Supporting Information

Synthesis of Functionalized α-Pyrone and Butenolide Derivatives by Rhodium-Catalyzed Oxidative Coupling of Substituted Acrylic Acids with Alkynes and Alkenes

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List of Contents for Experimental Section

General: S2

Characterization Data of Products: S2 – S5

Figure S1: S6

References: S6

^{1}H and ^{13}C NMR Spectra of Products: S7 – S30

Experimental Section

General. ^{1}H and ^{13}C NMR spectra were recorded at 400 and 100 MHz, respectively, for $CDCl_3$ solutions. MS data were obtained by EI, unless noted. GC analysis was carried out using a silicon OV-17 column (i. d. 2.6 mm x 1.5 m) or a CBP-1 capillary column (i. d. 0.5 mm x 25 m). GC-MS analysis was carried out using a CBP-1 capillary column (i. d. 0.25 mm x 25 m). The structures of all products listed below were unambiguously determined by ^{1}H and ^{13}C NMR with the aid of NOE, COSY, HMQC, and HMBC experiments.

2-Arylacrylic acids **1b**-**d**[10,11] and diarylacetylenes **2b**-**e**[12] were prepared according to published procedures. Other starting materials were commercially available.

Characterization Data of Products.

3-Methyl-5,6-diphenyl-2*H*-pyran-2-one (3a):[3a] mp 124-126 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.19 (d, *J* = 1.1 Hz, 3H), 7.16-7.35 (m, 11H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.4, 117.9, 123.7, 127.7, 128.0, 128.9, 129.1, 129.2, 129.5, 132.2, 136.6, 144.0, 155.4, 163.1; HRMS *m/z* Calcd for $C_{18}H_{14}O_2$ (M^+) 262.0994. Found 262.0996.

3-Methyl-5,6-bis(4-methylphenyl)-2*H*-pyran-2-one (3b): mp 114-116 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.21 (s, 3H), 2.33 (s, 3H), 2.38 (s, 3H) 7.05- 7.11 (m, 4H) 7.14 (d, *J* = 8.1 Hz, 2H), 7.27-7.29 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.4, 21.1, 21.3 117.4, 123.1, 128.7, 128.8, 128.9, 129.4, 129.5, 133.7, 137.4, 139.6, 144.3, 155.3, 163.2; MS *m/z* 290 (M^+). Anal. Calcd for $C_{20}H_{18}O_2$: C, 82.73; H, 6.25. Found: C, 82.58; H, 6.06.

5,6-Bis(4-methoxyphenyl)-3-methyl-2*H*-pyran-2-one (3c): mp 98-100 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.16 (d, *J* = 1.1Hz, 3H), 3.78 (s, 3H) 3.81 (s, 3H), 6.73 (d, *J* = 9.2 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 7.08 (d, *J* = 8.8 Hz, 2H), 7.22 (s, 1H) 7.29 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.4, 55.22, 55.26, 113.5, 114.3, 116.6, 122.6, 124.8, 129.1, 130.3, 130.5, 144.5, 155.1, 159.1, 160.4, 163.3; MS *m/z* 322 (M^+). Anal. Calcd for $C_{20}H_{18}O_4$: C, 74.52; H, 5.63. Found: C, 74.34; H, 5.62.

5,6-Bis(4-chlorophenyl)-3-methyl-2*H*-pyran-2-one (3d): mp 119-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (d, *J* = 1.1 Hz, 3H) 7.09 (d, *J* = 8.4 Hz, 2H), 7.20-7.32 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.5, 117.0, 124.4, 128.6, 129.3, 130.2, 130.3, 130.4, 134.1, 134.7, 135.9, 143.2, 154.3, 162.5; MS *m/z* 330, 332, 334 (M^+). Anal. Calcd for $C_{18}H_{12}Cl_2O_2$: C, 65.28; H, 3.65; Cl, 21.41. Found: C, 65.25; H, 3.66; Cl, 21.56.

3-Methyl-5,6-bis(2-thienyl)-2*H*-pyran-2-one (3e): mp 158-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) 2.14 (s, 3H), 6.95 (t, *J* = 5.0 Hz, 1H) 7.04-7.05 (d, *J* = 3.6 Hz, 1H), 7.11 (t, *J* = 4.0 Hz, 1H), 7.15 (s, 1H), 7.31 (d, *J* = 5.1 Hz, 1H), 7.35 (d, *J* = 4.0 Hz, 1H), 7.47 (d, *J* = 5.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 16.3, 109.1, 122.3 127.1, 127.7, 127.8, 128.8, 129.5, 129.7, 133.9, 136.3, 144.0, 152.0, 161.9; MS *m/z* 274 (M^+). Anal. Calcd for $C_{14}H_{10}O_2S_2$: C, 61.29; H, 3.67; S, 23.37. Found: C, 61.01; H, 3.58; S, 23.31.

3-Methyl-5,6-dipropyl-2*H*-pyran-2-one (3f): oil; ^{1}H NMR (400 MHz, $CDCl_3$) 0.92-0.98 (m, 6H), 1.46-1.55 (m, 2H), 1.63-1.72 (m, 2H), 2.07 (s, 3H), 2.22 (t, *J* = 7.7 Hz, 2H), 2.43 (t, *J* = 7.7 Hz, 2H), 6.97 (d, *J* = 1.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 13.5, 13.6, 16.3, 21.1, 23.3, 31.2, 32.2, 115.0, 122.5, 143.2, 158.8, 164.2; HRMS *m/z* Calcd for $C_{12}H_{18}O_2$ (M^+) 194.1307. Found 194.1304.

5,6-Diheptyl-3-methyl-2*H*-pyran-2-one (3g): oil; ^{1}H NMR (400 MHz, $CDCl_3$) 0.87-0.91 (m, 6H), 1.30 (m, 16H), 1.46-1.47 (m, 2H), 1.62-1.66 (m, 2H), 2.06 (s, 3H) 2.23 (t, *J* = 7.7 Hz, 2H), 2.44 (t, *J* = 7.4 Hz, 2H), 6.97 (d, *J* = 1.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 13.9 (overlapped), 16.2, 22.5 (overlapped), 27.7, 28.9, 29.0, 29.1, 29.16, 29.18, 30.2, 30.3, 31.6, 31.7, 115.0, 122.3, 143.1, 158.9, 164.1; HRMS *m/z* Calcd for $C_{20}H_{34}O_2$ (M^+) 306.2559. Found 306.2563.

3,5-Dimethyl-6-phenyl-2*H*-pyran-2-one (3h): mp 98-100 °C; ^{1}H NMR (400 MHz, $CDCl_3$) 2.14 (s, 6H), 7.11 (s, 1H) 7.41-7.45 (m, 3H), 7.55-7.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 16.3, 16.7, 111.3, 123.8, 128.3, 128.6, 129.4, 132.6, 144.7, 154.9, 163.5; HRMS *m/z* Calcd for $C_{13}H_{12}O_2$ (M^+) 200.0837. Found 200.0839.

5-Butyl-3-methyl-6-phenyl-2*H*-pyran-2-one (3i): mp 68-70 °C; ^{1}H NMR (400 MHz, $CDCl_3$) 0.87 (t, *J* = 7.3 Hz, 3H) 1.28-1.33 (m, 2H) 1.48-1.56 (m, 2H) 2.15 (d, *J* = 1.1 Hz, 3H) 2.40 (t, *J* = 7.7 Hz, 2H), 7.15 (d, *J* = 1.4 Hz, 1H), 7.41-7.44 (m, 3H), 7.49-7.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 13.7, 16.5, 22.2, 29.1, 32.2, 116.3, 124.1, 128.2, 128.6, 129.3, 132.5, 143.1, 155.3, 163.5 ; MS *m/z* 242 (M^+). Anal. Calcd for $C_{16}H_{18}O_2$: C, 79.31; H, 7.49. Found: C, 79.33; H, 7.47.

6-Butyl-3-methyl-5-phenyl-2*H*-pyran-2-one (3i'): mp 60-62 °C; ^{1}H NMR (400 MHz, $CDCl_3$) 0.83 (t, *J* = 7.3 Hz 3H) 1.24-1.30 (m, 2H) 1.57- 1.66 (m, 2H) 2.11 (d, *J* = 1.1Hz, 3H) 2.48 (t, *J* = 7.7 Hz, 2H), 7.11 (d, *J* = 1.1 Hz, 1H), 7.21-7.26 (m, 2H), 7.36-7.43 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) 13.6, 16.3, 22.2, 29.8, 30.8, 117.9, 122.3, 127.7, 128.6, 128.8, 136.3, 143.1, 160.1, 163.8; HRMS *m/z* Calcd for $C_{16}H_{18}O_2$ (M^+) 242.1307. Found 242.1311.

3,5,6-Triphenyl-2*H*-pyran-2-one (3j):[3a] mp 143-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) 7.23-7.45 (m, 13H), 7.61 (s, 1H), 7.75-7.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 118.5, 125.6, 127.9, 128.1, 128.2, 128.4, 128.6, 128.9, 129.1, 129.2, 129.8, 131.9, 134.4,

136.4, 144.2, 156.7, 161.1; HRMS *m/z* Calcd for $C_{23}H_{16}O_2$ (M^+) 324.1150. Found 324.1154.

3-(4-Methoxyphenyl)-5,6-diphenyl-2*H*-pyran-2-one (3k): mp 172-173 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.84 (s, 3H), 6.96 (d, *J* = 8.8 Hz, 2H), 7.23-7.41 (m, 10H), 7.55 (s, 1H), 7.73 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.3, 113.9, 118.6, 125.2, 126.8, 127.9, 128.1, 128.9, 129.1, 129.3, 129.5, 129.7, 132.0, 136.6, 142.9, 156.0, 160.0, 161.4; HRMS *m/z* Calcd for $C_{24}H_{18}O_3$ (M^+) 354.1256. Found 354.1259.

3-(4-Chlorophenyl)-5,6-diphenyl-2*H*-pyran-2-one (3l): mp 160-161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23-7.41 (m, 12H), 7.60 (s, 1H), 7.71 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.6, 124.3, 128.0, 128.2, 128.7, 129.0, 129.16, 129.22, 129.5, 130.0, 131.8, 132.8, 134.6, 136.3, 144.3, 157.1, 160.9; HRMS *m/z* Calcd for $C_{23}H_{15}ClO_2$ (M^+) 358.0761. Found 358.0768.

2-Oxo-5,6-diphenyl-2*H*-pyran-3-carboxylic acid (3m): mp 179-181 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 2H), 7.28-7.36 (m, 11H), 7.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 35.4, 118.1, 119.5, 127.9, 128.1, 128.9, 129.1, 129.2, 129.9, 131.7, 135.9, 146.5, 157.1, 162.5, 174.7; MS *m/z* 306 (M^+). Anal. Calcd for $C_{19}H_{14}O_4$: C, 74.50; H, 4.61. Found: C, 74.29; H, 4.54.

Butyl 2-Oxo-5,6-diphenyl-2*H*-pyran-3-carboxylate (3n): oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.93 (t, *J* = 7.3 Hz, 3H), 1.34-1.44 (m, 2H), 1.61-1.68 (m, 2H), 3.56 (s, 2H), 4.15 (t, *J* = 6.6 Hz, 2H), 7.17-7.42 (m, 11H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.6, 19.0, 30.5, 35.3, 65.1, 117.9, 120.3, 127.8, 128.1, 128.8, 129.1, 129.2, 129.8, 131.9, 136.2, 145.9, 156.7, 162.1, 170.1; HRMS *m/z* Calcd for $C_{23}H_{22}O_4$ (M^+) 362.1518. Found 362.1526.

5,6-Diphenyl-2*H*-pyran-2-one (3o):[13] mp 85-88 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.37 (d, *J* = 9.6 Hz, 1H), 7.15-7.38 (m, 10H), 7.46 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 114.0, 117.8, 127.9, 128.1, 128.9, 129.1, 129.2, 129.9, 132.0, 136.1, 147.8, 158.0, 161.7; HRMS *m/z* Calcd for $C_{17}H_{12}O_2$ (M^+) 248.0837. Found 248.0833.

3,4-Dimethyl-5,6-diphenyl-2*H*-pyran-2-one (3p):[3a] mp 117-119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.91 (s, 3H), 2.18 (s, 3H) 7.10-7.23 (m, 7H), 7.33-7.35 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.1, 18.1, 120.2 (overlapped), 127.7, 127.8, 128.8, 128.9 (overlapped), 130.7, 132.7, 135.6, 150.7, 153.9, 163.0; MS *m/z* 276 (M^+). Anal. Calcd for $C_{19}H_{16}O_2$: C, 82.58; H, 5.84. Found: C, 82.37; H, 5.55.

3,4,5,6-Tetraphenyl-2*H*-pyran-2-one (3q):[3a] mp 163-165 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.71-6.74 (m, 2H), 6.85-6.88 (m, 2H), 6.91-7.27 (m, 14H), 7.31-7.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 119.6, 125.1, 127.2, 127.3 (overlapped), 127.7, 127.8, 128.1, 129.3, 129.4, 130.6, 131.4, 132.7, 134.2, 135.0, 136.2, 155.3, 156.6, 162.2;

HRMS *m/z* Calcd for $C_{29}H_{20}O_2$ (M^+) 400.1463. Found 400.1464.

3,4-Diphenyl-5,6,7,8-tetrahydroisocoumarin (3r): mp 162-164 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) 1.61-1.67 (m, 2H), 1.71-1.76 (m, 2H), 2.13-2.16 (m, 2H), 2.58-2.61 (m, 2H), 7.10-7.35 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) 21.3, 21.7, 23.8, 28.6, 119.5, 121.5, 127.7, 127.8, 128.7, 128.88, 128.91, 130.6, 132.6, 134.8, 151.7, 153.5, 162.7; HRMS *m/z* Calcd for $C_{21}H_{18}O_2$ (M^+) 302.1307. Found 302.1305.

Butyl 2,5-Dihydro-4-methyl-5-oxo-2-furanacetate (5a): oil; ^{1}H NMR (400 MHz, $CDCl_3$) 0.94 (t, *J* = 7.3 Hz, 3H), 1.35-1.41 (m, 2H), 1.59-1.66 (m, 2H), 1.92-1.93 (t, *J* = 1.5 Hz, 3H), 2.59 (dd, *J* = 16.1, 7.0 Hz, 1H), 2.79 (dd, *J* = 16.1, 7.0 Hz, 1H) 4.13 (t, *J* = 7.0 Hz, 2H), 5.24-5.28 (m, 1H), 7.16-7.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 10.5, 13.5, 19.0, 30.5, 38.2, 65.0, 76.7, 130.6, 147.6, 169.1, 173.4; HRMS *m/z* Calcd for $C_{11}H_{16}O_4$ (M^+) 212.1049. Found 212.1046.

Cyclohexyl 2,5-Dihydro-4-methyl-5-oxo-2-furanacetate (5b): oil; ^{1}H NMR (400 MHz, $CDCl_3$) 1.25-1.94 (m, 13H), 2.57 (dd, *J* = 16.1, 7.3 Hz, 1H), 2.78 (dd, *J* = 16.1, 7.0 Hz, 1H), 4.78-4.83 (m, 1H), 5.23-5.28 (m, 1H), 7.15-7.16 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 10.6, 23.6, 25.2, 31.5, 38.5, 73.7, 76.8, 130.6, 147.7, 168.5, 173.5; HRMS *m/z* Calcd for $C_{13}H_{18}O_4$ (M^+) 238.1205. Found 238.1210.

***tert*-Butyl 2,5-Dihydro-4-methyl-5-oxo-2-furanacetate (5c):** oil; ^{1}H NMR (400 MHz, $CDCl_3$) 1.46 (s, 9H), 1.92 (t, *J* = 1.5 Hz, 3H), 2.50 (dd, *J* = 16.1, 7.0 Hz, 1H), 2.71 (dd, *J* = 16.1, 6.6 Hz, 1H), 5.18-5.23 (m, 1H), 7.14-7.15 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 10.5, 28.0, 39.3, 77.0, 81.8, 130.5, 147.8, 168.3, 173.5; HRMS (CI) *m/z* Calcd for $C_{11}H_{17}O_4$ (M+H) 213.1127. Found 213.1120.

Butyl 2,5-Dihydro-3,4-dimethyl-5-oxo-2-furanacetate (5d): oil; ^{1}H NMR (400 MHz, $CDCl_3$) 0.93 (t, *J* = 7.3 Hz, 3H), 1.35-1.41 (m, 2H), 1.58-1.65 (m, 2H), 1.82 (s, 3H), 1.98 (s, 3H), 2.53 (dd, *J* = 16.1, 8.0 Hz, 1H), 2.79 (dd, *J* = 16.1, 4.4 Hz, 1H), 4.13 (t, *J* = 6.6 Hz, 2H), 5.13-5.17 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 8.3, 11.7, 13.5, 18.9, 30.4, 37.4, 64.9, 79.1, 124.1, 157.7, 169.2, 173.6; HRMS (CI) *m/z* Calcd for $C_{12}H_{19}O_4$ (M+H) 227.1283. Found 227.1292.

Butyl 2,5-Dihydro-4-methyl-5-oxo-3-phenyl-2-furanacetate (5e): oil; ^{1}H NMR (400 MHz, $CDCl_3$) 0.91 (t, *J* = 7.3 Hz, 3H), 1.31-1.37 (m, 2H), 1.53-1.61 (m, 2H), 2.05 (d, *J* = 1.8 Hz, 3H), 2.42 (dd, *J* = 16.1, 9.2 Hz, 1H), 2.71 (dd, *J* = 16.1, 3.6 Hz, 1H), 4.07 (t, *J* = 6.6 Hz, 2H), 5.75-5.79 (m, 1H), 7.35-7.52 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) 10.0, 13.6, 18.9, 30.5, 38.4, 65.0, 77.9, 124.4, 127.8, 129.1, 130.0, 130.8, 158.1, 169.4, 173.7; HRMS (CI) *m/z* Calcd for $C_{17}H_{21}O_4$ (M+H) 289.1440. Found 289.1437.

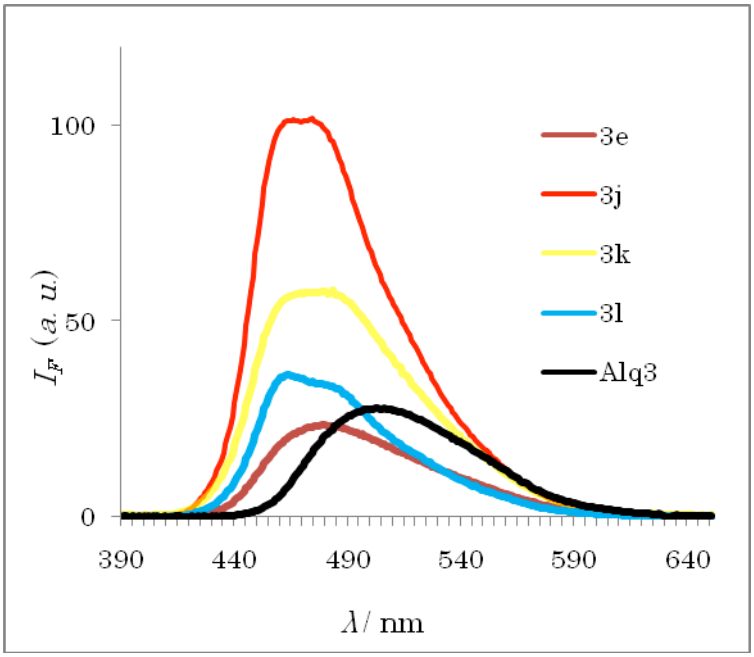

FIGURE S1. Fluorescence spectra of **3e**,**j**-**l** and Alq_3 in the solid state upon excitation at 380 nm.

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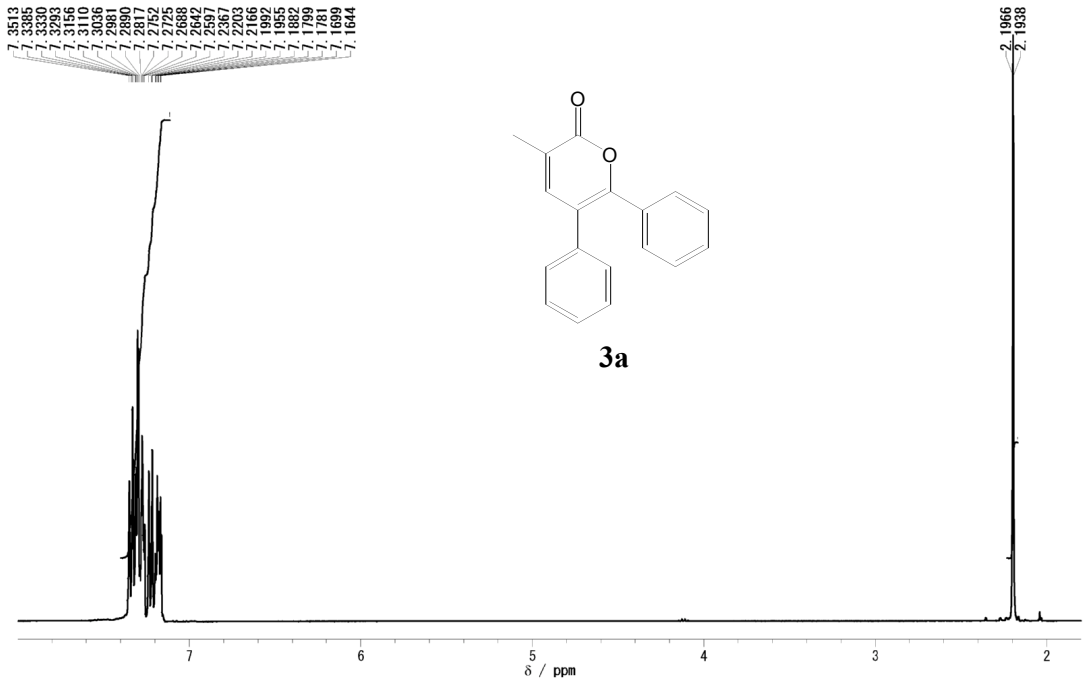
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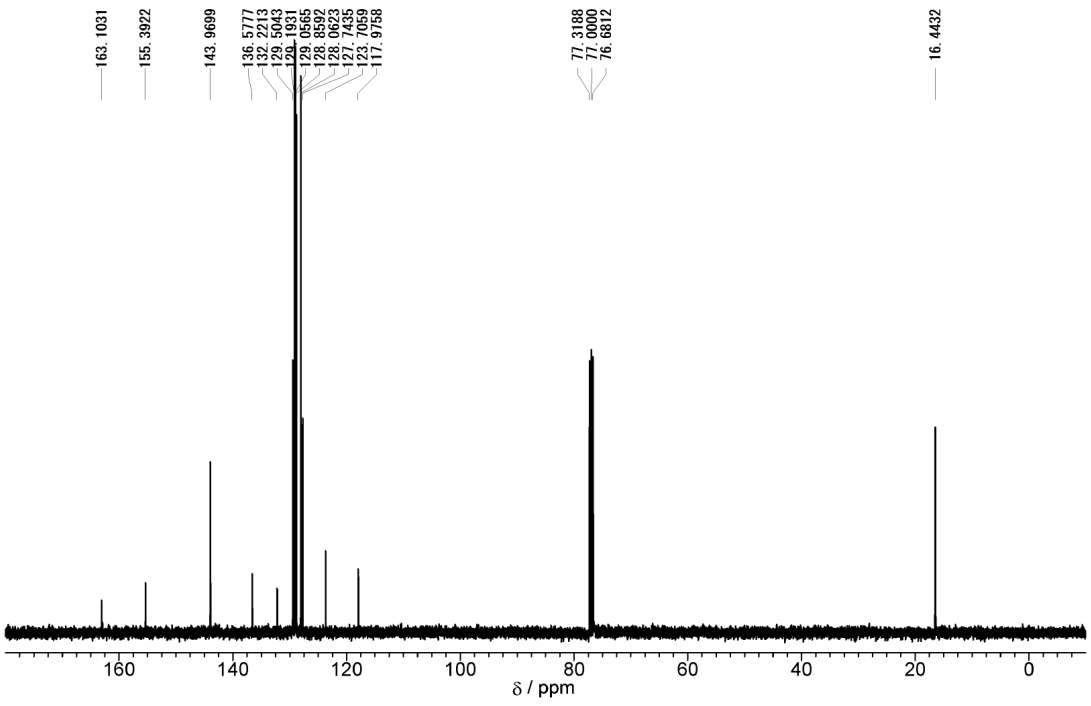
3a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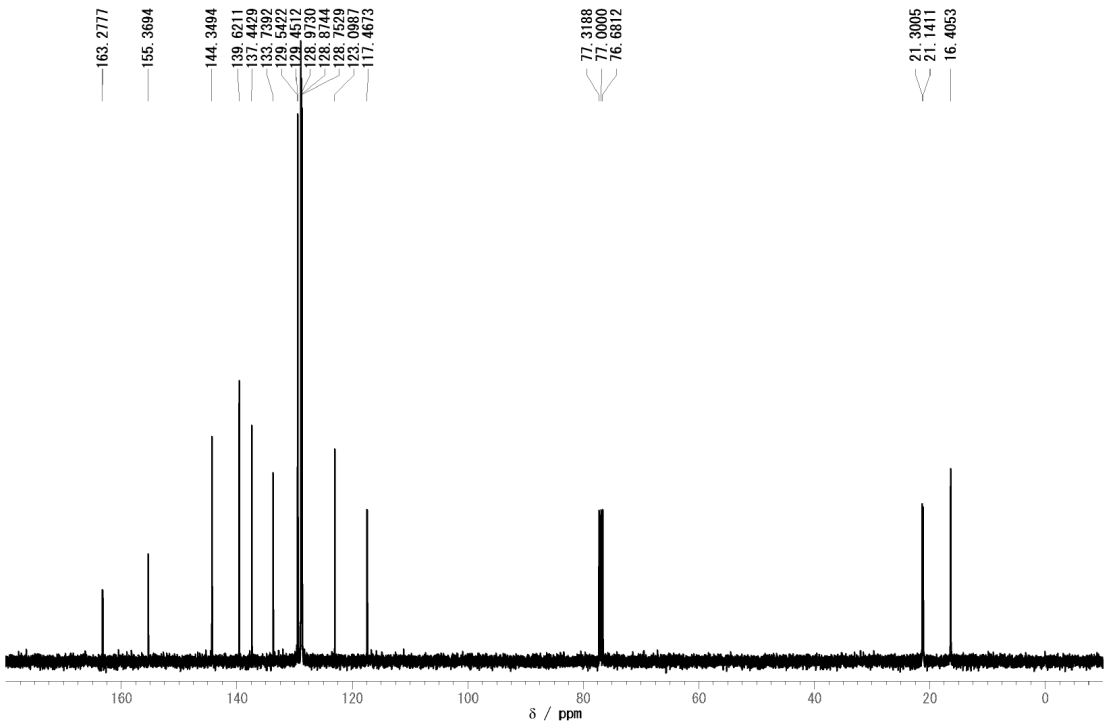
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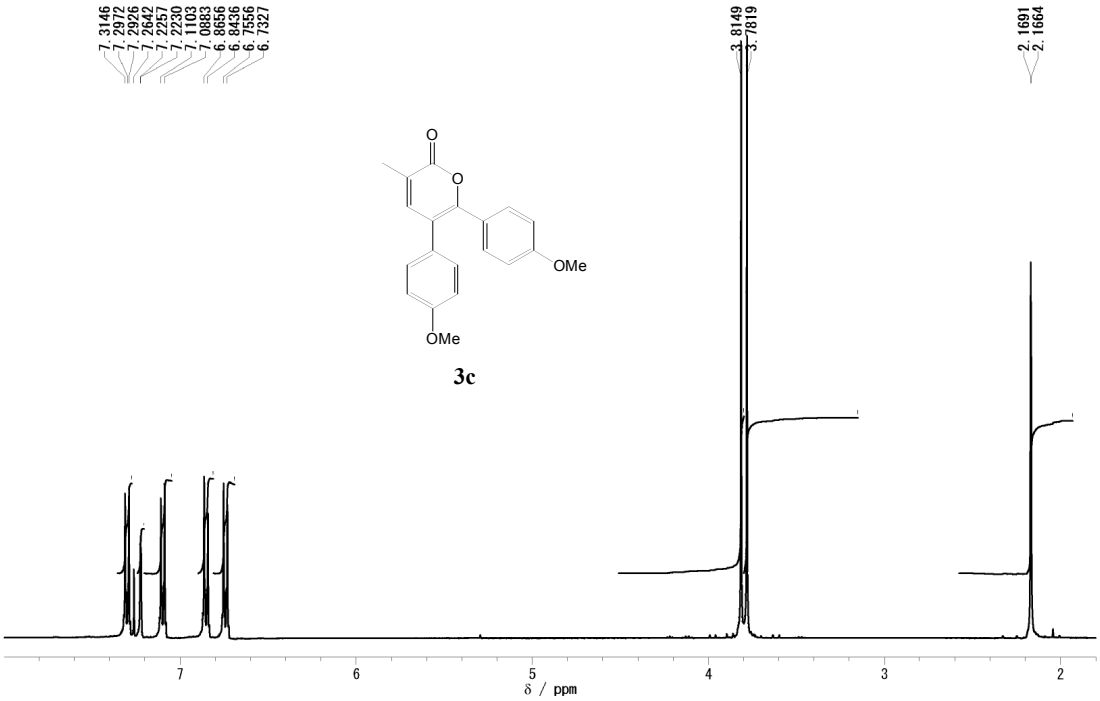
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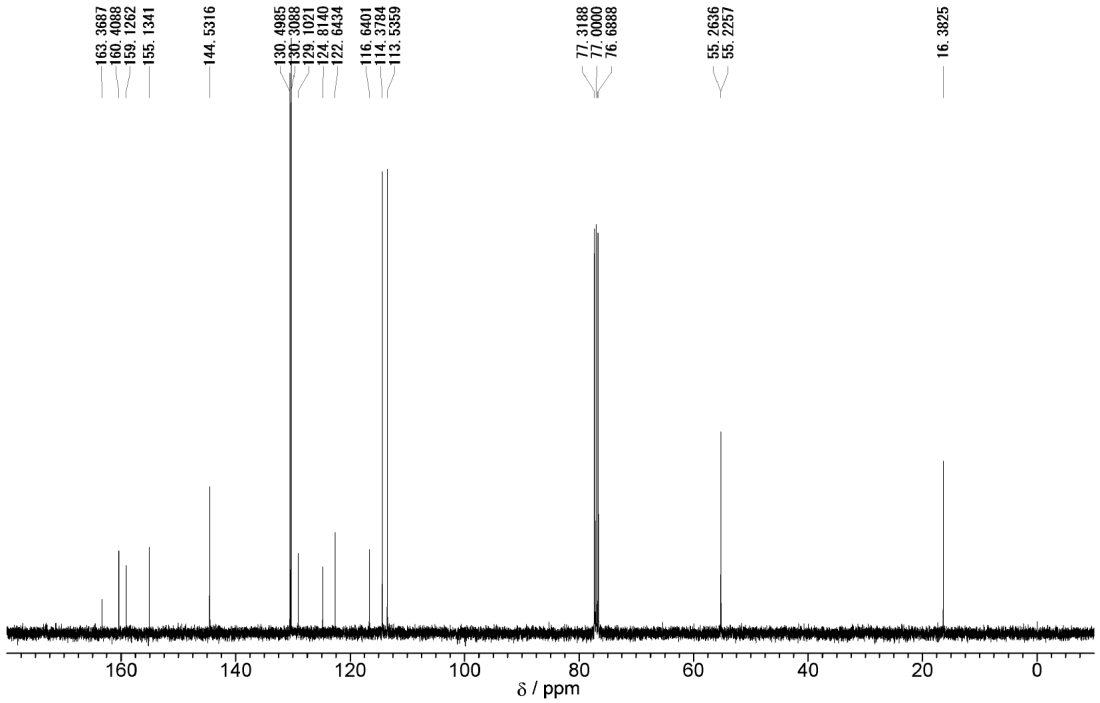
δ / ppm

3c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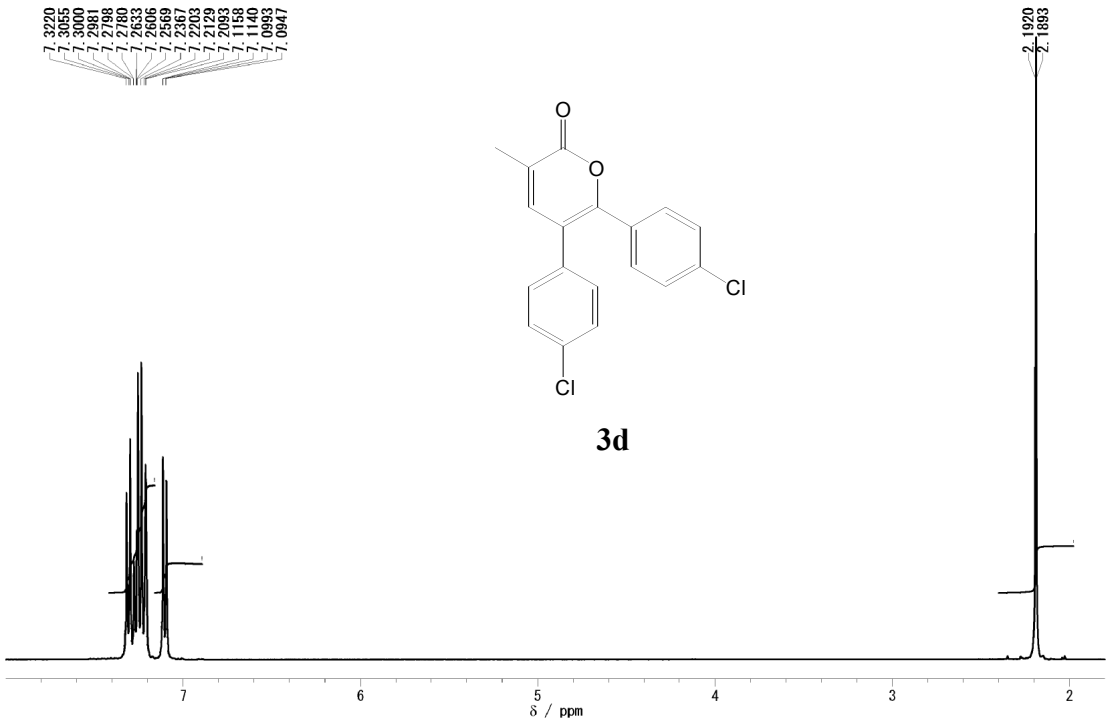
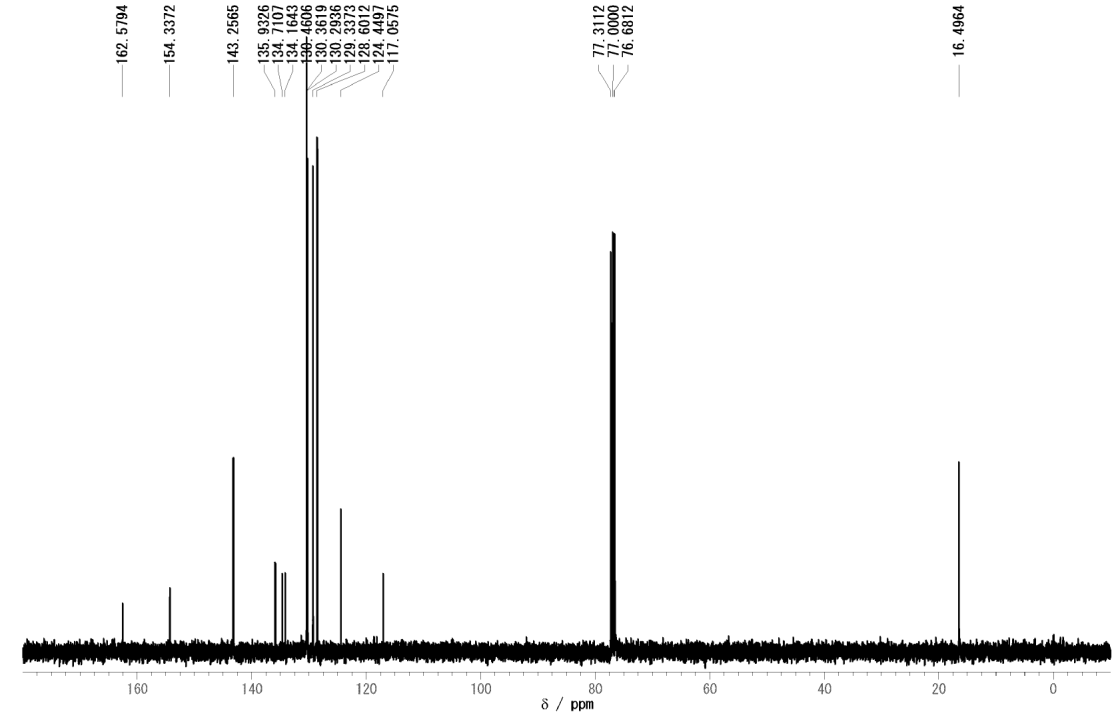
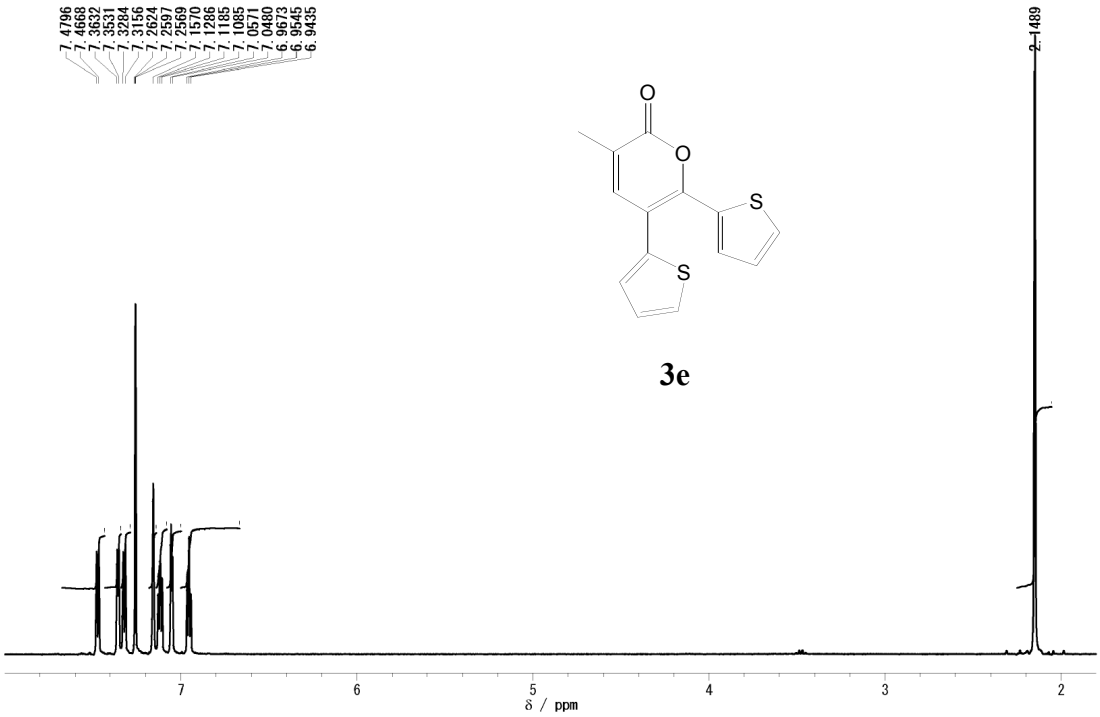
159.1262
155.1341
144.5316
130.4985
130.3088
129.1021
124.8140
122.6434
116.6401
114.3784
113.5359
77.3188
77.0000
76.6888
55.2636
55.2257
16.3825
160
140
120
100
80
60
40
20
0
δ / ppm


7.3220
7.3055
7.3000
7.2981
7.2798
7.2780
7.2633
7.2606
7.2569
7.2367
7.2203
7.2129
7.2093
7.1158
7.1140
7.0993
7.0947
2.1920
2.1893
O
O
Cl
Cl
7
6
5
4
3
2
δ / ppm

3d


162.5794
154.3372
143.2565
135.9326
134.7107
134.1643
130.4606
130.3619
130.2936
129.3373
128.6012
124.4497
117.0575
77.3112
77.0000
76.6812
16.4964
160
140
120
100
80
60
40
20
0
δ / ppm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7.3632
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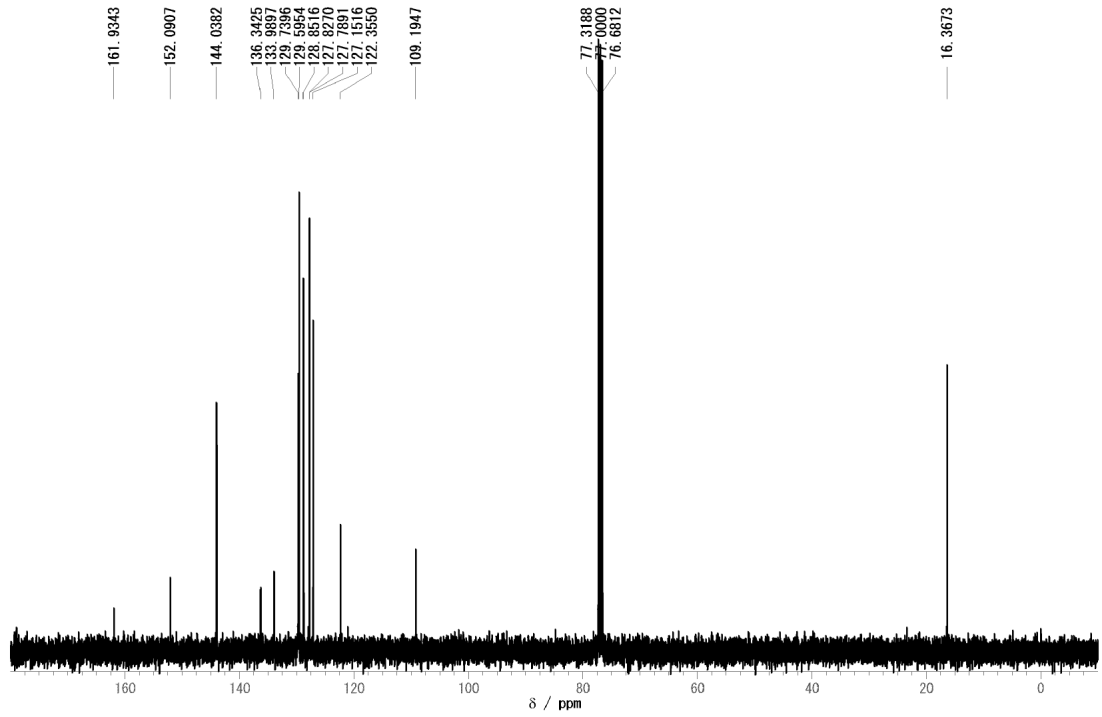
7.3284
7.3156
7.2624
7.2597
7.2569
7.1570
7.1286
7.1185
7.1085
7.0571
7.0480
6.9673
6.9545
6.9435
2.1489
O
O
S
S
7
6
5
4
3
2
δ / ppm

3e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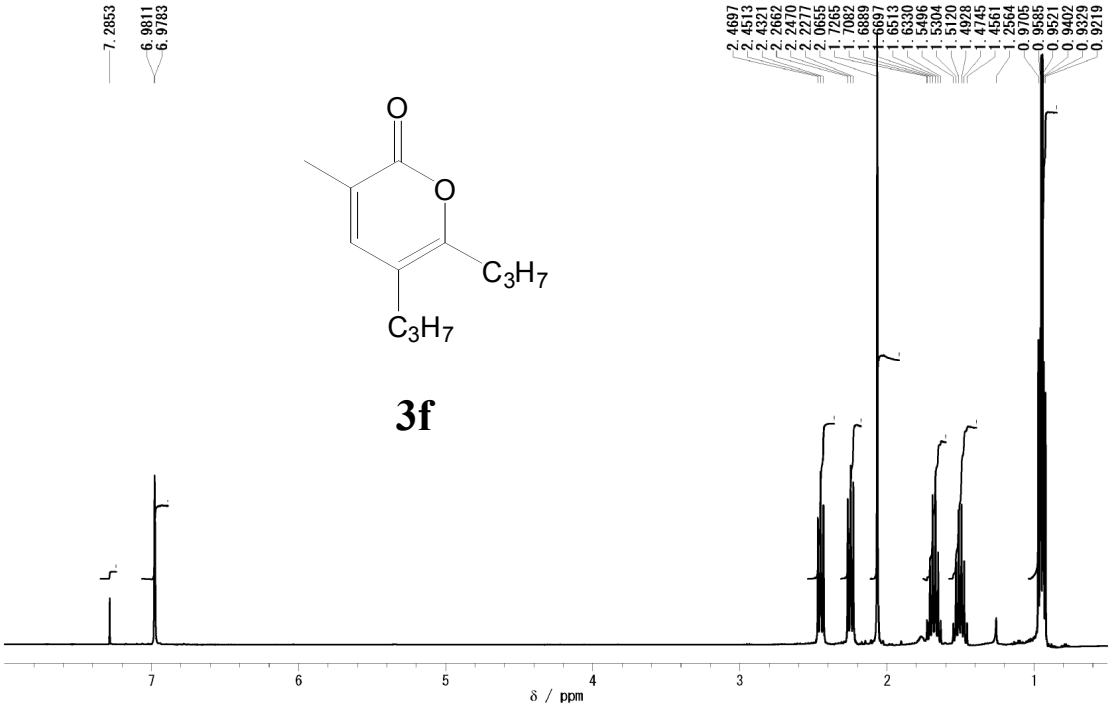
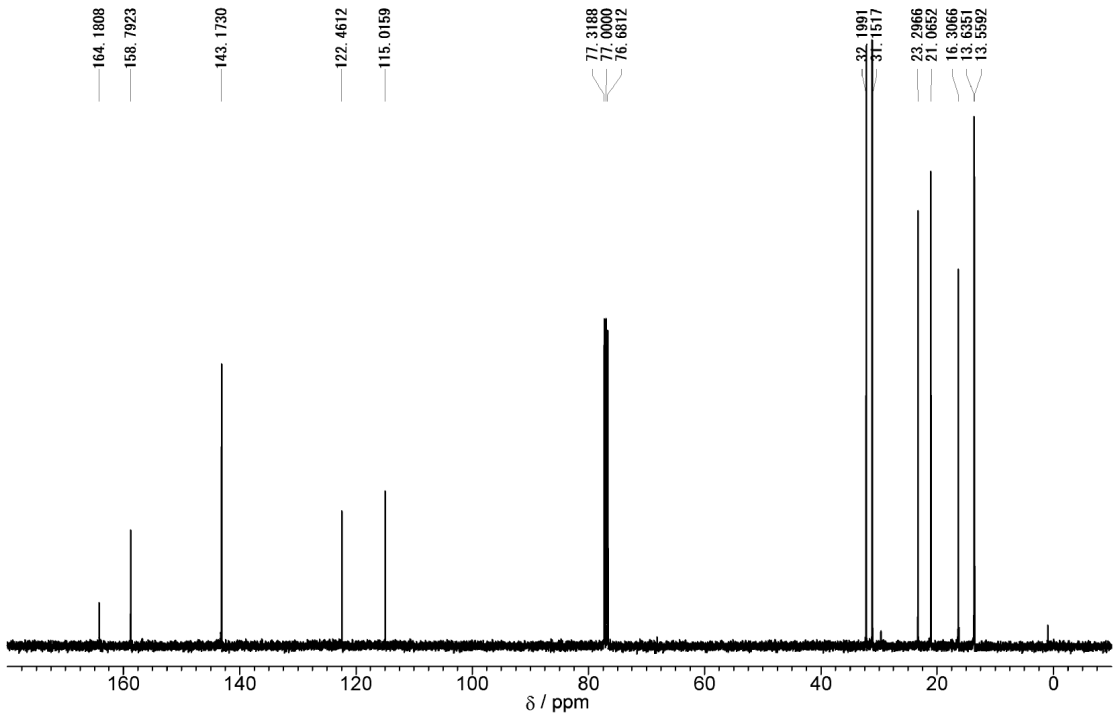
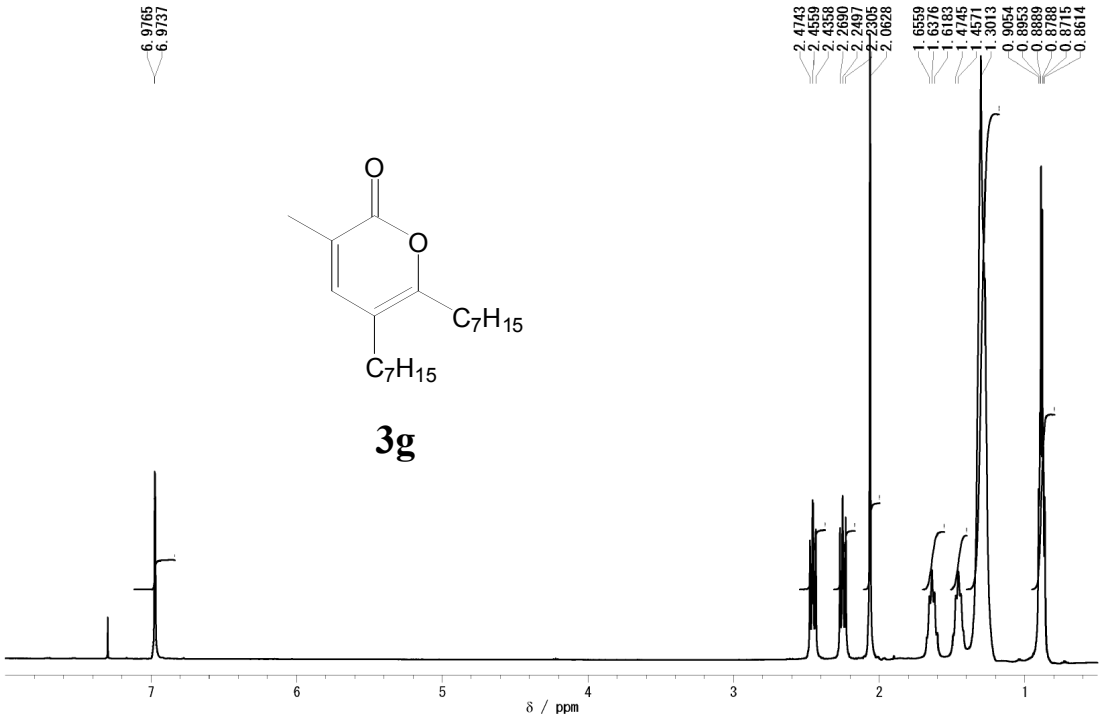
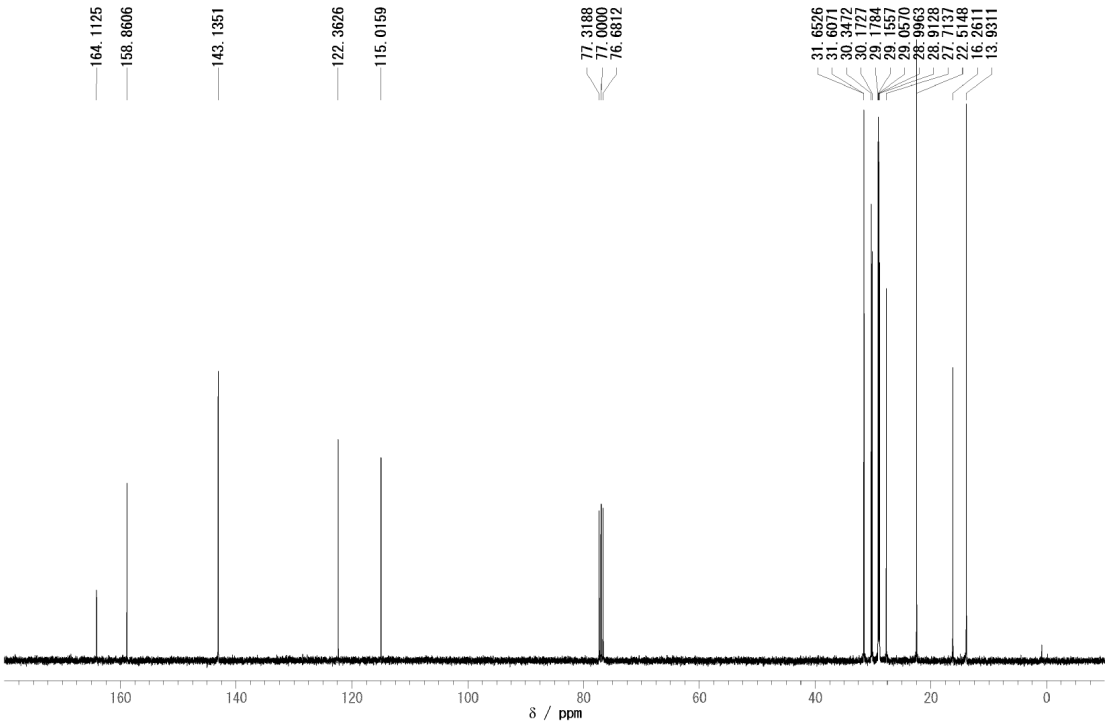
152.0907
144.0382
136.3425
133.9897
129.7396
129.5954
128.8516
127.8270
127.7891
127.1516
122.3550
109.1947
77.3188
77.0000
76.6812
16.3673
160
140
120
100
80
60
40
20
0
δ / ppm


7.2853
6.9811
6.9783
2.4697
2.4513
2.4321
2.2662
2.2470
2.2277
2.0655
1.7265
1.7082
1.6889
1.6697
1.6513
1.6330
1.5496
1.5304
1.5120
1.4928
1.4745
1.4561
1.2564
0.9705
0.9685
0.9521
0.9402
0.9329
0.9219
O
O
C3H7
C3H7
3f
δ / ppm


164.1808
158.7923
143.1730
122.4612
115.0159
77.3188
77.0000
76.6812
32.1991
31.1517
23.2966
21.0652
16.3066
13.6351
13.5592
δ / ppm


6.9765
6.9737
2.4743
2.4559
2.4358
2.2690
2.2497
2.2305
2.0628
1.6559
1.6376
1.6183
1.4746
1.4571
1.3013
0.9054
0.8953
0.8889
0.8788
0.8715
0.8614
O
O
C7H15
C7H15
7
6
5
4
3
2
1
δ / ppm

3g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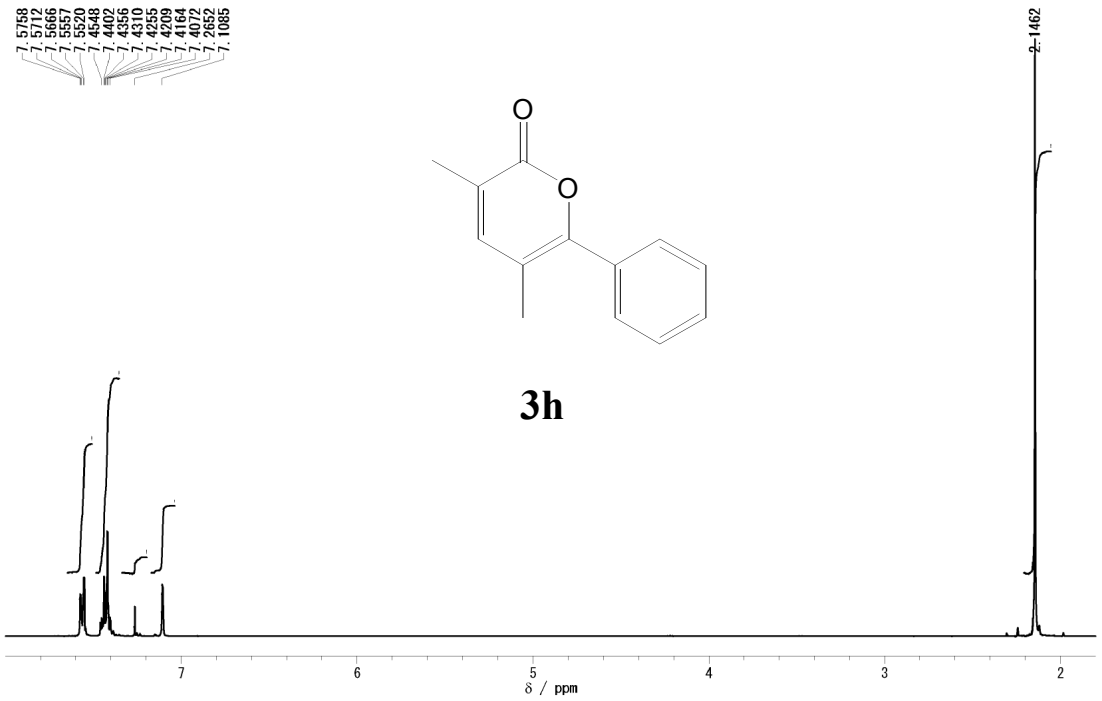
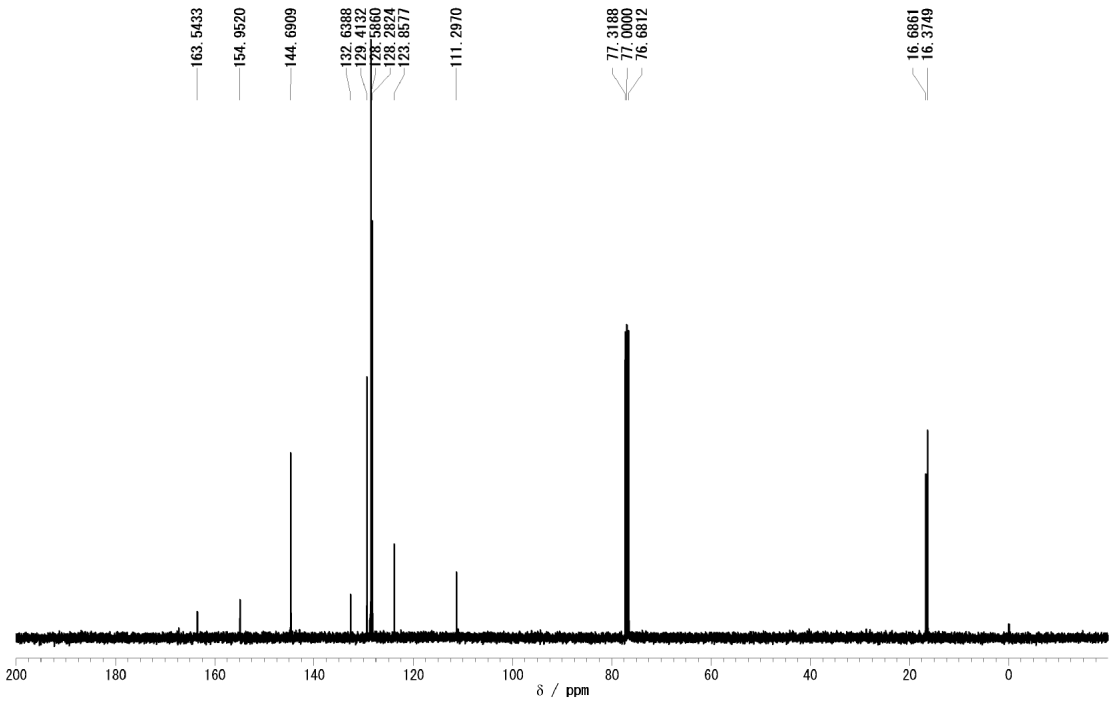
143.1351
122.3626
115.0159
77.3188
77.0000
76.6812
31.6526
31.6071
30.3472
30.1727
29.1784
29.1557
29.0570
28.9963
28.9128
27.7137
22.5148
16.2611
13.9311
160
140
120
100
80
60
40
20
0
δ / ppm


7.5758
7.5712
7.5666
7.5557
7.5520
7.4548
7.4462
7.4402
7.4356
7.4310
7.4255
7.4209
7.4164
7.4072
7.2652
7.1085
2.1462
O
O
δ / ppm

3h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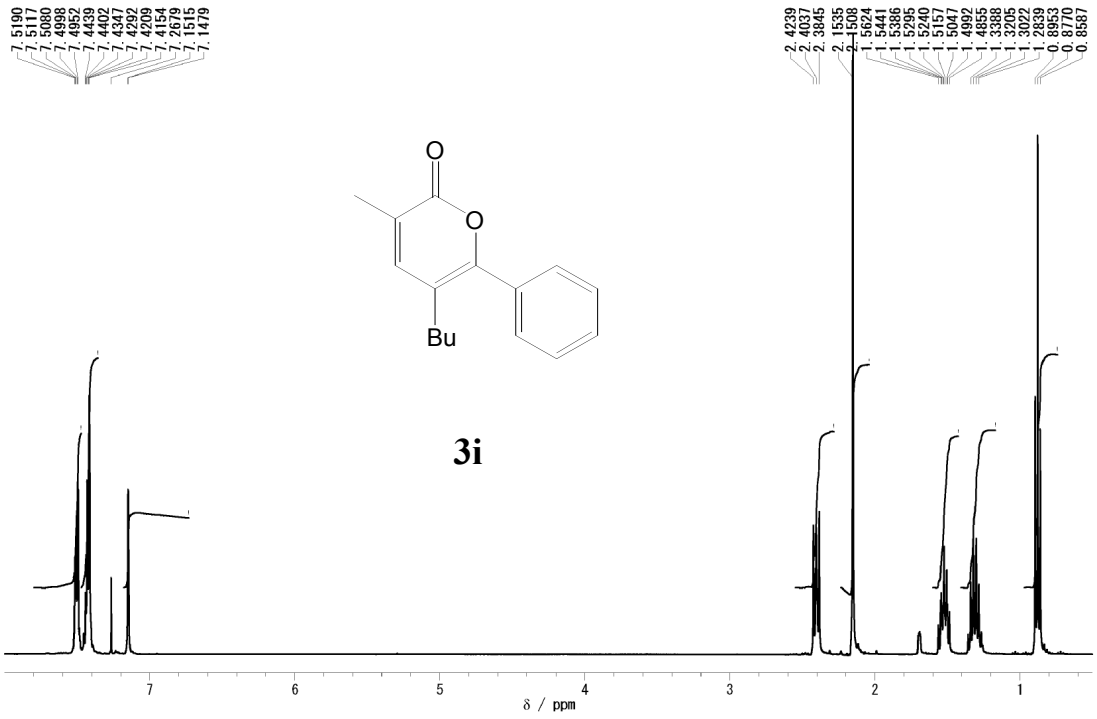
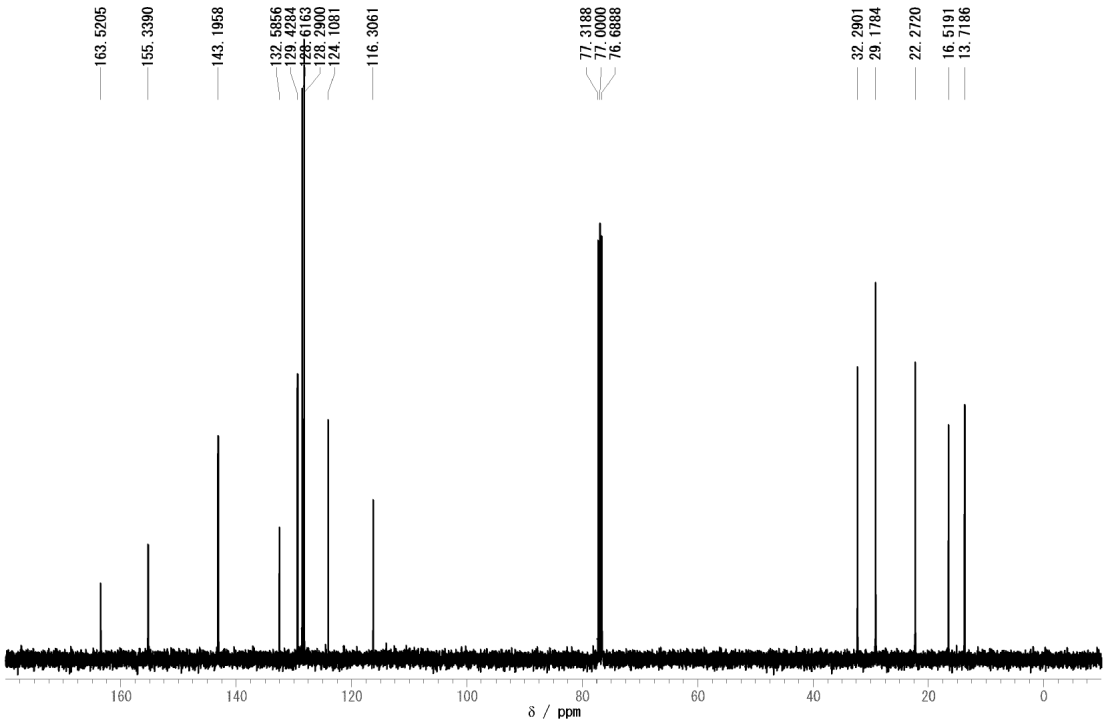
154.9520
144.6909
132.6388
129.4132
128.5860
128.2824
123.8577
111.2970
77.3188
77.0000
76.6812
16.6861
16.3749
δ / ppm


7.5190
7.5117
7.5080
7.4998
7.4952
7.4439
7.4402
7.4347
7.4292
7.4209
7.4154
7.2679
7.1515
7.1479
2.4239
2.4037
2.3845
2.1535
2.1508
1.5624
1.5441
1.5386
1.5295
1.5240
1.5157
1.5047
1.4992
1.4855
1.3388
1.3205
1.3022
1.2839
0.8953
0.8770
0.8587
O
O
Bu
7
6
5
4
3
2
1
δ / ppm

3i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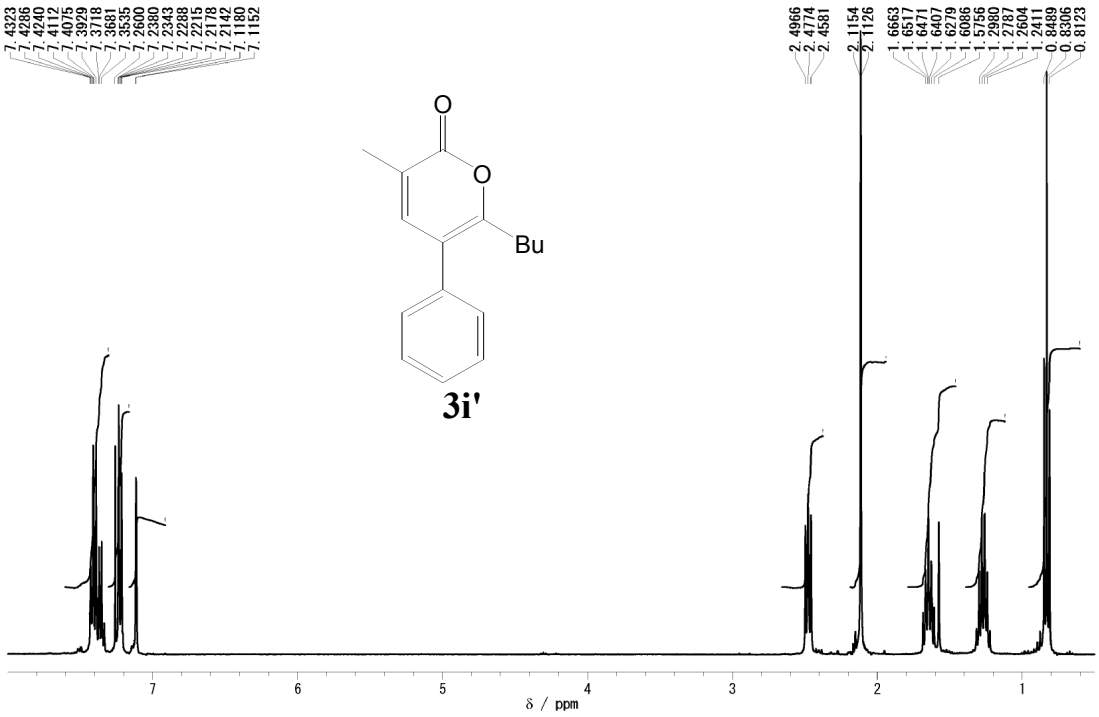
155.3390
143.1958
132.5856
129.4284
128.6163
128.2900
124.1081
116.3061
77.3188
77.0000
76.6888
32.2901
29.1784
22.2720
16.5191
13.7186
160
140
120
100
80
60
40
20
0
δ / ppm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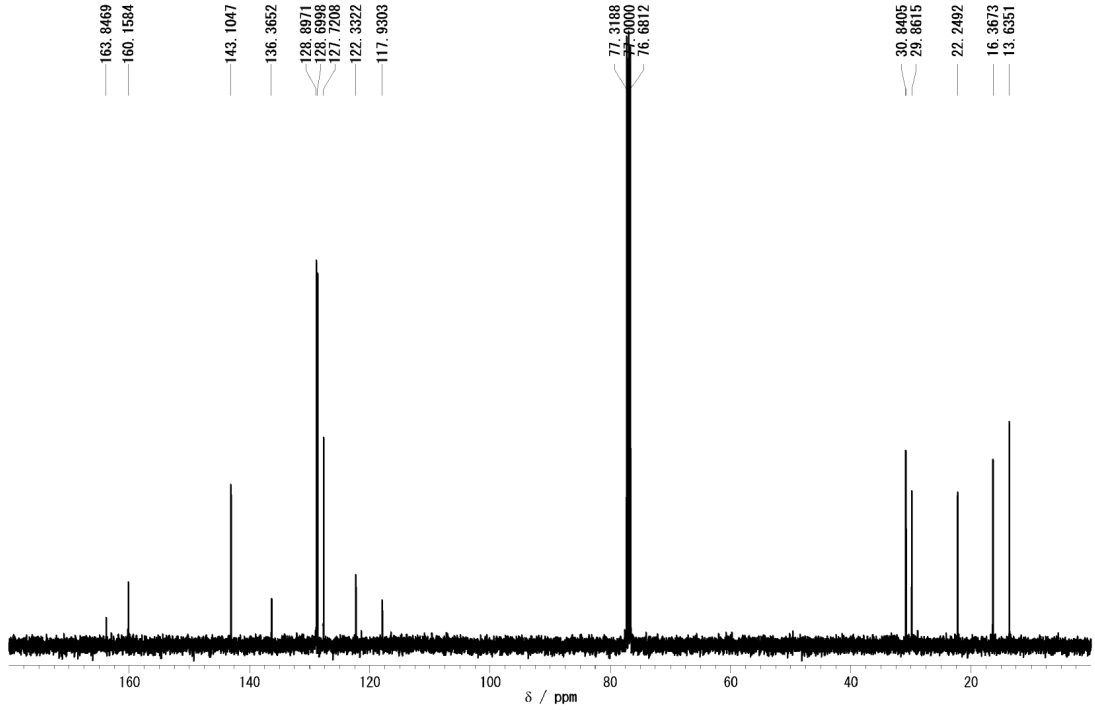
7.4286
7.4240
7.4112
7.4075
7.3929
7.3718
7.3681
7.3535
7.2600
7.2380
7.2343
7.2288
7.2215
7.2178
7.2142
7.1180
7.1152
2.4966
2.4774
2.4581
2.1154
2.1126
1.6663
1.6517
1.6471
1.6407
1.6279
1.6066
1.5756
1.5560
1.2980
1.2787
1.2604
1.2411
0.8489
0.8306
0.8123
O
O
Bu
7
6
5
4
3
2
1
δ / ppm

3i'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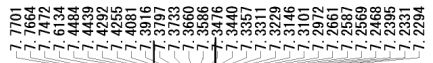
160.1584
143.1047
136.3652
128.8971
128.6998
127.7208
122.3322
117.9303
77.3188
77.0000
76.6812
30.8405
29.8615
22.2492
16.3673
13.6351
160
140
120
100
80
60
40
20
δ / ppm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7.7664
7.7472
7.6134
7.4484
7.4439
7.4292
7.4255
7.4081
7.3916
7.3797
7.3733
7.3660
7.3586
7.3476
7.3440
7.3357
7.3311
7.3229
7.3146
7.3101
7.2972
7.2661
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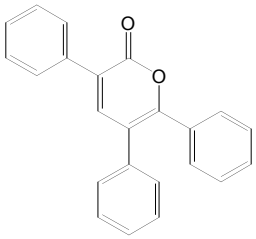
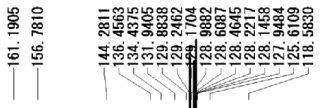
7.2569
7.2468
7.2395
7.2331
7.2294


O
O

3j

8
7
6
5
4
3
δ / ppm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156.7810
144.2811
136.4563
134.4375
131.9405
129.8838
129.2462
128.9882
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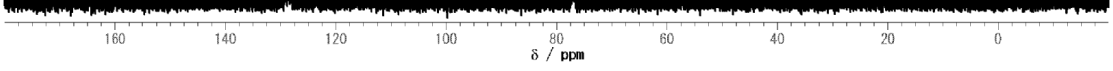
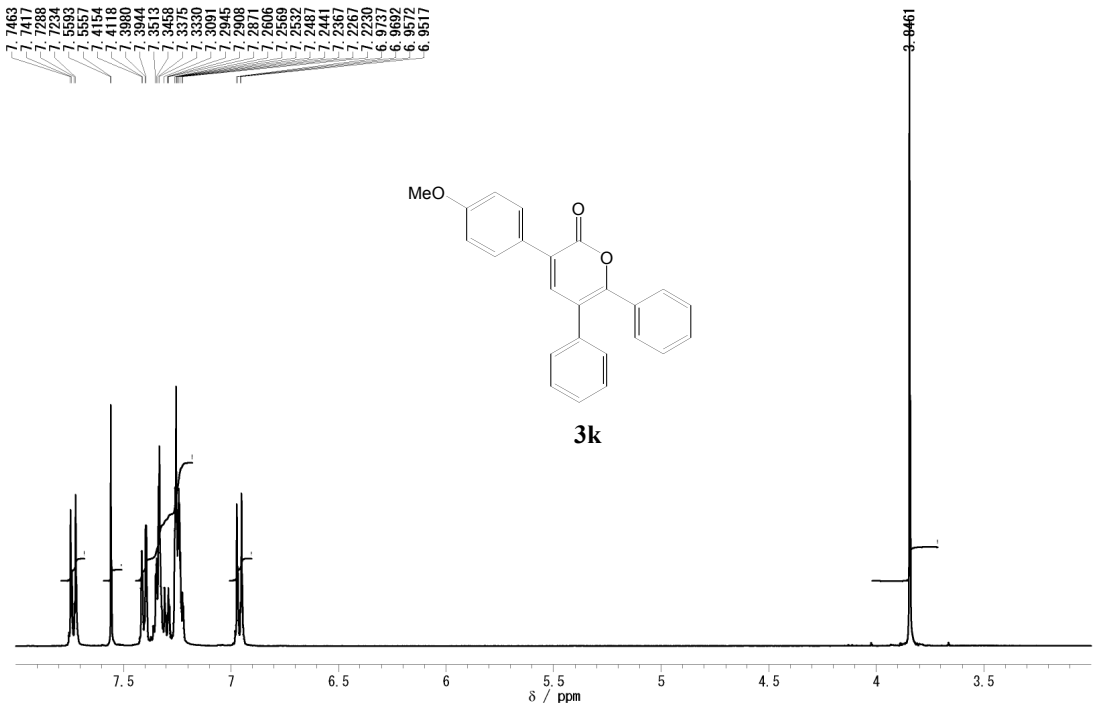
128.2217
128.1458
127.9484
125.6109
118.5830


77.3188
77.0000
76.6812


160
140
120
100
80
60
40
20
0
δ / ppm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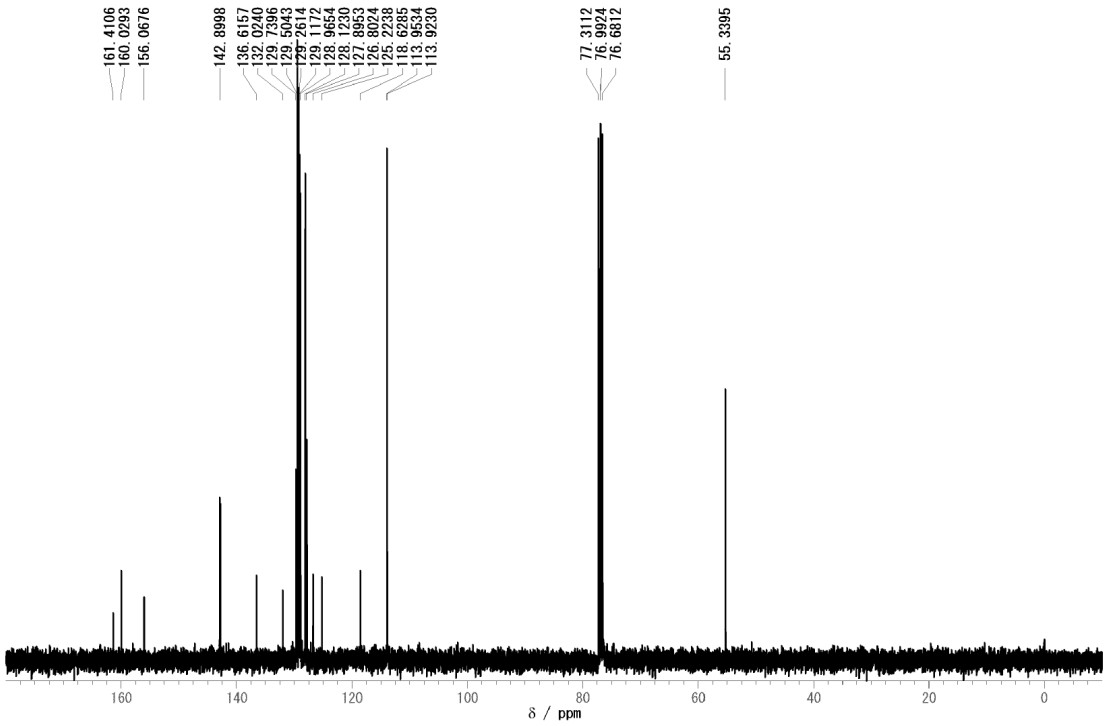
7.7417
7.7288
7.7234
7.5593
7.5557
7.4154
7.4118
7.3980
7.3944
7.3513
7.3458
7.3375
7.3330
7.3091
7.2945
7.2908
7.2871
7.2606
7.2569
7.2532
7.2487
7.2441
7.2367
7.2267
7.2230
6.9737
6.9692
6.9572
6.9517
3.8461
MeO
O
O
7.5
7
6.5
6
5.5
5
4.5
4
3.5
δ / ppm

3k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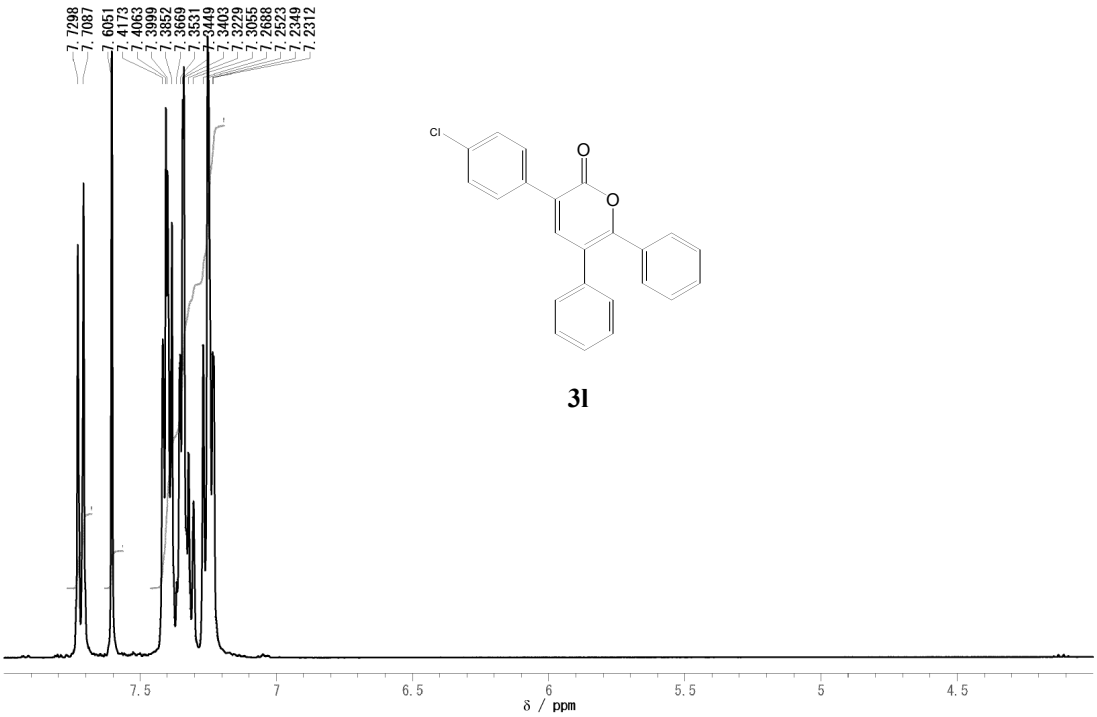
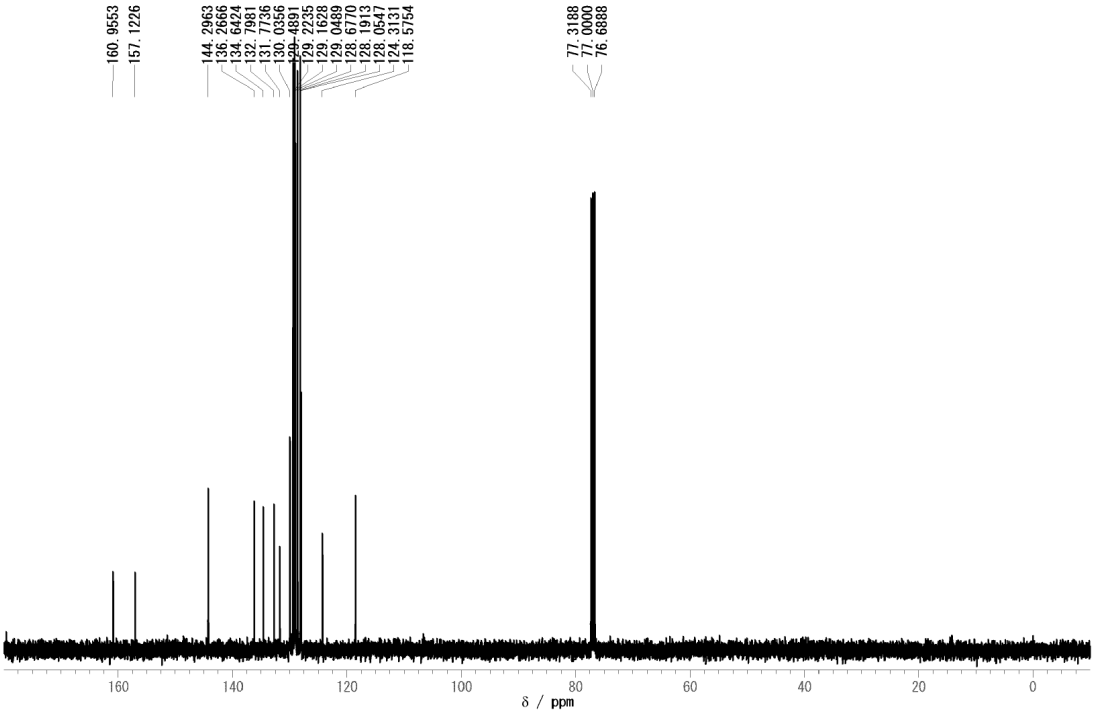
160.0293
156.0676
142.8998
136.6157
132.0240
129.7396
129.5043
129.2614
129.1172
128.9654
128.1230
127.8953
126.8024
125.2238
118.6285
113.9534
113.9230
77.3112
76.9924
76.6812
55.3395
160
140
120
100
80
60
40
20
0
δ / ppm


7.7298
7.7087
7.6051
7.4173
7.4063
7.3999
7.3852
7.3669
7.3531
7.3449
7.3403
7.3229
7.3055
7.2688
7.2523
7.2349
7.2312
Cl
O
O
7.5
7
6.5
6
5.5
5
4.5
δ / ppm

3l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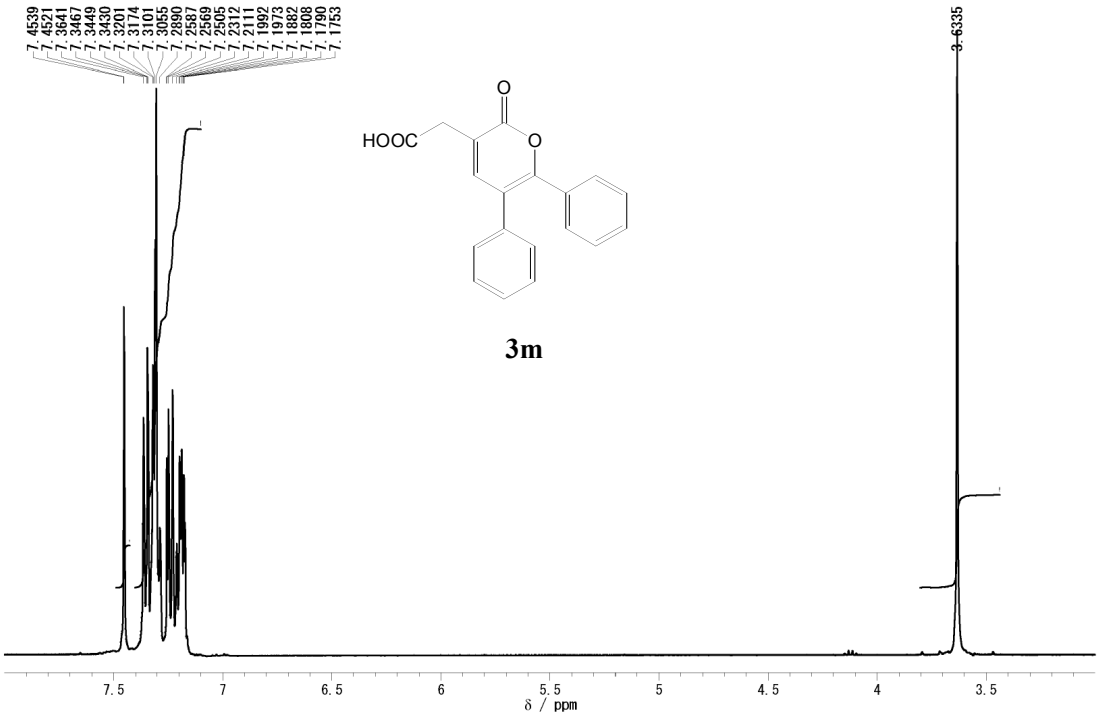
157.1226
144.2963
136.2666
134.6424
132.7981
131.7736
130.0356
129.4891
129.2235
129.1628
129.0489
128.6770
128.1913
128.0547
124.3131
118.5754
77.3188
77.0000
76.6888
160
140
120
100
80
60
40
20
0
δ / ppm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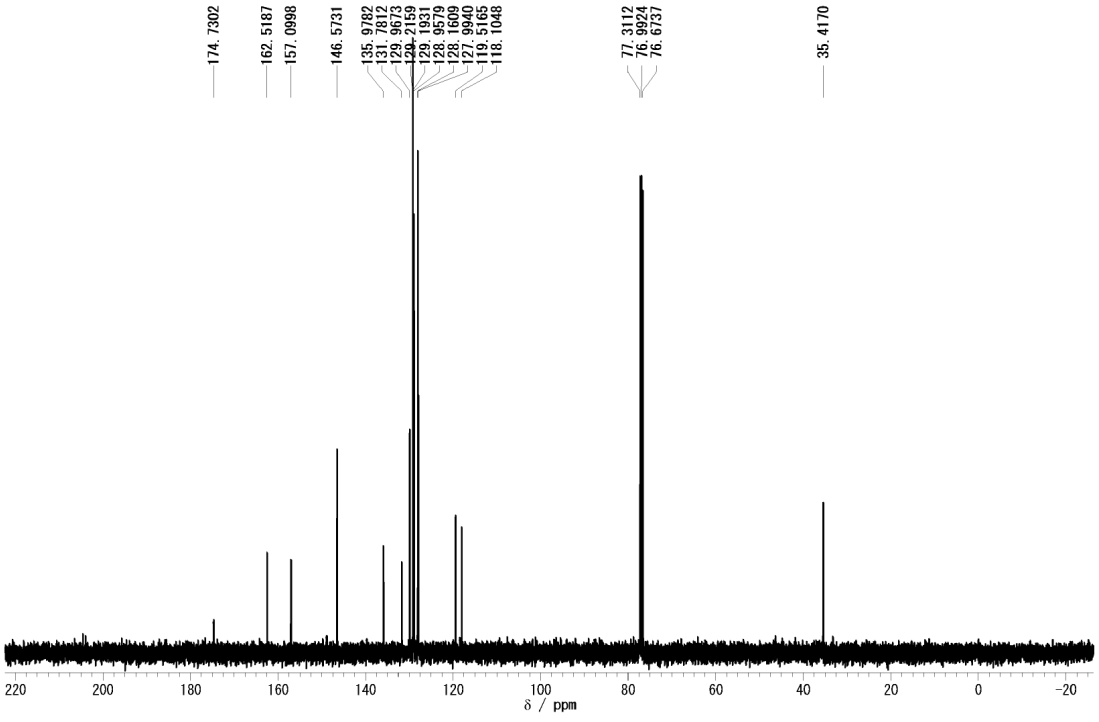
7.4521
7.3641
7.3467
7.3449
7.3430
7.3201
7.3174
7.3101
7.3055
7.2890
7.2587
7.2569
7.2505
7.2312
7.2111
7.1992
7.1973
7.1882
7.1808
7.1790
7.1753
3.6335
HOOC
O
O
7.5
7
6.5
6
5.5
5
4.5
4
3.5
δ / ppm

3m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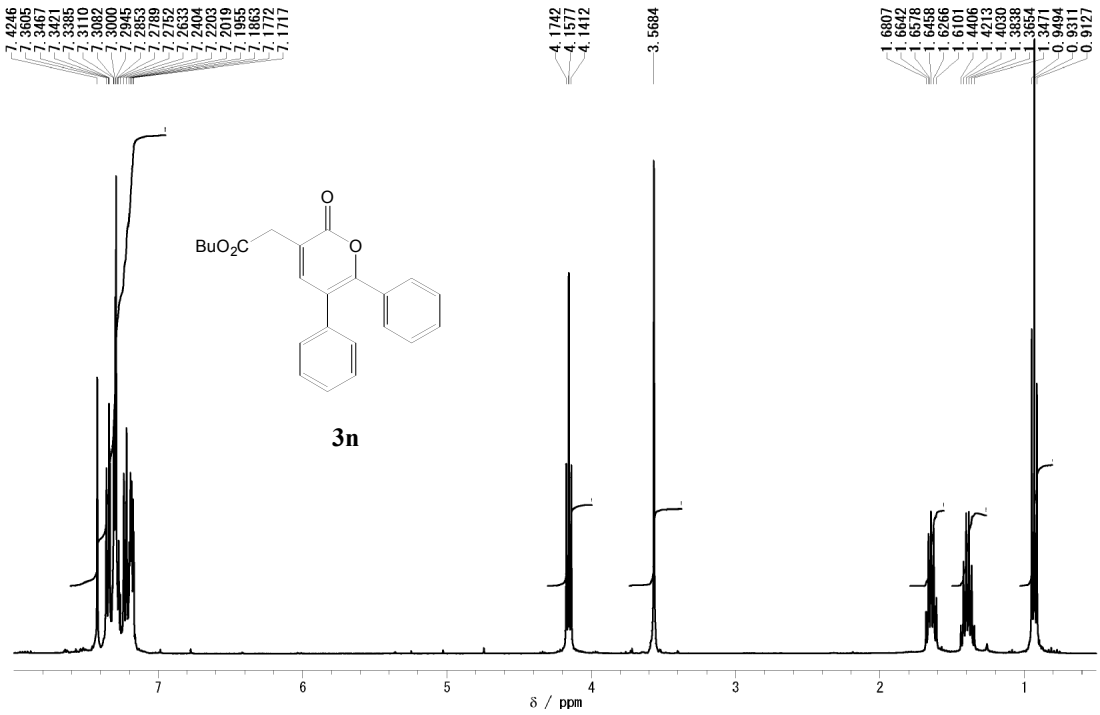
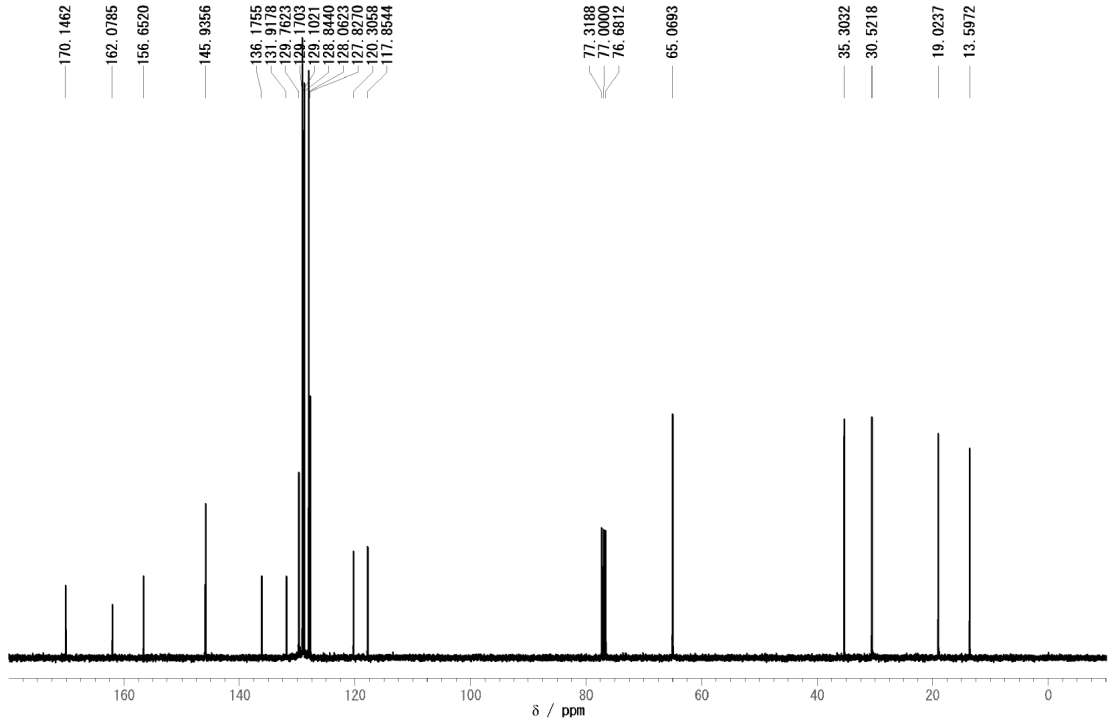
157.0998
146.5731
135.9782
131.7812
129.9673
129.2159
129.1931
128.9579
128.1609
127.9940
119.5165
118.1048
77.3112
76.9924
76.6737
35.4170
220
200
180
160
140
120
100
80
60
40
20
0
-20
δ / ppm


7.4246
7.3605
7.3467
7.3421
7.3385
7.3110
7.3082
7.3000
7.2945
7.2853
7.2789
7.2752
7.2633
7.2404
7.2203
7.2019
7.1955
7.1863
7.1772
7.1717
4.1742
4.1577
4.1412
3.5684
1.6807
1.6642
1.6578
1.6458
1.6266
1.6101
1.4406
1.4213
1.4030
1.3838
1.3654
1.3471
0.9494
0.9311
0.9127
O
O
BuO2C
3n
7
6
5
4
3
2
1
δ / ppm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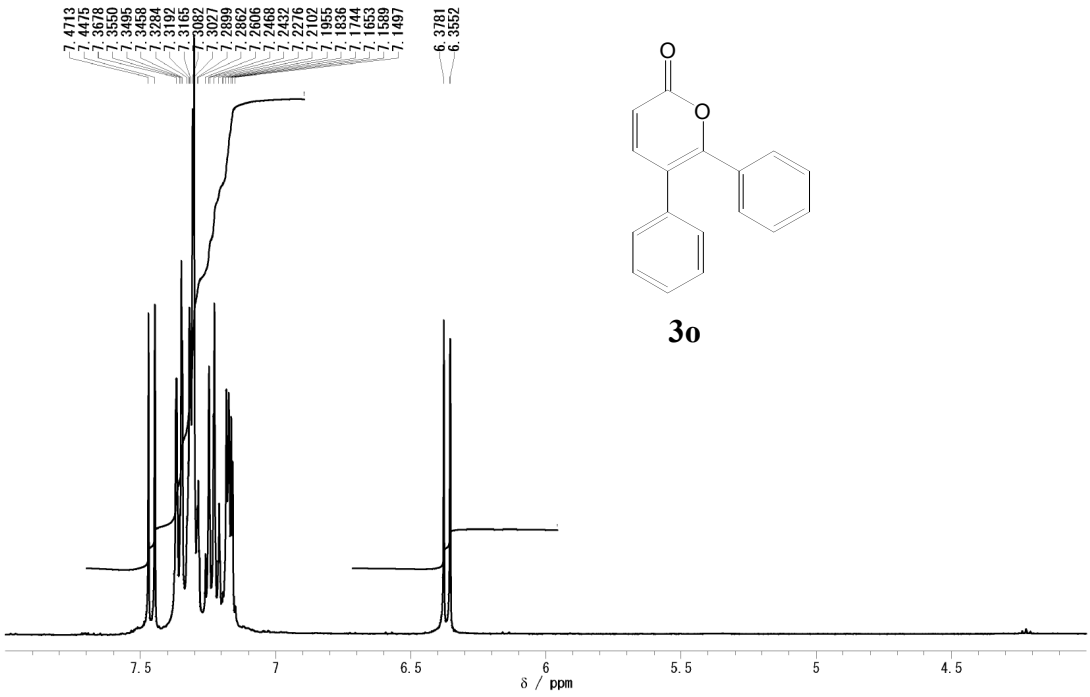
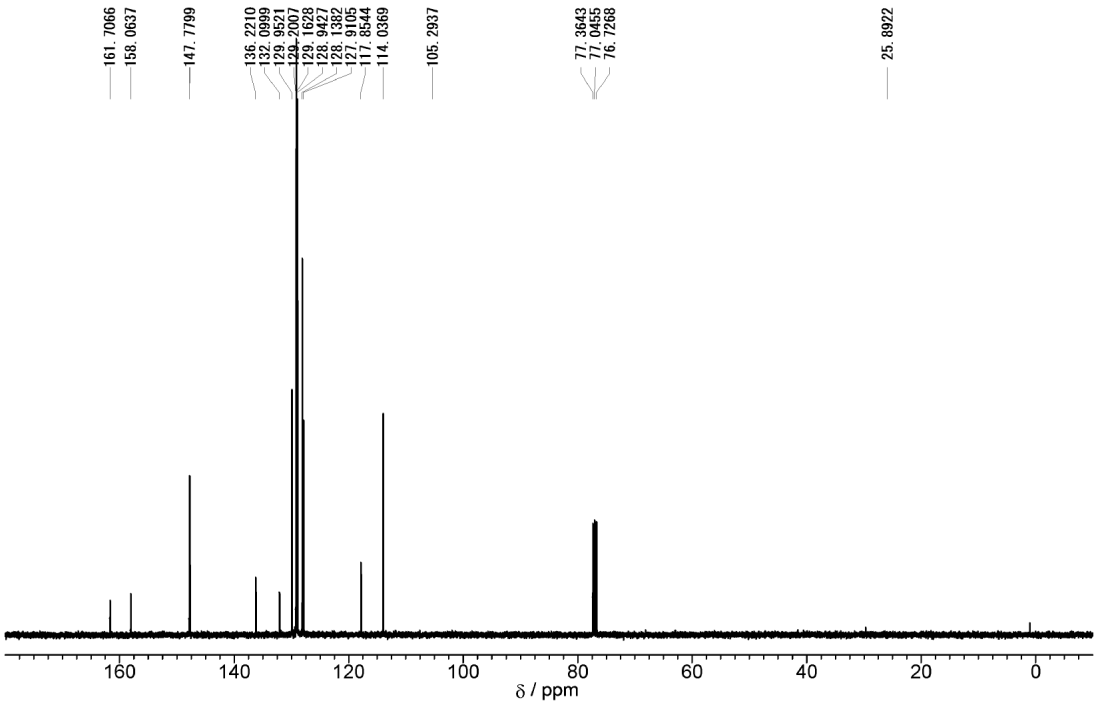
162.0785
156.6520
145.9356
136.1755
131.9178
129.7623
129.1703
129.1021
128.8440
128.0623
127.8270
120.3058
117.8544
77.3188
77.0000
76.6812
65.0693
35.3032
30.5218
19.0237
13.5972
160
140
120
100
80
60
40
20
0
δ / ppm


7.4713
7.4475
7.3678
7.3550
7.3495
7.3458
7.3284
7.3192
7.3165
7.3082
7.3027
7.2899
7.2862
7.2606
7.2468
7.2432
7.2276
7.2102
7.1955
7.1836
7.1744
7.1653
7.1589
7.1497
6.3781
6.3552
O
O
7.5
7
6.5
6
5.5
5
4.5
δ / ppm

3o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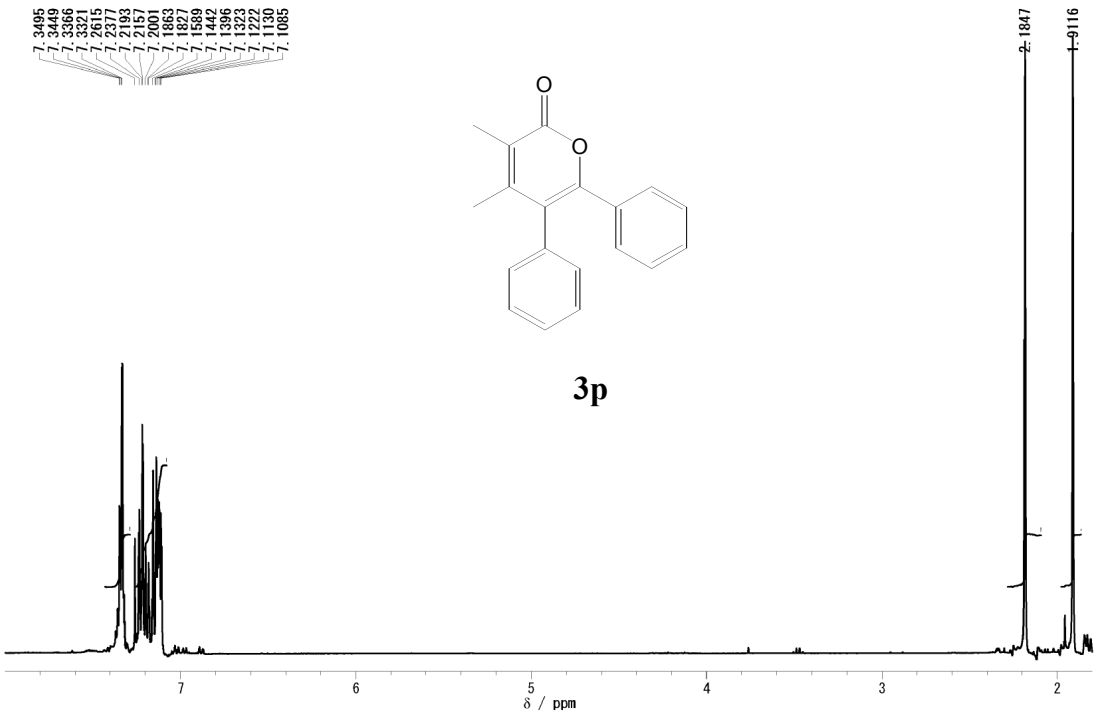
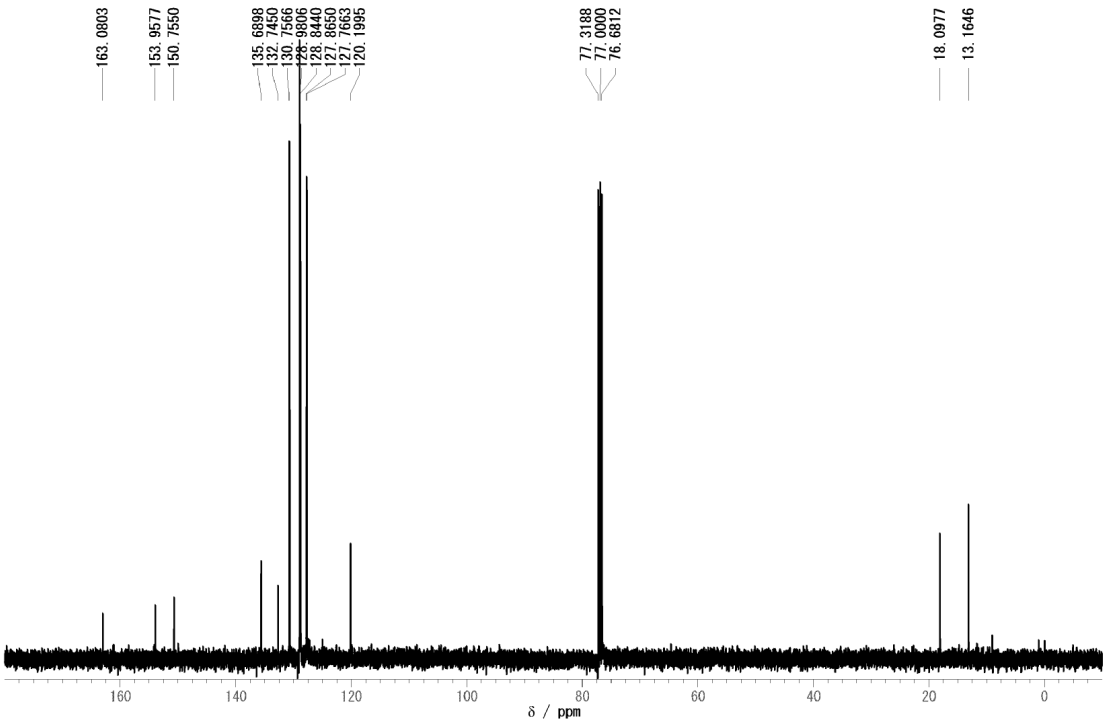
147.7799
136.2210
132.0999
129.9521
129.2007
129.1628
128.9427
128.1382
127.9105
117.8544
114.0369
105.2937
77.3643
77.0455
76.7268
25.8922
160
140
120
100
80
60
40
20
0
δ / ppm


7.3495
7.3449
7.3366
7.3321
7.2615
7.2377
7.2193
7.2157
7.2001
7.1863
7.1827
7.1589
7.1442
7.1396
7.1323
7.1222
7.1130
7.1085
2.1847
1.9116
O
O
7
6
5
4
3
2
δ / ppm

3p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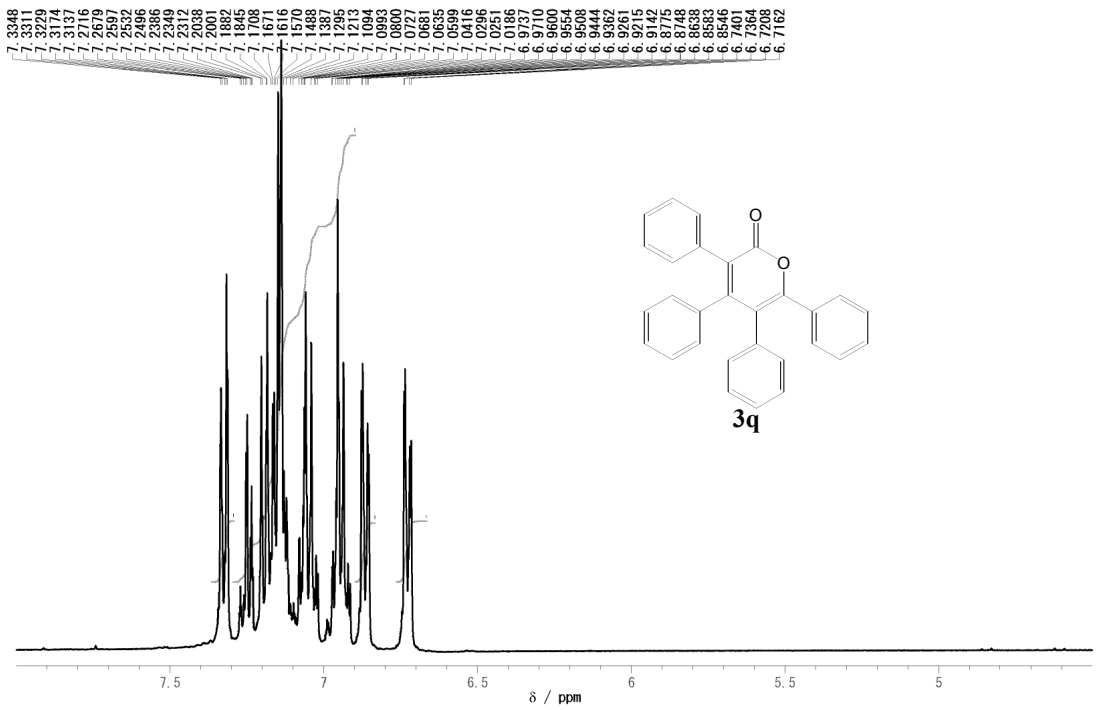
153.9577
150.7550
135.6898
132.7450
130.7566
128.9806
128.8440
127.8650
127.7663
120.1995
77.3188
77.0000
76.6812
18.0977
13.1646
160
140
120
100
80
60
40
20
0
δ / ppm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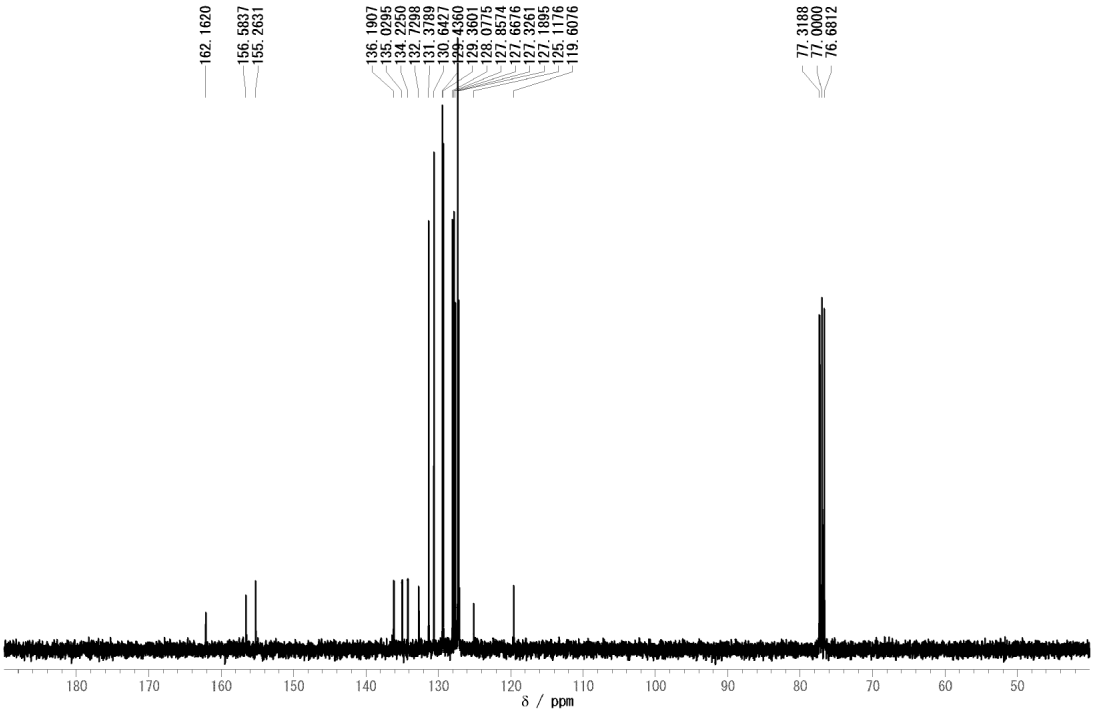
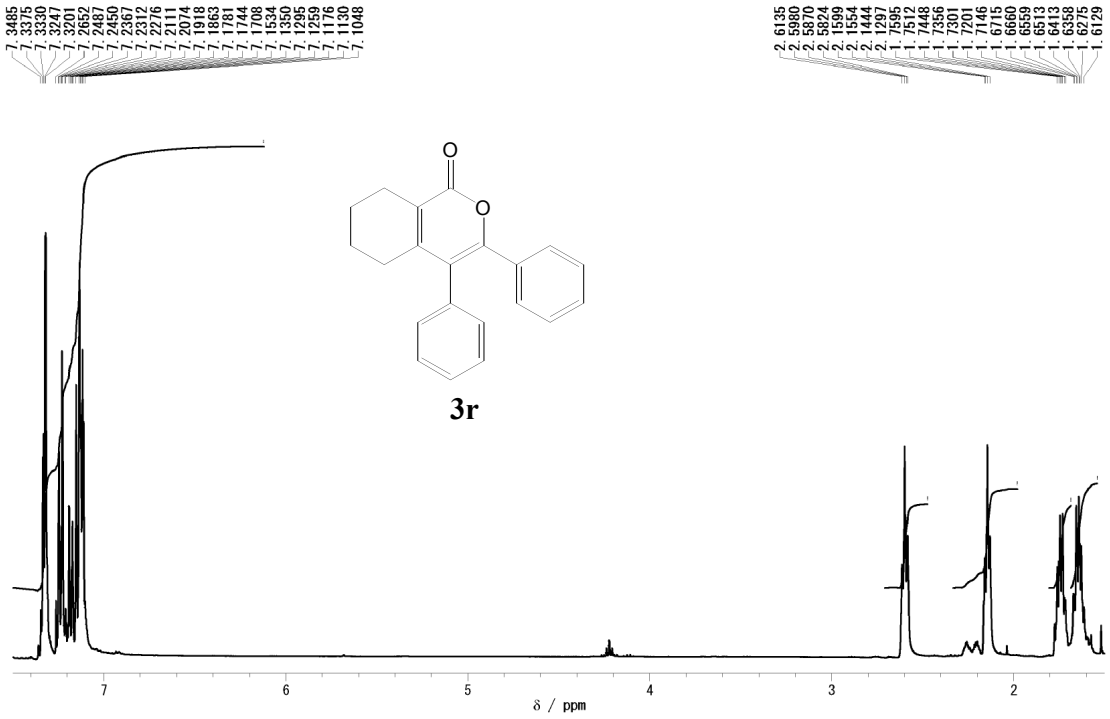
7.3311
7.3229
7.3174
7.3137
7.2716
7.2679
7.2597
7.2532
7.2496
7.2386
7.2349
7.2312
7.2038
7.2001
7.1882
7.1845
7.1708
7.1671
7.1616
7.1570
7.1488
7.1387
7.1295
7.1213
7.1094
7.0993
7.0800
7.0727
7.0681
7.0635
7.0599
7.0416
7.0296
7.0251
7.0186
6.9737
6.9710
6.9600
6.9554
6.9508
6.9444
6.9362
6.9261
6.9215
6.9142
6.8775
6.8748
6.8638
6.8563
6.8546
6.7401
6.7364
6.7208
6.7162
O
O
3q
7.5
7
6.5
6
5.5
5
δ / ppm


162.1620
156.5837
155.2631
136.1907
135.0295
134.2250
132.7298
131.3789
130.6427
129.4360
129.3601
128.0775
127.8574
127.6676
127.3261
127.1895
125.1176
119.6076
77.3188
77.0000
76.6812
180
170
160
150
140
130
120
110
100
90
80
70
60
50
δ / ppm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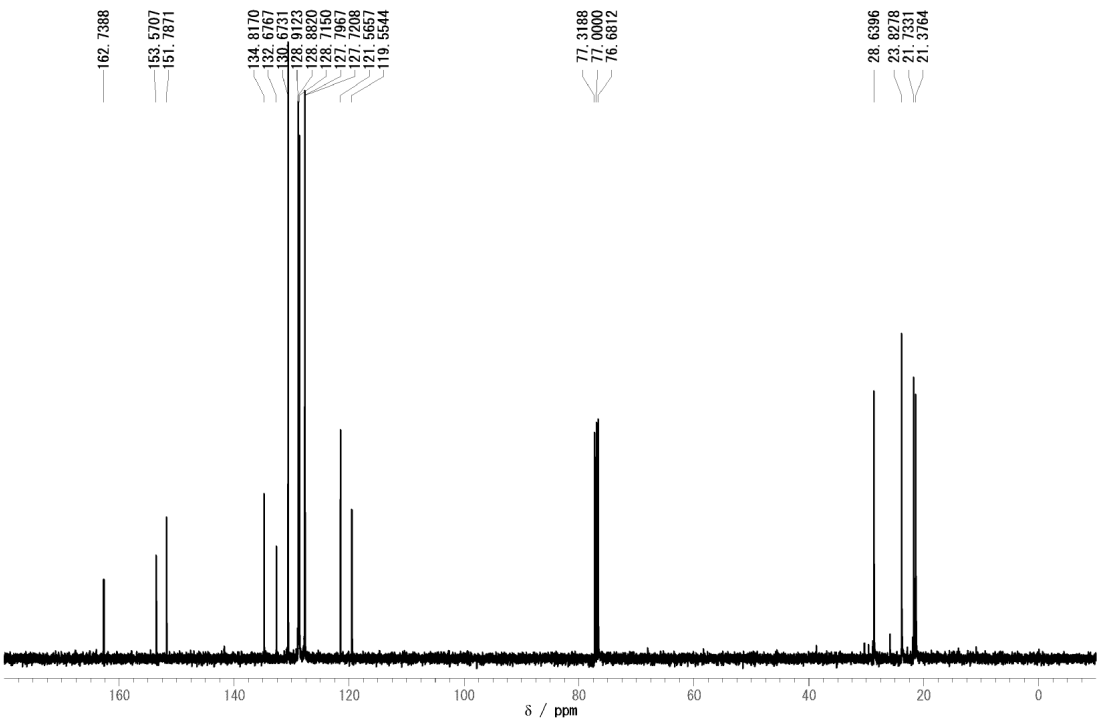
7.3375
7.3330
7.3247
7.3201
7.2652
7.2487
7.2450
7.2367
7.2312
7.2276
7.2111
7.2074
7.1918
7.1863
7.1781
7.1744
7.1708
7.1534
7.1350
7.1295
7.1259
7.1176
7.1130
7.1048
2.6135
2.5980
2.5870
2.5824
2.1599
2.1554
2.1444
2.1297
1.7595
1.7512
1.7448
1.7356
1.7301
1.7201
1.7146
1.6715
1.6660
1.6559
1.6513
1.6413
1.6358
1.6275
1.6129
O
O
7
6
5
4
3
2
δ / ppm

3r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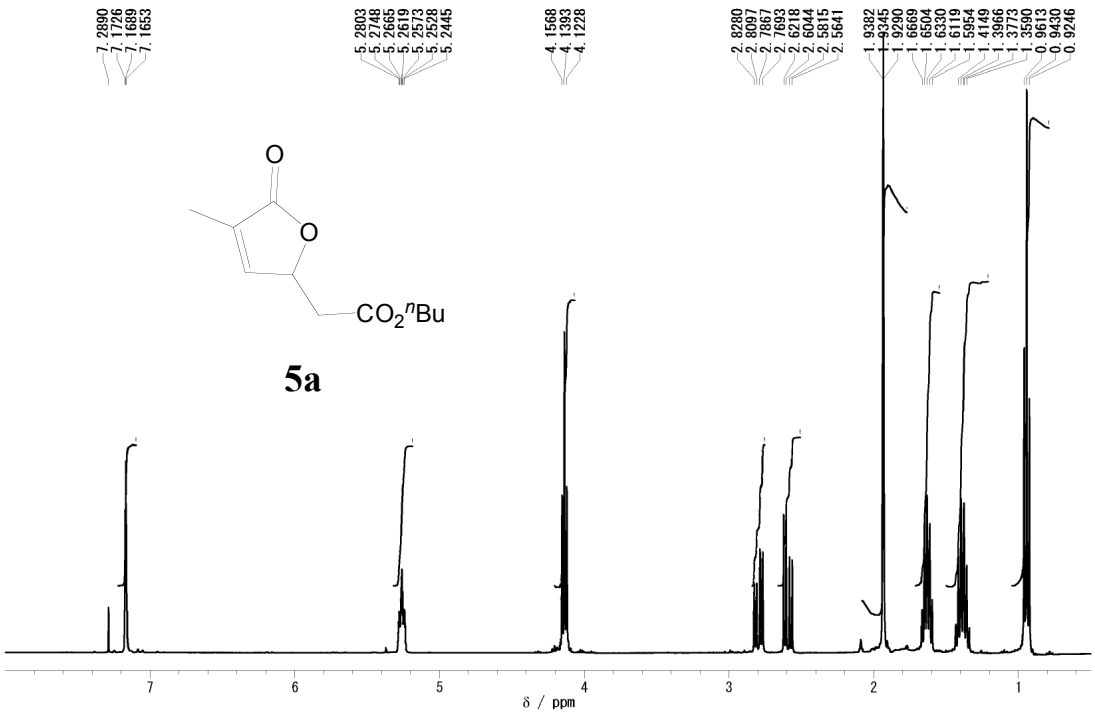
153.5707
151.7871
134.8170
132.6767
130.6731
128.9123
128.8820
128.7150
127.7967
127.7208
121.5657
119.5544
77.3188
77.0000
76.6812
28.6396
23.8278
21.7331
21.3764
160
140
120
100
80
60
40
20
0
δ / ppm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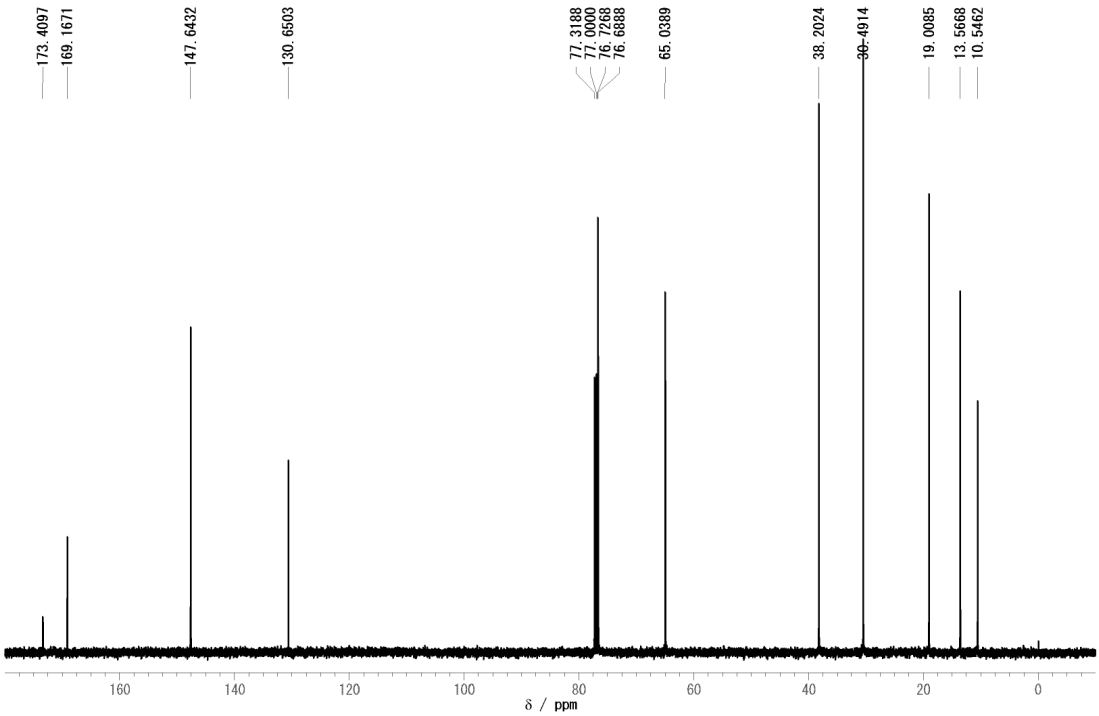
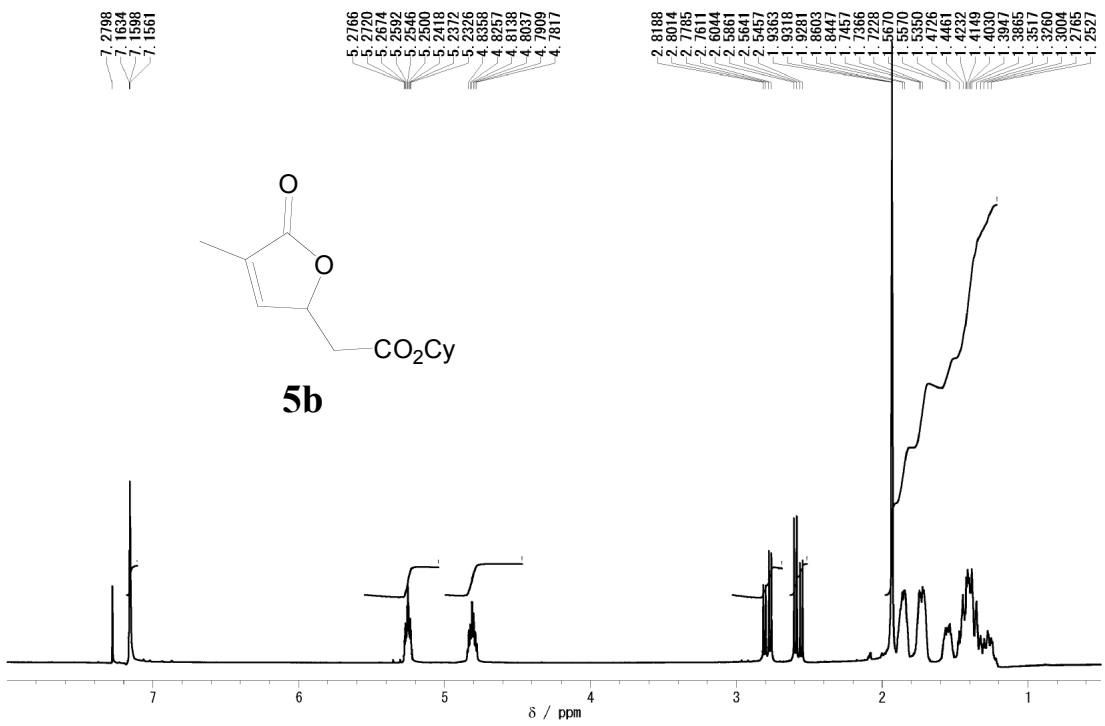
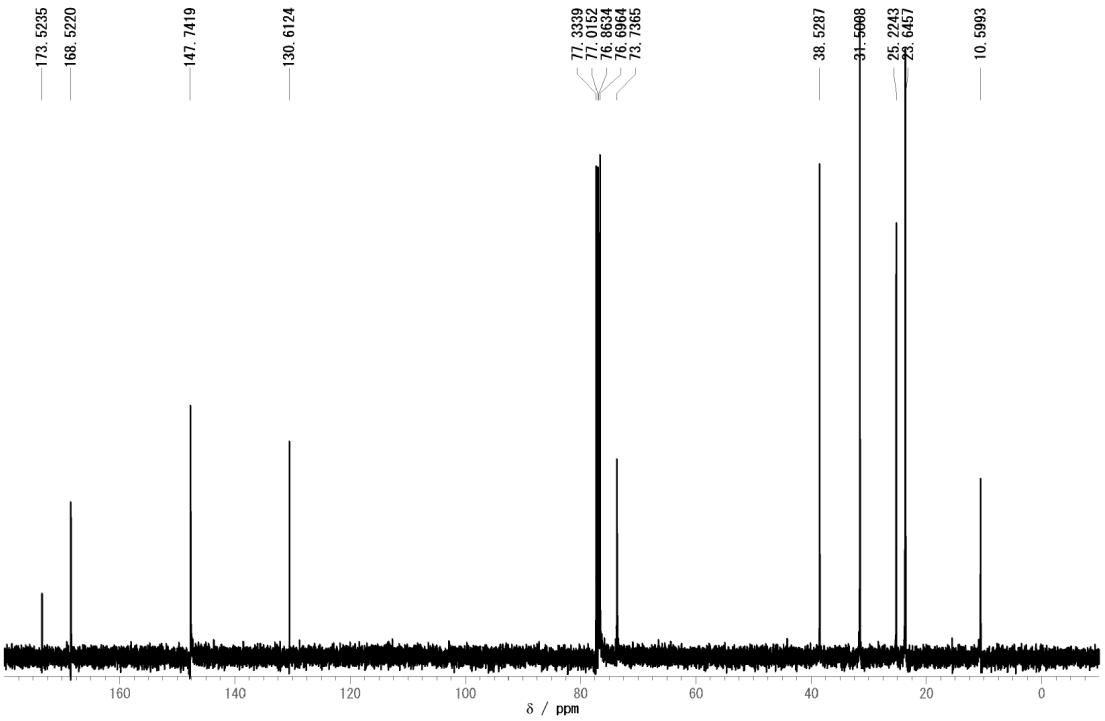
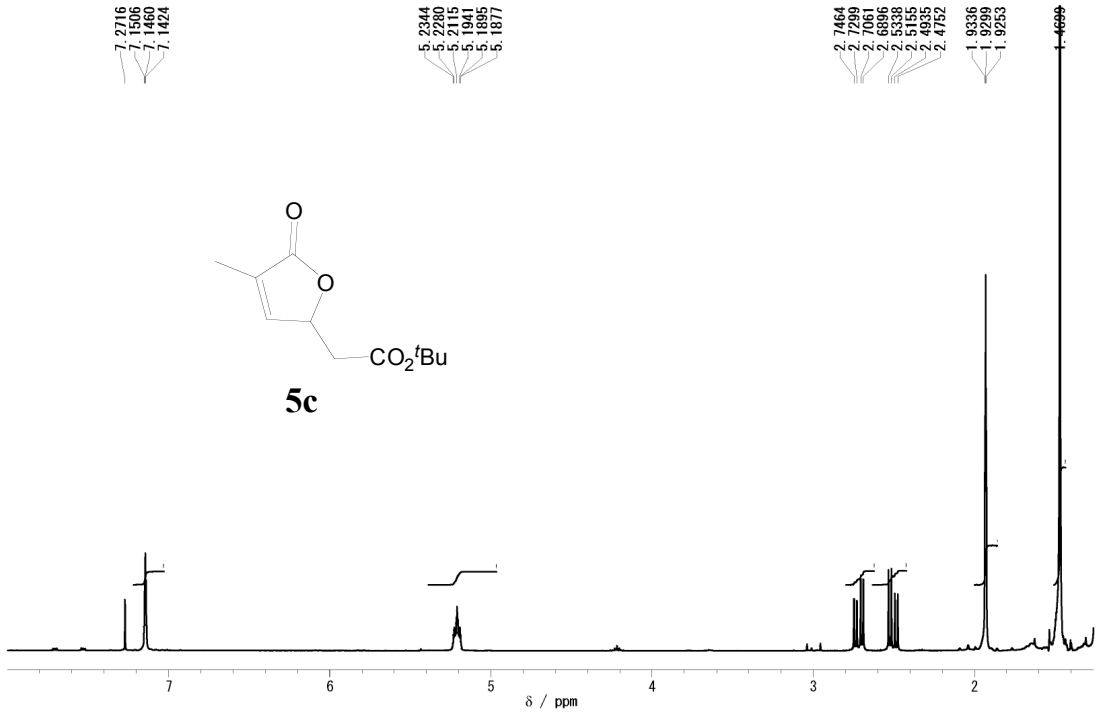
7.1726
7.1689
7.1653
5.2803
5.2748
5.2665
5.2619
5.2573
5.2528
5.2445
4.1568
4.1393
4.1228
2.8280
2.8097
2.7867
2.7693
2.6218
2.6044
2.5815
2.5641
1.9382
1.9345
1.9290
1.6669
1.6504
1.6330
1.6119
1.5954
1.4149
1.3966
1.3773
1.3590
0.9613
0.9430
0.9246
O
O
CO2nBu
5a
δ / ppm


173.4097
169.1671
147.6432
130.6503
77.3188
77.0000
76.7268
76.6888
65.0389
38.2024
30.4914
19.0085
13.5668
10.5462
δ / ppm


7.2798
7.1634
7.1598
7.1561
5.2766
5.2720
5.2674
5.2592
5.2546
5.2500
5.2418
5.2372
5.2326
4.8358
4.8257
4.8138
4.8037
4.7909
4.7817
2.8188
2.8014
2.7785
2.7611
2.6044
2.5861
2.5641
2.5457
2.9363
1.9318
1.9281
1.8603
1.8447
1.7457
1.7366
1.7228
1.5670
1.5570
1.5350
1.4726
1.4461
1.4232
1.4149
1.4030
1.3947
1.3865
1.3517
1.3260
1.3004
1.2765
1.2527
O
O
CO2Cy
5b
δ / ppm


173.5235
168.5220
147.7419
130.6124
77.3339
77.0152
76.8634
76.6964
73.7365
38.5287
31.5088
25.2243
23.6457
10.5993
δ / ppm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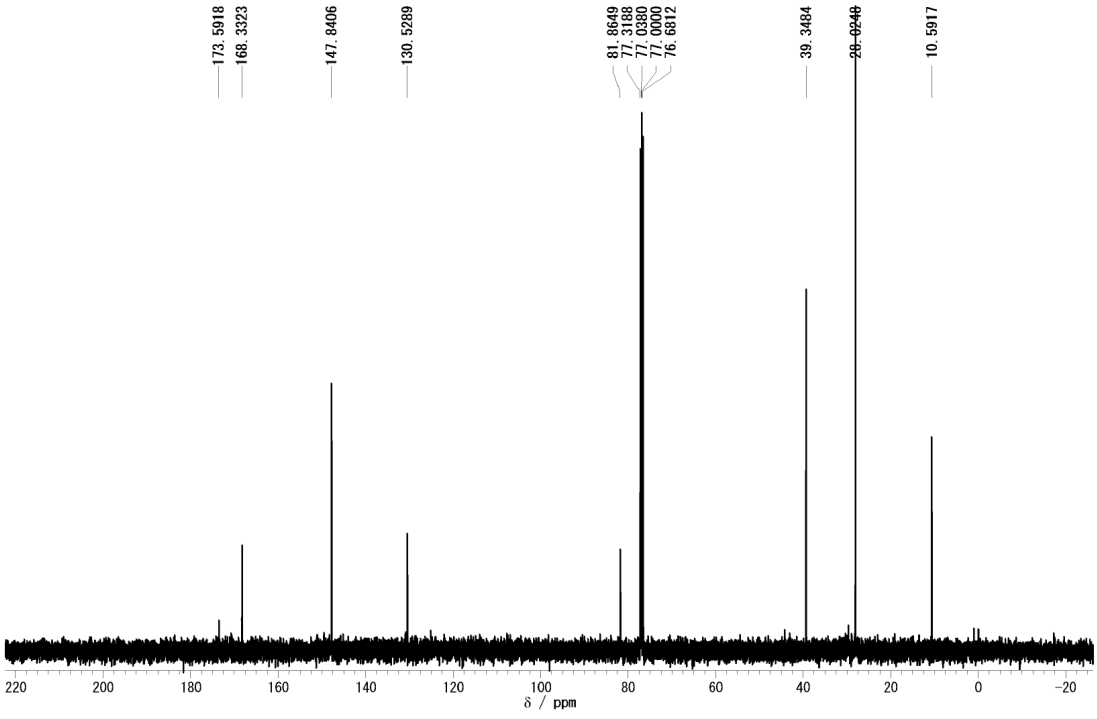
7.1506
7.1460
7.1424
5.2344
5.2280
5.2115
5.1941
5.1895
5.1877
2.7464
2.7299
2.7061
2.6896
2.5338
2.5155
2.4935
2.4752
1.9336
1.9299
1.9253
1.4699
O
O
CO2tBu
5c
δ / ppm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168.3323
147.8406
130.5289
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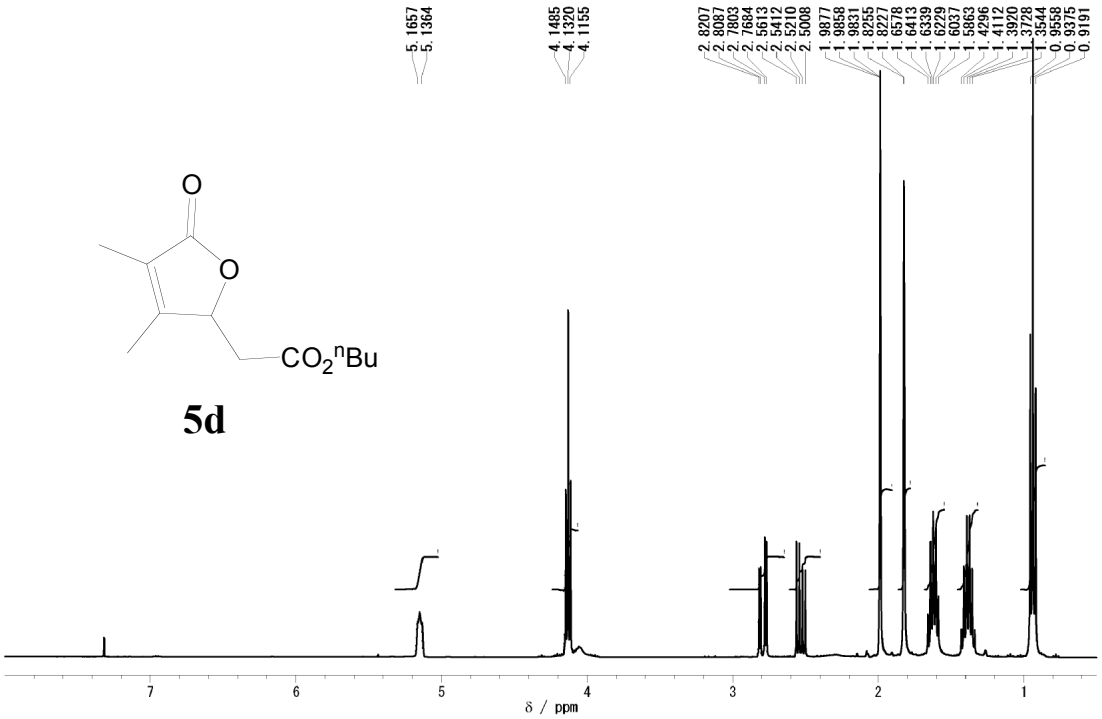
77.3188
77.0380
77.0000
76.6812
39.3484
28.0248
10.5917
δ / ppm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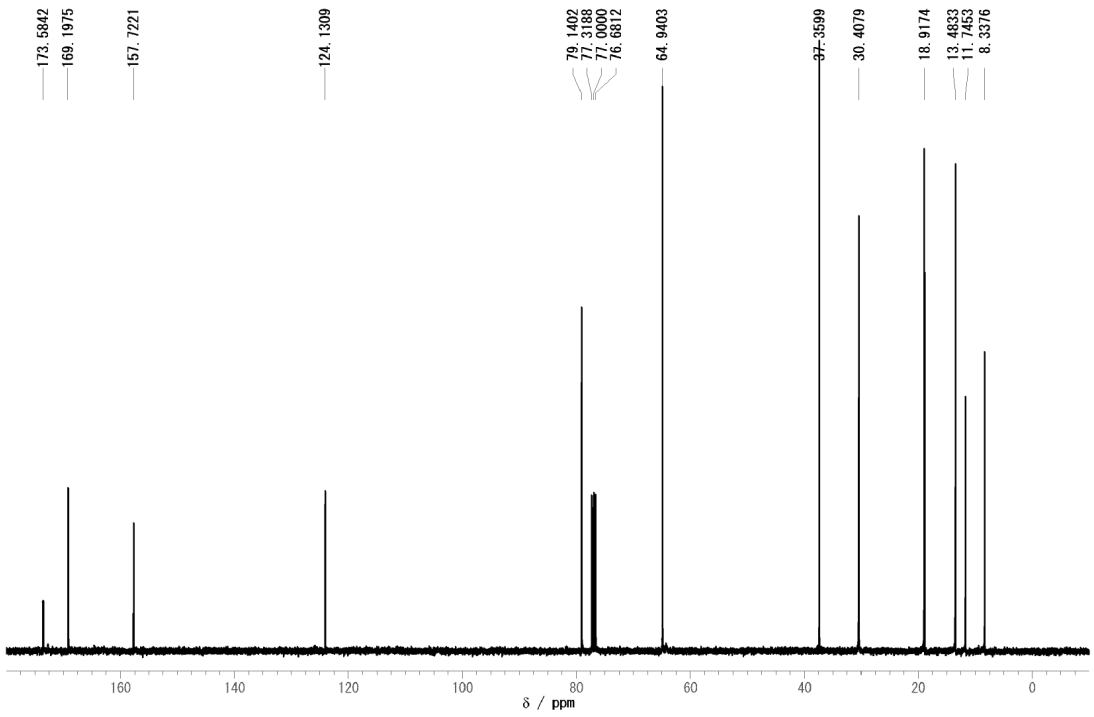
5.1364
4.1485
4.1320
4.1155
2.8207
2.8087
2.7803
2.7684
2.5613
2.5412
2.5210
2.5008
1.9877
1.9858
1.9831
1.8255
1.8227
1.6578
1.6413
1.6339
1.6229
1.6037
1.5863
1.4296
1.4112
1.3920
1.3728
1.3544
0.9558
0.9375
0.9191
O
O
CO2nBu
5d
δ / ppm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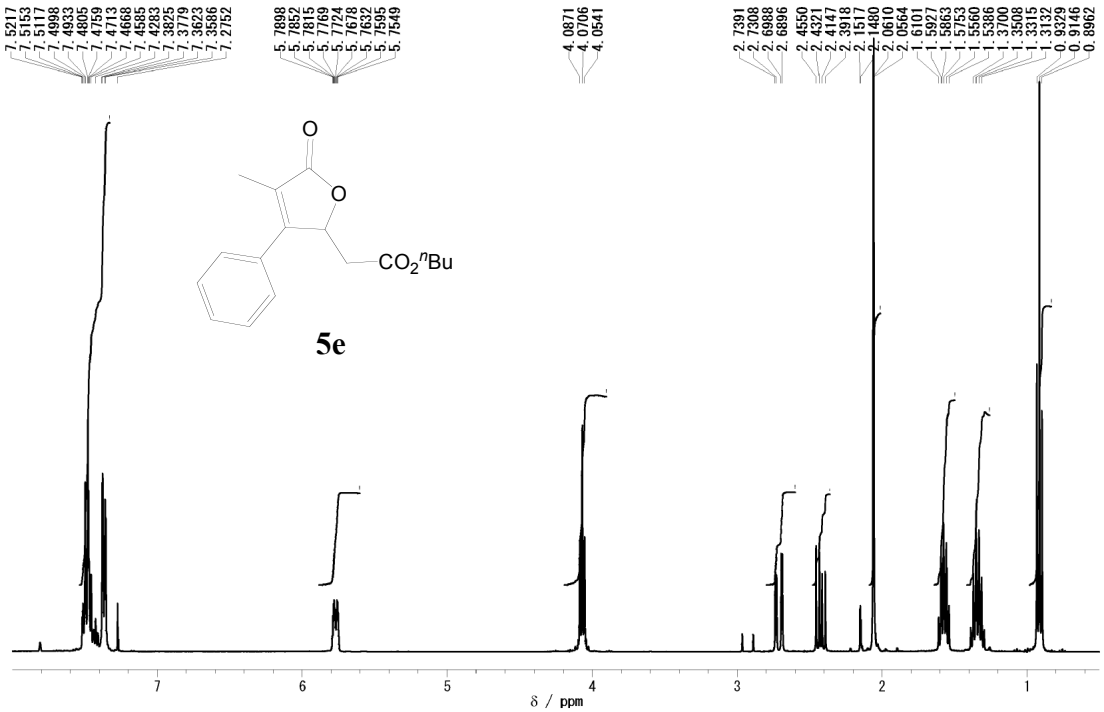
157.7221
124.1309
79.1402
77.3188
77.0000
76.6812
64.9403
37.3599
30.4079
18.9174
13.4833
11.7453
8.3376
δ / ppm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7.5153
7.5117
7.4998
7.4933
7.4805
7.4759
7.4713
7.4668
7.4585
7.4283
7.3825
7.3779
7.3623
7.3586
7.2752
5.7898
5.7852
5.7815
5.7769
5.7724
5.7678
5.7632
5.7595
5.7549
4.0871
4.0706
4.0541
2.7391
2.7308
2.6988
2.6896
2.4550
2.4321
2.4147
2.3918
2.1517
2.1480
2.0610
2.0564
1.6101
1.5927
1.5863
1.5753
1.5560
1.5386
1.3700
1.3508
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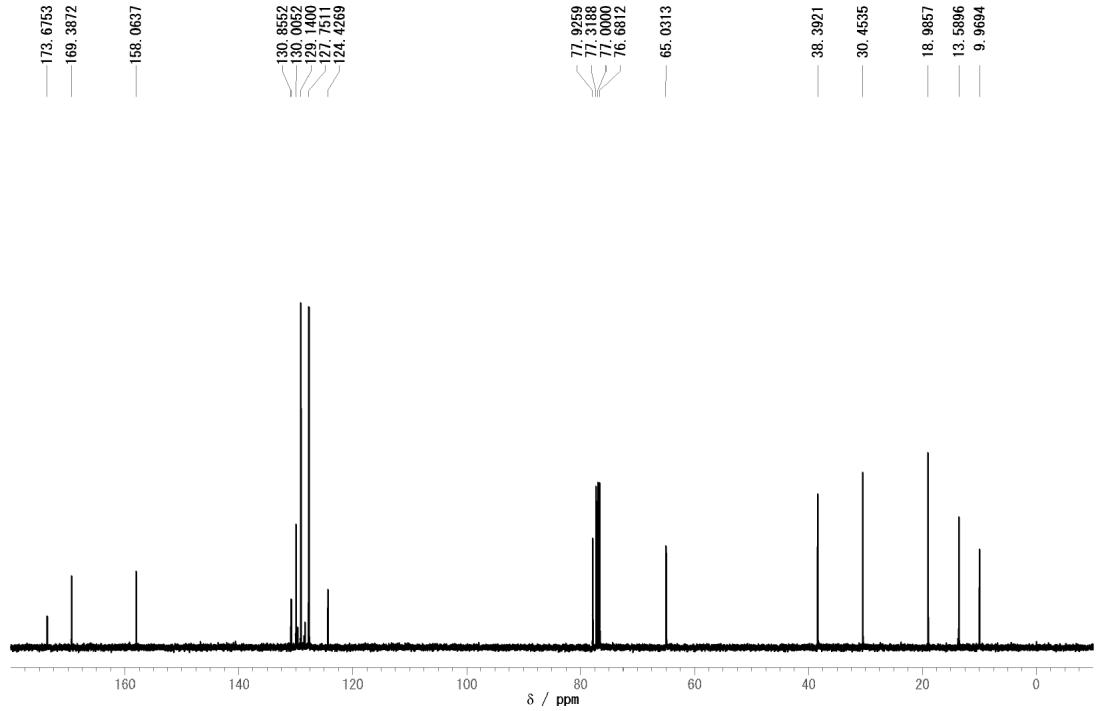
1.3132
0.9329
0.9146
0.8962
O
O
CO2nBu
5e
δ / ppm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130.0052
129.1400
127.7511
124.4269
77.9259
77.3188
77.0000
76.6812
65.0313
38.3921
30.4535
18.9857
13.5896
9.9694
δ / ppm