ELECTRONIC SUPPLEMENTARY INFORMATION

Synthesis of 2,4,5-trisubstituted oxazoles through tin(IV) chloride-mediated reaction of *trans*-2-aryl-3-nitro-cyclopropane-1,1-dicarboxylates with nitriles

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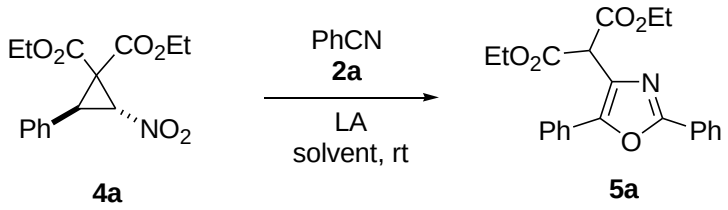
A. Optimisation of reaction conditions for the synthesis of oxazoles[a]



4a **5a**

Entry	Lewis acid (equiv)	Solvent	Time (h)	Yield (%)[b]
1	$SnCl_4$ (1.0)	1,2-DCE	5	89
2	$AlCl_3$ (1.0)	1,2-DCE	48	7[c]
3	$FeCl_3$ (1.0)	1,2-DCE	48	5
4	$BF_3.OEt_2$ (1.0)	1,2-DCE	48	NR[d]
5	$InCl_3$ (1.0)	1,2-DCE	48	NR[e]
6	MgI_2 (1.0)	1,2-DCE	4	NR[e]
7	$TiCl_4$ (1.0)	1,2-DCE	48	NR[e]
8	$Cu(OTf)_2$ (1.0)	1,2-DCE	48	NR[e]
9	$In(OTf)_3$ (1.0)	1,2-DCE	48	NR[e]
10	$Sc(OTf)_3$ (1.0)	1,2-DCE	48	NR[e]
11	$Yb(OTf)_3$ (1.0)	1,2-DCE	48	NR[e]
12	$SnCl_4$ (0.5)	1,2-DCE	12	62
13	$SnCl_4$ (1.5)	1,2-DCE	3	79
14	$SnCl_4$ (1.0)	DCM	9	68
15	$SnCl_4$ (1.0)	Toluene	48	42
16	$SnCl_4$ (1.0)	THF	48	NR[e]

[a]The reaction was conducted with **4a** (1 mmol), **2a** (1 mmol), Lewis acid (x mmol) and solvent (3 mL). [b]Isolated yield. [c]Diethyl phenacylmalonate is produced as byproduct in 65% yield. [d]Only benzoylmethylidene malonate **6a** (82%) is produced (no trace of oxazole). [e]No reaction.

B. Experimental Procedures

I. General Methods: Melting points were determined by the open capillary tube method and are uncorrected. The ^{1}H and ^{13}C NMR spectra were recorded on a *400 MHz* NMR spectrometer. High resolution mass spectra (ESI) were recorded on a Q-TOF mass spectrometer. The IR spectra were recorded on a FT-IR spectrometer. Low resolution mass spectra (ESI) were recorded on a LC mass spectrometer. Elemental analyses were performed on a CHN analyzer. X-ray crystallographic data were collected on a CCD diffractometer using graphite-monochromated Mo-Kα radiation. Thin layer chromatography (TLC) was performed on pre-coated alumina sheets and detected under UV light. *S*ilica gel (100-200 mesh) was used for column chromatography.

II. General procedure for the synthesis of oxazoles 5a-5ad:

To a mixture of nitrocyclopropane **4** (1 mmol) and nitrile **2** (1 mmol) in 1,2-dichloroethane (3 mL) was added $SnCl_4$ (1 mmol). The reaction mixture was stirred at room temperature for 1 to 7 h. After the reaction was complete, the reaction mixture was quenched with water and extracted with dichloromethane. The organic layer was washed with water, dried (anhydrous Na_2SO_4) and the solvent was removed under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane to give pure oxazole **5**. (This procedure when applied for cyclopropane **4a** and thiophene-2-acetonitrile (**2k**), the Michael adduct **8** was produced).

C. Characterization Data for Compounds 5a-5ad & 8:

Diethyl 2-(2,5-diphenyl-oxazol-4-yl)malonate (5a):

White solid; Yield: 337 mg (89%); M.p. 80-82 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12-8.10 (m, 2H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.49-7.38 (m, 6H), 4.98 (s, 1H), 4.30-4.19 (m, 4H), 1.25 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 160.1, 148.4, 130.4, 129.6, 128.9, 128.7, 127.9, 127.2, 126.6, 126.5, 62.1, 51.3, 14.0 ppm; IR (KBr): 2925, 2853, 1735, 1596, 1545 cm^{-1}; HRMS (ESI) calcd. for $C_{22}H_{21}NO_5$: 380.1493 [$M+H^+$], found: 380.1500.

Diethyl 2-[5-(4-methylphenyl)-2-phenyl-oxazol-4-yl]malonate (5b):

White solid; Yield: 346 mg (88%); M.p. 76-78 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11-8.08 (m, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.46-7.43 (m, 3H), 7.28 (d, *J* = 8.8 Hz, 2H), 4.95 (s, 1H), 4.28-4.21 (m, 4H), 2.40 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 159.8, 148.6, 139.0, 130.3, 129.6, 129.1, 128.6, 127.4, 126.6, 126.5, 125.1, 62.1, 51.3, 21.4, 14.0 ppm; IR (KBr): 2923, 2852, 1735, 1605, 1553 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{23}NO_5$: 394.1649 [$M+H^+$], found: 394.1649.

Diethyl 2-[5-(4-methoxyphenyl)-2-phenyl-oxazol-4-yl]malonate (5c):

Pale yellow solid; Yield: 368 mg (90%); M.p. 84-86 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10-8.07 (m, 2H), 7.61-7.58 (m, 2H), 7.46-7.43 (m, 3H), 6.99 (d, *J* = 8.8 Hz, 2H), 4.93 (s, 1H), 4.28-4.20 (m, 4H), 3.86 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 160.2, 159.6, 148.5, 130.2, 128.6, 128.4, 128.2, 127.4, 126.5, 120.6, 114.3, 62.1, 55.4, 51.3, 14.0

ppm; IR (KBr): 2931, 2850, 1731, 1604, 1510 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{23}NO_6$: 410.1598 [$M+H^+$], found: 410.1595.

Diethyl 2-[5-(4-chlorophenyl)-2-phenyl-oxazol-4-yl]malonate (5d):

White solid; Yield: 351 mg (85%); M.p. 70-72 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10-8.08 (m, 2H), 7.65-7.60 (m, 2H), 7.48-7.44 (m, 5H), 4.94 (s, 1H), 4.30-4.20 (m, 4H), 1.25 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 160.2, 146.6, 130.6, 130.5, 129.2, 129.1, 128.8, 128.7, 127.8, 127.0, 126.6, 126.4, 62.2, 51.4, 14.0 ppm; IR (KBr): 2983, 2922, 1730, 1546, 1488 cm^{-1}; HRMS (ESI) calcd. for $C_{22}H_{20}ClNO_5$: 414.1103 [$M+H^+$], found: 414.1110.

Diethyl 2-[5-(3,4-dimethoxyphenyl)-2-phenyl-oxazol-4-yl]malonate (5f):

White solid; Yield: 391 mg (89%); M.p. 94-96 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10-8.08 (m, 2H), 7.47-7.44 (m, 3H), 7.24-7.22 (m, 2H), 6.96 (d, *J* = 8.0 Hz, 1H), 4.95 (s, 1H), 4.29-4.17 (m, 4H), 3.94 (d, *J* = 8.0Hz, 6H), 1.24 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 159.6, 149.7, 149.1, 148.6, 130.3, 128.7, 128.6, 127.3, 126.5, 120.7, 119.6, 111.3, 110.0, 62.1, 56.0, 51.5, 14.0 ppm; IR (KBr): 2933, 2834, 1743, 1606, 1514 cm^{-1}; HRMS (ESI) calcd. for $C_{24}H_{25}NO_7$: 440.1704 [$M+H^+$], found: 440.1714.

Diethyl 2-[2-phenyl-5-(3,4,5-trimethoxyphenyl)-oxazol-4-yl]malonate (5g):

Brown semisolid; Yield: 328 mg (70%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10-8.08 (m, 2H),7.46-7.45 (m, 3H), 6.93 (s, 2H), 4.97 (s, 1H), 4.26-4.18 (m, 4H), 3.93 (s, 6H), 3.89 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 159.8, 153.6, 148.6, 138.8, 130.5, 129.3, 128.7, 127.2, 126.6, 123.3, 104.1, 62.2, 61.0, 56.2, 51.7, 14.0 ppm; IR (KBr): 2937, 2848,

1732, 1579, 1505 cm^{-1}; HRMS (ESI) calcd. for $C_{25}H_{27}NO_8$: 492.1629 [M+Na^+], found: 492.1637.

Diethyl 2-[5-(2-iodo-4,5-dimethoxyphenyl)-2-phenyl-oxazol-4-yl]malonate (5i):

Yellow semisolid; Yield: 322 mg (57%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12-8.09 (m, 2H), 7.46-7.44 (m, 3H), 7.35 (s, 1H), 7.19 (s, 1H), 4.79 (s, 1H), 4.21-4.05 (m, 4H), 3.92 (s, 3H), 3.87 (s, 3H), 1.23 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 160.5, 150.5, 149.2, 149.0, 131.1, 130.5, 128.7, 127.3, 126.6, 125.3, 122.1, 115.4, 86.9, 62.1, 56.3, 56.1, 51.3, 14.0 ppm ; IR (KBr): 2925, 2854, 1733, 1586, 1501 cm^{-1}; MS (ESI): *m/z* 566.10 [M+H^+]. Anal. calcd. for $C_{24}H_{24}INO_7$: C 50.99, H 4.28, N 2.48; found: C 50.74, H 4.38, N 2.62.

Diethyl 2-(5-naphthalen-1-yl-2-phenyl-oxazol-4-yl)malonate (5j)

Brown oil; Yield: 356 mg (83%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14-8.11 (m, 2H), 7.98-7.91 (m, 3H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.57-7.53 (m, 3H), 7.46 (t, *J* = 6.4 Hz, 3H), 4.78 (s, 1H), 4.15-4.09 (m, 2H), 4.07-3.97 (m, 2H), 1.13 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 161.1, 147.9, 133.7, 132.1, 132.0, 130.49, 130.47, 129.2, 128.7, 128.4, 127.4, 127.1, 126.7, 126.4, 125.6, 125.2, 124.8, 61.9, 50.9, 13.8 ppm; IR (KBr): 2927, 2853, 1732, 1591, 1512 cm^{-1}; MS (ESI): *m/z* 452.05 [M+Na^+]. Anal. calcd. for $C_{26}H_{23}NO_5$: C 72.71, H 5.40, N 3.26, found: C 72.97, H 5.55, N 3.33.

Diethyl 2-(2-phenyl-5-thiophen-2-yl-oxazol-4-yl)malonate (5l):

Yellow oil; Yield: 35 mg (9%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.07 (m, 2H), 7.46-7.37 (m, 5H), 7.14-7.11 (m, 1H), 4.97 (s, 1H), 4.27 (q, *J* = 7.2 Hz, 4H), 1.27 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C

NMR (100 MHz, $CDCl_3$): δ 166.7, 159.8, 143.9, 130.5, 129.4, 129.1, 128.7, 127.9, 127.0, 126.8, 126.6, 126.3, 62.2, 51.2, 14.0 ppm; IR (KBr): 2925, 2853, 1735, 1605, 1545 cm^{-1}; MS (ESI): *m/z* 407.99 [M+Na^+]. Anal. calcd. for $C_{20}H_{19}NO_5S$: C 62.32, H 4.97, N 3.63, found: C 62.47, H 5.15, N 3.53.

Diethyl 2-[2-(4-methylphenyl)-5-phenyl-oxazol-4-yl]malonate (5m):

Yellow semisolid; Yield: 338 mg (86%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.48-7.4 5 (m, 2H), 7.41-7.37 (m, 1H), 7.27-7.25 (m, 2H), 4.97 (s, 1H), 4.27-4.22 (m, 4H), 2.41 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 160.3, 148.0, 140.7, 129.5, 129.4, 128.9, 128.8, 128.0, 126.6, 126.5, 124.5, 62.1, 51.4, 21.6, 14.0 ppm; IR (KBr): 2923, 2853, 1745, 1646, 1489 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{23}NO_5$: 394.1649 [M+H^+], found: 394.1651.

Diethyl 2-[2-(4-methoxyphenyl)-5-phenyl-oxazol-4-yl]malonate (5n):

Yellow oil; Yield: 356 mg (87%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.8 Hz, 2H), 7.65-7.63 (m, 2H), 7.48-7.44 (m, 2H), 7.40-7.38 (m, 1H), 6.97 (d, *J* = 8.8 Hz, 2H), 4.96 (s, 1H), 4.27-4.21 (m, 4H), 3.87 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 161.6, 160.4, 147.9, 144.2, 129.1, 128.9, 128.4, 126.6, 125.8, 119.8, 114.2, 62.2, 55.4, 51.2, 14.0 ppm; IR (KBr): 2927, 2852, 1738, 1606, 1499 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{23}NO_6$: 432.1418 [M+Na^+], found: 432.1421.

Diethyl 2-[2-(4-chlorophenyl)-5-phenyl-oxazol-4-yl]malonate (5o):

White solid; Yield: 322 mg (78%); M.p. 94-96 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.49-7.39 (m, 5H), 4.95 (s, 1H), 4.29-4.21 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 159.2, 148.7 136.5, 129.8, 129.04, 129.01, 128.9, 127.9, 127.8, 126.6, 125.8, 62.2, 51.3, 14.0 ppm; IR (KBr): 2930, 2872, 1738, 1590, 1546, 1488 cm^{-1}; HRMS (ESI) calcd. for $C_{22}H_{20}ClNO_5$: 436.0922 [$M+Na^+$], found: 436.0932.

Diethyl 2-[2-(4-nitrophenyl)-5-phenyl-oxazol-4-yl]malonate (5p):

Yellow semisolid; Yield: 318 mg (75%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34-8.26 (m, 4H), 7.70-7.66 (m, 2H), 7.52-7.45 (m, 3H), 4.98 (s, 1H), 4.30-4.25 (m, 4H), 1.27 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.7, 158.0, 148.7, 132.6, 130.6, 129.6, 129. 1, 127.2, 127.0, 126.7, 126.2, 124.1, 62.3, 51.1, 14.0 ppm; IR (KBr): 2923, 2852, 1742, 1682, 1602, 1522 cm^{-1}; MS (ESI): *m/z* 425.13 [$M+H^+$]. Anal. calcd. for $C_{22}H_{20}N_2O_7$: C 62.26, H 4.75, N 6.60; found: C 62.45, H 4.86, N 6.78.

Diethyl 2-(2-naphthalen-1-yl-5-phenyl-oxazol-4-yl)malonate (5q):

Brown oil; Yield: 352 mg (82%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.26 (d, *J* = 8.8 Hz, 1H), 8.21 (d, *J* = 7.2 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.57-7.34 (m, 6H), 4.99 (s, 1H), 4.24-4.16 (m, 4H), 1.21 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0, 158.9, 147.0, 132.9, 130.3, 129.2, 128.6, 127.9, 127.5, 126.94, 126.88,

126.5, 125.5, 125.4, 125.2, 123.9, 122.6, 61.1, 50.6, 13.0 ppm; IR (KBr): 2981, 2848, 1734, 1623, 1596 cm^{-1}; HRMS (ESI) calcd. for $C_{26}H_{23}NO_5$: 430.1649 [M+H^+], found: 430.1649.

Diethyl 2-(5-phenyl-2-thiophen-2-yl-oxazol-4-yl)malonate (5r):

Dark brown semisolid; Yield: 339 mg (88%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 3.6 Hz, 1H), 7.64 (d, *J* = 7.2 Hz, 2H), 7.48-7.38 (m, 4H), 7.12 (t, *J* = 8.4 Hz, 1H) 4.95 (s, 1H), 4.27-4.19 (m, 4H), 1.24 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 156.4, 147.9, 129.6, 129.5, 129.0, 128.9, 128.5, 128.2, 127.9, 127.7, 126.6, 62.2, 51.3, 14.0 ppm; IR (KBr): 2925, 2853, 1733, 1597, 1448 cm^{-1}; HRMS (ESI) calcd. for $C_{20}H_{19}NO_5S$: 386.1057 [M+H^+], found: 386.1057.

Diethyl 2-[2-(4-bromo-benzyl)-5-phenyl-oxazol-4-yl]malonate (5s):

Yellow oil; Yield: 358 mg (76%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.50 (m, 2H), 7.46-7.33 (m, 5H), 7.22 (d, *J* = 8.0 Hz, 2H), 4.87 (s, 1H), 4.26-4.19 (m, 4H), 4.13 (s, 2H), 1.24 (t, *J* = 7.4 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 160.9, 148.9, 134.4, 131.84, 131.78, 130.6, 128.9, 128.8, 128.4, 126.5, 125.9, 62.1, 50.9, 33.5, 14.0 ppm; IR (KBr): 2925, 2853, 1732, 1620, 1596 cm^{-1}; MS (ESI): *m/z* 493.96 [M+Na^+]. Anal. calcd. for $C_{23}H_{22}BrNO_5$: C 58.49, H 4.69, N 2.97, found: C 58.45, H 4.86, N 3.18.

Diethyl 2-(2-methyl-5-phenyloxazol-4-yl)malonate (5t):

Yellow oil; Yield: 238 mg (75%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 7.6 Hz, 2H), 7.45-7.42 (m, 2H), 7.38-7.35 (m, 1H), 4.86 (s, 1H), 4.29-4.18 (m, 4H), 2.52 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 160.3, 148.3, 128.9, 128.7, 127.9, 127.8,

126.4, 62.1, 50.8, 14.1, 14.0 ppm; IR (KBr): 2940, 2866, 1745, 1587, 1449 cm^{-1}; HRMS (ESI) calcd. for $C_{17}H_{19}NO_5$: 318.1336 [$M+H^+$], found: 318.1335.

Diethyl 2-[2-(4-methoxyphenyl)-5-(4-methyphenyl)-oxazol-4-yl]malonate (5u):

White solid; Yield: 330 mg (78%); M.p. 84-86 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.8 Hz, 2H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 4.93 (s, 1H), 4.28-4.21 (m, 4H), 3.86 (s, 3H), 2.40 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 161.4, 160.0, 148.0, 138.8, 129.5, 128.8, 128.2, 126.4, 125.3, 120.2, 114.1, 62.1, 55.4, 51.3, 21.4, 14.0 ppm; IR (KBr): 2923, 2852, 1746, 1647, 1516 cm^{-1}; HRMS (ESI) calcd. for $C_{24}H_{25}NO_6$: 424.1755 [$M+H^+$], found: 424.1750.

Diethyl 2-[2, 5-bis-(4-methoxyphenyl)-oxazol-4-yl]malonate (5v):

Yellow semisolid; Yield: 391 mg (89%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.00-6.94 (m, 4H), 4.91 (s, 1H), 4.27-4.20 (m, 4H), 3.86 (d, *J* = 2.8 Hz, 6H), 1.25 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 161.3, 160.0, 159.7, 147.9, 128.2, 128.1, 120.7, 120.2, 114.3, 114.1, 62.1, 55.4, 51.3, 14.0 ppm; IR (KBr): 2929, 2845, 1742, 1609, 1502 cm^{-1}; HRMS (ESI) calcd. for $C_{24}H_{25}NO_7$: 462.1523 [$M+Na^+$], found: 462.1510.

Diethyl 2-[5-(4-methoxyphenyl)-2-methyl-oxazol-4-yl]malonate (5w):

Yellow oil; Yield: 281 mg (81%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 4.80 (s, 1H), 4.27-4.20 (m, 4H), 3.84 (s, 3H), 2.50 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 160.0, 159.7, 148.4, 128.1, 126.6, 120.6,

114.3, 62.0, 55.3, 50.8, 14.03, 13.99 ppm; IR (KBr): 2925, 2853, 1740, 1603, 1511 cm^{-1}; MS (ESI): *m/z* 348.14 [$M+H^+$]. Anal. calcd. for $C_{18}H_{21}NO_6$: C 62.24, H 6.09, N 4.03; found: C 62.52, H 6.22, N 4.28.

Diethyl 2-[2-(3-cyanophenyl)-5-(4-methoxyphenyl)-oxazol-4-yl]malonate (5x):

White solid; Yield: 312 mg (72%); M.p. 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (s, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.59-7.55 (m, 3H), 7.01 (d, *J* = 8.4 Hz, 2H), 4.92 (s, 1H), 4.29-4.20 (m, 4H), 3.86 (s, 3H), 1.26 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 160.5, 157.4, 149.6, 133.2, 130.3, 129.9, 129.6, 128.9, 128.6, 128.3, 119.9, 118.1, 114.5, 113.2, 62.2, 55.4, 51.1, 14.0 ppm; IR (KBr): 2927, 2853, 2226, 1744, 1612, 1511 cm^{-1}; MS (ESI): *m/z* 457.09 [$M+Na^+$]. Anal. calcd. for $C_{24}H_{22}N_2O_6$: C 66.35, H 5.10, N 6.45; found: C 66.63, H 5.25, N 6.26.

Diethyl 2-[5-(4-chlorophenyl)-2-(4-methoxy-phenyl)-oxazol-4-yl]malonate (5y):

White semisolid; Yield: 381 mg (86%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J* = 9.2 Hz, 2H), 8.00 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 4.93 (s, 1H), 4.28-4.20 (m, 4H), 3.86 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 161.6, 160.4, 146.8, 134.7, 129.8, 129.1, 128.3, 127.7, 126.6, 119.8, 114.1, 62.2, 55.4, 51.4, 14.0 ppm; IR (KBr): 2937, 2837, 1730, 1611, 1498 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{22}ClNO_6$: 466.1028 [$M+Na^+$], found: 466.1038.

Diethyl 2-[5-(4-chlorophenyl)-2-methyl-oxazol-4-yl]malonate (5z):

Yellow oil; Yield: 267 mg (76%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (d, *J* = 8.8 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 4.81 (s, 1H), 4.26-4.20 (m, 4H), 2.52 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 160.5, 147.3, 134.7, 129.1, 128.3, 127.7, 126.9, 62.2, 50.9, 14.04, 13.98 ppm; IR (KBr): 2927, 2853, 1740, 1586, 1490 cm^{-1}; MS (ESI): *m/z* 352.12 [$M+H^+$]. Anal. calcd. for $C_{17}H_{18}ClNO_5$: C 58.04, H 5.16, N 3.98; found: C 58.33, H 5.28, N 3.71.

Diethyl 2-[5-(3,4-dimethoxy-phenyl)-2-(4-methylphenyl)-oxazol-4-yl]malonate (5aa):

White semisolid; Yield: 371 mg (82%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.25-7.21 (m, 4H), 6.95 (d, *J* = 8.0 Hz, 1H), 4.94 (s, 1H), 4.28-4.17 (m, 4H), 3.94 (d, *J* = 8.4 Hz, 6H), 2.41 (s, 3H), 1.23 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 159.9, 149.6, 149.1, 148.3, 140.6, 129.4, 128.5, 126.5, 124.6, 120.8, 119.6, 111.3, 110.0, 62.1, 56.0, 51.5, 21.6, 14.0 ppm; IR (KBr): 2929, 2856, 1741, 1615, 1519 cm^{-1}; MS (ESI): *m/z* 454.21 [$M+H^+$], Anal. calcd. for $C_{25}H_{27}NO_7$: C 66.21, H 6.00, N 3.09; found: C 66.35, H 6.11, N 3.22.

Diethyl 2-[5-(3,4-dimethoxy-phenyl)-2-(4-methoxy-phenyl)-oxazol-4-yl]malonate (5ab):

Yellow semisolid; Yield: 380 mg (81%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 9.2 Hz, 2H), 7.23-7.20 (m, 2H), 6.98-6.94 (m, 3H), 4.94 (s, 1H), 4.28-4.17 (m, 4H), 3.94 (d, *J* = 8.4 Hz, 6H), 3.87 (s, 3H), 1.24 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 161.4, 159.8, 149.5, 149.1, 148.0, 128.4, 128.2, 120.9, 120.1, 119.5, 114.1, 111.3, 109.9, 62.1, 56.0,

55.4, 51.5, 14.0 ppm; IR (KBr): 2923, 2853, 1734, 1613, 1499 cm^{-1}; HRMS (ESI) calcd. for $C_{25}H_{27}NO_8$: 470.1809 [M+H^+], found: 470.1808.

Diethyl 2-[2-(4-methylphenyl)-5-(3,4,5-trimethoxy-phenyl)-oxazol-4-yl]malonate (5ac):

White solid; Yield: 285 mg (59%); M.p. 122-124 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 6.94 (s, 2H), 4.96 (s, 1H), 4.26-4.18 (m, 4H), 3.93 (s, 6H), 3.89 (s, 3H), 2.41 (s, 3H), 1.22 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 160.1, 153.6, 148.3, 140.8, 138.9, 129.4, 129.3, 126.6, 124.6, 123.4, 104.3, 62.1, 61.0, 56.3, 51.8, 21.5, 14.0 ppm; IR (KBr): 2976, 2836, 1744, 1576, 1502 cm^{-1}; MS (ESI): *m/z* 484.20 [M+H^+]. Anal. calcd. $C_{26}H_{29}NO_8$: C 64.59, H 6.05, N 2.90; found: C 64.40, H 6.19, N 3.00.

Diethyl 2-(2,5-di-naphthalen-1-yl-oxazol-4-yl)malonate (5ad):

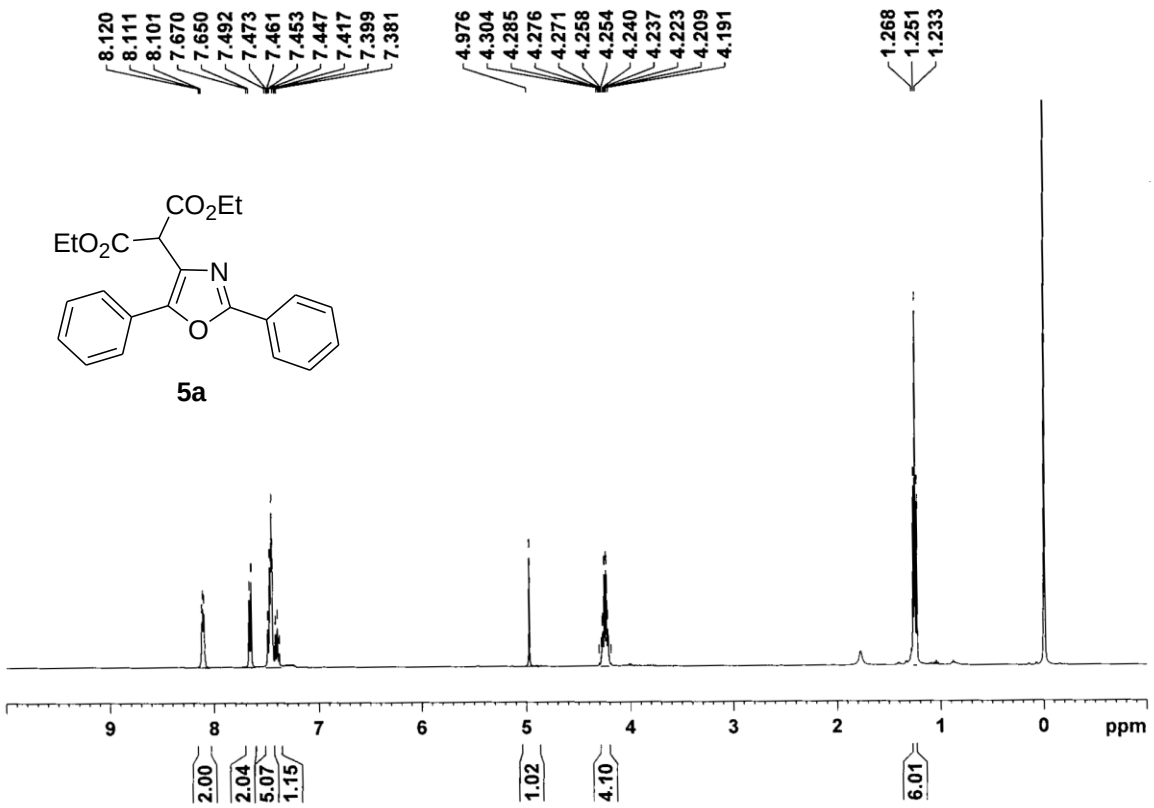
Brown oil; Yield: 297 mg (62%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.38 (d, *J* = 8.8 Hz, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.28 (d, *J* = 0.8 Hz, 1H), 8.26 (d, *J* = 0.8 Hz, 1H), 8.04-8.00 (m, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.70-7.52 (m, 8H), 4.85 (s, 1H), 4.20-4.00 (m, 4H), 1.16 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 161.1, 146.8, 134.6, 134.0, 133.1, 132.5, 131.6, 131.0, 130.2, 129.0, 128.6, 128.1, 127.9, 127.7, 127.6, 126.44, 126.35, 126.1, 125.7, 125.00, 124.95, 124.2, 123.5, 62.1, 51.2, 13.9 ppm; IR (KBr): 2925, 2852, 1730, 1680, 1510 cm^{-1}; HRMS (ESI) calcd. for $C_{30}H_{25}NO_5$: 480.1800 [M+H^+], found: 480.1804.

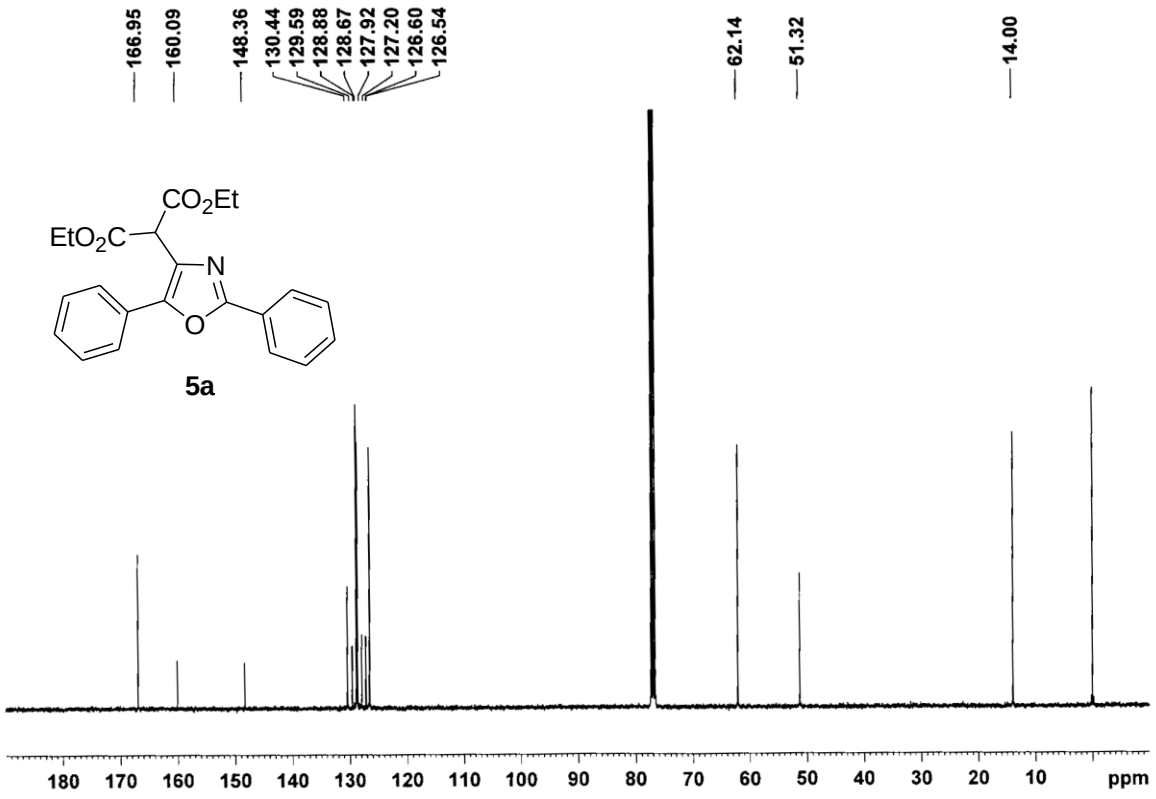
Diethyl 2-[1-(5-cyanomethylthiophen-2-yl)-2-oxo-2-phenyl-ethyl]malonate (8)

Dark brown oil; Yield: 299 mg (75%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.0 (d, *J* = 8.0 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 6.84 (s, 2H), 5.55 (d, *J* =11.2 Hz, 1H), 4.43 (d,

J =11.2 Hz, 1H), 4.18-4.07 (m, 4H), 3.78 (s, 2 H), 1.19 (t, *J* = 7.0 Hz, 3H), 1.14 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.0, 167.6, 137.3, 135.4, 133.6, 131.9, 128.9, 128.7, 127.9, 127.4, 116.4, 62.1, 61.8, 56.4, 47.4, 18.7, 13.93, 13.90 ppm; IR (KBr): 2935, 2813, 2215, 1741, 1698, 1680, 1540 cm^{-1}; MS (ESI): *m/z* 421.98 [$M+Na^+$]. Anal. calcd. $C_{21}H_{21}NO_5S$: C 63.14, H 5.30, N 3.51; found: C 63.40, H 5.19, N 3.66.

D. NMR spectra

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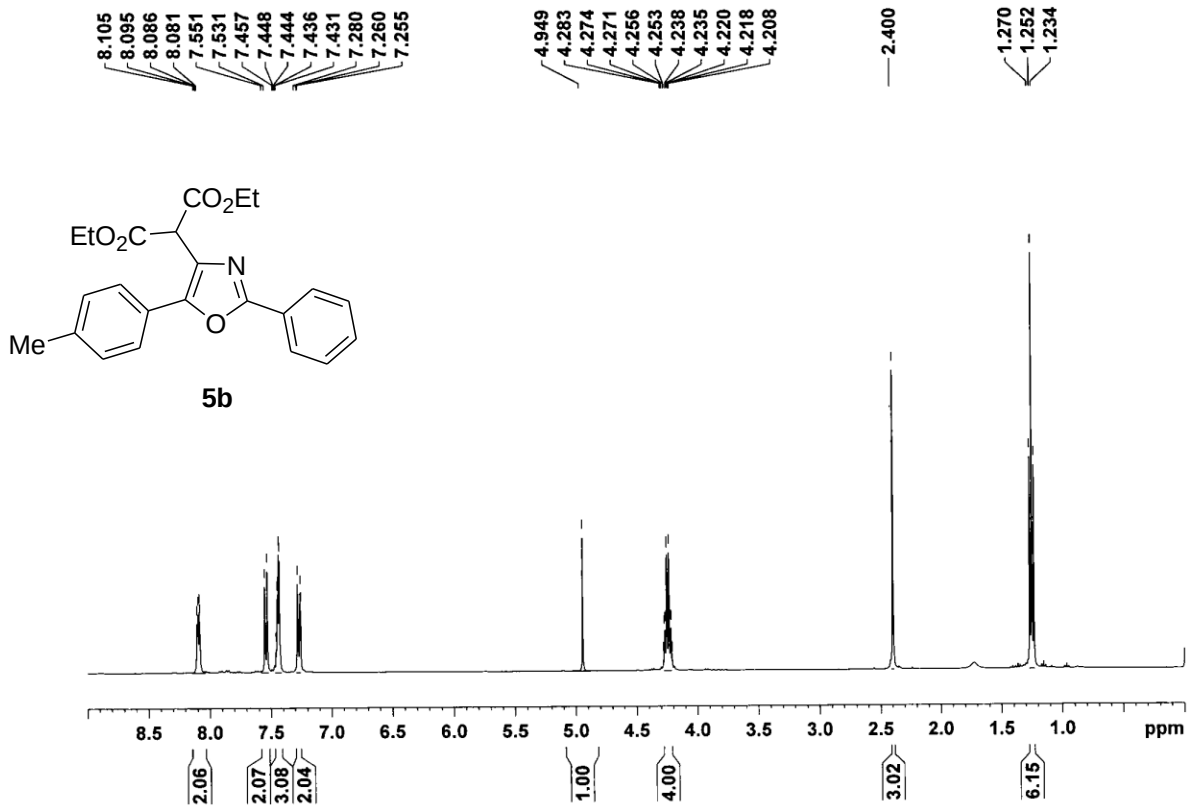
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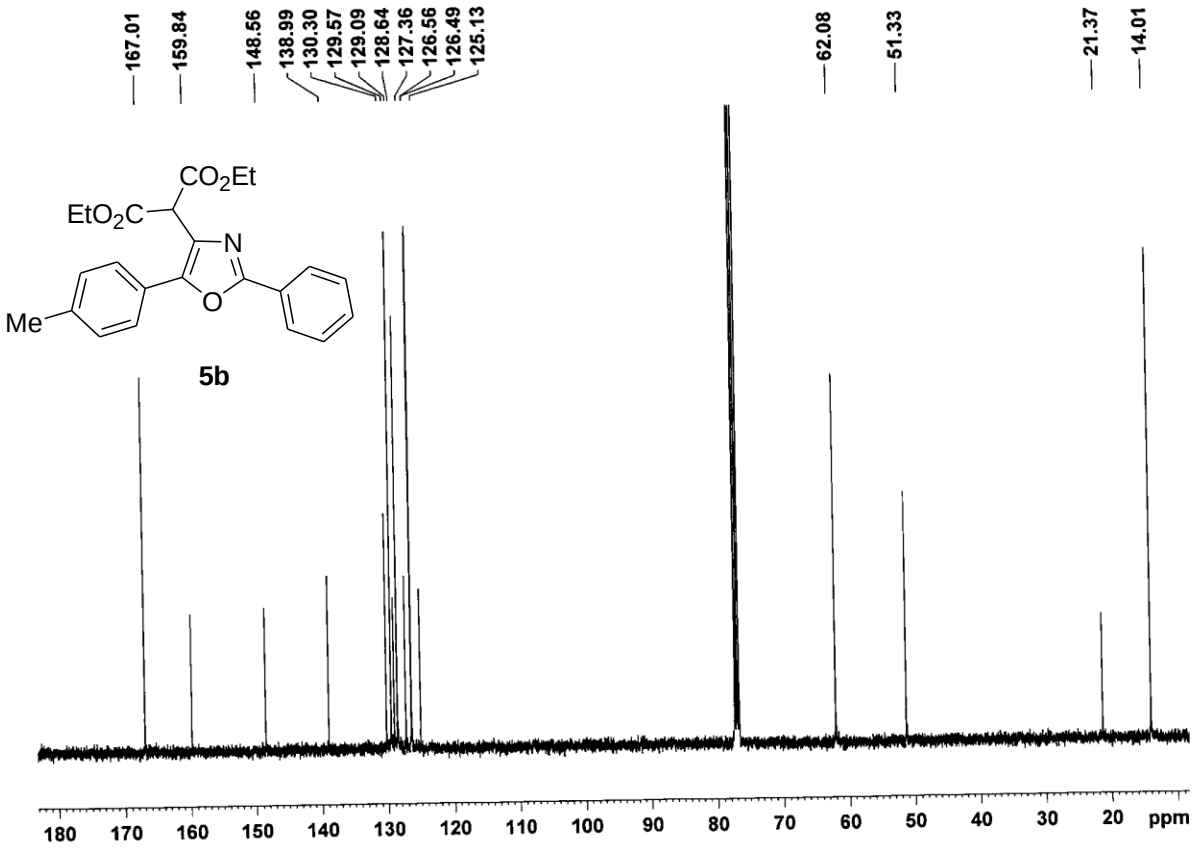
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21.37
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EtO2C
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O
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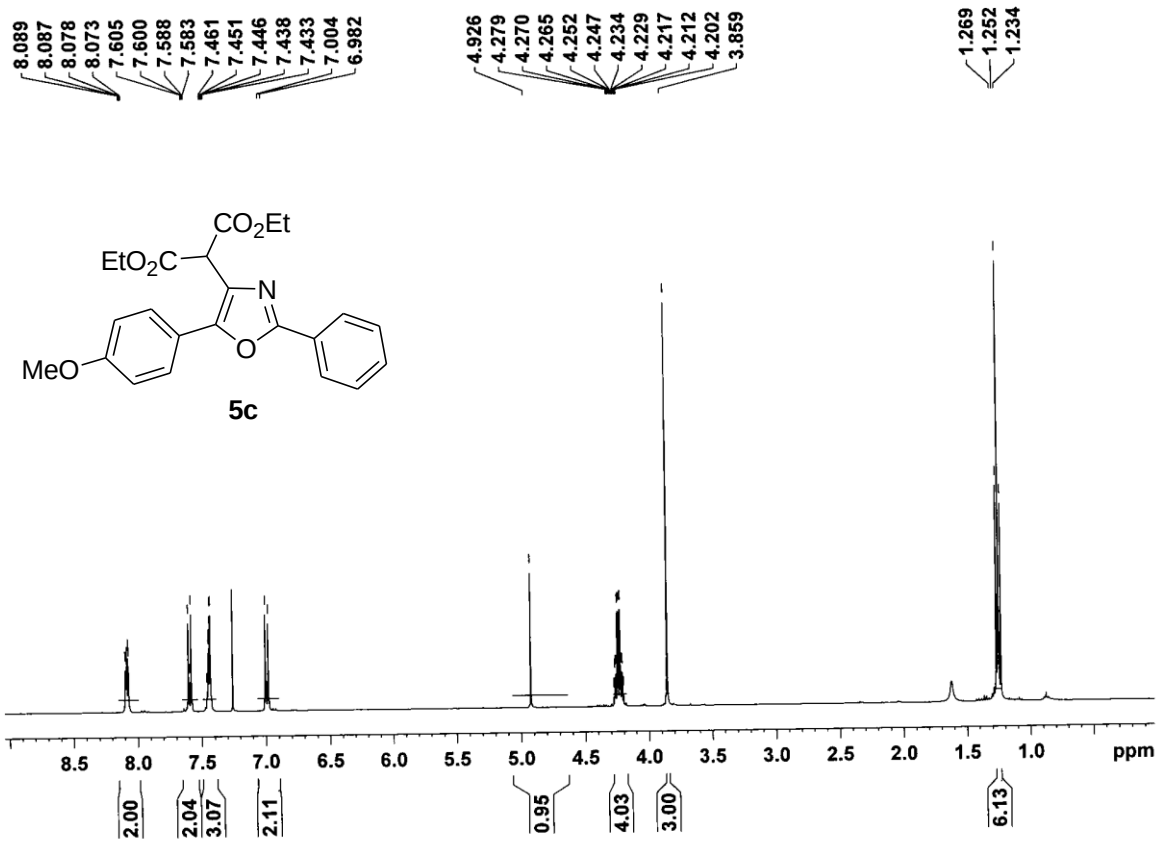
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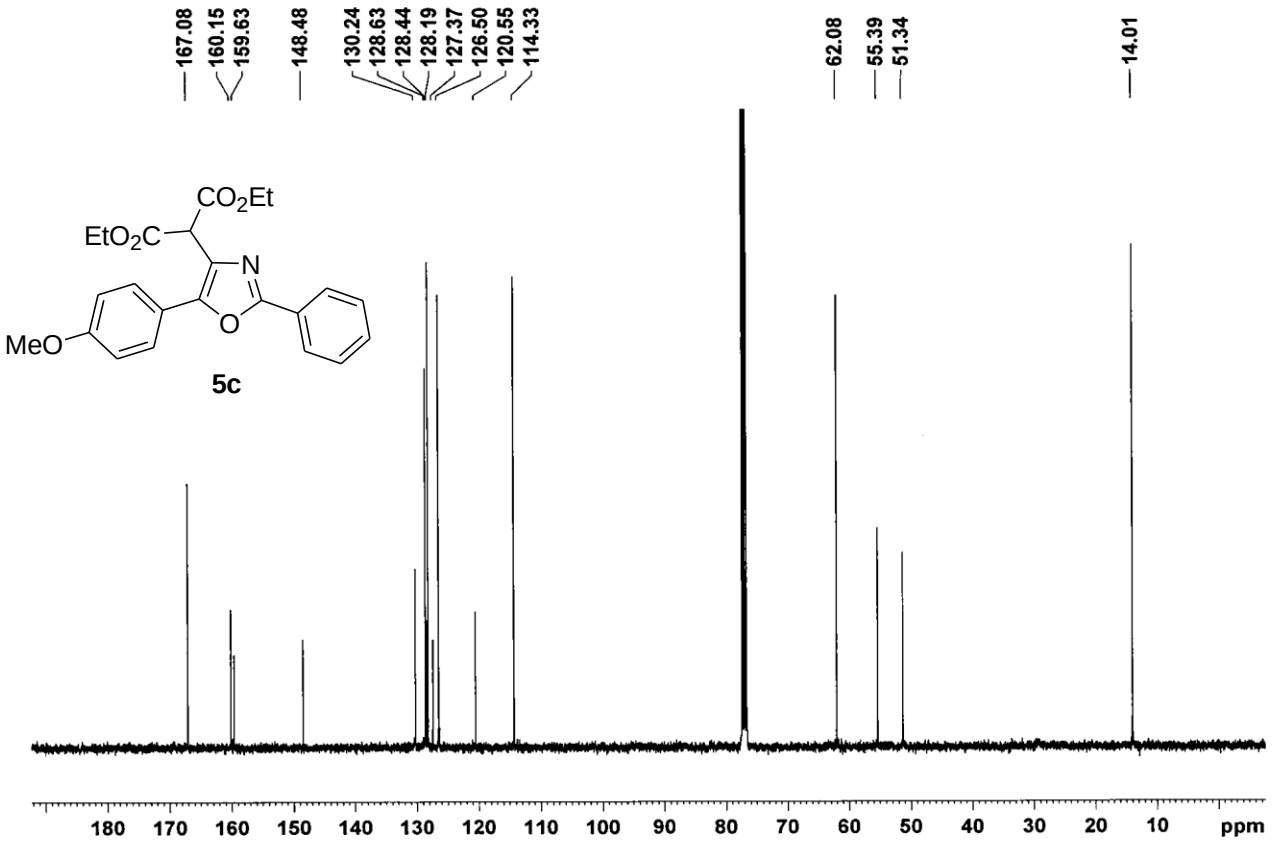
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O
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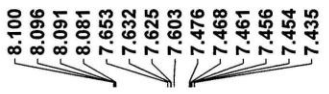
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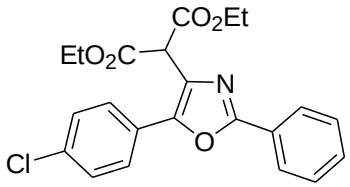
1.236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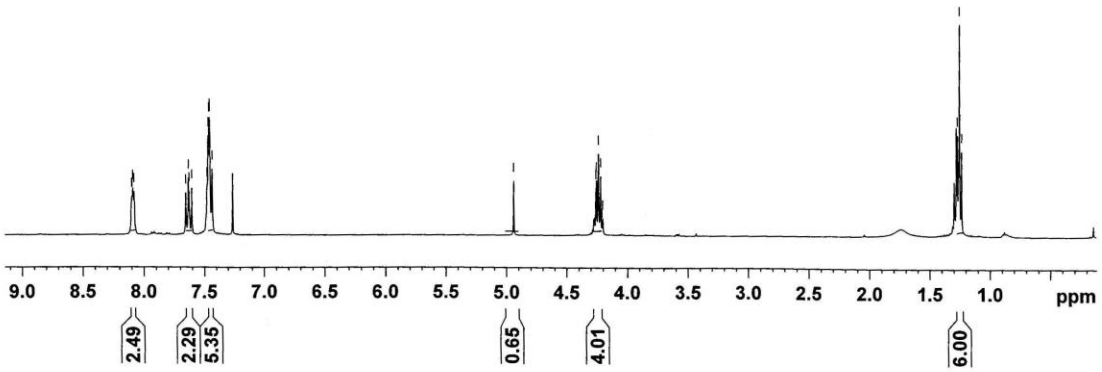
5d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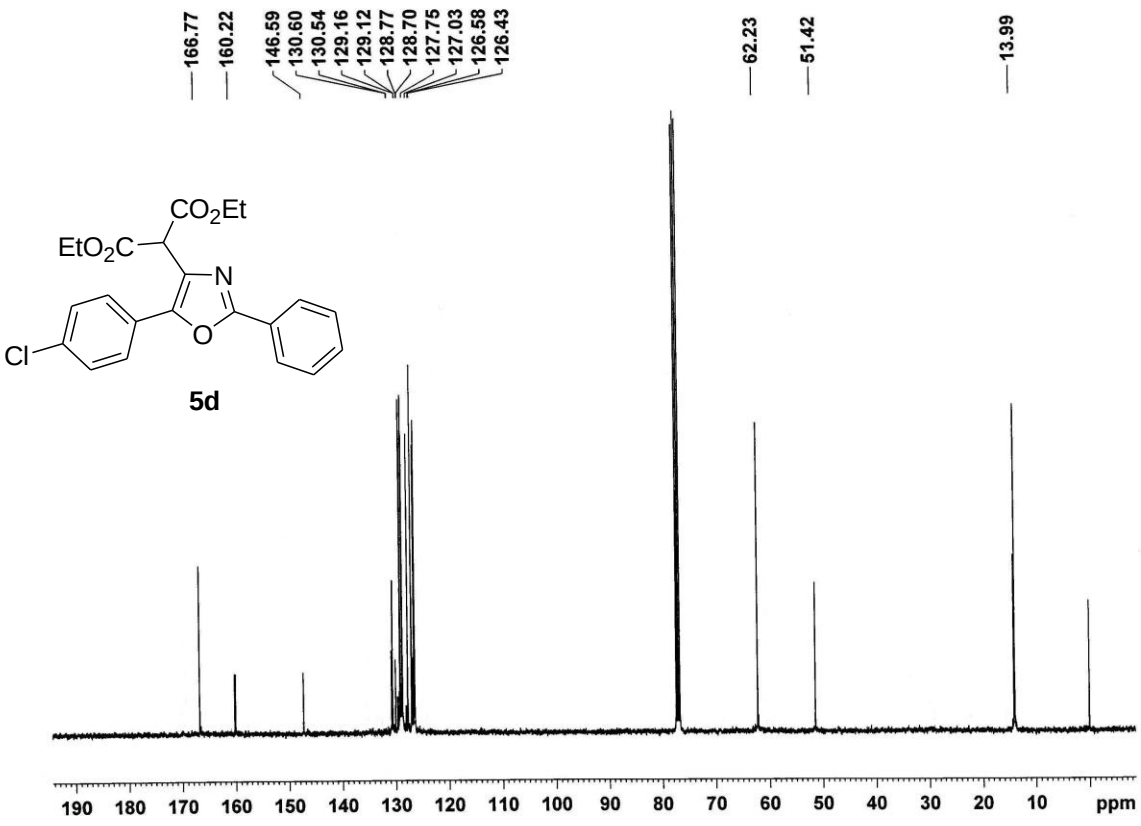
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O
Cl
5d
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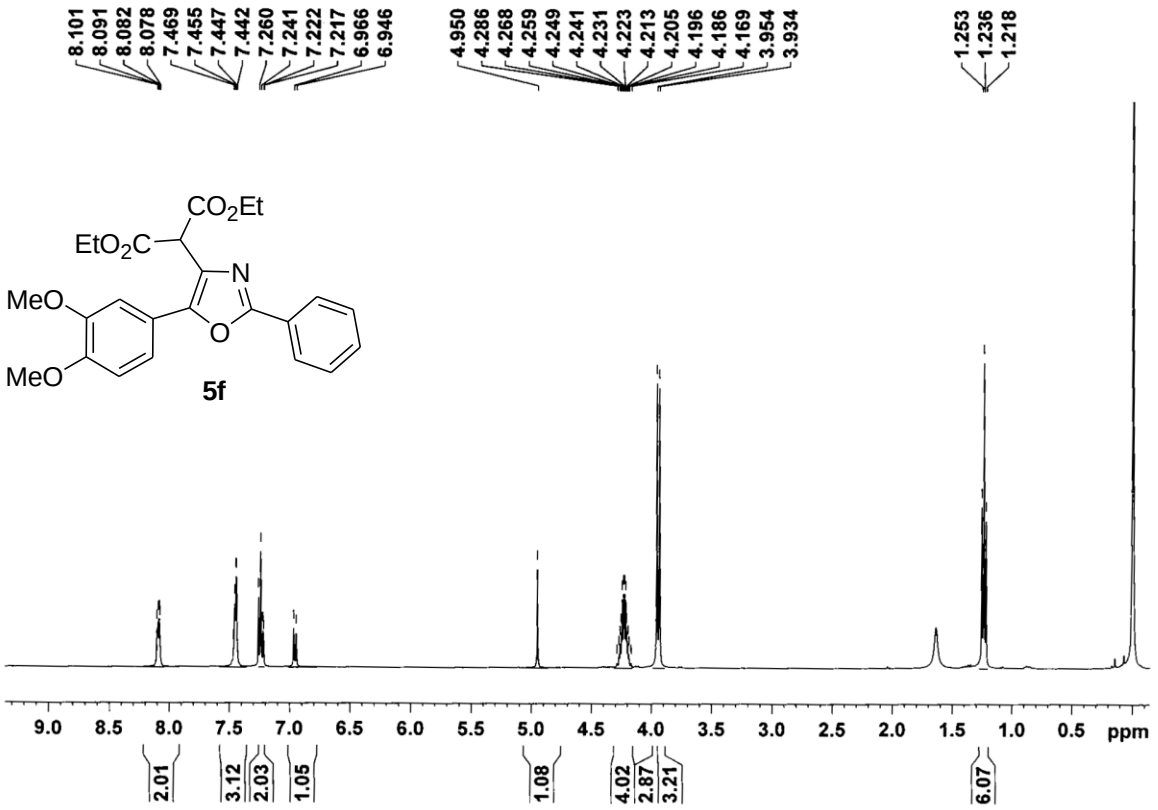
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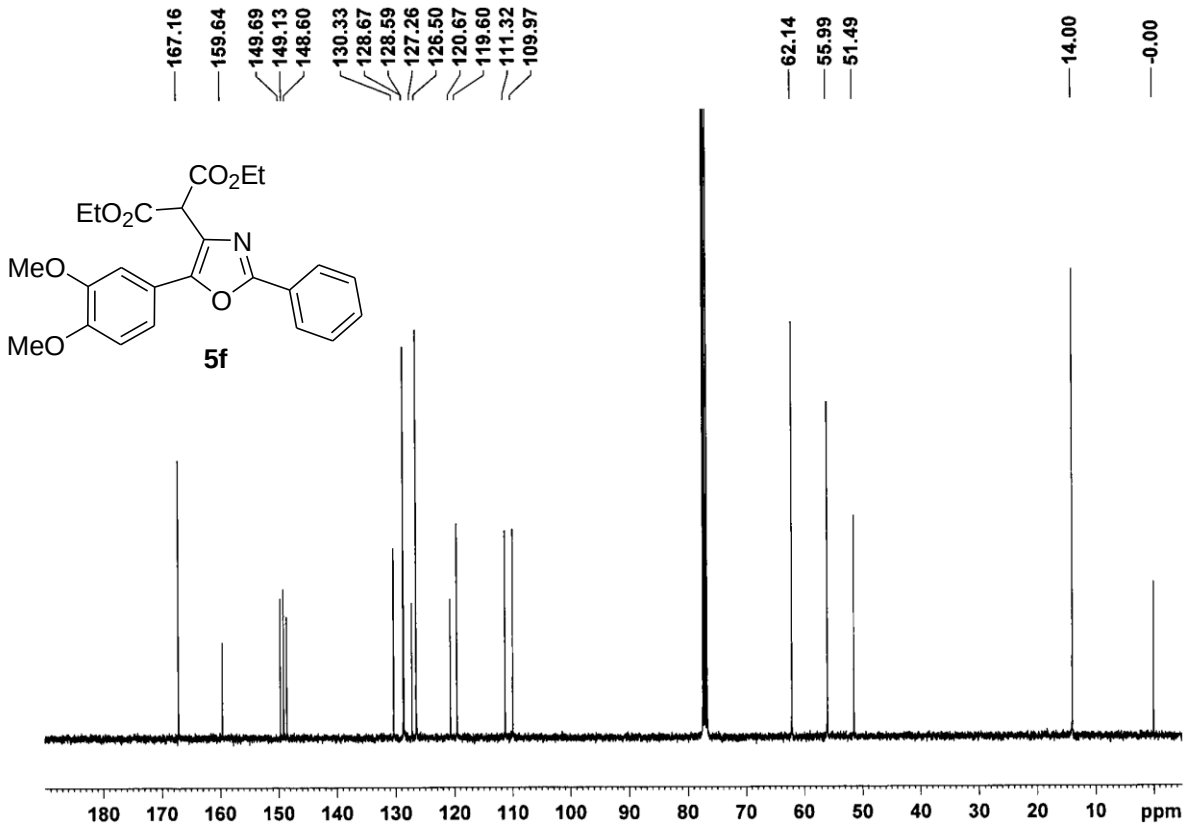
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55.99
51.49
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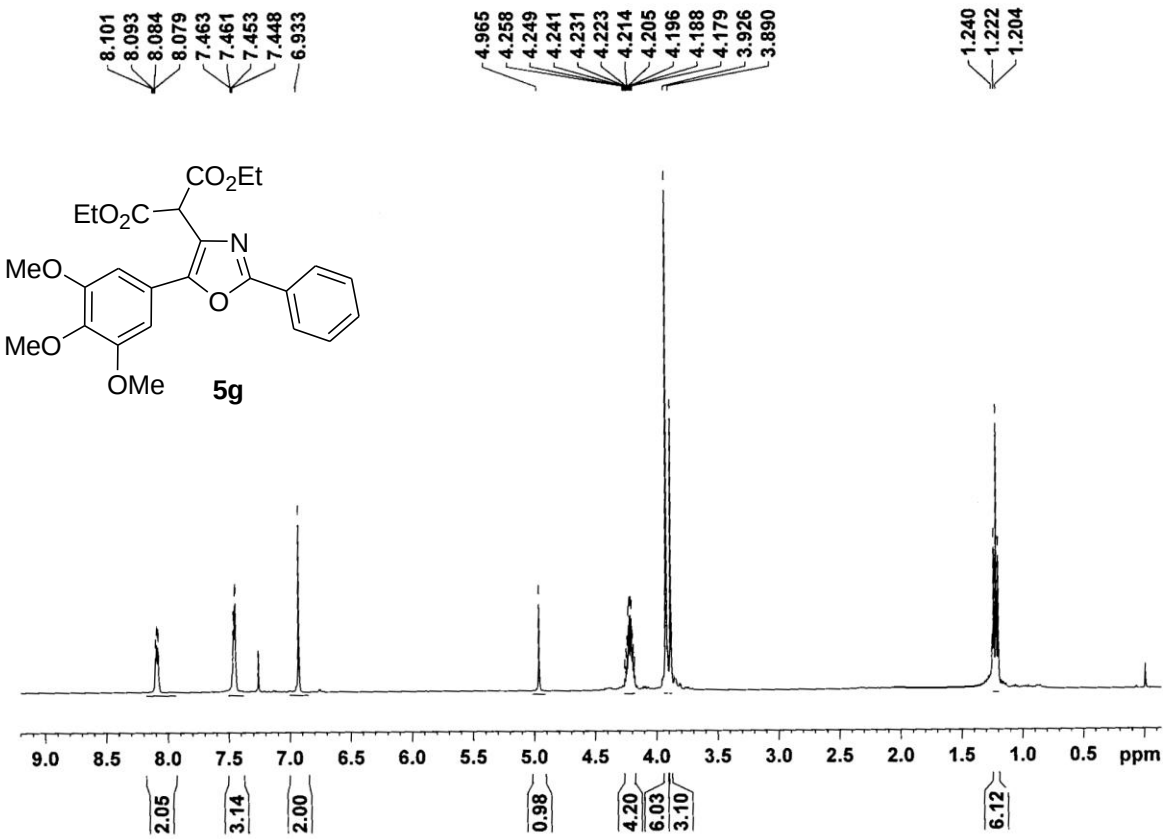
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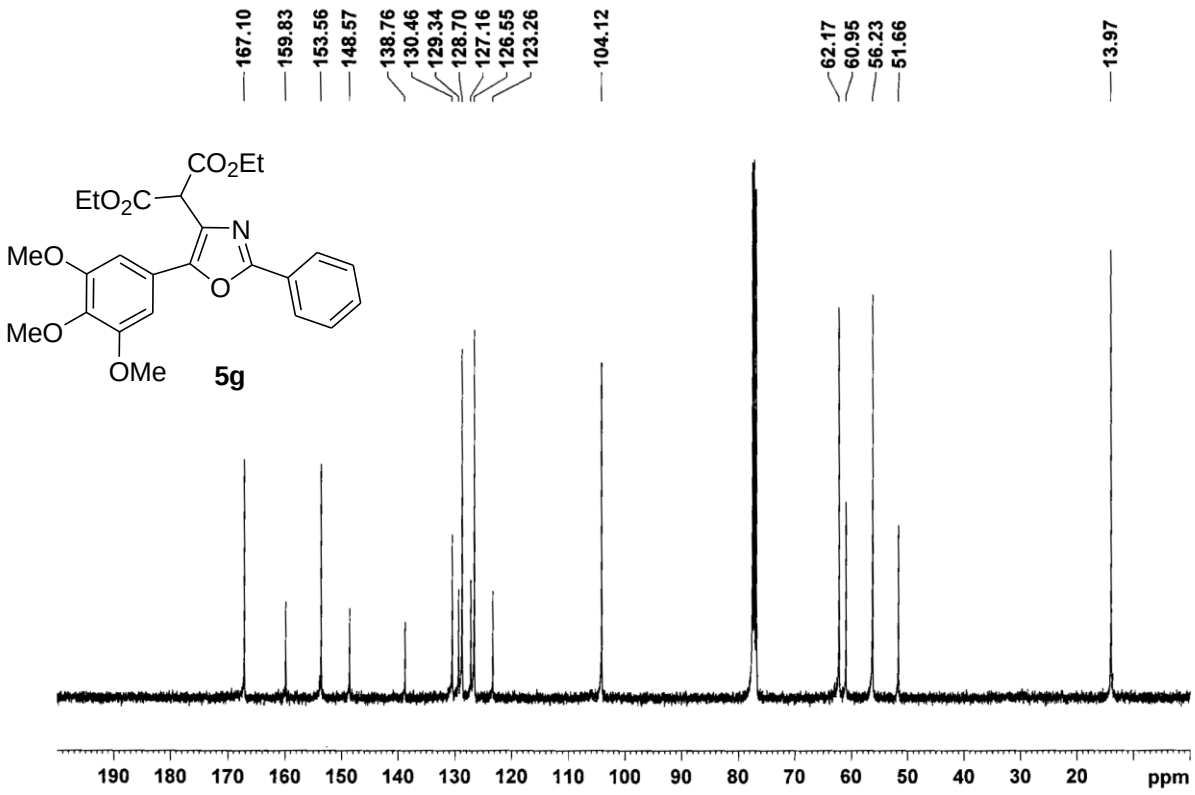
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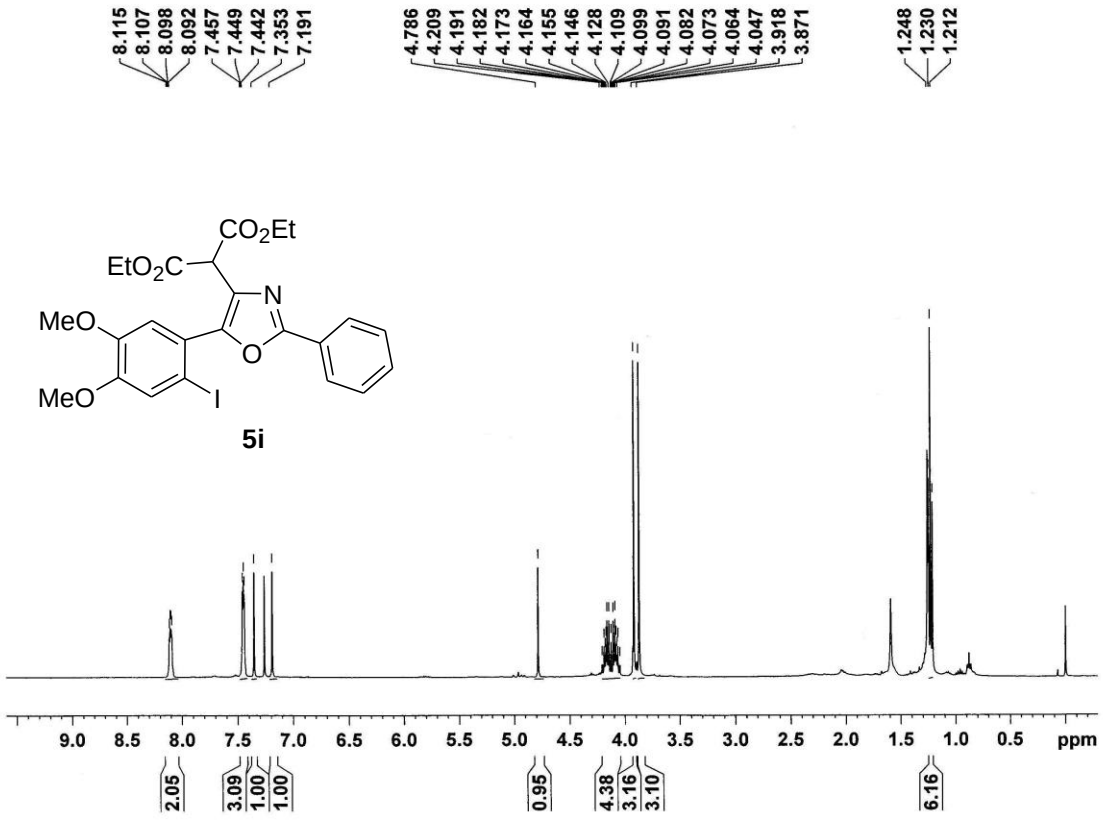
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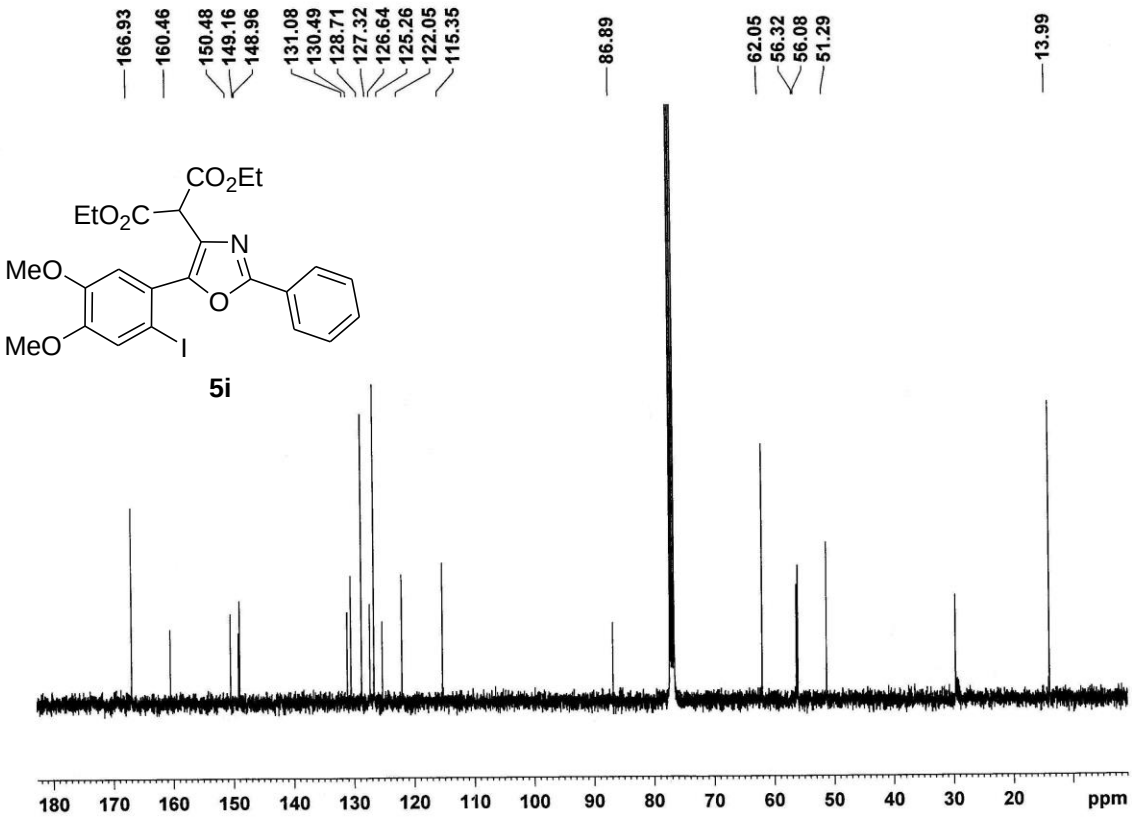
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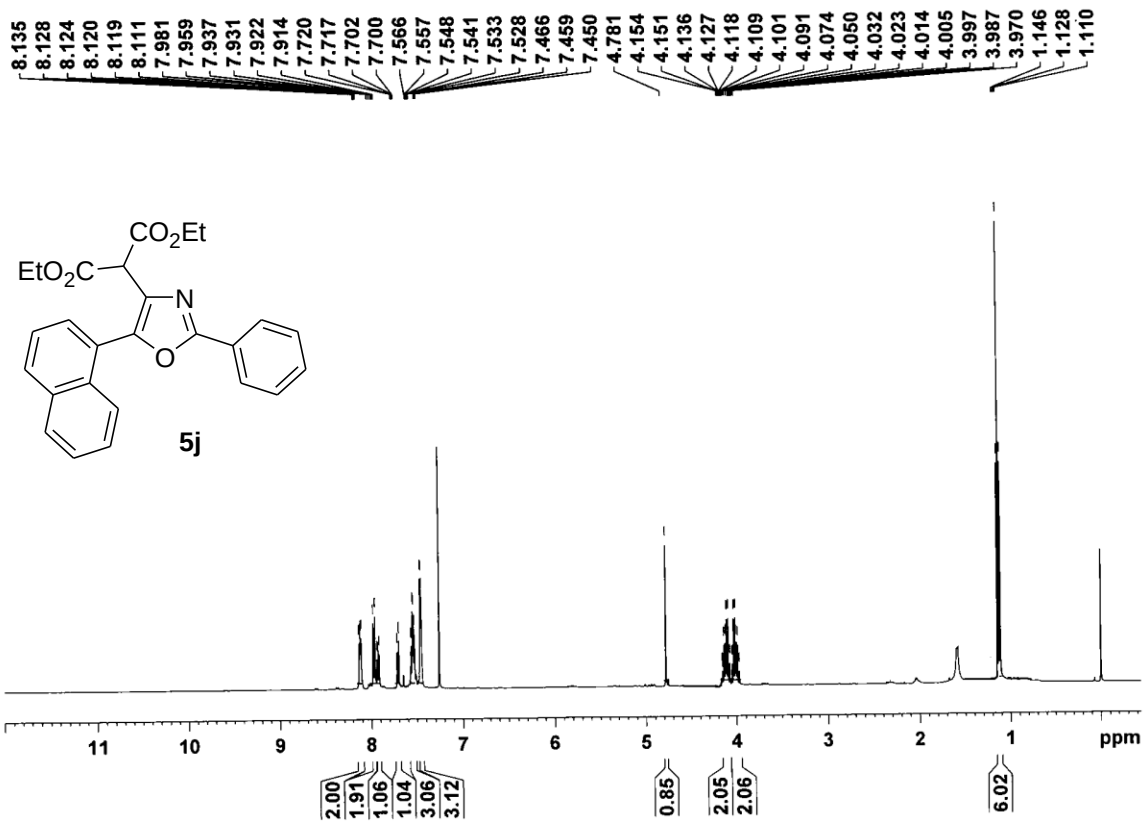
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7.700
7.566
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7.548
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7.528
7.466
7.459
7.450
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4.154
4.151
4.136
4.127
4.118
4.109
4.101
4.091
4.074
4.050
4.032
4.023
4.014
4.005
3.997
3.987
3.970
1.146
1.128
1.110
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EtO2C
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O
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9
8
7
6
5
4
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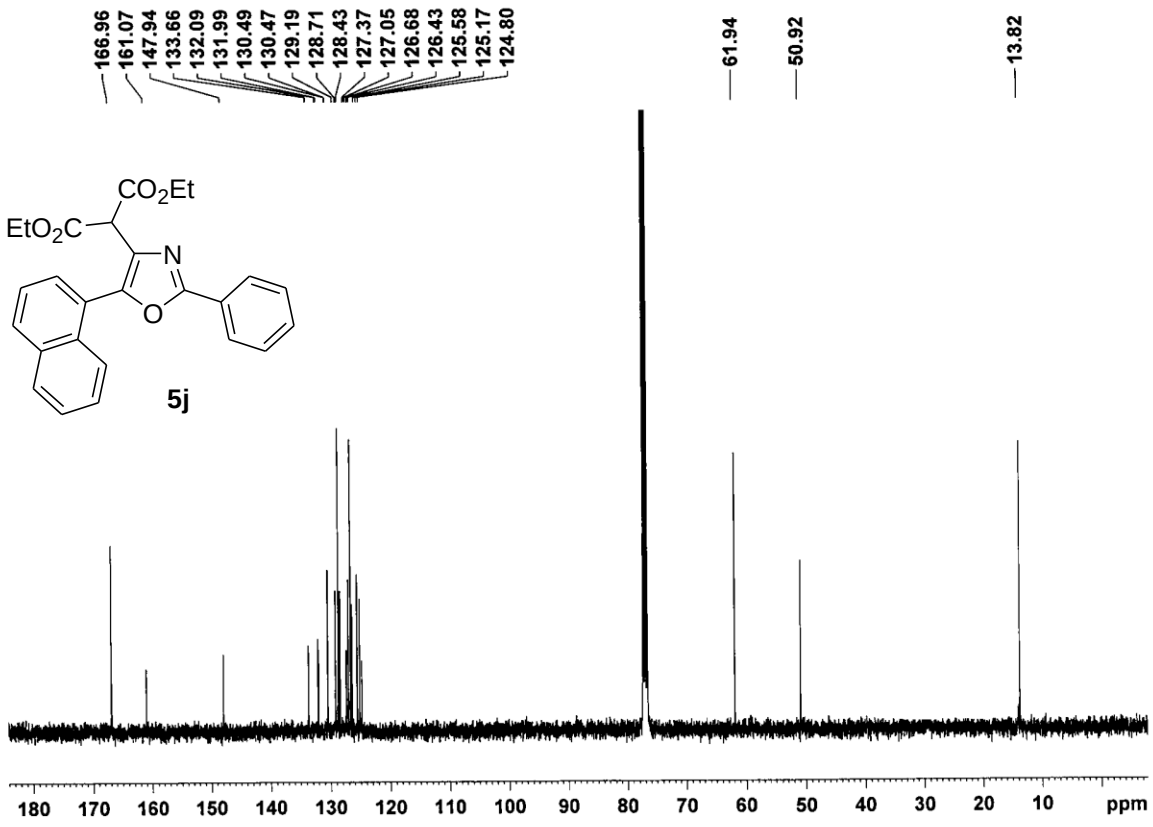
2.06
6.02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126.68
126.43
125.58
125.17
124.80
61.94
50.92
13.82
CO2Et
EtO2C
N
O
5j
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20
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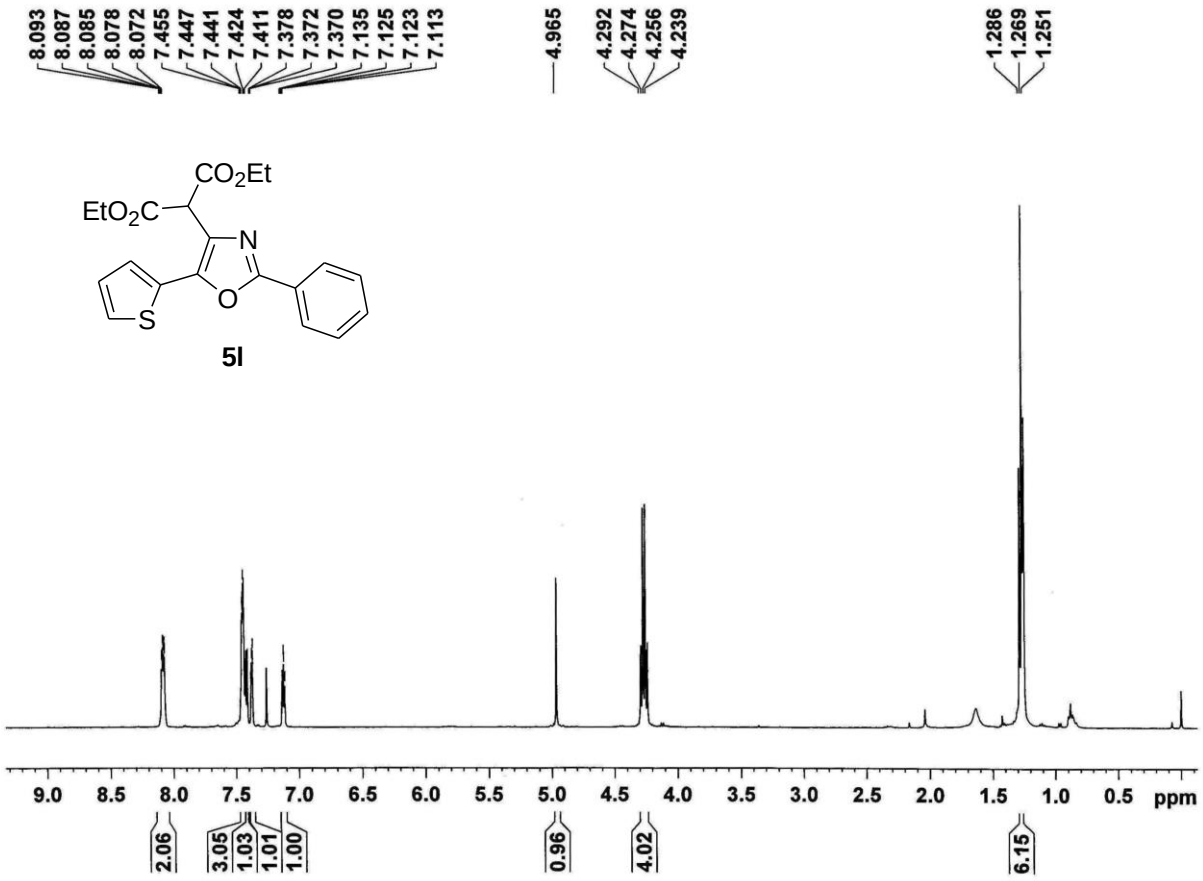
ppm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7.370
7.135
7.125
7.123
7.113
4.965
4.292
4.274
4.256
4.239
1.286
1.269
1.251
CO2Et
EtO2C
N
O
S
5l
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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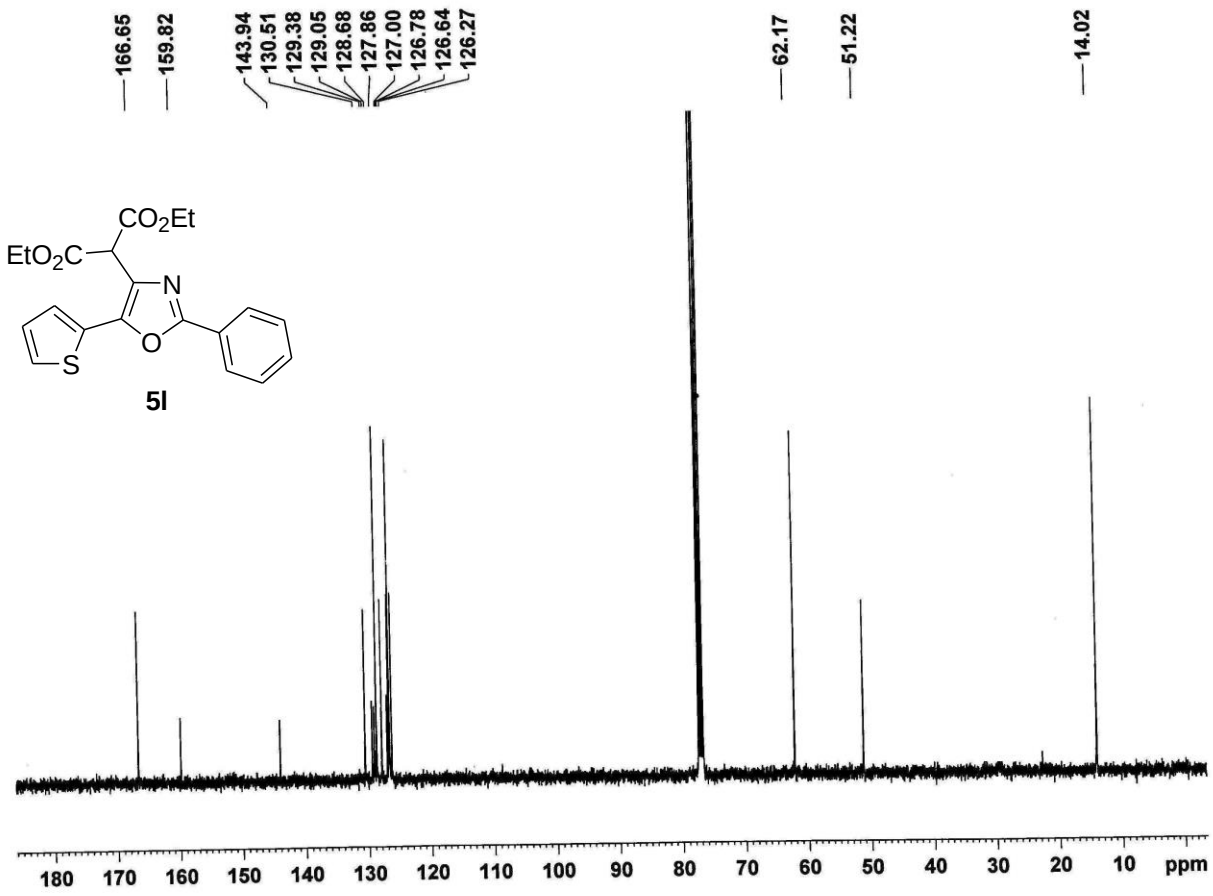
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126.78
126.64
126.27
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CO2Et
EtO2C
N
O
S
5l
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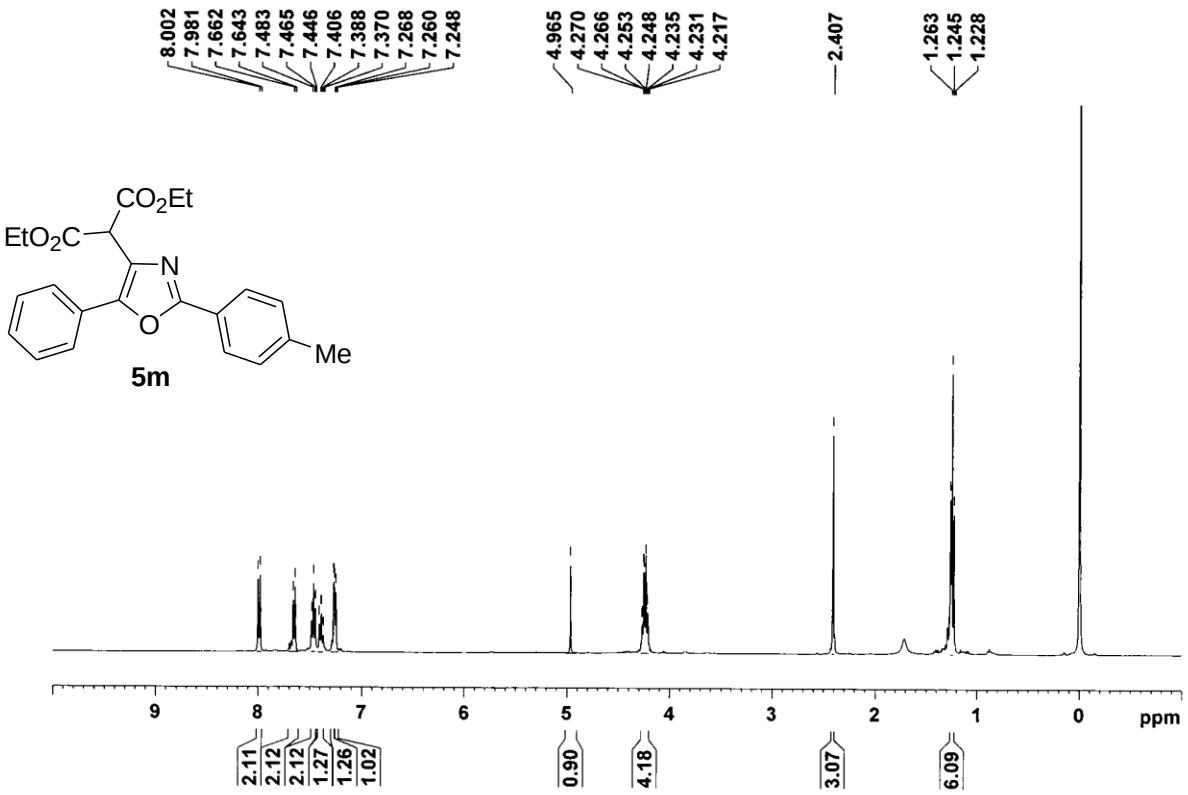
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7.446
7.406
7.388
7.370
7.268
7.260
7.248
4.965
4.270
4.266
4.253
4.248
4.235
4.231
4.217
2.407
1.263
1.245
1.228
CO2Et
EtO2C
N
O
Me
5m
9
8
7
6
5
4
3
2
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ppm
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2.12
2.12
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1.26
1.02
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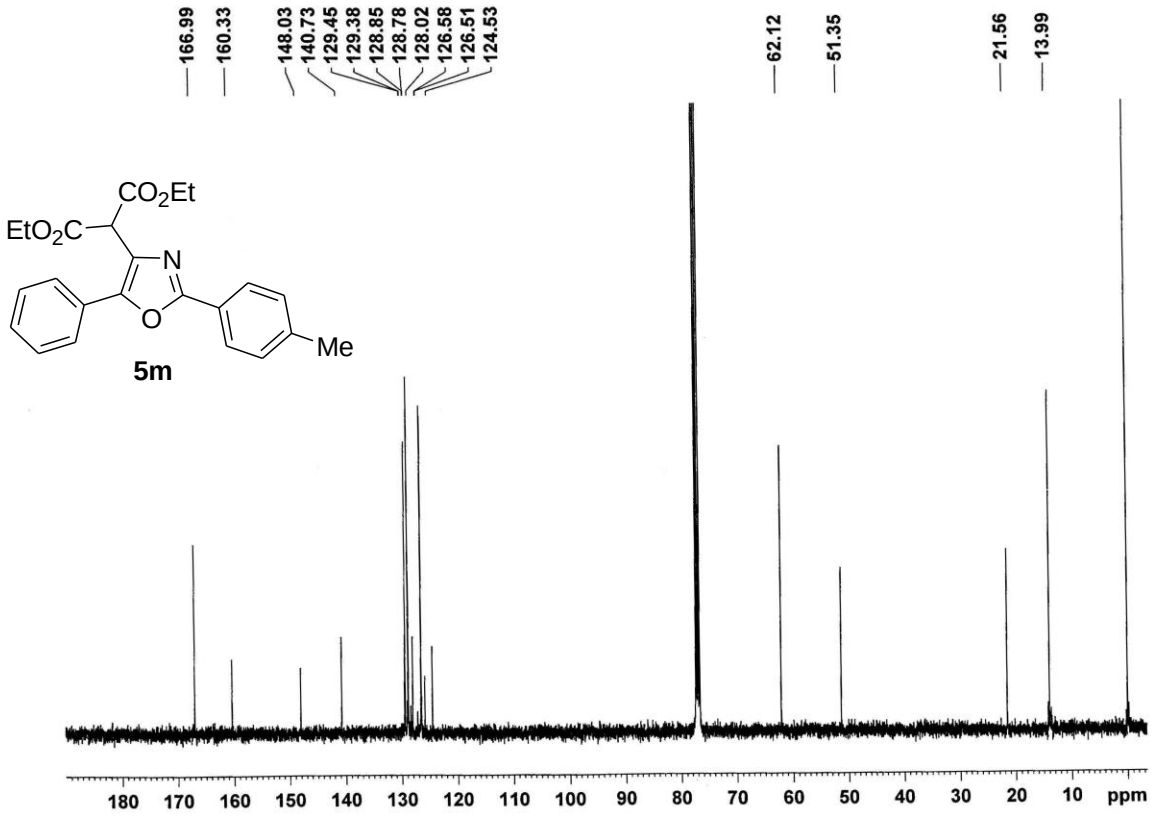
3.07
6.09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126.58
126.51
124.53
62.12
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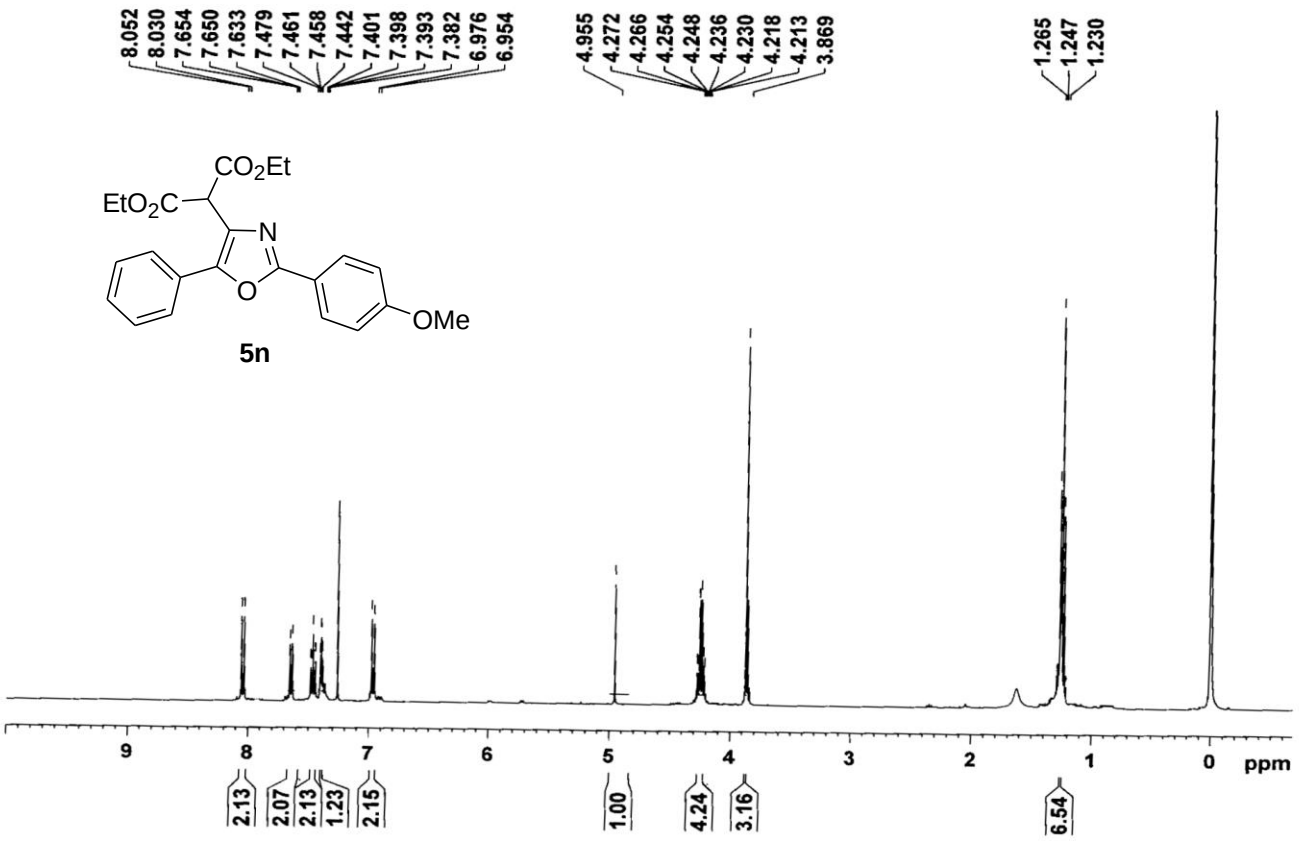
21.56
13.99
CO2Et
EtO2C
N
O
Me
5m
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.458
7.442
7.401
7.398
7.393
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6.976
6.954
4.955
4.272
4.266
4.254
4.248
4.236
4.230
4.218
4.213
3.869
1.265
1.247
1.230
CO2Et
EtO2C
N
O
OMe
5n
9
8
7
6
5
4
3
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ppm
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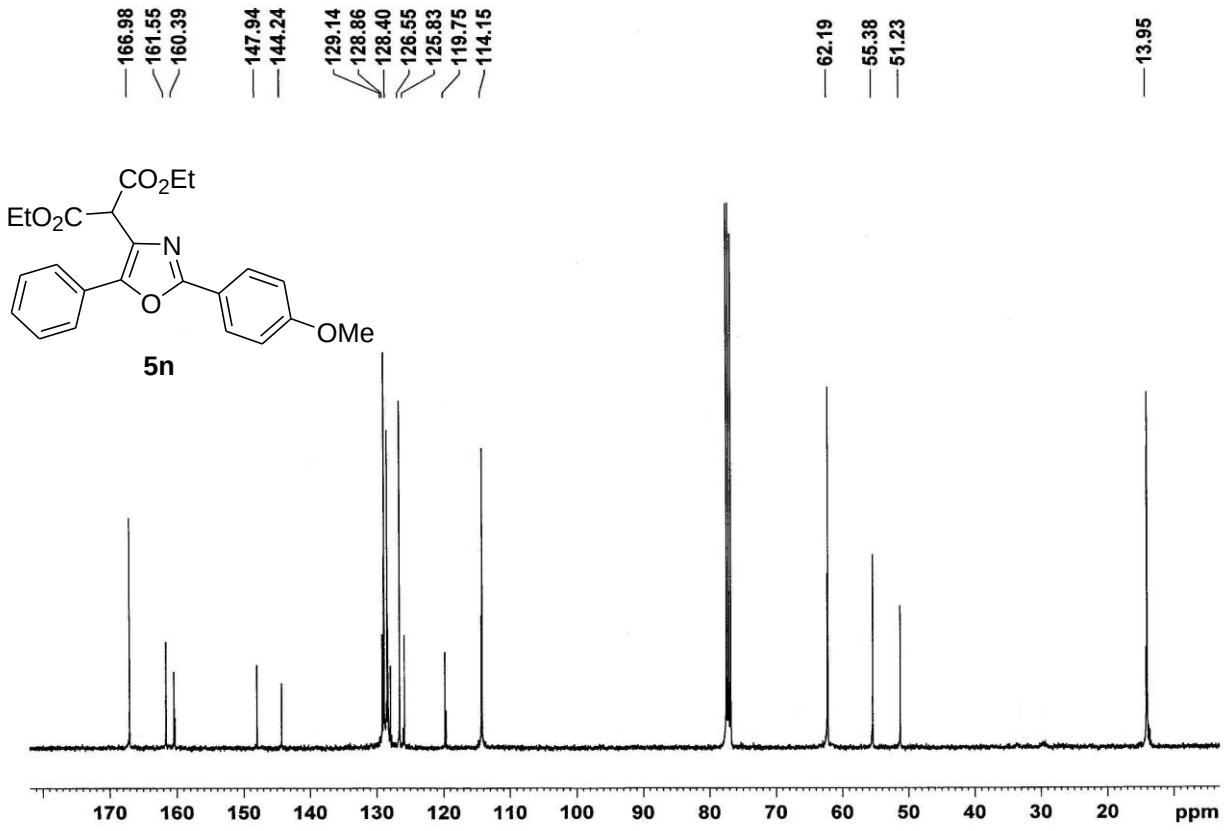
6.54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144.24
129.14
128.86
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125.83
119.75
114.15
62.19
55.38
51.23
13.95
CO2Et
EtO2C
N
O
OMe
5n
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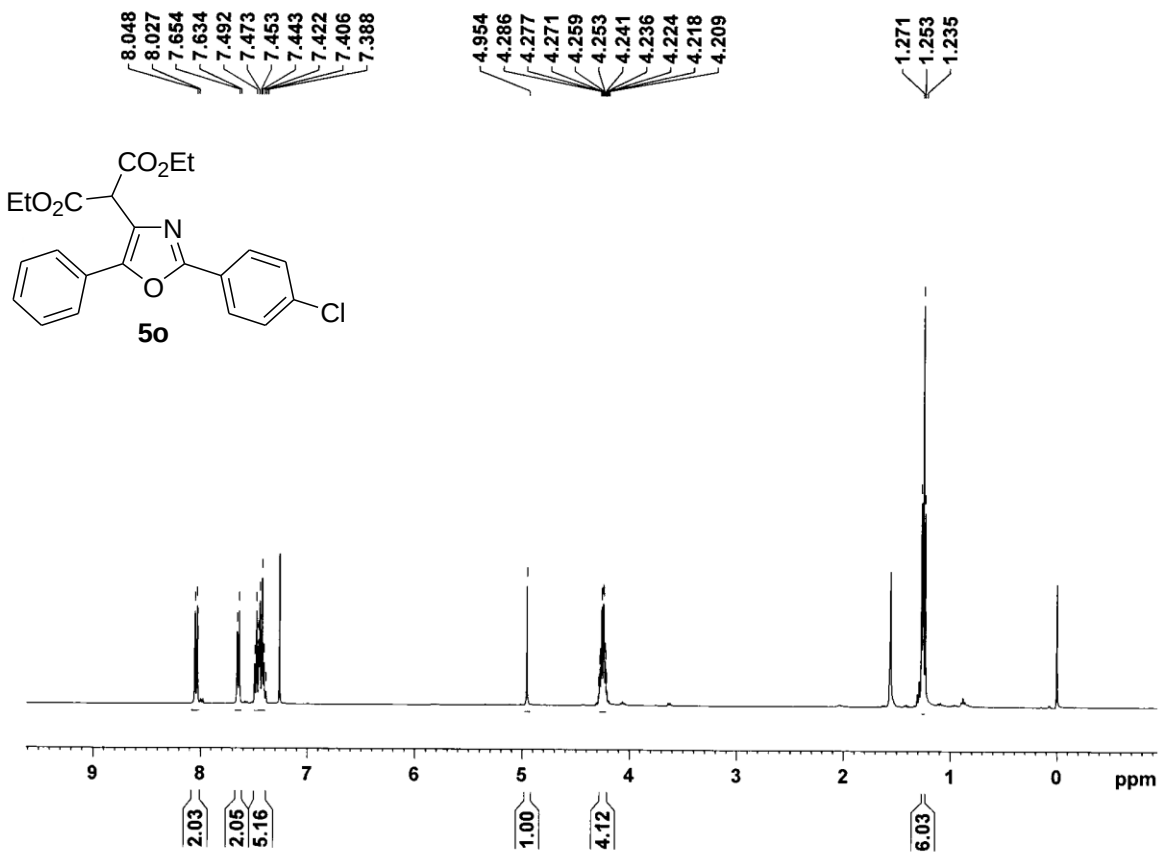
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.406
7.388
4.954
4.286
4.277
4.271
4.259
4.253
4.241
4.236
4.224
4.218
4.209
1.271
1.253
1.235
CO2Et
EtO2C
N
O
Cl
5o
9
8
7
6
5
4
3
2
1
0
ppm
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2.05
5.16
1.00
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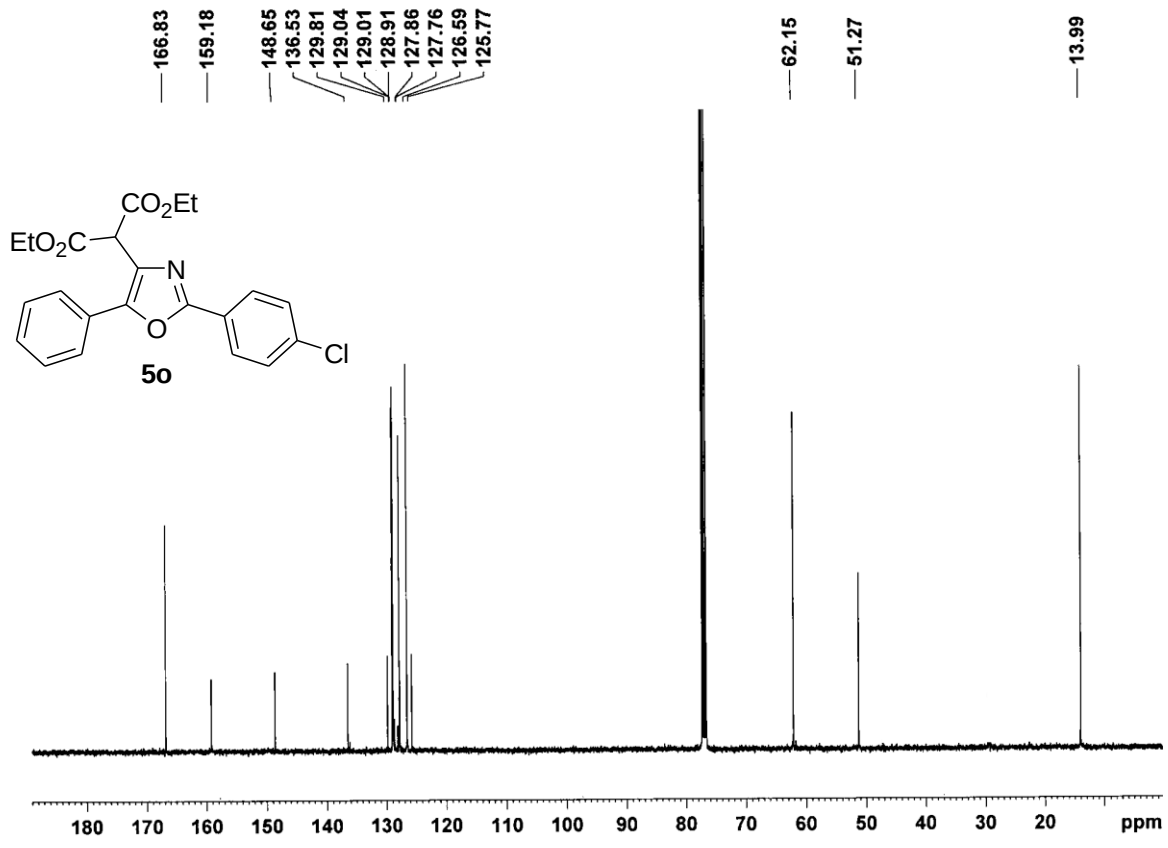
6.03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128.91
127.86
127.76
126.59
125.77
62.15
51.27
13.99
CO2Et
EtO2C
N
O
Cl
5o
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160
150
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80
70
60
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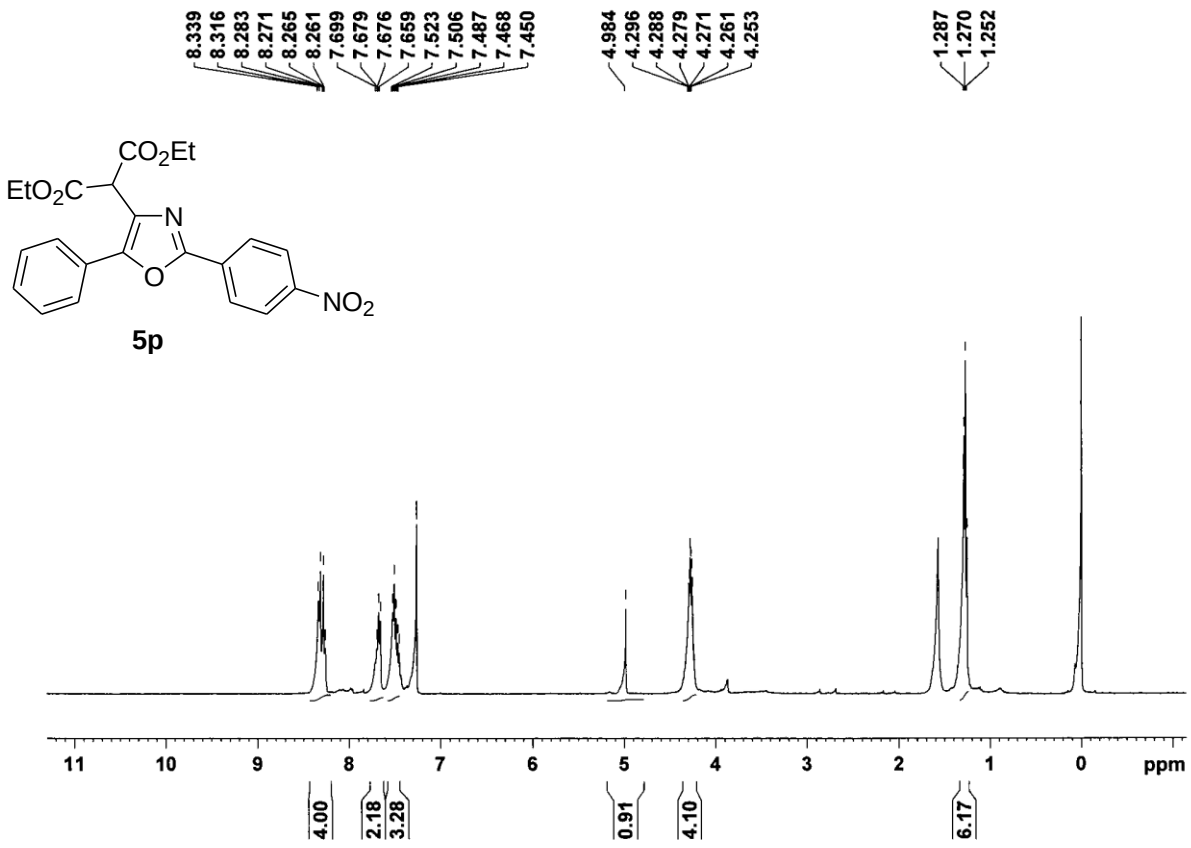
40
30
20
ppm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7.659
7.523
7.506
7.487
7.468
7.450
4.984
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4.288
4.279
4.271
4.261
4.253
1.287
1.270
1.252
CO2Et
EtO2C
N
O
NO2
5p
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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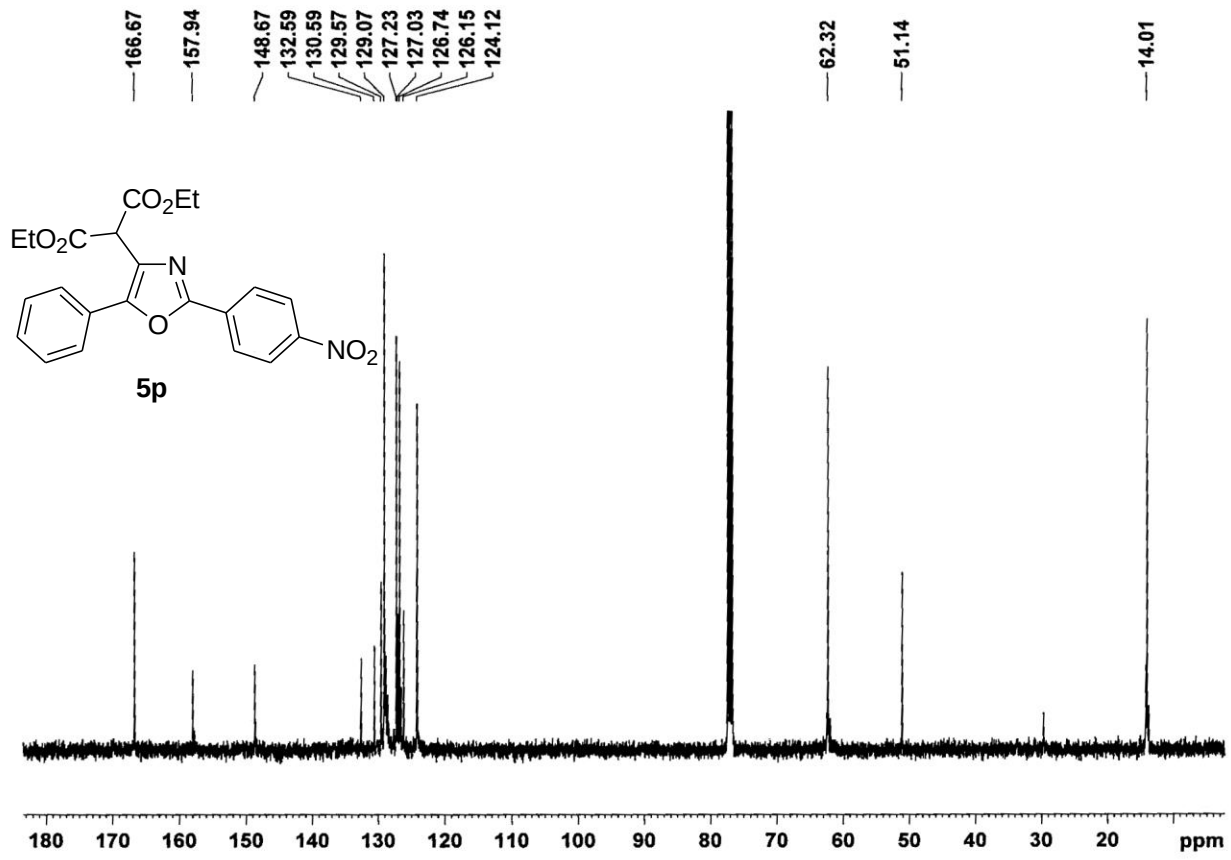
0.91
4.10
6.17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129.57
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127.23
127.03
126.74
126.15
124.12
62.32
51.14
14.01
CO2Et
EtO2C
N
O
NO2
5p
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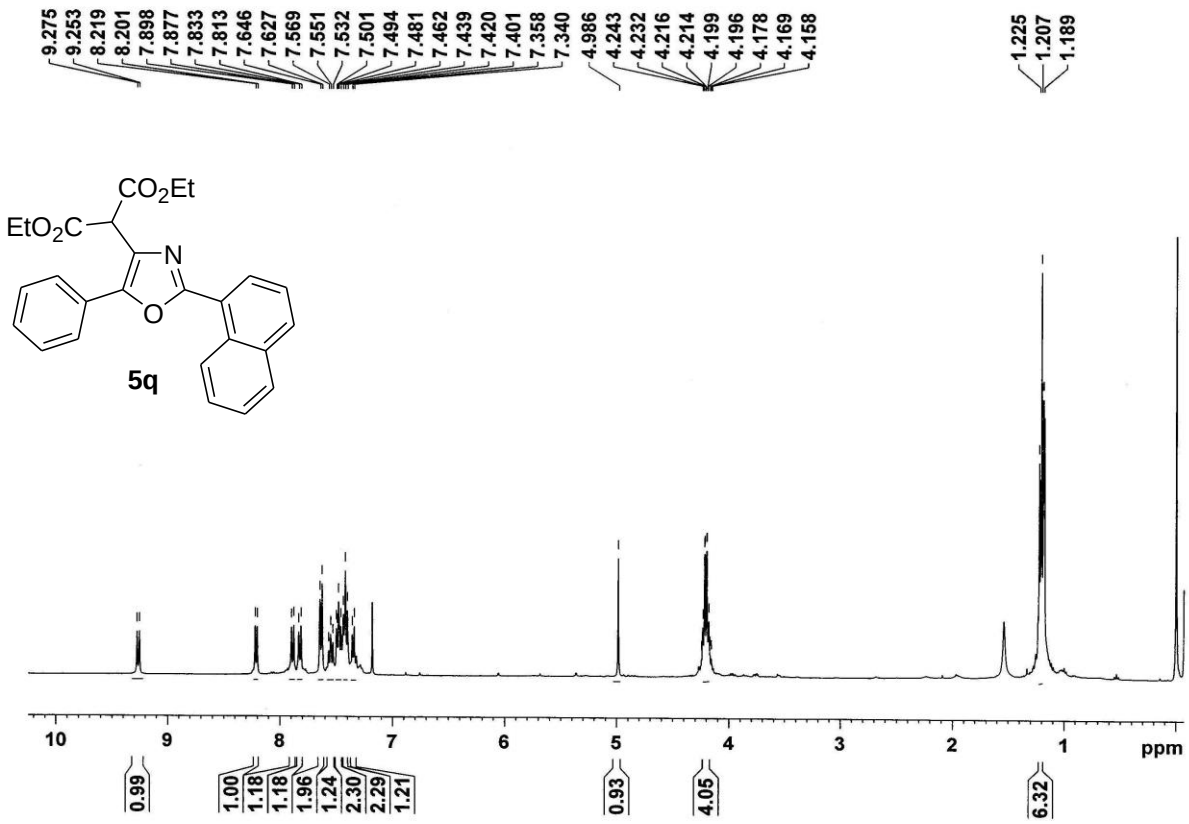
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.833
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7.627
7.569
7.551
7.532
7.501
7.494
7.481
7.462
7.439
7.420
7.401
7.358
7.340
4.986
4.243
4.232
4.216
4.214
4.199
4.196
4.178
4.169
4.158
1.225
1.207
1.189
CO2Et
EtO2C
N
O
5q
10
9
8
7
6
5
4
3
2
1
ppm
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1.18
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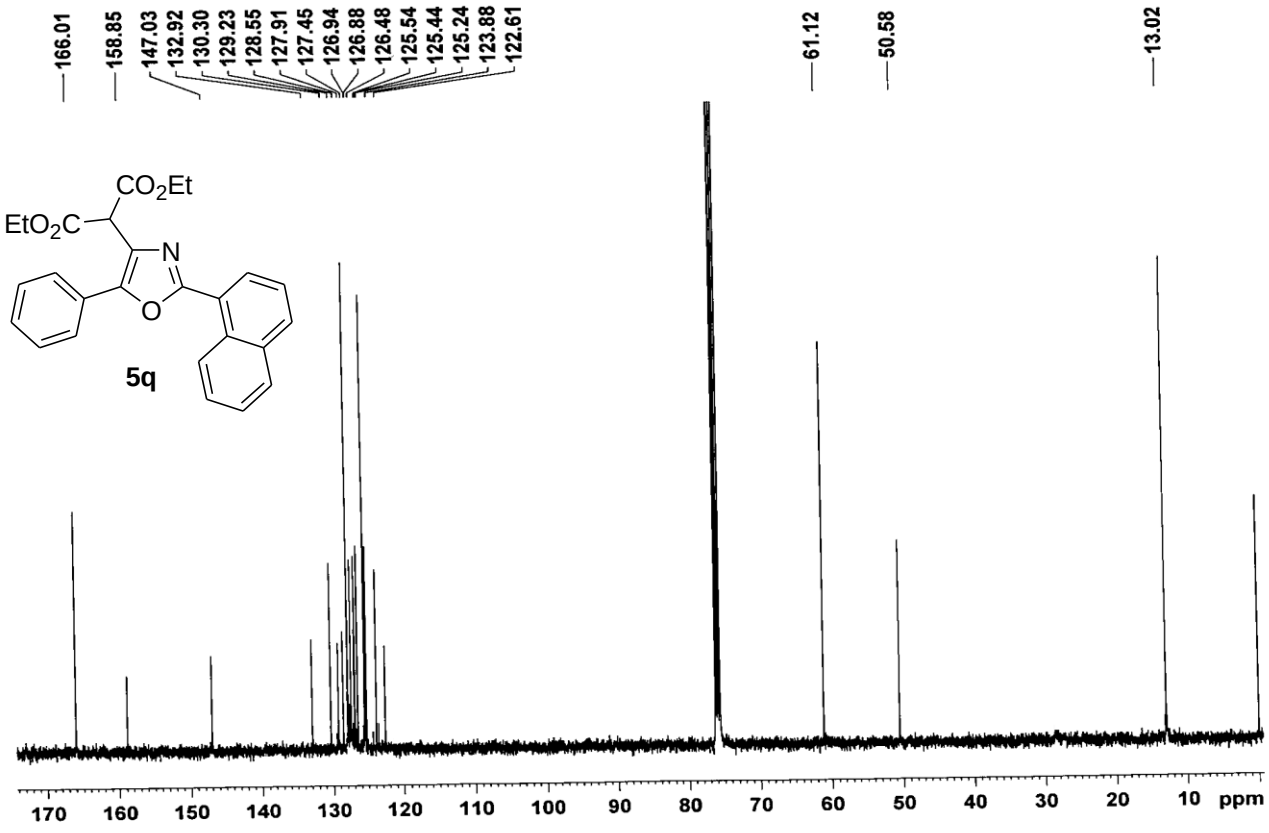
6.32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125.44
125.24
123.88
122.61
61.12
50.58
13.02
CO2Et
EtO2C
N
O
5q
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150
140
130
120
110
100
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80
70
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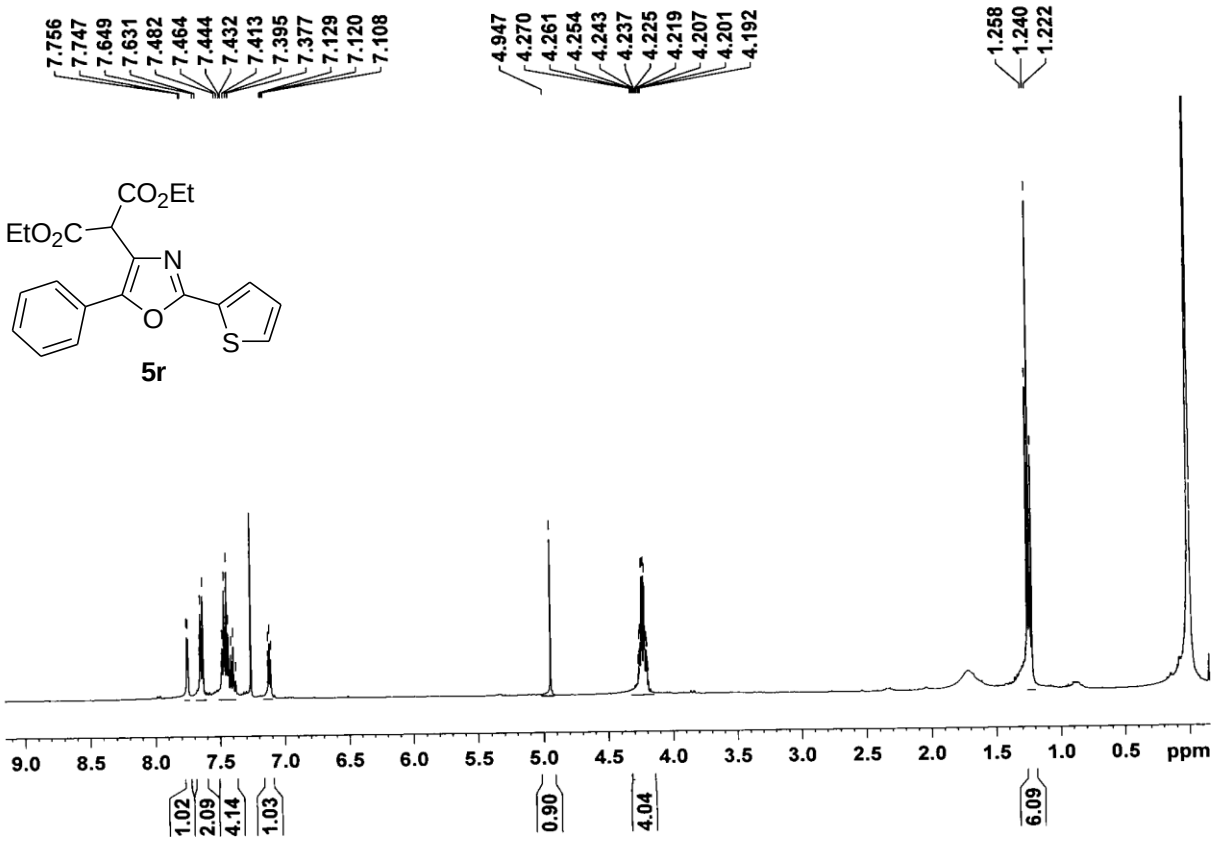
30
20
10
ppm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7.108
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4.270
4.261
4.254
4.243
4.237
4.225
4.219
4.207
4.201
4.192
1.258
1.240
1.222
CO2Et
EtO2C
N
O
S
5r
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.0
0.5
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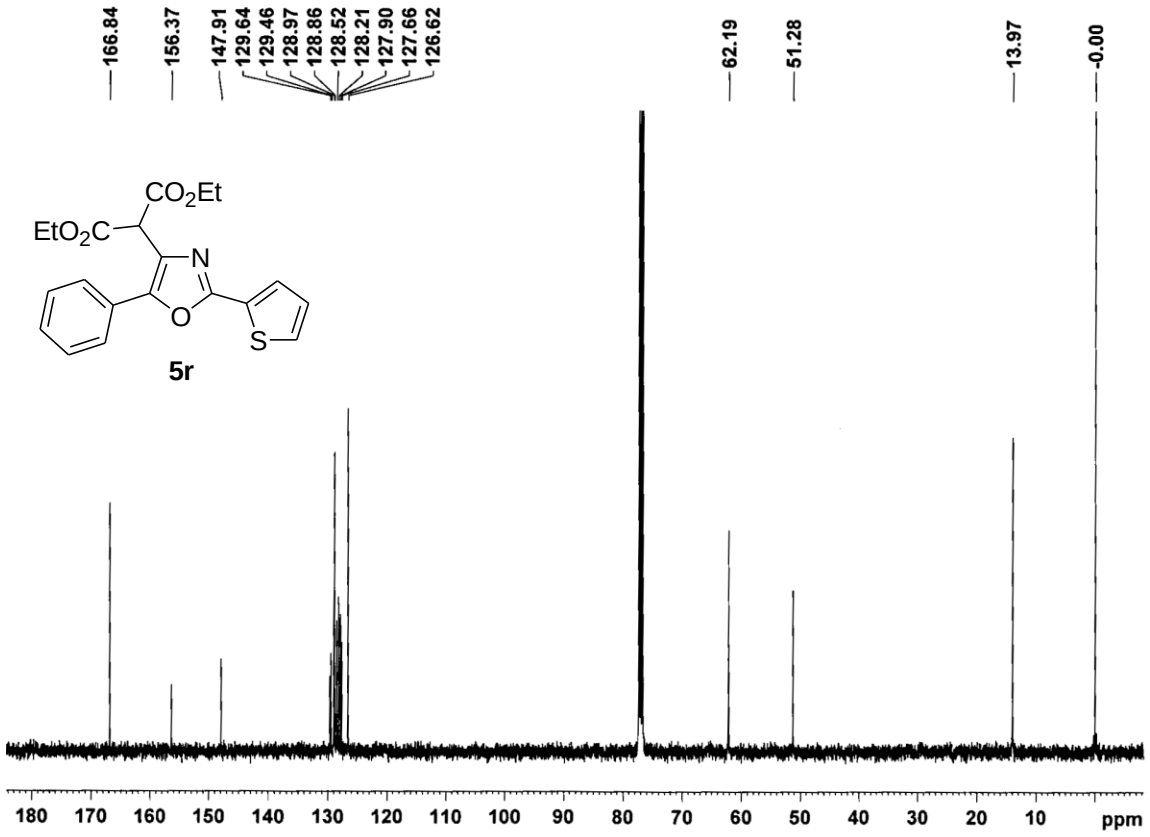
6.09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128.21
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62.19
51.28
13.97
-0.00
CO2Et
EtO2C
N
O
S
5r
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150
140
130
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80
70
60
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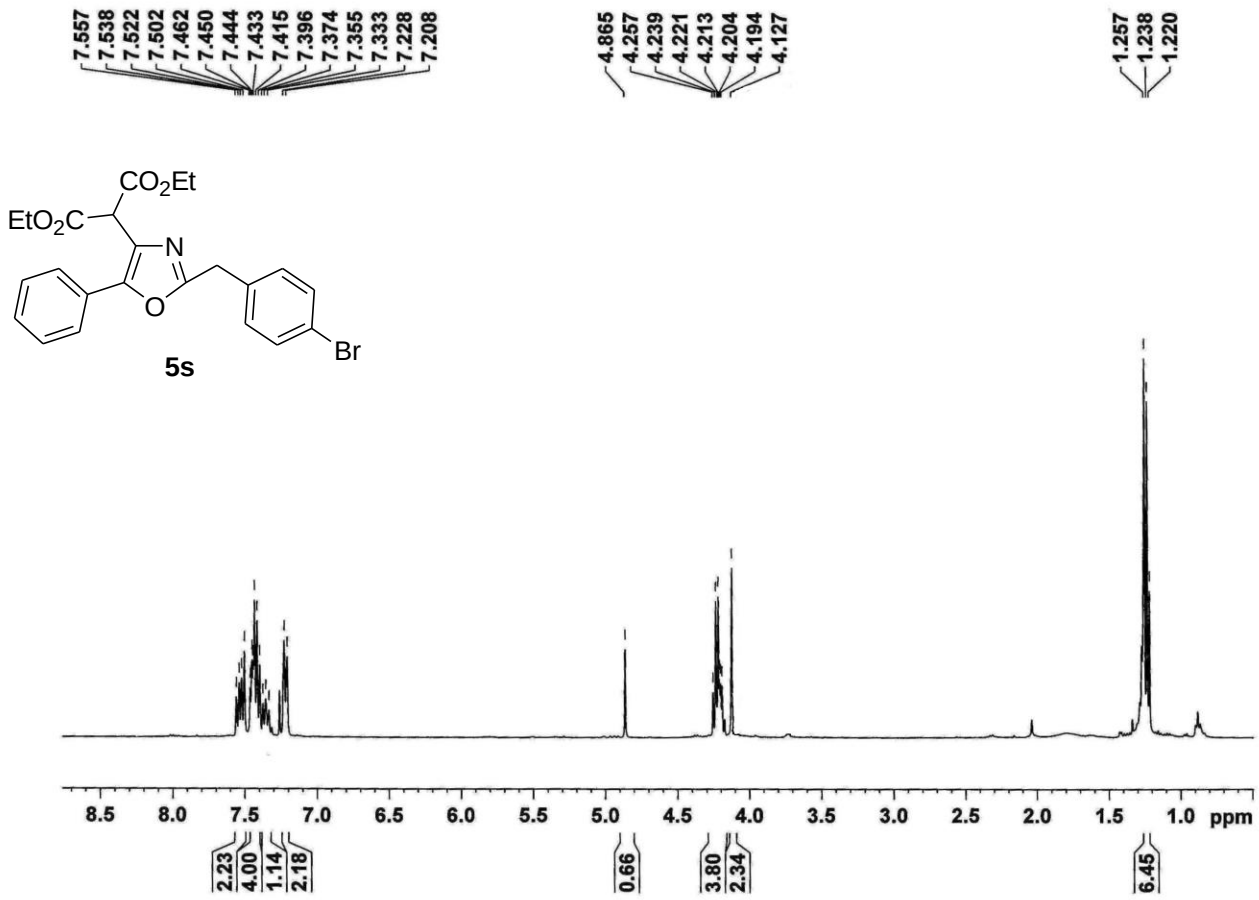
40
30
20
10
ppm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7.333
7.228
7.208
4.865
4.257
4.239
4.221
4.213
4.204
4.194
4.127
1.257
1.238
1.220
CO2Et
EtO2C
N
O
Br
5s
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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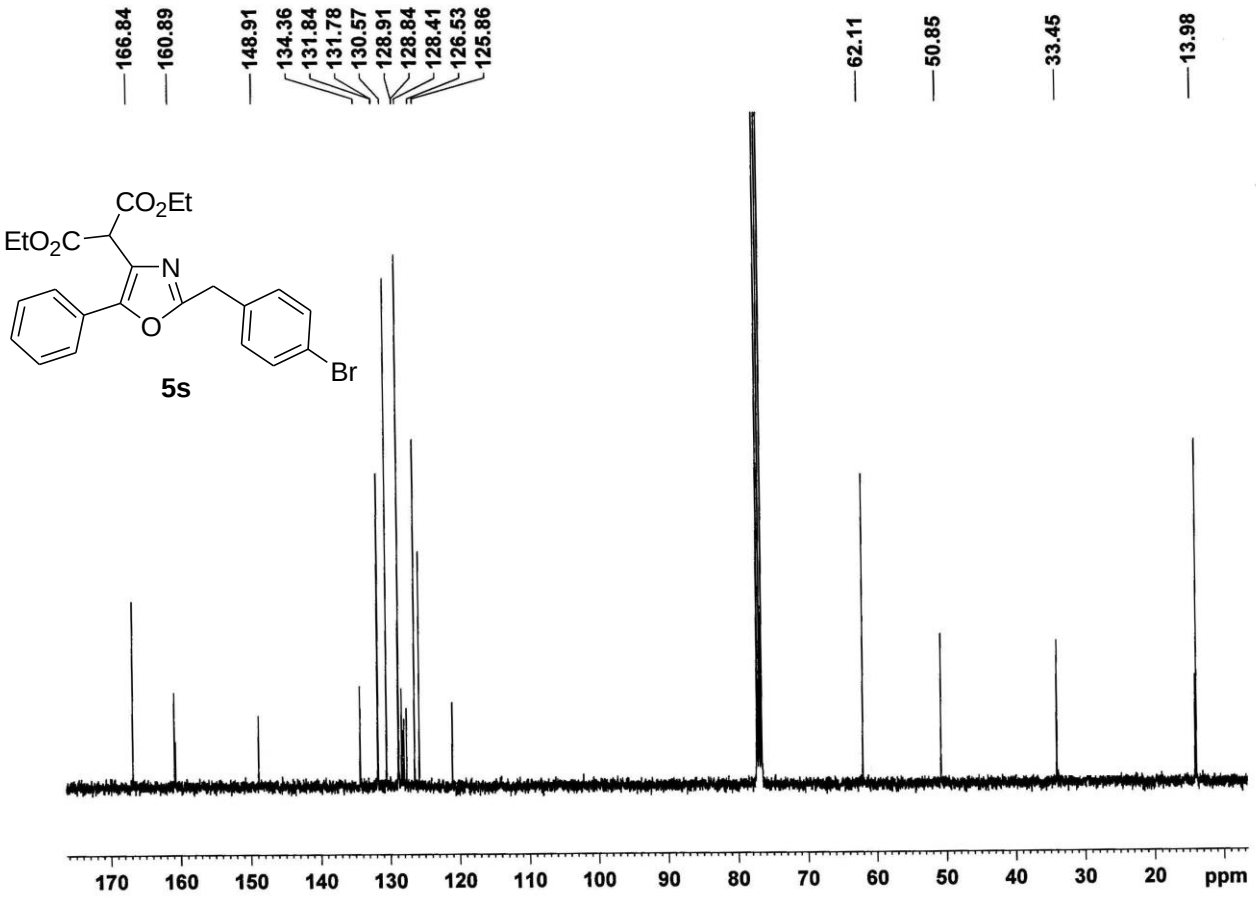
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62.11
50.85
33.45
13.98
CO2Et
EtO2C
N
O
Br
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150
140
130
120
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100
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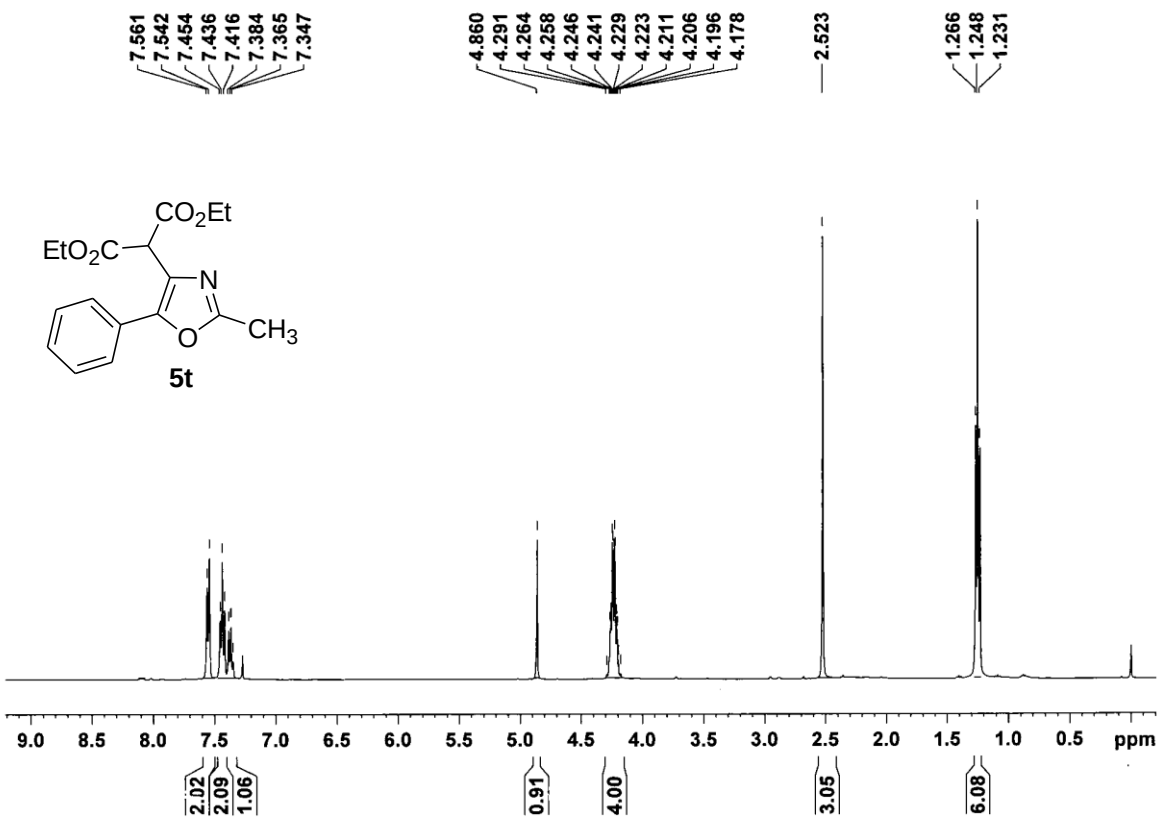
80
70
60
50
40
30
20
ppm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4.246
4.241
4.229
4.223
4.211
4.206
4.196
4.178
2.523
1.266
1.248
1.231
CO2Et
EtO2C
N
O
CH3
5t
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.06
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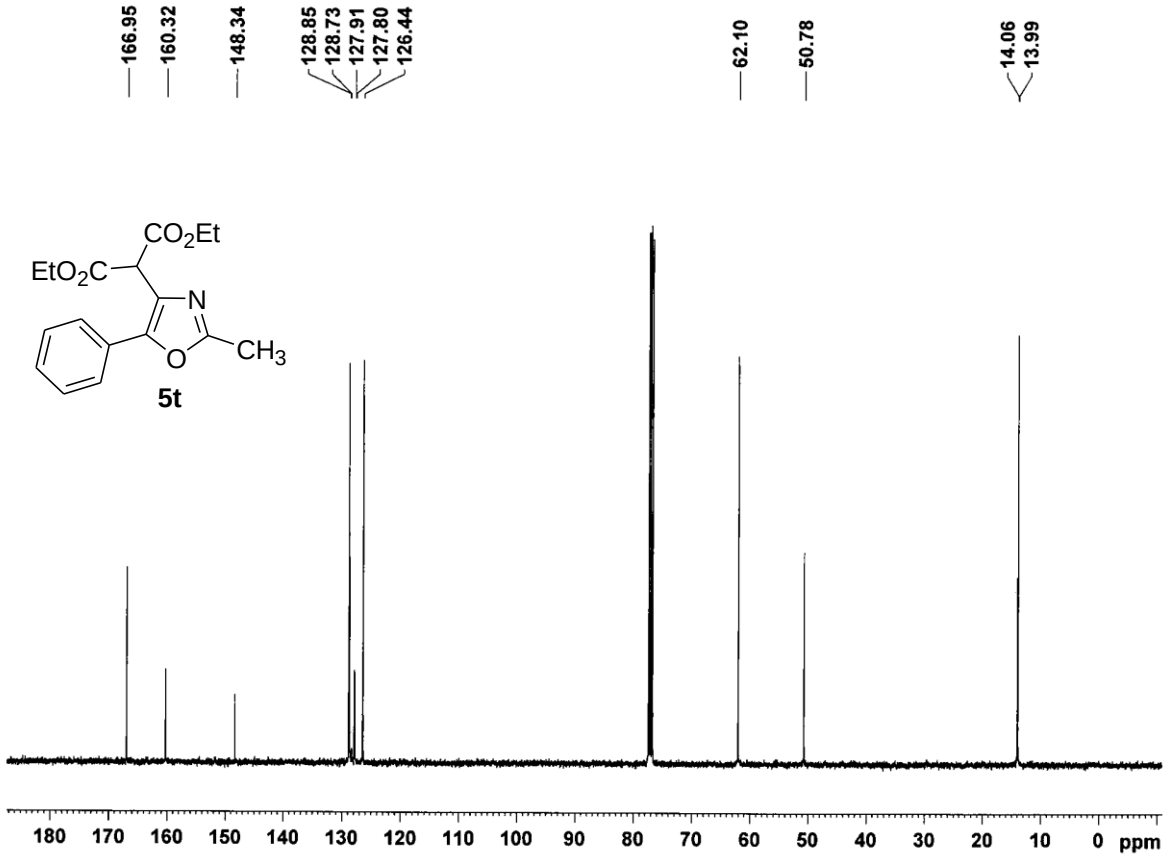
6.08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127.80
126.44
62.10
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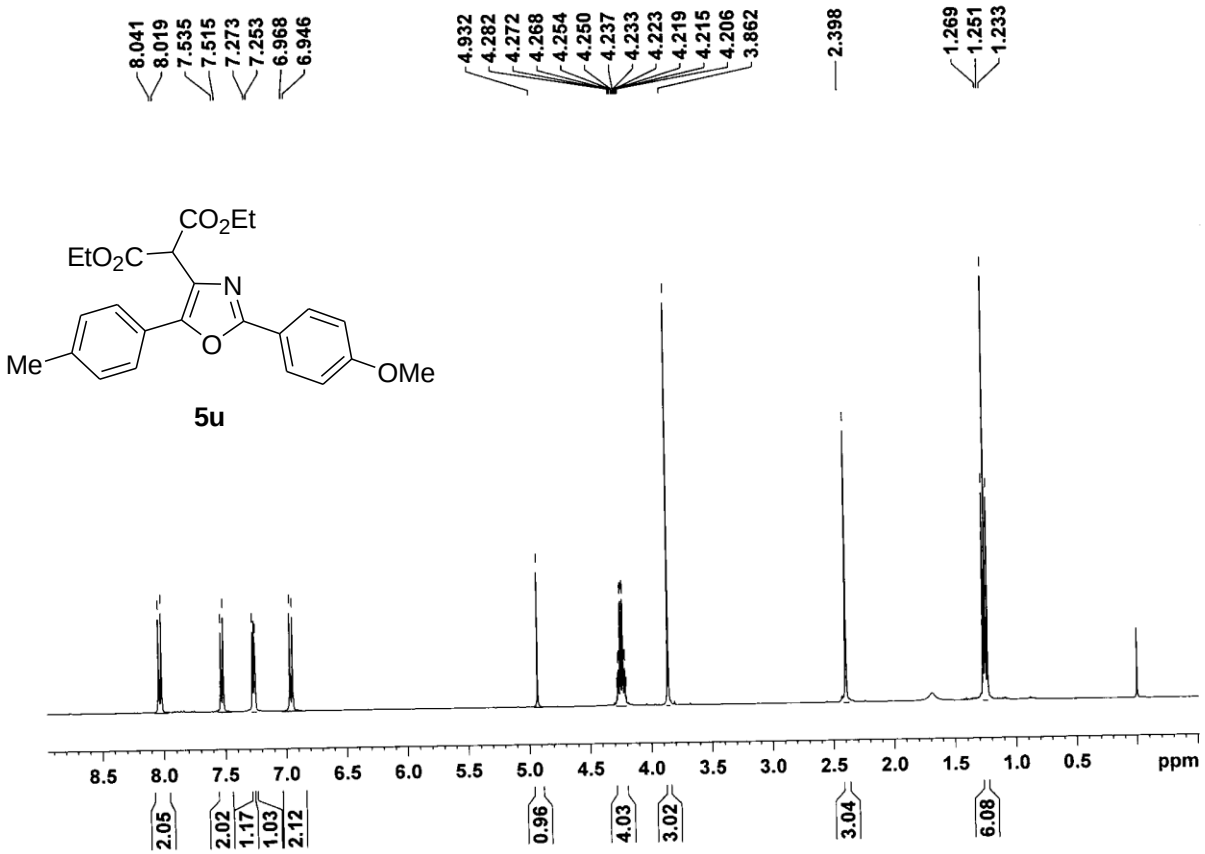
EtO2C
N
O
CH3
5t
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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6.946
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4.268
4.254
4.250
4.237
4.233
4.223
4.219
4.215
4.206
3.862
2.398
1.269
1.251
1.233
CO2Et
EtO2C
N
O
Me
OMe
5u
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
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1.03
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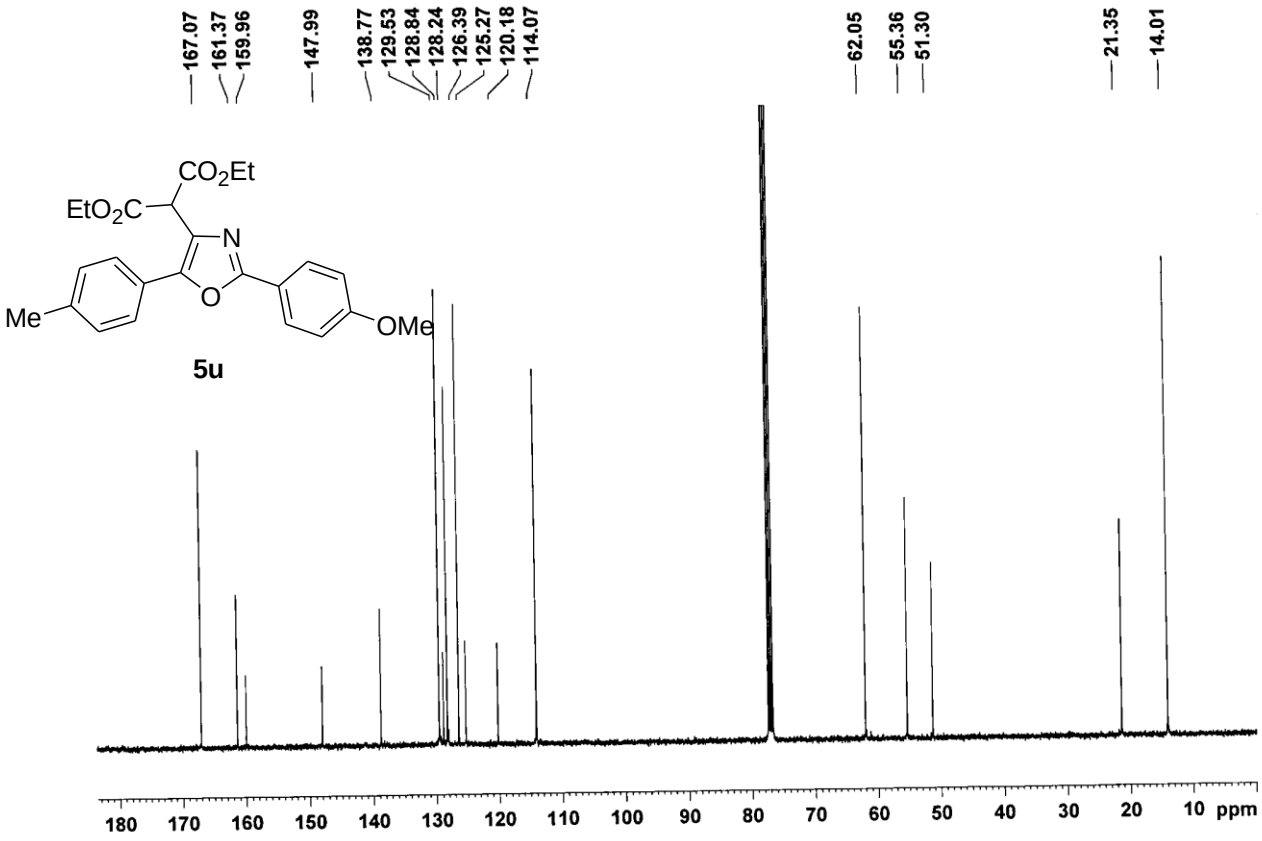
3.02
3.04
6.08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128.24
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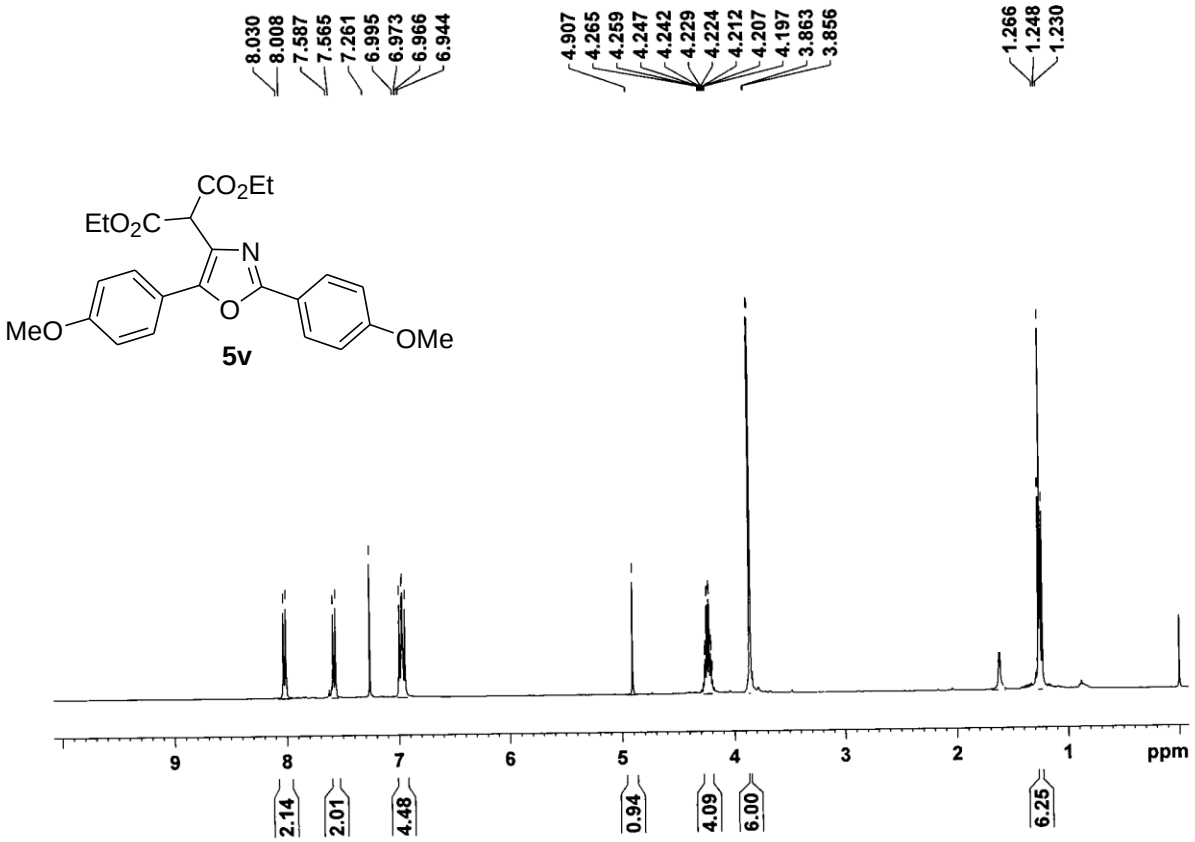
125.27
120.18
114.07
62.05
55.36
51.30
21.35
14.01
CO2Et
EtO2C
N
O
Me
OMe
5u
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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4.259
4.247
4.242
4.229
4.224
4.212
4.207
4.197
3.863
3.856
1.266
1.248
1.230
CO2Et
EtO2C
N
O
MeO
OMe
5v
9
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2
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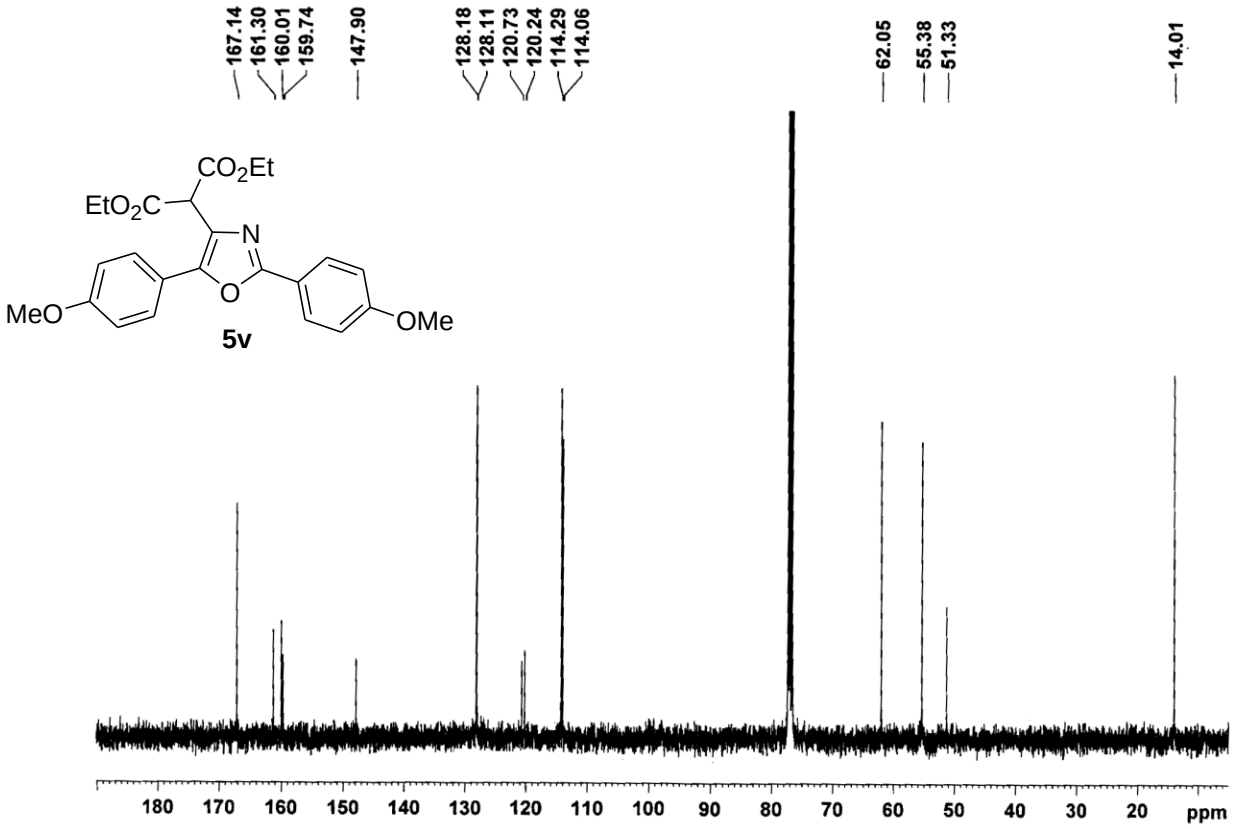
6.25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114.29
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62.05
55.38
51.33
14.01
CO2Et
EtO2C
N
O
MeO
OMe
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80
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40
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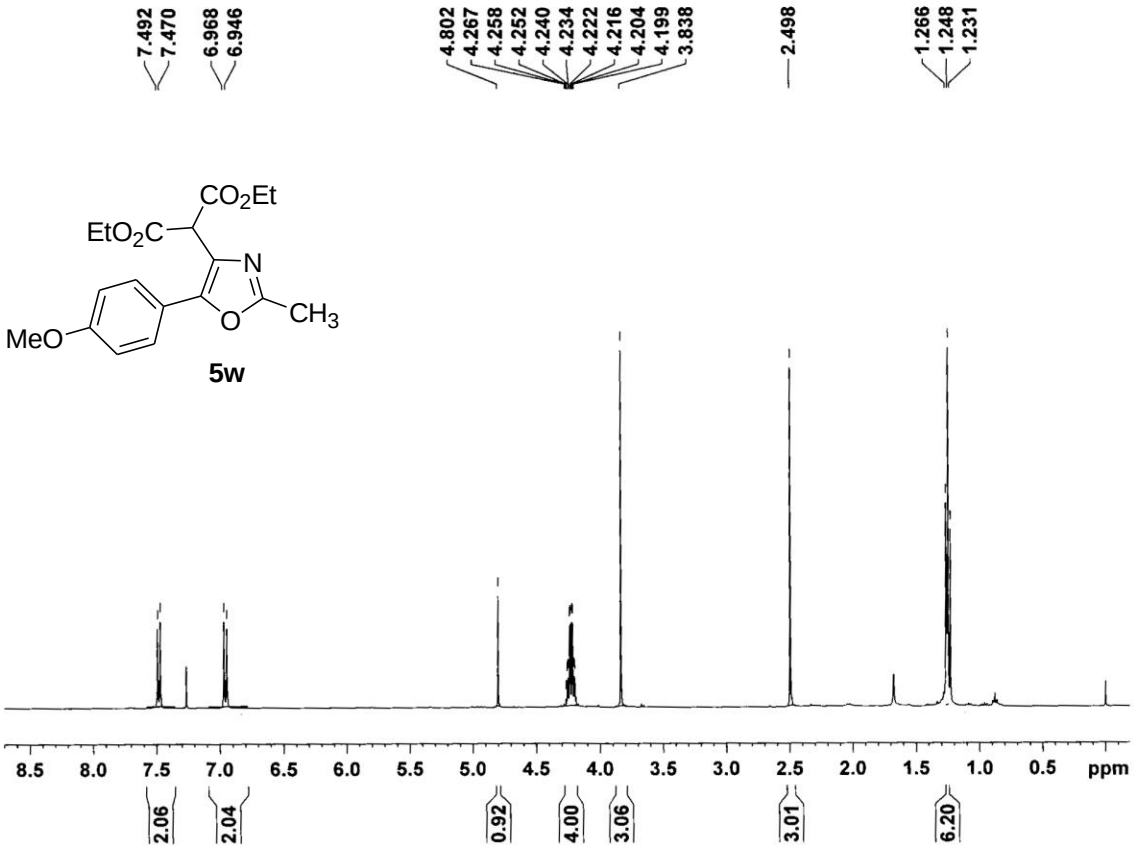
20
ppm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4.252
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4.222
4.216
4.204
4.199
3.838
2.498
1.266
1.248
1.231
CO2Et
EtO2C
N
O
CH3
MeO
5w
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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ppm
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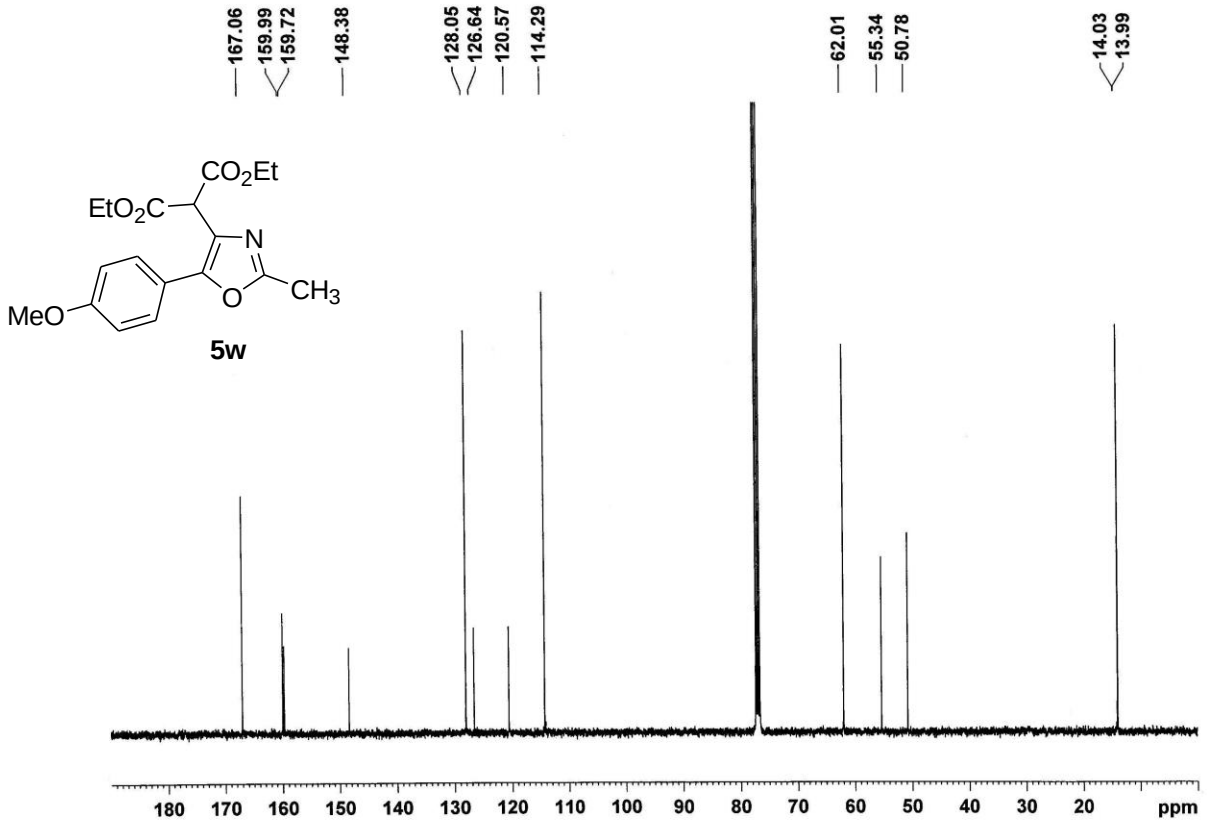
2.04
0.92
4.00
3.06
3.01
6.20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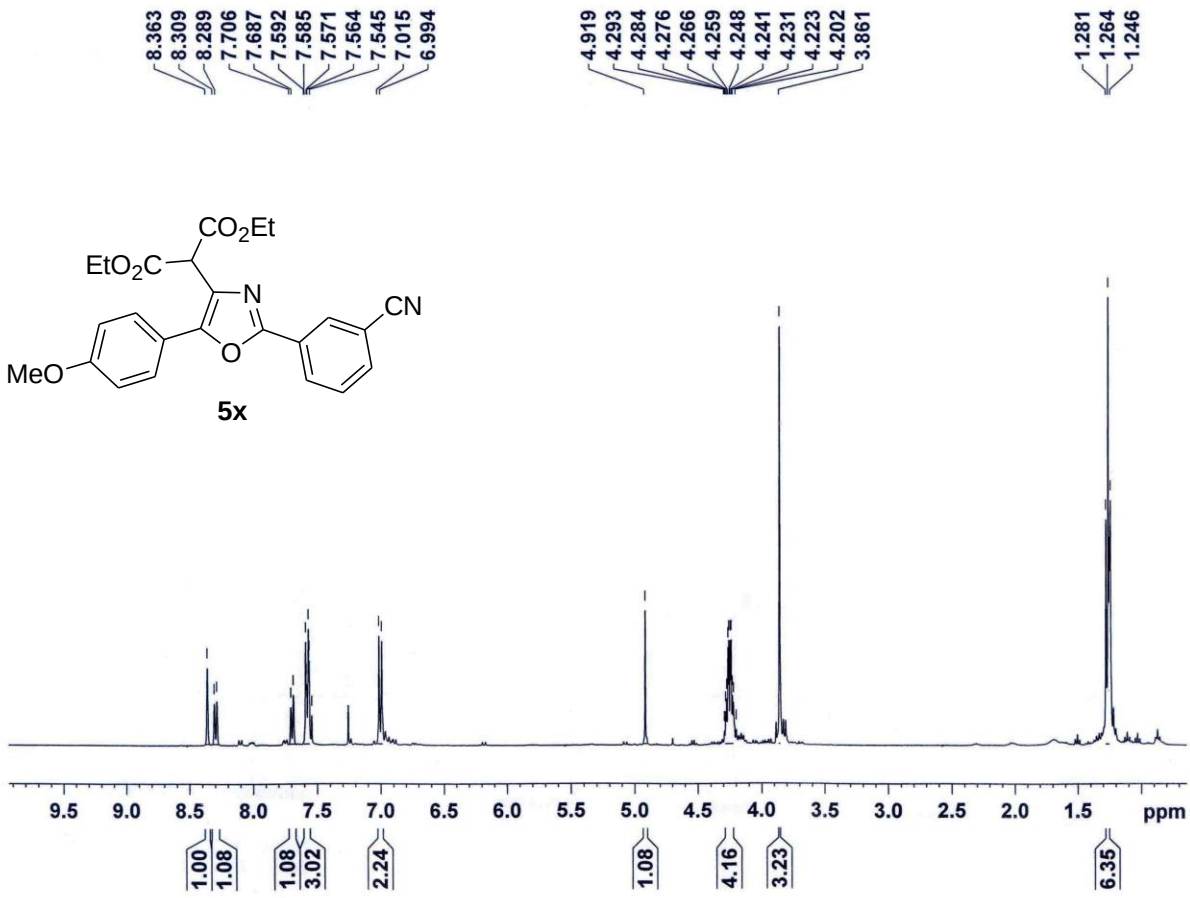
159.99
159.72
148.38
128.05
126.64
120.57
114.29
62.01
55.34
50.78
14.03
13.99
CO2Et
EtO2C
N
O
CH3
MeO
5w
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.706
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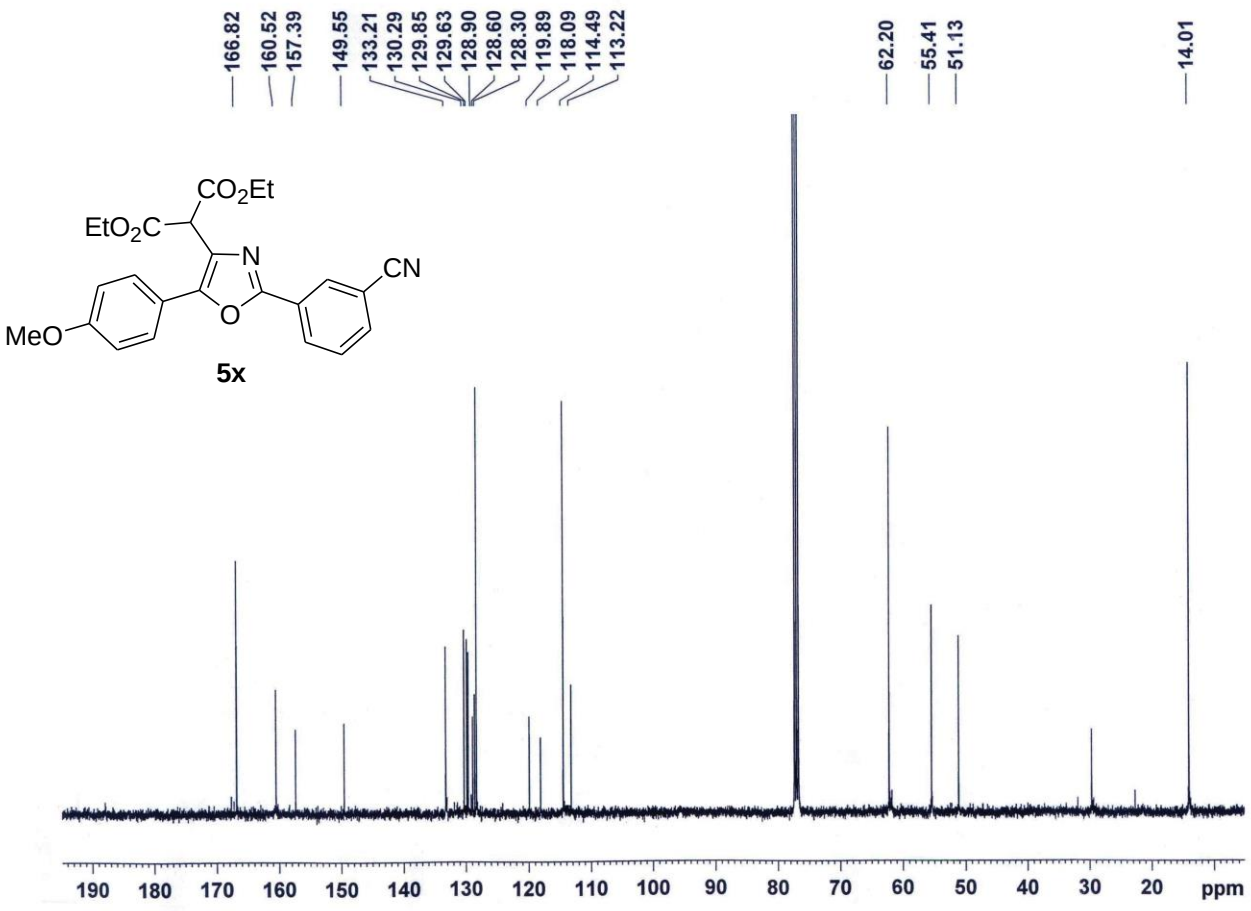
7.592
7.585
7.571
7.564
7.545
7.015
6.994
4.919
4.293
4.284
4.276
4.266
4.259
4.248
4.241
4.231
4.223
4.202
3.861
1.281
1.264
1.246
CO2Et
EtO2C
N
CN
O
MeO
5x
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
1.08
1.08
3.02
2.24
1.08
4.16
3.23
6.35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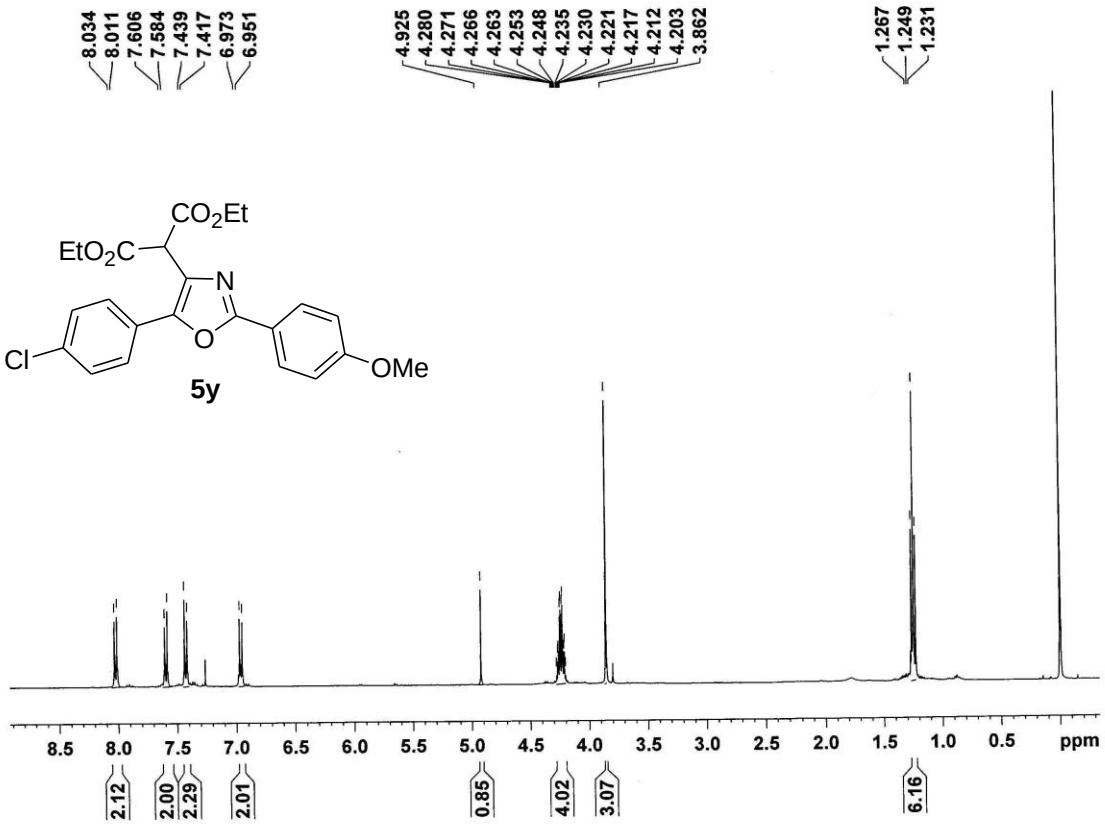
160.52
157.39
149.55
133.21
130.29
129.85
129.63
128.90
128.60
128.30
119.89
118.09
114.49
113.22
62.20
55.41
51.13
14.01
CO2Et
EtO2C
N
CN
O
MeO
5x
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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8.011
7.606
7.584
7.439
7.417
6.973
6.951
4.925
4.280
4.271
4.266
4.263
4.253
4.248
4.235
4.230
4.221
4.217
4.212
4.203
3.862
1.267
1.249
1.231
CO2Et
EtO2C
N
O
Cl
OMe
5y
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
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0.5
ppm
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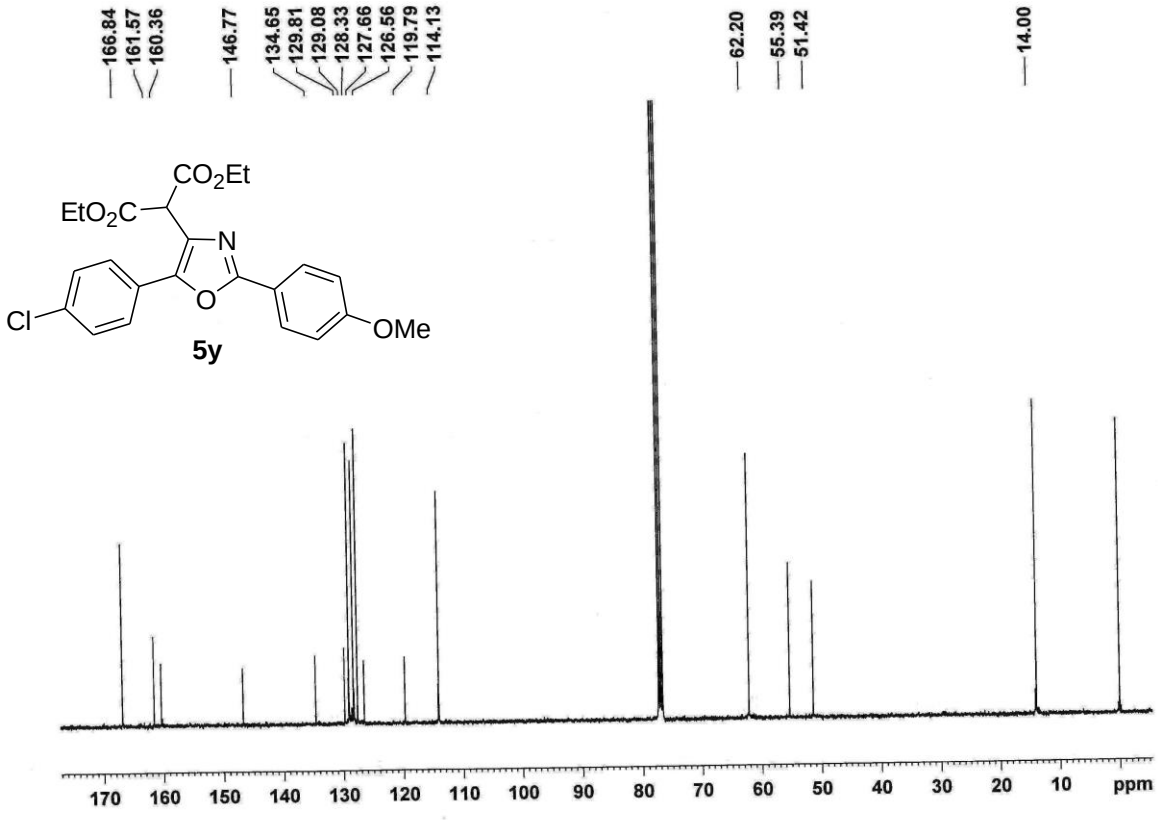
2.29
2.01
0.85
4.02
3.07
6.16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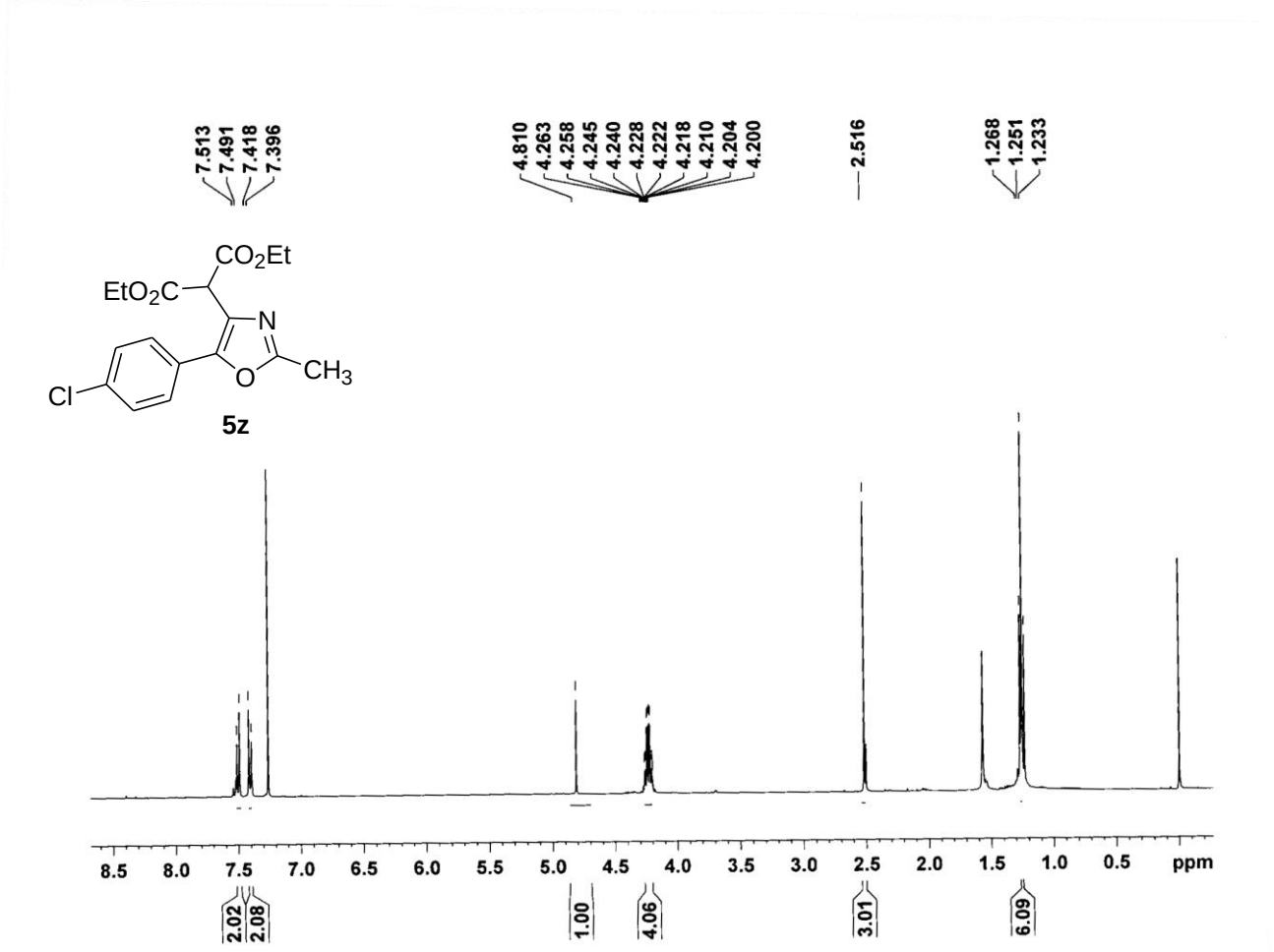
161.57
160.36
146.77
134.65
129.81
129.08
128.33
127.66
126.56
119.79
114.13
62.20
55.39
51.42
14.00
CO2Et
EtO2C
N
O
Cl
OMe
5y
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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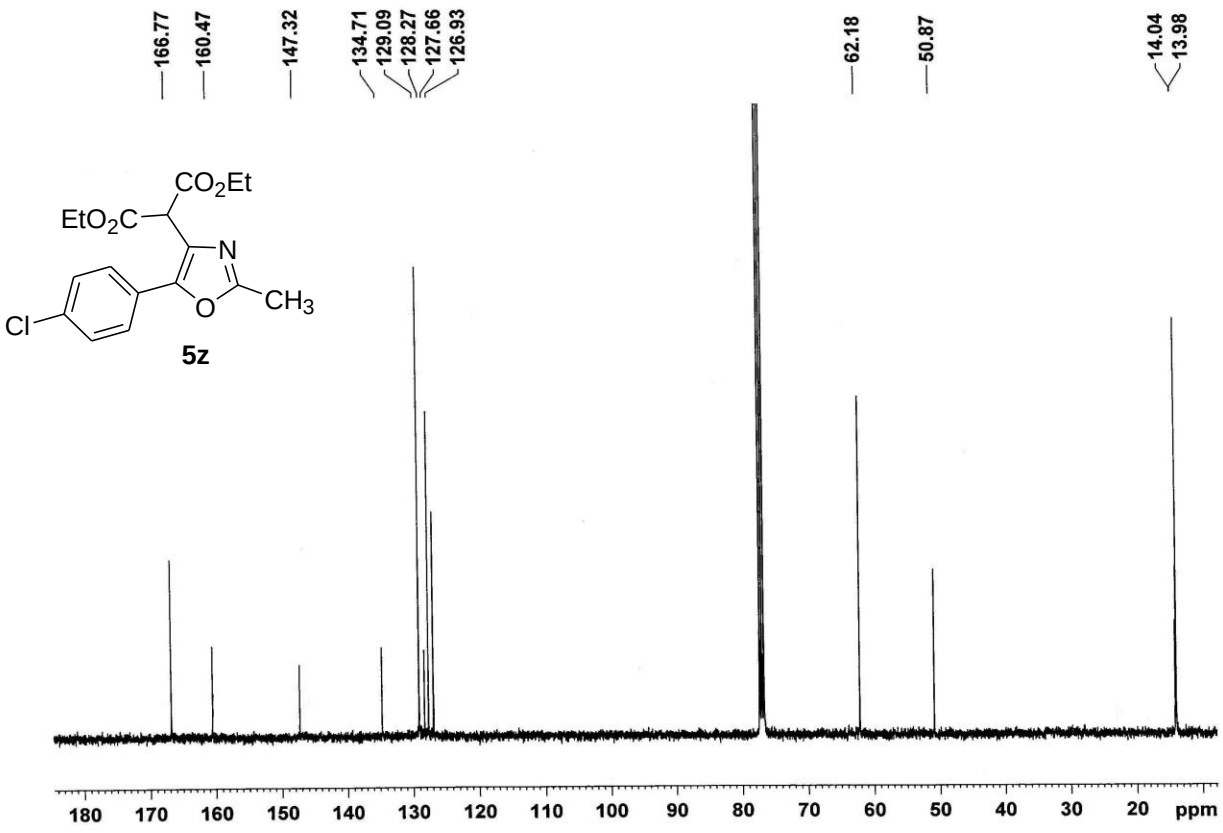
7.491
7.418
7.396
4.810
4.263
4.258
4.245
4.240
4.228
4.222
4.218
4.210
4.204
4.200
2.516
1.268
1.251
1.233
CO2Et
EtO2C
N
O
CH3
Cl
5z
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.02
2.08
1.00
4.06
3.01
6.09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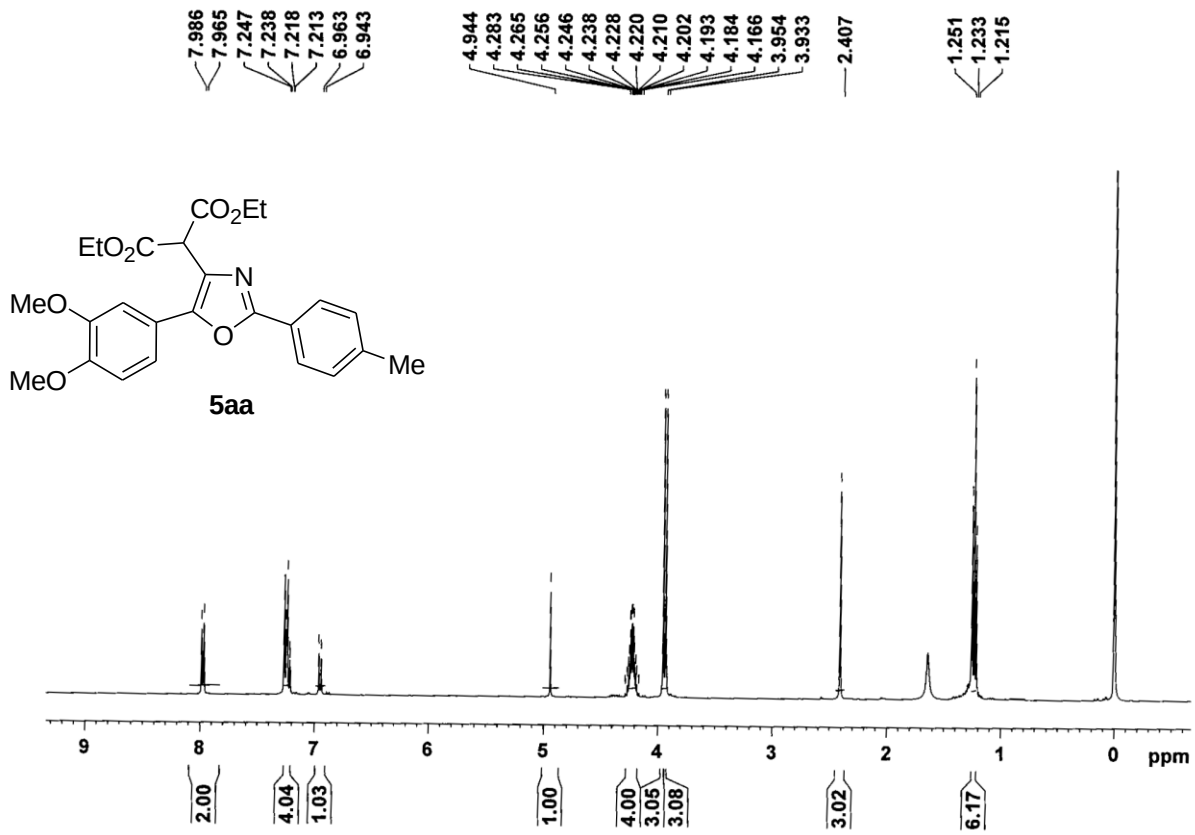
147.32
134.71
129.09
128.27
127.66
126.93
62.18
50.87
14.04
13.98
CO2Et
EtO2C
N
O
CH3
Cl
5z
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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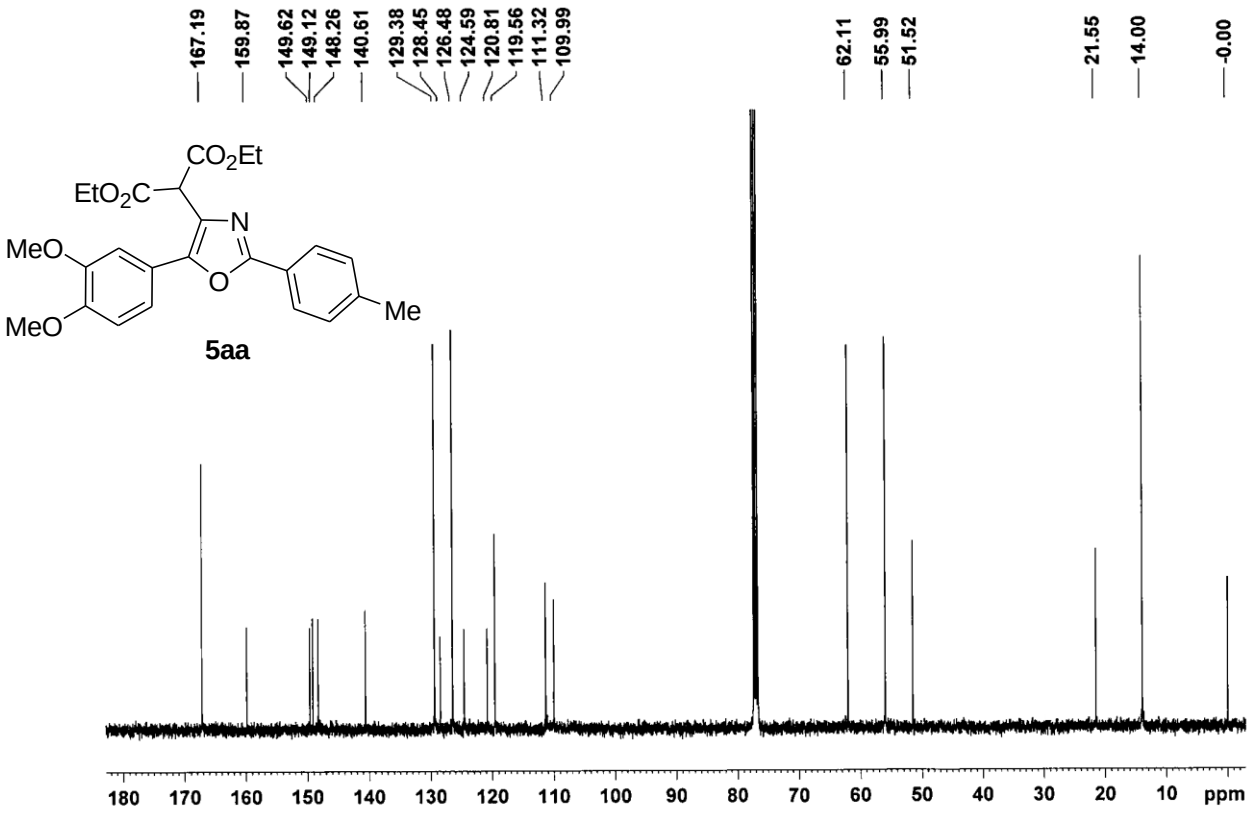
7.965
7.247
7.238
7.218
7.213
6.963
6.943
4.944
4.283
4.265
4.256
4.246
4.238
4.228
4.220
4.210
4.202
4.193
4.184
4.166
3.954
3.933
2.407
1.251
1.233
1.215
CO2Et
EtO2C
N
MeO
O
MeO
Me
5aa
9
8
7
6
5
4
3
2
1
0
ppm
2.00
4.04
1.03
1.00
4.00
3.05
3.08
3.02
6.17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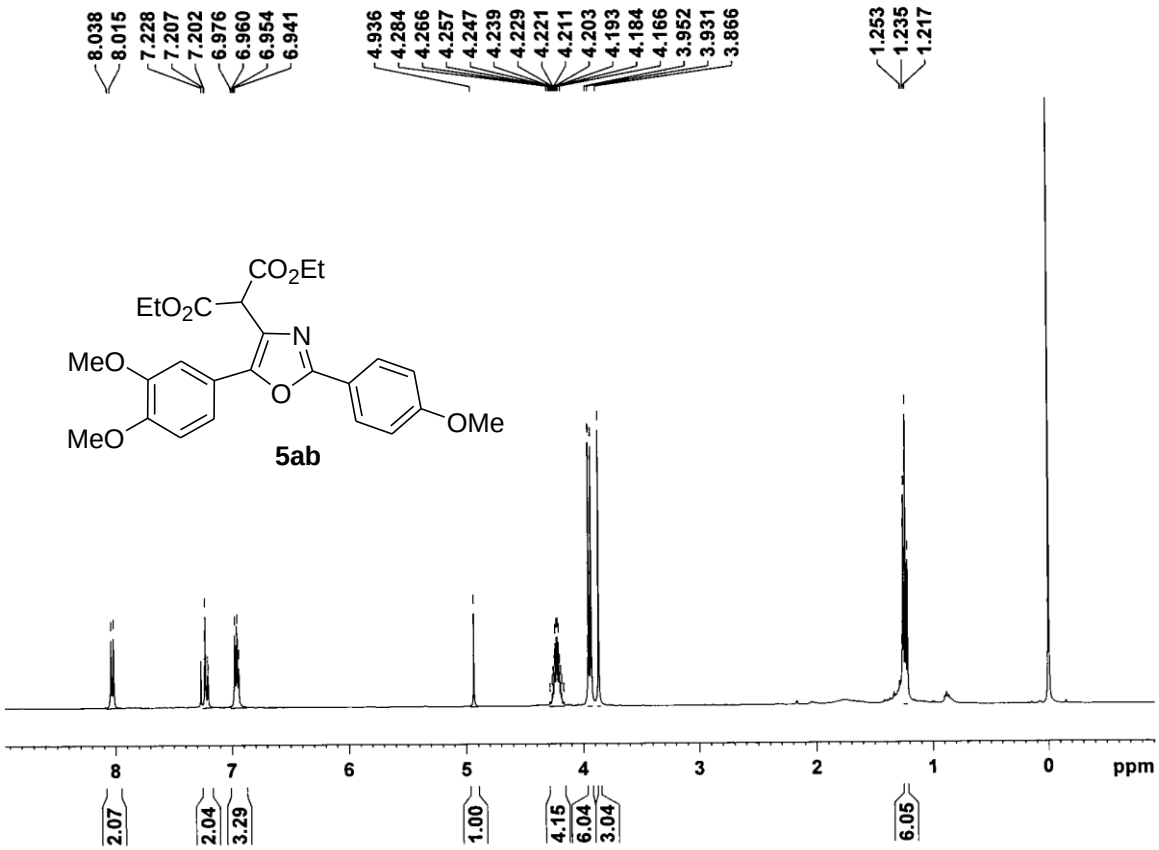
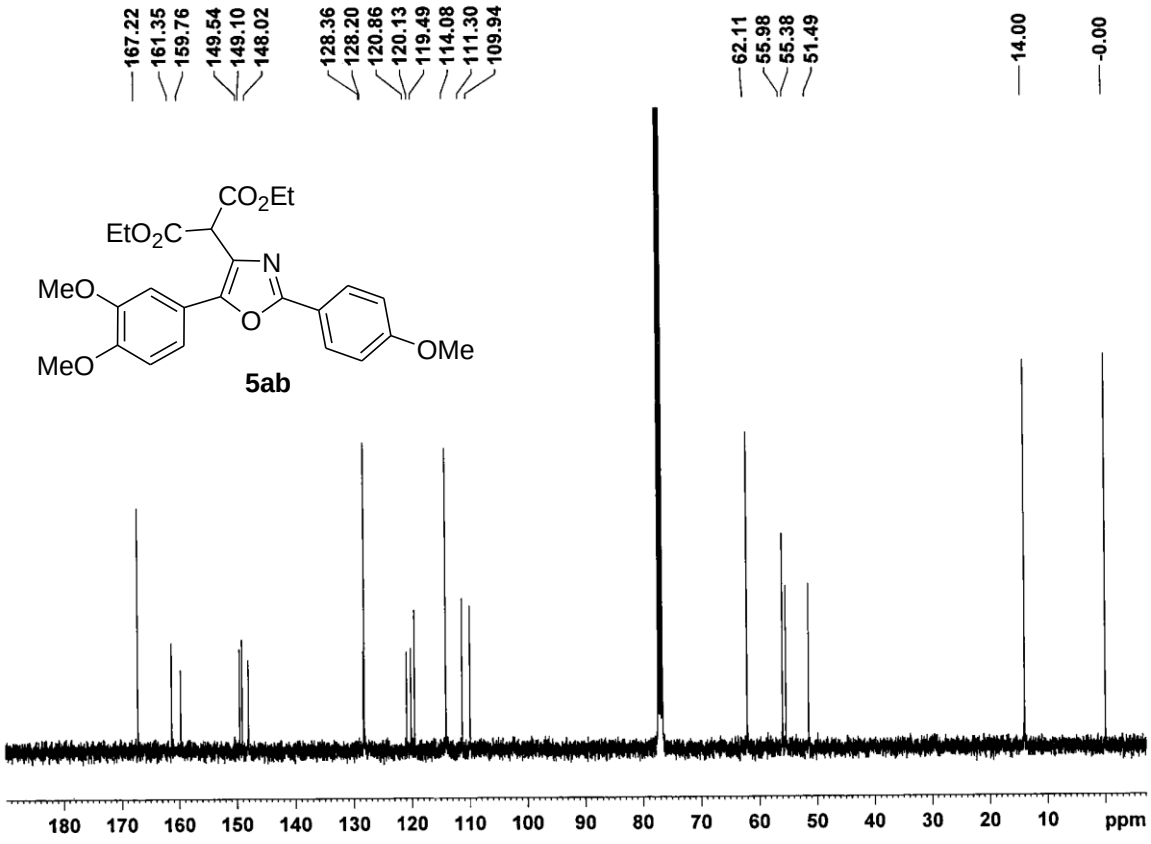
159.87
149.62
149.12
148.26
140.61
129.38
128.45
126.48
124.59
120.81
119.56
111.32
109.99
62.11
55.99
51.52
21.55
14.00
-0.00
CO2Et
EtO2C
N
MeO
MeO
O
Me
5aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.038
8.015
7.228
7.207
7.202
6.976
6.960
6.954
6.941
4.936
4.284
4.266
4.257
4.247
4.239
4.229
4.221
4.211
4.203
4.193
4.184
4.166
3.952
3.931
3.866
1.253
1.235
1.217
CO2Et
EtO2C
N
MeO
MeO
O
OMe
5ab
8
7
6
5
4
3
2
1
0
ppm
2.07
2.04
3.29
1.00
4.15
6.04
3.04
6.05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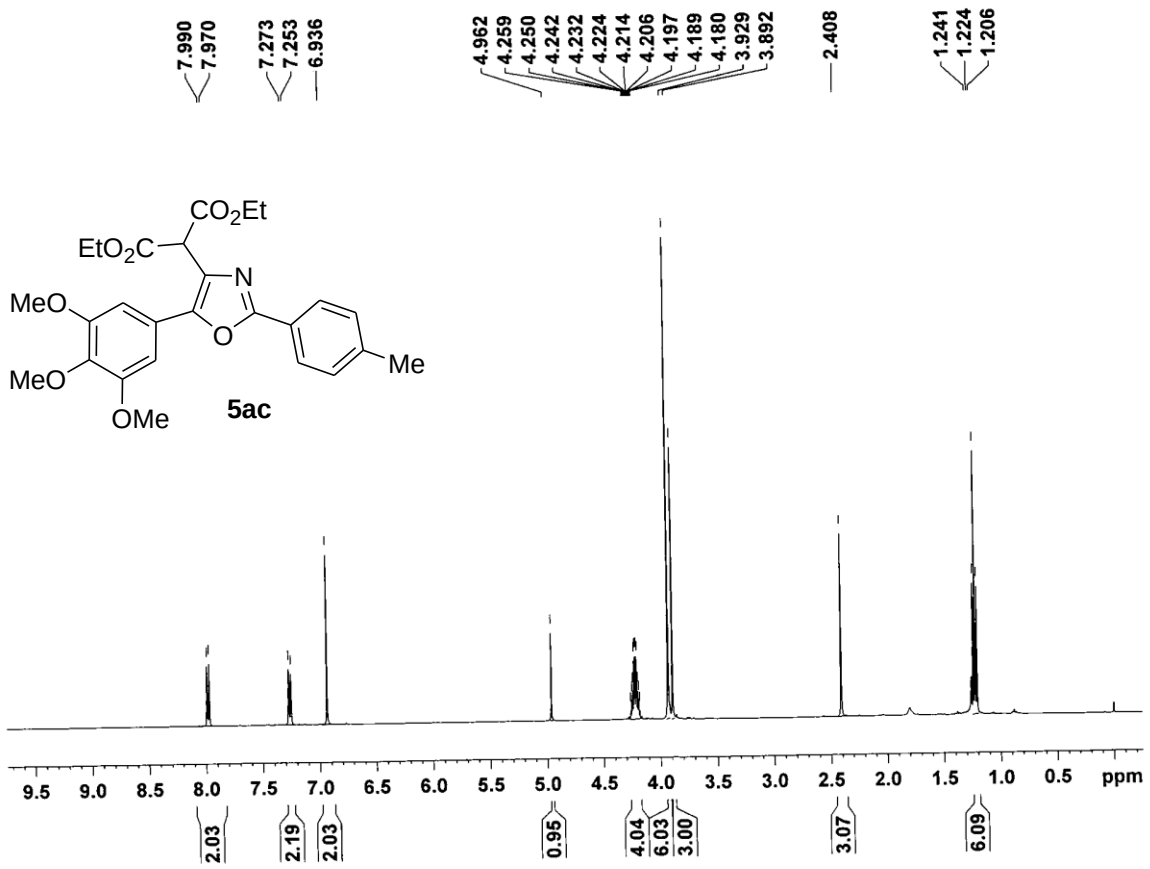
161.35
159.76
149.54
149.10
148.02
128.36
128.20
120.86
120.13
119.49
114.08
111.30
109.94
62.11
55.98
55.38
51.49
14.00
-0.00
CO2Et
EtO2C
N
MeO
O
MeO
OMe
5ab
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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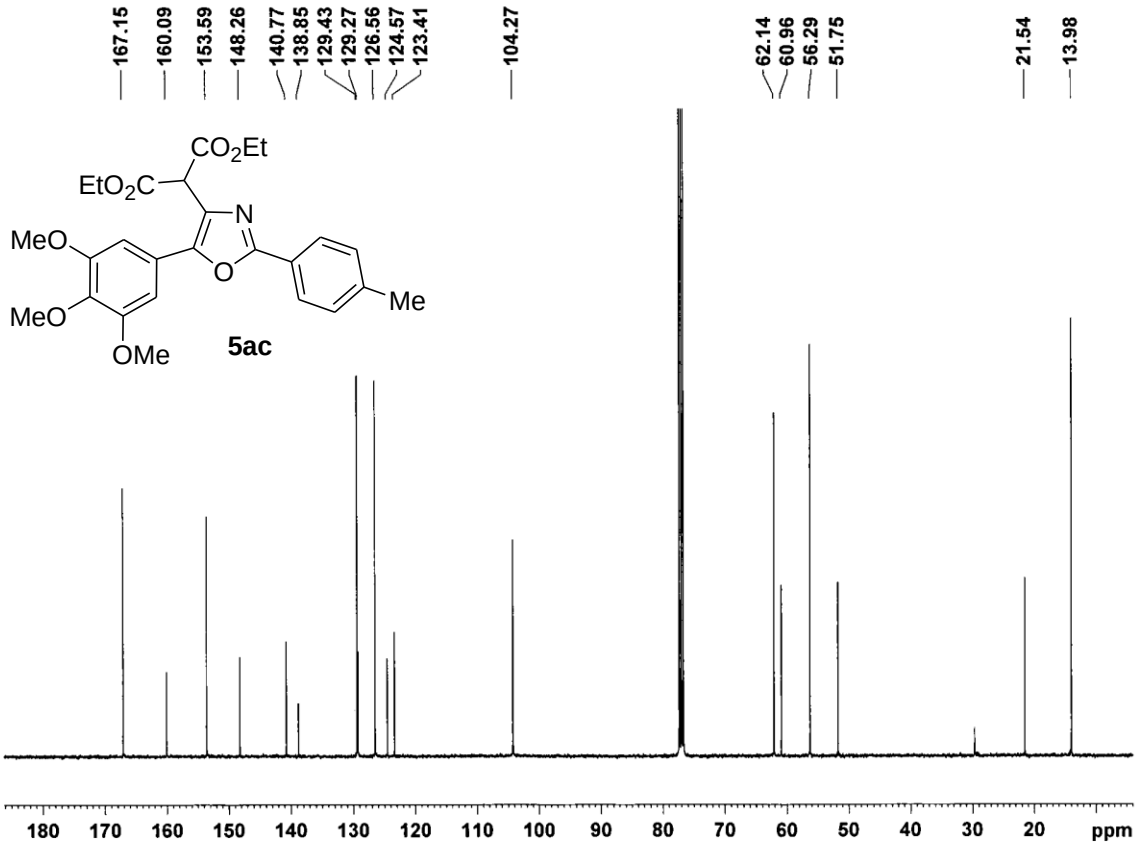
7.970
7.273
7.253
6.936
4.962
4.259
4.250
4.242
4.232
4.224
4.214
4.206
4.197
4.189
4.180
3.929
3.892
2.408
1.241
1.224
1.206
CO2Et
EtO2C
N
MeO
O
MeO
Me
OMe
5ac
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.03
2.19
2.03
0.95
4.04
6.03
3.00
3.07
6.09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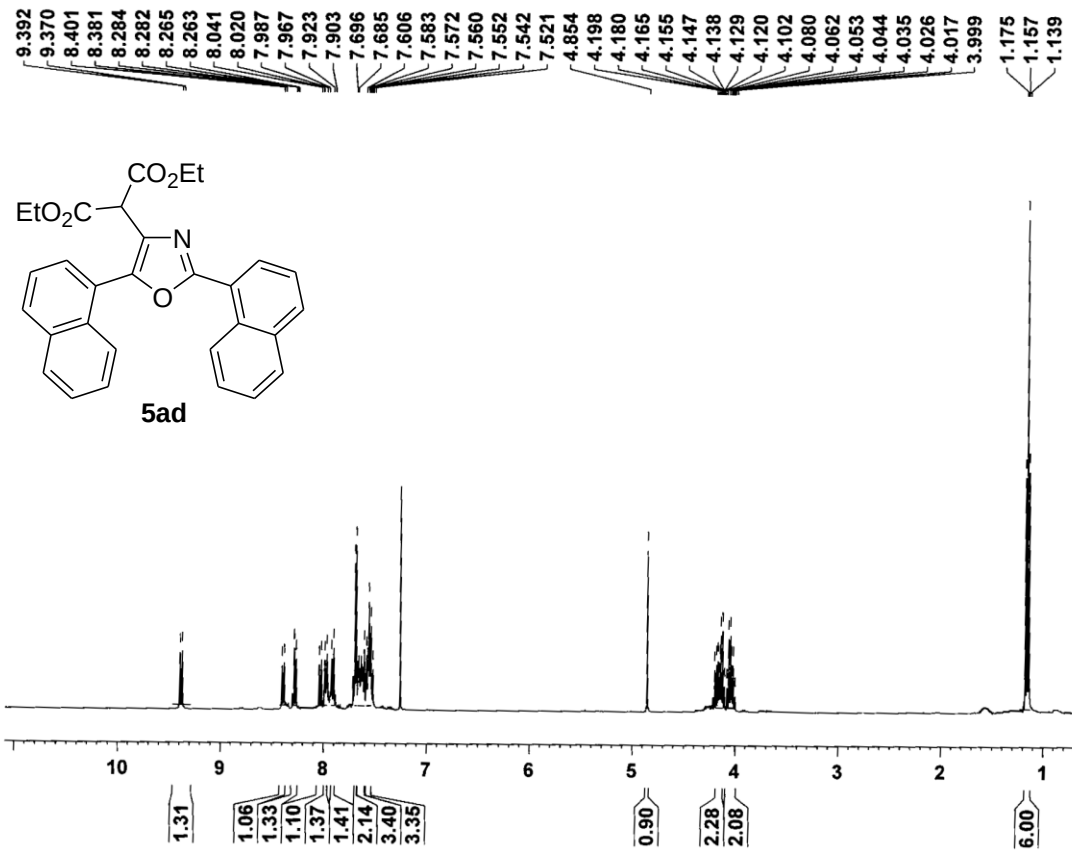
153.59
148.26
140.77
138.85
129.43
129.27
126.56
124.57
123.41
104.27
62.14
60.96
56.29
51.75
21.54
13.98
CO2Et
EtO2C
N
MeO
O
MeO
Me
OMe
5ac
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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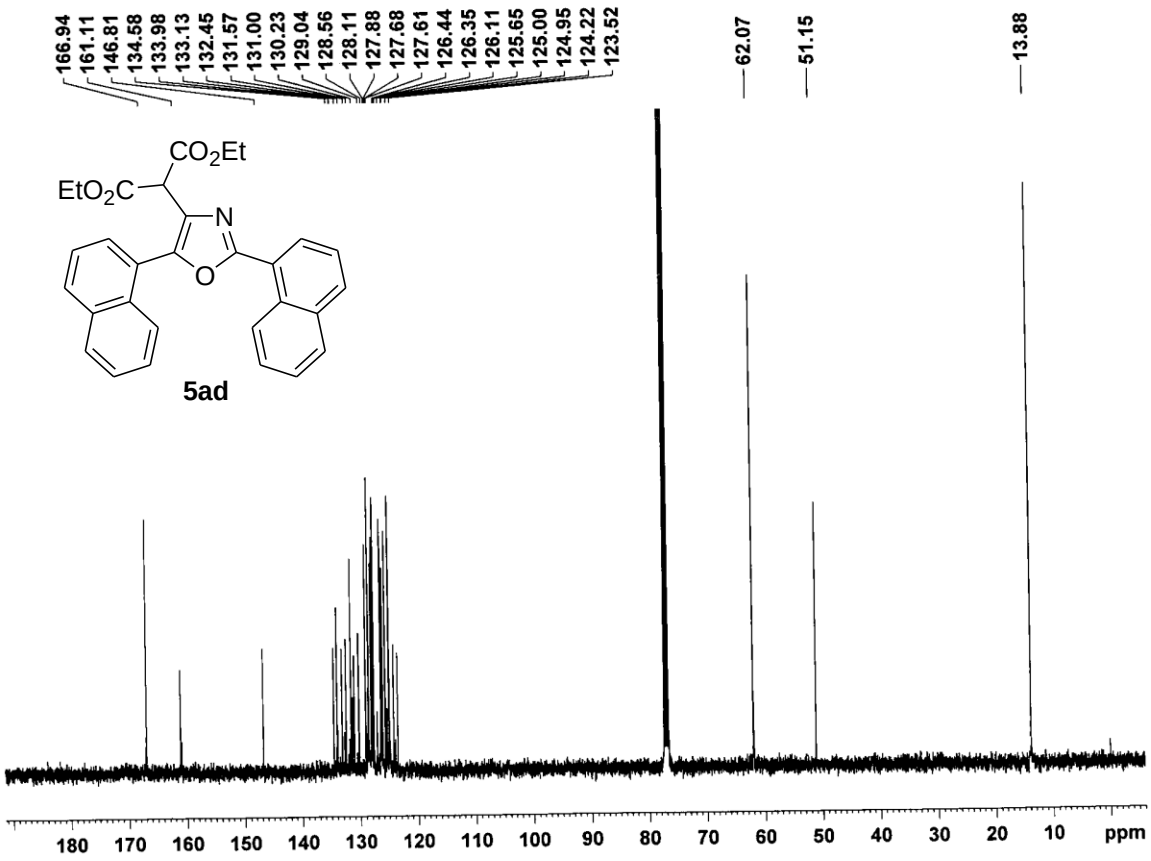
8.263
8.041
8.020
7.987
7.967
7.923
7.903
7.696
7.685
7.606
7.583
7.572
7.560
7.552
7.542
7.521
4.854
4.198
4.180
4.165
4.155
4.147
4.138
4.129
4.120
4.102
4.080
4.062
4.053
4.044
4.035
4.026
4.017
3.999
1.175
1.157
1.139
CO2Et
EtO2C
N
O
5ad
10
9
8
7
6
5
4
3
2
1
ppm
1.31
1.06
1.33
1.10
1.37
1.41
2.14
3.40
3.35
0.90
2.28
2.08
6.00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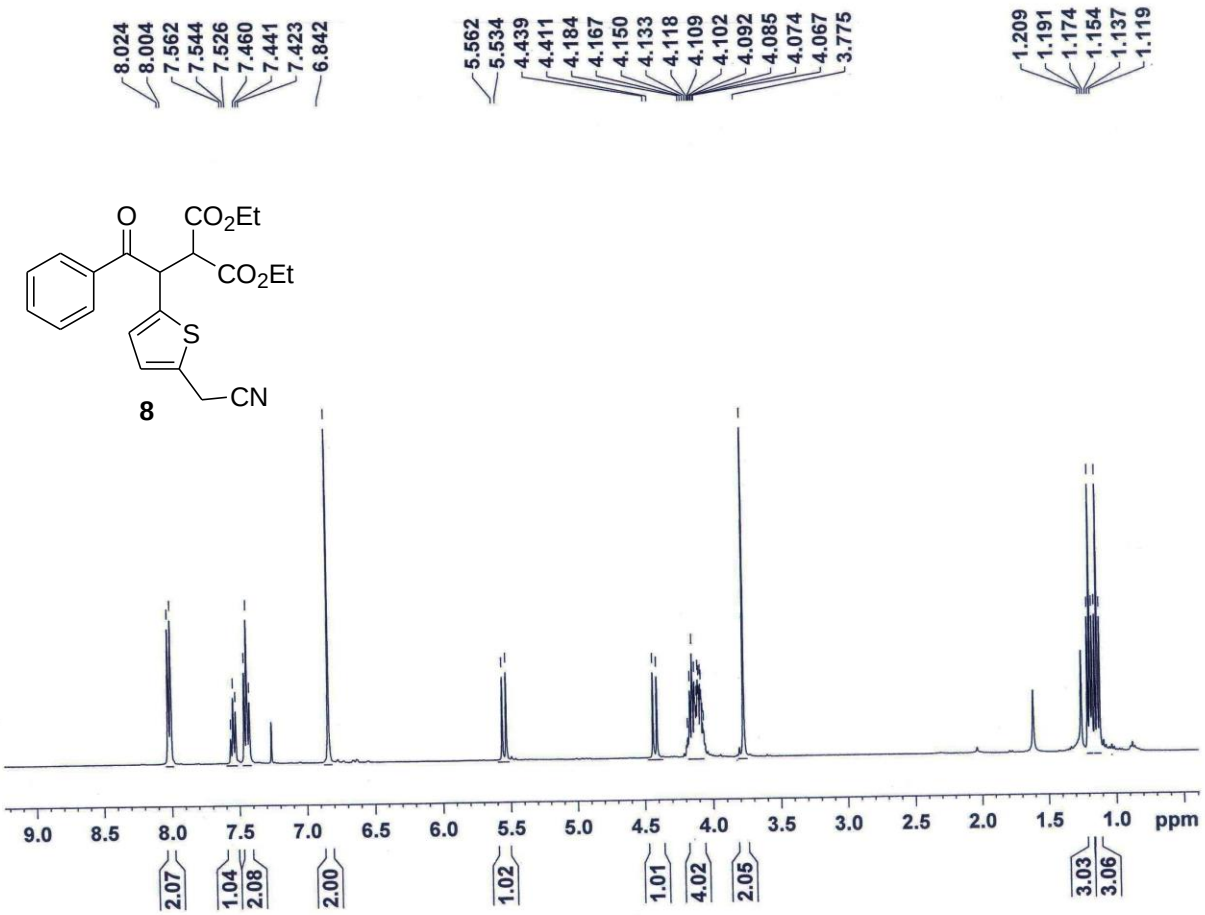
131.00
130.23
129.04
128.56
128.11
127.88
127.68
127.61
126.44
126.35
126.11
125.65
125.00
124.95
124.22
123.52
62.07
51.15
13.88
CO2Et
EtO2C
N
O
5ad
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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5.534
4.439
4.411
4.184
4.167
4.150
4.133
4.118
4.109
4.102
4.092
4.085
4.074
4.067
3.775
1.209
1.191
1.174
1.154
1.137
1.119
O
CO2Et
CO2Et
S
CN
8
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
ppm
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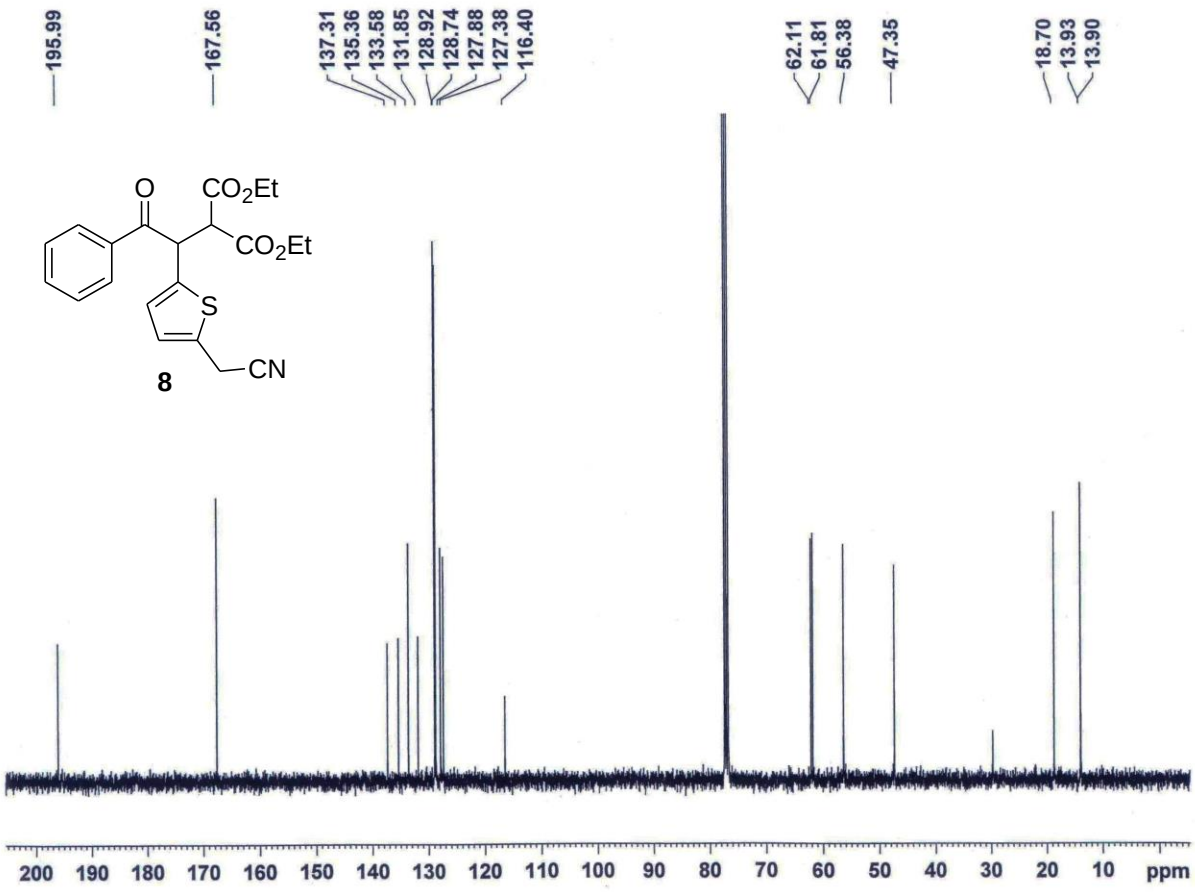
1.04
2.08
2.00
1.02
1.01
4.02
2.05
3.03
3.06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135.36
133.58
131.85
128.92
128.74
127.88
127.38
116.40
62.11
61.81
56.38
47.35
18.70
13.93
13.90
O
CO2Et
CO2Et
S
CN
8
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm