

## Supplementary information

### Two Step, One-Pot Sequential Synthesis of Functionalized Hybrid Polyheterocyclic Scaffolds *via* Solid State Melt Reaction

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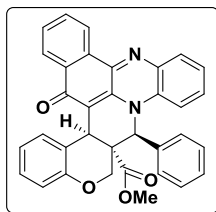
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## 1) Experimental Section

**General Remarks:** Melting points were recorded on a Superfit (India) capillary melting point apparatus and were uncorrected. IR spectra were recorded on a Bruker-FT-IR spectrometer using solid samples as KBr plates. For compounds (**4a-q**, **6a-f** & **8a-d**) spectra were recorded  $^1\text{H}$  NMR (300 MHz and 400 MHz) and  $^{13}\text{C}$  NMR (75 MHz and 100 MHz) in deuteriochloroform ( $\text{CDCl}_3$ ) on a Bruker 300 MHz and 400 MHz spectrometer using tetramethylsilane (TMS,  $\delta = 0$ ) as an internal standard at room temperature. Mass spectra were recorded on Agilent 6530 ESI-MS mass spectrometer.

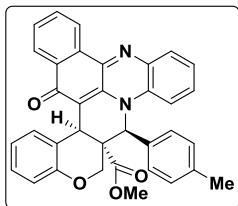
### Typical experimental procedure for the synthesis of Methyl-5-oxo-16-phenyl-4b,5-dihydro-16H-benzo[a]chromeno [4',3':4,5] pyrido[3,2,1-de]phenazine-16a (17H)-carboxylate (**4a**)

A mixture of 2-hydroxynaphthalene-1,4-dione (**2**) (0.35 g, 2 mmol) and *o*-phenylenediamine (**1**) (0.21 g, 2 mmol) melted at 180 °C over the period 10 min to form the benzo[a]phenazin-5-ol after that (*E*)-methyl 2-((2-formylphenoxy)methyl)-3-phenylacrylate (**3a**) (0.6 g, 2 mmol) was added to the reaction mixture and raise the temperature to 180 °C for 1 h. After completion of the reaction as indicated by TLC, The crude product obtained was purified by column chromatography on silica gel (Acme 60-120 mesh), using ethylacetate and hexane (1:9) to afford the compound (**4a**).



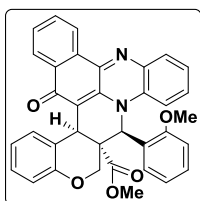
Red color solid; Yield: 78%; mp.: 210 – 212 °C; IR (KBr):  $\nu$  1734, 1708, 1649  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.60 (s, 3H), 4.66 (d, 1H,  $J = 11.7$  Hz), 4.85 (d, 1H,  $J = 11.7$  Hz), 5.51 (s, 1H), 5.90 (d, 1H,  $J = 9.3$  Hz), 6.44 (s, 1H), 6.61 – 9.04 (m, 16H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.9, 45.1, 53.6, 62.1, 66.9, 107.5, 114.1, 114.9, 120.8, 121.5, 124.0, 125.0, 125.8, 126.9, 127.2, 127.7, 128.2, 130.6, 130.9, 131.0, 131.3, 131.5, 131.7, 132.4, 134.9, 135.1, 135.4, 145.7, 151.1, 172.4, 180.8; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{25}\text{N}_2\text{O}_4$  ( $[\text{M}+\text{H}]^+$ ): 525.1814, found: 525.1803.

**Methyl-5-oxo-16-(*p*-tolyl)-4b, 5-dihydro-16*H*-benzo [a] chromeno [4',3':4,5] pyrido [3,2,1-de] phenazine-16a(17*H*)-carboxylate (4b)**



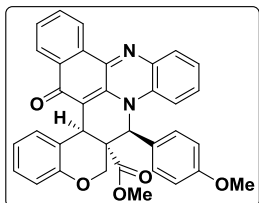
Red color solid; Yield: 74%; mp.: 208-210 °C; IR (KBr):  $\nu$  1732, 1708, 1650  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.07 (s, 3H), 3.59 (s, 3H), 4.64 (d, 1H,  $J = 12$  Hz), 4.82 (d, 1H,  $J = 11.7$  Hz), 5.49 (s, 1H), 5.90 (d, 1H,  $J = 7.5$  Hz), 6.41 (s, 1H), 6.61 – 9.03 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  20.8, 30.9, 45.1, 53.6, 61.9, 66.9, 107.5, 114.2, 114.7, 120.8, 121.6, 124.0, 124.9, 125.8, 126.8, 127.4, 127.9, 128.2, 130.7, 130.9, 131.0, 131.3, 131.5, 131.7, 132.1, 132.4, 135.0, 135.1, 137.5, 151.1, 172.4, 180.8; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{35}\text{H}_{27}\text{N}_2\text{O}_4$  ( $[\text{M}+\text{H}]^+$ ): 539.1971, found: 539.1952.

**Methyl-16-(2-methoxyphenyl)-5-oxo-4b,5-dihydro-16*H*-benzo[a] chromeno[4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17*H*)-carboxylate (4c)**



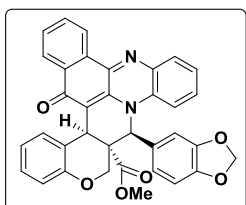
Red colour solid; Yield: 72%; mp.: 212-214 °C; IR (KBr):  $\nu$  1732, 1709, 1648  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$   $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.04 – 9.01 (m, 1H), 8.60 – 8.58 (m, 1H), 7.97 (dd,  $J = 7.9, 1.4$  Hz, 1H), 7.86 – 7.83 (m, 2H), 7.41 (d,  $J = 7.1$  Hz, 1H), 7.32 – 7.28 (m, 2H), 7.12 (d,  $J = 7.1$  Hz, 1H), 7.04 (d,  $J = 2.0$  Hz, 1H), 6.88 – 6.84 (m, 1H), 6.78 (d,  $J = 8.1$  Hz, 1H), 6.70 – 6.64 (m, 2H), 6.06 (dd,  $J = 7.8, 1.4$  Hz, 1H), 5.95 (dd,  $J = 7.7, 1.6$  Hz, 1H), 5.88 (t,  $J = 7.5$  Hz, 1H), 5.51 (s, 1H), 4.96 (d,  $J = 11.1$  Hz, 1H), 4.54 (d,  $J = 11.1$  Hz, 1H), 4.11 (s, 3H), 3.59 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  181.02, 172.75, 157.16, 151.89, 145.67, 135.62, 135.21, 132.67, 131.91, 131.83, 131.45, 131.07, 130.97, 130.88, 129.10, 128.71, 128.48, 127.24, 125.94, 125.10, 124.63, 124.22, 122.07, 120.90, 119.14, 114.95, 113.95, 109.06, 107.63, 77.48, 77.16, 76.84, 67.50, 55.87, 54.65, 53.68, 45.35, 31.73; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{35}\text{H}_{27}\text{N}_2\text{O}_5$  ( $[\text{M}+\text{H}]^+$ ): 555.1920, found: 555.1906.

**Methyl-16-(4-methoxyphenyl) -5-oxo-4b,5-dihydro-16H-benzo [a] chromeno [4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4d)**



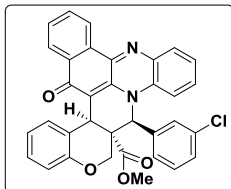
Red color solid; Yield: 73%; mp.: 218-220 °C; IR (KBr):  $\nu$  1734, 1706, 1642  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.59 (s, 6H), 4.64 (d, 1H,  $J = 11.7$  Hz), 4.81 (d, 1H,  $J = 11.7$  Hz), 5.49 (s, 1H), 5.98 (d, 1H,  $J = 7.5$  Hz), 6.39 (s, 1H), 6.64 – 9.04 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.9, 45.0, 53.6, 55.1, 61.6, 66.9, 107.5, 114.2, 114.8, 120.9, 121.7, 124.0, 125.0, 125.8, 127.1, 127.2, 128.2, 129.2, 130.6, 130.9, 131.0, 131.3, 131.5, 131.7, 132.4, 134.9, 135.1, 145.7, 151.1, 159.0, 172.4, 180.8; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{35}\text{H}_{27}\text{N}_2\text{O}_5$  ( $[\text{M}+\text{H}]^+$ ): 555.1920, found: 555.1907.

**Methyl-16-(benzo[d][1,3]dioxol-5-yl) -5-oxo-4b,5-dihydro-16H-benzo [a] chromeno [4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4e)**



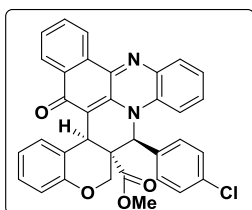
Red color solid; Yield: 76%; mp.: 208-210 °C; IR (KBr):  $\nu$  1739, 1705, 1650  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.05 – 9.03 (m, 1H), 8.61 – 8.59 (m, 1H), 8.01 (d,  $J = 8.0$  Hz, 1H), 7.87 (d,  $J = 4.0$  Hz, 3H), 7.46 – 7.38 (m, 4H), 7.07 (d,  $J = 7.4$  Hz, 1H), 6.74 (dt,  $J = 36.5, 7.3$  Hz, 3H), 6.39 (s, 2H), 6.15 (d,  $J = 8.0$  Hz, 1H), 5.68 (s, 2H), 5.51 (s, 1H), 4.82 (d,  $J = 11.9$  Hz, 1H), 4.67 (d,  $J = 11.9$  Hz, 1H), 3.61 (s, 3H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.8, 45.2, 53.6, 61.8, 66.9, 100.9, 106.7, 107.5, 114.1, 114.9, 121.0, 121.6, 124.1, 125.0, 125.8, 127.0, 128.3, 128.9, 130.6, 130.9, 131.0, 131.4, 131.5, 131.7, 132.3, 134.8, 135.0, 145.7, 146.7, 147.2, 151.3, 172.3, 180.9; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{35}\text{H}_{25}\text{N}_2\text{O}_6$  ( $[\text{M}+\text{H}]^+$ ): 569.1713, found: 569.1708.

**Methyl-16-(3-chlorophenyl)-5-oxo-4b,5-dihydro-16H-benzo [a] chromeno[4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4f)**



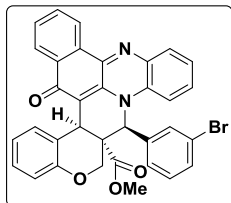
Red colour solid; Yield: 76%; mp.: 230-232 °C; IR (KBr):  $\nu$  1749, 1706, 1649  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.61 (s, 3H), 4.67 (d, 1H,  $J = 11.7$  Hz), 4.83 (d, 1H,  $J = 12$  Hz), 5.49 (s, 1H), 6.01 (d, 1H,  $J = 8.1$  Hz), 6.41 (s, 1H), 6.68 – 9.05 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.9, 45.1, 53.7, 61.5, 66.8, 107.6, 113.8, 115.0, 121.3, 124.2, 125.0, 125.8, 127.7, 128.2, 130.4, 131.0, 131.2, 131.4, 131.6, 131.7, 132.3, 133.2, 134.7, 135.0, 137.6, 145.8, 151.0, 172.1, 180.9; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{24}\text{ClN}_2\text{O}_4$  ( $[\text{M}+1]^+$ ): 559.1425, found: 559.1407.

**Methyl-16-(4-chlorophenyl)-5-oxo-4b,5-dihydro-16H-benzo [a] chromeno[4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4g)**



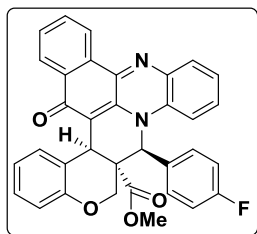
Red colour solid; Yield: 80%; mp.: 215-217 °C; IR (KBr):  $\nu$  1712, 1634, 1598  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.60 (s, 3H), 4.66 (d, 1H,  $J = 11.7$  Hz), 4.82 (d, 1H,  $J = 12$  Hz), 5.49 (s, 1H), 5.97 (d, 1H,  $J = 8.1$  Hz), 6.41 (s, 1H), 6.63 - 9.04 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.9, 45.1, 53.7, 61.4, 66.9, 107.6, 113.8, 114.9, 121.1, 121.6, 124.2, 125.0, 125.8, 126.9, 127.3, 128.2, 129.3, 130.4, 131.0, 131.1, 131.4, 131.5, 131.7, 132.3, 133.8, 133.9, 134.7, 135.0, 145.8, 151.0, 172.1, 180.9; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{24}\text{ClN}_2\text{O}_4$  ( $[\text{M}+1]^+$ ): 559.1425, found: 559.1424.

**Methyl-16-(3-bromophenyl)-5-oxo-4b,5-dihydro-16H-benzo [a] chromeno[4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4h)**



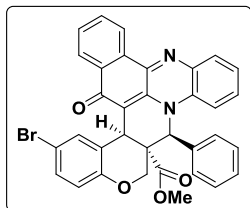
Red color solid; Yield: 75%; mp.: 230-232 °C; IR (KBr):  $\nu$  1724, 1649, 1611  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.60 (s, 3H), 4.66 (d, 1H,  $J = 12$  Hz), 4.82 (d, 1H,  $J = 11.7$  Hz), 5.49 (s, 1H), 6.02 (d, 1H,  $J = 7.8$  Hz), 6.38 (s, 1H), 6.68 - 9.03 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.9, 45.1, 53.7, 61.5, 66.8, 107.6, 113.8, 115.0, 121.3, 124.2, 125.0, 125.8, 127.8, 128.1, 130.4, 131.0, 131.2, 131.4, 131.6, 131.7, 132.3, 134.7, 135.0, 137.9, 145.8, 151.0, 172.1, 180.9; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{24}\text{BrN}_2\text{O}_4$  ( $[\text{M}+\text{H}]^+$ ): 603.0919, found: 603.0898.

**Methyl-16-(4-fluorophenyl)-5-oxo-4b,5-dihydro-16H-benzo [a] chromeno[4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4i)**



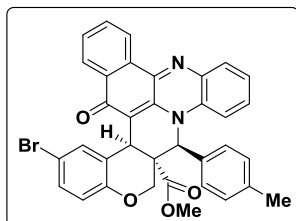
Red color solid; Yield: 73%; mp.: 223-225 °C; IR (KBr):  $\nu$  1730, 1660, 1618  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.60 (s, 3H), 4.66 (d, 1H,  $J = 11.7$  Hz), 4.82 (d, 1H,  $J = 12$  Hz), 5.50 (s, 1H), 5.98 (d, 1H,  $J = 7.8$  Hz), 6.42 (s, 1H), 6.63 - 9.03 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.9, 45.0, 53.7, 61.4, 66.9, 107.6, 113.9, 114.9, 121.0, 121.6, 124.1, 125.0, 125.8, 127.3, 128.2, 129.7, 130.4, 131.0, 131.1, 131.4, 131.5, 131.7, 132.3, 134.8, 135.0, 145.7, 151.0, 172.2, 180.9; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{24}\text{FN}_2\text{O}_4$  ( $[\text{M}+\text{H}]^+$ ): 543.1720, found: 543.1709.

**Methyl-3-bromo-5-oxo-16-phenyl-4b,5-dihydro-16H-benzo [a] chromeno[4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4j)**



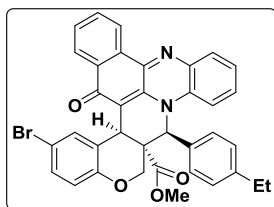
Red color solid; Yield: 78%; mp.: 205 – 207 °C; IR (KBr):  $\nu$  1728, 1662, 1619  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.60 (s, 3H), 4.62 (d, 1H,  $J = 12$  Hz), 4.85 (d, 1H,  $J = 11.7$  Hz), 5.47 (s, 1H), 5.80 (d, 1H,  $J = 8.4$  Hz), 6.42 (s, 1H), 6.75 - 9.03 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  31.0, 45.0, 53.8, 62.0, 67.0, 106.8, 113.1, 114.1, 116.7, 123.9, 124.2, 125.0, 126.0, 127.2, 128.1, 130.3, 130.5, 130.6, 131.1, 131.5, 131.6, 131.8, 132.3, 135.1, 145.7, 149.2, 150.4, 172.0, 180.7; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{24}\text{BrN}_2\text{O}_4$  ( $[\text{M}+\text{H}]^+$ ): 603.0919, found: 603.0905.

**Methyl-3-bromo-5-oxo-16-(p-tolyl)-4b,5-dihydro-16H-benzo [a] chromeno[4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4k)**



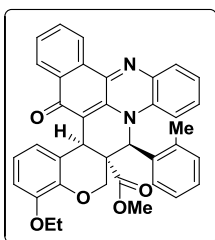
Red colour solid; Yield: 76%; mp.: 235 – 237 °C; IR (KBr):  $\nu$  1731, 1669, 1619  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.06 (dd,  $J = 6.0, 3.2$  Hz, 1H), 8.61 (dd,  $J = 6.0, 3.0$  Hz, 1H), 8.01 (dd,  $J = 7.9, 1.4$  Hz, 1H), 7.90 – 7.61 (m, 2H), 7.38 – 7.34 (m, 6H), 7.14 (d,  $J = 1.2$  Hz, 1H), 6.81 (dd,  $J = 8.7, 1.9$  Hz, 1H), 6.42 (s, 1H), 5.82 (d,  $J = 8.7$  Hz, 1H), 5.47 (s, 1H), 4.85 (d,  $J = 11.9$  Hz, 1H), 4.63 (d,  $J = 11.9$  Hz, 1H), 3.61 (s, 3H), 2.12 (s, 3H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  20.9, 30.9, 45.0, 53.7, 61.8, 67.0, 106.7, 113.0, 114.1, 116.5, 124.0, 124.1, 125.0, 125.9, 127.7, 129.5, 129.7, 130.5, 130.7, 131.0, 131.1, 131.4, 131.5, 131.7, 131.8, 132.3, 135.1, 137.9, 145.6, 150.4, 172.0, 180.6; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{35}\text{H}_{26}\text{BrN}_2\text{O}_4$  ( $[\text{M}+\text{H}]^+$ ): 617.1076, found: 617.1062.

**Methyl-3-bromo-16-(4-ethylphenyl)-5-oxo-4b,5-dihydro-16H-benzo [a] chromeno [4',3':4,5] pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4l)**



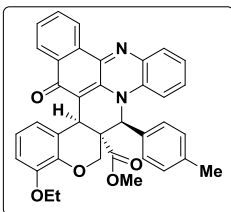
Red color solid; Yield: 71%; mp.: 217 – 219 °C; IR (KBr):  $\nu$  1739, 1665, 1610  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.06 (t, 3H,  $J = 7.8$  Hz), 2.38 (q,  $J = 7.5$  Hz, 2H), 3.58 (s, 3H), 4.60 (d,  $J = 12$  Hz, 1H), 4.83 (d,  $J = 11.7$  Hz, 1H), 5.45 (s, 1H), 5.79 (d,  $J = 8.7$  Hz, 1H), 6.40 (s, 1H), 6.73 - 9.04 (m, 14H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  180.78, 172.18, 150.47, 145.71, 144.40, 135.22, 135.20, 132.42, 132.11, 131.84, 131.78, 131.57, 131.21, 131.18, 130.72, 130.62, 130.19, 126.08, 125.14, 124.35, 124.12, 116.74, 114.29, 113.07, 106.80, 67.12, 61.93, 53.93, 45.03, 31.01, 28.56, 15.69.

**Methyl-1-ethoxy-5-oxo-16-(o-tolyl)-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4m)**



Red color solid; Yield: 75%; mp.: 211 – 213 °C; IR (KBr):  $\nu$  1721, 1659, 1621  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.25 (t, 3H,  $J = 7.2$  Hz), 2.85 (s, 3H), 3.59 (s, 3H), 3.79 (q, 2H,  $J = 5.4$  Hz), 4.61 (d, 1H,  $J = 11.7$  Hz), 4.97 (d, 1H,  $J = 12$  Hz), 5.55 (s, 1H), 6.08 – 9.03 (m, 16H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  14.7, 20.1, 32.1, 45.9, 53.6, 64.2, 65.1, 67.9, 107.8, 110.9, 115.8, 117.6, 120.3, 125.8, 127.6, 130.2, 130.8, 130.9, 131.0, 131.3, 131.5, 131.6, 131.7, 132.4, 134.2, 135.1, 135.6, 141.9, 146.5, 172.5, 180.9; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{37}\text{H}_{31}\text{N}_2\text{O}_5$  ( $[\text{M}+\text{H}]^+$ ): 583.2233, found: 583.2211.

**Methyl-1-ethoxy-5-oxo-16-(p-tolyl)-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4n)**

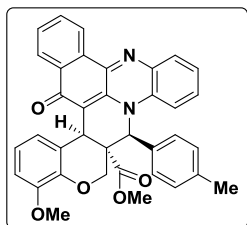


Red color solid; Yield: 74%; mp.: 216 – 218 °C; IR (KBr):  $\nu$  1734, 1663, 1610  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.25 (t, 3H,  $J = 7.2$  Hz), 2.85 (s, 3H), 3.59 (s, 3H), 3.79 (q, 2H,  $J = 6.9$  Hz), 4.67 (d, 1H,  $J = 11.7$  Hz), 4.97 (d, 1H,  $J = 12$  Hz), 5.48 (s, 1H), 6.30 (d, 1H,  $J = 7.8$  Hz), 6.41 (s, 1H), 6.52 – 9.03 (m, 14H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  14.7,



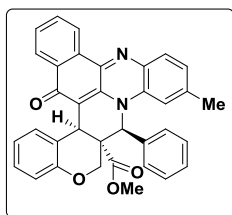
20.8, 30.9, 45.0, 53.6, 61.9, 63.8, 67.2, 107.6, 110.0, 114.2, 120.1, 122.4, 123.9, 124.9, 125.8, 127.5, 130.7, 130.8, 130.9, 131.3, 131.5, 131.7, 132.2, 132.4, 134.9, 135.0, 137.0, 141.1, 146.3, 172.5, 180.8; HRMS (ESI-MS)  $m/z$  calcd for  $C_{37}H_{31}N_2O_5$  ( $[M+H]^+$ ): 583.2233, found: 583.2225.

**Methyl-1-methoxy-5-oxo-16-(p-tolyl)-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4o)**



Red color solid; Yield: 78%; mp.: 222 – 224 °C; IR (KBr):  $\nu$  1734, 1664, 1619  $cm^{-1}$ ;  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta$  2.08 (s, 3H), 3.53 (s, 3H), 3.59 (s, 3H), 4.68 (d, 1H,  $J = 11.7$  Hz), 4.97 (d, 1H,  $J = 11.7$  Hz), 5.48 (s, 1H), 6.32 (d, 1H,  $J = 7.8$  Hz), 6.41 (s, 1H), 6.55 - 9.04 (m, 14H);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ ):  $\delta$  20.9, 30.9, 45.0, 53.6, 55.4, 61.9, 67.2, 107.5, 108.8, 114.2, 120.1, 120.3, 122.4, 124.0, 124.9, 125.8, 127.4, 130.7, 130.9, 131.0, 131.3, 131.5, 131.7, 132.1, 132.4, 135.0, 135.1, 137.1, 140.8, 145.7, 147.0, 172.4, 180.8; HRMS (ESI-MS)  $m/z$  calcd for  $C_{36}H_{28}N_2O_5$  ( $[M+H]^+$ ): 569.2076, found: 569.2066.

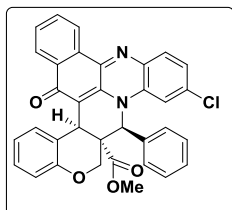
**Methyl-13-methyl-5-oxo-16-phenyl-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carboxylate (4p)**



Red color solid; Yield: 76%; mp.: 312 – 316 °C; IR (KBr):  $\nu$  1734, 1664, 1619  $cm^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$   $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  9.04- 9.02 (m, 1H), 8.61 (dd,  $J = 6.0, 2.7$  Hz, 1H), 7.89- 7.64 (m, 3H), 7.27 – 6.80 (m, 8H), 6.77 – 6.61 (m, 2H), 6.46 (s, 1H), 5.98 – 5.83 (m, 1H), 5.54 (s, 1H), 4.88 (dd,  $J = 11.8, 1.1$  Hz, 1H), 4.69 (d,  $J = 11.9$  Hz, 1H), 3.62 (d,  $J = 1.8$  Hz, 3H), 2.40 (d,  $J = 15.7$  Hz, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  180.82, 180.66, 172.56, 172.47, 151.14, 145.60, 144.53, 142.72, 135.55, 135.46, 135.13, 134.99, 134.92, 134.16, 133.49, 133.00, 132.47, 132.32, 131.83, 131.72, 131.31, 131.12, 130.85, 130.81, 130.73, 130.49, 128.52, 128.28, 127.77, 127.25, 125.81,

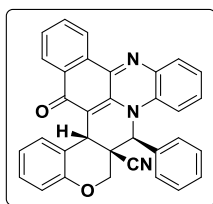
124.93, 124.84, 121.60, 120.87, 114.88, 113.94, 107.29, 107.03, 66.91, 62.13, 62.00, 53.78, 53.75, 45.15, 45.11, 30.96, 30.90, 22.64, 20.60; HRMS (ESI-MS)  $m/z$  calcd for  $C_{35}H_{26}N_2O_4$  ( $[M+H]^+$ ): 539.1971, found: 539.1970.

**Methyl-13-chloro-5-oxo-16-phenyl-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido [3,2,1-de]phenazine-16a(17H)-carboxylate (4q)**



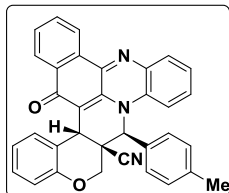
Red color solid; Yield: 72%; mp.: 308 – 310 °C; IR (KBr):  $\nu$  1734, 1664, 1619  $cm^{-1}$ ;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.99 (d,  $J = 6.9$  Hz, 1H), 8.59 (d,  $J = 6.9$  Hz, 1H), 7.92 (d,  $J = 33.9$  Hz, 3H), 7.27 (d,  $J = 12.6$  Hz, 5H), 7.04 – 6.88 (m, 3H), 6.67 (d,  $J = 5.8$  Hz, 2H), 6.39 (s, 1H), 5.93 (d,  $J = 7.6$  Hz, 1H), 5.51 (s, 2H), 4.85 (d,  $J = 11.8$  Hz, 2H), 4.67 (d,  $J = 11.8$  Hz, 1H), 3.63 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  181.12, 172.46, 151.22, 147.13, 135.78, 135.28, 134.76, 132.50, 131.95, 131.58, 131.46, 131.32, 130.09, 129.45, 129.39, 128.23, 128.09, 127.53, 126.03, 125.28, 121.38, 121.02, 115.40, 115.11, 108.10, 66.90, 62.43, 53.94, 45.12, 31.04; HRMS (ESI-MS)  $m/z$  calcd for  $C_{34}H_{23}ClN_2O_4$  ( $[M+H]^+$ ): 559.1424, found: 559.1414.

**5-oxo-16-phenyl-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carbonitrile (6a)**



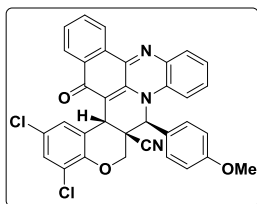
Red color solid; Yield: 68%; mp.: 245 – 247 °C; IR (KBr):  $\nu$  2242, 1701, 1640  $cm^{-1}$ ;  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta$  4.48 (d, 1H,  $J = 11.4$  Hz), 4.61 (d, 1H,  $J = 11.7$  Hz), 5.47 (s, 1H), 5.73 (s, 1H), 6.83 – 8.97 (m, 17H);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ ):  $\delta$  33.9, 40.2, 59.4, 67.7, 108.6, 116.7, 117.1, 117.5, 120.8, 123.0, 123.9, 125.0, 125.9, 127.7, 128.8, 129.4, 129.5, 129.9, 130.4, 130.5, 131.4, 131.6, 131.7, 132.3, 135.4, 147.1, 151.8, 180.0; HRMS (ESI-MS)  $m/z$  calcd for  $C_{33}H_{21}N_3O_2$  ( $[M+H]^+$ ): 492.1712, found: 492.1704.

**16-(4-ethylphenyl)-5-oxo-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido  
[3,2,1-de]phenazine-16a(17H)-carbonitrile (6b)**



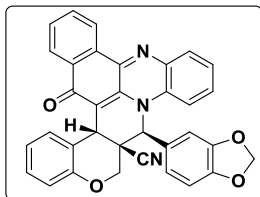
Red color solid; Yield: 66%; mp.: 235 – 237 °C; IR (KBr):  $\nu$  2244, 1706, 1648  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.98 (dd,  $J = 6.0, 2.9$  Hz, 1H), 8.76 – 8.39 (m, 1H), 8.21 – 7.69 (m, 3H), 7.25 – 6.53 (m, 11H), 5.72 (s, 1H), 5.49 (s, 1H), 4.63 (d,  $J = 11.5$  Hz, 1H), 4.50 (d,  $J = 11.4$  Hz, 1H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  180.03, 151.78, 147.36, 139.67, 136.58, 136.01, 132.44, 131.82, 131.70, 131.53, 130.62, 130.12, 130.00, 129.65, 129.01, 126.07, 125.09, 124.04, 123.00, 120.93, 117.82, 117.44, 116.92, 108.93, 67.36, 58.64, 40.72, 34.83, 21.38; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{23}\text{N}_3\text{O}_2$  ( $[\text{M}+\text{H}]^+$ ): 506.1868, found: 506.1875.

**16-(4-isopropylphenyl)-5-oxo-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido  
[3,2,1-de]phenazine-16a(17H)-carbonitrile (6c)**



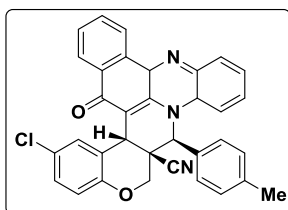
Red color solid; Yield: 69%; mp.: 235 – 237 °C; IR (KBr):  $\nu$  2244, 1706, 1648  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.00 – 8.98 (m, 1H), 8.55 – 8.53 (m, 1H), 7.98 – 7.78 (m, 3H), 7.265 – 7.16(m, 5H), 6.96- 6.91 (m, 4H), 5.58 (s, 1H), 5.46 (s, 1H), 4.75 (d,  $J = 11.6$  Hz, 1H), 4.54 (d,  $J = 11.6$  Hz, 1H), 3.80 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  179.83, 160.47, 147.05, 146.44, 136.66, 136.09, 132.23, 131.82, 131.76, 130.82, 130.27, 129.88, 129.62, 128.30, 127.79, 126.54, 126.15, 125.19, 124.37, 123.95, 122.69, 117.49, 117.16, 114.92, 107.58, 67.88, 58.44, 55.45, 40.57, 34.78; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{21}\text{Cl}_2\text{N}_3\text{O}_3$  ( $[\text{M}+\text{H}]^+$ ): 590.1038, found: 590.1022.

**16-(benzo[d][1,3]dioxol-5-yl)-5-oxo-4b,5-dihydro-16H-benzo[a]chromeno[4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carbonitrile (6d)**



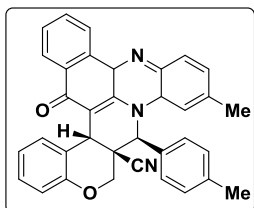
Red color solid; Yield: 65%; mp.: 238 – 240 °C; IR (KBr):  $\nu$  2249, 1707, 1649  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.48 (d, 1H,  $J = 11.1$  Hz), 4.63 (d, 1H,  $J = 11.1$  Hz), 5.45 (s, 1H), 5.63 (s, 1H), 5.96 (s, 2H), 6.64-8.95 (m, 15H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  34.7, 40.6, 58.4, 67.3, 101.6, 107.8, 108.7, 108.9, 116.7, 117.0, 117.6, 120.7, 121.8, 122.9, 123.9, 124.9, 125.9, 128.8, 128.9, 129.3, 129.8, 130.5, 130.6, 131.4, 131.5, 131.7, 132.3, 135.9, 136.3, 147.3, 148.6, 151.6, 179.9; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{21}\text{N}_3\text{O}_2$  ( $[\text{M}+\text{H}]^+$ ): 536.1610, found: 536.1614.

**3-bromo-5-oxo-16-(p-tolyl)-4b,5,9b,14a-tetrahydro-16H-benzo [a] chromeno [4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carbonitrile (6e)**



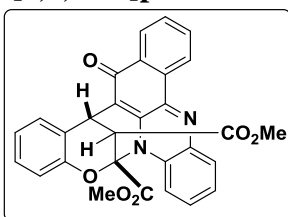
Red color solid; Yield: 70%; mp.: 238 – 240 °C; IR (KBr):  $\nu$  2249, 1707, 1649  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.05 – 8.90 (m, 1H), 8.66 – 8.42 (m, 1H), 8.08 – 7.70 (m, 4H), 7.23 – 6.64 (m, 9H), 5.62 (s, 1H), 5.43 (s, 1H), 4.60 (d,  $J = 11.5$  Hz, 1H), 4.45 (d,  $J = 11.5$  Hz, 1H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  179.87, 150.38, 147.23, 139.82, 136.66, 136.08, 132.34, 132.16, 131.83, 131.78, 131.66, 130.76, 130.47, 130.18, 129.95, 129.77, 129.55, 129.48, 129.25, 128.02, 126.16, 125.15, 124.22, 122.58, 118.35, 117.49, 117.34, 108.13, 67.44, 58.63, 40.50, 34.71, 21.37; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{34}\text{H}_{24}\text{ClN}_3\text{O}_2$  ( $[\text{M}+\text{H}]^+$ ): 542.1635, found: 542.1679.

**13-Methyl-5-oxo-16-(p-tolyl)-4b,5,9b,14a-tetrahydro-16H-benzo[a]chromeno[4',3':4,5]pyrido[3,2,1-de]phenazine-16a(17H)-carbonitrile (6f)**



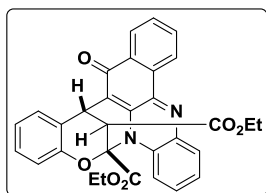
Red color solid; Yield: 69%; mp.: 206 – 210 °C; IR (KBr):  $\nu$  2249, 1707, 1649  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.94 (dd,  $J = 6.2, 3.0$  Hz, 1H), 8.53 (dd,  $J = 6.0, 3.2$  Hz, 1H), 8.02 – 7.56 (m, 4H), 7.20 – 6.14 (m, 10H), 5.68 (d,  $J = 1.3$  Hz, 1H), 5.46 (s, 1H), 4.86 – 4.55 (m, 1H), 4.52 – 4.28 (m, 1H), 2.32 (s, 3H), 2.17 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  179.85, 151.80, 147.19, 140.74, 139.63, 136.60, 136.03, 134.06, 132.59, 132.56, 132.51, 131.62, 131.42, 131.00, 130.39, 130.08, 128.97, 128.48, 126.05, 125.03, 123.00, 121.08, 117.87, 117.19, 116.89, 108.67, 108.45, 96.26, 67.40, 58.64, 40.76, 40.73, 34.83, 34.80, 31.74, 22.80, 22.22, 21.40, 20.71; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{35}\text{H}_{27}\text{N}_3\text{O}_2$  ( $[\text{M}+\text{H}]^+$ ): 522.2181, found: 522.2096.

**Dimethyl-13-oxo-12,13-dihydro-6H-6,12-methanobenzo[a]benzo[7,8][1,3] oxazocino [5,4,3-de]phenazine-6,19-dicarboxylate (8a)**



Red colour solid; Yield: 94%; mp.: 243 – 245 °C; IR (KBr):  $\nu$  1789, 1566, 1556  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.30 (s, 1H), 3.70 (s, 3H), 3.76 (d, 1H,  $J = 1.8$  Hz), 5.32 (d, 1H,  $J = 1.6$  Hz), 6.97 – 8.84 (m, 12H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  14.1, 21.0, 27.5, 45.4, 52.8, 53.9, 60.3, 87.1, 114.5, 114.7, 117.2, 122.3, 123.7, 124.8, 124.9, 125.7, 127.8, 129.7, 130.7, 130.8, 130.9, 131.3, 131.4, 132.0, 135.1, 135.8, 147.9, 149.5, 167.2, 167.4, 179.3; HRMS (ESI-MS)  $m/z$  calcd for  $\text{C}_{29}\text{H}_{21}\text{N}_2\text{O}_6$  ( $[\text{M}+\text{H}]^+$ ): 493.1400, found: 493.1394.

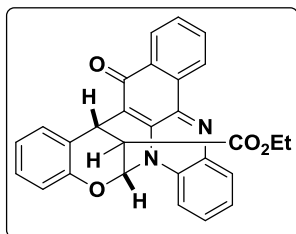
**Diethyl-13-oxo-12,13-dihydro-6H-6,12-methanobenzo[a]benzo [7,8][1,3] oxazocino [5,4,3-de]phenazine-6,19-dicarboxylate (8b)**



Red color solid; Yield: 95%; mp.: 253 – 255 °C; IR (KBr):  $\nu$  1758, 1591, 1538  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.03 (t, 3H,  $J = 7.2$  Hz), 1.16 (t, 3H,  $J = 7.2$  Hz), 3.25 (d, 1H,  $J = 1.8$  Hz), 4.11 – 4.23 (m, 4H), 5.31 (d, 1H,  $J = 1.5$  Hz), 6.96 – 8.81 (m, 12H);  $^{13}\text{C}$

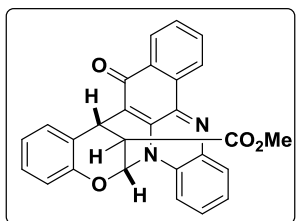
NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  13.6, 13.8, 27.6, 45.1, 61.9, 63.2, 87.1, 114.5, 115.2, 117.1, 122.4, 123.6, 124.7, 124.9, 125.7, 127.7, 129.6, 130.5, 130.7, 130.8, 131.3, 131.4, 132.1, 135.1, 135.8, 149.7, 166.2, 167.0, 177.9; HRMS (ESI-MS)  $m/z$  calcd for C<sub>31</sub>H<sub>25</sub>N<sub>2</sub>O<sub>6</sub> ([M+H]<sup>+</sup>): 521.1713, found: 521.1706.

**Ethyl-13-oxo-12,13-dihydro-6H-6,12-methanobenzo[a]benzo[7,8][1,3]oxazocino [5,4,3-de] phenazine-19-carboxylate (8c)**



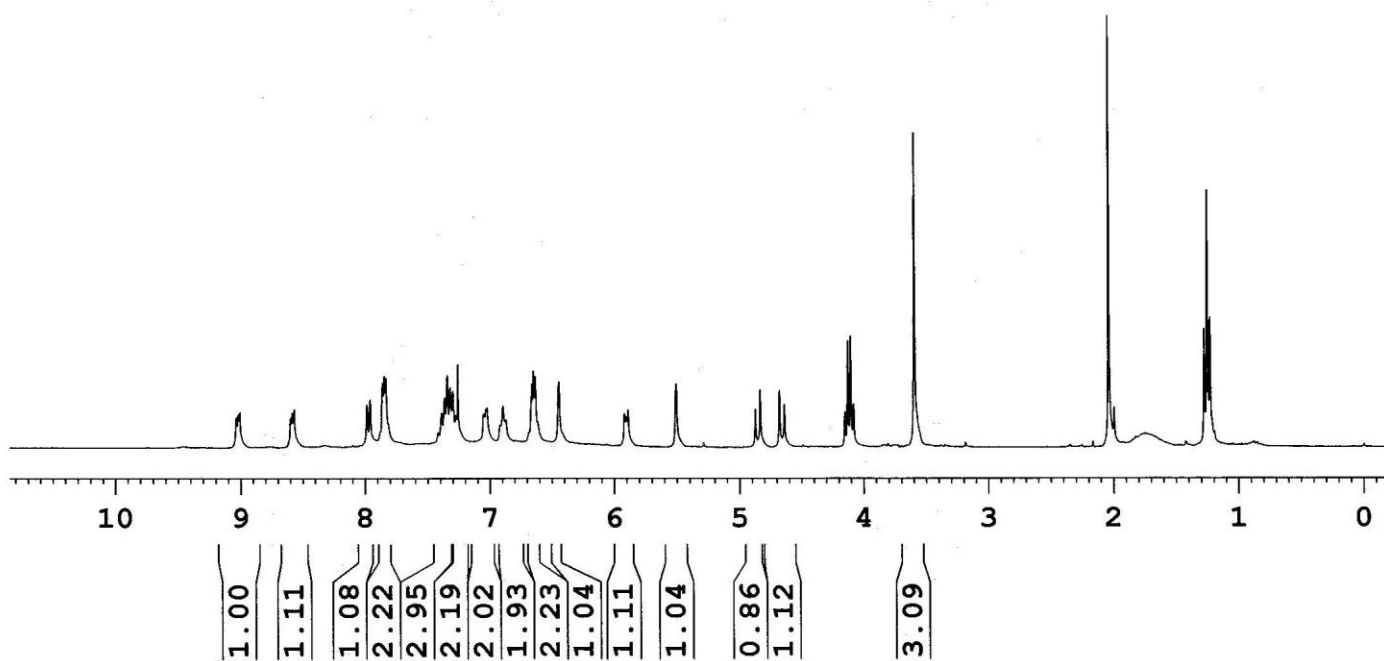
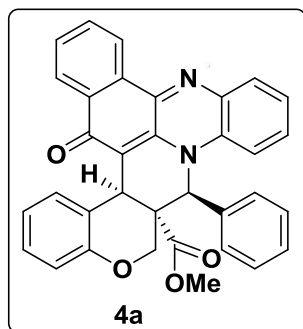
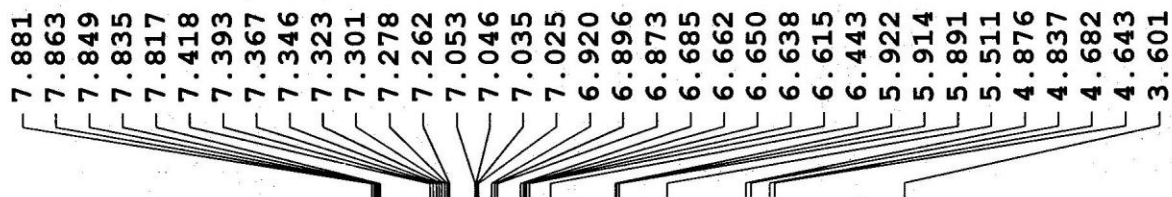
Red color solid; Yield 93%; mp.: 246 – 248 °C; IR (KBr):  $\nu$  1729, 1578, 1546 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.86 – 8.84 (m, 1H), 8.43 – 8.41 (m, 1H), 7.99 (d,  $J$  = 7.9 Hz, 1H), 7.92 (d,  $J$  = 8.4 Hz, 1H), 7.76 – 7.61 (m, 2H), 7.62 (d,  $J$  = 6.8 Hz, 1H), 7.45 (t,  $J$  = 7.5 Hz, 1H), 7.10 (dd,  $J$  = 11.4, 4.0 Hz, 1H), 6.96 (dd,  $J$  = 7.5, 3.6 Hz, 2H), 6.78 (s, 1H), 5.41 (s, 1H), 4.03 (dd,  $J$  = 7.1, 2.0 Hz, 1H), 3.58 (s, 1H), 1.03 (t,  $J$  = 7.1 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  178.55, 168.62, 150.14, 146.71, 135.13, 133.31, 132.31, 131.61, 131.40, 131.32, 131.10, 129.79, 128.11, 125.71, 124.88, 124.76, 124.72, 122.63, 116.85, 113.62, 110.25, 61.64, 38.44, 27.70, 14.03; HRMS (ESI-MS)  $m/z$  calcd for C<sub>28</sub>H<sub>21</sub>N<sub>2</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 449.1501, found: 449.1423.

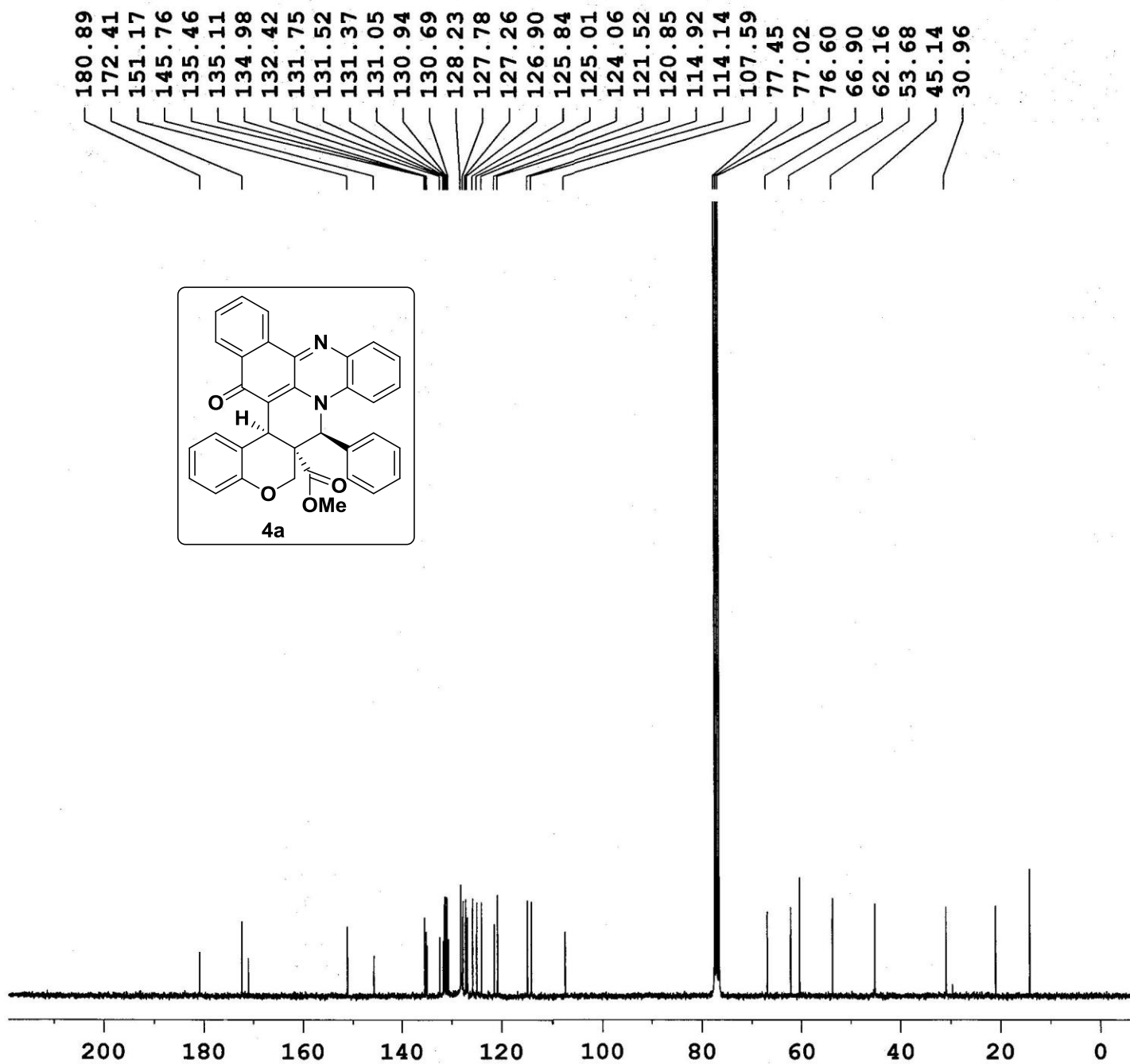
**Methyl-13-oxo-12,13-dihydro-6H-6,12-methanobenzo[a]benzo[7,8][1,3]oxazocino [5,4,3-de]phenazine-19-carboxylate (8d)**



Red color solid; Yield: 95%; mp.: 246 – 248 °C; IR (KBr):  $\nu$  1729, 1578, 1546 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  3.56 (s, 4H), 5.38 (s, 1H), 6.76 – 8.83 (m, 13H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  27.5, 38.3, 52.6, 110.0, 113.4, 116.7, 122.5, 124.5, 124.7, 125.6, 127.9, 129.6, 130.9, 131.0, 131.2, 131.4, 132.2, 133.1, 135.0, 146.6, 150.0, 168.9, 178.4; HRMS (ESI-MS)  $m/z$  calcd for C<sub>27</sub>H<sub>19</sub>N<sub>2</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 435.1345, found: 435.1338.

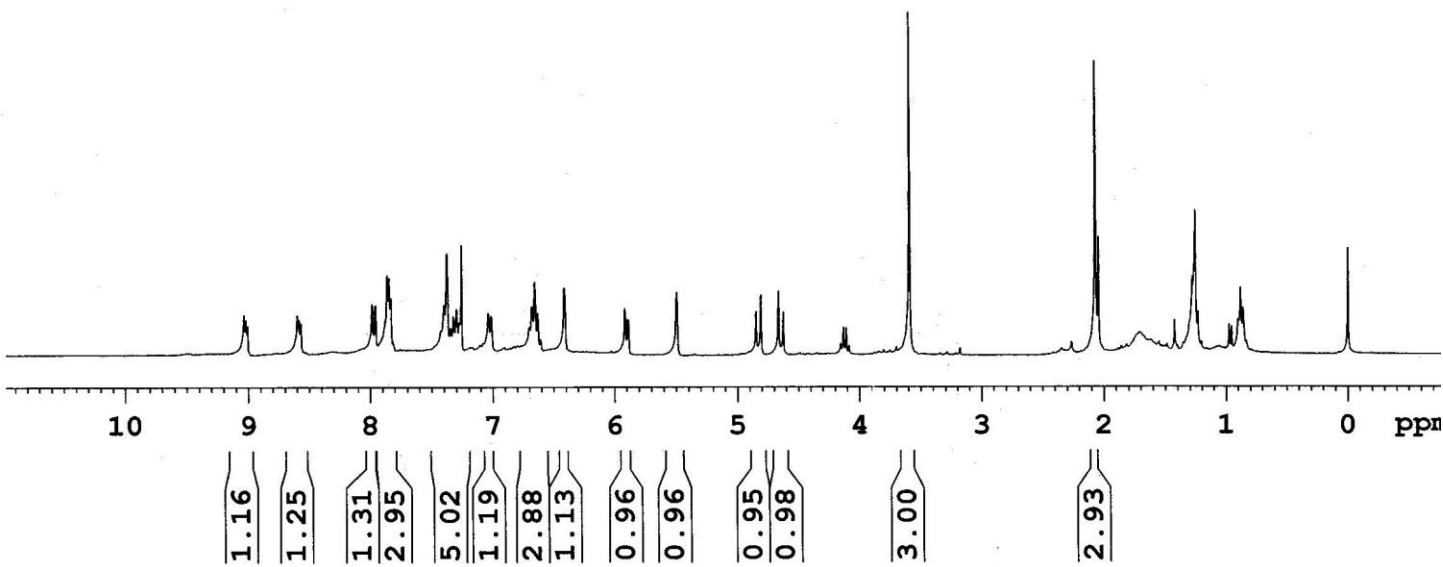
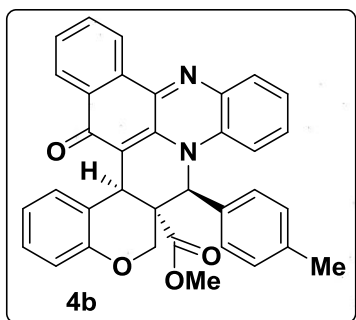
2)  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for compounds **4a-q**, **6a-f** & **8a-d**

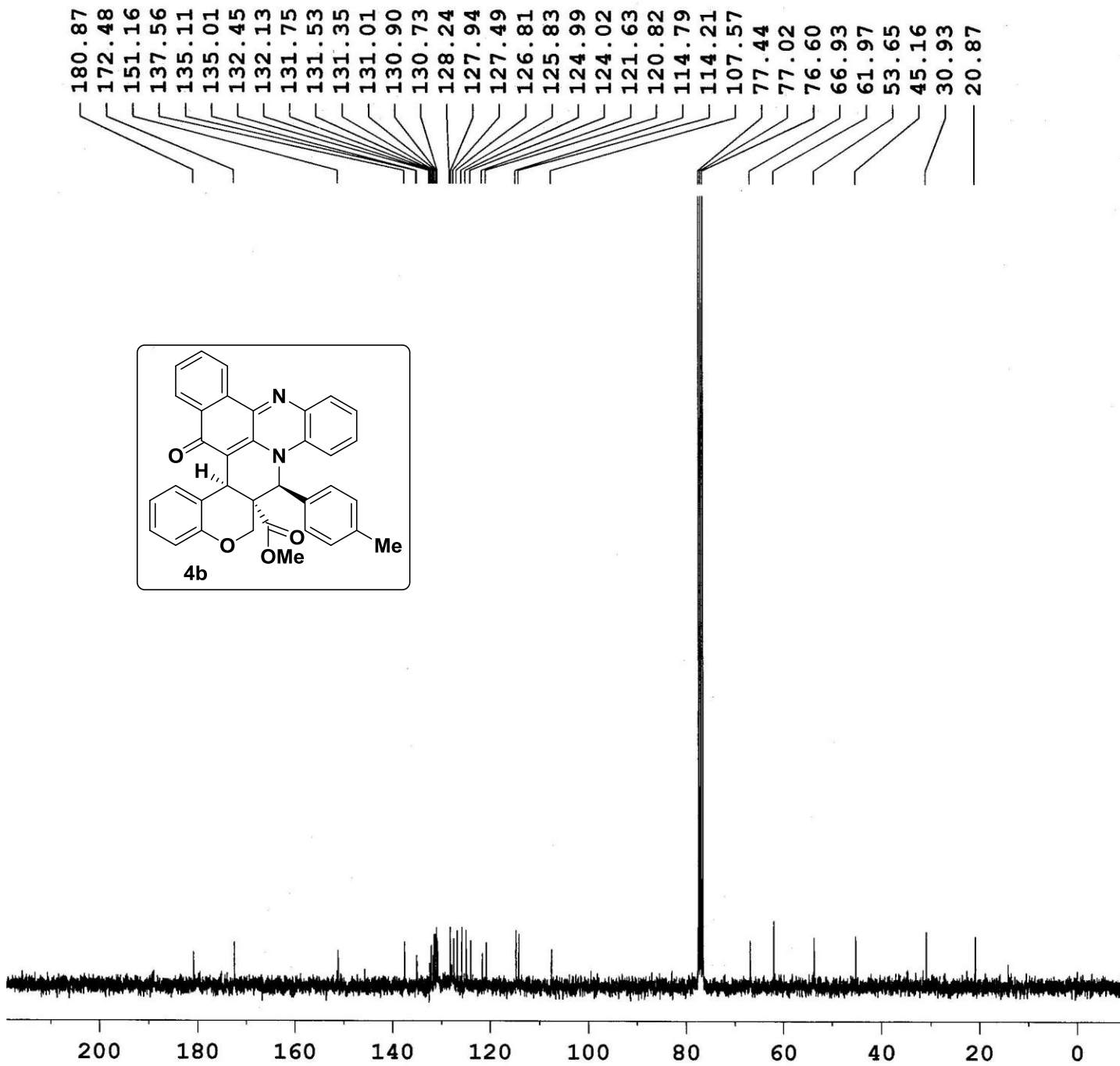


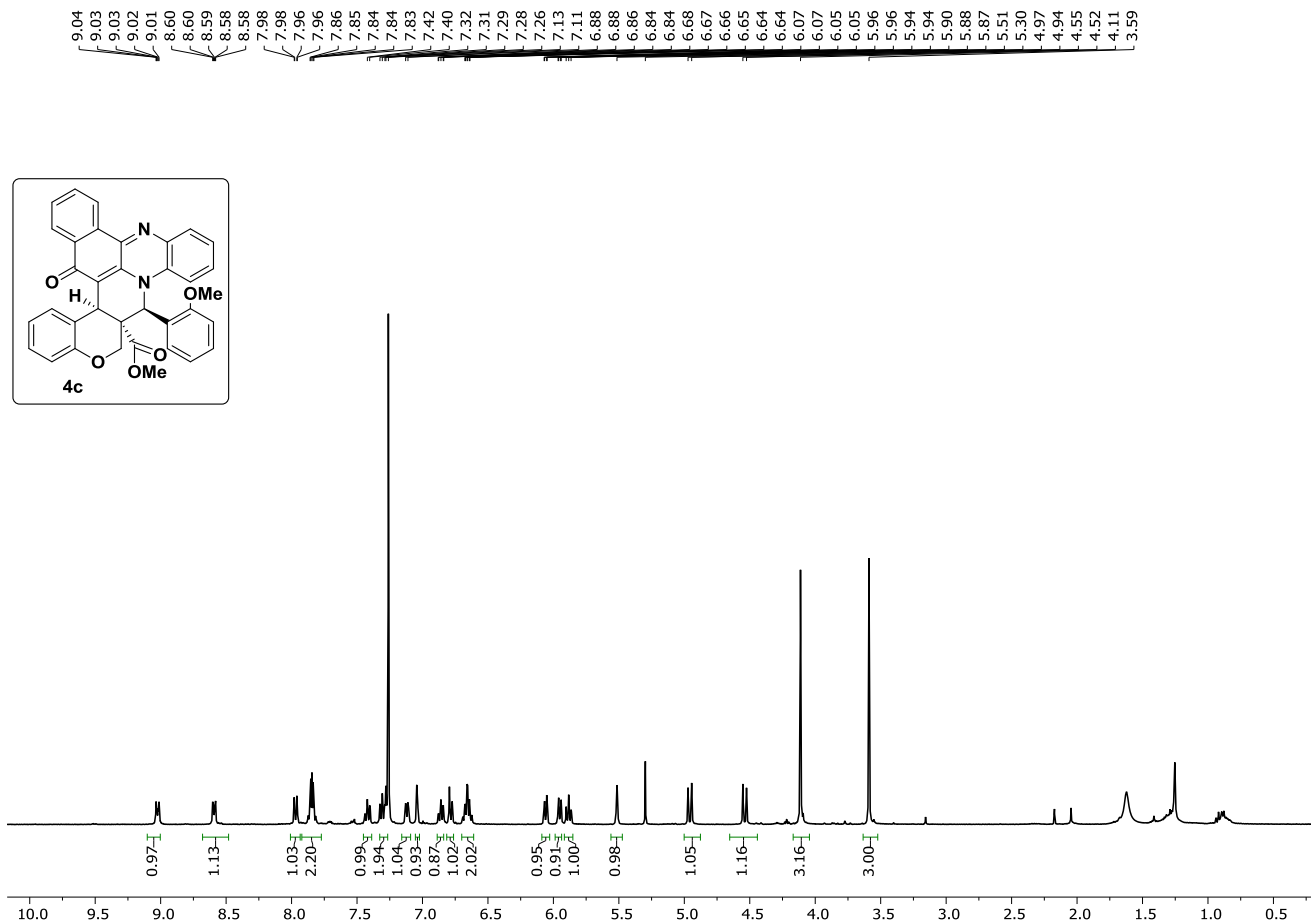


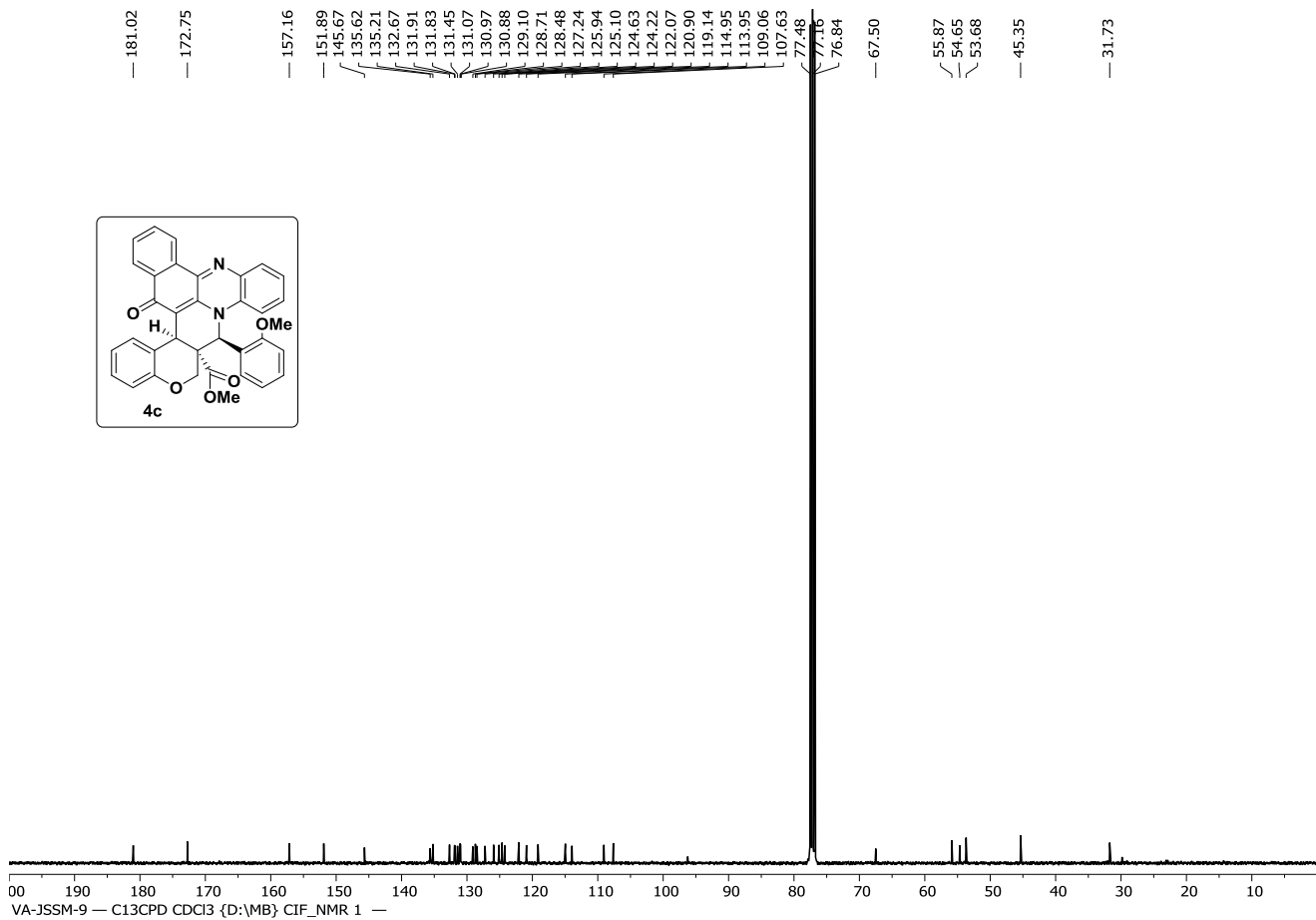


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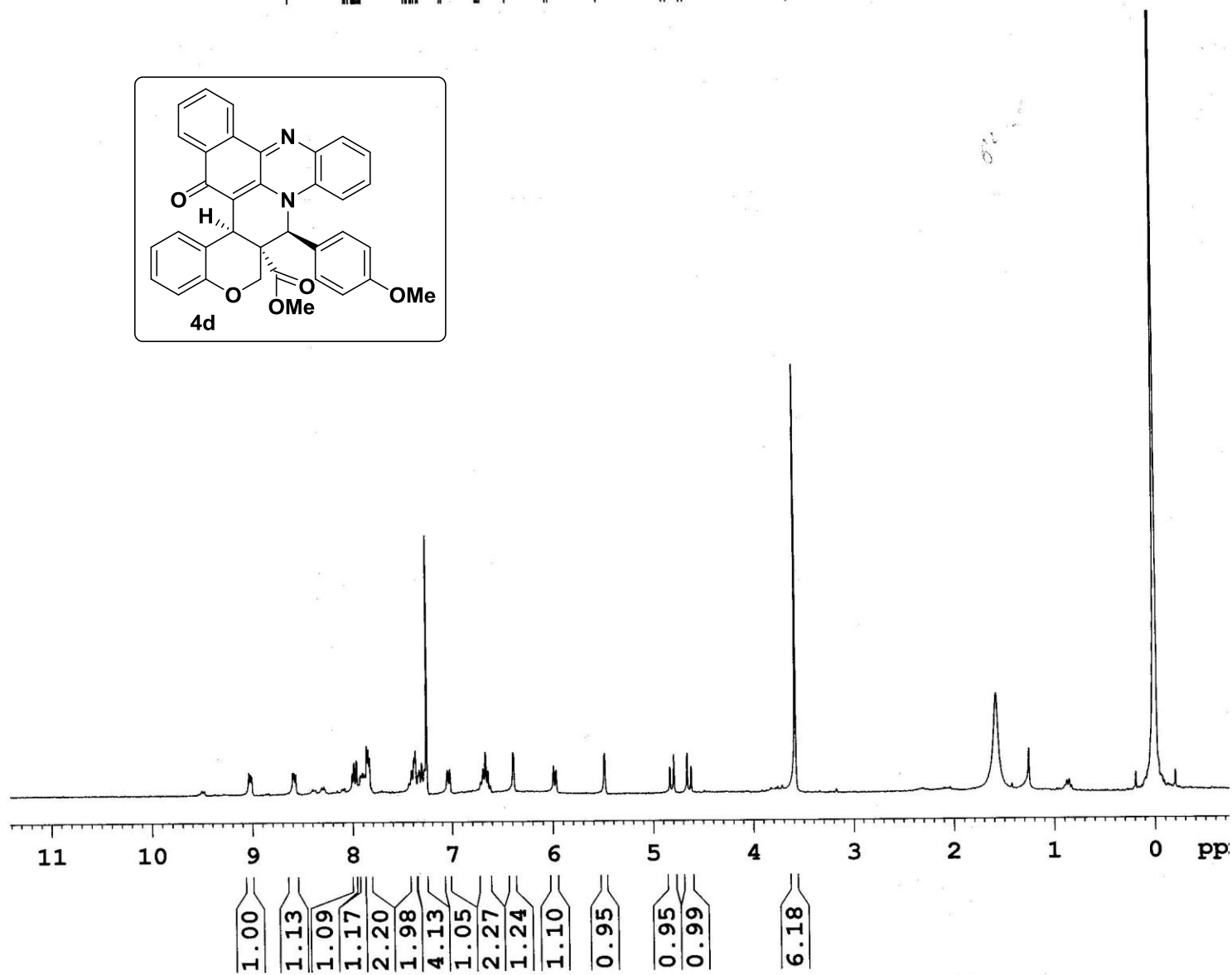
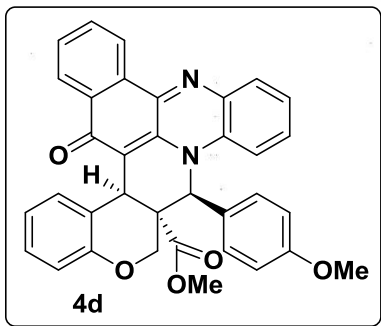


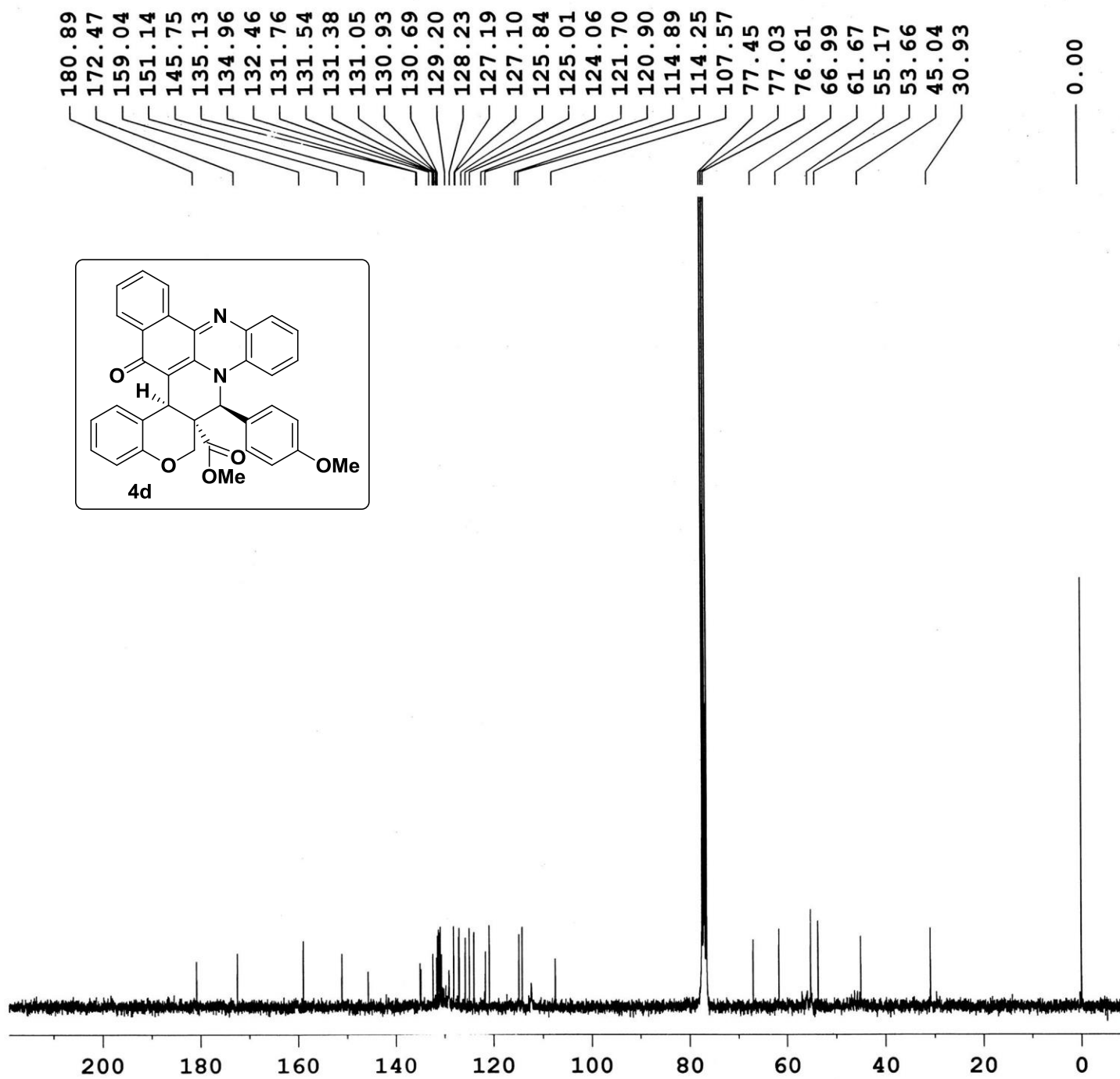


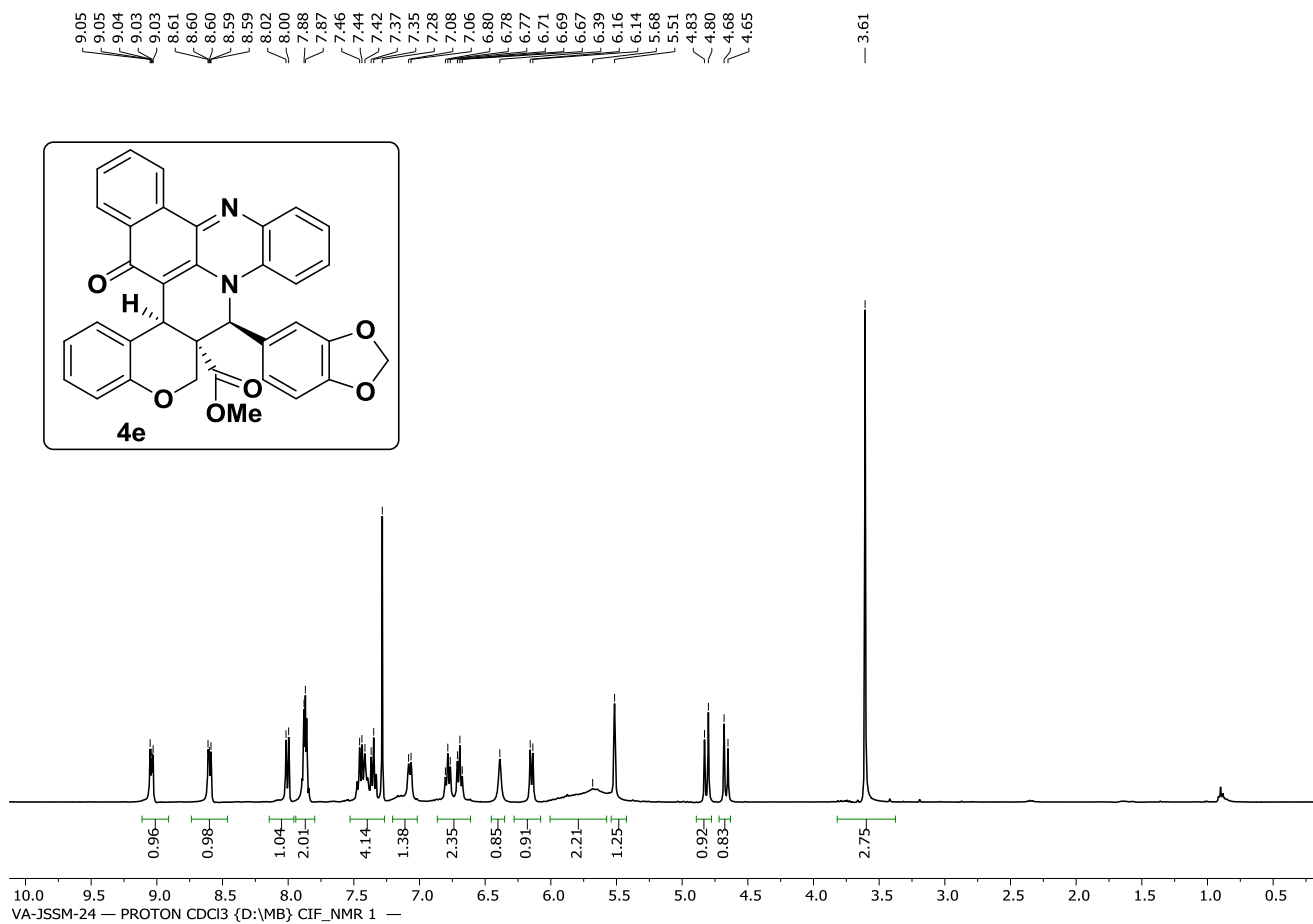




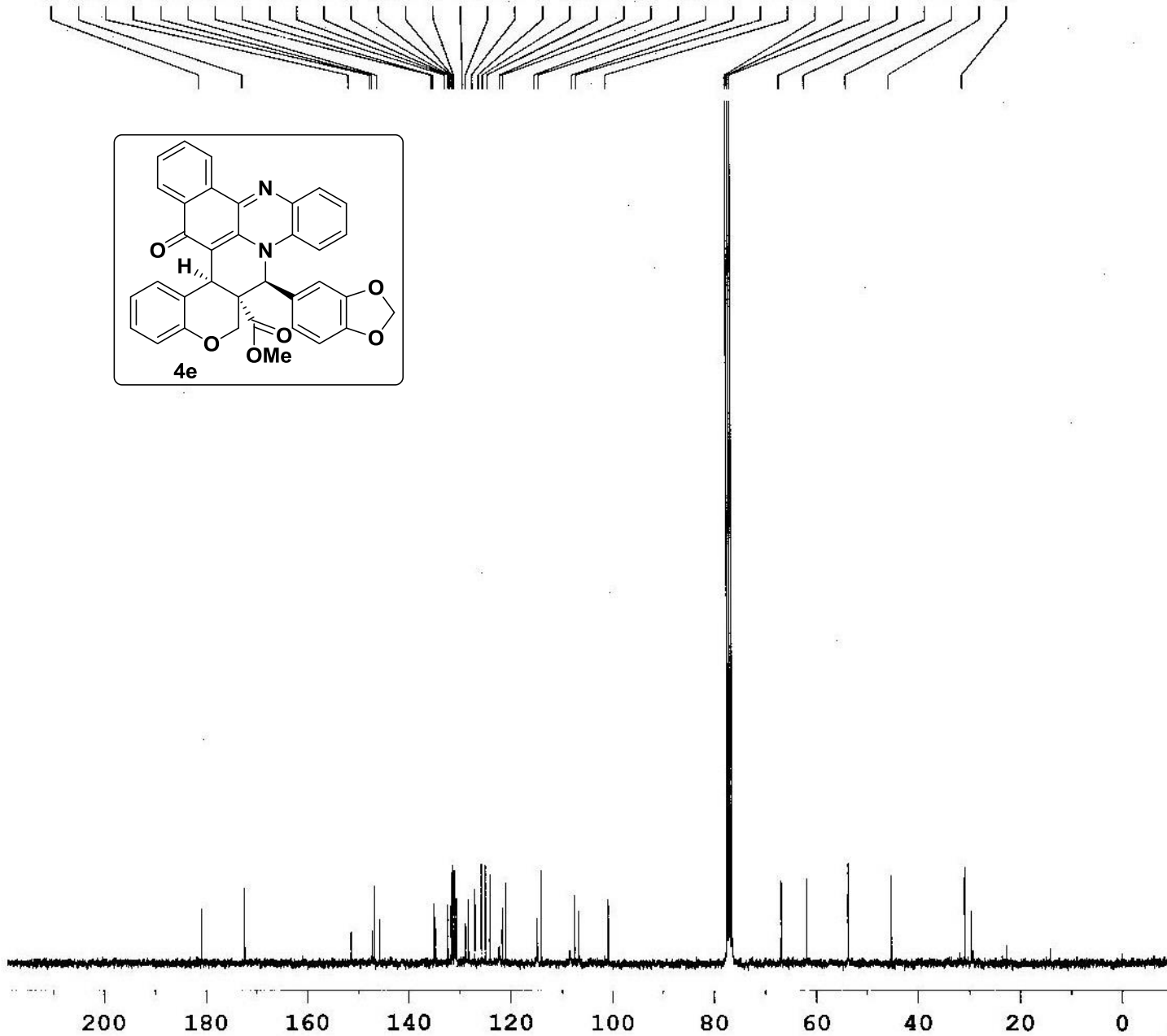
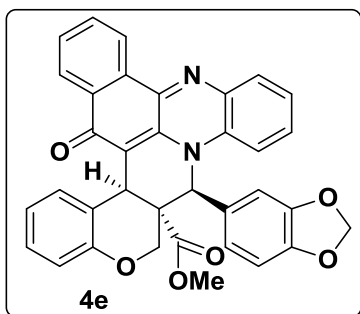
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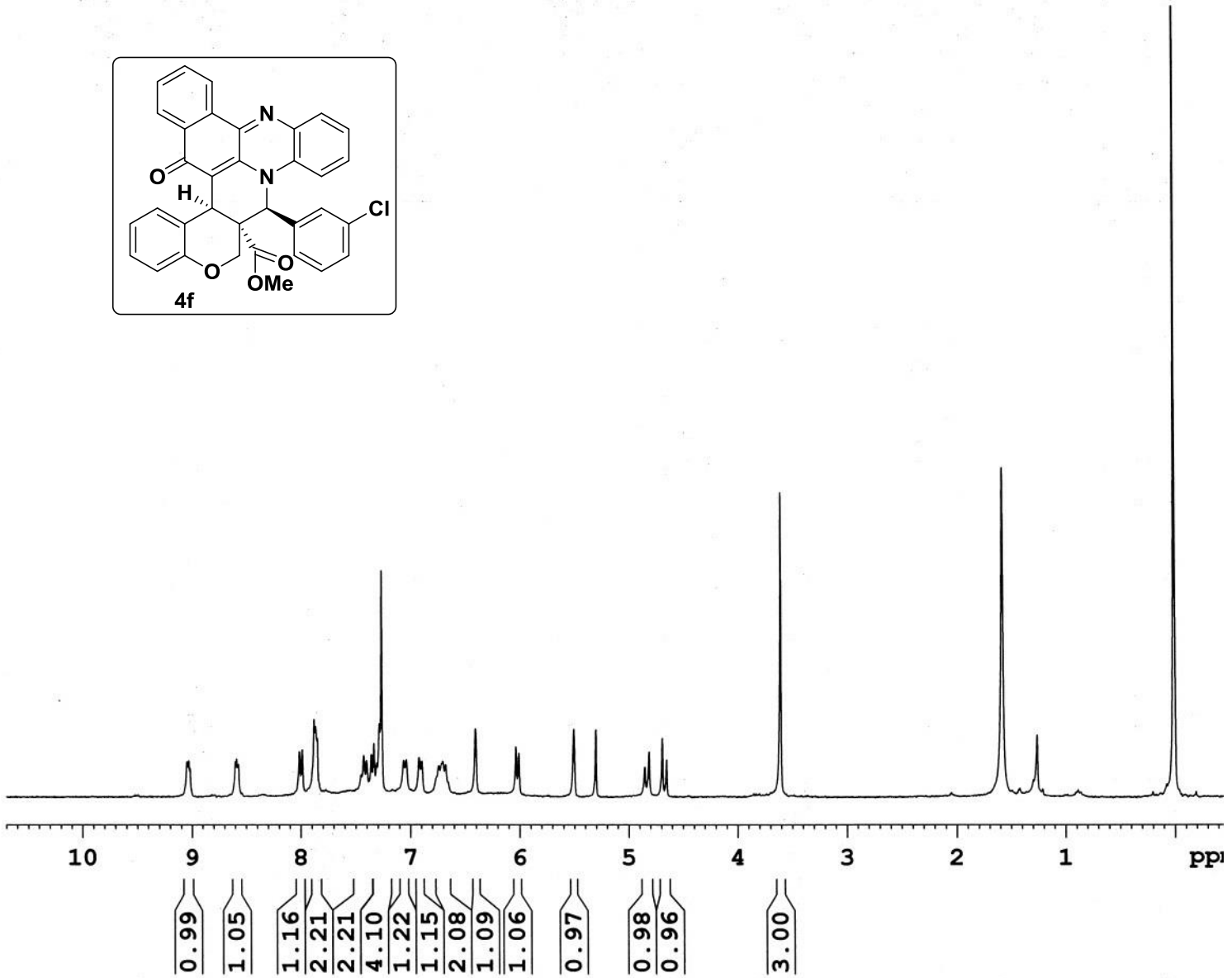
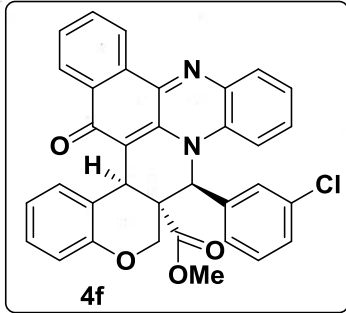


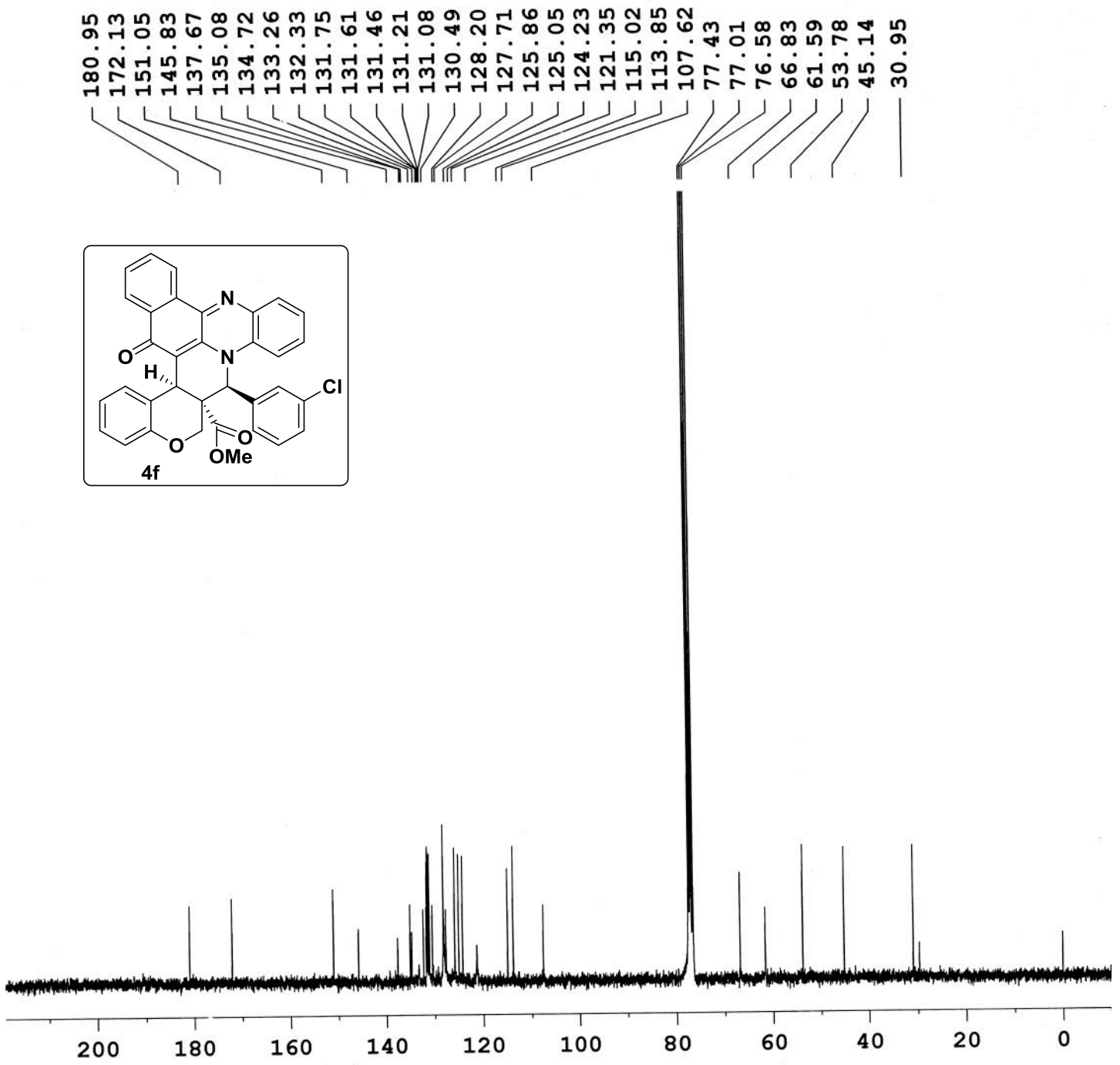
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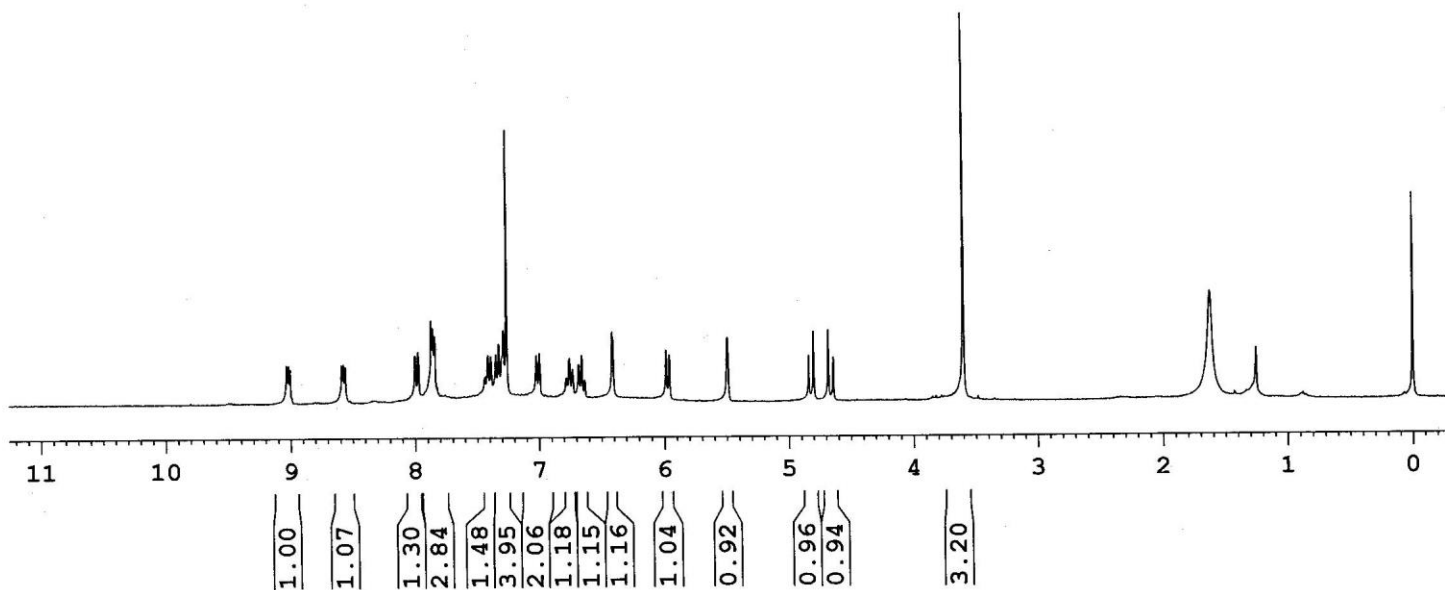
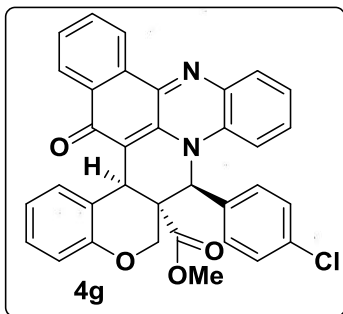


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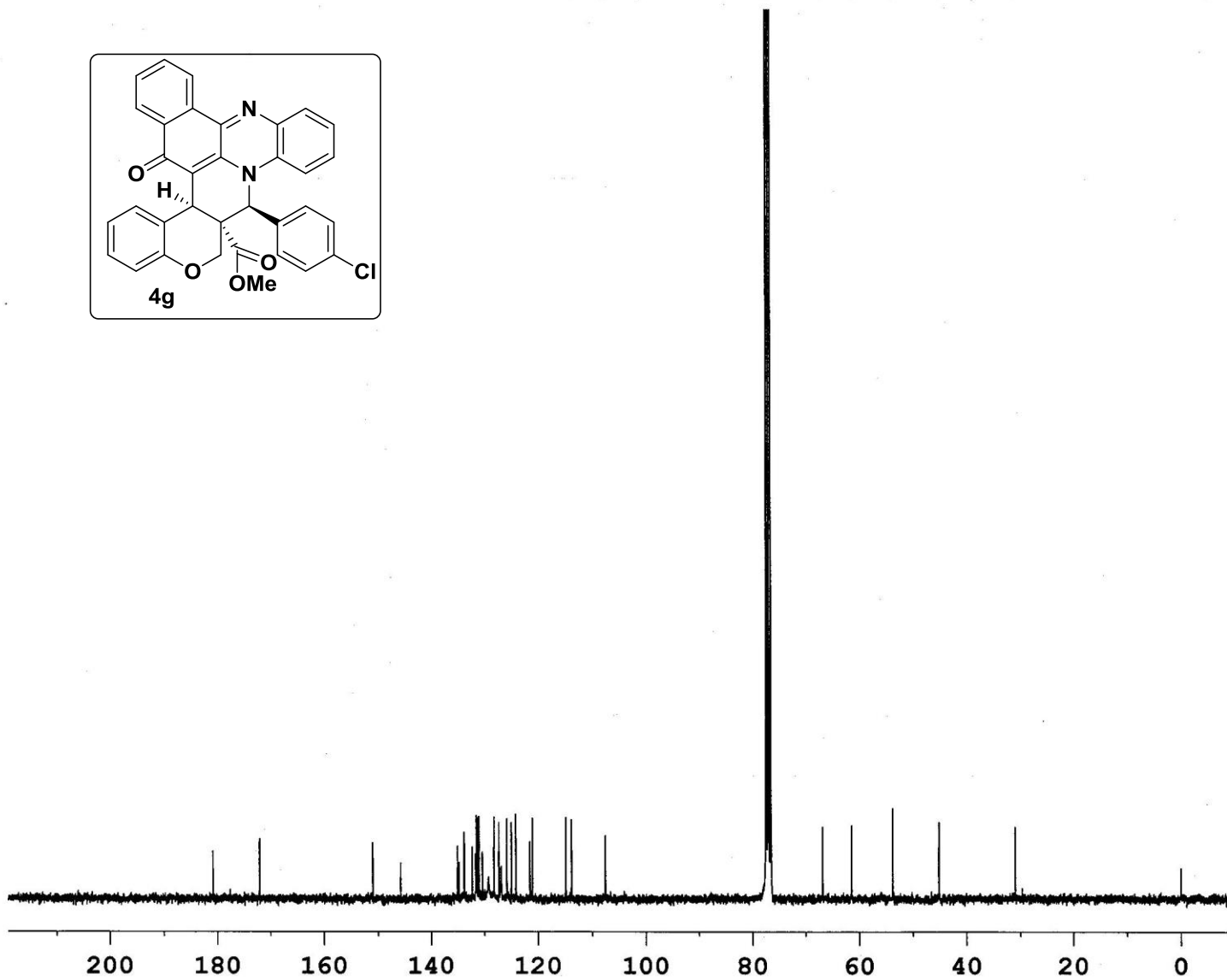
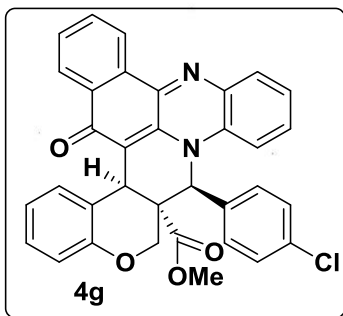




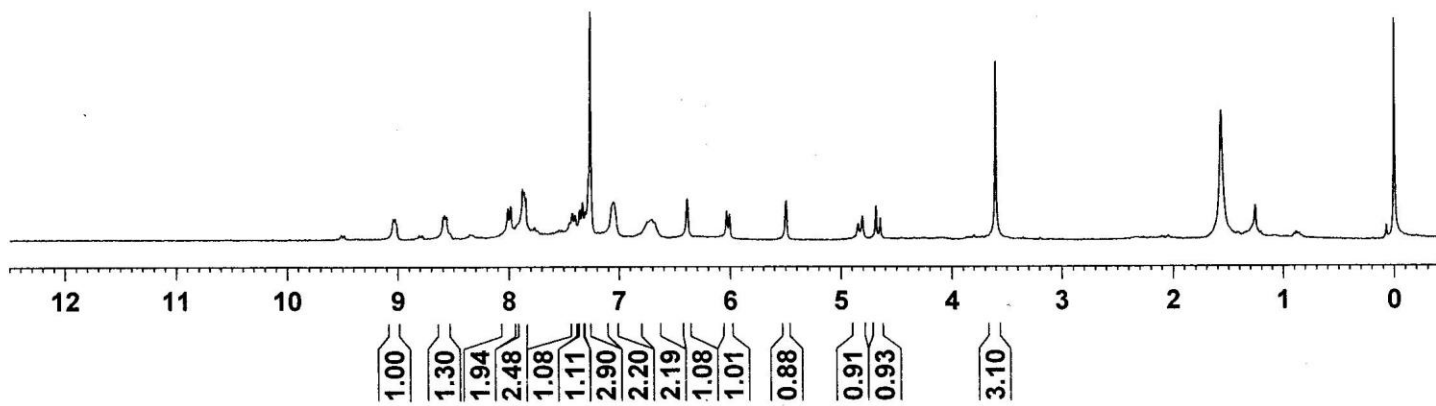
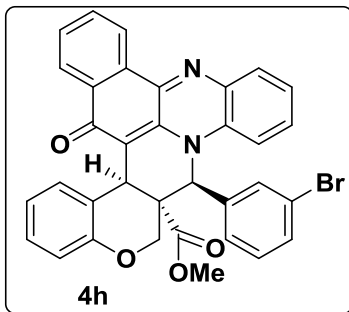
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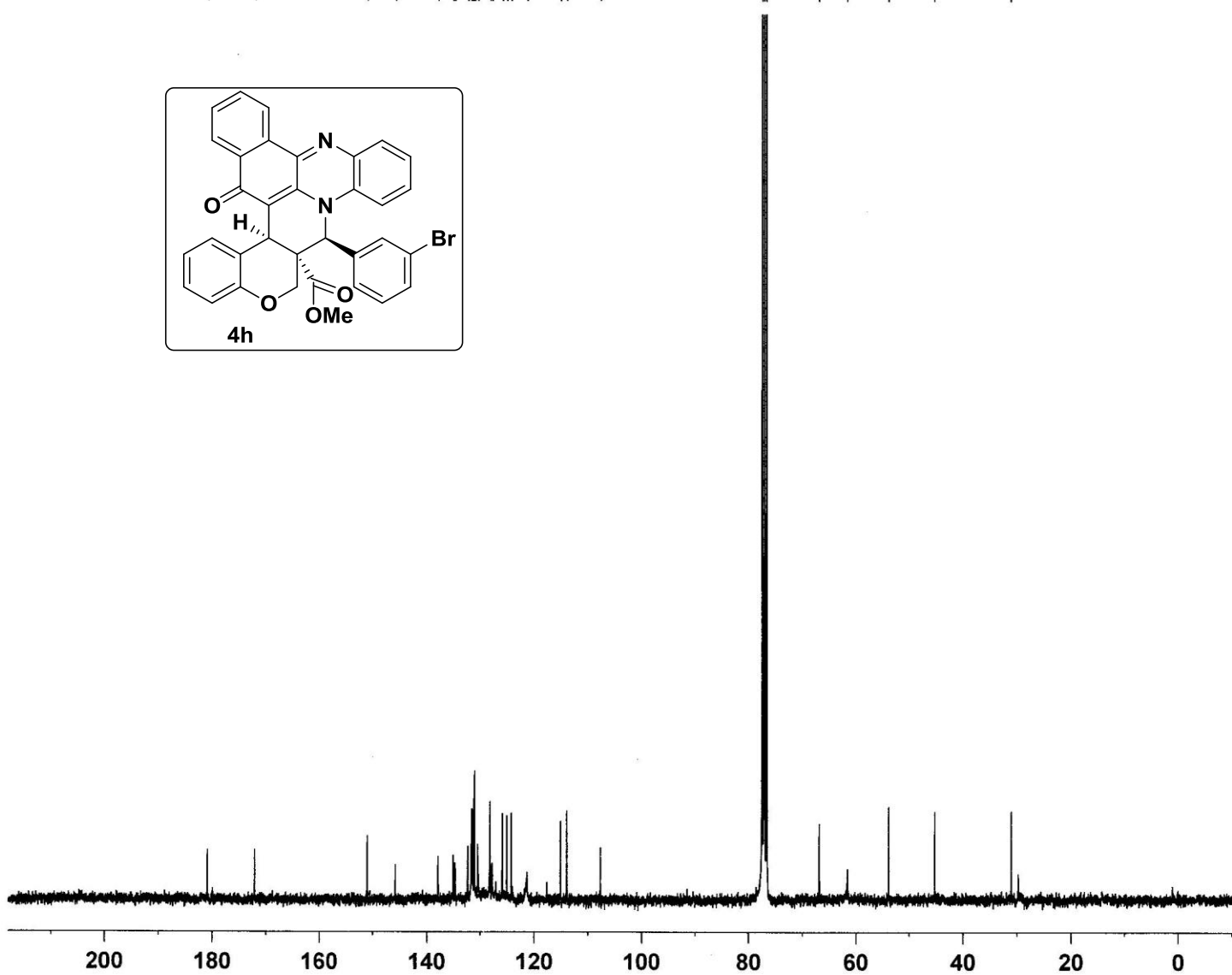
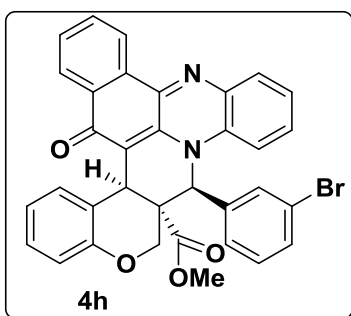
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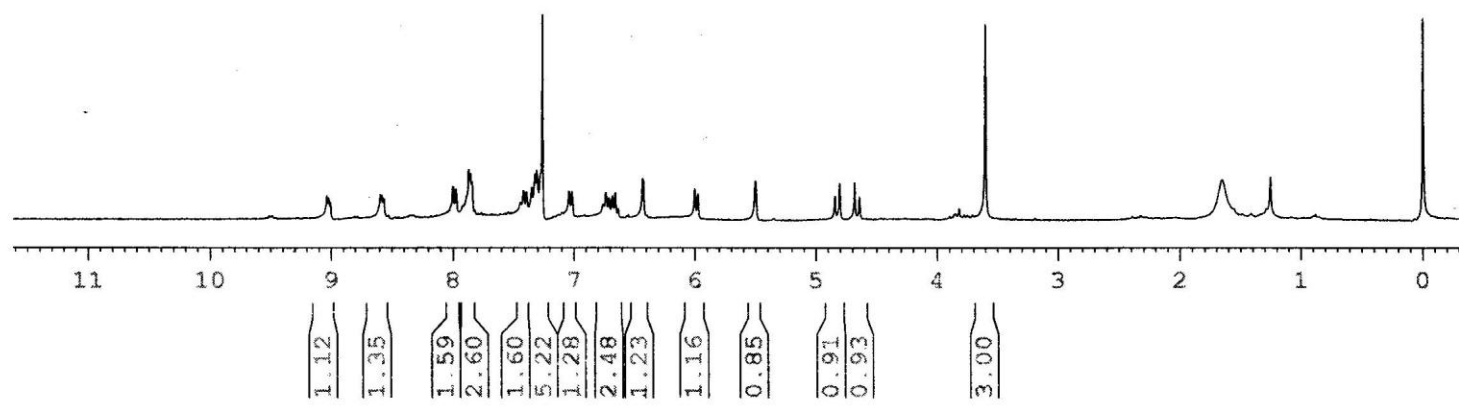
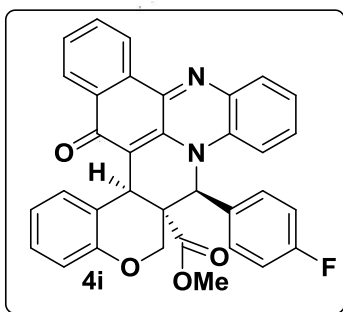
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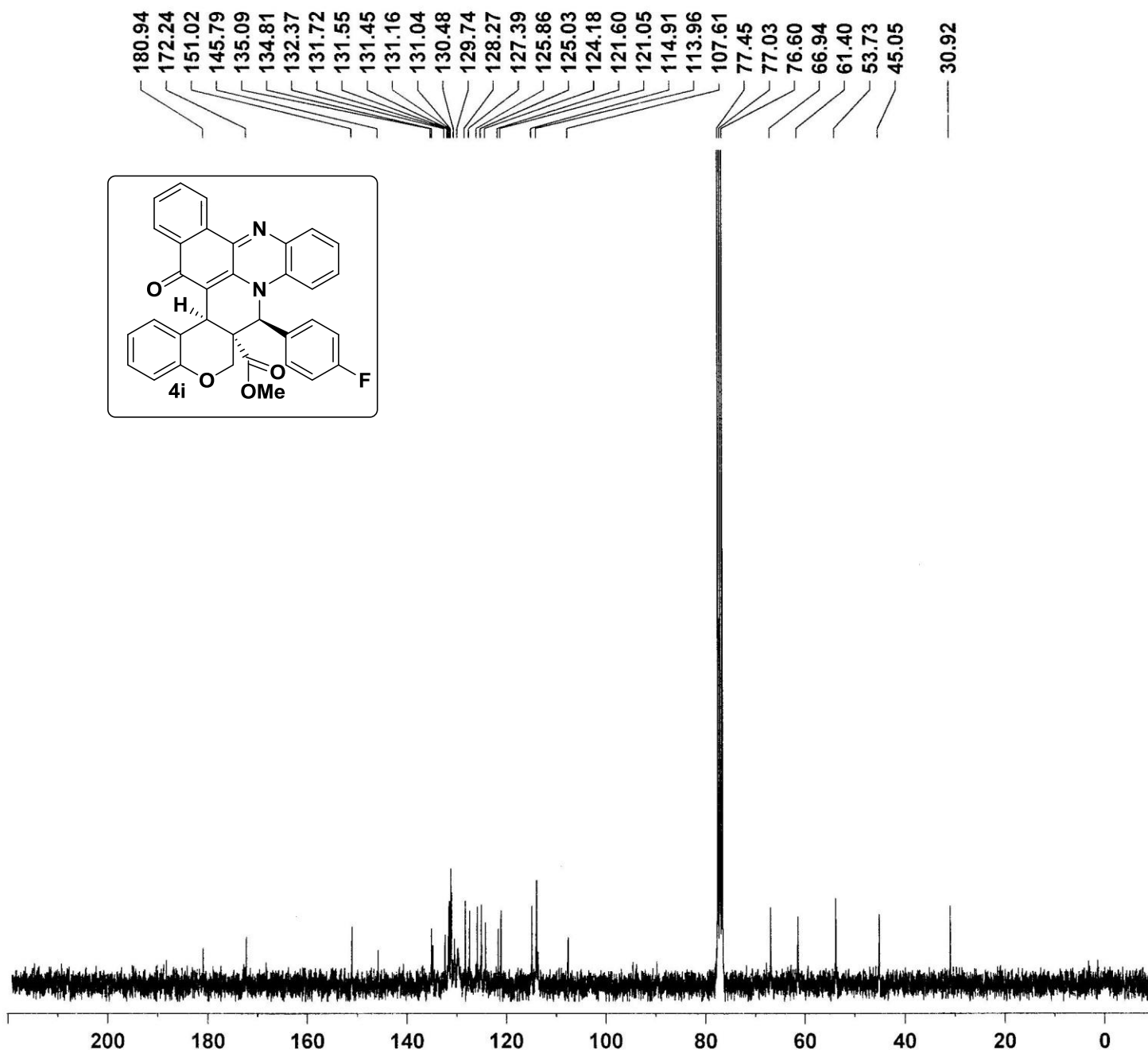


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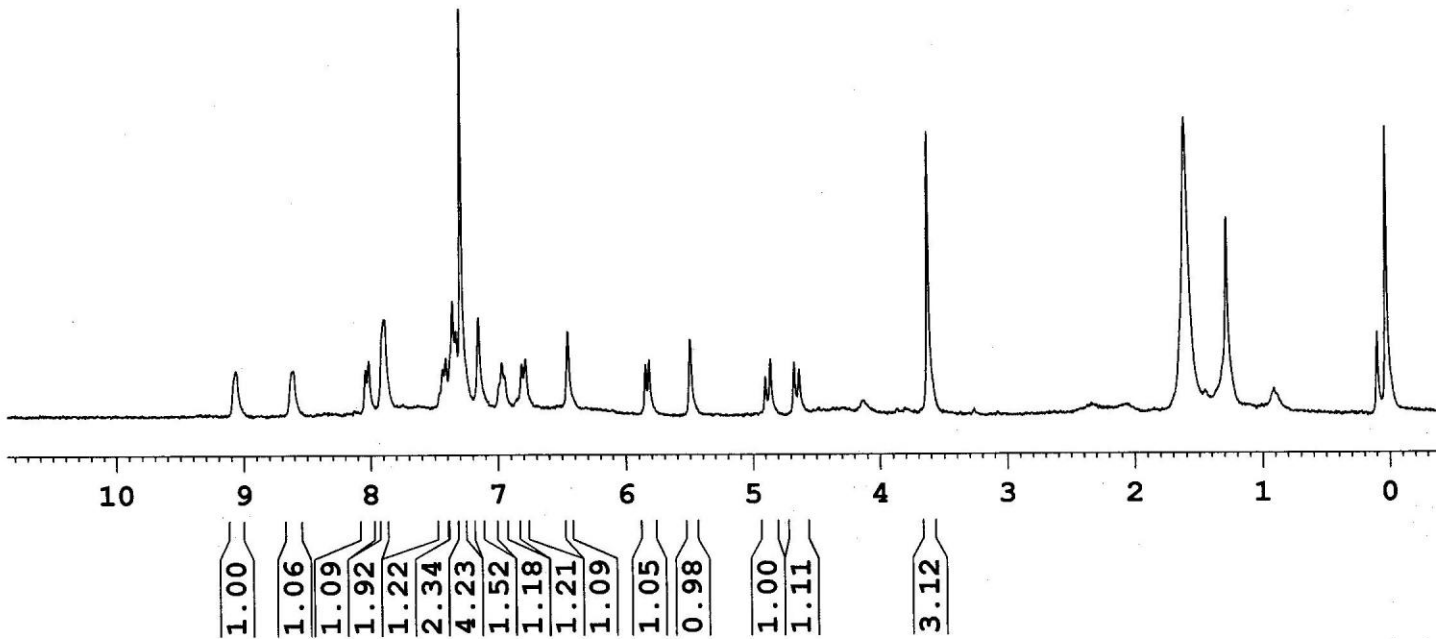
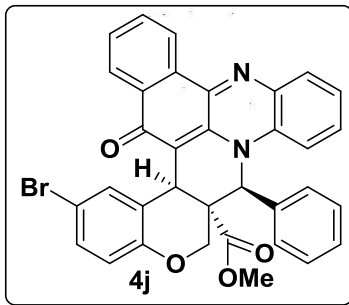
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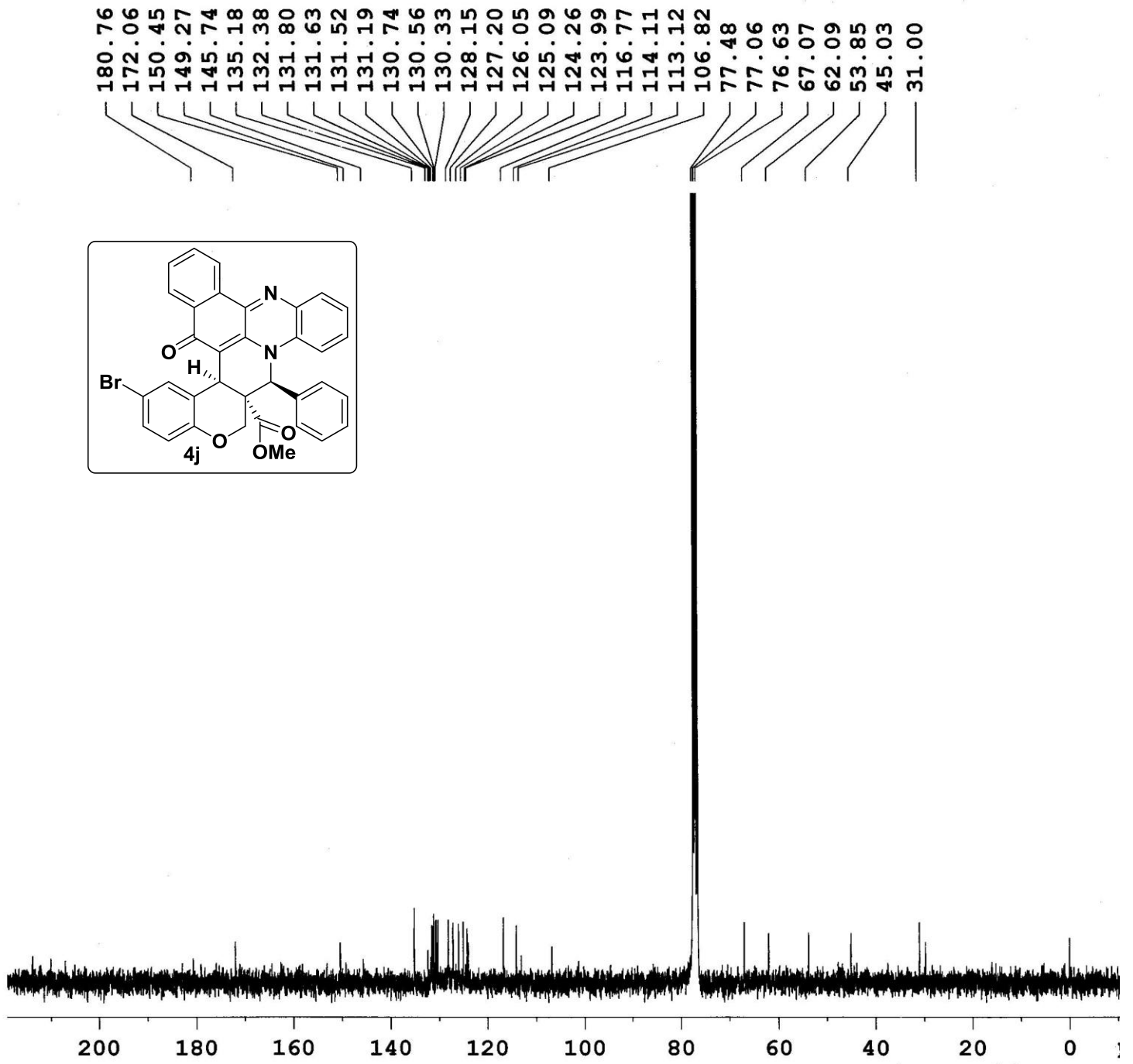


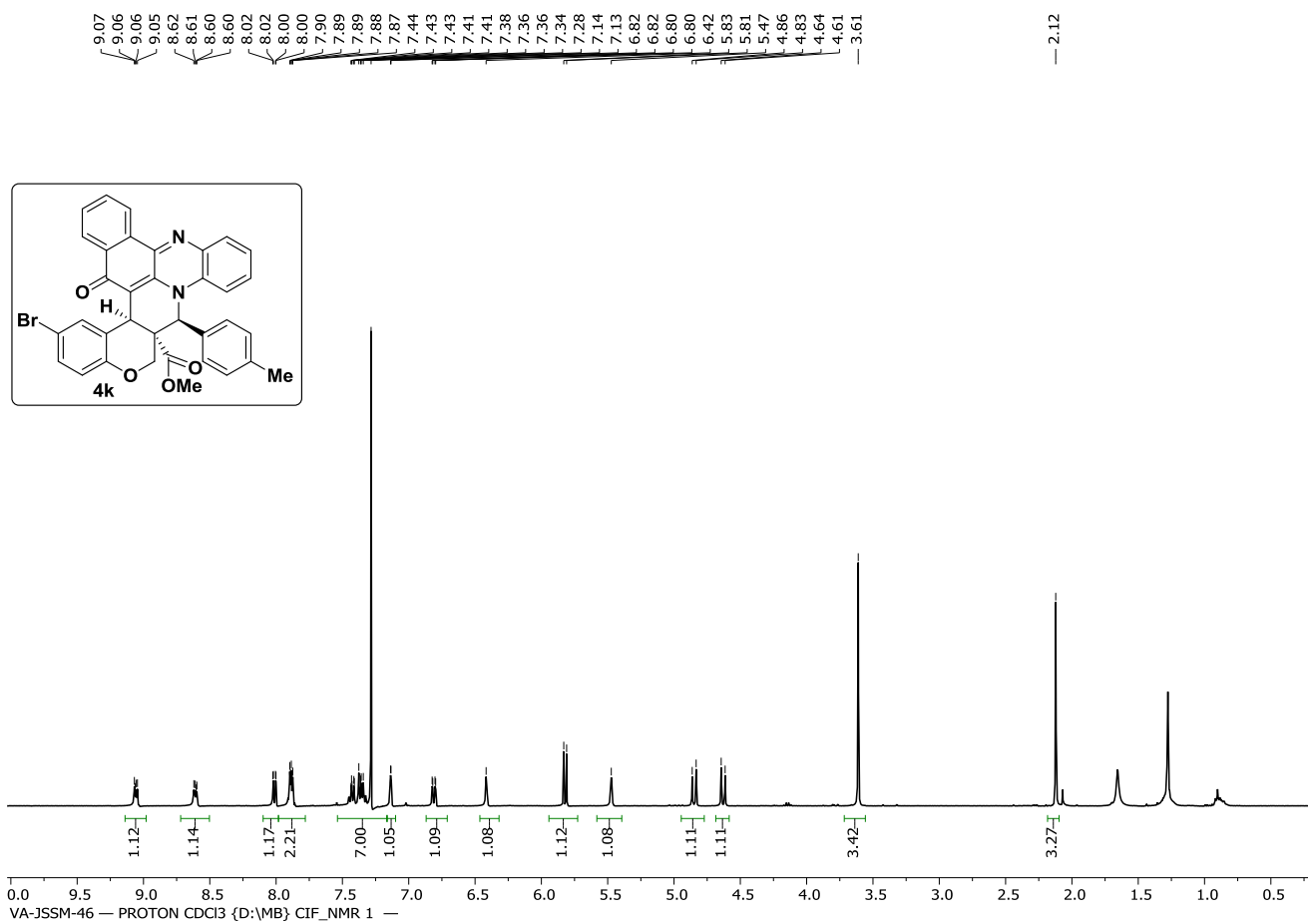




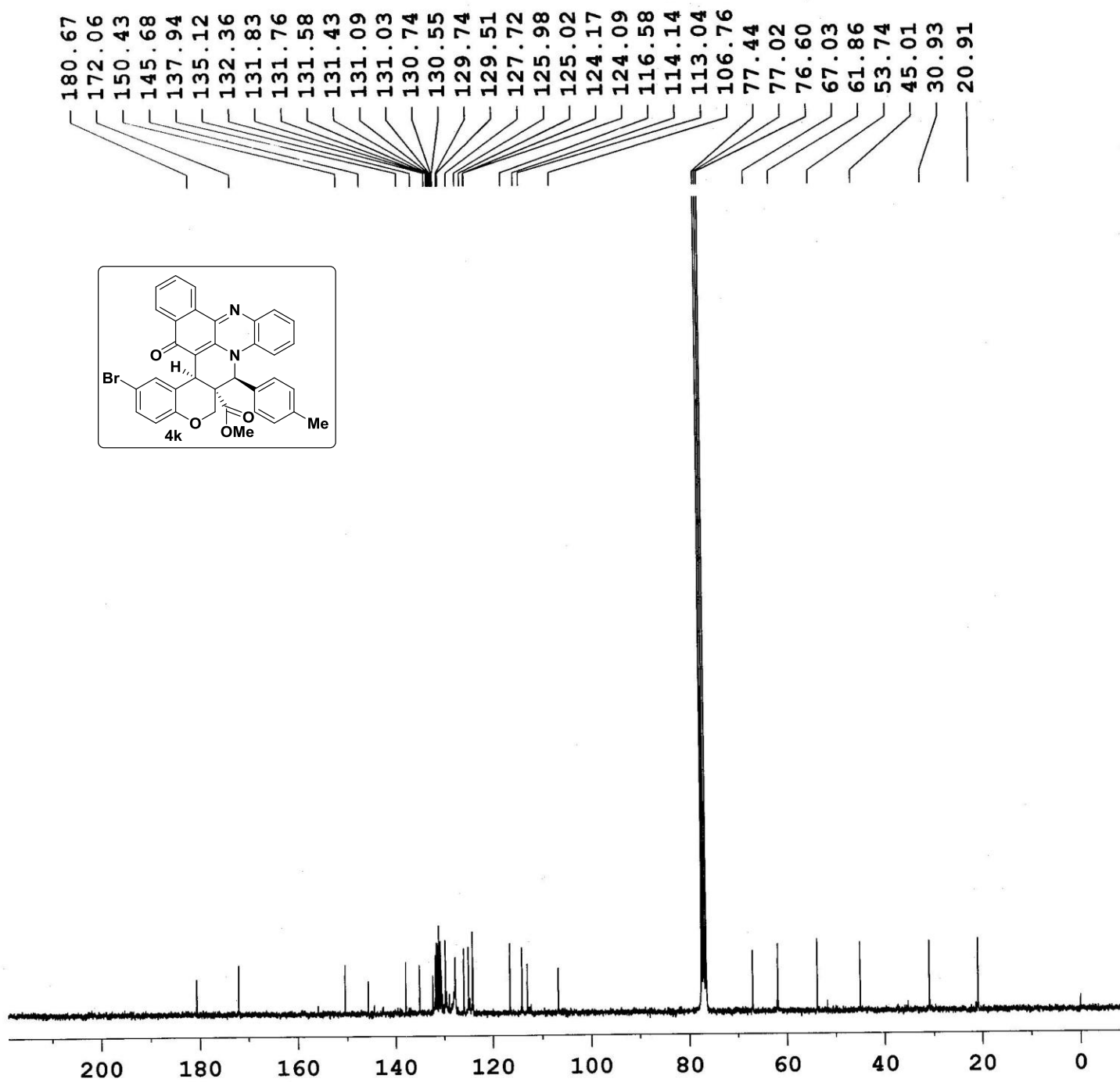
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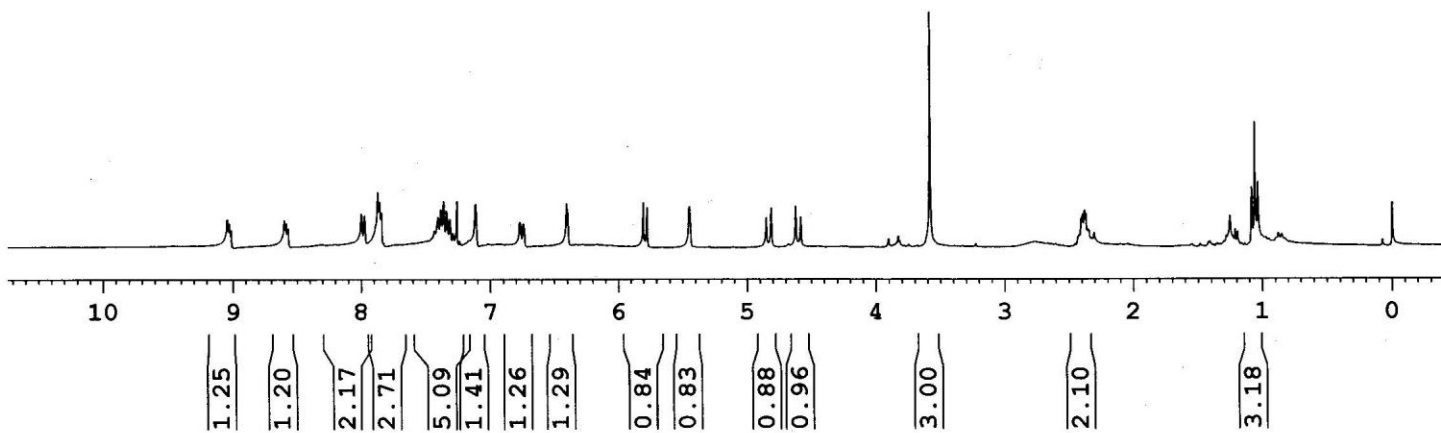
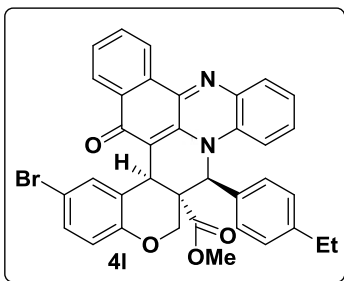


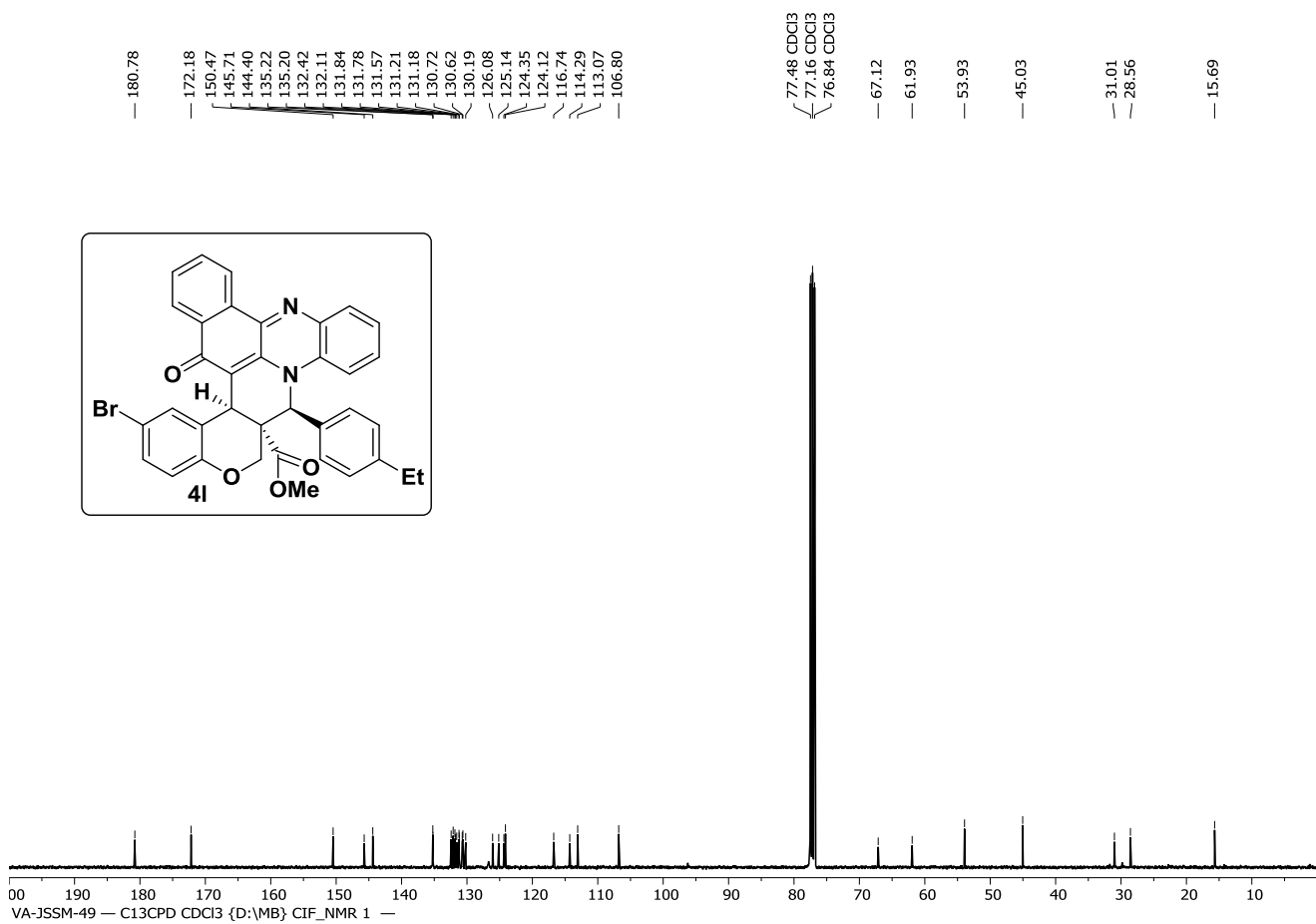


— 2.12

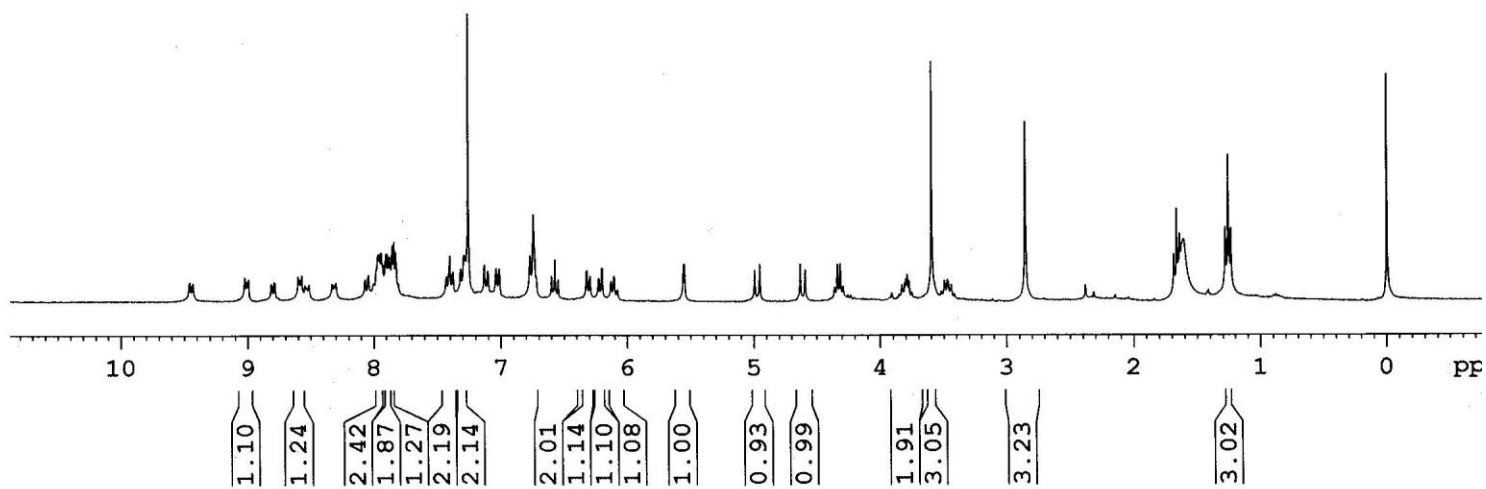
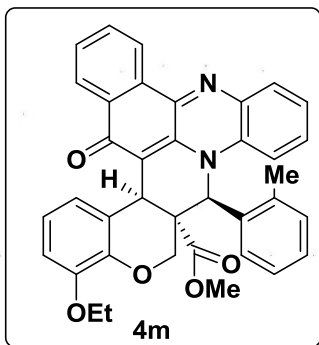


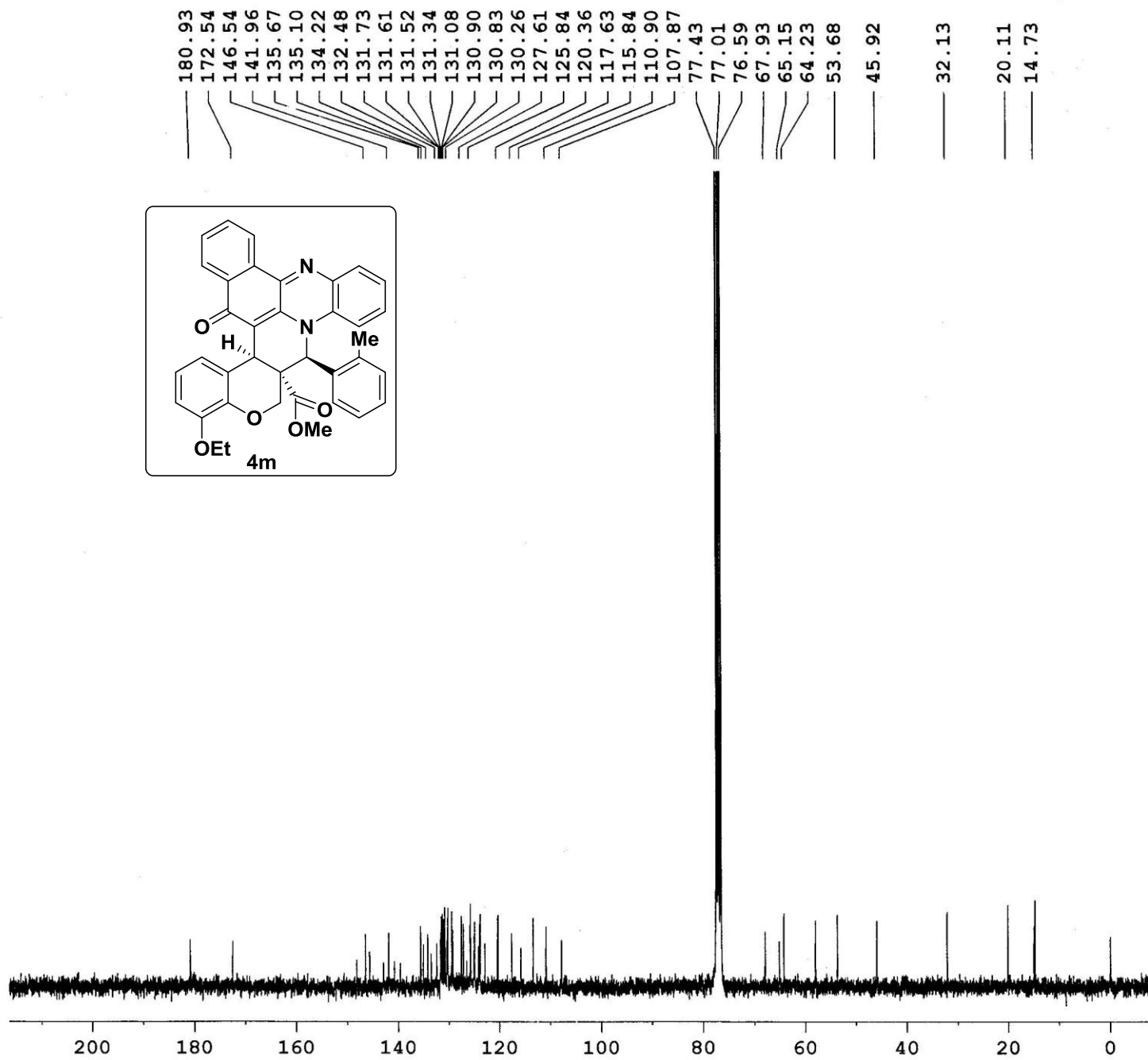
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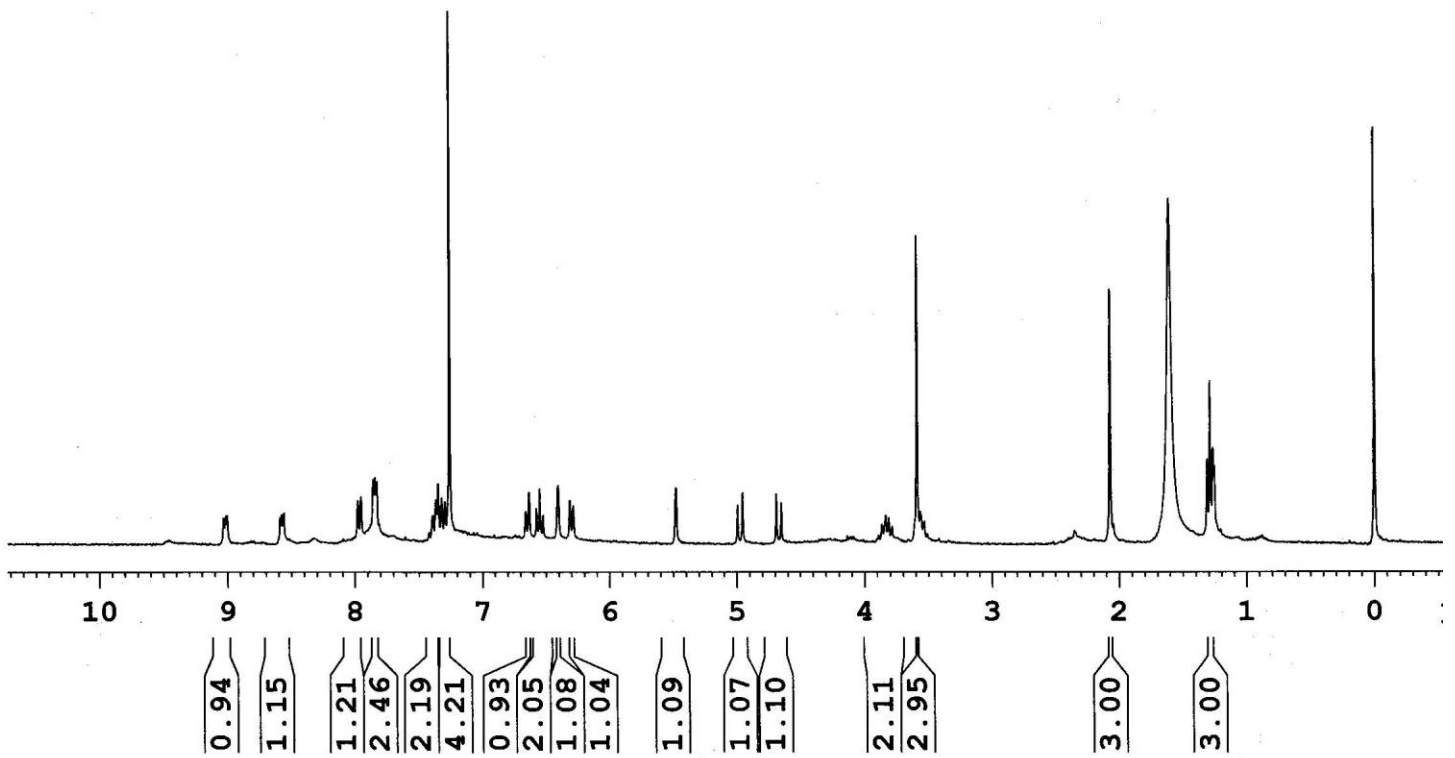
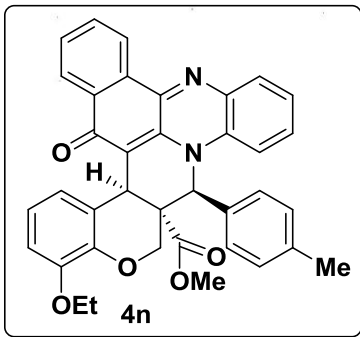
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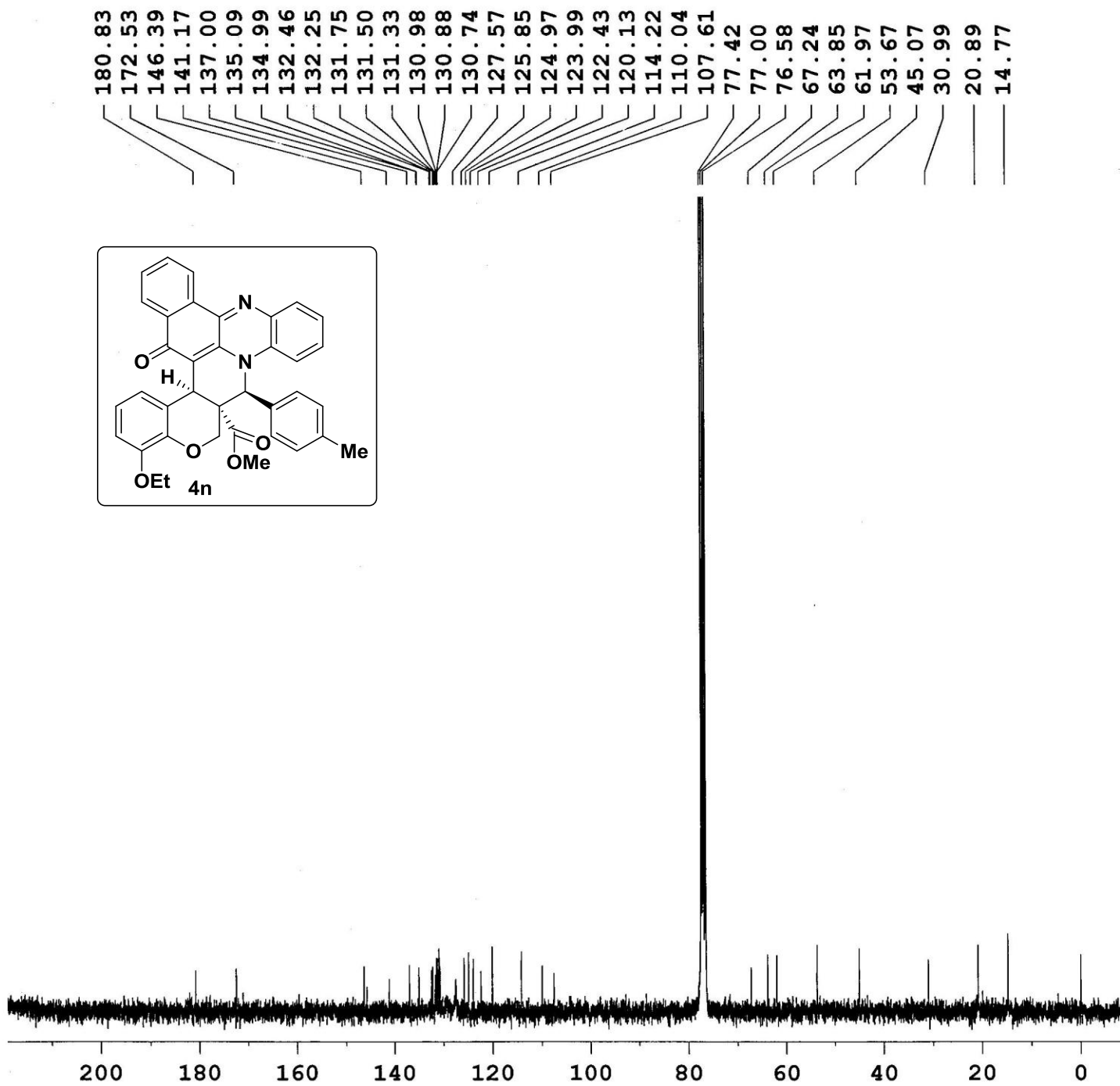




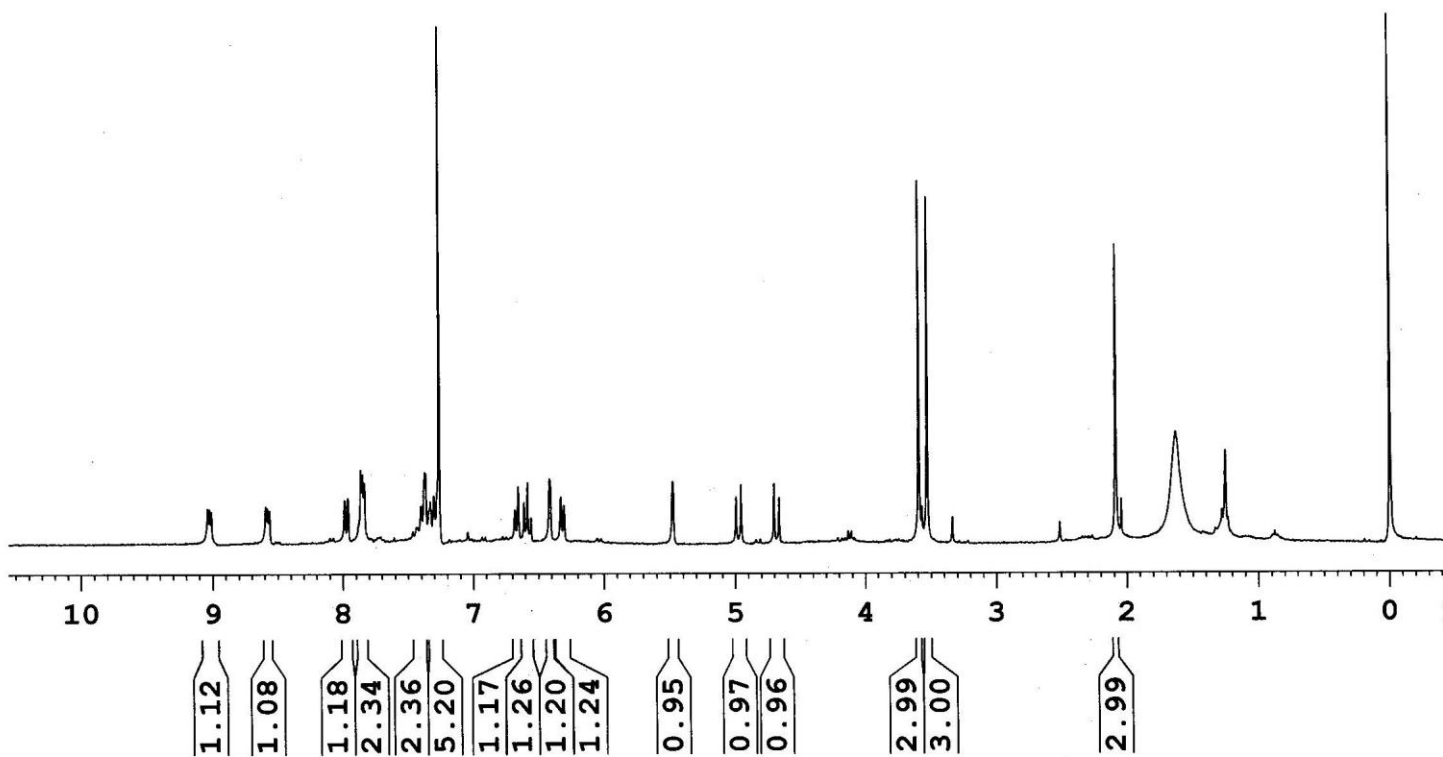
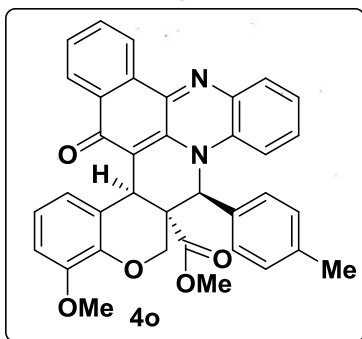


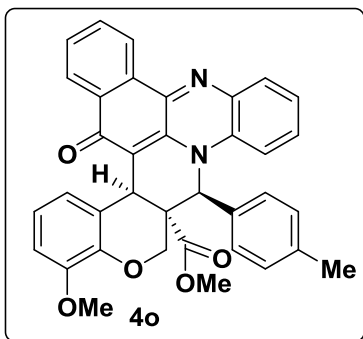
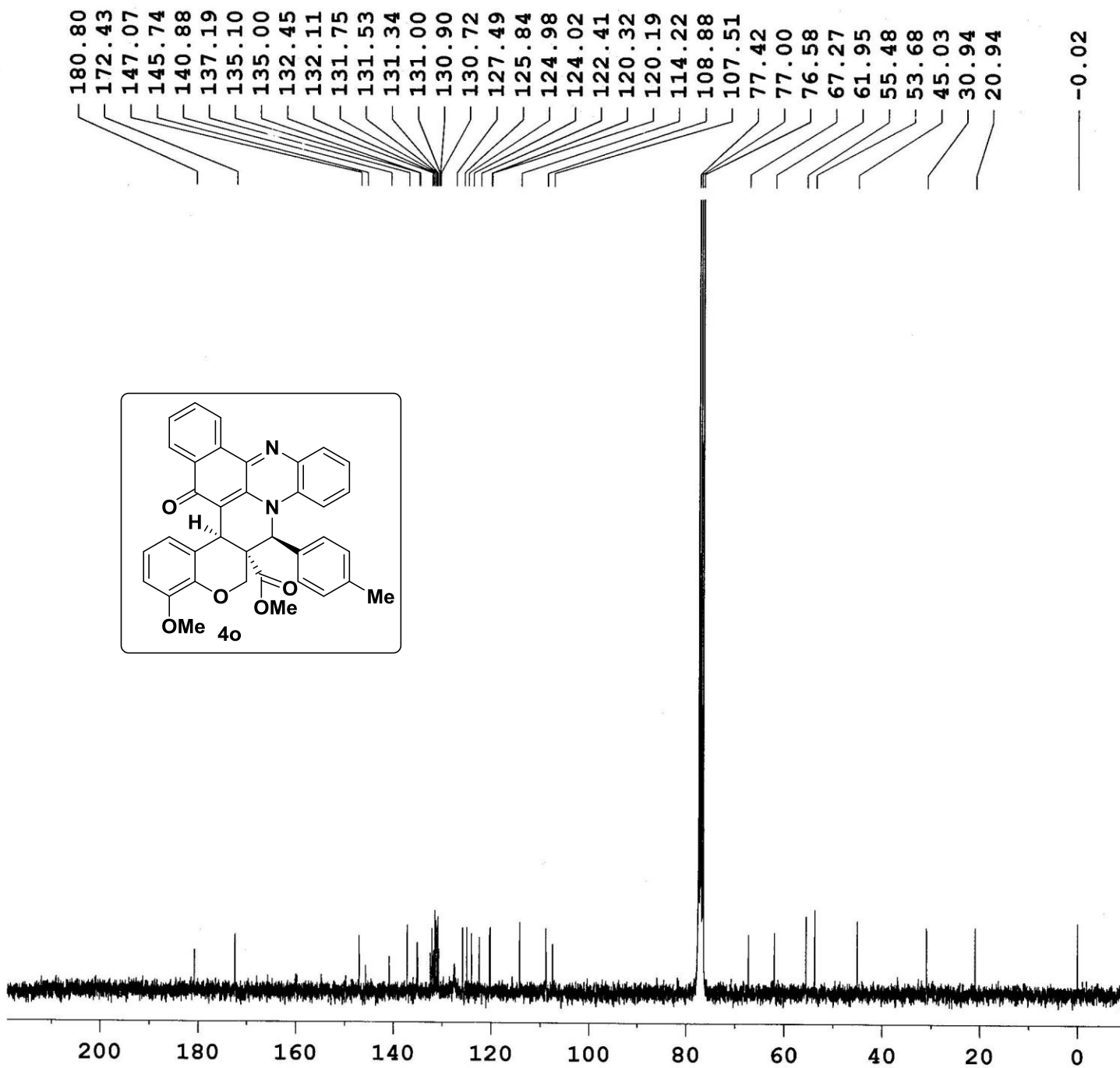
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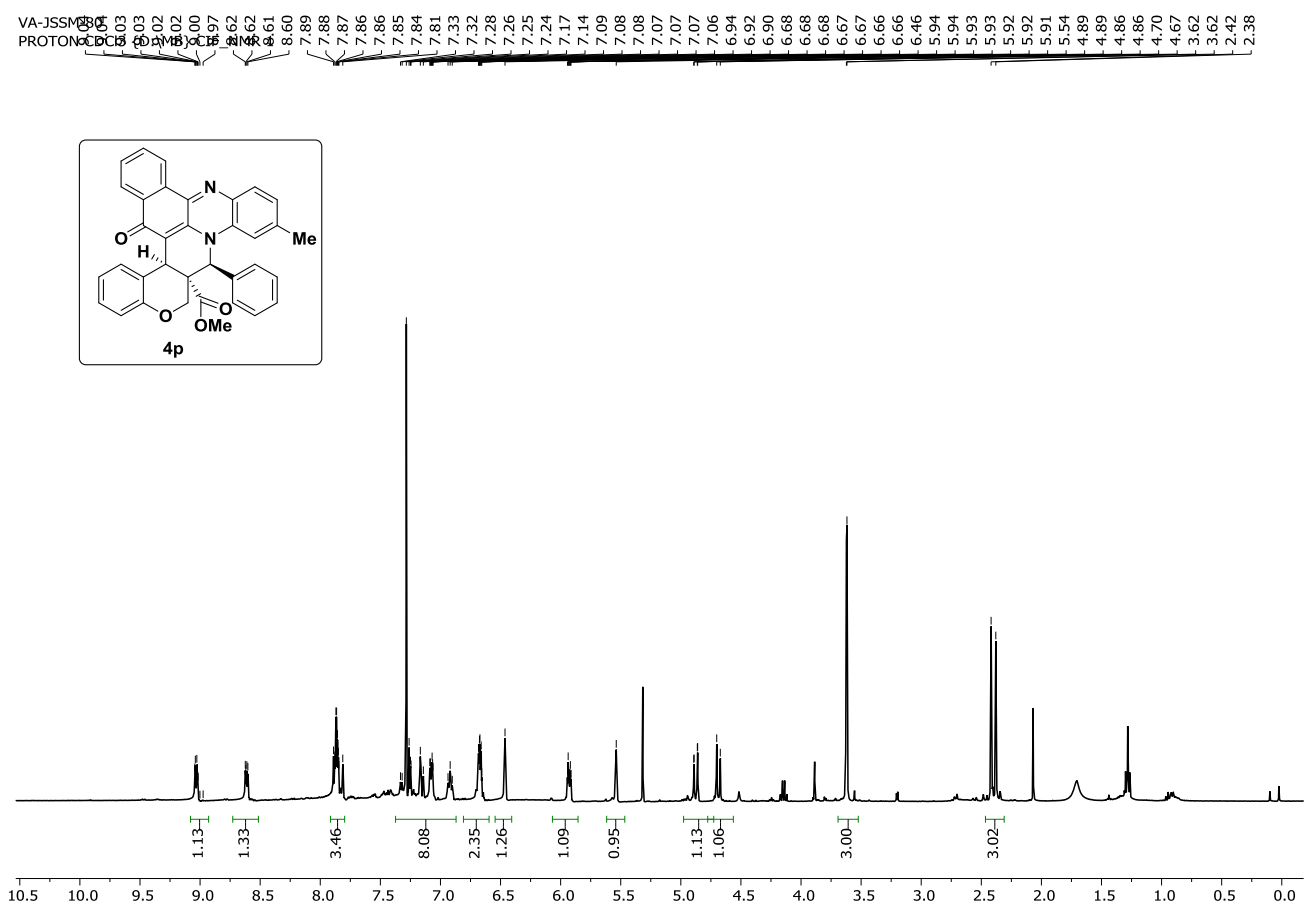


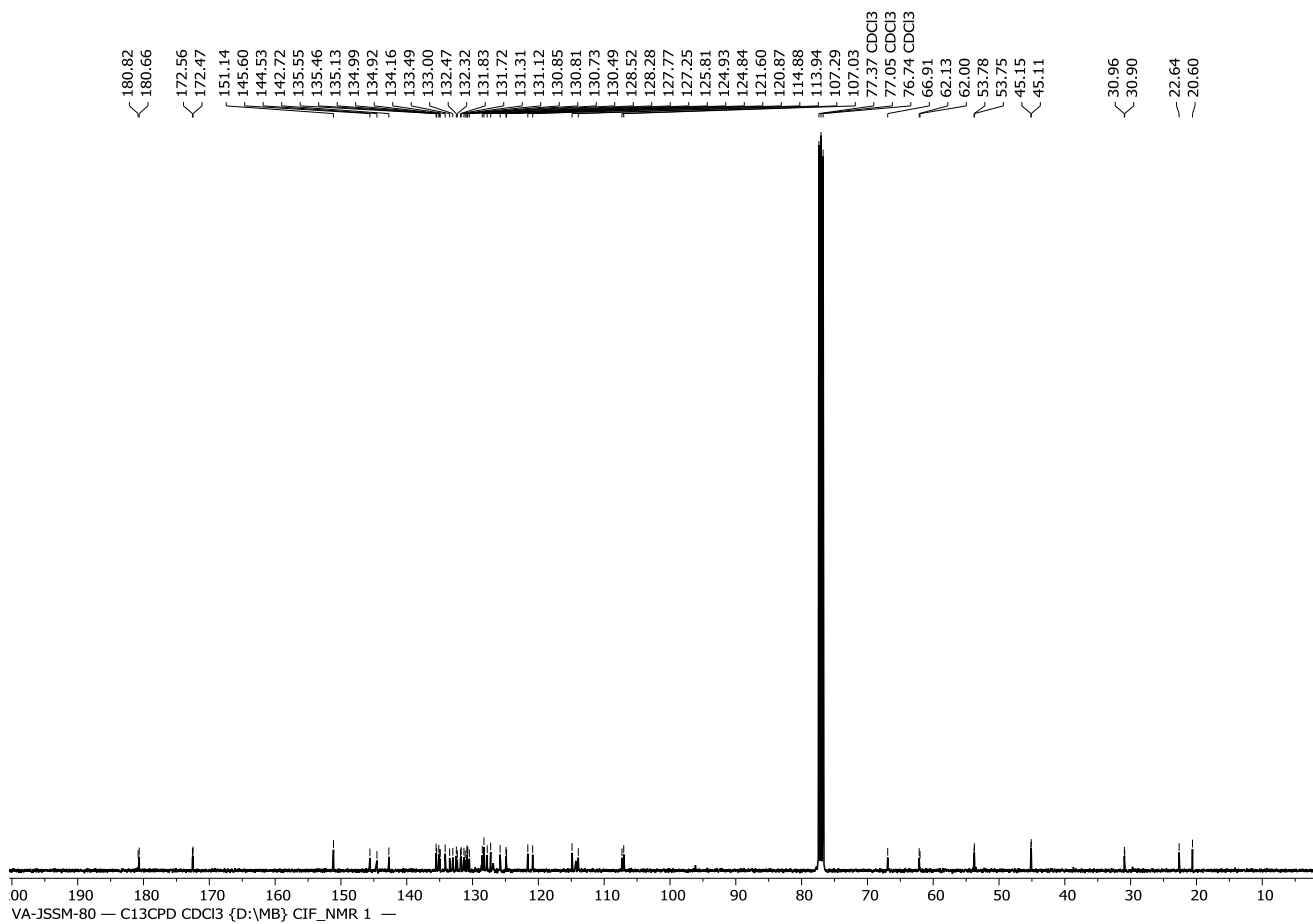


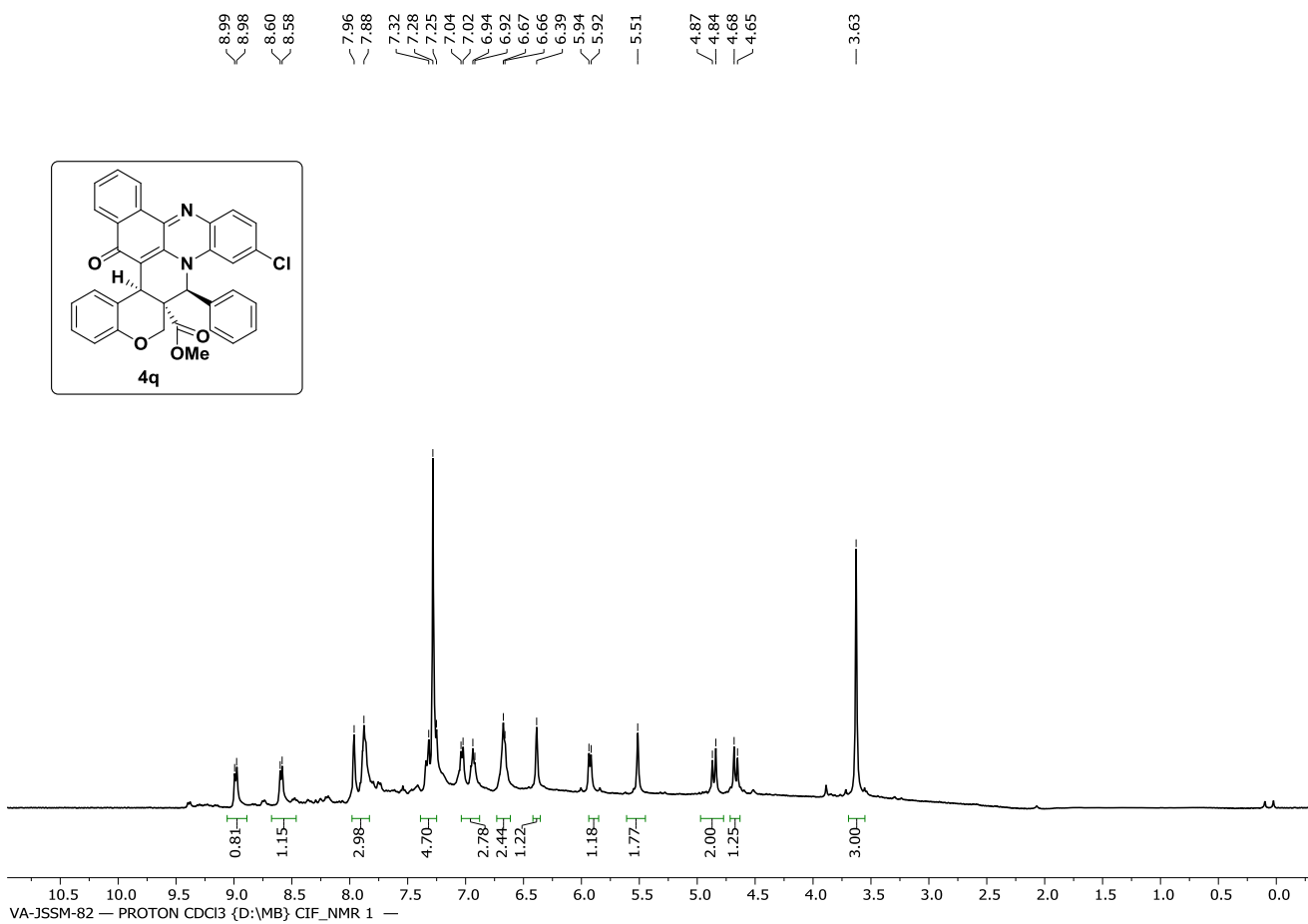
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7.864  
7.857  
7.849  
7.840  
7.834  
7.466  
7.431  
7.402  
7.374  
7.331  
7.304  
7.262  
7.044  
6.681  
6.655  
6.609  
6.583  
6.557  
6.415  
6.329  
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5.482  
4.997  
4.958  
4.705  
4.666  
3.595  
3.531  
2.088

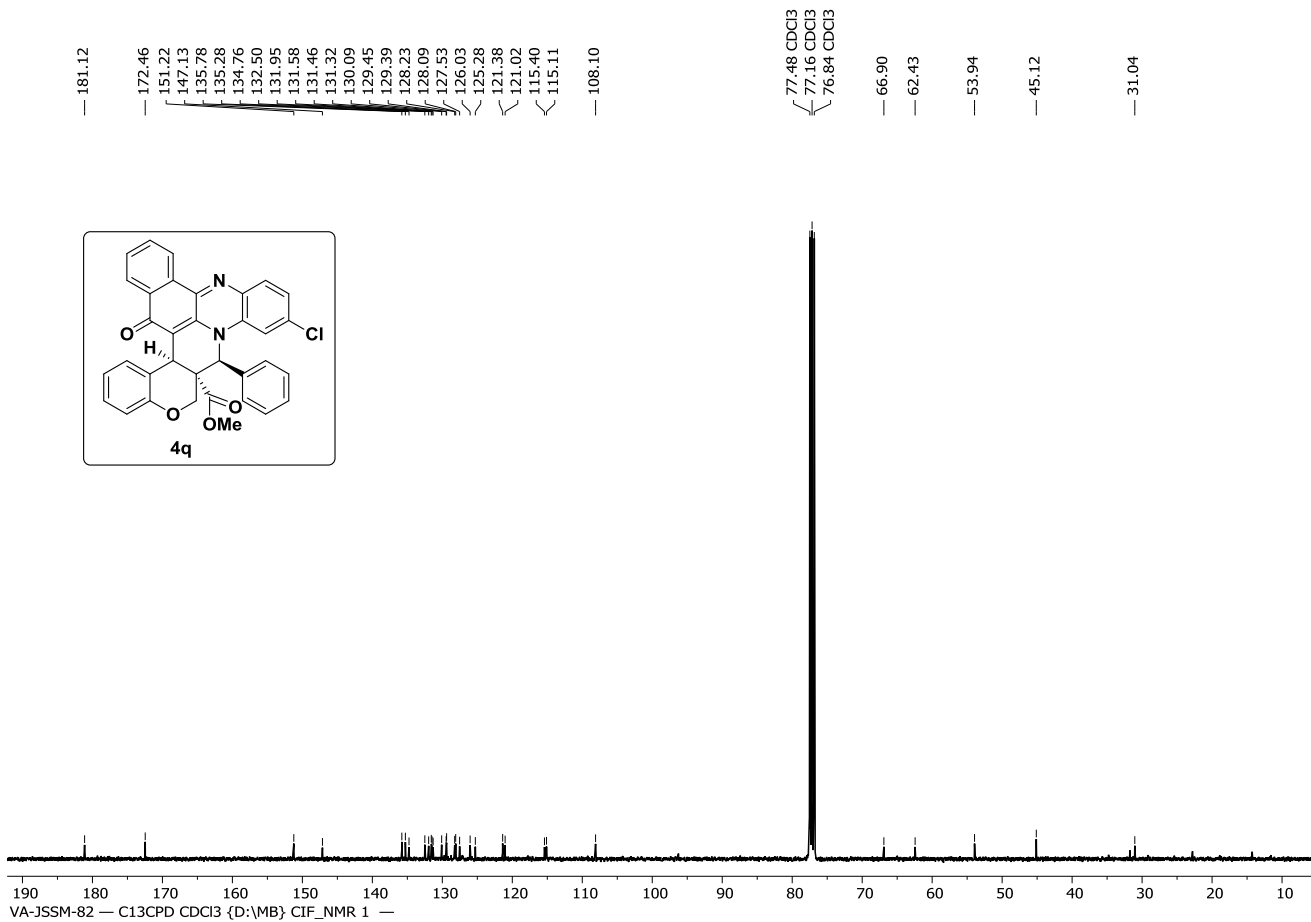






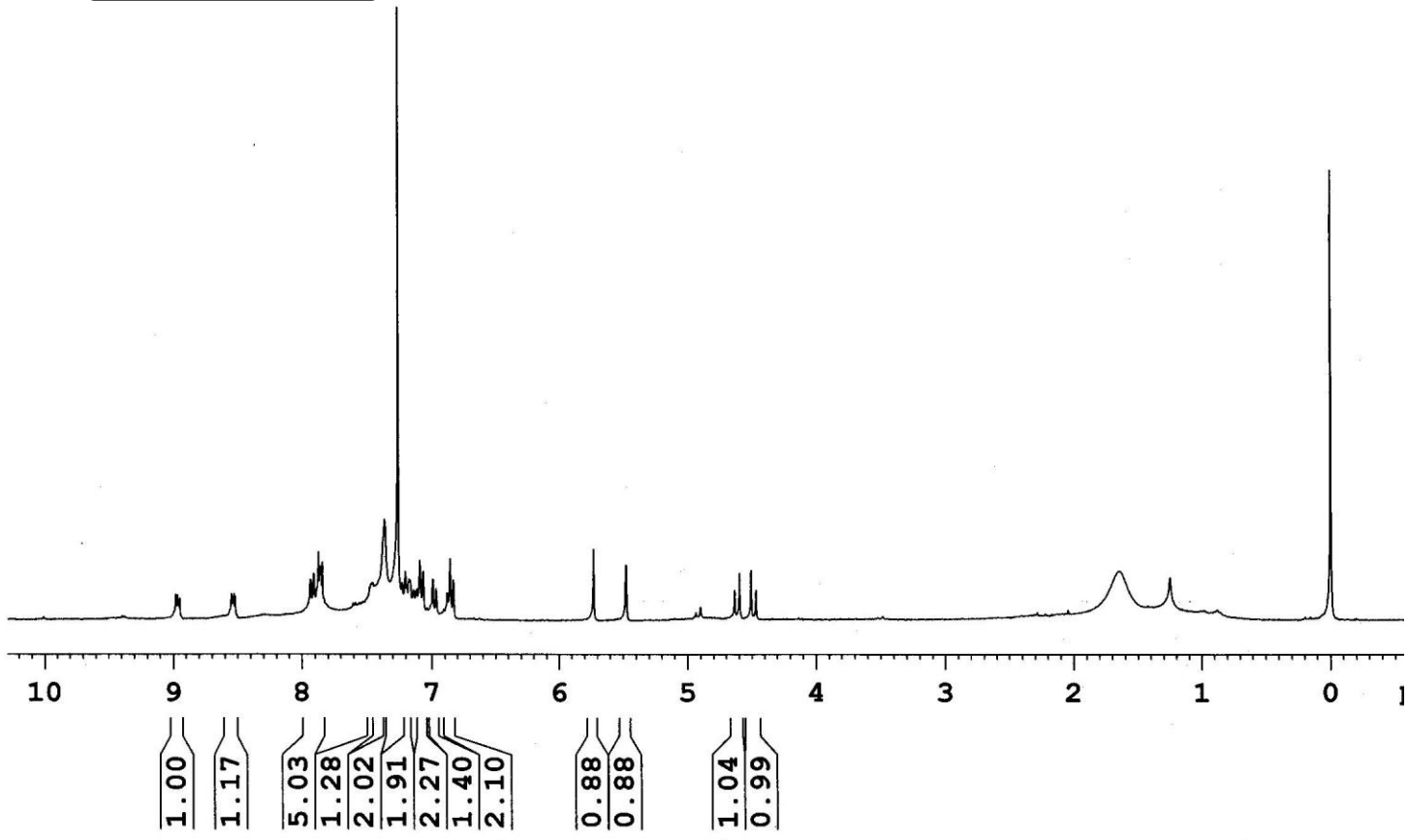
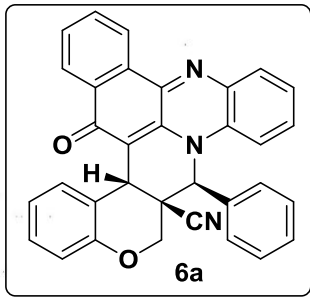




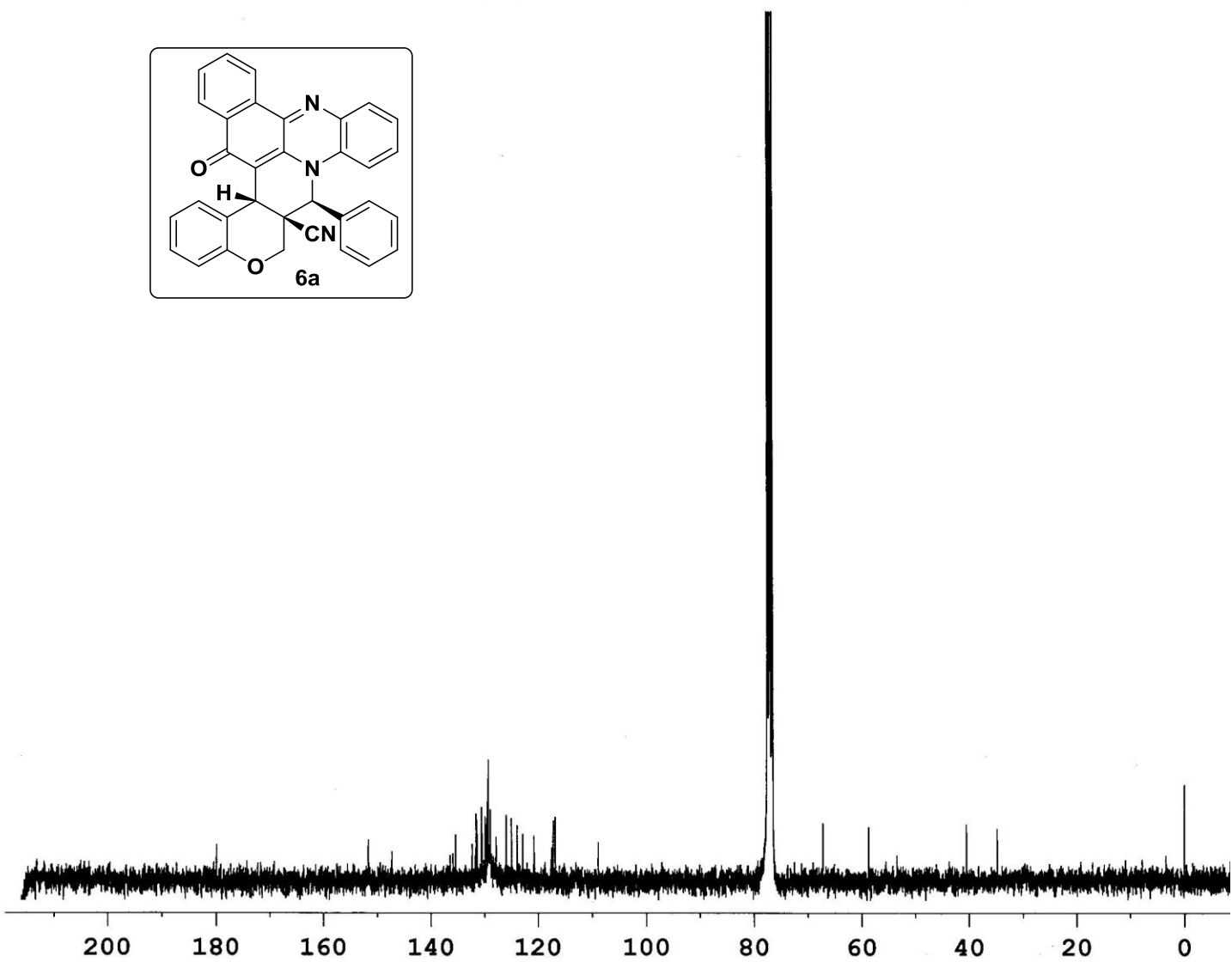
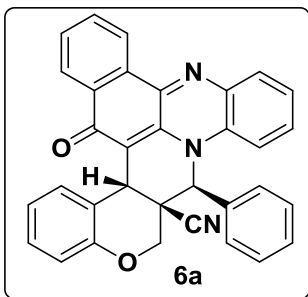


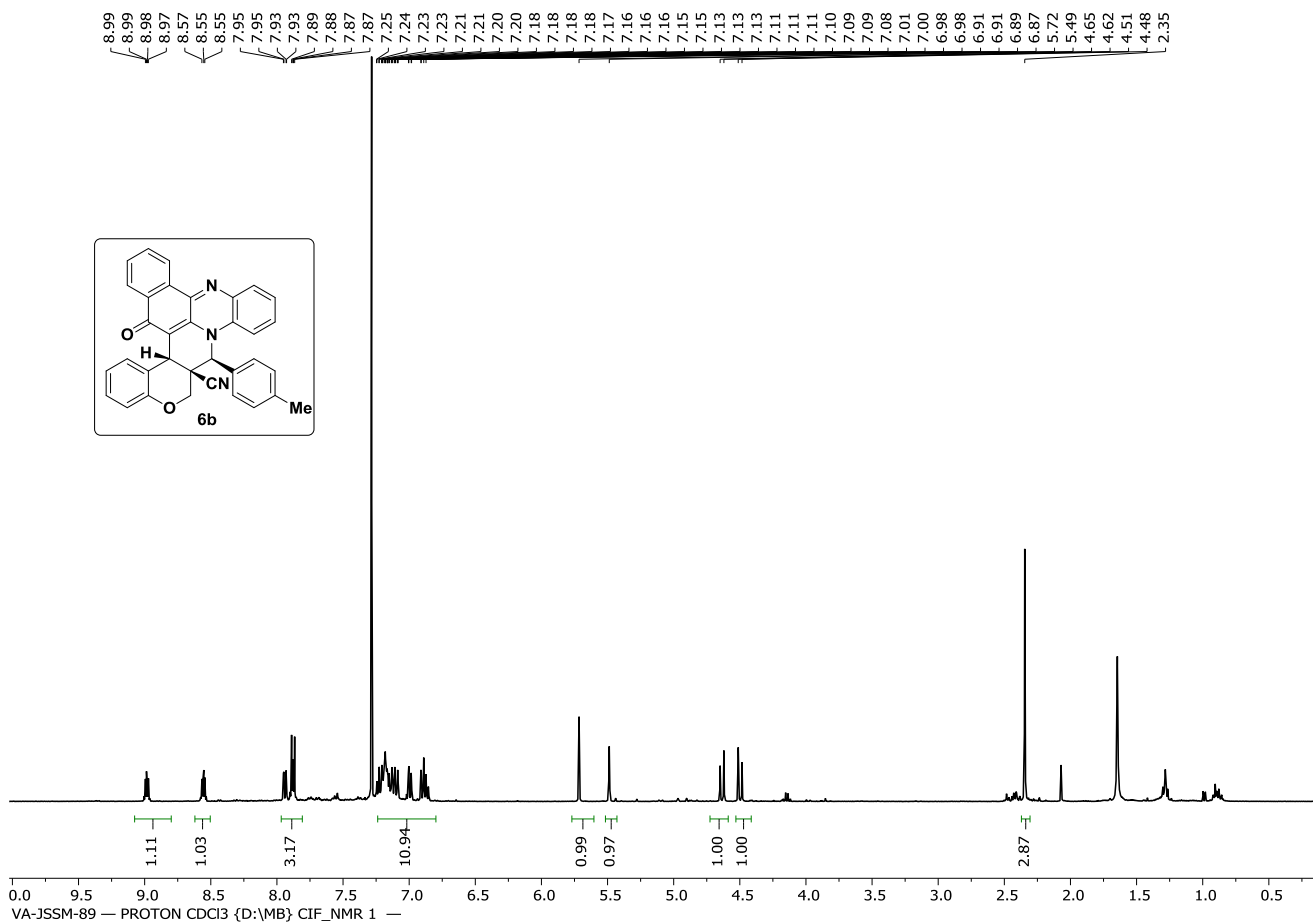


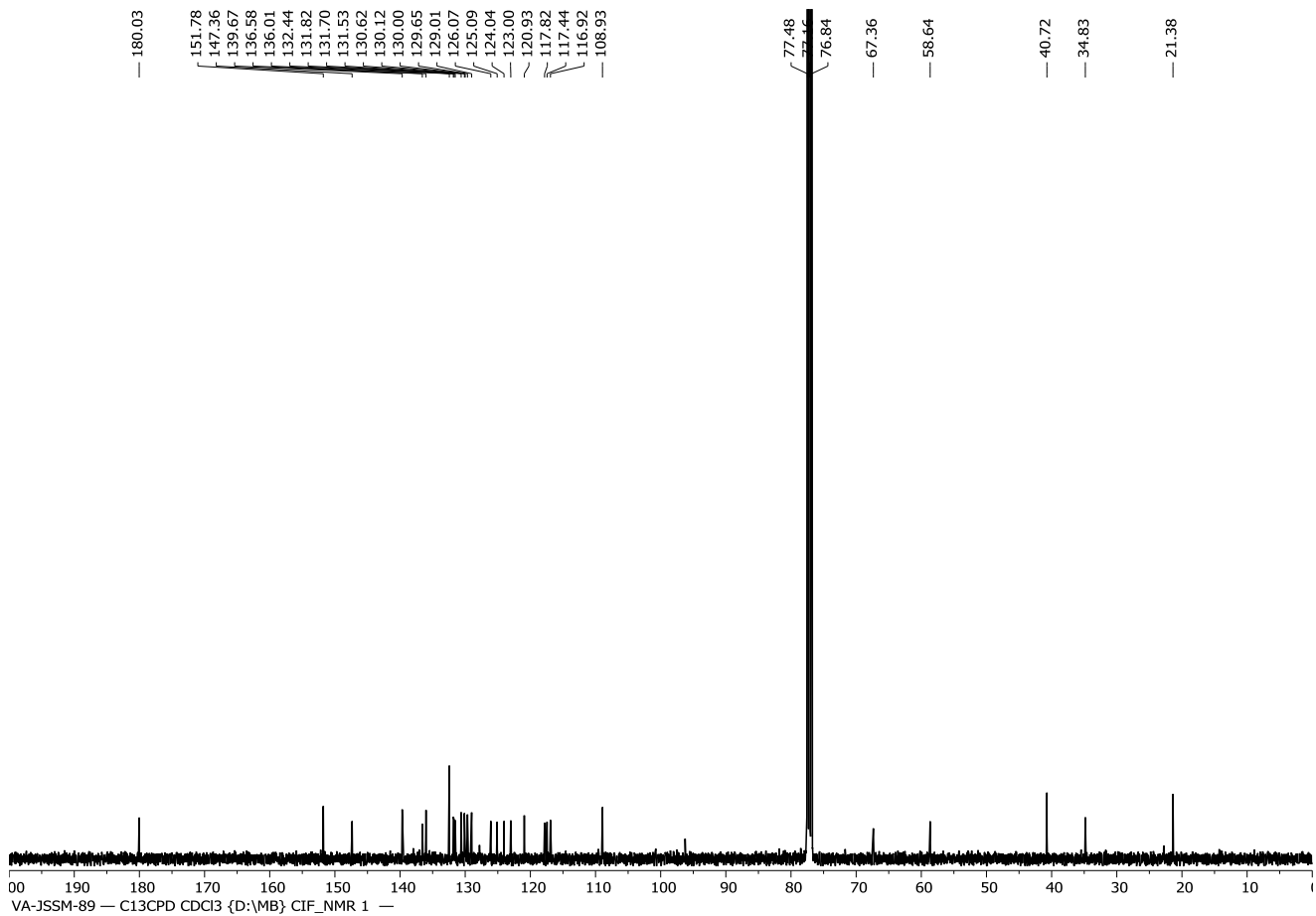
8.532  
8.521  
7.938  
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7.911  
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7.875  
7.863  
7.856  
7.844  
7.457  
7.366  
7.203  
7.176  
7.168  
7.143  
7.121  
7.116  
7.093  
7.068  
6.882  
6.858  
6.832  
5.731  
5.477  
4.636  
4.598  
4.507  
4.469

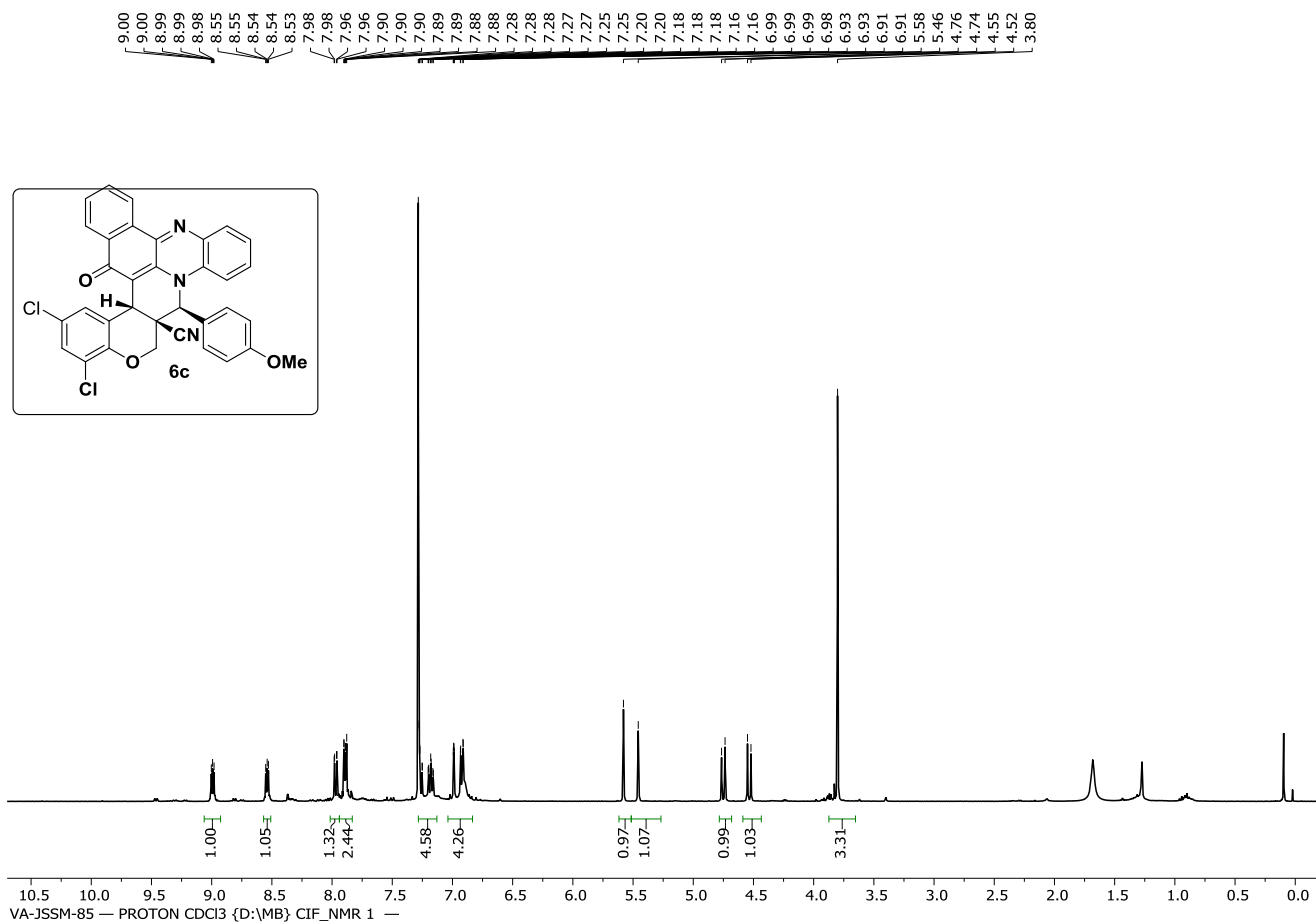


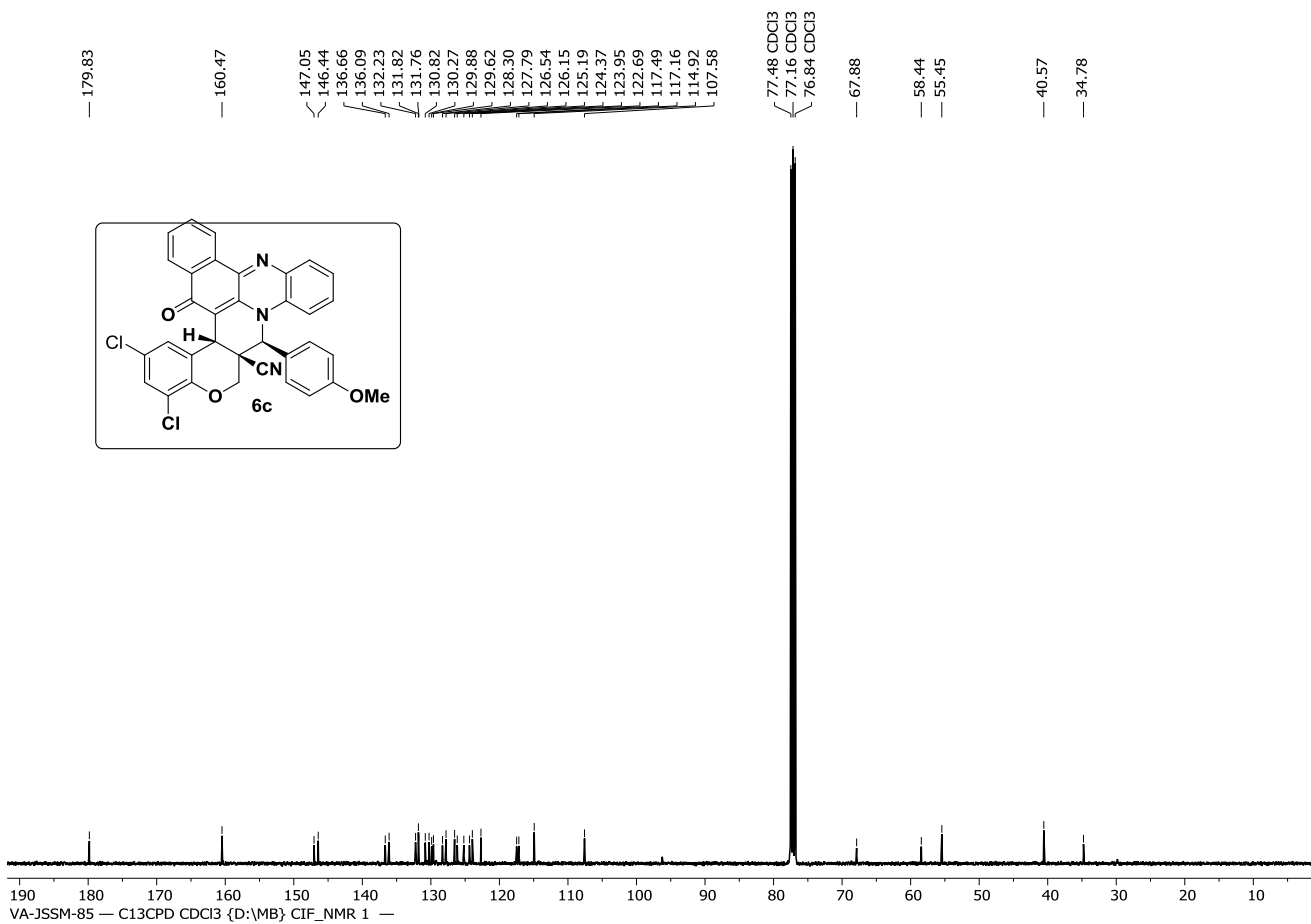
180.08  
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147.18  
135.40  
132.32  
131.72  
131.61  
131.41  
130.56  
130.45  
129.93  
129.55  
129.40  
128.86  
127.79  
125.99  
125.02  
123.95  
123.01  
120.82  
117.58  
117.19  
116.78  
108.64  
77.43  
77.01  
76.59  
67.73  
59.41  
40.22  
33.98



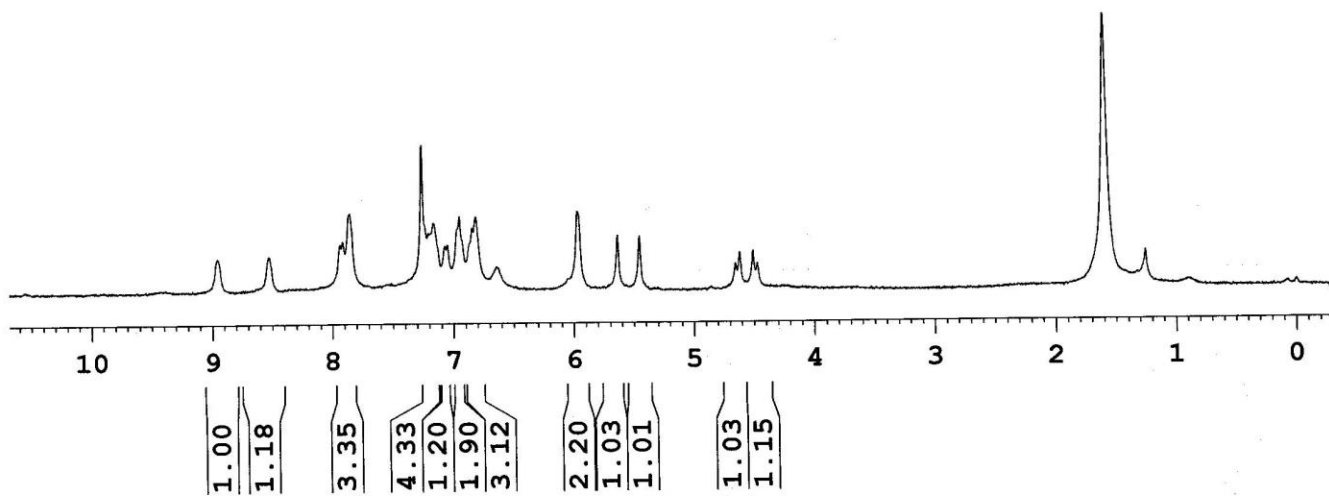
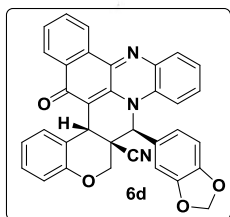


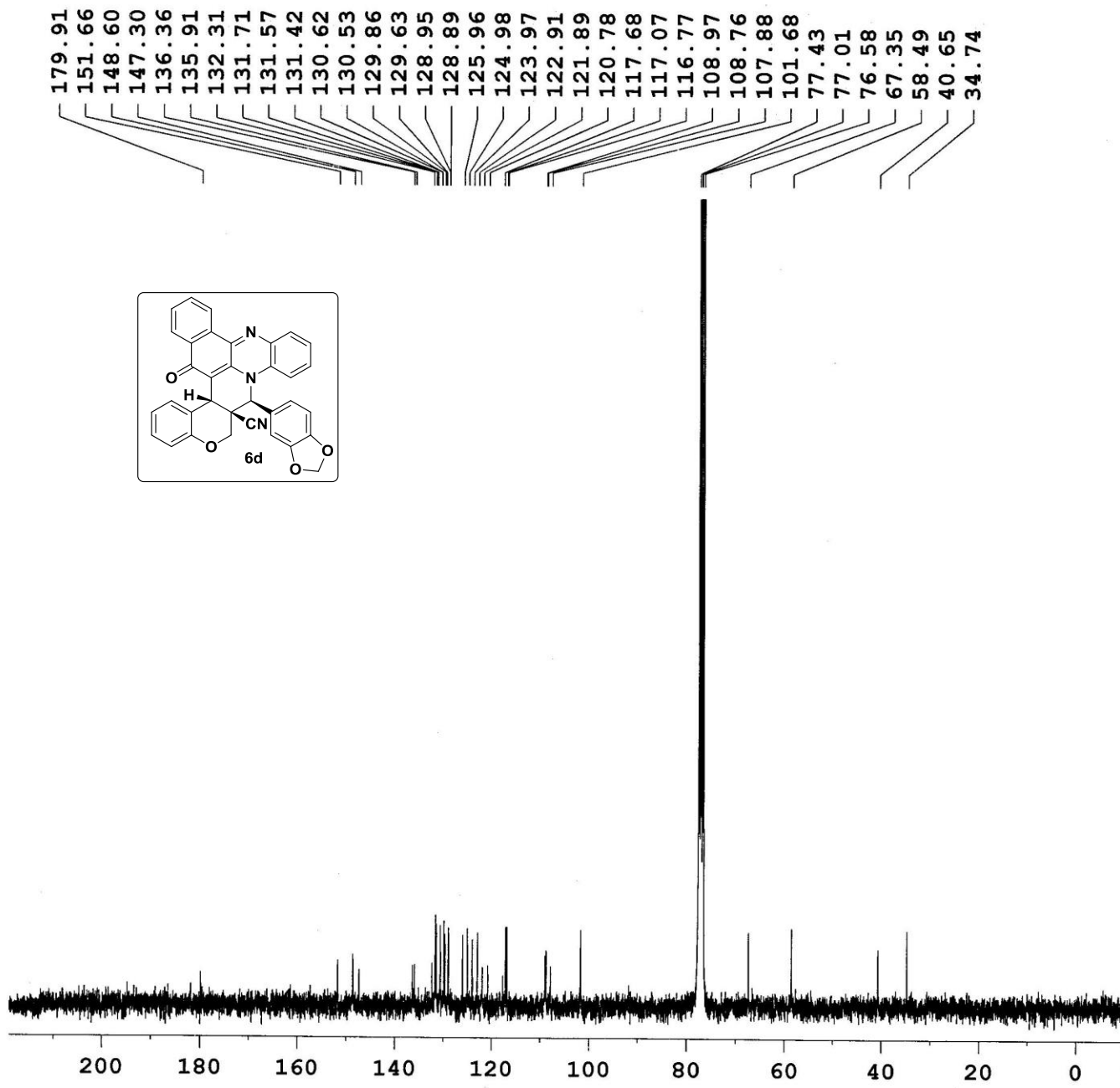




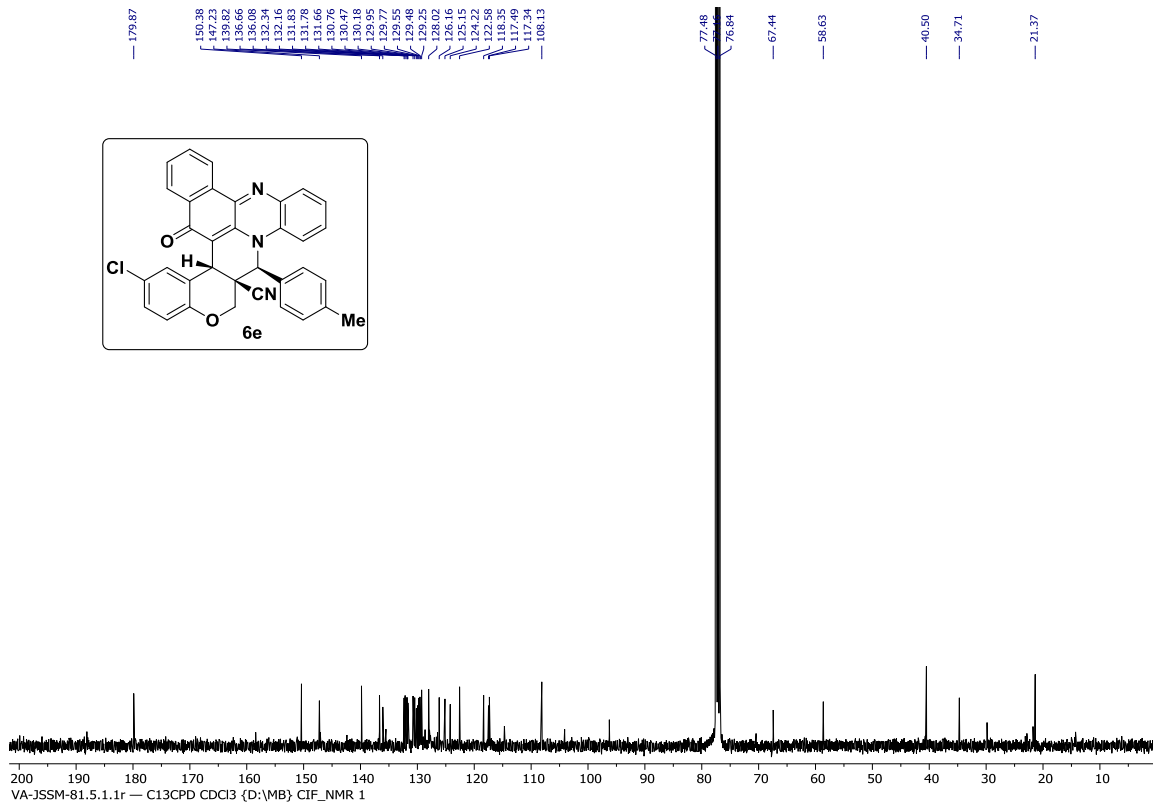
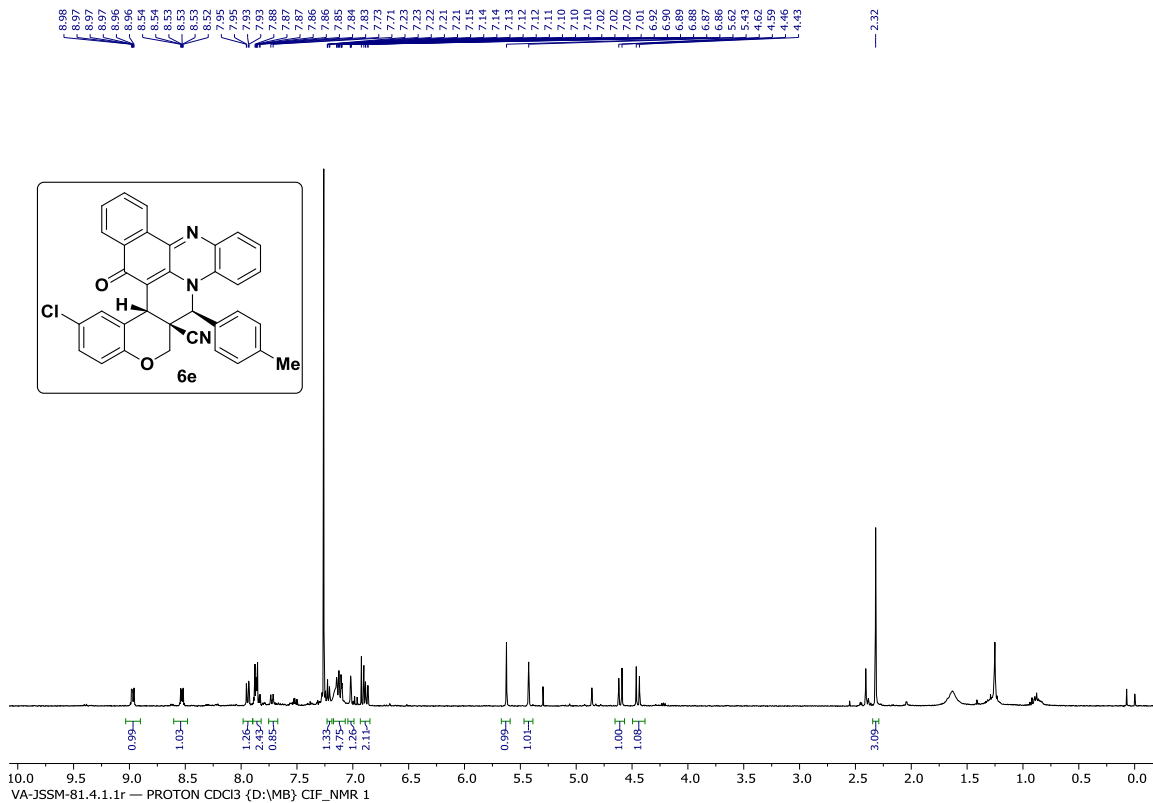


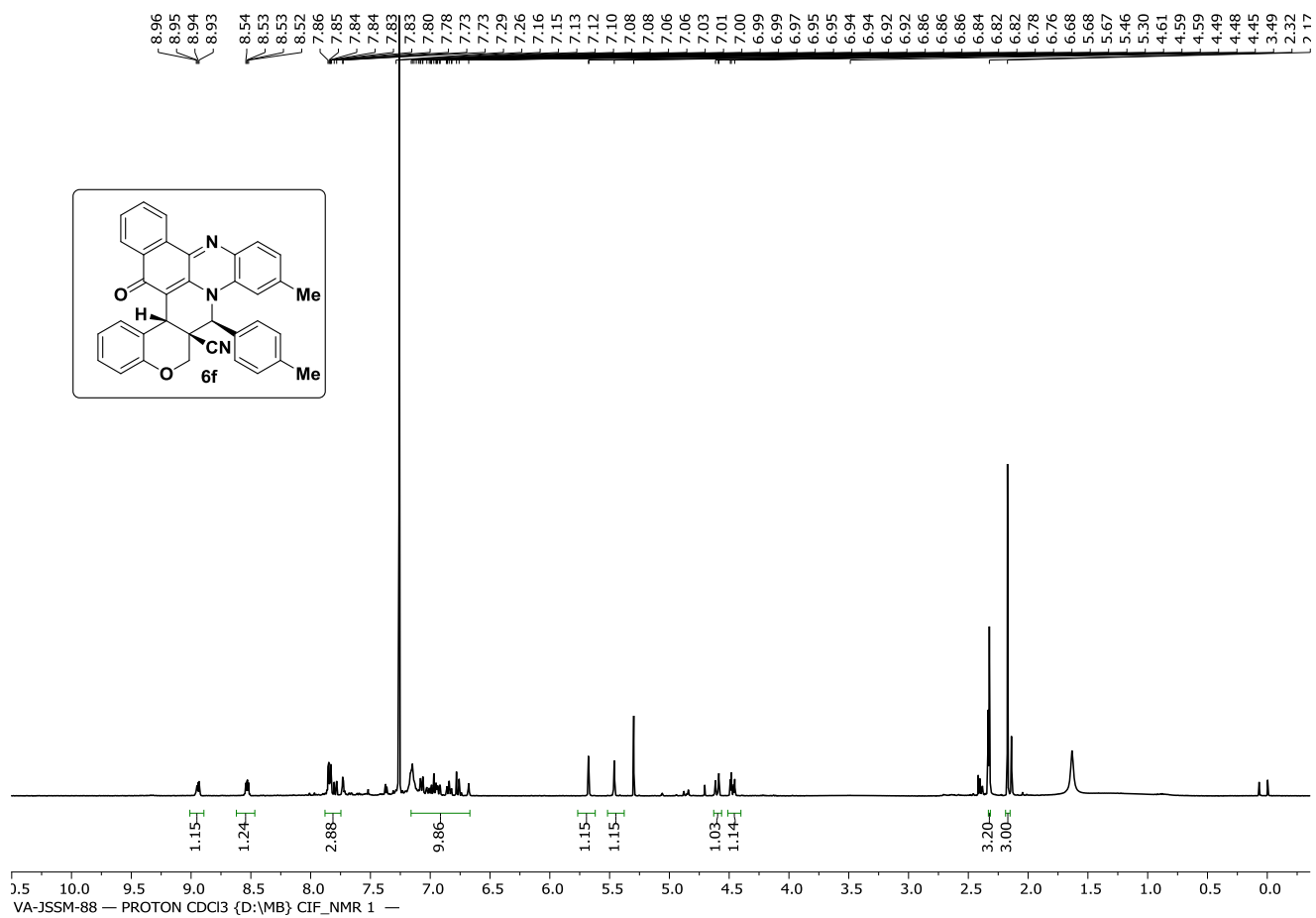
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7.207  
7.163  
7.069  
7.049  
6.949  
6.843  
6.812  
6.643  
5.967  
5.635  
5.453  
4.654  
4.617  
4.506  
4.469

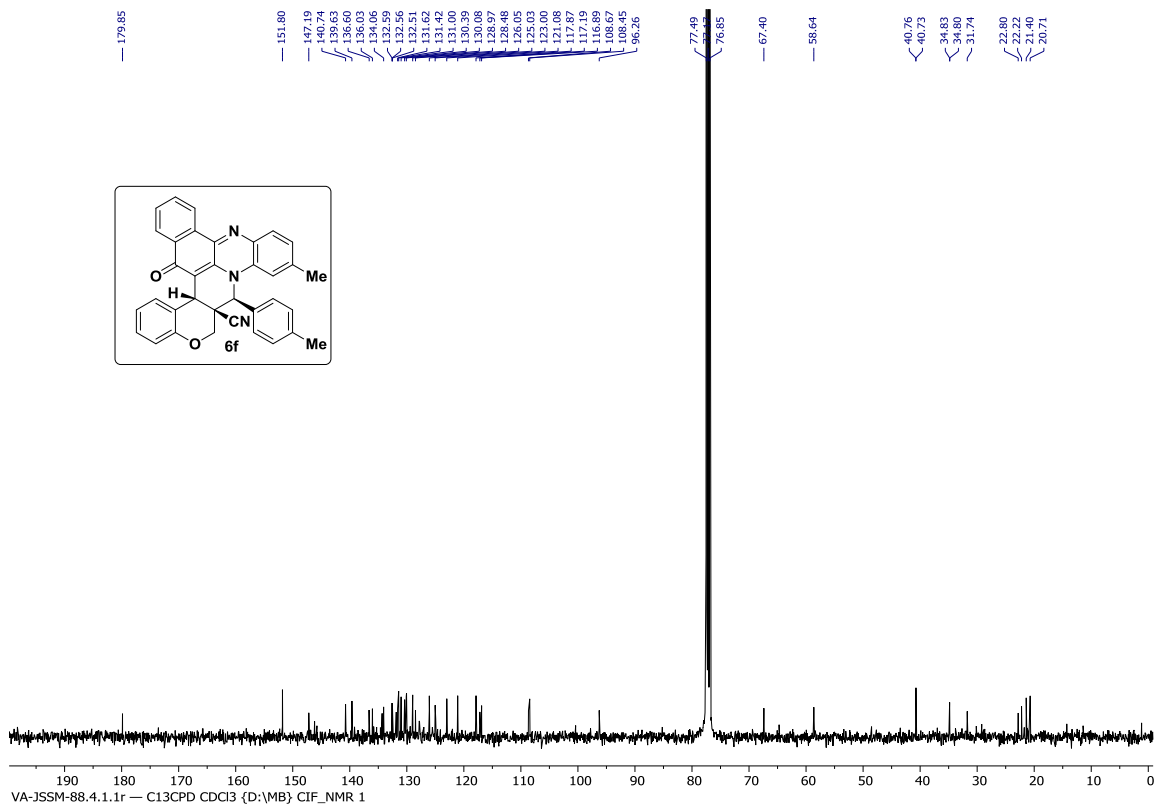




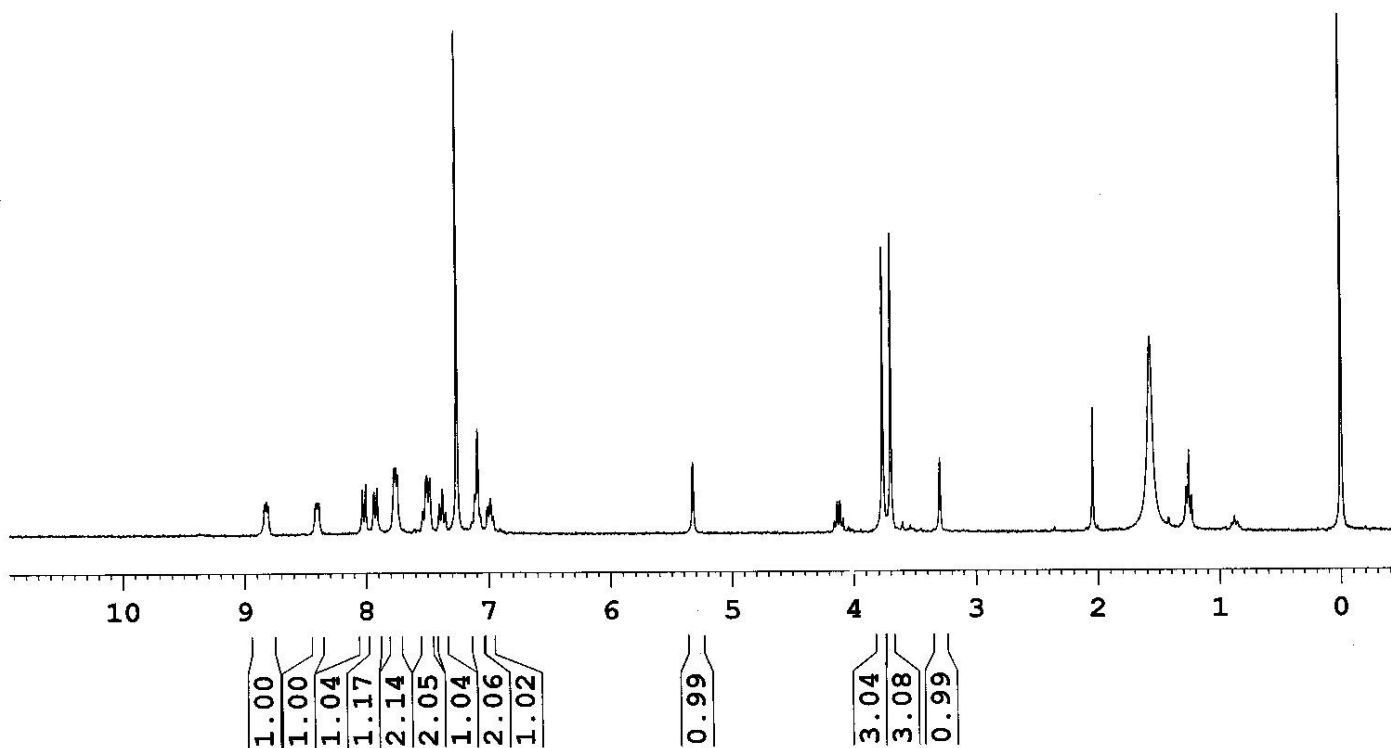
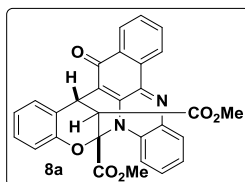


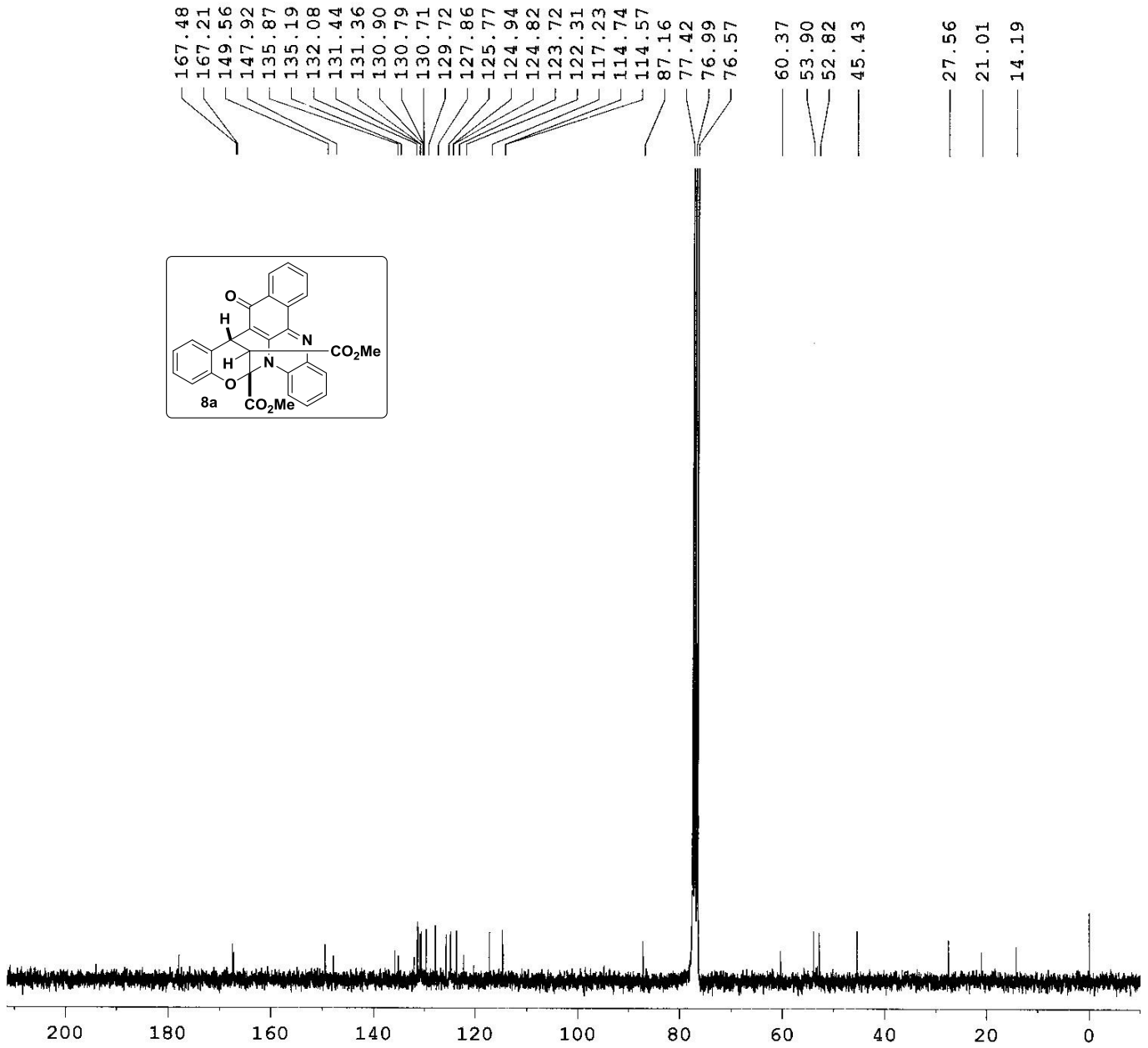




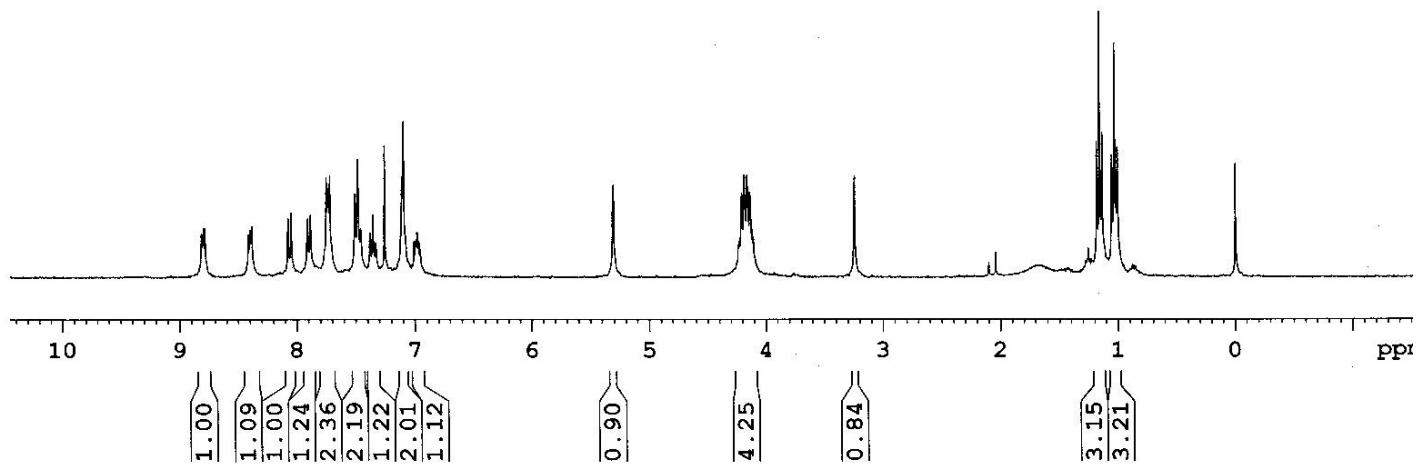
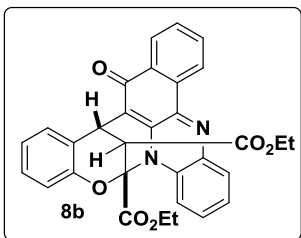


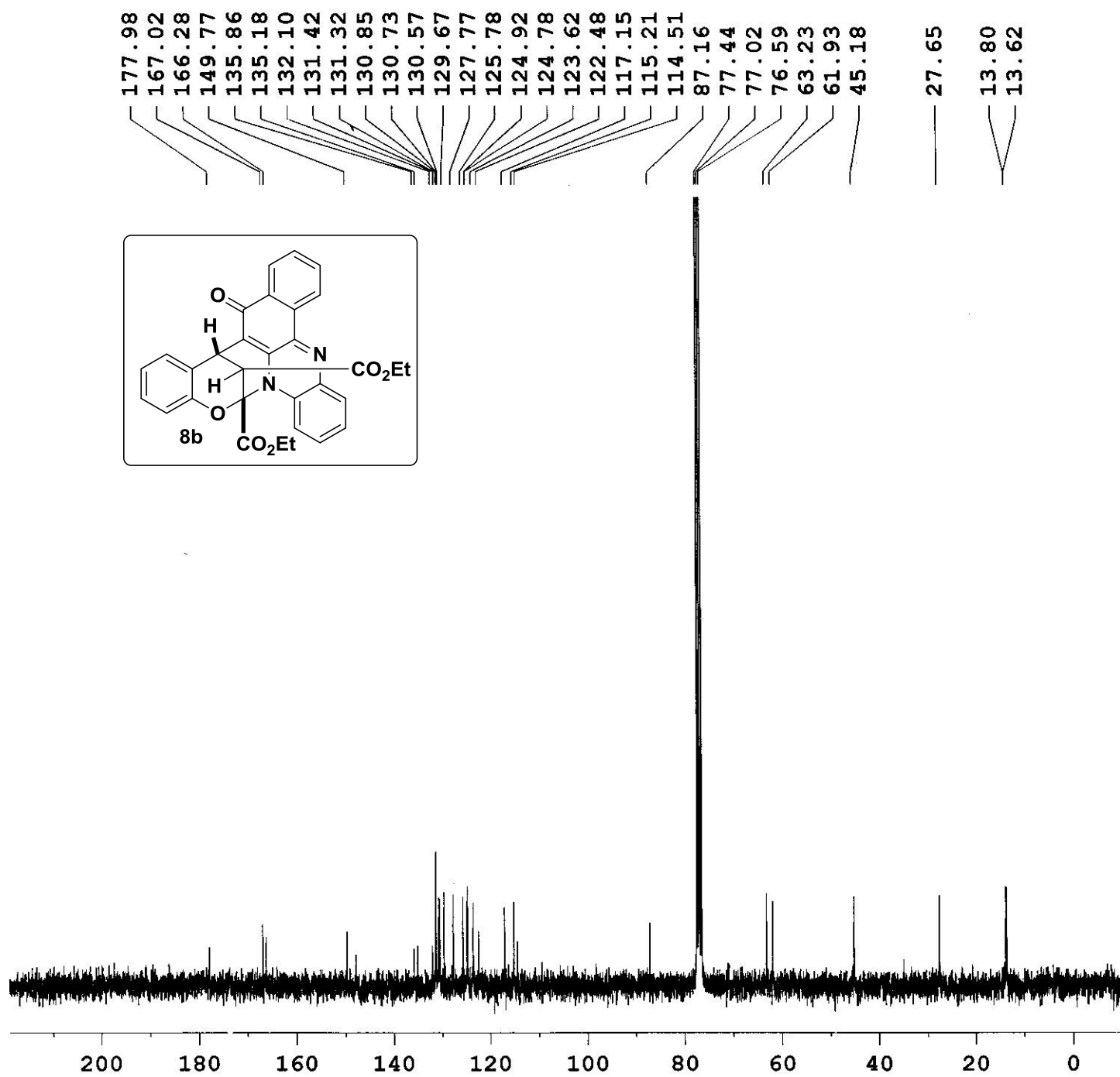
8.420  
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8.390  
8.031  
8.003  
7.938  
7.911  
7.775  
7.763  
7.757  
7.745  
7.540  
7.508  
7.482  
7.405  
7.381  
7.356  
7.261  
7.114  
7.093  
7.069  
7.011  
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6.968  
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3.767  
3.701  
3.300

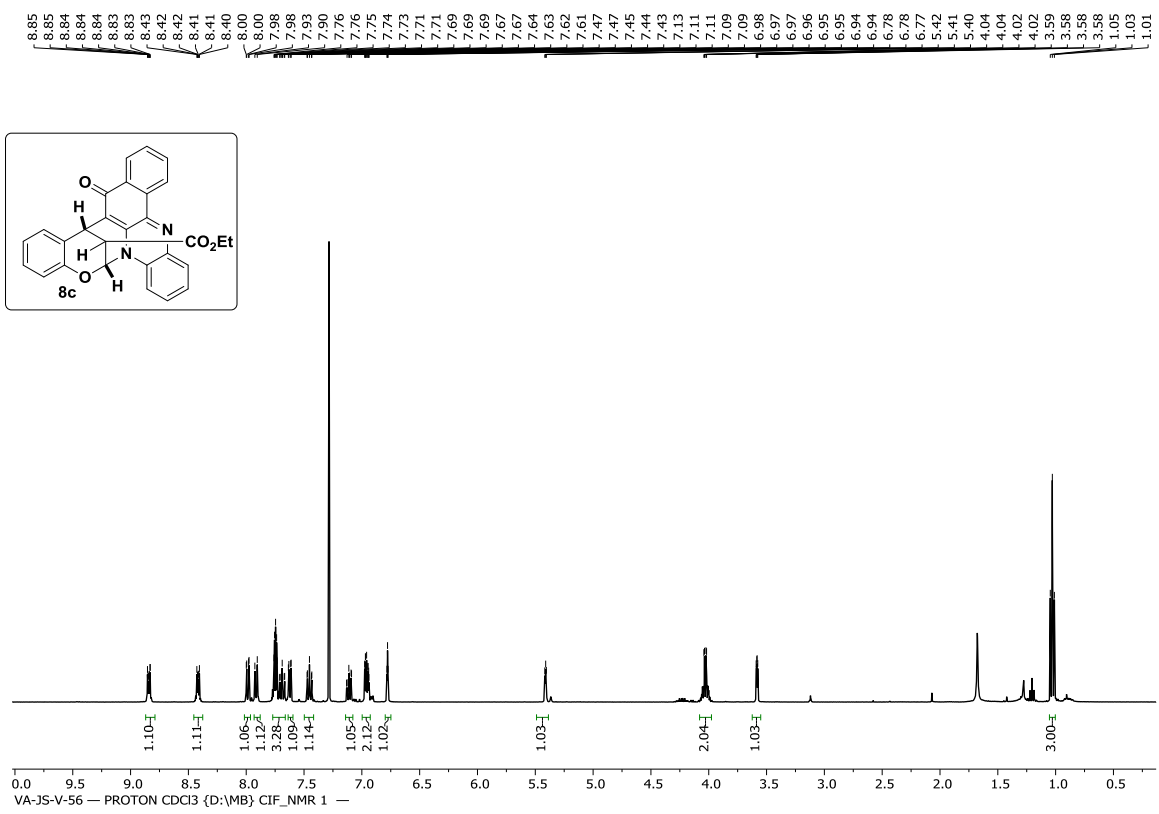




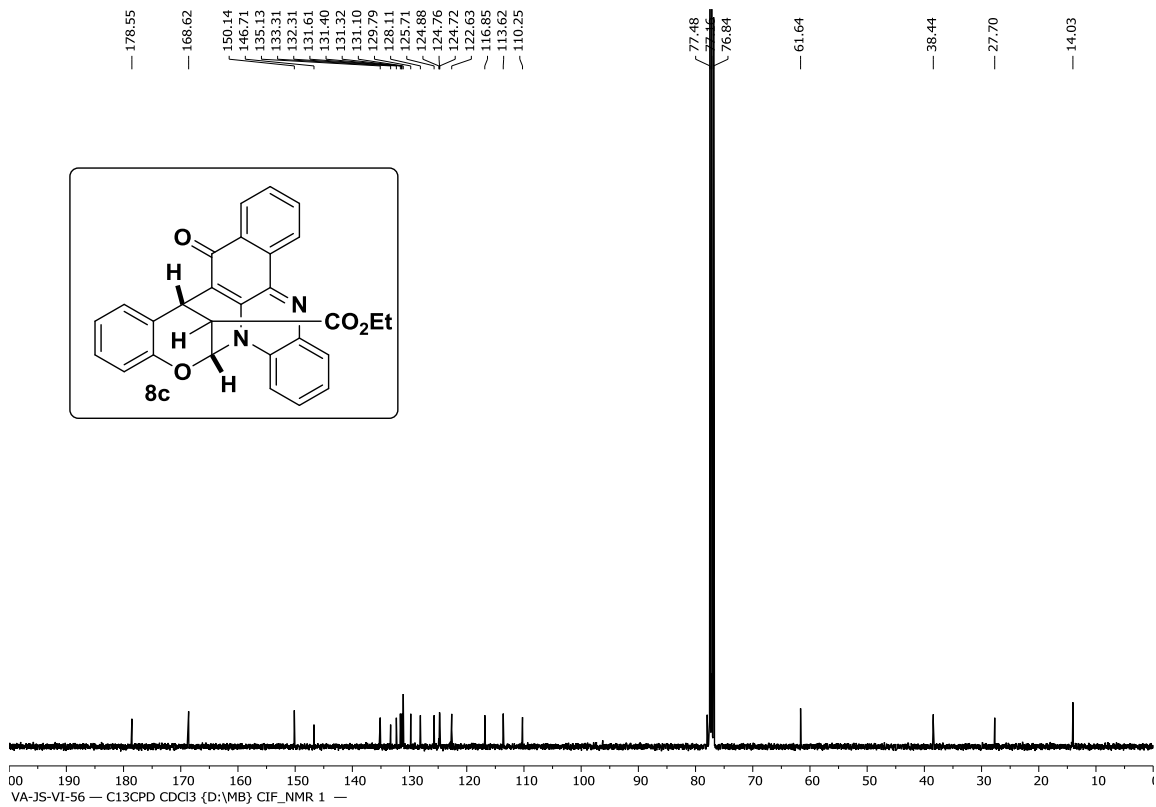
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8.076  
8.048  
7.915  
7.910  
7.889  
7.884  
7.753  
7.740  
7.736  
7.732  
7.723  
7.509  
7.485  
7.462  
7.456  
7.380  
7.357  
7.259  
7.111  
7.100  
7.000  
6.985  
6.969  
5.311  
5.306  
4.234  
4.215  
4.210  
4.191  
4.187  
4.180  
4.166  
4.156  
4.142  
4.132  
4.119  
4.109  
3.251  
3.245  
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1.162  
1.138  
1.057  
1.033  
1.009



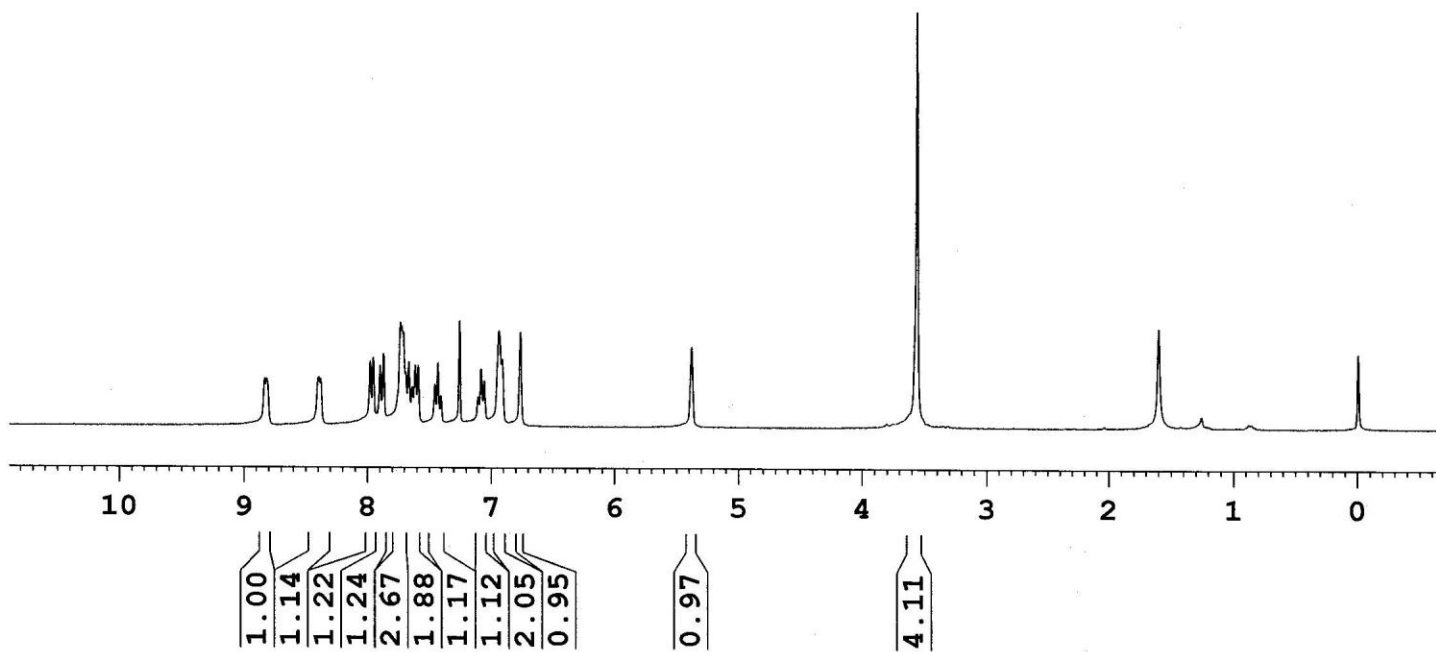
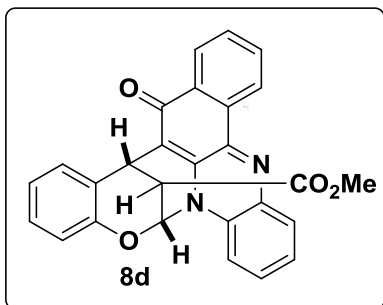


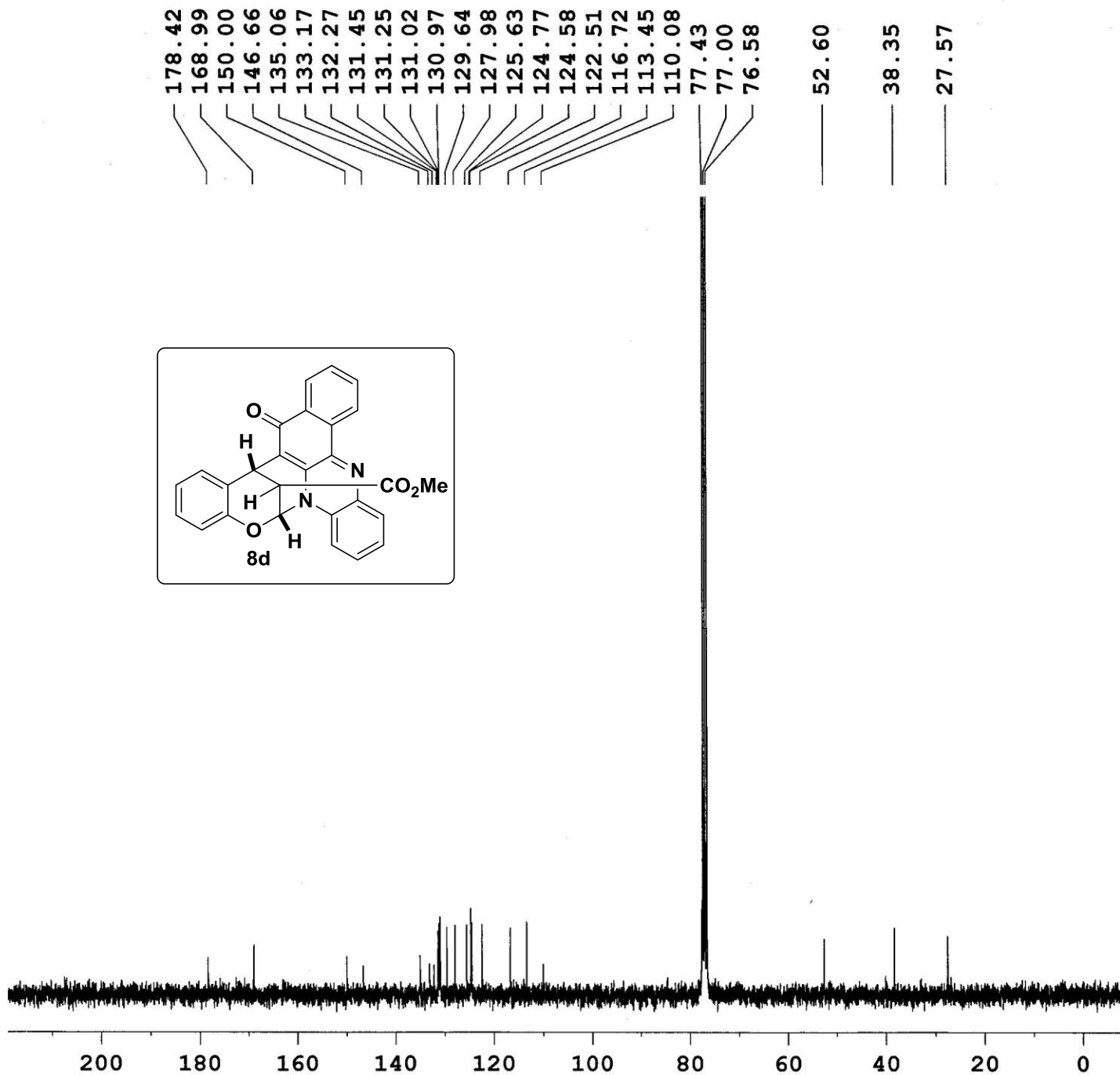




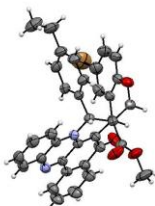
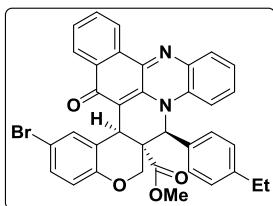


8.403  
8.396  
8.380  
7.981  
7.955  
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7.872  
7.734  
7.725  
7.710  
7.692  
7.667  
7.639  
7.615  
7.590  
7.457  
7.431  
7.406  
7.257  
7.107  
7.082  
7.056  
6.939  
6.912  
6.766  
5.382  
3.563



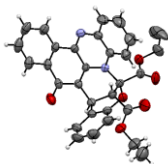
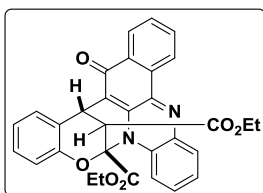


### 3) Crystal data and structure refinement for Compound 4l.



Identification code	MB-2-29-03-14
Empirical formula	C <sub>35</sub> H <sub>27</sub> BrN <sub>2</sub> O <sub>4</sub>
Formula weight	630.11
Temperature/K	298
Crystal system	triclinic
Space group	P-1
a/Å	10.8736(11)
b/Å	11.2191(11)
c/Å	12.8583(13)
α/°	70.525(9)
β/°	84.720(8)
γ/°	84.754(8)
Volume/Å <sup>3</sup>	1469.5(3)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.400
μ/mm <sup>-1</sup>	1.441
F(000)	636.0
Crystal size/mm <sup>3</sup>	0.38 × 0.24 × 0.16
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	7.54 to 58.42
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 15, -16 ≤ l ≤ 17
Reflections collected	15946
Independent reflections	6803 [R <sub>int</sub> = 0.0439, R <sub>sigma</sub> = 0.0643]
Data/restraints/parameters	6803/0/390
Goodness-of-fit on F <sup>2</sup>	1.015
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0598, wR <sub>2</sub> = 0.1384
Final R indexes [all data]	R <sub>1</sub> = 0.1292, wR <sub>2</sub> = 0.1773
Largest diff. peak/hole / e Å <sup>-3</sup>	0.41/-0.68

## Crystal data and structure refinement for Compound 8b.



Identification code	MB-4-29-03-14
Empirical formula	C <sub>31</sub> H <sub>25</sub> N <sub>2</sub> O <sub>6</sub>
Formula weight	521.53
Temperature/K	293 (2)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	12.2139(7)
b/Å	10.5529(9)
c/Å	19.644(2)
α/°	90.00
β/°	96.522(7)
γ/°	90.00
Volume/Å <sup>3</sup>	2515.5(4)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.377
μ/mm <sup>-1</sup>	0.096
F(000)	1092.0
Crystal size/mm <sup>3</sup>	0.28 × 0.24 × 0.18
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	7.82 to 58.14
Index ranges	-15 ≤ h ≤ 16, -10 ≤ k ≤ 14, -19 ≤ l ≤ 25
Reflections collected	7487
Independent reflections	4410 [R <sub>int</sub> = 0.0290, R <sub>sigma</sub> = 0.0470]
Data/restraints/parameters	4410/0/363
Goodness-of-fit on F <sup>2</sup>	1.051
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0578, wR <sub>2</sub> = 0.1550
Final R indexes [all data]	R <sub>1</sub> = 0.0973, wR <sub>2</sub> = 0.1834
Largest diff. peak/hole / e Å <sup>-3</sup>	0.30/-0.23