Electronic Supplementary Material (ESI) for Organic .

Electronic Supplementary Information

Trifluoroacetic acid-Promoted Michael Addition-Cyclization Reactions of Vinylogous Carbamates

Ram Tilak Naganaboina, Amrita Nayak and Rama Krishna Peddinti*

Contents

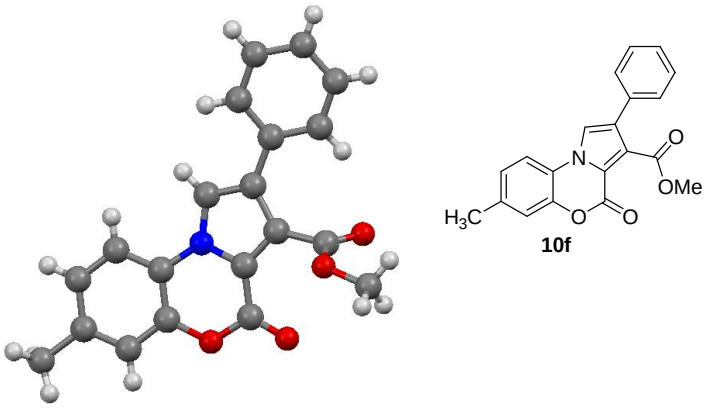


Figure 1. Single crystal X-ray structure of **10f**. (CCDC No: 982192)

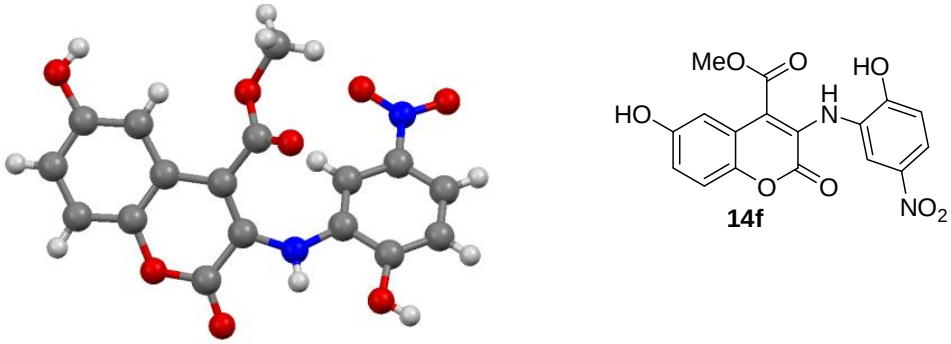


Figure 2. Single crystal X-ray structure of **14f**. (CCDC No: 982194)

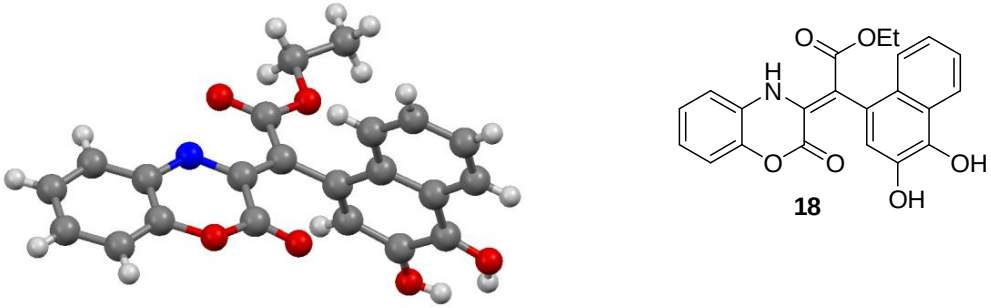
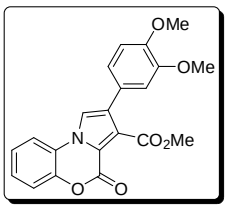


Figure 3. Single crystal X-ray structure of **18.** (CCDC NO: 982195)

General procedure for synthesis of pyrrolobenzoxazine derivatives: To a mixture of a 1,4-benzoxazinone derivative (0.5 mmol) and a β-nitrostyrene (0.6 mmol) in 4 mL of 1,2-dichloroethane (DCE), trifluoroacetic acid (TFA) (0.75 mmol) was added dropwise, and the mixture was allowed reflux for 5 h. After completion of the reaction as shown by TLC, the reaction was quenched with 4 mL of sat. $NaHCO_3$ solution. The organic layer was separated, washed with water twice, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude reaction mixture was purified by column chromatography on silica gel (100−200 Mesh) using 20-40% ethyl acetate/hexanes as the eluting system.

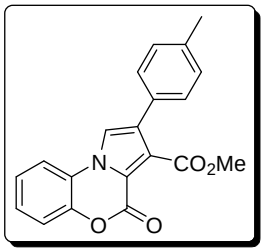
General procedure for synthesis of 3-aminocoumarin derivatives: To a mixture of 1,4-benzoxazinone derivative (0.5 mmol) and *p*-benzoquinone (**12**)/naphthoquinone (**13**) (0.6 mmol) in 4 mL of CH_2Cl_2, trifluoroacetic acid (TFA) (0.6 mmol) was added dropwise, and the mixture was allowed stir at room temperature for 3 h. As the reaction proceeded the desired product precipitated out. After completion of the reaction, as shown by TLC, the reaction mixture was filtered and the resultant precipitate was washed with 5 mL of CH_2Cl_2, and dried under vacuum to furnish a yellow coloured solid.

Compound 9a:



Yield: 156 mg (82%) as yellow solid, Mp.: 150-151 ^{o}C, IR (KBr): ν_{max} 1732, 1721, 1598, 1410, 1256, 1116, 1031 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.65 (s, 1H), 7.60 (d, *J* = 7.0 Hz, 1H), 7.32-7.26 (m, 3H), 6.99-6.95 (m, 2H), 6.82 (d, *J* = 8.5 Hz, 1H), 3.93 (s, 3H), 3.87 (s, 3H), 3.86 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 151.9, 148.8, 148.7, 142.8, 128.8, 126.9, 124.9, 124.4, 121.5, 121.3, 119.9, 118.1, 115.4, 115.4, 114.4, 111.1, 110.7, 55.7, 52.8 ppm. HRMS (ES+): *m/z* calcd for $[C_{21}H_{17}NO_6+Na]^{+}$: 402.0948, found: 402.0945.

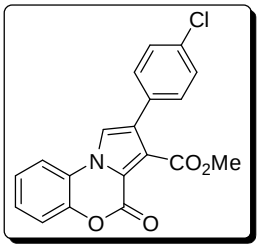
Compound 9b:



Yield: 128 mg (77%) as yellow solid, Mp.: 162-163 ^{o}C, IR (KBr): ν_{max} 1743, 1724, 1595, 1400, 1238, 1112, 1023 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.65 (s, 1H), 7.61-7.59 (m, 1H), 7.36-7.27 (m, 5H), 7.17 (d, *J* = 8.0 Hz, 2H), 3.92 (s, 3H), 2.34 (s, 3H) ppm. ^{13}C NMR

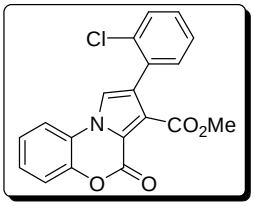
(125 MHz, $CDCl_3$): δ 165.3, 152.1, 142.9, 137.8, 129.4, 129.2, 128.9, 127.4, 127.1, 125.0, 121.8, 121.5, 118.3, 115.6, 115.5, 114.4, 52.8, 21.1 ppm. HRMS (ES+): *m/z* calcd for $[C_{20}H_{15}NO_4+Na]^+$: 356.0893, found: 356.0888.

Compound 9c:



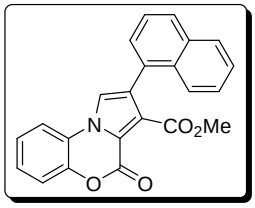
Yield: 132 mg (75%) as orange solid, Mp.: 178-179 ^oC, IR (KBr): ν_{max} 1748, 1726, 1598, 1409, 1240, 1125, 1010 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 7.67 (s, 1H), 7.64-7.62 (m, 1H), 7.38-7.36 (m, 2H), 7.36-7.35 (m, 1H), 7.34-7.33 (m, 2H), 7.33-7.29 (m, 2H), 3.91 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.0, 151.9, 143.0, 134.0, 130.4, 129.0, 128.9, 128.1, 127.3, 125.1, 121.8, 121.4, 118.4, 115.9, 115.7, 114.4, 52.9 ppm. HRMS (ES+): *m/z* calcd for $[C_{19}H_{12}ClNO_4+Na]^+$: 376.0347, found: 376.0346.

Compound 9d:



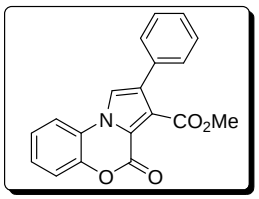
Yield: 126 mg (71%) as yellow solid, Mp.: 160-161 ^oC, IR (KBr): ν_{max} 1730, 1721, 1606, 1524, 1412, 1372, 1247, 1068 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.44 (dd, *J* = 3.0, 5.5 Hz, 1H), 7.38-7.28 (m, 6 H), 3.80 (s, 3H), ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.8, 151.6, 143.1, 133.3, 131.4, 131.2, 129.7, 129.3, 127.3, 127.1, 126.7, 125.0, 123.1, 121.4, 118.2, 117.6, 115.7, 114.5, 52.5 ppm. HRMS (ES+): *m/z* calcd for $[C_{19}H_{12}ClNO_4+Na]^+$: 376.0347, found: 376.0343.

Compound 9e:



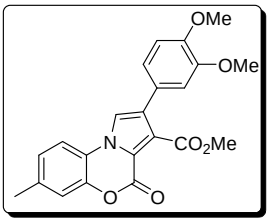
Yield: 149 mg (81%) as yellow solid, Mp.: 136-137 ^oC, IR (KBr): ν_{max} 1745, 1725, 1598, 1381, 1259, 1089 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.88-7.85 (m, 3H), 7.71 (s, 1H), 7.60 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.51-7.40 (m, 5H), 7.36 (dt, *J* = 1.5, 7.0 Hz, 1H), 7.30 (dt, *J* = 1.5, 8.0 Hz, 1H), 3.59 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.1, 151.8, 143.1, 133.4, 132.0, 129.9, 128.5, 128.3, 128.2, 127.8, 127.2, 126.3, 125.9, 125.1, 125.0, 123.8, 121.5, 118.3, 117.7, 115.6, 114.5, 52.3 ppm. HRMS (ES+): *m/z* calcd for $[C_{23}H_{15}NO_4+Na]^+$: 392.0893, found: 392.0883.

Compound 9f:



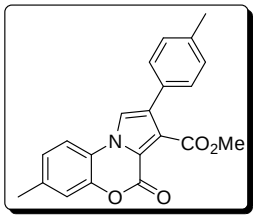
Yield: 134 mg (84%) as brown solid, Mp.: 168-169 ^{o}C, IR (KBr): ν_{max} 1741, 1722, 1530, 1468, 1384, 1250, 1138 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.68 (s, 1H), 7.62-7.60 (m, 1H), 7.45 - 7.43 (m, 2H), 7.38-7.35 (m, 2H), 7.34-7.29 (m, 4H), 3.91 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 152.0, 142.9, 131.9, 129.2, 128.7, 127.8, 127.6, 127.1, 125.0, 121.9, 121.4, 118.3, 115.7, 115.7, 114.4, 52.8 ppm. HRMS (ES+): *m/z* calcd for $[C_{19}H_{13}NO_4+Na]^+$: 342.0737, found: 342.0735.

Compound 10a:



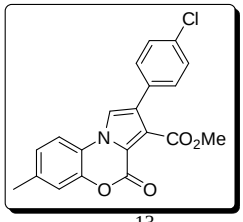
Yield: 151 mg (76%) as brown solid. Mp.: 143-144 ^{o}C, IR (KBr): ν_{max} 1738, 1716, 1595, 1397, 1261, 1115, 1032 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.58 (s, 1H), 7.36 (d, *J* = 1.0 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 1H), 7.06 (dd, *J* = 1.5, 8.5 Hz, 1H), 6.97 (d, *J* = 2.0 Hz, 1H), 6.95 (dd, *J* = 2.0, 8.0 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 3.91 (s, 3H), 3.86 (s, 3H), 3.85 (s, 3H), 2.40 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.5, 152.1, 148.8, 148.7, 140.7, 135.2, 128.6, 127.7, 124.5, 121.4, 120.8, 119.9, 117.7, 115.4, 115.2, 114.5, 111.1, 110.6, 55.7, 52.8, 20.9 ppm. HRMS (ES+): *m/z* calcd for $[C_{22}H_{19}NO_6+Na]^+$: 416.1105, found: 416.1105.

Compound 10b:



Yield: 131 mg (75%) as brown solid, Mp.: 182-183 ^{o}C, IR (KBr): ν_{max} 1739, 1719, 1594, 1410, 1272, 1119, 1029 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.59 (s, 1H), 7.46 (d, *J* = 8.5 Hz, 1H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.13 (s, 1H), 7.08 (dd, *J* = 1.0, 8.0 Hz, 1H), 3.92 (s, 3H), 2.40 (s, 3H), 2.35 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 152.2, 142.8, 137.7, 129.4, 129.1, 129.0, 127.5, 125.7, 121.5, 119.2, 118.4, 115.5, 115.3, 114.0, 52.8, 21.1, 21.0 ppm. HRMS (ES+): *m/z* calcd for $[C_{21}H_{17}NO_4+Na]^+$: 370.1050, found: 370.1048.

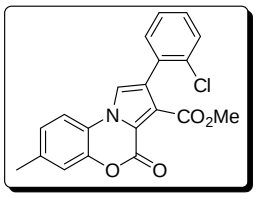
Compound 10c:



Yield: 131 mg (71%) as yellow solid, Mp.: 180-181 ^{o}C, IR (KBr): ν_{max} 1739, 1721, 1539, 1368, 1235, 1124, 1024 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.63 (s, 1H), 7.50 (d, *J* = 8.5 Hz, 1H), 7.37 (q, *J* = 7.5 Hz, 4H), 7.18-7.17 (m, 1H), 7.12 (d, *J* = 8.0Hz, 1H), 3.91 (s, 3H), 2.42 (s, 3H) ppm. ^{13}C NMR

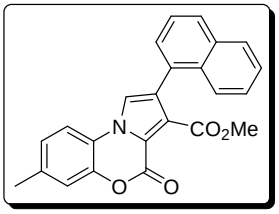
(125 MHz, $CDCl_3$): δ 165.1, 152.2, 142.9, 138.1, 134.0, 130.7, 129.1, 129.0, 128.0, 125.9, 121.6, 119.1, 118.6, 115.9, 115.5, 114.1, 52.9, 21.2 ppm. HRMS (ES+): *m/z* calcd for $[C_{20}H_{14}ClNO_4+Na]^+$: 390.0504, found: 390.0505.

Compound 10d:



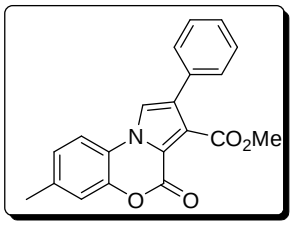
Yield: 122 mg (66%) as yellow solid, Mp: 168-169 ^oC, IR (KBr): ν_{max} 1744, 1728, 1576, 1382, 1264, 1058 cm^{-1}, ^1H NMR (500 MHz, CDCl3): δ 7.66 (s, 1H), 7.48 (d, J = 8.0 Hz, 1H), 7.45 (dd, *J* = 3.5, 5.5 Hz, 1H), 7.37 (dd, *J* = 3.5, 5.5 Hz, 1H), 7.31-7.27 (m, 2H), 7.17 (s, 1H), 7.10 (d, *J* = 8.5 Hz, 1H), 3.80 (s, 3H), 2.42 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.9, 151.8, 142.9, 138.0, 133.3, 131.5, 131.4, 129.7, 129.3, 126.9, 126.7, 125.7, 122.8, 119.1, 118.3, 117.4, 115.3, 114.2, 52.4, 21.1 ppm. HRMS (ES+): m/z calcd for $[C_{20}H_{14}ClNO_4+Na]^+$: 390.0505, found: 390.0509.

Compound 10e:



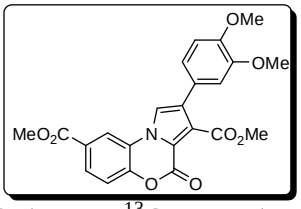
Yield: 149mg (78%) as yellow solid, Mp.: 167-168 ^oC, IR (KBr): ν_{max} 1744, 1724, 1593, 1394, 1259, 1075 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 7.89-7.86 (m, 3H), 7.67 (s, 1H), 7.51-7.43 (m, 5H), 7.22 (s, 1H), 7.10 (d, *J* = 8.5 Hz, 1H), 3.59 (s, 3H), 2.44 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.2, 152.0, 143.0, 137.9, 133.5, 132.1, 130.0, 128.5, 128.3, 128.1, 127.8, 126.3, 125.9, 125.8, 125.2, 125.1, 123.5, 119.2, 118.4, 117.4, 115.5, 114.2, 52.3, 21.1 ppm. HRMS (ES+): *m/z* calcd for $[C_{24}H_{17}NO_4+Na]^+$: 406.1050, found: 406.1049.

Compound 10f:



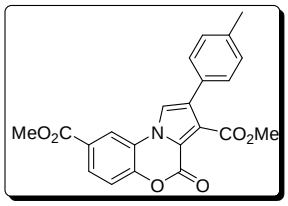
Yield: 137 mg (82%) as yellow solid, Mp.: 166-167 ^oC, IR (KBr): ν_{max} 1734, 1716, 1594, 1409, 1265, 1117, 1028 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 7.64 (s, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.47 - 7.46 (m, 2H), 7.39 (t, *J* = 7.0 Hz, 2H), 7.35-7.32 (m, 1H), 7.16 (s, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 3.92 (s, 3H), 2.41 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.3, 152.3, 142.9, 137.8, 132.1, 129.1, 128.8, 127.9, 127.7, 125.8, 121.6, 119.2, 118.5, 115.6, 115.5, 114.1, 52.8, 21.1 ppm. HRMS (ES+): *m/z* calcd for $[C_{20}H_{15}NO_4+Na]^+$: 356.0893, found: 356.0893.

Compound 11a:



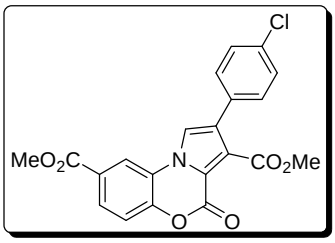
Yield: 148 mg (68%) as yellow solid, Mp.: 180-181 ^{o}C, IR (KBr): ν_{max} 1742, 1722, 1595, 1397, 1262, 1119, 1015 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.30 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.74 (s, 1H), 7.40 (d, *J* = 8.5 Hz, 1H), 6.98 (d, *J* = 7.5 Hz, 2H), 6.84 (d, *J* = 8.5 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H), 3.88 (s, 3H), 3.87 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.3, 165.2, 151.2, 149.0, 148.9, 146.0, 129.4, 128.2, 127.0, 124.2, 122.3, 121.5, 120.0, 118.3, 116.1, 115.9, 115.1, 111.2, 110.7, 55.8, 55.8, 52.9, 52.6 ppm. HRMS (ES+): *m/z* calcd for $[C_{23}H_{19}NO_8+Na]^+$: 460.1003, found: 460.1014.

Compond 11b:



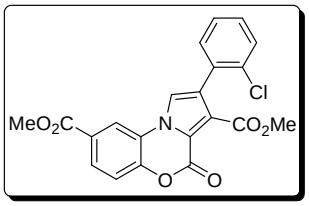
Yield: 129 mg (66%) as brown solid, Mp.: 150-151 ^{o}C, IR (KBr): ν_{max} 1749, 1726, 1604, 1391, 1254, 1117, 1058 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.75 (s, 1H), 7.38 (d, *J* = 8.5 Hz, 1H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 3.96 (s, 3H), 3.95 (s, 3H), 2.33 (s, 3H)ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 165.1, 151.2, 145.9, 137.8, 129.4, 129.4, 128.5, 128.1, 127.2, 126.9, 122.3, 121.4, 118.2, 116.1, 116.1, 115.1, 52.8, 52.5, 21.0 ppm. HRMS (ES+): *m/z* calcd for $[C_{22}H_{17}NO_6+Na]^+$: 414.0948, found: 414.0948.

Compound 11c:



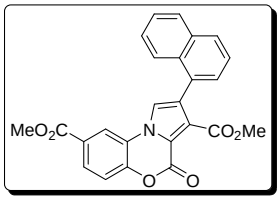
Yield: 128 mg (62%) as orange solid, Mp.: 154-155 ^{o}C, IR (KBr): ν_{max} 1746, 1724, 1604, 1398, 1260, 1119, 1069 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.33 (d, *J* = 1.5 Hz, 1H), 8.03 (dd, *J* = 1.5, 8.5 Hz, 1H), 7.78 (s, 1H), 7.44 (d, *J* = 8.5 Hz, 1H), 7.39 (q, *J* = 8.0 Hz, 4 H), 3.97 (s, 3H), 3.93 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 164.7, 151.1, 146.1, 134.2, 130.2, 129.1, 129.0, 128.6, 128.5, 127.1, 122.5, 121.4, 118.5, 116.2, 115.6, 53.0, 52.7 ppm. HRMS (ES+): *m/z* calcd for $[C_{21}H1_4ClNO_6+Na]^+$: 434.0402 , found: 434.0403.

Compound 11d:



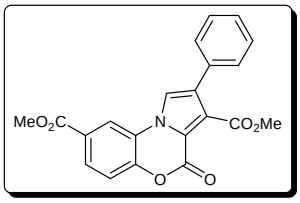
Yield: 116 mg (56%) as white solid, Mp.: 184-185 ^{o}C, IR (KBr): ν_{max} 1736, 1712, 1595, 1398, 1259, 1115, 1062 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.33 (d, *J* = 1.5 Hz, 1H), 8.02 (dd, *J* = 1.5, 8.5 Hz, 1H), 7.82 (s, 1H), 7.46-7.43 (m, 2H), 7.38-7.36 (m, 1H), 7.32-7.29 (m, 2H), 3.95 (s, 3H), 3.81 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 163.6, 150.8, 146.2, 133.3, 131.4, 131.0, 129.7, 129.5, 128.5, 127.6, 127.0, 126.7, 123.8, 121.5, 118.3, 118.1, 116.3, 115.3, 52.6, 52.6 ppm. HRMS (ES+): *m/z* calcd for $[C_{21}H_{14}ClNO_6+Na]^+$: 434.0402, found: 434.0402.

Compound 11e:



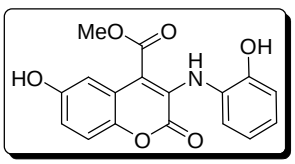
Yield: 152 mg (71%) as brown solid, Mp.: 208-209 ^{o}C, IR (KBr): ν_{max} 1738, 1723, 1593, 1393, 1263, 1118, 1076 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.32 (d, *J* = 2.0 Hz, 1H), 8.04 (dd, *J* = 1.5, 8.5 Hz, 1H), 7.89-7.84 (m, 3H), 7.83 (s, 1H), 7.52-7.44 (m, 5H), 3.95 (s, 3H), 3.61 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 163.8, 151.0, 146.2, 133.5, 131.9, 129.5, 128.7, 128.5, 128.4, 127.9, 127.1, 126.4, 126.0, 125.1, 125.1, 124.6, 121.6, 118.4, 118.2, 116.3, 115.3, 52.6, 52.3 ppm. HRMS (ES+): *m/z* calcd for $[C_{25}H_{17}NO_6+Na]^+$: 450.0948, found: 450.0955.

Compound 11f:



Yield: 142 mg (75%) as yellow solid, Mp.: 158-159 ^{o}C, IR (KBr): ν_{max} 1730, 1714, 1603 1465, 1364, 1261, 1006 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (d, *J* = 1.5 Hz, 1H), 7.96 (dd, *J* = 2.0, 9.0 Hz, 1H), 7.77 (s, 1H), 7.41 (d, *J* = 7.0 Hz, 2H), 7.37 (d, *J* = 9.0 Hz, 1H), 7.33 (t, *J* = 7.0 Hz, 2H), 7.28 (d, *J* = 7.5 Hz, 1H), 3.93 (s, 3H), 3.92 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.1, 164.9, 151.1, 145.9, 131.4, 129.4, 128.6, 128.2, 127.9, 127.4, 126.9, 122.4, 121.4, 118.2, 116.2, 116.1, 115.2, 52.8, 52.5 ppm. HRMS (ES+): *m/z* calcd for $[C_{21}H_{15}NO_6+Na]^+$: 400.0792, found: 400.0791.

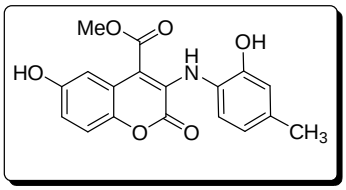
Compound 14a:



Yield: 144 mg (88%) as yellow solid. Mp.: 154-155 ^{o}C, IR (KBr): ν_{max} 3334, 1712, 1663, 1506, 1497, 1350, 1247, 1024cm^{-1}.^{1}H NMR (500 MHz, $CDCl_3$): δ 9.54 (s, 2H), 7.82 (s, 1H), 7.22 (d, *J* = 9.0 Hz, 1H), 6.97 (d, *J* = 6.5 Hz, 2H), 6.87-6.83 (m, 2H), 6.78-6.73 (m, 2H), 3.17 (s, 3H) ppm.

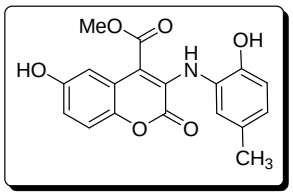
^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 159.5, 154.5, 151.0, 141.1, 130.0, 127.3, 126.1, 124.9, 119.4, 119.2, 117.5, 116.4, 115.2, 111.6, 105.2, 51.9 ppm. HRMS (ES+): *m/z* calcd for $[C_{17}H_{13}NO_6+Na]^+$: 350.0635, found: 350.0637.

Compound 14b:



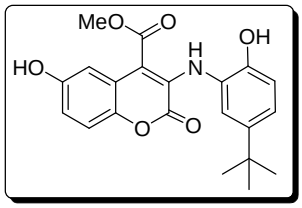
Yield: 138 mg (81%) as yellow solid, Mp.: 178-179 ^{o}C, IR (KBr): ν_{max} 3375, 1727, 1689, 1524, 1500, 1344, 1274, 1028 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.74 (br s, 1H), 9.57 (br s, 1H), 7.61 (s, 1H), 7.19 (d, *J* = 8.5 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.75-6.72 (m, 2H), 6.64-6.63 (m, 1H), 6.55 (dd, *J* = 1.5, 8.0 Hz, 1H), 3.18 (s, 3H), 2.17 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.7, 159.6, 154.6, 151.3, 141.0, 136.2, 130.4, 125.6, 124.5, 120.1, 119.4, 117.6, 117.0, 115.2, 110.9, 108.2, 52.1, 21.2 ppm. HRMS (ES+): *m/z* calcd for $[C_{18}H_{15}NO_6+Na]^+$: 364.0792, found: 364.0791.

Compound 14c:



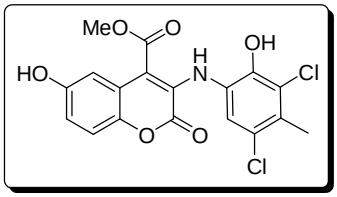
Yield: 133 mg (78%) as yellow solid, Mp.: 164-165 ^{o}C, IR (KBr): ν_{max} 3358, 1724, 1683, 1577, 1524, 1450, 1344, 1257, 1021 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.69 (br s, 1H), 9.41 (br s, 1H), 7.59 (s, 1H), 7.10 (d, *J* = 9.0 Hz, 1H), 6.83 (d, *J* = 2.5 Hz, 1H), 6.77-6.70 (m, 4H), 3.20 (s, 3H), 2.13 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.4, 159.4, 154.5, 148.3, 141.0, 129.8, 128.0, 126.9, 126.2, 124.5, 119.1, 117.4, 116.1, 115.2, 111.5, 108.2, 51.7, 20.4 ppm. HRMS (ES+): *m/z* calcd for $[C_{18}H_{15}NO_6+Na]^+$: 364.0792, found: 364.0789.

Compound 14d:



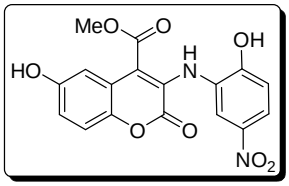
Yield: 132 mg (68%) as yellow solid, Mp: 184-185 ^{o}C, IR (KBr): ν_{max} 3359, 1714, 1649, 1563, 1526, 1344, 1241, 1042 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$: δ 9.51 (br s, 1H), 9.32 (br s, 1H), 7.69 (s, 1H), 7.21 (d, *J* = 9.0 Hz, 1H), 6.99 (dd, *J* = 2.0, 8.0 Hz, 1H), 6.96 (d, *J* = 2.5 Hz, 1H), 6.92 (d, *J* = 3.0 Hz, 1H), 6.78 (d, *J* = 8.5 Hz, 1H), 6.76 (dd, *J* = 2.5, 8.5 Hz, 1H), 3.08 (s, 3H), 1.22 (s, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.0, 159.2, 154.2, 148.0, 141.2, 140.6, 129.9, 126.2, 122.3, 120.4, 119.0, 117.0, 115.7, 114.5, 109.8, 107.5, 51.2, 33.7, 31.2 ppm. HRMS (ES^+): *m/z* calcd for $[C_{21}H_{21}NO_6+Na]^+$: 406.1261, found: 406.1273.

Compound 14e:



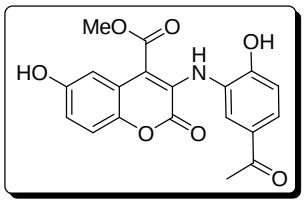
Yield: 152 mg (72%) as yellow solid, Mp.: 198-199 ^{o}C, IR (KBr): ν_{max} 3387, 1718, 1674, 1603, 1530, 1444, 206, 1017 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.74 (br s, 1H), 7.91 (s, 1H), 7.21 9d, *J* = 9.0 Hz, 1H), 7.02 (s, 1H), 6.79 (dd, *J* = 3.0, 9.0 Hz, 1H), 6.76 (d, *J* = 2.5 Hz, 1H), 3.29 (s, 3H), 2.33 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.8, 158.6, 154.2, 146.7, 141.1, 130.3, 129.6, 127.5, 123.5, 122.8, 122.4, 118.5, 117.1, 115.3, 113.0, 107.9, 51.5, 17.3 ppm. HRMS (ES+): *m/z* calcd for $[C_{18}H_{13}C_{l2}NO_6+Na]^+$: 432.0012, found: 432.0017.

Compound 14f:



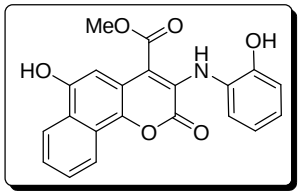
Yield: 132 mg (71%) as yellow solid, Mp.: 171-172 ^{o}C, IR (KBr): ν_{max} 3326, 1712, 1674, 1592, 1527, 1361, 1241, 1079 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 11.38 (br s, 1H), 8.05 (br s, 1H), 7.89 (d, *J* = 9.0 Hz, 1H), 7.87-7.85 (m, 1H), 7.24 (d, *J* = 8.5 Hz, 1H), 7.00 (d, *J* = 9.0 Hz, 1H), 6.91 (s, 1H), 6.84 (dd, *J* = 2.5, 8.5 Hz, 1H), 3.36 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165, 158.7, 156.7, 156.7, 154.3, 141.7, 139.3, 128.9, 128.8, 121.1, 118.5, 118.2, 117.4, 116.1, 115.6, 108.5, 52.0 ppm. HRMS (ES+): *m/z* calcd for $[C_{17}H_{12}N_2O_8+Na]^+$: 395.0486, found: 395.0497.

Compound 14g:



Yield: 137 mg (74%) as yellow solid, Mp.: 184-185 ^{o}C, (KBr): ν_{max} 3361, 1709, 1653, 1586, 1506, 1450, 1338, 1074 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.67 (br s, 1H), 9.65 (br s, 1H), 7.84 (s, 1H), 7.63 (dd, *J* = 2.0, 8.5 Hz, 1H), 7.58 (d, *J* = 2.0 Hz, 1H), 7.23 (d, *J* = 8.5 Hz, 1H), 6.93 (d, *J* = 8.5 Hz, 1H), 6.84 (d, *J* = 2.5 Hz, 1H), 6.80 (dd, *J* = 2.5, 8.5 Hz, 1H), 3.20 (s, 3H), 2.45 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.2, 165.2, 159.0, 155.4, 154.4, 141.1, 129.5, 128.6, 127.4, 126.6, 124.6, 118.7, 117.3, 115.8, 115.3, 112.7, 108.1, 51.7, 26.4 ppm. IR HRMS (ES+): *m/z* calcd for $[C_{19}H_{15}NO_7+Na]^+$: 392.0741, found: 392.0746.

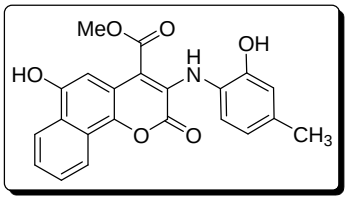
Compound 15a:



Yield: 162 mg (86%) as yellow solid, Mp.: 176-177 ^{o}C, IR (KBr): ν_{max} 3382, 1711, 1677, 1592, 1577, 1409, 1245, 1078 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.29 (br s, 1H), 9.56 (br s, 1H), 8.23

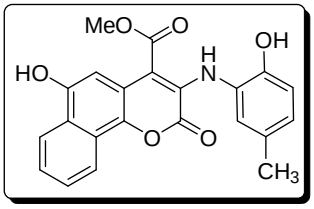
(d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.89 (s, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.02-6.97 (m, 2H), 6.95 (s, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.76 (t, *J* = 7.5 Hz, 1H), 3.23 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 158.9, 150.7, 150.0, 135.8, 130.1, 127.6, 127.1, 125.7, 125.5, 124.6, 123.6, 123.3, 122.4, 120.1, 118.8, 116.0, 114.4, 112.3, 100.8, 51.4 ppm. HRMS (ES+): *m/z* calcd for $[C_{21}H_{15}NO_6+Na]^+$: 400.0792, found: 400.0800.

Compound 15b:



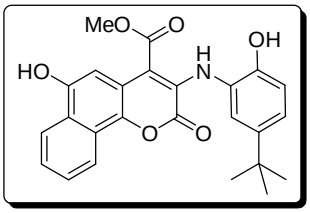
Yield: 159 mg (81%) as yellow solid, Mp.: 216-217 ^{o}C, IR (KBr): ν_{max} 3358, 1709, 1674, 1592, 1559, 1421, 1232, 1085 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.29 (br s, 1H), 9.43 (br s, 1H), 8.22 (d, *J* = 8.5 Hz, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.81 (s, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 1H), 6.94 (s, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.70 (s, 1H), 6.58 (d, *J* = 8.0 Hz, 1H), 3.25 (s, 3H), 2.22 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.3, 159.0, 151.0, 150.1, 135.6, 135.3, 130.4, 127.6, 125.6, 125.1, 124.3, 123.5, 123.4, 122.4, 120.0, 119.4, 116.6, 114.6, 111.5, 100.8, 51.5, 20.7 ppm. HRMS (ES+): *m/z* calcd for $[C_{22}H_{17}NO_6+Na]^+$: 414.0948, found: 414.0960.

Compound 15c:



Yield: 164 mg (84%) as yellow solid, Mp.: 208-209 ^{o}C, IR (KBr): ν_{max} 3352, 1712, 1689, 1589, 1562, 1430, 1206, 1085 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.31 (br s, 1H), 9.33 (br s, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.79 (s, 1H), 7.67 (t, *J* = 7.0 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 6.97 (s, 1H), 6.81-6.74 (m, 3H), 3.25 (s, 3H), 2.17 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.3, 159.1, 150.1, 148.2, 136.0, 130.0, 127.7, 127.6, 126.8, 125.8, 124.3, 123.7, 123.4, 122.5, 120.2, 115.9, 114.4, 112.5, 101.0, 51.5, 20.2 ppm. HRMS (ES+): *m/z* calcd for $[C_{22}H_{17}NO_6+Na]^+$: 414.0948, found: 414.0963

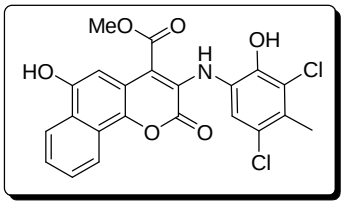
Compound 15d:



Yield: 162 mg (75%) as yellow solid, Mp.: 202-203 ^{o}C, IR (KBr): ν_{max} 3364, 1721, 1657, 1572, 1509, 1352, 1238, 1063 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.27 (br s, 1H), 9.38 (br s, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.78 (s, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.07 (s, 1H), 7.03 (s, 1H), 6.99 (d, *J* = 8.5 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 1H), 3.15 (s, 3H), 1.20 (s, 9H) ppm. ^{13}C NMR (125 MHz,

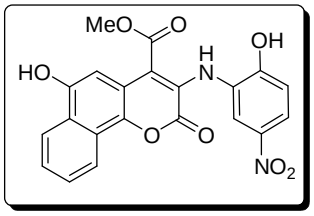
$CDCl_3$): δ 165.2, 159.2, 150.1, 148.1, 141.3, 135.8, 130.3, 127.5, 126.3, 125.6, 123.7, 123.4, 122.4, 122.3, 120.4, 120.1, 115.8, 114.6, 111.3, 101.0, 51.3, 33.7, 31.2 ppm. HRMS (ES+): *m/z* calcd for $[C_{25}H_{23}NO_6+Na]^+$: 456.1418, found: 456.1428.

Compound 15e:



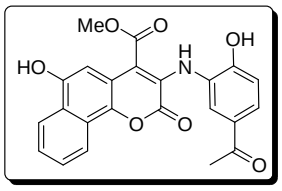
Yield: 182 mg (79%) as yellow solid, Mp.: 220-221 ^oC, IR (KBr): ν_{max} 3368, 1714, 1689, 1546, 1468, 1268, 1082 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 10.32 (br s, 1H), 9.75 (br s, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 8.05 (s, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.11 (s, 1H), 6.89 (s, 1H), 3.39 (s, 3H), 2.37 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.1, 158.6, 150.1, 146.7, 136.6, 130.2, 129.8, 127.7, 127.6, 126.0, 124.0, 123.3, 123.3, 122.9, 122.5, 122.5, 120.2, 114.8, 113.9, 100.8, 51.7, 17.3 ppm. HRMS (ES+): *m/z* calcd for $[C_{22}H_{15}C_{l2}NO_6+Na]^+$: 482.0169, found: 482.0178.

Compound 15f:



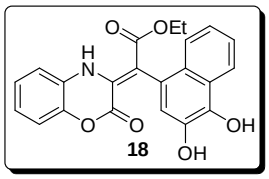
Yield: 152 mg (72%) as yellow solid, Mp.: 194-195 ^oC, IR (KBr): ν_{max} 3364, 1724, 1677, 1589, 1559, 1421, 1318, 1079 cm^{-1}.^1H NMR (500 MHz, $CDCl_3$): δ 11.40 (br s, 1H), 10.35 (br s, 1H), 8.19-8.05 (m, 2H), 8.05 (s, 1H), 7.86 (s, 2H), 7.61-7.53 (m, 2H), 7.01-6.94 (m, 2H), 3.42 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.3, 157.7, 155.6, 149.3, 138.5, 136.6, 128.1, 128.0, 126.8, 125.4, 123.5, 122.5, 121.6, 119.9, 119.6, 117.2, 117.0, 114.7, 112.8, 100.2, 51.1 ppm. HRMS (ES+): *m/z* calcd for $[C_{21}H_{14}N_2O_8+Na]^+$: 445.0642, found: 445.0647.

Compound 15g:



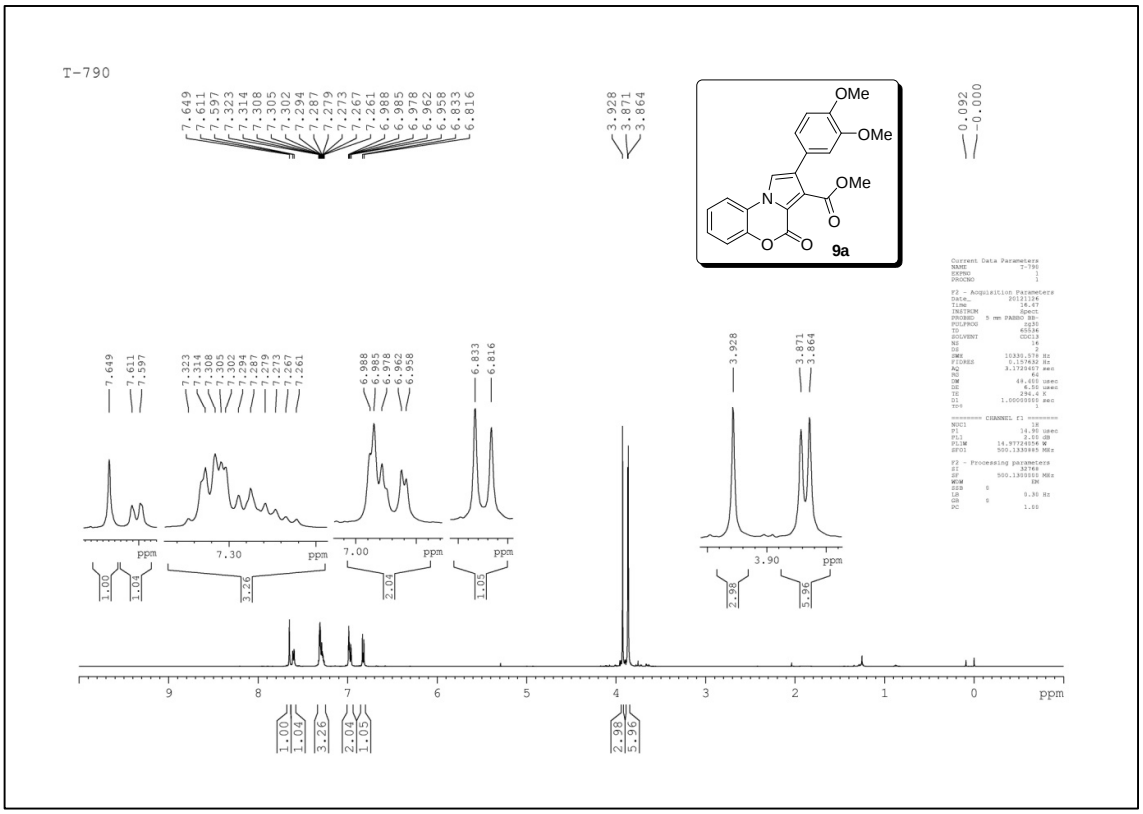
Yield: 162 mg (77%) as yellow solid, Mp.: 202-203 ^oC, IR (KBr): ν_{max} 3387, 1706, 1656, 1586, 1562, 1415, 1321 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 10.34 (br s, 1H), 8.24 (d, *J* = 8.5Hz, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.93 (s, 1H), 7.68-7.64 (m, 3H), 7.56 (t, *J* = 8.0 Hz, 1H), 6.96-6.94 (m, 2H), 3.26 (s, 3H), 2.47 (s, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 195.9, 165.2, 158.8, 155.3, 150.1, 136.3, 129.7, 128.5, 127.6, 127.4, 126.3, 125.9, 124.5, 123.9, 123.3, 122.4, 120.2, 115.7, 114.1, 114.0, 100.9, 51.6, 26.2 ppm. HRMS (ES+): *m/z* calcd for $[C_{23}H_{17}NO_7+Na]^+$: 442.0897, found: 442.0905.

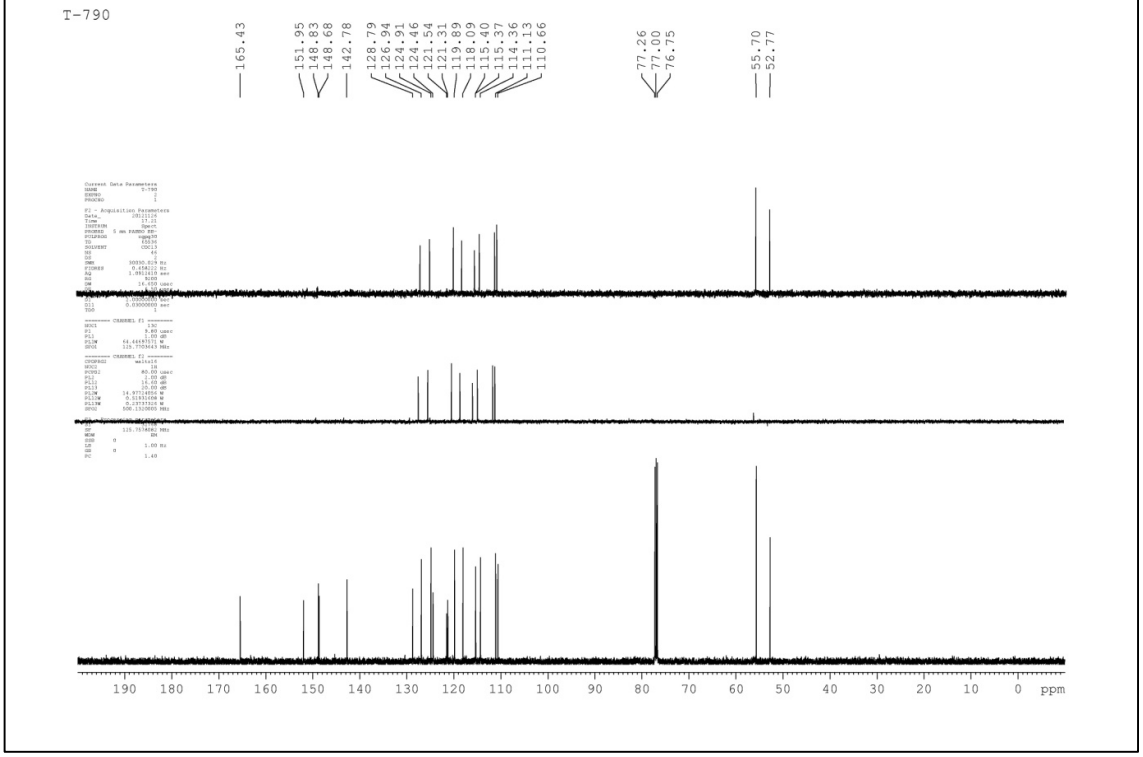
Synthesis of 1,4-benzoxazinone derivative 18: To a mixture of 1,4-benzoxazinone derivative **16** (0.5 mmol) and naphthoquinone monoketal **17** (0.6 mmol) in 4 mL of CH_2Cl_2, trifluoroacetic acid (TFA) (0.6 mmol) was added dropwise, and the mixture was allowed to stir at room temperature for 4 h. After completion of the reaction, as shown by TLC, The crude reaction mixture was purified by column chromatography on silica gel (100−200 mesh) using 30-50% ethyl acetate/hexanes as the eluting system.

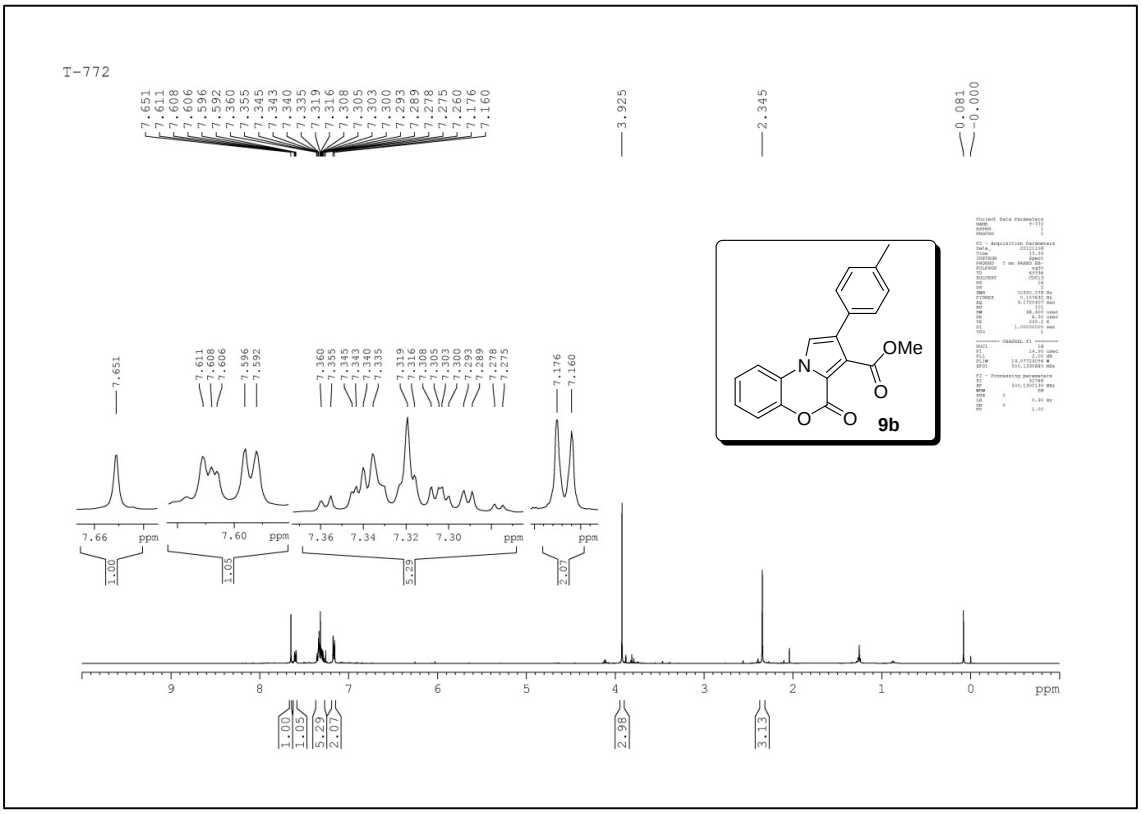


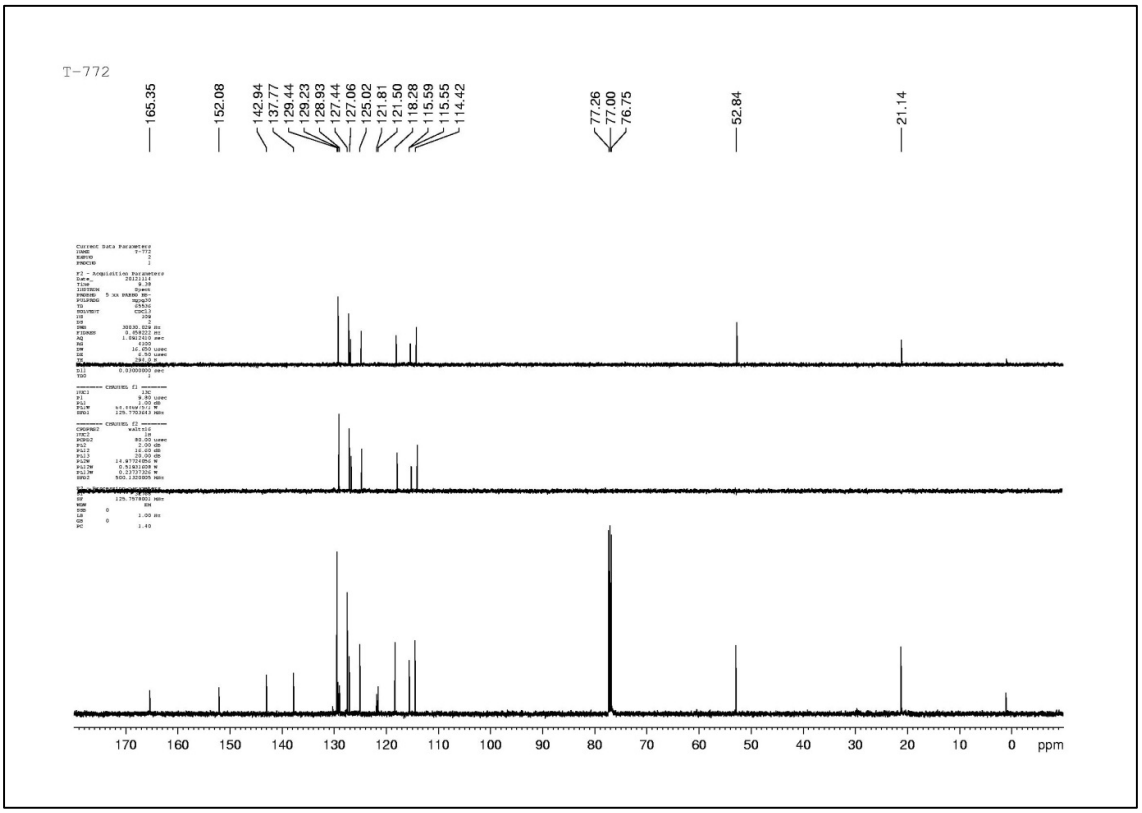
18

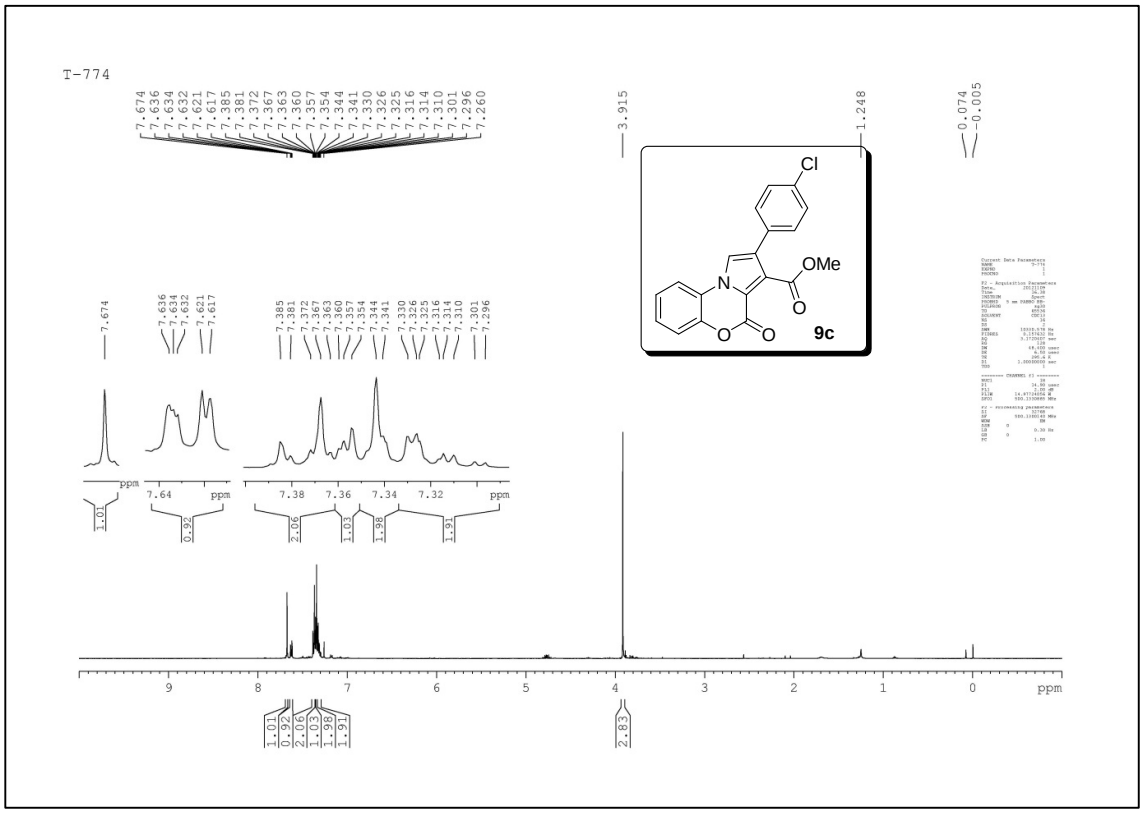
Yield: 153 mg (78%) as brown solid, Mp.: 168-169 ^{o}C, IR (KBr): ν_{max} 3352, 1726, 1678, 1593, 1394, 1279, 1085 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 11.97 (br s, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.26 (d, *J* = 7.5 Hz, 1H), 7.19-7.14 (m, 1H), 7.12-7.03 (m, 3H), 6.27 (s, 1H), 4.20-4.15 (m, 2H), 1.12-1.09 (m, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.7, 179.6, 168.5, 154.0, 153.1, 140.4, 136.7, 136.3, 135.3, 131.1, 130.1, 129.9, 128.1, 127.0, 125.8, 123.6, 123.5, 116.7, 115.4, 100.0, 61.5, 13.9 ppm. HRMS (ES+): *m/z* calcd for $[C_{22}H_{17}NO_6+Na]^+$: 414.0948, found: 414.0938.

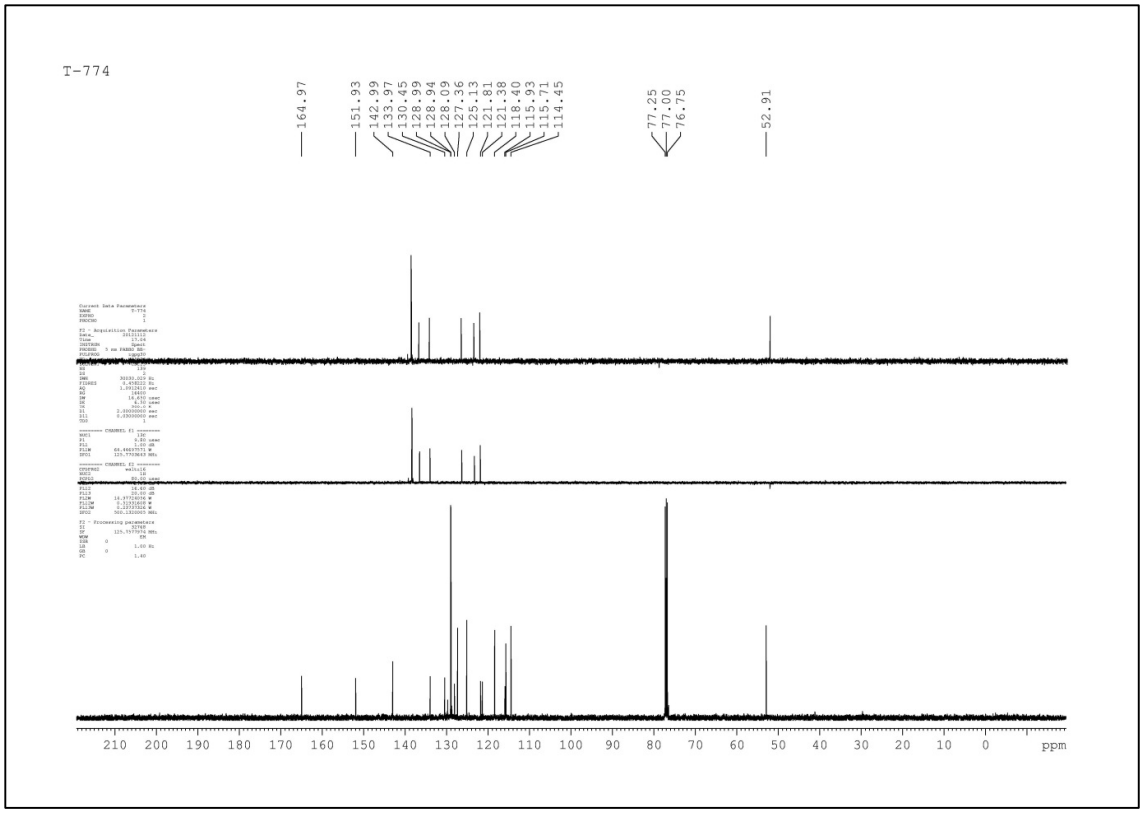

T-790
7.649
7.611
7.597
7.323
7.314
7.308
7.305
7.302
7.294
7.287
7.279
7.273
7.267
7.261
6.988
6.985
6.978
6.962
6.958
6.833
6.816
3.928
3.871
3.864
0.092
0.000
OMe
OMe
OMe
N
O
O
O
9a
ppm
7.30
7.00
3.90
1.00
1.04
3.26
2.04
1.05
2.98
5.96

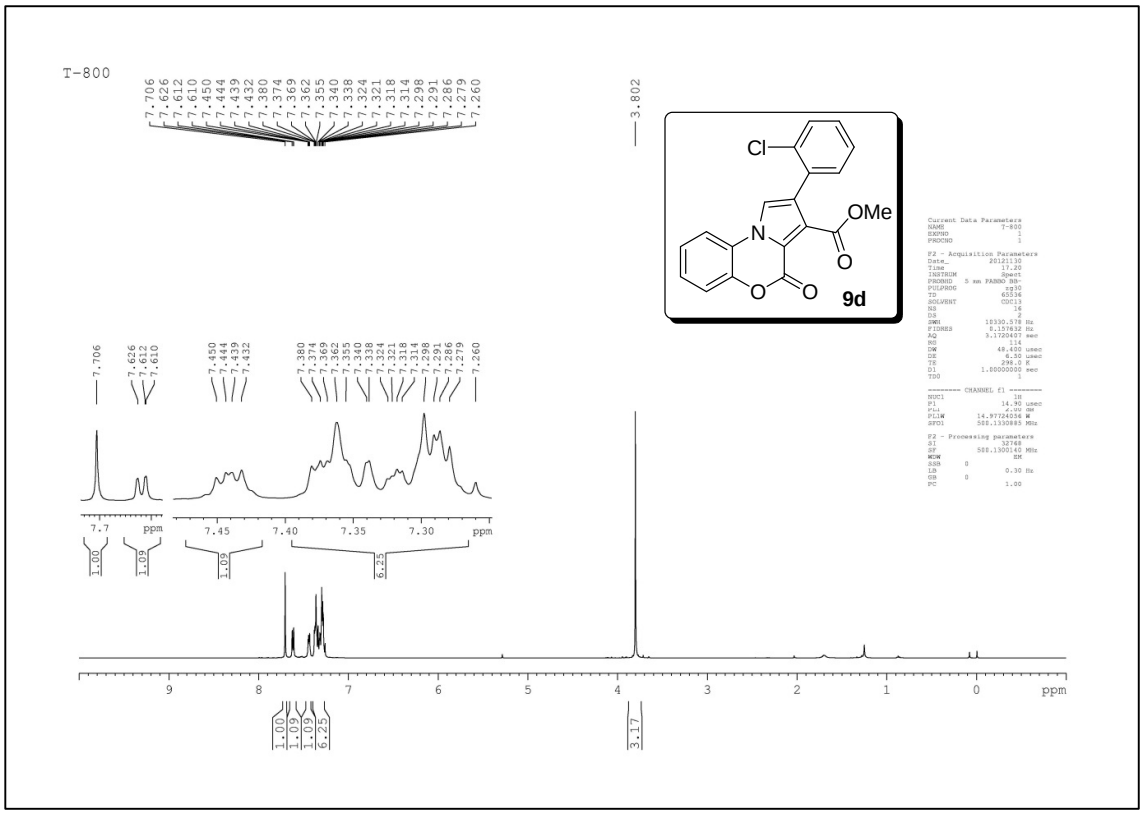

T-790
165.43
151.95
148.83
148.68
142.78
128.79
126.94
124.91
124.46
121.54
121.31
119.89
118.09
115.40
115.37
114.36
111.13
110.66
77.26
77.00
76.75
55.70
52.77
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

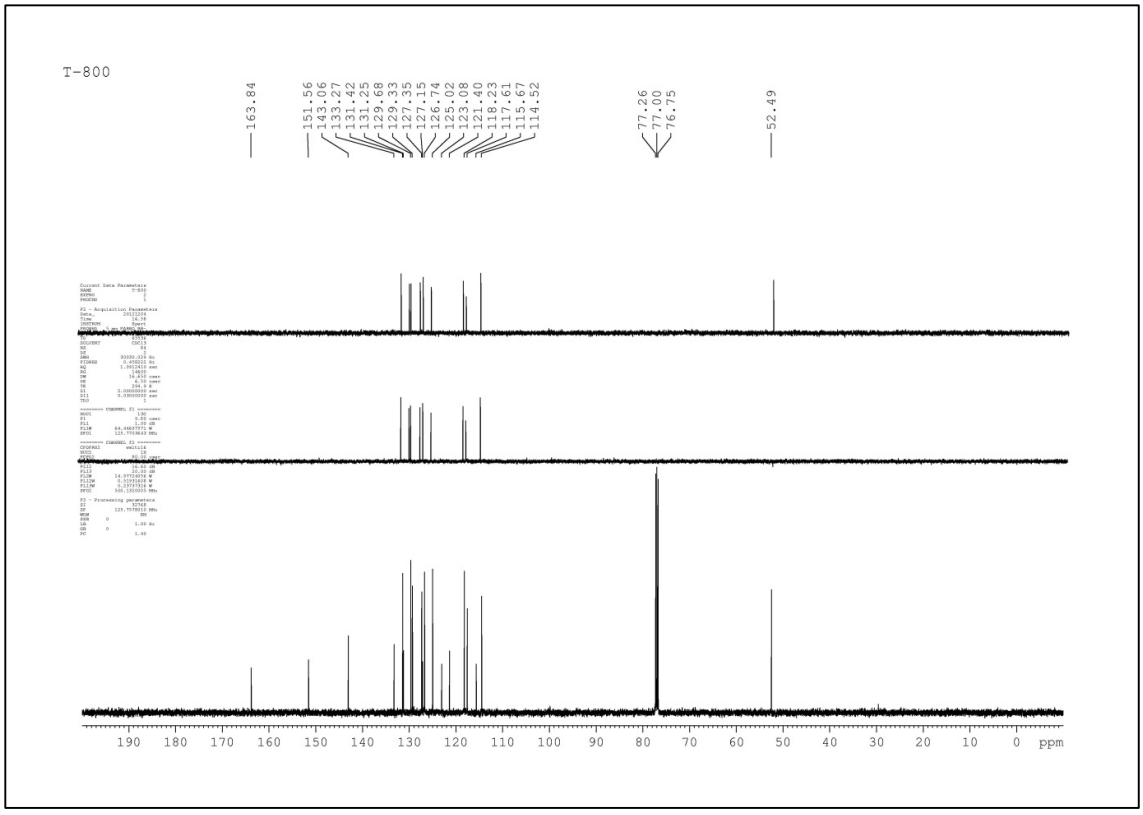

T-772
7.651
7.611
7.608
7.606
7.596
7.592
7.360
7.355
7.345
7.343
7.340
7.335
7.319
7.316
7.308
7.305
7.303
7.300
7.293
7.289
7.278
7.275
7.260
7.176
7.160
3.925
2.345
0.081
-0.000
OMe
O
O
O
N
9b
7.66 ppm
7.60 ppm
7.36 7.34 7.32 7.30 ppm
ppm
1.00
1.05
5.29
2.07
2.98
3.13

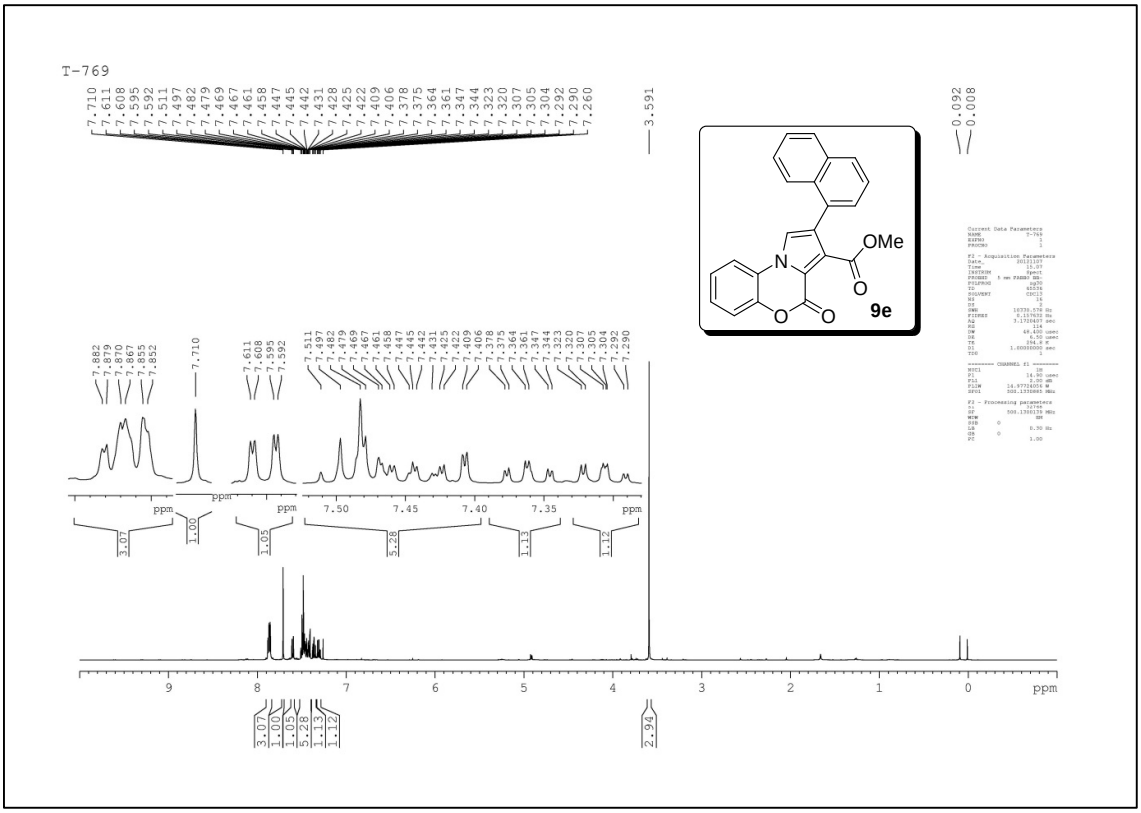

T-772
165.35
152.08
142.94
137.77
129.44
129.23
128.93
127.44
127.06
125.02
121.81
121.50
118.28
115.59
115.55
114.42
77.26
77.00
76.75
52.84
21.14
ppm

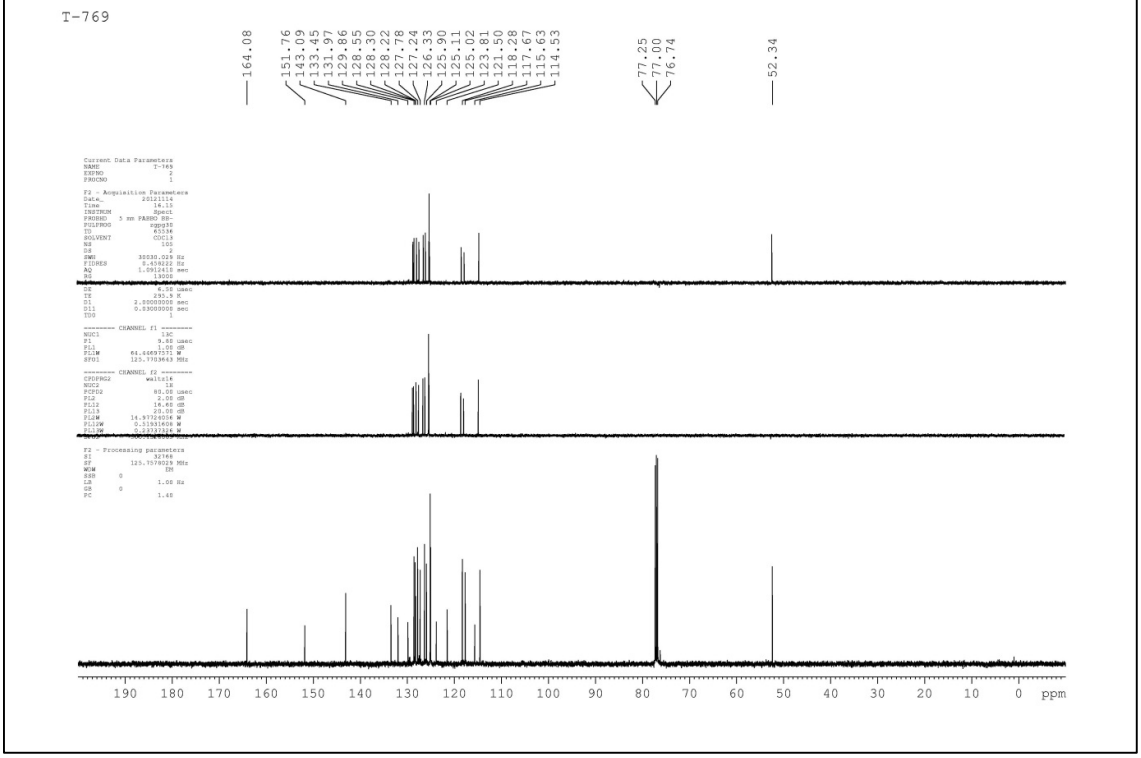

T-774
7.674
7.636
7.634
7.632
7.621
7.617
7.385
7.381
7.372
7.367
7.363
7.360
7.357
7.354
7.344
7.341
7.330
7.326
7.325
7.316
7.314
7.310
7.301
7.296
7.260
3.915
1.248
0.074
0.005
Cl
OMe
N
O
O
O
9c
ppm
7.64
7.38
7.36
7.34
7.32
1.01
0.92
2.06
1.03
1.98
1.91
2.83

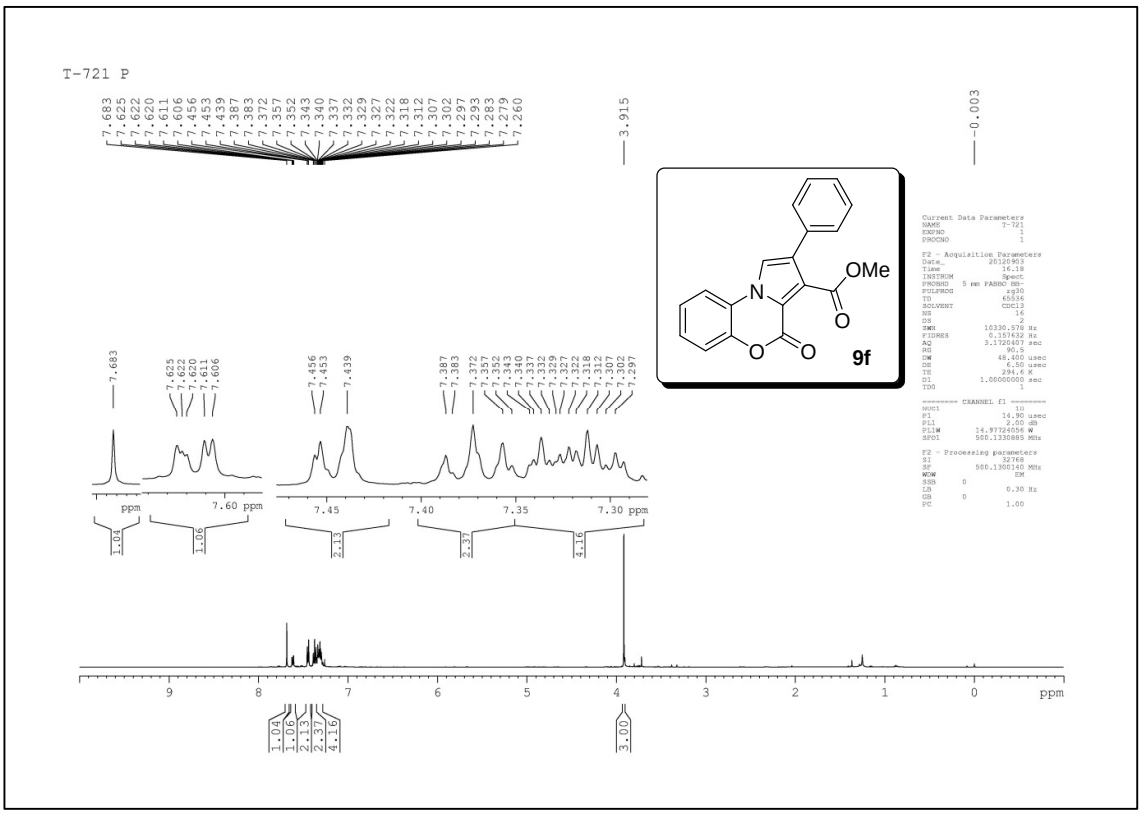

T-774
164.97
151.93
142.99
133.97
130.45
128.99
128.94
128.09
127.36
125.13
121.81
121.38
118.40
115.93
115.71
114.45
77.25
77.00
76.75
52.91
ppm

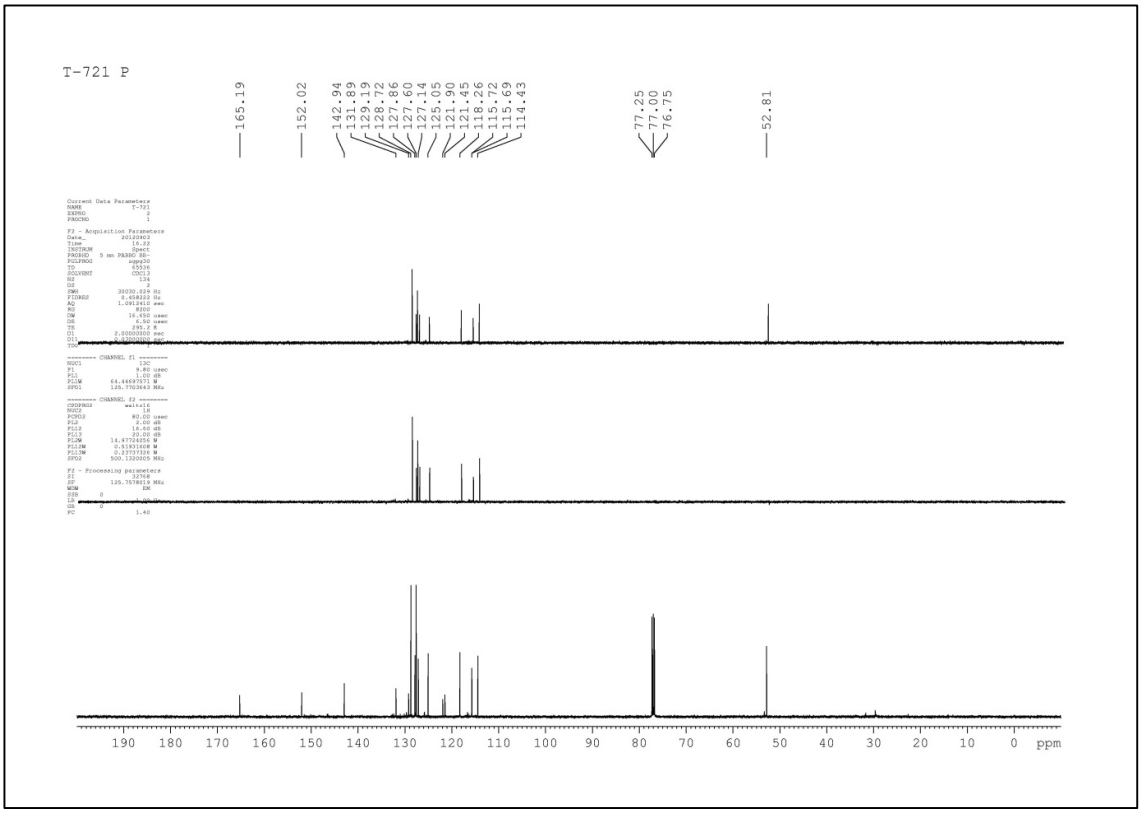

T-800
7.706
7.626
7.612
7.610
7.450
7.444
7.439
7.432
7.380
7.374
7.369
7.362
7.355
7.340
7.338
7.324
7.321
7.318
7.314
7.298
7.291
7.286
7.279
7.260
3.802
Cl
OMe
N
O
O
O
9d
ppm
1.00
1.09
1.09
6.25
3.17

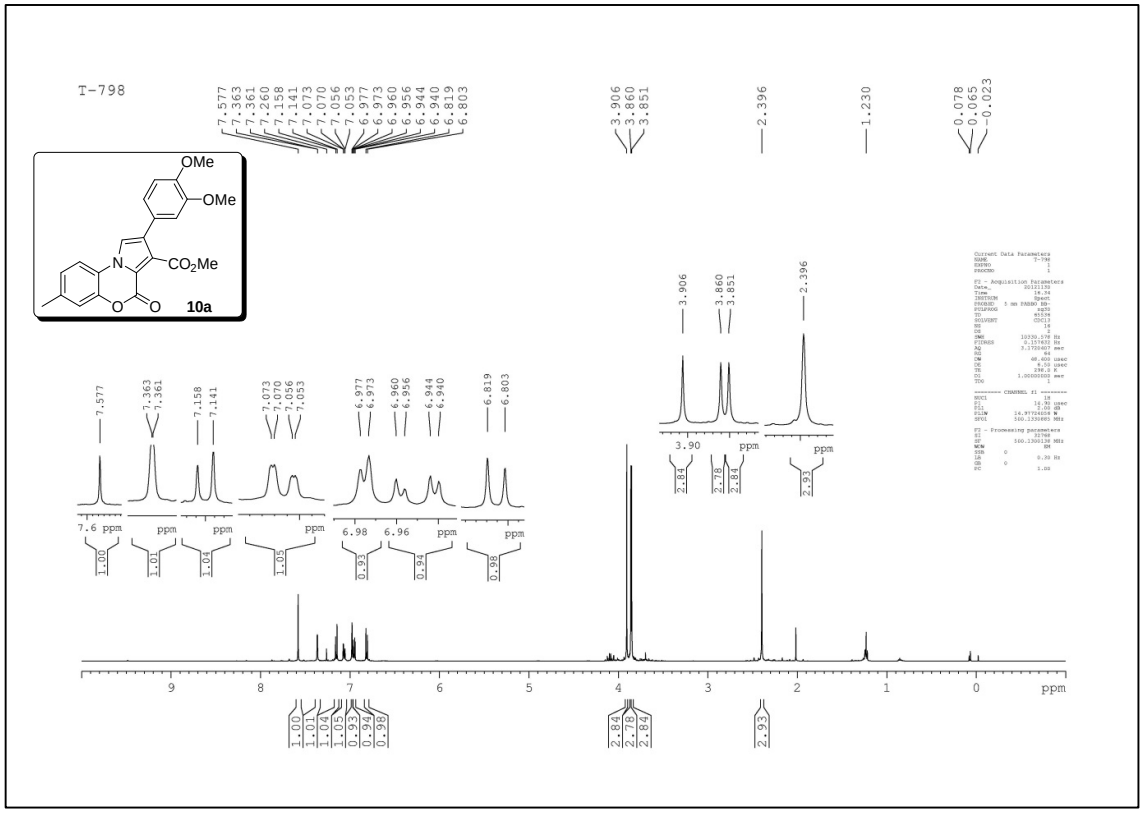

T-800
163.84
151.56
143.06
133.27
131.42
131.25
129.68
129.33
127.35
127.15
126.74
125.02
123.08
121.40
118.23
117.61
115.67
114.52
77.26
77.00
76.75
52.49
ppm

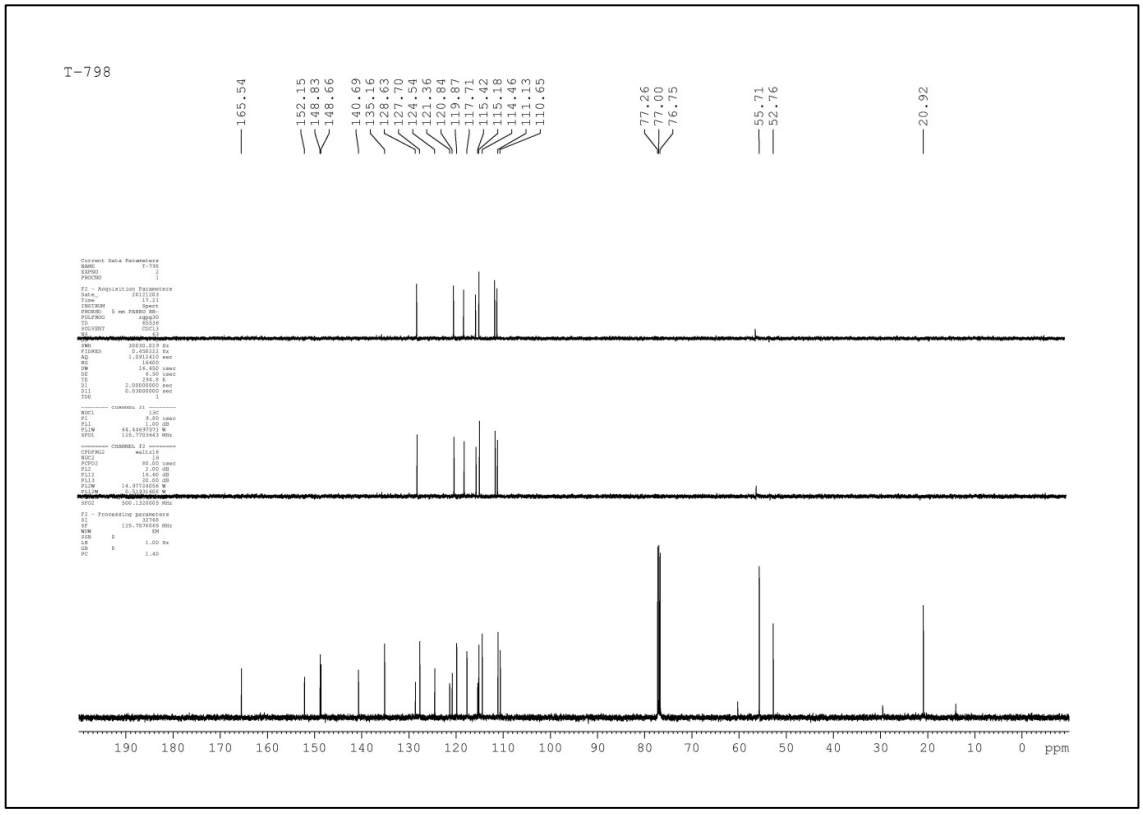

T-769
7.710 7.611 7.608 7.595 7.592 7.511 7.497 7.482 7.479 7.469 7.467 7.461 7.458 7.447 7.445 7.442 7.431 7.428 7.425 7.422 7.409 7.406 7.378 7.375 7.364 7.361 7.347 7.344 7.323 7.320 7.307 7.305 7.304 7.292 7.290 7.260
3.591
0.092
0.008
OMe
O
O
O
9e
7.882 7.879 7.870 7.857 7.855 7.852
7.710
7.611 7.608 7.595 7.592
7.511 7.497 7.482 7.479 7.469 7.467 7.461 7.458 7.447 7.445 7.442 7.431 7.425 7.422 7.409 7.406 7.378 7.375 7.364 7.361 7.344 7.323 7.320 7.307 7.305 7.304 7.292 7.290
ppm
7.50 7.45 7.40 7.35
3.07 1.00 1.05 5.28 1.13 1.12
2.94
9 8 7 6 5 4 3 2 1 0 ppm

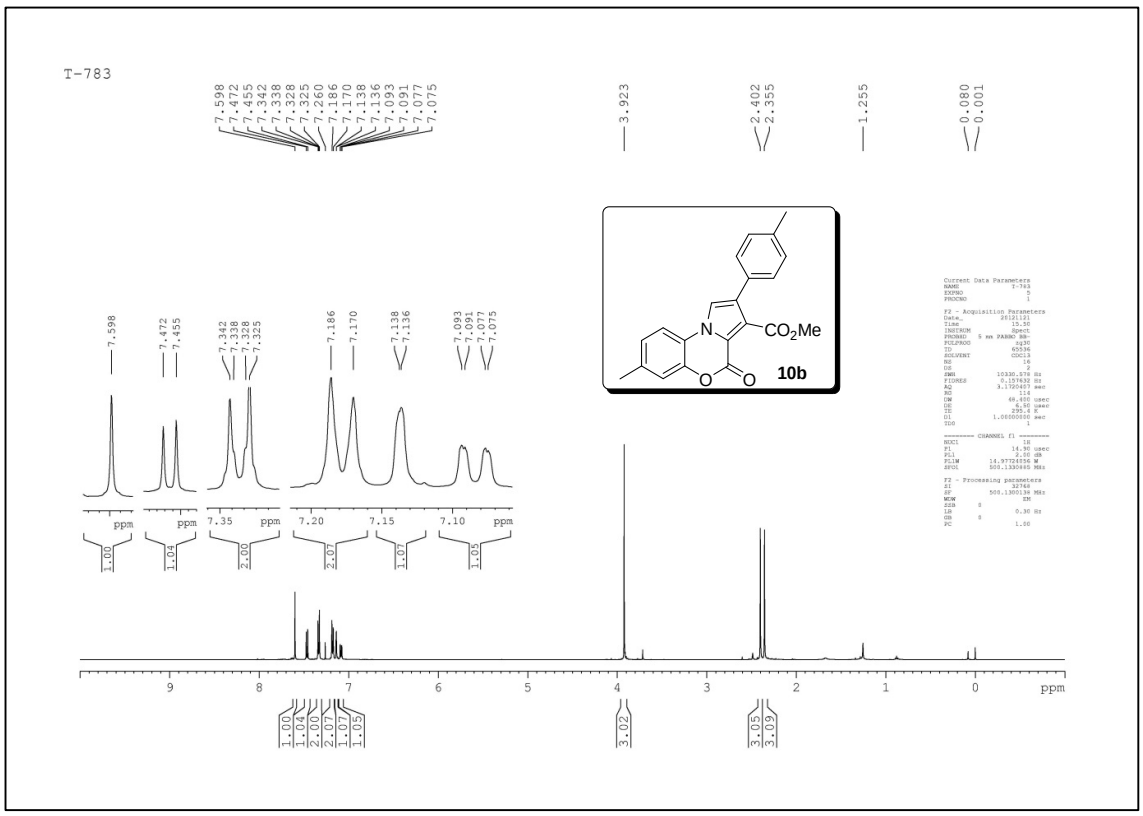

T-769
164.08
151.76 143.09 133.45 131.97 129.66 128.55 128.30 128.22 127.78 127.24 126.33 125.90 125.11 125.02 123.81 121.50 118.28 117.67 115.63 114.53
77.25 77.00 76.74
52.34
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

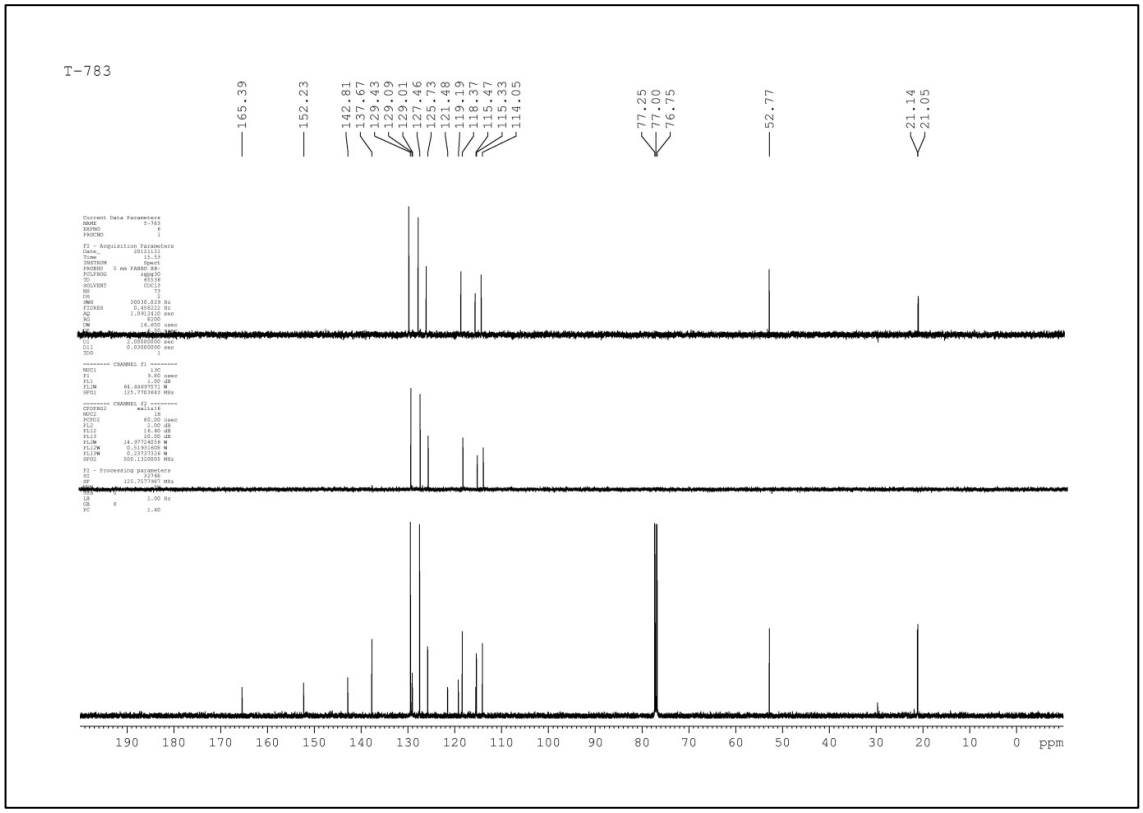

T-721 P
7.683
7.625
7.622
7.620
7.611
7.606
7.456
7.453
7.439
7.387
7.383
7.372
7.357
7.352
7.343
7.340
7.337
7.332
7.329
7.327
7.322
7.318
7.312
7.307
7.302
7.297
7.293
7.283
7.279
7.260
3.915
-0.003
OMe
O
N
O
O
9f
ppm
7.60 ppm
7.45
7.40
7.35
7.30 ppm
1.04
1.06
2.13
2.37
4.16
3.00

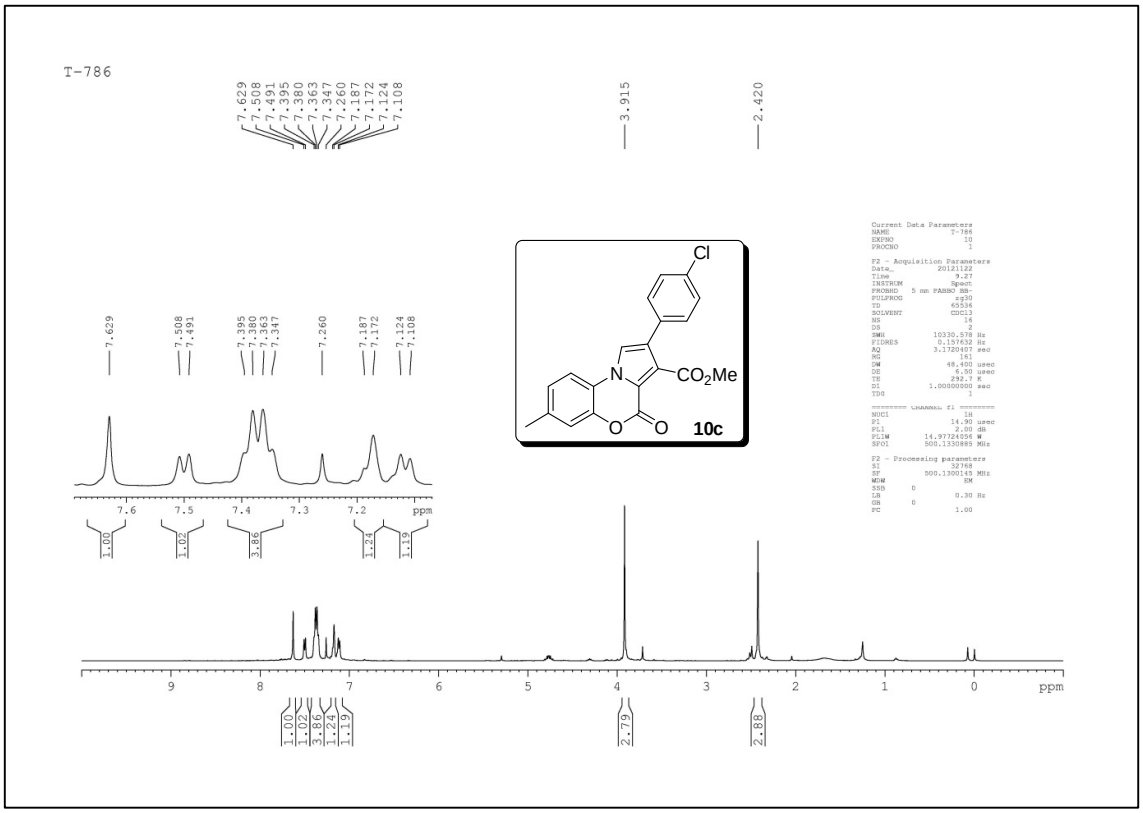

T-721 P
165.19
152.02
142.94
131.89
129.19
128.72
127.86
127.60
127.14
125.05
121.90
121.45
118.26
115.72
115.69
114.43
77.25
77.00
76.75
52.81
ppm

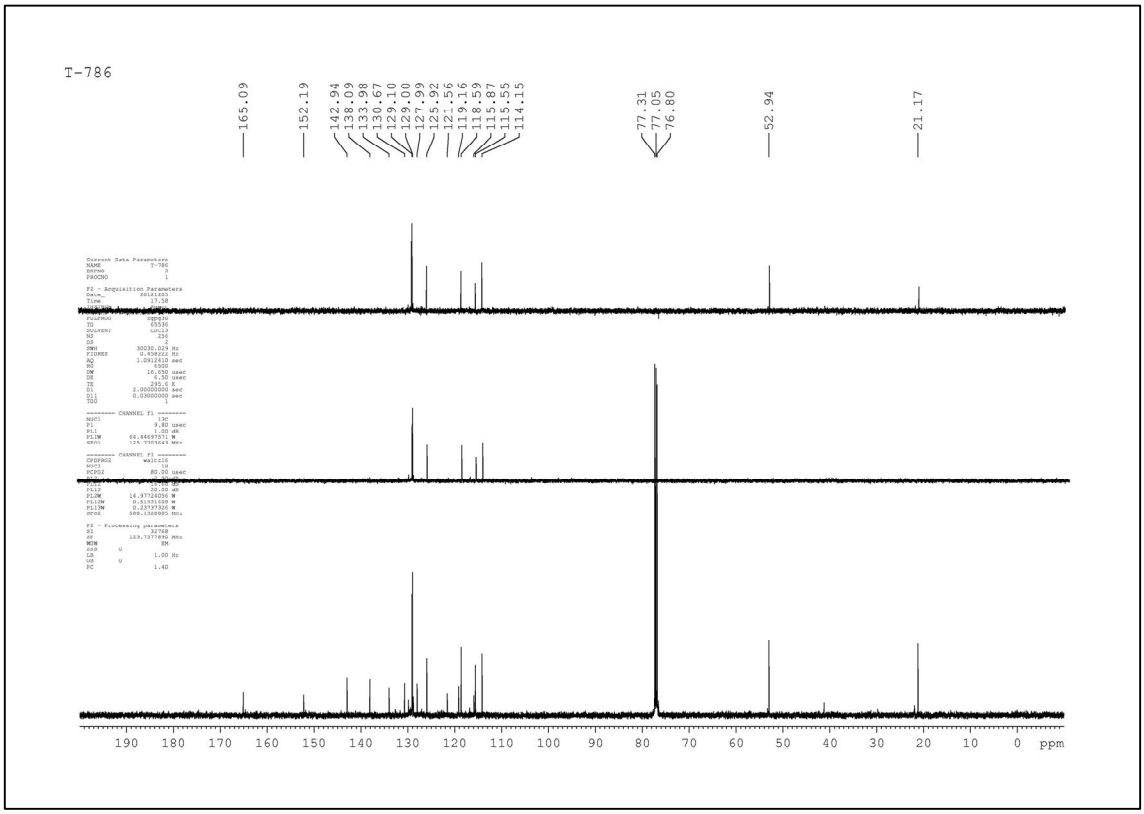

T-798
7.577
7.363
7.361
7.260
7.158
7.141
7.073
7.070
7.056
7.053
6.977
6.973
6.960
6.956
6.944
6.940
6.819
6.803
3.906
3.860
3.851
2.396
1.230
0.078
0.065
-0.023
OMe
OMe
CO2Me
N
O
O
10a
7.6 ppm
6.98
6.96
ppm
3.90
1.00
1.01
1.04
1.05
0.93
0.94
0.98
2.84
2.78
2.84
2.93
9
8
7
6
5
4
3
2
1
0
ppm

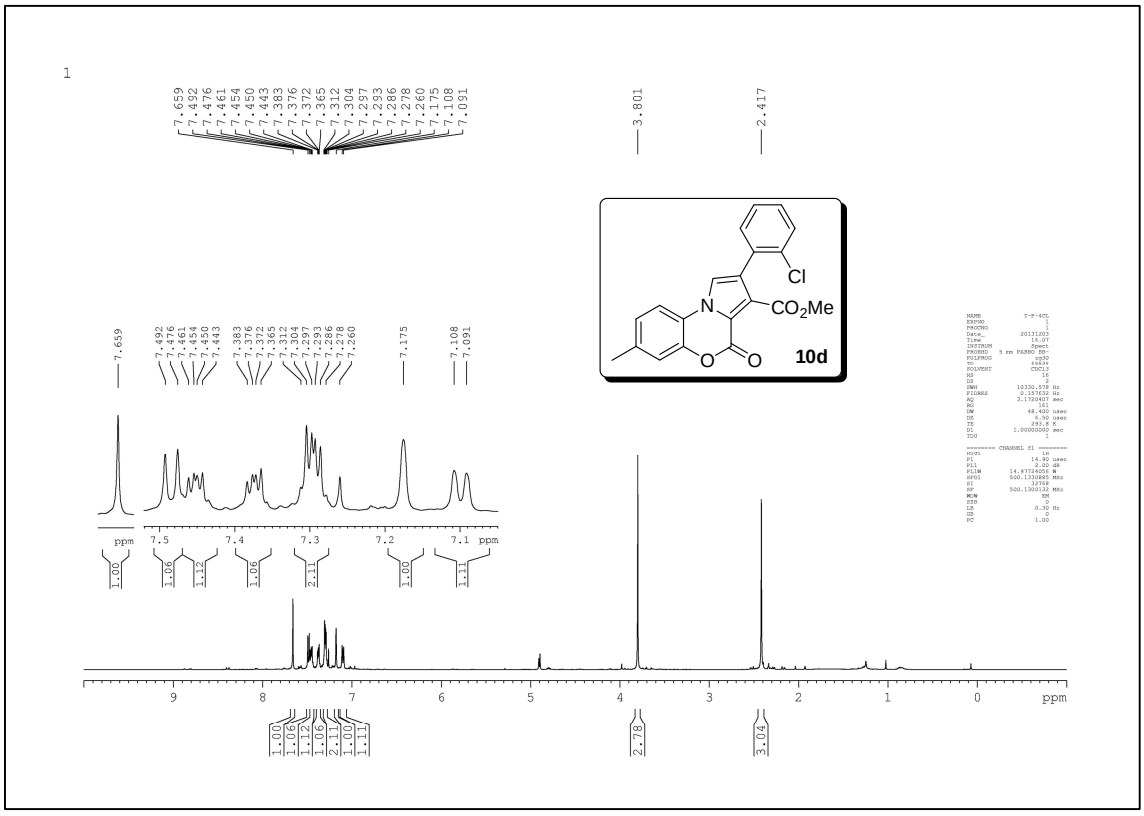

T-798
165.54
152.15
148.83
148.66
140.69
135.16
128.63
127.70
124.54
121.36
120.84
119.87
117.71
115.42
115.18
114.46
111.43
110.65
77.26
77.00
76.75
55.71
52.76
20.92
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

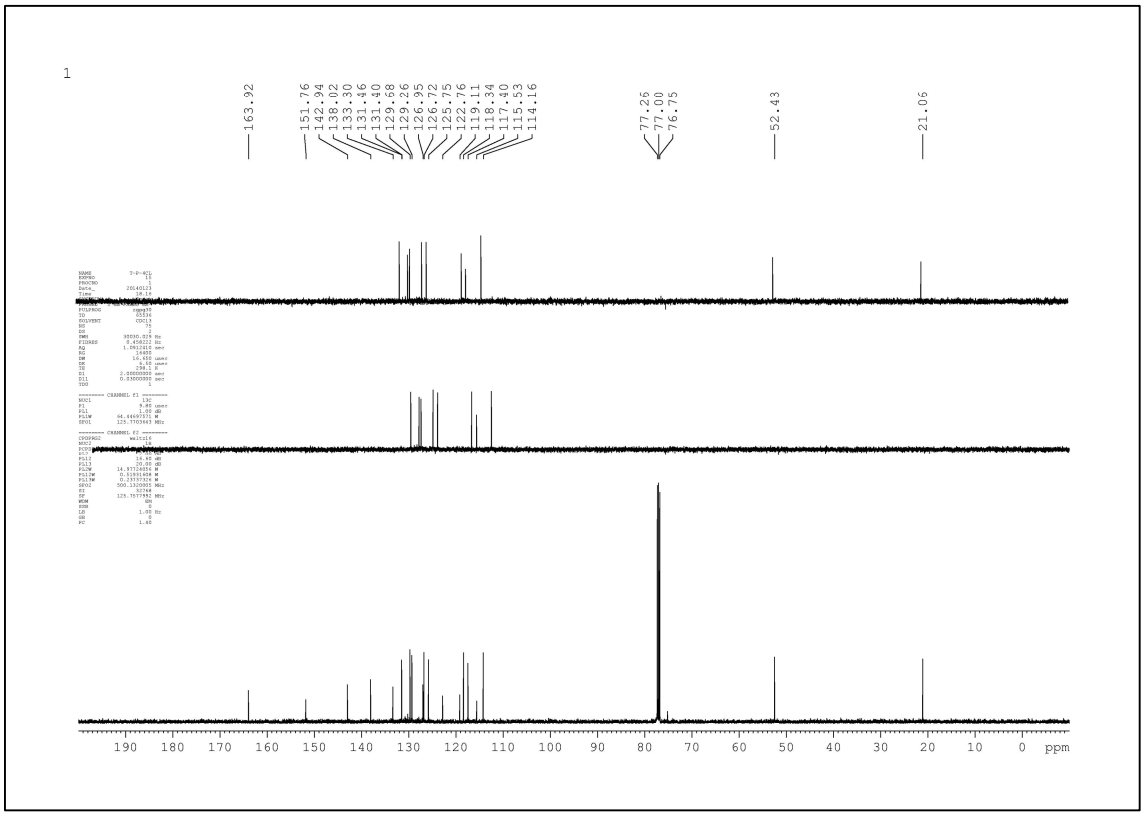

T-783
7.598
7.472
7.455
7.342
7.338
7.328
7.325
7.260
7.186
7.170
7.138
7.136
7.093
7.091
7.077
7.075
3.923
2.402
2.355
1.255
0.080
0.001
CO2Me
10b
ppm
1.00
1.04
2.00
2.07
1.07
1.05
3.02
3.05
3.09

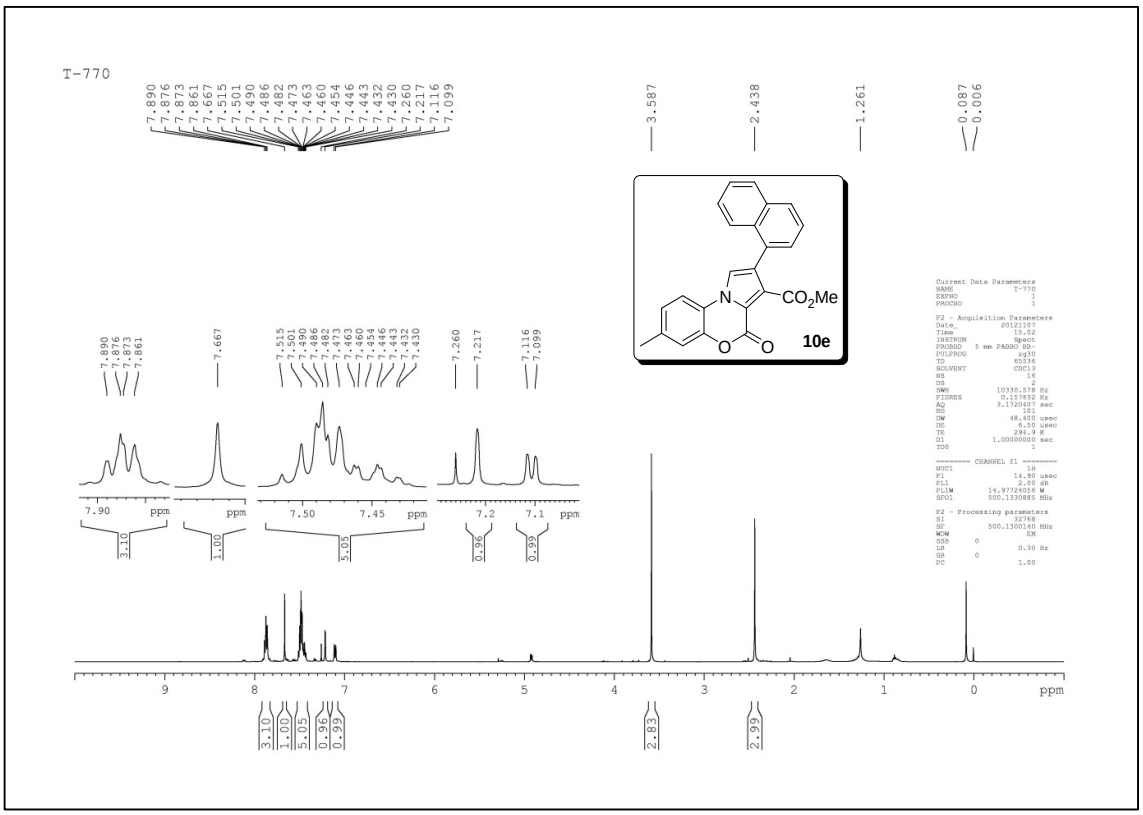

T-783
165.39
152.23
142.81
137.67
129.43
129.09
129.01
127.46
125.73
121.48
119.19
118.37
115.47
115.33
114.05
77.25
77.00
76.75
52.77
21.14
21.05
ppm

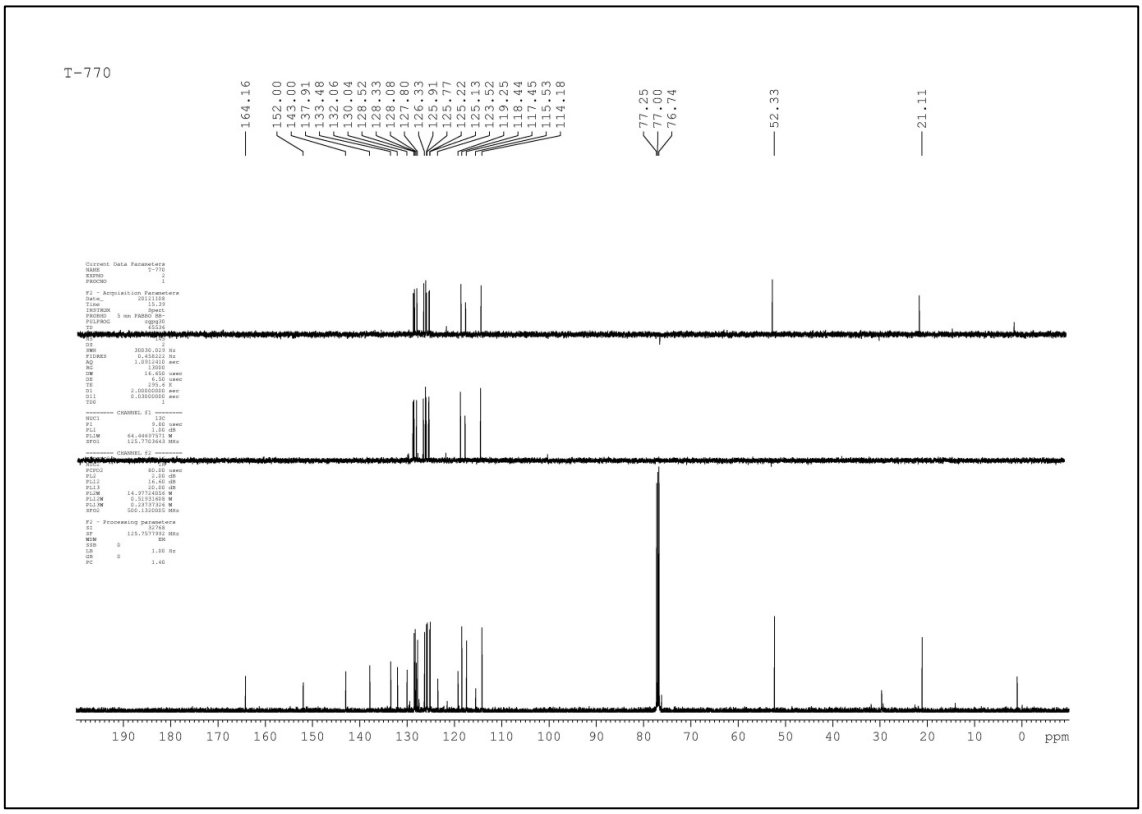

T-786
7.629
7.508
7.491
7.395
7.380
7.363
7.347
7.260
7.187
7.172
7.124
7.108
3.915
2.420
Cl
N
CO2Me
O
O
10c
ppm
1.00
1.02
3.86
1.24
1.19
2.79
2.88

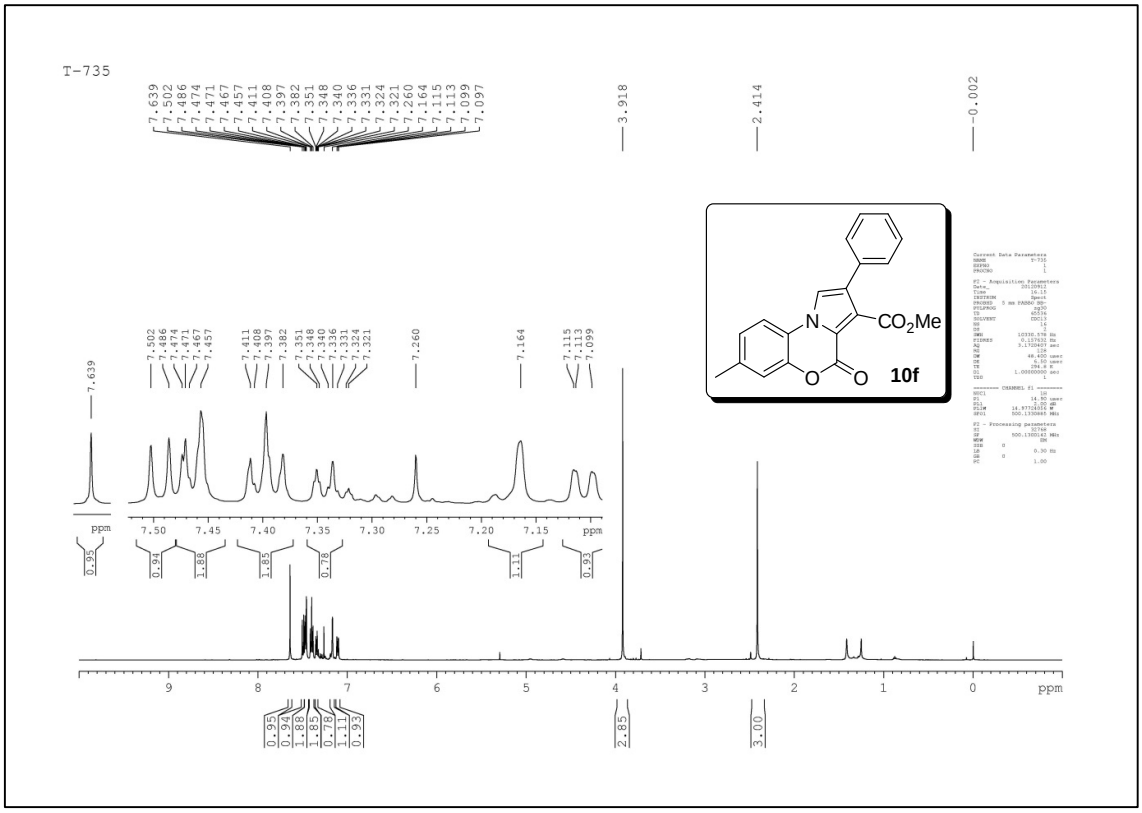

T-786
165.09
152.19
142.94
138.09
133.98
130.67
129.10
129.00
127.99
125.92
123.56
119.16
118.59
116.87
115.55
114.15
77.31
77.05
76.80
52.94
21.17
ppm

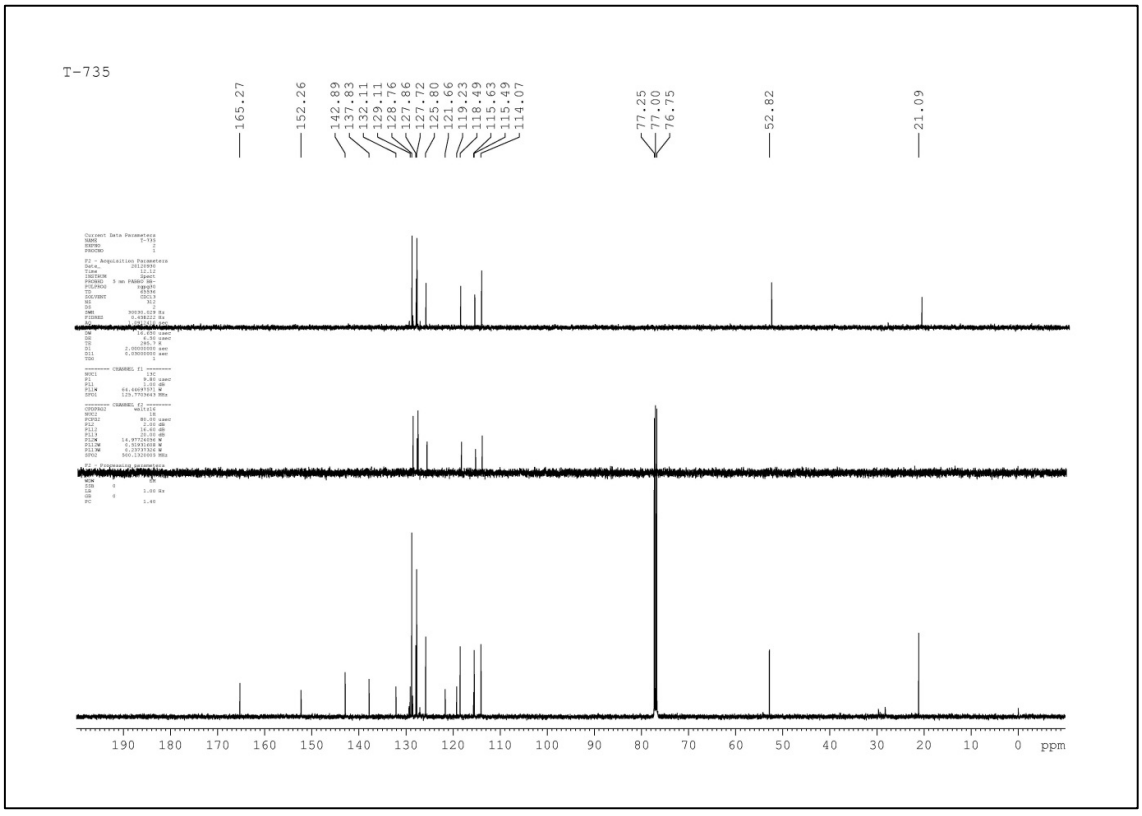

7.659
7.492
7.476
7.461
7.454
7.450
7.443
7.383
7.376
7.372
7.365
7.312
7.304
7.297
7.293
7.286
7.278
7.260
7.175
7.108
7.091
3.801
2.417
Cl
N
CO2Me
O
O
10d
ppm
1.00
1.06
1.12
1.06
2.11
1.00
1.11
2.78
3.04

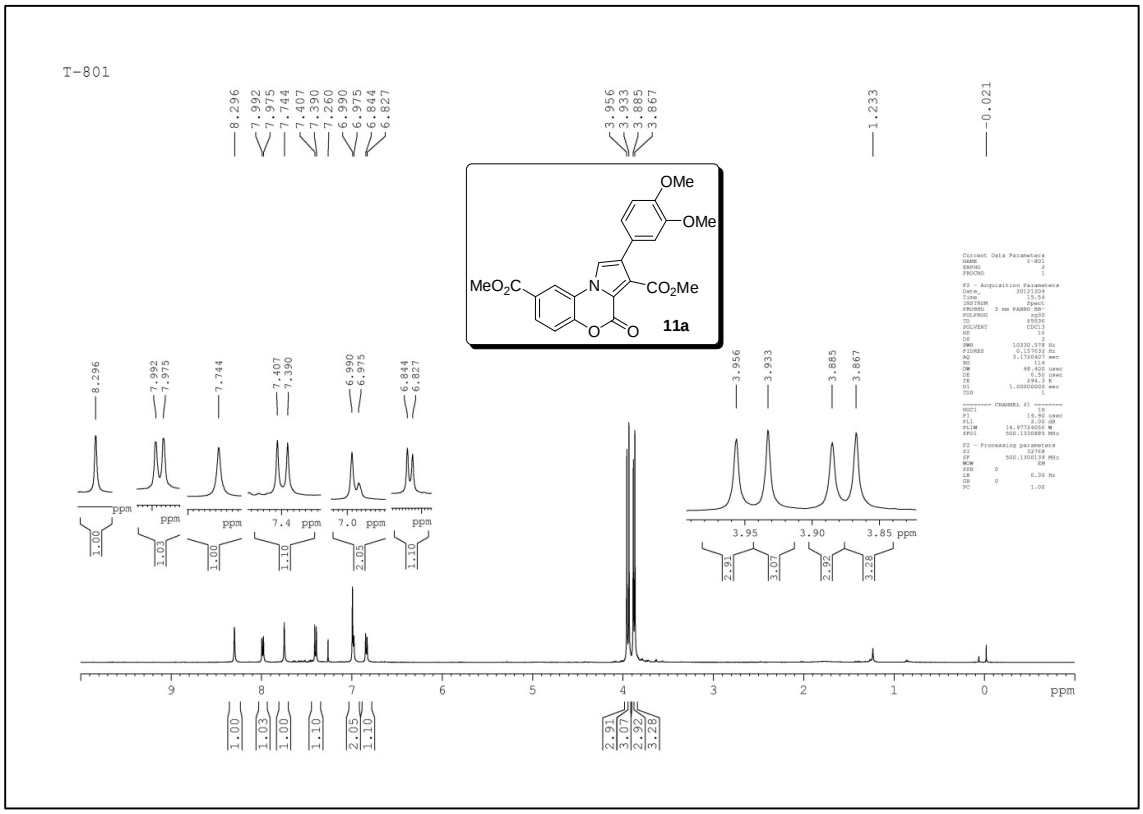

163.92
151.76
142.94
138.02
133.30
131.46
131.40
129.68
129.26
126.95
126.72
125.75
122.76
119.11
118.34
117.40
115.53
114.16
77.25
77.00
76.75
52.43
21.05
ppm

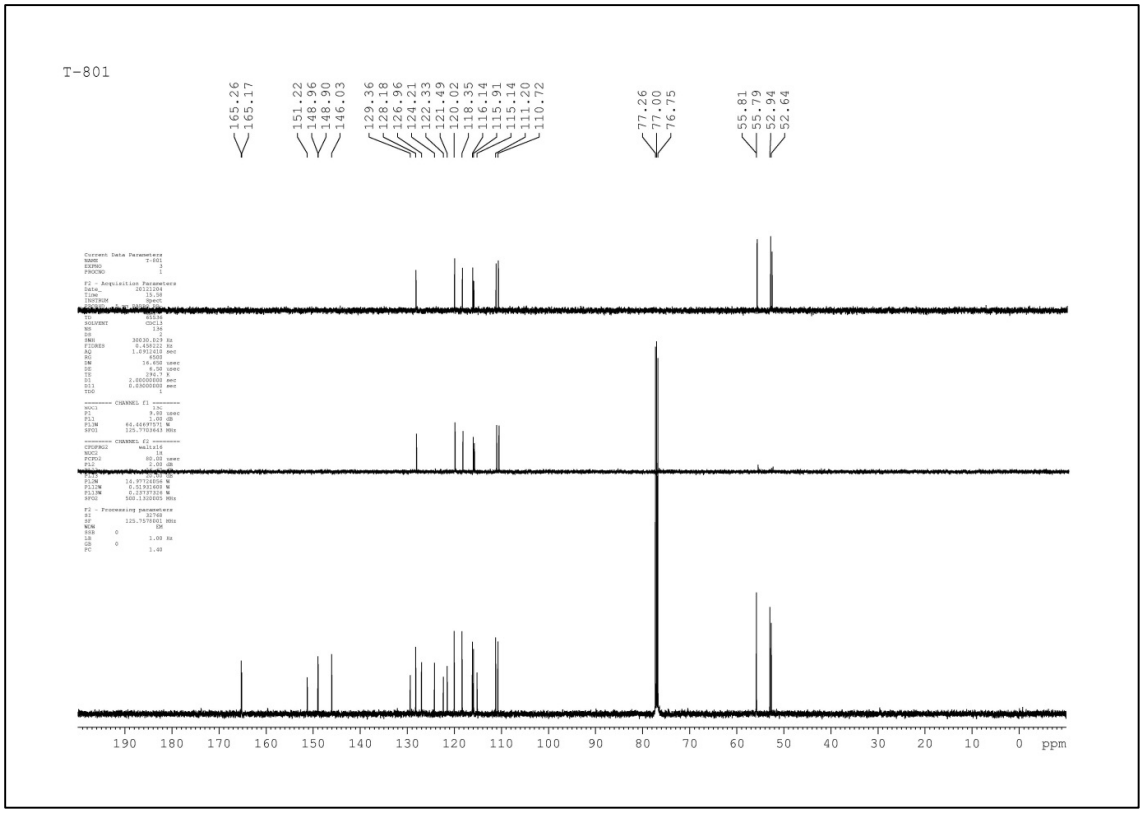

T-770
7.890
7.876
7.873
7.861
7.667
7.515
7.501
7.490
7.486
7.482
7.473
7.463
7.460
7.454
7.446
7.443
7.432
7.430
7.260
7.217
7.116
7.099
3.587
2.438
1.261
0.087
0.006
CO2Me
10e
ppm


T-770
164.16
152.00
143.00
137.91
133.48
132.06
130.04
128.52
128.33
128.08
127.80
126.33
125.91
125.77
125.22
125.13
123.52
119.25
118.44
117.45
117.53
114.18
77.25
77.00
76.74
52.33
21.11
ppm

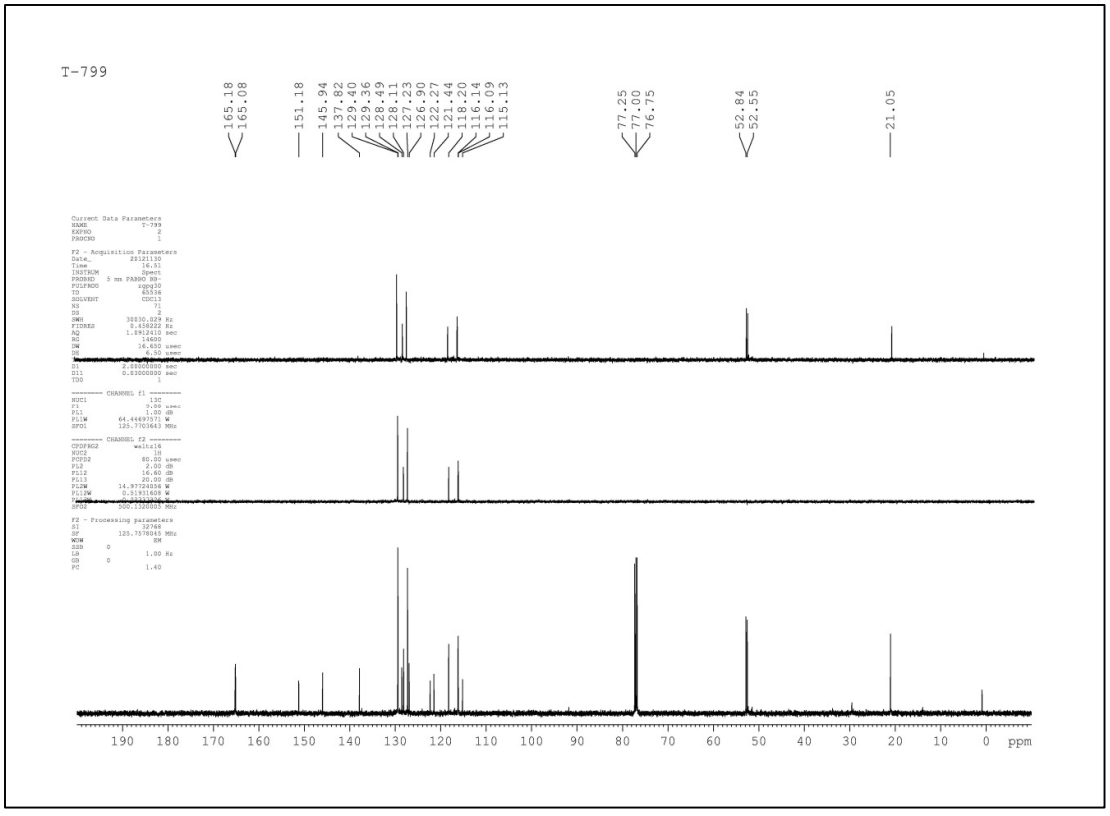

T-735
7.639
7.502
7.486
7.474
7.471
7.467
7.457
7.411
7.408
7.397
7.382
7.351
7.348
7.340
7.336
7.331
7.324
7.321
7.260
7.164
7.115
7.113
7.099
7.097
3.918
2.414
0.002
CO2Me
O
O
10f
ppm
0.95
0.94
1.88
1.85
0.78
1.11
0.93
2.85
3.00

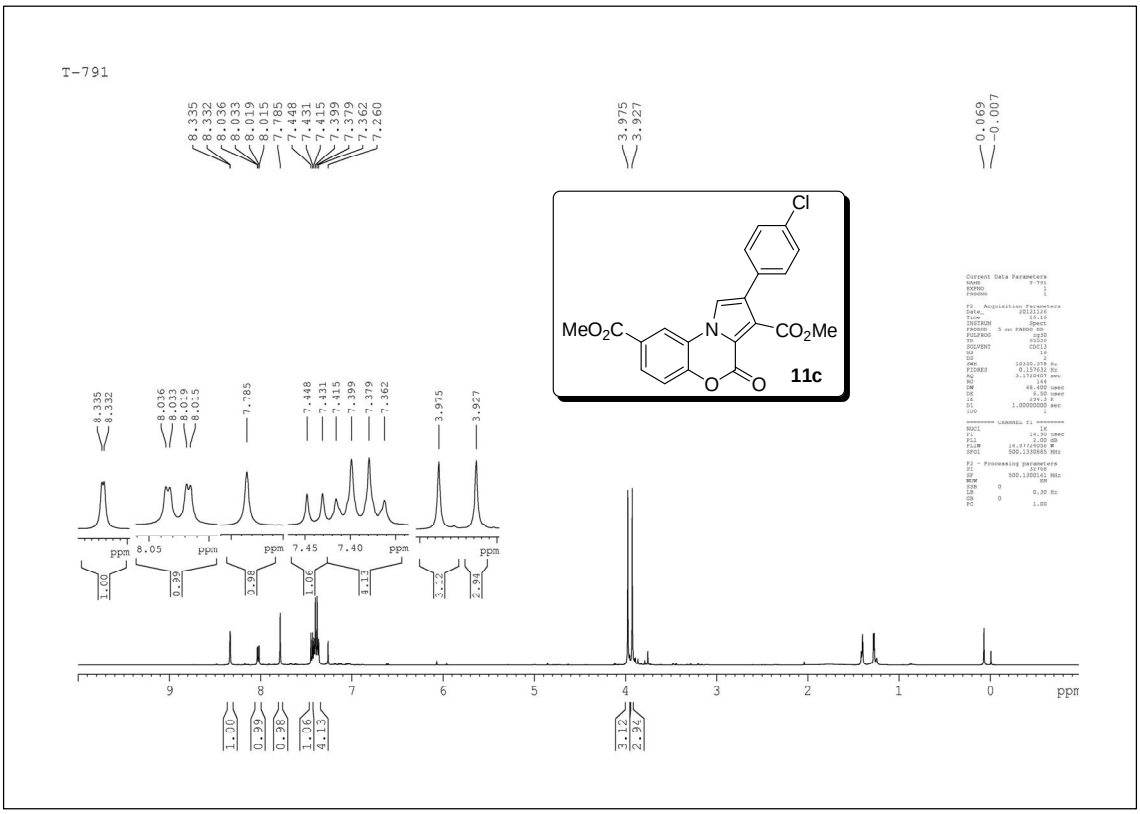

T-735
165.27
152.26
142.89
137.83
132.11
129.11
128.76
127.86
127.72
125.80
121.66
119.23
118.49
115.63
115.49
114.07
77.25
77.00
76.75
52.82
21.09
ppm

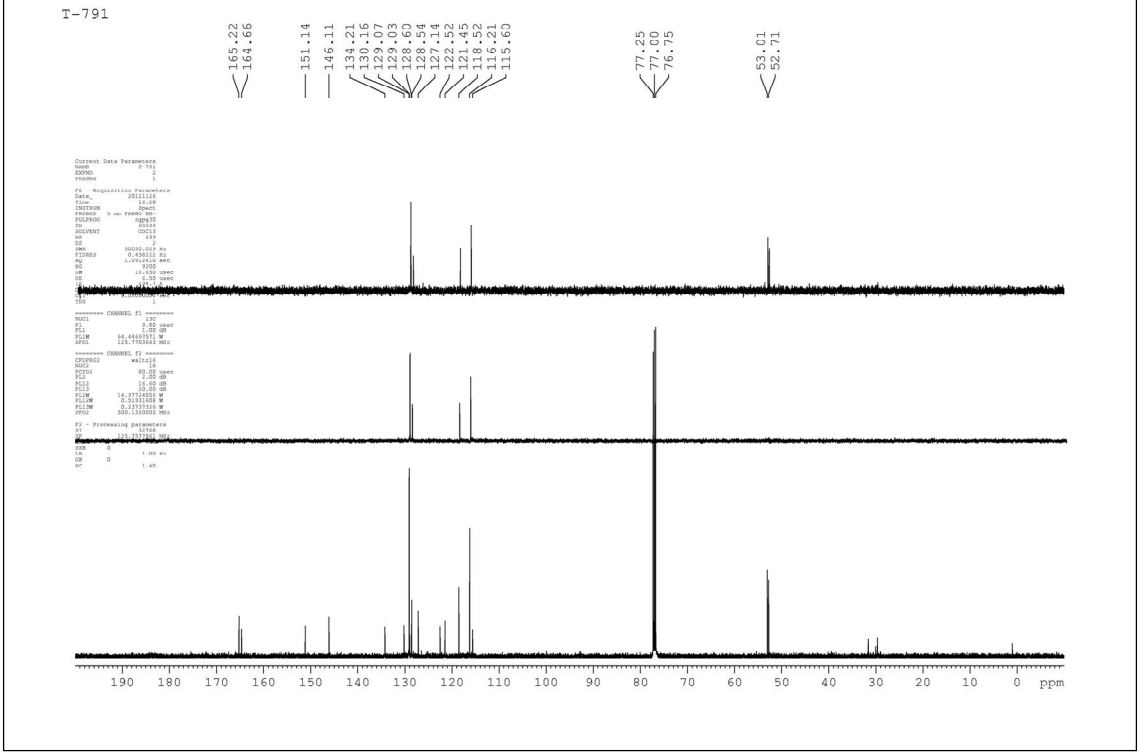

T-801
8.296
7.992
7.975
7.744
7.407
7.390
7.260
6.990
6.975
6.844
6.827
3.956
3.933
3.885
3.867
1.233
0.021
OMe
OMe
MeO2C
N
CO2Me
O
O
11a
ppm

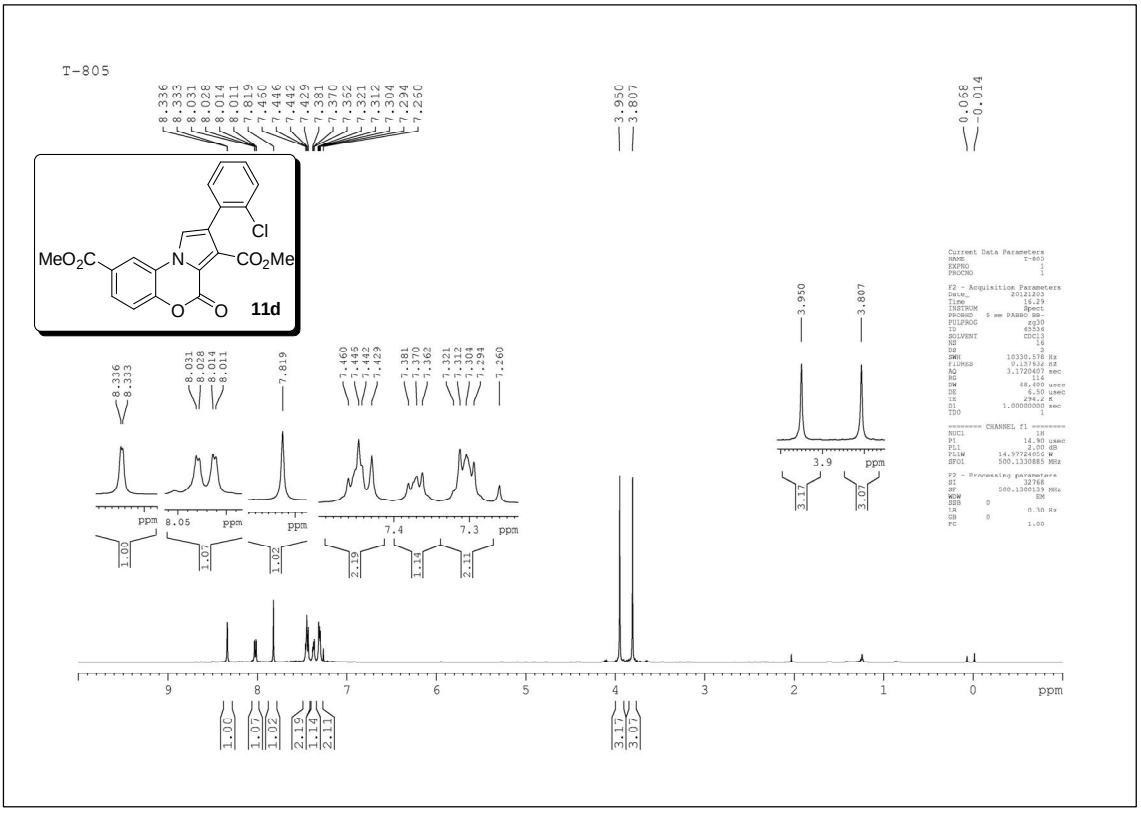

T-801
165.26
165.17
151.22
148.96
148.90
146.03
129.36
128.18
126.96
124.21
122.33
121.49
120.02
118.35
116.14
115.91
115.14
111.20
110.72
77.26
77.00
76.75
55.81
55.79
52.94
52.64
ppm

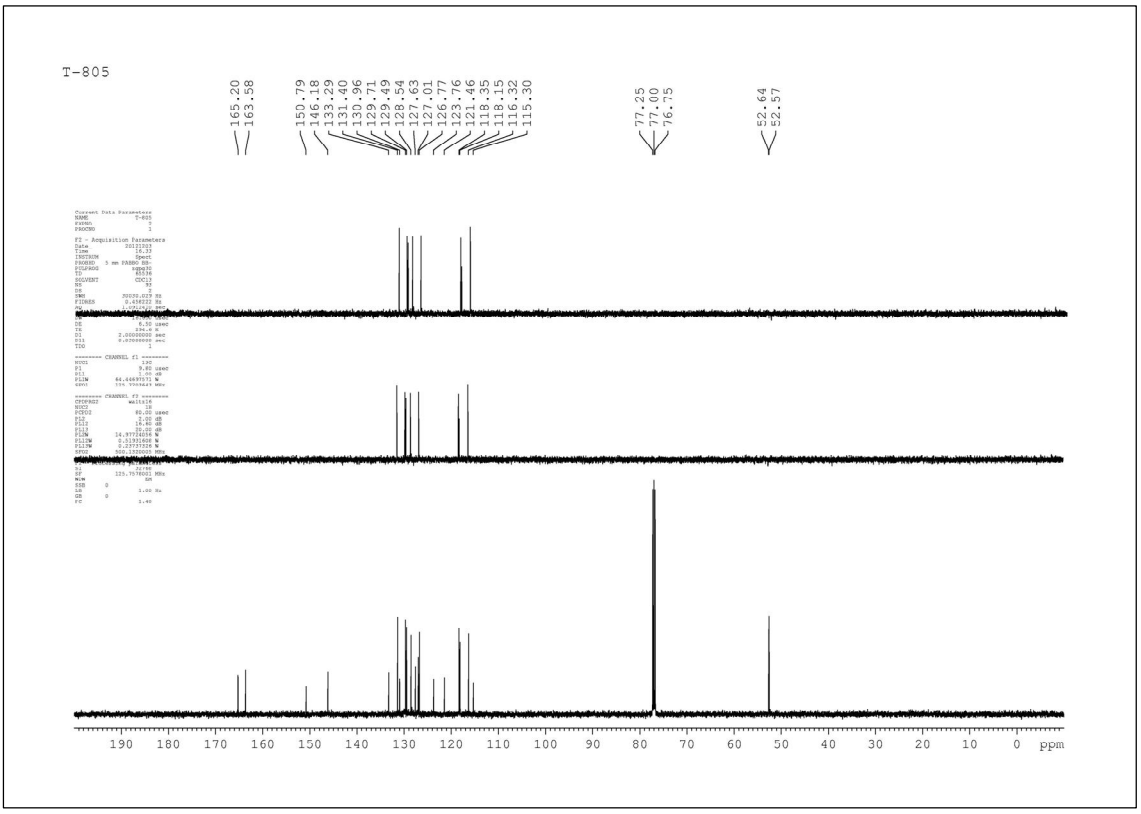

T-799
8.281
7.986
7.969
7.755
7.393
7.376
7.309
7.294
7.147
7.131
3.959
3.946
2.329
1.266
0.106
0.013
MeO2C
CO2Me
11b
ppm
1.00
1.09
1.07
1.11
2.24
2.26
2.83
2.89
3.35

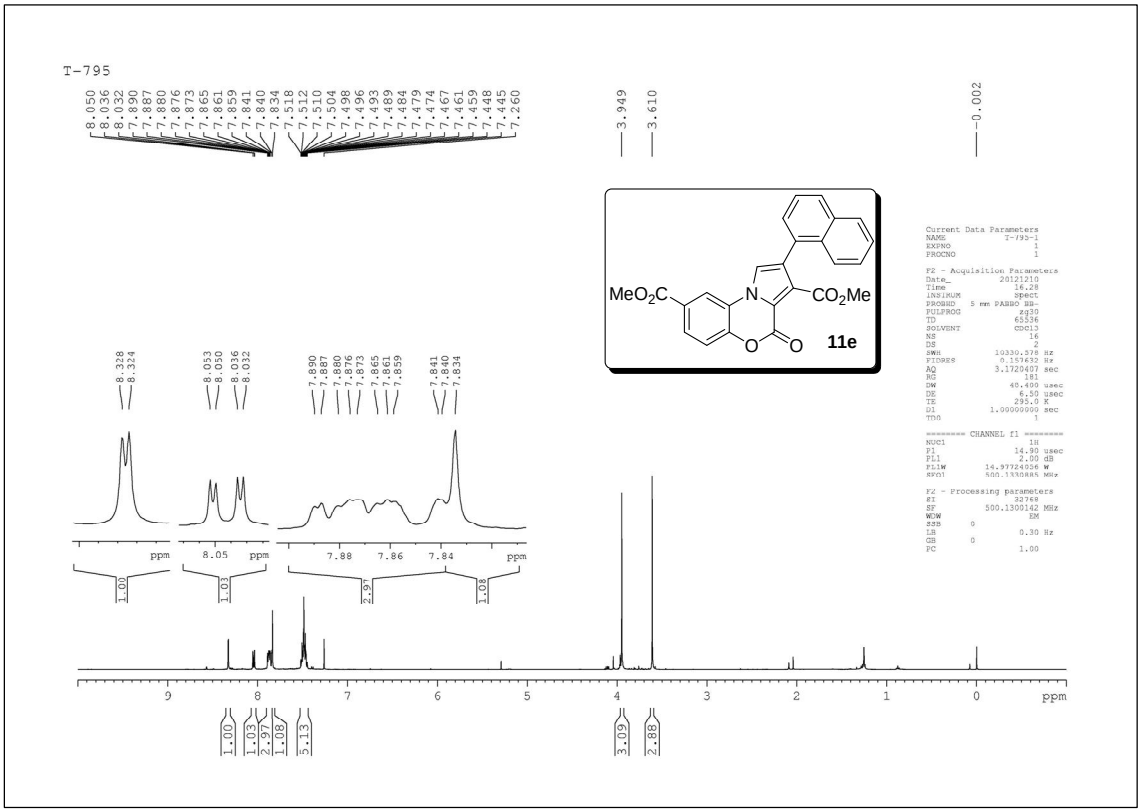

T-799
165.18
165.08
151.18
145.94
137.82
129.40
129.36
128.49
128.11
127.23
126.90
122.27
118.24
116.14
116.03
115.13
77.25
77.00
76.75
52.84
52.55
21.05
ppm

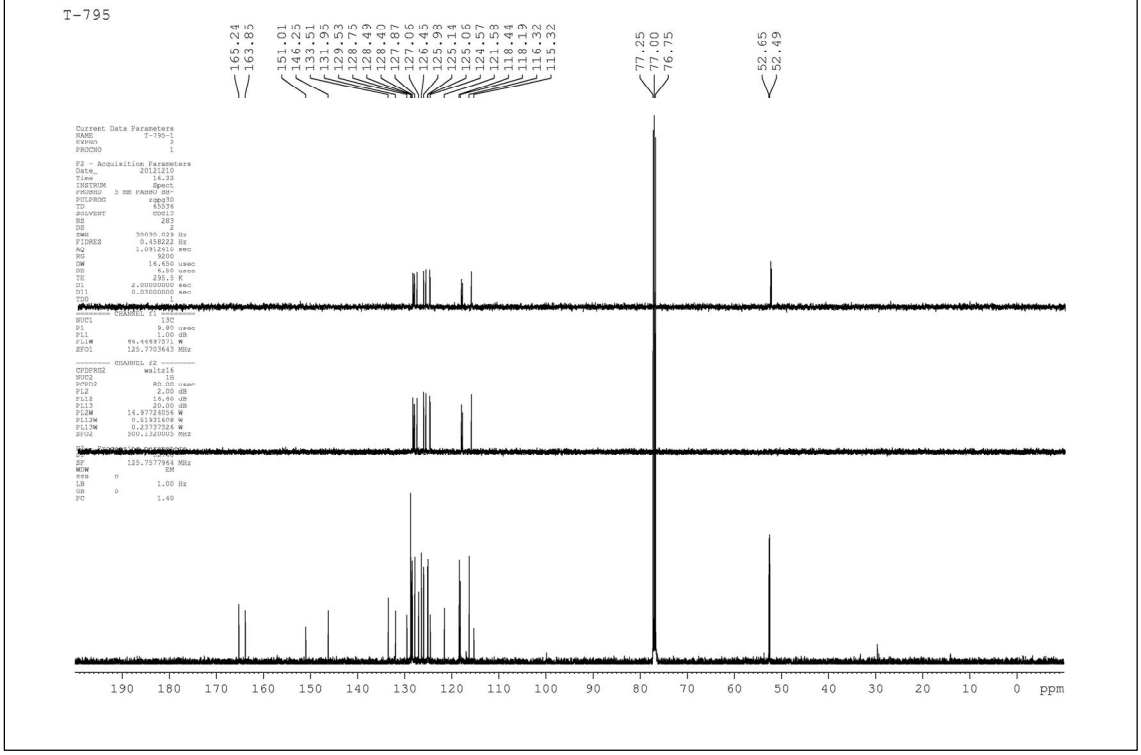

T-791
8.335
8.332
8.036
8.033
8.019
8.015
7.785
7.448
7.431
7.415
7.399
7.379
7.362
7.260
3.975
3.927
0.069
-0.007
Cl
MeO2C
N
CO2Me
O
O
11c
ppm
1.00
0.99
0.98
1.06
4.13
3.12
2.94

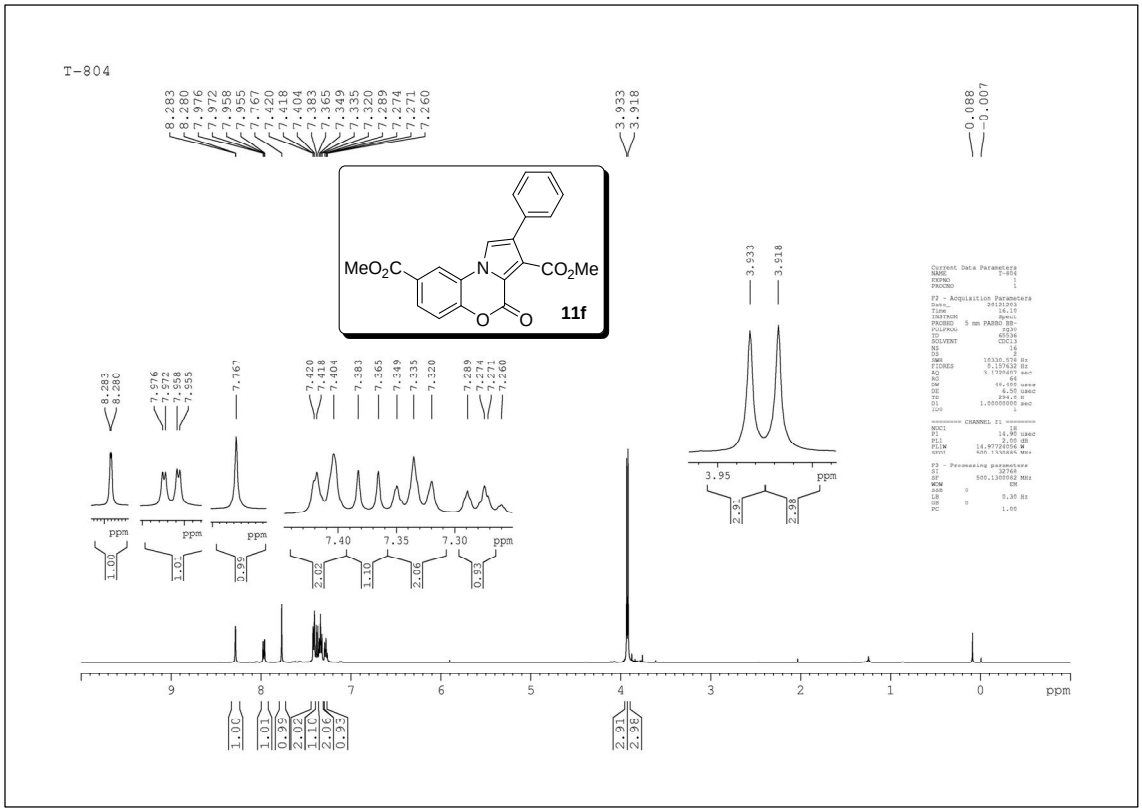

T-791
165.22
164.66
151.14
146.11
134.21
130.16
129.07
129.03
128.60
128.54
127.14
122.52
121.45
118.52
116.21
115.60
77.25
77.00
76.75
53.01
52.71
ppm

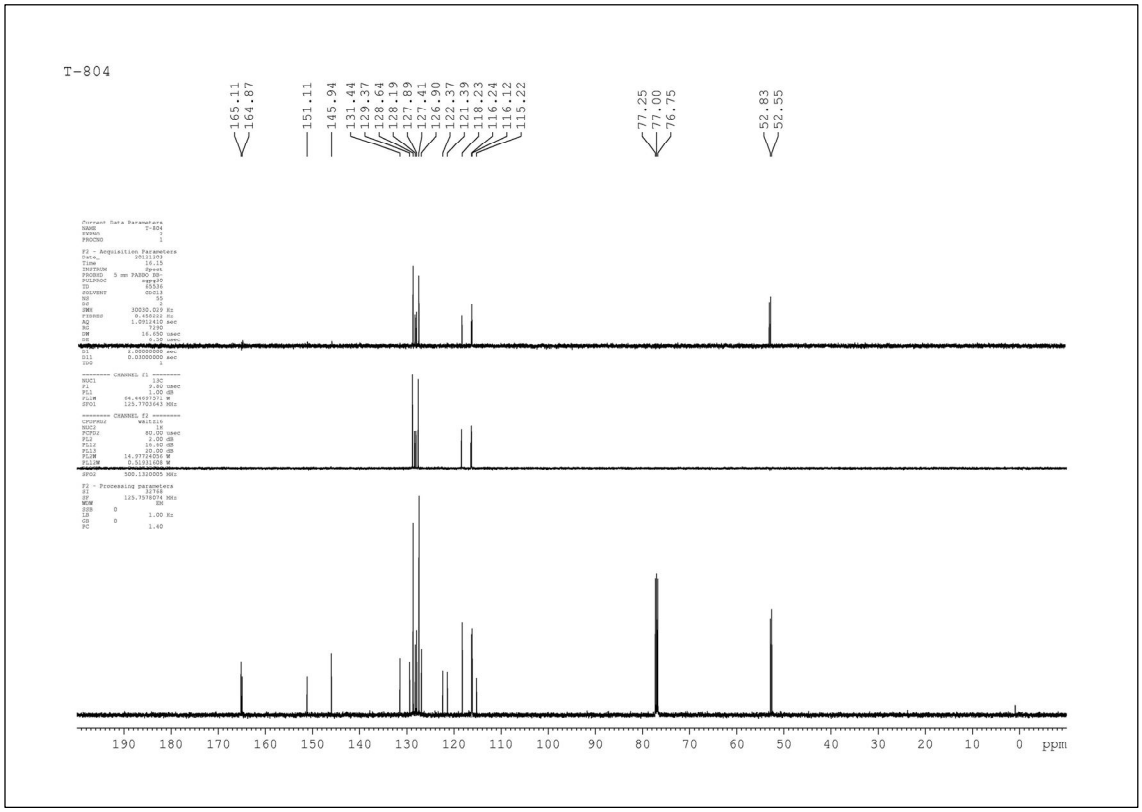

T-805
11d


T-805


T-795
8.050
8.036
8.032
7.890
7.887
7.880
7.876
7.873
7.865
7.861
7.859
7.841
7.840
7.834
7.518
7.512
7.510
7.504
7.498
7.496
7.493
7.489
7.484
7.479
7.474
7.467
7.461
7.459
7.448
7.445
7.260
3.949
3.610
0.002
MeO2C
CO2Me
11e
8.328
8.324
8.053
8.050
8.036
8.032
7.890
7.887
7.880
7.875
7.865
7.861
7.859
7.841
7.840
7.834
ppm
8.05
7.88
7.86
7.84
1.00
1.03
2.97
1.08
5.13
3.09
2.88


T-795
165.24
163.85
151.01
146.25
133.51
131.95
129.53
128.75
128.49
128.40
127.87
127.05
126.45
125.98
125.14
125.05
124.57
121.53
118.44
118.19
116.32
115.32
77.25
77.00
76.75
52.65
52.49
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


T-804
8.283
8.280
7.976
7.972
7.958
7.955
7.767
7.420
7.418
7.404
7.383
7.365
7.349
7.335
7.320
7.289
7.274
7.271
7.260
3.933
3.918
0.088
0.007
MeO2C
N
CO2Me
O
O
11f
ppm
1.00
1.01
0.98
2.02
1.10
2.06
0.93
2.91
2.98


T-804
165.11
164.87
151.11
145.94
131.44
129.37
128.64
128.19
127.89
127.41
126.90
122.37
121.39
118.23
116.24
116.12
115.22
77.25
77.00
76.75
52.83
52.55
ppm