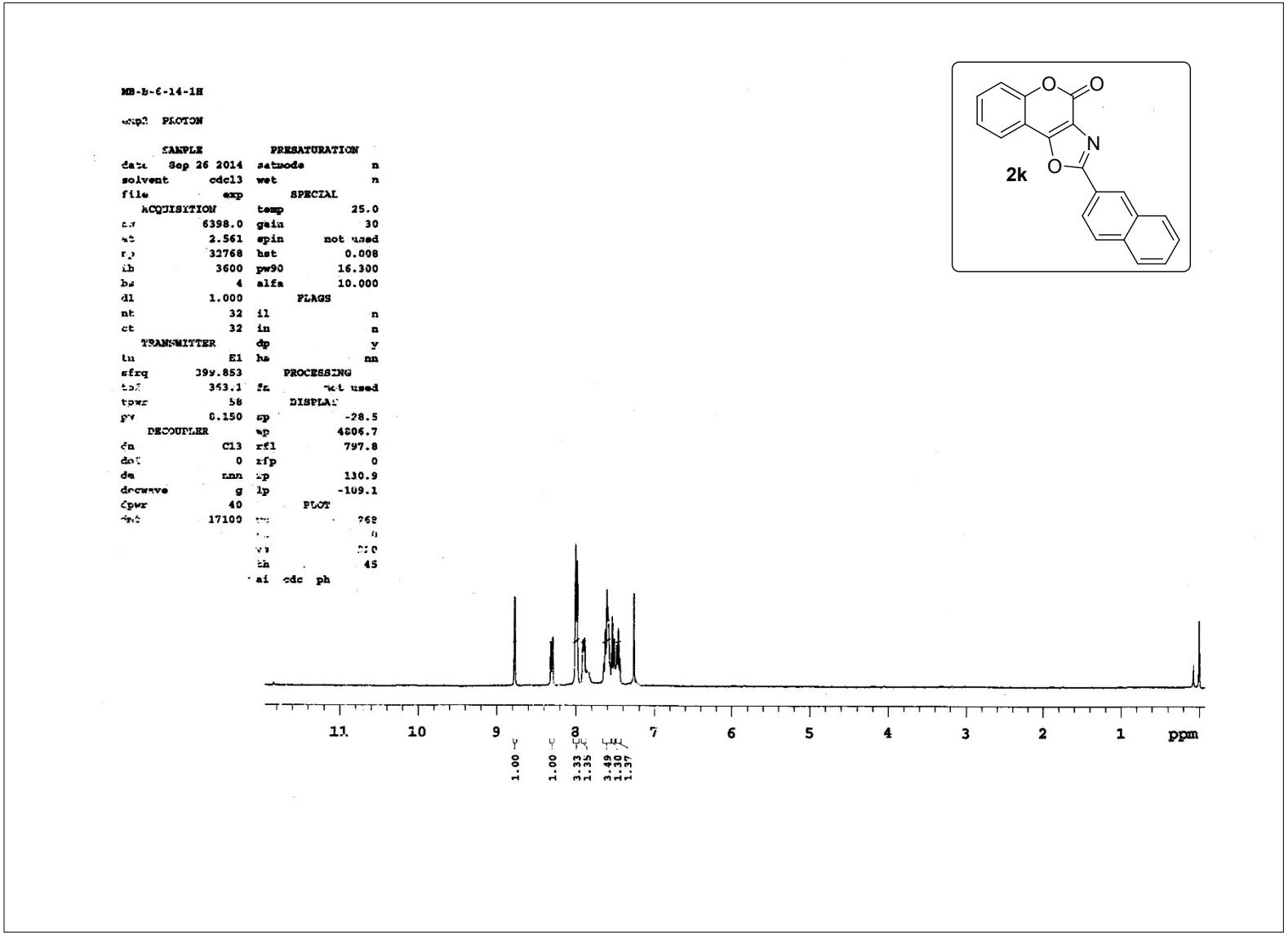
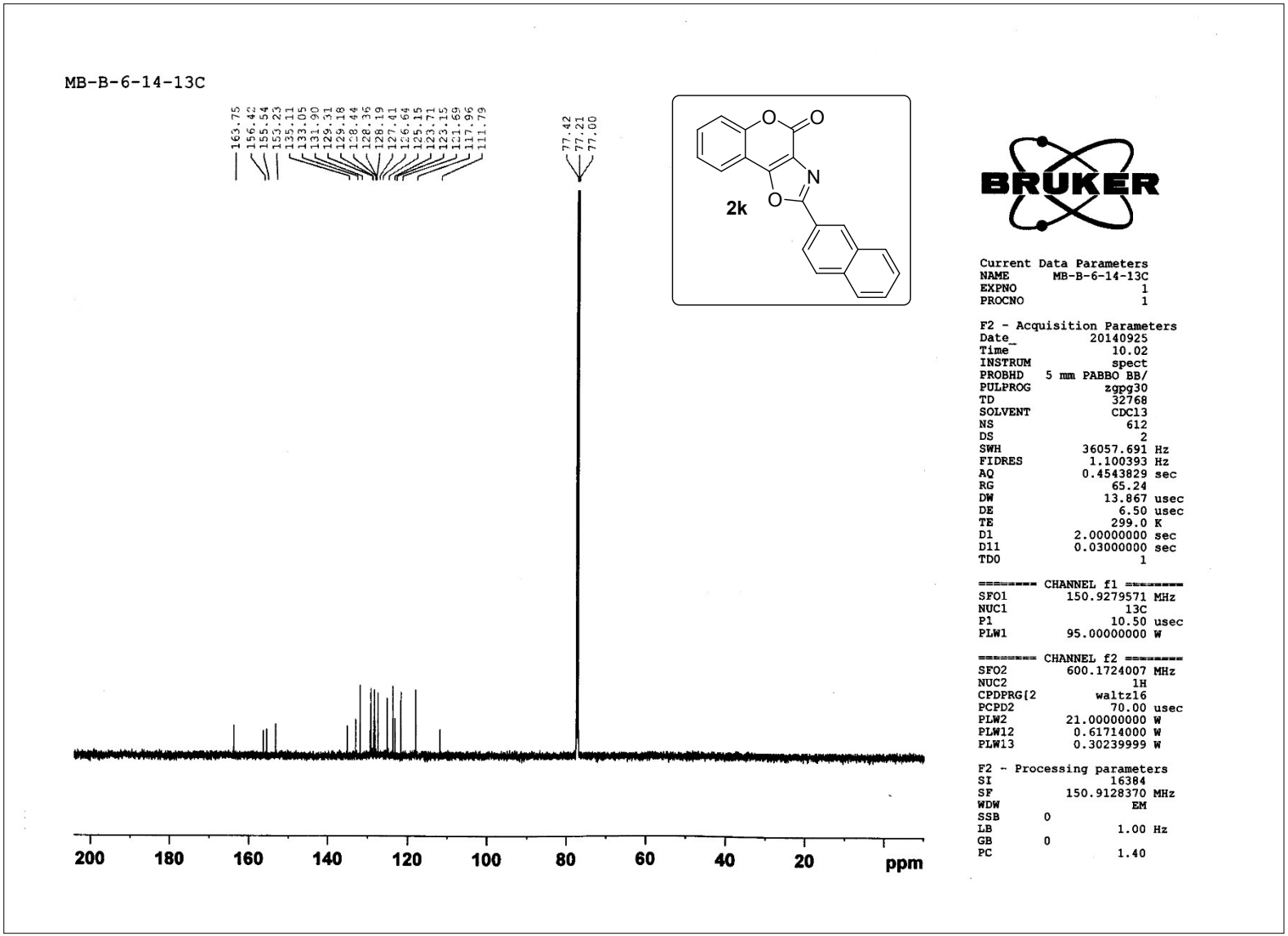


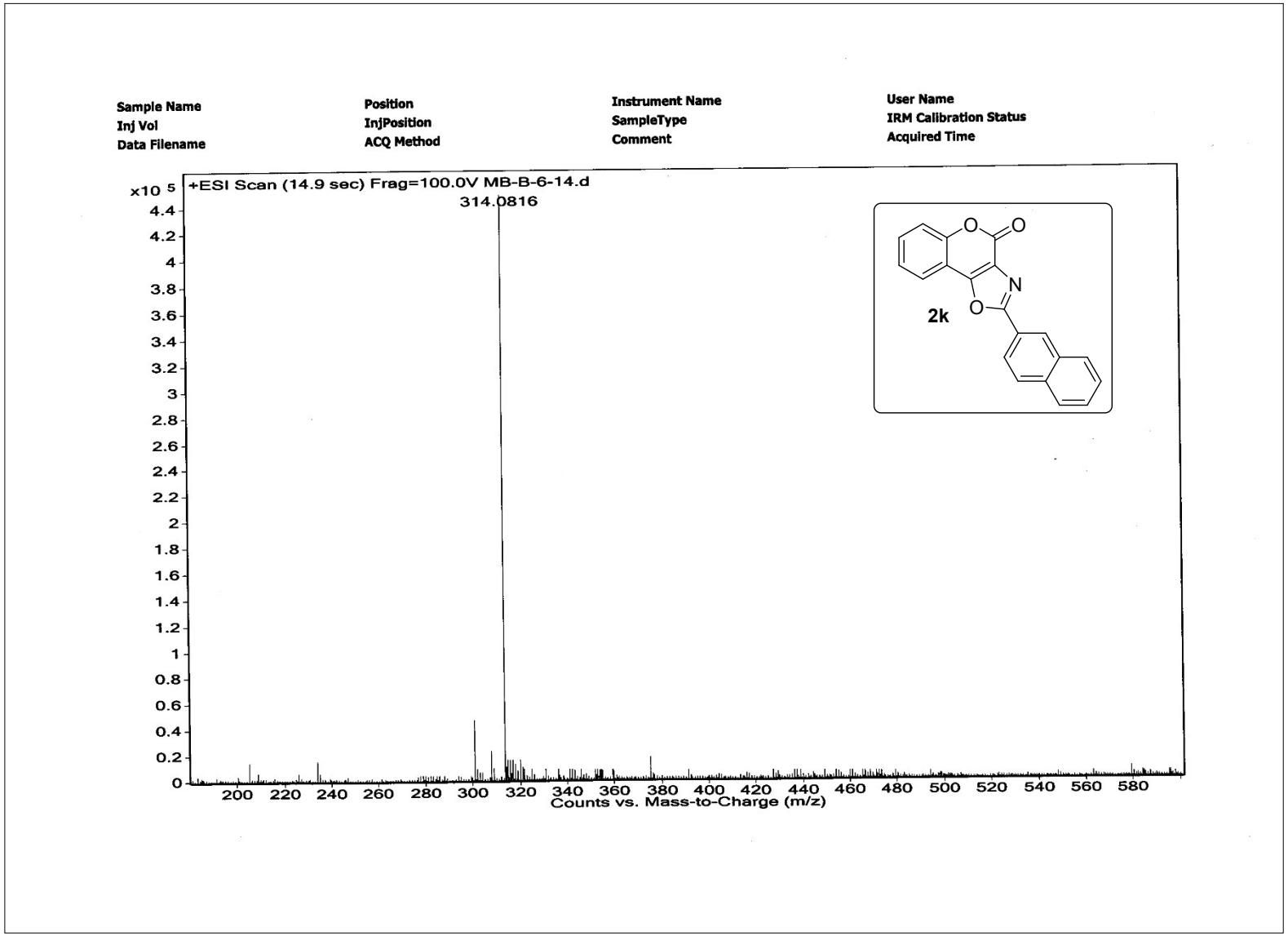
H[1] NMR spectra of **2k**



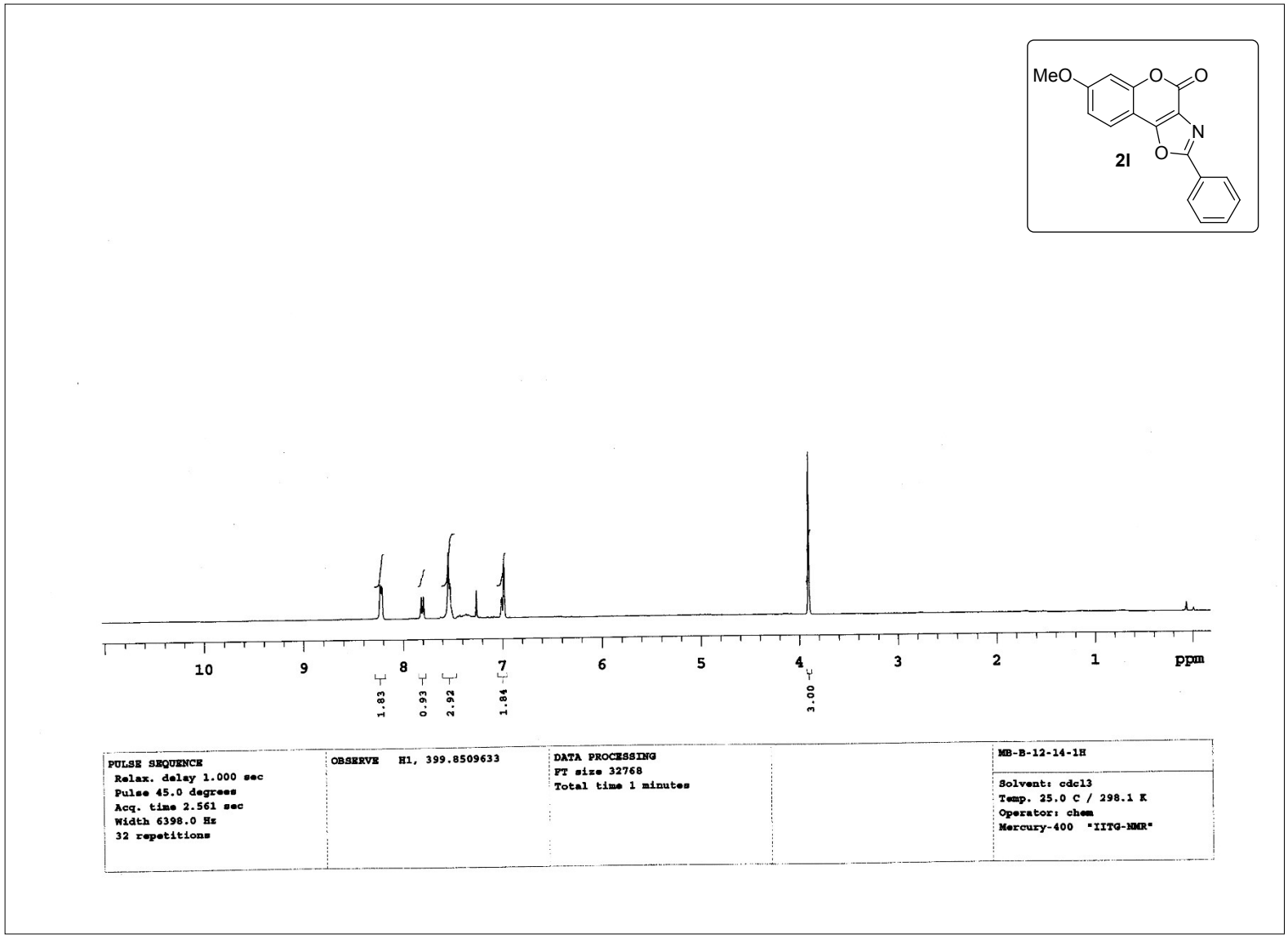
^{13}C NMR spectra of **2k**



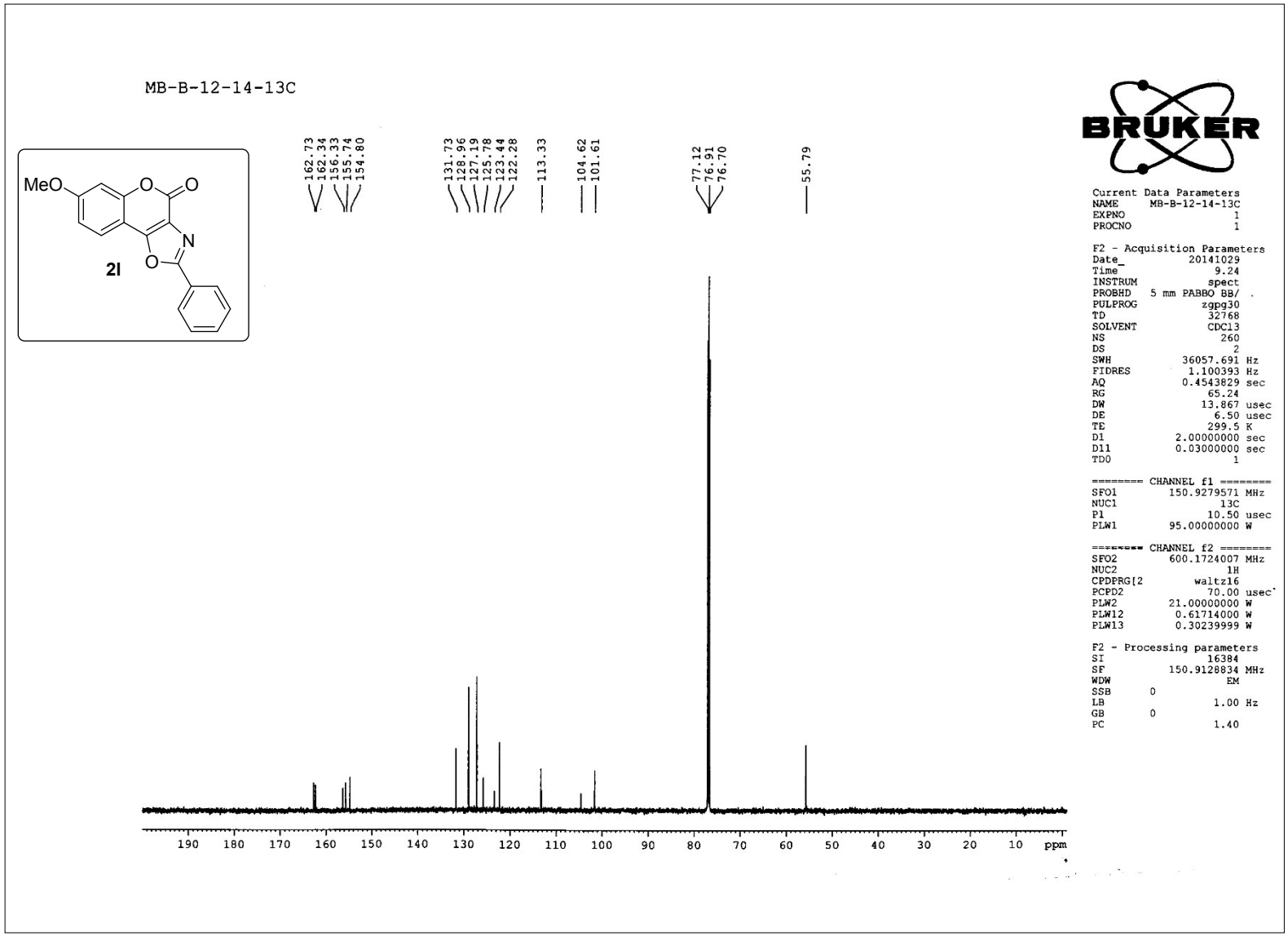
HRMS spectra of **2k**



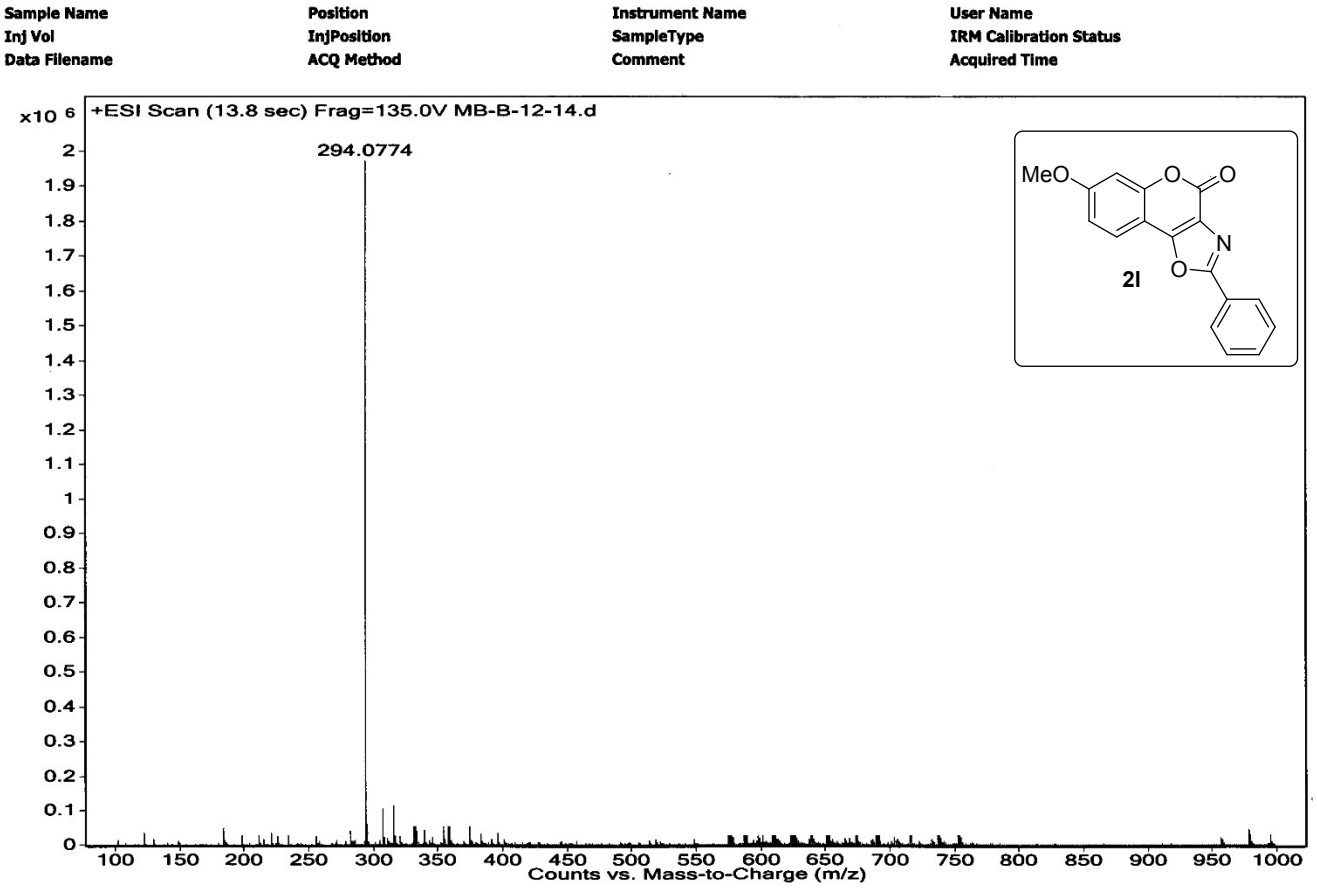
H[1] NMR spectra of **2l**



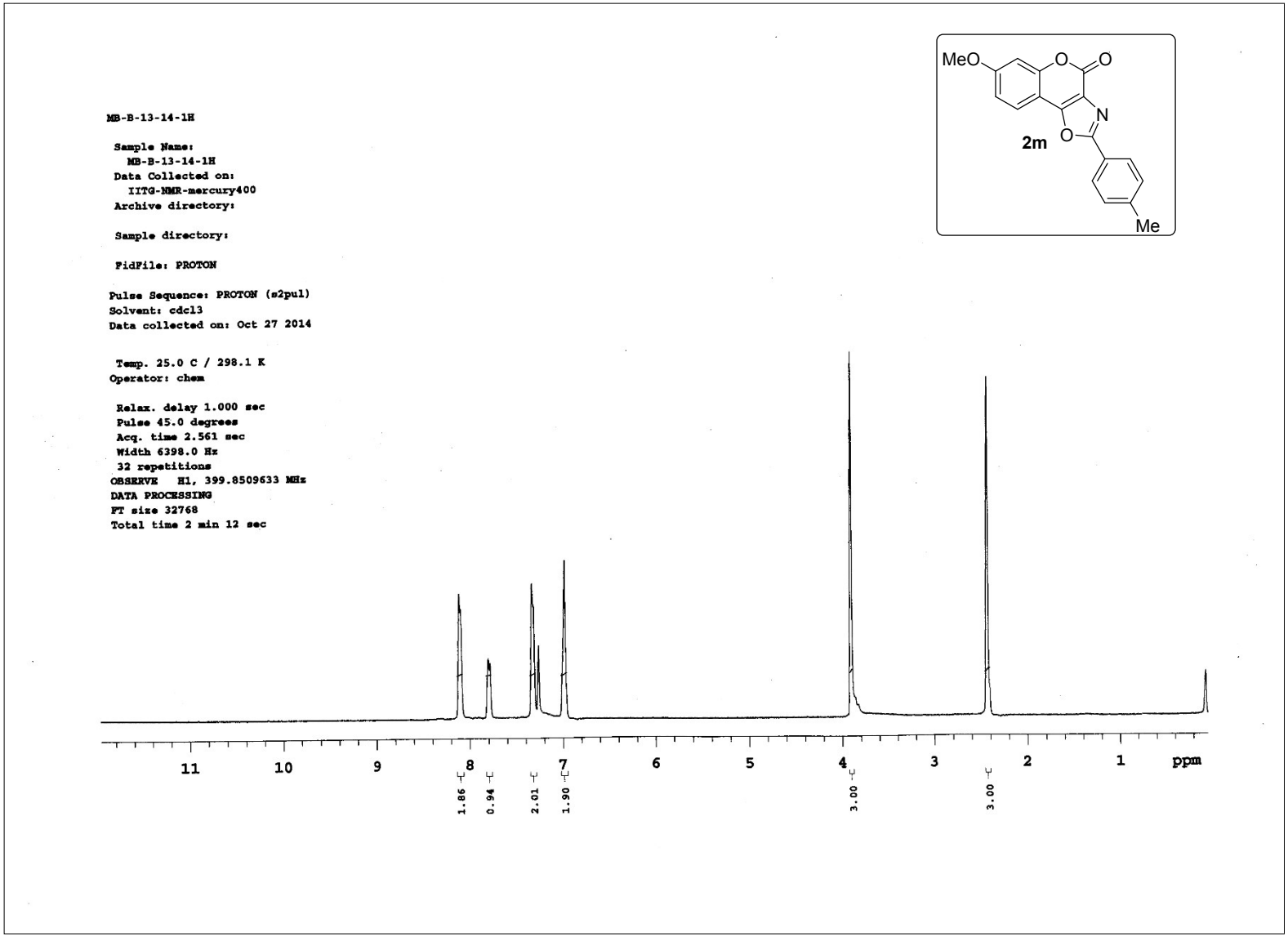
^{13}C NMR spectra of **2l**



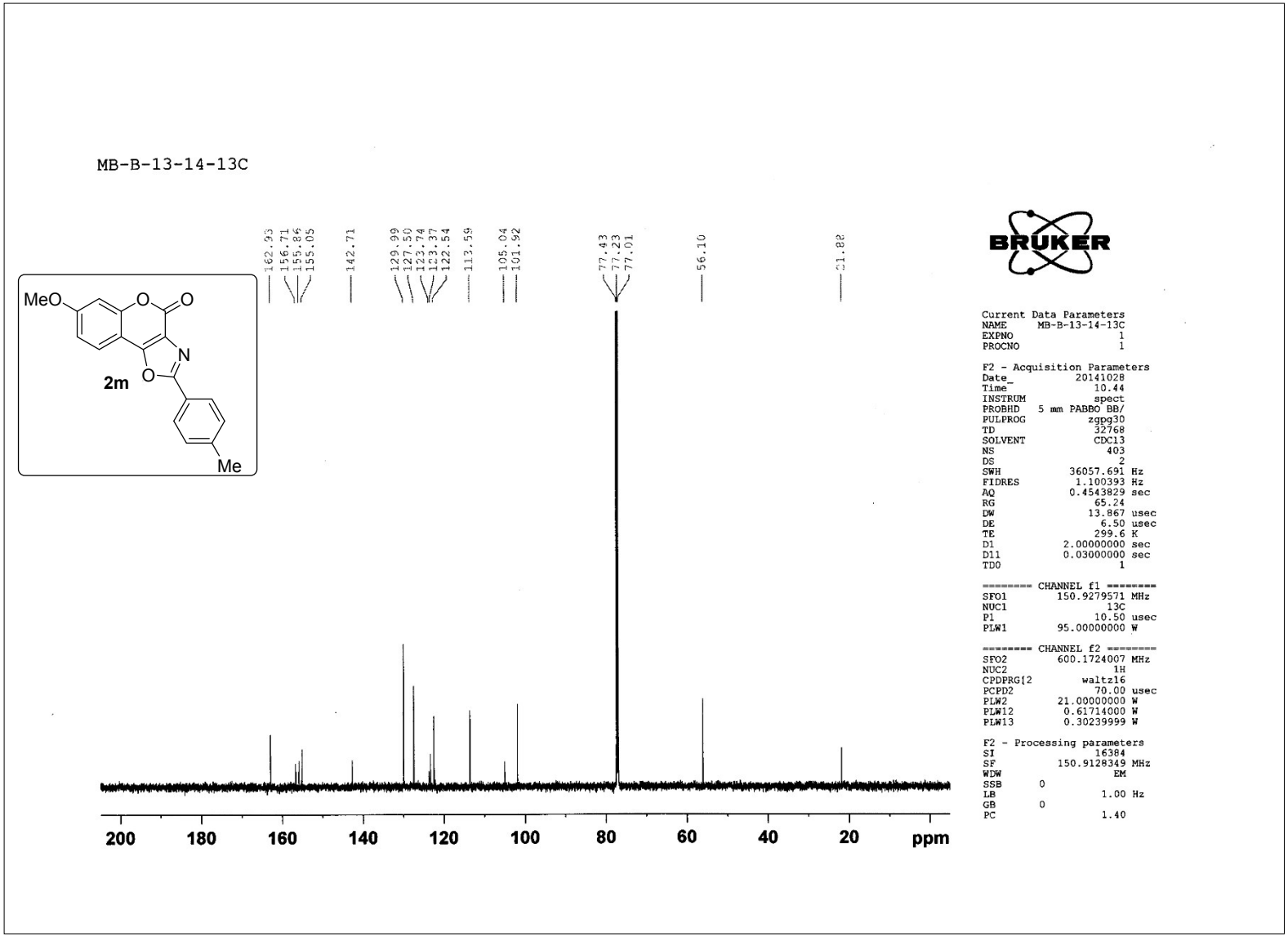
HRMS spectra of **2l**



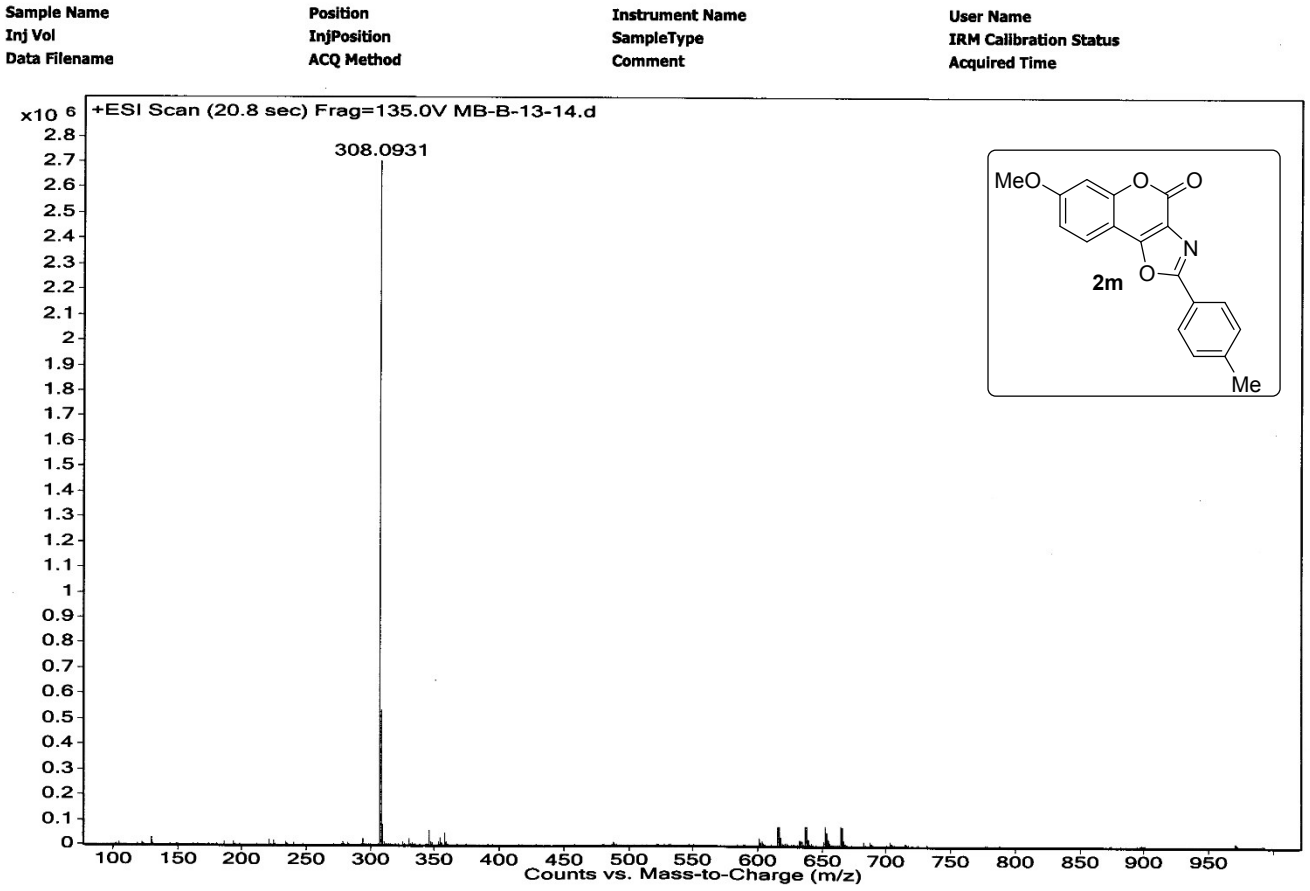
H[1] NMR spectra of **2m**



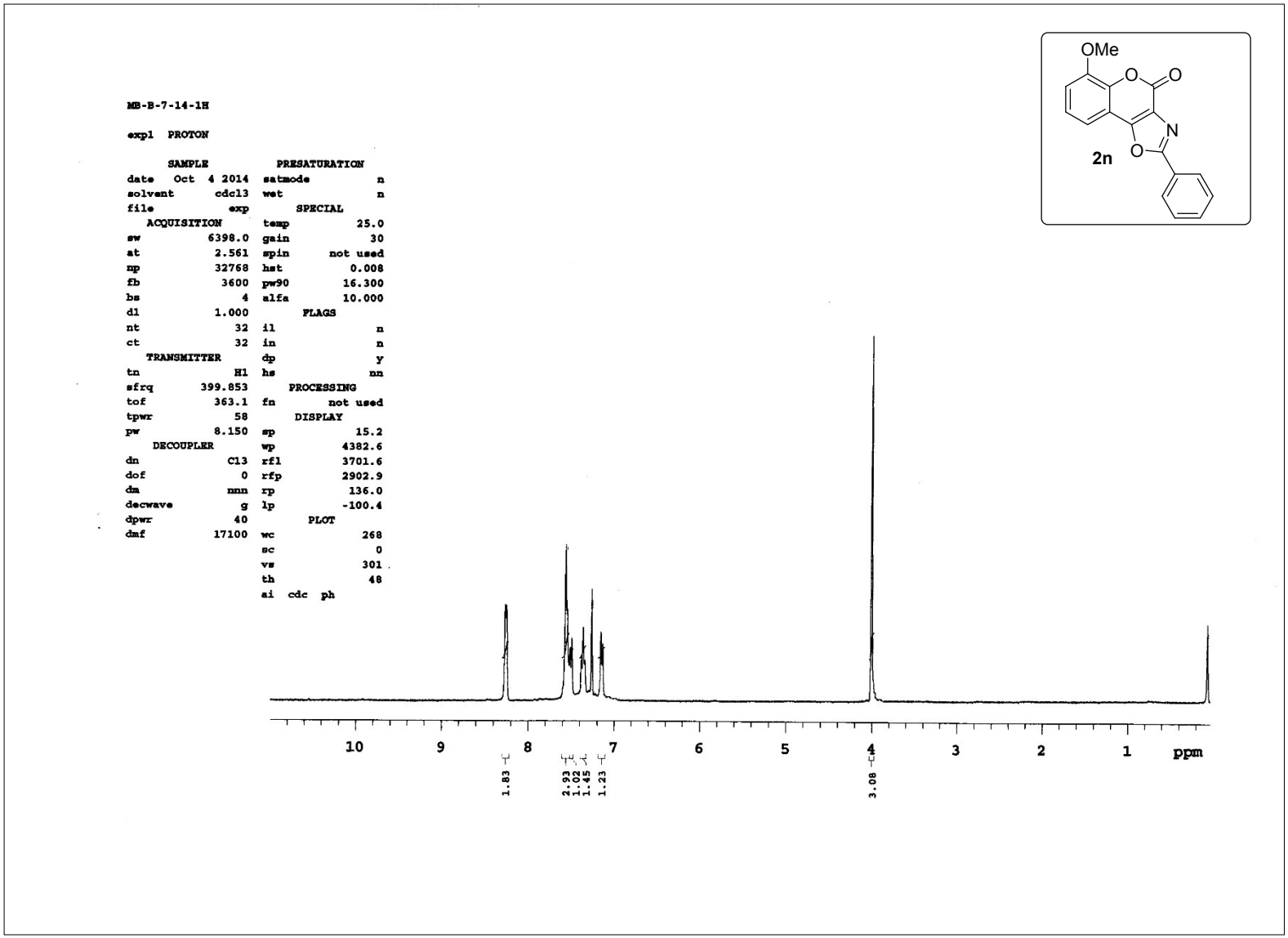
^{13}C NMR spectra of **2m**



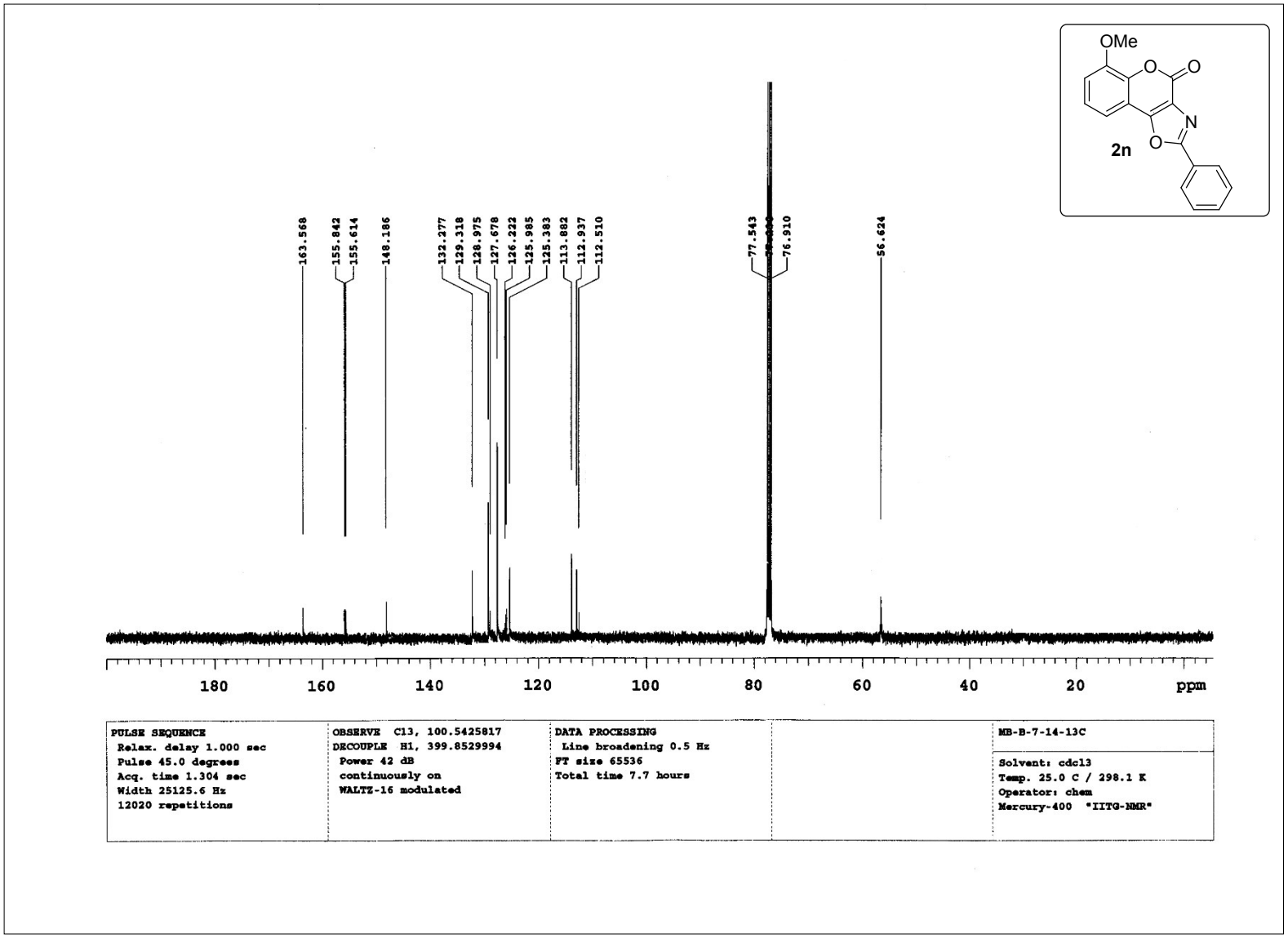
HRMS spectra of **2m**



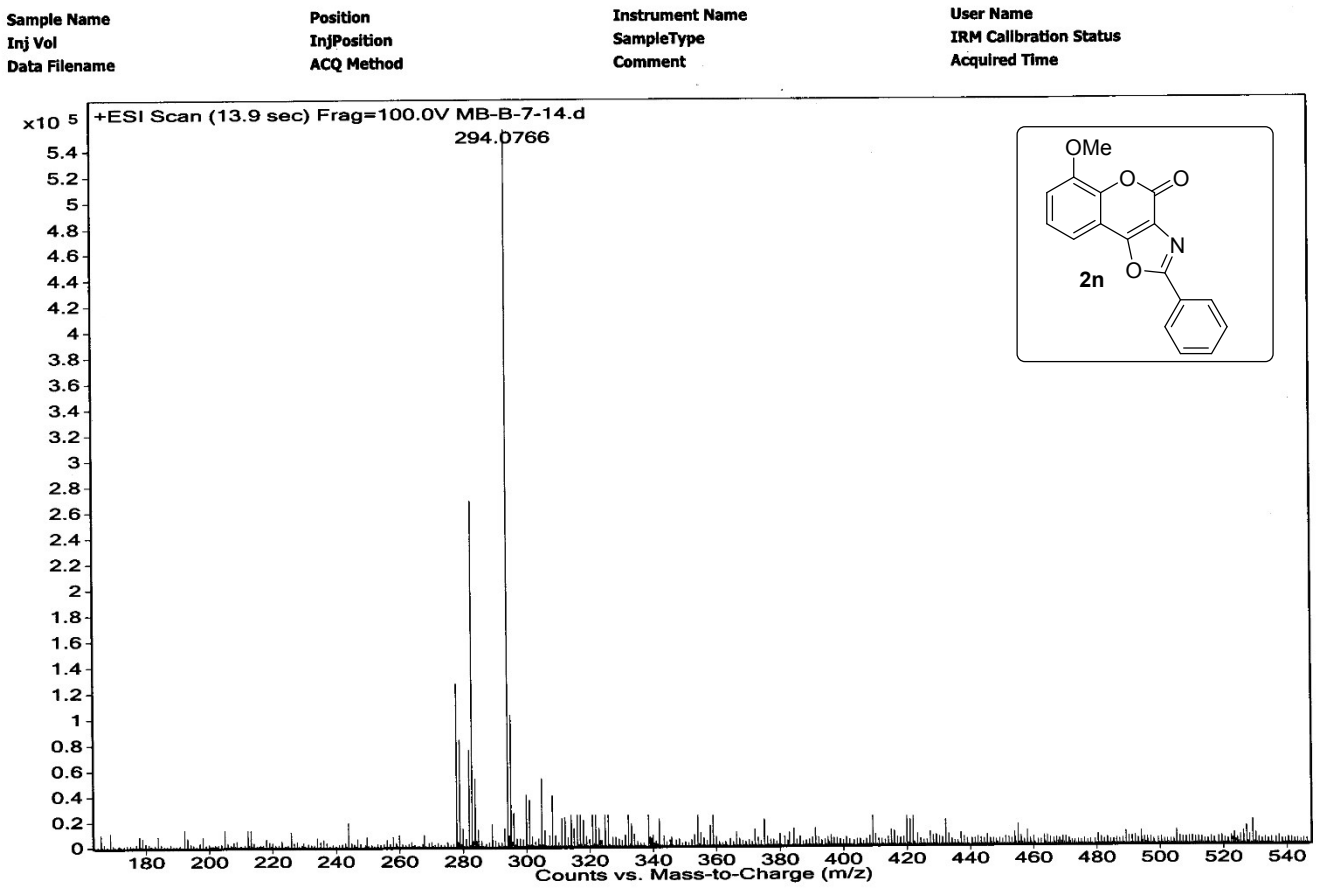
H[1] NMR spectra of **2n**



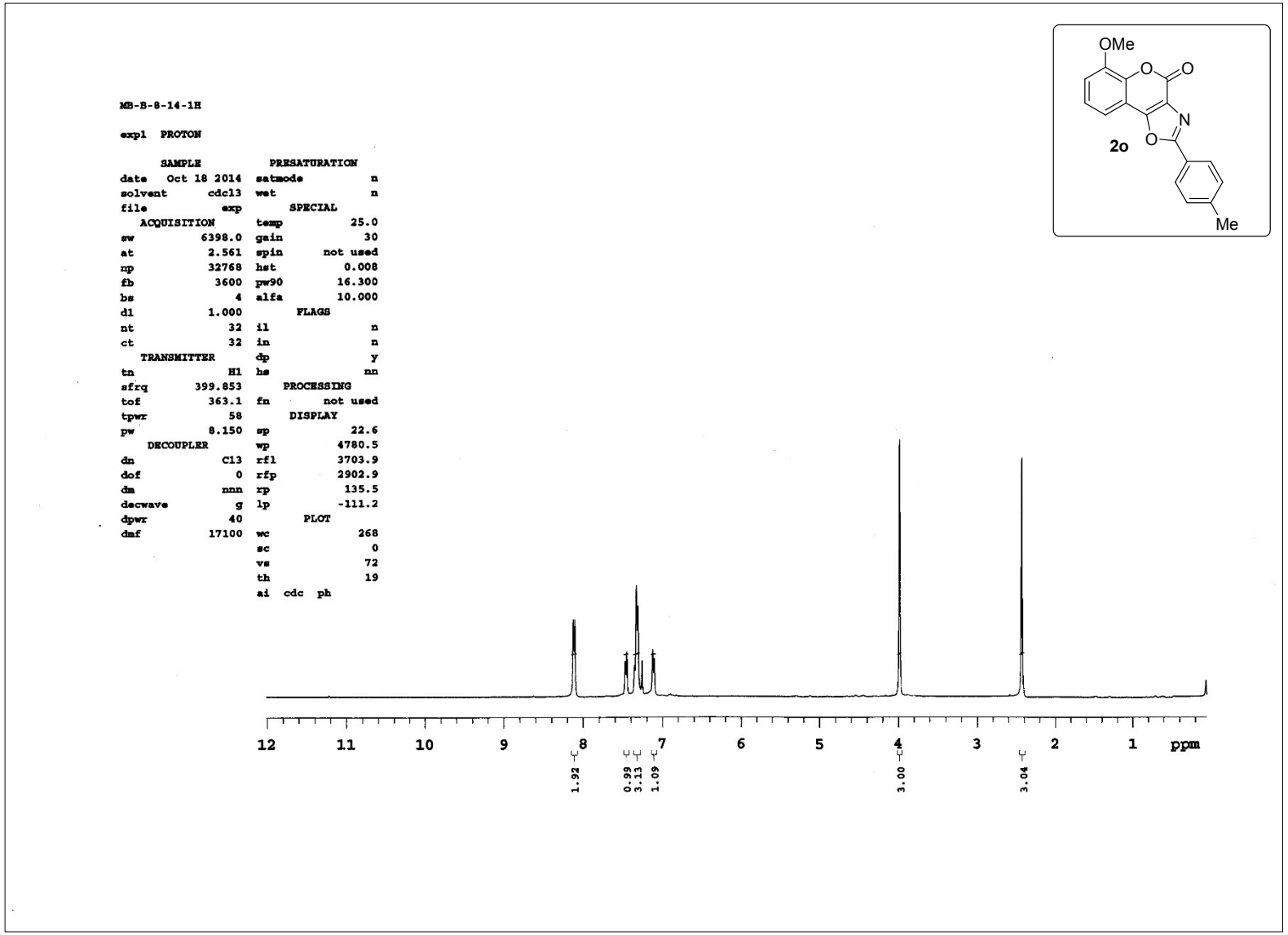
^{13}C NMR spectra of **2n**



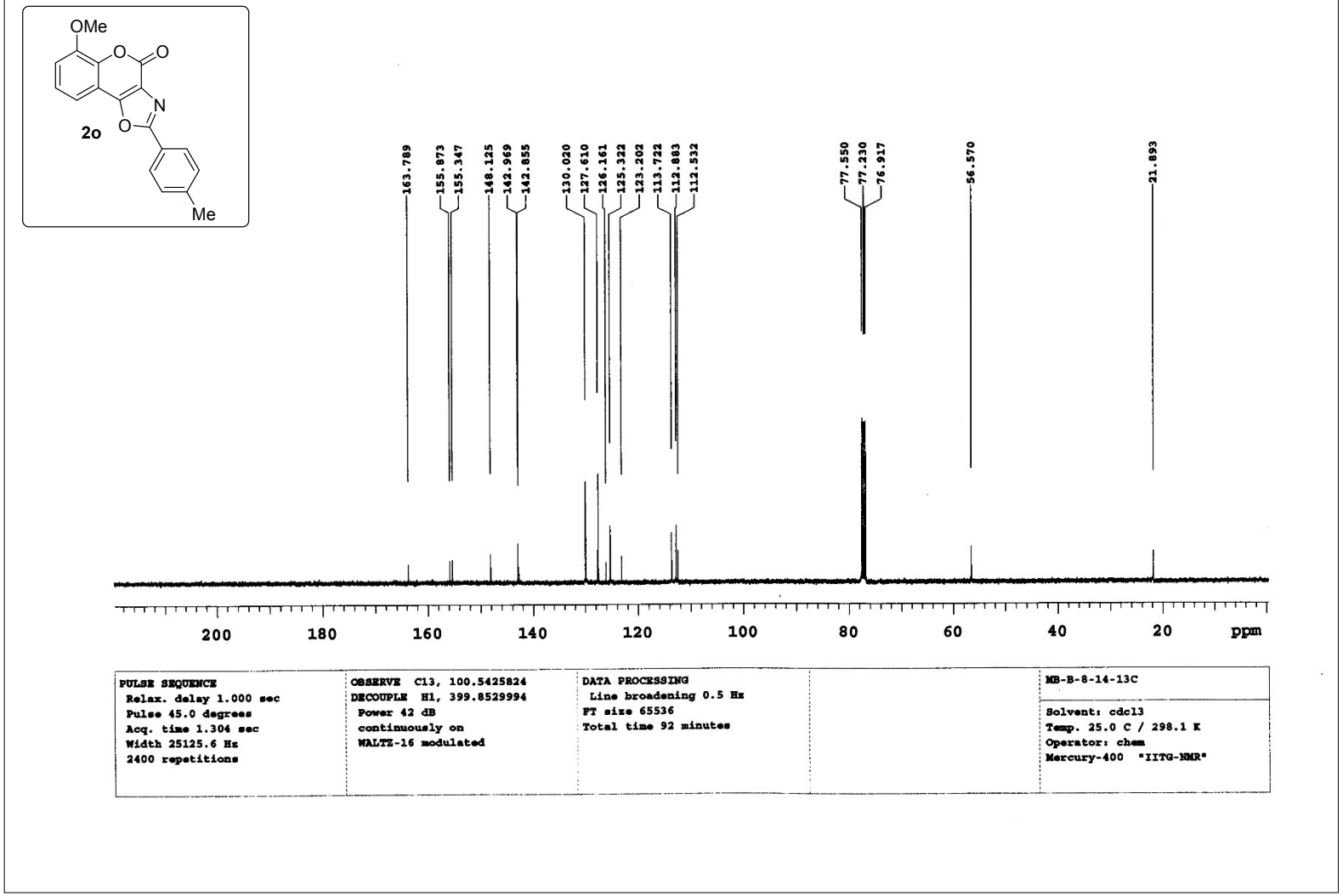
HRMS spectra of **2n**



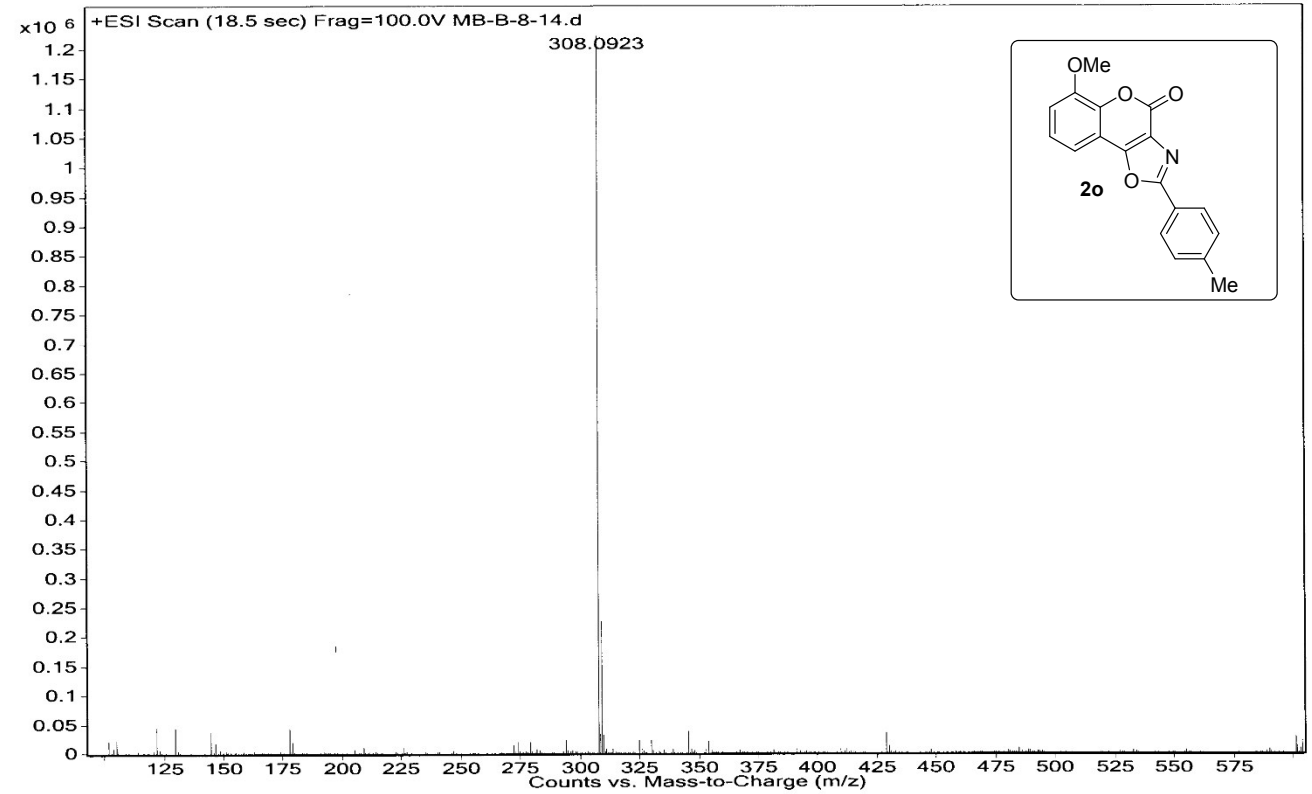
H[1] NMR spectra of **2o**



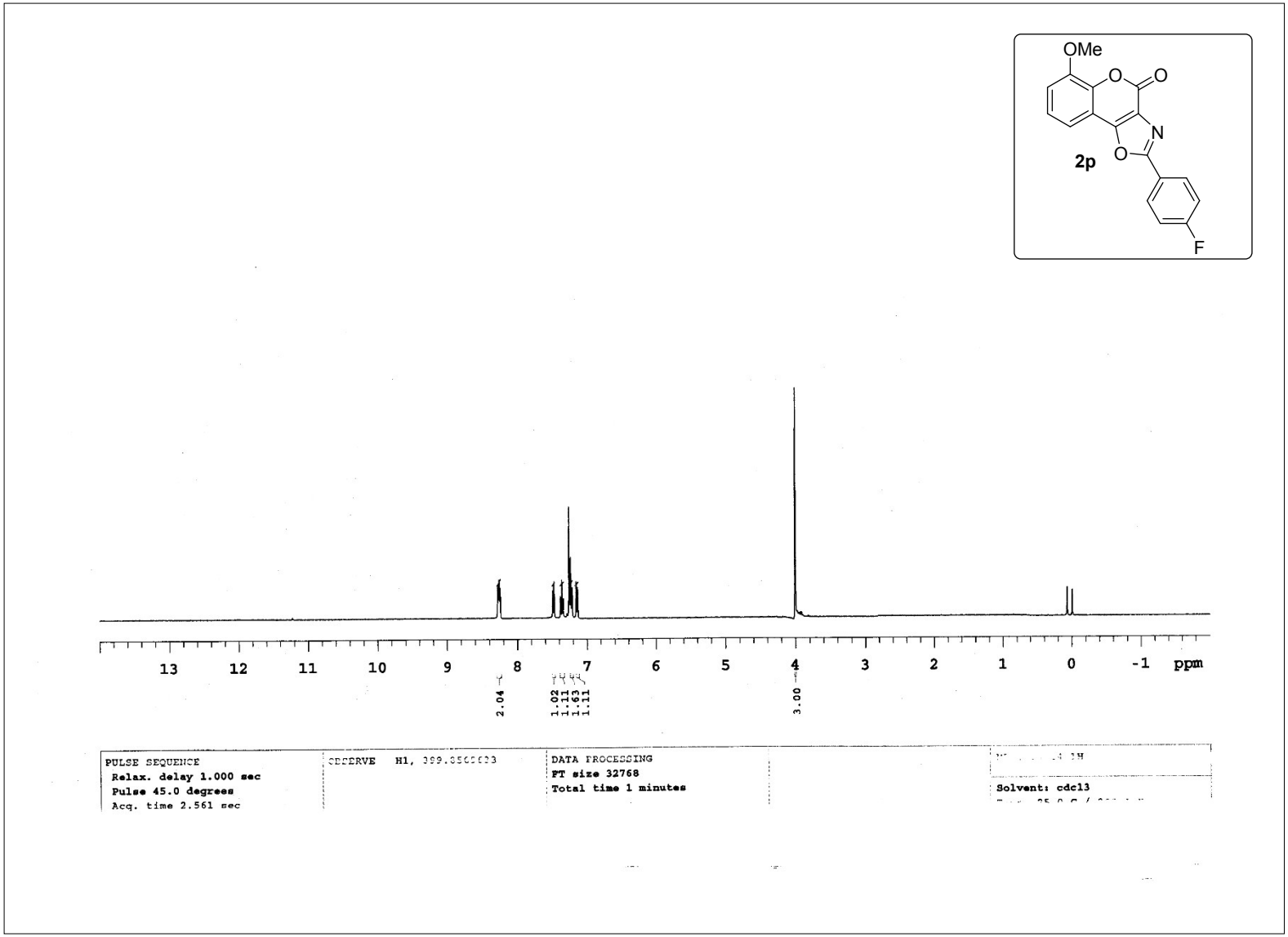
^{13}C NMR spectra of **2o**



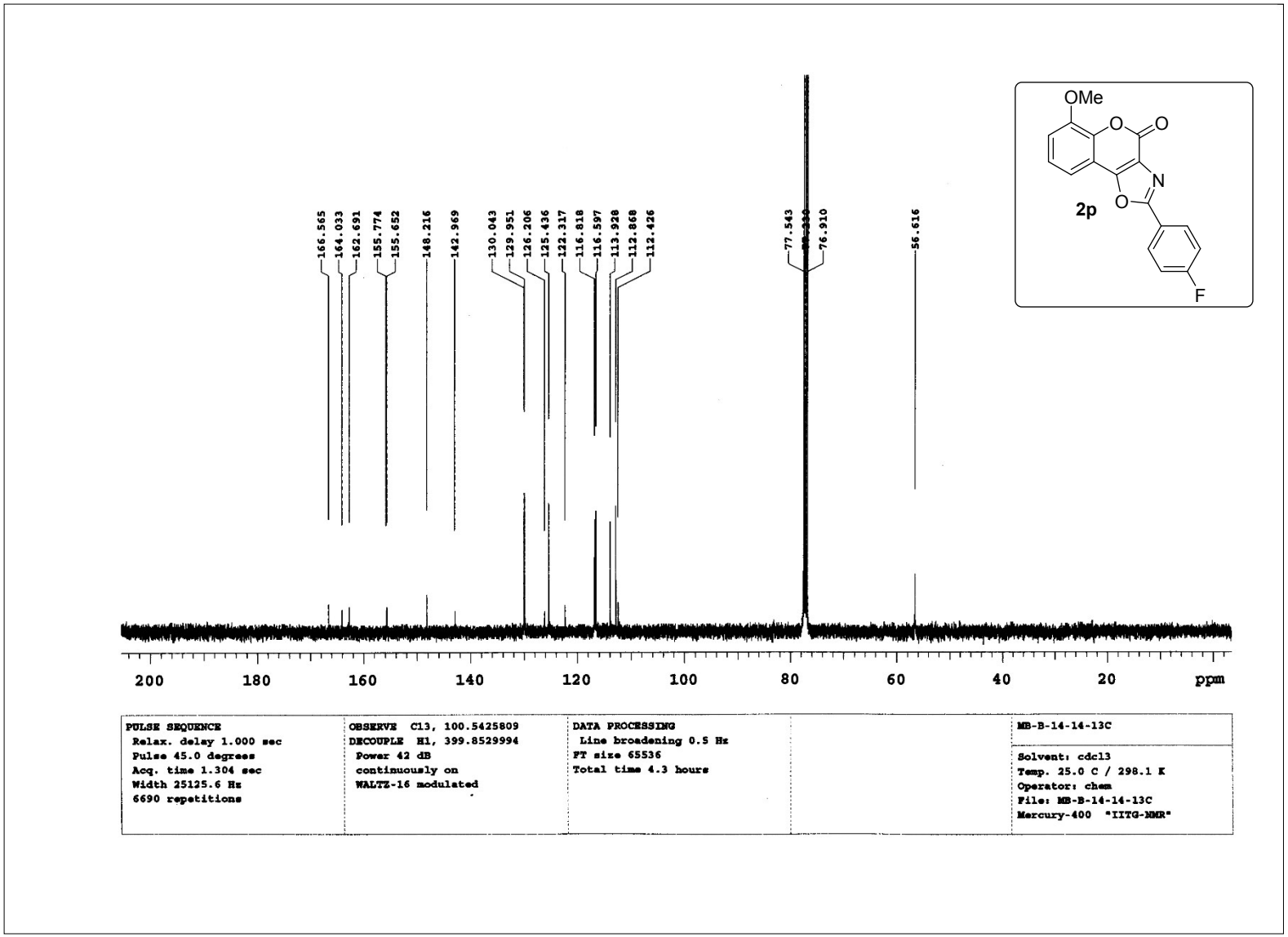
HRMS spectra of **2o**



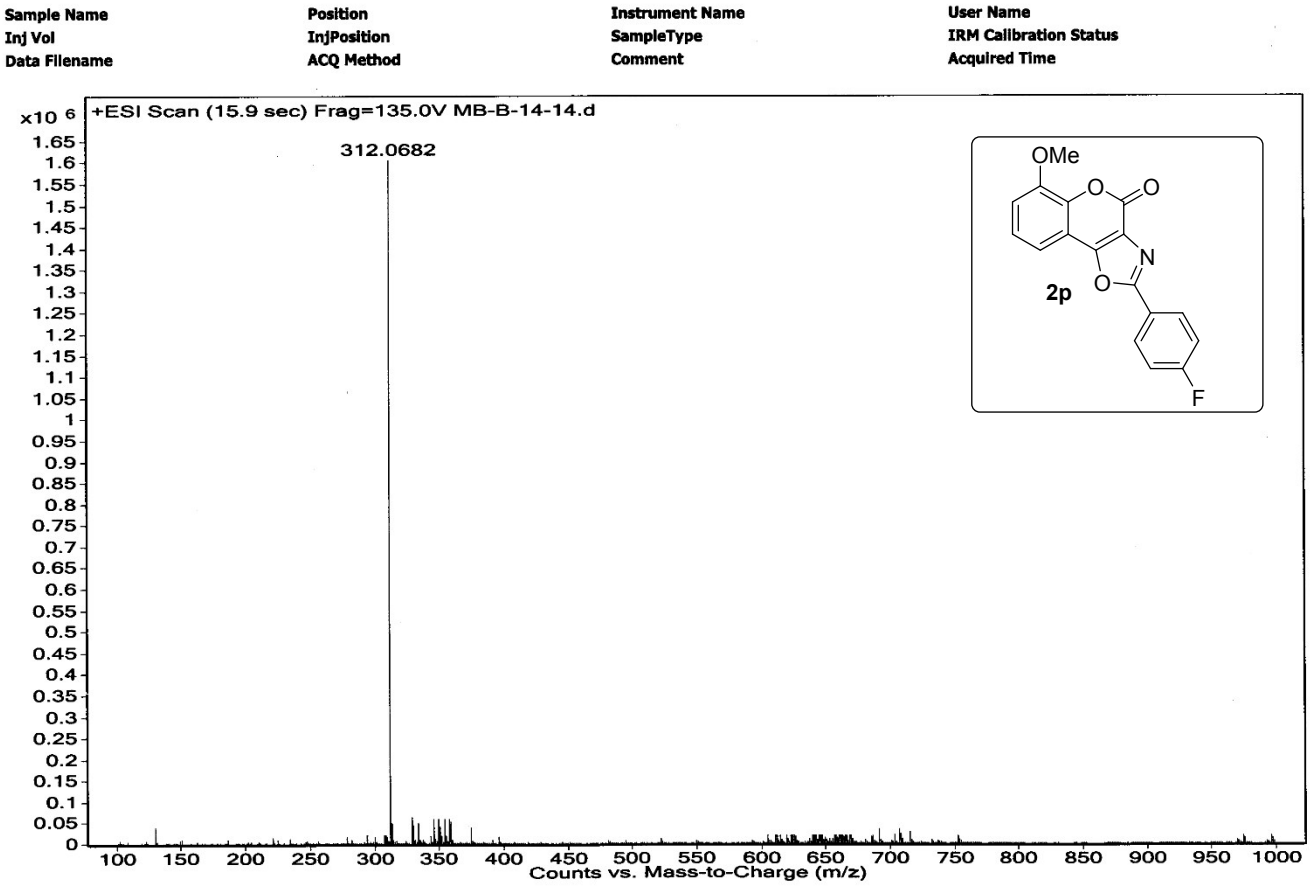
H[1] NMR spectra of **2p**



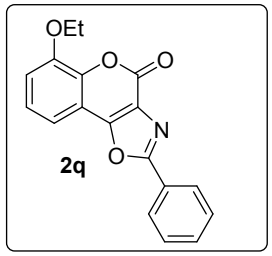
^{13}C NMR spectra of **2p**

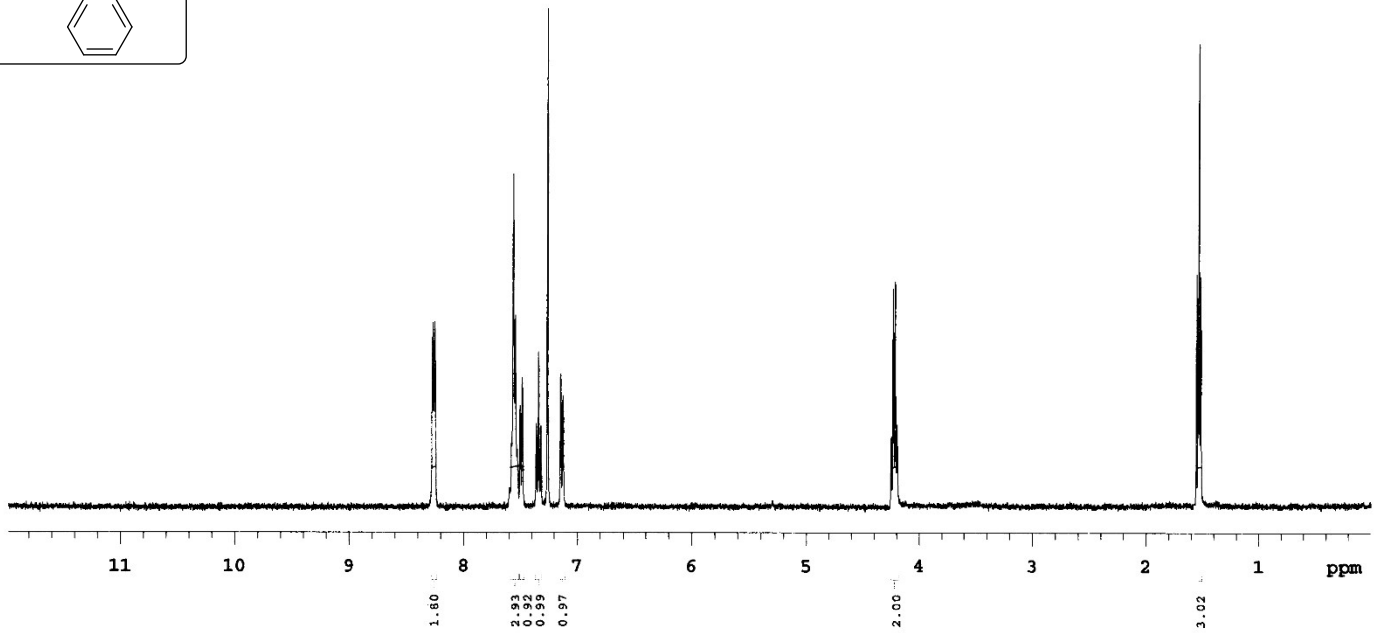


HRMS spectra of **2p**

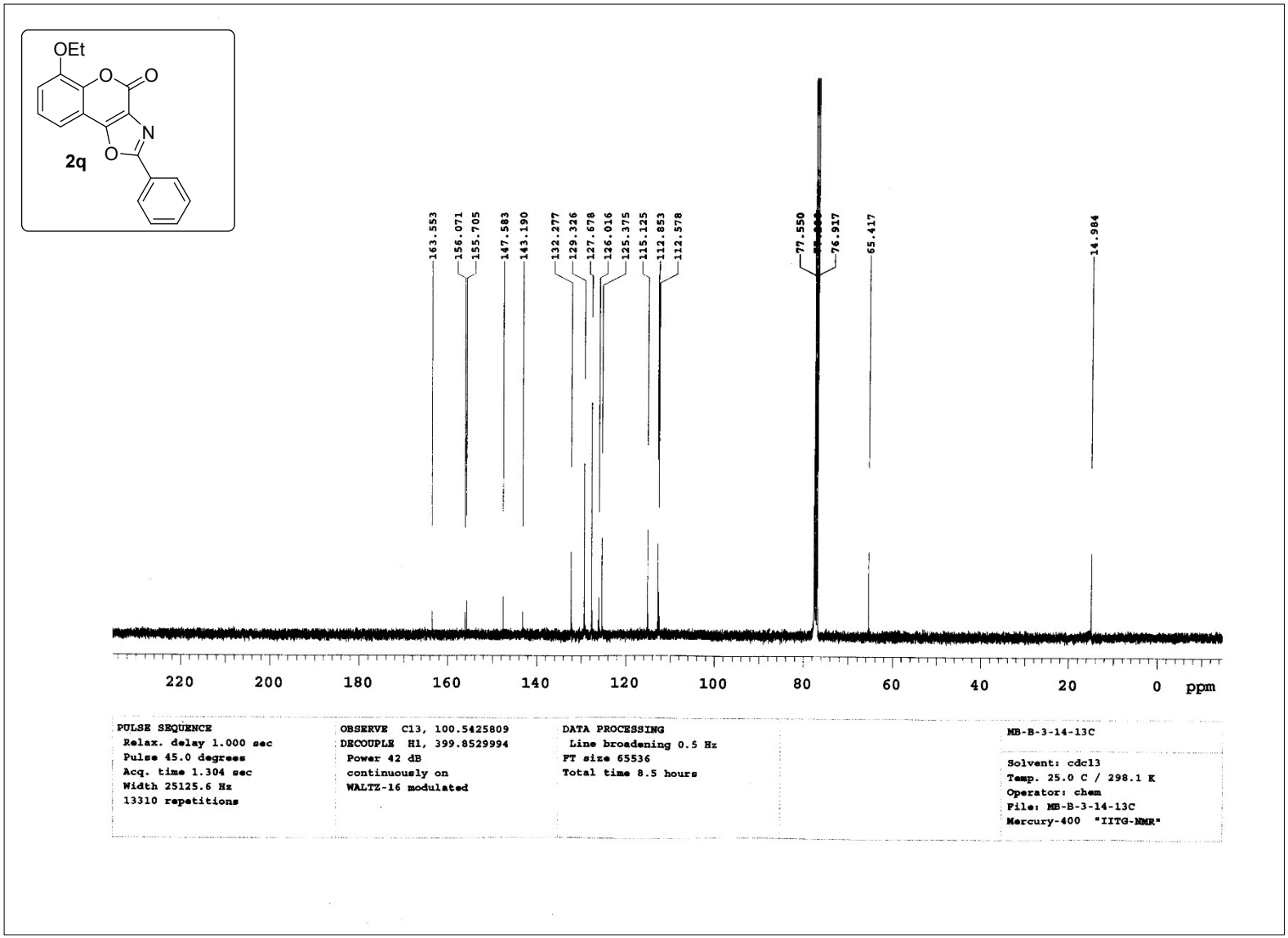


H[1] NMR spectra of **2q**



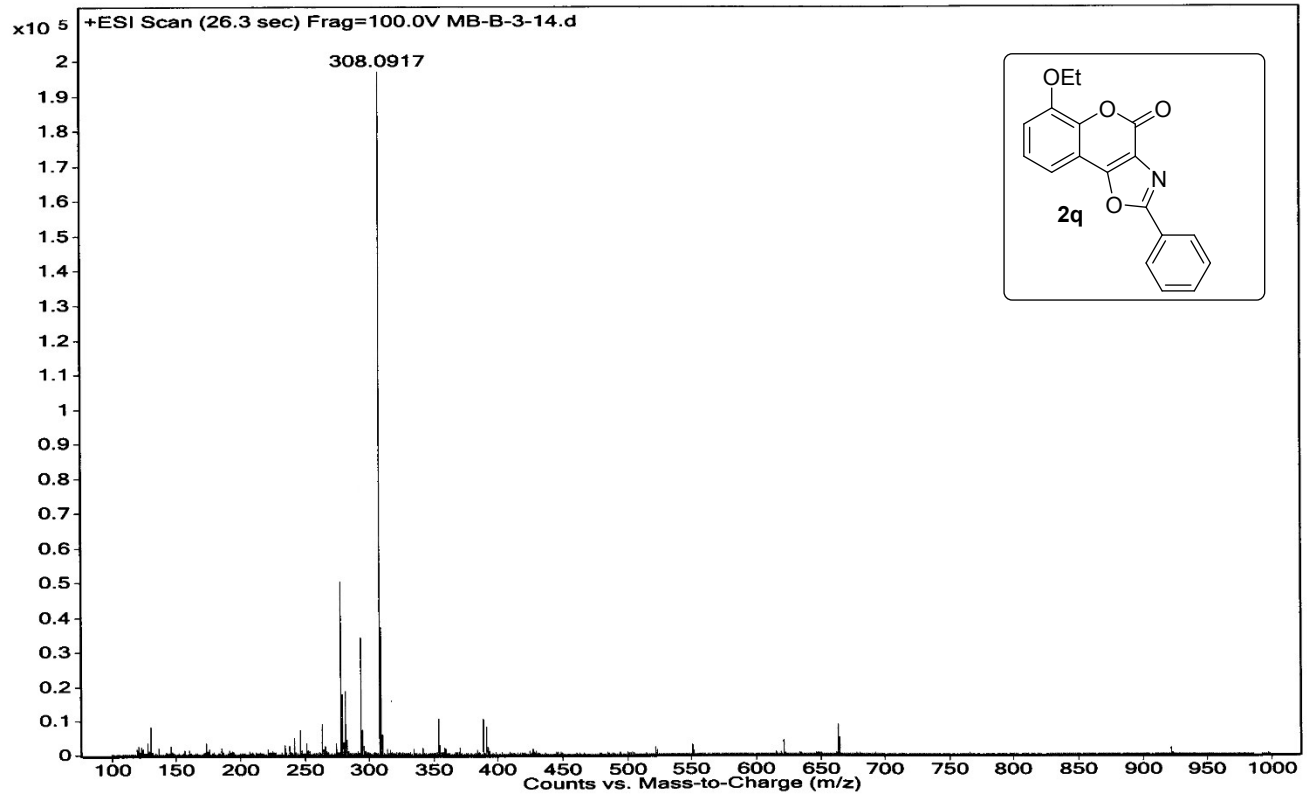


^{13}C NMR spectra of **2q**

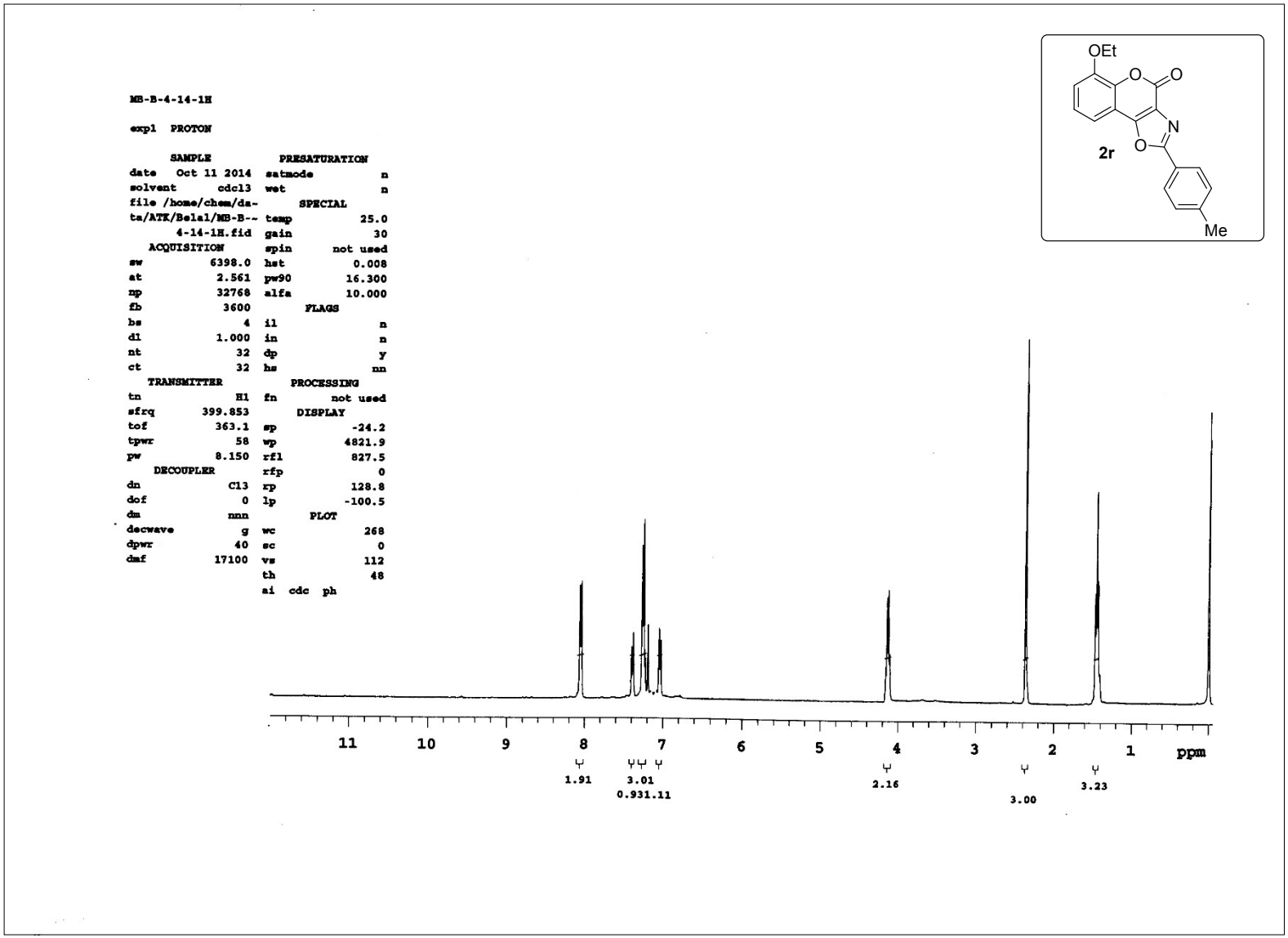


HRMS spectra of **2q**

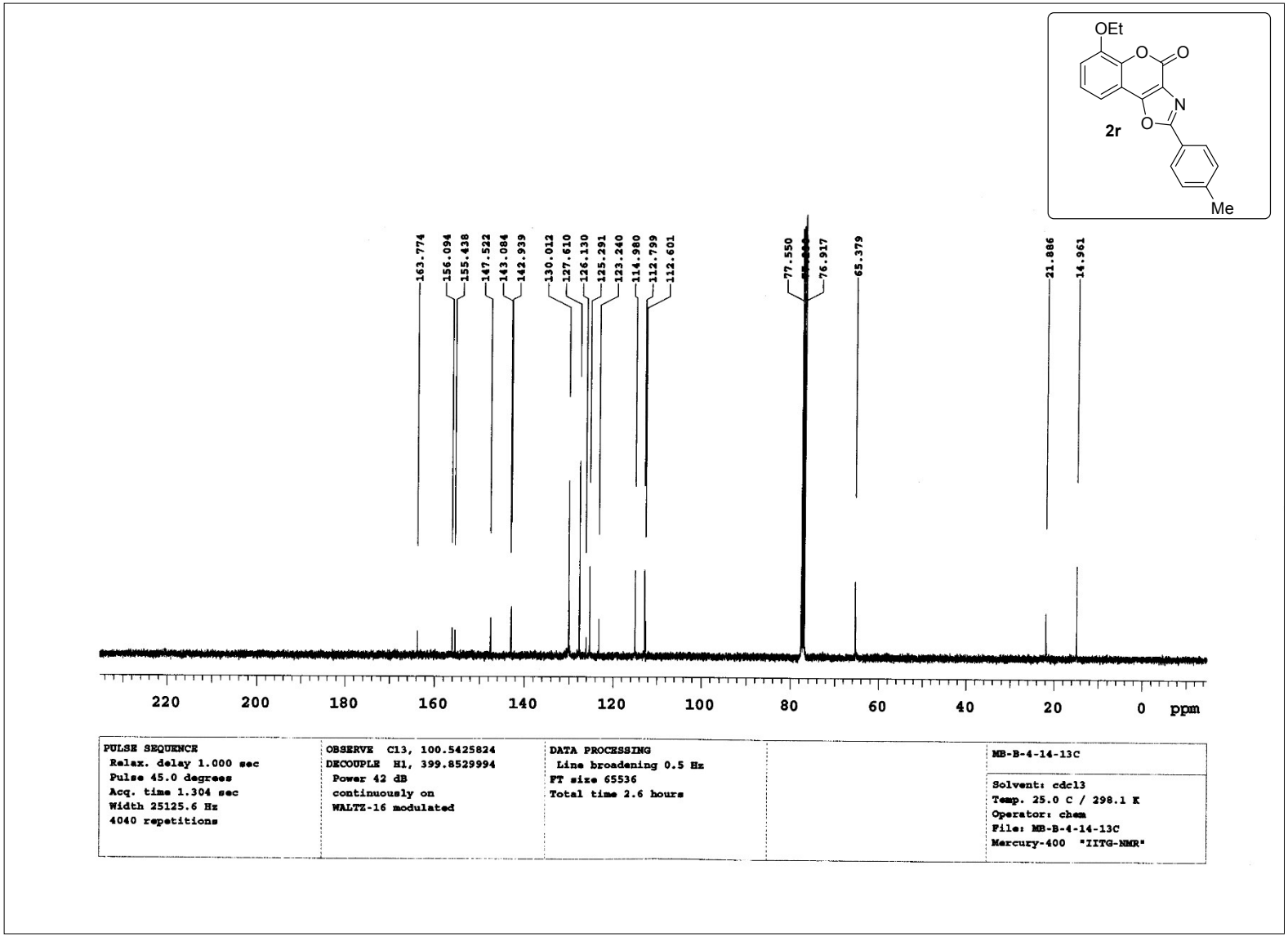
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	MB-B-3-14.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



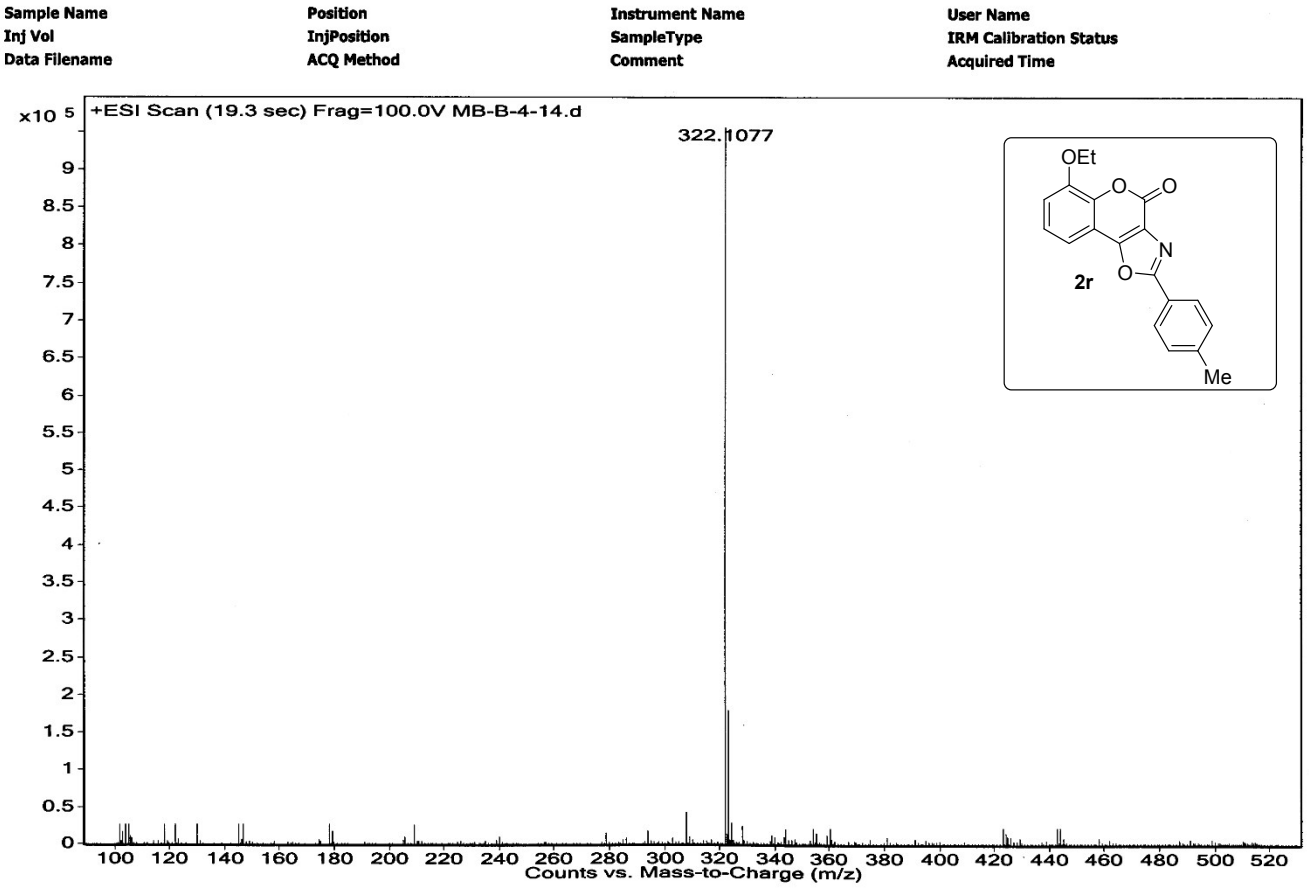
H[1] NMR spectra of **2r**



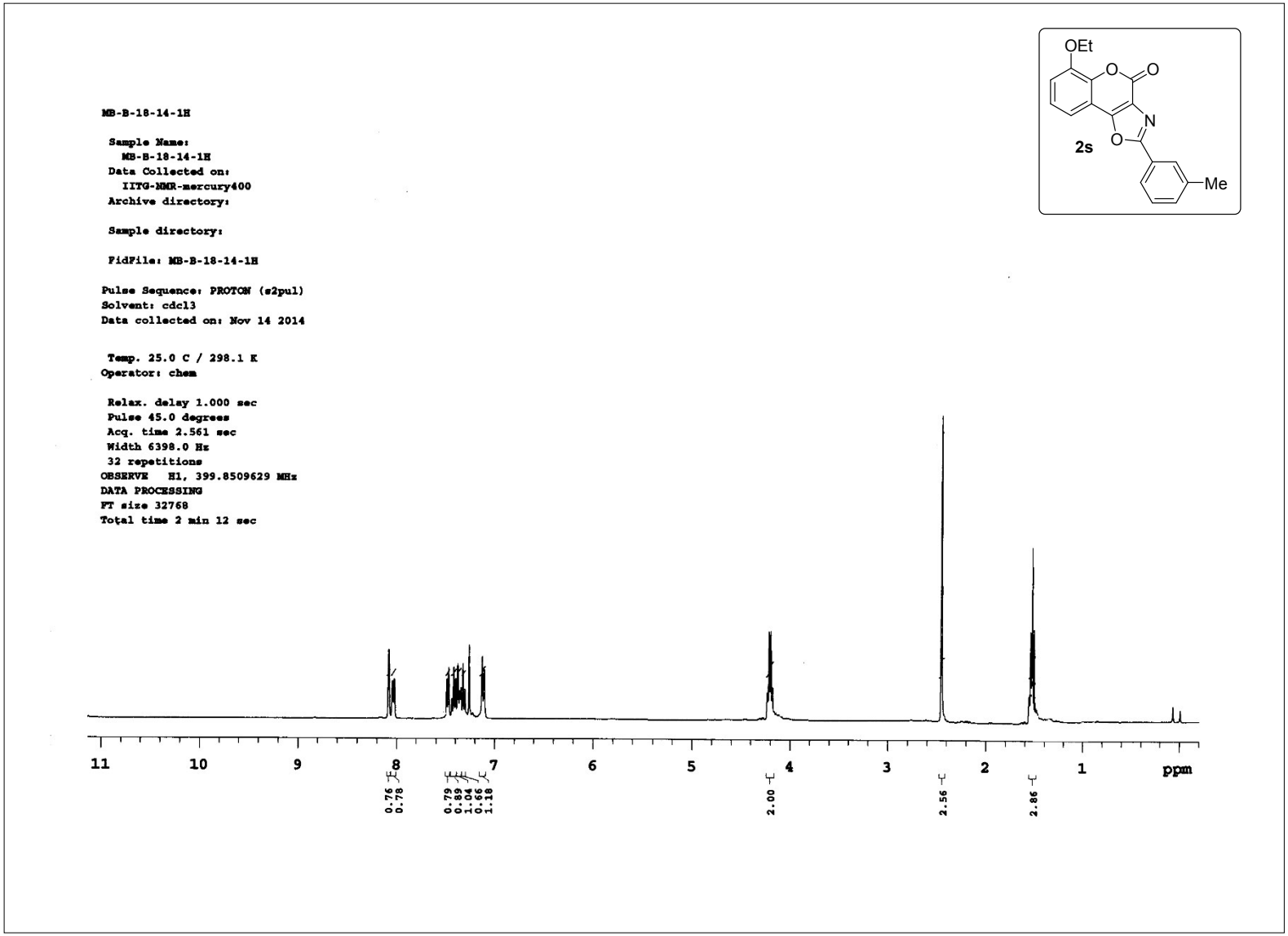
^{13}C NMR spectra of **2r**



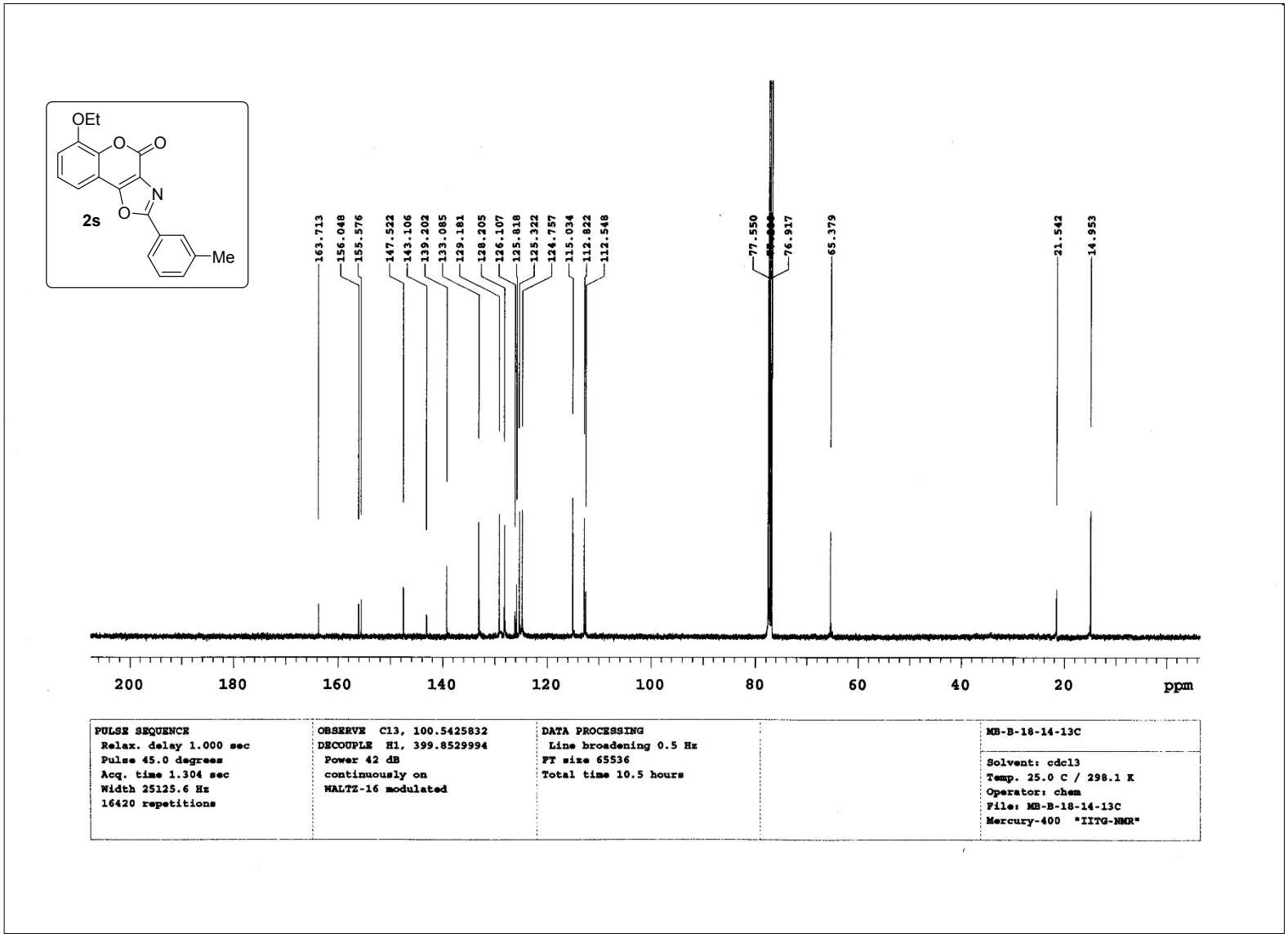
HRMS spectra of **2r**



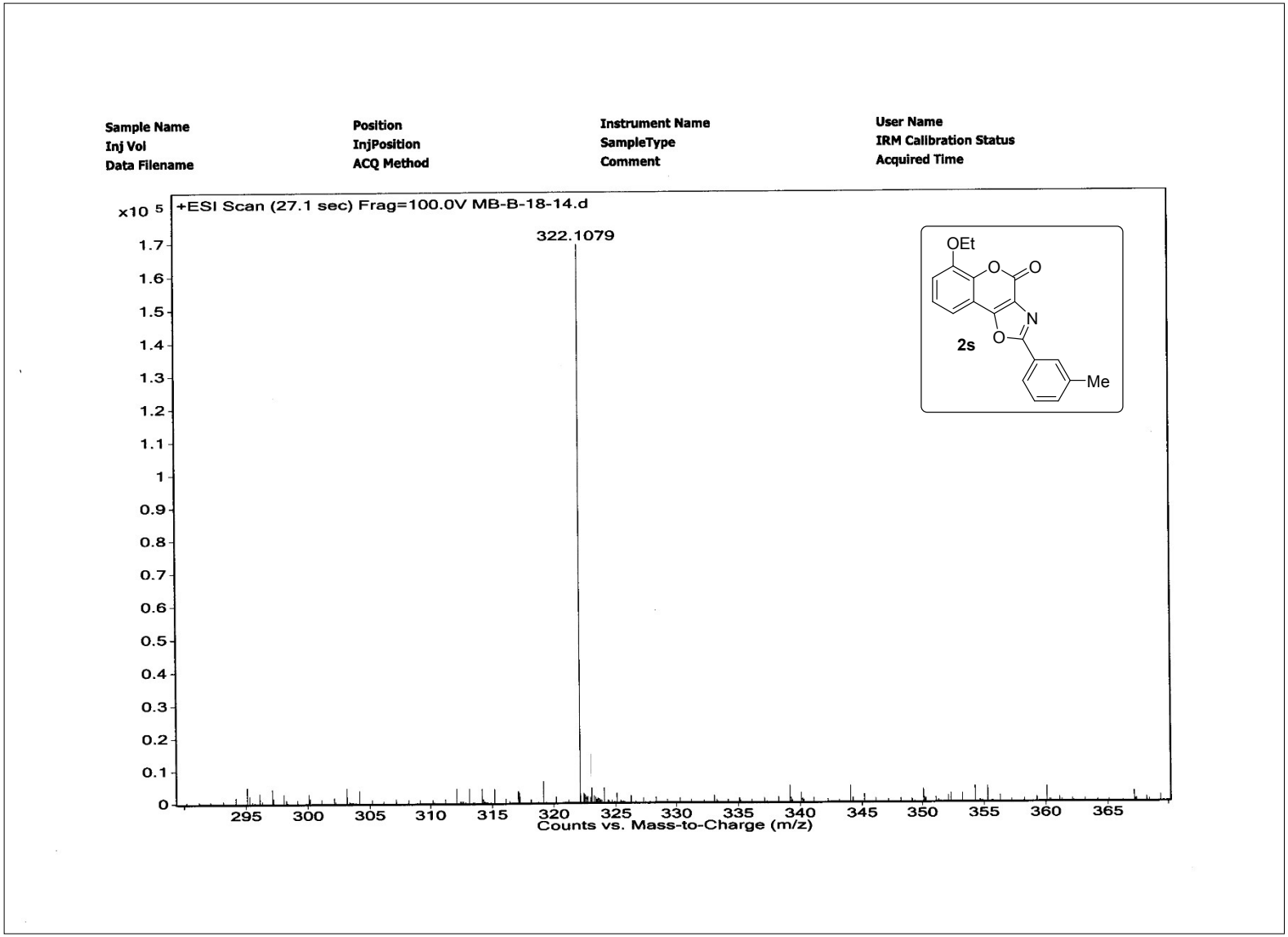
H[1] NMR spectra of **2s**



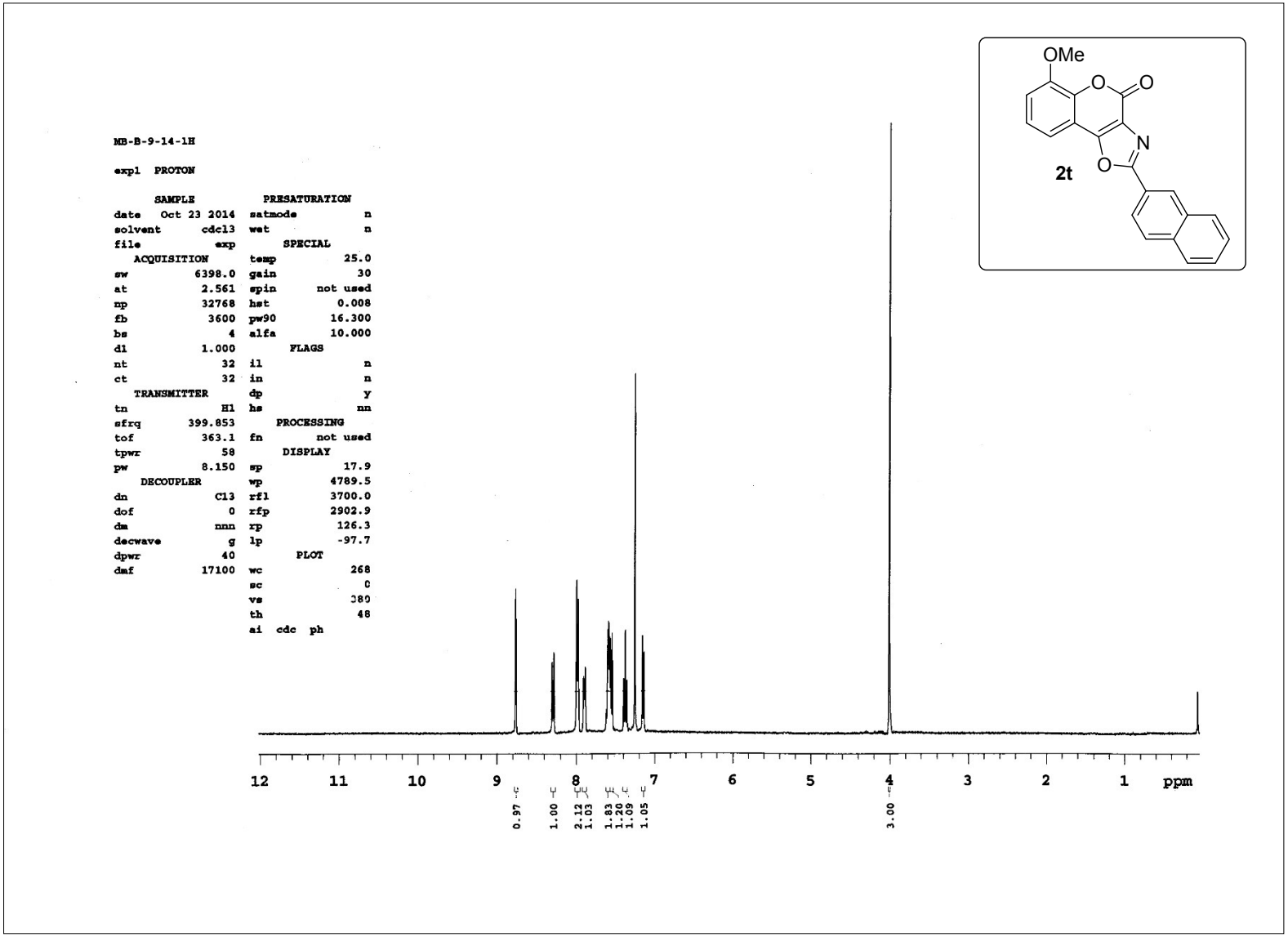
^{13}C NMR spectra of **2s**



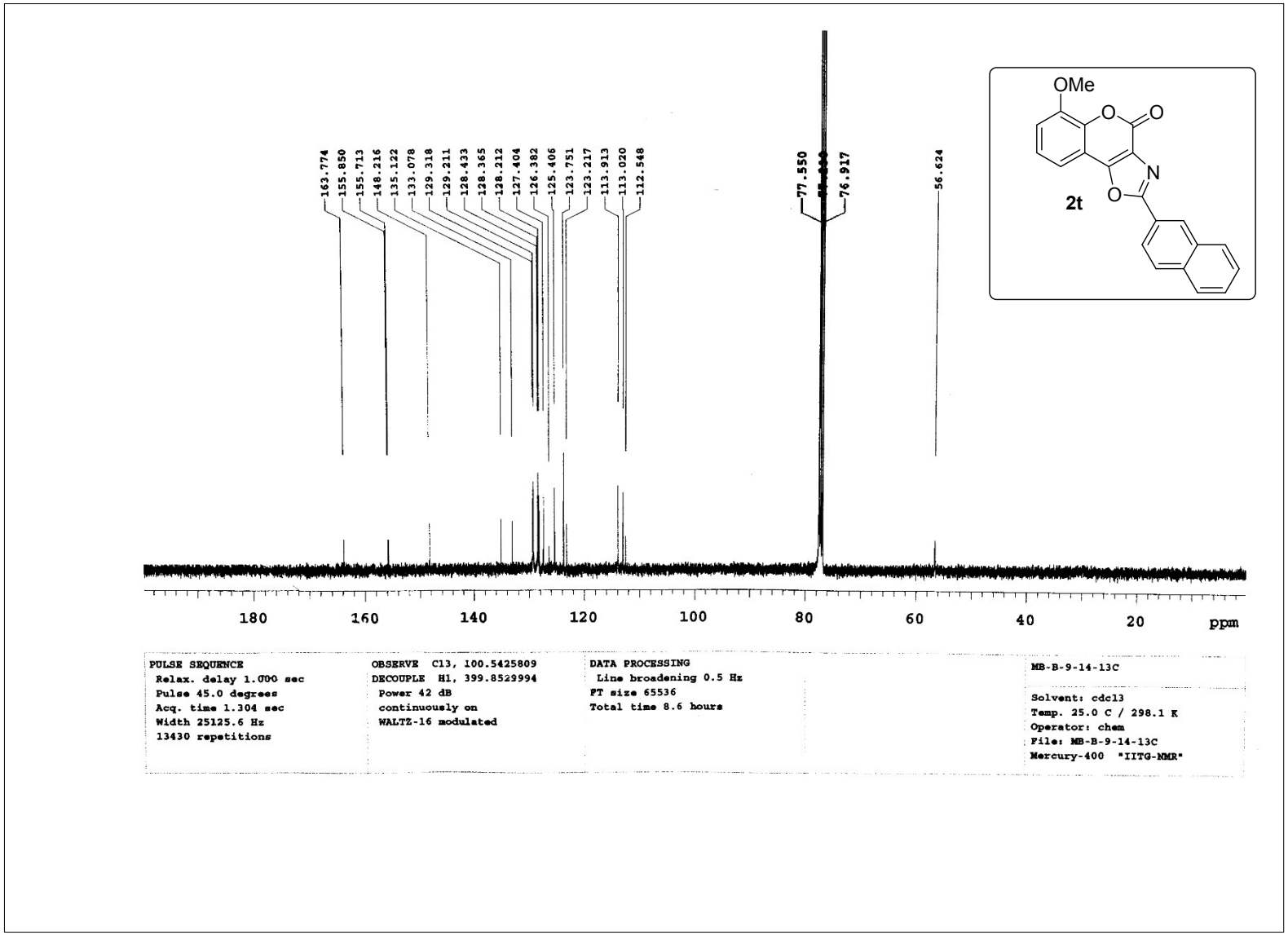
HRMS spectra of **2s**



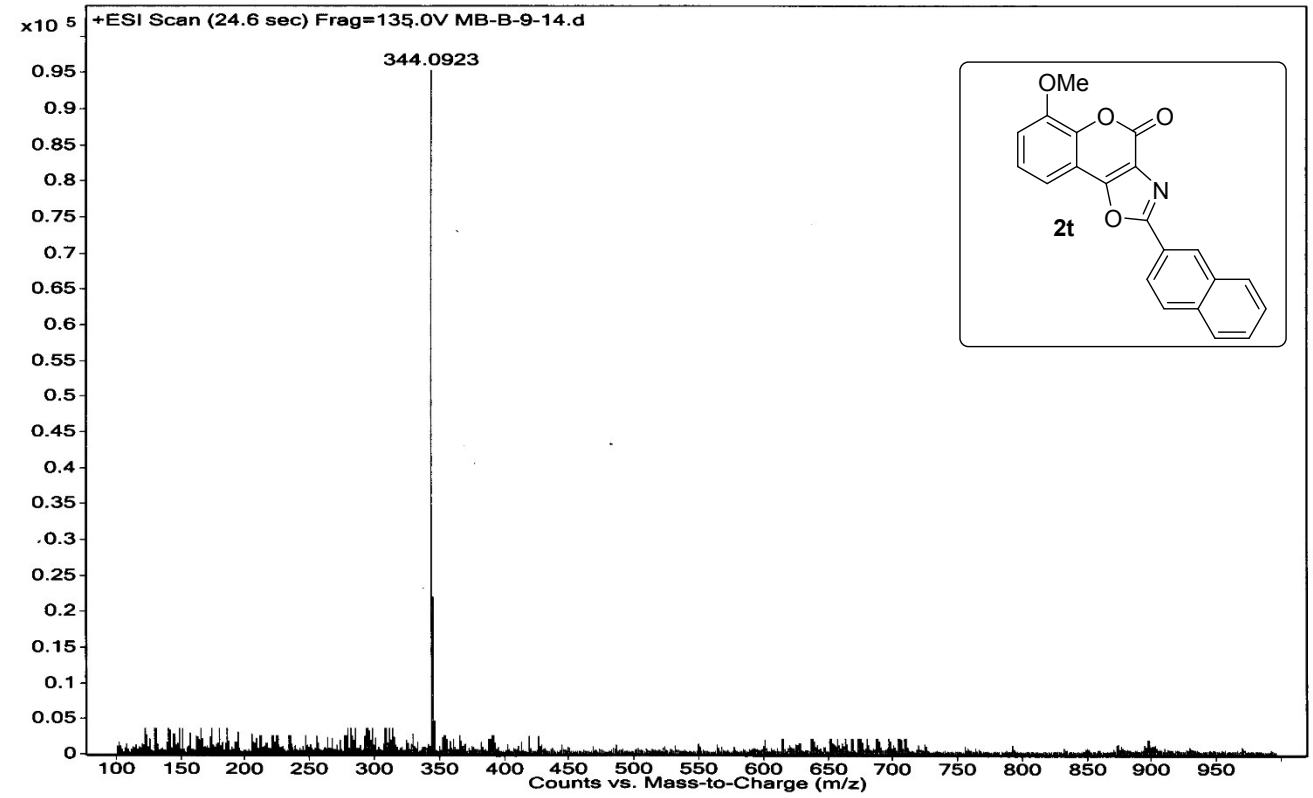
H[1] NMR spectra of **2t**



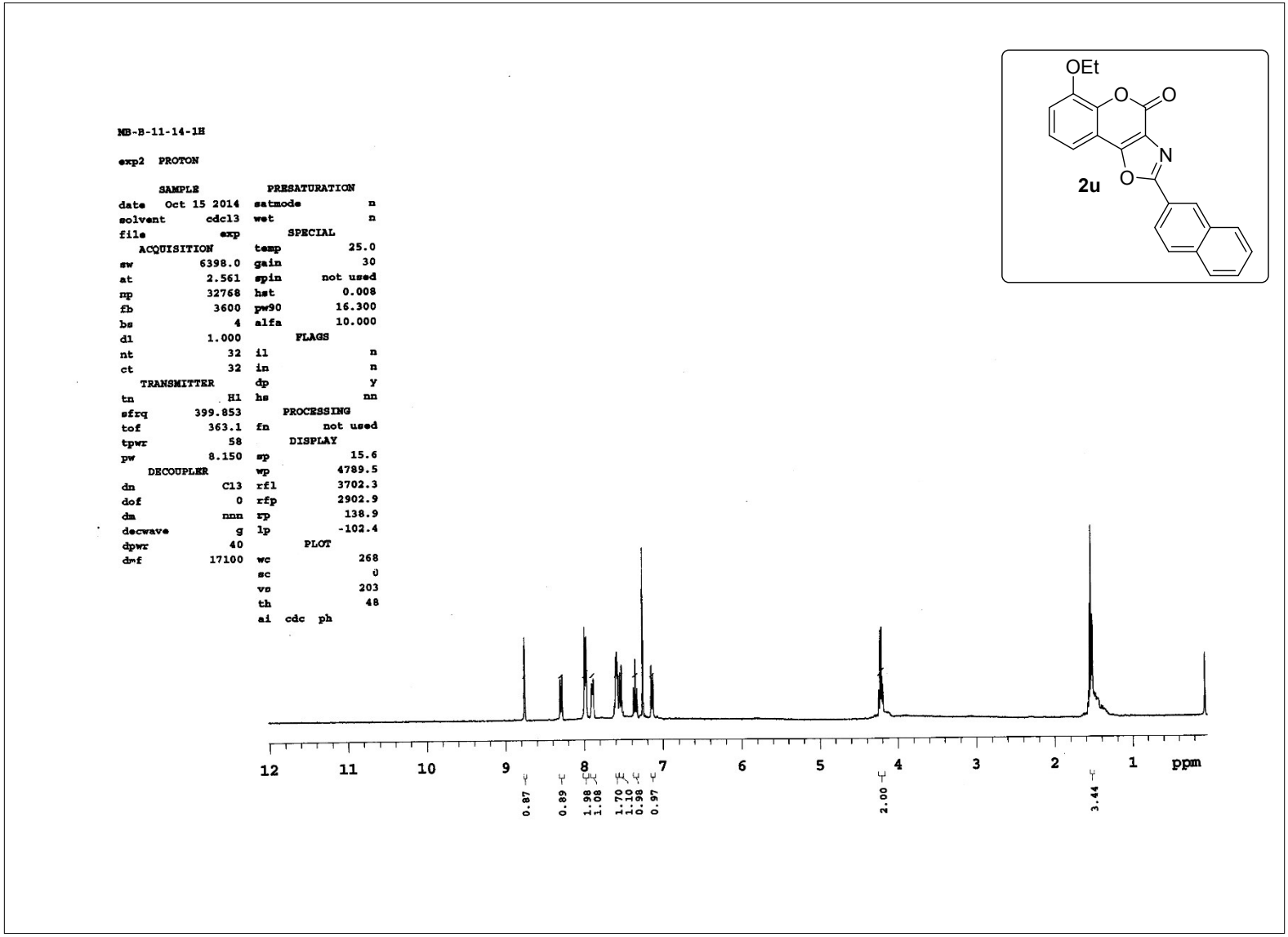
^{13}C NMR spectra of **2t**



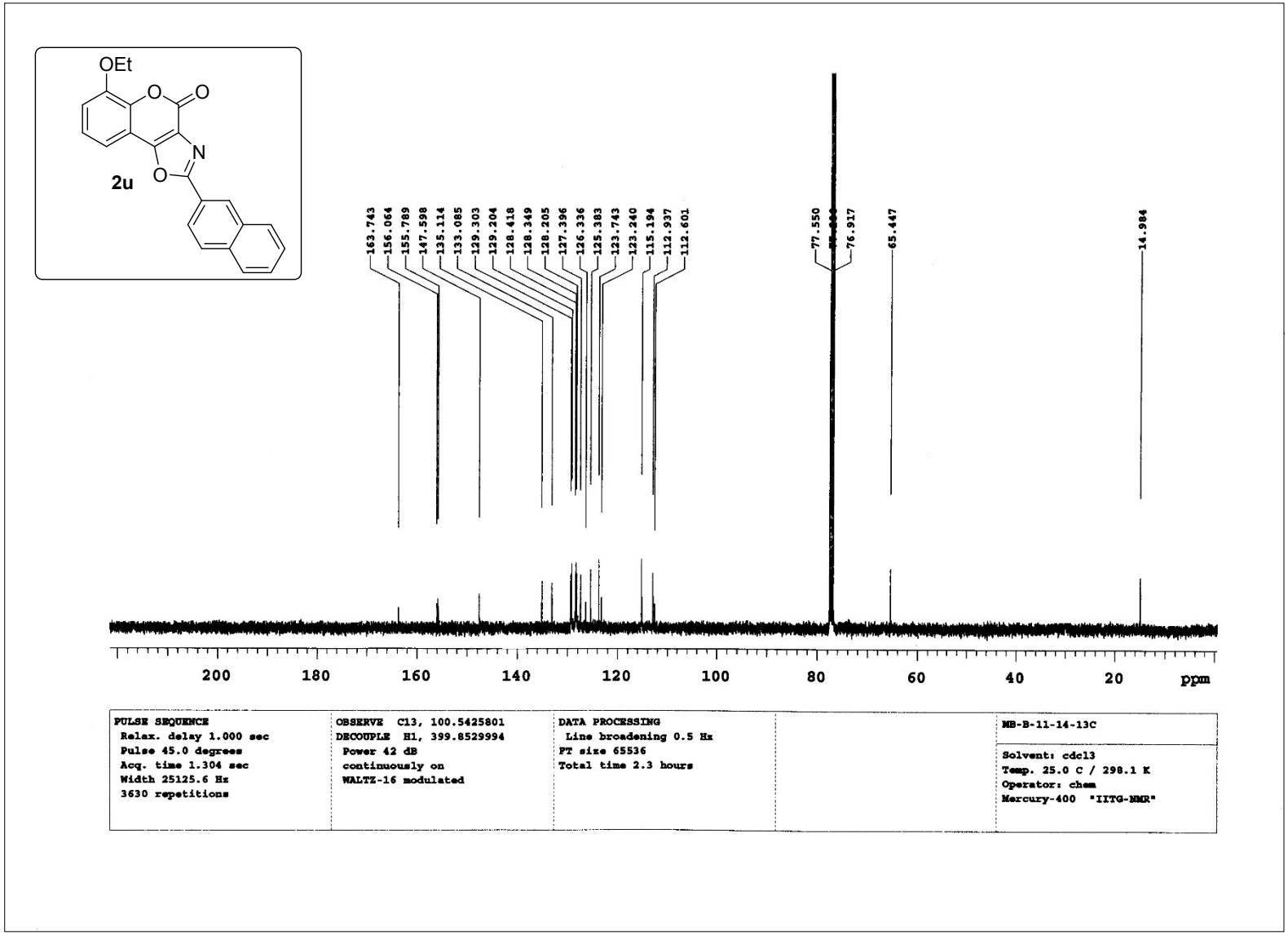
HRMS spectra of **2t**



H[1] NMR spectra of **2u**



^{13}C NMR spectra of **2u**



HRMS spectra of **2u**