

## Supporting information

Synthesis of fused oxazole containing coumarin derivatives via oxidative cross coupling reaction using a combination of CuCl<sub>2</sub> and TBHP

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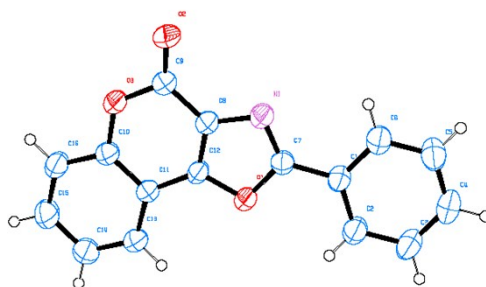
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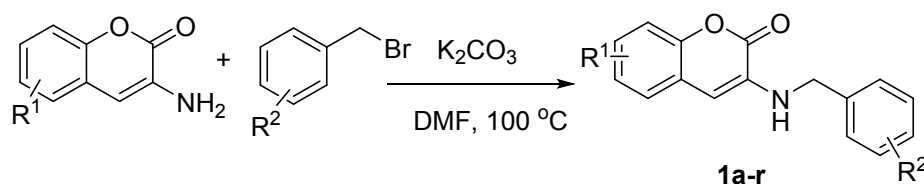
**Experimental General:** Melting points were determined on a Büchi melting point apparatus. IR spectra were recorded on Perkin-Elmer 281 IR spectrophotometer.  $^1\text{H}$  NMR spectra were recorded on Bruker 600 MHz and Varian 400 MHz spectrometer with TMS as internal reference; chemical shifts ( $\delta$  scale) are reported in parts per million (ppm).  $^1\text{H}$  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  $\text{MoK}\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) 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  $\text{C}_{16}\text{H}_9\text{NO}_3$ , pale yellow crystal, formula wt 263.24, Monoclinic, P2(1)/n,  $a = 7.1596(4) \text{ \AA}$ ,  $b = 13.3572(7) \text{ \AA}$ ,  $c = 13.0999(6) \text{ \AA}$ ,  $V = 1239.47(11) \text{ \AA}^3$ ,  $Z = 4$ ,  $F(000) = 544$ ,  $\text{GOF}(S) = 0.976$ . Final indices  $R_{\text{obs}} = 0.0501$ ,  $wR_{\text{obs}} = 0.1013$  with  $I > 2\sigma(I)$ ;  $R_{\text{all}} = 0.1039$ ,  $wR_{\text{all}} = 0.1238$  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):**

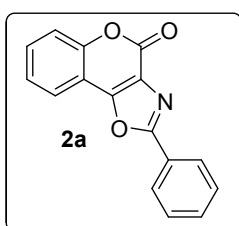


Into a 25 mL round bottom flask was taken a mixture of 3-aminochromen-2-one (1 mmol), benzyl bromide (1 mmol) and  $K_2CO_3$  (1.2 mmol) in 3 mL of DMF. The reaction mixture was heated at 100 °C for 2-8 h and after completion of the reaction, the reaction mixture was worked-up with ethyl acetate. The 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.

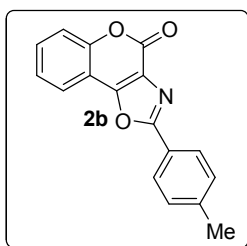
**2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (2a).** Pale yellow solid; Yield = 72% (57 mg); MP = 188-



190 °C; IR(KBr)  $\nu_{max}$  = 2958.00, 2923.26, 1756.03, 1606.03, 1261.51, 1156.54, 1103.31, 1064.16  $cm^{-1}$ ;  $H^1$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  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,  $CDCl_3$ )  $\delta$  163.6, 156.4, 155.5, 153.2, 132.3, 131.9,

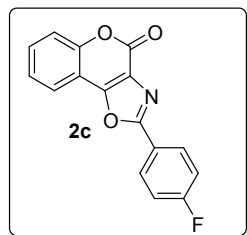
129.3, 127.7, 126.1, 125.9, 125.2, 121.7, 117.9, 111.7 ppm. HRMS [ESI+]  $m/z$ : calcd for  $C_{16}H_9NO_3$   $[M+H]^+ = 264.0655$  (found 264.0655).

**2-(*p*-tolyl)-4*H*-chromeno[3,4-*d*]oxazol-4-one (2b)**. Pale yellow solid; Yield = 68% (56 mg); MP = 246



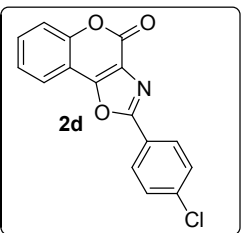
$^{\circ}C$ ; IR(KBr)  $\nu_{max} = 3062.59, 2920.20, 1756.65, 1639.88, 1261.33, 1155.35, 1101.03, 1065.66 \text{ cm}^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.13 (d,  $J = 8 \text{ Hz}$ , 2 H), 7.92 (d,  $J = 7.6 \text{ Hz}$ , 1 H), 7.60 (t,  $J = 7.6 \text{ Hz}$ , 1 H), 7.50 (d,  $J = 8 \text{ Hz}$ , 1 H), 7.42 (t,  $J = 4.8 \text{ Hz}$ , 1 H), 7.34 (d,  $J = 8 \text{ Hz}$ , 2 H), 2.44 (s, 3 H) ppm.  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  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)-4*H*-chromeno[3,4-*d*]oxazol-4-one (2c)**. Pale yellow solid; Yield = 64% (54 mg);



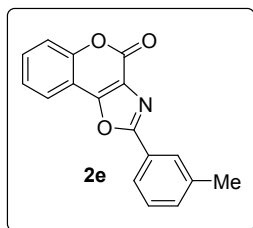
MP = 233  $^{\circ}C$ ; IR(KBr)  $\nu_{max} = 2924.10, 2853.13, 1737.29, 1634.64, 1229.50, 1097.64, 1068.25, 1027.01 \text{ cm}^{-1}$ ;  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  8.27 (t,  $J = 7.8 \text{ Hz}$ , 2 H), 7.93 (d,  $J = 7.8 \text{ Hz}$ , 1 H), 7.62 (t,  $J = 7.8 \text{ Hz}$ , 1 H), 7.53 (d,  $J = 8.4 \text{ Hz}$ , 1 H), 7.44 (t,  $J = 7.8 \text{ Hz}$ , 1 H), 7.25 (t,  $J = 8.4 \text{ Hz}$ , 2 H) ppm.  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  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)-4*H*-chromeno[3,4-*d*]oxazol-4-one (2d)**. Pale yellow solid; Yield = 60% (54 mg);



MP = 226-229  $^{\circ}C$ ; IR(KBr)  $\nu_{max} = 2963.49, 2925.09, 2845.34, 1760.06, 1604.80, 1261.57, 1093.47, 1020.06 \text{ cm}^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.18 (d,  $J = 8.4 \text{ Hz}$ , 2 H), 7.92 (d,  $J = 8 \text{ Hz}$ , 1 H), 7.61 (t,  $J = 7.6 \text{ Hz}$ , 1 H), 7.51 (t,  $J = 7.6 \text{ Hz}$ , 3 H), 7.43 (t,  $J = 7.6 \text{ Hz}$ , 1 H) ppm.  $^{13}C$  NMR (100 MHz,  $CDCl_3:CD_2Cl_2 = 5:1$ )  $\delta$  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)

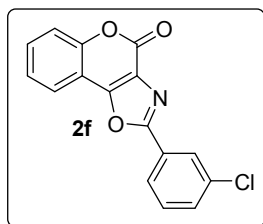
**2-(*m*-tolyl)-4*H*-chromeno[3,4-*d*]oxazol-4-one (2e)**. Pale yellow solid; Yield = 62% (52 mg); MP = 188



$^{\circ}C$ ; IR(KBr)  $\nu_{max} = 2956.72, 2918.40, 1753.81, 1639.30, 1102.98, 1060.65, 1031.94 \text{ cm}^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.08 (s, 1 H), 8.04 (d,  $J = 6.8 \text{ Hz}$ , 1 H), 7.93 (d,  $J = 7.6 \text{ Hz}$ , 1 H), 7.60 (t,  $J = 7.2 \text{ Hz}$ , 1 H), 7.50 (d,  $J = 8.4 \text{ Hz}$ , 1 H), 7.42 (t,  $J = 7.6 \text{ Hz}$ , 2 H), 7.37 (d,  $J = 7.2 \text{ Hz}$ , 1 H), 2.45 (s, 3 H) ppm.  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  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

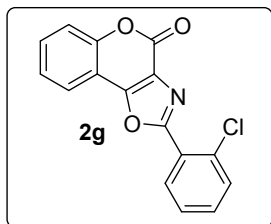
278.0817)

**2-(3-chlorophenyl)-4*H*-chromeno[3,4-*d*]oxazol-4-one (2f)**. Pale yellow solid; Yield = 56% (50 mg);



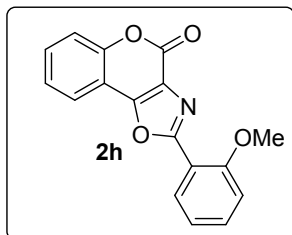
MP = 232-234  $^{\circ}C$ ; IR(KBr)  $\nu_{max} = 2923.34, 2852.57, 1755.61, 1638.29, 1286.06, 1096.19, 1052.92, 1029.17 \text{ cm}^{-1}$ ;  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  8.26 (t,  $J = 1.8 \text{ Hz}$ , 1 H), 8.16 (d,  $J = 7.8 \text{ Hz}$ , 1 H), 7.95 (dd,  $J = 7.8, 1.8 \text{ Hz}$ , 1 H), 7.64 (m, 1 H), 7.55 (d,  $J = 7.5 \text{ Hz}$ , 1 H), 7.53 (d,  $J = 8.4 \text{ Hz}$ , 1 H), 7.50 (t,  $J = 8.4 \text{ Hz}$ , 1 H), 7.45 (t,  $J = 7.2 \text{ Hz}$ , 1 H) ppm.  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  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);



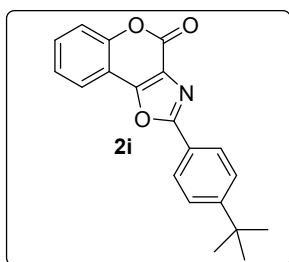
MP = 171-173 °C; IR(KBr)  $\nu_{\max}$  = 2924.13, 2852.45, 1757.06, 1641.27, 1167.90, 1068.50, 1034.42;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.23 (d,  $J$  = 8.4 Hz, 1 H), 7.95 (d,  $J$  = 7.6 Hz, 1 H), 7.63 (t,  $J$  = 8.8 Hz, 1 H), 7.59 (d,  $J$  = 8.4 Hz, 1 H), 7.53 (d,  $J$  = 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;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) 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  $\text{C}_{16}\text{H}_8\text{ClNO}_3$  [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



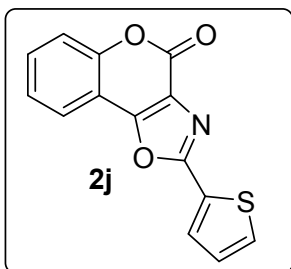
mg); MP = 168-170 °C; IR 2956.26, 2924.46, 2853.39, 1751.49, 1652.71, 1265.42, 1161.69, 1069.43, 1021.09  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.16 (d,  $J$  = 7.2 Hz, 1 H), 7.93 (d,  $J$  = 8 Hz, 1 H), 7.59 (m, 1 H), 7.52 (t,  $J$  = 8.4 Hz, 2 H), 7.42 (t,  $J$  = 7.6 Hz, 1 H), 7.11 (m, 2 H), 4.02 (s, 3 H) ppm;  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{17}\text{H}_{11}\text{NO}_4$  [M+H] $^+$  = 294.0761 (found 294.0778).

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



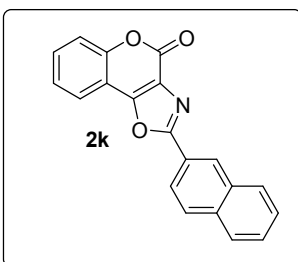
mg); MP = 207-209 °C; IR 3066.92, 2949.93, 1753.50, 1684.67, 1285.19, 1167.19, 1063.56, 1041.90  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.19 (d,  $J$  = 8.4 Hz, 2 H), 7.94 (d,  $J$  = 7.6 Hz, 1 H), 7.61 (t,  $J$  = 7.4 Hz, 1 H), 7.56 (d,  $J$  = 8.4 Hz, 2 H), 7.51 (d,  $J$  = 8.8 Hz, 1 H), 7.43 (t,  $J$  = 7.2 Hz, 1 H), 1.38 (s, 9 H) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{19}\text{H}_{17}\text{NO}_3$  [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



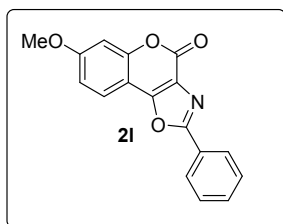
= 170-172 °C; IR 3095.65, 2924.28, 2853.43, 1752.86, 1634.11, 1210.78, 1101.71, 1068.24, 1032.66  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J$  = 3.2 Hz, 1 H), 7.90 (dd,  $J$  = 7.6, 1.2 Hz, 1 H), 7.60 (m, 2 H), 7.50 (d,  $J$  = 8 Hz, 1 H), 7.42 (t,  $J$  = 7.6 Hz, 1 H), 7.21 (t,  $J$  = 4.8 Hz, 1 H) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{14}\text{H}_7\text{NO}_3\text{S}$  [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 °C; IR(KBr)  $\nu_{\max}$  = 2925.03, 2852.61, 1755.81, 1605.26, 1101.74, 1067.46, 1029.24  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{20}\text{H}_{11}\text{NO}_3$  [M+H] $^+$  = 314.0812 (found 314.0816)

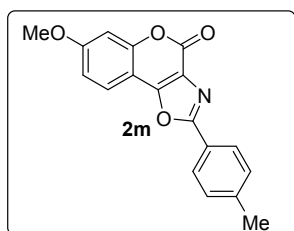
**7-methoxy-2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (2l).** Pale yellow solid; Yield = 54% (47 mg);



MP = 209 °C; IR(KBr)  $\nu_{\max}$  = 2924.88, 2852.86, 1748.58, 1638.71, 1151.36, 1117.36, 1061.23, 1029.99  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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;  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{17}\text{H}_{11}\text{NO}_4$  [M+H] $^+$  = 294.0761 (found

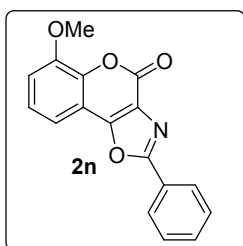
294.0774)

**7-methoxy-2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2m).** Pale yellow solid; Yield = 58% (53



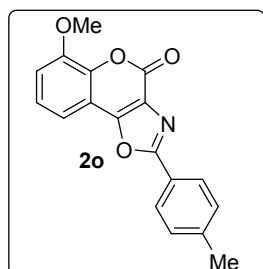
mg); MP = 220 °C; IR(KBr)  $\nu_{\max}$  = 2923.23, 2854.65, 1767.39, 1638.09, 1270.71, 1103.27, 1059.04, 1023.23  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.10 (d,  $J$  = 6.4 Hz, 2 H), 7.79 (d,  $J$  = 8.4 Hz, 1 H), 7.32 (d,  $J$  = 6.4 Hz, 2 H), 6.98 (s, 2 H) 3.83 (s, 3 H), 2.36 (s, 3 H) ppm;  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{18}\text{H}_{13}\text{NO}_4$  [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);



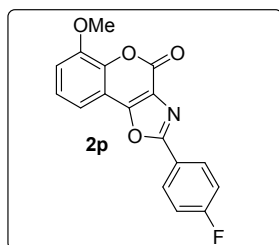
MP = 220 °C; IR(KBr)  $\nu_{\max}$  = 3063.33, 2997.68, 2928.07, 2844.55, 1759.97, 1640.76, 1277.78, 1075.41, 1043.28, 1002.19  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.26 (d,  $J$  = 6 Hz, 2 H), 7.56 (m, 3 H), 7.50 (d,  $J$  = 8 Hz, 1 H), 7.36 (t,  $J$  = 7.6 Hz, 1 H), 7.14 (d,  $J$  = 8.4 Hz, 1 H), 4.00(s, 3 H) ppm.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{17}\text{H}_{11}\text{NO}_4$  [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 °C; IR(KBr)  $\nu_{\max}$  = 2923.41, 2850.78, 1753.51, 1610.64, 1275.99, 1081.42, 1048.66, 996.21  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{18}\text{H}_{13}\text{NO}_4$  [M+H] $^+$  = 308.0917 (found 308.0923)

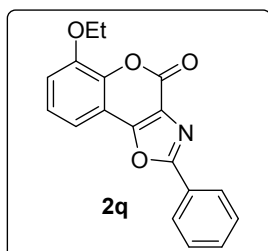
**2-(4-fluorophenyl)-6-methoxy-4H-chromeno[3,4-d]oxazol-4-one (2p).** Pale yellow solid; Yield = 56



% (52 mg); MP = 248 °C; IR(KBr)  $\nu_{\max}$  = 2923.84, 2852.00, 1751.45, 1637.57, 1277.09, 1100.90, 1081.26, 1046.33  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{17}\text{H}_{16}\text{NO}_4$

[M+H] $^+$  = 312.0667 (found 312.0682)

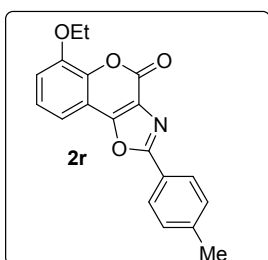
**6-ethoxy-2-phenyl-4H-chromeno[3,4-d]oxazol-4-one(2q).** Pale yellow solid; Yield = 64 % (59 mg);



MP = 218 °C; IR(KBr)  $\nu_{\max}$  = 2967.46, 2920.28, 2845.34, 1752.51, 1603.25, 1276.85, 1081.11, 1045.09, 1017.41  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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,  $J$

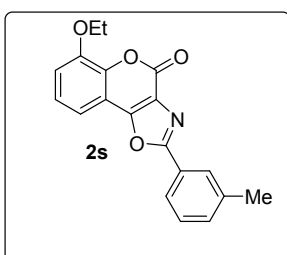
= 6.8 Hz, 3 H) ppm;  $^{13}\text{C}$  NMR; (100 MHz,  $\text{CDCl}_3$ )  $\delta$  163.6, 156.1, 155.7, 147.6, 143.2, 132.3, 129.3, 127.7, 126.0, 125.4, 115.1, 112.9, 112.6, 65.4, 15.0 ppm. HRMS [ESI+]  $m/z$ : calcd for  $\text{C}_{18}\text{H}_{13}\text{NO}_4$   $[\text{M}+\text{H}]^+ = 308.0917$  (found 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  $^{\circ}\text{C}$ ; IR(KBr)  $\nu_{\text{max}}$  = 2959.14, 2923.05, 2844.49, 1752.97, 1637.36, 1276.51, 1262.41, 1081.73, 1102.88, 1017.50  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{19}\text{H}_{15}\text{NO}_4$   $[\text{M}+\text{H}]^+ = 322.1074$  (found 322.1077)

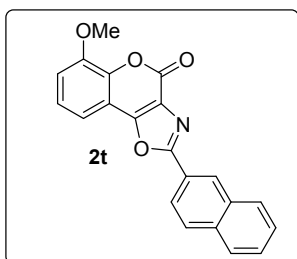
**6-ethoxy-2-(*m*-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2s)** Pale yellow solid; Yield = 59% (57 mg);



MP = 189  $^{\circ}\text{C}$ ; IR(KBr)  $\nu_{\text{max}}$  = 2924.09, 2852.21, 1747.07, 1640.50, 1278.12, 1104.94, 1047.03, 1019.35  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{19}\text{H}_{15}\text{NO}_4$   $[\text{M}+\text{H}]^+ = 322.1074$  (found 322.1079)

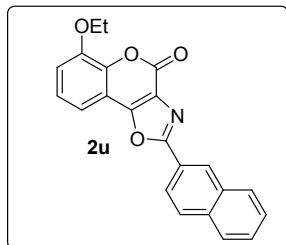
**6-methoxy-2-(naphthalen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one (2t).** Pale yellow solid; Yield = 7



8% (80 mg); MP = 270  $^{\circ}\text{C}$  IR(KBr)  $\nu_{\text{max}}$  = 2924.69, 2852.94, 1759.34, 1603.15, 1603.15, 1273.60, 1111.62, 1048.71  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{21}\text{H}_{13}\text{NO}_4$   $[\text{M}+\text{H}]^+ =$

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  $^{\circ}\text{C}$ ; IR(KBr)  $\nu_{\text{max}}$  = 2924.43, 2852.64, 1760.02, 1605.56, 1272.39, 2080.36, 1051.17, 1013.12  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  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;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  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  $\text{C}_{22}\text{H}_{15}\text{NO}_4$   $[\text{M}+\text{H}]^+ = 358.1074$  (found 358.1096).

# <sup>1</sup>H NMR spectra of 2a

MB-B-1-14-1H

Sample Name:  
MB-B-1-14-1H  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:

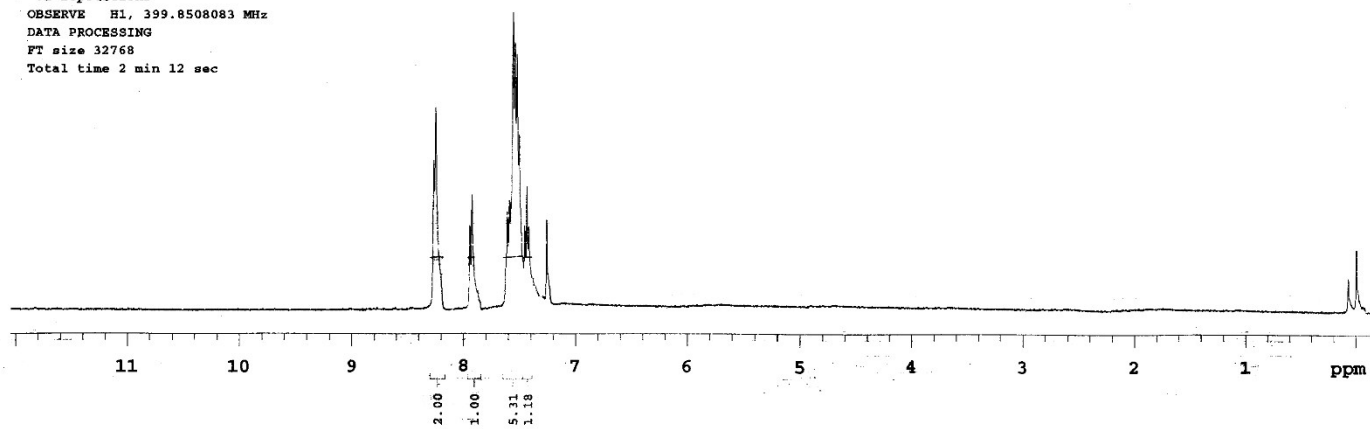
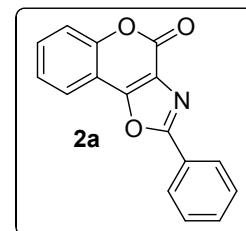
Sample directory:

FidFile: MB-B-1-14-1H

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 17 2014

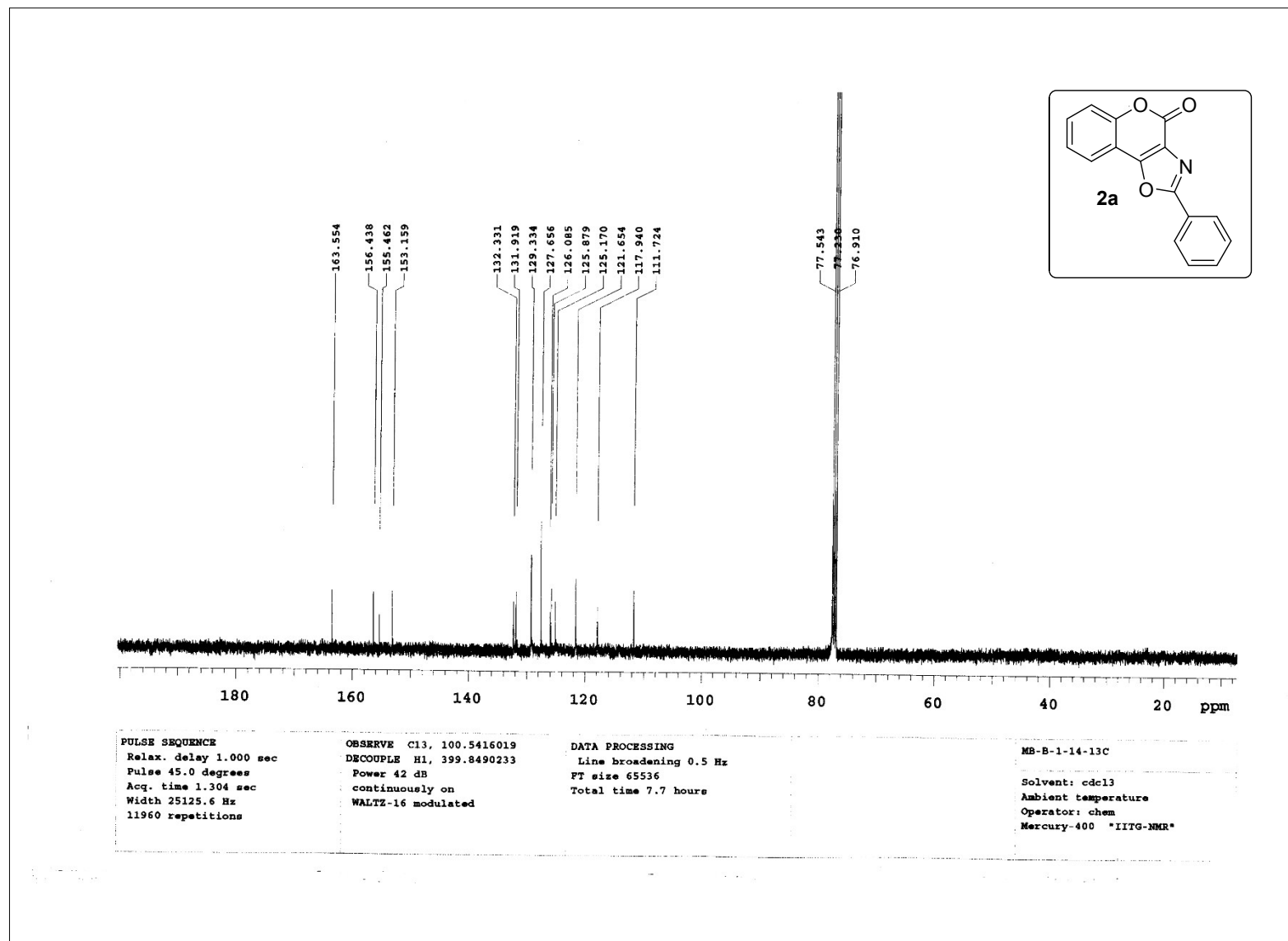
Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8508083 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



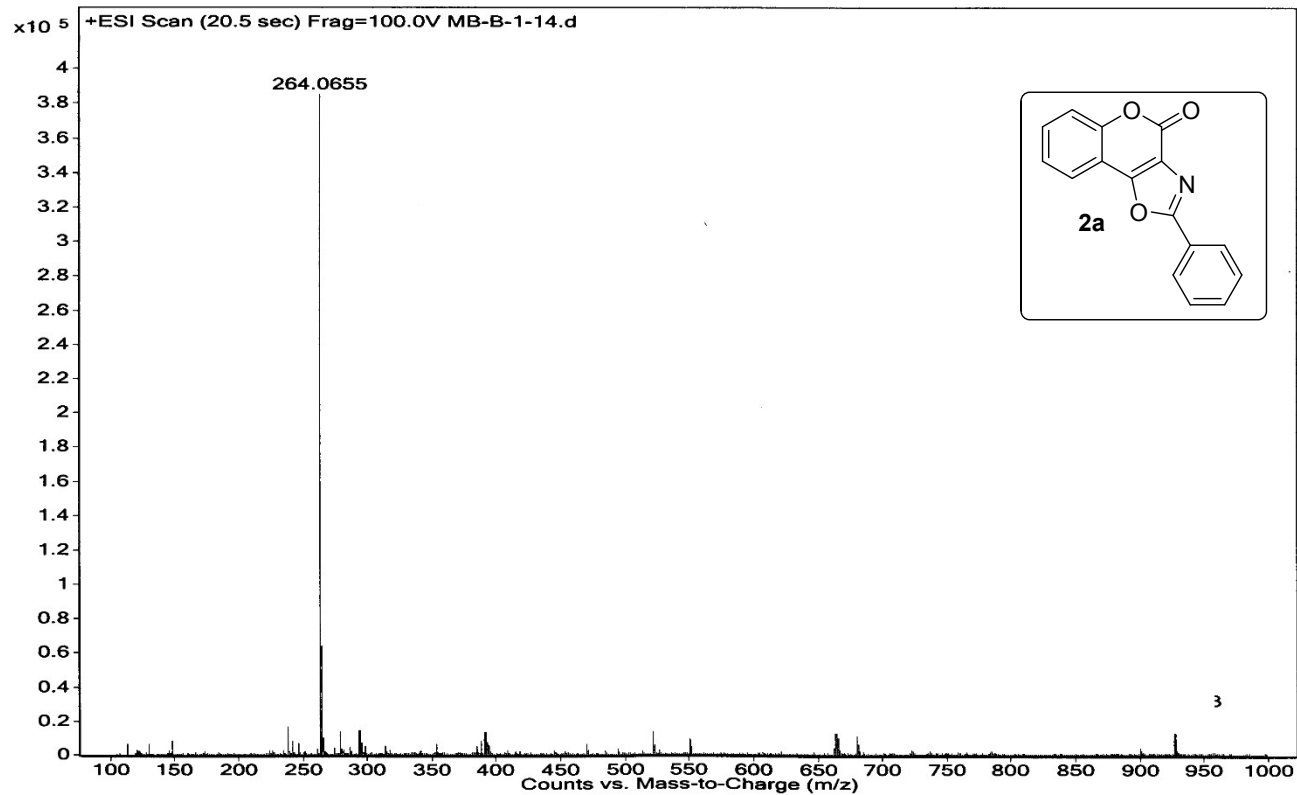


<sup>13</sup>C NMR spectra of **2a**

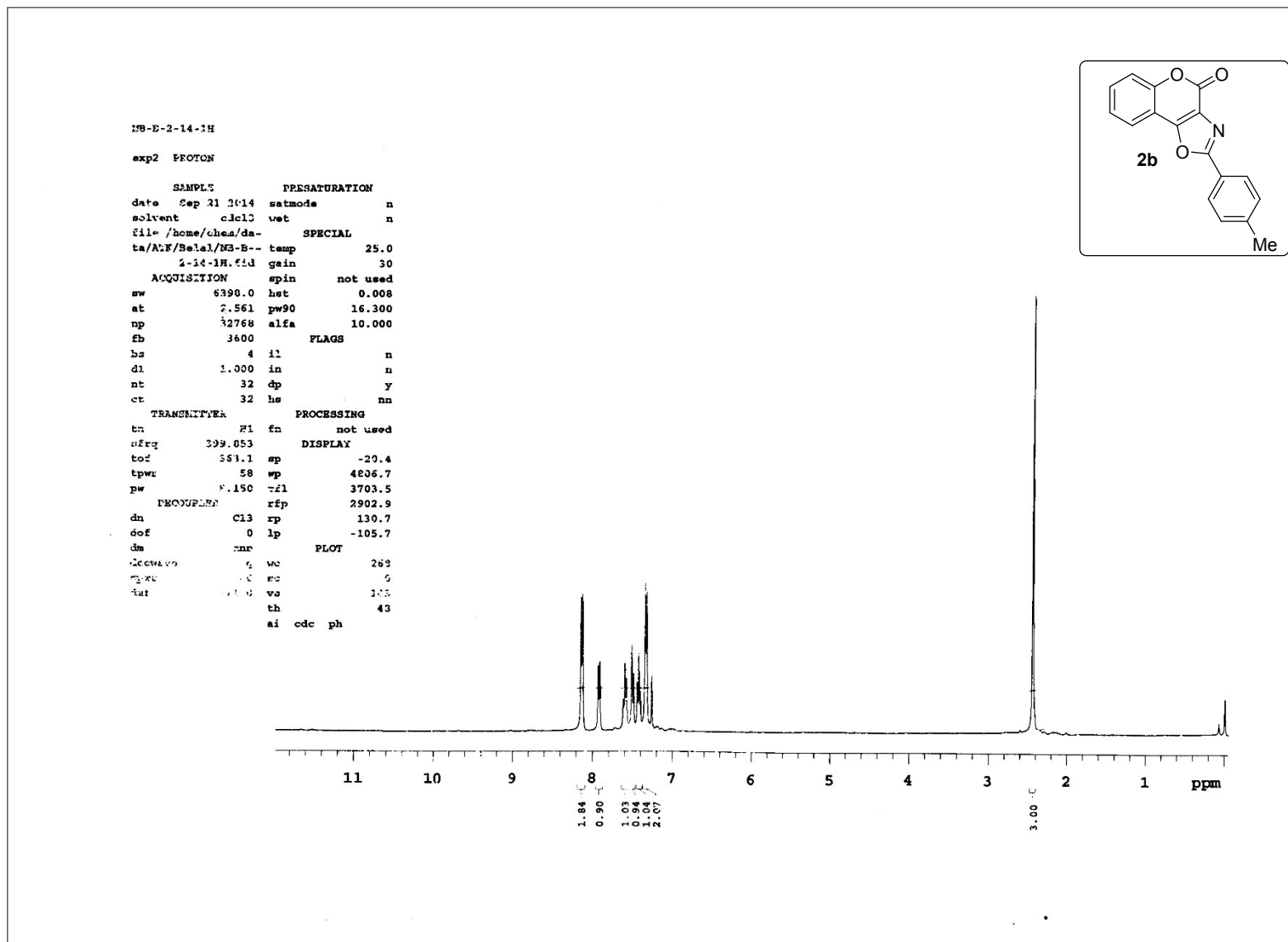


# HRMS spectra of 2a

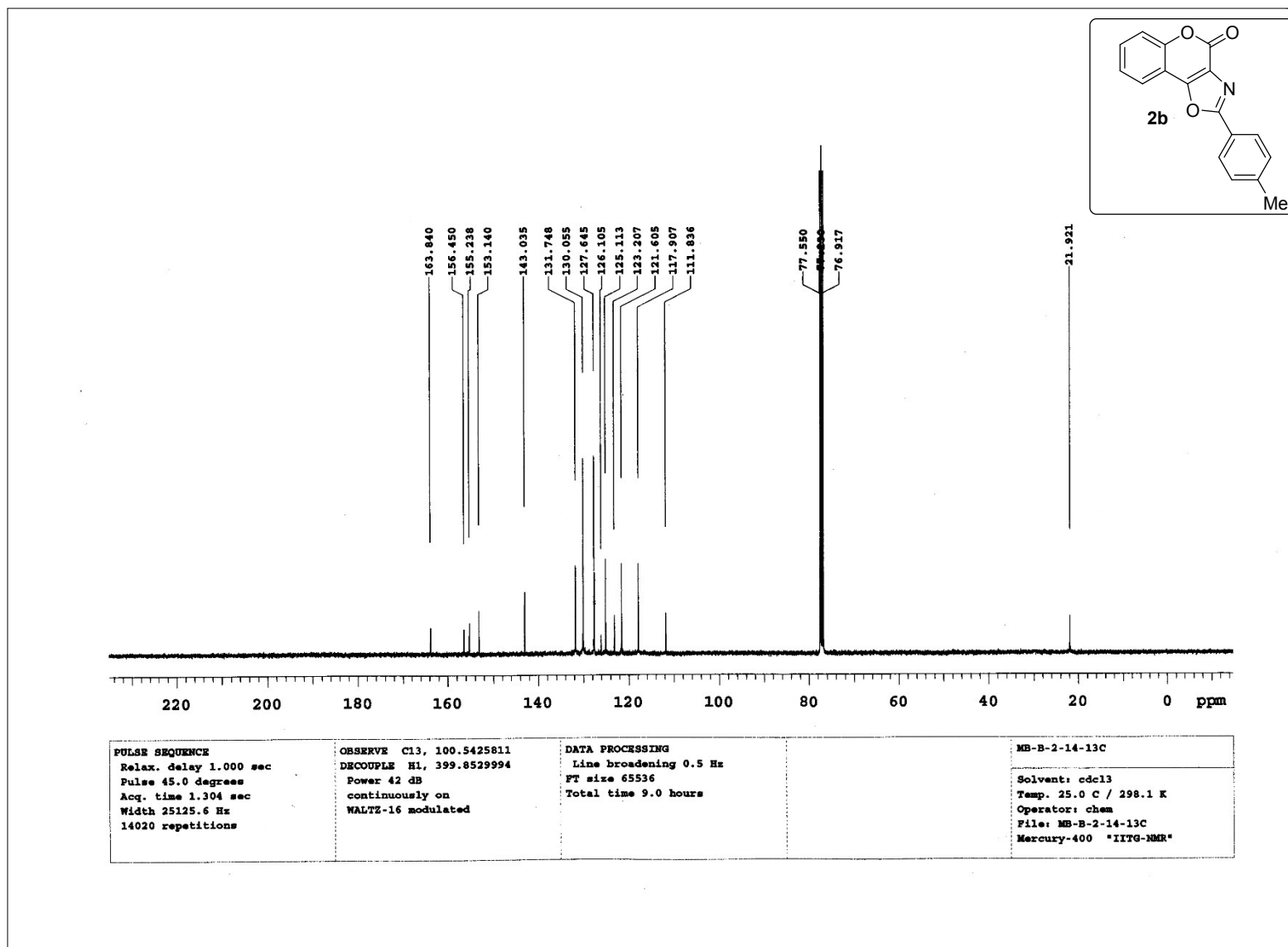
<b>Sample Name</b>	MB-B-1-14	<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	MB-B-1-14.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	1/13/2015 11:05:17 AM



# <sup>1</sup>H NMR spectra of 2b

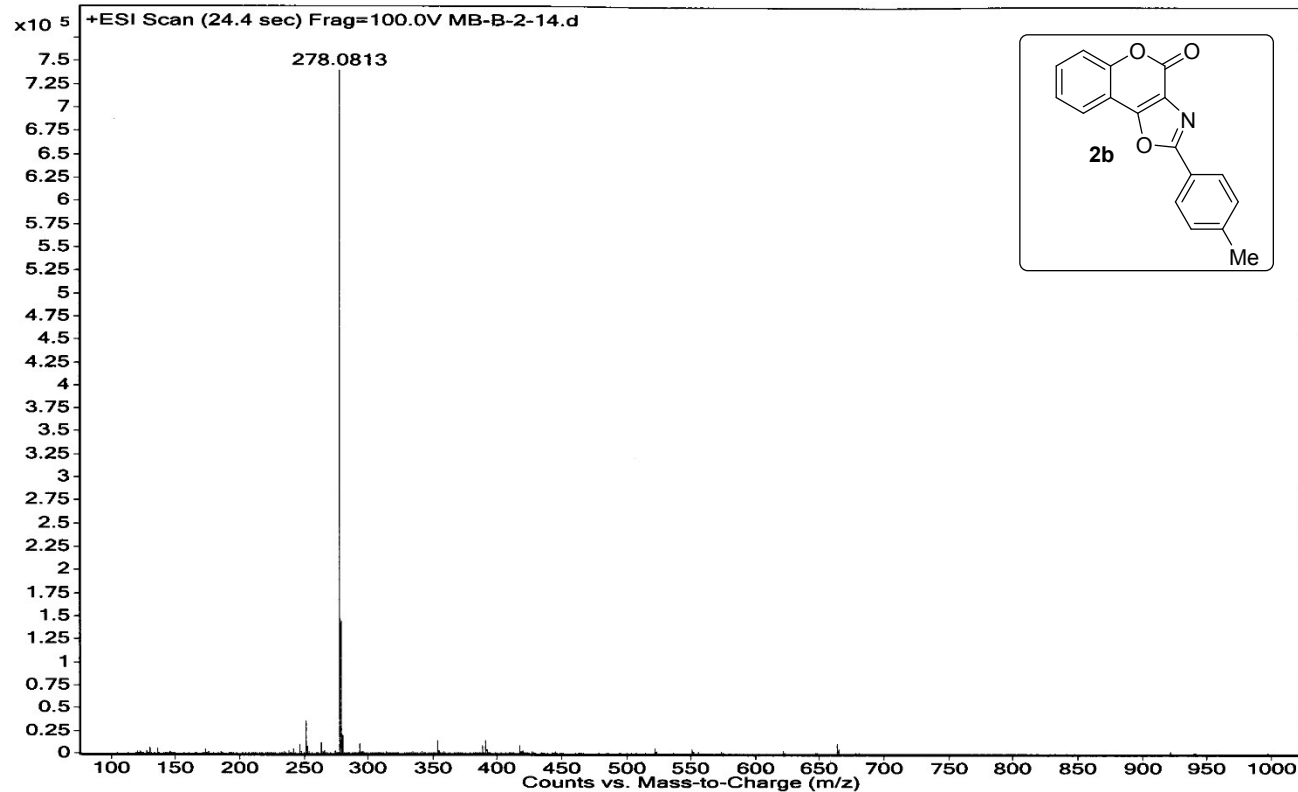


<sup>13</sup>C NMR spectra of **2b**

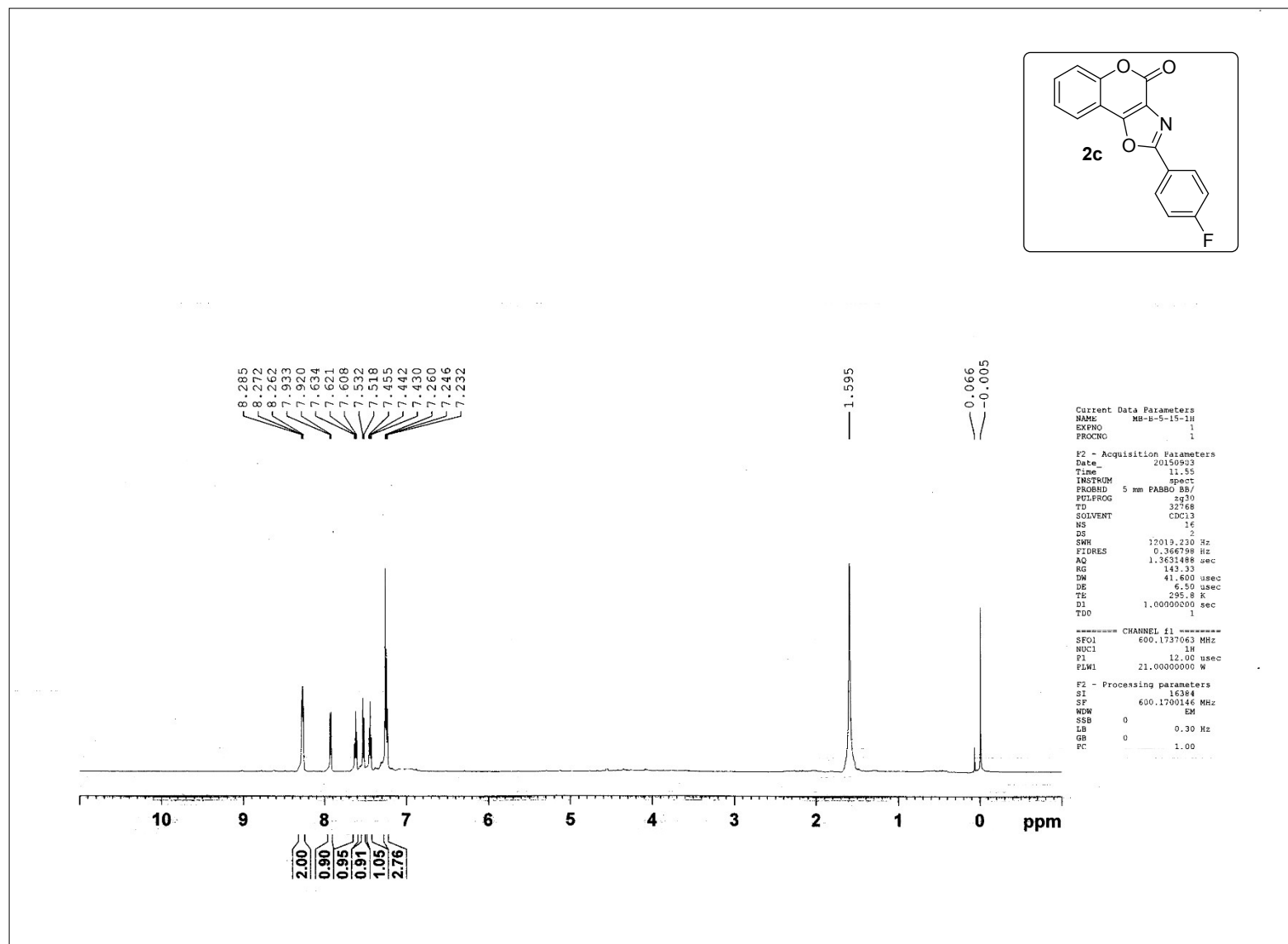


# HRMS spectra of 2b

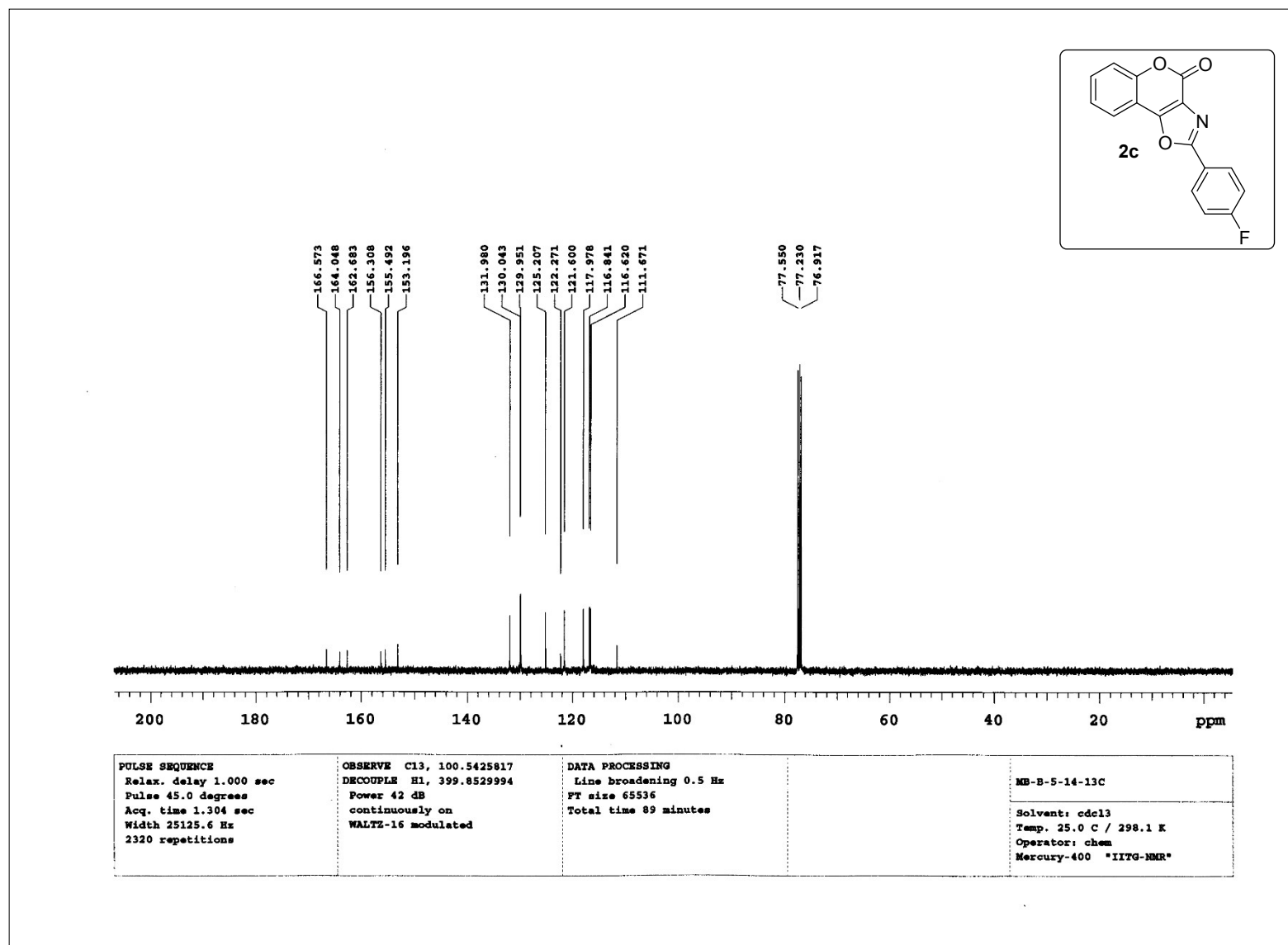
<b>Sample Name</b>	MB-B-2-14	<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	MB-B-2-14.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	1/13/2015 11:10:42 AM



$^1\text{H}$  NMR spectra of **2c**

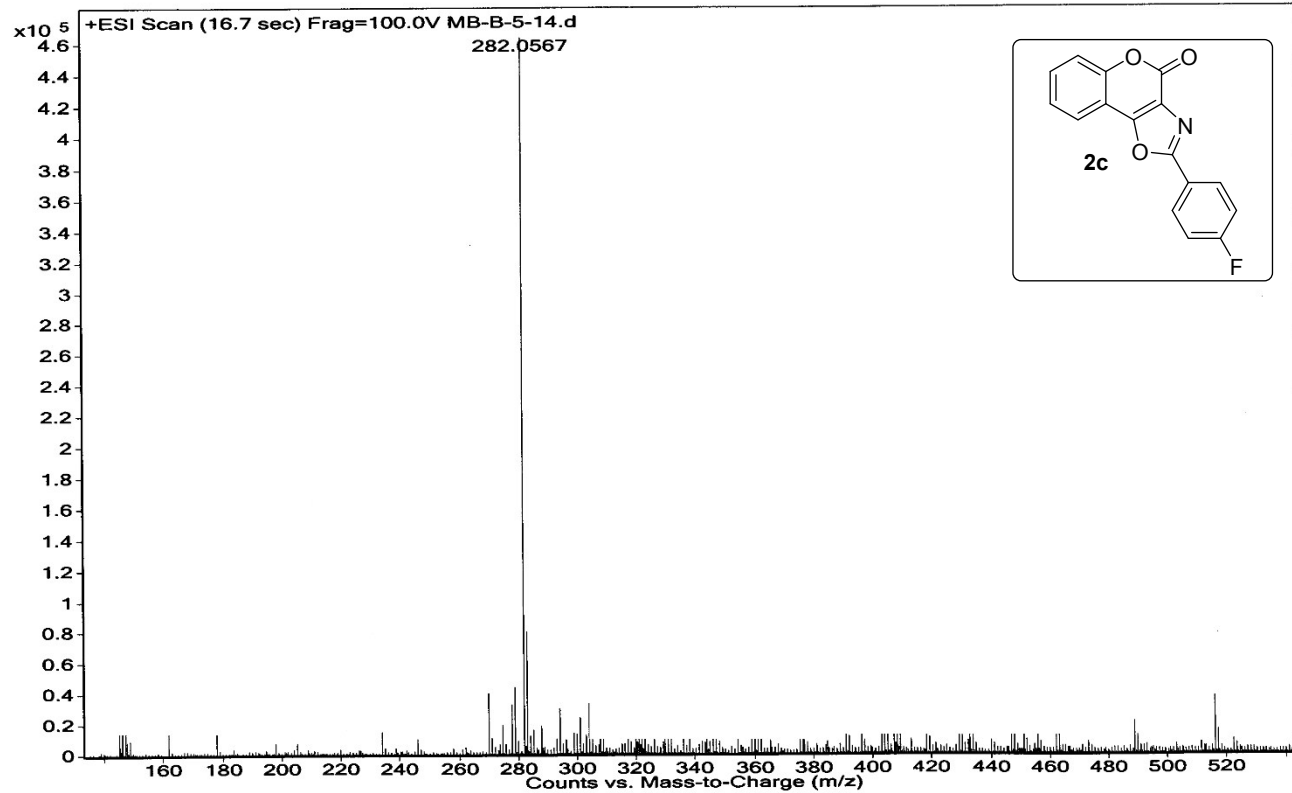


<sup>13</sup>C NMR spectra of 2c



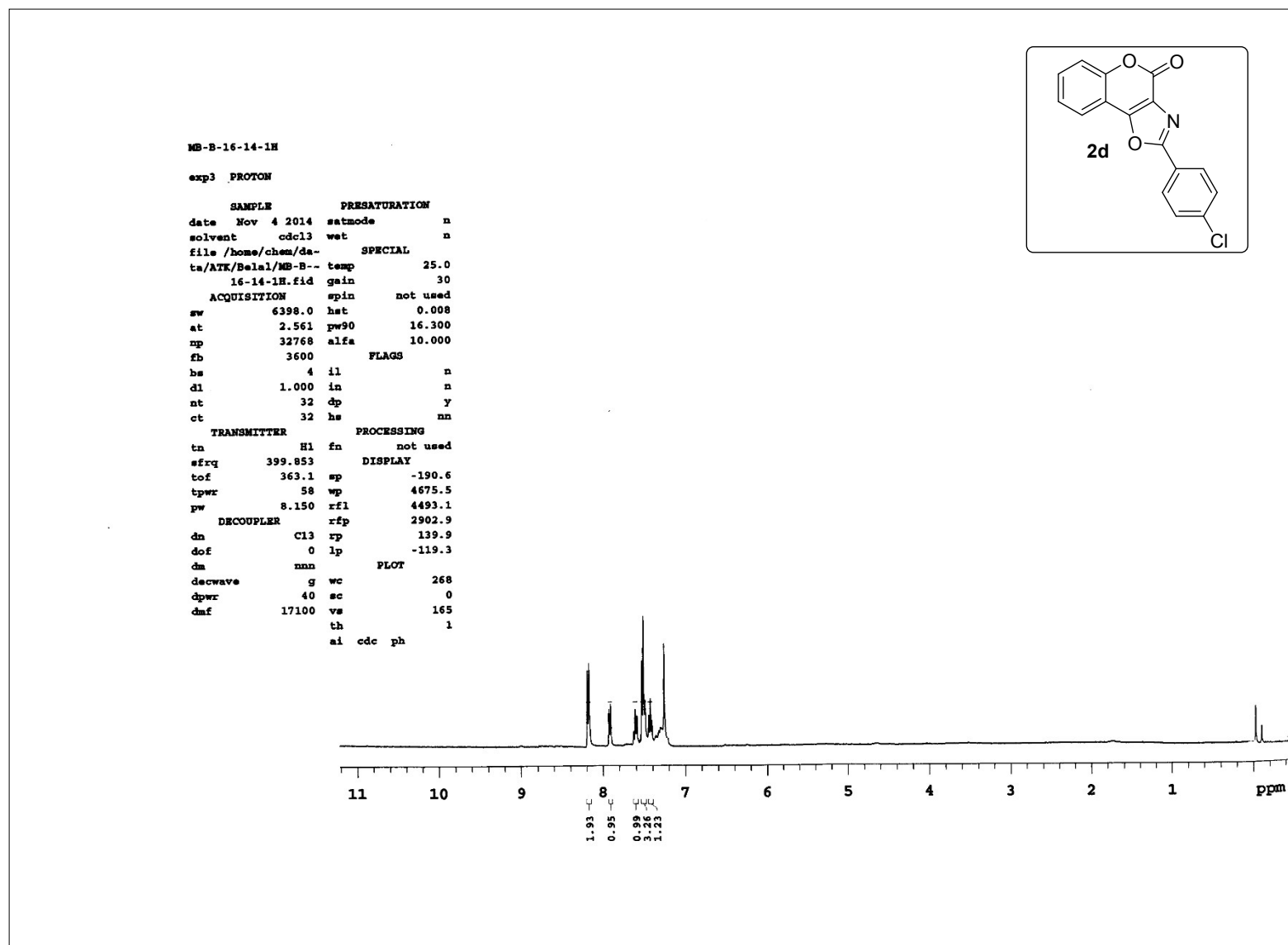
# HRMS spectra of 2c

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

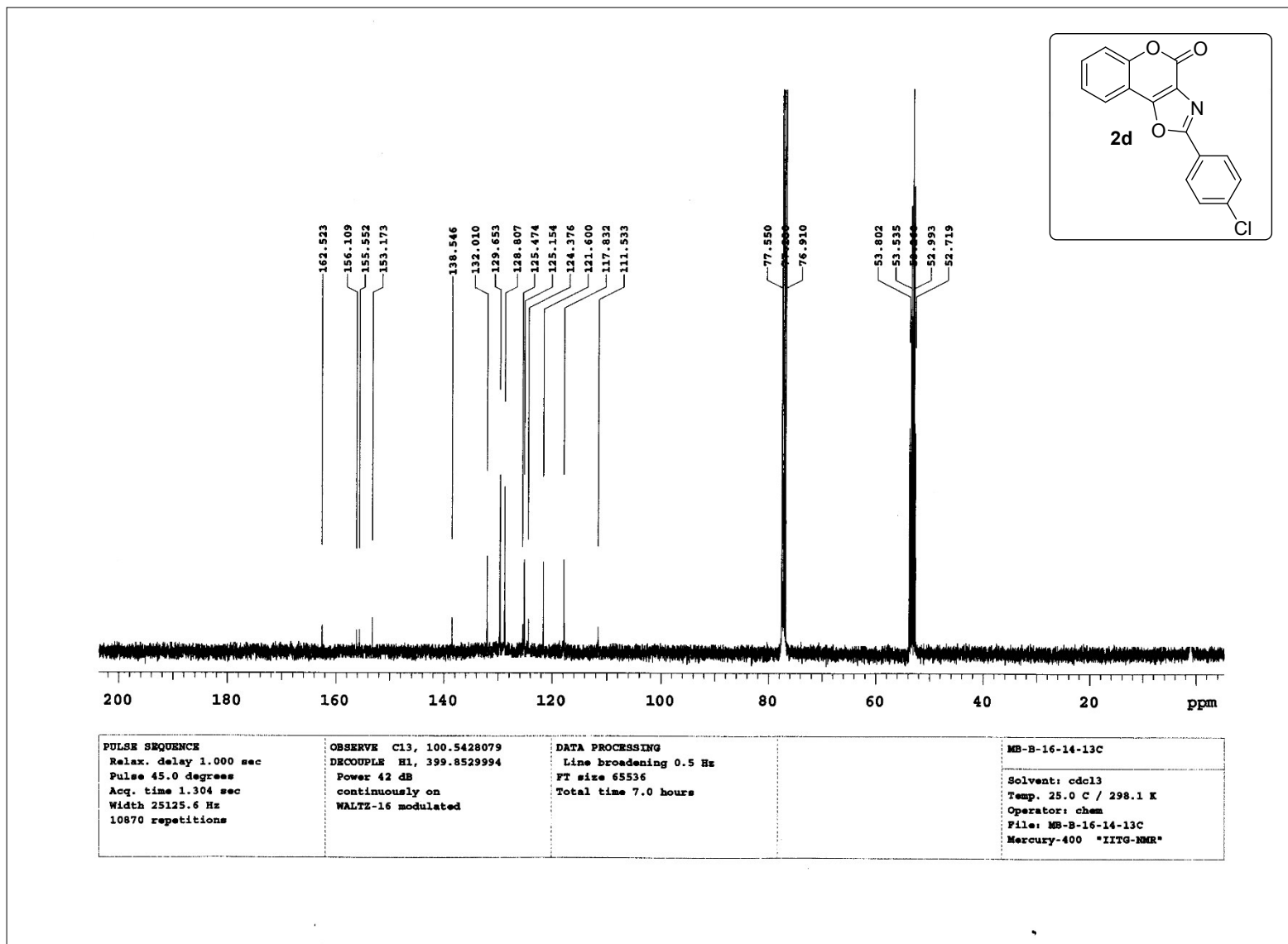




# <sup>1</sup>H NMR spectra of 2d

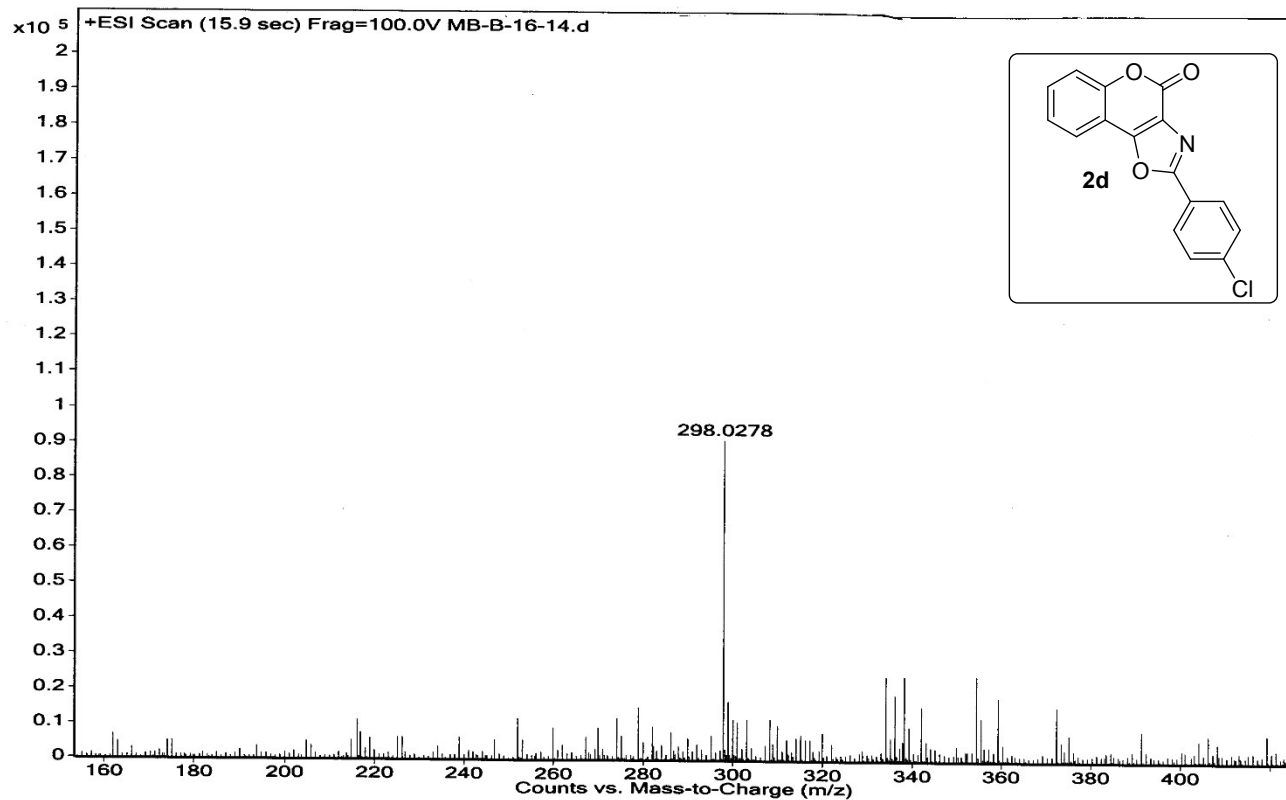


<sup>13</sup>C NMR spectra of **2d**

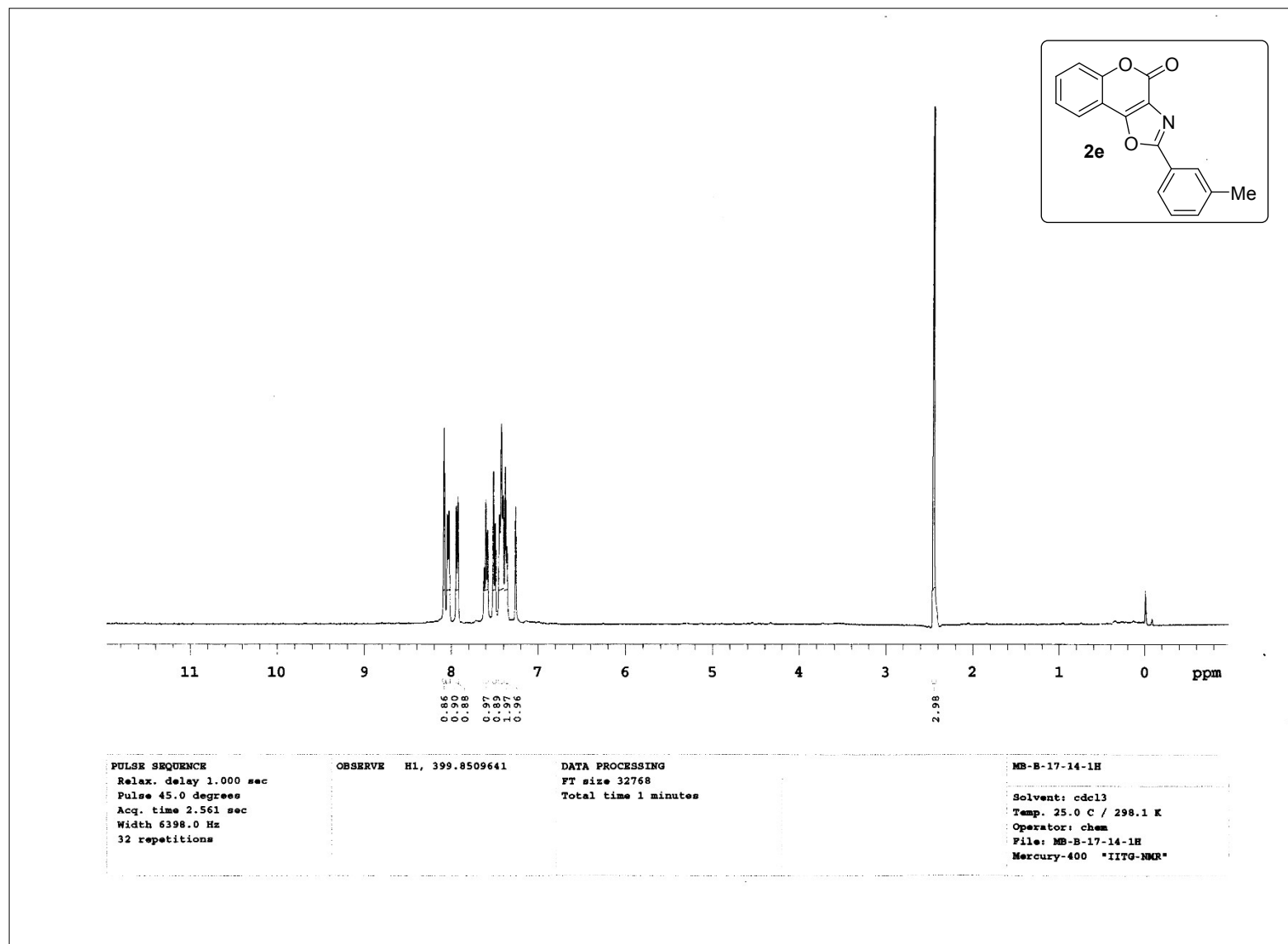


# HRMS spectra of 2d

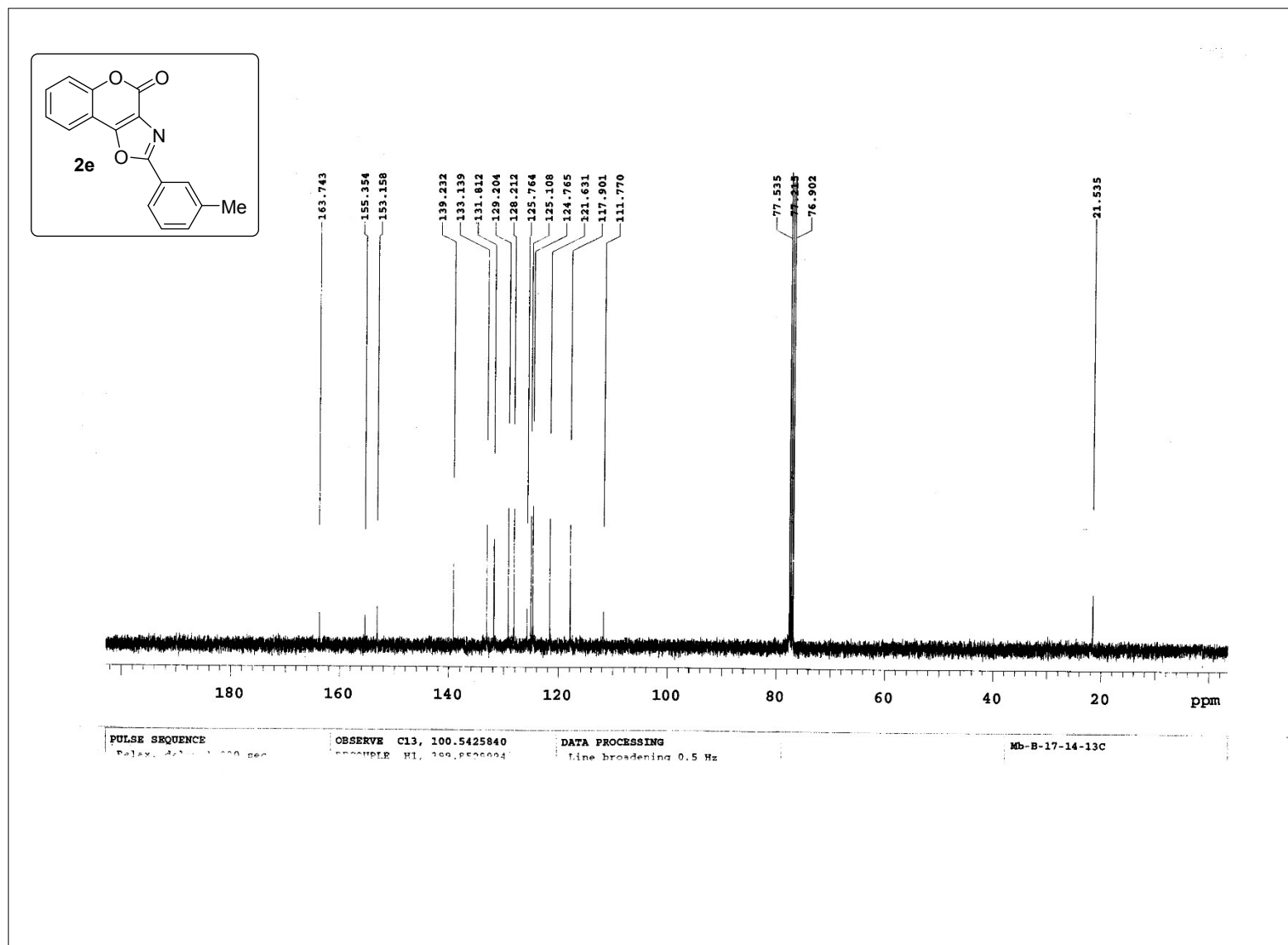
Sample Name	Position	Instrument Name	User Name
Inj Vol	Inj Position	Sample Type	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra of 2e

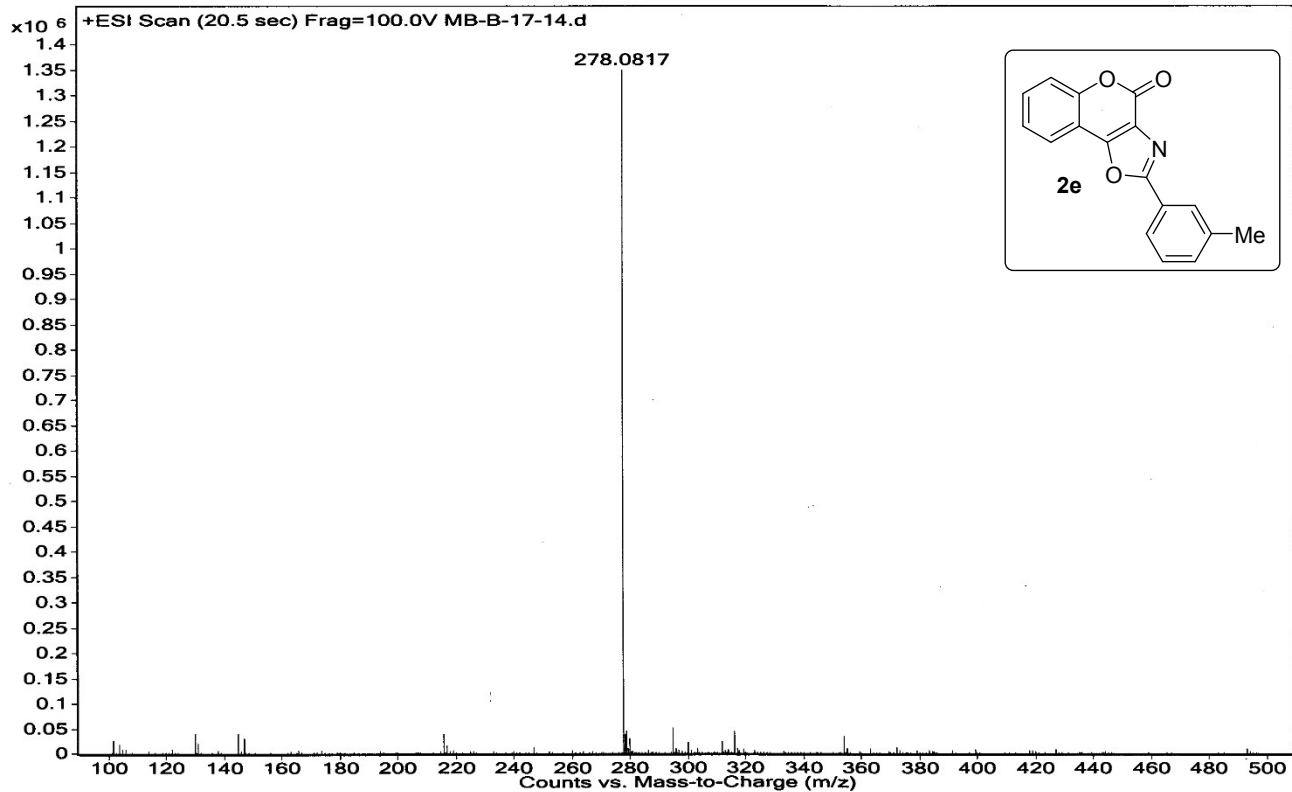


# <sup>13</sup>C NMR spectra of 2e

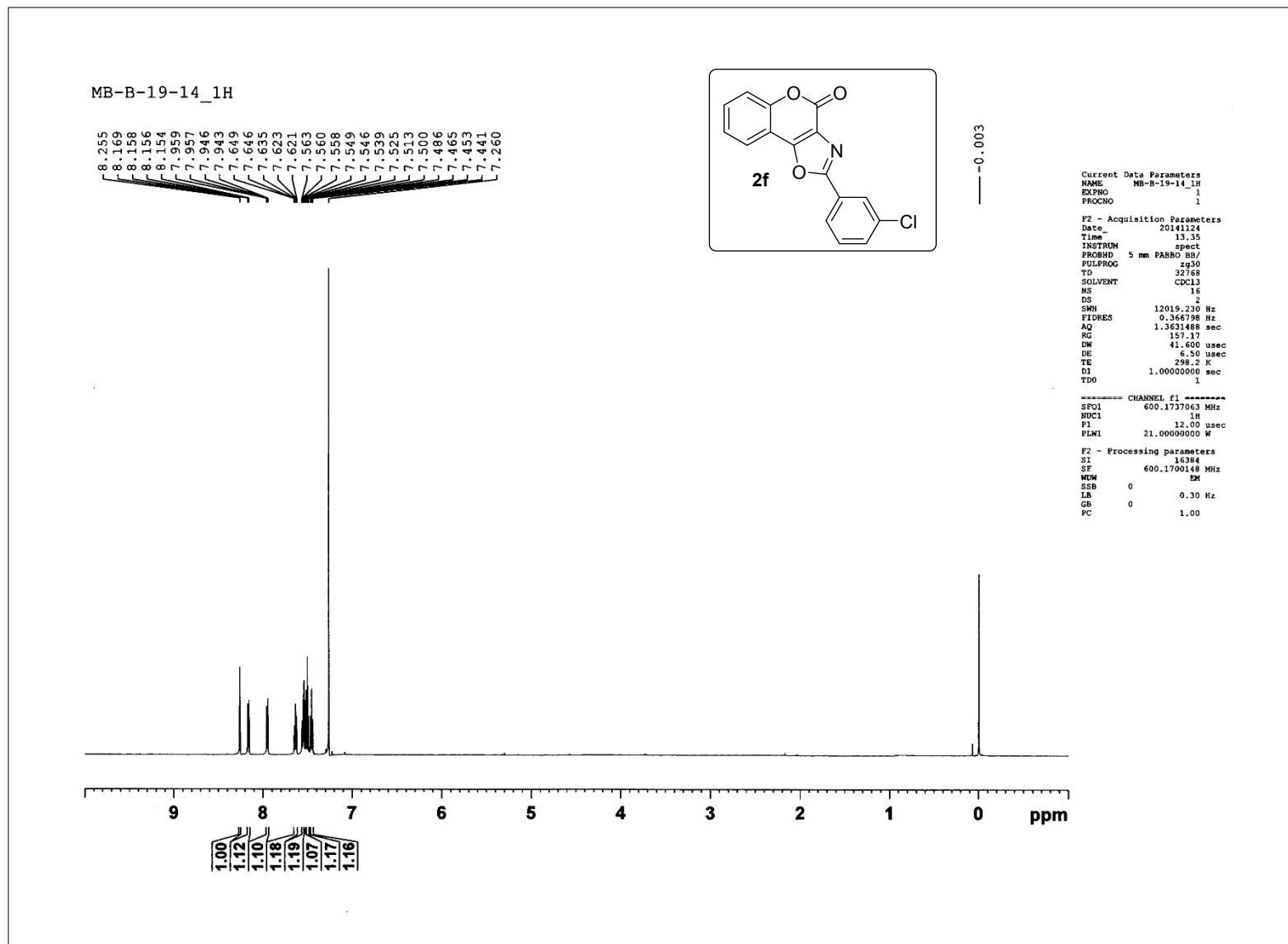


HRMS spectra of 2e

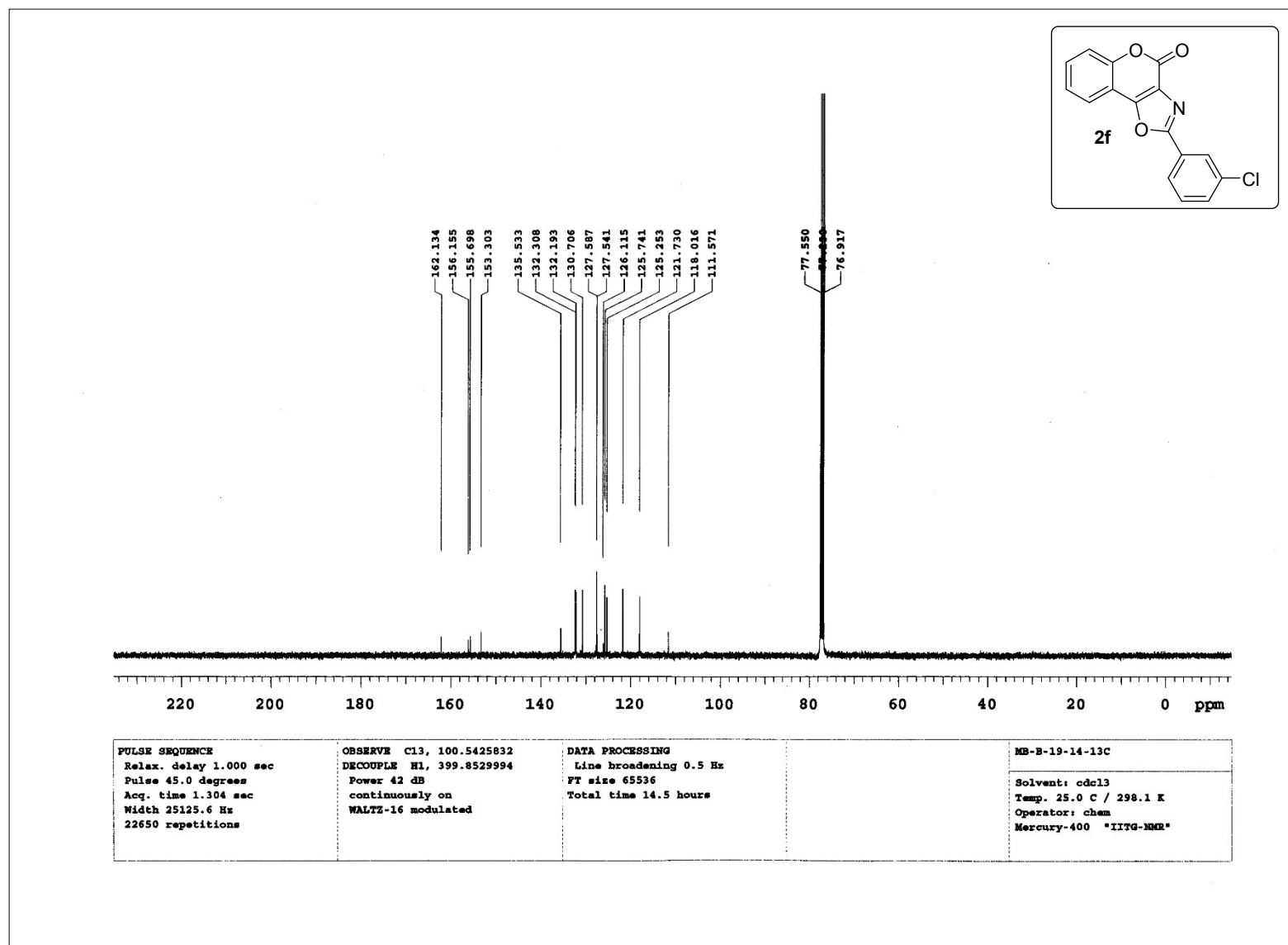
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



H<sup>1</sup> NMR spectra of **2f**

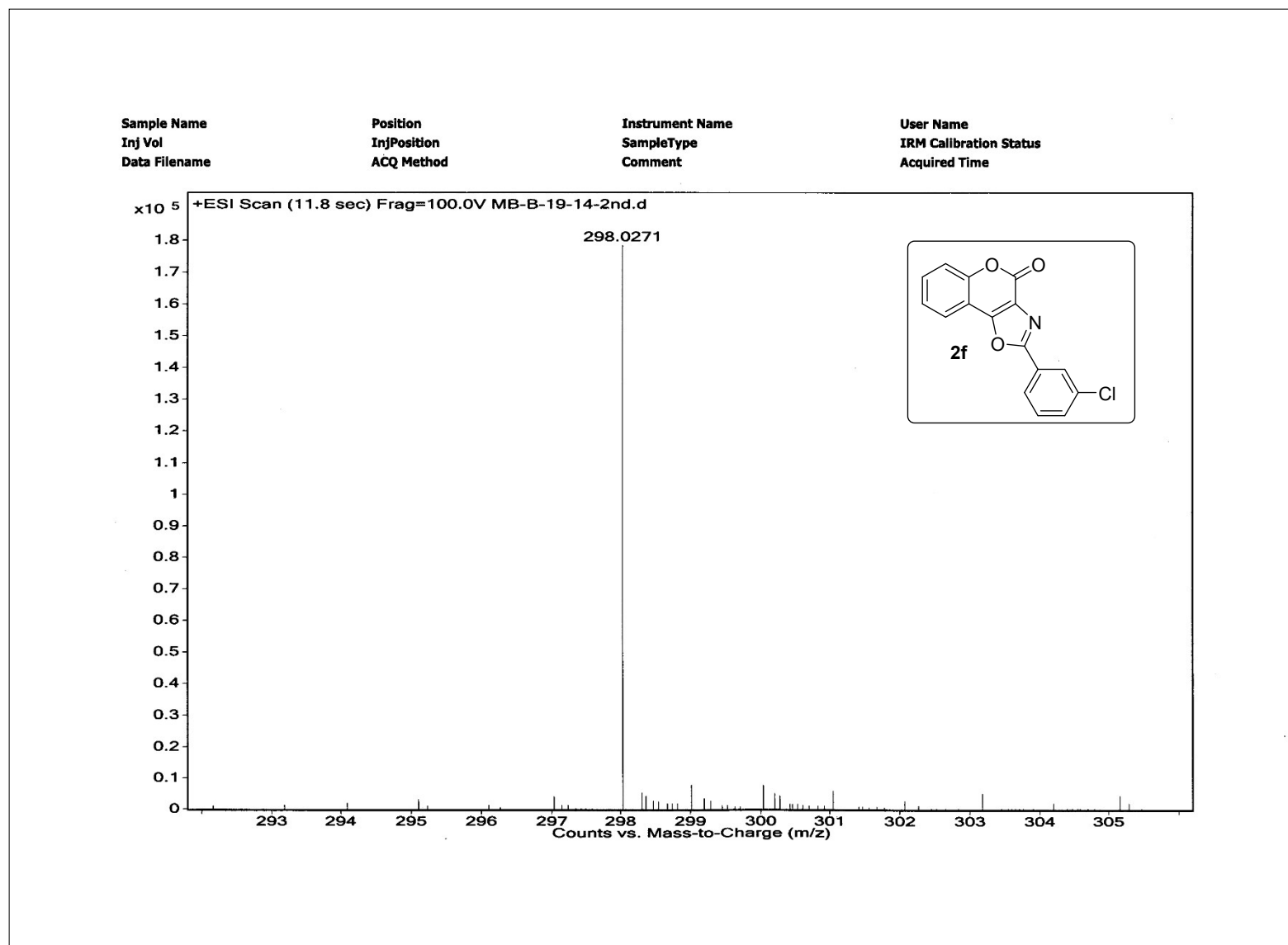


<sup>13</sup>C NMR spectra of 2f

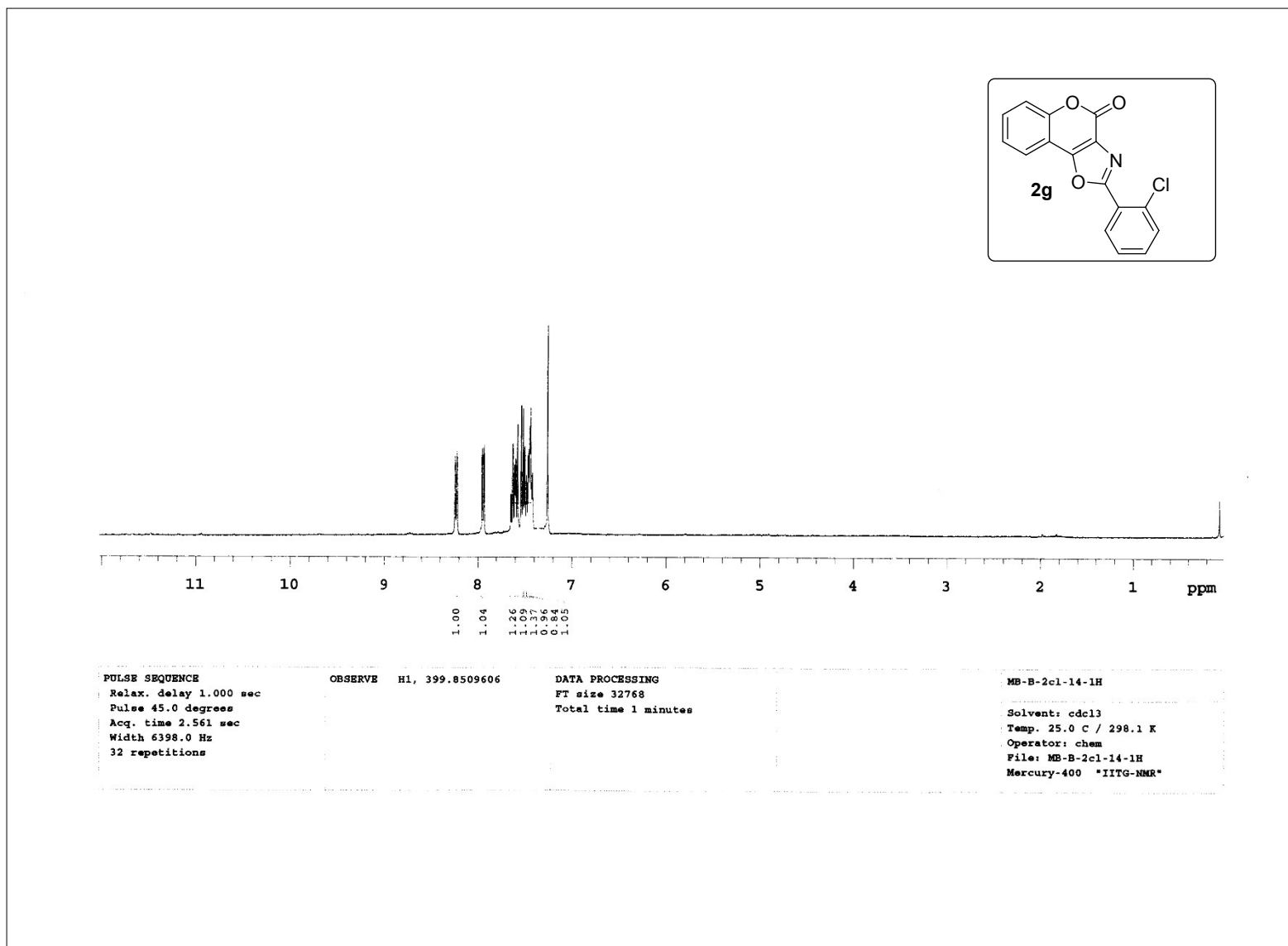




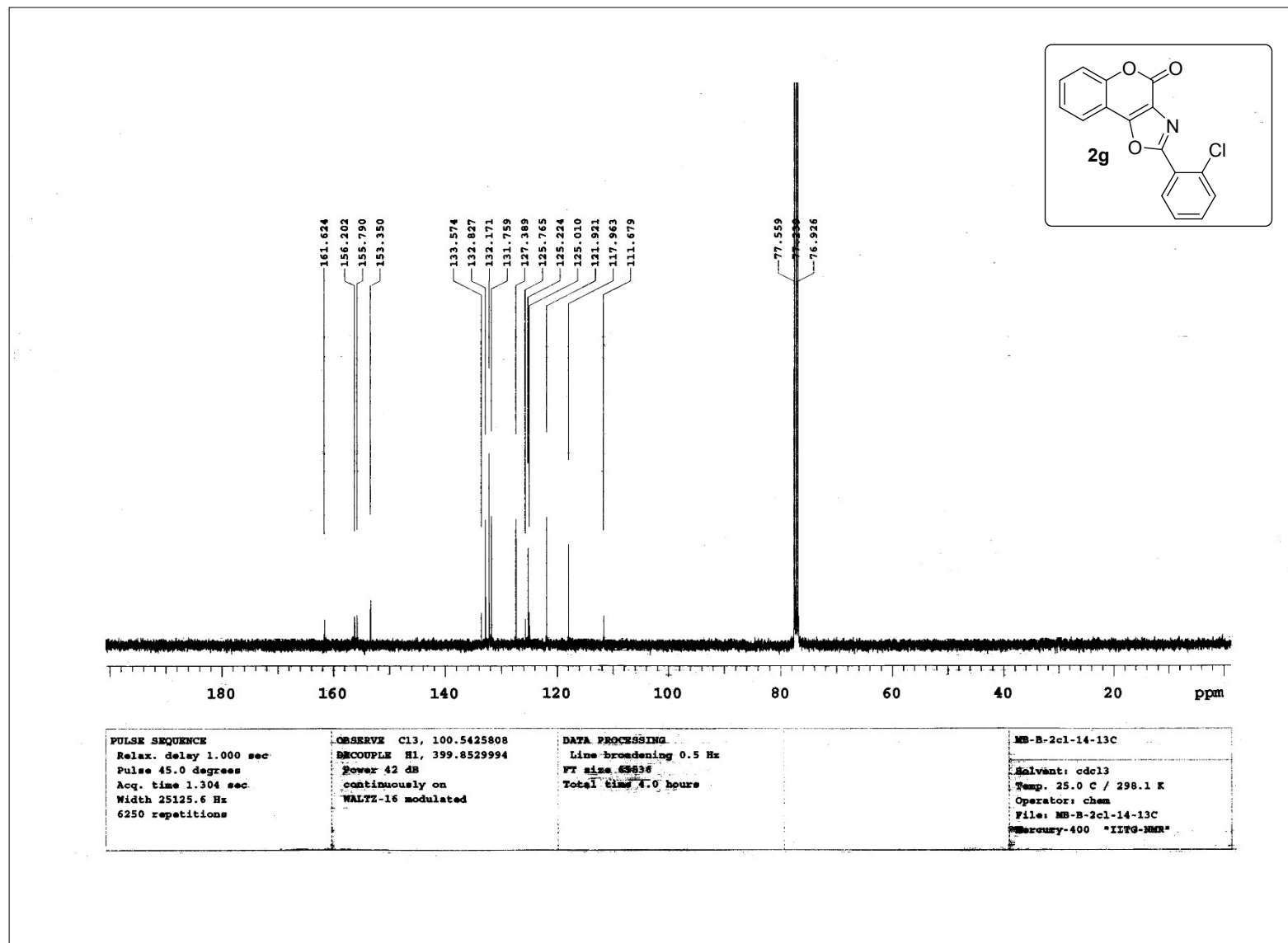
# HRMS spectra of 2f



# H<sup>1</sup> NMR spectra of **2g**

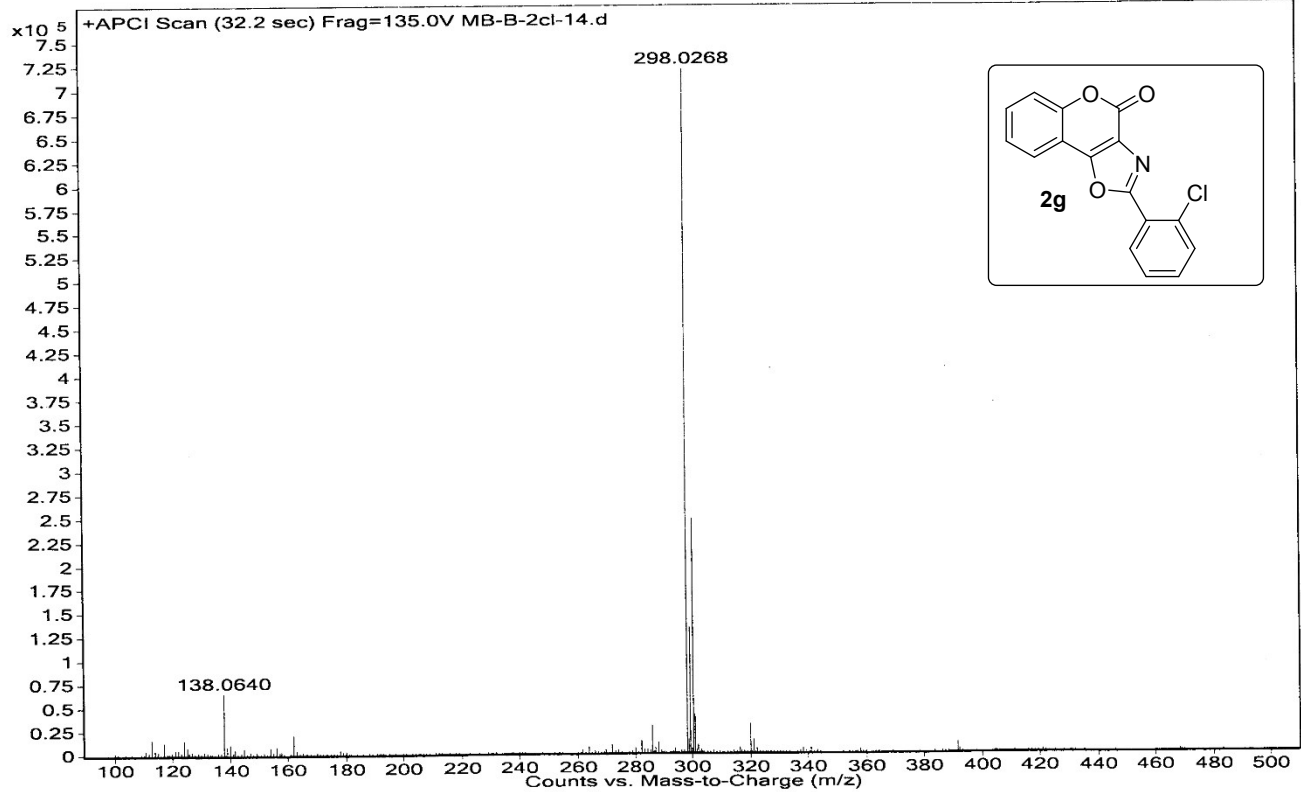


<sup>13</sup>C NMR spectra of 2g

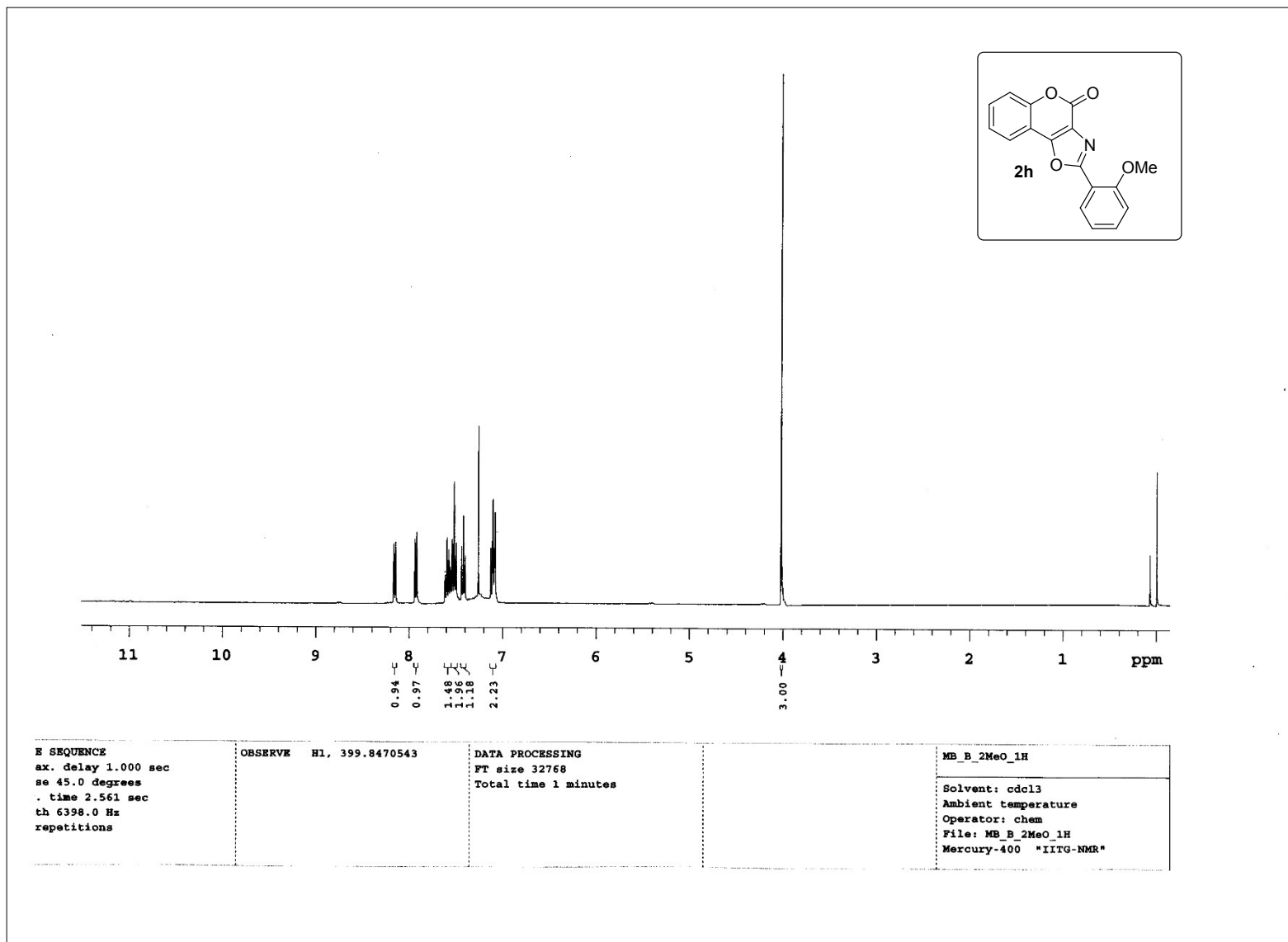


HRMS spectra of 2g

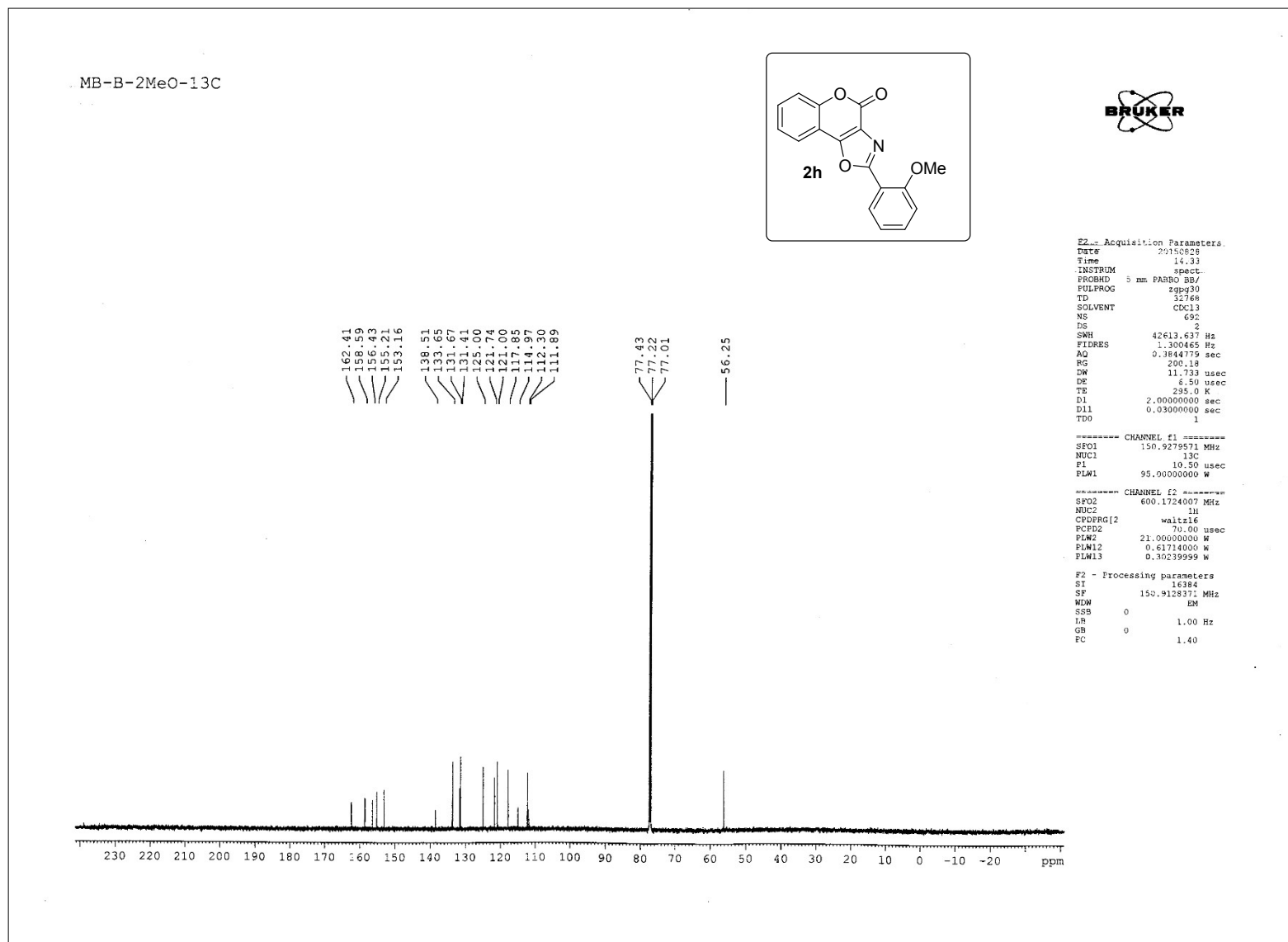
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra of 2h

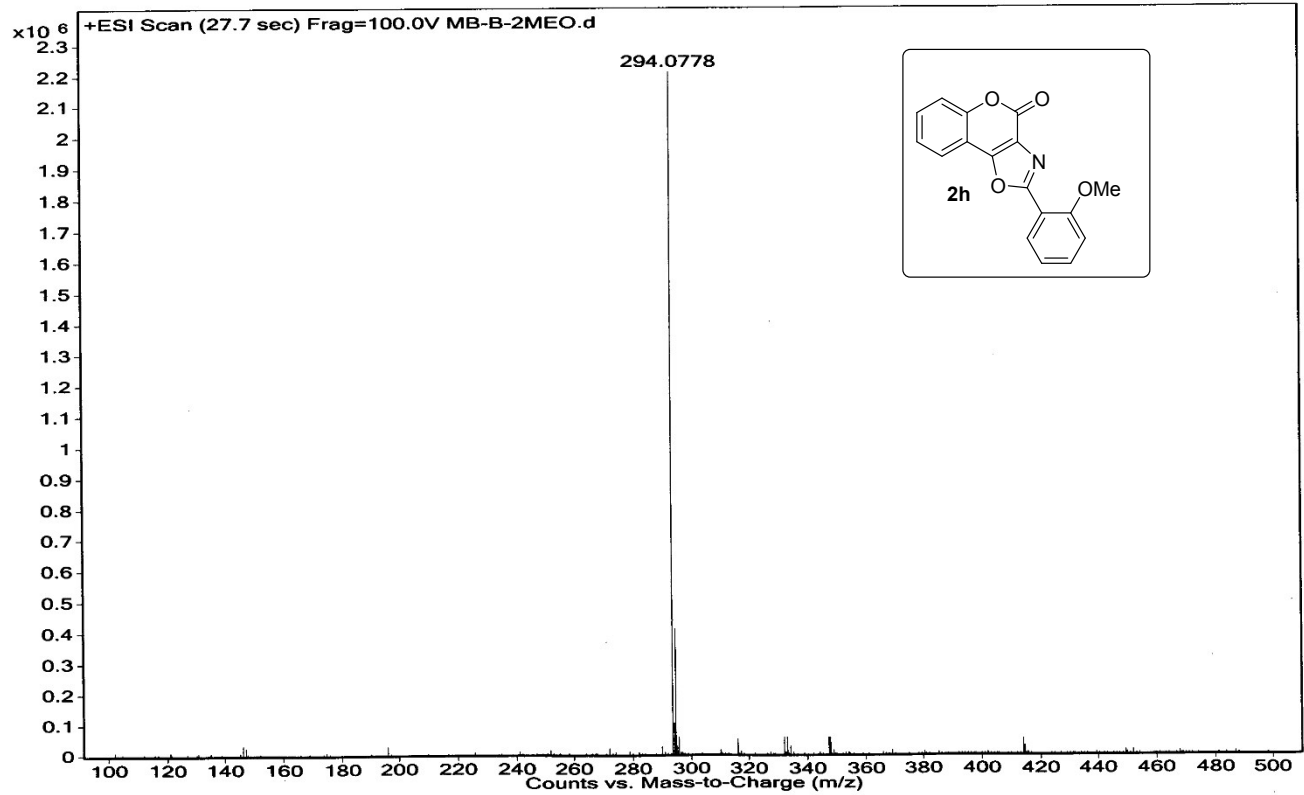


<sup>13</sup>C NMR spectra of 2h

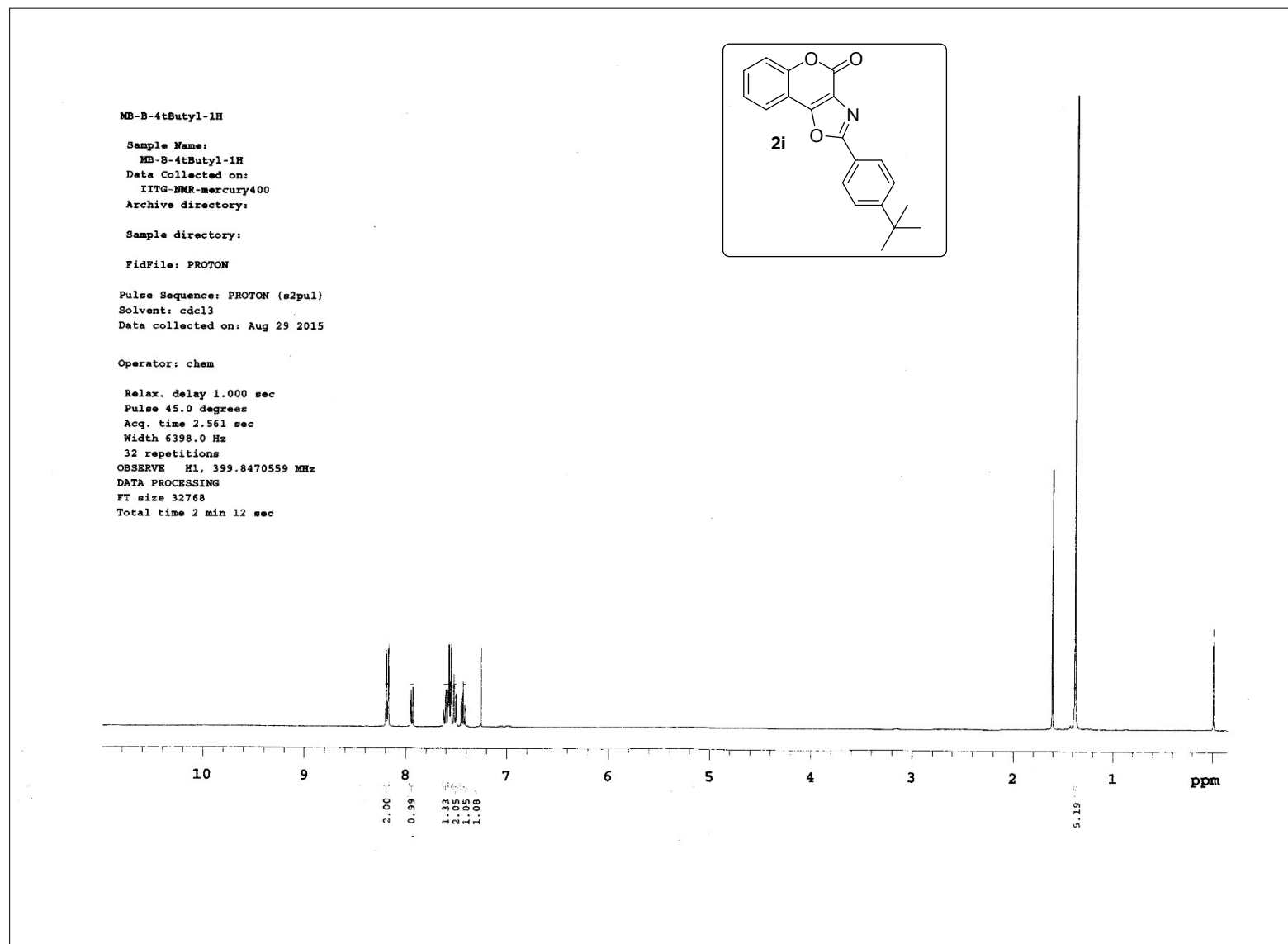


# HRMS spectra of 2h

<b>Sample Name</b>	Unavailable	<b>Position</b>	Unavailable	<b>Instrument Name</b>	Unavailable	<b>User Name</b>	Unavailable
<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
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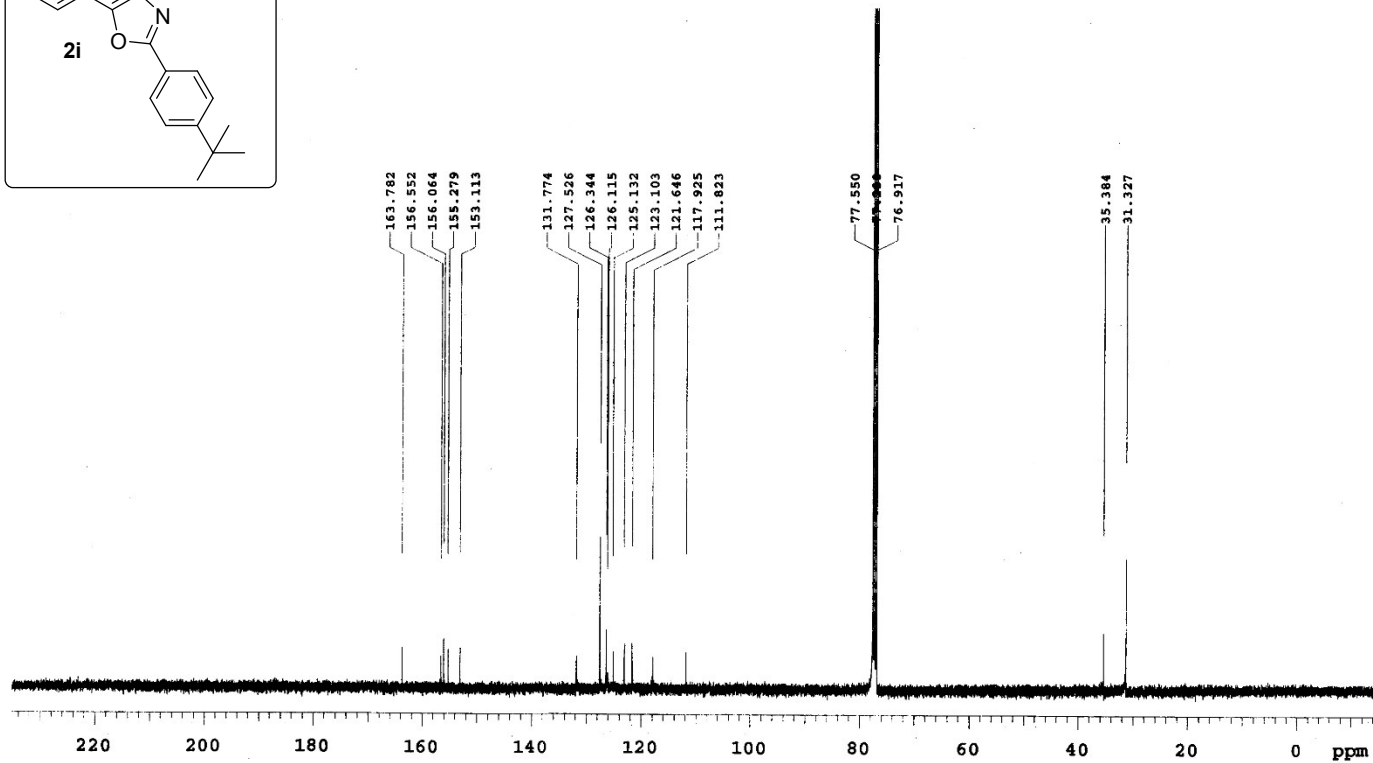
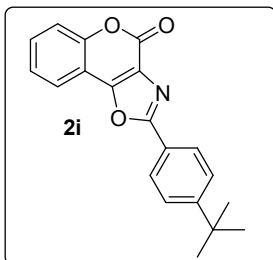


# H<sup>1</sup> NMR spectra of 2i





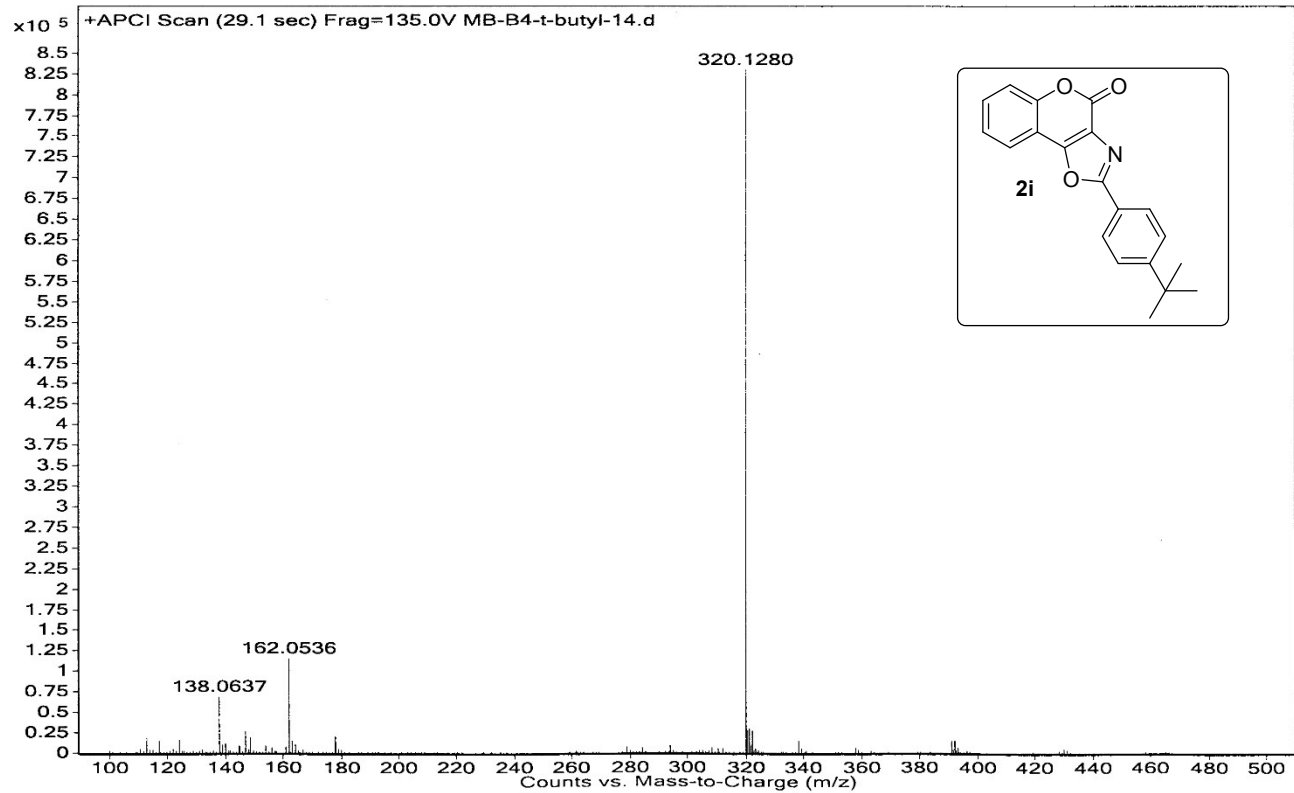
<sup>13</sup>C NMR spectra of **2i**



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 16000 repetitions	<b>OBSERVE</b> C13, 100.5416011 <b>DECOUPLE</b> H1, 399.8490233 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 10.2 hours	<b>MS-B-4tButyl-13c</b> Solvent: cdcl3 Ambient temperature Operator: chem Mercury-400 "IITG-NMR"
---	--	--	--

# 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**

MB-B-THIO-14-1H

Sample Name:  
MB-B-THIO-14-1H  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:

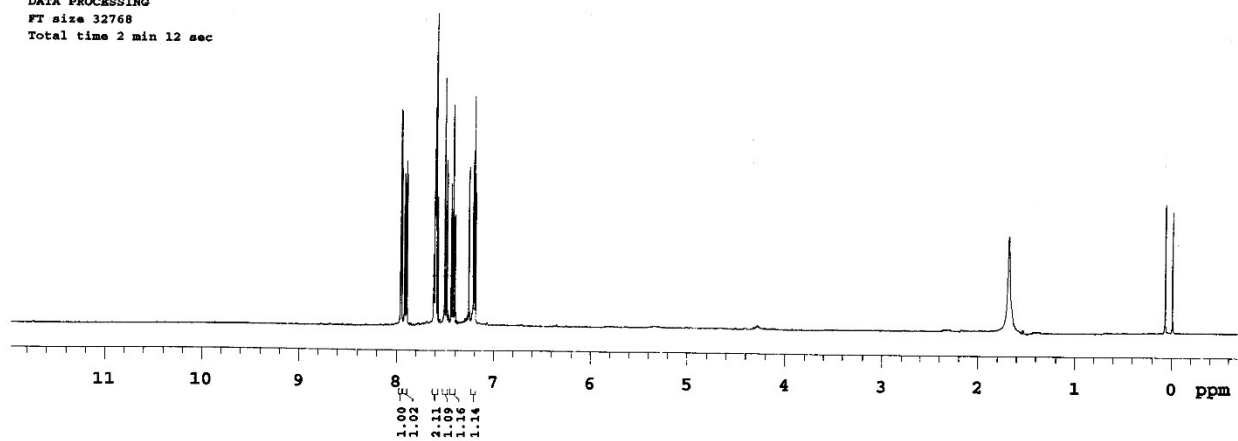
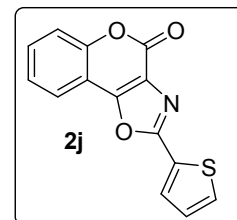
Sample directory:

FidFile: PROTON

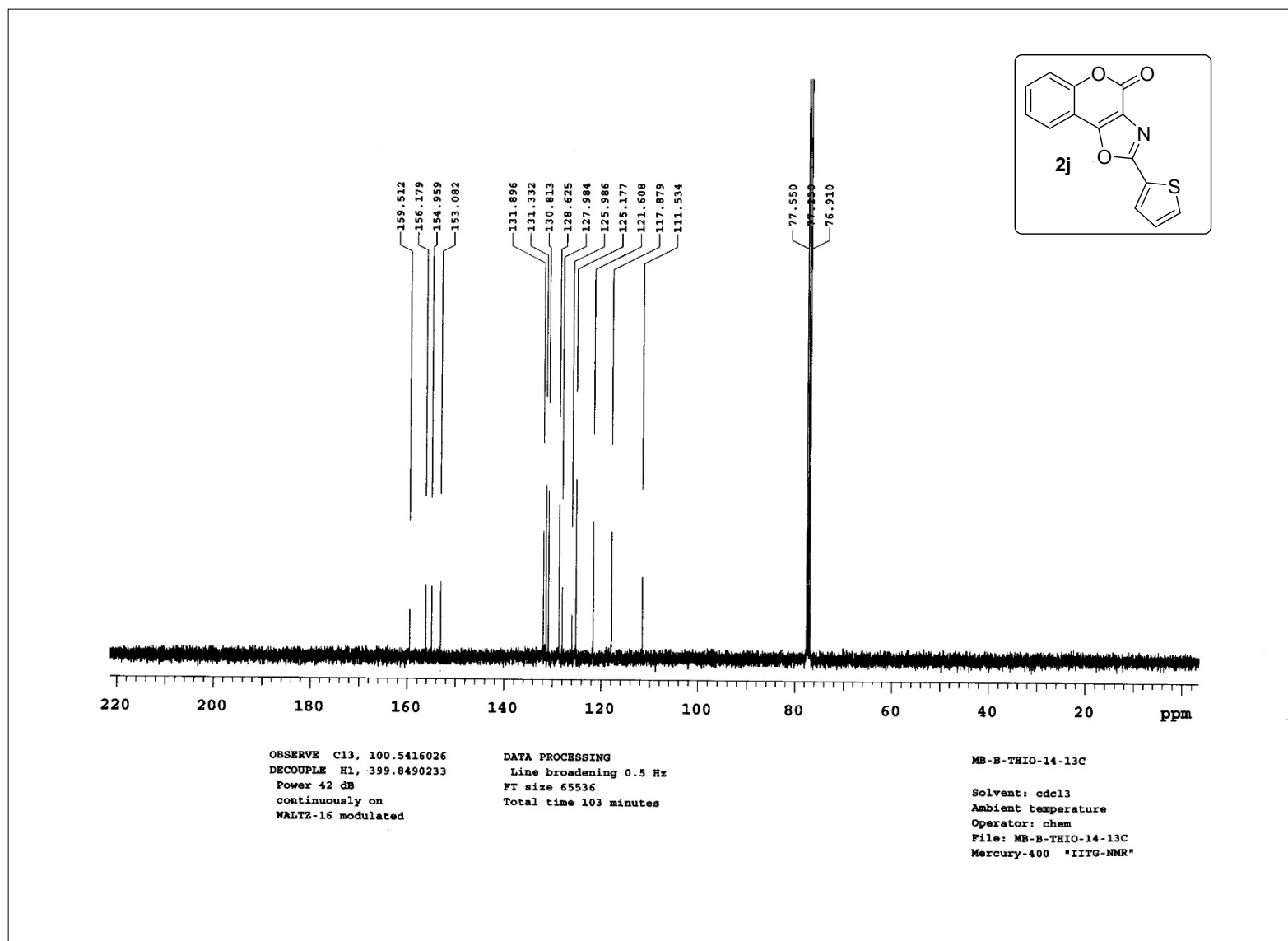
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Aug 21 2015

Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8470543 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec

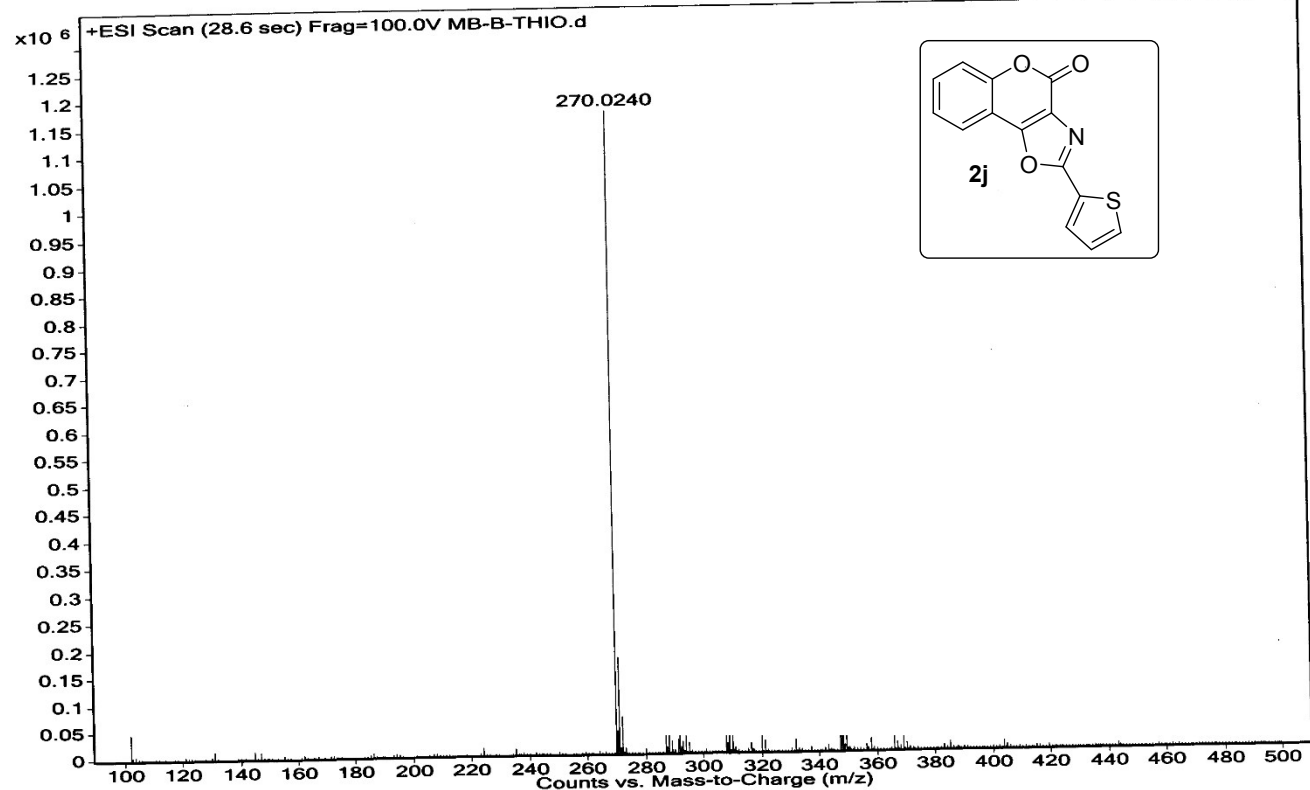


<sup>13</sup>C NMR spectra of **2j**



# HRMS spectra of 2j

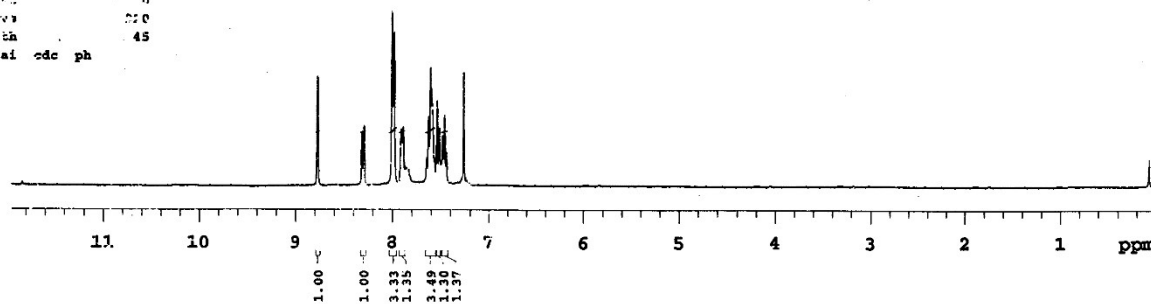
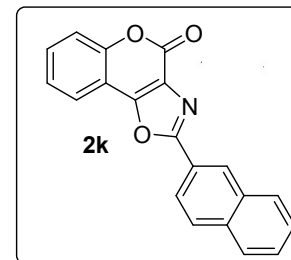
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-B-THIO.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



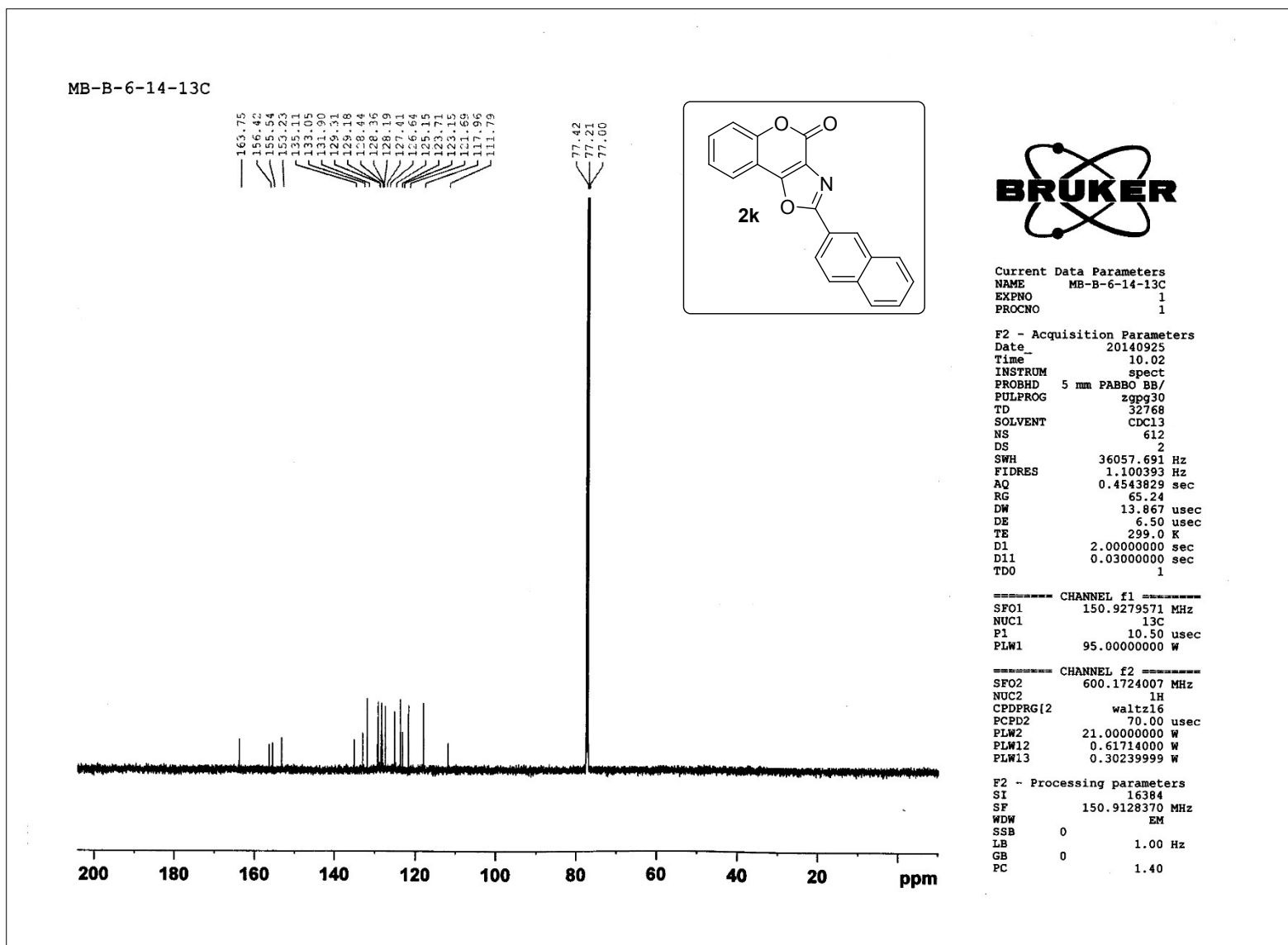
H<sup>1</sup> NMR spectra of 2k

```

MB-b-6-14-1E
exp: PROTON
SAMPLE          PRESATURATION
date Sep 26 2014 satmode      n
solvent cdcl3  wet          n
file          exp          SPECIAL
ACQUISITION    temp        25.0
nu          6398.0 gain      30
wt          2.561 spin      not used
rg          32768 hst        0.008
lh          3600 pw90       16.300
ds          4   alfa        10.000
dl          1.000          FLAGS
nt          32 il          n
ct          32 in          n
TRANSMITTER    dp          y
lu          E1 ha          nn
sfrq          399.853      PROCESSING
tsc          343.1   fa      not used
tscr          58          DISPLAY
pv          0.150   sp      -28.5
DECOUPLER      wp          4806.7
ca          C13 rfl        797.8
dcf          0   rfp        0
da          mm   sp        130.9
dcrwave        g   lp      -109.1
cpr          40          PLOT
ntc          17100          262
          0
          0
          0
          45
          al cdc ph
  
```

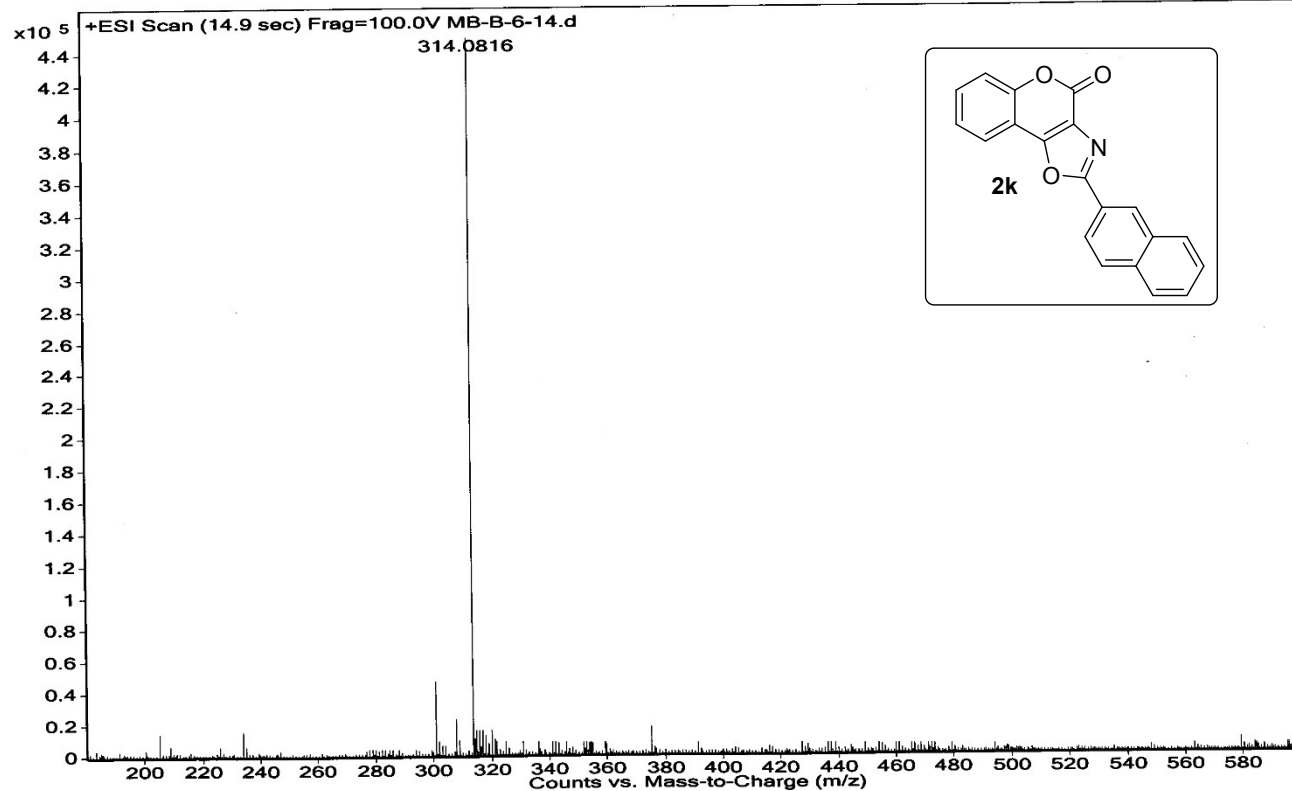


<sup>13</sup>C NMR spectra of 2k



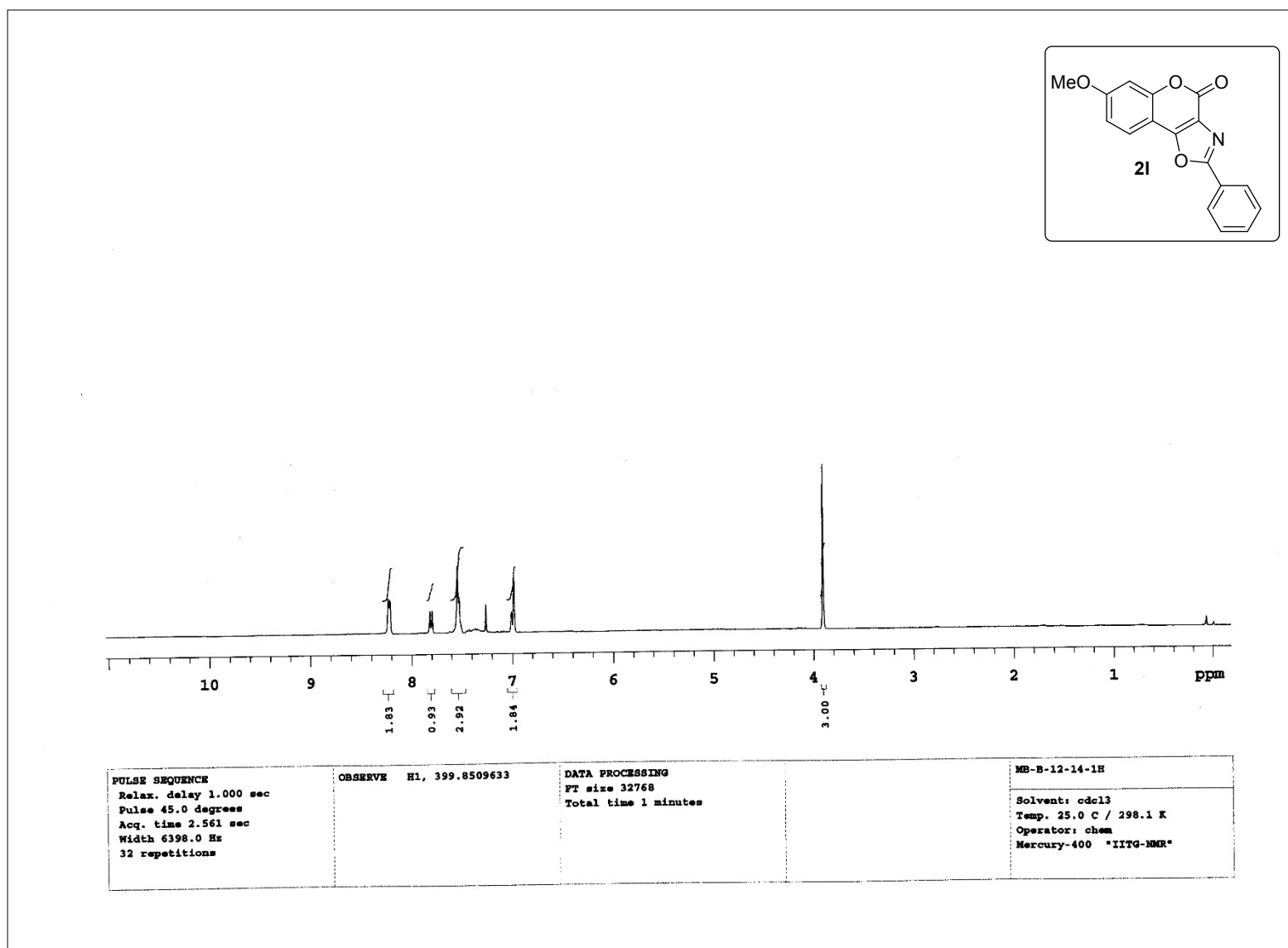
# HRMS spectra of 2k

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

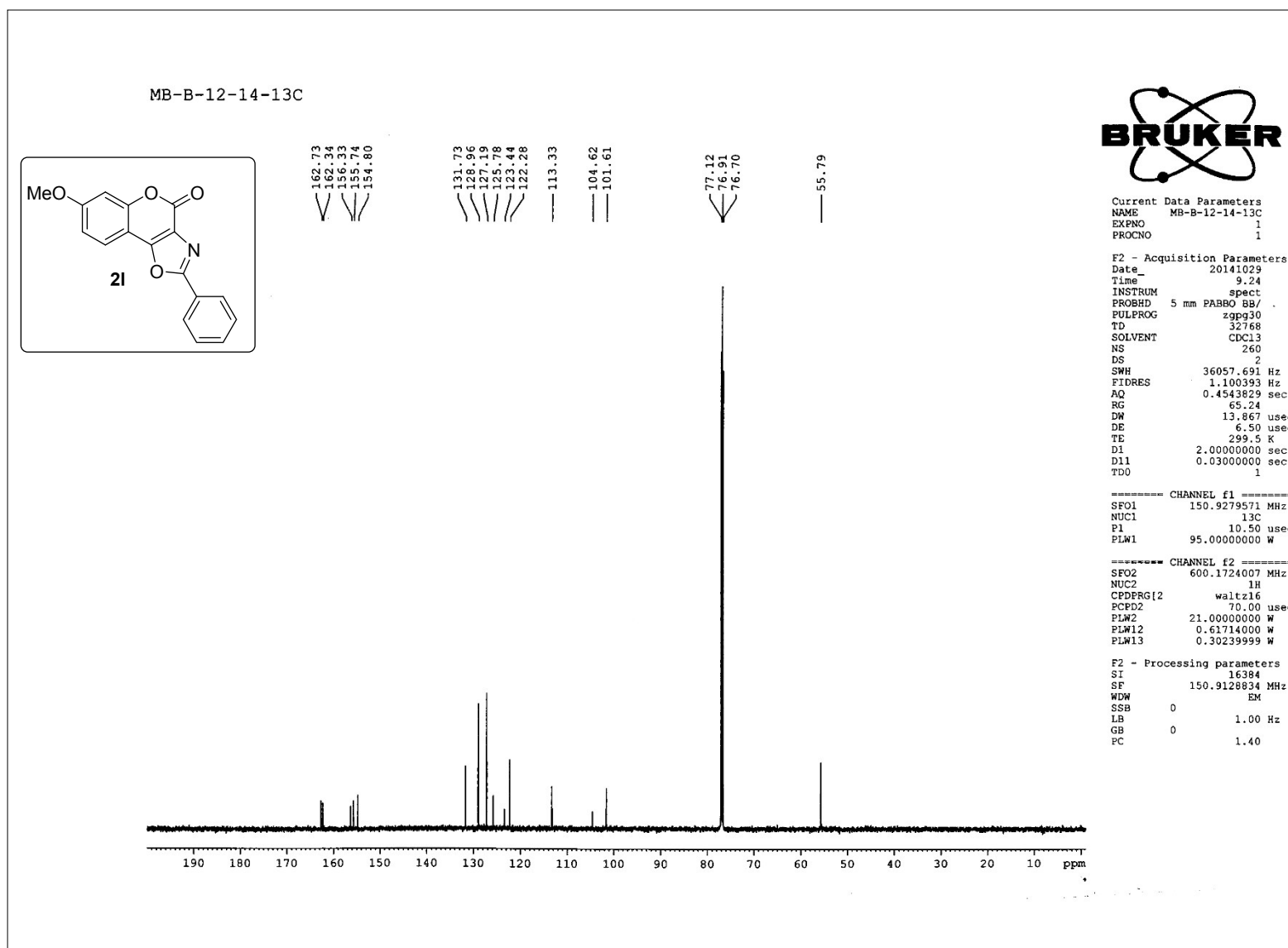




# H<sup>1</sup> NMR spectra of 21

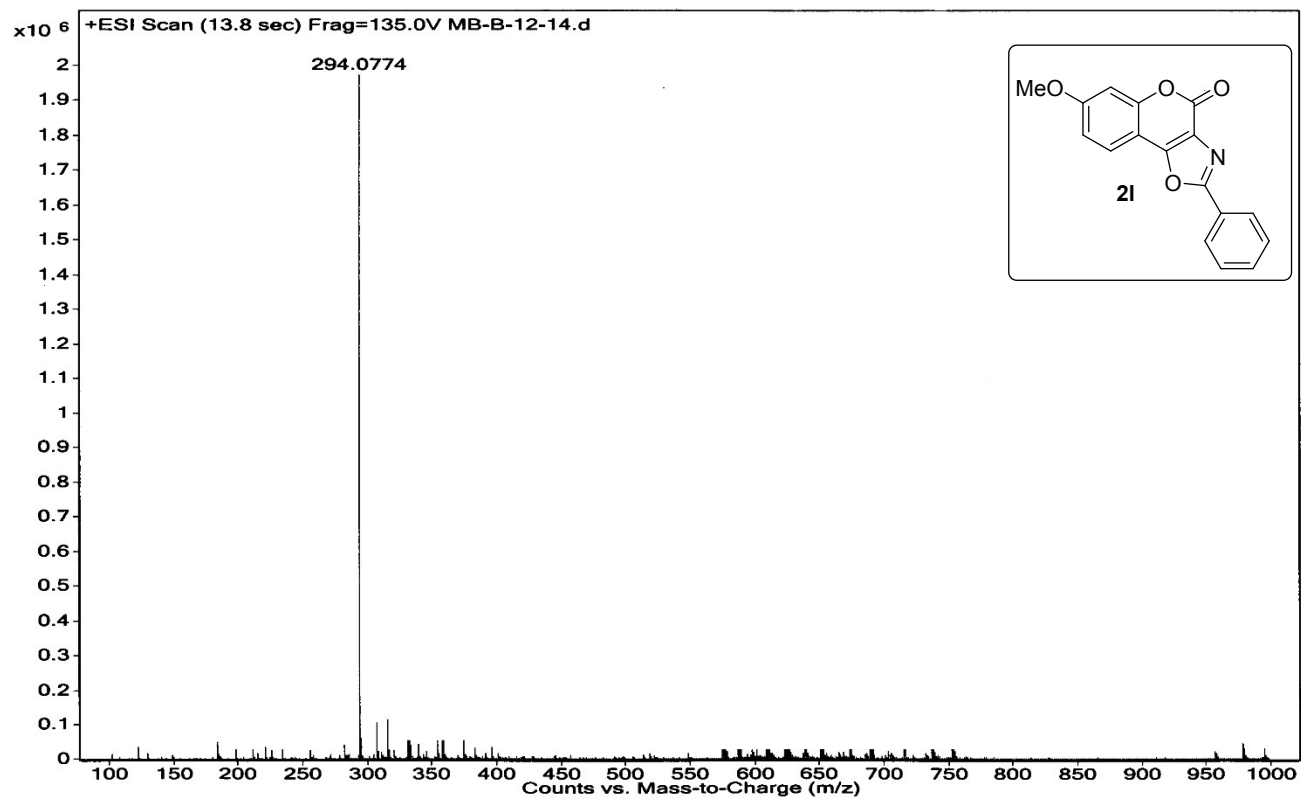


<sup>13</sup>C NMR spectra of **21**



# HRMS spectra of 2l

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



# $^1\text{H}$ NMR spectra of 2m

MB-B-13-14-1H

Sample Name:  
MB-B-13-14-1H  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:

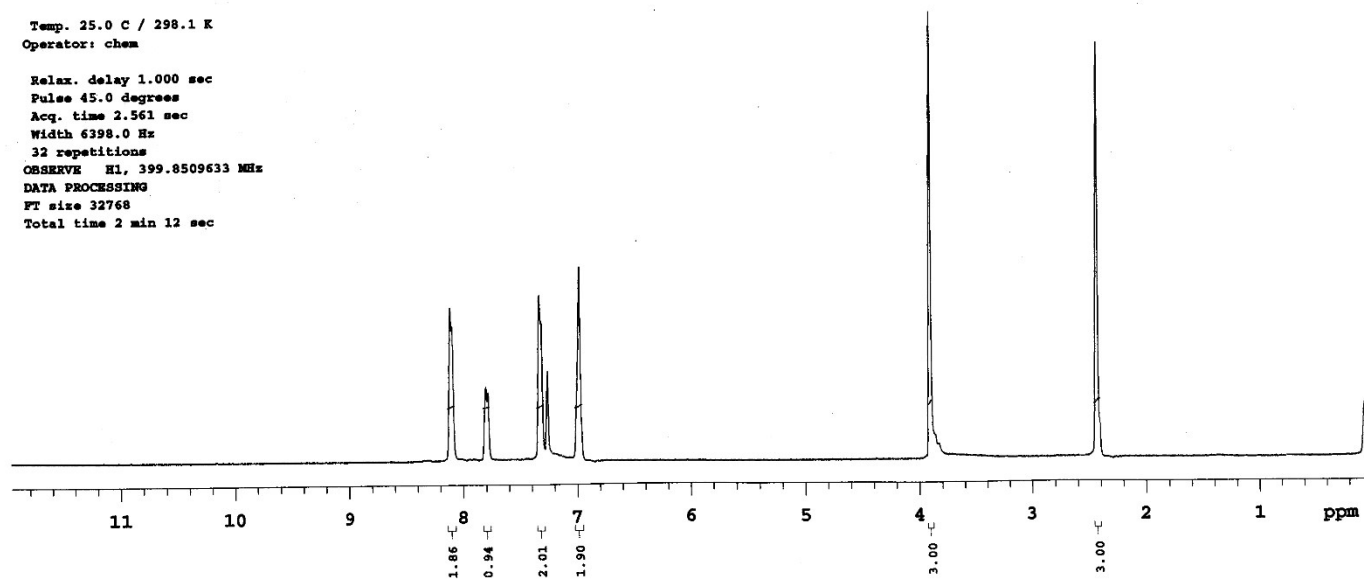
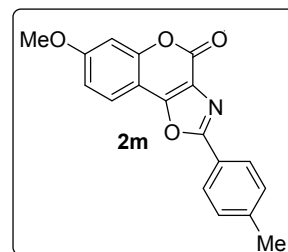
Sample directory:

FidFile: PROTON

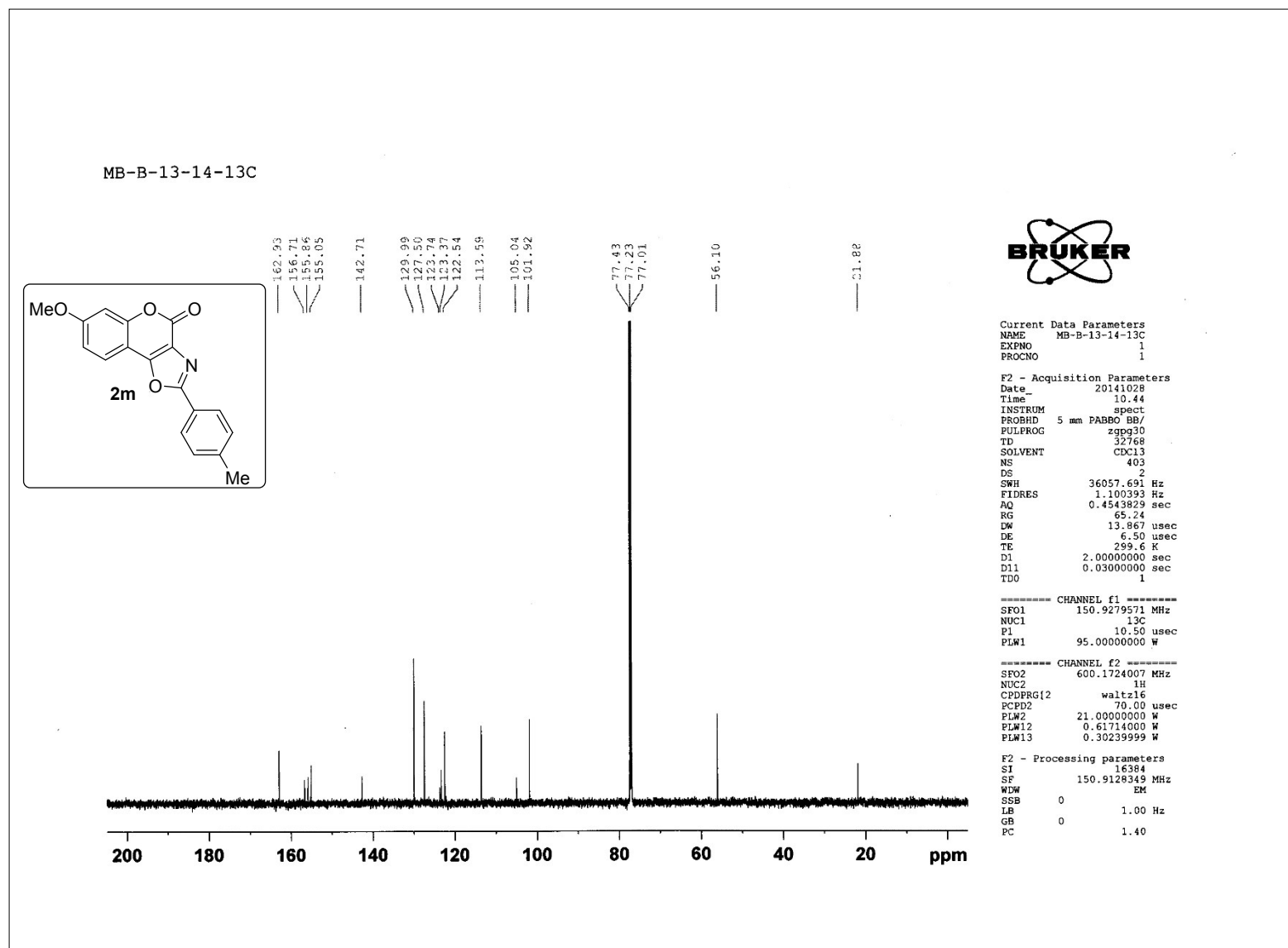
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Oct 27 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

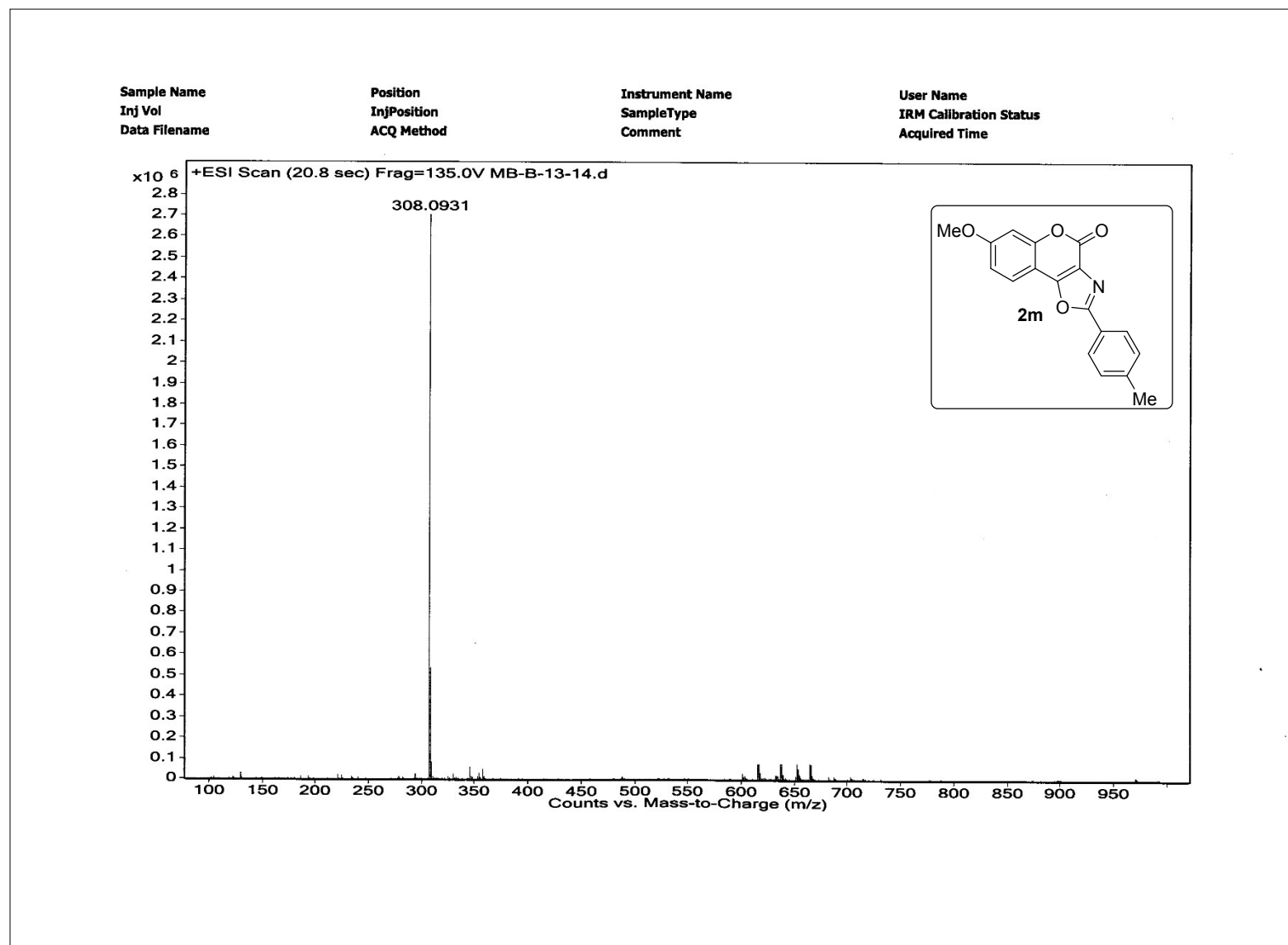
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509633 MHz  
DATA PROCESSING  
F1 size 32768  
Total time 2 min 12 sec



<sup>13</sup>C NMR spectra of **2m**



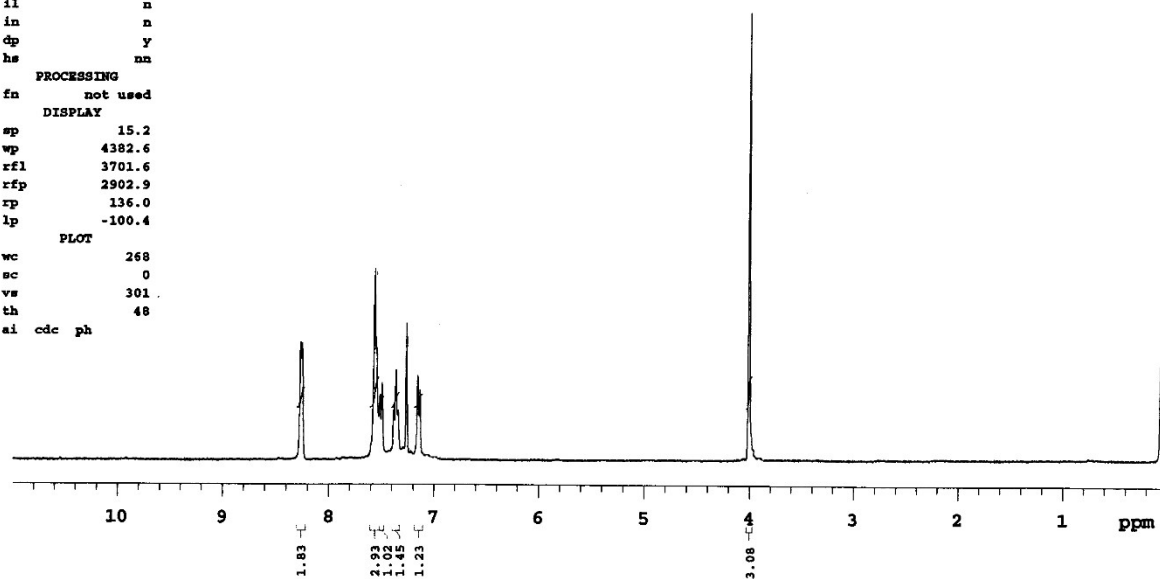
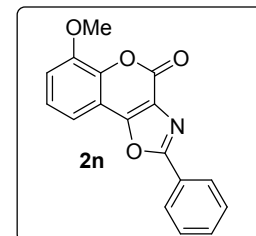
# HRMS spectra of 2m



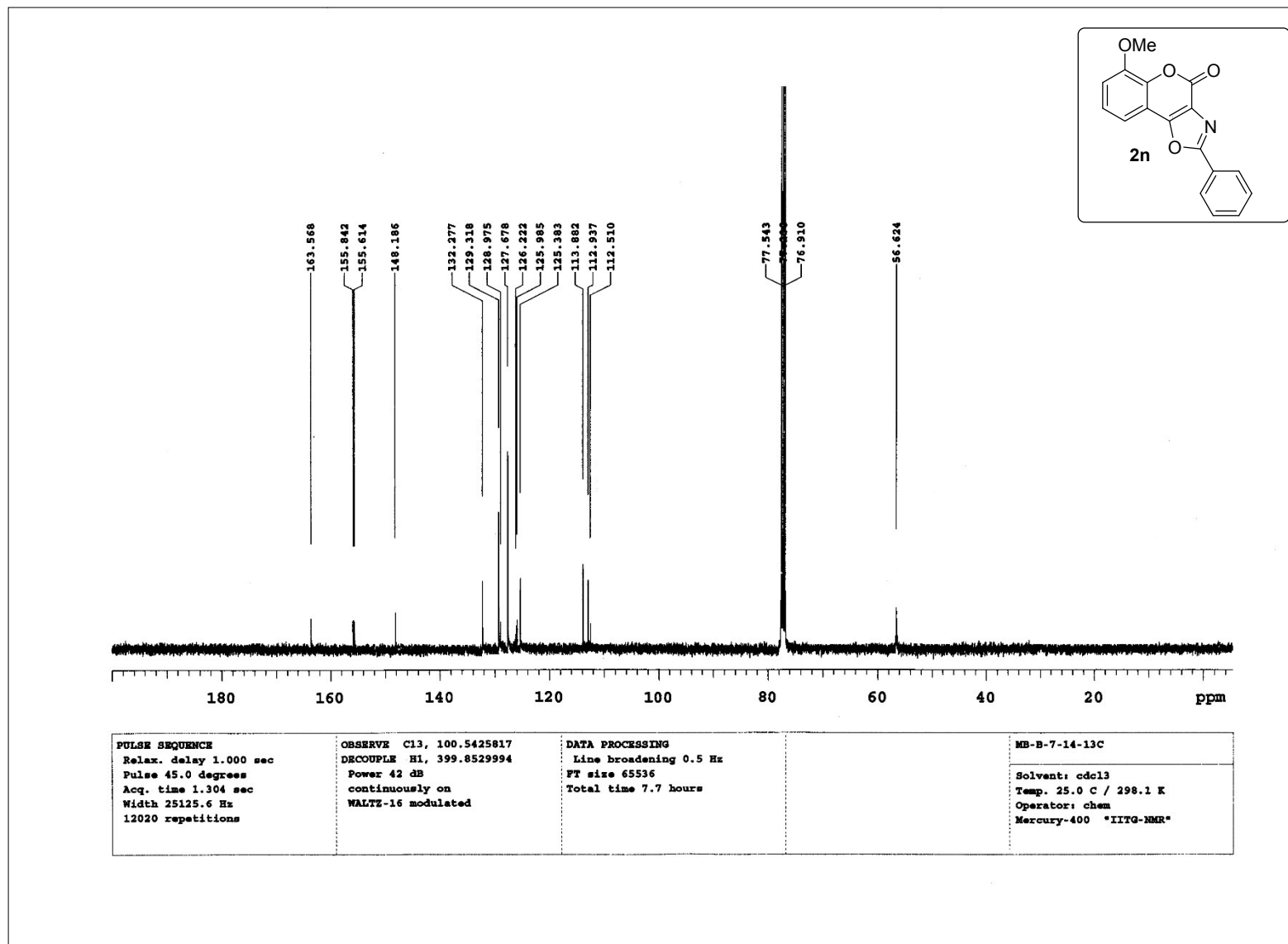
# H<sup>1</sup> NMR spectra of 2n

```

MB-B-7-14-1H
expl PROTON
SAMPLE          PRESATURATION
date Oct 4 2014 satmode n
solvent cdcl3   wet      n
file           exp      SPECIAL
ACQUISITION    temp     25.0
sw            6398.0 gain   30
at            2.561 spin   not used
np            32768 hst    0.008
fb            3600 pw90   16.300
bs            4   alfa    10.000
d1            1.000      FLAGS
nt            32 il      n
ct            32 in      n
TRANSMITTER    dp      y
tn            H1 hs     nn
sfrq          399.853 PROCESSING
tof           363.1 fn   not used
tpwr          58      DISPLAY
pw            8.150 sp   15.2
DECOUPLER     wp     4382.6
dm            C13 rf1   3701.6
dof           0   rfp   2902.9
dm            mn rp    136.0
decwave       g lp    -100.4
dpwr          40      PLOT
dmf           17100 wc   268
                   sc   0
                   vs  301
                   th   48
                   ai cdc ph
    
```



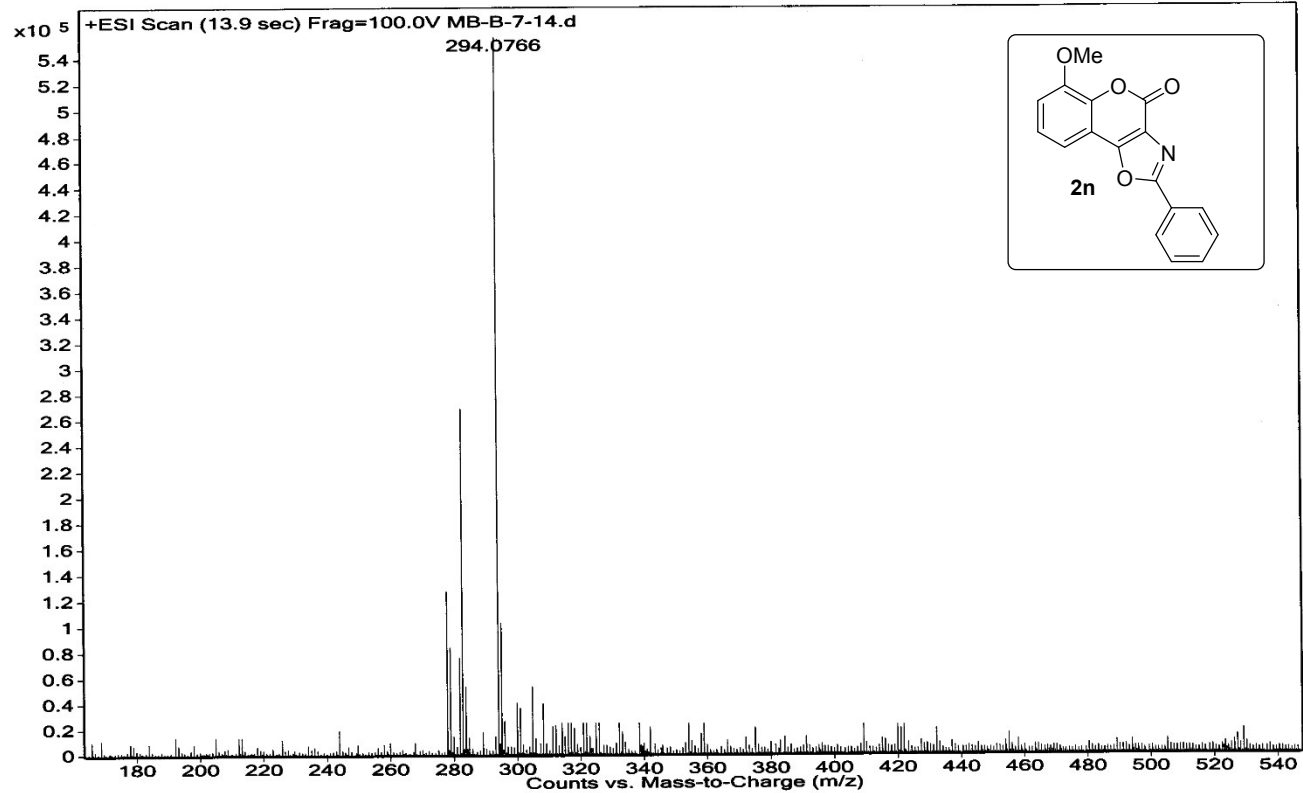
<sup>13</sup>C NMR spectra of **2n**



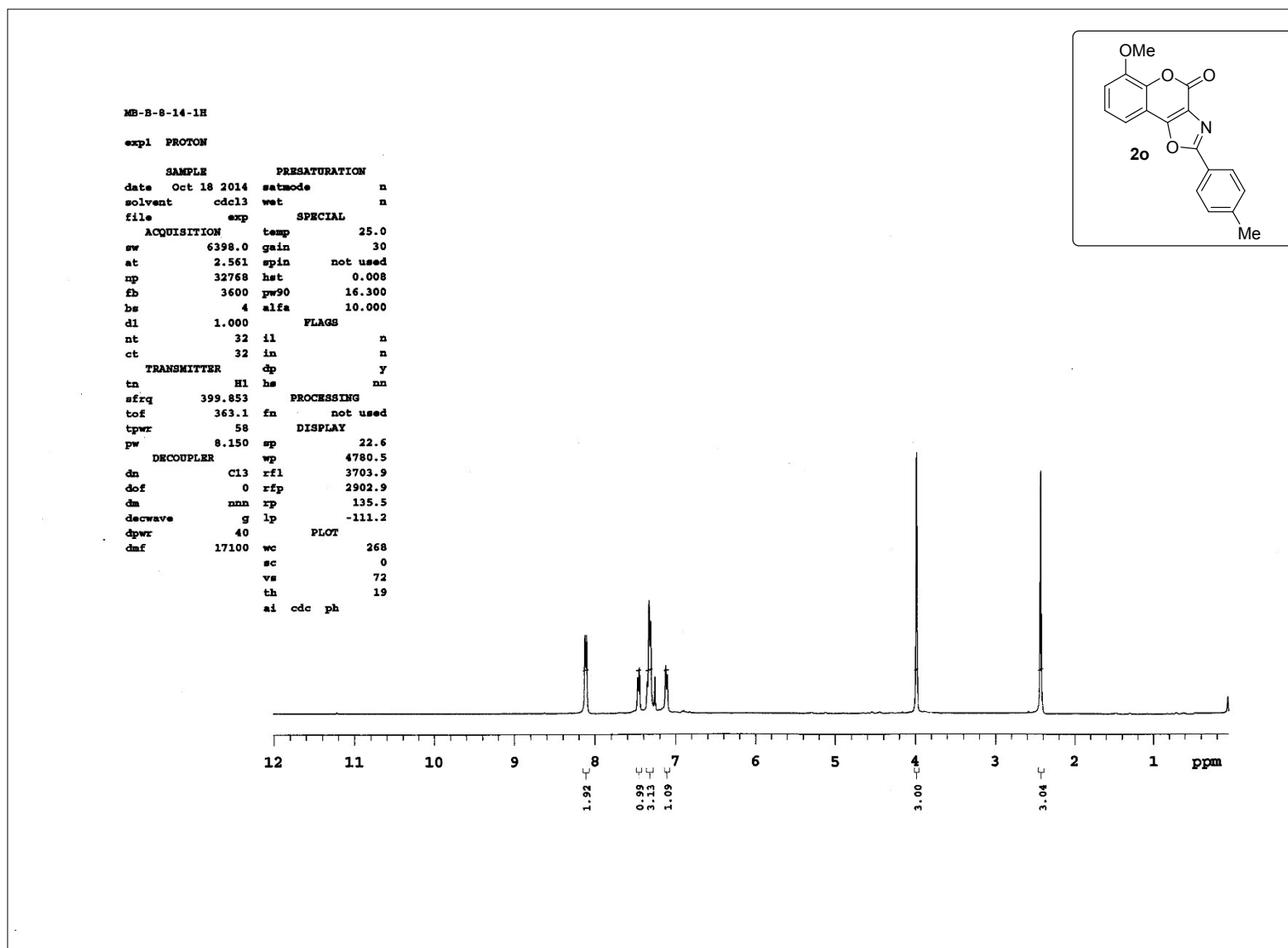


# HRMS spectra of 2n

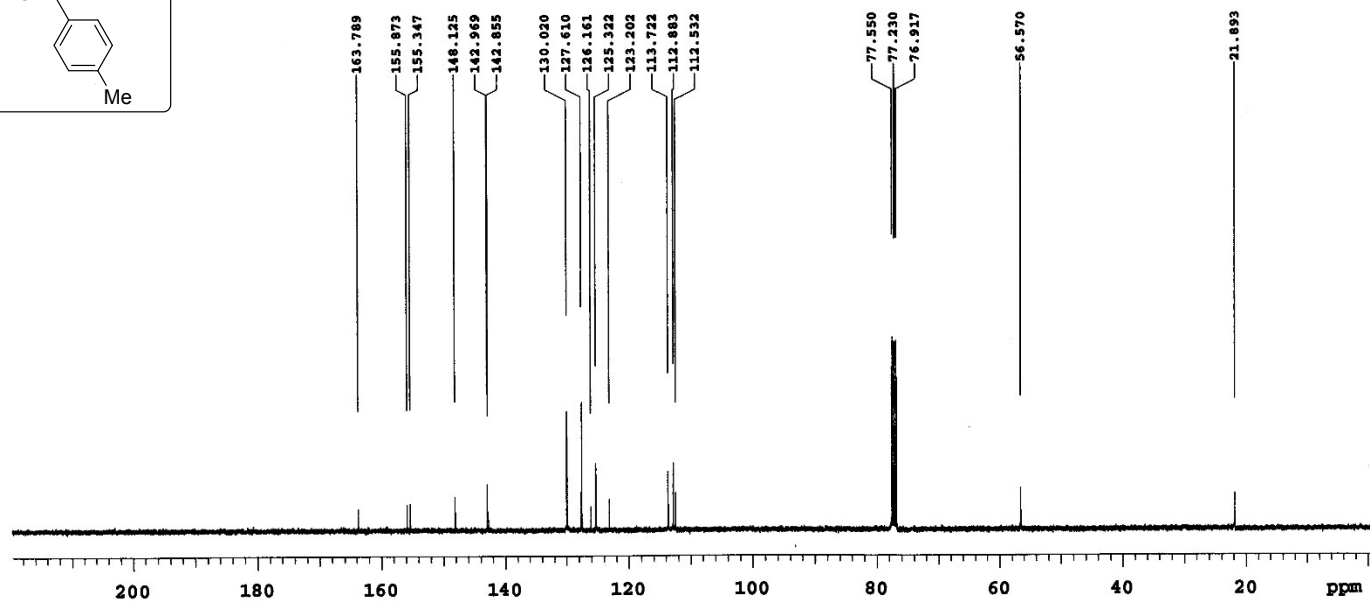
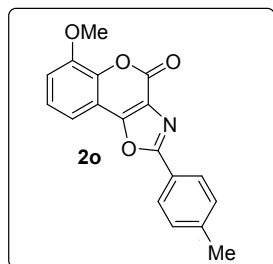
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra of 2o

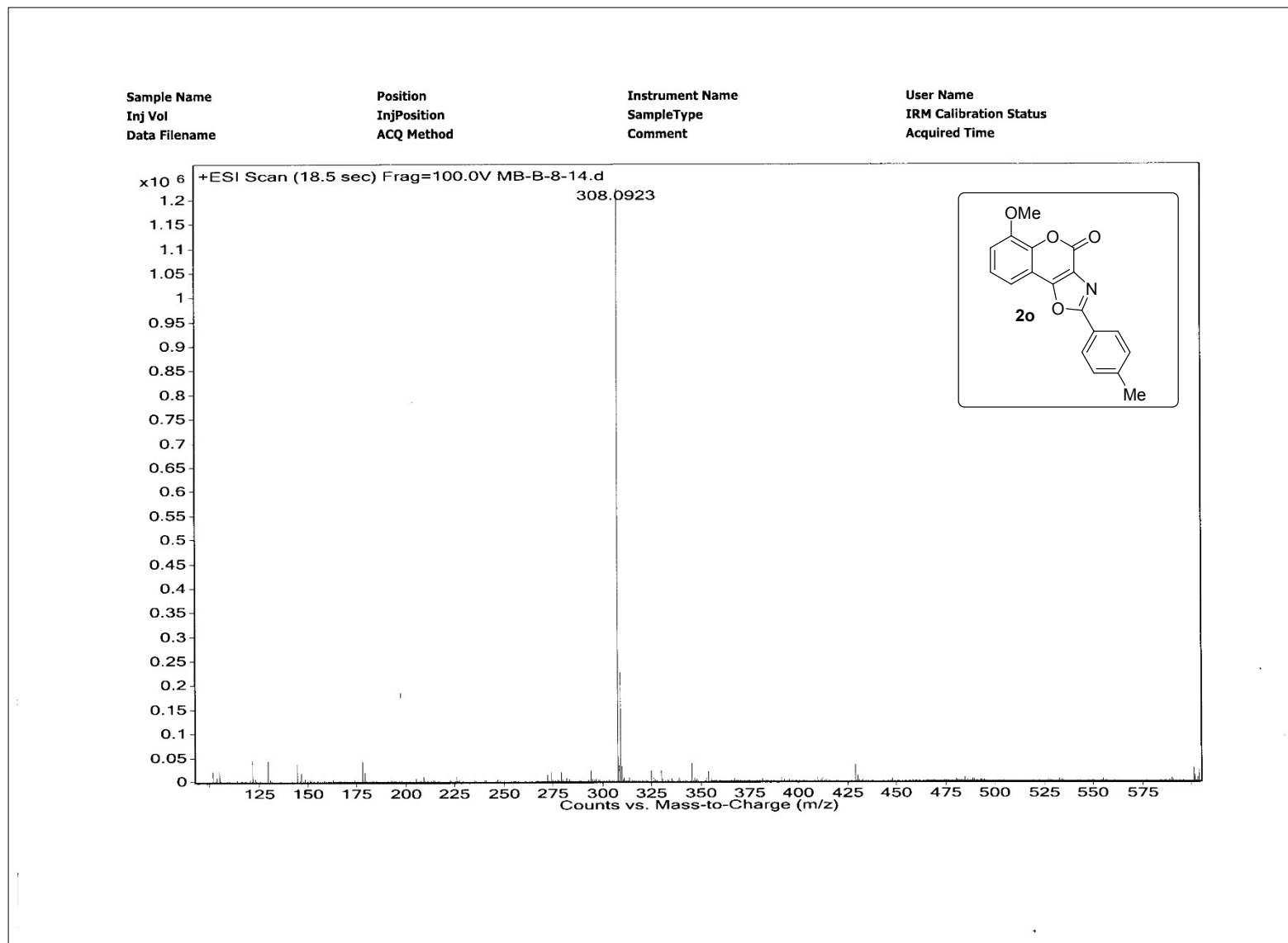


<sup>13</sup>C NMR spectra of 2o

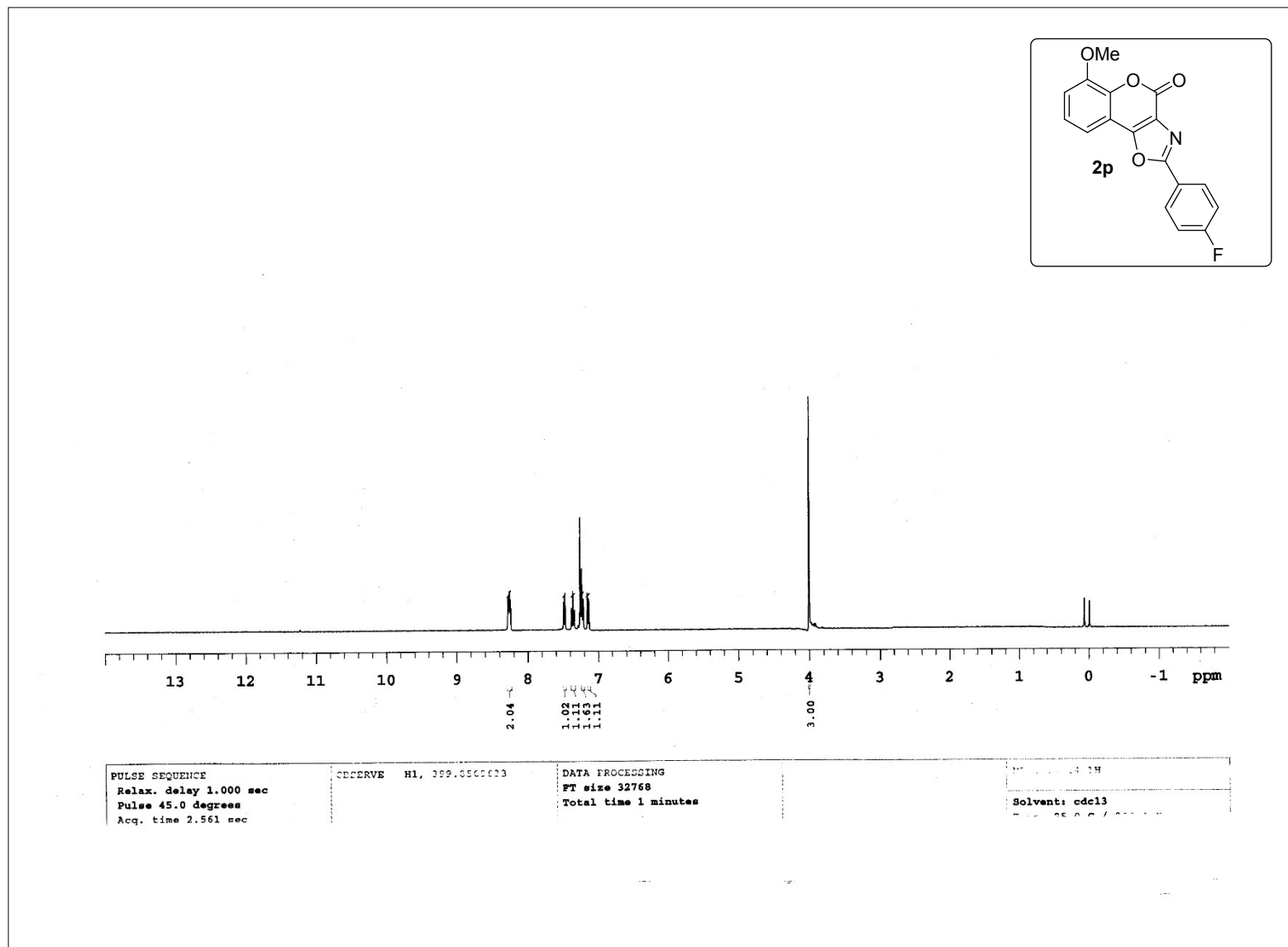


<p><b>PULSE SEQUENCE</b>                  Relax. delay 1.000 sec                  Pulse 45.0 degrees                  Acq. time 1.304 sec                  Width 25125.6 Hz                  2400 repetitions</p>	<p><b>OBSERVE</b> C13, 100.5425824  <b>DECOUPLE</b> H1, 399.8529994                  Power 42 dB                  continuously on  <b>WALTZ-16</b> modulated</p>	<p><b>DATA PROCESSING</b>                  Line broadening 0.5 Hz                  FT size 65536                  Total time 92 minutes</p>	<p>MB-B-8-14-13C                  Solvent: cdcl3                  Temp. 25.0 C / 298.1 K                  Operator: chem                  Mercury-400 "IITG-NMR"</p>
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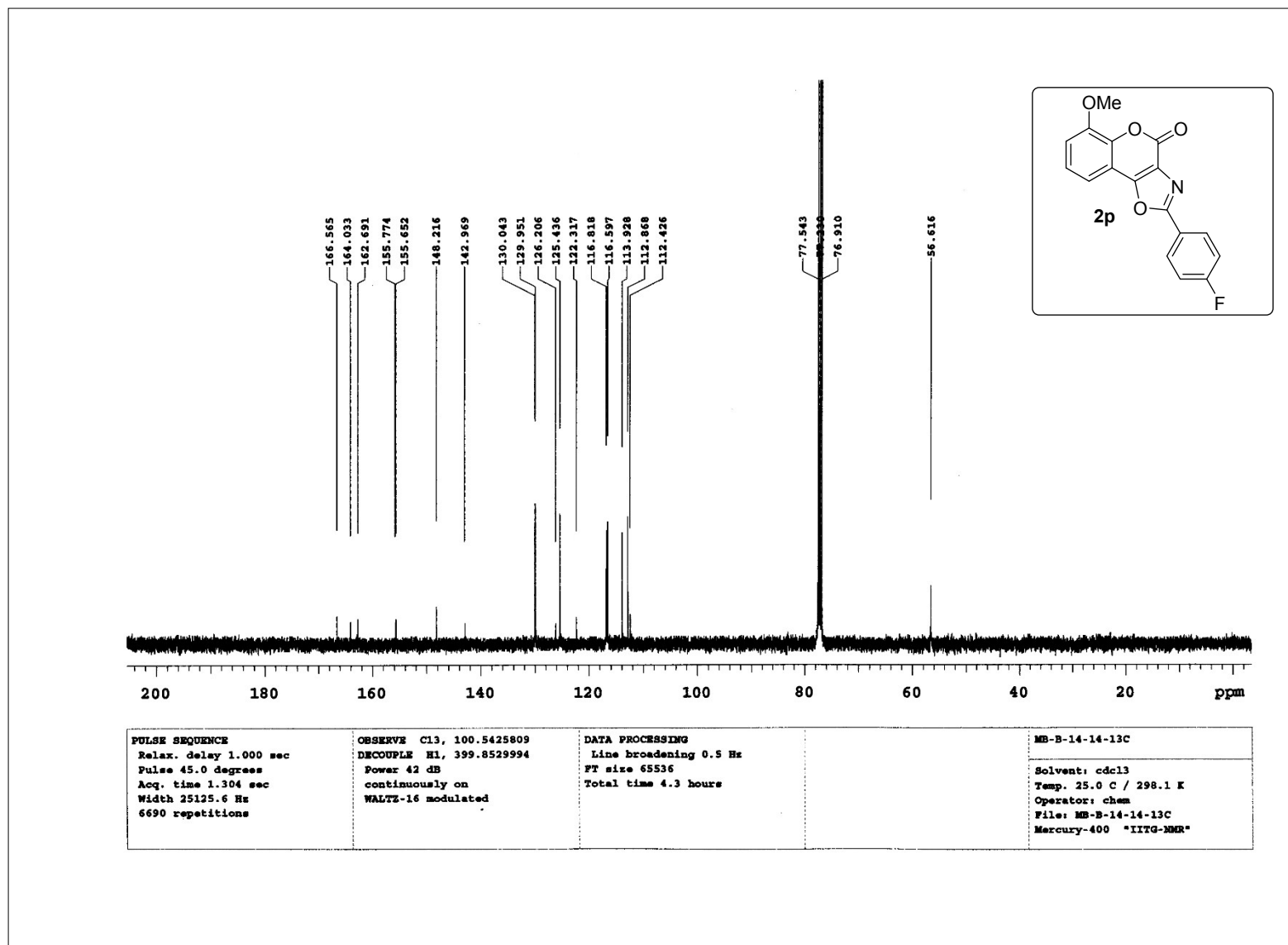
# HRMS spectra of 2o



H<sup>1</sup> NMR spectra of **2p**

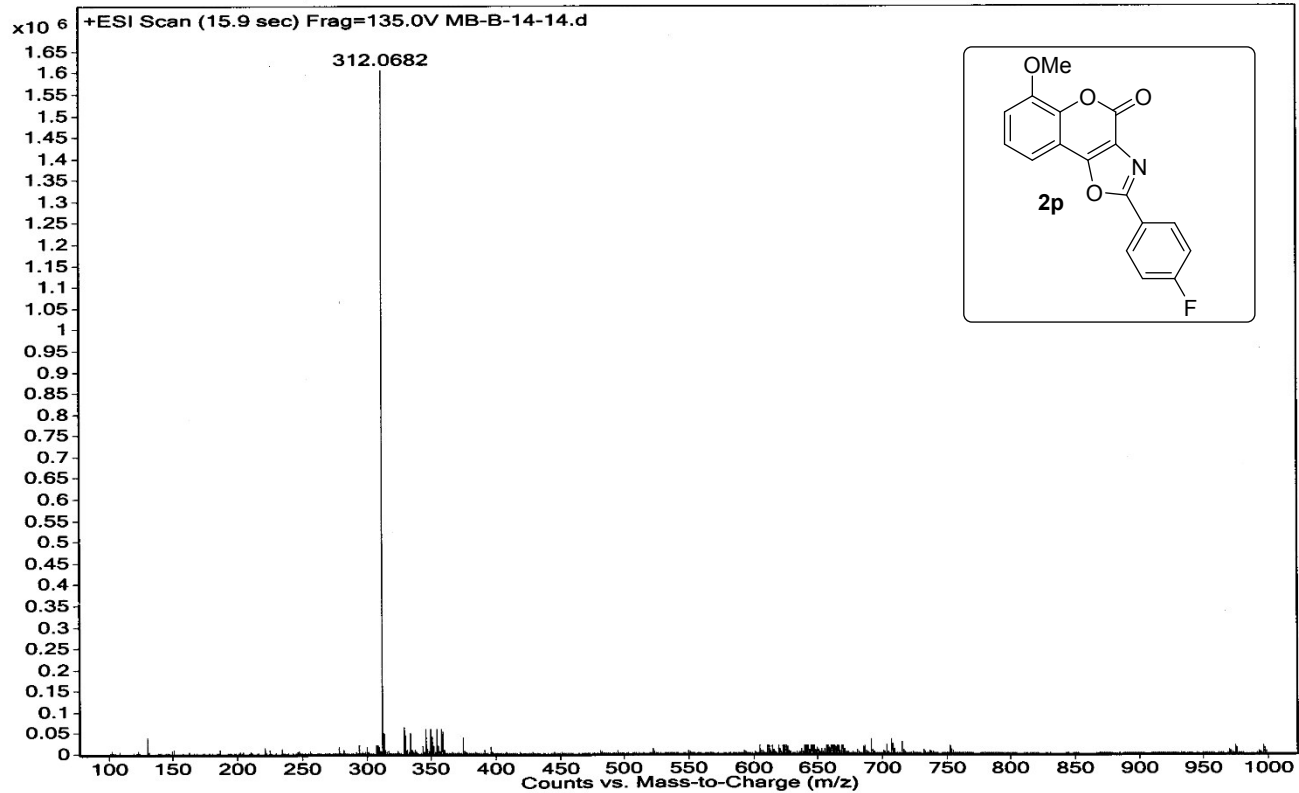


<sup>13</sup>C NMR spectra of **2p**

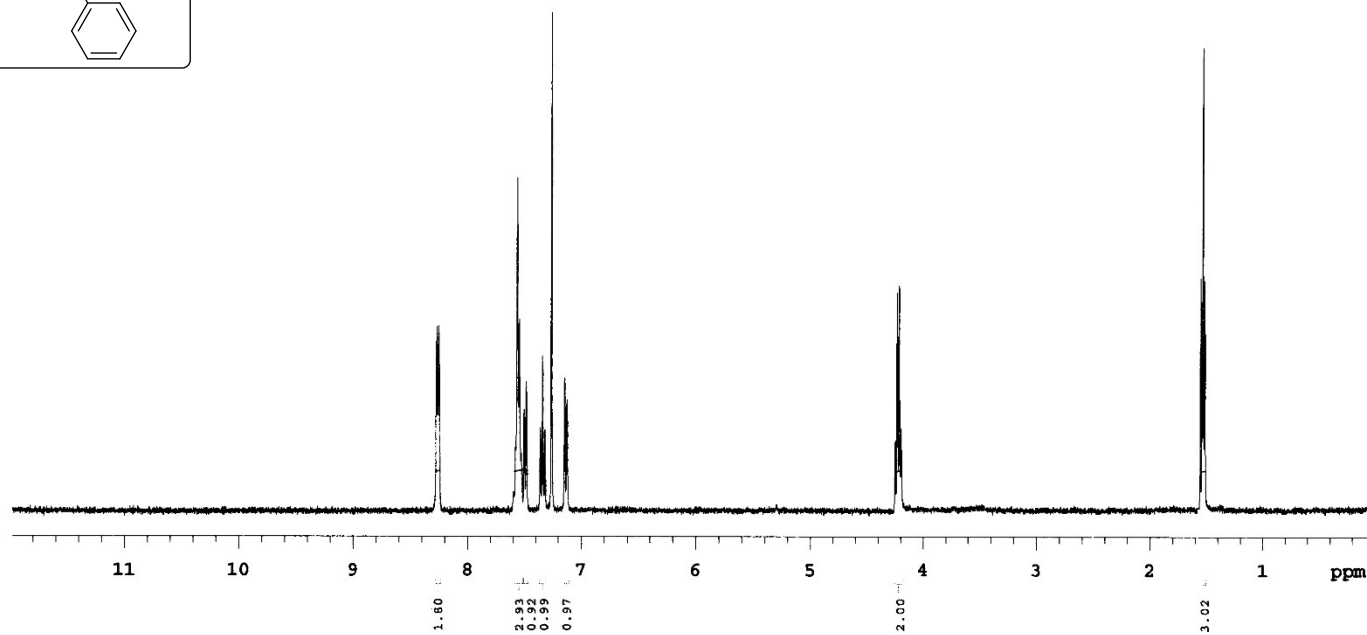
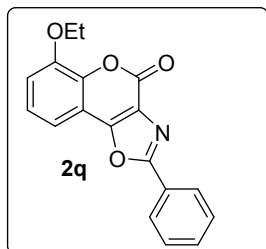


# HRMS spectra of 2p

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



H<sup>1</sup> NMR spectra of **2q**



PULSE SEQUENCE  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.561 sec  
 Width 6398.0 Hz  
 32 repetitions

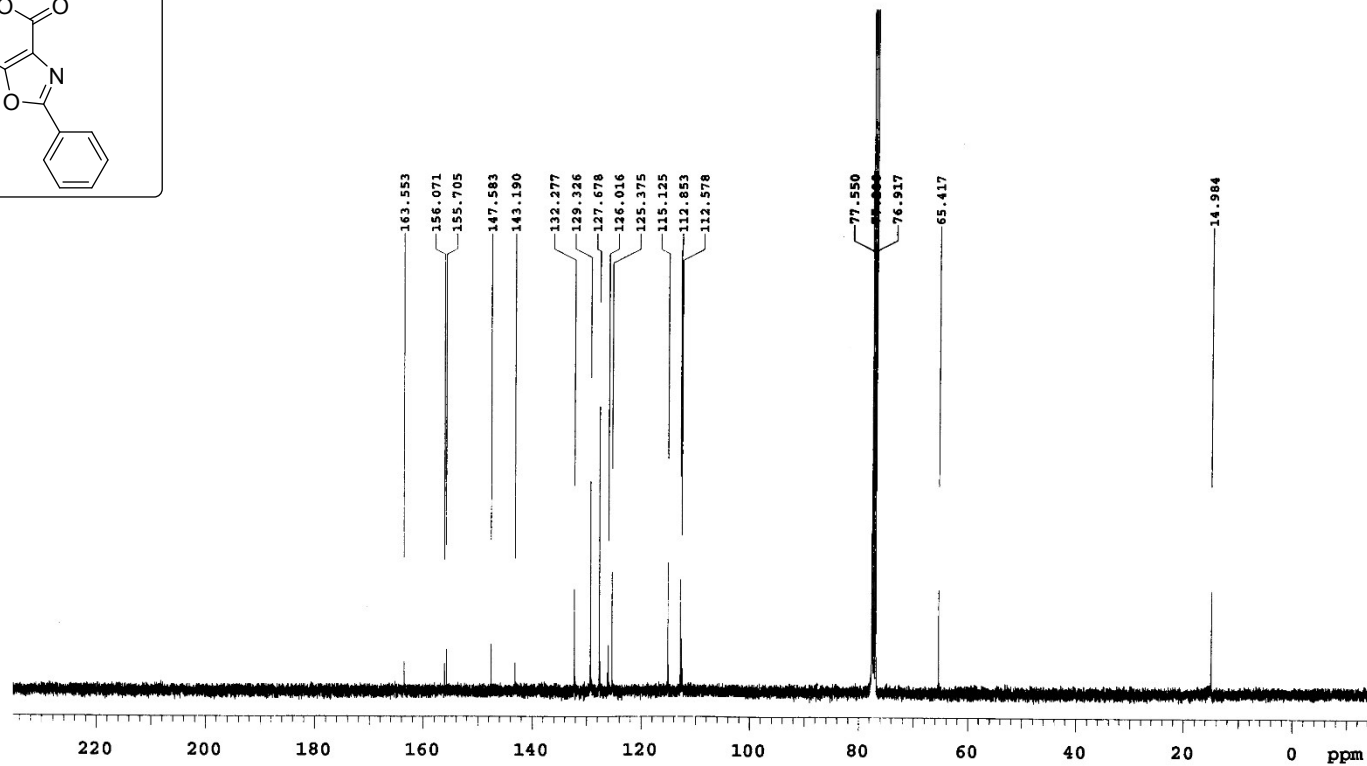
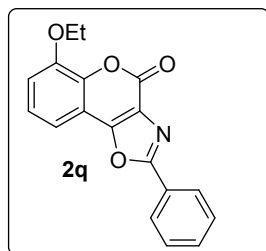
OBSERVE H1, 399.8509633

DATA PROCESSING  
 FT size 32768  
 Total time 1 minutes

MB\_B\_3\_14\_1H  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 File: MB\_B\_3\_14\_1H  
 Mercury-400 "IITG-MMR"



<sup>13</sup>C NMR spectra of **2q**



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
13310 repetitions

OBSERVE C13, 100.5425809  
DECOUPLE H1, 399.8529994  
Power 42 dB  
continuously on  
WALTZ-16 modulated

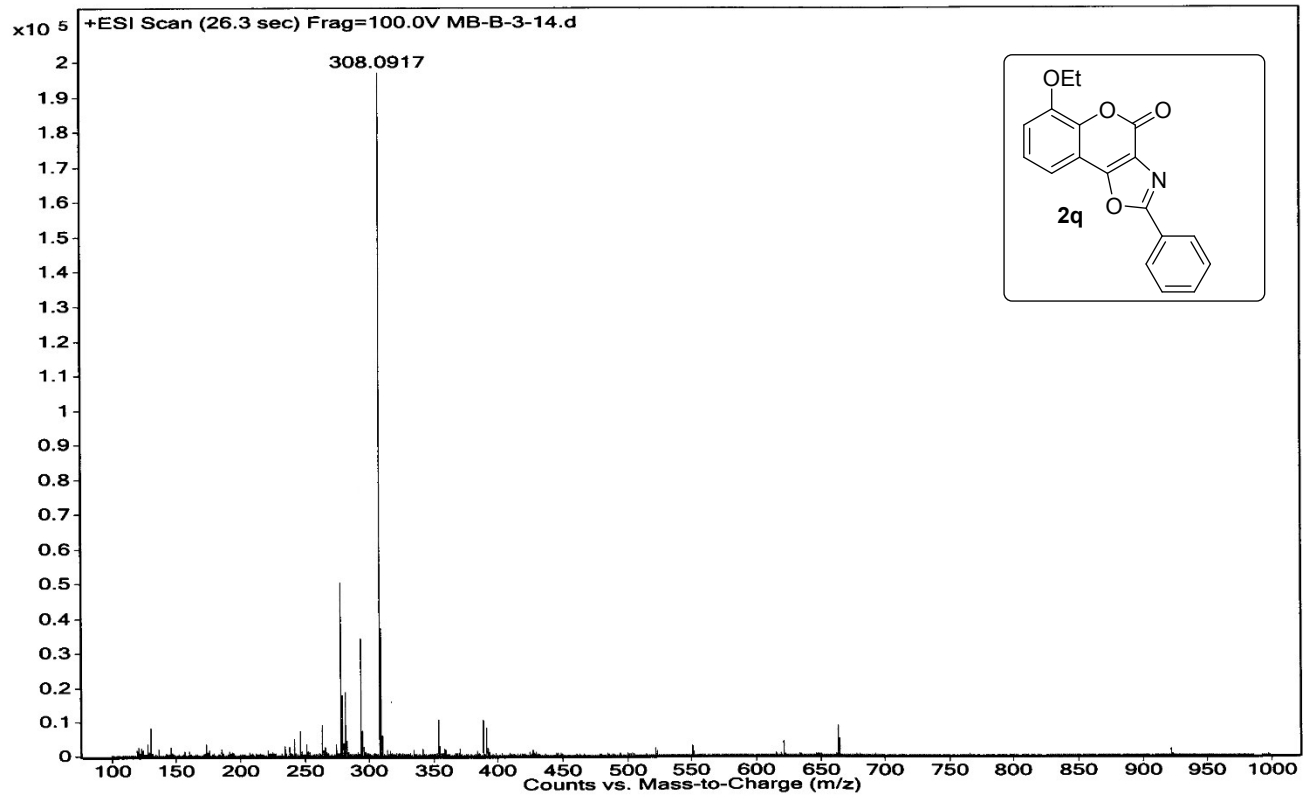
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 8.5 hours

MB-B-3-14-13C

Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: MB-B-3-14-13C  
Mercury-400 "IITG-NMR"

# HRMS spectra of 2q

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



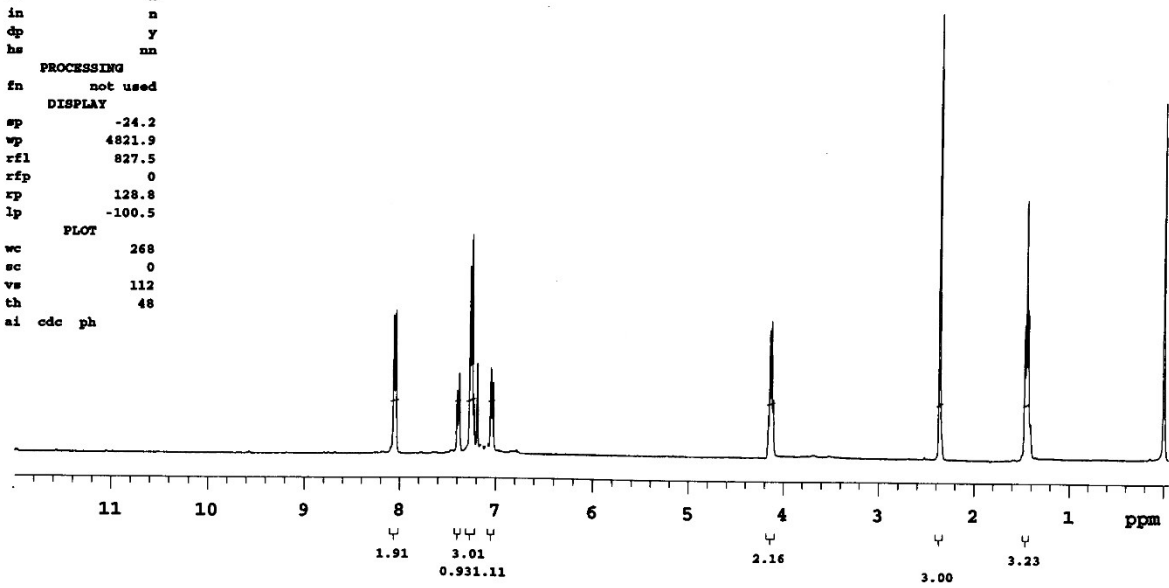
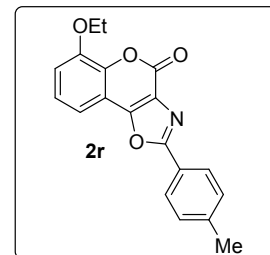
# H<sup>1</sup> NMR spectra of 2r

```

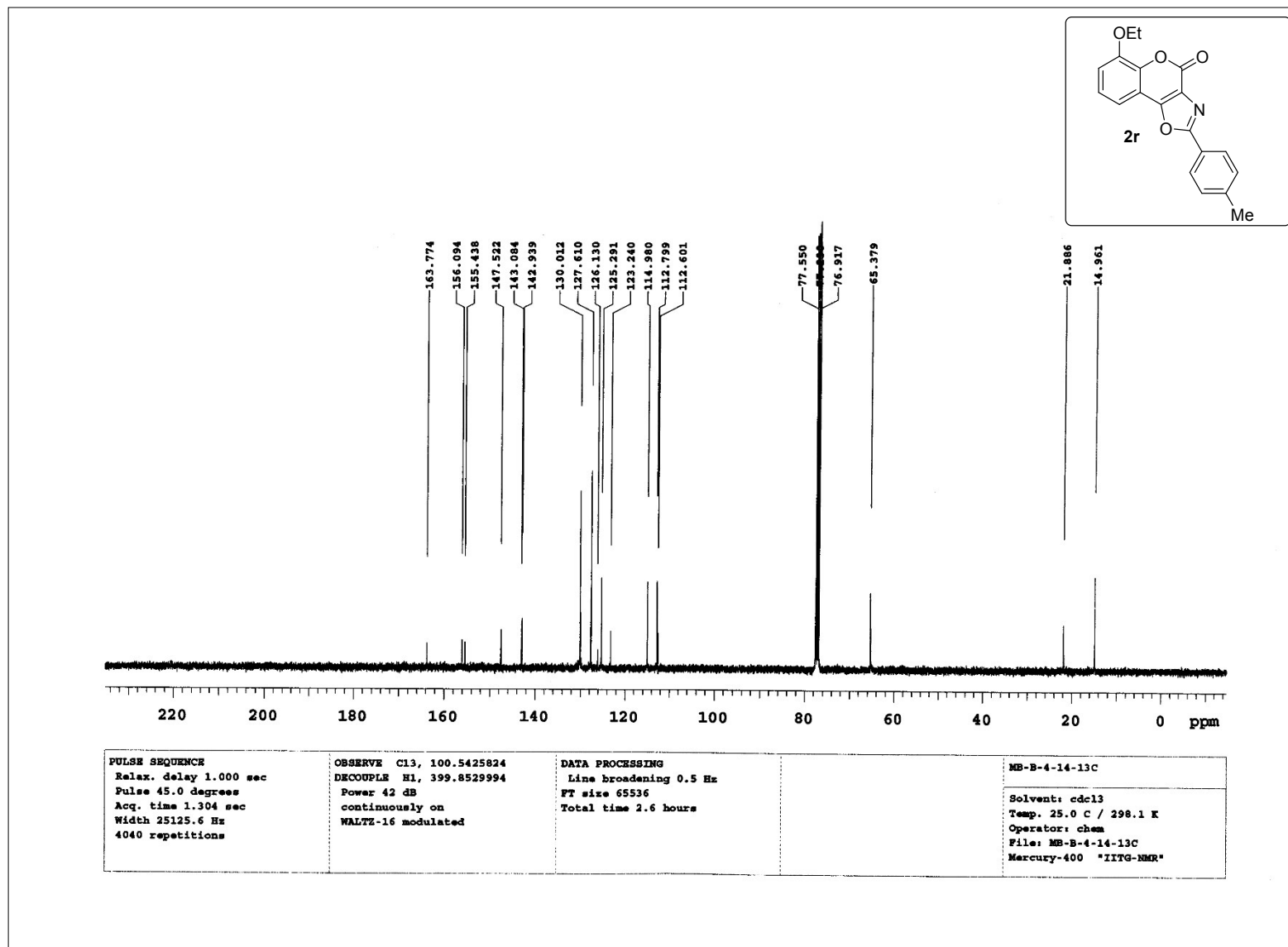
MB-B-4-14-1H
expl  PROTON

SAMPLE      PRESATURATION
date  Oct 11 2014  satmode      n
solvent  cdcl3      wet          n
file /home/chem/ds-
ta/ATK/Bela1/MB-B-
4-14-1H.fid  gain          30
ACQUISITION  spin      not used
sw         6398.0  hst         0.008
at         2.561  pw90        16.300
np         32768  alfa         10.000
fb         3600
bs         4      il          n
dl         1.000  in          n
nt         32     dp          y
ct         32     hs          nn

TRANSMITTER  PROCESSING
tn           H1     fn      not used
sfrq        399.853  DISPLAY
tof         363.1   sp       -24.2
tpwr        58     wp       4821.9
pw          8.150  rfl      827.5
DECOUPLER   rfp      0
dn          C13   xp      128.8
dof         0     lp     -100.5
dm          nnn
decwave     g     wc      268
dpwr        40    sc       0
dmf         17100 vs      112
                th      48
                ai cdc ph
  
```

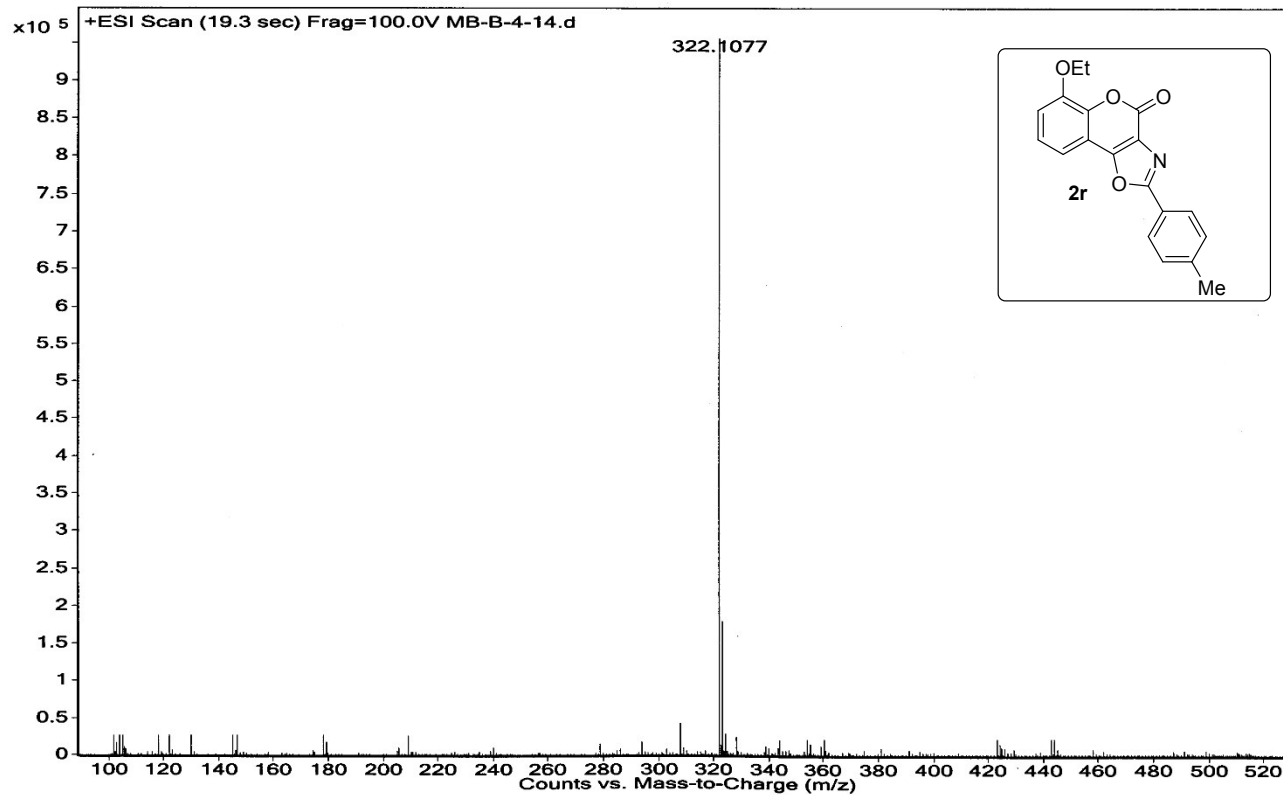


<sup>13</sup>C NMR spectra of **2r**



HRMS spectra of 2r

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 2s

MB-B-18-14-1H

Sample Name:  
MB-B-18-14-1H  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:

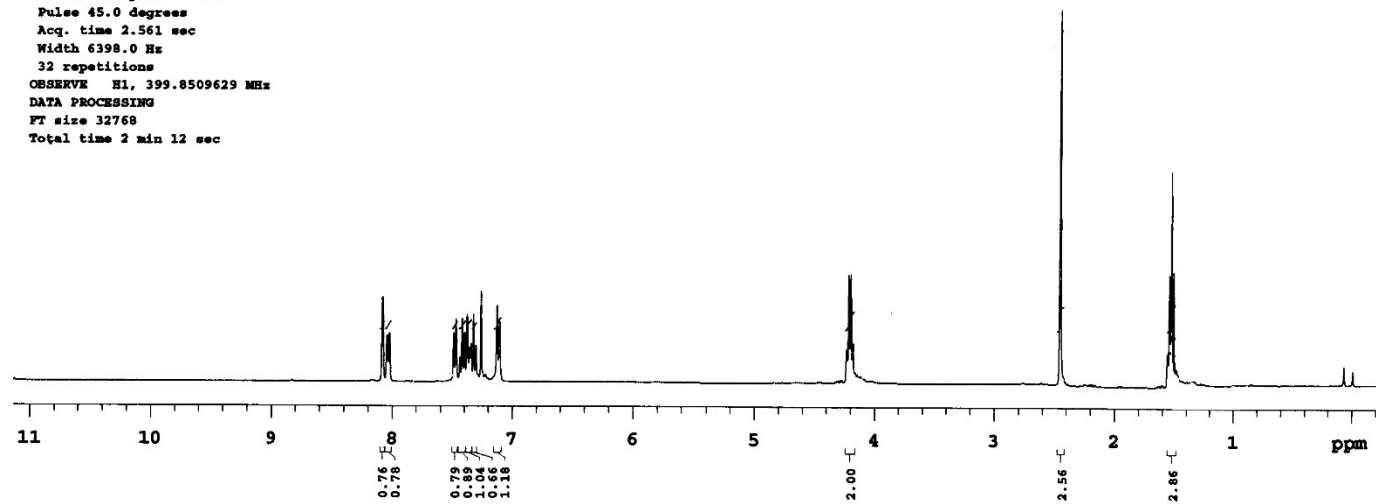
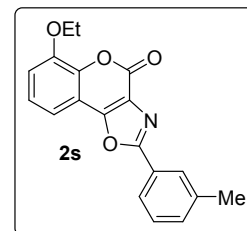
Sample directory:

FidFile: MB-B-18-14-1H

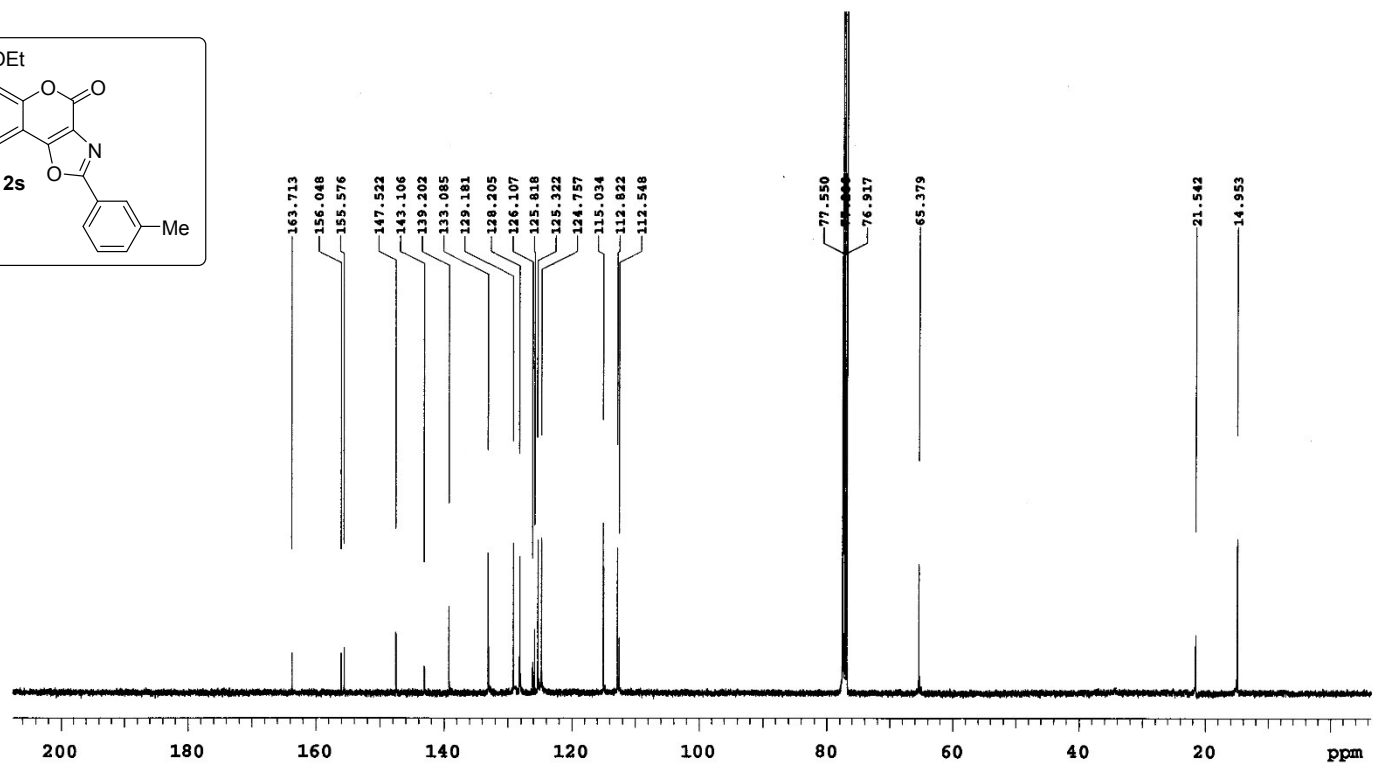
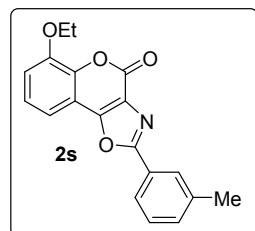
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 14 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509629 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



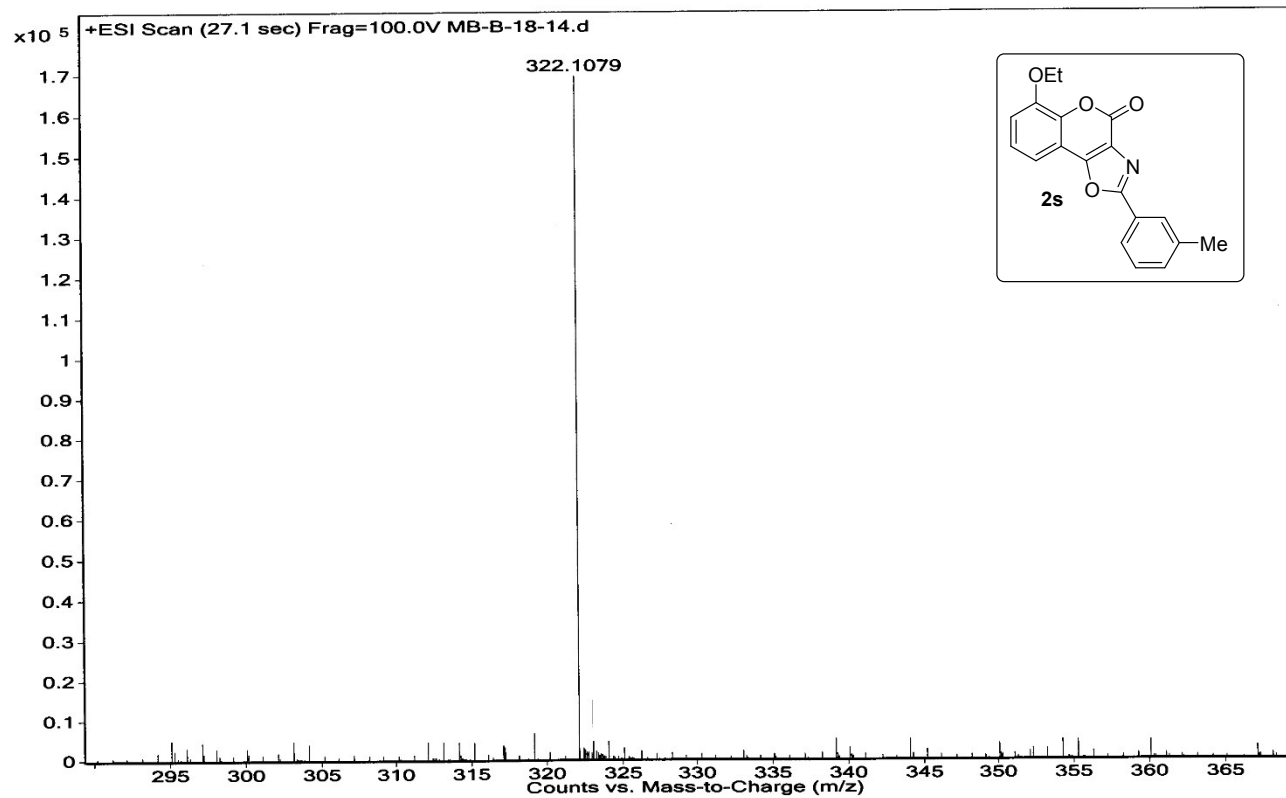
<sup>13</sup>C NMR spectra of 2s



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 16420 repetitions	<b>OBSERVE</b> C13, 100.5425832 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 10.5 hours	<b>MB-B-18-14-13C</b> Solvent: cdc13 Temp. 25.0 C / 298.1 K Operator: chem File: MB-B-18-14-13C Mercury-400 *IITG-NMR*
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# HRMS spectra of 2s

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



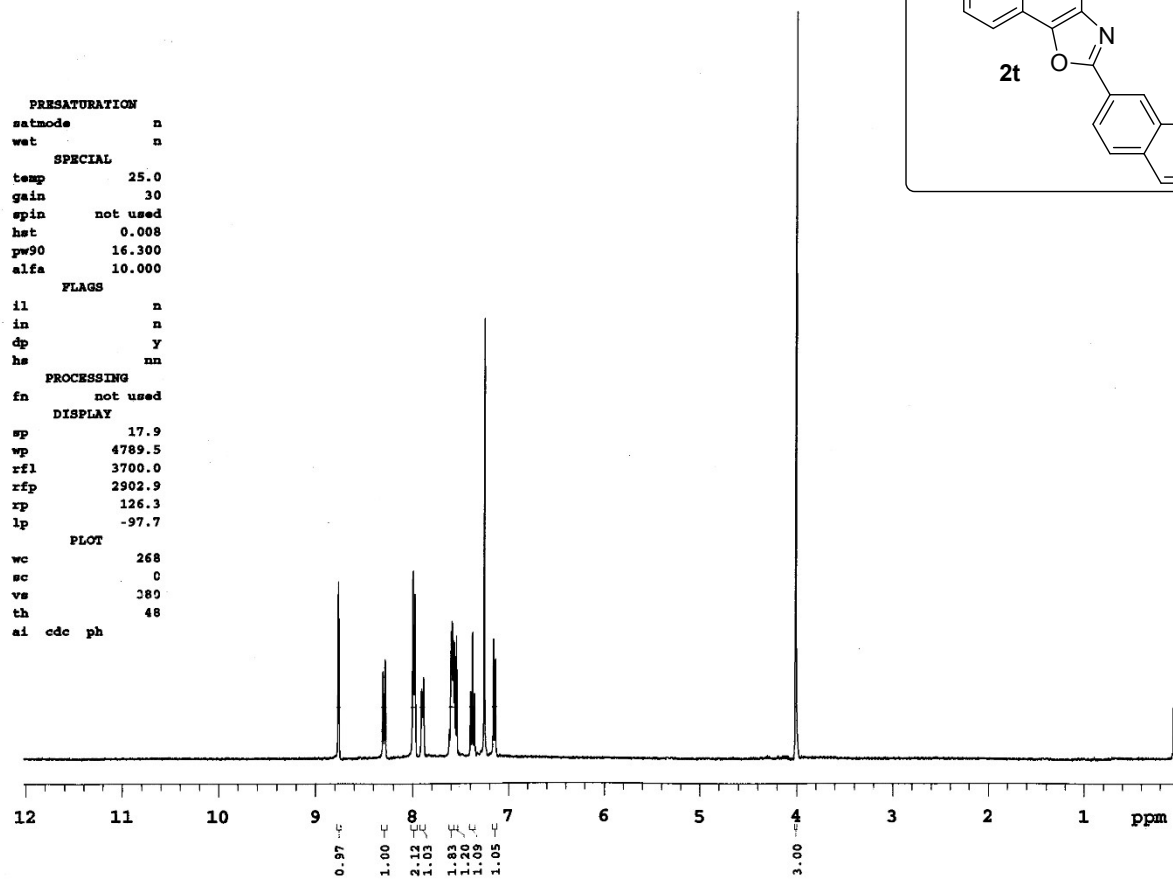
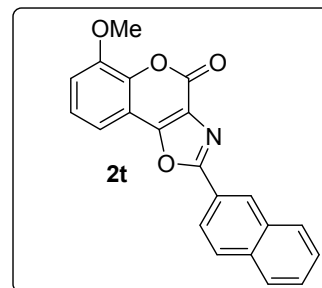


# H<sup>1</sup> NMR spectra of 2t

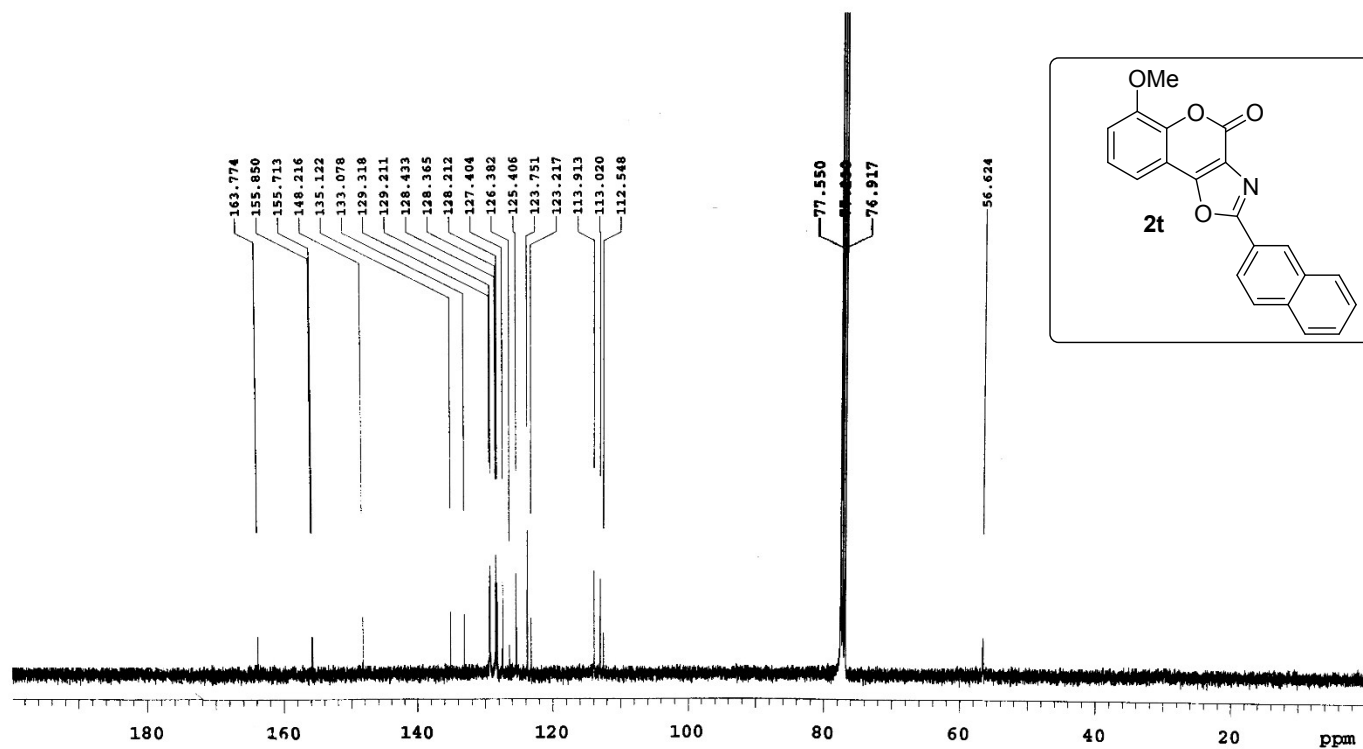
```

MB-B-9-14-1H
expl  PROTON

SAMPLE          PRESATURATION
date  Oct 23 2014  satmode      n
solvent  cdcl3  wet          n
file     exp     SPECIAL
ACQUISITION  temp      25.0
sw       6398.0  gain       30
at       2.561  spin       not used
np       32768  hst        0.008
fb       3600  pw90       16.300
bs       4     a1fa     10.000
d1       1.000  FLAGS
nt       32    il      n
ct       32    in      n
TRANSMITTER   dp        y
tn          H1    hs     mn
sfrq       399.853  PROCESSING
tof        363.1  fn      not used
tpwr       58    DISPLAY
pw         8.150  sp      17.9
DECOUPLER    wp      4789.5
dn         C13   rfl    3700.0
dof        0    rfp    2902.9
da         nnn   xp    126.3
decwave     g    lp    -97.7
dpwr       40    PLOT
daf        17100  wc      268
              sc      0
              vs     380
              th      48
              ai  cdc  ph
  
```



<sup>13</sup>C NMR spectra of **2t**



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
13430 repetitions

OBSERVE C13, 100.5425809  
DECOUPLE H1, 399.8529994  
Power 42 dB  
continuously on  
WALTZ-16 modulated

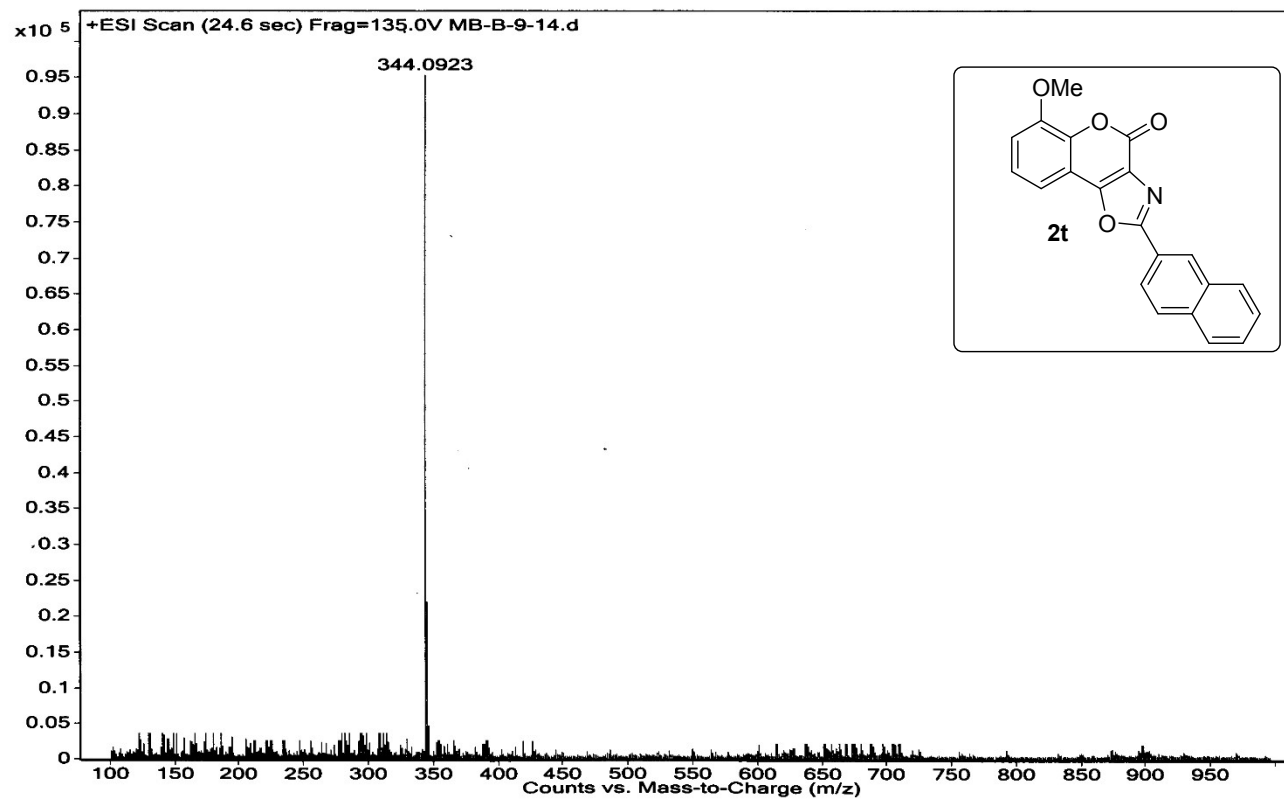
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 8.6 hours

MB-B-9-14-13C

Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: MB-B-9-14-13C  
Mercury-400 \*IITG-NMR\*

# HRMS spectra of 2t

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

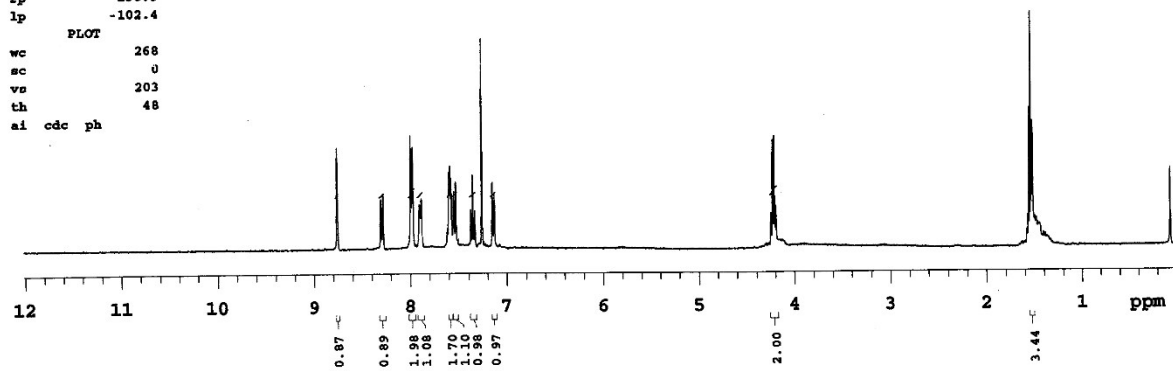
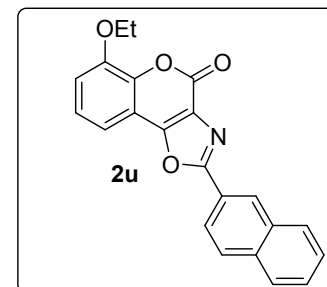


# H<sup>1</sup> NMR spectra of **2u**

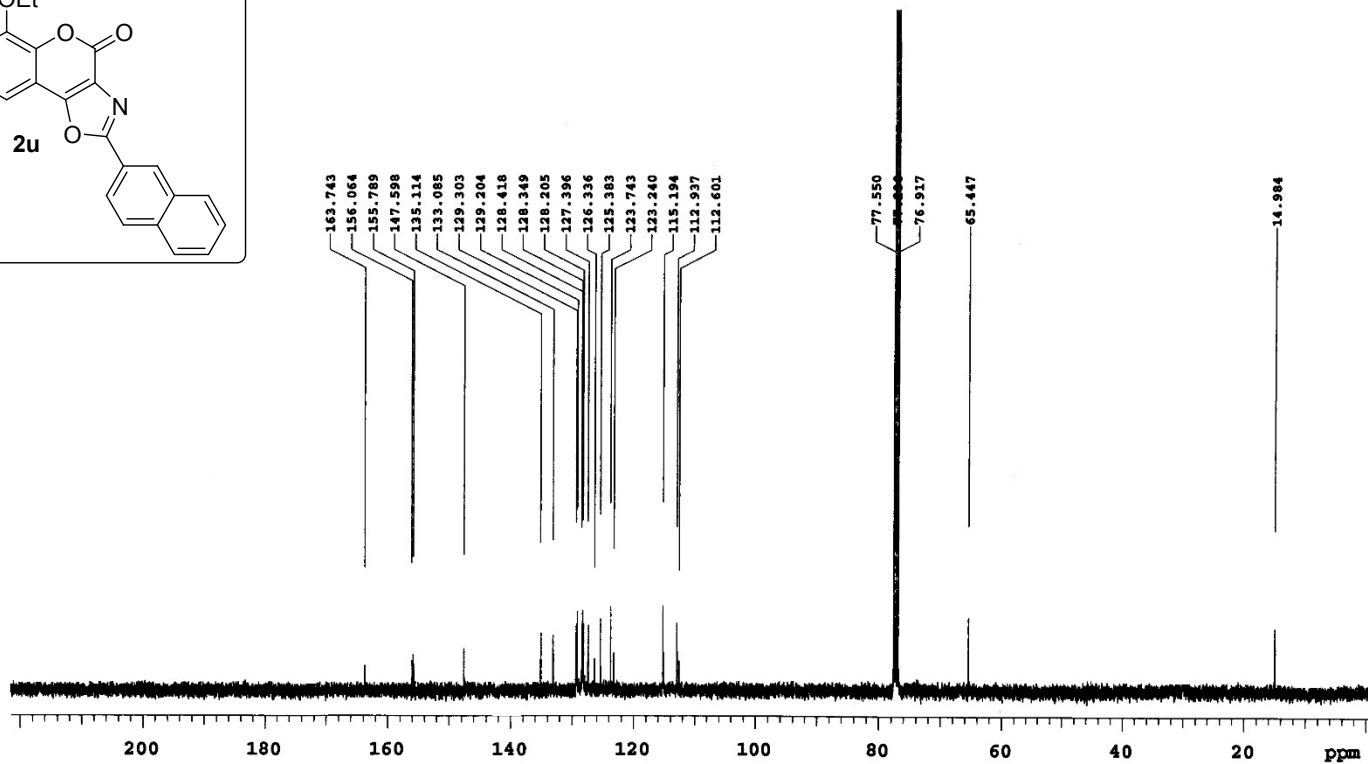
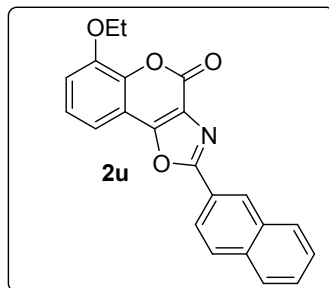
MB-B-11-14-1H

exp2 PROTON

SAMPLE		PRESATURATION	
date	Oct 15 2014	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	
sw	6398.0	gain	30
at	2.561	spin	not used
rp	32768	hst	0.008
fb	3600	pw90	16.300
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	32	il	n
ct	32	in	n
TRANSMITTER		dp	
tn	H1	hs	nn
sfrq		PROCESSING	
tof	363.1	fn	not used
tpwr	58	DISPLAY	
pw	8.150	sp	15.6
DECOUPLER		wp	4789.5
dm	C13	rfl	3702.3
dof	0	rfp	2902.9
dm	nnn	rp	138.9
decwave	g	lp	-102.4
dpwr	40	PLOT	
dof	17100	wc	268
		sc	0
		vs	203
		th	48
		ai	odc ph



<sup>13</sup>C NMR spectra of **2u**



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
3630 repetitions

OBSERVE C13, 100.5425801  
DECOUPLE H1, 399.8529994  
Power 42 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 2.3 hours

MB-B-11-14-13C  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
Mercury-400 "IITG-NMR"

# HRMS spectra of **2u**

Sample Name  
Inj Vol  
Data Filename

Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time

