Competitive intramolecular C-C *vs.* C-O bond coupling reactions toward C_6 Ring-Fused 2-Pyridones Synthesis

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Supporting Information

1) General Procedure 1: precursor synthesis.

To a stirred solution containing α,β-unsaturated chromone derivates and CsF (10.0 mol%) in dichloromethane or ethanol, the corresponding amine (1.1 equiv.) was slowly added. The reaction mixture was stirred under reflux until full consumption of substrates was observed (followed by TLC). After concentration under reduced pressure, the resulting mixture yielded pure *N*,3,5-trisubstituted pyridin-2-ones by simple filtration of the formed precipitate or by purification on silica gel column chromatography.

Ethyl 1-(2-bromophenethyl)-5-(2-hydroxybenzoyl)pyridin-2(1H)-one-3-carboxylate (1a). White powder (precipitation in Et_2O), R_f = 0.40, eluent (50% ethyl acetate in cyclohexane), mp = 213 °C, 3.00 g scale reaction (in 15 mL of CH_2Cl_2) for 5 h, 3.92 g was isolated, 88% yield. IR (ν_{max} / cm^{-1}): 1724, 1660, 1619, 1215 and 758. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.54 (d, *J* = 2.7 Hz, 1H), 7.65 (d, *J* = 2.7 Hz, 1H), 7.62 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.46 - 7.53 (m, 1H), 7.24 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.19 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.13 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.04 (d, *J* = 8.3 Hz, 1H), 6.93 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.80 (t, *J* = 7.6 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 4.30 (t, *J* = 6.7 Hz, 2H), 3.33 (t, *J* = 6.7 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 194.0, 164.1, 162.4, 158.7, 146.8, 143.9, 136.5, 136.3, 133.2, 131.7, 131.0, 129.1, 128.1, 124.6, 120.4, 119.0, 118.8, 118.3, 115.2, 61.6, 51.6, 34.6, 14.3. HRMS (ESI^+): calcd for $C_{23}H_{21}BrNO_5$ $[M+H]^+$ 471.0603, found 471.0590.

Ethyl 5-(2-hydroxybenzoyl)-1-(phenethyl)pyridin-2(1H)-one-3-carboxylate (1c). White powder (precipitation in Et_2O), R_f = 0.40, eluent (80% ethyl acetate in cyclohexane), mp = 158 °C, 1.00 g scale reaction (in 5 mL of CH_2Cl_2) for 4 h, 1.09 g was isolated, 88% yield. IR (ν_{max} / cm^{-1}): 1725, 1650, 1624, 1536, 1344, 1269, 1220. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.58 (d, *J* = 2.7 Hz, 1H), 7.57 (d, *J* = 2.7 Hz, 1H),. 7.45 – 7.53 (m, 1H), 7.31 – 7.41 (m, 3H), 7.17 (d, *J* = 7.6 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.74 – 6.83 (m, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 4.27 (t, *J* = 6.6 Hz, 2H), 3.20 (t, *J* = 6.6 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 194.0, 164.1, 162.3, 158.6, 147.0, 144.0, 137.2, 136.1, 131.0, 129.2 (x2), 129.1 (x2), 127.1, 120.3, 119.1, 118.6, 118.3, 114.9, 61.6, 54.1, 34.2, 14.2. HRMS (ESI^+) calcd for $C_{23}H_{22}NO_5$ $[M+H]^+$ 392.1497, found 392.1492.

Ethyl 1-(2-bromophenethyl)-5-(2-hydroxy-5-methylbenzoyl)pyridin-2(1H)-one-3-carboxylate (5a). Pale yellow powder (column chromatography), R_f = 0.35, eluent (50% ethyl acetate in cyclohexane), mp = 156-158 °C, 250 mg scale reaction (in 4 mL of CH_2Cl_2) for 2 h, 273 mg was isolated, 74% yield. IR (ν_{max} / cm^{-1}): 1726, 1529, 1340, 1238. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 11.12 (s, 1H), 8.54 (d, *J* = 2.7 Hz, 1H), 7.89 (d, *J* = 2.7 Hz, 1H), 7.56 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.35 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.18 – 7.27 (m, 3H), 7.13 (dt, *J* = 9.1, 6.7, 2.4 Hz, 1H), 6.99 (d, *J* = 8.5 Hz, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 4.30 (q, *J* = 7.3 Hz, 2H), 3.31 (t, *J* = 7.3 Hz, 2H), 2.32 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 194.0, 164.1, 160.3, 158.7, 146.6, 144.0, 137.5, 136.4, 133.1, 131.5, 130.9, 129.1, 128.3, 128.1, 124.5, 120, 118.6, 118.2, 115.7, 61.6, 51.4, 35.2, 20.7, 14.3. HRMS (ESI^+): calcd for $C_{24}H_{23}BrNO_5$ $[M+H]^+$ 484.0760, found 484.0757

Ethyl 5-[5-(benzyloxy)-2-hydroxybenzoyl]-1-(2-bromophenethyl)pyridin-2(1H)-one-3-carboxylate (5b). Yellow powder (precipitation in Et_2O), R_f = 0.49, eluent (50% ethyl acetate in cyclohexane), mp = 179 °C, 700 mg scale reaction (in 5 mL of dichloromethane) for 4 h, 869 mg was isolated, 91% yield. IR (ν_{max} / cm^{-1}): 1721, 1647, 1584, 1218, 1020 and 761. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 10.85 (s, 1H), 8.55 (d, *J* = 2.7 Hz, 1H), 7.80 (d, *J* = 2.7 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.37 – 7.44 (m, 4H), 7.34 (dd, *J* = 5.5, 2.9 Hz, 1H), 7.24 (dd, *J* = 9.1, 2.9 Hz, 1H), 7.13 – 7.21 (m, 2H), 7.06 – 7.12 (m, 1H), 7.03 (d, *J* = 9.1 Hz, 1H), 6.93 (d, *J* = 3.0 Hz, 1H), 5.04 (s, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 4.26 (t, *J* = 7.2 Hz, 2H), 3.29 (t, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 193.7, 164.1, 158.6, 156.7, 151.0, 146.6, 143.8, 136.5, 136.2, 133.18, 131.4, 129.1, 128.7 (x2), 128.3, 128.0, 127.4 (x2), 124.8, 124.5, 119.9, 119.7, 118.1, 115.7, 115.5, 71.1, 61.7, 51.4, 35.1, 14.3. HRMS (ESI^+): calcd for $C_{30}H_{27}BrNO_6$ $[M+H]^+$ 576.1016, found. 576.1016

Ethyl 1-(2-bromophenethyl)-5-(2-hydroxy-6-methoxybenzoyl)pyridin-2(1H)-one-3-carboxylate (5c). Pale yellow powder (column chromatography), R_f = 0.54, eluent (70% ethyl acetate in cyclohexane), mp = 80 - 82 °C , 300 mg scale reaction (in 3 mL of CH_2Cl_2) for 4 h, 343 mg was isolated, 79% yield. IR (ν_{max} / cm^{-1}): 1741, 1697,1654, 1535, 1473 and 1282. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 10.11 (s, 1H), 8.32 (d, *J* = 2.7 Hz, 1H), 7.87 (d, *J* = 2.7 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 8.3 Hz, 1H), 7.14 – 7.25 (m, 2H), 7.10 (ddd, *J* = 7.8, 6.7, 2.4 Hz, 1H), 6.67 (d, *J* = 8.3 Hz, 1H), 6.47 (d, *J* = 8.3 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 4.27 (t, *J* = 7.3 Hz, 2H), 3.72 (s, 3H), 3.25 (t, *J* = 7.3 Hz, 2H), 1.37 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 192.2, 164.5, 161.2, 159.1, 158.9,

146.4, 144.8, 136.4, 135.6, 133.1, 131.4, 129.0, 128.0, 124.5, 118.6, 117.9, 110.9, 110.8, 102.3, 61.4, 55.6, 50.9, 35.3, 14.3. HRMS (ESI^+): calcd for $C_{24}H_{23}BrNO_6$ $[M+H]^+$ 502.0688, found 502.0708.

Ethyl 1-(2-bromophenethyl)-5-(5-chloro-2-hydroxy-4-methylben-zoyl)pyridin-2(1H)-one-3-carboxylate (5d). Pale yellow powder, R_f = 0.59, eluent (50% ethyl acetate in cyclohexane),mp = 161-163 °C, 500 mg scale reaction (in 5 mL of CH_2Cl_2) for 3 h, 597 mg was isolated, 84% yield. IR (ν_{max} / cm^{-1}): 1737, 1653, 1531, 1469 and 1231. ^1H NMR (300 MHz, $CDCl_3$): δ_H 11.25 (s, 1H), 8.51 (d, *J* = 2.7 Hz, 1H), 7.87 (d, *J* = 2.8 Hz, 1H), 7.59 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.38 (s, 1H), 7.18 – 7.26 (m, 2H), 7.14 (ddd, *J* = 8.0, 6.9, 2.2 Hz, 1H), 6.99 (s, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 4.31 (t, *J* = 7.3 Hz, 2H), 3.33 (t, *J* = 7.3 Hz, 2H), 2.43 (s, 3H), 1.43 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 192.8, 163.9, 160.9, 158.6, 146.5, 145.9, 143.6, 136.3, 133.2, 131.4, 130.6, 129.1, 128.0, 124.5 (x2), 120.9, 120.3, 117.4, 115.3, 61.7, 51.5, 35.1, 20.9, 14.3. HRMS (ESI^+): calcd for $C_{24}H_{22}BrClNO_5$ $[M+H]^+$ 518.0375, found 518.0361.

Ethyl 1-(2-bromophenethyl)-5-(2-hydroxy-1-naphthoyl)pyridin-2(1H)-one-3-carboxylate (5e). Yellow solid (column chromatography), R_f = 0.22, eluent (50% ethyl acetate in cyclohexane), mp = 101 °C, 400 mg scale reaction (in 5 mL of dichloromethane) for 5 h, 487 mg was isolated, 85% yield. IR (ν_{max} / cm^{-1}): 1732, 1660, 1591, 1341, 1217 and 753. ^1H NMR (300 MHz, $CDCl_3$): δ_H 8.52 (d, *J* = 2.7 Hz, 1H), 7.77 (d, *J* = 2.6 Hz, 1H), 7.43 - 7.57 (m, 2H), 7.09 – 7.24 (m, 4H), 6.95 – 7.06 (m, 2H), 4.38 (q, *J* = 7.1 Hz, 2H), 4.23 (t, *J* = 7.2 Hz, 2H), 3.77 (s, 3H), 3.22 (t, *J* = 7.2 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_c 182.2, 166.7, 166.6, 157.3, 152.8, 137.1, 135.2, 133.1, 131.6, 131.2, 130.0, 128.6, 128.3 (x2), 127.8, 126.4, 124.5, 124.4, 118.9, 115.4, 98.5, 61.7, 61.6, 56.0, 48.9, 38.3, 14.1. HRMS (ESI^+): calcd for $C_{27}H_{23}BrNO_5$ $[M+H]^+$ 520.0754, found 520.0754

Ethyl 5-(5-bromo-2-hydroxybenzoyl)-1-(2-bromophenethyl)pyridin-2(1H)-one-3-carboxylate (5f). Pale yellow powder (column chromatography), R_f = 0.35, eluent (50% ethyl acetate in cyclohexane), mp = 140 - 142 °C, 300 mg scale reaction (in 4 mL of CH_2Cl_2) for 3 h, 352 mg was isolated, 84% yield. IR (ν_{max} / cm^{-1}): 1739, 1622, 1530, 1333, 1207. ^1H NMR **(**300 MHz, $CDCl_3$)**:** δ_H 11.17 (s, 1H), 8.52 (d, *J* = 2.7 Hz, 1H), 7.89 (d, *J* = 2.7 Hz, 1H), 7.63 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.54 – 7.60 (m, 2H), 7.19 – 7.27 (m, 2H), 7.14 (dt, *J* = 9.1, 6.7, 2.4 Hz, 1H), 7.01 (d, *J* = 8.8 Hz, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 4.28 – 4.36 (m, 2H), 3.32 (t, *J* = 7.3 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 193.0, 163.9, 161.2, 158.5, 146.8, 143.5, 139.0, 136.2, 133.2, 133.1, 131.4, 129.2, 128.1, 124.5, 120.9, 120.3, 119.9, 115.0, 110.7, 61.7, 51.4, 35.2, 14.3. HRMS (ESI^+): calcd for $C_{23}H_{20}Br_2NO_5$ $[M+H]^+$ 549.9691, found 549.9683

***Ethyl 1-(2-bromophenethyl)-5-(2-hydroxy-5-nitrobenzoyl)pyridin-2(1H)-one-3-carboxylate* (*5g*).** Yellow solid (column chromatography), R_f = 0.39, eluent (50% ethyl acetate in cyclohexane), mp = 134 °C, 1.00 g scale reaction (in 5 mL of CH_2Cl_2) for 5 h, 1.01 g was isolated, 71% yield. IR (ν_{max} / cm^{-1}): 1732, 1539, 1337, 1247 and 751. ^1H NMR (300 MHz, $CDCl_3$): δ_H 11.94 (s, 1H), 8.52 (d, *J* = 2.7 Hz, 1H), 8.48 (d, *J* = 2.7 Hz, 1H), 8.42 (dd, *J* = 9.1, 2.7 Hz, 1H), 7.93 (d, *J* = 2.7 Hz, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.16 – 7.29 (m, 3H), 7.12 (t, *J* = 7.3 Hz, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 4.35 (t, *J* = 7.3 Hz, 2H), 3.32 (t, *J* = 7.3 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 193.1, 167.1, 163.7, 158.4, 147.1, 143.1, 139.6, 136.1, 133.1, 131.4, 131.1, 129.2, 128.1, 127.3, 124.5, 120.4, 119.9, 117.5, 114.4, 61.9, 51.4, 35.2, 14.3. HRMS (ESI^+): calcd for $C_{23}H_{20}BrN_2O_7$ $[M+H]^+$ 515.0448, found 515.0449.

Ethyl 1-(2-bromophenethyl)-5-(1-hydroxy-2-naphthoyl)pyridin-2(1H)-one-3-carboxylate (5h). Yellow solid (column chromatography), R_f = 0.44, eluent (50% ethyl acetate in cyclohexane), mp = 77 °C, 500mg scale reaction (in 5 mL of dichloromethane) for 6 h, 463 mg was isolated, 64% yield. IR (ν_{max} / cm^{-1}): 1733, 1660, 1590, 1342, 1217 and 752. ^1H NMR (300 MHz, $CDCl_3$): δ_H 13.33 (s, 1H), 8.57 (d, *J* = 2.7 Hz, 1H), 8.45 (d, *J* = 8.3 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.61 – 7.75 (m, 3H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.09 – 7.30 (m, 4H), 6.93 (d, *J* = 8.8 Hz, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 4.31 (t, *J* = 6.8 Hz, 2H), 3.35 (t, *J* = 6.7 Hz, 2H), 1.41 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 193.9, 164.1, 163.3, 158.7, 146.6, 144.1, 137.1, 136.6, 133.2, 131.7, 130.5, 129.1, 128.1, 127.5, 126.3, 125.3, 125.1, 124.7, 124.5, 120.3, 118.50, 115.6, 111.7, 61.6, 51.6, 34.8, 14.3. HRMS (ESI^+): calcd for $C_{27}H_{23}BrNO_5$ $[M+H]^+$ 520.0754, found. 520.0754

1-(2-bromophenethyl)-5-(2-hydroxybenzoyl)pyridin-2(1H)-one-3-carbonitrile (5i). Yellow powder (precipitation in Et_2O), R_f = 0.59, eluent (50% ethyl acetate in cyclohexane), mp = 173 °C, 500 mg scale reaction (in 4 mL of ethanol) for 4 h, 397 mg was isolated, 51% yield. IR (ν_{max} / cm^{-1}): 2233, 1664, 1596, 1251 and 757. ^1H NMR (300 MHz, $CDCl_3$): δ_H 11.13 (s, 1H), 8.24 (s, 1H), 7.63 (d, *J* = 5.4 Hz, 2H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.16 – 7.35 (m, 4H),

7.13 (d, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 8.5 Hz, 1H), 6.76 – 6.92 (m, 2H), 4.33 (t, *J* = 6.6 Hz, 2H), 3.33 (t, *J* = 6.6 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 192.8, 162.5, 158.9, 147.1, 146.9, 136.8, 136.0, 133.3, 131.7, 130.7, 129.4, 128.3, 124.7, 119.3, 119.1, 118.0, 116.0, 114.50, 105.40, 52.1, 34.4. HRMS (ESI^+): calcd for $C_{21}H_{15}BrN_2O_3$ $[M+H]^+$ 423.0339, found 423.0339.

3-benzoyl-1-(2-bromophenethyl)-5-(2-hydroxybenzoyl)pyridin-2(1H)-one (5j). Pale yellow powder (column chromatography), R_f = 0.49, eluent (33% ethyl acetate in cyclohexane), mp = 175-177 °C, 200 mg scale reaction (in 3 mL of CH_2Cl_2) for 7 h, 147 mg was isolated, 51% yield. IR (ν_{max} / cm^{-1}): 1677, 1590, 1540, 1341, 1271. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 11.33 (s, 1H), 8.13 (d, *J* = 2.6 Hz, 1H), 7.85 – 7.92 (m, 2H), 7.70 (d, *J* = 2.6 Hz, 1H), 7.60 – 7.68 (m, 2H), 7.47 – 7.56 (m, 3H), 7.32 (td, *J* = 7.4, 1.4 Hz, 1H), 7.22 (dd, *J* = 7.7, 2.0 Hz, 1H), 7.18 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.05 (ddd, *J* = 11.0, 8.2, 1.4 Hz, 2H), 6.83 (ddd, *J* = 8.1, 7.3, 1.2 Hz, 1H), 4.34 (t, *J* = 6.7 Hz, 2H), 3.35 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 194.2, 193.2, 162.5, 159.6, 145.8, 141.2, 136.7, 136.5, 136.4, 133.5, 133.2, 131.7, 131.1, 129.6, 129.5 (x2), 129.2, 128.5 (x2), 128.2, 124.7, 119.1, 118.8, 118.4, 116.1, 51.4, 34.74. HRMS (ESI^+): calcd for $C_{27}H_{21}BrNO_4$ $[M+H]^+$ 502.0649, found 502.0660

1-(2-bromophenethyl)-5-(2-hydroxy-1-naphthoyl)pyridin-2(1H)-one-3-carbonitrile (5k). Yellow solid (column chromatography), R_f = 0.17, eluent (50% ethyl acetate in cyclohexane), mp = 117 °C, 700 mg scale reaction (in 5 mL of ethanol) for 6 h, 550 mg was isolated, 53% yield. IR (ν_{max} / cm^{-1}): 2232, 1627, 1543, 1241, 1342 and 759. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 9.88 (s, 1H), 7.92 – 8.03 (m, 2H), 7.84 (d, *J* = 5.5 Hz, 1H), 7.72 (d, *J* = 2.5 Hz, 1H), 7.38 – 7.50 (m, 4H), 7.19 – 7.27 (m, 2H), 7.03 – 7.17 (m, 2H), 4.23 (t, *J* = 7.1 Hz, 2H), 3.20 (t, *J* = 7.1 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C) 191.4, 159.3, 158.1, 148.1, 146.8, 135.7, 135.5, 133.1, 131.4, 131.3, 129.2, 129.1, 128.5, 128.0, 127.9, 124.6, 124.5, 124.4, 118.9, 118.2, 114.7, 114.1, 104.4, 51.2, 34.8. HRMS (ESI^+): calcd for $C_{25}H_{18}BrN_2O_3$ $[M+H]^+$ 473.0495, found 473.0495

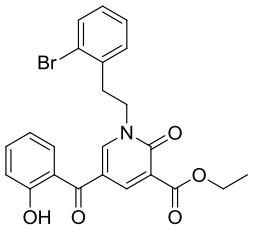
1-(2-bromophenethyl)-5-(1-hydroxy-2-naphthoyl)pyridin-2(1H)-one-3-carbonitrile (5l). Pale green solid (column chromatography), R_f = 0.38, eluent (50% ethyl acetate in cyclohexane), mp = 199 °C, 600 mg scale reaction (in 5 mL of ethanol) for 4 h, 561 mg was isolated, 63% yield. IR (ν_{max} / cm^{-1}): 2236, 1663, 1597, 1273 and 759. ^{1}H NMR (300 MHz, $CDCl_3$) : δ_H 13.18 (s, 1H), 8.48 (d, *J* = 8.3 Hz, 1H), 8.28 (d, *J* = 2.5 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.64 – 7.75 (m, 3H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.29 – 7.36 (m, 1H), 7.22 – 7.26 (m, 1H), 7.15 – 7.22 (m, 2H), 6.88 (d, *J* = 8.8 Hz, 1H), 4.35 (t, *J* = 6.7 Hz, 2H), 3.36 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 192.6, 163.6, 158.9, 147.0, 146.8, 137.2, 136.0, 133.3, 131.6, 130.9, 129.4, 128.3, 127.6, 126.6, 125.2, 124.7, 124.5 (x2), 118.9, 116.4, 114.7, 111.3, 105.3, 52.0, 34.5. HRMS (ESI^+): calcd for $C_{25}H_{18}BrN_2O_3$ $[M+H]^+$ 473.0495, found 473.0495

2) General Procedure 2: O-methylated benzoylpyridones synthesis.

To a heated solution containing the appropriated pyridin-2-ones, K_2CO_3 (2.5 equiv.), KI (10.0 mol% equiv.) and 18-crown-6 (1.0 mol%) in dichloromethane, methyl iodide (2.0 equiv.) was added dropwise and the mixture allowed to stir at 40 °C for 2 hours then left at room temperature during overnight. The reaction mixture was filtered through celite and rinsed with dichloromethane, and then the filtrate concentrated. The crude product was purified by using silica gel column chromatography (cyclohexane / ethyl acetate) to yield pure *O*-alkylated pyridones.

Ethyl 1-(2-bromophenethyl)-5-(2-methoxybenzoyl)pyridin-2(1H)-one-3-carboxylate (1b). Pale yellow solid (column chromatography), R_f = 0.23, eluent (50% ethyl acetate in cyclohexane), mp = 191 °C, 150 mg scale reaction (in 5 mL of toluene) for 24 h, 130 mg was isolated, 81% yield. IR (ν_{max} / cm^{-1}): 1737, 1705, 1644, 1436 and 1231. ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.52 (d, *J* = 2.7 Hz, 1H), 7.77 (d, *J* = 2.6 Hz, 1H), 7.43 - 7.57 (m, 2H), 7.09 – 7.24 (m, 4H), 6.95 – 7.06 (m, 2H), 4.38 (q, *J* = 7.1 Hz, 2H), 4.23 (t, *J* = 7.2 Hz, 2H), 3.77 (s, 3H), 3.22 (t, *J* = 7.2 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 190.3, 164.4, 159.0, 156.8, 147.6, 143.8, 136.4, 133.0, 132.6, 131.5, 129.5, 129.0, 127.9, 126.8, 124.4, 120.9, 119.7, 116.4, 111.8, 61.4, 55.6, 50.9, 35.2, 14.3. HRMS (ESI^+): calcd for $C_{24}H_{23}BrNO_5$ $[M+H]^+$ 484.0760, found 484.0754.

3) Copies of ^{1}H and ^{13}C NMR spectra of starting materials, arylated and aryloxylated products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O

(1a)

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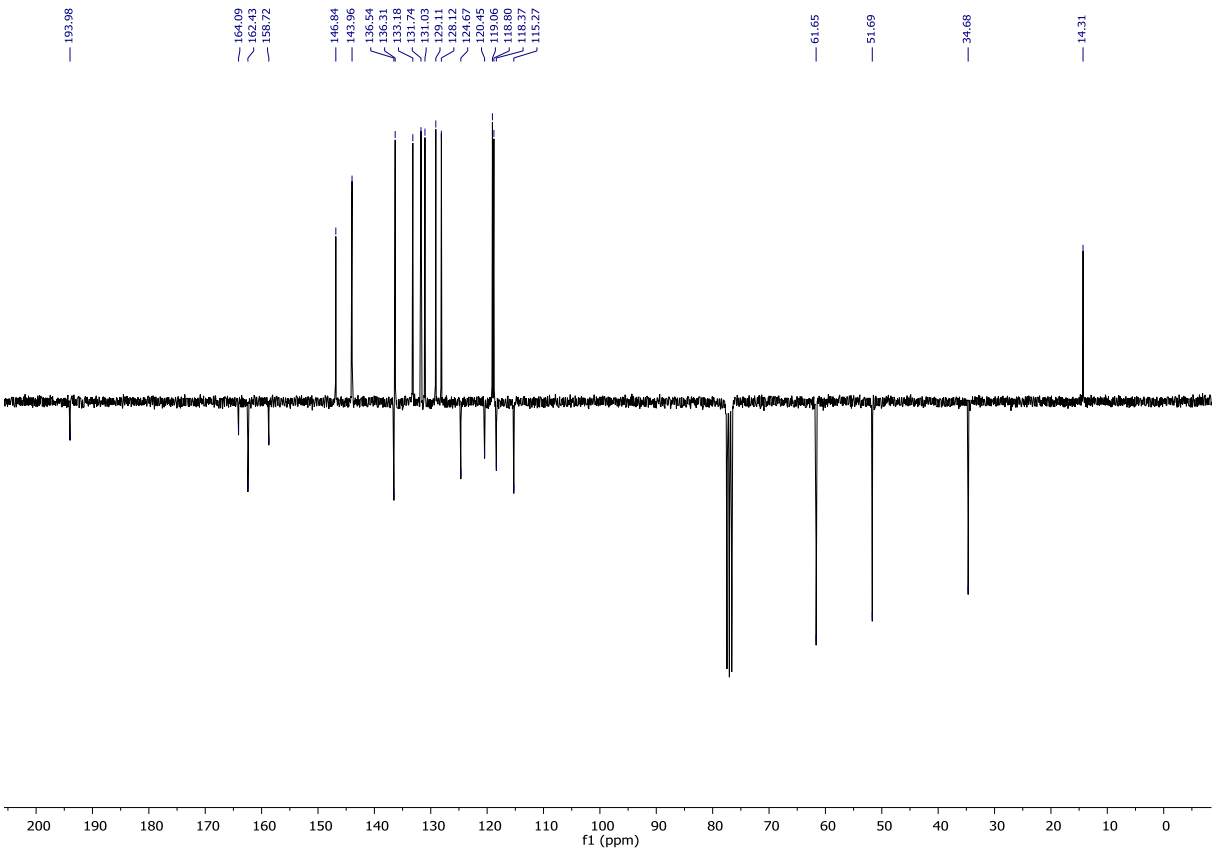
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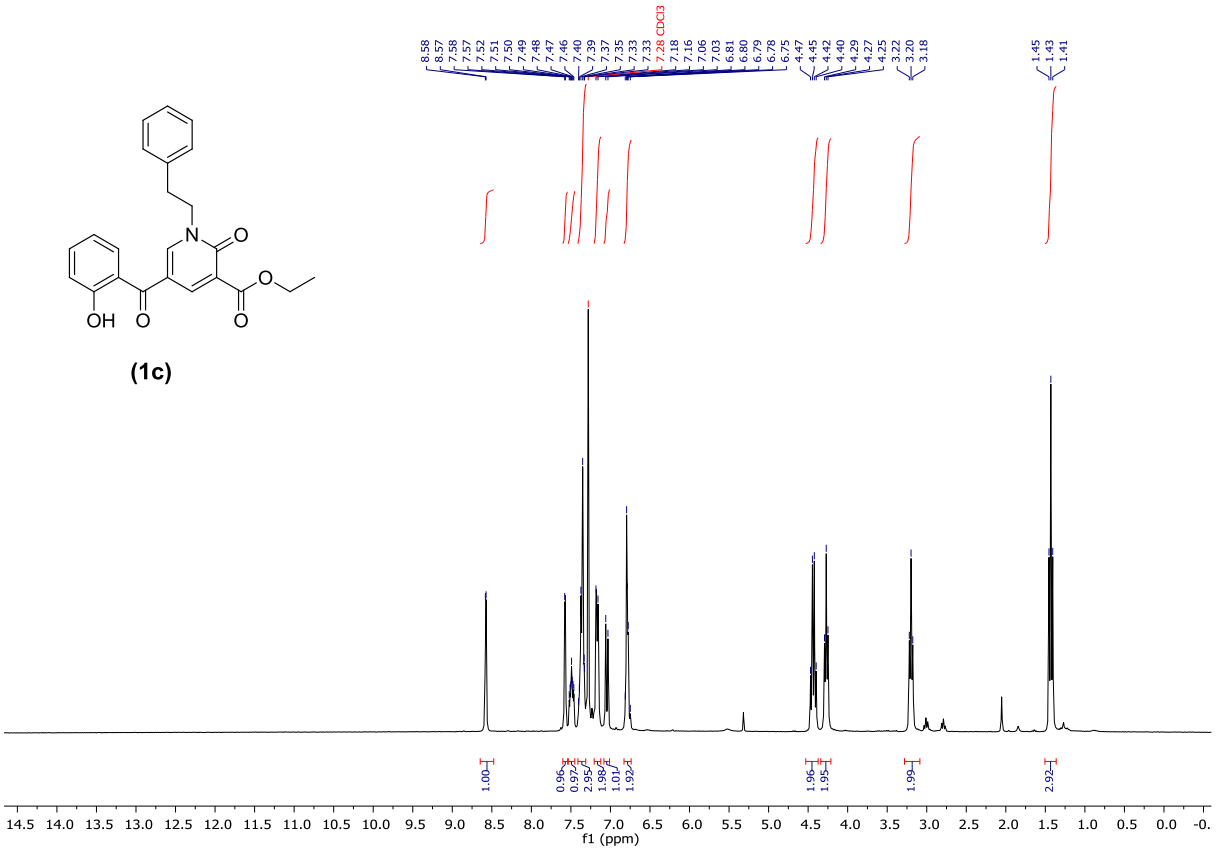
f1 (ppm)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4.29
4.27
4.25
3.22
3.20
3.18
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1.41
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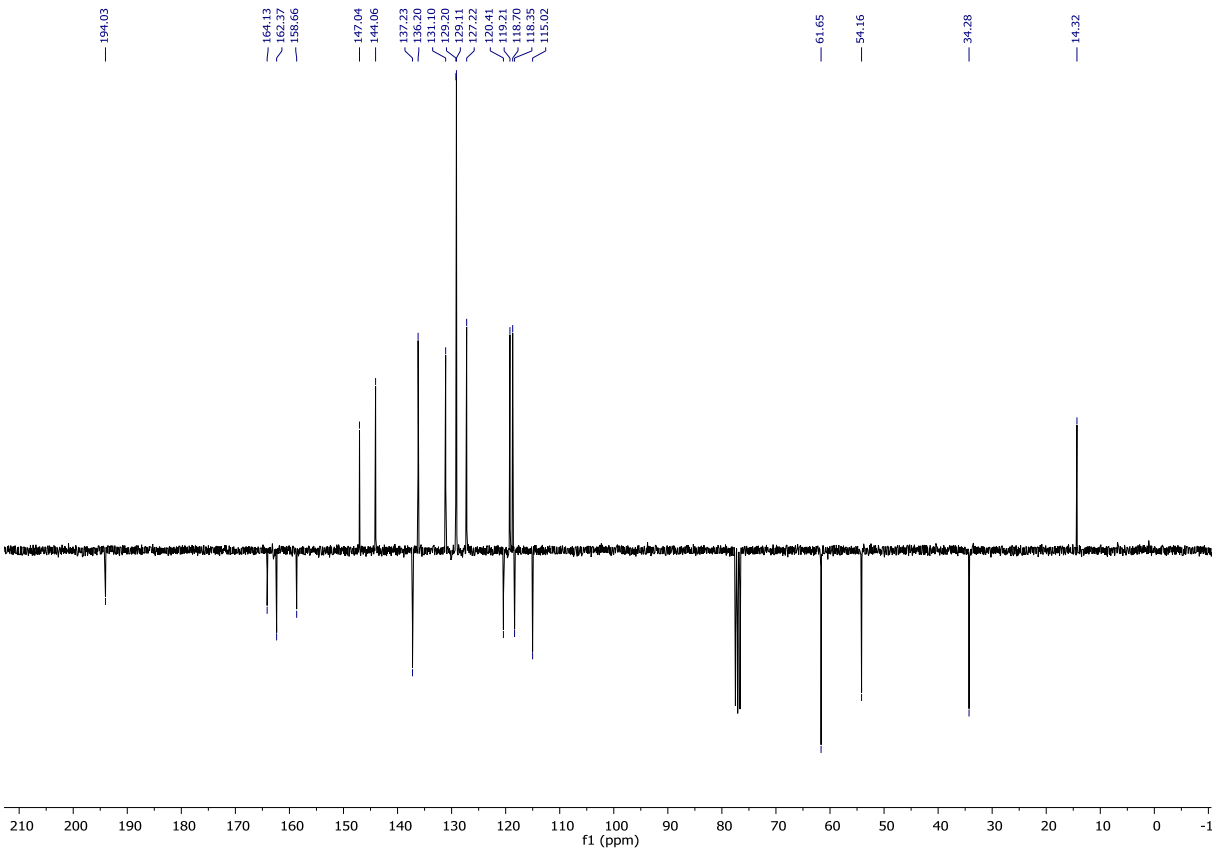
1.99
2.92
f1 (ppm)

(1c)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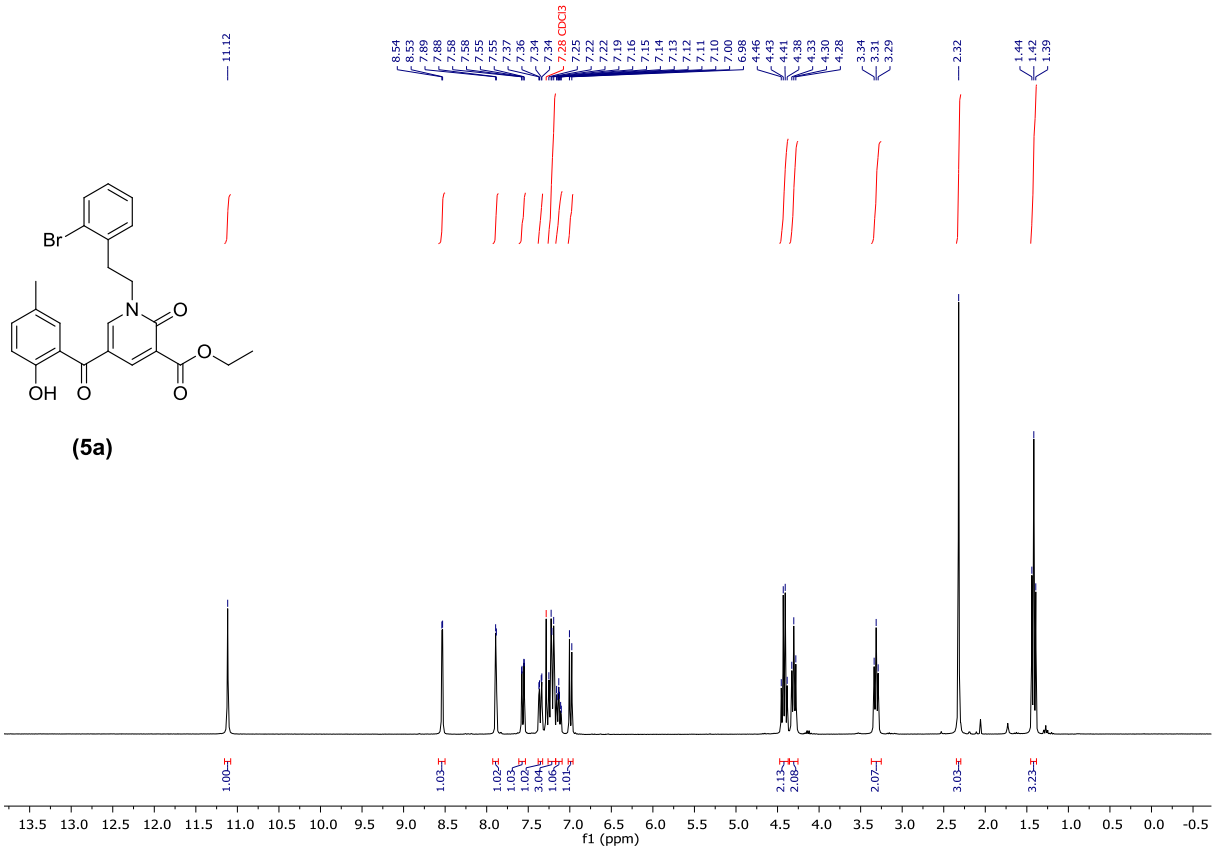
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3.29
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O
OH
O
O
(5a)
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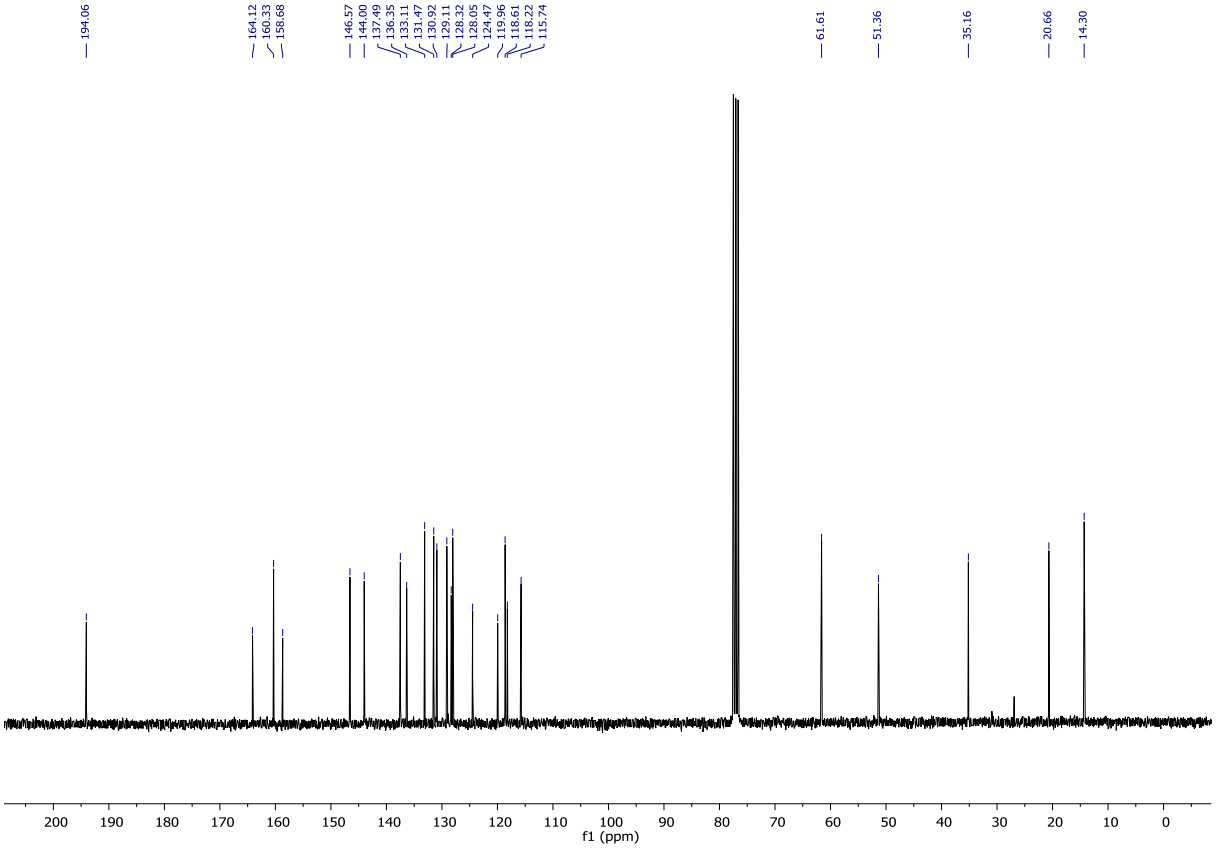
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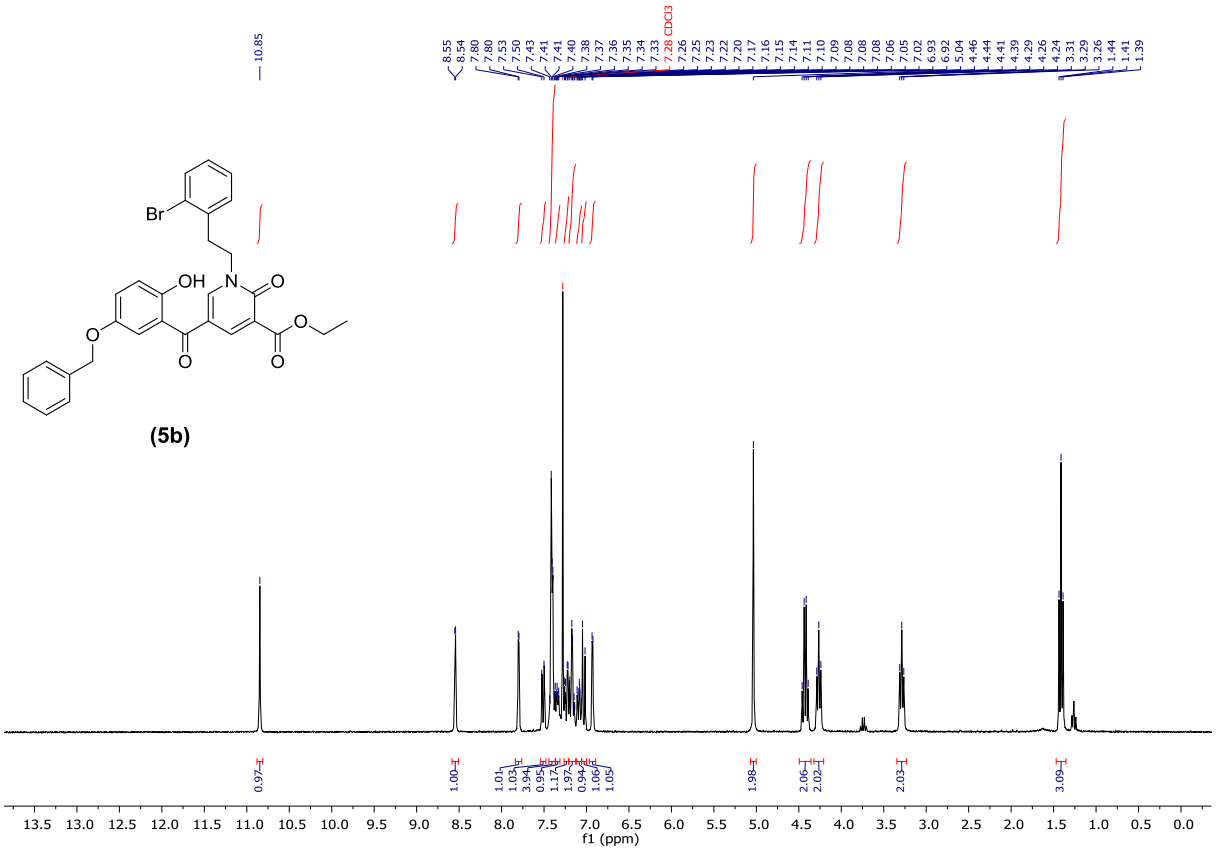
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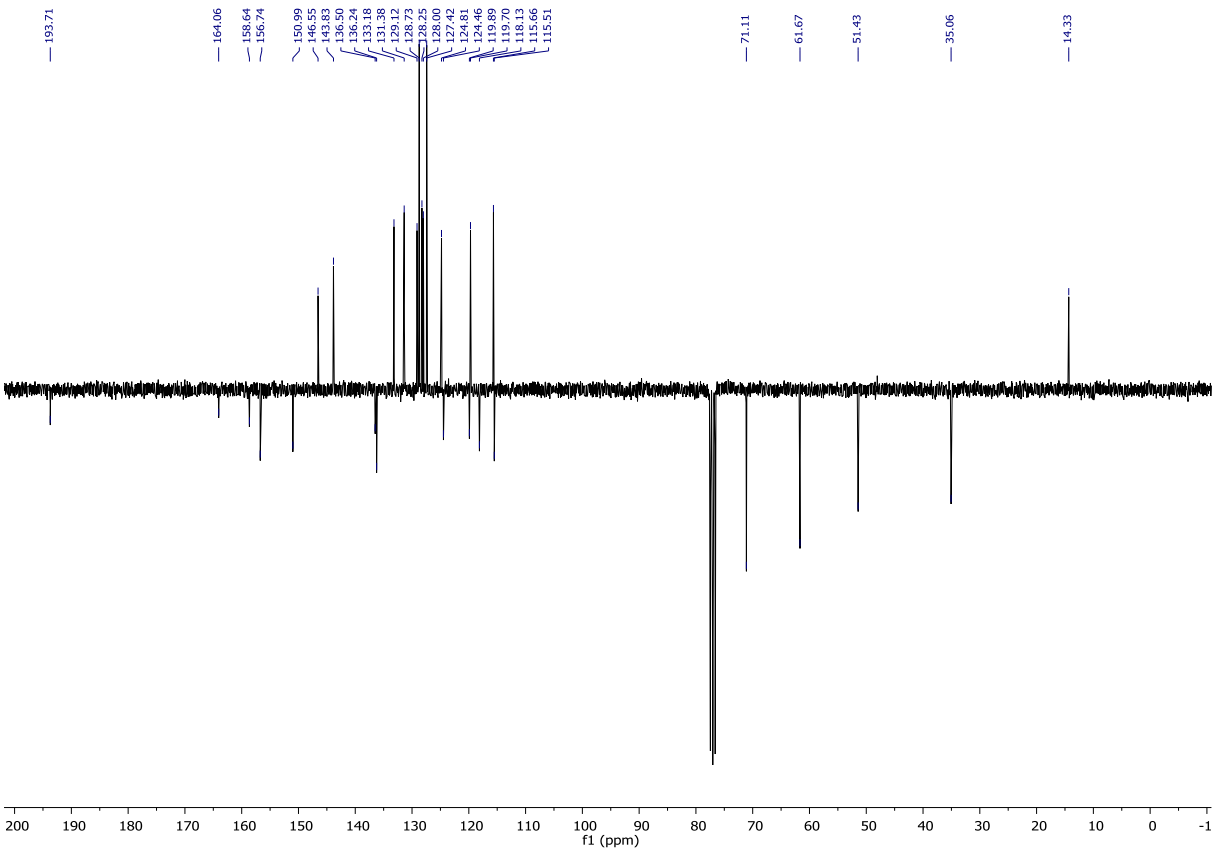
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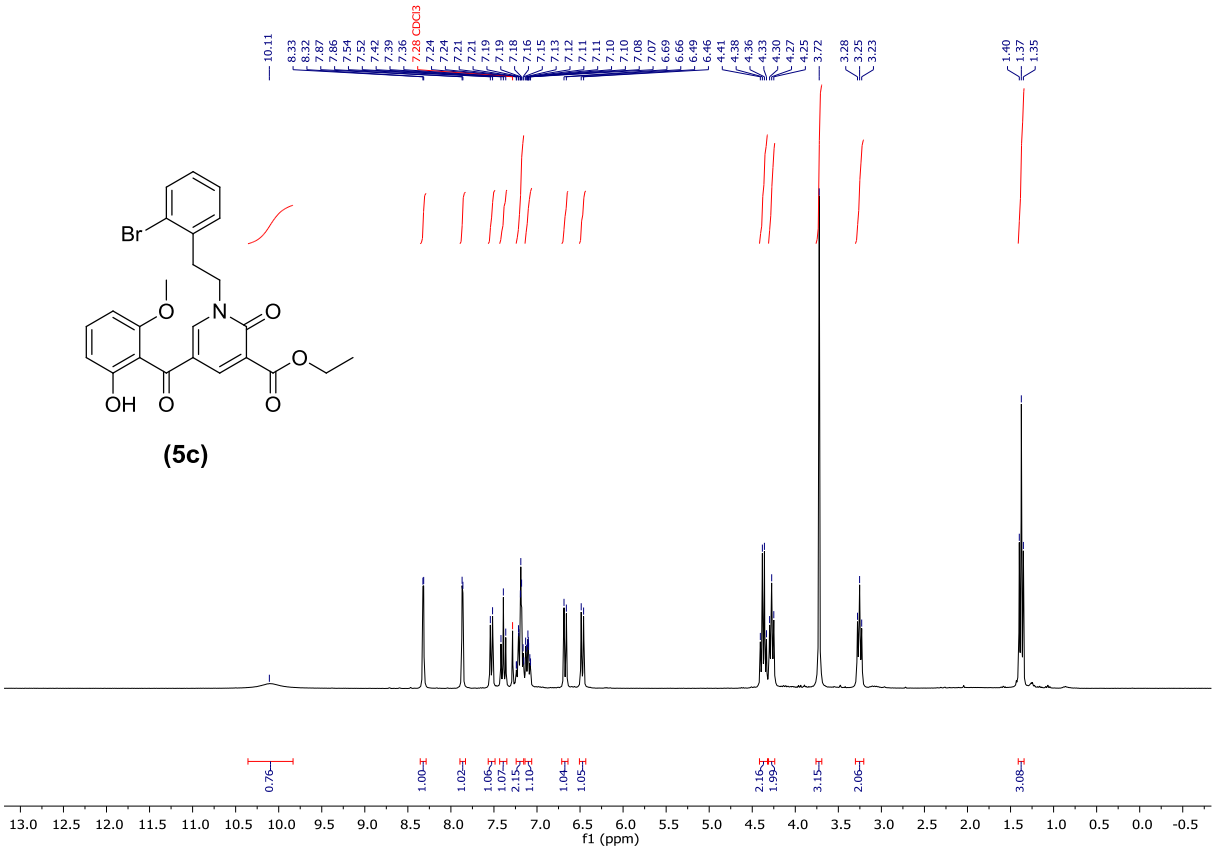
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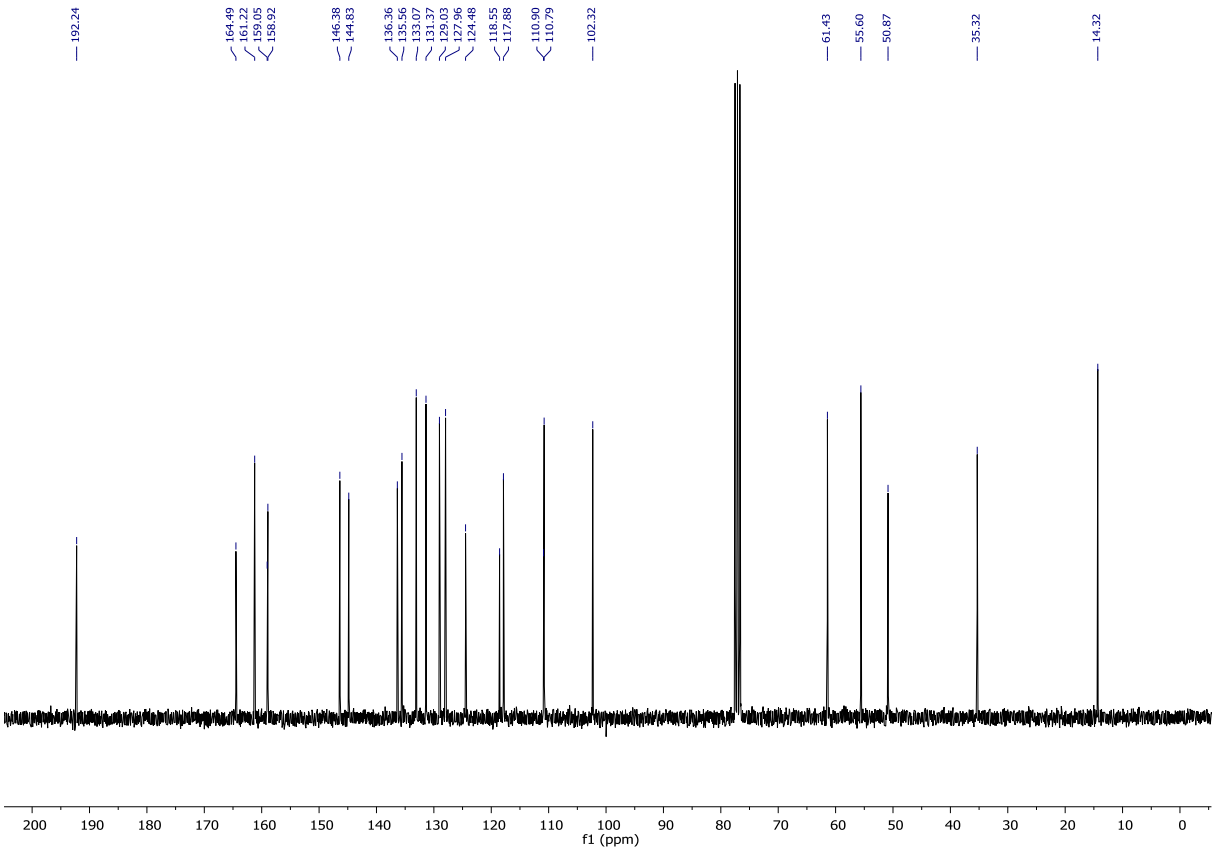
(5c)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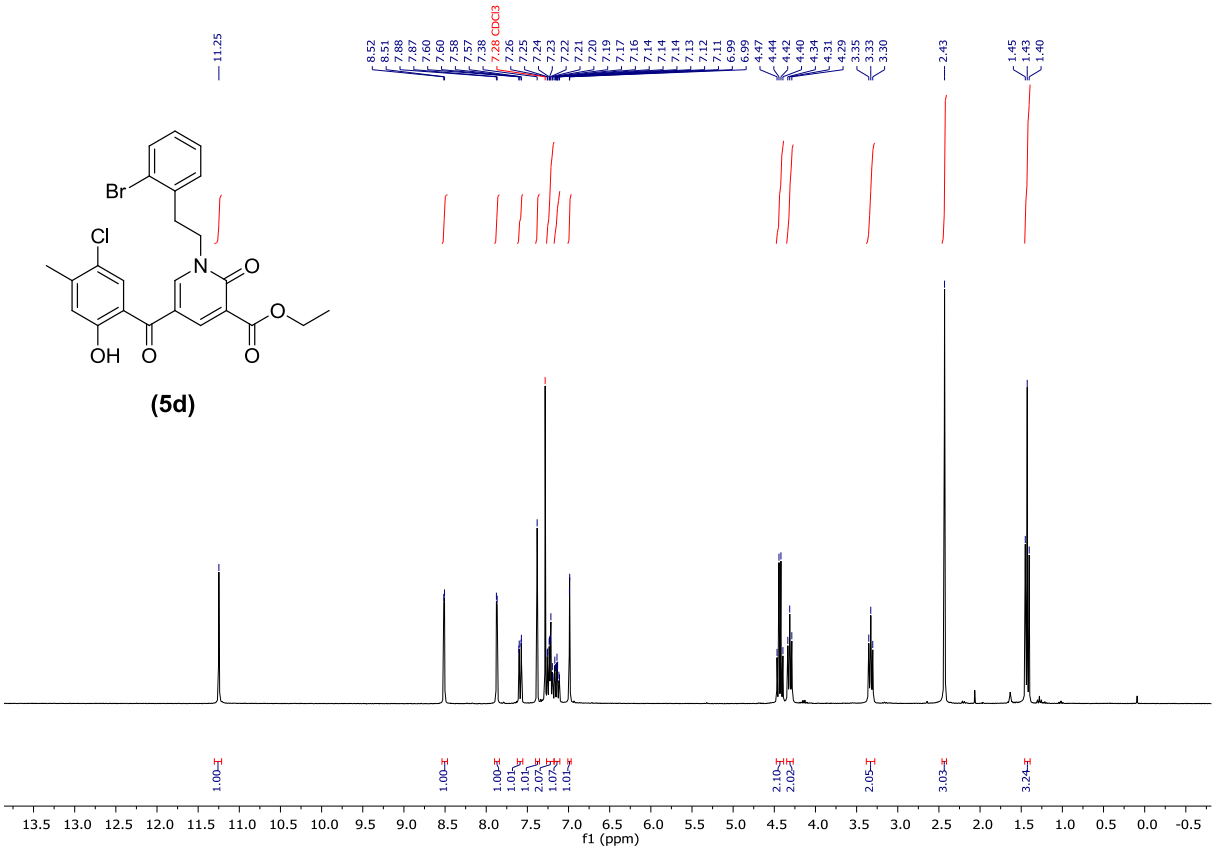
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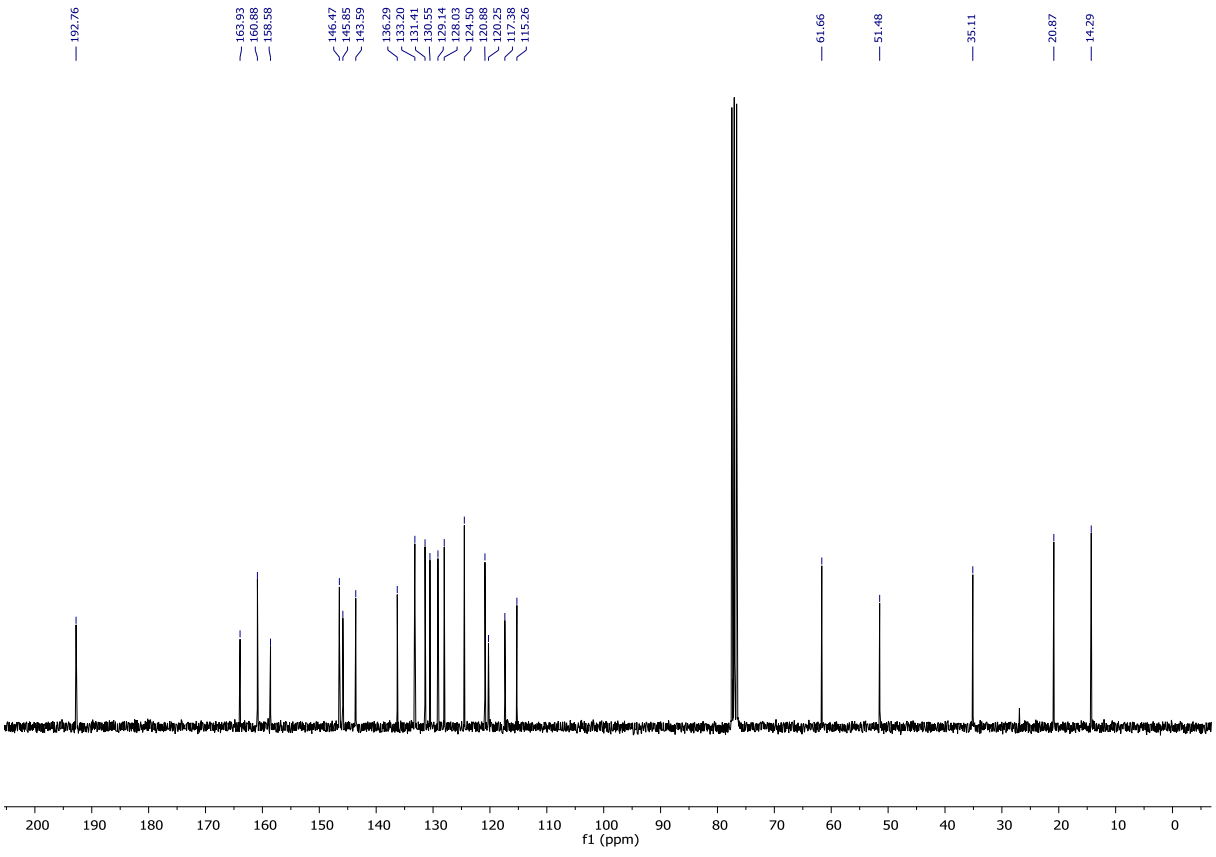
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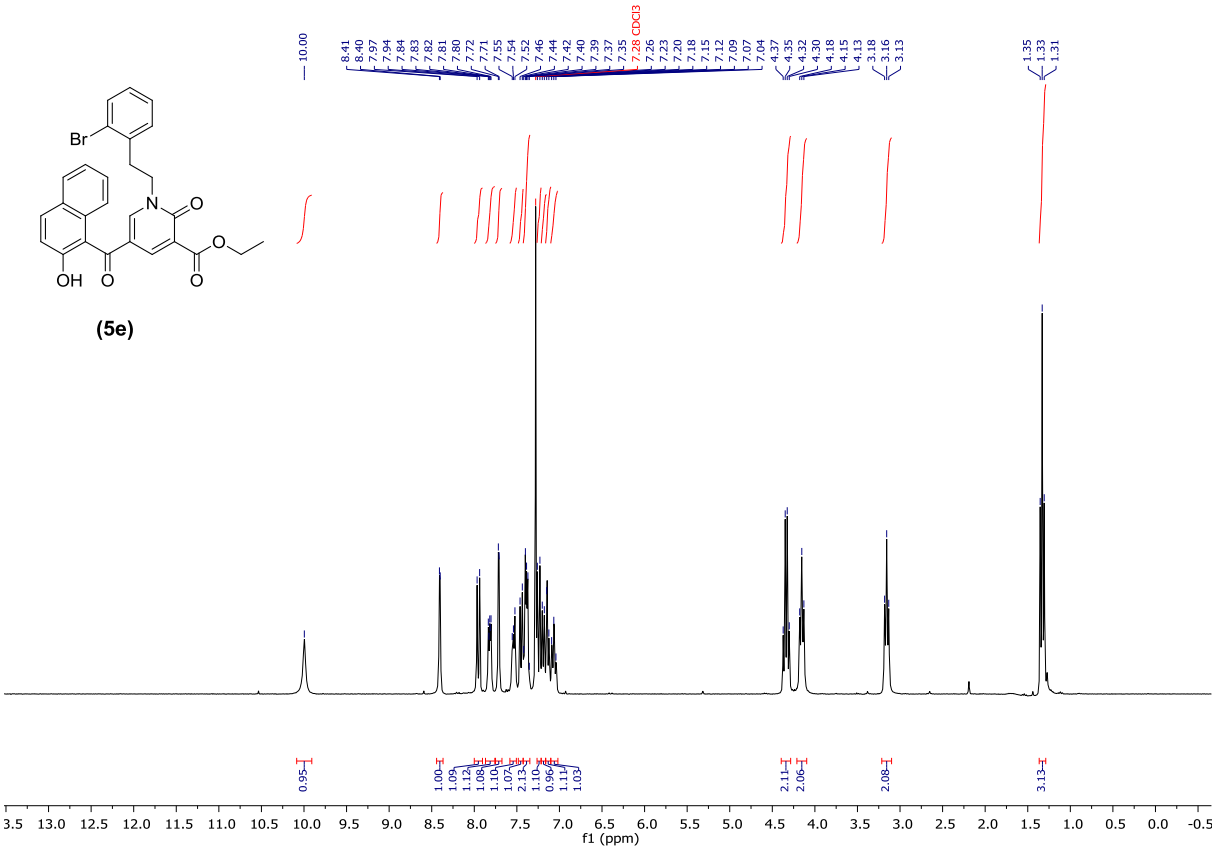
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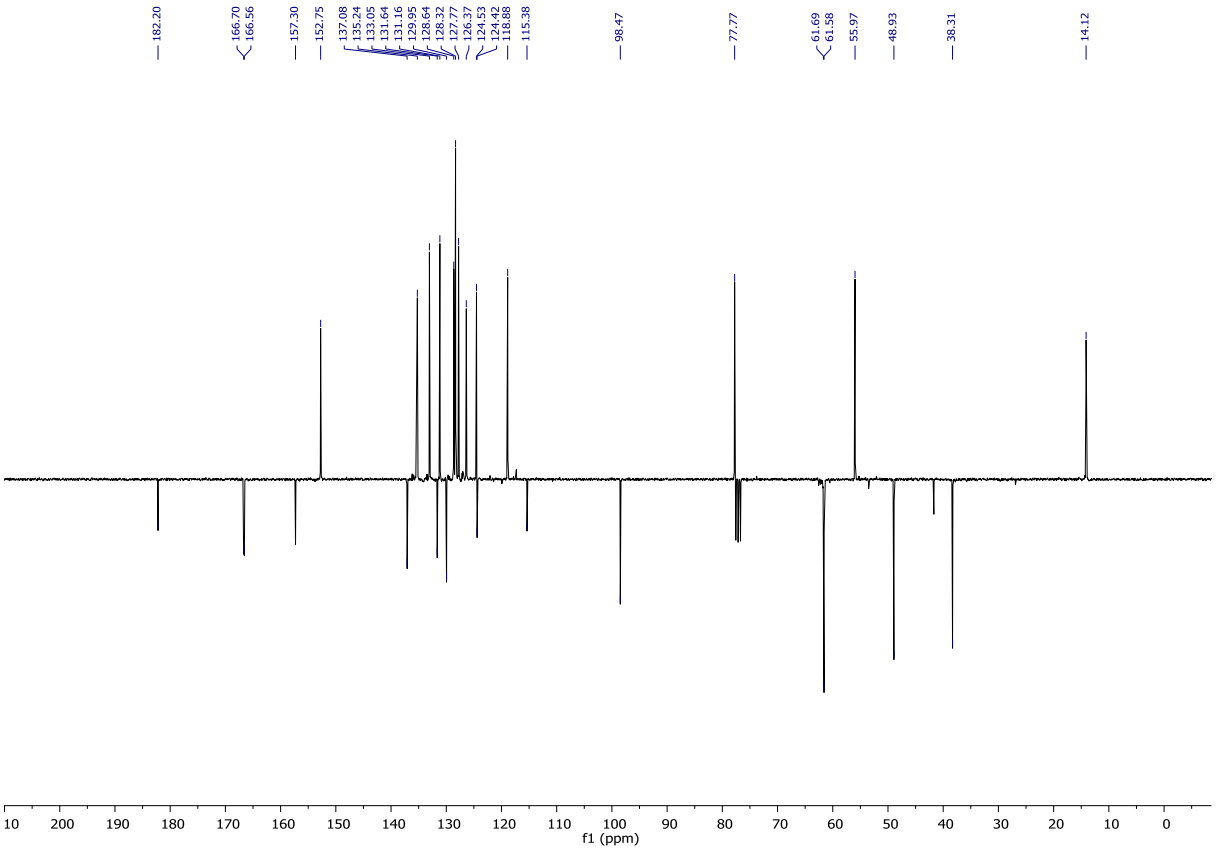
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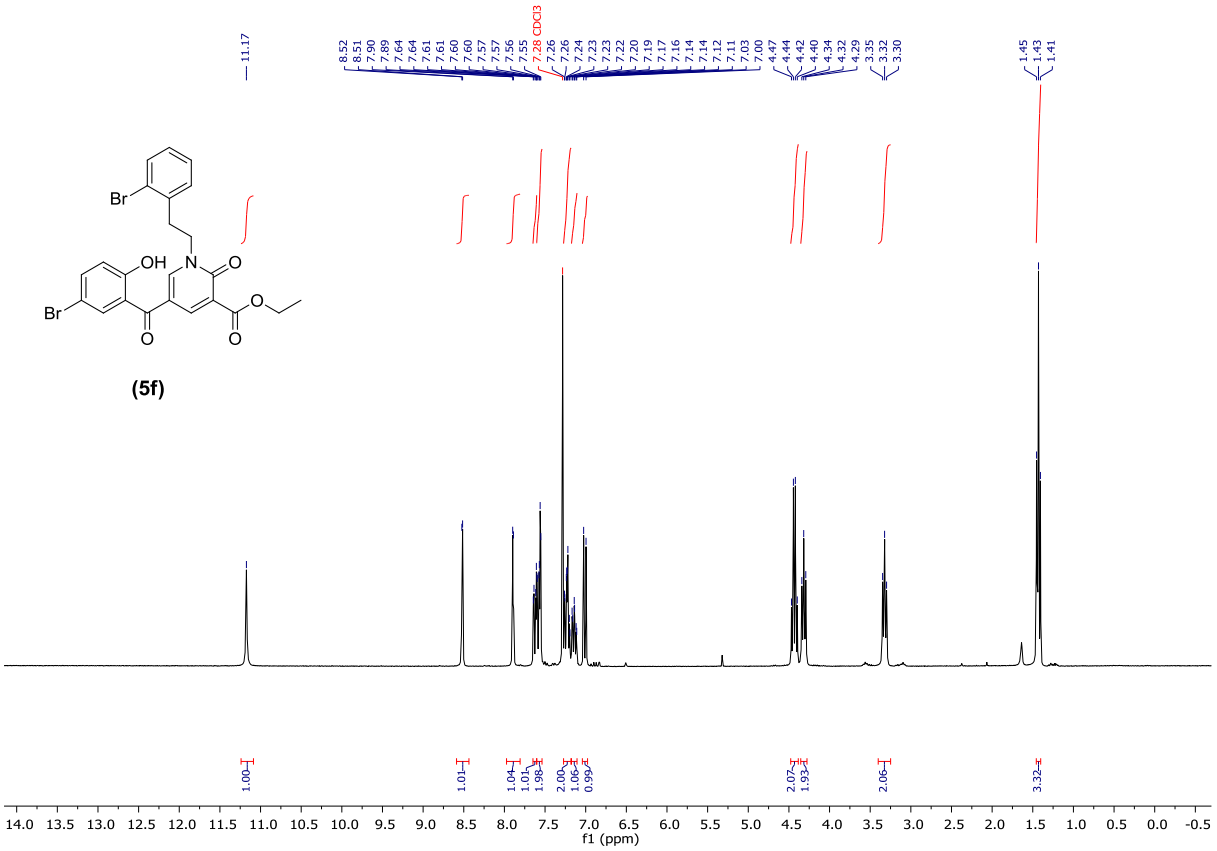
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7.57
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1.01
1.04
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0.99
2.07
1.93
2.06
3.32
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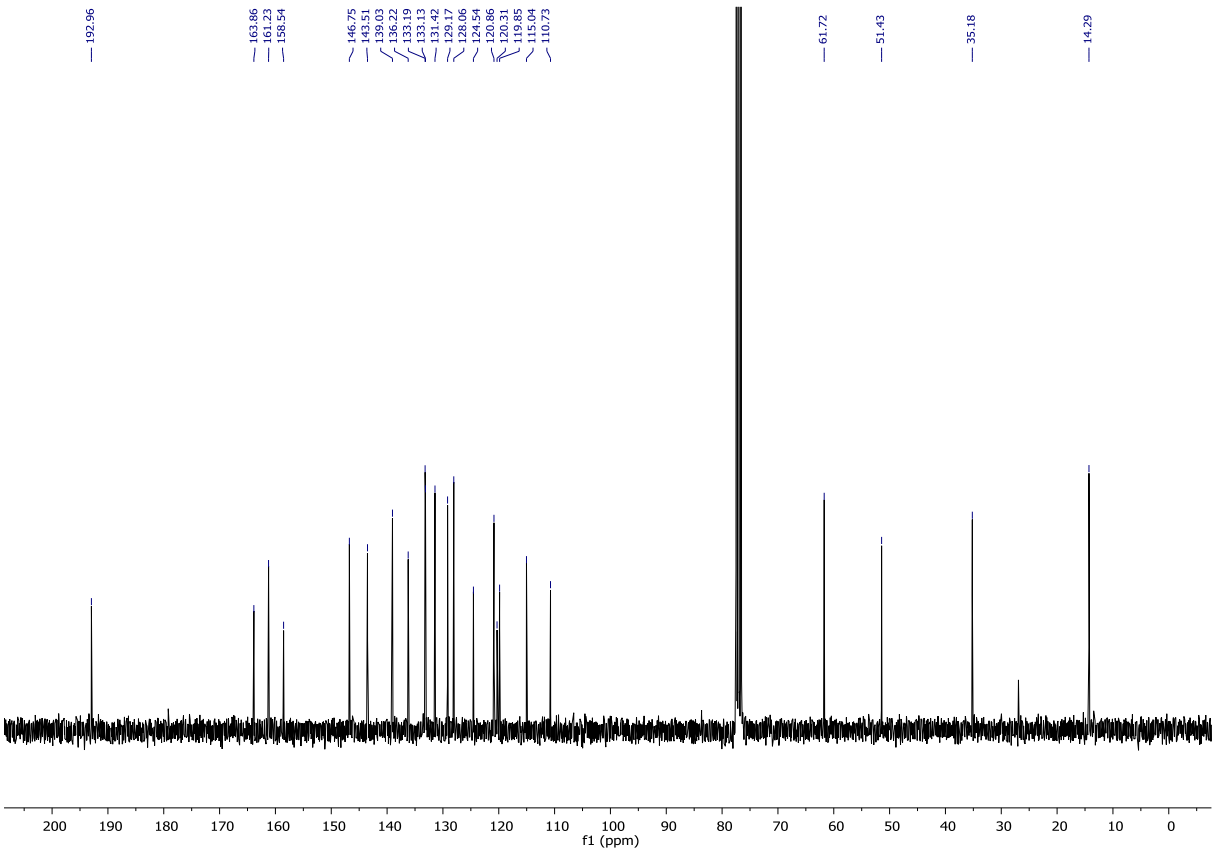
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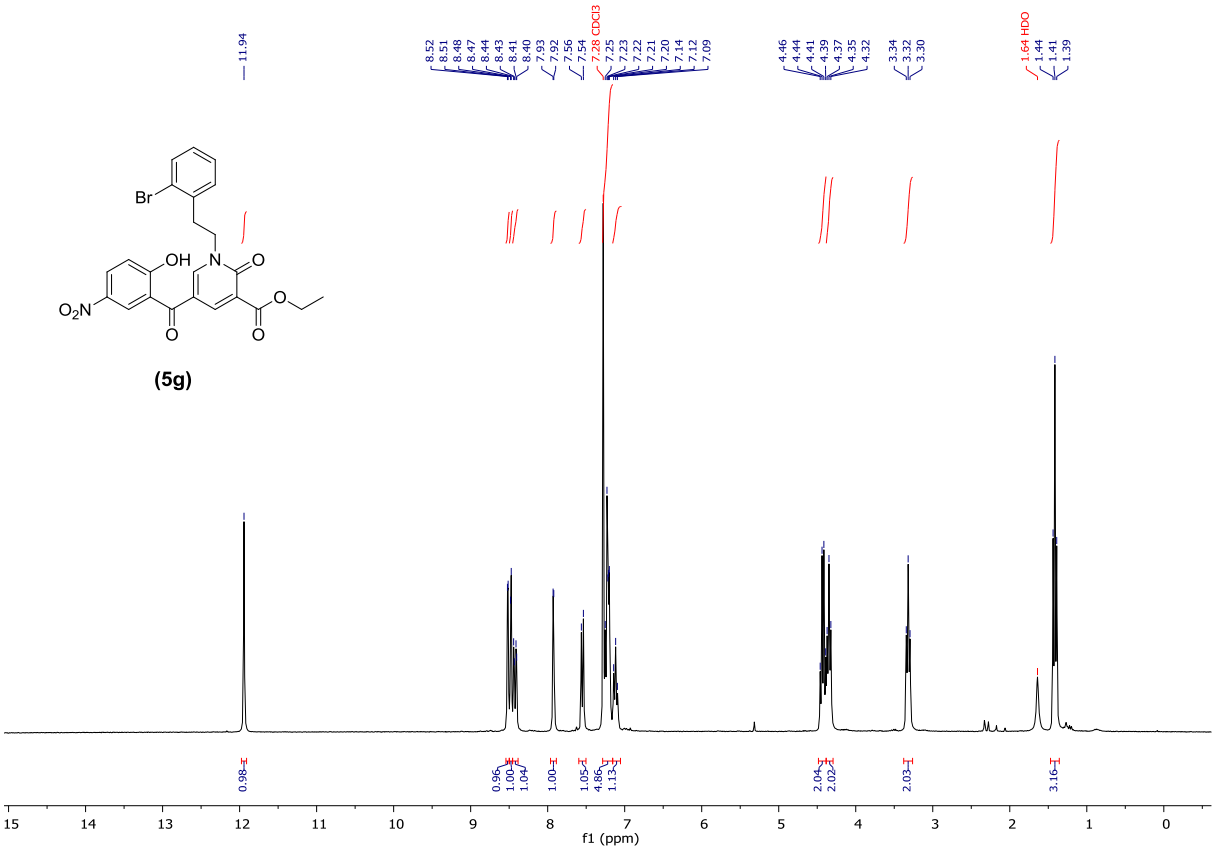
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7.21
7.20
7.14
7.12
7.09
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4.39
4.37
4.35
4.32
3.34
3.32
3.30
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1.41
1.39
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OH
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O
O
O2N
O
O
O
(5g)
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2.02
2.03
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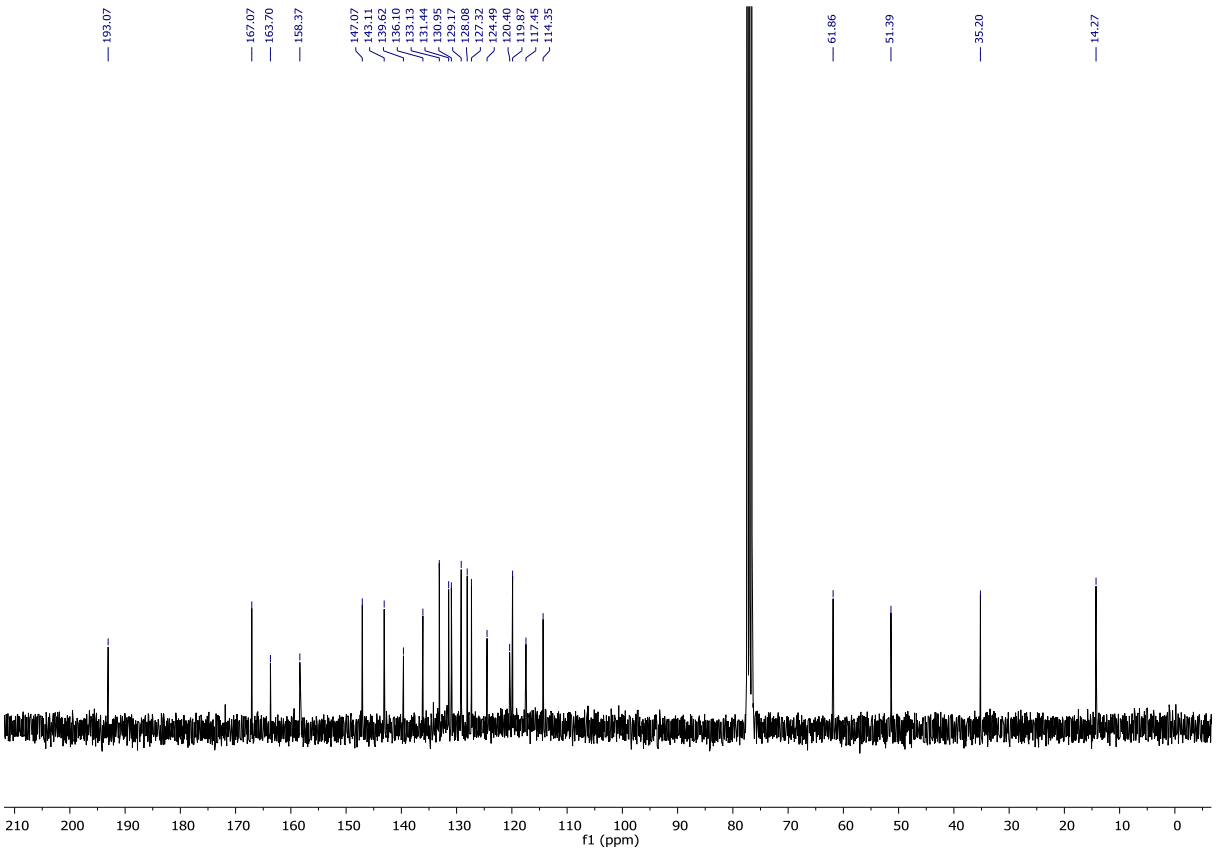
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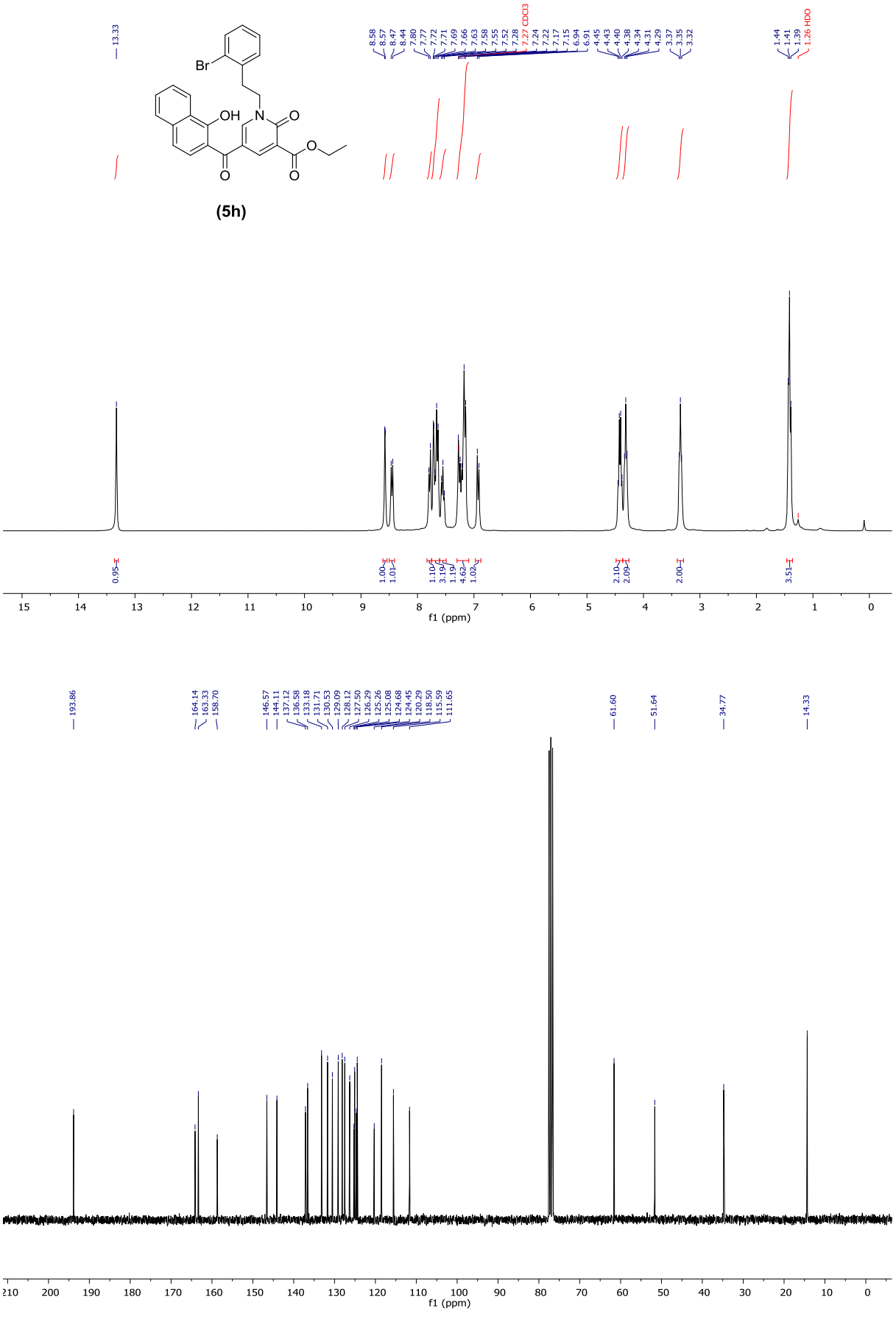
f1 (ppm)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7.28
7.27 CDCl3
7.24
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4.43
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4.38
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4.31
4.29
3.37
3.35
3.32
1.44
1.41
1.39
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Br
OH
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O
O
O
O
(5h)
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1.10
3.19
1.19
4.62
1.02
2.10
2.09
2.00
3.51
f1 (ppm)
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136.58
135.18
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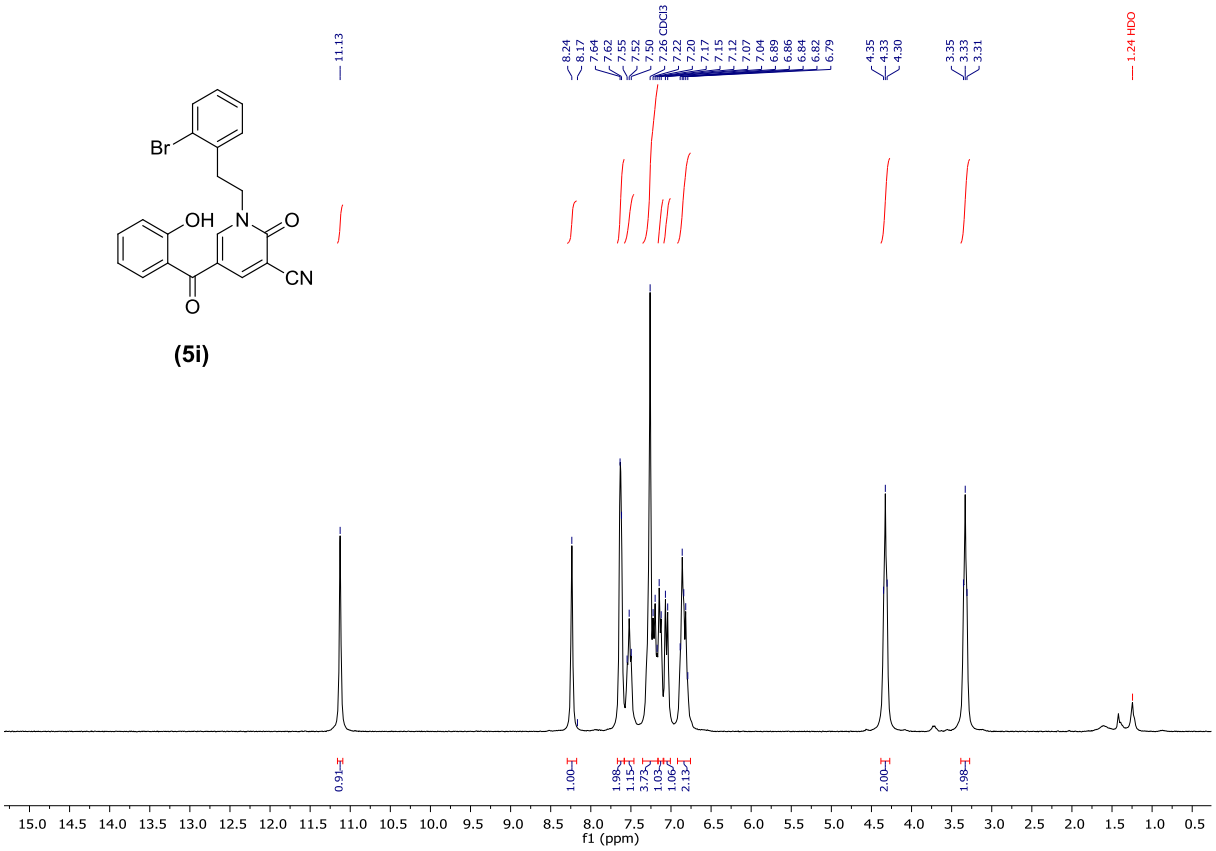
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6.86
6.84
6.82
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4.35
4.33
4.30
3.35
3.33
3.31
1.24 H2O
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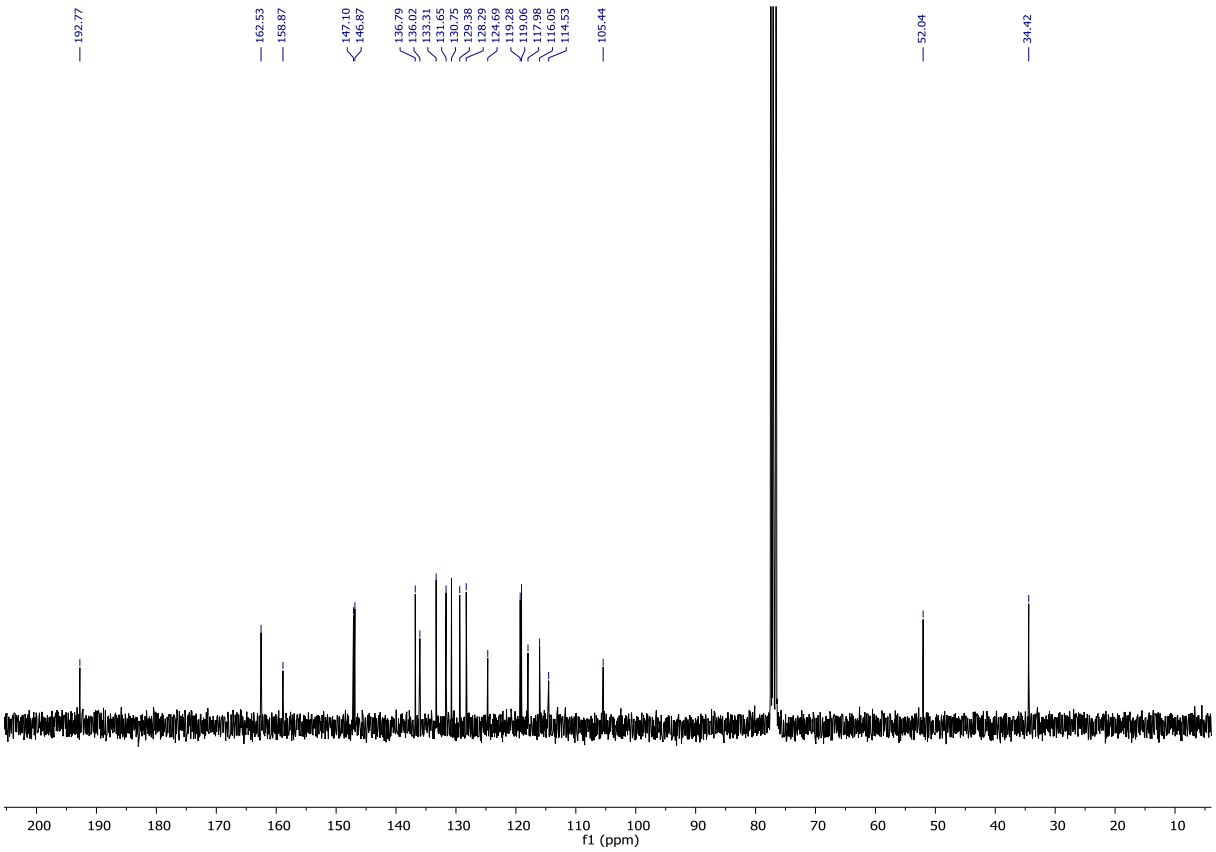
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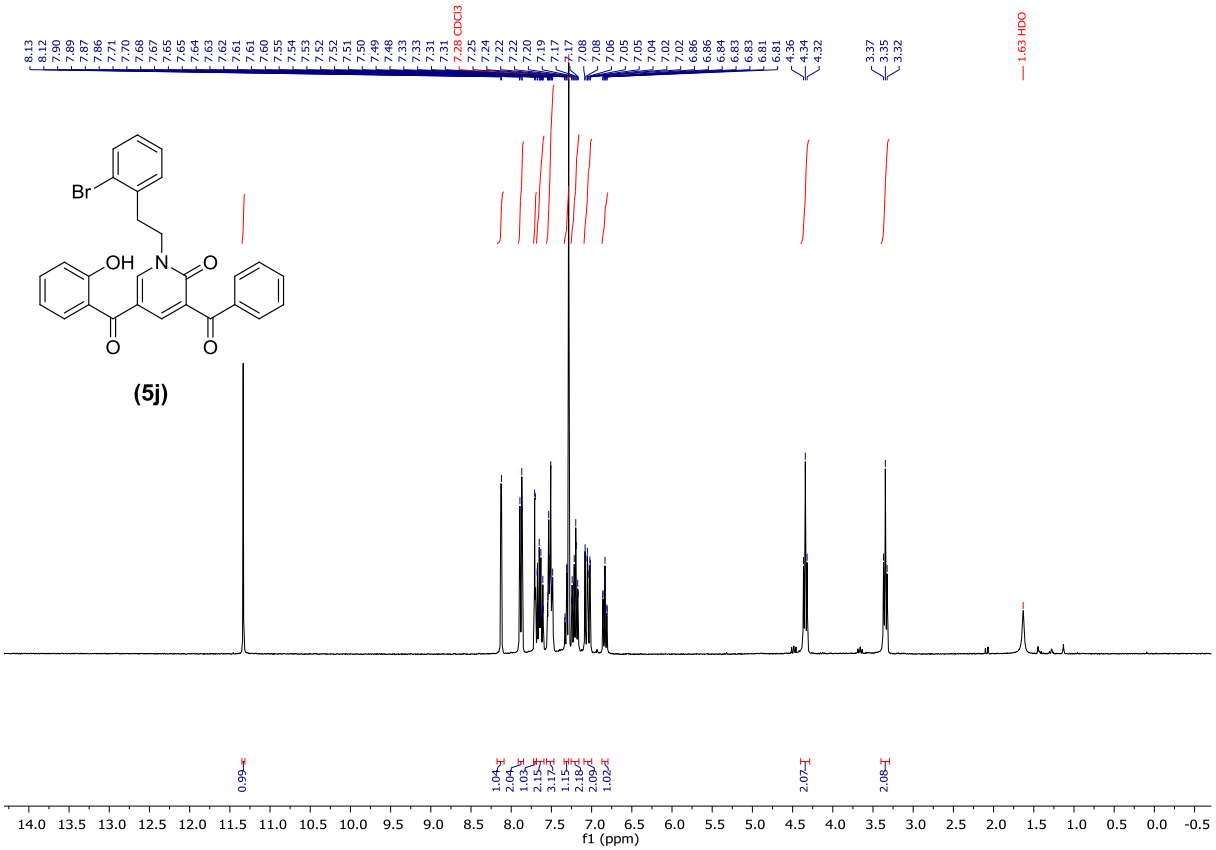
f1 (ppm)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7.48
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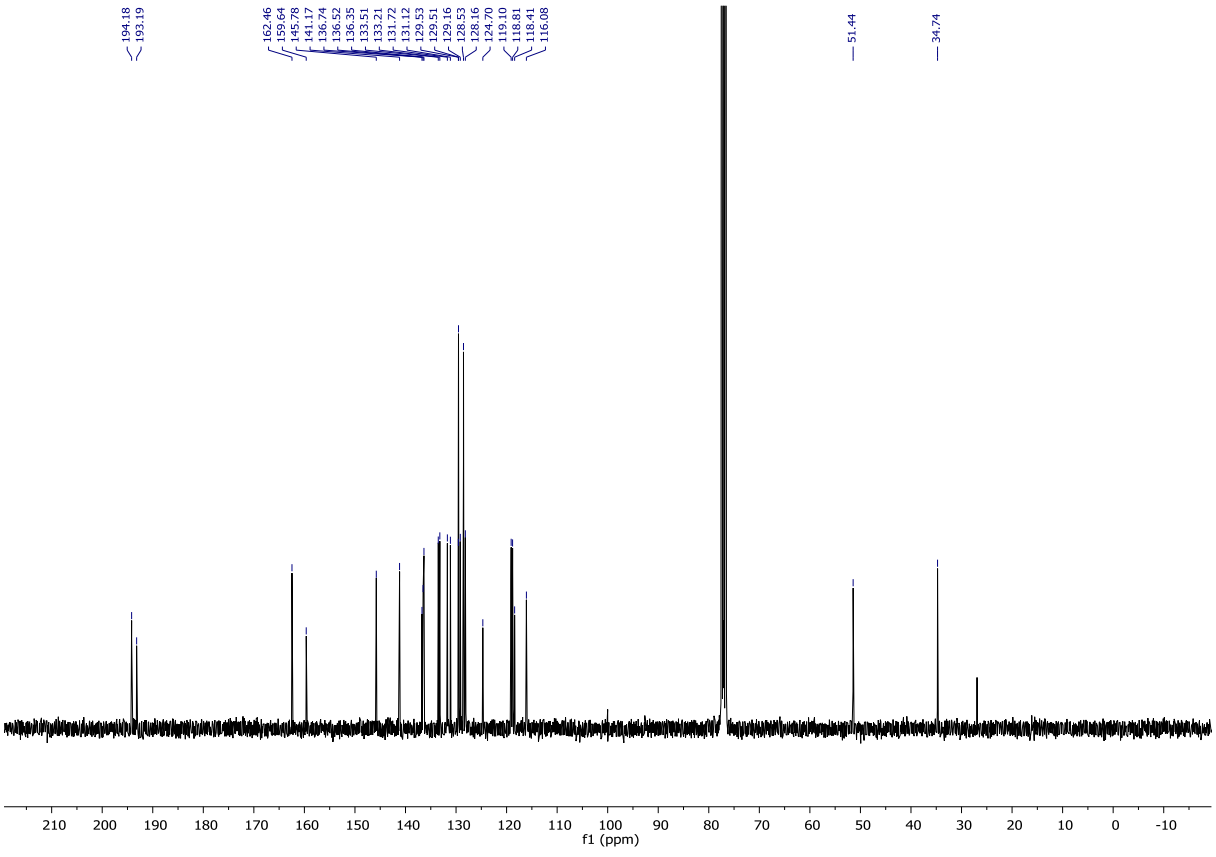
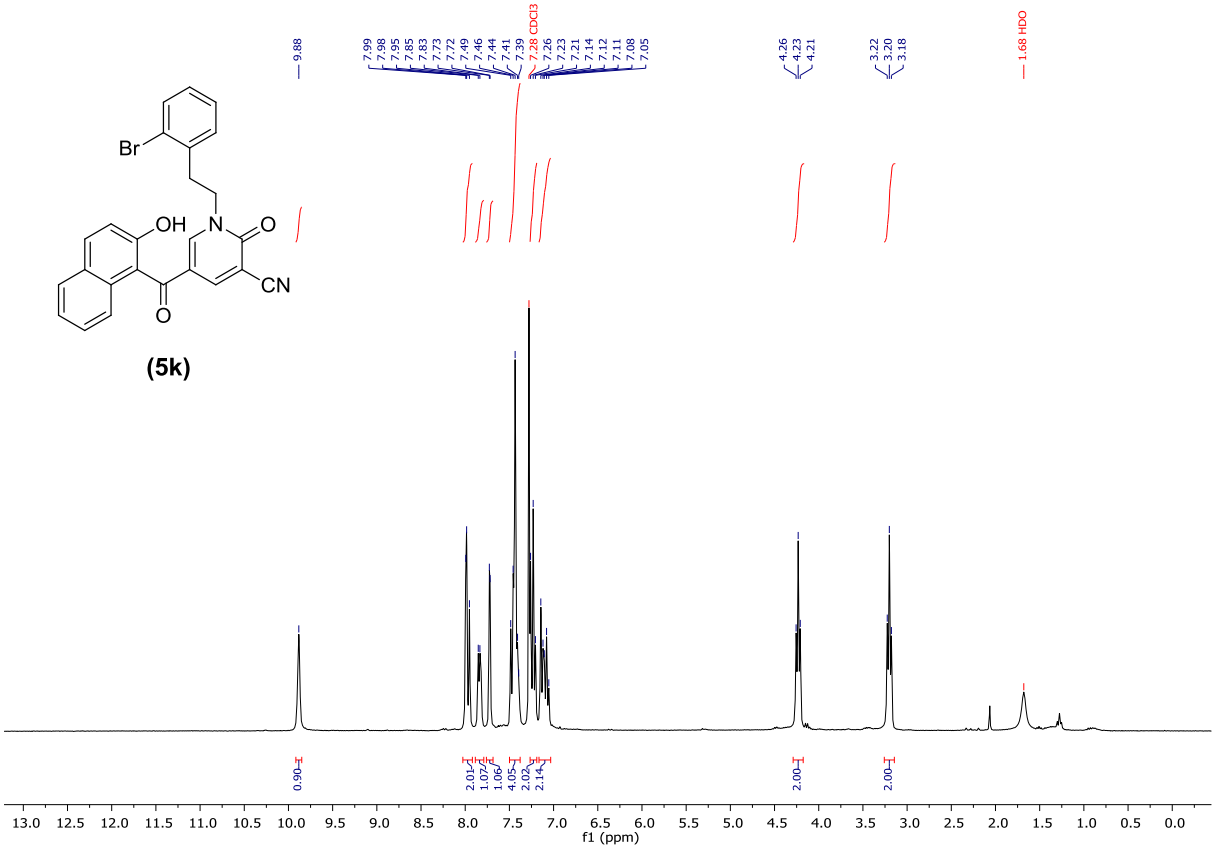
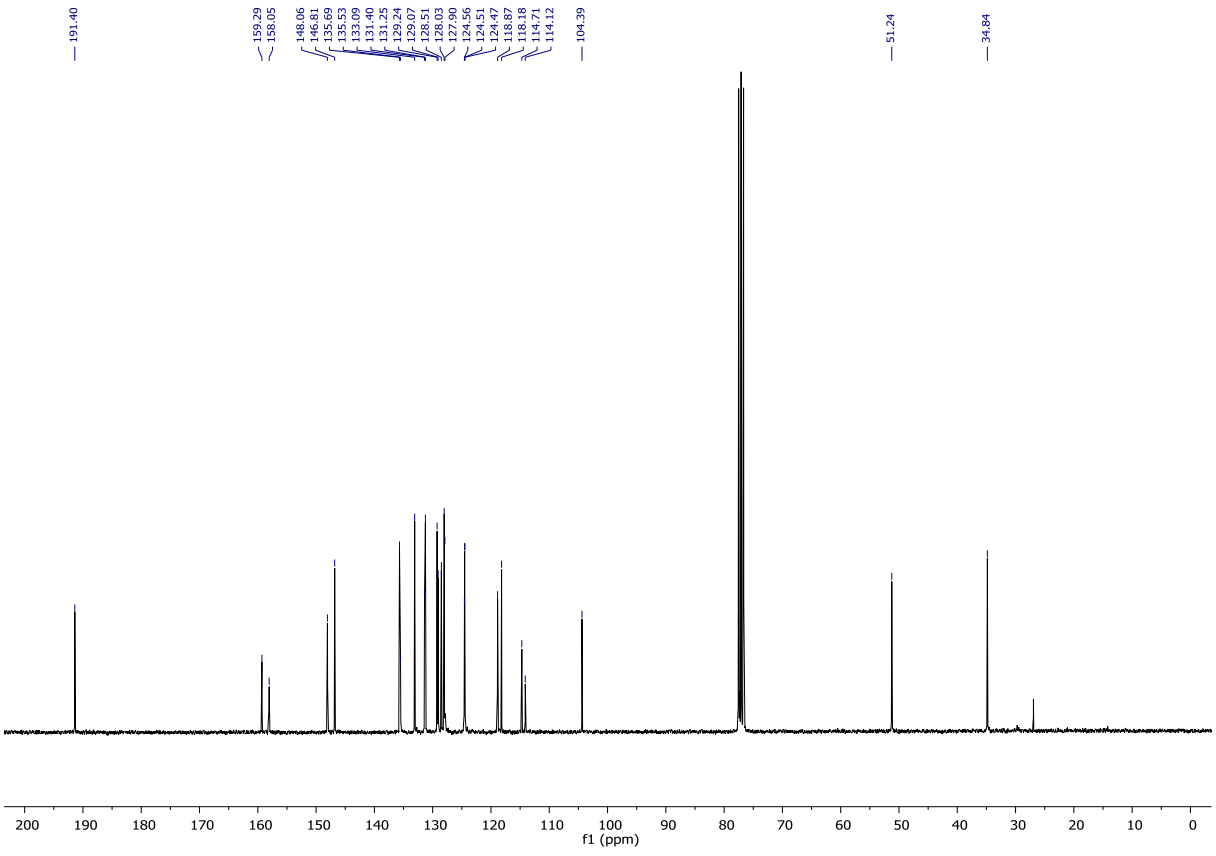
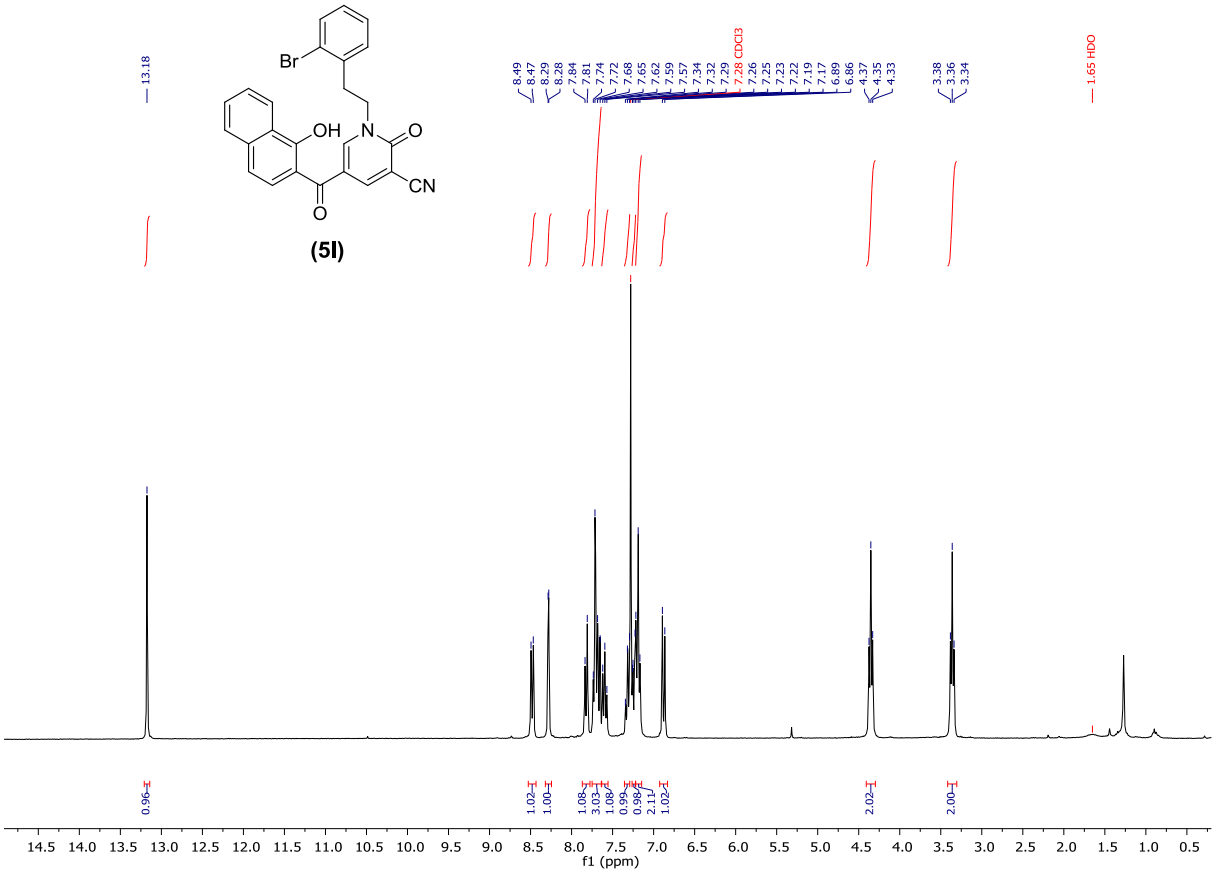
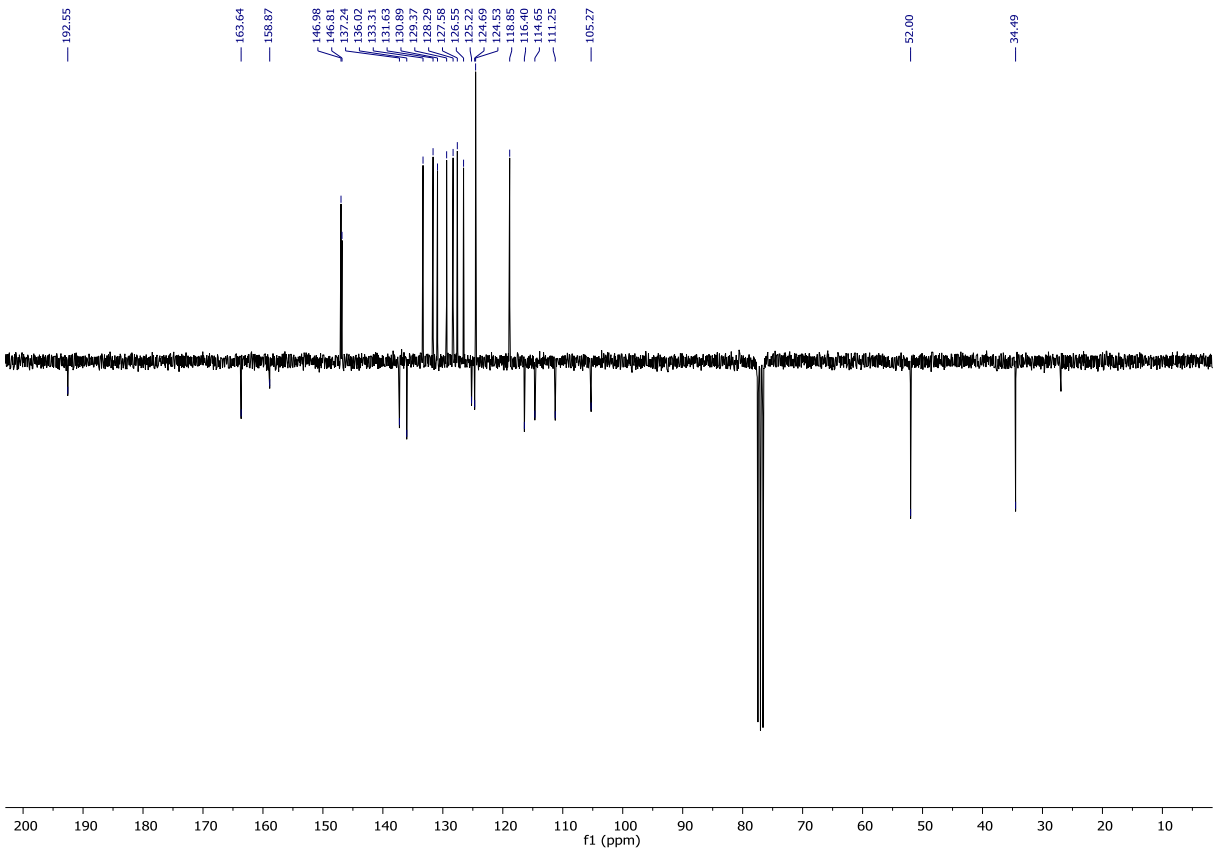
7.31
7.31
7.28 CDCl3
7.25
7.24
7.22
7.22
7.20
7.19
7.17
7.17
7.08
7.08
7.06
7.05
7.05
7.04
7.02
7.02
6.86
6.86
6.84
6.83
6.83
6.81
6.81
4.36
4.34
4.32
3.37
3.35
3.32
1.63 HDO
Br
OH
N
O
O
O
(5j)
0.99
1.04
2.04
1.03
2.15
3.17
1.15
2.18
2.09
1.02
2.07
2.08
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


194.18
193.19
162.46
159.64
145.78
141.17
136.74
136.52
136.35
133.51
133.21
131.72
131.12
129.53
129.51
129.16
128.53
128.16
124.70
119.10
118.81
118.41
116.08
51.44
34.74
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Br
OH
N
O
CN
O
(5k)
9.88
7.99
7.98
7.95
7.85
7.83
7.73
7.72
7.49
7.46
7.44
7.41
7.39
7.28 CDCl3
7.26
7.23
7.21
7.14
7.12
7.11
7.08
7.05
4.26
4.23
4.21
3.22
3.20
3.18
1.68 HDO
0.90
2.01
1.07
1.06
4.05
2.02
2.14
2.00
2.00
f1 (ppm)


191.40
159.29
158.05
148.06
146.81
135.69
135.53
133.09
131.40
131.25
129.24
129.07
128.51
128.03
127.90
124.56
124.51
124.47
118.87
118.18
114.71
114.12
104.39
51.24
34.84
f1 (ppm)


Br
OH
N
O
O
CN
O
(5l)
13.18
8.49
8.47
8.29
8.28
7.84
7.81
7.74
7.72
7.68
7.65
7.62
7.59
7.57
7.34
7.32
7.30
7.28 CDCl3
7.26
7.25
7.23
7.22
7.19
7.17
6.89
6.86
4.37
4.35
4.33
3.38
3.36
3.34
1.65 HDO
0.96
1.02
1.00
1.08
3.03
1.08
0.99
0.98
2.11
1.02
2.02
2.00
14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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163.64
158.87
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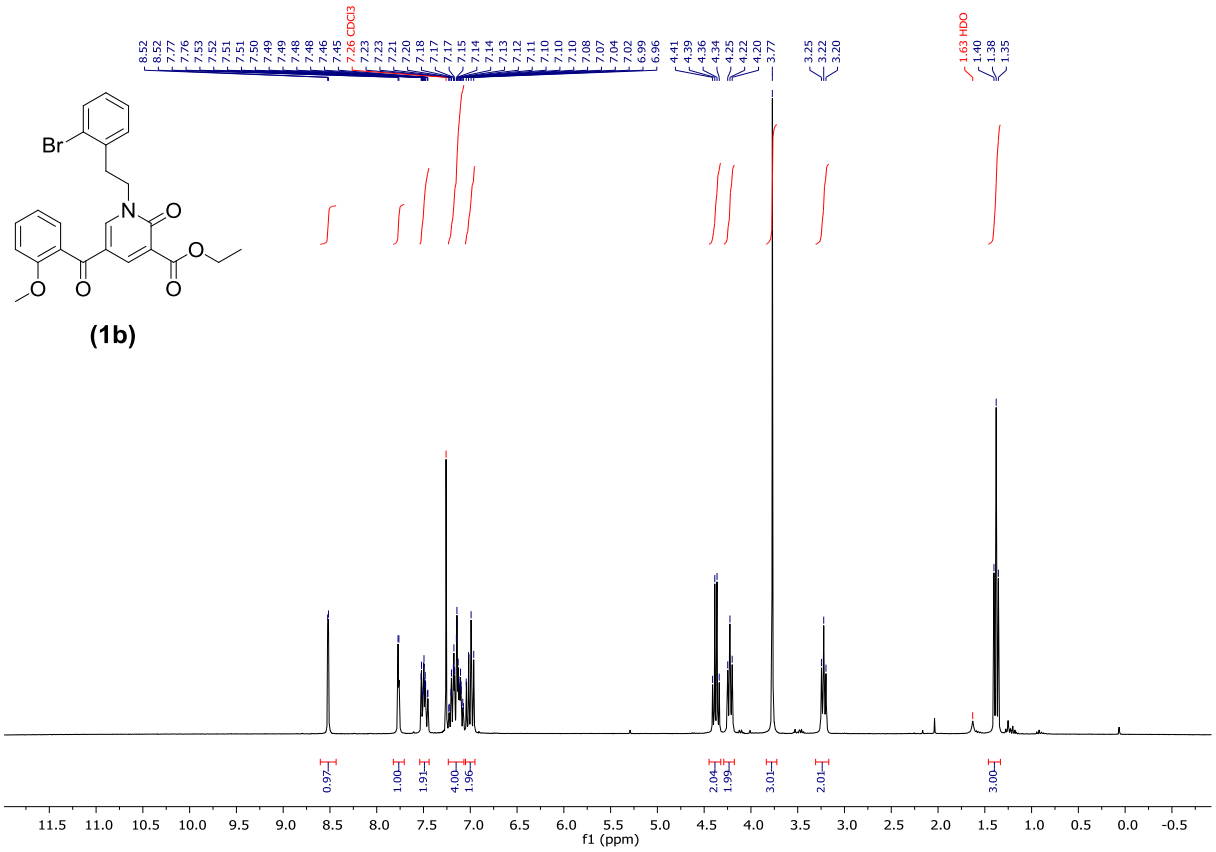
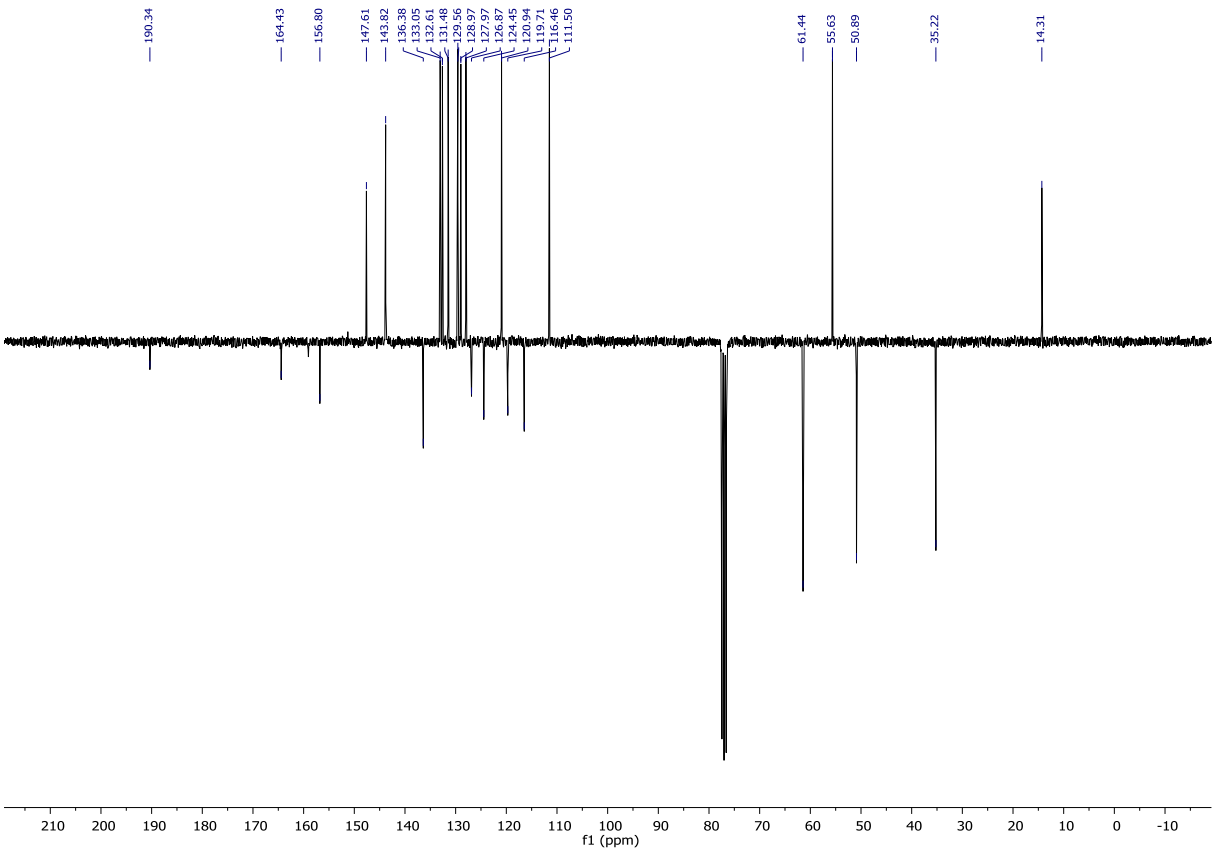
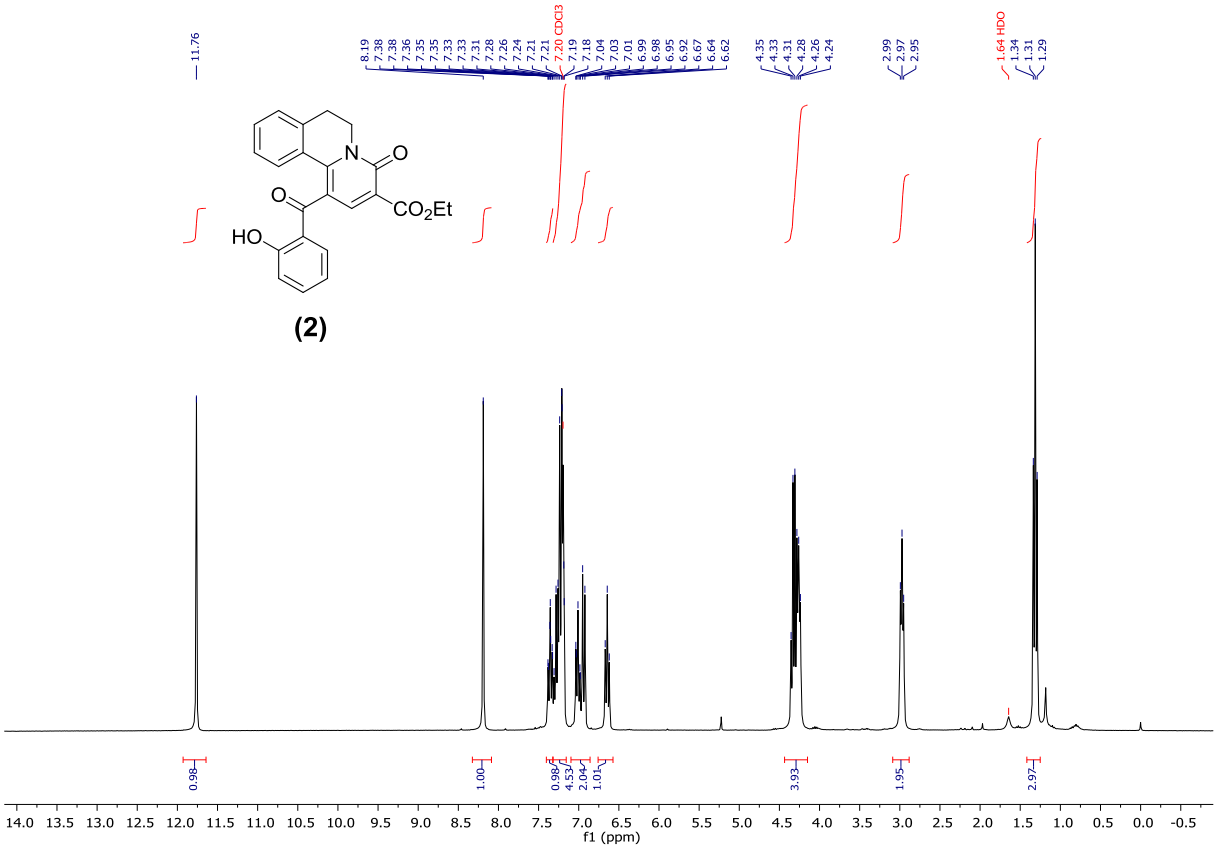
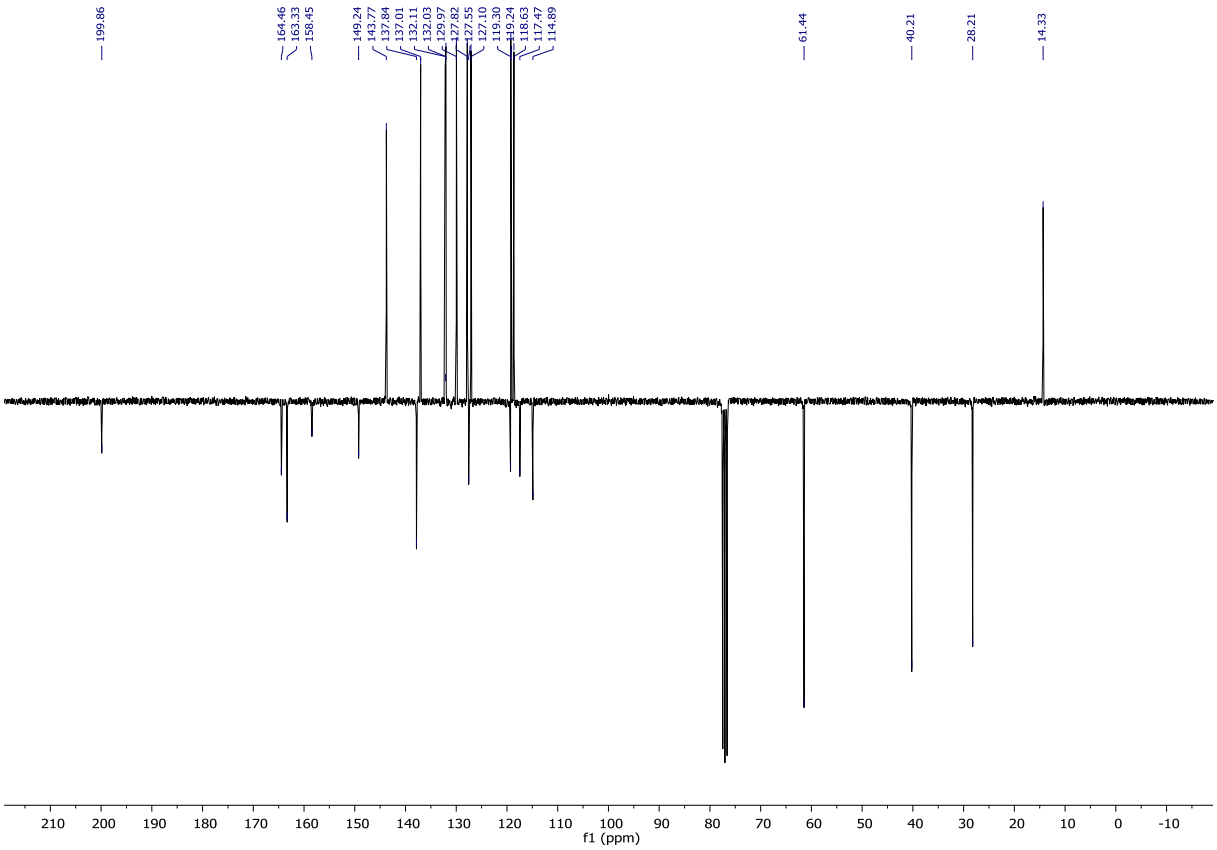
146.81
137.24
136.02
133.31
131.63
130.89
129.37
128.29
127.58
126.55
125.22
124.69
124.53
118.85
116.40
114.65
111.25
105.27
52.00
34.49
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.52
8.52
7.77
7.76
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.48
7.48
7.46
7.45
7.26 CDCl3
7.23
7.23
7.21
7.20
7.18
7.17
7.17
7.15
7.14
7.14
7.13
7.12
7.11
7.10
7.10
7.08
7.07
7.04
7.02
6.99
6.96
4.41
4.39
4.36
4.34
4.25
4.22
4.20
3.77
3.25
3.22
3.20
1.63 HDO
1.40
1.38
1.35
Br
N
O
O
O
O
O
(1b)
0.97
1.00
1.91
4.00
1.96
2.04
1.99
3.01
2.01
3.00
f1 (ppm)


190.34
164.43
156.80
147.61
143.82
136.38
133.05
132.61
131.48
129.56
128.97
127.97
126.87
124.45
120.94
119.71
116.46
111.50
61.44
55.63
50.89
35.22
14.31
f1 (ppm)


11.76
8.19
7.38
7.38
7.36
7.35
7.35
7.33
7.33
7.31
7.28
7.26
7.24
7.21
7.21
7.20 CDCl3
7.19
7.18
7.04
7.03
7.01
6.99
6.98
6.95
6.92
6.67
6.64
6.62
4.35
4.33
4.31
4.28
4.26
4.24
2.99
2.97
2.95
1.64 HDO
1.34
1.31
1.29
N
O
O
CO2Et
HO
(2)
0.98
1.00
0.98
4.53
2.04
1.01
3.93
1.95
2.97
f1 (ppm)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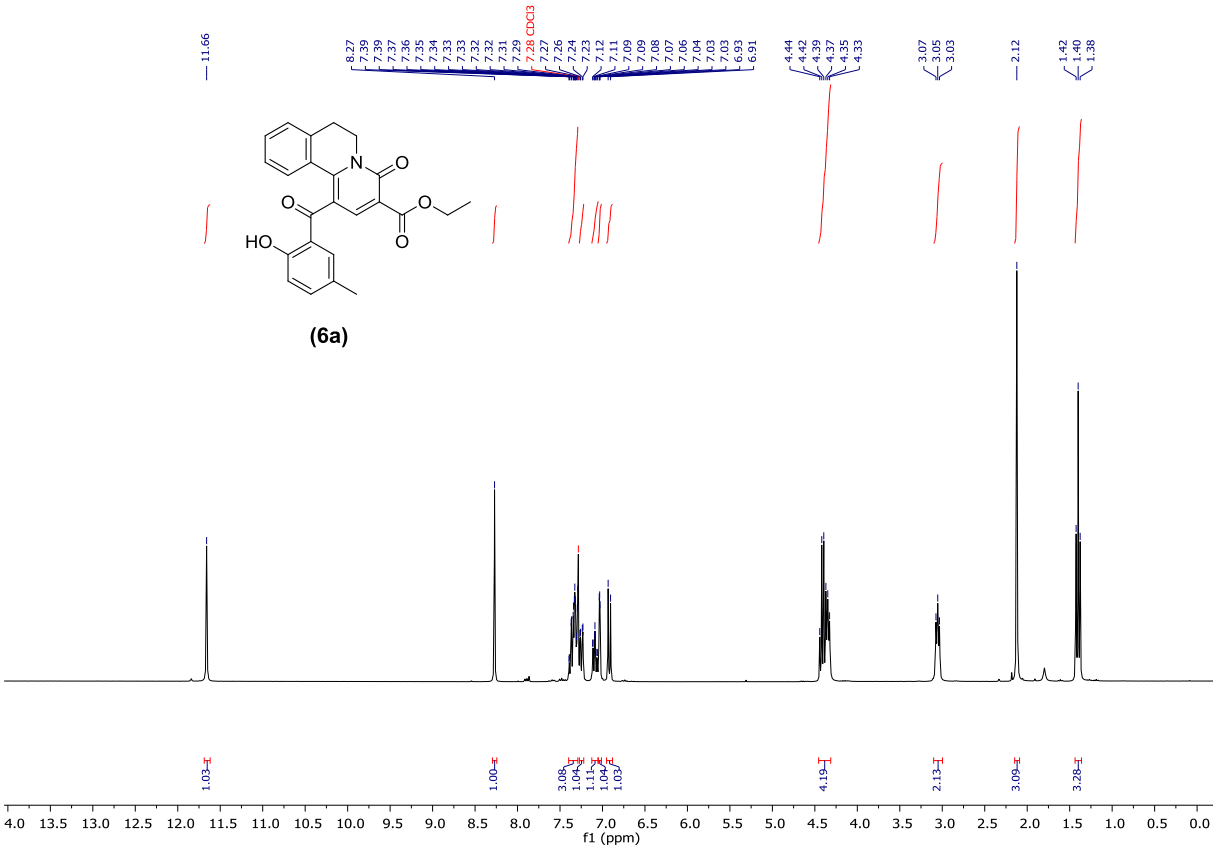
164.46
163.33
158.45
149.24
143.77
137.84
137.01
132.11
132.03
129.97
127.82
127.55
127.10
119.30
119.24
118.63
117.47
114.89
61.44
40.21
28.21
14.33
f1 (ppm)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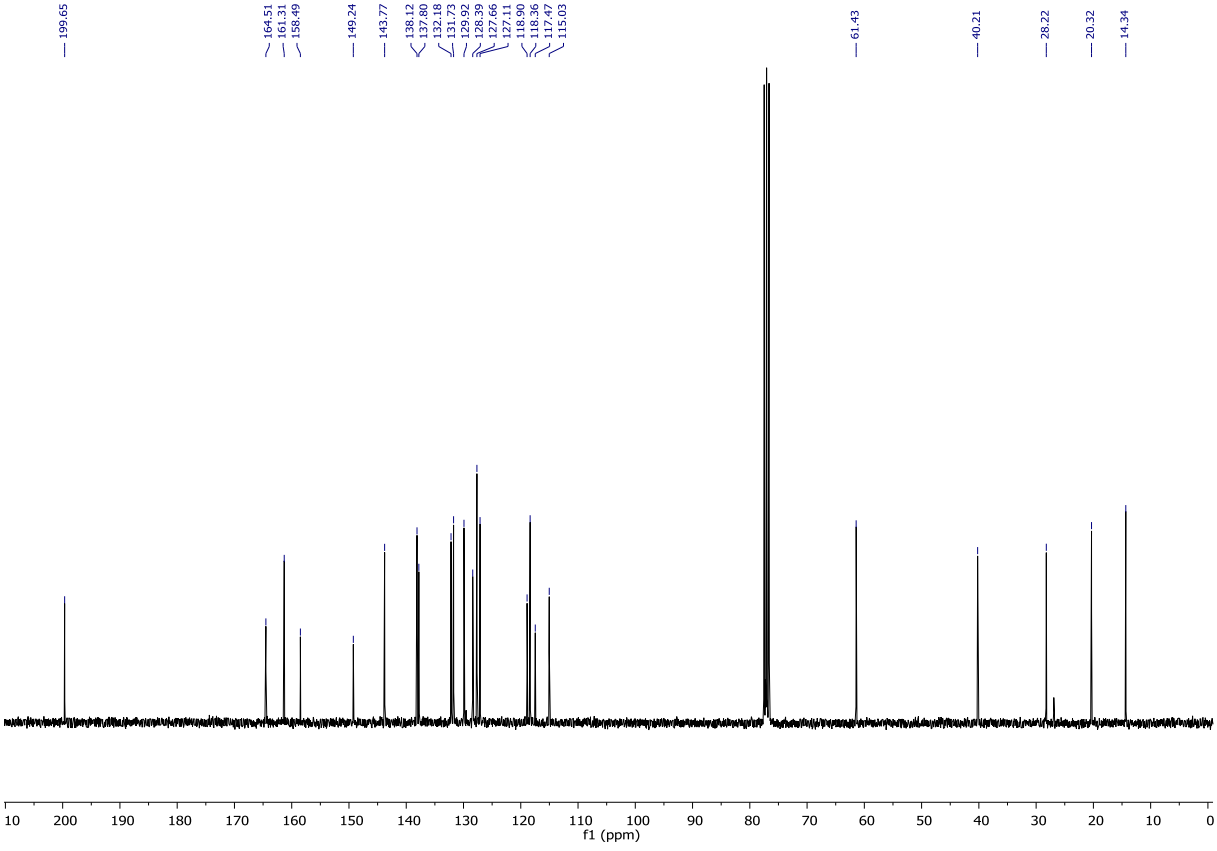
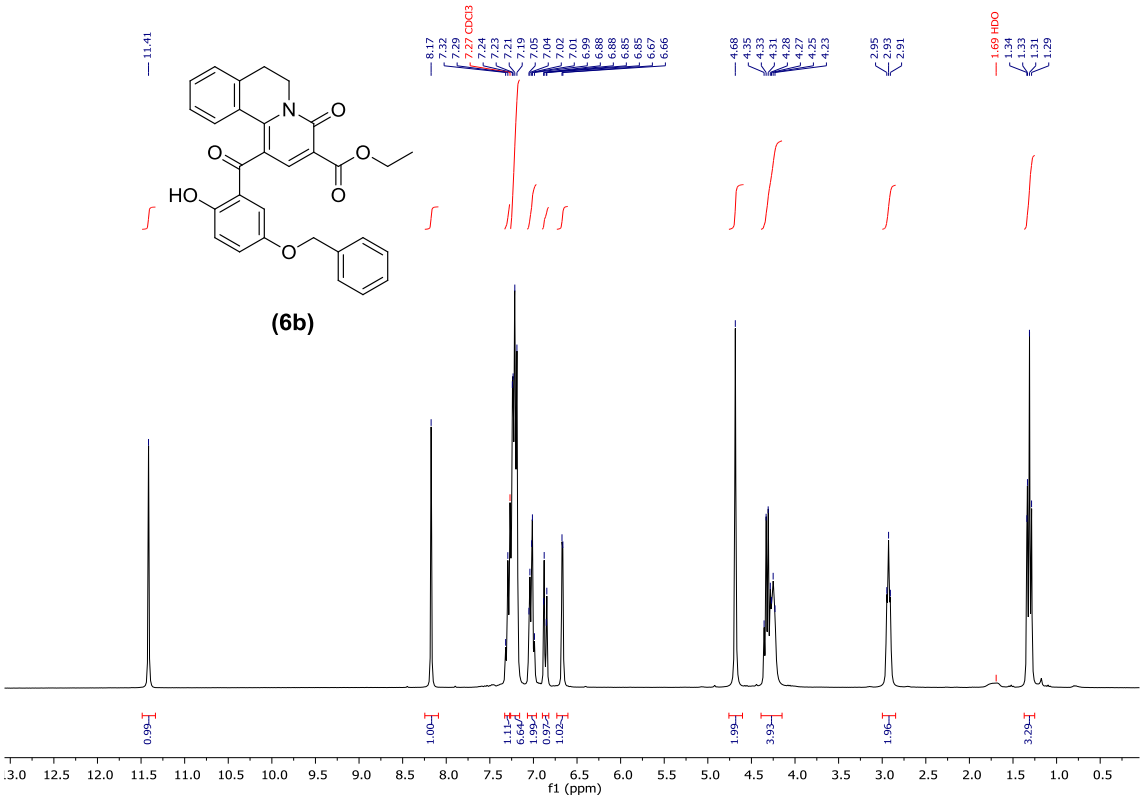
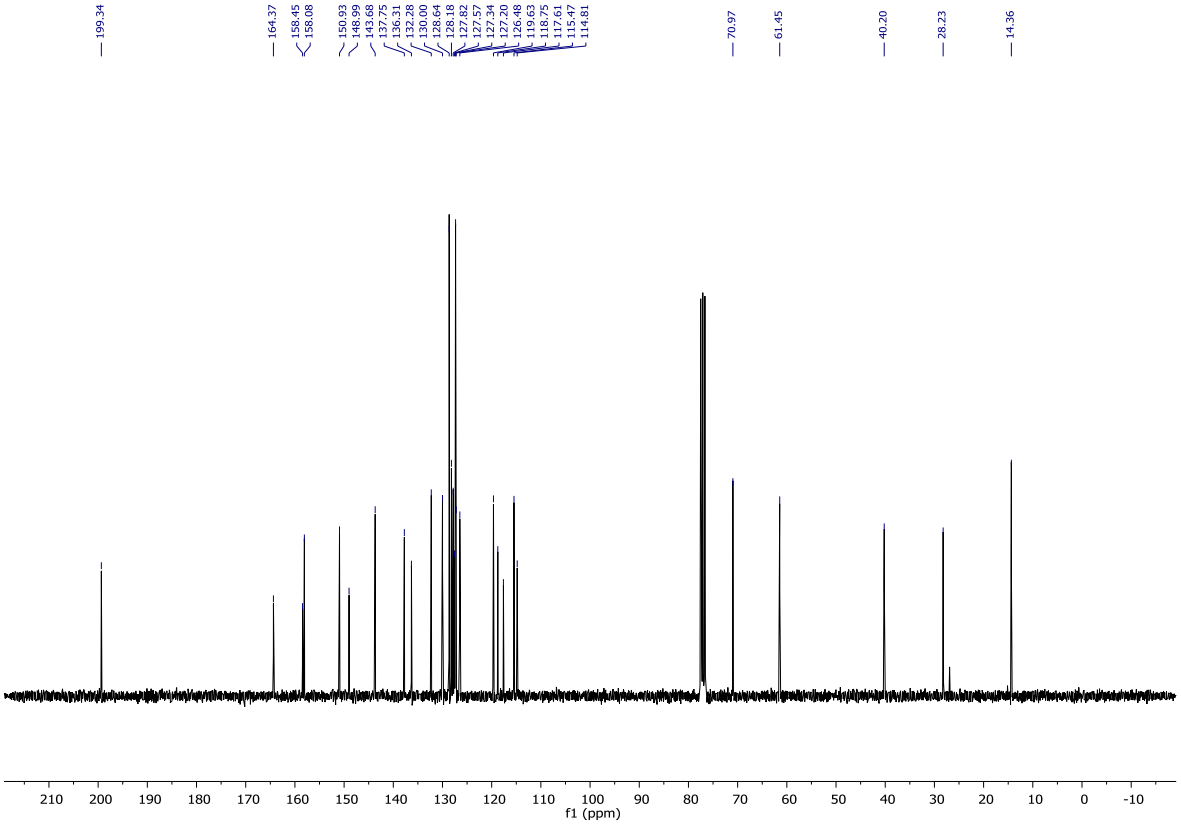
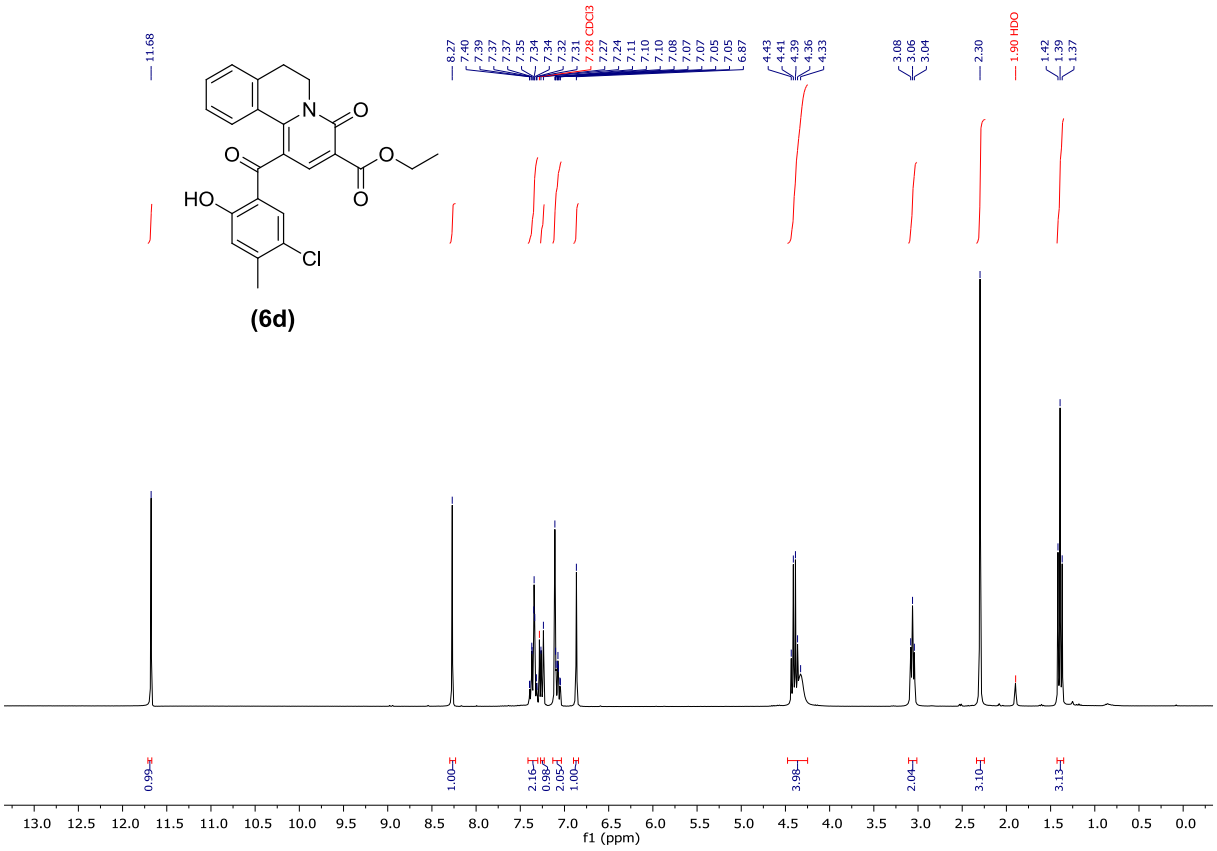
8.27
7.39
7.39
7.37
7.36
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.29
7.26 CDCl3
7.27
7.26
7.24
7.23
7.12
7.11
7.09
7.09
7.08
7.07
7.07
7.06
7.04
7.03
7.03
6.93
6.91
4.44
4.42
4.39
4.37
4.35
4.33
3.07
3.05
3.03
2.12
1.42
1.40
1.38
N
O
O
O
O
HO
1.03
1.00
3.08
1.04
1.11
1.04
1.03
4.19
2.13
3.09
3.28
4.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

(6a)

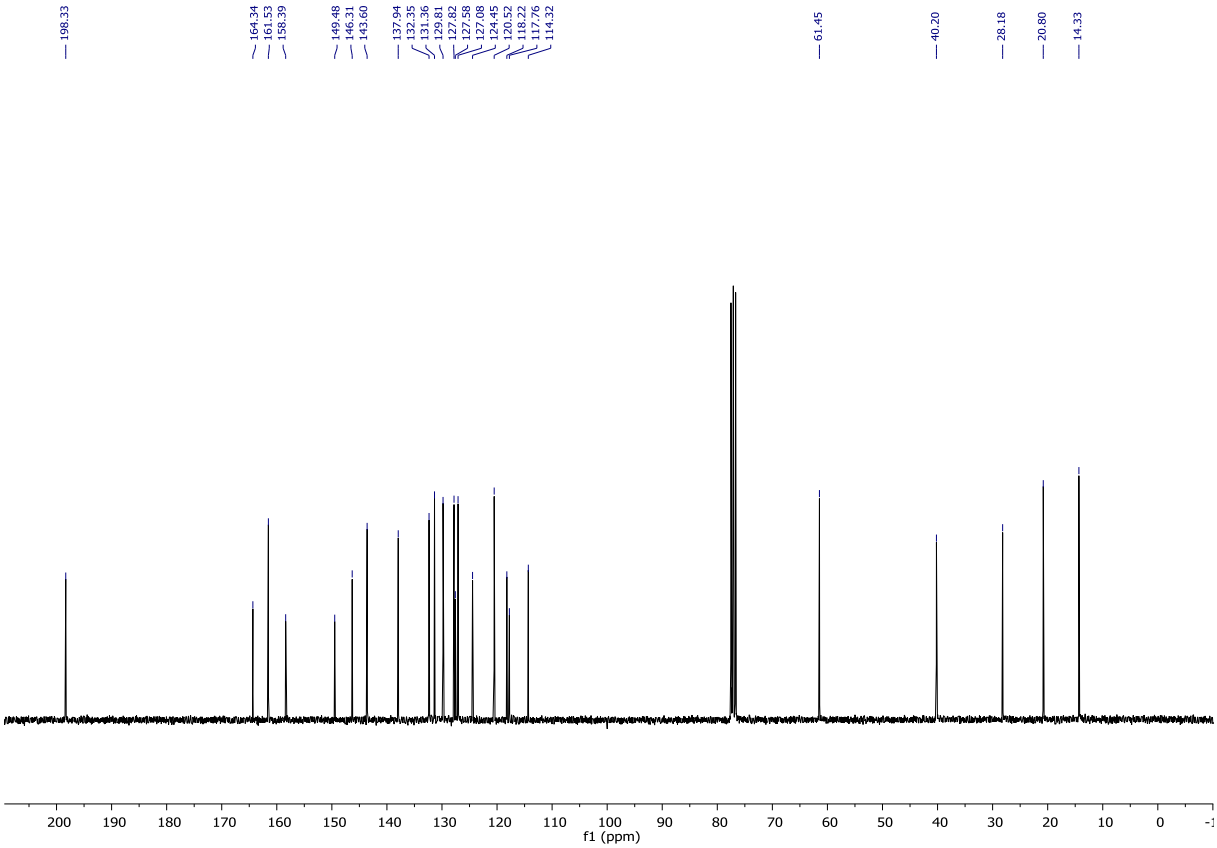

199.65
164.51
161.31
158.49
149.24
143.77
138.12
137.80
132.18
131.73
129.92
128.39
127.66
127.11
118.90
118.36
117.47
115.03
61.43
40.21
28.22
20.32
14.34
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


11.41
8.17
7.32
7.29
7.27 CDCl3
7.24
7.23
7.21
7.19
7.05
7.04
7.02
7.01
6.99
6.88
6.88
6.85
6.85
6.67
6.66
4.68
4.35
4.33
4.31
4.28
4.27
4.25
4.23
2.95
2.93
2.91
1.69 HDO
1.34
1.33
1.31
1.29
HO
O
N
O
O
O
O
(6b)
0.99
1.00
1.14
6.64
1.99
0.97
1.02
1.99
3.93
1.96
3.29
f1 (ppm)


199.34
164.37
158.45
158.08
150.93
148.99
143.68
137.75
136.31
132.28
130.00
128.64
128.18
127.82
127.57
127.34
127.20
126.48
119.63
118.75
117.61
115.47
114.81
70.97
61.45
40.20
28.23
14.36
f1 (ppm)


11.68
8.27
7.40
7.39
7.37
7.37
7.35
7.34
7.34
7.32
7.31
7.28 CDCl3
7.27
7.24
7.11
7.10
7.10
7.08
7.07
7.07
7.05
7.05
6.87
4.43
4.41
4.39
4.36
4.33
3.08
3.06
3.04
2.30
1.90 HDO
1.42
1.39
1.37
HO
Cl
O
N
O
O
O
0.99
1.00
2.16
0.98
2.05
1.00
3.98
2.04
3.10
3.13
f1 (ppm)

(6d)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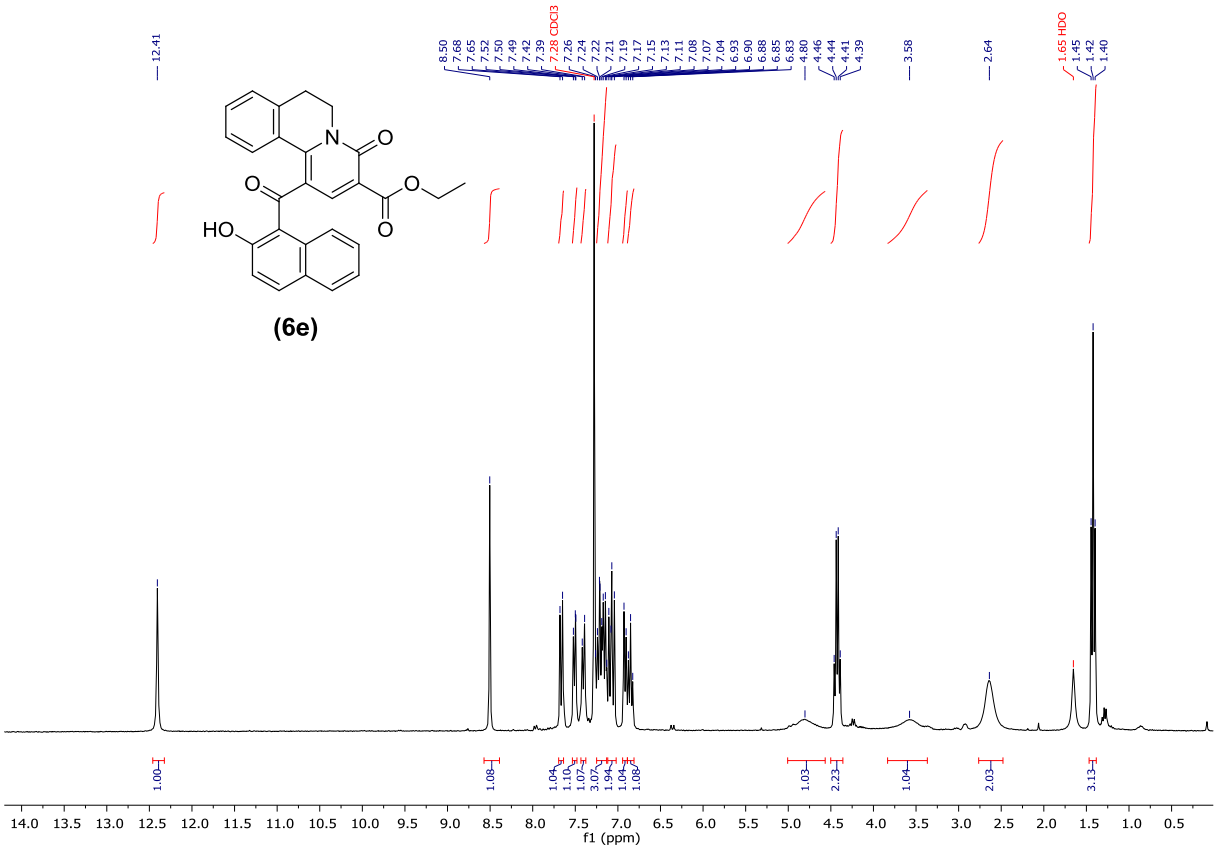
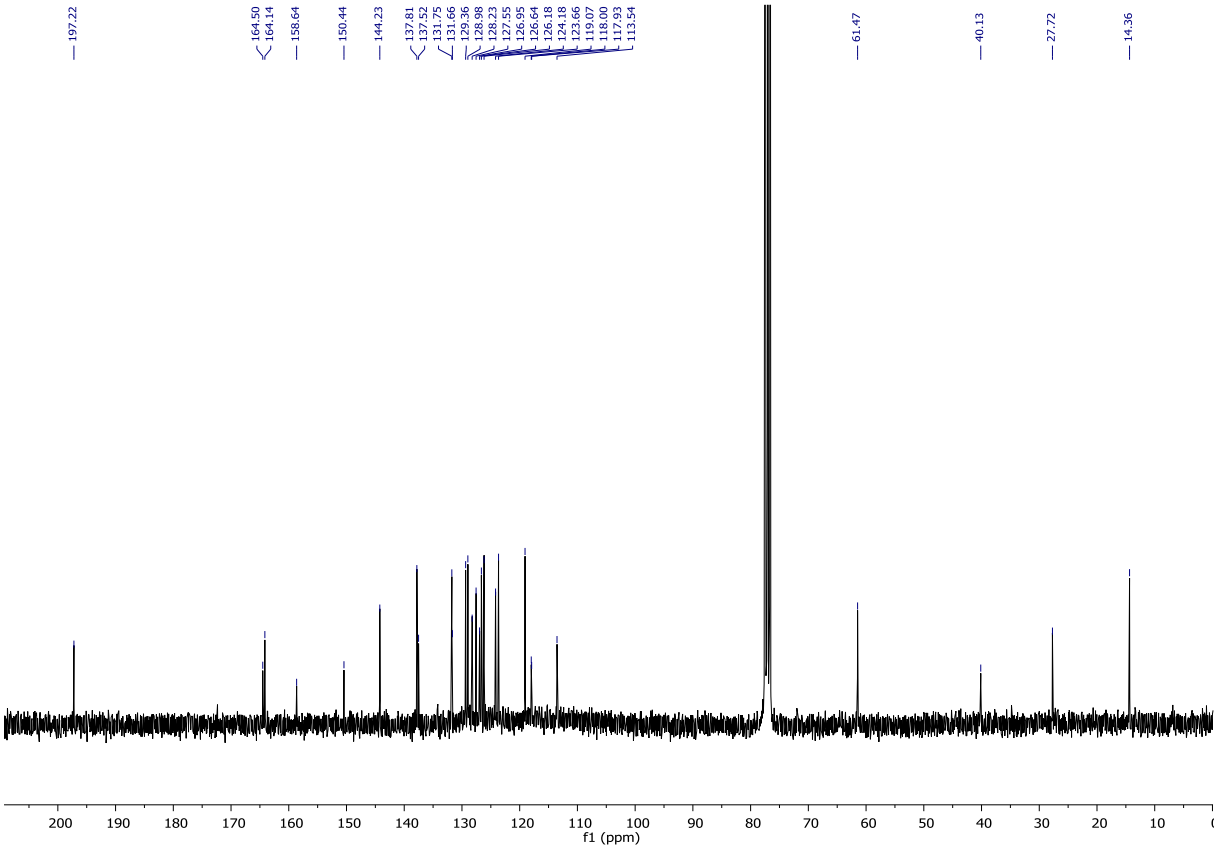
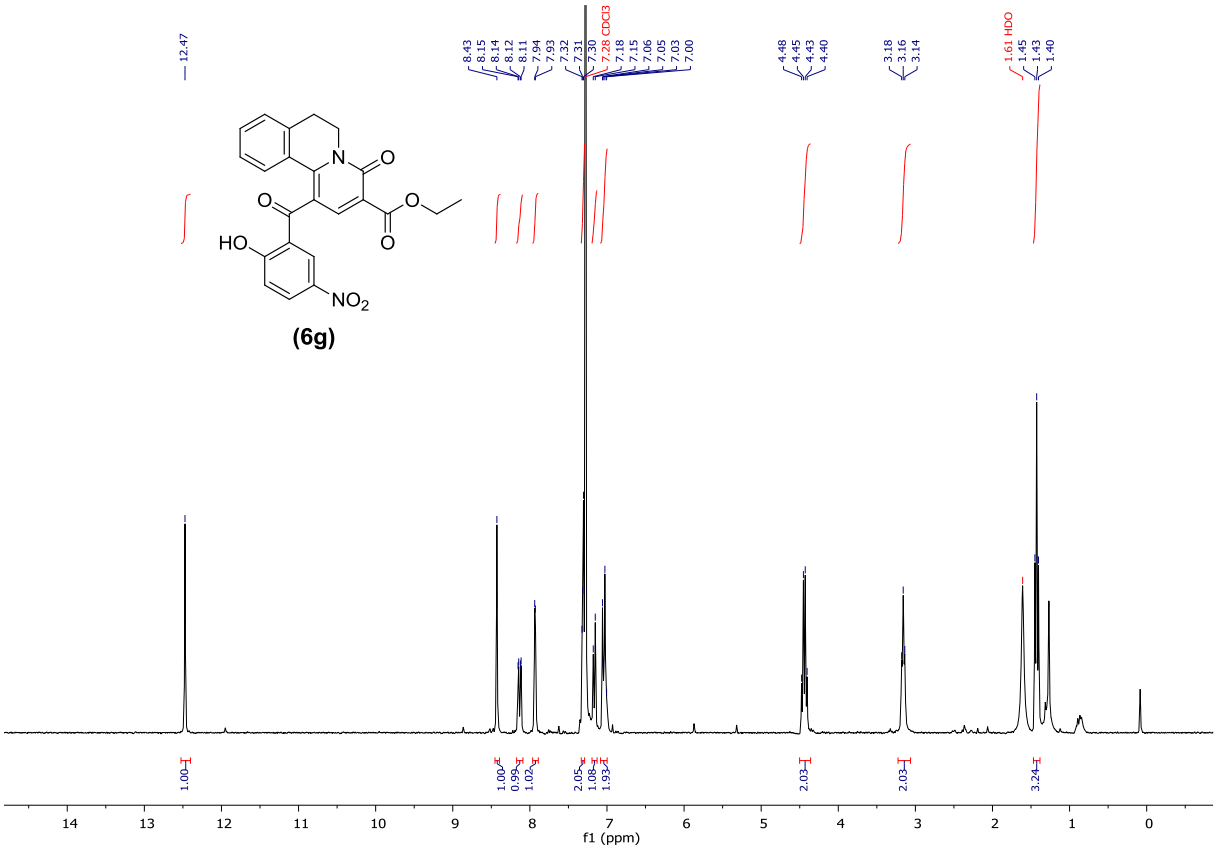
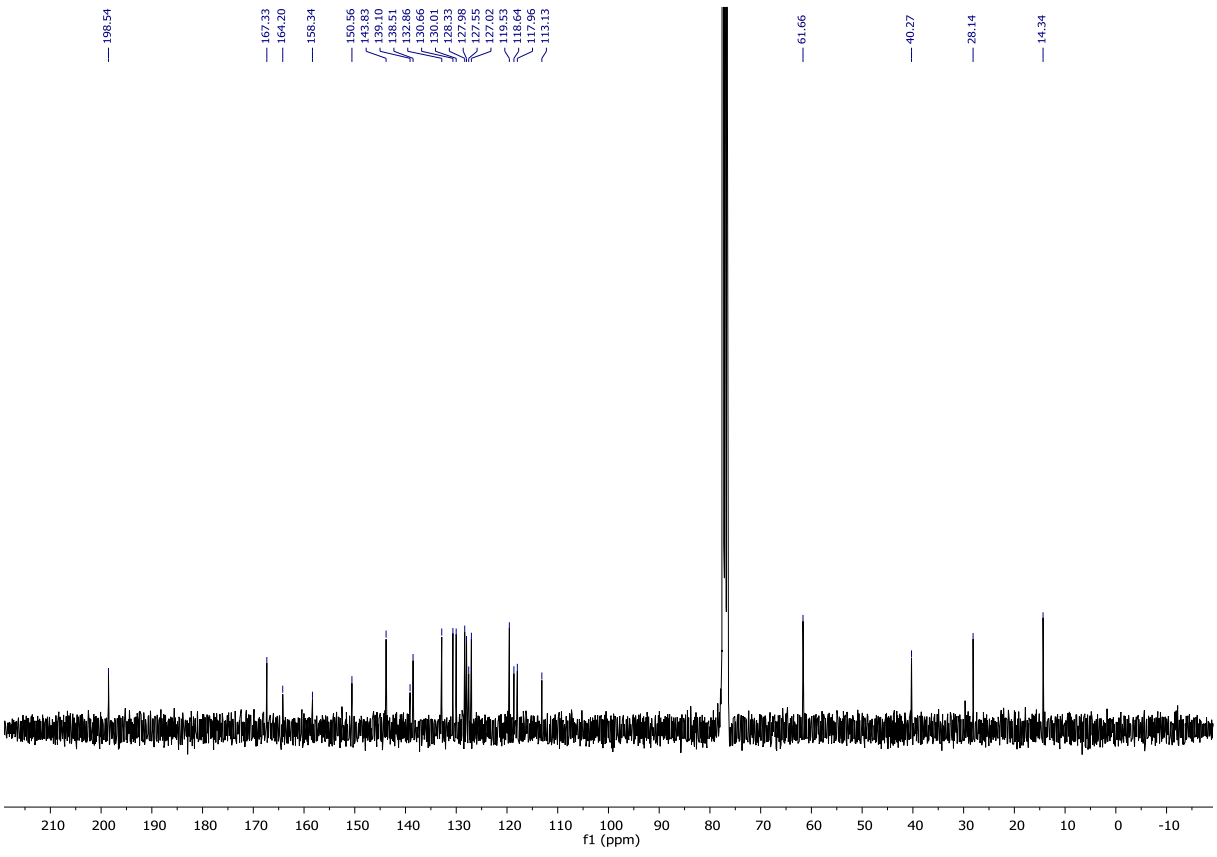
158.39
149.48
146.31
143.60
137.94
132.35
131.36
129.81
127.82
127.58
127.08
124.45
120.52
118.22
117.76
114.32
61.45
40.20
28.18
20.80
14.33
f1 (ppm)


(6e)
f1 (ppm)


f1 (ppm)


12.47
8.43
8.15
8.14
8.12
8.11
7.94
7.93
7.32
7.31
7.30
7.28 CDCl3
7.18
7.15
7.06
7.05
7.03
7.00
4.48
4.45
4.43
4.40
3.18
3.16
3.14
1.61 HDO
1.45
1.43
1.40
1.00
0.99
1.02
2.05
1.08
1.93
2.03
2.03
3.24
f1 (ppm)

(6g)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167.33
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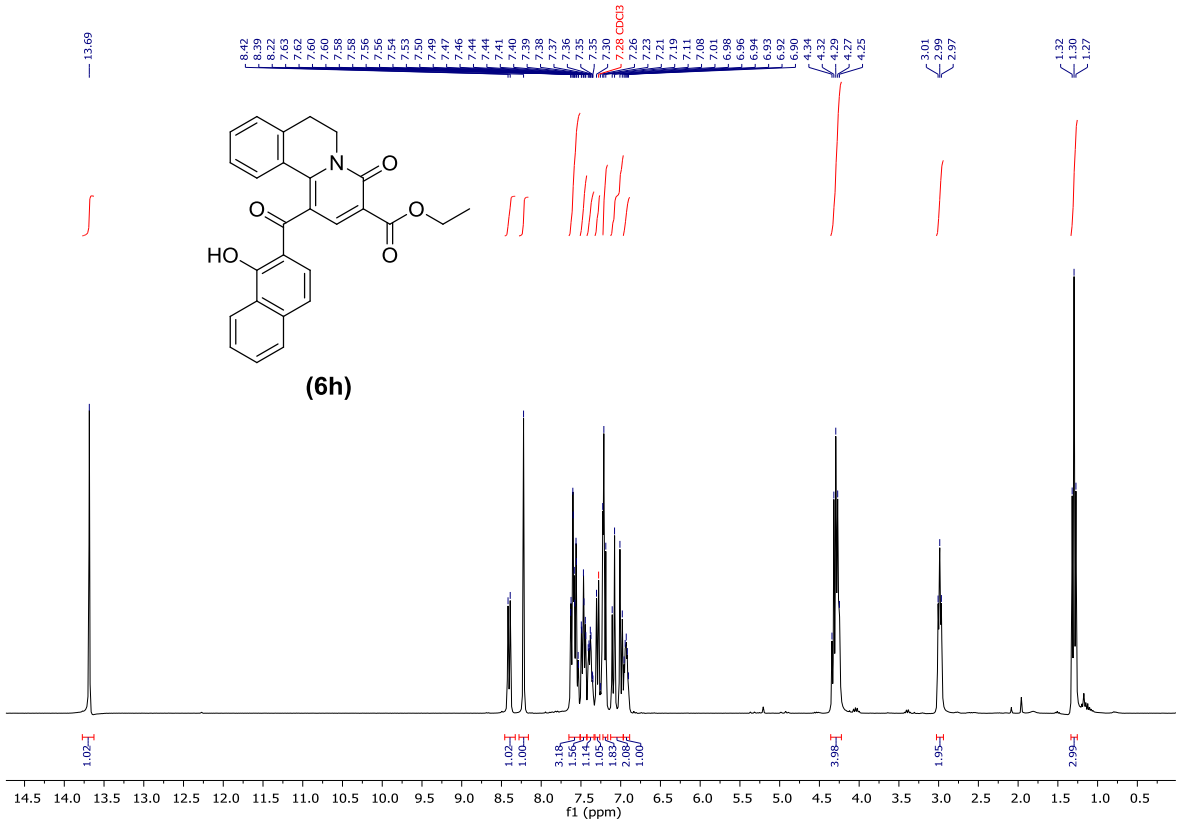
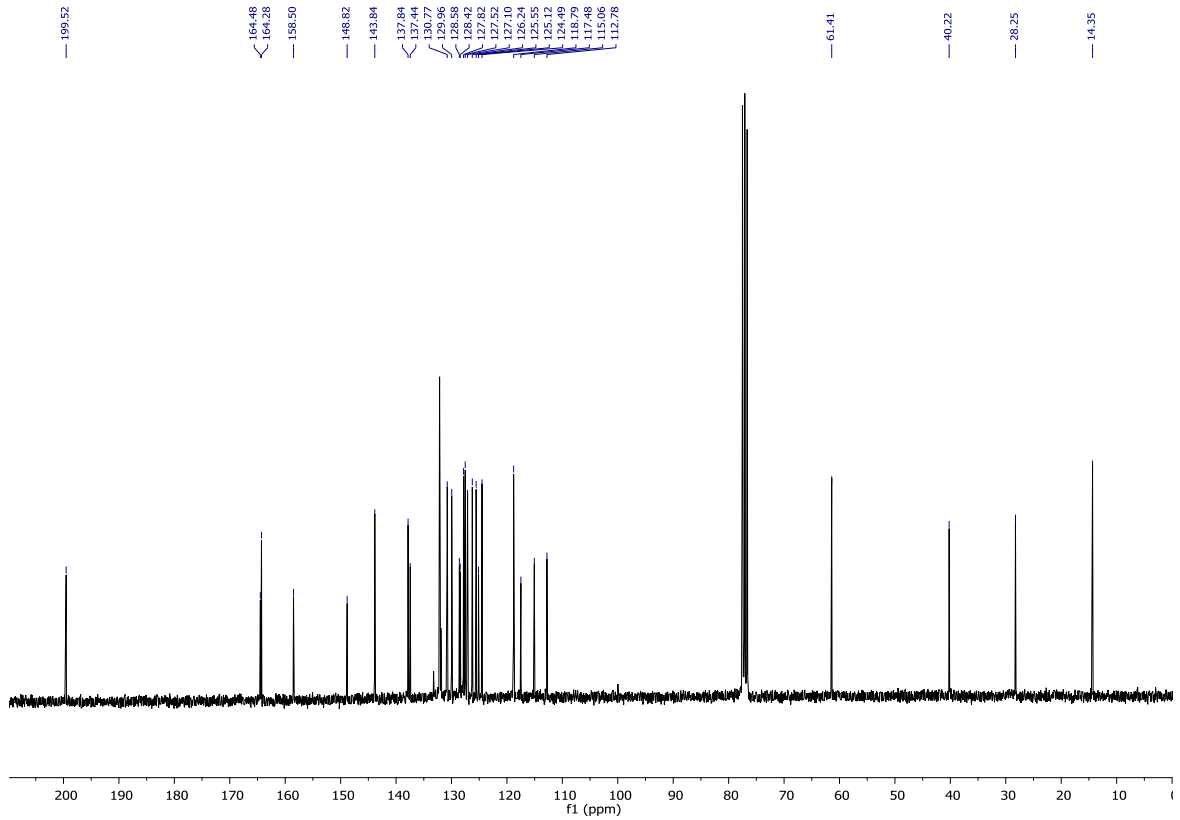
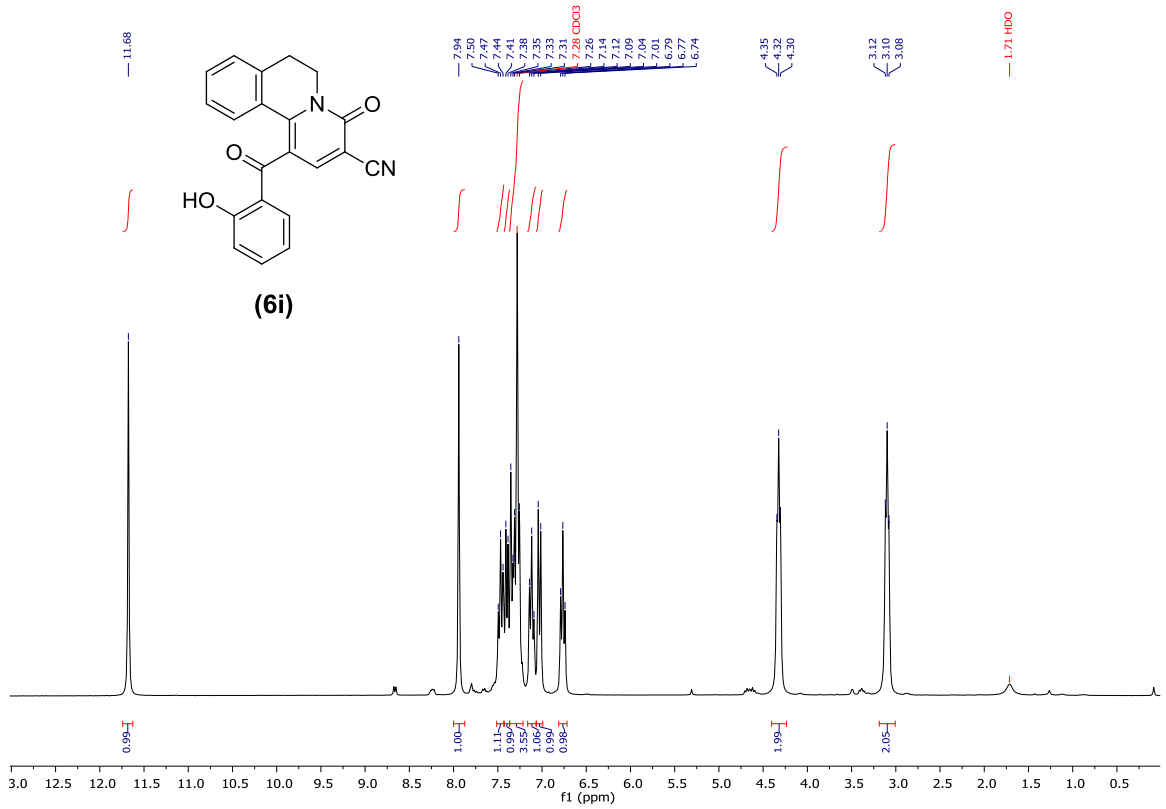
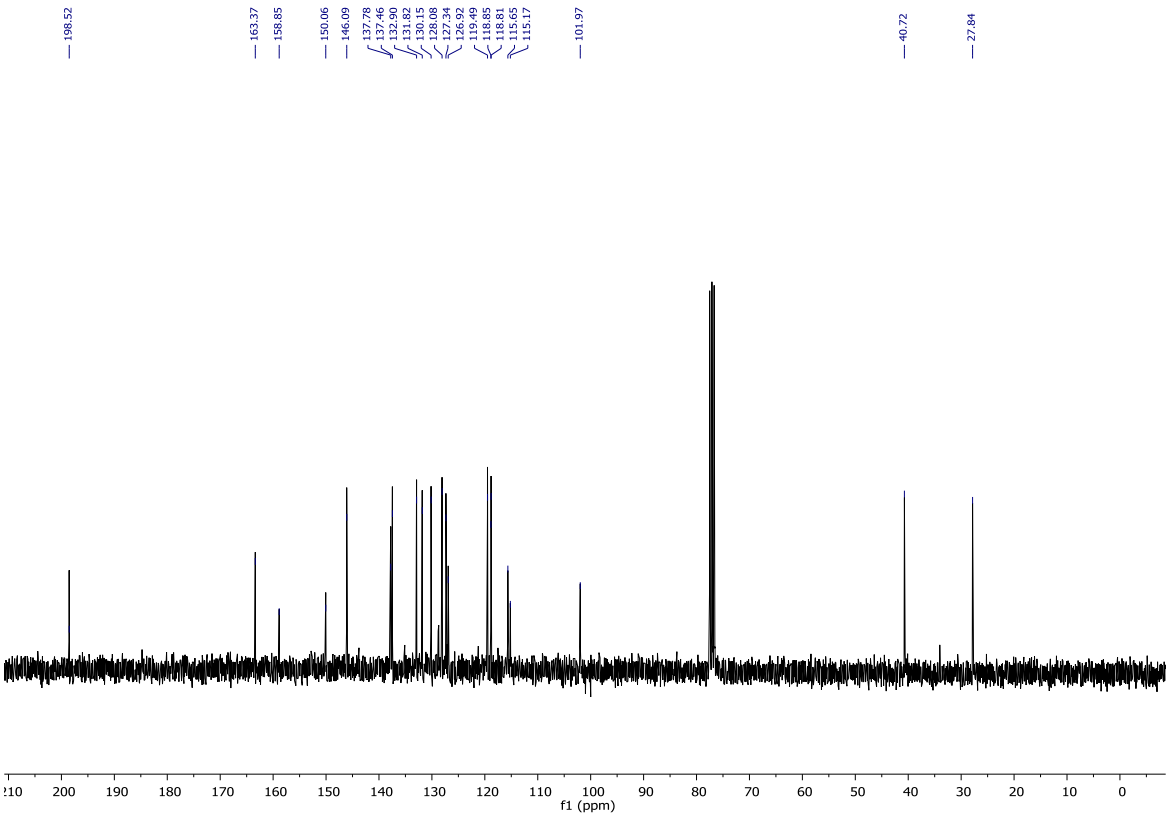
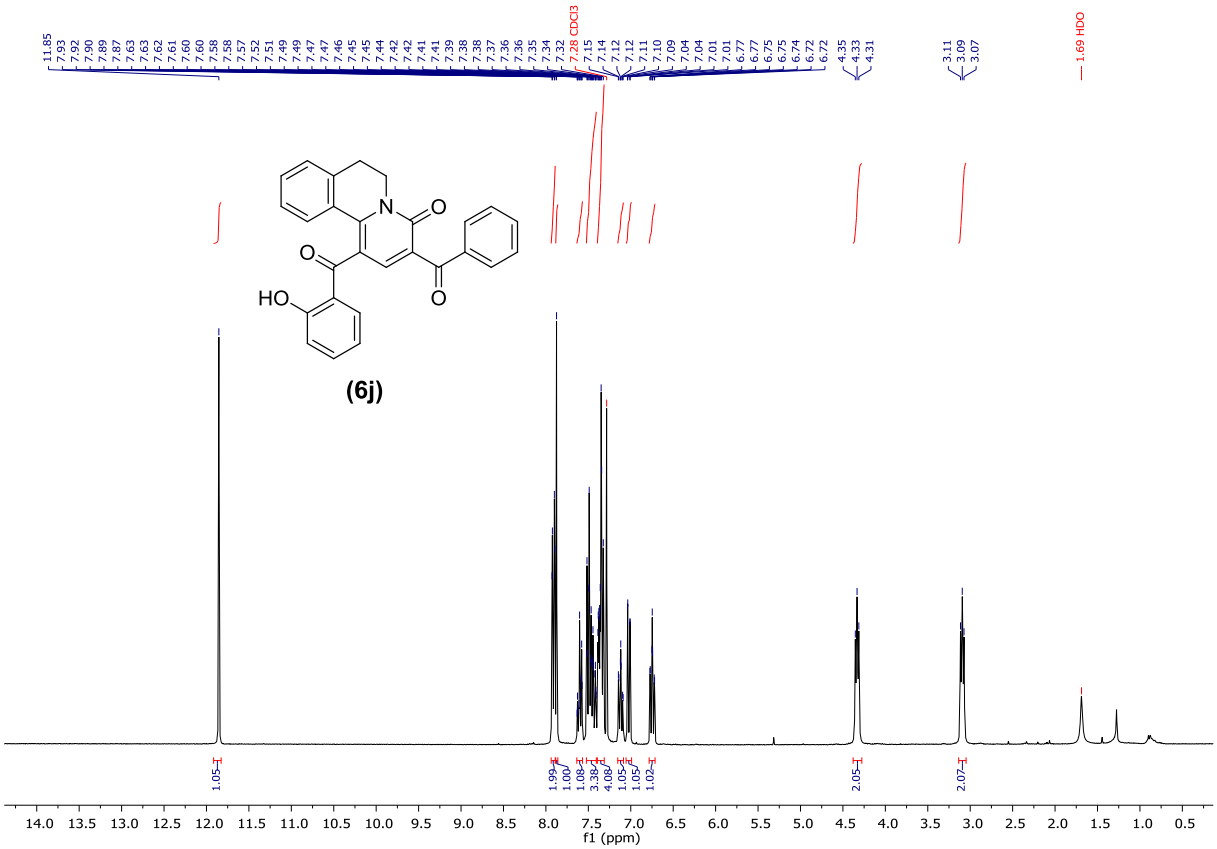
143.83
139.10
138.51
132.86
130.66
130.01
128.33
127.98
127.55
127.02
119.53
118.64
117.96
113.13
61.66
40.27
28.14
14.34
f1 (ppm)


HO
N
O
O
O
O
(6h)
f1 (ppm)


f1 (ppm)


11.68
7.94
7.50
7.47
7.44
7.41
7.38
7.35
7.33
7.31
7.28 CDCl3
7.26
7.14
7.12
7.09
7.04
7.01
6.79
6.77
6.74
4.35
4.32
4.30
3.12
3.10
3.08
1.71 HDO
O
N
O
O
CN
HO
(6i)
0.99
1.00
1.11
0.99
3.55
1.06
0.99
0.98
1.99
2.05
f1 (ppm)


198.52
163.37
158.85
150.06
146.09
137.78
137.46
132.90
131.82
130.15
128.08
127.34
126.92
119.49
118.85
118.81
115.65
115.17
101.97
40.72
27.84
f1 (ppm)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7.93
7.92
7.90
7.89
7.87
7.63
7.63
7.62
7.61
7.60
7.60
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7.58
7.57
7.52
7.51
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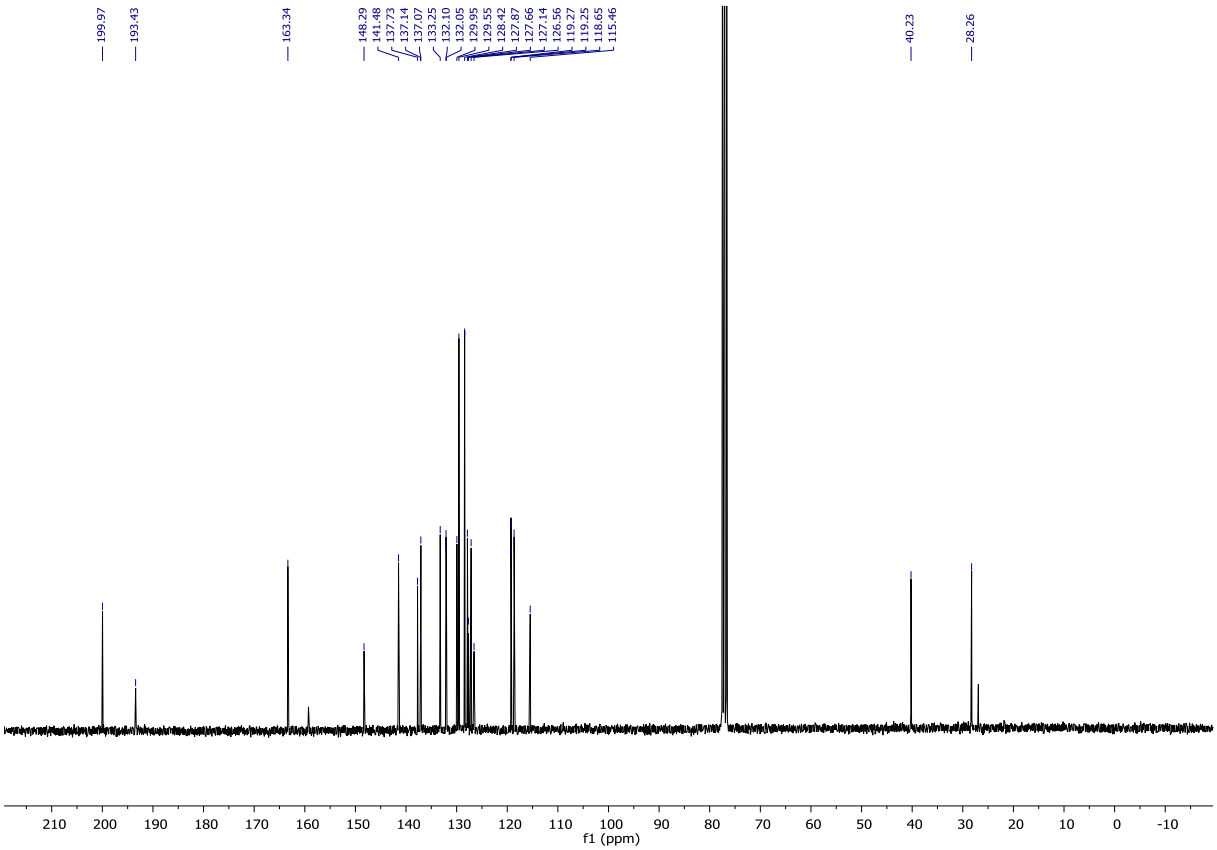
7.49
7.47
7.47
7.46
7.45
7.45
7.44
7.42
7.42
7.41
7.41
7.39
7.38
7.38
7.37
7.36
7.36
7.35
7.34
7.32
7.28 CDCl3
7.15
7.14
7.12
7.12
7.11
7.10
7.09
7.04
7.04
7.01
7.01
6.77
6.77
6.75
6.75
6.74
6.72
6.72
4.35
4.33
4.31
3.11
3.09
3.07
1.69 HDO
N
O
O
O
HO
(6j)
1.05
1.99
1.00
1.08
3.38
4.08
1.05
1.05
1.02
2.05
2.07
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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193.43
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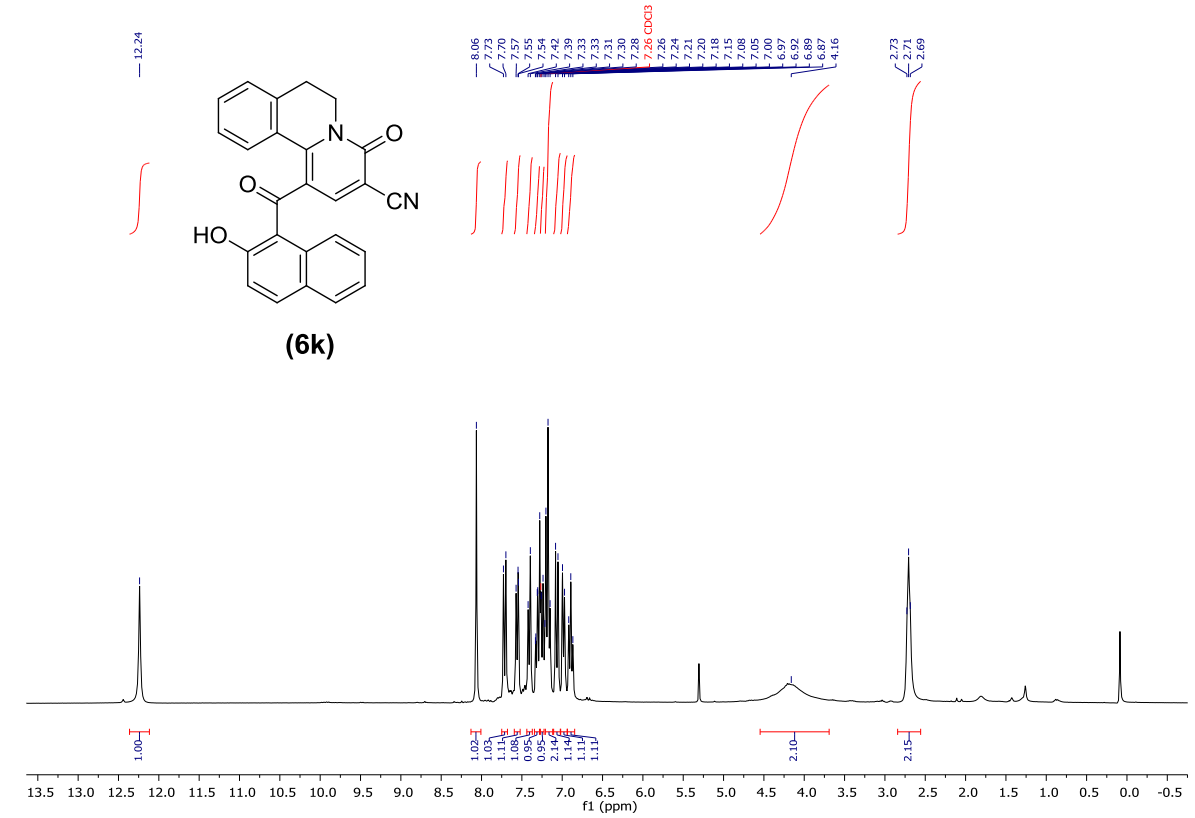
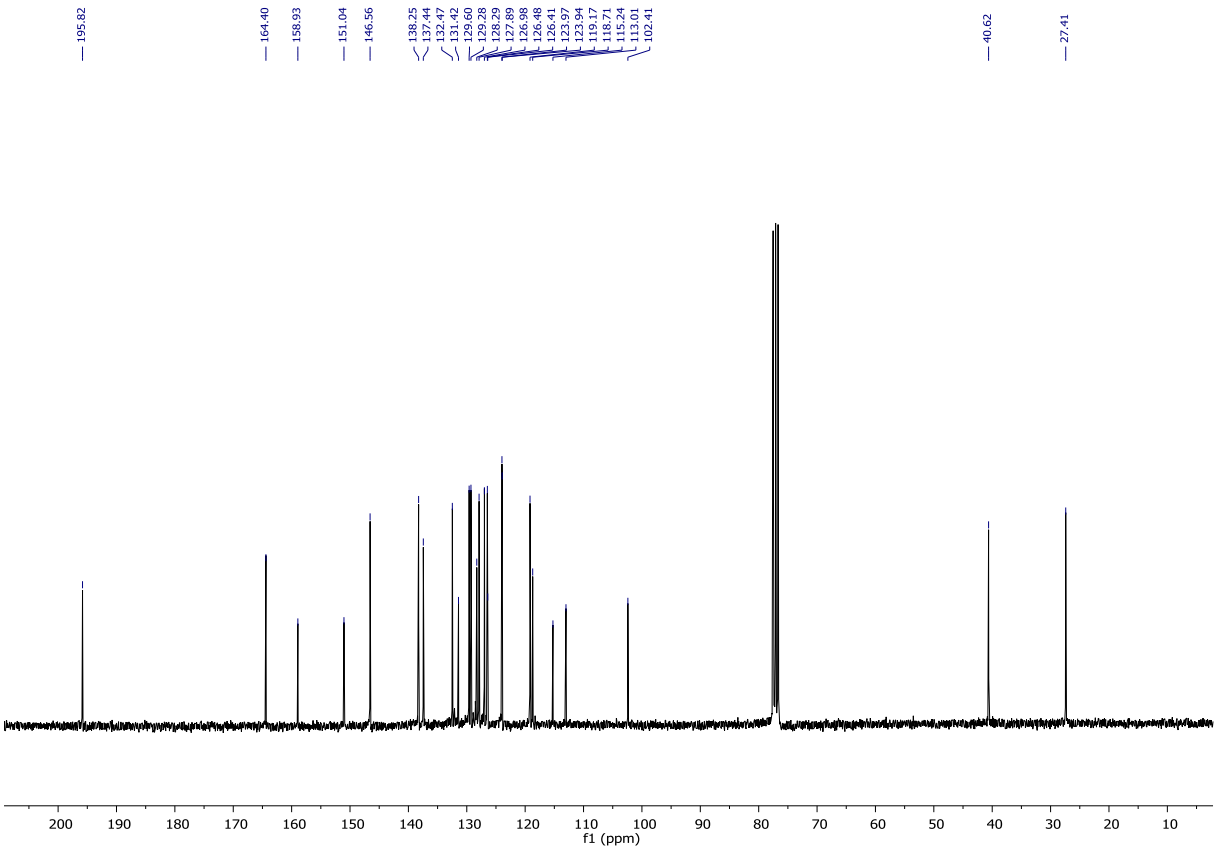
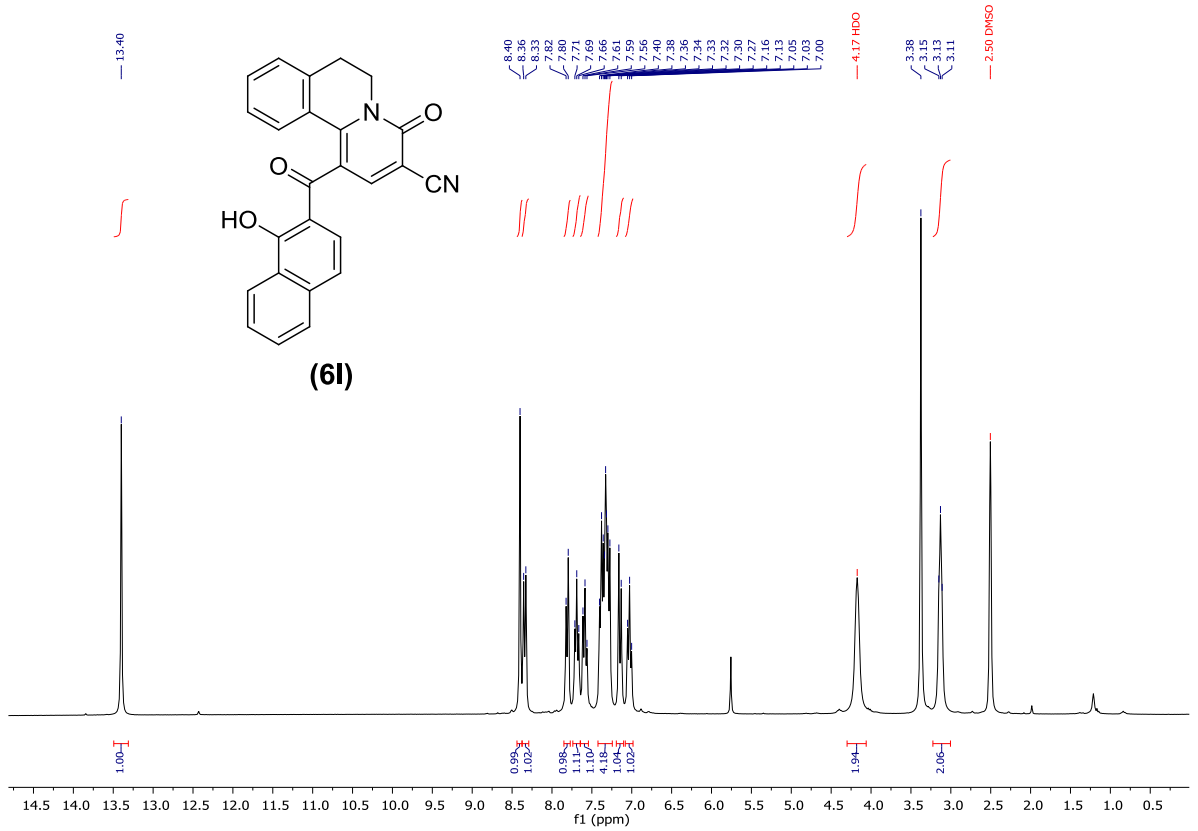
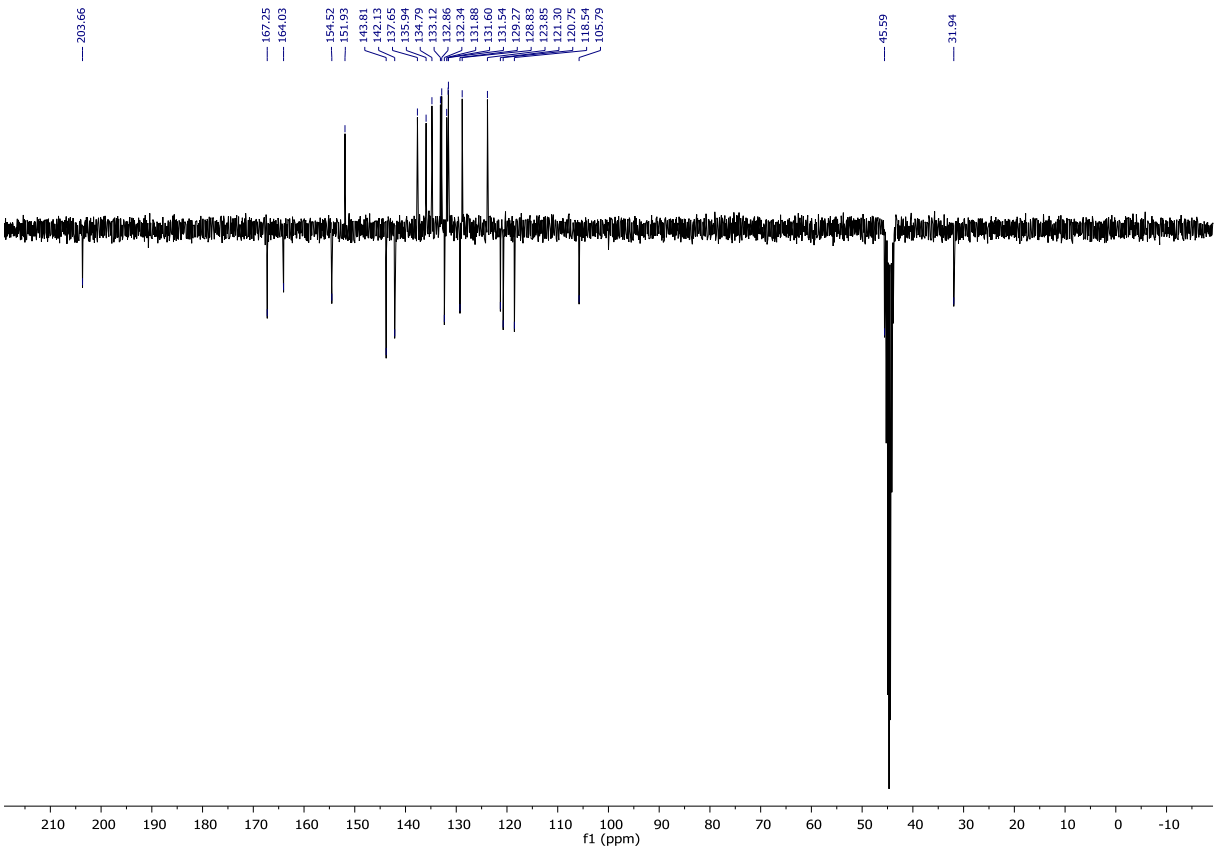
148.29
141.48
137.73
137.14
137.07
133.25
132.10
132.05
129.95
129.55
128.42
127.87
127.66
127.14
126.55
119.27
119.25
118.65
115.46
40.23
28.26
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

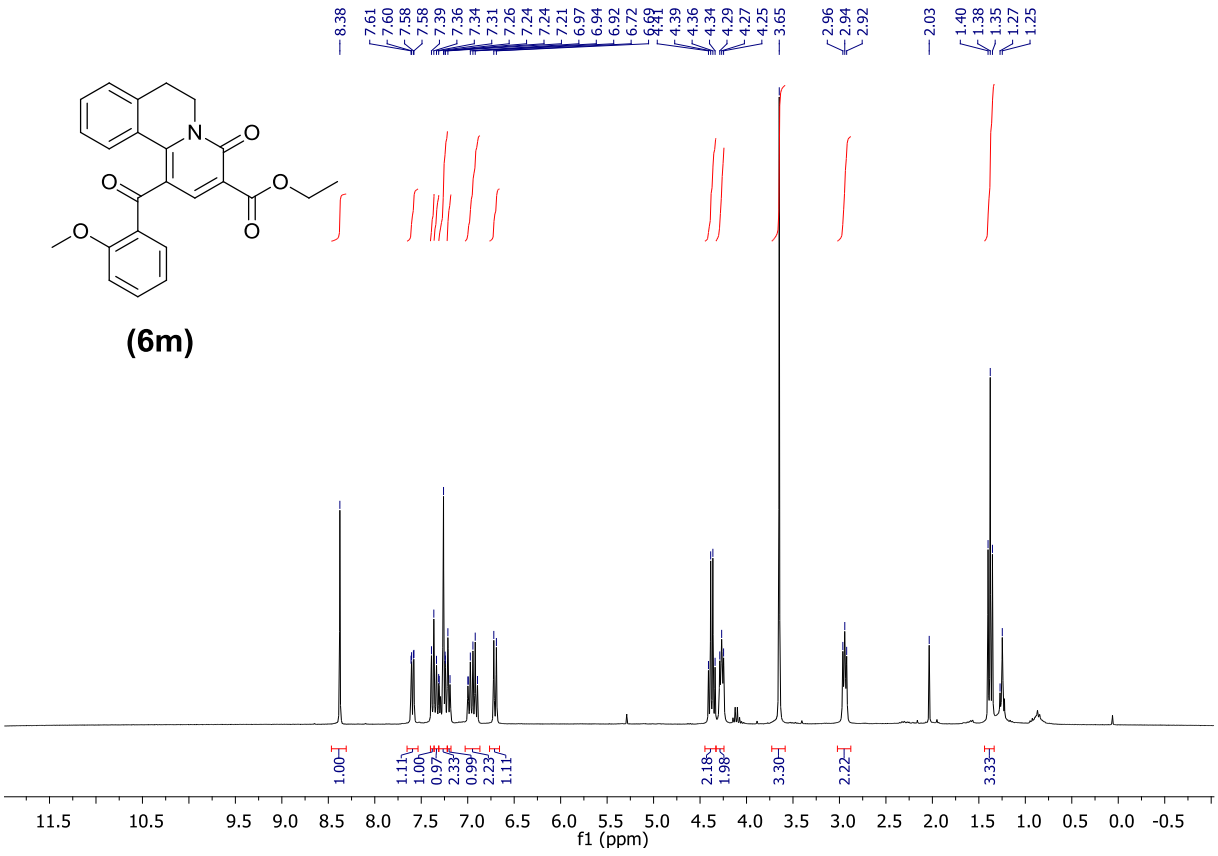

12.24
8.06
7.73
7.70
7.57
7.55
7.54
7.42
7.39
7.33
7.31
7.30
7.28
7.26 CDCl3
7.26
7.24
7.21
7.20
7.18
7.15
7.08
7.05
7.00
6.97
6.92
6.89
6.87
4.16
2.73
2.71
2.69
N
O
O
CN
HO
1.00
1.02
1.03
1.11
1.08
0.95
0.95
1.44
1.11
1.11
2.10
2.15
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

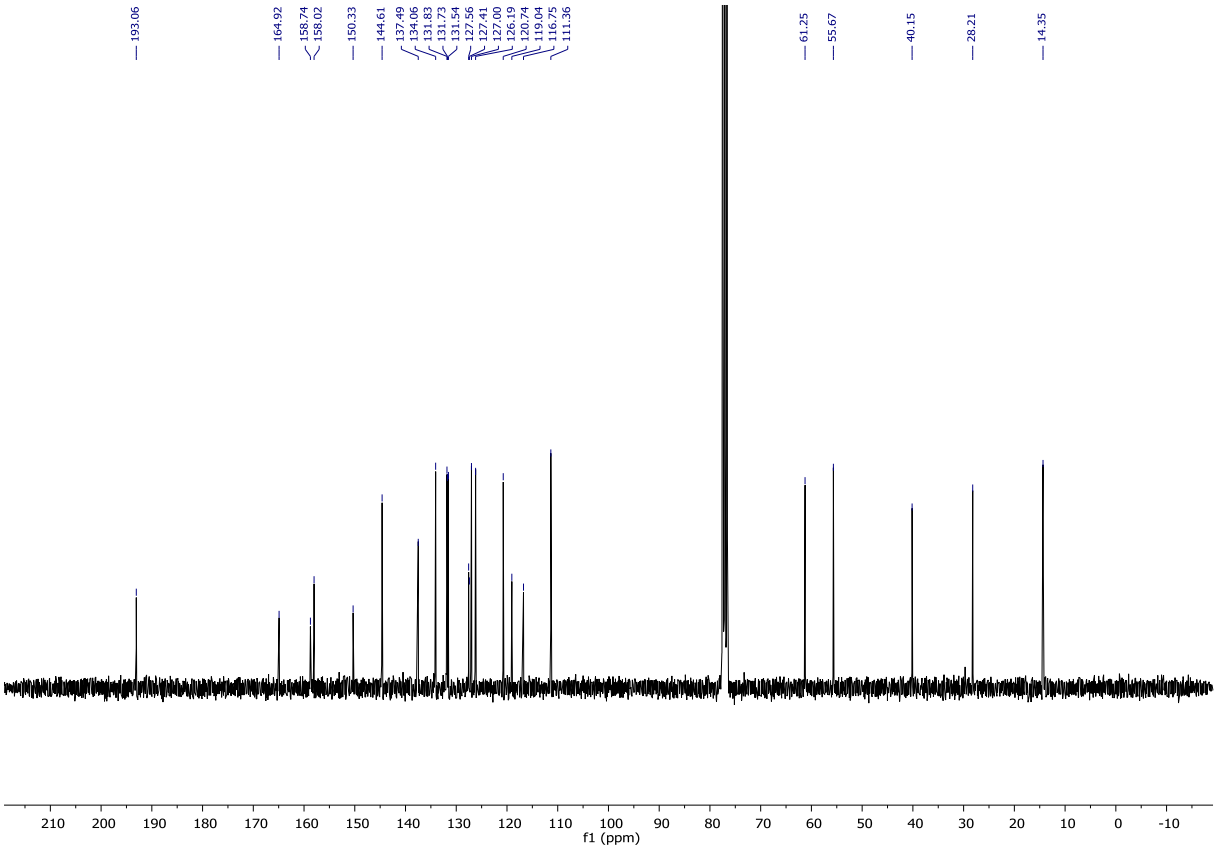
(6k)

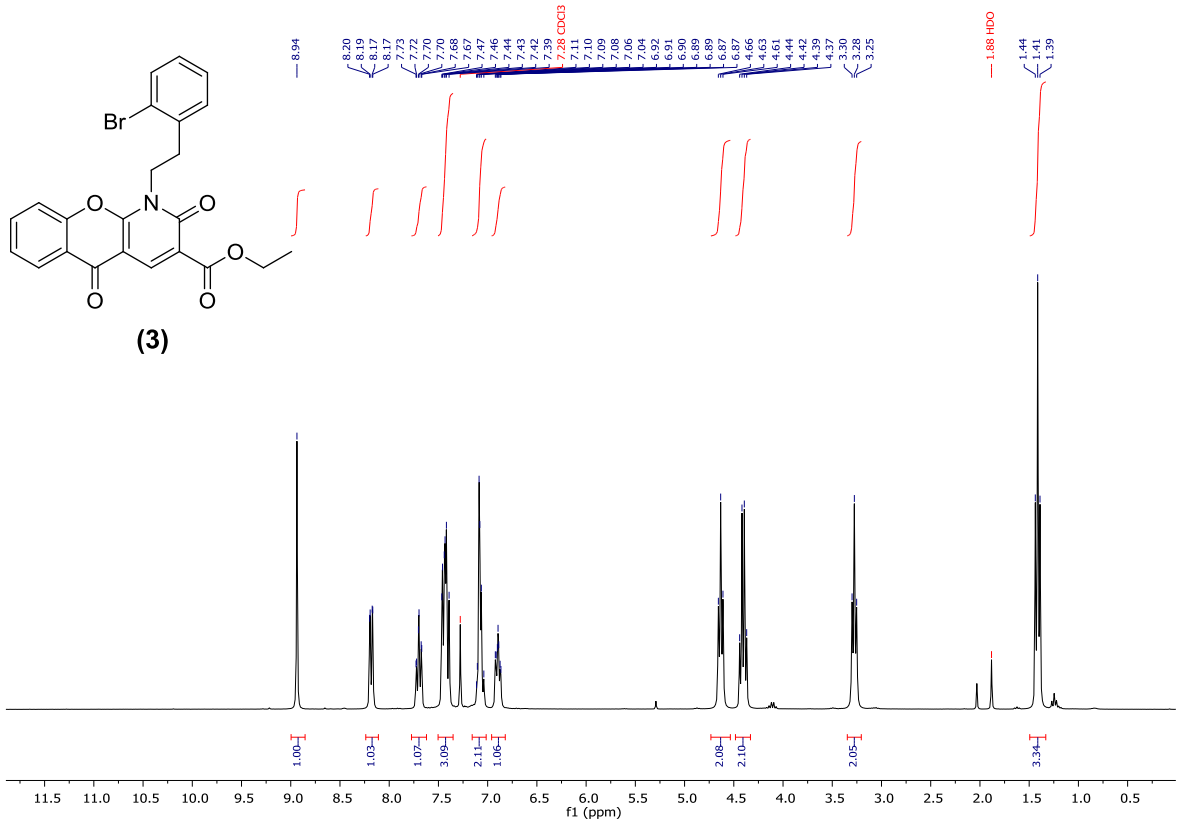

195.82
164.40
158.93
151.04
146.56
138.25
137.44
132.47
131.42
129.60
129.28
128.29
127.89
126.98
126.48
126.41
123.97
123.94
119.17
118.71
115.24
113.01
102.41
40.62
27.41
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

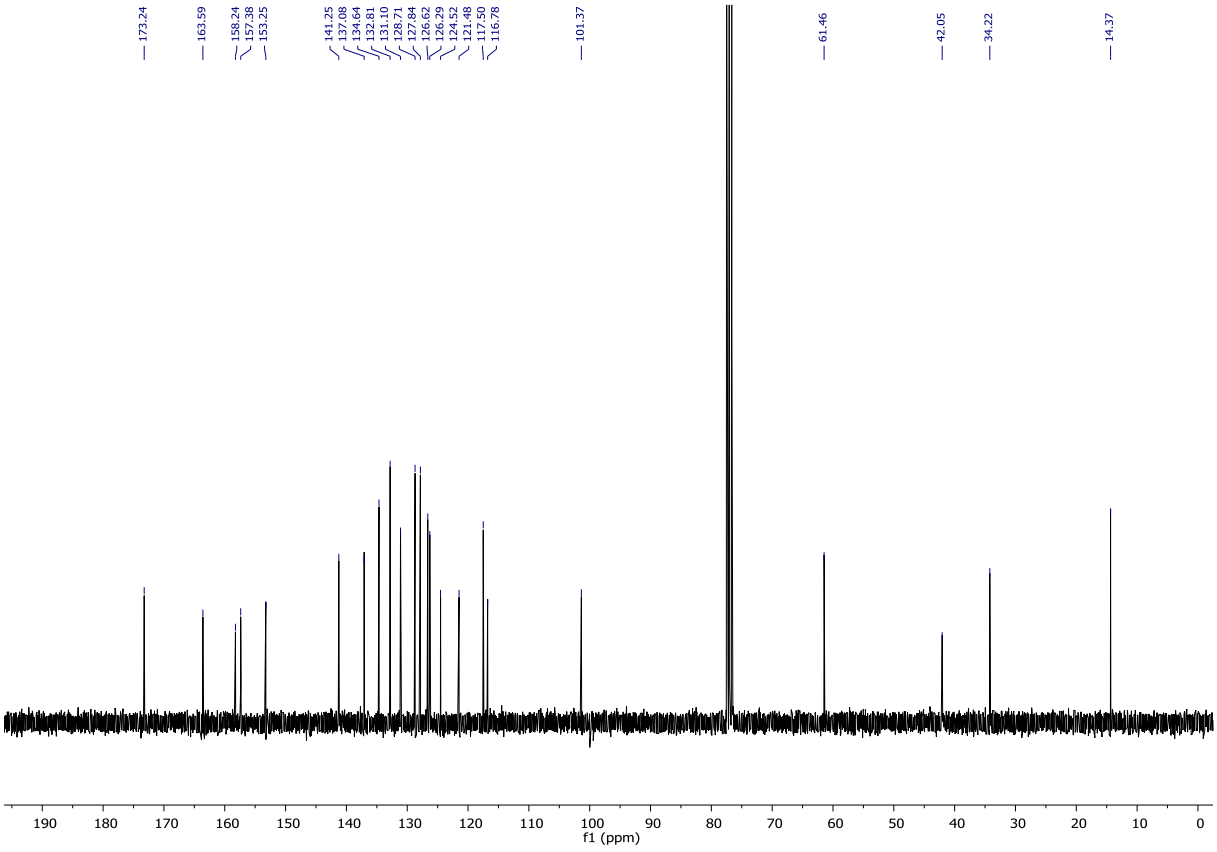

13.40
8.40
8.36
8.33
7.82
7.80
7.71
7.69
7.66
7.61
7.59
7.56
7.40
7.38
7.36
7.34
7.33
7.32
7.30
7.27
7.16
7.13
7.05
7.03
7.00
4.17 HDO
3.38
3.15
3.13
3.11
2.50 DMSO
N
O
O
CN
HO
(6l)
1.00
0.99
1.02
0.98
1.11
1.10
4.18
1.04
1.02
1.94
2.06
14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

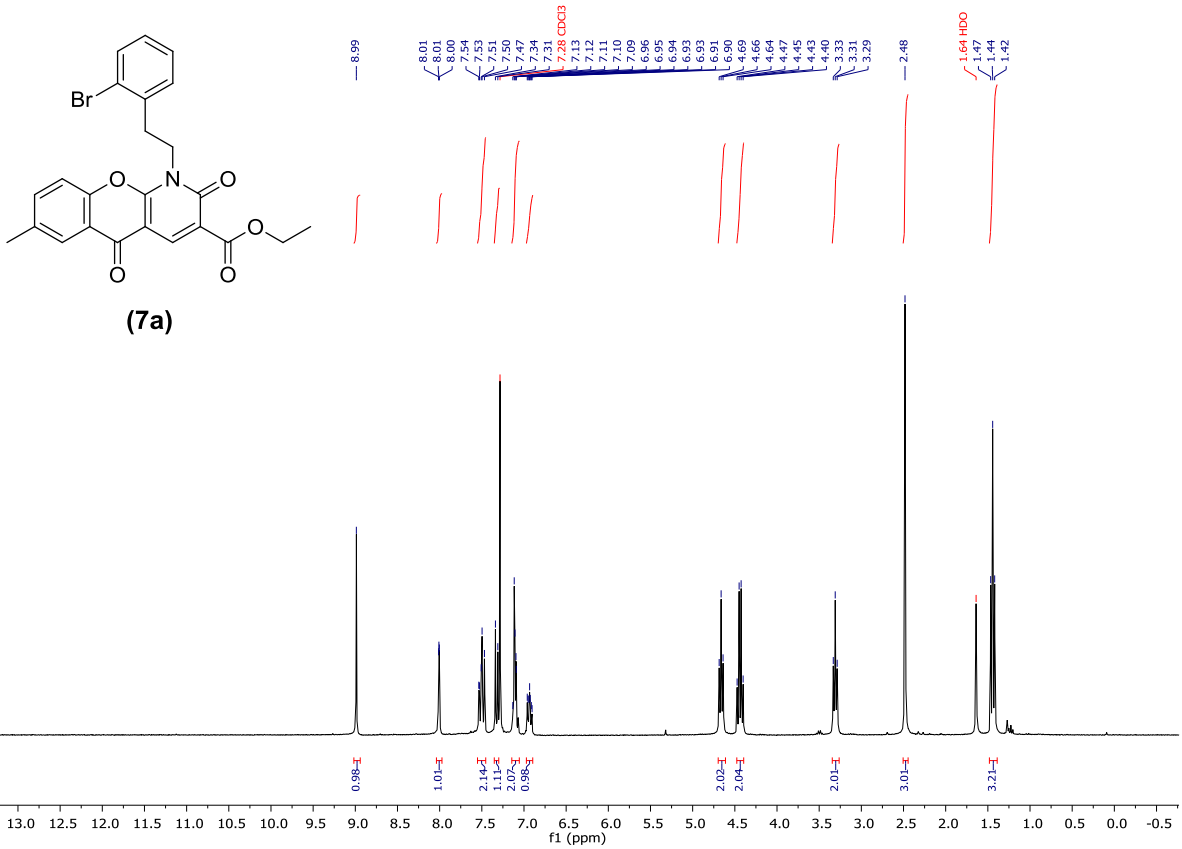

203.66
167.25
164.03
154.52
151.93
143.81
142.13
137.65
135.94
134.79
133.12
132.86
132.34
131.88
131.60
131.54
129.27
128.83
123.85
121.30
120.75
118.54
105.79
45.59
31.94
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

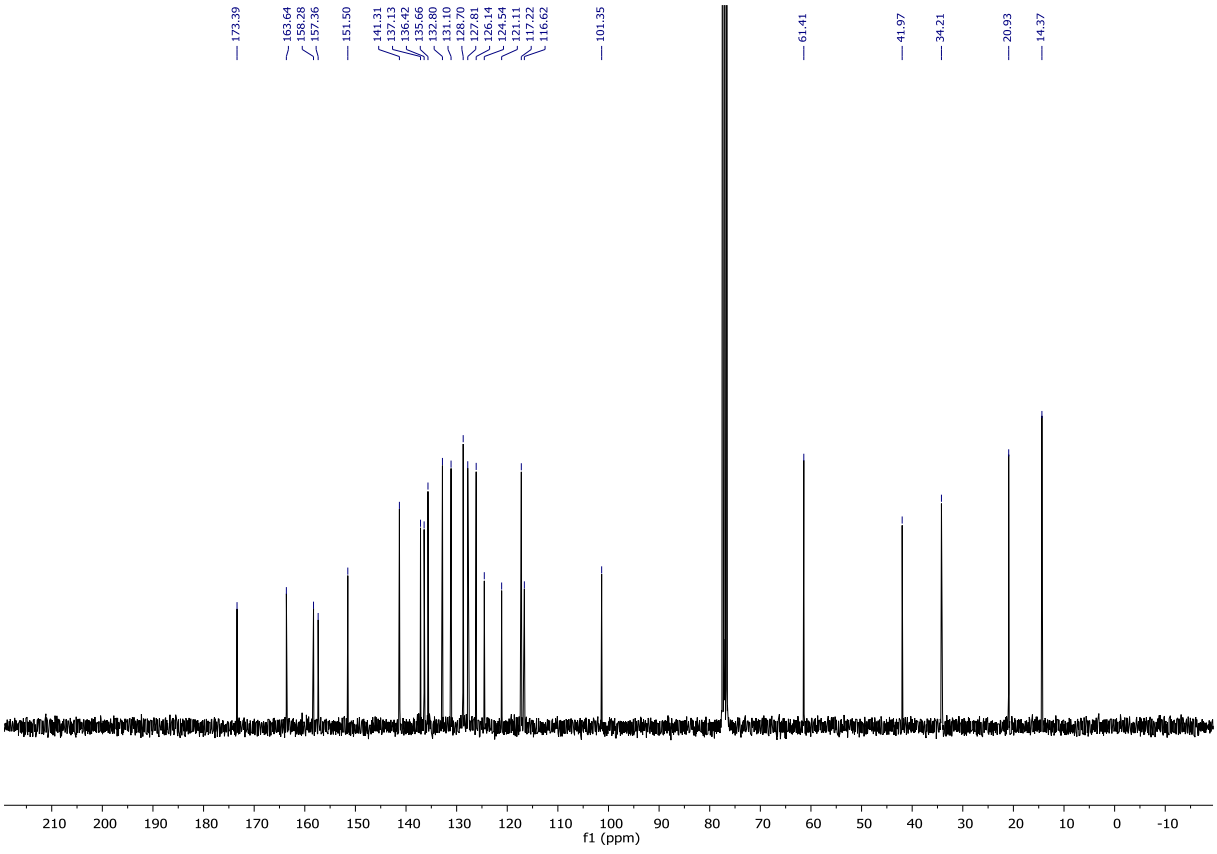

(6m)
f1 (ppm)

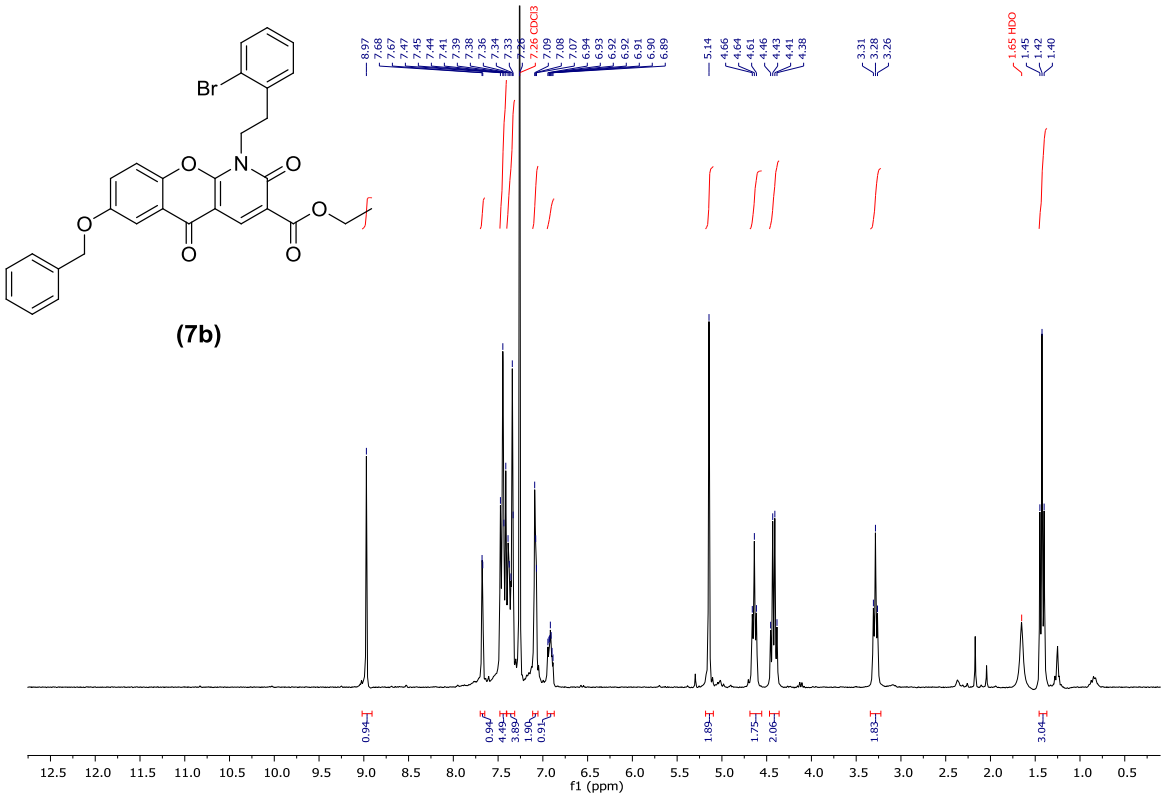

f1 (ppm)

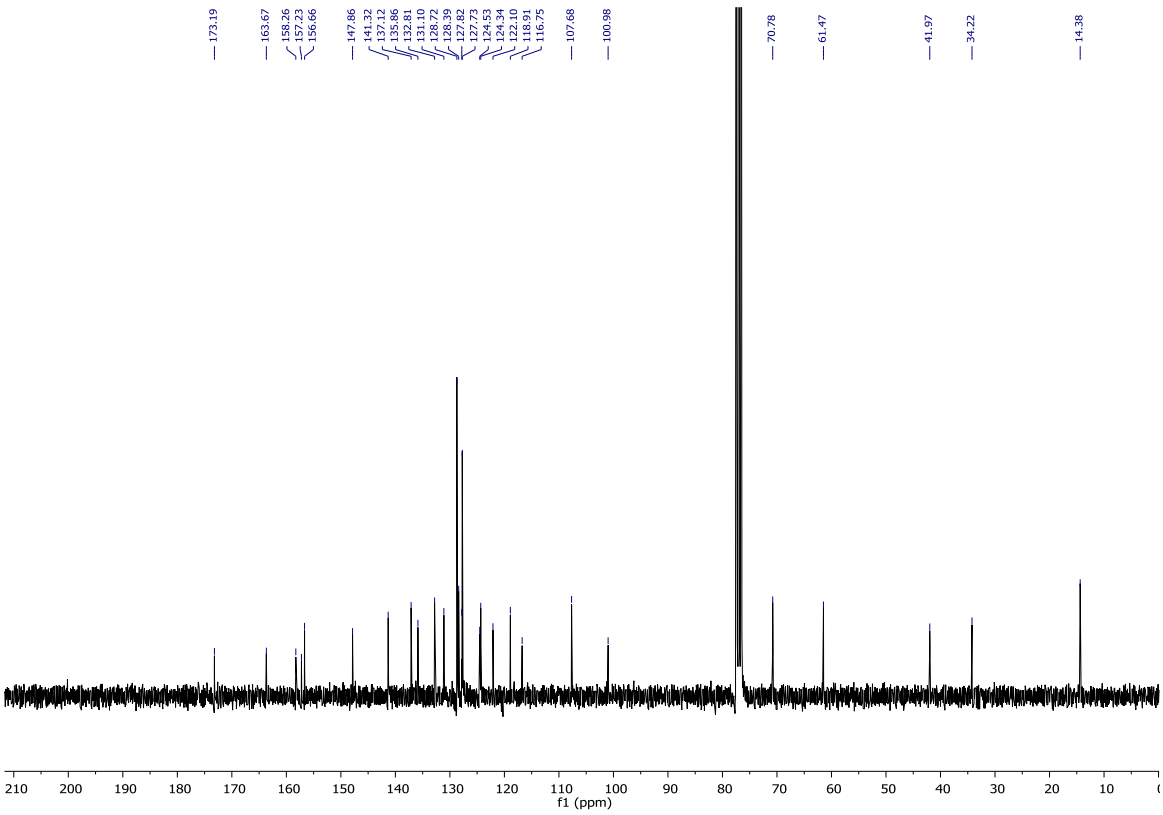

Br
O
N
O
O
O
O
(3)
8.94
8.20
8.19
8.17
8.17
7.73
7.72
7.70
7.70
7.68
7.67
7.47
7.46
7.44
7.43
7.42
7.39
7.28 CDCl3
7.11
7.10
7.09
7.08
7.06
7.04
6.92
6.91
6.90
6.89
6.89
6.87
6.87
4.66
4.65
4.61
4.44
4.42
4.39
4.37
3.30
3.28
3.25
1.88 HDO
1.44
1.41
1.39
1.00
1.03
1.07
3.09
2.11
1.06
2.08
2.10
2.05
3.34
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

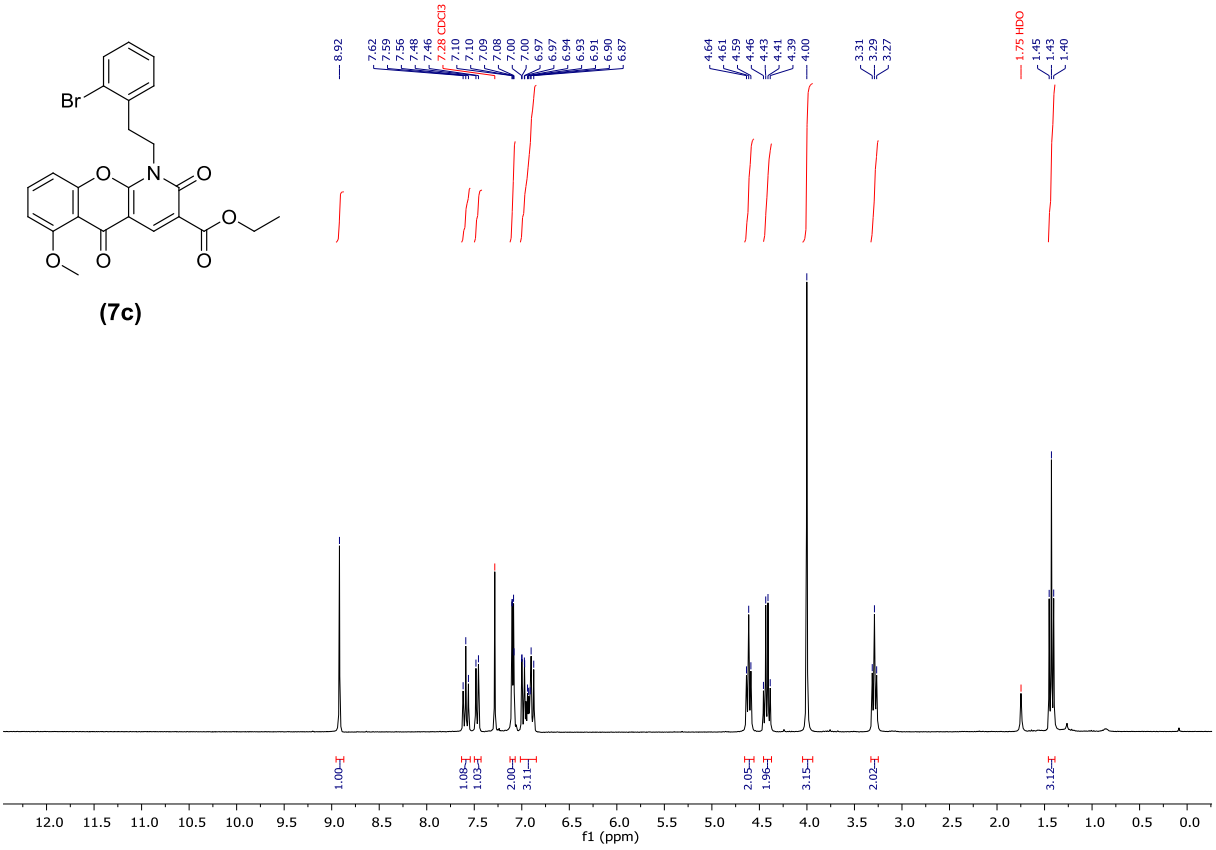

173.24
163.59
158.24
157.38
153.25
141.25
137.08
134.64
132.81
131.10
128.71
127.84
126.62
126.29
124.52
121.48
117.50
116.78
101.37
61.46
42.05
34.22
14.37
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

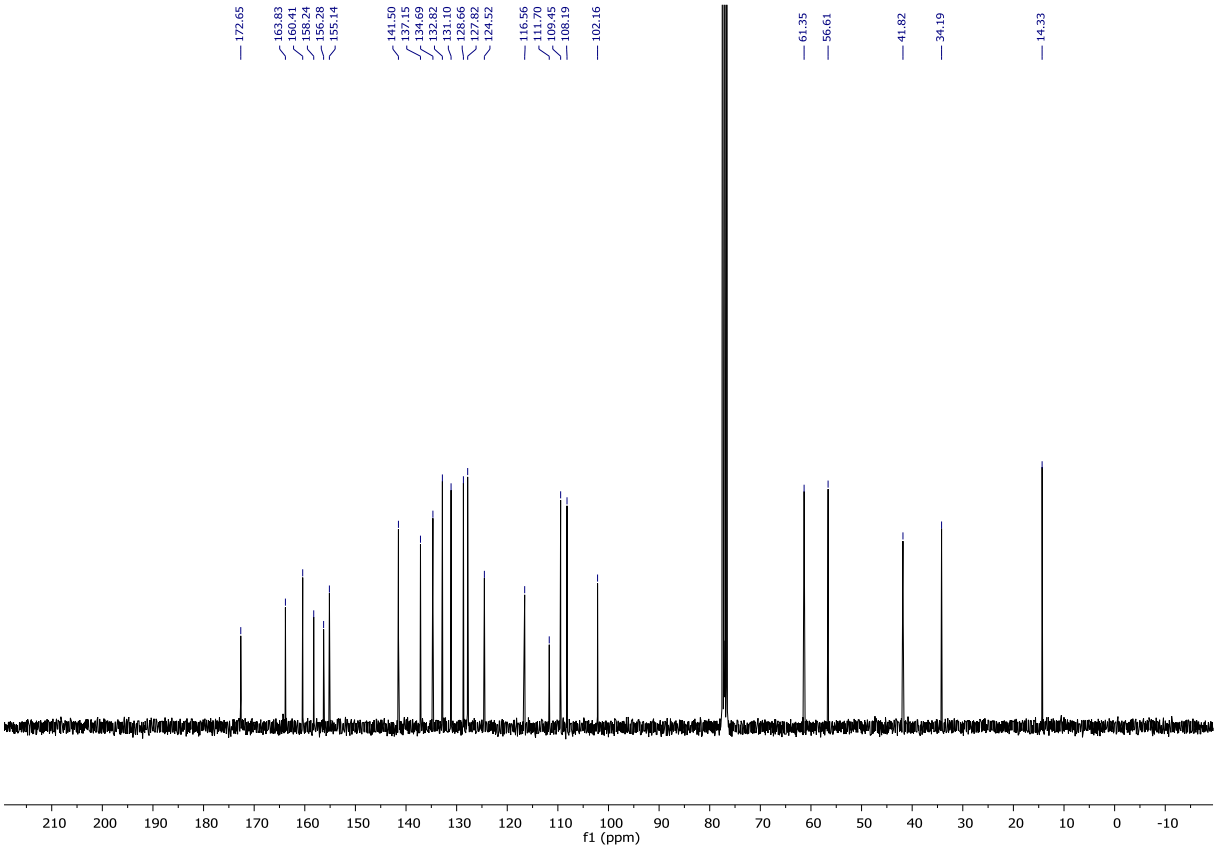

Br
O
N
O
O
O
O
(7a)
8.99
8.01
8.01
8.00
7.54
7.53
7.51
7.50
7.47
7.34
7.31
7.28 CDCl3
7.13
7.12
7.11
7.10
7.09
6.96
6.95
6.94
6.93
6.93
6.91
6.90
4.69
4.66
4.64
4.47
4.45
4.43
4.40
3.33
3.31
3.29
2.48
1.64 HDO
1.47
1.44
1.42
0.98
1.01
2.14
1.11
2.07
0.98
2.02
2.04
2.01
3.01
3.21
f1 (ppm)

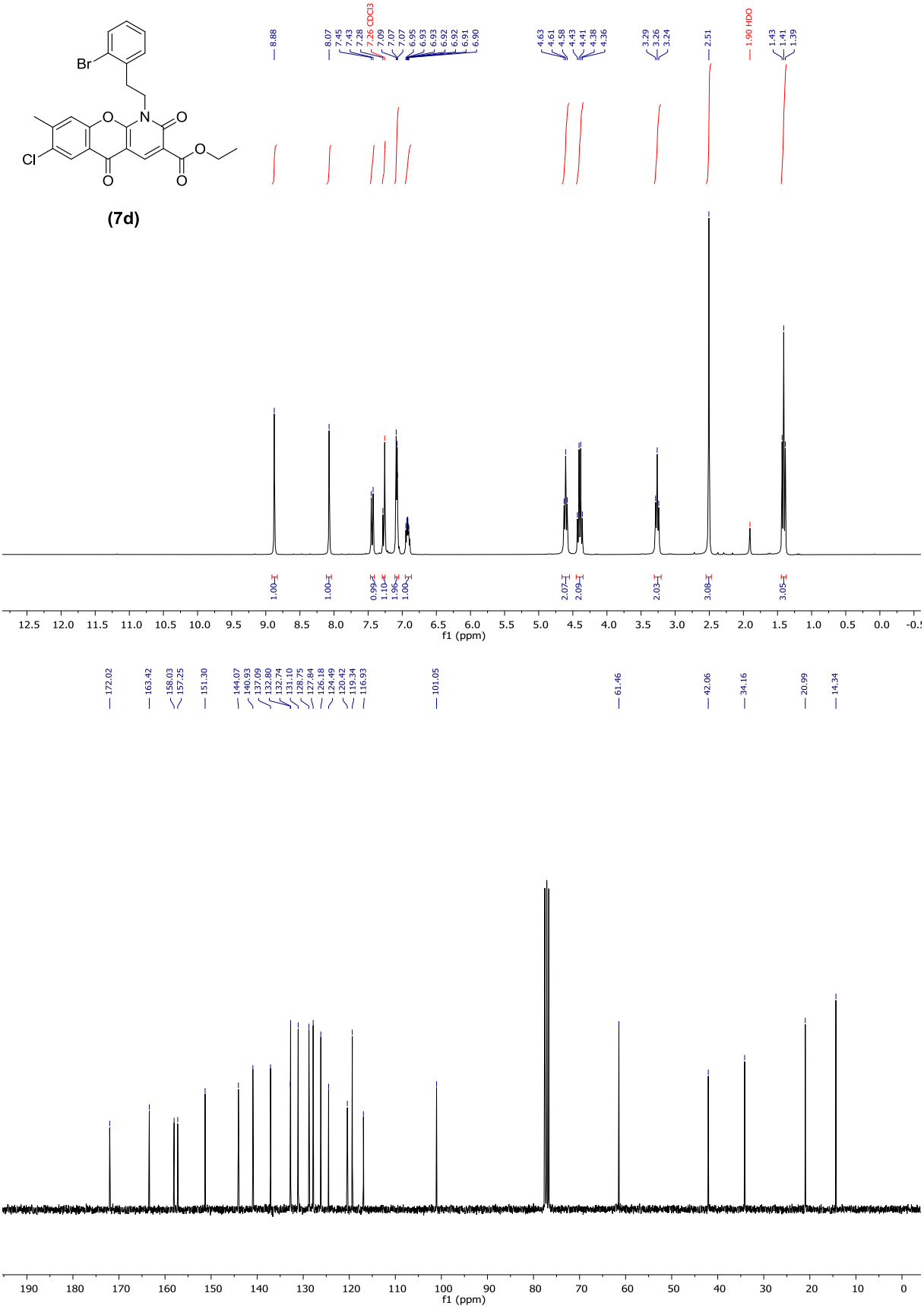

173.39
163.64
158.28
157.36
151.50
141.31
137.13
136.42
135.66
132.80
131.10
128.70
127.81
126.14
124.54
121.11
117.22
116.62
101.35
61.41
41.97
34.21
20.93
14.37
f1 (ppm)


Br
O
N
O
O
O
O
O
(7b)
8.97
7.68
7.67
7.47
7.45
7.44
7.41
7.39
7.38
7.36
7.34
7.33
7.26
7.26 CDCl3
7.09
7.08
7.07
6.94
6.93
6.92
6.92
6.91
6.90
6.89
5.14
4.66
4.64
4.61
4.46
4.43
4.41
4.38
3.31
3.28
3.26
1.65 HDO
1.45
1.42
1.40
0.94
0.94
4.49
3.89
1.90
0.91
1.89
1.75
2.06
1.83
3.04
f1 (ppm)

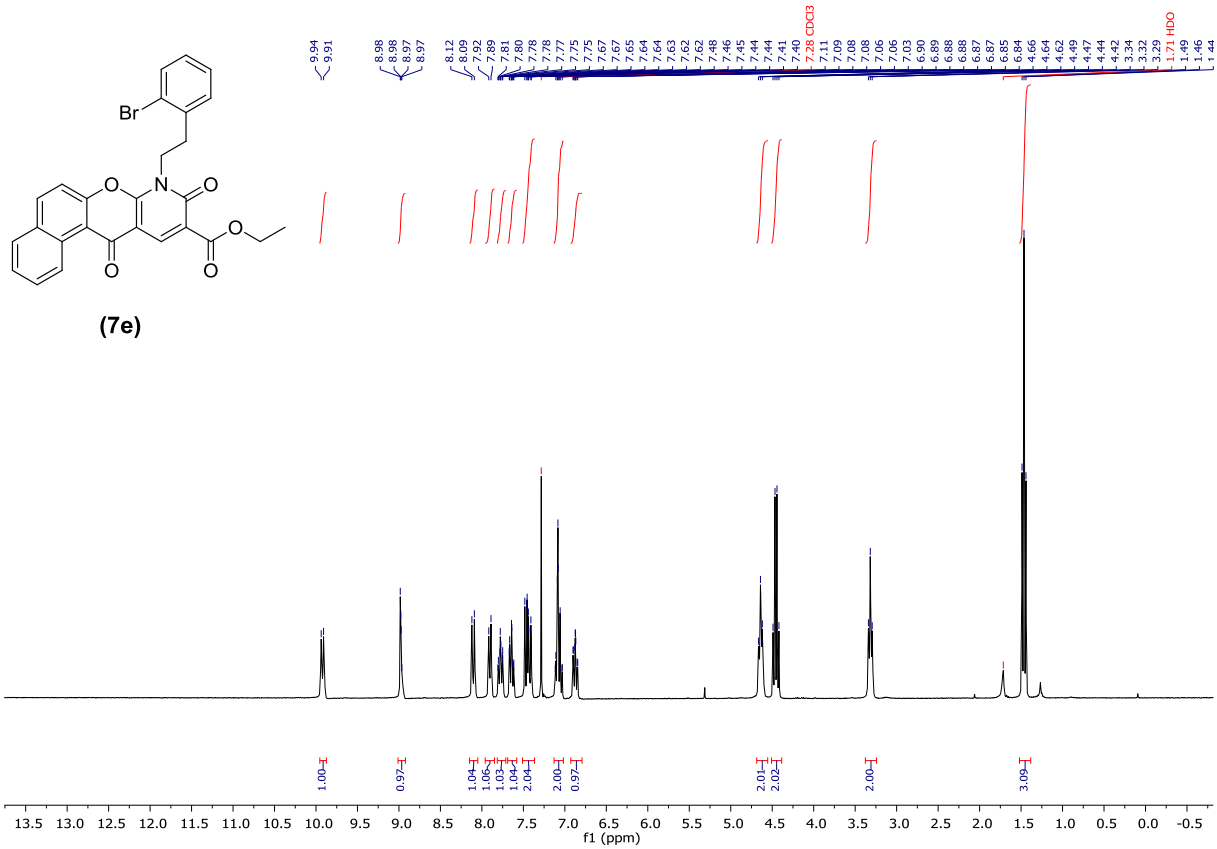

173.19
163.67
158.26
157.23
156.66
147.86
141.32
137.12
135.86
132.81
131.10
128.72
128.39
127.82
127.73
124.53
124.34
122.10
118.91
116.75
107.68
100.98
70.78
61.47
41.97
34.22
14.38
f1 (ppm)

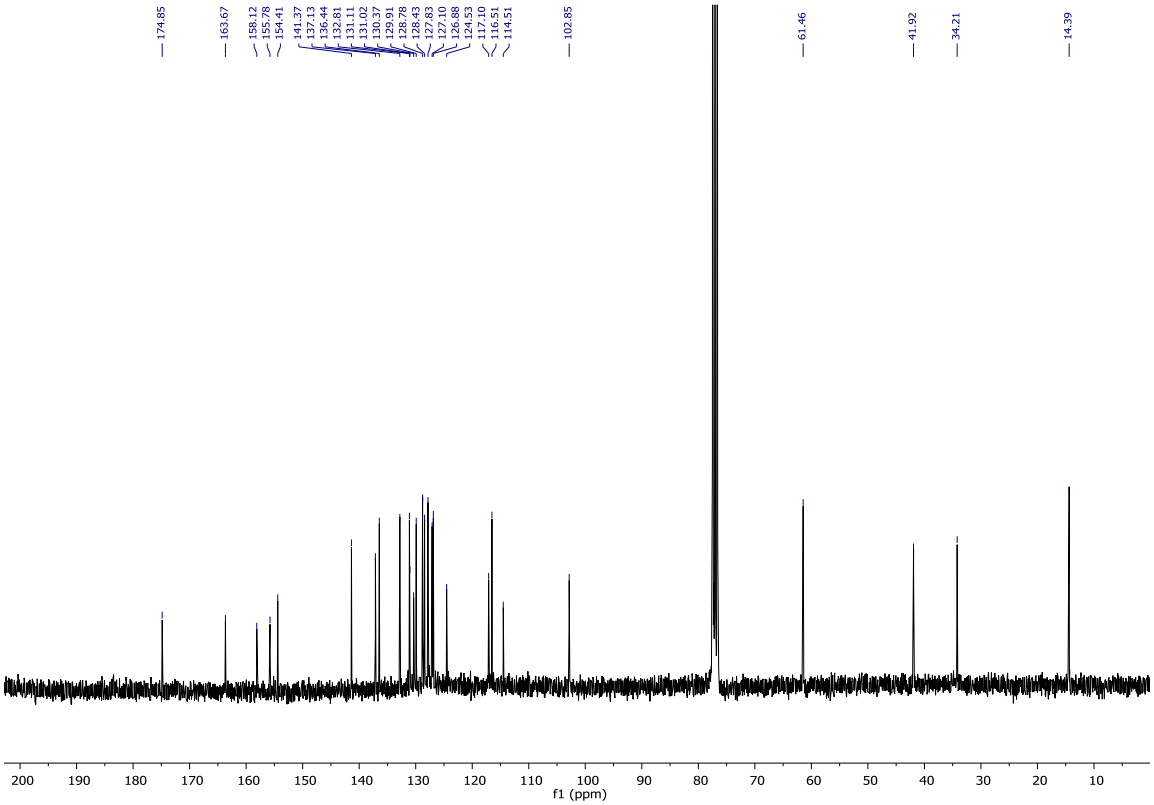

Br
O
N
O
O
O
O
O
O
(7c)
8.92
7.62
7.59
7.56
7.48
7.46
7.28 CDCl3
7.10
7.10
7.09
7.08
7.00
7.00
6.97
6.97
6.94
6.93
6.91
6.90
6.87
4.64
4.61
4.59
4.46
4.43
4.41
4.39
4.00
3.31
3.29
3.27
1.75 HDO
1.45
1.43
1.40
1.00
1.08
1.03
2.00
3.11
2.05
1.96
3.15
2.02
3.12
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

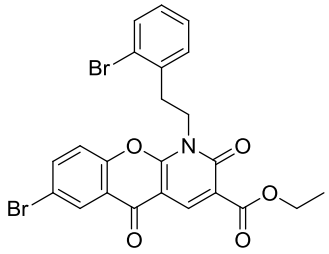

172.65
163.83
160.41
158.24
156.28
155.14
141.50
137.15
134.69
132.82
131.10
128.66
127.82
124.52
116.56
111.70
109.45
108.19
102.16
61.35
56.61
41.82
34.19
14.33
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Br
O
N
O
O
Cl
O
O
O
8.88
8.07
7.45
7.43
7.28
7.26 CDCl3
7.09
7.07
7.07
6.95
6.93
6.92
6.92
6.91
6.90
4.63
4.61
4.58
4.43
4.41
4.38
4.36
3.29
3.26
3.24
2.51
1.90 HDO
1.43
1.41
1.39
1.00
1.00
0.99
1.10
1.96
1.00
2.07
2.09
2.03
3.08
3.05
f1 (ppm)
172.02
163.42
158.03
157.25
151.30
144.07
140.93
137.09
132.80
132.74
131.10
128.75
127.84
126.18
124.49
120.42
119.34
116.93
101.05
61.46
42.06
34.16
20.99
14.34
f1 (ppm)

(7d)

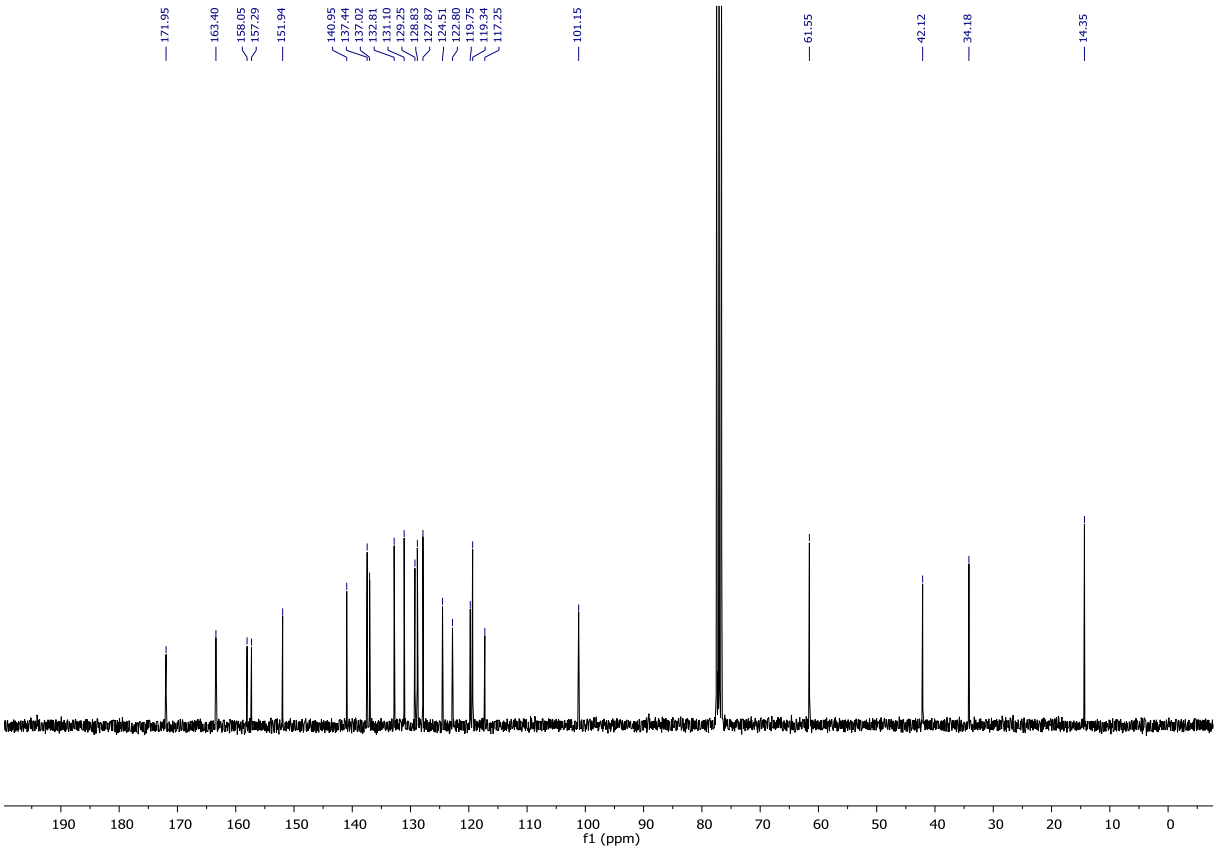

Br
O
N
O
O
O
O
(7e)
9.94
9.91
8.98
8.98
8.97
8.97
8.12
8.09
7.92
7.89
7.81
7.80
7.78
7.78
7.77
7.75
7.75
7.67
7.67
7.65
7.64
7.64
7.63
7.62
7.62
7.48
7.46
7.45
7.44
7.44
7.41
7.40
7.26 CDCl3
7.11
7.09
7.08
7.08
7.06
7.06
7.03
6.90
6.89
6.88
6.88
6.87
6.87
6.85
6.84
4.66
4.64
4.62
4.49
4.47
4.44
4.42
3.34
3.32
3.29
1.71 HDO
1.49
1.46
1.44
1.00
0.97
1.04
1.06
1.03
1.04
2.04
2.00
0.97
2.01
2.02
2.00
3.09
f1 (ppm)

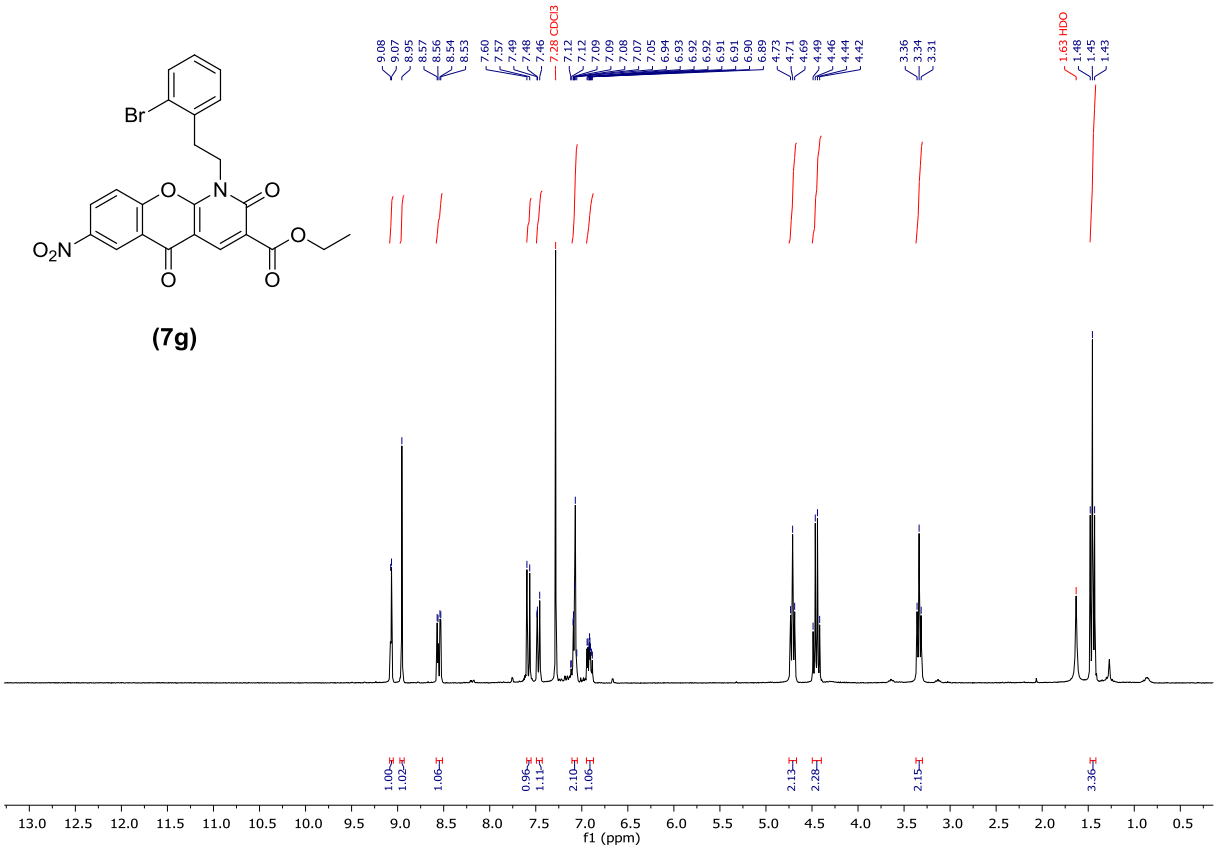

174.85
163.67
158.12
155.78
154.41
141.37
137.13
136.44
132.81
131.11
131.02
130.37
129.91
128.78
128.43
127.83
127.10
126.88
124.53
117.10
116.51
114.51
102.85
61.46
41.92
34.21
14.39
f1 (ppm)

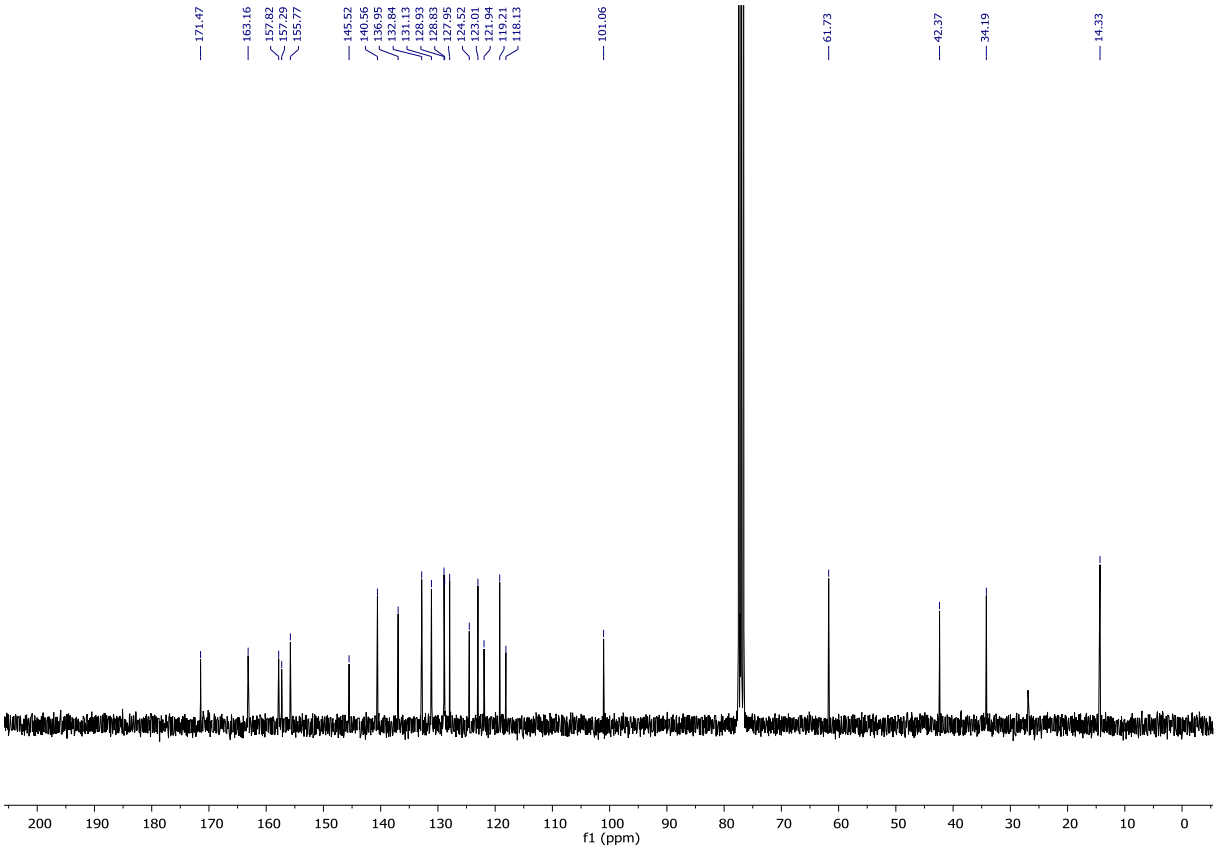

Br
O
N
O
Br
O
O
O

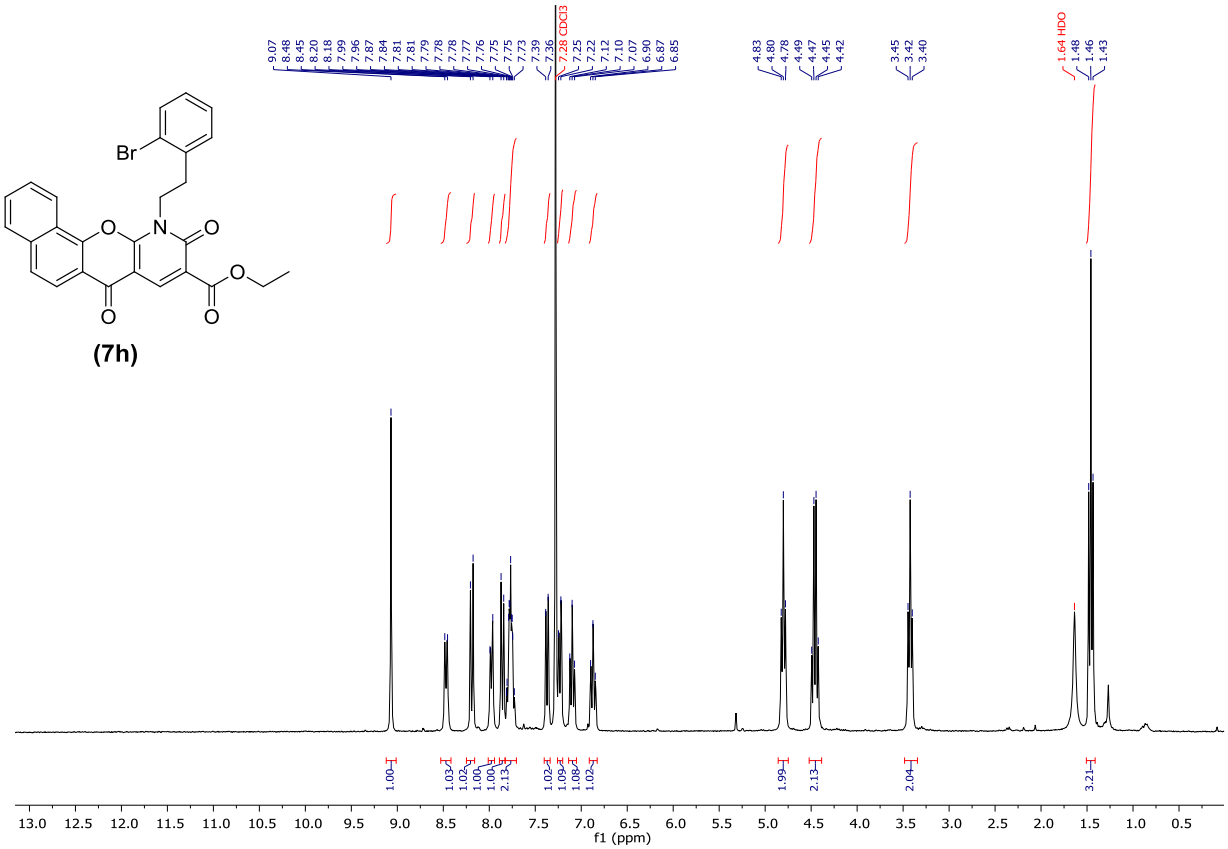
(7f)

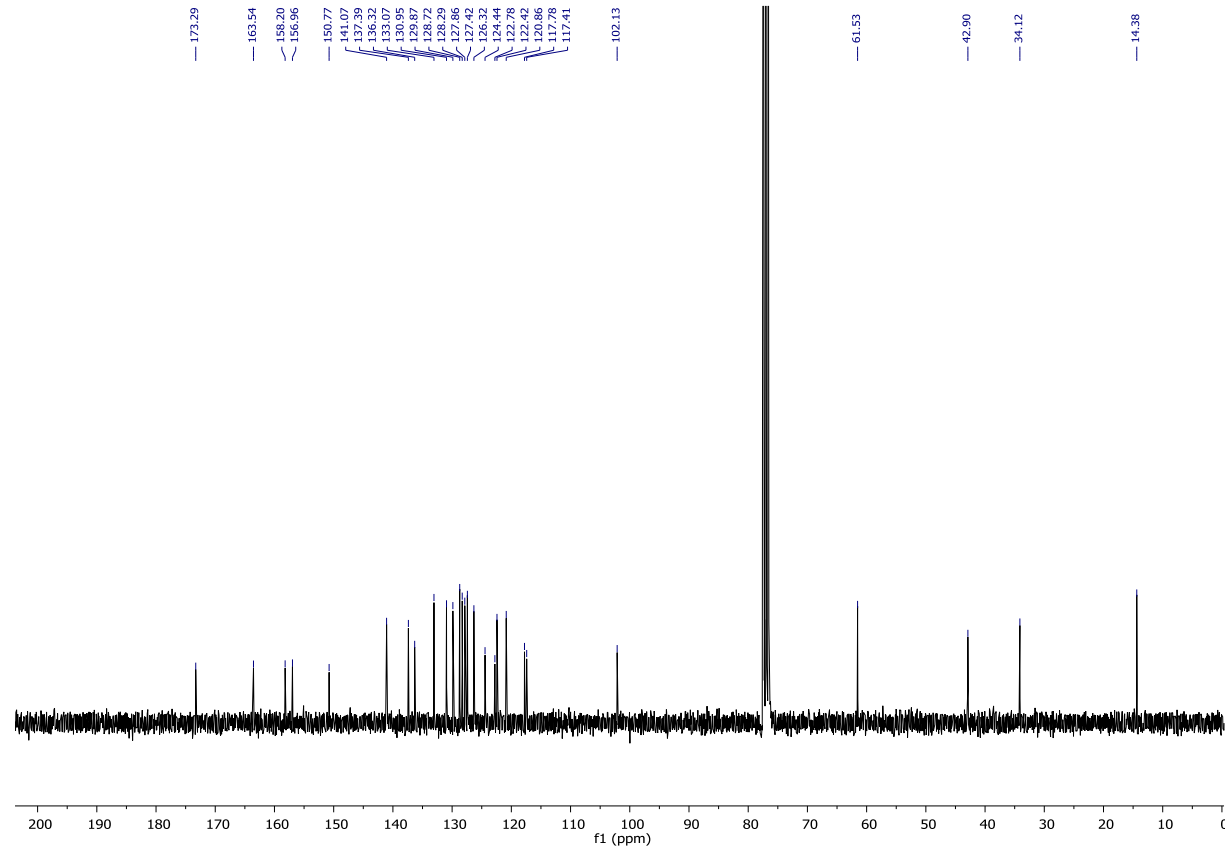
8.94
8.32
8.31
7.81
7.80
7.78
7.77
7.48
7.45
7.32
7.29
7.28 CDCl3
7.07
7.06
6.95
6.94
6.94
6.93
6.91
6.90
4.68
4.66
4.63
4.47
4.44
4.42
4.39
3.32
3.30
3.28
1.70 HDO
1.46
1.44
1.41
1.00
0.98
1.04
1.00
1.07
2.04
1.02
2.01
2.14
2.00
3.17
f1 (ppm)

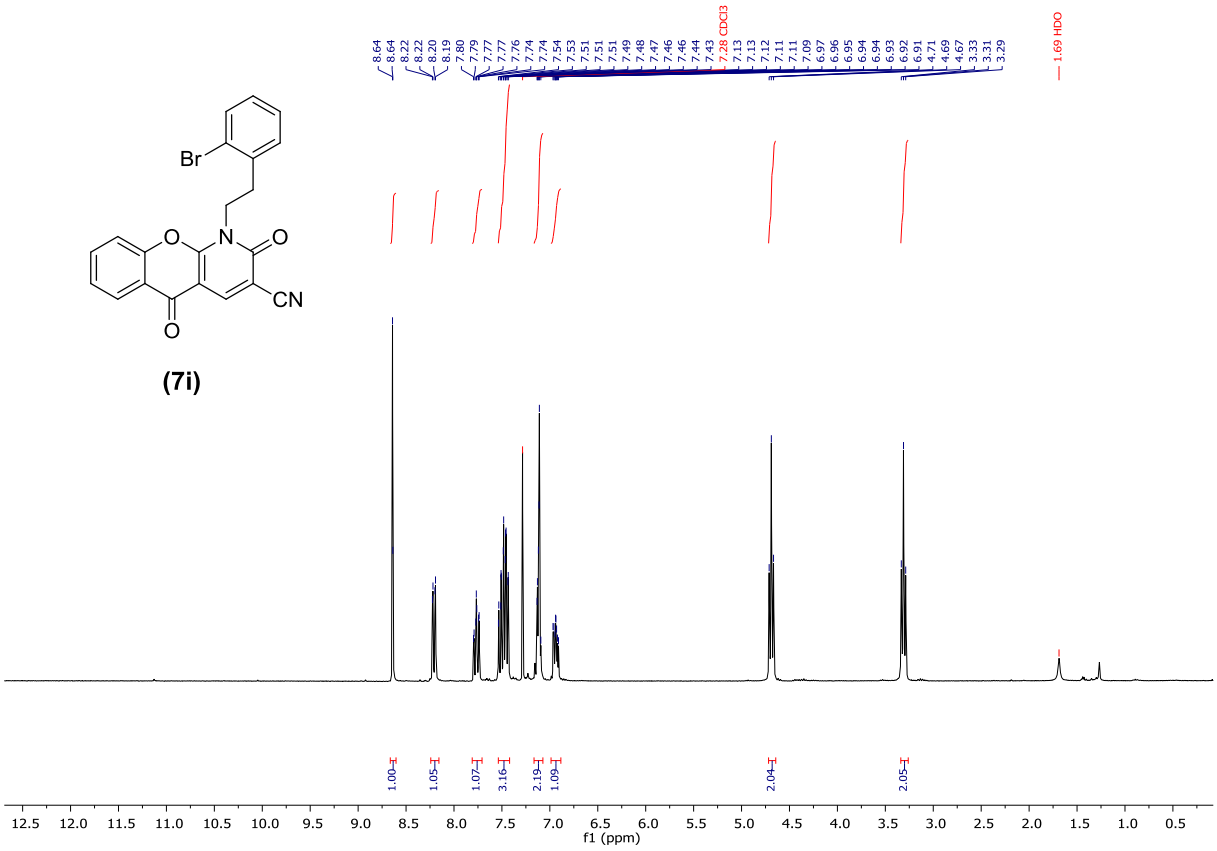

171.95
163.40
158.05
157.29
151.94
140.95
137.44
137.02
132.81
131.10
129.25
128.83
127.87
124.51
122.80
119.75
119.34
117.25
101.15
61.55
42.12
34.18
14.35
f1 (ppm)


Br
O
N
O
O
O
O
O2N
O
(7g)
9.08
9.07
8.95
8.57
8.56
8.54
8.53
7.60
7.57
7.49
7.48
7.46
7.28 CDCl3
7.12
7.12
7.09
7.09
7.08
7.07
7.05
6.94
6.93
6.92
6.92
6.91
6.91
6.90
6.89
4.73
4.71
4.69
4.49
4.46
4.44
4.42
3.36
3.34
3.31
1.63 HDO
1.48
1.45
1.43
1.00
1.02
1.06
0.96
1.11
2.10
1.06
2.13
2.28
2.15
3.36
f1 (ppm)


171.47
163.16
157.82
157.29
155.77
145.52
140.56
136.95
132.84
131.13
128.93
128.83
127.95
124.52
123.01
121.94
119.21
118.13
101.06
61.73
42.37
34.19
14.33
f1 (ppm)


Br
O
N
O
O
O
O
(7h)
9.07
8.48
8.45
8.20
8.18
7.99
7.96
7.87
7.84
7.81
7.81
7.79
7.78
7.78
7.77
7.76
7.75
7.75
7.73
7.39
7.36
7.28 CDCl3
7.25
7.22
7.12
7.10
7.07
6.90
6.87
6.85
4.83
4.80
4.78
4.49
4.47
4.45
4.42
3.45
3.42
3.40
1.64 HDO
1.48
1.46
1.43
1.00
1.03
1.02
1.00
1.00
2.13
1.02
1.09
1.08
1.02
1.99
2.13
2.04
3.21
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


173.29
163.54
158.20
156.96
150.77
141.07
137.39
136.32
133.07
130.95
129.87
128.72
128.29
127.86
127.42
126.32
124.44
122.78
122.42
120.86
117.78
117.41
102.13
61.53
42.90
34.12
14.38
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


Br
O
N
O
CN
O
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8.64
8.22
8.22
8.20
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7.77
7.77
7.76
7.74
7.74
7.54
7.53
7.51
7.51
7.49
7.48
7.47
7.46
7.46
7.44
7.43
7.28 CDCl3
7.13
7.13
7.12
7.11
7.11
7.09
6.97
6.96
6.95
6.94
6.94
6.93
6.92
6.91
4.71
4.69
4.67
3.33
3.31
3.29
1.69 HDO
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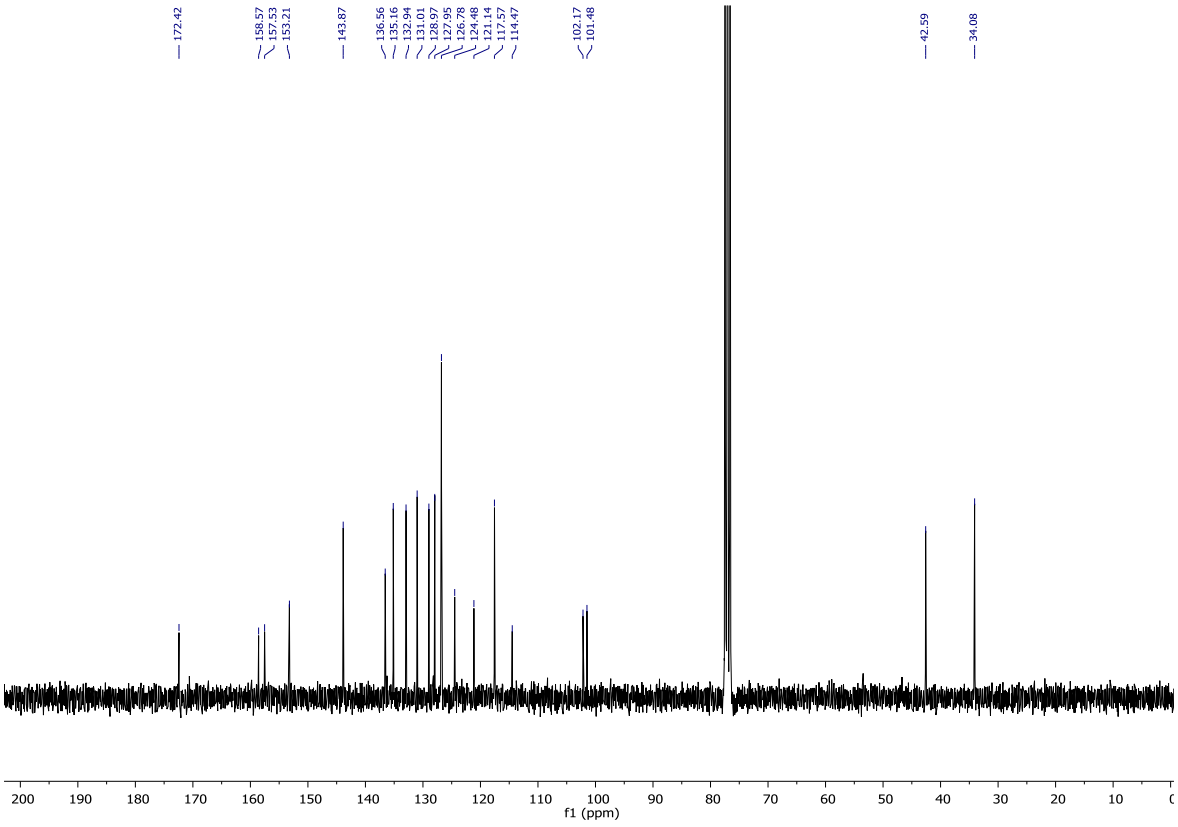
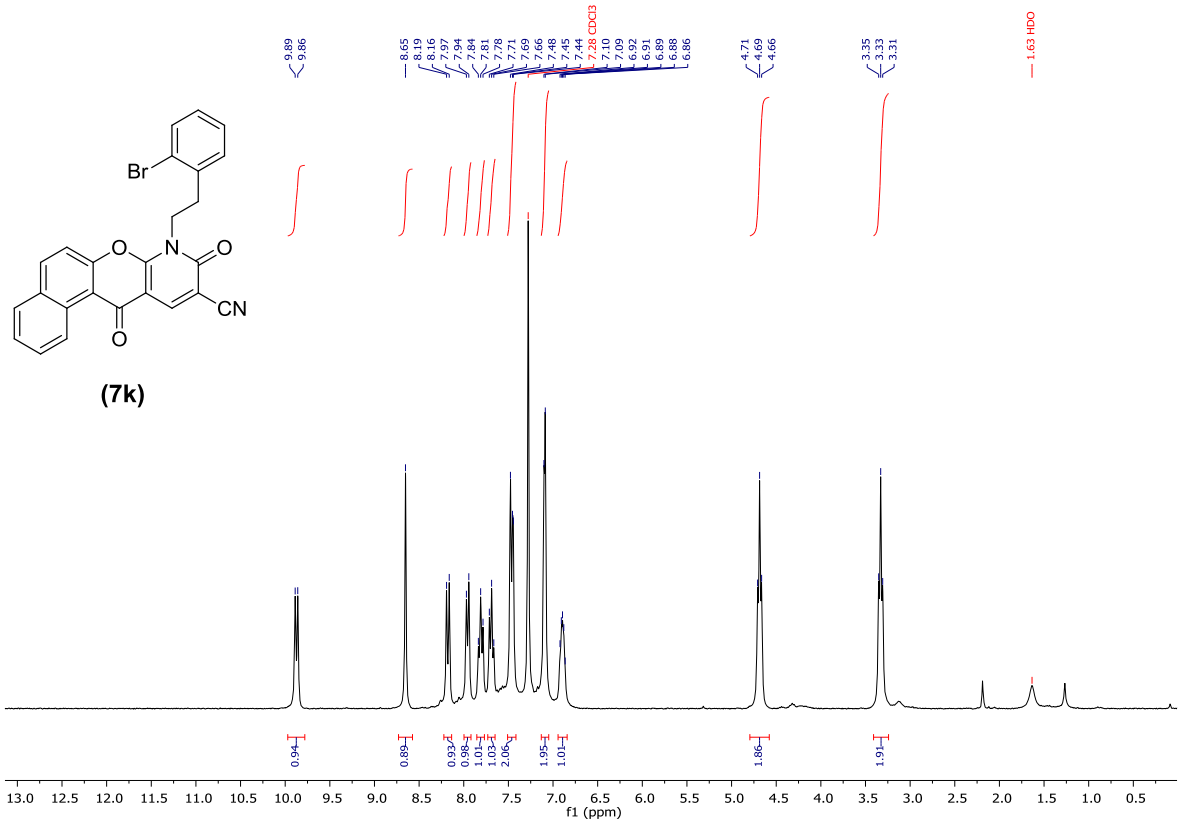
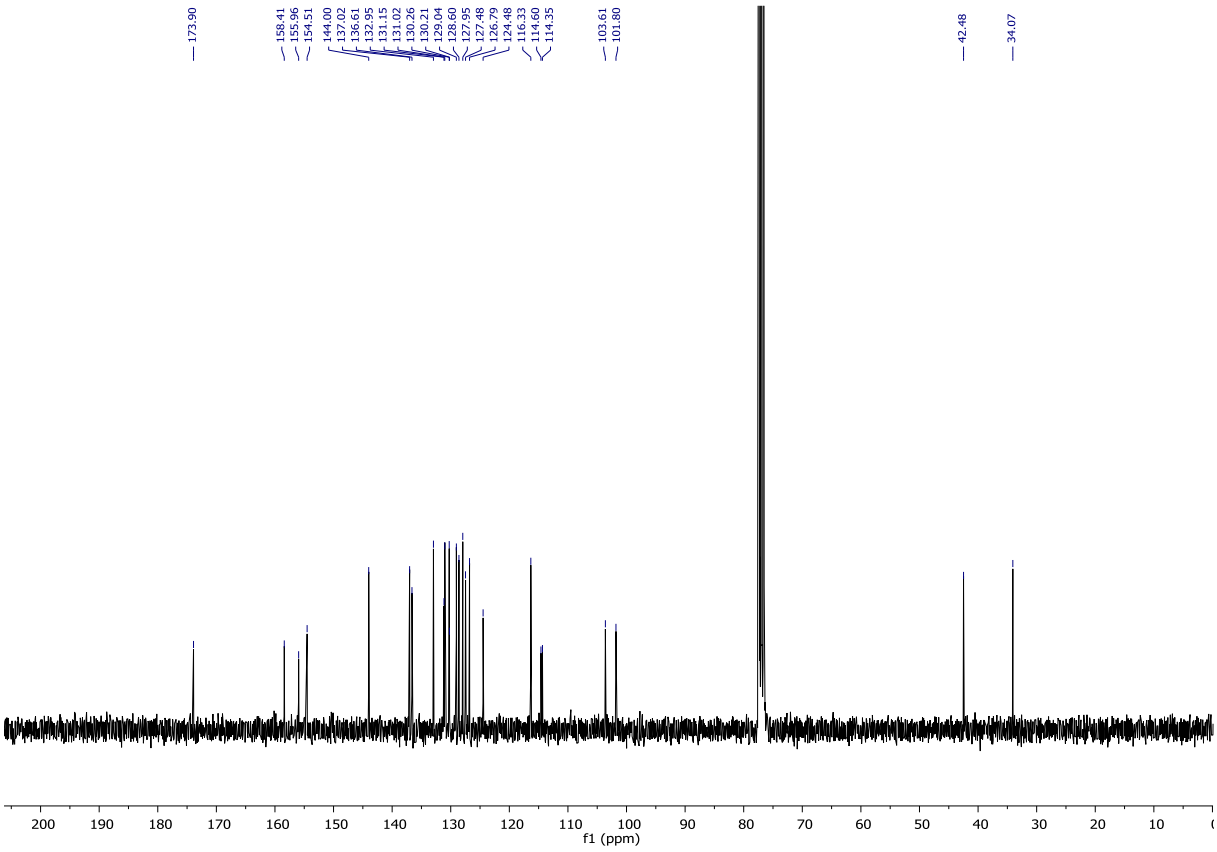
1.05
1.07
3.16
2.19
1.09
2.04
2.05
f1 (ppm)

(7i)


172.42
158.57
157.53
153.21
143.87
136.56
135.16
132.94
131.01
128.97
127.95
126.78
124.48
121.14
117.57
114.47
102.17
101.48
42.59
34.08
f1 (ppm)


Br
O
N
O
CN
O
(7k)
9.89
9.86
8.65
8.19
8.16
7.97
7.94
7.84
7.81
7.78
7.71
7.69
7.66
7.48
7.45
7.44
7.28 CDCl3
7.10
7.09
6.92
6.91
6.89
6.88
6.86
4.71
4.69
4.66
3.35
3.33
3.31
1.63 HDO
0.94
0.89
0.93
0.98
1.01
1.03
2.06
1.95
1.01
1.86
1.91
f1 (ppm)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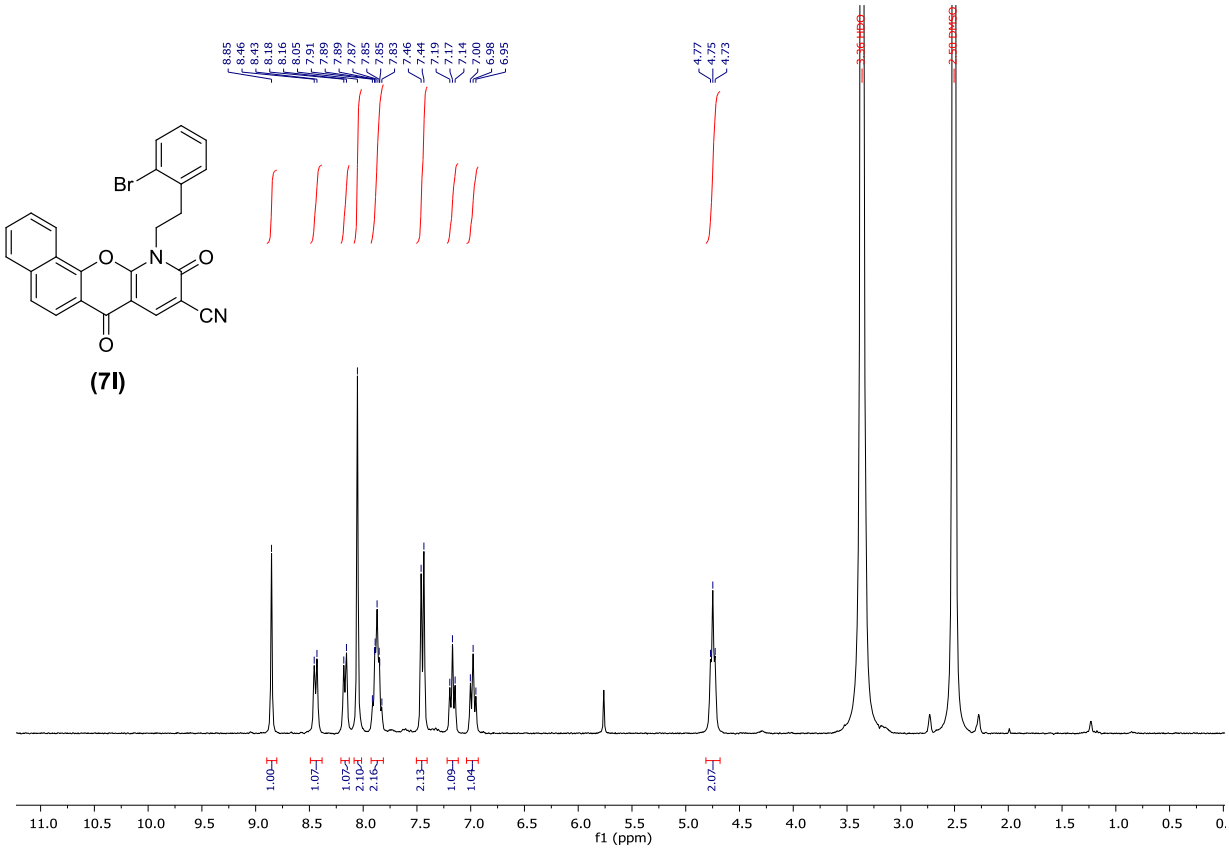
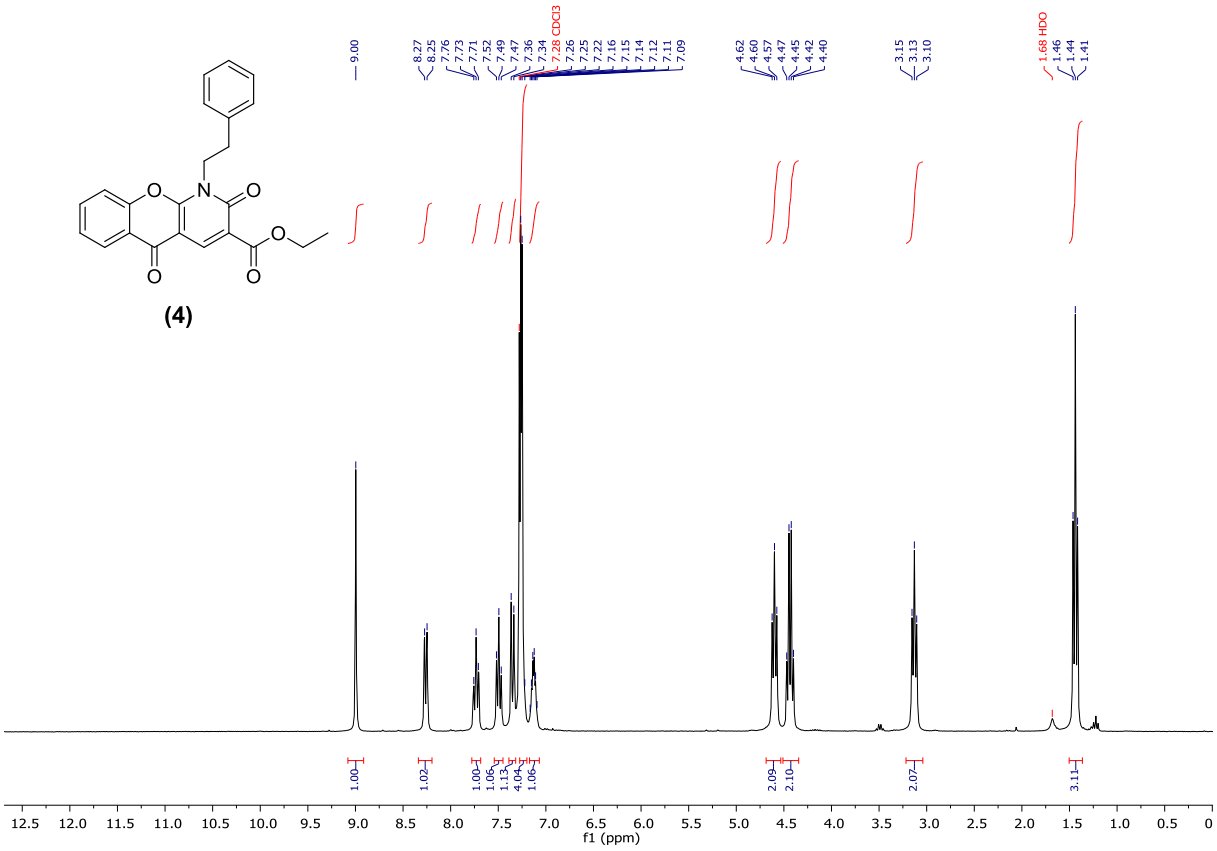
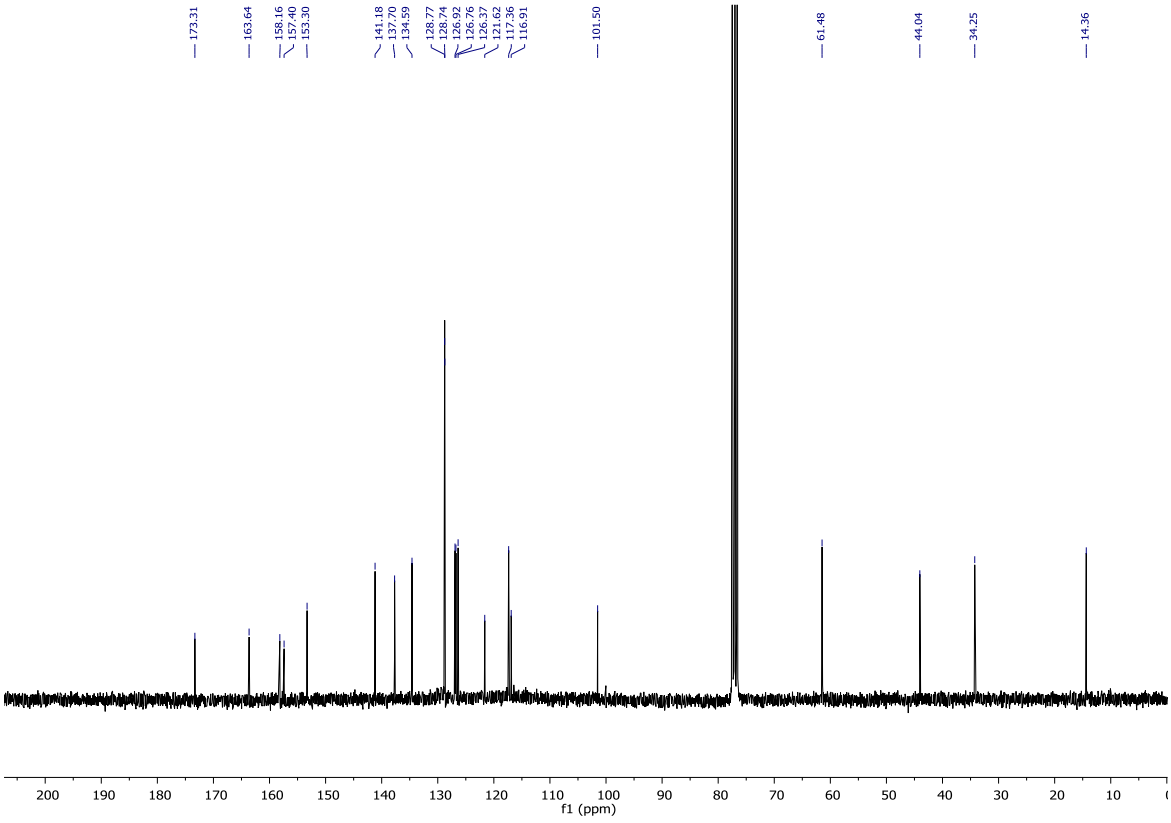
158.41
155.96
154.51
144.00
137.02
136.61
132.95
131.15
131.02
130.26
130.21
129.04
128.60
127.95
127.48
126.79
124.48
116.33
114.60
114.35
103.61
101.80
42.48
34.07
f1 (ppm)


Br
O
N
O
CN
O
(7l)
8.85
8.46
8.43
8.18
8.16
8.05
7.91
7.89
7.89
7.87
7.85
7.85
7.83
7.46
7.44
7.19
7.17
7.14
7.00
6.98
6.95
4.77
4.75
4.73
3.36 HDO
2.50 DMSO
1.00
1.07
1.07
2.10
2.16
2.13
1.09
1.04
2.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


(4)
9.00
8.27
8.25
7.76
7.73
7.71
7.52
7.49
7.47
7.36
7.34
7.28 CDCl3
7.26
7.25
7.22
7.16
7.15
7.14
7.12
7.11
7.09
4.62
4.60
4.57
4.47
4.45
4.42
4.40
3.15
3.13
3.10
1.68 HDO
1.46
1.44
1.41
1.00
1.02
1.00
1.06
1.13
4.04
1.06
2.09
2.10
2.07
3.11
f1 (ppm)


173.31
163.64
158.16
157.40
153.30
141.18
137.70
134.59
128.77
128.74
126.92
126.76
126.37
121.62
117.36
116.91
101.50
61.48
44.04
34.25
14.36
f1 (ppm)