Supporting Information

Organocatalysed Michael addition on arylmethylidenemalonates involving 4-(2-nitrophenyl)acetoacetate: a diversity-oriented access to 8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one and salicylate scaffolds

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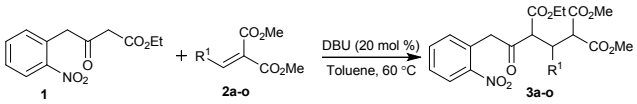
General information :

All reactions were carried out under air and monitored by TLC using Merck 60 F_{254} pre coated silica gel plates (0.25 mm thickness) and the products were visualized by UV detection. Flash chromatography was carried out with silica gel (200-300 mesh). FT-IR spectra were recorded on a Bruker Tensor-27 spectrometer. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance (III) 400 MHz spectrometer. Data for ^{1}H NMR are reported as a chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, q = quartet, m = multiplet), coupling constant *J* (Hz), integration, and assignment, data for ^{13}C are reported as a chemical shift. High resolutions mass spectral analyses (HRMS) were carried out using ESI-TOF-MS.

General experimental procedure for the synthesis of various Michael adducts (3a-o):

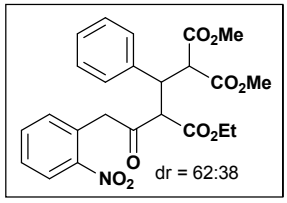


To a stirred mixture of ethyl 4-(2-nitrophenyl)acetoacetate (**1**, 0.25 mmol) and alkylidene malonates (**2a-o**, 0.3 mmol) in dry toluene (0.5 mL) was added catalyst DBU (20 mol%) and heated to 60 ˚C for 22-28h (monitored by TLC). After completion of the reaction, the reaction mixture was extracted with ethyl acetate before being quenched with aqueous diluted HCl, washed with brine and dried over Na_2SO_4. The evaporation of the solvent left the crude product which was purified by column chromatography over silica-gel 230-400 mesh using

EtOAc/hexane as eluent to furnish the pure product. All the products were fully characterized by their corresponding spectroscopic data (IR, ^{1}H and ^{13}C NMR and HRMS). The diastereomeric ratio was determined by ^{1}H NMR data of crude product.

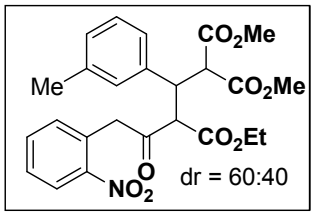
All the products in Table 2 were followed the above procedure.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-phenyl-pentan-4-one (3a):



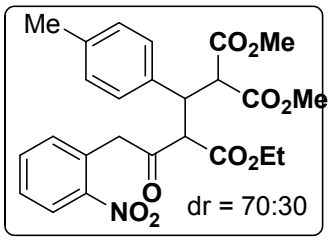
Yield 71%; **IR** (KBr) ν 3443, 2953, 1752, 1731, 1714, 1614, 1581, 1525, 1497, 1453, 1405, 1352, 1326, 1259 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 62:38**)** 8.11-8.13 (m, 0.62H), 8.02-8.04 (m, 0.38H), 7.57-7.61 (m, 0.76H), 7.42-7.48 (m, 1.24H), 7.36-7.40 (m, 0.62H), 7.28-7.32 (m, 4H), 7.21-7.24 (m, 1H), 6.70-6.72 (m, 0.38H), 4.65 (d, *J* = 10.5 Hz, 0.62H), 4.55 (d, *J* = 9.5 Hz, 0.38H), 4.44-4.48 (m, 0.76H), 4.32-4.36 (m, 1H), 4.22-4.27 (m, 1.24H), 4.16-4.21 (m, 1H), 3.93-3.98 (m, 1.24H), 3.82-3.87 (m, 0.76H), 3.67 (s, 1.14H), 3.58 (s, 1.86H), 3.53 (s, 1.14H), 3.51 (s, 1.86H), 1.29 (t, *J* = 7.28 Hz, 1.14H), 0.98 (t, *J* = 7.28 Hz, 1.86H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 199.1, 168.7, 168.2, 167.0, 148.7, 137.8, 133.7, 133.5, 129.4, 129.0, 128.4, 128.3, 127.7, 125.2, 62.3, 61.8, 55.2, 52.6, 52.5, 47.5, 43.5, 13.6; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.1, 168.5, 168.2, 167.8, 148.7, 137.5, 133.3, 133.2, 129.4, 128.9, 128.5, 128.5, 127.8, 125.1, 62.1, 61.0, 54.6, 52.7, 52.4, 48.4, 44.3, 13.9; HRMS (ESI) m/z calcd For $C_{24}H_{25}NO_9$ $[M+Na]^+$: 494.1422. Found 494.1412.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(3-methylphenyl)-pentan-4-one (3b):



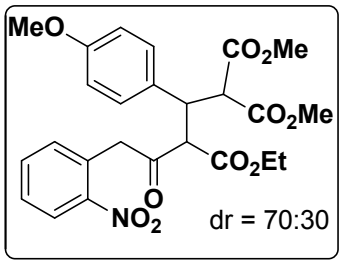
Yield 77%; IR (KBr) ν 3449, 2956, 1748, 1745, 1611, 1528, 1437, 1349, 1154 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 60:40) 8.11 (d, *J* = 8.0 Hz, 0.60H), 8.02 (d, *J* = 8.0 Hz, 0.40H), 7.57-7.60 (m, 0.60H), 7.42-7.48 (m, 1H), 7.36-7.40 (m, 0.6H) 7.31-7.32 (m, 0.4H), 7.11-7.16 (m, 1H), 7.01-7.09 (m, 3H), 6.69-6.71 (m, 0.40H), 4.63 (d, *J* = 10.5 Hz, 0.60H), 4.44-4.52 (m, 1H), 4.27-4.32 (m, 1.40H), 4.17-4.22(m, 1.6H), 4.13-4.15 (m, 0.4H), 3.94-3.99 (m, 1H), 3.81-3.86 (m, 1H), 3.67 (s, 1.20H), 3.58 (s, 1.80H), 3.55 (s, 1.20H), 3.52 (s, 1.80H), 2.30 (s, 3H), 1.29 (t, *J* = 7.28 Hz, 1.20H), 0.99 (t, *J* = 7.0 Hz, 1.80H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 199.2, 168.7, 168.2, 167.0, 148.7, 137.8, 137.8, 133.7, 133.5, 129.7, 129.4, 128.5, 128.4, 128.4, 125.8, 125.2, 62.3, 61.8, 55.2, 52.6, 52.4, 47.6, 43.4, 21.4, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.2, 168.5, 168.3, 167.9, 148.8, 138.1, 137.4, 133.3, 133.2, 130.2, 129.0, 128.5, 128.4, 128.1, 126.1, 125.1, 62.0, 61.1, 54.6, 52.7, 52.4, 48.3, 44.2, 21.4, 14.0; **HRMS** (ESI) m/z calcd For $C_{25}H_{27}NO_9$[M+K]: 524.1317. Found 524.1309.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-methylphenyl)-pentan-4-one (3c):



Yield 76%; **IR** (KBr) ν 3062, 3030, 2984, 2951, 2917, 1755, 1734, 1710, 1662, 1553, 1518, 1447, 1431, 1414, 1399, 1363, 1336, 1297, 1247, 1227 cm^{-1}; **^{1}H NMR (400 MHz, $CDCl_3$)** δ **(mixture of diastereomers dr = 70:30)** 8.10-8.13 (m, 0.70H), 8.01-8.04 (m, 0.30H), 7.57-7.61 (m, 0.70H), 7.42-7.48 (m, 1.3H), 7.36-7.40 (m, 0.3H), 7.29-7.32 (m, 0.70H), 7.16-7.21 (m, 2.0H), 7.05-7.08 (m, 1.7H), 6.71-6.74 (m, 0.3H), 4.62 (d, *J* = 10.5 Hz, 0.7H), 4.52 (d, *J* = 9.3 Hz, 0.30H), 4.44-4.48 (m, 0.7H), 4.30-4.32 (m, 1H), 4.27-4.28 (m, 0.30H), 4.18-4.24 (m, 1.0H), 4.13-4.17 (m, 0.60H), 3.94-4.00 (m, 1.4H), 3.82-3.89 (m, 1.0H), 3.67 (s, 0.9H), 3.58 (s, 2.10H), 3.55 (s, .90H), 3.52 (s, 2.10H), 2.29 (s, 0.90H), 2.28 (s, 2.10H), 1.29 (t, *J* = 7.28 Hz, 0.90H), 1.01 (t, *J* = 7.28 Hz, 2.10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 199.2, 168.7, 168.2, 167.1, 148.7, 137.3, 134.7, 133.7, 133.5, 133.3, 129.4, 129.0, 128.8, 125.2, 62.4, 61.8, 55.2, 52.6, 52.4, 47.6, 43.1, 21.1, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.2, 168.5, 168.3, 168.0, 148.7, 137.4, 134.2, 133.7, 133.5, 133.3, 129.2, 128.5, 128.4, 125.1, 62.1, 61.1, 54.6, 52.7, 52.4, 48.2, 43.9, 21.1, 14.0 ; HRMS (ESI) m/z calcd For $C_{25}H_{27}NO_9$ $[M+Na]^+$: 508.1578. Found 508.1576.

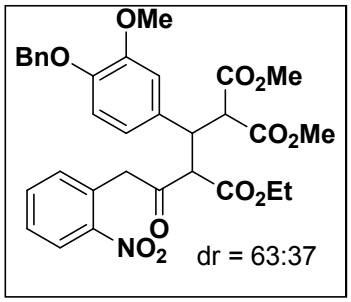
3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-methoxyphenyl)-pentan-4-one (3d):



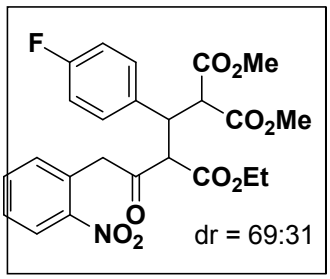
Yield 71%; **IR** (KBr) ν 3443, 2956, 2929, 2843, 2360, 2340, 1745, 1742, 1613, 1582, 1528, 1463, 1437, 1410, 1350, 1306 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 70:30) 8.10-8.13 (m, 0.70H), 8.01-8.04 (m, 0.3H), 7.56-7.60 (m, 0.70H), 7.43-7.48 (m, 1H), 7.37-7.40 (m, 0.30H), 7.29-7.32 (m, 0.7H), 7.21-7.25 (m, 2H), 6.77-6.80 (m, 2.30H), 4.59 (d, *J* = 10.3 Hz, 0.7H), 4.51 (d, *J* = 9.3 Hz, 0.30H), 4.41-4.46 (m, 0.70H), 4.26-4.31 (m, 1H), 4.20-4.22 (m, 1H), 4.13-4.18 (m, 0.70H), 3.95-4.00 (m, 1.70H), 3.88-3.92 (0.7H), 3.82-3.84 (m, 0.3H), 3.77 (s, 0.90H), 3.76 (s, 2.10H), 3.67 (s, 0.90H), 3.58 (s, 2.10H), 3.55 (s, 0.90H), 3.53 (s, 2.10H), 1.29 (t, *J* = 7.04 Hz, 0.90H), 1.03 (t, *J* = 7.28 Hz, 2.10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 199.2, 168.7, 168.2, 167.1, 158.9, 148.8, 133.7, 133.3, 130.2, 129.7, 129.4, 128.5, 125.2, 113.6, 62.5, 61.8, 55.1, 52.6, 52.4, 47.5, 42.8, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.2, 168.5, 168.3, 168.0, 159.0, 148.8, 133.4, 133.3, 130.6, 129.2, 129.0, 128.4, 125.1, 113.8, 62.0, 61.1, 55.2, 54.6, 52.6, 52.4, 48.2, 43.6, 14.0; HRMS (ESI) m/z calcd For $C_{25}H_{27}NO_{10}$$[M+K]^+$: 540.1267. Found 540.1267.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-benzyloxy-3-methoxyphenyl)-pentan-4-one (3e):

Yield 67%; **IR** (KBr) ν 3462, 2936, 1745, 1728, 1591, 1521, 1455, 1424, 1382, 1348, 1291, 1263, 1217, 1173 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 63:37) 8.11-8.13 (m, 0.63H), 8.02-8.04 (m, 0.37H), 7.56-7.60 (m, 0.63H), 7.46-7.48 (m, 0.63H), 7.40-7.44 (m, 3H), 7.33-7.36 (m, 2.37H), 7.28-7.30 (m, 1.37H), 6.90-6.91 (m, 0.63H), 6.75-6.77 (m, 2H), 6.71-6.73 (m, 0.37H), 5.12 (s, 0.74H), 5.11 (s, 1.26H), 4.62 (d, *J* = 10.3 Hz, 0.63H), 4.49 (d, *J* = 8.8 Hz, 0.37H), 4.39-4.44 (m, 0.63H), 4.22-4.30 (m, 1.63H), 4.11-4.22 (m, 2.37H), 3.94-3.99 (m, 1.37H), 3.86 (m, 1.89H), 3.82 (s, 1.11H), 3.66 (s, 1.11H), 3.57 (s, 1.89H), 3.53 (s, 1.11H), 3.51 (s, 1.89H), 1.28 (t, *J* = 7.28 Hz, 1.11H), 0.99 (t, *J* = 7.0 Hz, 1.89H; ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 199.1, 168.8, 168.2, 167.0, 149.1, 148.6, 147.3, 137.0, 133.6, 133.4, 130.7, 129.3, 128.5, 128.4, 127.8, 127.3, 125.2, 120.9, 113.4, 113.0, 70.8, 62.3, 61.8, 55.9, 55.2, 52.6, 52.4, 47.5, 43.1, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.2, 168.4, 168.2, 167.8, 149.3, 148.7, 147.4, 137.0, 133.3, 133.2, 130.2, 128.9, 128.5, 128.4, 127.8, 127.2, 125.0, 121.3, 113.5, 113.3, 70.8, 62.0, 61.1, 55.9, 54.6, 52.6, 52.4, 48.2, 43.9, 13.9; HRMS (ESI) m/z calcd For $C_{32}H_{33}NO_{11}[M+Na]^+$: 630.1946. Found 630.1962.



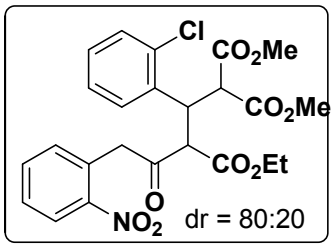
3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-fluorophenyl)-pentan-4-one (3f):



Yield 82%; IR (KBr) ν 3444, 2954, 1753, 1718, 1607, 1529, 1513, 1436, 1402, 1359, 1264, 1225, 1180, 1164, 1148, 1102, 1078 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 69:31) 8.12-8.14 (m, 0.69H), 8.04-8.06 (m, 0.31H), 7.58-7.62 (m, 0.69H), 7.45-7.49 (m, 1.0H), 7.41-7.43 (m, 0.31H), 7.28-7.34 (m, 3.0H), 6.93-6.98 (m, 1.69H), 6.86-6.88 (m, 0.31H), 4.62 (d, *J* = 10.3 Hz, 0.69H), 4.56 (d, *J* = 9.04 Hz, 0.31H), 4.40-4.45 (m, 0.69H), 4.30-4.35 (m, 1.31H), 4.19-4.27 (m, 1.30H), 3.95-4.01 (m, 1.69H), 3.83-3.92 (m, 1H), 3.68 (s, 0.93H), 3.58 (s, 2.07H), 3.54 (s, 3H), 1.28 (t, *J* = 7.0 Hz, 0.93H), 1.02 (t, *J* = 7.0 Hz, 2.07H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 199.0, 168.5, 168.3, 166.9, 163.3, 160.9, 148.6, 133.7, 133.6, 133.5, 133.0, 130.9, 130.8, 129.3, 128.7, 125.3, 115.3, 115.0, 62.3, 62.0, 54.9, 52.7, 52.5, ,47.6, 42.6, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.1, 168.2, 168.1, 167.8, 148.6, 133.5, 133.3, 131.3, 131.2, 128.9, 128.6, 125.2, 115.4, 115.2,

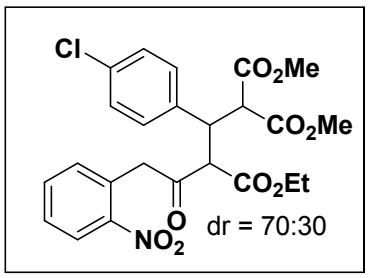
60.7, 54.2, 52.7, 52.5, 48.4, 43.5, 14.0; HRMS (ESI) m/z calcd For $C_{24}H_{24}F\ NO_9[M+Na]^+$: 512.1327. Found 512.1322.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(2-chlorophenyl)-pentan-4-one (3g):



Yield 80%; IR (KBr) ν 3449, 2950, 1749, 1719, 1527, 1480, 1436, 1356, 1315, 1261, 1227, 1201, 1180, 1154, 1083 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.11 (d, *J* = 8.3 Hz, 1H), 7.58-7.61 (m, 1H), 7.44-7.48 (m, 1H), 7.36-7.39 (m, 3H), 7.15-7.22 (m, 2H), 4.96 (s, 2H), 4.63 (d, *J* = 18 Hz, 1H), 4.25-4.29 (m, 1H), 3.97-3.99 (m, 2H), 3.67-3.87 (m, 1H), 3.58 (s, 3H), 3.54 (s, 3H), 1.00 (t, *J* = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major distereomer) 198.7, 168.4 (2C), 166.5, 148.8, 136.3, 134.9, 133.8, 133.4, 130.0, 129.4, 128.7, 128.5, 127.1, 126.9, 125.1, 62.0, 61.2, 53.8, 52.7, 52.5, 47.8, 39.1, 13.6; HRMS (ESI) m/z calcd For $C_{24}H_{24}NClO_9[M+K]^+$: 544.0771. Found 544.0777.

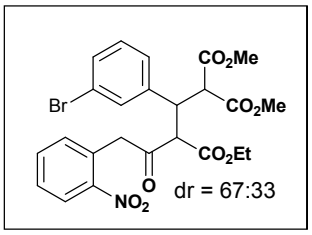
3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-chlorophenyl)-pentan-4-one (3h):



Yield 84%; IR (KBr) ν 3033, 2997, 2951, 1751, 1715, 1633, 1599, 1527, 1492, 1433, 1414, 1399, 1338, 1314, 1295, 1258, 1243, 1195, 1181, 1147, 1094 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 70:30) 8.13 (d, *J* = 8.0 Hz, 0.70H), 8.05 (d, *J* = 8 Hz, 0.30H), 7.58-7.62 (m, 0.7H), 7.47-7.51 (m, 1.3H), 7.40-7.44 (m, 0.3H), 7.27-7.31 (m, 2.0H), 7.24-7.25 (m, 1.7H), 7.21-7.23 (m, 0.7H) 6.86-6.88 (m, 0.3H), 4.63 (d, *J* = 10.3 Hz, 0.70H), 4.56 (d, *J* = 8.3 Hz, 0.30H), 4.41-4.45 (m, 0.70H), 4.29-4.34 (m, 1.30H), 4.16-4.26 (m, 1.7H), 3.92-4.02 (m, 2.0H), 3.83-3.85 (m, 0.30H), 3.68 (s, 0.90H), 3.59 (s, 2.10H), 3.55 (s, 3H), 1.28 (t, *J* = 7.28 Hz, 0.90H), 1.03 (t, *J* = 7.0 Hz, 2.10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.9, 168.4, 168.1, 166.8, 148.6, 136.3, 133.7, 133.6, 133.6, 130.5, 129.3, 128.7, 128.4, 125.3, 62.0, 61.9, 54.7, 52.7, 52.6, 47.7, 42.7, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.1, 168.3, 168.2, 167.7, 148.6, 135.9, 133.5, 133.5, 133.3, 131.0, 128.8, 128.6, 128.6, 125.2, 62.2, 60.6, 54.1, 52.8, 52.5, 48.3, 43.6, 14.0; HRMS (ESI) m/z calcd For $C_{24}H_{24}NO_9Cl\ [M+Na]^+$: 528.1032. Found 528.1042.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(3-bromophenyl)-pentan-4-one (3i):

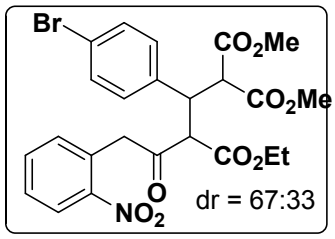
Yield 81%; **IR** (KBr) ν 3444, 2955, 1747, 1728,1613, 1527, 1435, 1349, 1155 cm^{-1}; ^1H NMR



(400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 67:33) 8.13 (d, *J* = 7.28 Hz, 0.67H), 8.06 (d, *J* = 8.3 Hz, 0.33H), 7.58-7.62 (m, 0.67H), 7.44-7.52 (m, 2.67H), 7.29-7.37 (m, 2.33H), 7.11-7.16 (m 1H), 6.89-6.91 (m, 0.33H), 4.64 (d, *J* = 10.3 Hz, 0.67H), 4.57 (d, *J* = 8.5 Hz, 0.33H), 4.42-4.46 (m, 0.67H), 4.27-4.32 (m, 1.67H), 4.17-4.23 (m, 1H), 4.15-4.14 (m, 0.33H), 3.97-4.03 (m, 1.33H), 3.83-3.93 (m, 1H), 3.69 (s, 0.99H), 3.60 (s, 2.01H), 3.57 (s, 3H), 1.29 (t, *J* = 7.28 Hz, 0.99H), 1.04 (t, *J* = 7.0 Hz, 2.01H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.8, 168.4, 168.0, 166.7, 148.6, 140.2, 133.7, 133.6, 132.1, 130.8, 129.8, 129.3, 128.7, 127.9, 125.3, 122.2, 62.1, 61.8, 54.6, 52.7, 52.6, 47.7, 42.9, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 198.9, 168.2, 168.1, 167.6, 148.6, 139.8, 133.5, 133.3, 132.3, 130.9, 130.0, 128.8, 128.6, 128.4, 125.2, 122.3, 62.3, 60.4, 54.0, 52.8, 52.5, 48.5, 43.8, 14.0; HRMS (ESI) m/z calcd For $C_{24}H_{24}BrNO_9[M+K]^+$: 588.0266. Found 588.0259.

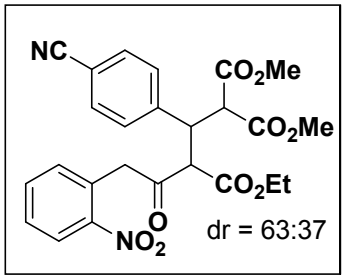
3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-bromophenyl)-pentan-4-one (3j):

Yield 79%; IR (KBr) ν 3061, 2997, 2976, 2949, 2921, 1747, 1712, 1631, 1606, 1526, 1488,



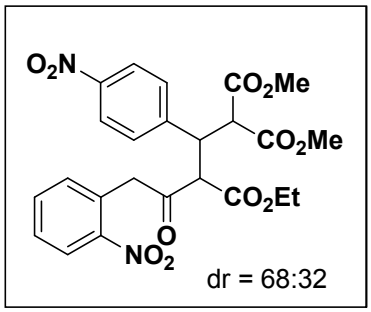
1450, 1434, 1401, 1341, 1314, 1295, 1257 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 67:33) 8.12-8.14 (m, 0.67H), 8.04-8.06 (m, 0.33H), 7.58-7.62 (m, 0.67H), 7.43-7.52 (m, 1.33H), 7.37-7.40 (m, 2.0H), 7.29-7.31 (m, 0.67H), 7.18-7.23 (m, 2.0), 6.85-6.87 (m, 0.33H), 4.63 (d, *J* = 10.3 Hz, 0.67H), 4.55-4.57 (m, 0.33H), 4.41-4.45 (m, 0.67H), 4.26-4.32 (m, 1.33H), 4.18-4.23 (m, 1.67H), 3.96-4.02 (m, 1.33H), 3.91-3.96 (m, 0.33H), 3.82-3.84 (m, 0.67H), 3.68 (s, 0.99H), 3.59 (s, 2.01H), 3.56 (s, 0.99H), 3.55 (s, 2.01H), 1.28 (t, *J* = 7.28 Hz, 0.99H), 1.04 (t, *J* = 7.28 Hz, 2.01H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.9, 168.4, 168.1, 166.8, 148.6, 136.8, 133.7, 133.6, 131.4, 130.9, 129.3, 128.7, 125.3, 121.7, 62.1, 61.8, 54.6, 52.7, 52.6, 47.7, 42.8, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 199.0, 168.3, 168.1, 167.7, 148.6, 136.4, 133.5, 133.3, 131.5, 131.3, 128.8, 128.6, 125.2, 121.9, 62.2, 60.5, 54.0, 52.8, 52.5, 48.3, 43.7, 14.0; HRMS (ESI) m/z calcd For $C_{24}H_{24}NO_9Br$ $[M+Na]^+$: 572.0527. Found 572.0488.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-cyanophenyl)-pentan-4-one (3k):



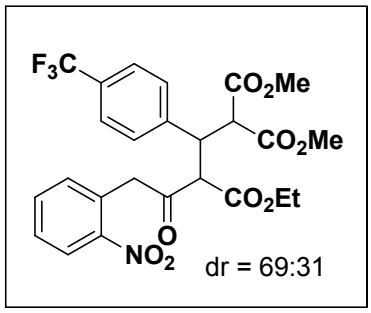
Yield 83%; **IR** (KBr) ν 3457, 2956, 2230, 1746, 1610, 1580, 1528, 1437, 1351, 1262, 1158 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 63:37) 8.12 (d, *J* = 8 Hz, 0.63H), 8.03 (d, *J* = 8 Hz, 0.37H), 7.50-7.61 (m, 3.63H), 7.44-7.48 (m, 2.37H), 7.40-7.42 (m, 0.37H), 7.28-7.30 (m, 0.63H), 6.95-6.97 (m, 0.37H), 4.68 (d, *J* = 10.3 Hz, 0.63H), 4.63 (d, *J* = 9.0 Hz, 0.37H), 4.35-4.45 (m, 1.63H), 4.24-4.30 (m, 1.37H), 4.17-4.22 (m, 1H), 3.95-4.02 (m, 1.63H), 3.86-3.88 (m, 0.37H), 3.66 (s, 1.11H), 3.58 (s, 1.89H), 3.54 (s, 1.89H), 3.53 (s, 1.11H), 1.26 (t, *J* = 7.0 Hz, 1.11H), 1.01 (t, *J* = 7.0 Hz, 1.89H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.4, 168.1, 167.8, 166.5, 148.5, 143.4, 133.6, 133.5, 133.2, 131.9, 130.1, 129.0, 128.7, 125.2, 111.5, 62.1, 61.3, 54.1, 52.7, 52.6, 47.7, 43.0, 13.6; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 198.7, 167.9, 167.9, 167.3, 148.5, 142.9, 131.9, 130.4, 128.7, 128.6, 125.1, 118.4, 62.3, 60.2, 53.6, 52.8, 52.5, 48.2, 43.9, 13.9; HRMS (ESI) m/z calcd For $C_{25}H_{24}N_2O_9[M+Na]^+$: 519.1374. Found 519.1373.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-nitrophenyl)-pentan-4-one (3l):



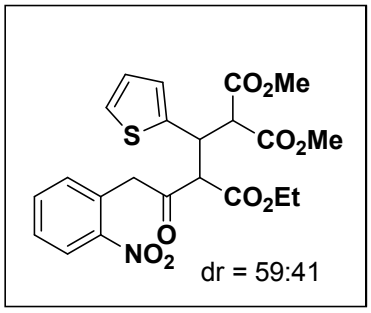
Yield 85%; IR (KBr) ν 2956, 2852, 2360, 2340, 1744, 1739, 1608, 1580, 1526, 1437, 1406, 1349, 1244, 1157, 1111 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 68:32) 8.13-8.16 (m, 1.68H), 8.09-8.11 (m, 0.68H), 8.04-8.07 (m, 0.32H), 7.59-7.63 (m, 0.68H), 7.51-7.58 (m, 2.32H), 7.41-7.51 (m, 1.32H), 7.30-7.32 (m, 0.68H), 6.99-7.01 (m, 0.32H), 4.73 (d, *J* = 10.3 Hz, 0.68H), 4.68 (d, *J* = 9.04 Hz, 0.32H), 4.41-4.47 (m, 1.32H), 4.29-4.36 (m, 1H), 4.20-4.24 (m, 1H), 4.07-4.18 (m, 0.68H), 3.97-4.03 (m, 1.32H), 3.90-3.92 (m, 0.68H), 3.69 (s, 0.96H), 3.61 (s, 2.04H), 3.58 (s, 2.04H), 3.56 (s, 0.96H), 1.29 (t, *J* = 7.28 Hz, 0.96H), 1.04 (t, *J* = 7.28 Hz, 2.04H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.5, 168.1, 167.9, 166.5, 148.5, 147.3, 145.5, 133.7, 133.6, 130.3, 128.8, 128.8, 125.3, 123.3, 62.3, 61.3, 54.1, 52.8, 52.7, 47.8, 42.8, 13.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 198.7, 168.0, 167.9, 167.4, 148.5, 147.3, 145.1, 133.3, 130.7, 129.1, 128.7, 125.3, 123.4, 62.5, 60.2, 53.6, 52.9, 52.7, 48.2, 43.7, 14.0; HRMS (ESI) m/z calcd For $C_{24}H_{24}N_2O_{11}[M+Na]^+$: 539.1272. Found 539.1272.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(4-trifluoromethylphenyl)-pentan-4-one (3m):



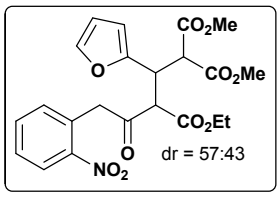
Yield 74%; IR (KBr) ν 2961, 1748, 1722, 1617, 1580, 1531, 1460, 1439, 1422, 1407, 1350, 1325, 1268 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 69:31) 8.12-8.15 (m, 0.69H), 8.04-8.06 (m, 0.31H), 7.58-7.62 (m, 0.69H), 7.50-7.54 (m, 2.31H), 7.44-7.48 (m, 2.69H), 7.41-7.43 (m, 0.31H), 7.29-7.32 (m, 0.69H), 6.81-6.84 (m, 0.31H), 4.70 (d, *J* = 10.3 Hz, 0.69H), 4.62 (d, *J* = 9.3 Hz, 0.31H), 4.38-4.46 (m, 1.31H), 4.28-4.32 (m, 1H), 4.18-4.24 (m, 1.31H), 3.95-4.00 (m, 1.69H), 3.87-3.92 (m, 0.69H), 3.68 (s, 0.93H), 3.60 (s, 2.07H), 3.55 (s, 3H), 1.28 (t, *J* = 7.04 Hz, 0.93H), 0.99 (t, *J* = 7.28 Hz, 2.07H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.7, 168.3, 168.0, 166.7, 148.6, 142.0, 133.7, 133.6, 130.0, 129.7 (m), 129.6, 129.2, 128.7, 125.3, 125.2, 62.1, 61.7, 54.5, 52.7, 52.6, 47.7, 43.0, 13.6; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 198.9, 168.2, 168.1, 167.5, 148.6, 141.6, 133.5, 133.2, 129.7, 128.7, 125.3, 125.1, 122.6, 62.3, 60.4, 53.9, 52.8, 52.6, 48.4, 43.9, 13.9; HRMS (ESI) m/z calcd For $C_{25}H_{24}F_3NO_9[M+K]^+$: 578.1035. Found 578.1049.

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(thiophen-2-yl)-pentan-4-one (3n):



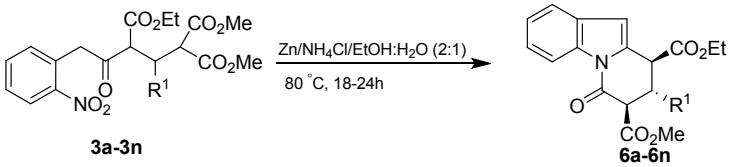
Yield 81%; IR (KBr) ν 3443, 3113, 2957, 2924, 2853, 2359, 2335, 1746, 1662, 1614, 1578, 1527, 1437, 1406, 1349, 1263, 1158, 1096 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 59:41) 8.11-8.14 (m, 0.59H), 8.05-8.08 (m, 0.41H), 7.57-7.61 (m, 0.82H), 7.47-7.52 (m, 1.18H), 7.41-7.44 (m, 0.59H), 7.27-7.29 (m, 0.41H), 7.16-7.20 (m, 1.0H), 6.96-6.97 (m, 0.41H), 6.92-6.95 (m, 0.59H), 6.87-6.89 (m,1H), 4.69-4.71 (m, 0.59H), 4.60-4.64 (m, 1H), 4.51-4.56 (m, 0.41H), 4.36-4.40 (m, 0.82H), 4.27-4.32 (m, 1H), 4.2-4.25 (m, 1.17H), 4.05-4.07 (m, 1H), 3.93-3.99 (m, 1.0H), 3.70 (s, 1.23H), 3.64 (s, 1.77H), 3.62 (s, 1.23H), 3.61 (s, 1.77H), 1.29 (t, *J* = 7.0 Hz, 1.23H), 1.10 (t, *J* = 7.28 Hz, 1.77H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.9, 168.3, 168.1, 166.8, 148.6, 139.7, 133.7, 133.6, 129.3, 128.6, 127.3, 126.4, 125.3, 125.2, 62.5, 62.0, 54.8, 52.6, 52.6, 47.7, 38.7, 13.7 (minor diastereomer) 199.1, 168.2, 168.1, 167.5, 148.7, 138.9, 133.5, 133.4, 129.1, 128.5, 128.5, 126.5, 125.7, 125.1, 62.2, 60.8, 54.4, 52.7, 52.5, 48.5, 39.8, 13.9; HRMS (ESI) m/z calcd For $C_{22}H_{23}SNO_9[M+Na]^+$: 500.0986. Found 500.0966

3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-5-(2-nitrophenyl)-2-(2-furyl)-pentan-4-one (3o):



Yield 78%; IR (KBr) ν 3448, 2957, 2927, 2852, 2361, 2340, 1746, 1613, 1580, 1528, 1437, 1409, 1349, 1265, 1159, 1097 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (mixture of diastereomers dr = 57:43) 8.11-8.13 (m, 0.57H), 8.05-8.07 (m, 0.43H), 7.57-7.61 (m, 0.57H), 7.49-7.53 (m, 0.43H), 7.44-7.48 (m, 0.57H), 7.39-7.43 (m, 0.43H), 7.28-7.32 (m, 1.43H), 6.99-7.01 (m, 0.57H), 6.28-6.30 (m, 0.43H), 6.24-6.29 (m, 1.57H), 4.60 (d, *J* = 9.8 Hz, 0.57H), 4.55 (d, *J* = 9.5 Hz, 0.43H), 4.45-4.49 (m, 0.86H), 4.37-4.43 (m, 1.14H), 4.31-4.32 (m, 0.86H), 4.23-4.29 (m, 1.14H), 4.10-4.13 (m, 1H), 4.00-4.03 (m, 0.57H), 3.87-3.88 (m, 0.43H), 3.72 (s, 1.29H), 3.67 (s, 1.71H), 3.64 (s, 1.29H), 3.62 (s, 1.71H), 1.31 (t, *J* = 7.28 Hz, 1.29H), 1.16 (t, *J* = 7.0 Hz, 1.71H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 198.7, 168.2, 168.0, 166.9, 151.2, 148.7, 141.8, 133.7, 133.3, 129.3, 128.6, 125.2, 110.4, 108.5, 62.0, 60.1, 52.8, 52.6, 52.6, 47.6, 37.2, 13.8; ^{13}C NMR (100 MHz, $CDCl_3$) δ (minor diastereomer) 198.6, 168.1, 168.0, 167.5, 150.9, 148.9, 141.8, 133.5, 129.0, 128.5, 125.1, 110.8, 109.5, 62.2, 58.9, 52.8, 52.7, 47.9, 37.8, 13.9; HRMS (ESI) m/z calcd For $C_{22}H_{23}NO_{10}[M+Na]^+$: 484.1214. Found 484.1214.

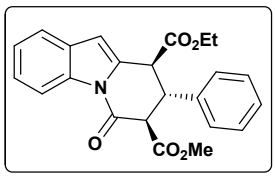
General procedure for the diastereoselective synthesis of substituted 8,9-dihydropyrido[1,2-*a*]indole-6(7*H*)-ones:



3a-3n **6a-6n**

To a stirred mixture of compound (**3a-n**, 0.1 mmol)] in EtOH/H_2O ratio (4.5 mL, 2:1) was added Zn-dust (0.3 mmol) and NH_4Cl (1.0 mmol) and heated at 80 °C for 18-24 h (monitored by TLC). After that, solvent was evaporated by rotary evaporator under reduced pressure. The crude product was diluted with ethyl acetate and filtered through celite-545, washed with ethyl acetate. The filtrate was concentrated under reduced pressure to leave the crude residue which was purified by column chromatography over silica-gel 230-400 mesh using EtOAc/hexane as eluent to furnish the pure product. All the products were fully characterized by their corresponding spectroscopic data (IR, ^1H and ^{13}C NMR and HRMS).

***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-phenyl-8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one (6a):**



Yield 80%; dr = 95:5; IR (KBr) ν 3443, 3286, 2924, 2852, 2361, 2340, 1746, 1702, 1595, 1572, 1496, 1455, 1380, 1355, 1262, 1149, 1096 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (major diastereomer **5a**) 8.44 (d, *J* = 8.5 Hz, 1H), 7.51 (d, *J* = 7.04 Hz, 1H), 7.27-7.38 (m, 7H), 6.43 (s, 1H), 4.26-4.29 (m, 1H), 4.05-4.18 (m, 4H), 3.61 (s, 3H), 1.09 (t, *J* = 7.24 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer **5a**) 169.2, 167.9, 164.3, 137.1, 134.9, 133.4, 129.6, 128.9, 128.3, 127.7, 125.3, 124.8, 120.5, 116.6, 107.0, 61.7, 57.0, 52.7, 47.7, 45.3, 13.9; HRMS (ESI) m/z calcd For $C_{23}H_{21}NO_5[M+Na]^+$: 414.1312. Found 414.1319.

The relative configuration of major diastereomer was confirmed by its single crystal x-ray diffraction data.

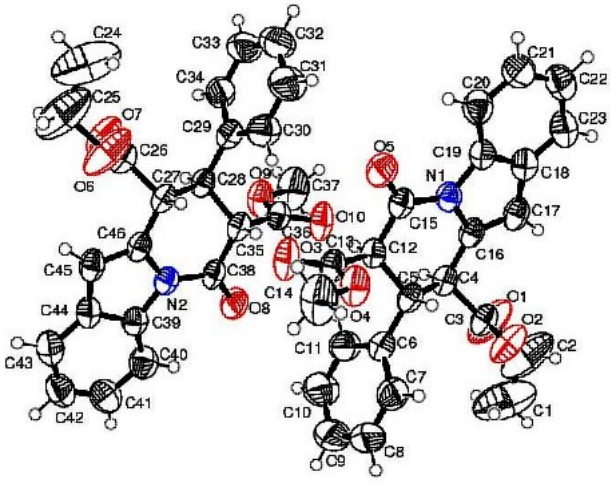
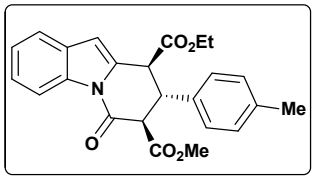


Figure 1. ORTEP diagram of compound **6a**, thermal ellipsoid drawn at the 50% probability level.

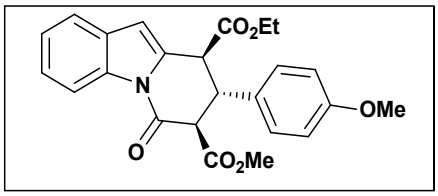
Table 1. Crystal data for compound 6a.

Compound	Compound **6a**
Empirical formula	C46 H42 N2 O10
Molecular weight	782.82
Temperature	150(2) K
Wavelength (Å)	0.71073 A
Crystal system, space group	Triclinic, P -1

a (Å) *b* (Å) *c* (Å) α (°) β (°) γ (°)	a = 9.8354(5) A b = 13.4213(8) A c = 16.8559(9) A alpha = 95.977(4) deg. beta = 103.638(4) deg. gamma = 102.512(4) deg.
Volume (Å^3)	2082.5(2) A^3
Z, Calculated density (mg/m^3)	2, 1.248 Mg/m^3
Absorption coefficient (mm^{-1})	0.088 mm^-1
F(000)	824
Crystal size (mm)	0.08 x 0.06 x 0.05 mm
θ range (deg)	2.92 to 25.00 deg.
Limiting indices	-11<=h<=11, -15<=k<=15, -20<=l<=19
Reflections collected / unique	19605 / 7324 [R(int) = 0.0325]
Completeness to θ = 25	99.8 %
Max. and min. transmission	0.9956 and 0.9930
Data / restraints / parameters	7324 / 0 / 527
Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0711, wR2 = 0.2285
R indices (all data)	R1 = 0.1252, wR2 = 0.2855
Largest diff. peak and hole (e.A^{-3})	0.581 and -0.409 e.A^-3
CCDC	**1045133**

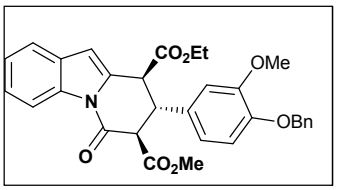
***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-(4-methylphenyl)-8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one (6c):** 

Yield 77%; dr = 96:4; **IR** (KBr) ν 3442, 2955, 2925, 2853, 2360, 2340, 1753, 1729, 1706, 1594, 1573, 1515, 1456, 1357, 1319, 1291, 1263, 1229, 1194, 1147, 1096 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.44 (d, *J* = 8.04 Hz, 1H), 7.50 (d, *J* = 7.28 Hz, 1H), 7.28-7.37 (m, 2H), 7.11-7.21 (m, 4H), 6.42 (s, 1H), 4.23-4.26 (m, 1H), 4.03-4.14 (m, 4H), 3.63 (s, 3H), 2.32 (s, 3H), 1.12 (t, *J* = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 169.3, 167.9, 164.5, 138.0, 135.0, 134.0, 133.6, 129.7, 129.6, 127.5, 125.3, 124.7, 120.5, 116.6, 107.0, 61.7, 57.1, 52.6, 47.8, 44.9, 21.1, 14.0; HRMS (ESI) m/z calcd For $C_{24}H_{23}NO_5$[M+Na]$^+$: 428.1468. Found 428.1469.

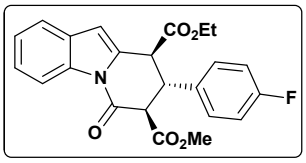
***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-(4-methoxyphenyl)-8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one (6d):** 

Yield 81%; dr = 93: 7; IR (KBr) ν 3443, 2955, 2924, 2852, 2360, 2340, 2267, 1740, 1699, 1611, 1572, 1514, 1455, 1382, 1250, 1213, 1179, 1153, 1108 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.47 (d, *J* = 8.04 Hz, 1H), 7.53 (d, *J* = 7.28 Hz, 1H), 7.29-7.40 (m, 3H), 7.23-7.24 (m, 1H), 6.88-

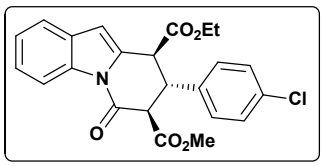
6.90 (m, 2H), 6.44 (s, 1H), 4.24-4.27 (m, 1H), 4.04-4.19 (m, 4H), 3.83 (s, 3H), 3.66 (s, 3H), 1.16 (t, J = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 169.3, 167.9, 164.4, 159.3, 135.0, 133.6, 129.7, 129.1, 128.8, 125.3, 124.7, 120.5, 116.6, 114.3, 106.9, 61.7, 57.2, 55.2, 52.6, 48.0, 44.6, 14.0; HRMS (ESI) m/z calcd For $C_{24}H_{23}NO_6[M+Na]^+$: 444.1418. Found 444.1431.

***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-(4-benzyloxy-3-methoxyphenyl)-8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one (6e):** 

Yield 78%; dr = 90:10; IR (KBr) ν 3440, 2926, 2852, 2360, 1744, 1704, 1594, 1573, 1517, 1454, 1374, 1264, 1144, 1107 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.44 (d, J = 8.04 Hz, 1H), 7.50 (d, J = 6.8 Hz, 1H), 7.42-7.43 (m, 2H), 7.28-7.38 (m, 5H), 6.76-6.86 (m, 3H), 6.42 (s, 1H), 5.13 (s, 2H), 4.21-4.24 (m, 1H), 4.01-4.15 (m, 4H), 3.87 (s, 3H), 3.63 (s, 3H), 1.11 (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 169.3, 168.0, 164.4, 149.6, 147.9, 136.9, 134.9, 133.5, 130.1, 129.6, 128.5, 127.9, 127.3, 125.3, 124.8, 120.5, 119.6, 116.5, 114.0, 111.5, 107.0, 70.9, 61.7, 57.1, 56.1, 52.7, 47.8, 44.9, 14.0; HRMS (ESI) m/z calcd For $C_{31}H_{29}NO_7[M+Na]^+$: 550.1836. Found 550.1836.

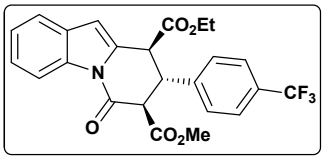
***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-(4-fluorophenyl)-8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one (6f):** 

Yield 73%; dr = 95:5; IR (KBr) ν 2926, 2853, 2380, 2349, 1742, 1698, 1654, 1601, 1577, 1509, 1456, 1379, 1265, 1223, 1156, 1101 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.43 (d, J = 8.04 Hz, 1H), 7.51 (d, J = 7.24 Hz, 1H), 7.27-7.38 (m, 4H), 7.02-7.06 (m, 2H), 6.43 (s, 1H), 4.20-4.24 (m, 1H), 4.01-4.17 (m, 4H), 3.63 (s, 3H), 1.12 (t, J = 7.28 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ(major diastereomer) 169.1, 167.7, 164.1, 134.9, 133.2, 129.6, 129.5, 129.4, 125.4, 124.8, 120.6, 116.5, 116.0, 115.8, 107.1, 61.8, 57.0, 52.7, 47.8, 44.6, 14.0; HRMS (ESI) m/z calcd For $C_{23}H_{20}FNO_5[M+Na]^+$: 432.1218. Found 432.1217.

***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-(4-chlorophenyl)-8,9-dihydropyrido[1,2*a*]indol-6(7*H*)-one (6h):** 

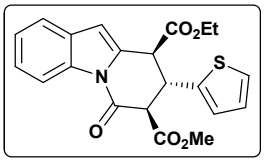
Yield 75%; dr = 95:5; IR (KBr) ν 3442, 2963, 2924, 2854, 2362, 2331, 1749, 1703, 1596, 1572, 1494, 1455, 1378, 1261, 1146, 1096 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.43 (d, J = 7.28 Hz, 1H), 7.51 (d, J = 7.28 Hz, 1H), 7.29-7.38 (m, 4H), 7.22-7.26 (m, 2H), 6.43 (s, 1H), 4.21-4.24 (m, 1H), 4.07-4.17 (m, 3H), 4.01-4.04 (m, 1H), 3.64 (s, 3H), 1.14 (t, J = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 169.0, 167.7, 164.0, 135.7, 135.0, 134.2, 133.0, 129.6, 129.2, 129.1, 125.4, 124.9, 120.6, 116.6, 107.2, 61.9, 56.8, 52.8, 47.6, 44.6, 14.0; HRMS (ESI) m/z calcd For $C_{23}H_{20}ClNO_5[M+Na]^+$: 448.0922. Found 448.0921.

***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-(4-trifluoromethylphenyl)-8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one (6m):**



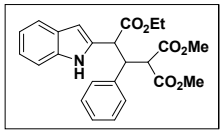
Yield 62%; dr = 93:7; IR (KBr) ν 3444, 2961, 2924, 2853, 2361, 2340, 1743, 1698, 1621, 1601, 1578, 1557, 1540, 1457, 1382, 1326, 1262, 1211, 1172, 1129, 1069 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.44 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.04 Hz, 2H), 7.52 (d, *J* = 7.04 Hz, 1H), 7.44 (d, *J* = 8.04 Hz, 2H), 7.30-7.39 (m, 2H), 6.45 (s, 1H), 4.21-4.30 (m, 2H), 4.06-4.16 (m, 3H), 3.64 (s, 3H), 1.12 (t, *J* = 7.28 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 168.8, 167.5, 163.7, 141.3, 135.0, 132.8, 129.5, 128.3, 126.0, 125.9, 125.5, 124.9, 122.5, 120.6, 116.6, 107.4, 61.9, 56.6, 52.8, 47.4, 44.9, 13.9; HRMS (ESI) m/z calcd For $C_{24}H_{20}NO_5F_3[M+K]^+$: 498.0925. Found 498.0946.

***(trans-trans-trans)*-9-Ethoxycarbonyl-7-methoxycarbonyl-8-(thiophen-2-yl)-8,9-dihydropyrido[1,2-*a*]indol-6(7*H*)-one (6n):**

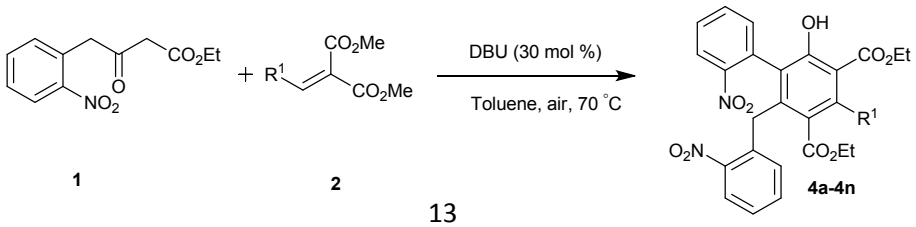


Yield 61%; dr = 4:1; IR (KBr) ν 3450, 2958, 2925, 2853, 2361, 2341, 1741, 1706, 1595, 1571, 1456, 1379, 1262, 1180, 1151, 1105 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (major diastereomer) 8.44 (d, *J* = 8.3 Hz, 1H), 7.51 (d, *J* = 6.8 Hz, 1H), 7.30-7.37 (m, 2H), 7.23-7.24 (m, 1H), 6.92-6.70 (m, 2H), 6.45 (s, 1H), 4.44-4.53 (m, 1H), 4.16-4.26 (m, 3H), 4.02-4.04 (m, 1H), 3.72 (s, 3H), 1.20 (t, *J* = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major diastereomer) 169.0, 167.7, 163.6, 140.4, 134.9, 132.8, 129.6, 127.0, 126.2, 125.4, 125.2, 124.8, 120.6, 116.6, 107.3, 62.0, 57.9, 52.8, 48.7, 40.6, 14.0; HRMS (ESI) m/z calcd For $C_{21}H_{19}NO_5S[M+Na]^+$: 420.0876. Found 420.0895.

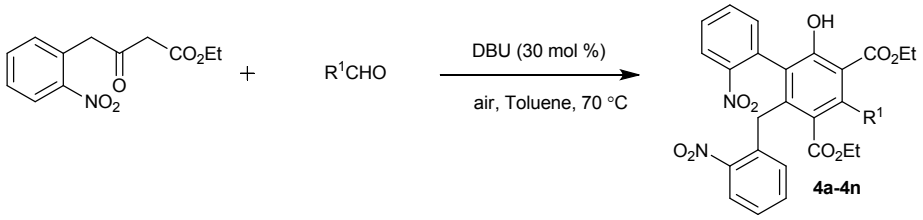
3-Ethoxycarbonyl-1,1-dimethoxycarbonyl-2-phenyl-3-(1H-indol-2-yl]propane (5a): ^1H NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 1H), 7.54-7.56 (m, 1H), 7.34-7.38 (m, 1H), 7.31-7.33 (m, 2H), 7.26-7.29 (m, 2H), 7.22-7.25 (m, 1H), 7.15-7.20 (m, 1H), 7.06-7.10 (m, 1H), 6.50-6.51 (m, 1H), 4.54 (d, *J* = 11.3 Hz, 1H), 4.17-4.21 (m, 1H), 3.80-3.93 (m, 2H), 3.75 (d, *J* = 7 Hz, 1H), 3.35 (s, 3H), 3.29 (s, 3H), 0.90 (t, *J* = 7.28 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.6, 168.9, 167.9, 137.9, 136.5, 131.9, 128.9, 128.3, 128.0, 127.8, 122.2, 120.3, 119.9, 111.1, 103.8, 61.2, 55.2, 52.4, 52.3, 49.5, 48.6, 13.7; **HRMS** (ESI) m/z calcd For $C_{24}H_{25}NO_6[M+Na]^+$: 446.1574. Found 446.1571



General procedure for the synthesis of ploy-substituted salicylate derivatives (4a-4n):

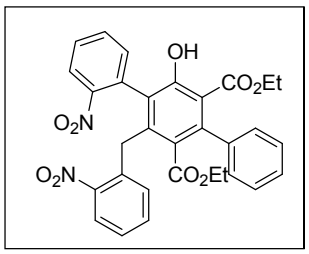


Method A: A mixture of ethyl-4-(2-nitrophenyl)-3-oxobutanoate(**1**, 0.5 mmol), alkylidene malonates (**2a-n**, 0.25 mmol), H_2O (0.25 mmol) and DBU (30 mol%) in toluene (0.5 mL) under air was heated at 70 ˚C for 24-28h (monitored by TLC). After that, toluene was evaporated by rotary evaporator under reduced pressure. The crude product was extracted with ethyl acetate, washed with aqueous diluted HCl, brine and dried over Na_2SO_4. The evaporation of the solvent gave the crude product which was purified by column chromatography over silica-gel 230-400 mesh using EtOAc/hexane as eluent (1:9 to 1:5) to furnish the pure product. All the products were fully characterized by their corresponding spectroscopic data (IR, ^1H and ^{13}C NMR and HRMS).



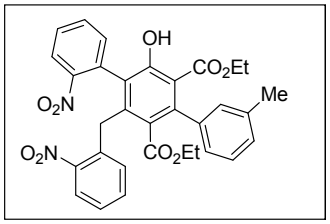
Method B: To a stirred mixture of ethyl-4-(2-nitrophenyl)-3-oxobutanoate(**1**, 0.5 mmol) and aldehydes (0.25 mmol) in toluene (0.5 mL) was added catalyst DBU (30 mol%) and heated at 70 ˚C under air. The reaction was monitored by TLC. After completion of the reaction, the reaction mixture was extracted with ethyl acetate, washed with aqueous diluted HCl, brine and dried over Na_2SO_4. The evaporation of the solvent gave the crude product which was purified by column chromatography over silica-gel 230-400 mesh using EtOAc/hexane as eluent (1:9 to 1:5) to furnish the pure product. All the products were fully characterized by their corresponding spectroscopic data (IR, ^1H and ^{13}C NMR and HRMS).

2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-phenylphenol(4a):



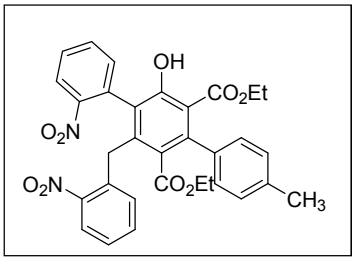
^1H NMR (400 MHz, $CDCl_3$) δ 11.4 (s, 1H), 8.02-8.05 (m, 1H), 7.66-7.68 (m, 1H), 7.56-7.60 (m, 1H), 7.49-7.53 (m, 1H), 7.41-7.45 (m, 1H), 7.27-7.35 (m, 5H), 7.21-7.25 (m, 2H), 7.15-7.17 (m, 1H), 4.26-4.30 (m, 1H), 4.09-4.13 (m, 1H), 3.91-3.97 (m, 2H), 3.62-3.69 (m, 2H), 0.69-0.73 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 168.4, 159.5, 148.6, 148.3, 142.2, 140.0, 139.1, 133.6, 133.4, 132.9, 132.1, 130.3, 129.6, 129.4, 129.0, 128.5, 128.0, 127.4, 127.4, 127.3, 127.1, 124.9, 123.9, 111.5, 61.6, 61.2, 33.4, 13.4, 12.8; HRMS (ESI) m/z calcd For $C_{31}H_{26}N_2O_9[M+Na]^+$: 593.1531. Found 593.1535.

2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(3-methylphenyl)phenol(4b):



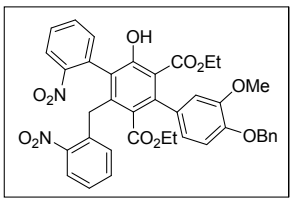
^{1}H NMR (400 MHz, $CDCl_3$) δ 11.4 (s, 1H), 8.02-8.04 (m, 1H), 7.66-7.68 (m, 1H), 7.56-7.60 (m, 1H), 7.49-7.53 (m, 1H), 7.41-7.45 (m, 1H), 7.29-7.31 (m, 1H), 7.19-7.26 (m, 2H), 7.12-7.16 (m, 3H), 7.00-7.03 (m, 1H), 4.25-4.30 (m, 1H), 4.08-4.12 (m, 1H), 3.88-4.00 (m, 2H), 3.66-3.69 (m, 2H), 2.35 (s, 3H), 0.69-0.74 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 170.5, 168.4, 159.4, 148.5, 148.3, 142.4, 139.6, 139.0, 136.8, 136.8, 133.6, 133.4, 133.4, 132.9, 132.2, 132.1, 130.3, 129.5, 129.5, 129.4, 129.1, 127.9, 127.8, 127.3, 127.3, 127.1, 126.0, 125.6, 124.9, 123.9, 111.5, 61.5, 61.1, 33.4, 21.3, 13.3, 12.8; **HRMS** (ESI) m/z calcd For $C_{32}H_{28}N_2O_9[M+Na]^+$: 607.1687. Found 607.1684.

2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(4-methylphenyl)phenol(4c):



^{1}H NMR (400 MHz, $CDCl_3$) δ 11.4 (s, 1H), 8.01-8.03 (m, 1H), 7.66-7.68 (m, 1H), 7.56-7.59 (m, 1H), 7.48-7.52 (m, 1H), 7.41-7.44 (m, 1H), 7.29-7.31 (m, 1H), 7.21-7.24 (m, 2H), 7.08-7.16 (m, 4H), 4.25-4.30 (m, 1H), 4.07-4.12 (m, 1H), 3.92-3.97 (m, 2H), 3.66-3.70 (m, 2H), 2.38 (s, 3H), 0.70-0.76 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 170.6, 168.5, 159.3, 148.5, 148.3, 142.3, 138.9, 137.0, 136.8, 133.6, 133.6, 133.4, 132.9, 132.1, 132.1, 130.3, 129.7, 129.4, 128.7, 128.3, 128.0, 128.0, 127.7, 127.1, 124.9, 123.9, 111.7, 61.6, 61.1, 33.4, 21.2, 13.4, 12.8; HRMS (ESI) m/z calcd For $C_{32}H_{28}N_2O_9[M+Na]^+$: 607.1687. Found 607.1694.

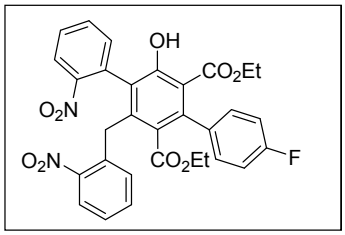
2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(3-methoxy-4-benzyloxyphenyl)phenol(4e):



^{1}H NMR (400 MHz, $CDCl_3$) δ 11.3 (s, 1H), 8.02-8.04 (m, 1H), 7.66-7.68 (m, 1H), 7.49-7.59 (m, 2H), 7.44-7.55 (m, 3H), 7.34-7.37 (m, 2H), 7.26-7.31 (m, 3H), 7.12-7.17 (m, 1H), 6.79-6.91 (m, 2H), 6.67-6.69 (m, 1H), 5.21 (s, 2H), 4.25-4.29 (m, 1H), 4.08-4.13 (m, 1H), 3.87-3.95 (m, 5H), 3.65-3.74 (m, 2H), 0.73-0.74 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 170.5, 168.5, 168.4, 159.3 (159.3*), 148.9 (148.8*), 148.5 (148.5*), 148.3 (148.3*), 147.3(147.3*), 141.7 (141.7*), 139.0 (139.0*), 137.0 (137.0*), 133.6(133.6*), 133.4, 133.2, 132.9(132.8*), 132.1, 132.1, 130.3 (130.3*), 129.8, 129.4, 128.5, 127.9, 127.1, 124.9 (124.9*), 124.0 (123.9*), 121.4, 120.8, 113.2, 113.1, 113.0, 112.6, 111.7, 70.9, 61.6, 61.2 (61.1*), 56.2(56.1*), 33.4(33.3*), 13.5, 13.2; **HRMS** (ESI) m/z calcd For $C_{39}H_{34}N_2O_{11}[M+Na]^+$: 729.2201. Found 729.2199

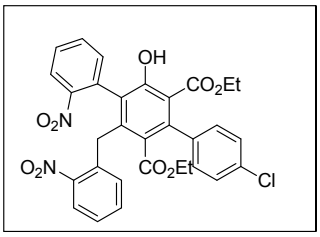
*the peak may be the existence of rotamer.

2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(4-flourophenyl)phenol(4f):



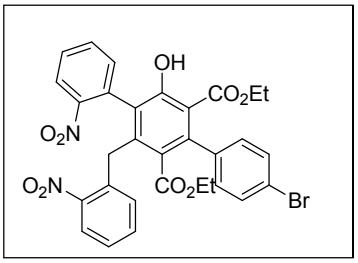
^{1}H NMR (400 MHz, $CDCl_3$) δ 11.5 (s, 1H), 8.03-8.05 (m, 1H), 7.67-7.69 (m, 1H), 7.57-7.61 (m, 1H), 7.50-7.54 (m, 1H), 7.41-7.45 (m, 1H), 7.31-7.34 (m, 1H), 7.26-7.29 (m, 2H), 7.15-7.24 (m, 2H), 7.03-7.09 (m, 2H), 4.26-4.30 (m, 1H), 4.08-4.13 (m, 1H), 3.95-4.00 (m, 2H), 3.67-3.70 (m, 2H), 0.76-0.81 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 170.4, 168.2, 162. 3 (d, *J* = 244.9 Hz), 159.7, 148.5, 148.3, 140.9, 139.1, 135.7, 135.6, 133.6, 133.2, 132.9, 132.0, 130.7 (2C), 130.2 (2C), 129.8, 129.5, 128.3, 127.2, 124.9, 124.0, 114.4 (d, *J* = 6.56 Hz), 114.2 (d, *J*= 5.83 Hz), 111.4, 61.7, 61.3, 33.4, 13.5, 13.0; **HRMS** (ESI) m/z calcd For $C_{31}H_{25}FN_2O_9[M+Na]^+$: 611.1436. Found 611.1440.

2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(4-chlorophenyl)phenol(4h):



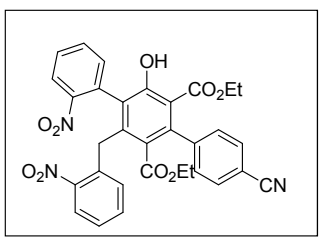
^{1}H NMR (400 MHz, $CDCl_3$) δ 11.5 (s, 1H), 8.03-8.05 (m, 1H), 7.67-7.69 (m, 1H), 7.57-7.61 (m, 1H), 7.50-7.54 (m, 1H), 7.41-7.45 (m, 1H), 7.31-7.37 (m, 3H), 7.24-7.28 (m, 2H), 7.14-7.18 (m, 2H), 4.26-4.30 (m, 1H), 4.09-4.13 (m, 1H), 3.96-3.99 (m, 2H), 3.69-3.71 (m, 2H), 0.78-0.79 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 170.2, 168.1, 159.7, 148.5, 148.2, 140.7, 139.3, 138.2, 133.6, 133.4, 133.2, 132.9, 132.0, 130.4, 130.1, 129.9, 129.5, 129.5, 128.5, 127.6, 127.5, 127.2, 124.9, 124.0, 111.1, 61.9, 61.3, 33.4, 13.4, 12.9; **HRMS** (ESI) m/z calcd For $C_{31}H_{25}ClN_2O_9[M+Na]^+$: 627.1141. Found 627.1148

2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(4-bromophenyl)phenol(4j):



^{1}H NMR (400 MHz, $CDCl_3$) δ 11.5 (s, 1H), 8.03-8.06 (m, 1H), 7.67-7.69 (m, 1H), 7.57-7.61 (m, 1H), 7.48-7.54 (m, 3H), 7.41-7.45 (m, 1H), 7.23-7.28 (m, 3H), 7.11-7.16 (m, 2H), 4.26-4.30 (m, 1H), 4.09-4.13 (m, 1H), 3.96-4.01 (m, 2H), 3.68-3.73 (m, 2H), 0.77-0.80 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 170.2, 168.1, 159.7, 148.5, 148.2, 140.7, 139.3, 138.7, 133.6, 133.2, 132.9, 132.0, 130.7, 130.5, 130.5, 130.3, 130.1, 129.5, 129.4, 128.5, 127.2, 124.9, 124.0, 121.5, 111.1, 61.9, 61.3, 33.4, 13.4, 12.9; **HRMS** (ESI) m/z calcd For $C_{31}H_{25}BrN_2O_9[M+Na]^+$: 671.0636. Found 671.0610.

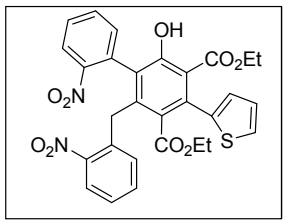
2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(4-cyanophenyl)phenol(4k):



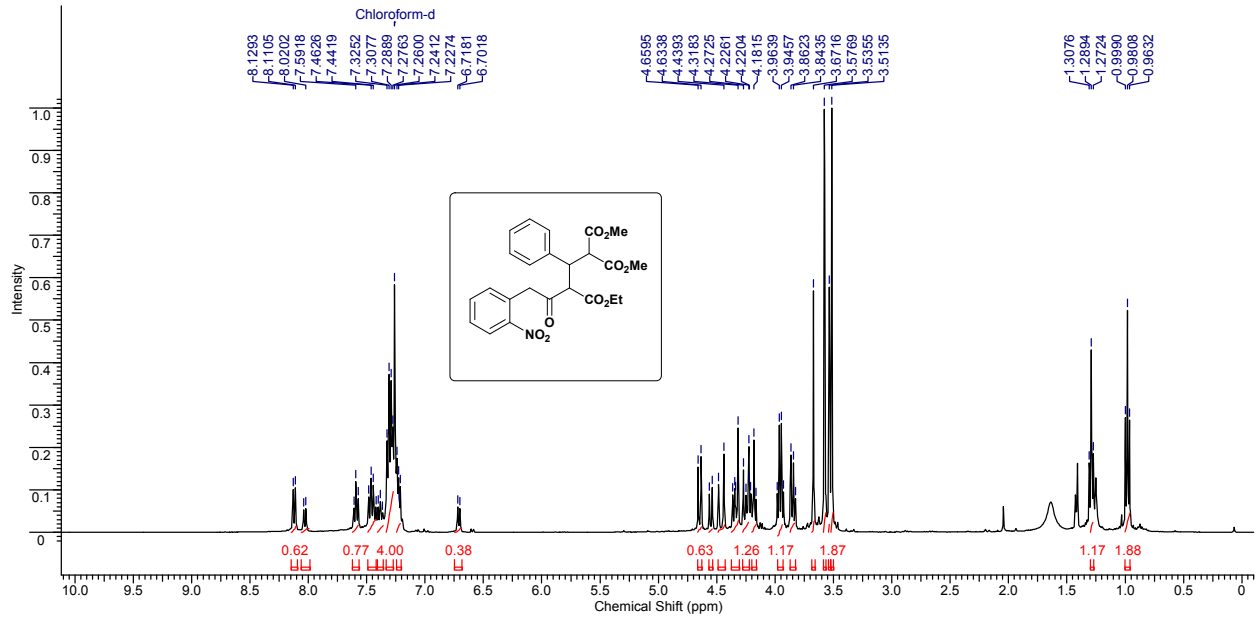
^{1}H NMR (400 MHz, $CDCl_3$) δ 11.6 (s, 1H), 8.05-8.07 (m, 1H), 7.66-7.70 (m, 3H), 7.59-7.63 (m, 1H), 7.49-7.56 (m, 2H), 7.41-7.45 (m, 1H), 7.37-7.39 (m, 1H), 7.23-7.28 (m, 2H), 7.15-7.17 (m, 1H), 4.27-4.31 (m, 1H), 4.11-4.15 (m, 1H), 3.95-4.00 (m, 2H), 3.62-3.67 (m, 2H), 0.72-0.76 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 169.8, 167.7, 160.0, 148.6, 148.2, 144.9, 139.7, 139.7, 133.7, 133.0, 132.9, 131.9, 131.9, 131.1, 131.1, 130.0, 129.9, 129.7, 129.5, 129.3, 129.0,

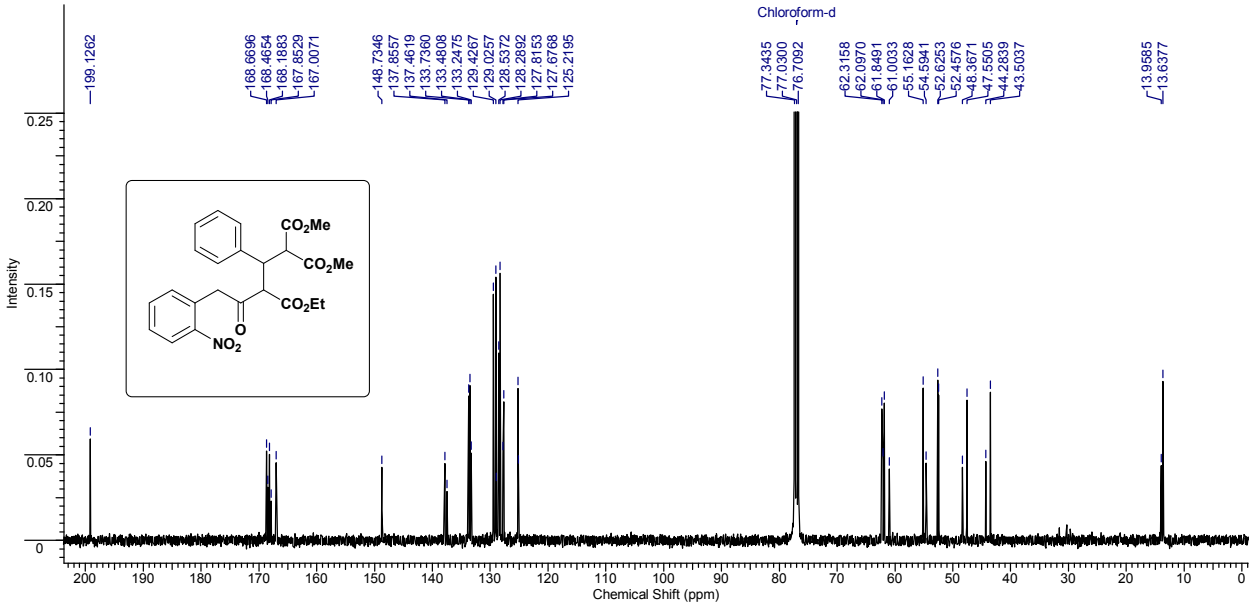
127.3, 125.0, 124.1, 118.7, 111.2, 110.5, 62.0, 61.4, 33.5, 13.4, 12.9; **HRMS** (ESI) m/z calcd For $C_{32}H_{25}N_3O_9[M+Na]^+$: 618.1483. Found 618.1485.

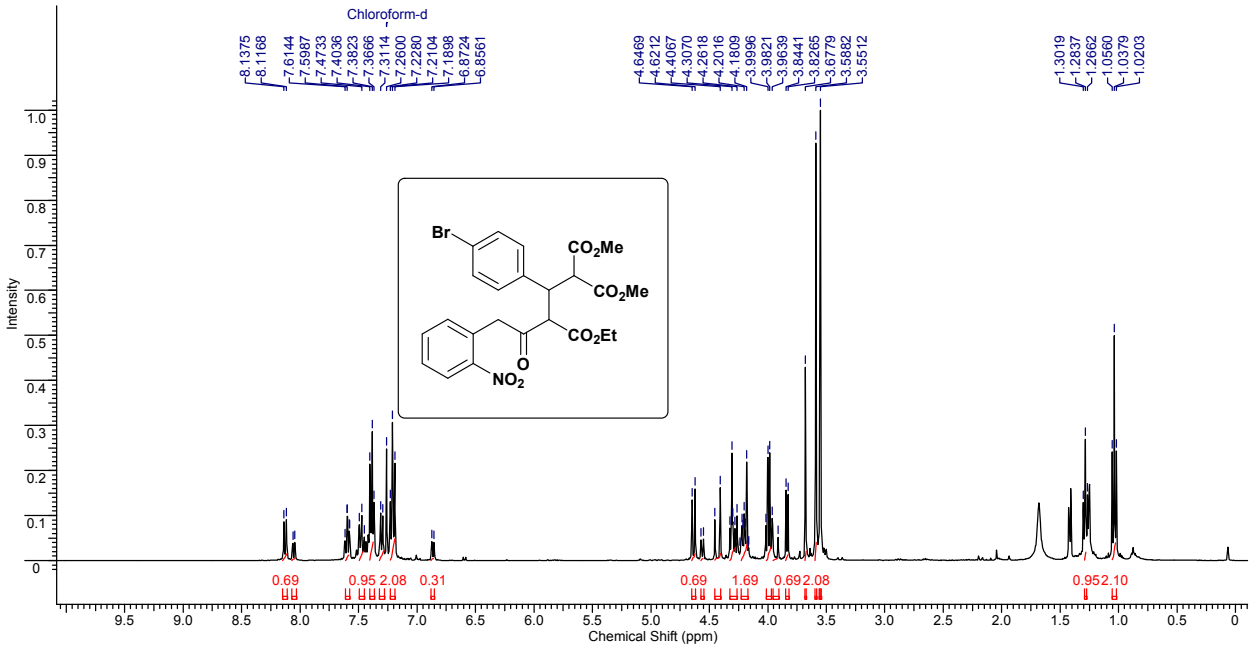
2,4-Diethoxycarbonyl-5-(2-nitrobenzyl)-6-(2-nitrophenyl)-3-(2-thiophenyl)phenol(4n):

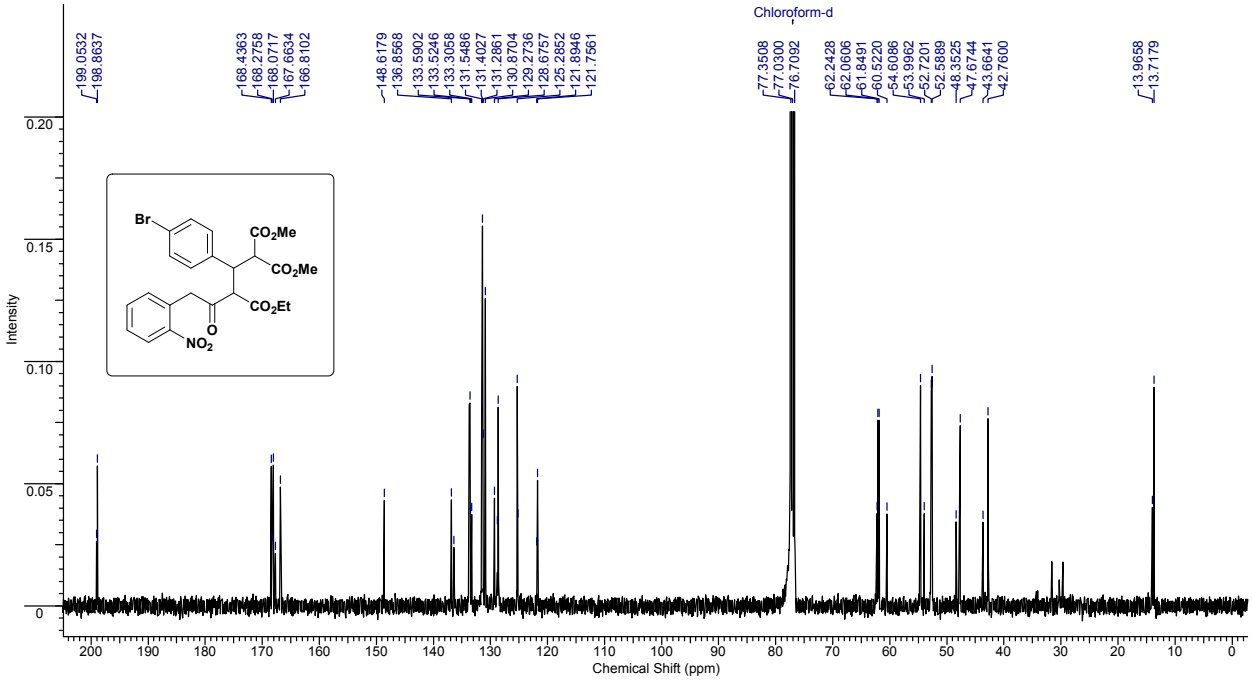


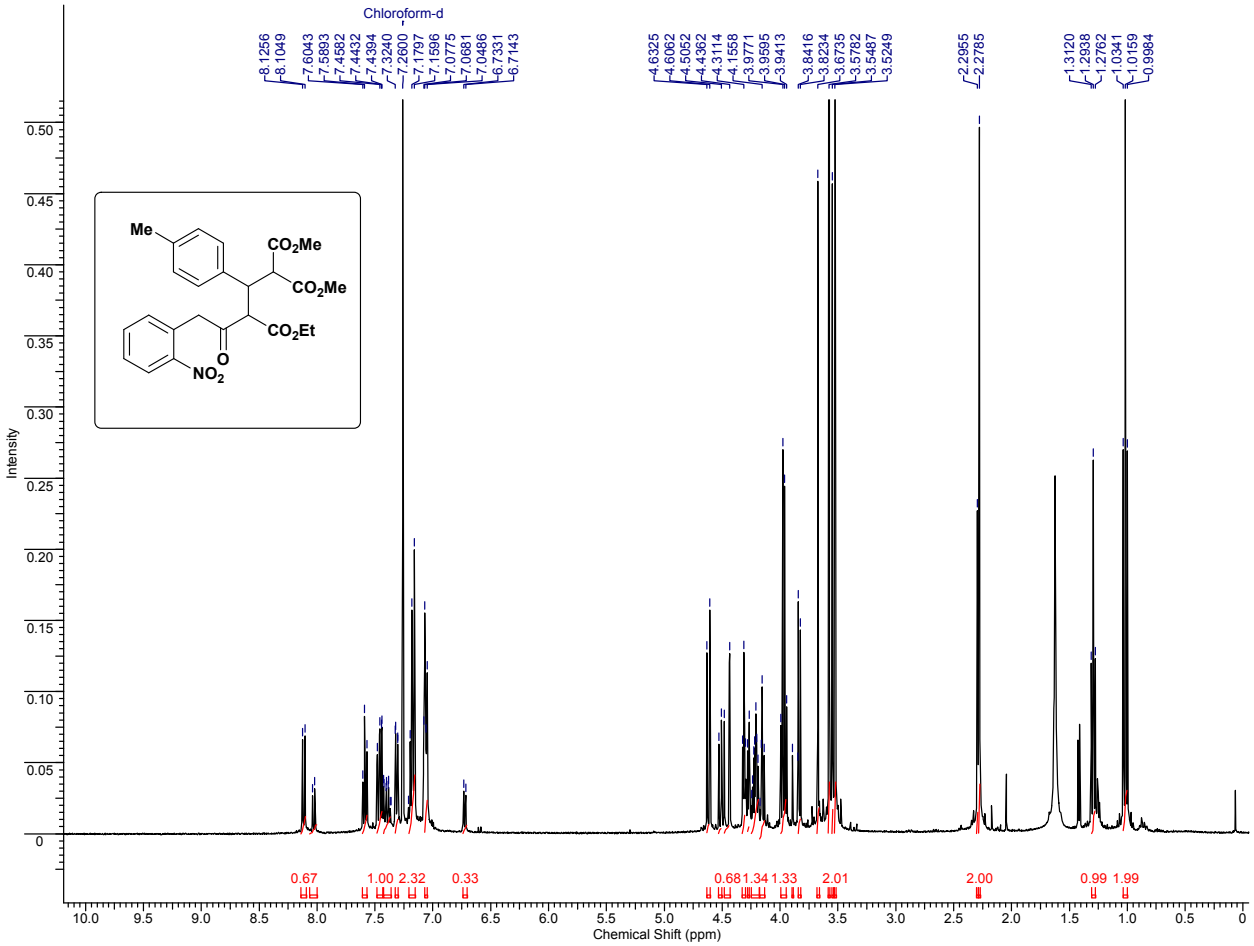
^{1}H NMR (400 MHz, $CDCl_3$) δ 11.3 (s, 1H), 8.03-8.05 (m, 1H), 7.67-7.68 (m, 1H), 7.52-7.59 (m, 2H), 7.38-7.44 (m, 2H), 7.26-7.30 (m, 2H), 7.14-7.15 (m, 1H), 7.00-7.01 (m, 2H), 4.27-4.31 (m, 1H), 4.05-4.12 (m, 3H), 3.80-3.81 (m, 2H), 0.87-0.89 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 170.2, 168.1, 159.3, 148.5, 148.1, 139.7, 138.8, 134.1, 133.7, 133.1, 132.9, 132.1, 131.9, 131.1, 130.1, 129.5, 129.1, 127.6, 127.2, 126.2, 126.1, 124.9, 123.9, 112.8, 61.8, 61.4, 33.4, 13.5, 13.0; **HRMS** (ESI) m/z calcd For $C_{29}H_{24}SN_2O_9[M+Na]^+$: 599.1095. Found 599.1095.

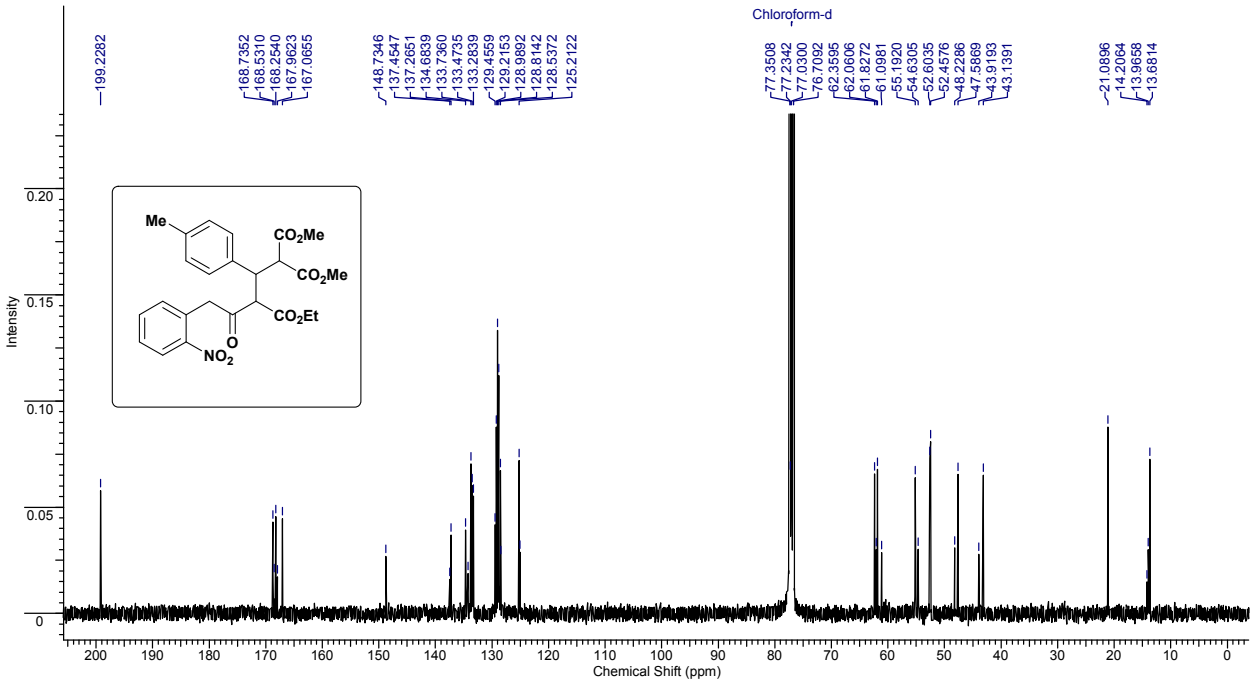

Chloroform-d
8.1293
8.1105
8.0202
7.5918
7.4626
7.4419
7.3252
7.3077
7.2889
7.2763
7.2600
7.2412
7.2274
6.7181
6.7018
4.6595
4.6338
4.4393
4.3183
4.2725
4.2261
4.2204
4.1815
3.9639
3.9457
3.8623
3.8435
3.6716
3.5769
3.5355
3.5135
1.3076
1.2894
1.2724
0.9990
0.9808
0.9632
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.62
0.77
4.00
0.38
0.63
1.26
1.17
1.87
1.17
1.88
Chemical Shift (ppm)

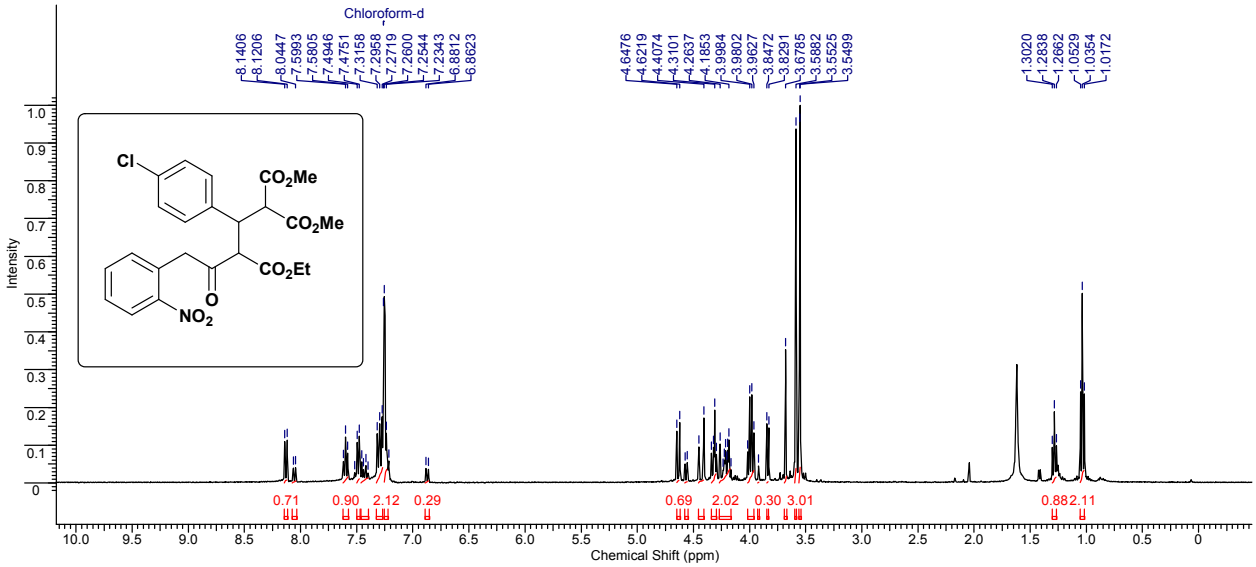

Chloroform-d
199.1262
168.6696
168.4654
168.1883
167.8529
167.0071
148.7346
137.8557
137.4619
133.7360
133.4808
133.2475
129.4267
129.0257
128.5372
128.2892
127.8153
127.6768
125.2195
77.3435
77.0300
76.7092
62.3158
62.0970
61.8491
61.0033
55.1628
54.5941
52.6253
52.4576
48.3671
47.5505
44.2839
43.5037
13.9585
13.6377
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)

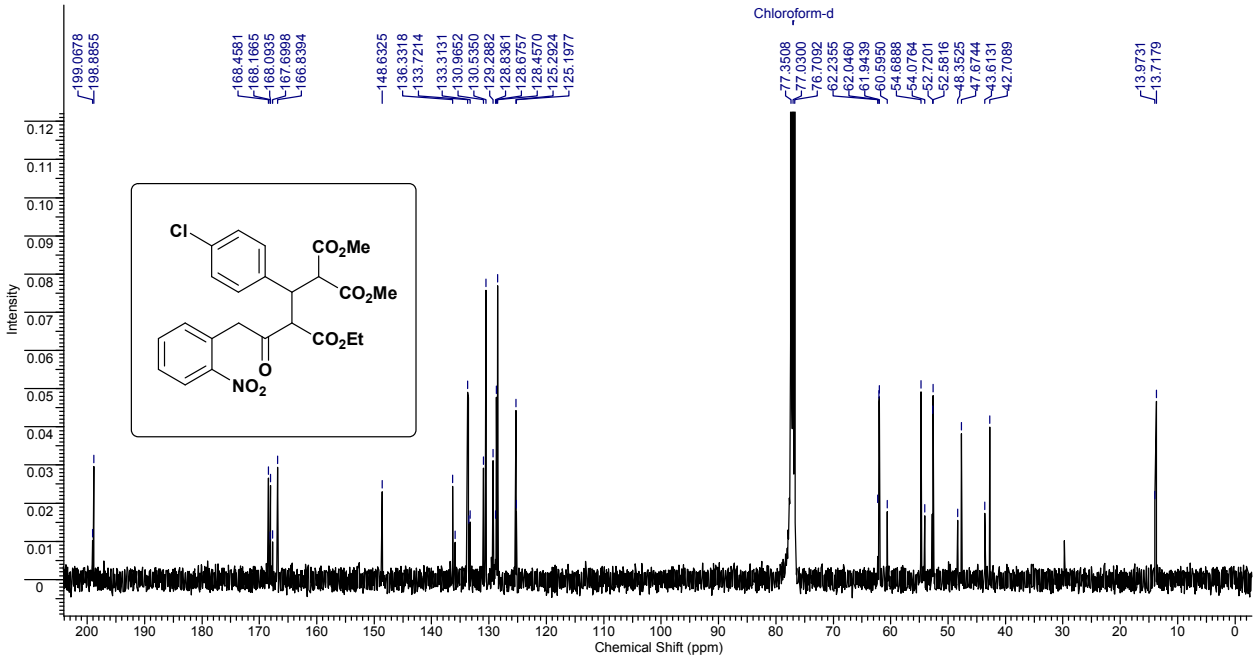

Chloroform-d
8.1375
8.1168
7.6144
7.5987
7.4733
7.4036
7.3823
7.3666
7.3114
7.2600
7.2280
7.2104
7.1898
6.8724
6.8561
4.6469
4.6212
4.4067
4.3070
4.2618
4.2016
4.1809
3.9996
3.9821
3.9639
3.8441
3.8265
3.6779
3.5882
3.5512
1.3019
1.2837
1.2662
1.0560
1.0379
1.0203
Br
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.69
0.95
2.08
0.31
0.69
1.69
0.69
2.08
0.95
2.10
Chemical Shift (ppm)

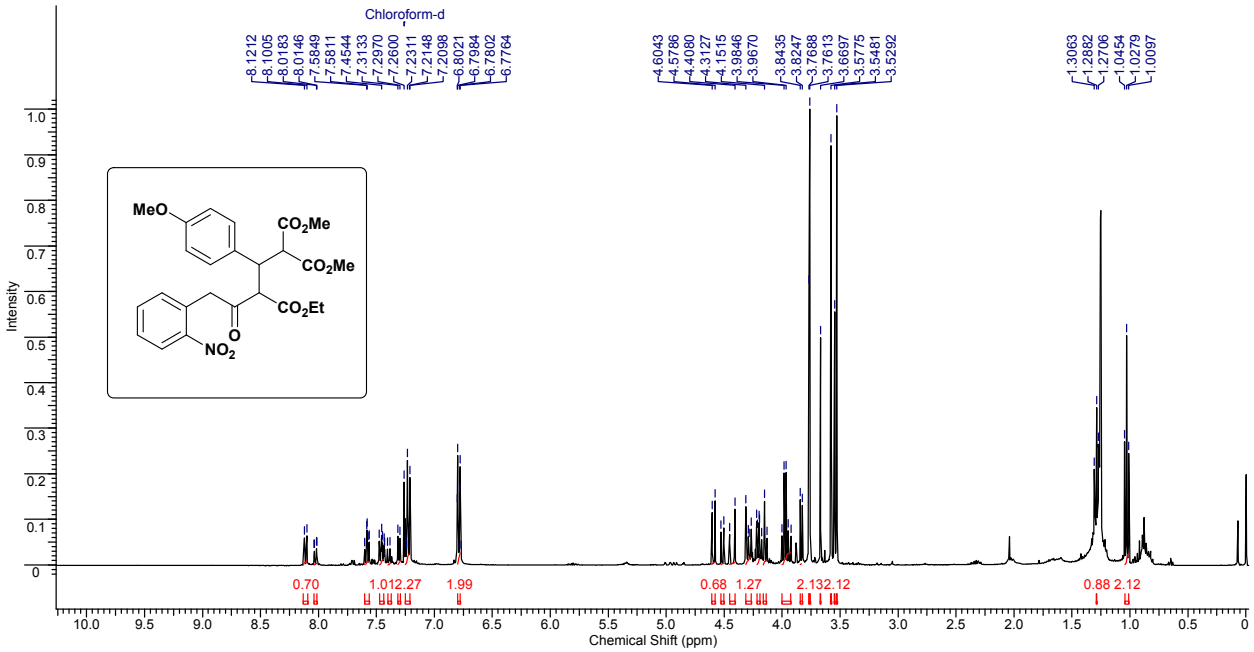

Chloroform-d
199.0532
198.8637
168.4363
168.2758
168.0717
167.6634
166.8102
148.6179
136.8568
133.5902
133.5246
133.3058
131.5486
131.4027
131.2861
130.8704
129.2736
128.6757
125.2852
121.8946
121.7561
77.3508
77.0300
76.7092
62.2428
62.0606
61.8491
60.5220
54.6086
53.9962
52.7201
52.5889
48.3525
47.6744
43.6641
42.7600
13.9658
13.7179
Br
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)

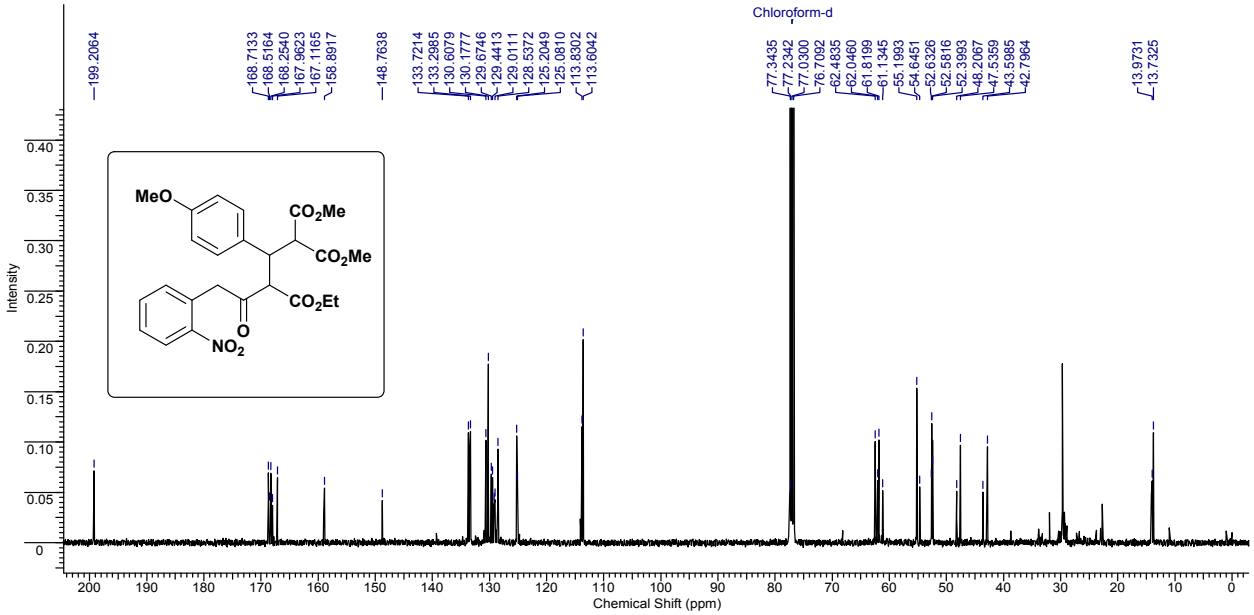

Chloroform-d
Me
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)

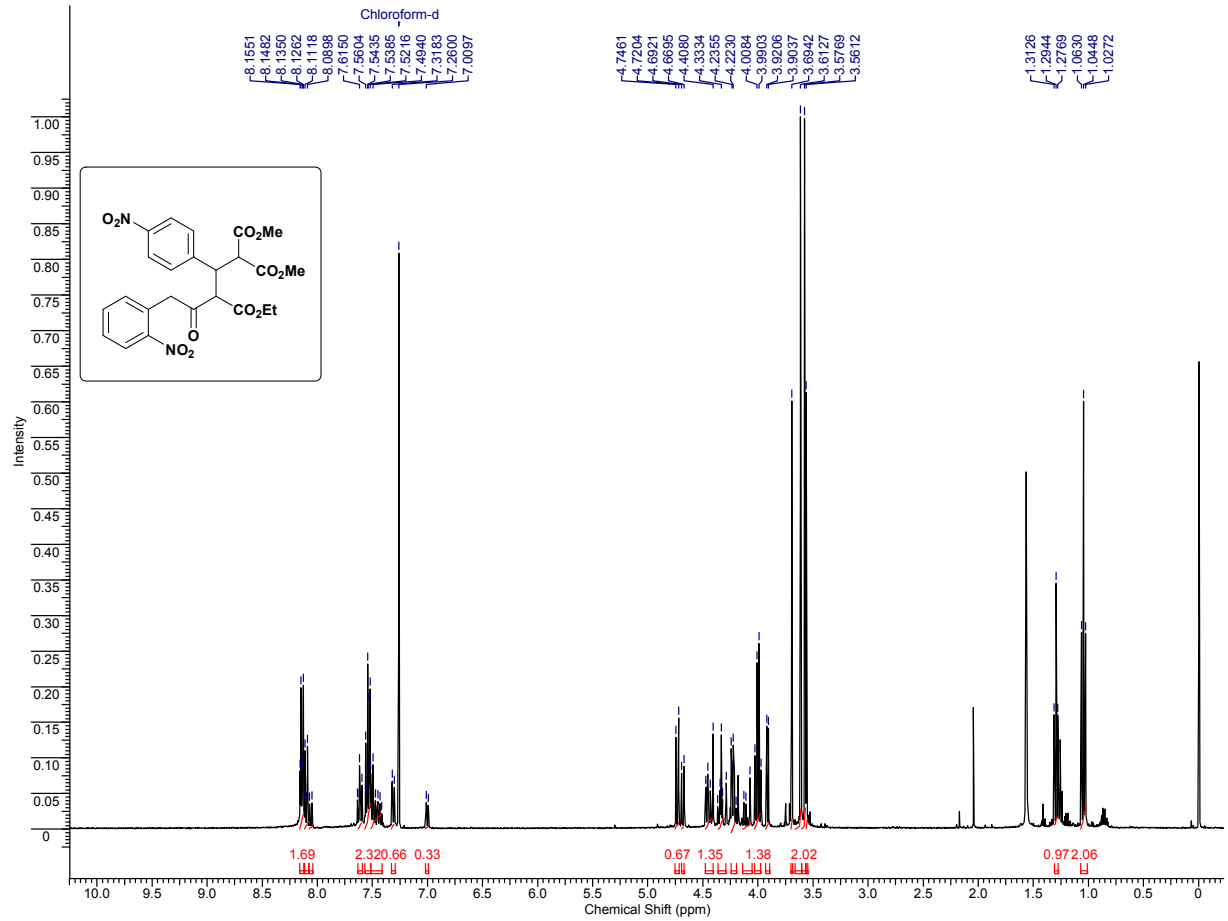

Chloroform-d
Me
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)


Chloroform-d
8.1406
8.1206
8.0447
7.5993
7.5805
7.4946
7.4751
7.3158
7.2958
7.2719
7.2600
7.2544
7.2343
6.8812
6.8623
4.6476
4.6219
4.4074
4.3101
4.2637
4.1853
3.9984
3.9802
3.9627
3.8472
3.8291
3.6785
3.5882
3.5525
3.5499
1.3020
1.2838
1.2662
1.0529
1.0354
1.0172
Cl
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.71
0.90
2.12
0.29
0.69
2.02
0.30
3.01
0.88
2.11
Chemical Shift (ppm)


Chloroform-d
199.0678
198.8855
168.4581
168.1665
168.0935
167.6998
166.8394
148.6325
136.3318
133.7214
133.3131
130.9652
130.5350
129.2882
128.8361
128.6757
128.4570
125.2924
125.1977
77.3508
77.0300
76.7092
62.2355
62.0460
61.9439
60.5950
54.6888
54.0764
52.7201
52.5816
48.3525
47.6744
43.6131
42.7089
13.9731
13.7179
Cl
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)


Chloroform-d
8.1212
8.1005
8.0183
8.0146
7.5849
7.5611
7.4544
7.3133
7.2970
7.2600
7.2311
7.2148
7.2098
6.8021
6.7984
6.7802
6.7764
4.6043
4.5786
4.4080
4.3127
4.1515
3.9846
3.9670
3.8435
3.8247
3.7688
3.7613
3.6697
3.5775
3.5481
3.5292
1.3063
1.2882
1.2706
1.0454
1.0279
1.0097
MeO
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.70
1.012.27
1.99
0.68
1.27
2.132.12
0.88
2.12
Chemical Shift (ppm)


199.2064
168.7133
168.5164
168.2540
167.9623
167.1165
158.8917
148.7638
133.7214
133.2985
130.6079
130.1777
129.6746
129.4413
129.0111
128.5372
125.2049
125.0810
113.8302
113.6042
Chloroform-d
77.3435
77.2342
77.0300
76.7092
62.4835
62.0460
61.8199
61.1345
55.1993
54.6451
52.6326
52.5816
52.3993
48.2067
47.5359
43.5985
42.7964
13.9731
13.7325
MeO
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)


Chloroform-d
8.1551
8.1482
8.1350
8.1262
8.1118
8.0898
7.6150
7.5604
7.5435
7.5385
7.5216
7.4940
7.3183
7.2600
7.0097
4.7461
4.7204
4.6921
4.6695
4.4080
4.3334
4.2355
4.2230
4.0084
3.9903
3.9206
3.9037
3.6942
3.6127
3.5769
3.5612
1.3126
1.2944
1.2769
1.0630
1.0448
1.0272
O2N
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
1.69
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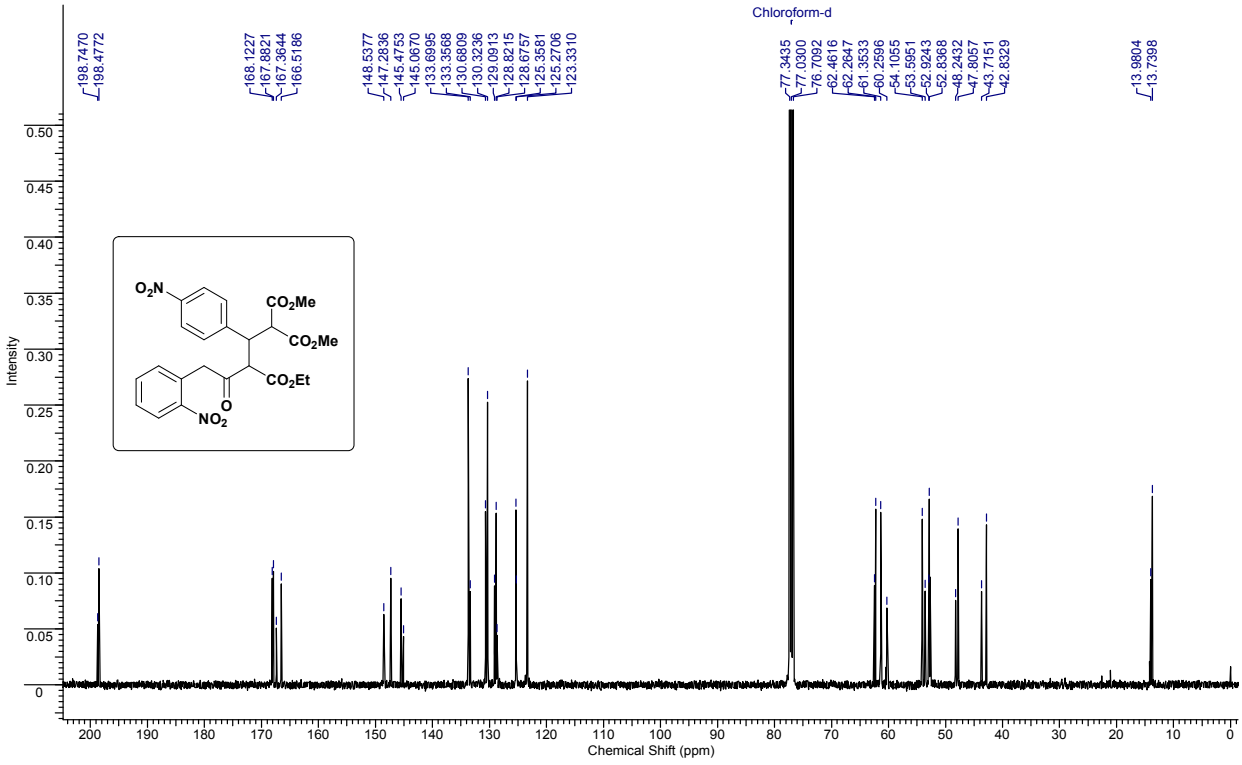
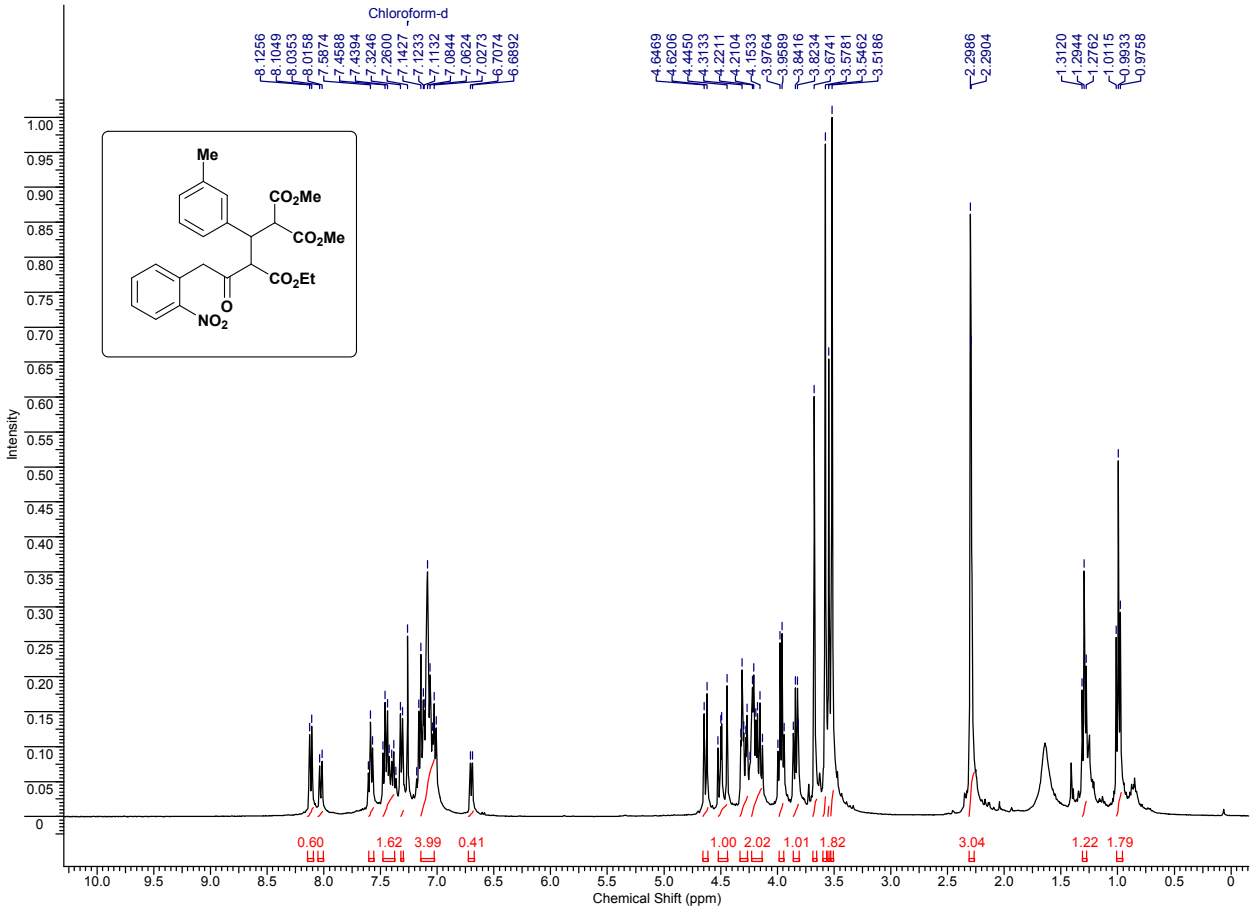
0.66
0.33
0.67
1.35
1.38
2.02
0.97
2.06
Chemical Shift (ppm)


Chloroform-d
198.7470
198.4772
168.1227
167.8821
167.3644
166.5186
148.5377
147.2836
145.4753
145.0670
133.6995
133.3568
130.6809
130.3236
129.0913
128.8215
128.6757
125.3581
125.2706
123.3310
77.3435
77.0300
76.7092
62.4616
62.2647
61.3533
60.2596
54.1055
53.5951
52.9243
52.8368
48.2432
47.8057
43.7151
42.8329
13.9804
13.7398
O2N
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)


Chloroform-d
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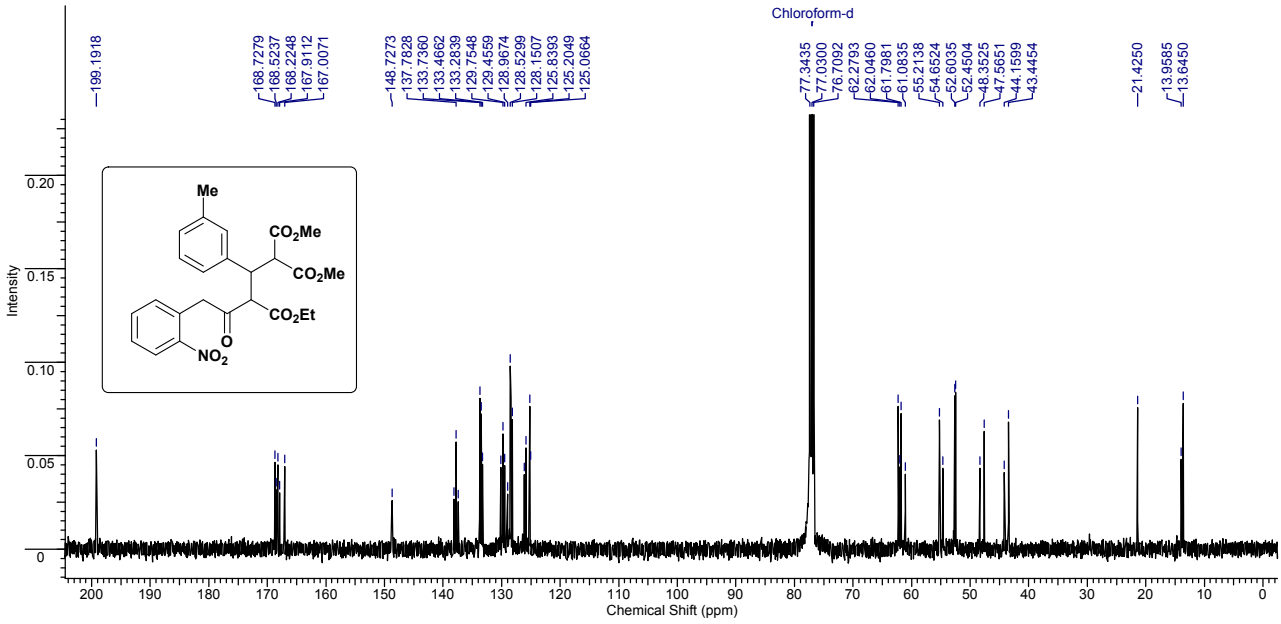
8.1049
8.0353
8.0158
7.5874
7.4588
7.4394
7.3246
7.2600
7.1427
7.1233
7.1132
7.0844
7.0624
7.0273
6.7074
6.6892
4.6469
4.6206
4.4450
4.3133
4.2211
4.2104
4.1533
3.9764
3.9589
3.8416
3.8234
3.6741
3.5781
3.5462
3.5186
2.2986
2.2904
1.3120
1.2944
1.2762
1.0115
0.9933
0.9758
Me
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.60
1.62
3.99
0.41
1.00
2.02
1.01
1.82
3.04
1.22
1.79
Chemical Shift (ppm)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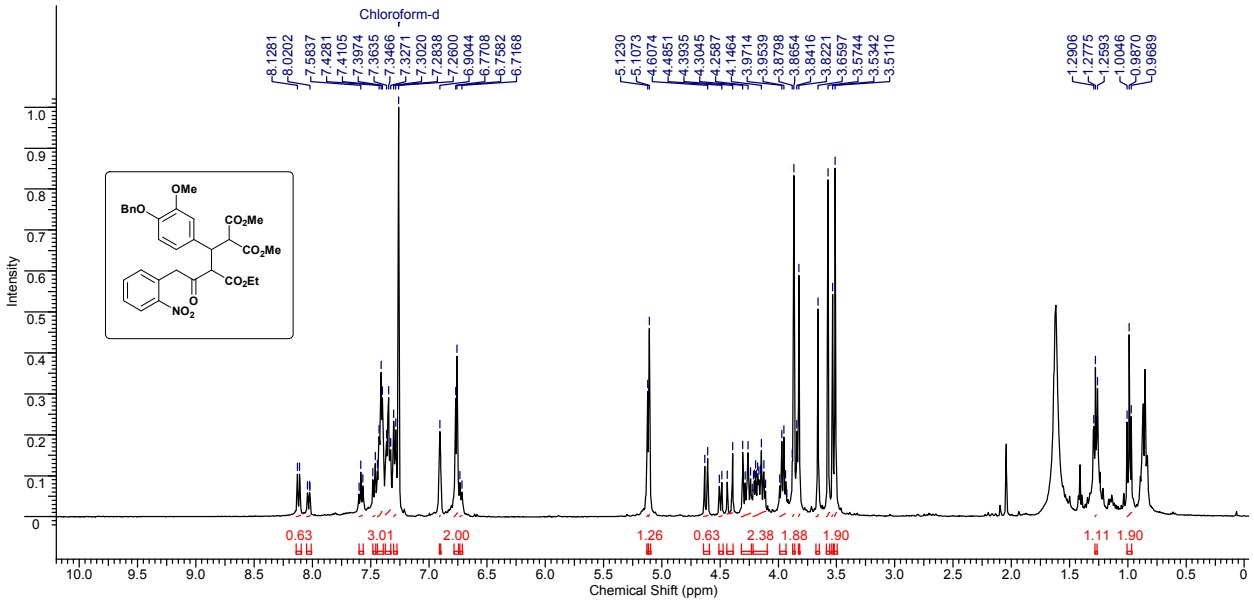
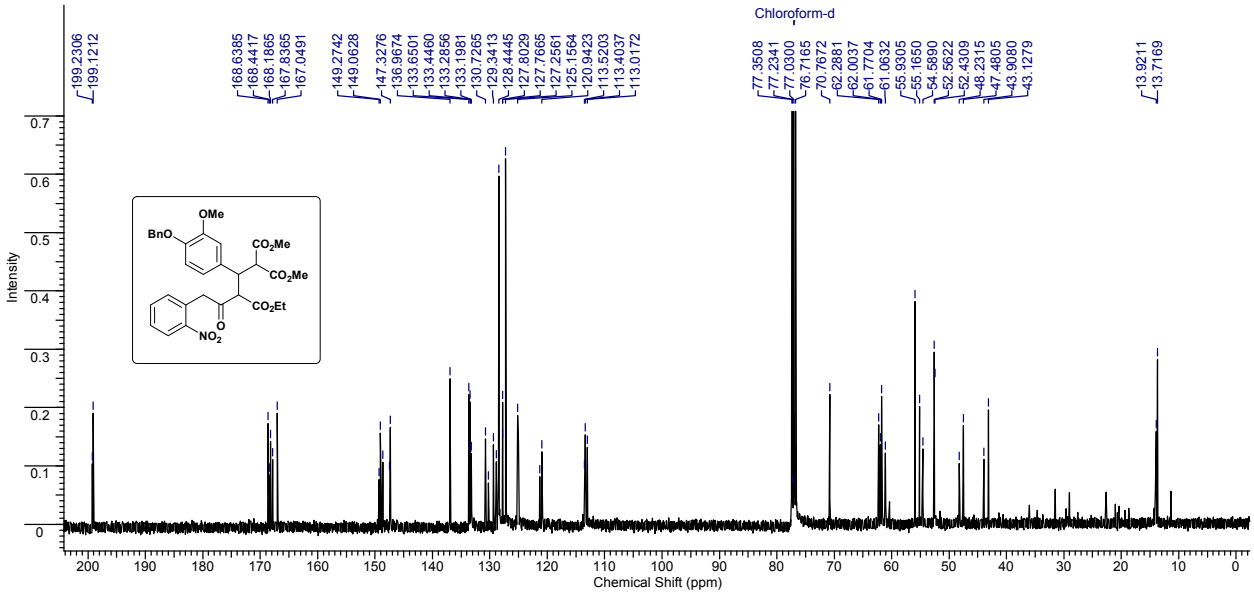
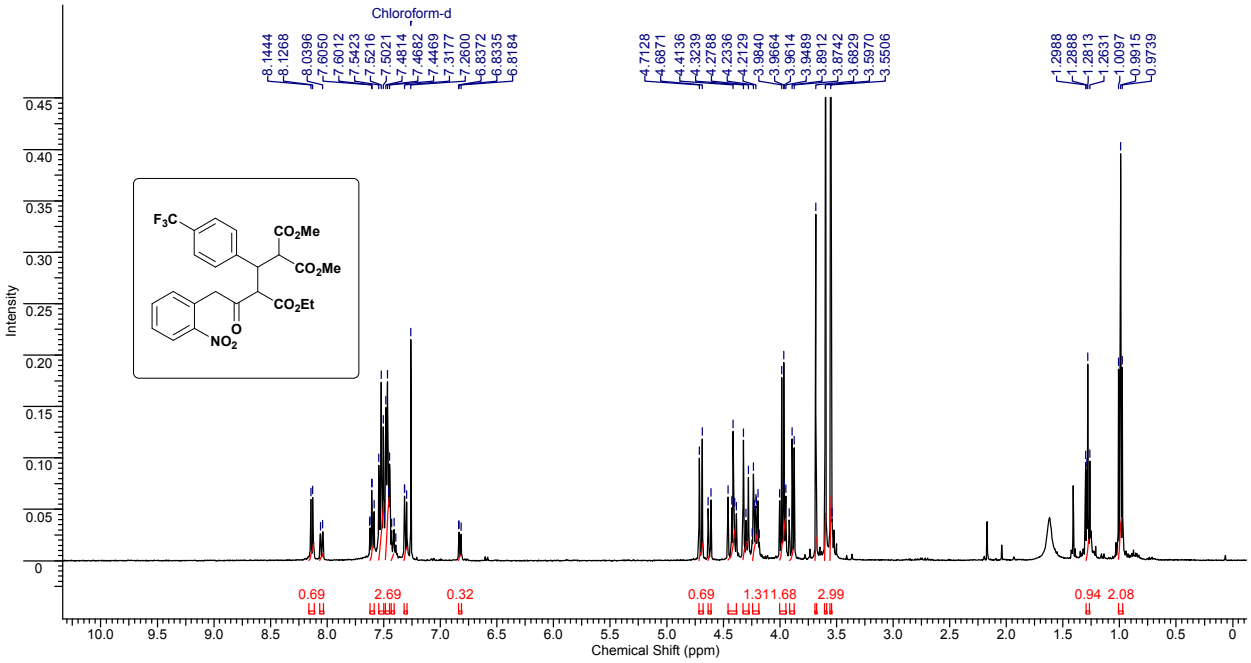
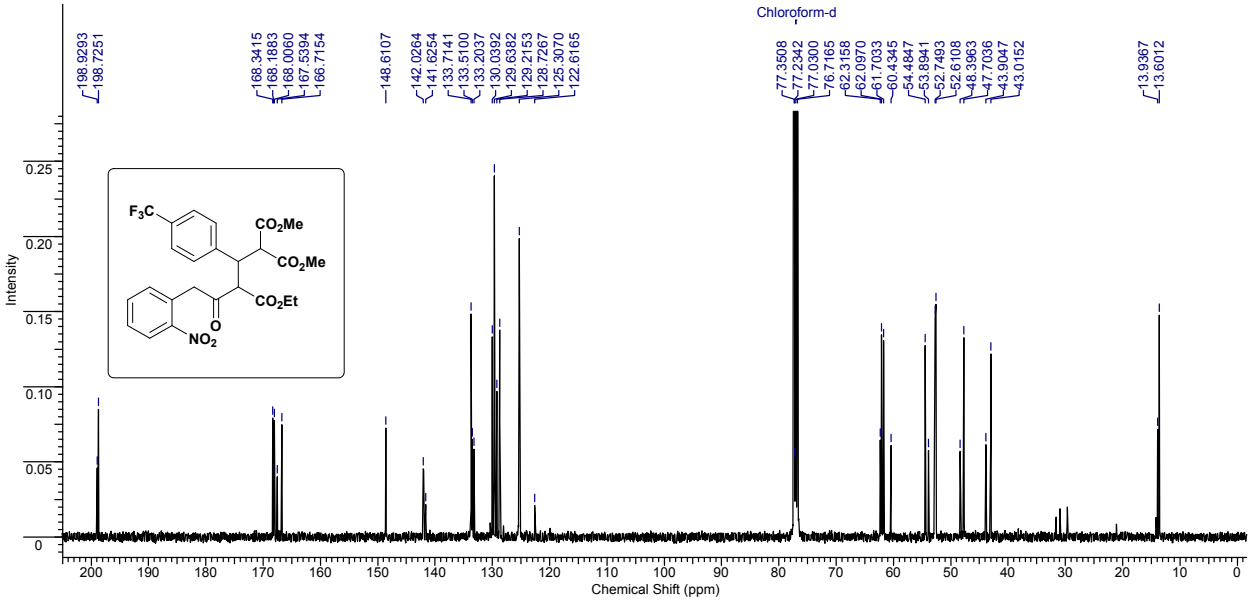
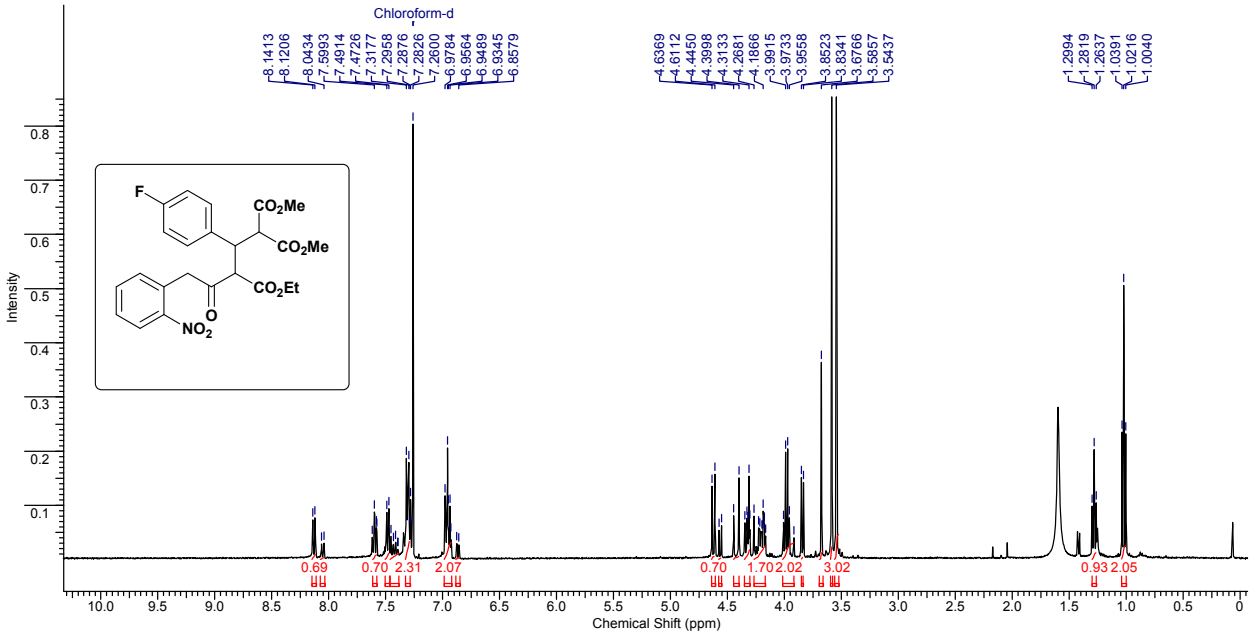
167.9112
167.0071
148.7273
137.7828
133.7360
133.4662
133.2839
129.7548
129.4559
128.9674
128.5299
128.1507
125.8393
125.2049
125.0664
Chloroform-d
77.3435
77.0300
76.7092
62.2793
62.0460
61.7981
61.0835
55.2138
54.6524
52.6035
52.4504
48.3525
47.5651
44.1599
43.4454
21.4250
13.9585
13.6450
Me
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)

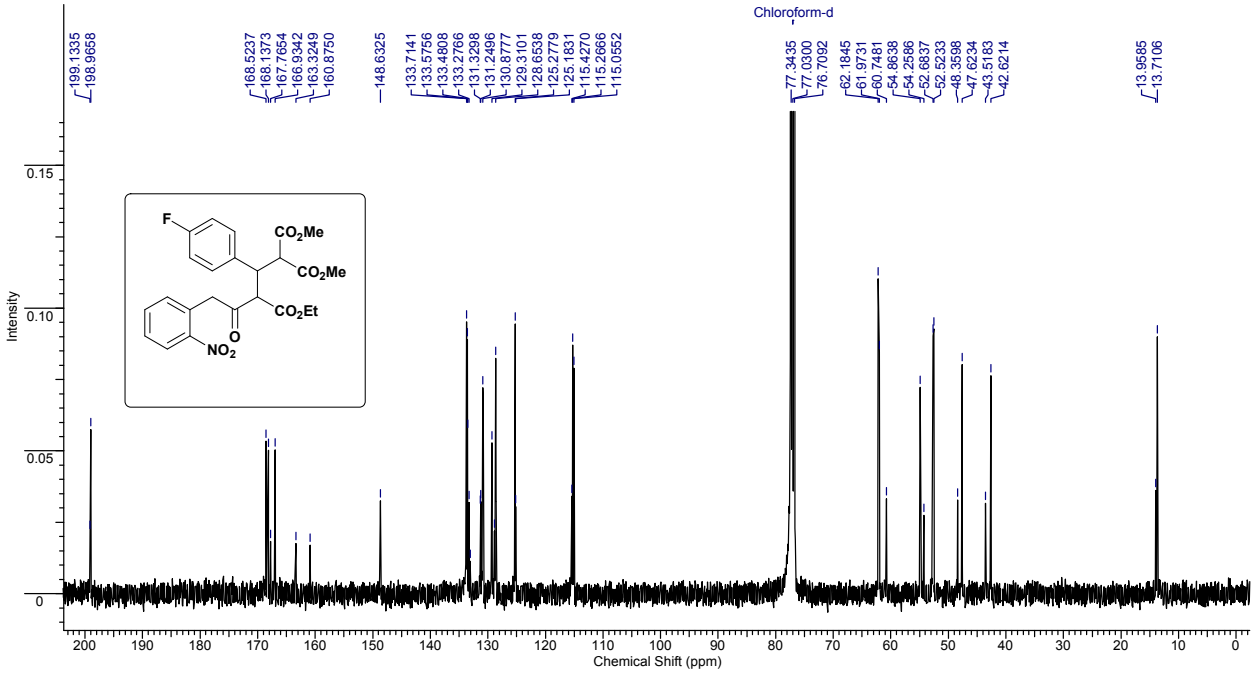

Chloroform-d
8.1281
8.0202
7.5837
7.4281
7.4105
7.3974
7.3635
7.3466
7.3271
7.3020
7.2838
7.2600
6.9044
6.7708
6.7582
6.7168
5.1230
5.1073
4.6074
4.4851
4.3935
4.3045
4.2587
4.1464
3.9714
3.9539
3.8798
3.8654
3.8416
3.8221
3.6597
3.5744
3.5342
3.5110
1.2906
1.2775
1.2593
1.0046
0.9870
0.9689
OMe
BnO
CO2Me
CO2Me
CO2Et
NO2
0.63
3.01
2.00
1.26
0.63
2.38
1.88
1.90
1.11
1.90
Intensity
Chemical Shift (ppm)

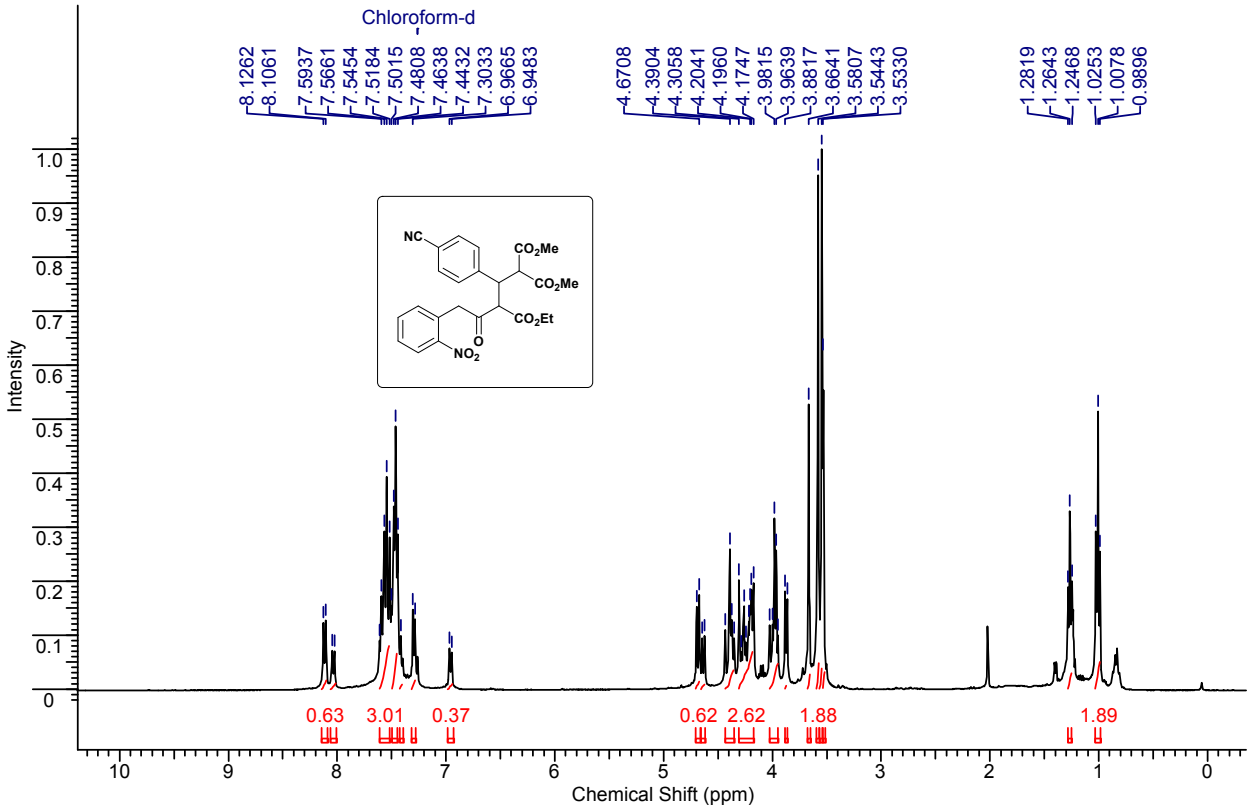

Chloroform-d
199.2306
199.1212
168.6385
168.4417
168.1865
167.8365
167.0491
149.2742
149.0628
147.3276
136.9674
133.6501
133.4460
133.2856
133.1981
130.7265
129.3413
128.4445
127.8029
127.7665
127.2561
125.1564
120.9423
113.5203
113.4037
113.0172
77.3508
77.2341
77.0300
76.7165
70.7672
62.2881
62.0037
61.7704
61.0632
55.9305
55.1650
54.5890
52.5622
52.4309
48.2315
47.4805
43.9080
43.1279
13.9211
13.7169
OMe
BnO
CO2Me
CO2Me
CO2Et
NO2
Intensity
Chemical Shift (ppm)

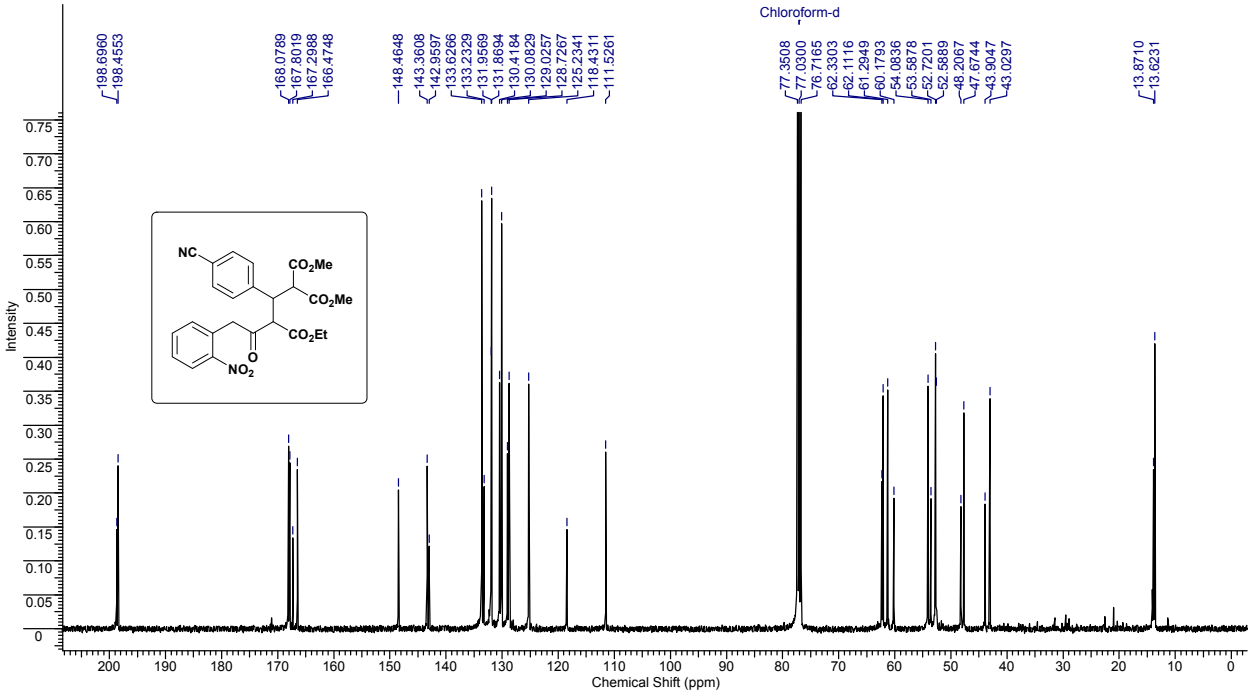

Chloroform-d
8.1444
8.1268
8.0396
7.6050
7.6012
7.5423
7.5216
7.5021
7.4814
7.4682
7.4469
7.3177
7.2600
6.8372
6.8335
6.8184
4.7128
4.6871
4.4136
4.3239
4.2788
4.2336
4.2129
3.9840
3.9664
3.9614
3.9489
3.8912
3.8742
3.6829
3.5970
3.5506
1.2988
1.2888
1.2813
1.2631
1.0097
0.9915
0.9739
F3C
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.69
2.69
0.32
0.69
1.31
1.68
2.99
0.94
2.08
Chemical Shift (ppm)

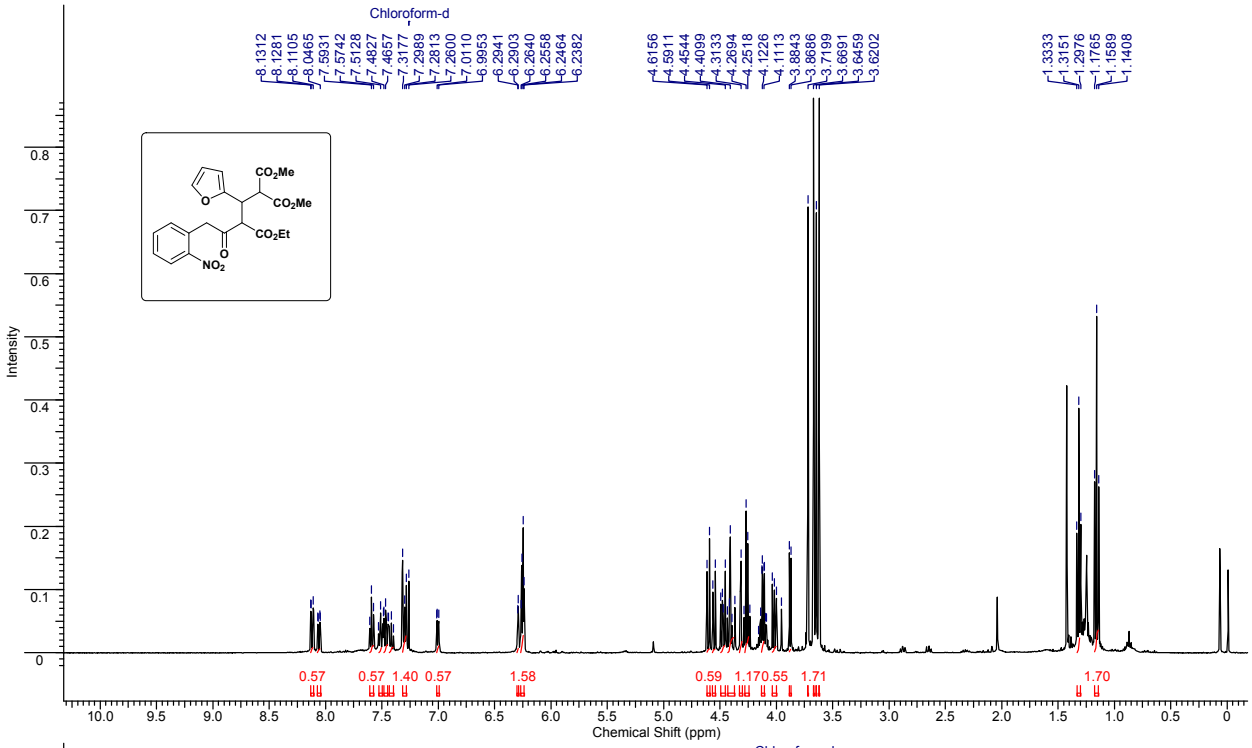

198.9293
198.7251
168.3415
168.1883
168.0060
167.5394
166.7154
148.6107
142.0264
141.6254
133.7141
133.5100
133.2037
130.0392
129.6382
129.2153
128.7267
125.3070
122.6165
Chloroform-d
77.3508
77.2342
77.0300
76.7165
62.3158
62.0970
61.7033
60.4345
54.4847
53.8941
52.7493
52.6108
48.3963
47.7036
43.9047
43.0152
13.9367
13.6012
F3C
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)

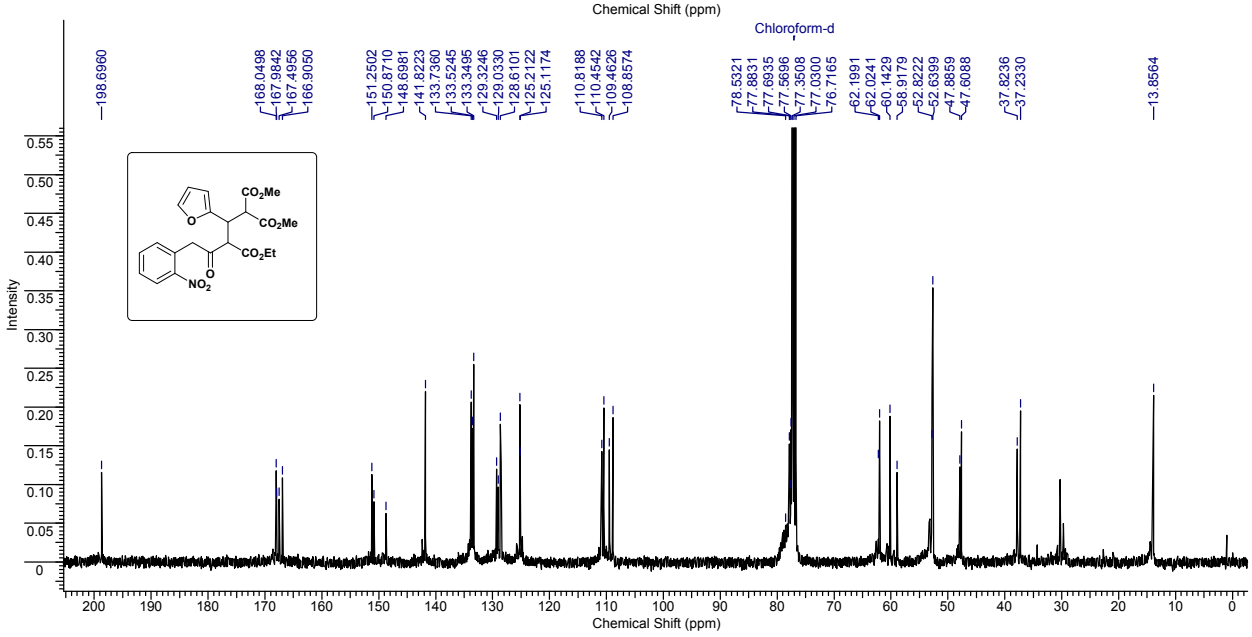

Chloroform-d
8.1413
8.1206
8.0434
7.5993
7.4914
7.4726
7.3177
7.2958
7.2876
7.2826
7.2600
6.9784
6.9564
6.9489
6.9345
6.8579
4.6369
4.6112
4.4450
4.3998
4.3133
4.2681
4.1866
3.9915
3.9733
3.9558
3.8523
3.8341
3.6766
3.5857
3.5437
1.2994
1.2819
1.2637
1.0391
1.0216
1.0040
F
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.69
0.70
2.31
2.07
0.70
1.70
2.02
3.02
0.93
2.05
Chemical Shift (ppm)

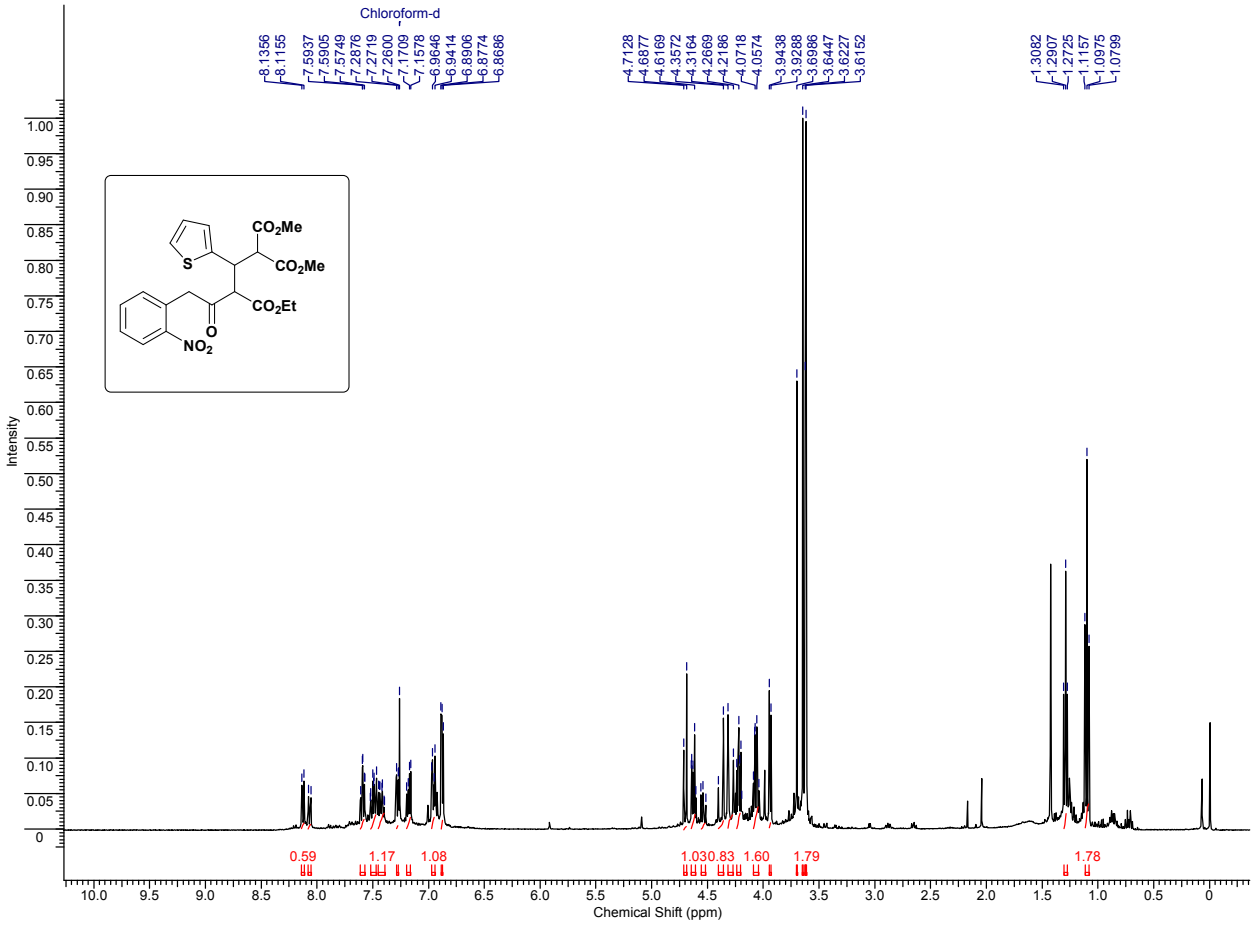

199.1335
198.9658
168.5237
168.1373
167.7654
166.9342
163.3249
160.8750
148.6325
133.7141
133.5756
133.4808
133.2766
131.3298
131.2496
130.8777
129.3101
128.6538
125.2779
125.1831
115.4270
115.2666
115.0552
Chloroform-d
77.3435
77.0300
76.7092
62.1845
61.9731
60.7481
54.8638
54.2586
52.6837
52.5233
48.3598
47.6234
43.5183
42.6214
13.9585
13.7106
F
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)

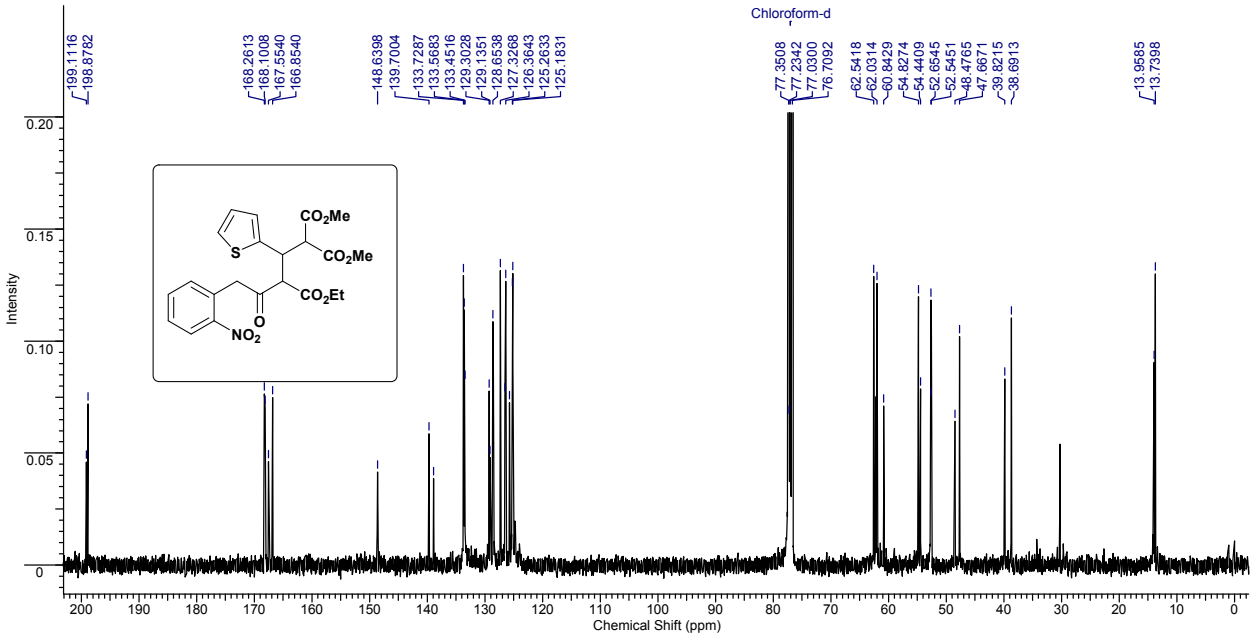

Chloroform-d
8.1262
8.1061
7.5937
7.5661
7.5454
7.5184
7.5015
7.4808
7.4638
7.4432
7.3033
6.9665
6.9483
4.6708
4.3904
4.3058
4.2041
4.1960
4.1747
3.9815
3.9639
3.8817
3.6641
3.5807
3.5443
3.5330
1.2819
1.2643
1.2468
1.0253
1.0078
0.9896
NC
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.63
3.01
0.37
0.62
2.62
1.88
1.89
Chemical Shift (ppm)

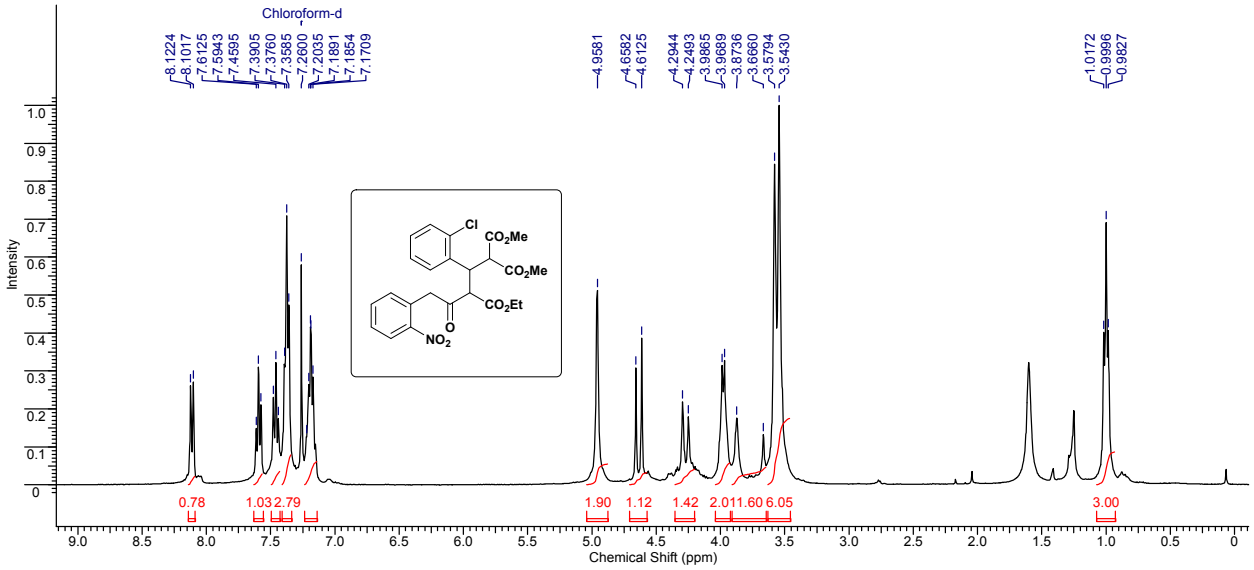

198.6960
198.4553
168.0789
167.8019
167.2988
166.4748
148.4648
143.3608
142.9597
133.6266
133.2329
131.9569
131.8694
130.4184
130.0829
129.0257
128.7267
125.2341
118.4311
111.5261
Chloroform-d
77.3508
77.0300
76.7165
62.3303
62.1116
61.2949
60.1793
54.0836
53.5878
52.7201
52.5889
48.2067
47.6744
43.9047
43.0297
13.8710
13.6231
NC
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)


Chloroform-d
8.1312
8.1281
8.1105
8.0465
7.5931
7.5742
7.5128
7.4827
7.4657
7.3177
7.2989
7.2813
7.2600
7.0110
6.9953
6.2941
6.2903
6.2640
6.2558
6.2464
6.2382
4.6156
4.5911
4.4544
4.4099
4.3133
4.2694
4.2518
4.1226
4.1113
3.8843
3.8686
3.7199
3.6691
3.6459
3.6202
1.3333
1.3151
1.2976
1.1765
1.1589
1.1408
CO2Me
CO2Me
CO2Et
NO2
Intensity
0.57
0.57
1.40
0.57
1.58
0.59
1.17
0.55
1.71
1.70
Chemical Shift (ppm)


Chloroform-d
198.6960
168.0498
167.9842
167.4956
166.9050
151.2502
150.8710
148.6981
141.8223
133.7360
133.5245
133.3495
129.3246
129.0330
128.6101
125.2122
125.1174
110.8188
110.4542
109.4626
108.8574
78.5321
77.8831
77.6935
77.5696
77.3508
77.0300
76.7165
62.1991
62.0241
60.1429
58.9179
52.8222
52.6399
47.8859
47.6088
37.8236
37.2330
13.8564
CO2Me
CO2Me
CO2Et
NO2
Intensity
Chemical Shift (ppm)


Chloroform-d
8.1356
8.1155
7.5937
7.5905
7.5749
7.2876
7.2719
7.2600
7.1709
7.1578
6.9646
6.9414
6.8906
6.8774
6.8686
4.7128
4.6877
4.6169
4.3572
4.3164
4.2669
4.2186
4.0718
4.0574
3.9438
3.9288
3.6986
3.6447
3.6227
3.6152
1.3082
1.2907
1.2725
1.1157
1.0975
1.0799
CO2Me
CO2Me
CO2Et
O
NO2
S
Intensity
0.59
1.17
1.08
1.03
0.83
1.60
1.79
1.78
Chemical Shift (ppm)


Chloroform-d
199.1116
198.8782
168.2613
168.1008
167.5540
166.8540
148.6398
139.7004
133.7287
133.5683
133.4516
129.3028
129.1351
128.6538
127.3268
126.3643
125.2633
125.1831
77.3508
77.2342
77.0300
76.7092
62.5418
62.0314
60.8429
54.8274
54.4409
52.6545
52.5451
48.4765
47.6671
39.8215
38.8913
13.9585
13.7398
CO2Me
CO2Me
CO2Et
O
NO2
S
Intensity
Chemical Shift (ppm)


Chloroform-d
8.1224
8.1017
7.6125
7.5943
7.4595
7.3905
7.3760
7.3585
7.2600
7.2035
7.1891
7.1854
7.1709
4.9581
4.6582
4.6125
4.2944
4.2493
3.9865
3.9689
3.8736
3.8660
3.5794
3.5430
1.0172
0.9996
0.9827
Cl
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.78
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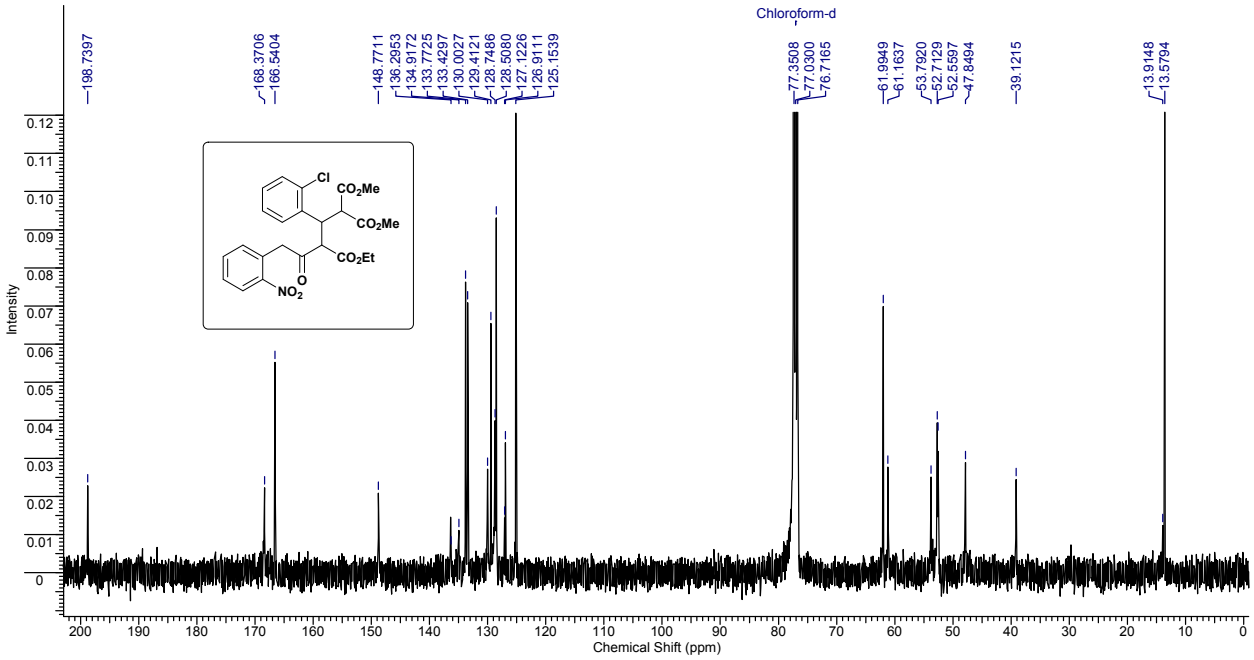
2.79
1.90
1.12
1.42
2.01
1.60
6.05
3.00
Chemical Shift (ppm)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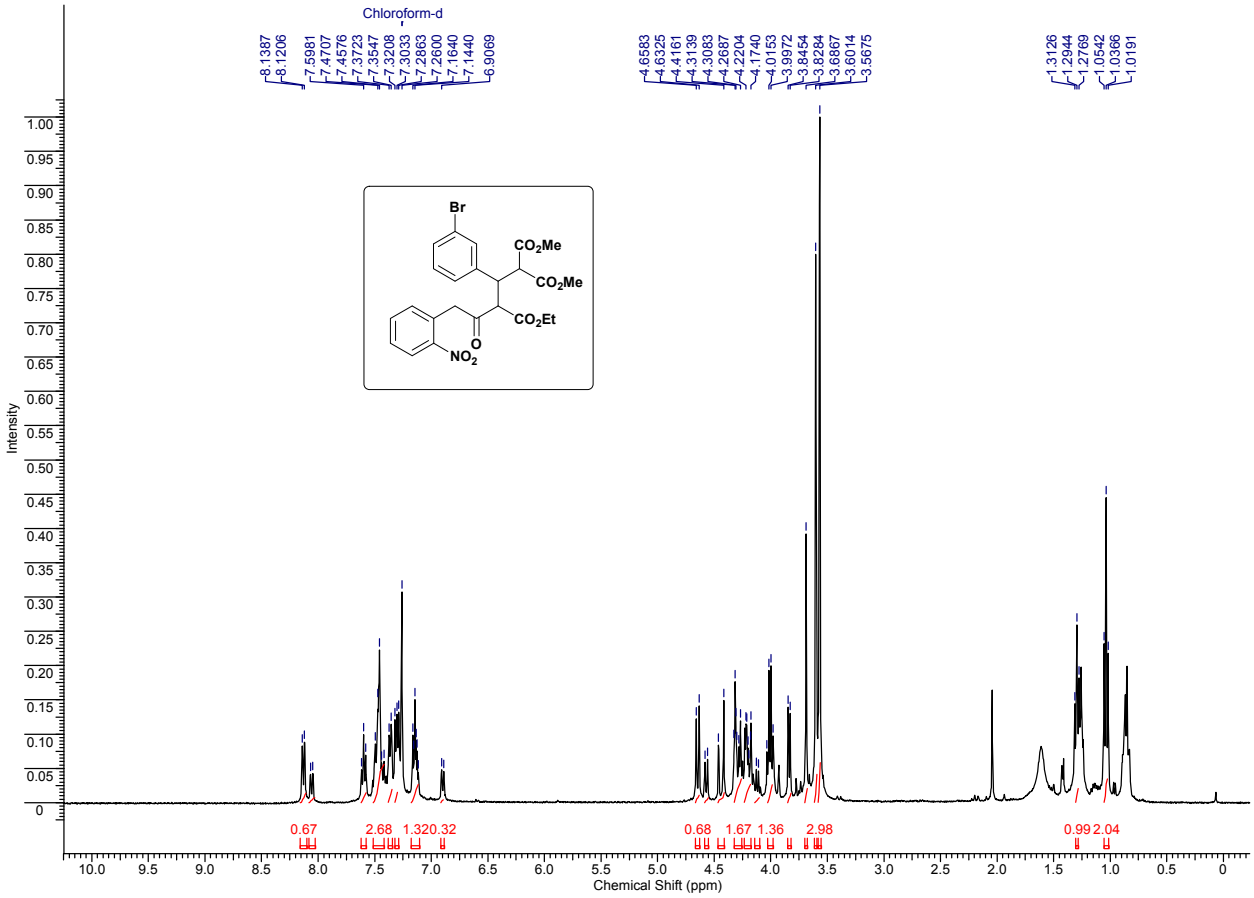
134.9172
133.7725
133.4297
130.0027
129.4121
128.7486
128.5080
127.1226
126.9111
125.1539
Chloroform-d
77.3508
77.0300
76.7165
61.9949
61.1637
53.7920
52.7129
52.5597
47.8494
39.1215
13.9148
13.5794
Cl
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)


Chloroform-d
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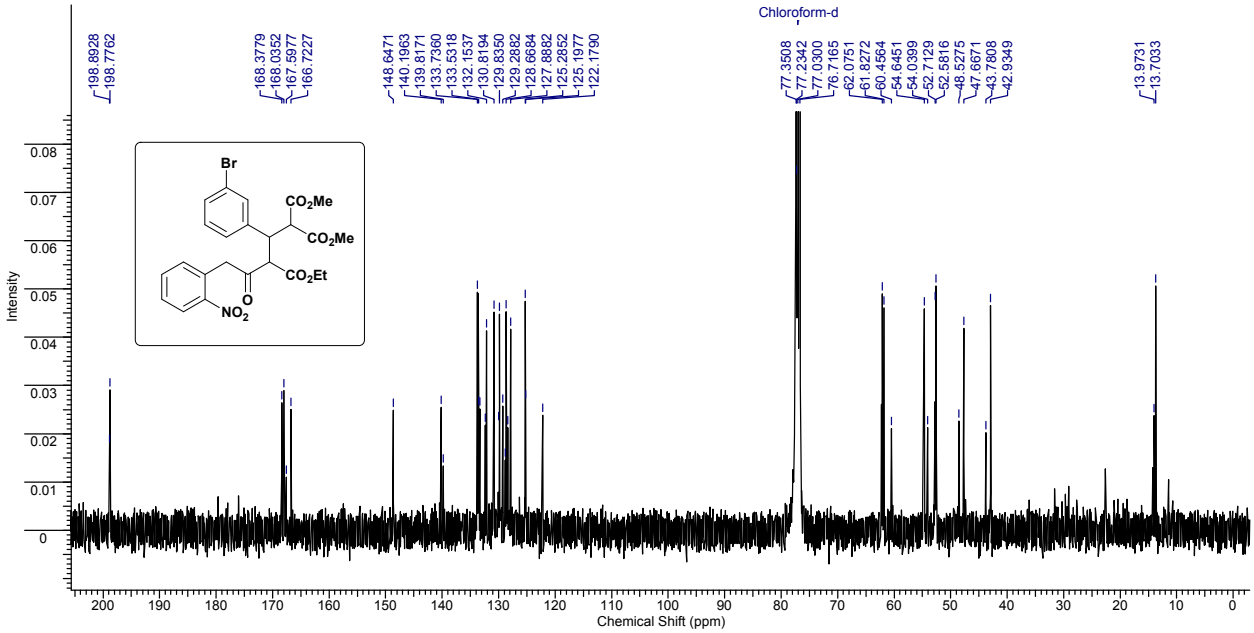
7.4707
7.4576
7.3723
7.3547
7.3208
7.3033
7.2863
7.2600
7.1640
7.1440
6.9069
4.6583
4.6325
4.4161
4.3139
4.3083
4.2687
4.2204
4.1740
4.0153
3.9972
3.8454
3.8284
3.8867
3.6014
3.5675
1.3126
1.2944
1.2769
1.0542
1.0366
1.0191
Br
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
0.67
2.68
1.32
0.32
0.68
1.67
1.36
2.98
0.99
2.04
Chemical Shift (ppm)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168.0352
167.5977
166.7227
148.6471
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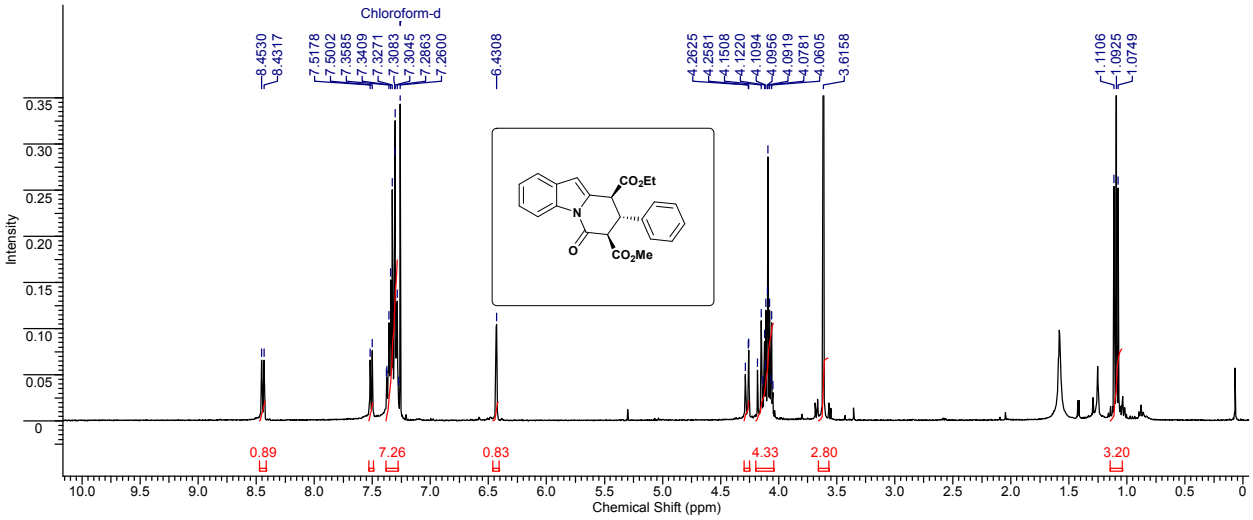
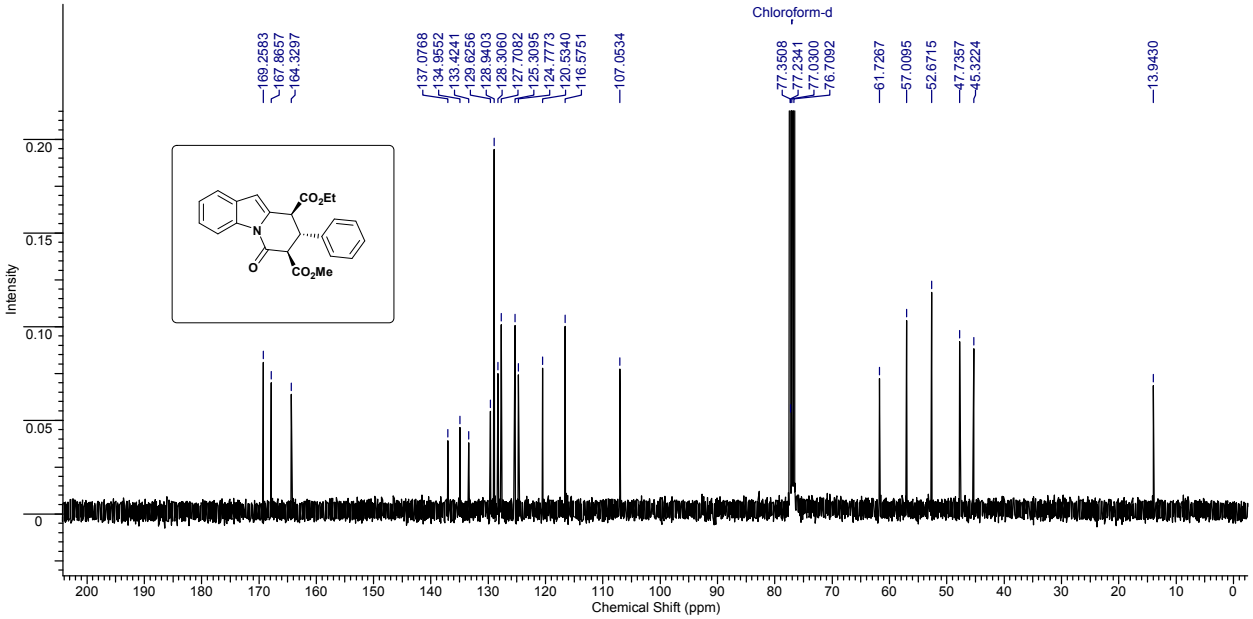
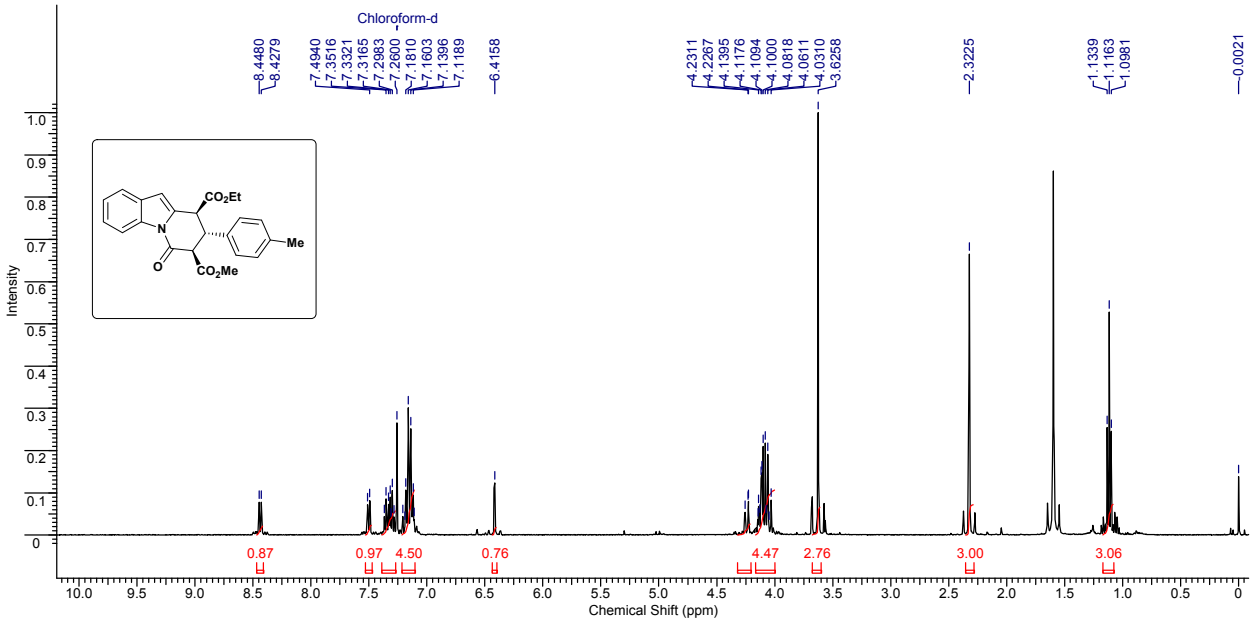
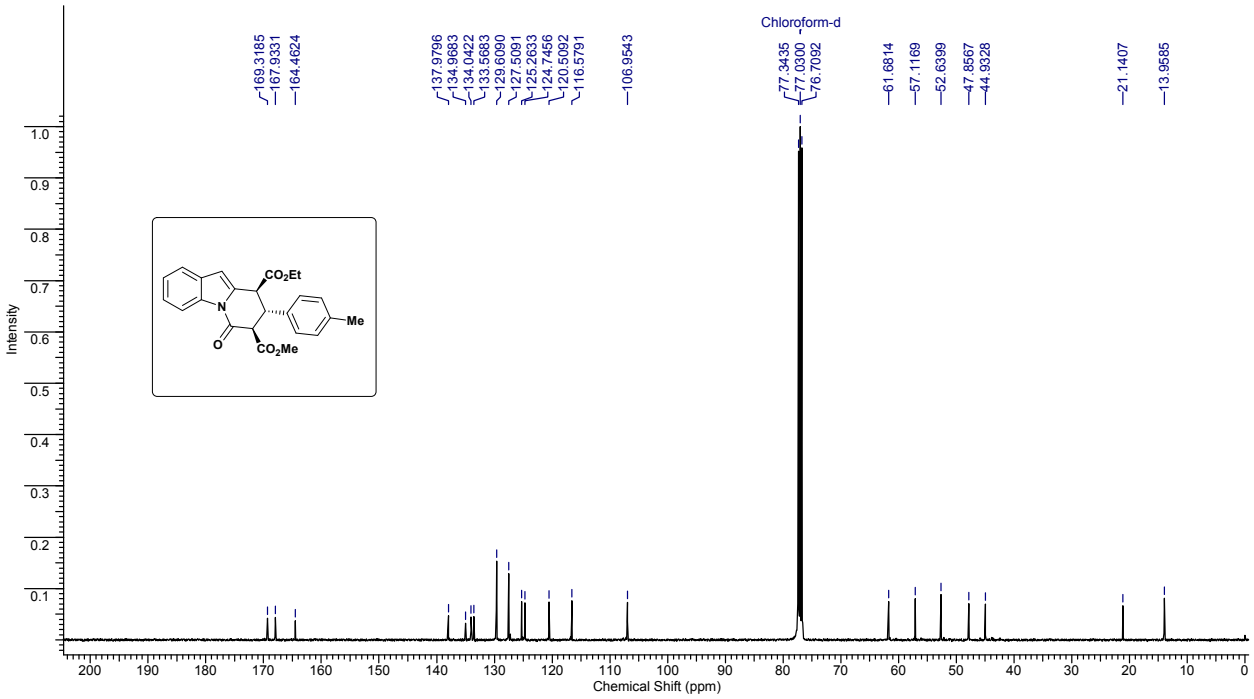
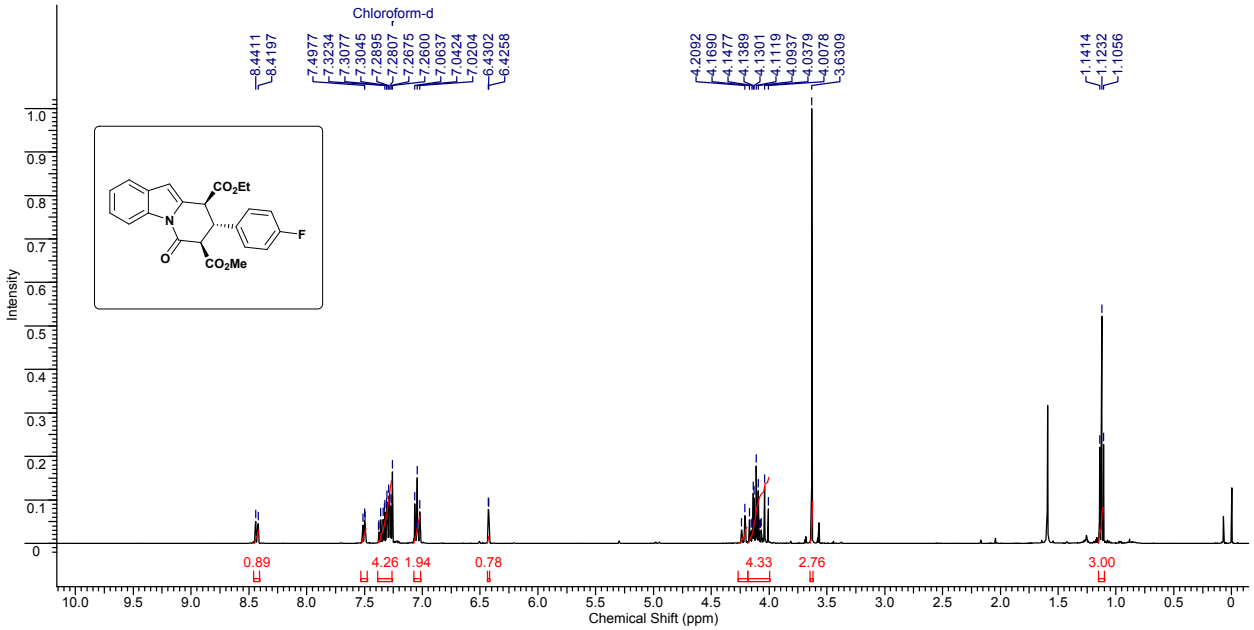
139.8171
133.7360
133.5318
132.1537
130.8194
129.8350
129.2882
128.6684
127.8882
125.2852
125.1977
122.1790
Chloroform-d
77.3508
77.2342
77.0300
76.7165
62.0751
61.8272
60.4564
54.6451
54.0399
52.7129
52.5816
46.5275
47.6671
43.7808
42.9349
13.9731
13.7033
Br
CO2Me
CO2Me
CO2Et
O
NO2
Intensity
Chemical Shift (ppm)

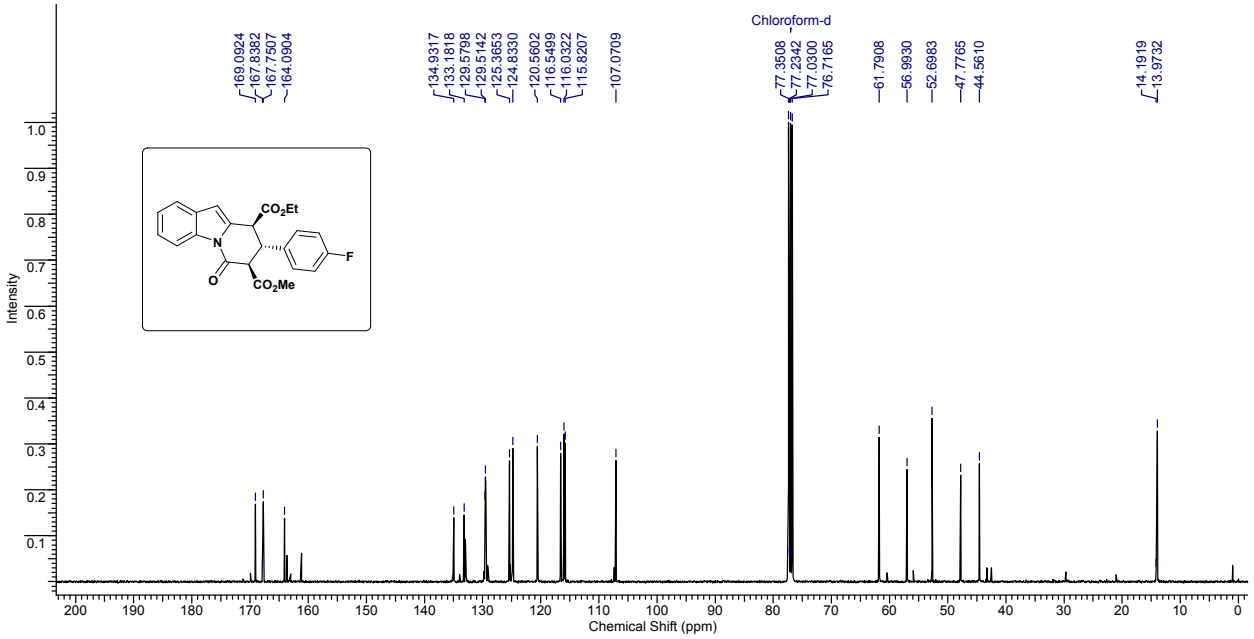

Chloroform-d
8.4530
8.4317
7.5178
7.5002
7.3585
7.3409
7.3271
7.3083
7.3045
7.2863
7.2600
6.4308
4.2625
4.2581
4.1508
4.1220
4.1094
4.0956
4.0919
4.0781
4.0605
3.6158
1.1106
1.0925
1.0749
Intensity
0.89
7.26
0.83
4.33
2.80
3.20
Chemical Shift (ppm)
CO2Et
CO2Me
N
O

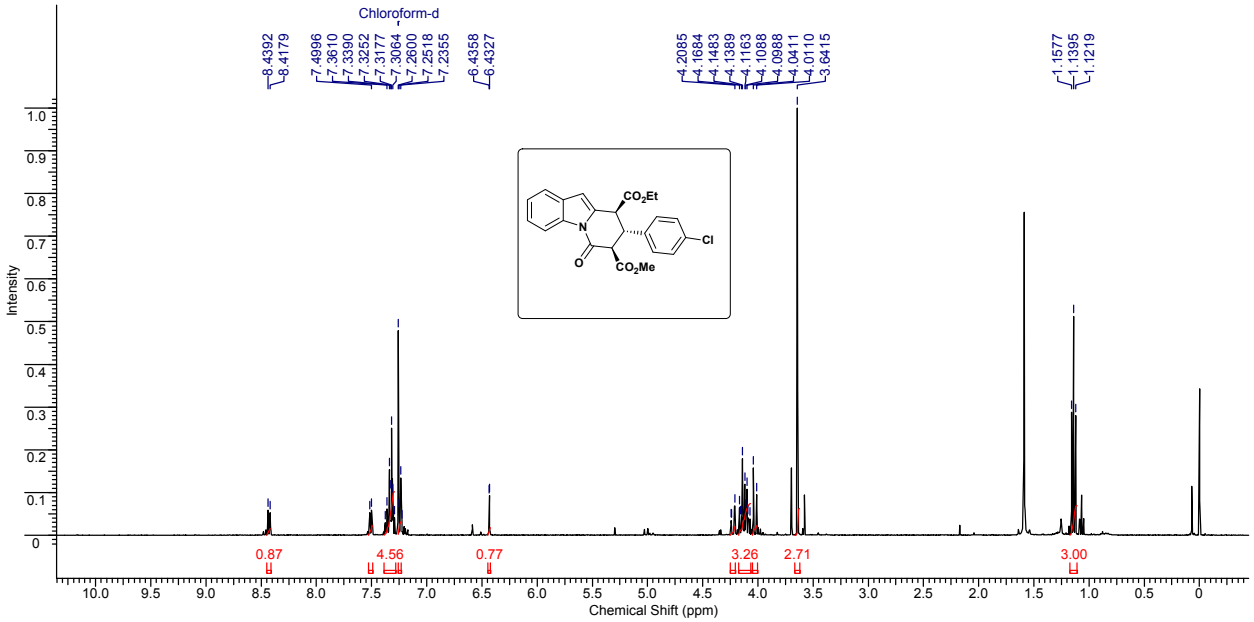

Chloroform-d
169.2583
167.8657
164.3297
137.0768
134.9552
133.4241
129.6256
128.9403
128.3060
127.7082
125.3095
124.7773
120.5340
116.5751
107.0534
77.3508
77.2341
77.0300
76.7092
61.7267
57.0095
52.6715
47.7357
45.3224
13.9430
Intensity
Chemical Shift (ppm)
CO2Et
CO2Me
N
O

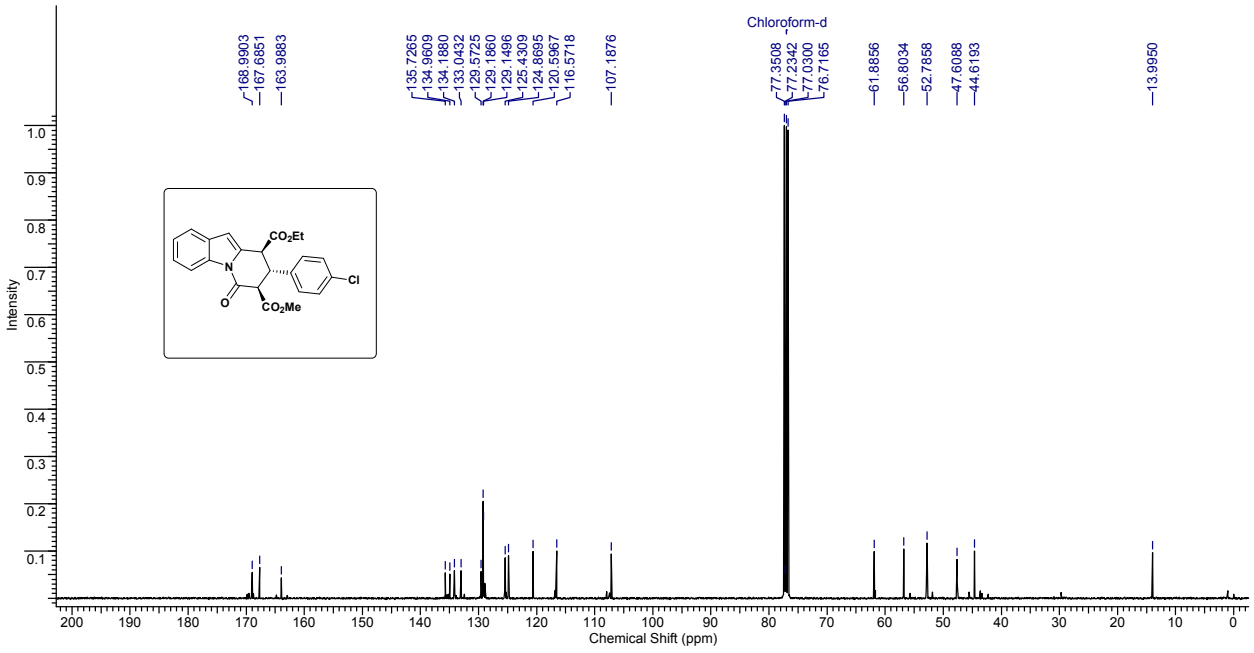

Chloroform-d
8.4480
8.4279
7.4940
7.3516
7.3321
7.3165
7.2983
7.2600
7.1810
7.1603
7.1396
7.1189
6.4158
4.2311
4.2267
4.1395
4.1176
4.1094
4.1000
4.0818
4.0611
4.0310
3.6258
2.3225
1.1339
1.1163
1.0981
0.0021
CO2Et
N
O
CO2Me
Me
Intensity
0.87
0.97
4.50
0.76
4.47
2.76
3.00
3.06
Chemical Shift (ppm)

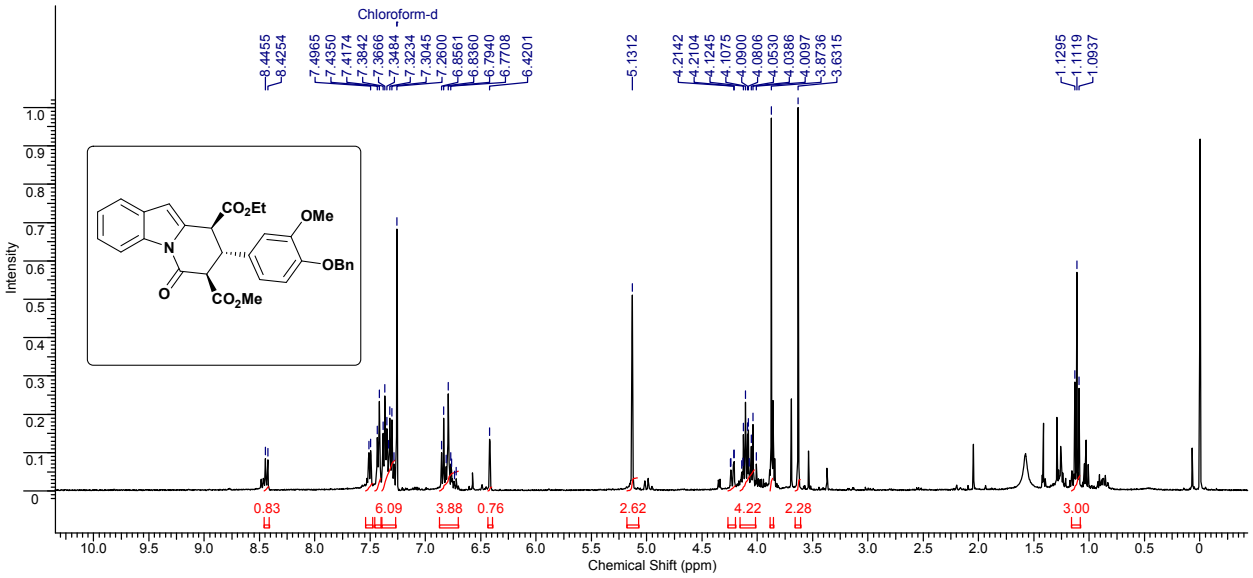

Chloroform-d
169.3185
167.9331
164.4624
137.9796
134.9683
134.0422
133.5683
129.6090
127.5091
125.2633
124.7456
120.5092
116.5791
106.9543
77.3435
77.0300
76.7092
61.6814
57.1169
52.6399
47.8567
44.9328
21.1407
13.9585
CO2Et
N
O
CO2Me
Me
Intensity
Chemical Shift (ppm)

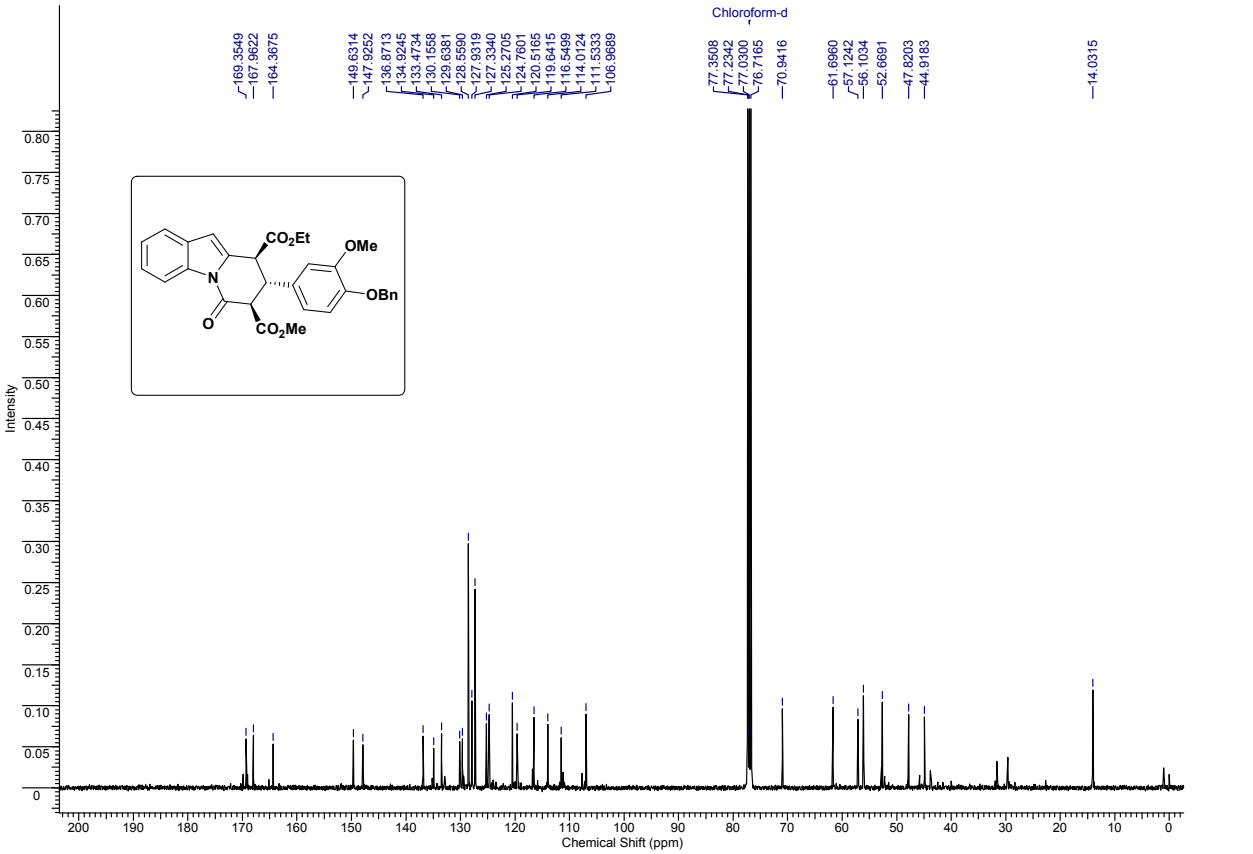

Chloroform-d
8.4411
8.4197
7.4977
7.3234
7.3077
7.3045
7.2895
7.2807
7.2675
7.2600
7.0637
7.0424
7.0204
6.4302
6.4258
4.2092
4.1690
4.1477
4.1389
4.1301
4.1119
4.0937
4.0379
4.0078
3.6309
1.1414
1.1232
1.1056
CO2Et
CO2Me
F
O
N
Intensity
0.89
4.26
1.94
0.78
4.33
2.76
3.00
Chemical Shift (ppm)

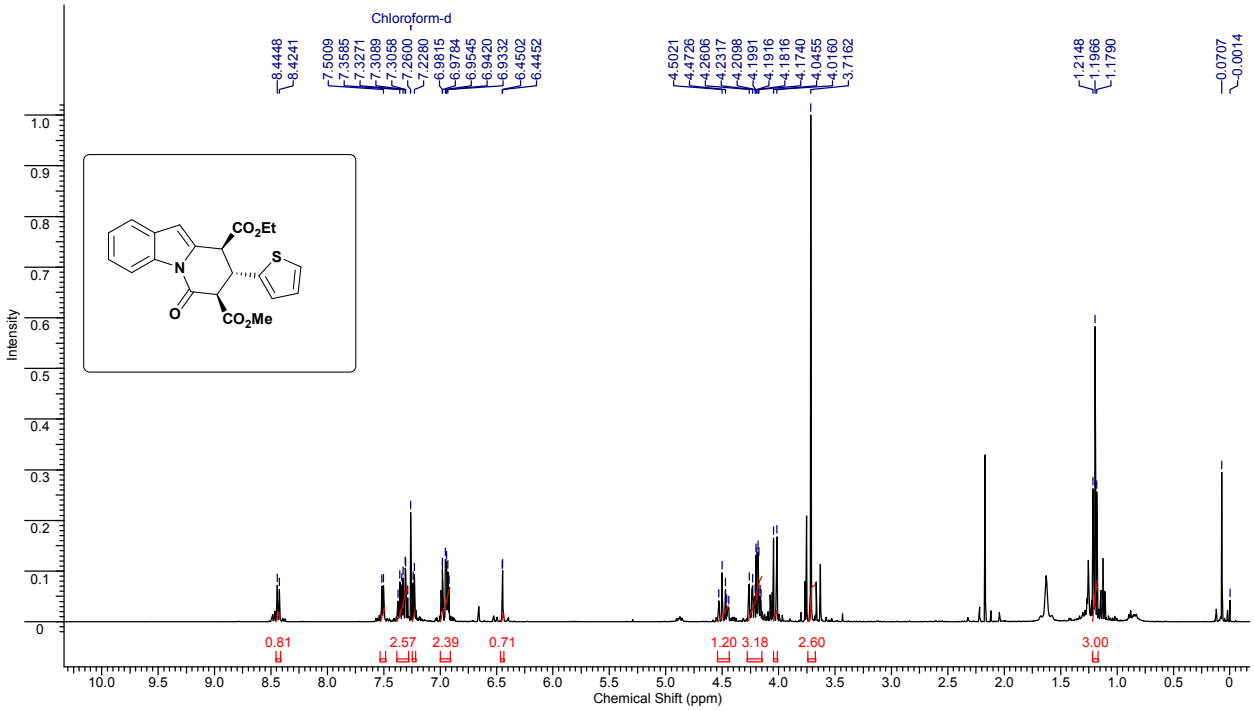

169.0924
167.8382
167.7507
164.0904
134.9317
133.1818
129.5798
129.5142
125.3653
124.8330
120.5602
116.5499
116.0322
115.8207
107.0709
Chloroform-d
77.3508
77.2342
77.0300
76.7165
61.7908
56.9930
52.6983
47.7765
44.5610
14.1919
13.9732
CO2Et
CO2Me
F
O
N
Intensity
Chemical Shift (ppm)

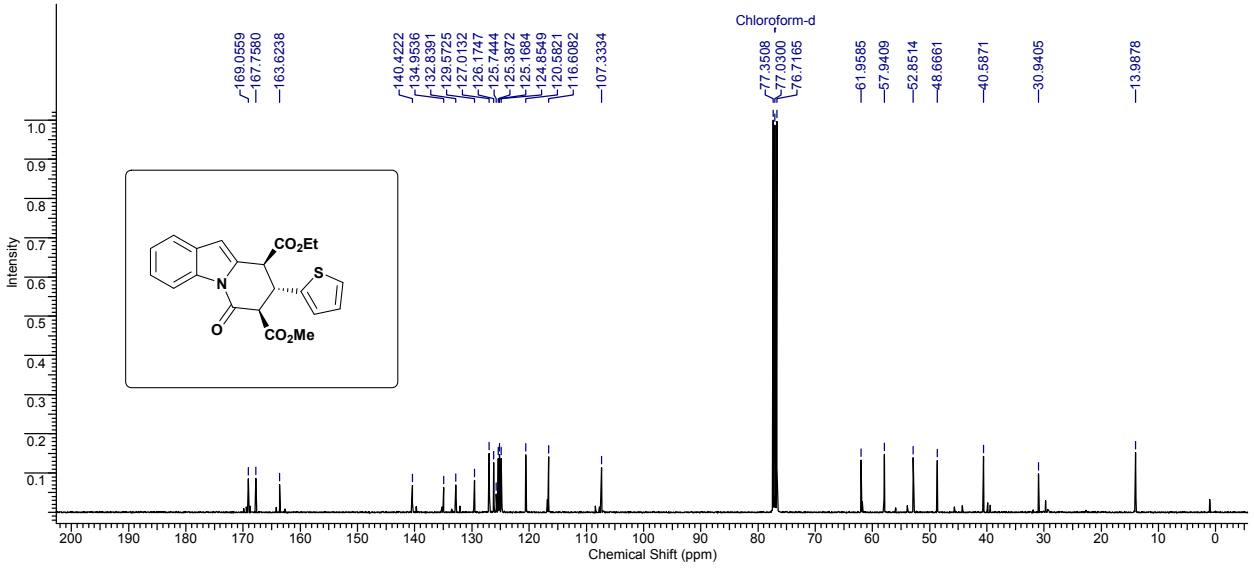

Chloroform-d
8.4392
8.4179
7.4996
7.3610
7.3390
7.3252
7.3177
7.3064
7.2600
7.2518
7.2355
6.4358
6.4327
4.2085
4.1684
4.1483
4.1389
4.1163
4.1088
4.0988
4.0411
4.0110
3.6415
1.1577
1.1395
1.1219
CO2Et
N
O
CO2Me
Cl
Intensity
0.87
4.56
0.77
3.26
2.71
3.00
Chemical Shift (ppm)

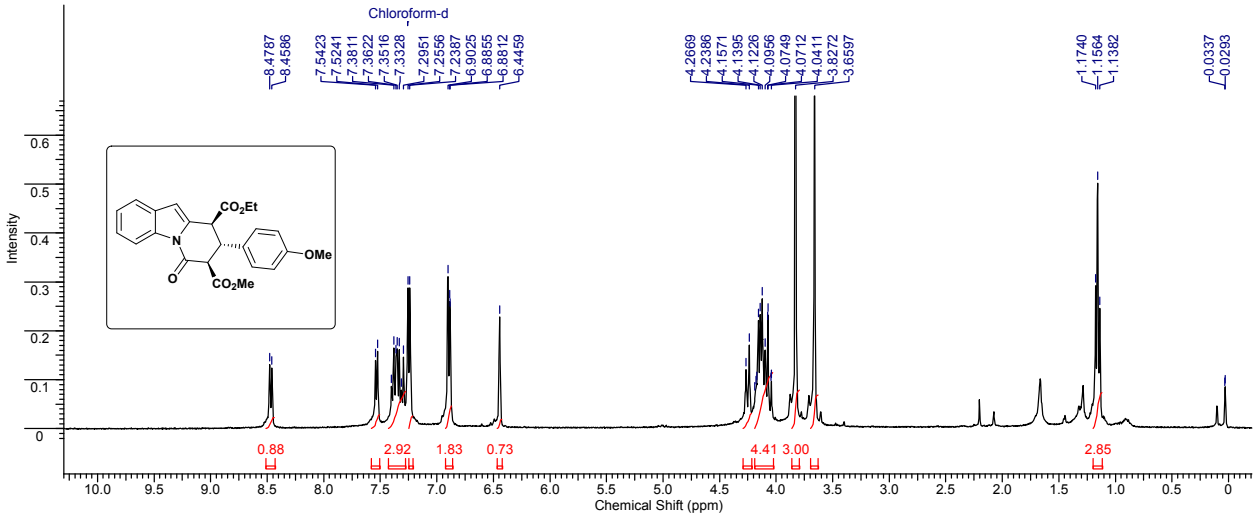

168.9903
167.6851
163.9883
135.7265
134.9609
134.1880
133.0432
129.5725
129.1860
129.1496
125.4309
124.8695
120.5967
116.5718
107.1876
Chloroform-d
77.3508
77.2342
77.0300
76.7165
61.8856
56.8034
52.7858
47.6088
44.6193
13.9950
CO2Et
N
O
CO2Me
Cl
Intensity
Chemical Shift (ppm)

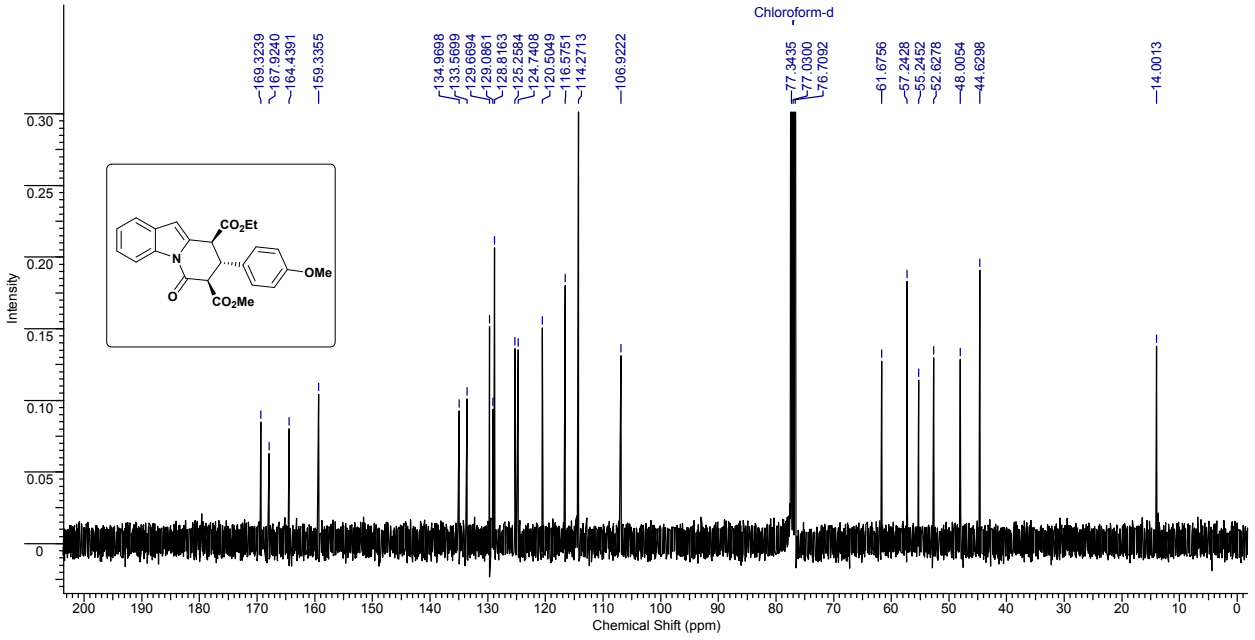

Chloroform-d
8.4455
8.4254
7.4965
7.4350
7.4174
7.3842
7.3666
7.3484
7.3234
7.3045
7.2600
6.8561
6.8360
6.7940
6.7708
6.4201
5.1312
4.2142
4.2104
4.1245
4.1075
4.0900
4.0806
4.0530
4.0386
4.0097
3.8736
3.6315
1.1295
1.1119
1.0937
CO2Et
OMe
OBn
N
O
CO2Me
Intensity
0.83
6.09
3.88
0.76
2.62
4.22
2.28
3.00
Chemical Shift (ppm)

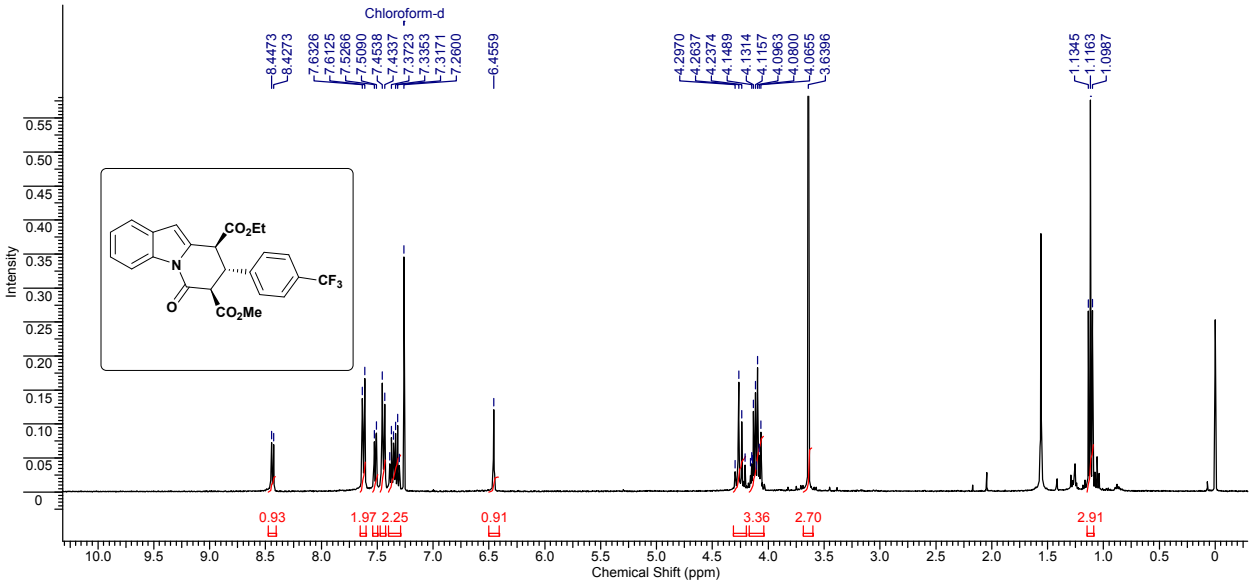

Chloroform-d
169.3549
167.9622
164.3675
149.6314
147.9252
136.8713
134.9245
133.4734
130.1558
129.6381
128.5590
127.9319
127.3340
125.2705
124.7601
120.5165
119.6415
116.5499
114.0124
111.5333
106.9689
77.3508
77.2342
77.0300
76.7165
70.9416
61.6960
57.1242
56.1034
52.6691
47.8203
44.9183
14.0315
CO2Et
OMe
OBn
N
O
CO2Me
Intensity
Chemical Shift (ppm)

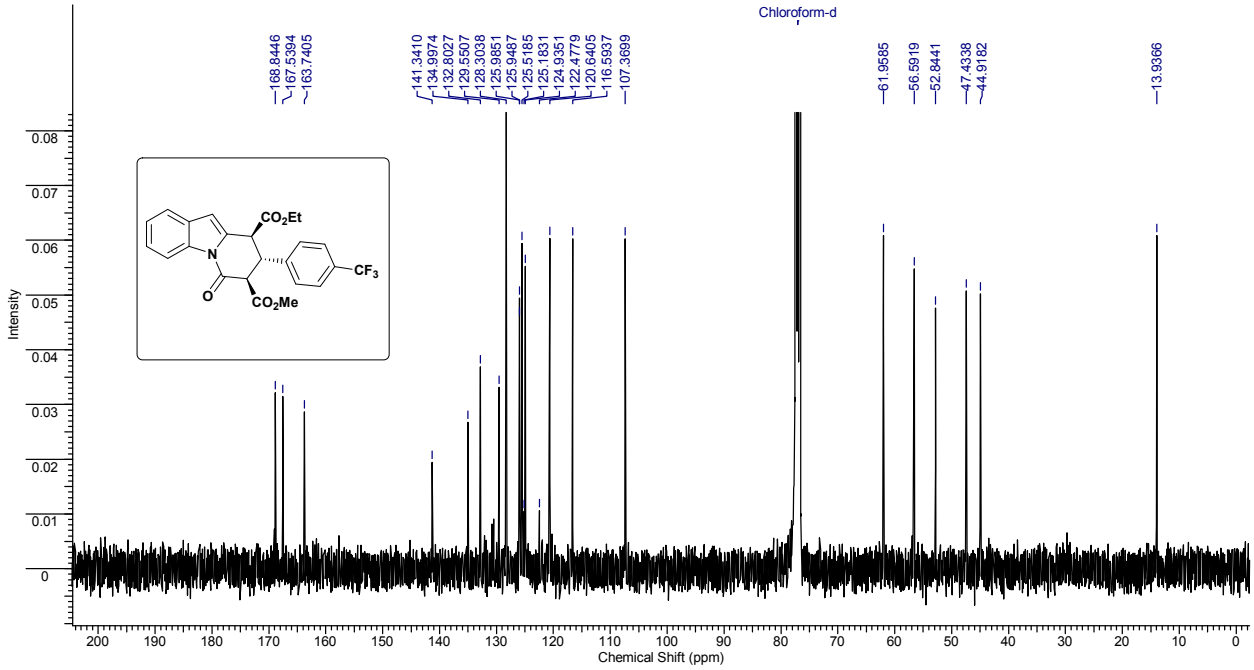

Chloroform-d
8.4448
8.4241
7.5009
7.3585
7.3271
7.3089
7.3058
7.2600
7.2280
6.9815
6.9784
6.9545
6.9420
6.9332
6.4502
6.4452
4.5021
4.4726
4.2606
4.2317
4.2098
4.1991
4.1916
4.1816
4.1740
4.0455
4.0160
3.7162
1.2148
1.1966
1.1790
0.0707
-0.0014
CO2Et
S
N
O
CO2Me
Intensity
0.81
2.57
2.39
0.71
1.20
3.18
2.60
3.00
Chemical Shift (ppm)

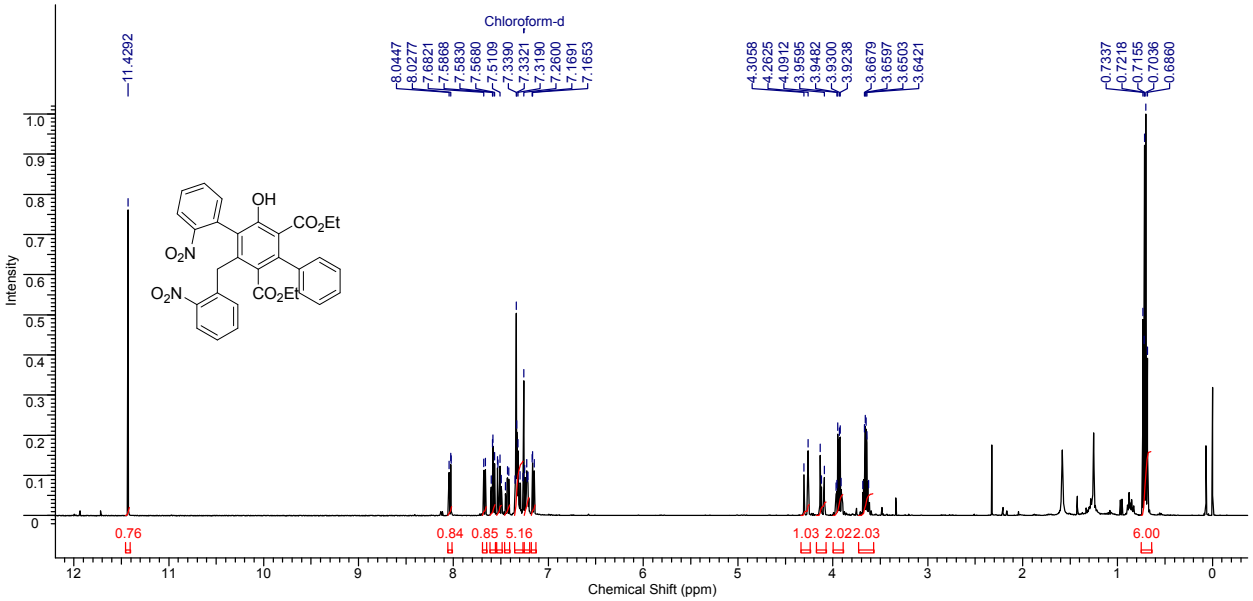

169.0559
167.7580
163.6238
140.4222
134.9536
132.8391
129.5725
127.0132
126.1747
125.7444
125.3872
125.1684
124.8549
120.5821
116.6082
107.3334
Chloroform-d
77.3508
77.0300
76.7165
61.9585
57.9409
52.8514
48.6661
40.5871
30.9405
13.9878
CO2Et
S
N
O
CO2Me
Intensity
Chemical Shift (ppm)

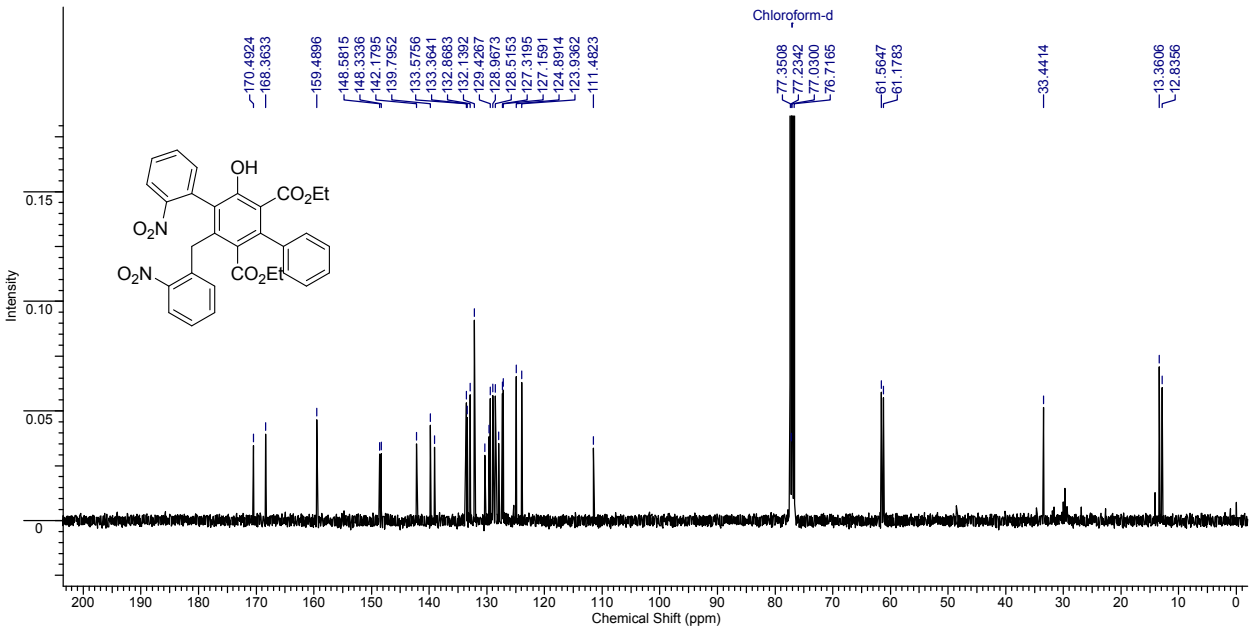

Chloroform-d
8.4787
8.4586
7.5423
7.5241
7.3811
7.3622
7.3516
7.3328
7.2951
7.2556
7.2387
6.9025
6.8855
6.8812
6.4459
4.2669
4.2386
4.1571
4.1395
4.1226
4.0956
4.0749
4.0712
4.0411
3.8272
3.6597
1.1740
1.1564
1.1382
0.0337
0.0293
CO2Et
OMe
CO2Me
Intensity
0.88
2.92
1.83
0.73
4.41
3.00
2.85
Chemical Shift (ppm)

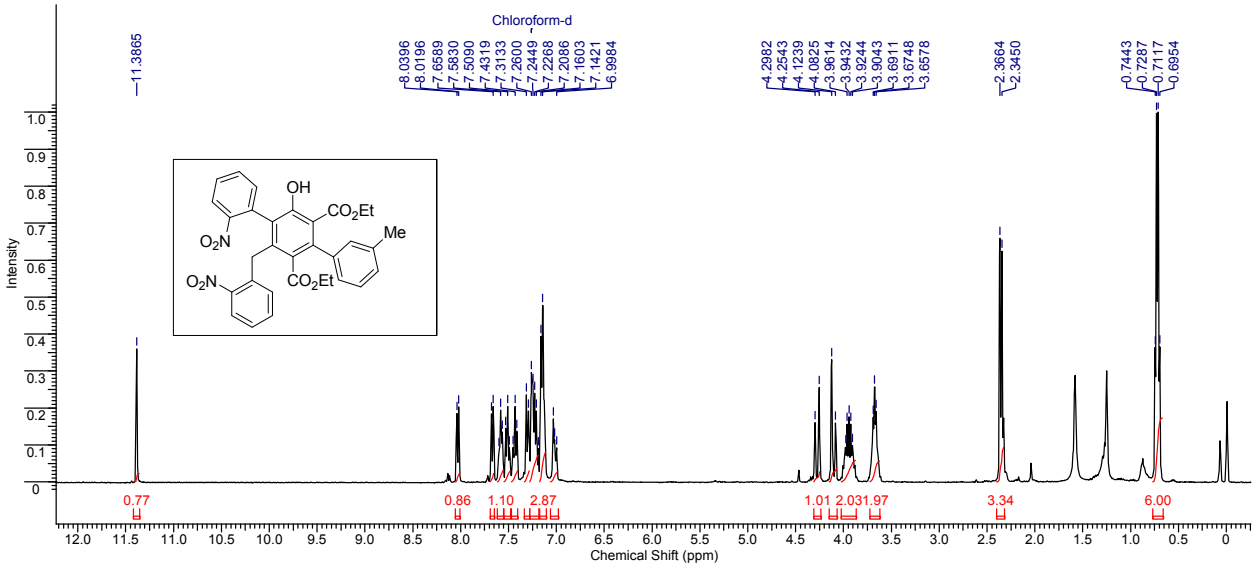

Chloroform-d
169.3239
167.9240
164.4391
159.3355
134.9698
133.5699
129.6694
129.0861
128.8163
125.2584
124.7408
120.5049
116.5751
114.2713
106.9222
77.3435
77.0300
76.7092
61.6756
57.2428
55.2452
52.6278
48.0054
44.6298
14.0013
CO2Et
OMe
CO2Me
Intensity
Chemical Shift (ppm)

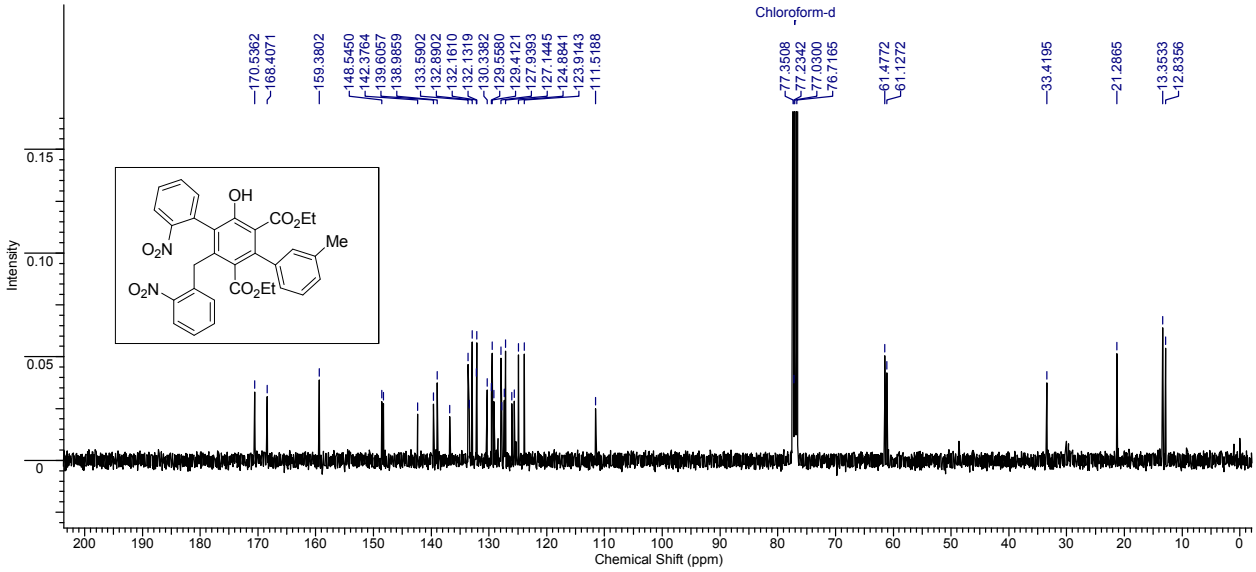

Chloroform-d
8.4473
8.4273
7.6326
7.6125
7.5266
7.5090
7.4538
7.4337
7.3723
7.3353
7.3171
7.2600
6.4559
4.2970
4.2637
4.2374
4.1489
4.1314
4.1157
4.0963
4.0800
4.0655
3.6396
1.1345
1.1163
1.0987
Intensity
Chemical Shift (ppm)
0.93
1.97
2.25
0.91
3.36
2.70
2.91
CO2Et
CF3
CO2Me

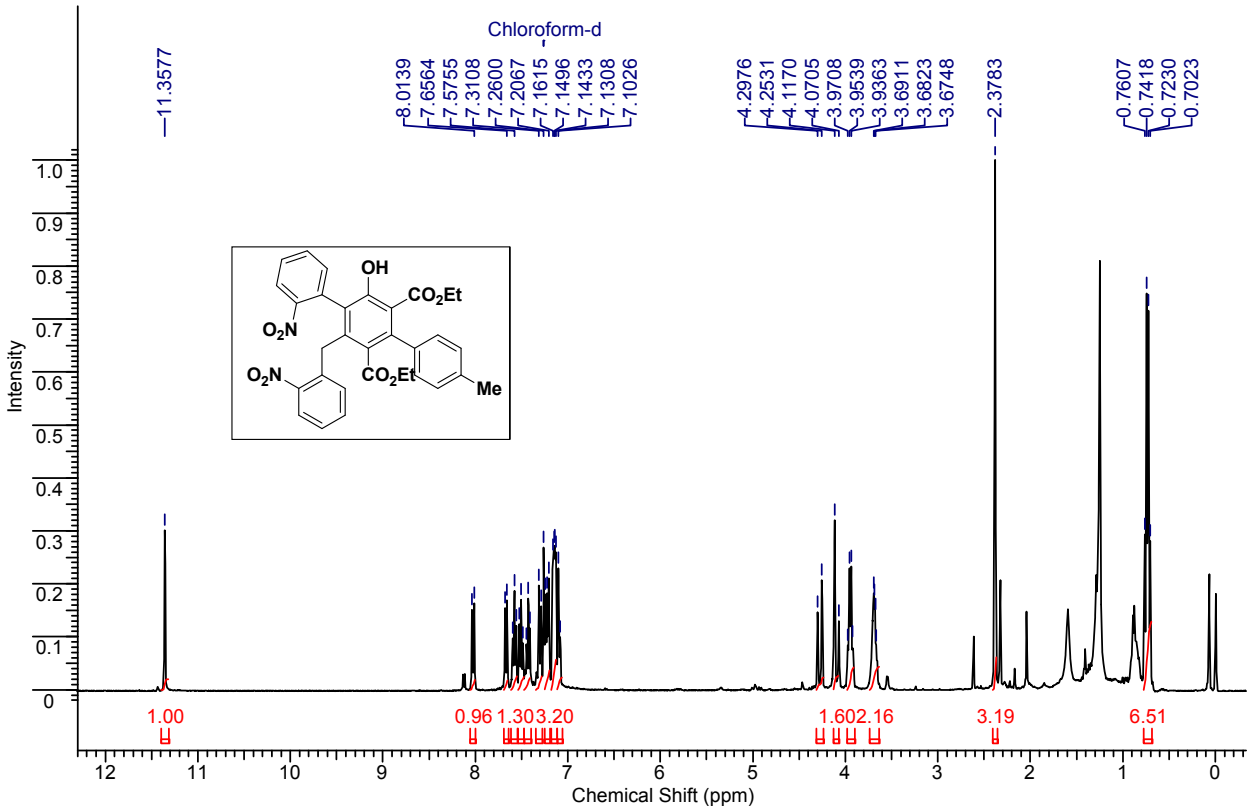

Chloroform-d
168.8446
167.5394
163.7405
141.3410
134.9974
132.8027
129.5507
128.3038
125.9851
125.9487
125.5185
125.1831
124.9351
122.4779
120.6405
116.5937
107.3699
61.9585
56.5919
52.8441
47.4338
44.9182
13.9366
Intensity
Chemical Shift (ppm)
CO2Et
CF3
CO2Me

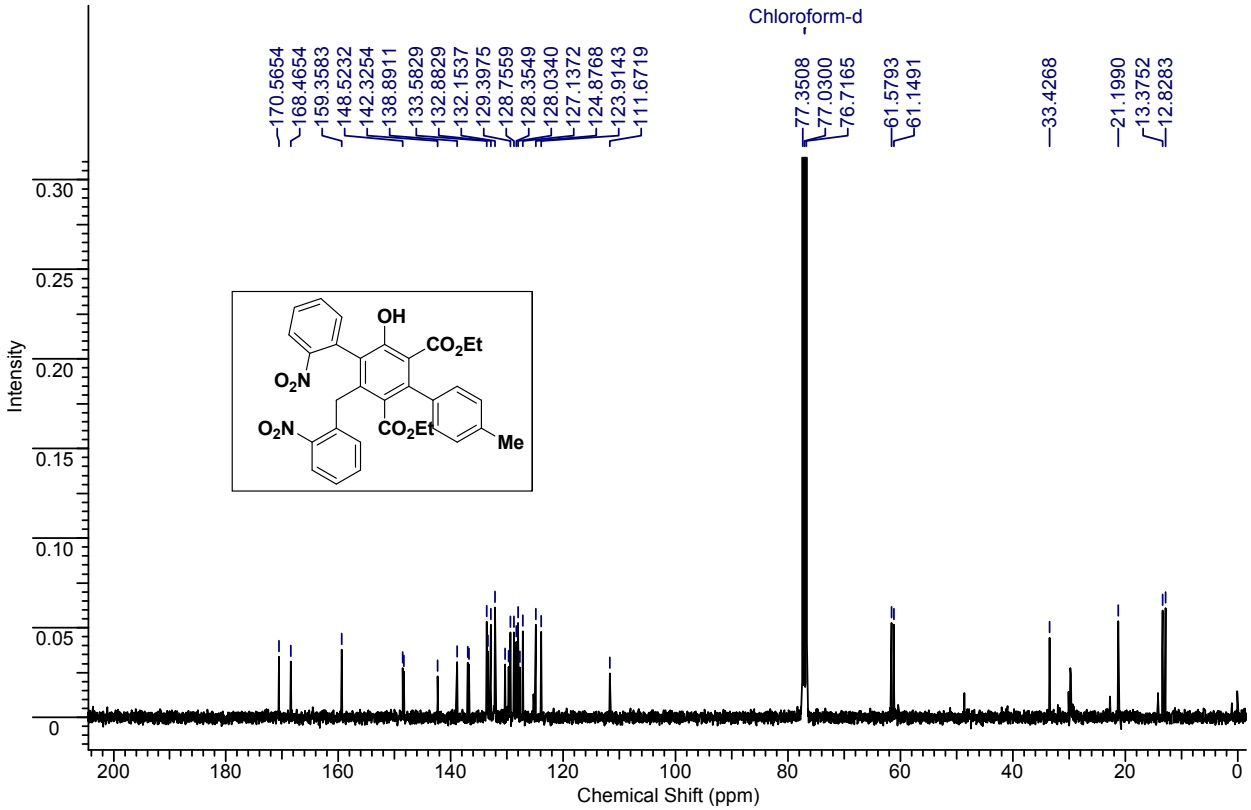

Chloroform-d
11.4292
8.0447
8.0277
7.6821
7.5868
7.5830
7.5680
7.5109
7.3390
7.3321
7.3190
7.2600
7.1691
7.1653
4.3058
4.2625
4.0912
3.9595
3.9482
3.9300
3.9238
3.6679
3.6597
3.6503
3.6421
0.7337
0.7218
0.7155
0.7036
0.6880
OH
CO2Et
O2N
O2N
CO2Et
Intensity
0.76
0.84
0.85
5.16
1.03
2.02
2.03
6.00
Chemical Shift (ppm)

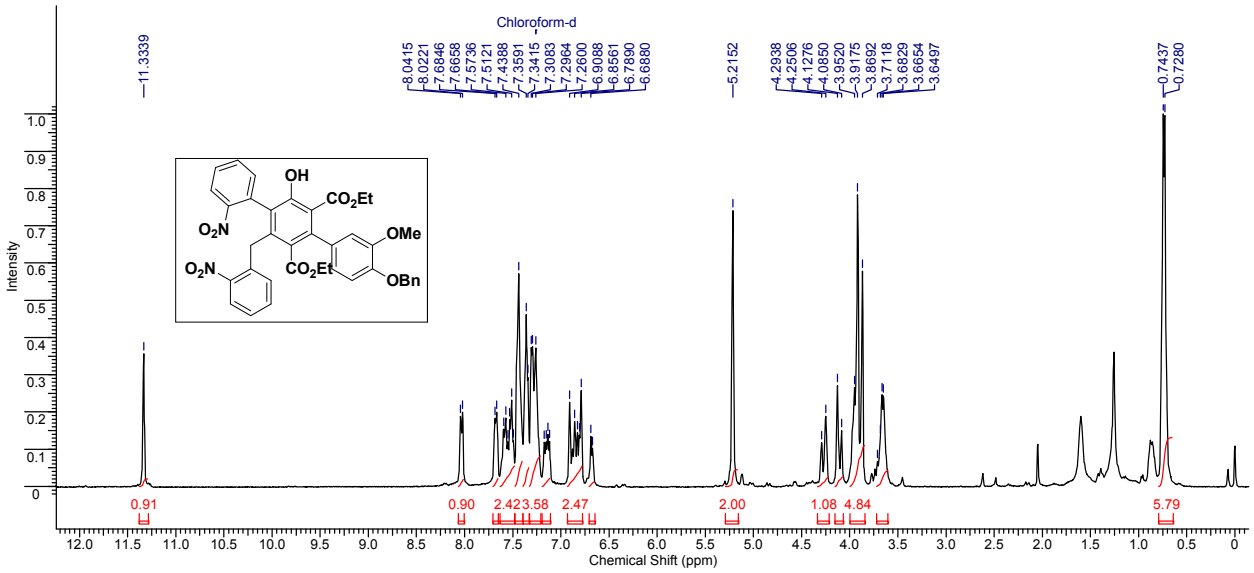

Chloroform-d
170.4924
168.3633
159.4896
148.5815
148.3336
142.1795
139.7952
133.5756
133.3641
132.8683
132.1392
129.4267
128.9673
128.5153
127.3195
127.1591
124.8914
123.9362
111.4823
77.3508
77.2342
77.0300
76.7165
61.5647
61.1783
33.4414
13.3606
12.8356
OH
CO2Et
O2N
O2N
CO2Et
Intensity
Chemical Shift (ppm)

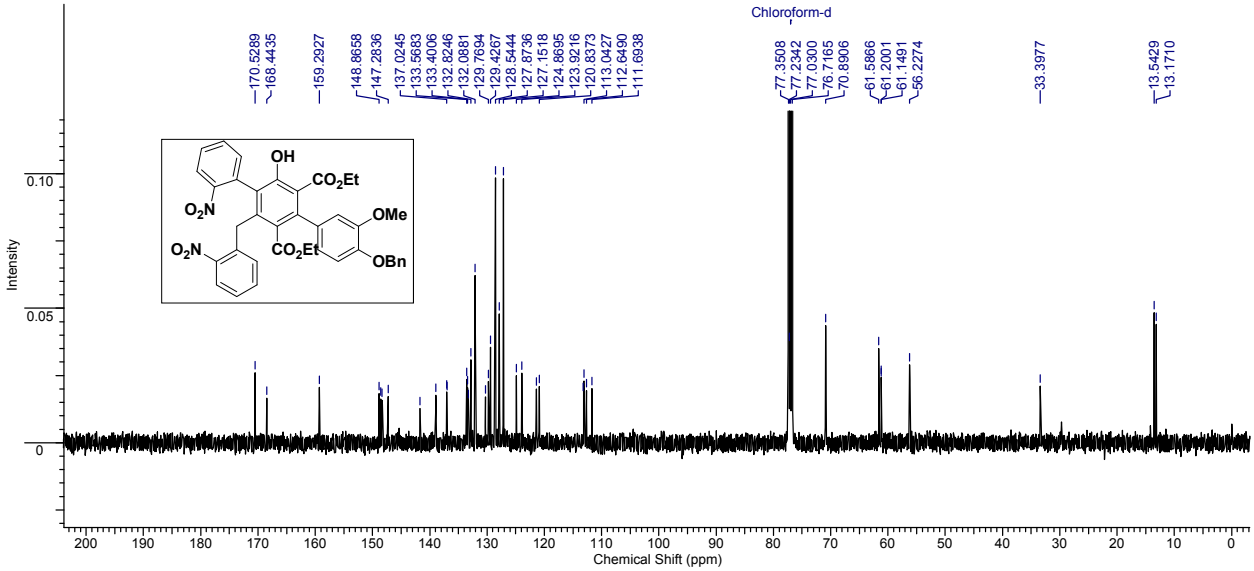

Chloroform-d
11.3865
8.0396
8.0196
7.6589
7.5830
7.5090
7.4319
7.3133
7.2600
7.2449
7.2268
7.2086
7.1603
7.1421
6.9984
4.2982
4.2543
4.1239
4.0825
3.9614
3.9432
3.9244
3.9043
3.6911
3.6748
3.6578
2.3664
2.3450
0.7443
0.7287
0.7117
0.6954
OH
CO2Et
Me
O2N
O2N
CO2Et
Intensity
0.77
0.86
1.10
2.87
1.01
2.03
1.97
3.34
6.00
Chemical Shift (ppm)

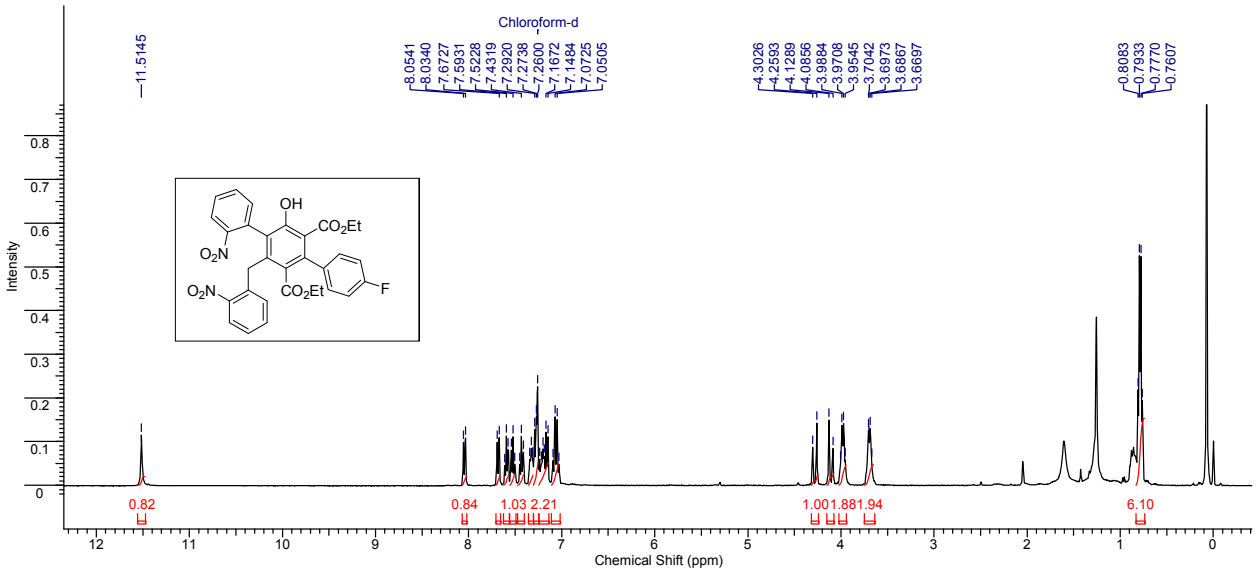

Chloroform-d
170.5362
168.4071
159.3802
148.5450
142.3764
139.6057
138.9859
133.5902
132.8902
132.1610
132.1319
130.3382
129.5580
129.4121
127.9393
127.1445
124.8841
123.9143
111.5188
77.3508
77.2342
77.0300
76.7165
61.4772
61.1272
33.4195
21.2865
13.3533
12.8356
OH
CO2Et
Me
O2N
O2N
CO2Et
Intensity
Chemical Shift (ppm)

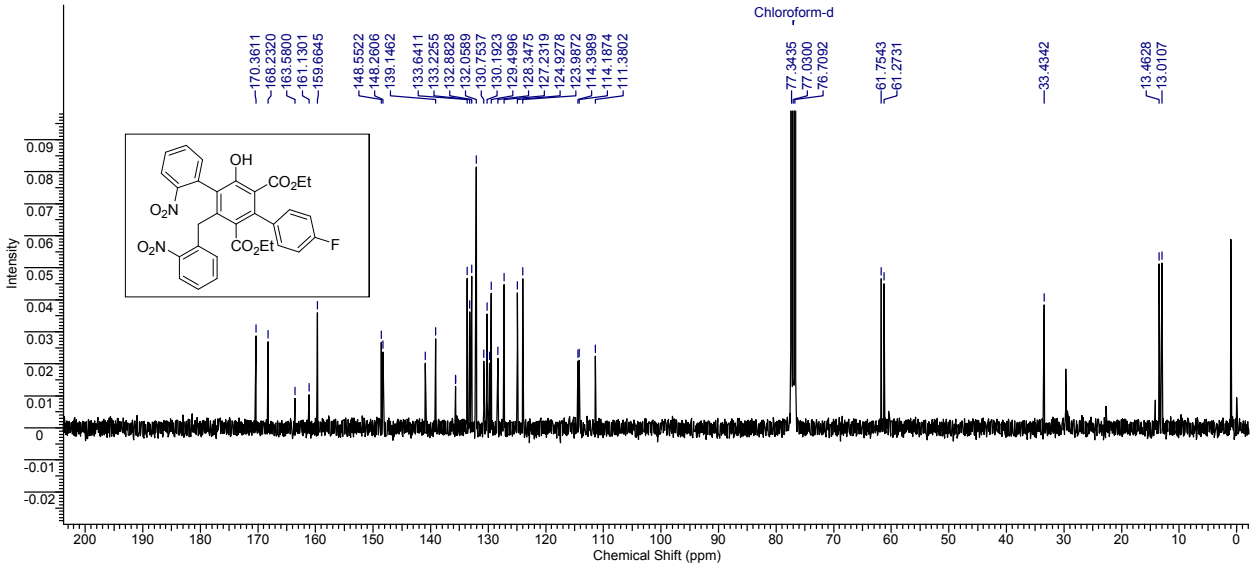

Chloroform-d
11.3577
8.0139
7.6564
7.5755
7.3108
7.2600
7.2067
7.1615
7.1496
7.1433
7.1308
7.1026
4.2976
4.2531
4.1170
4.0705
3.9708
3.9539
3.9363
3.6911
3.6823
3.6748
2.3783
0.7607
0.7418
0.7230
0.7023
OH
CO2Et
O2N
O2N
CO2Et
Me
Intensity
1.00
0.96
1.30
3.20
1.60
2.16
3.19
6.51
Chemical Shift (ppm)

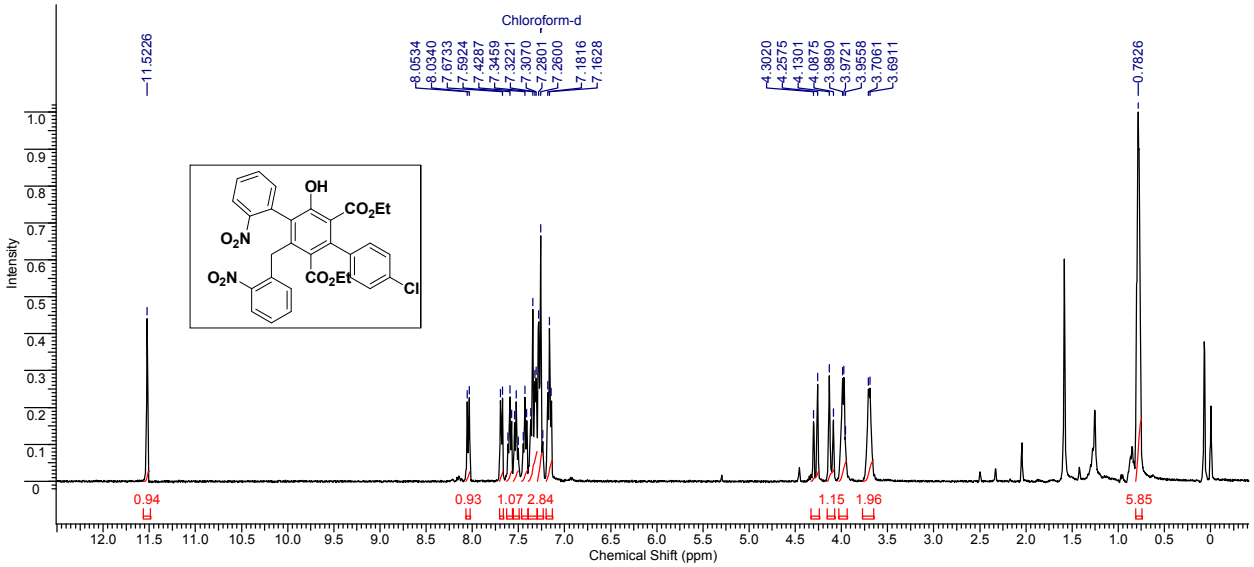

Chloroform-d
170.5654
168.4654
159.3583
148.5232
142.3254
138.8911
133.5829
132.8829
132.1537
129.3975
128.7559
128.3549
128.0340
127.1372
124.8768
123.9143
111.6719
77.3508
77.0300
76.7165
61.5793
61.1491
33.4268
21.1990
13.3752
12.8283
OH
CO2Et
O2N
O2N
CO2Et
Me
Intensity
Chemical Shift (ppm)

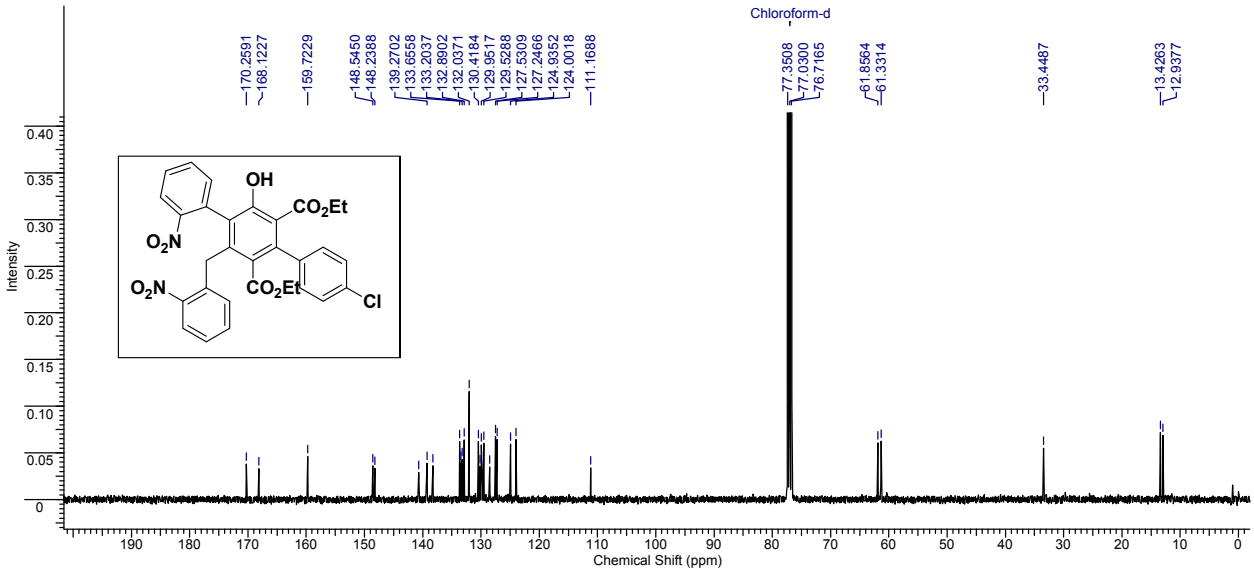

Chloroform-d
11.3339
8.0415
8.0221
7.6846
7.6658
7.5736
7.5121
7.4388
7.3591
7.3415
7.3083
7.2964
7.2600
6.9088
6.8561
6.7890
6.6880
5.2152
4.2938
4.2506
4.1276
4.0850
3.9520
3.9175
3.8692
3.7118
3.6829
3.6654
3.6497
0.7437
0.7280
OH
CO2Et
O2N
OMe
O2N
CO2Et
OBn
Intensity
0.91
0.90
2.42
3.58
2.47
2.00
1.08
4.84
5.79
Chemical Shift (ppm)

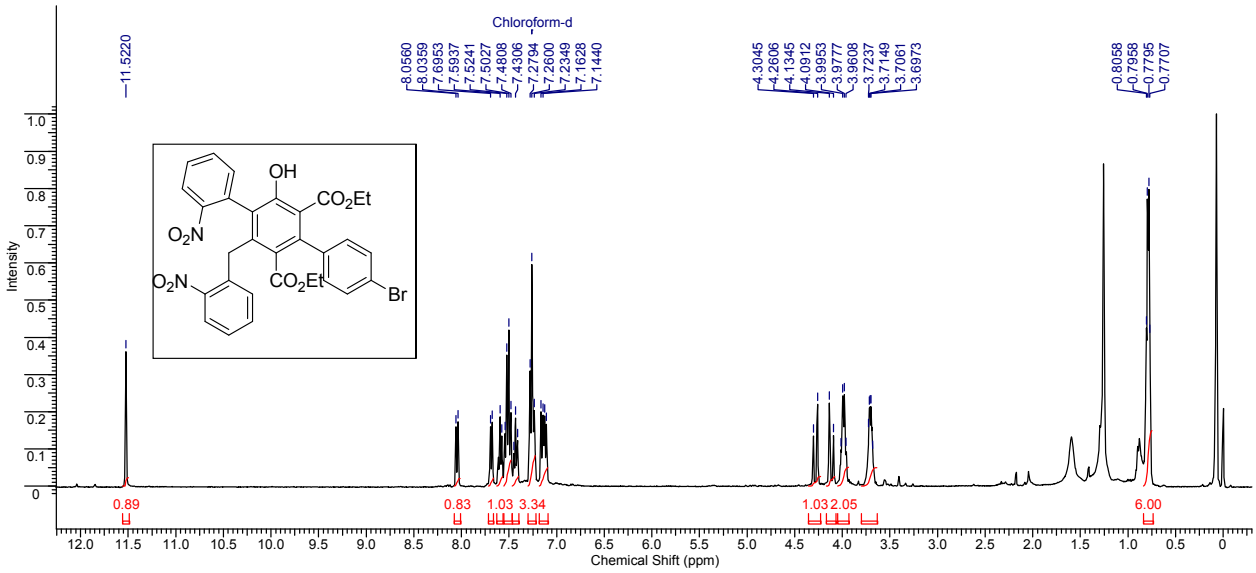

Chloroform-d
170.5289
168.4435
159.2927
148.8658
147.2836
137.0245
133.5683
133.4006
132.8246
132.0881
129.7694
129.4267
128.5444
127.8736
127.1518
124.8695
123.9216
120.8373
113.0427
112.6490
111.6938
77.3508
77.2342
77.0300
76.7165
70.8906
61.5886
61.2001
61.1491
56.2274
33.3977
13.5429
13.1710
OH
CO2Et
O2N
OMe
O2N
CO2Et
OBn
Intensity
Chemical Shift (ppm)

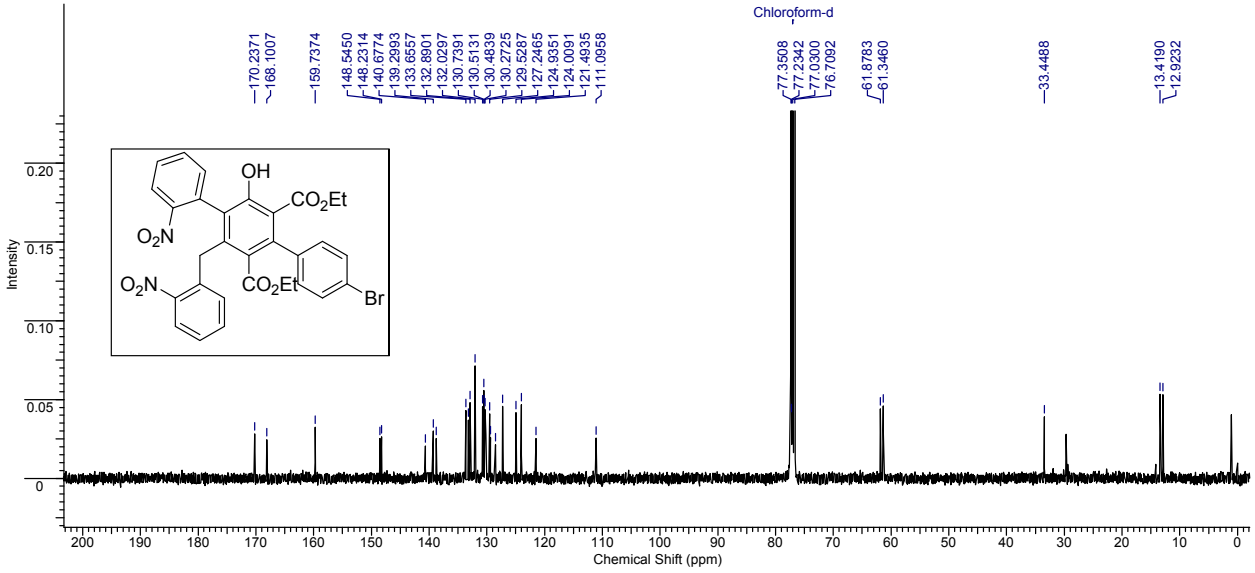

Chloroform-d
11.5145
8.0541
8.0340
7.6727
7.5931
7.5228
7.4319
7.2920
7.2738
7.2600
7.1672
7.1484
7.0725
7.0505
4.3026
4.2593
4.1289
4.0856
3.9884
3.9708
3.9545
3.7042
3.6973
3.6867
3.6697
0.8083
0.7933
0.7770
0.7607
OH
CO2Et
O2N
O2N
CO2Et
F
Intensity
0.82
0.84
1.03
2.21
1.00
1.88
1.94
6.10
Chemical Shift (ppm)

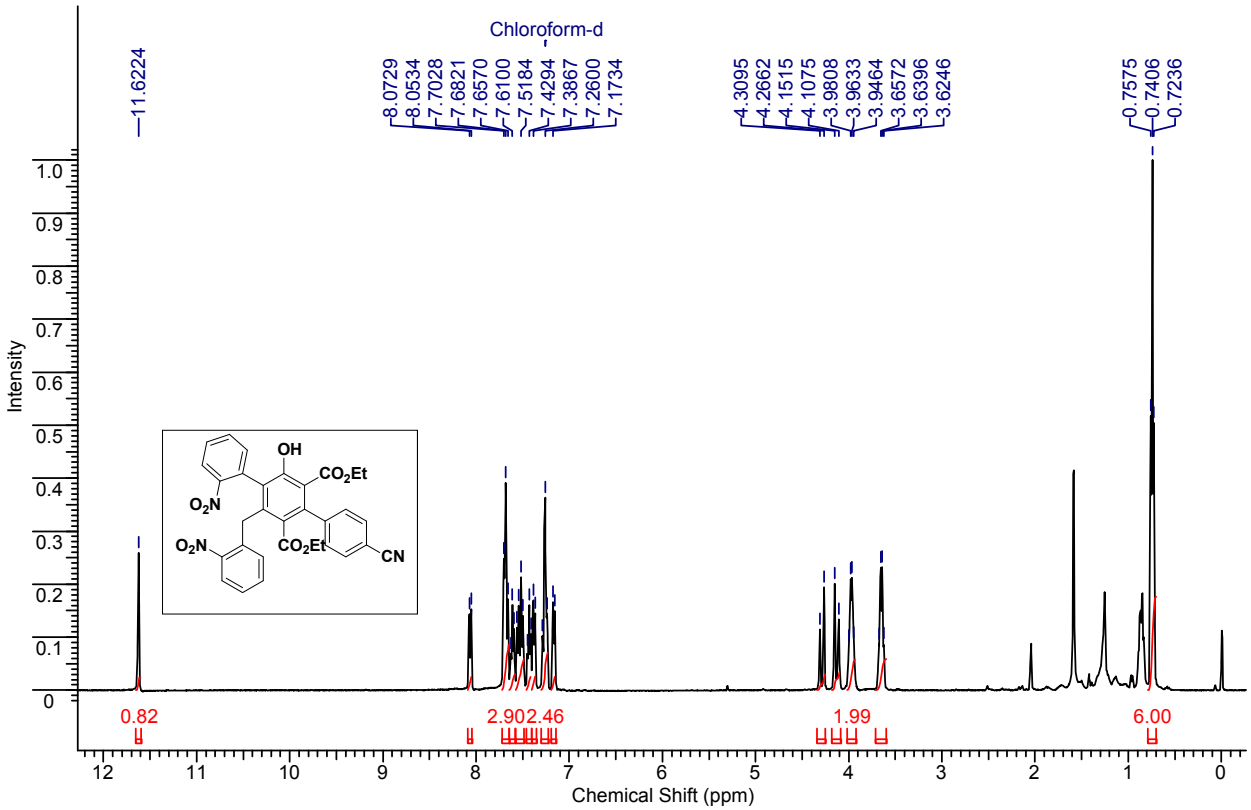

Chloroform-d
170.3611
168.2320
163.5800
161.1301
159.6645
148.5522
148.2606
139.1462
133.6411
133.2255
132.8828
132.0589
130.7537
130.1923
129.4996
128.3475
127.2319
124.9278
123.9872
114.3989
114.1874
111.3802
77.3435
77.0300
76.7092
61.7543
61.2731
33.4342
13.4628
13.0107
OH
CO2Et
O2N
O2N
CO2Et
F
Intensity
Chemical Shift (ppm)

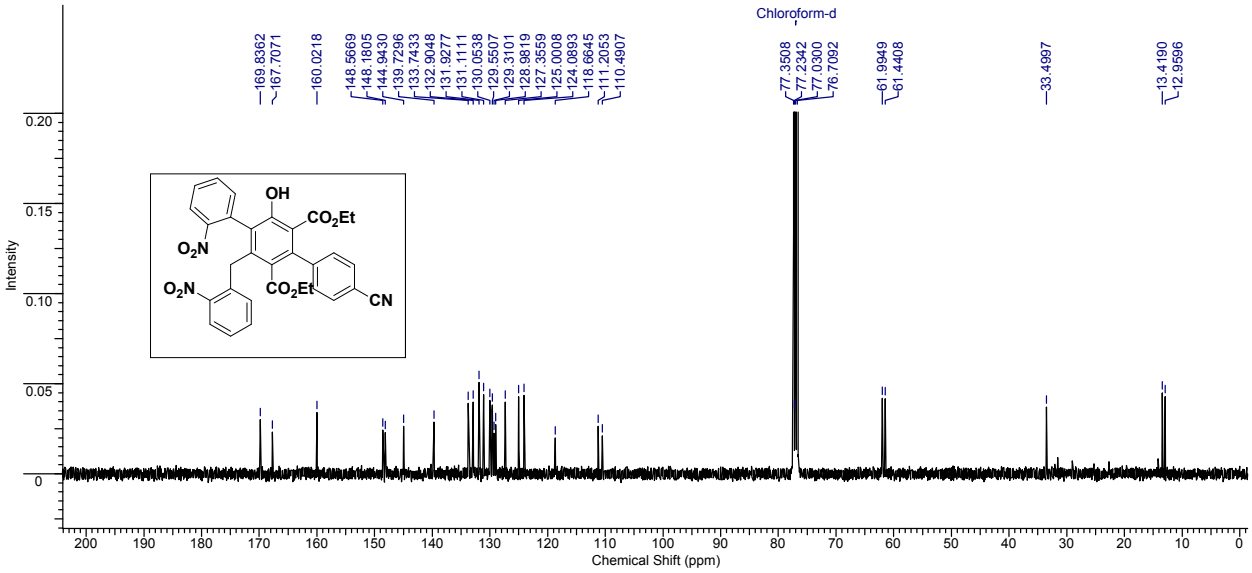

Chloroform-d
11.5226
8.0534
8.0340
7.6733
7.5924
7.4287
7.3459
7.3221
7.3070
7.2801
7.2600
7.1816
7.1628
4.3020
4.2575
4.1301
4.0875
3.9890
3.9721
3.9558
3.7061
3.6911
0.7826
OH
CO2Et
O2N
O2N
CO2Et
Cl
Intensity
0.94
0.93
1.07
2.84
1.15
1.96
5.85
Chemical Shift (ppm)

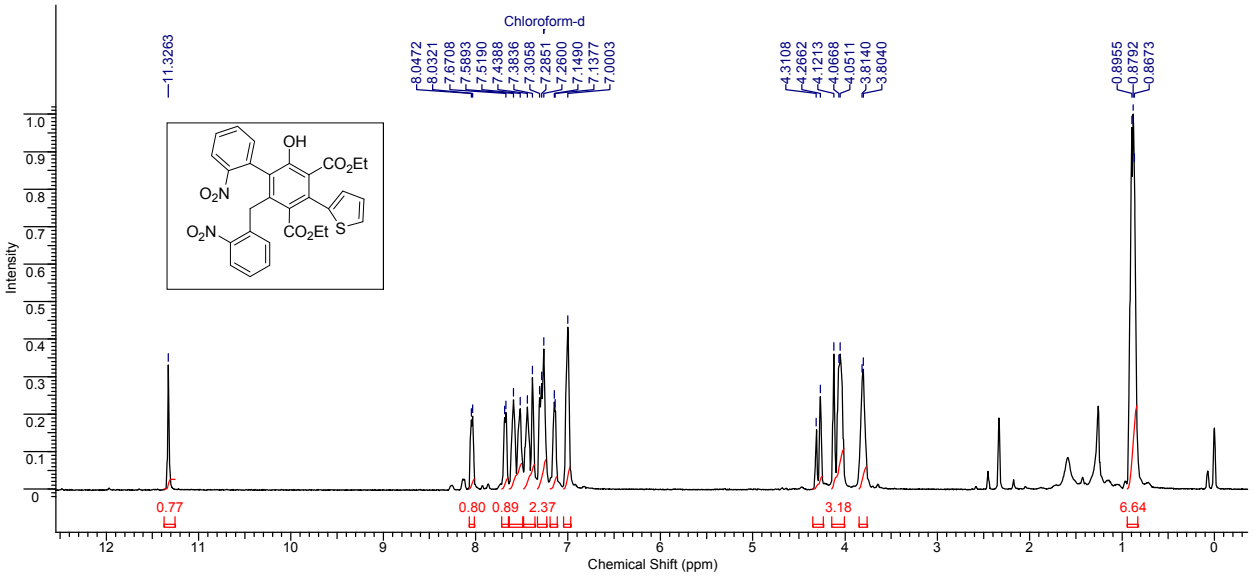

Chloroform-d
170.2591
168.1227
159.7229
148.5450
148.2388
139.2702
133.6558
133.2037
132.8902
132.0371
130.4184
129.9517
129.5288
127.5309
127.2466
124.9352
124.0018
111.1688
77.3508
77.0300
76.7165
61.8564
61.3314
33.4487
13.4263
12.9377
OH
CO2Et
O2N
O2N
CO2Et
Cl
Intensity
Chemical Shift (ppm)

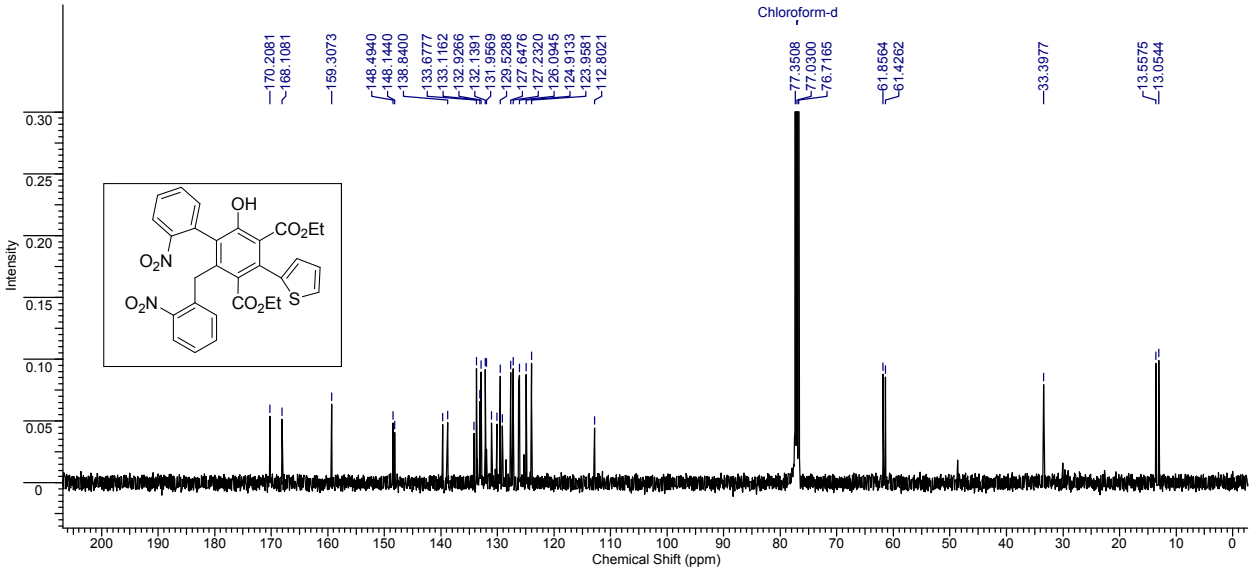

Chloroform-d
11.5220
8.0560
8.0359
7.6953
7.5937
7.5241
7.5027
7.4808
7.4306
7.2794
7.2600
7.2349
7.1628
7.1440
4.3045
4.2606
4.1345
4.0912
3.9953
3.9777
3.9608
3.7237
3.7149
3.7061
3.6973
0.8058
0.7958
0.7795
0.7707
OH
CO2Et
O2N
O2N
CO2Et
Br
Intensity
0.89
0.83
1.03
3.34
1.03
2.05
6.00
Chemical Shift (ppm)

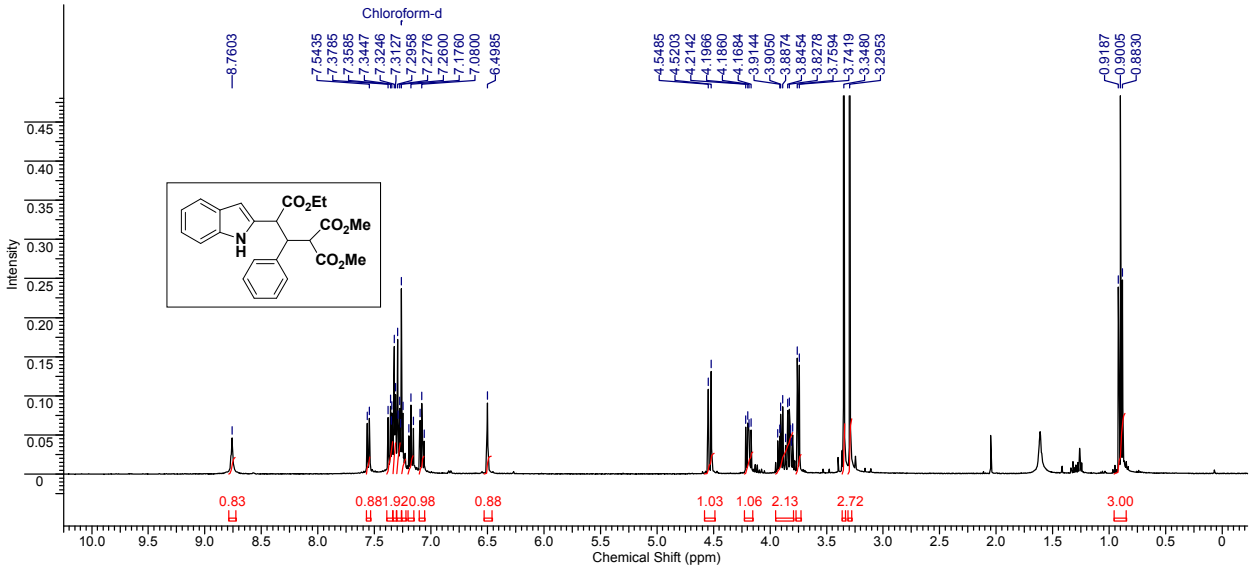

Chloroform-d
170.2371
168.1007
159.7374
148.5450
148.2314
140.6774
139.2993
133.6557
132.8901
132.0297
130.7391
130.5131
130.4839
130.2725
129.5287
127.2465
124.9351
124.0091
121.4935
111.0958
77.3508
77.2342
77.0300
76.7092
61.8783
61.3460
33.4488
13.4190
12.9232
OH
CO2Et
O2N
O2N
CO2Et
Br
Intensity
Chemical Shift (ppm)

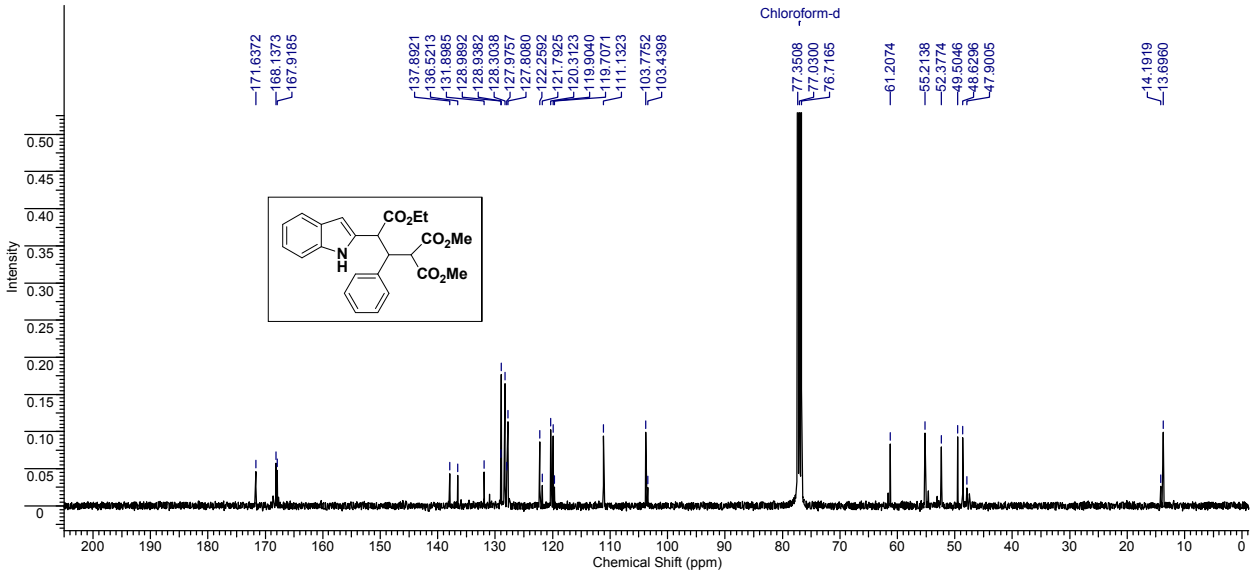

Chloroform-d
11.6224
8.0729
8.0534
7.7028
7.6821
7.6570
7.6100
7.5184
7.4294
7.3867
7.2600
7.1734
4.3095
4.2662
4.1515
4.1075
3.9808
3.9633
3.9464
3.6572
3.6396
3.6246
0.7575
0.7406
0.7236
Intensity
0.82
2.90
2.46
1.99
6.00
Chemical Shift (ppm)
OH
CO2Et
O2N
O2N
CO2Et
CN


Chloroform-d
169.8362
167.7071
160.0218
148.5669
148.1805
144.9430
139.7296
133.7433
132.9048
131.9277
131.1111
130.0538
129.5507
129.3101
128.9819
127.3559
125.0008
124.0893
118.6645
111.2053
110.4907
77.3508
77.2342
77.0300
76.7092
61.9949
61.4408
33.4997
13.4190
12.9596
Intensity
Chemical Shift (ppm)
OH
CO2Et
O2N
O2N
CO2Et
CN


Chloroform-d
11.3263
8.0472
8.0321
7.6708
7.5893
7.5190
7.4388
7.3836
7.3058
7.2851
7.2600
7.1490
7.1377
7.0003
4.3108
4.2662
4.1213
4.0668
4.0511
3.8140
3.8040
0.8955
0.8792
0.8673
OH
CO2Et
O2N
O2N
CO2Et
S
Intensity
0.77
0.80
0.89
2.37
3.18
6.64
Chemical Shift (ppm)


Chloroform-d
170.2081
168.1081
159.3073
148.4940
148.1440
138.8400
133.6777
133.1162
132.9266
132.1391
131.9569
129.5288
127.6476
127.2320
126.0945
124.9133
123.9581
112.8021
77.3508
77.0300
76.7165
61.8564
61.4262
33.3977
13.5575
13.0544
OH
CO2Et
O2N
O2N
CO2Et
S
Intensity
Chemical Shift (ppm)


Chloroform-d
8.7603
7.5435
7.3785
7.3585
7.3447
7.3246
7.3127
7.2958
7.2776
7.2600
7.1760
7.0800
6.4985
4.5485
4.5203
4.2142
4.1966
4.1860
4.1684
3.9144
3.9050
3.8874
3.8454
3.8278
3.7594
3.7419
3.3480
3.2953
0.9187
0.9005
0.8830
Intensity
Chemical Shift (ppm)
0.83
0.88
1.03
1.06
2.13
2.72
3.00


Chloroform-d
171.6372
168.1373
167.9185
137.8921
136.5213
131.8985
128.9892
128.9382
128.3038
127.9757
127.8080
122.2592
121.7925
120.3123
119.9040
119.7071
111.1323
103.7752
103.4398
77.3508
77.0300
76.7165
61.2074
55.2138
52.3774
49.5046
48.6296
47.9005
14.1919
13.6960
Intensity
Chemical Shift (ppm)