Dead Line: 8.11.2015

Determine structure by using following analytical data for three compounds. ^{1}H and ^{13}C NMR Spectra are also provided.

Total four molecules

Assignment 1:

Analytical data: **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.36-7.33 (m, 2H), 7.30-7.27 (m, 3H), 5.30 (t, *J* = 7.8 Hz, 1H), 3.92 (s, 3H), 3.56 (dd, *J* = 14.4, 7.8 Hz, 1H) 3.28 (dd, *J* = 14.4, 7.8 Hz, 1H); **^{13}C NMR** (150 MHz, CDCl3): δ 184.8, 160.4, 136.3, 129.3, 128.7, 127.3, 53.4, 47.3, 38.1; **IR** (thin film): 3031, 1733,1455, 1260, 1068, 1027, 699 cm^{-1}; **LRMS** (ESI): Calcd. for $C_{11}H_{11}BrO_3$: ([M+H]): 271.00, Found: 271.12; **TLC** (15% EtOAc/hexane): R*f* = 0.17.

Hints: This Molecule has two carbonyl functional groups.

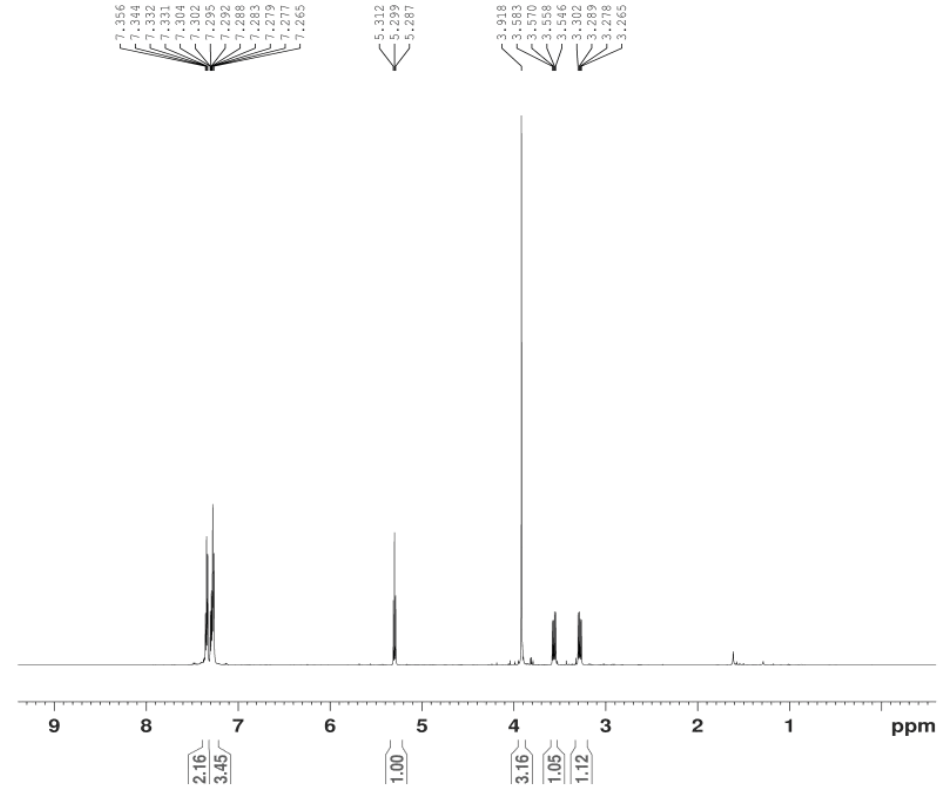
Assignment 2:

Analytical data: IR (neat, cm-1) 3324, 2931, 2806, 1495, 1452, 1028, 978, 748, 698; 1H NMR (400 MHz, $CDCl_3$) δ: 7.42 – 7.33 (m, 8H), 7.33 – 7.26 (m, 2H), 5.56 (s, 1H), 4.04 (d, *J* = 13.1 Hz, 2H), 3.64 (dd**d**, *J* = 10.5, 3.7, 2.2 Hz, 1H), 3.30 (dd, *J* = 10.5, 9.3 Hz, 1H), 3.19 (d, *J* = 13.1 Hz, 2H), 2.58 (d**d**, *J* = 12.6, 11.1 Hz, 1H), 2.41 (dd**d**, *J* = 12.7, 3.5, 2.2 Hz, 1H), 2.36 – 2.16 (m, 1H), 0.75 (d, *J* = 6.7 Hz, 3H); 13C NMR (100.6 MHz, CDCl3) δ: 138.1, 129.3, 128.6, 127.4, 70.5, 61.4, 59.1, 31.6, 15.0. HRMS (DART-TOF) calcd. for $C_{18}H_{23}NO$ [M+H]+ *m/z* 270.1852, found 270.1852. Anal. Calcd. for C18H23NO: C, 80.26; H, 8.61. Found: C, 80.00; H, 8.62.

Assignment 3:

Analytical data: IR (neat, cm-1) 2956, 1495, 1451, 1028, 735, 697; 1H NMR (400 MHz, CDCl3) δ: 7.58 – 7.21 (m, 10H), 5.72 (s, 1H), 4.05 (d, *J* = 13.1 Hz, 2H), 3.75 (d, *J* = 10.4 Hz, 1H), 3.37 (t, *J* = 10.0 Hz, 1H), 3.18 (d, *J* = 13.1 Hz, 2H), 2.72 (t, *J* = 12.1 Hz, 1H), 2.50 (dt, *J* = 12.7, 2.7 Hz, 1H), 2.03 – 1.80 (m, 1H), 1.64 – 1.37 (m, 1H), 0.87 (d, *J* = 6.9 Hz, 3H), 0.83 (d, *J* = 6.9 Hz, 3H); 13C NMR (100.6 MHz, CDCl3) δ: 137.8, 129.4, 128.5, 127.4, 66.9, 59.0, 57.7, 41.9, 28.60, 20.2, 19.8; HRMS (DART-TOF) calcd. for C20H27NO [M+H]+ *m/z* 298.2165, found 298.2158. [α]D 23 = + 101.4 (*c* = 1.00, CHCl3).

Assignment 1: ^{1}H and ^{13}C Spectra

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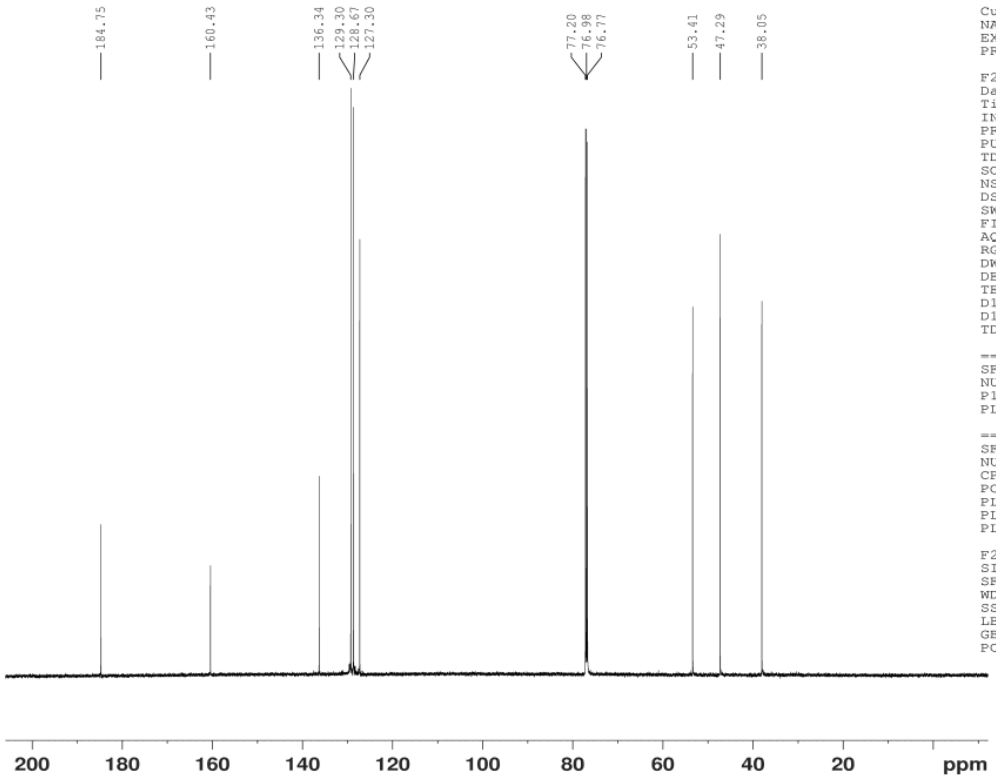


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NUC1                       13C
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======== CHANNEL f2 ========
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CPDPRG[2             waltz16
PCPD2               90.00 usec
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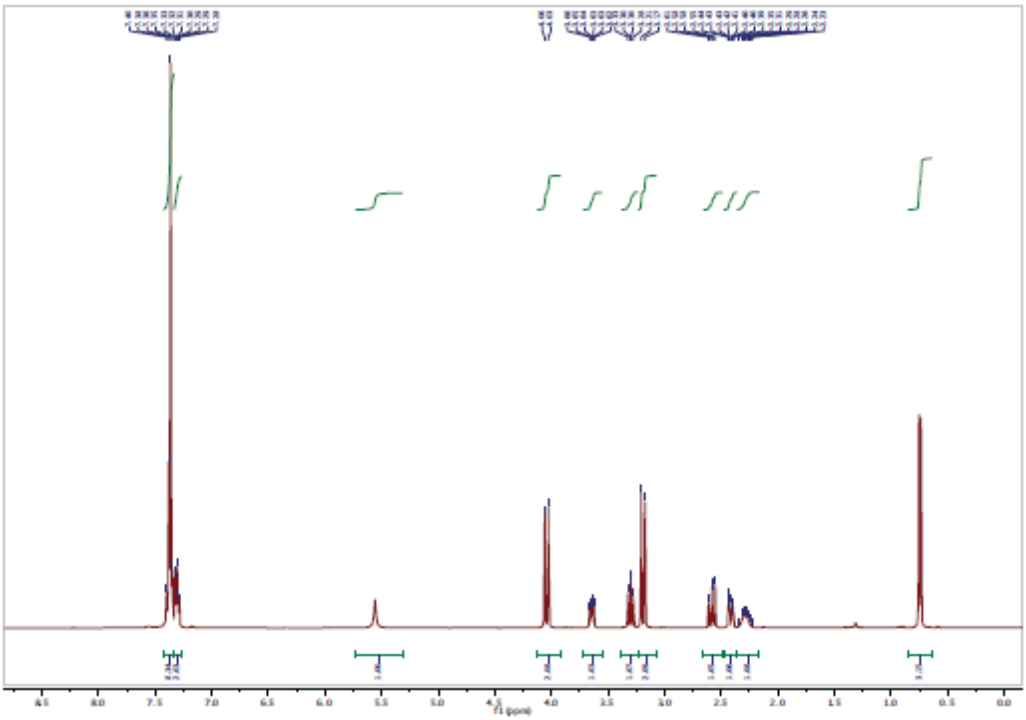
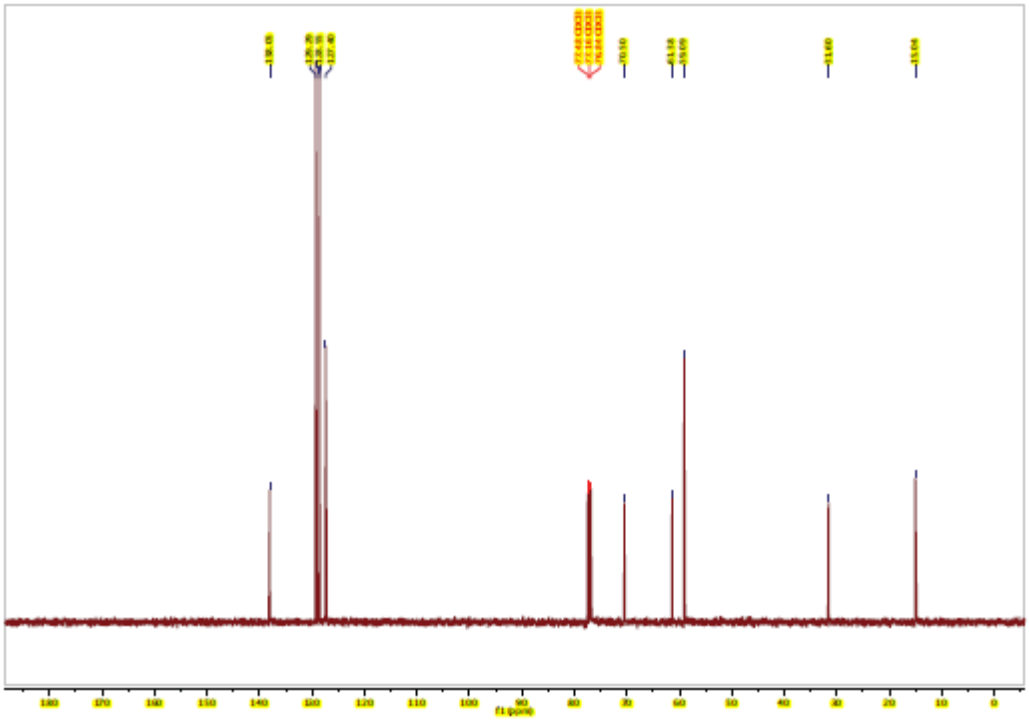
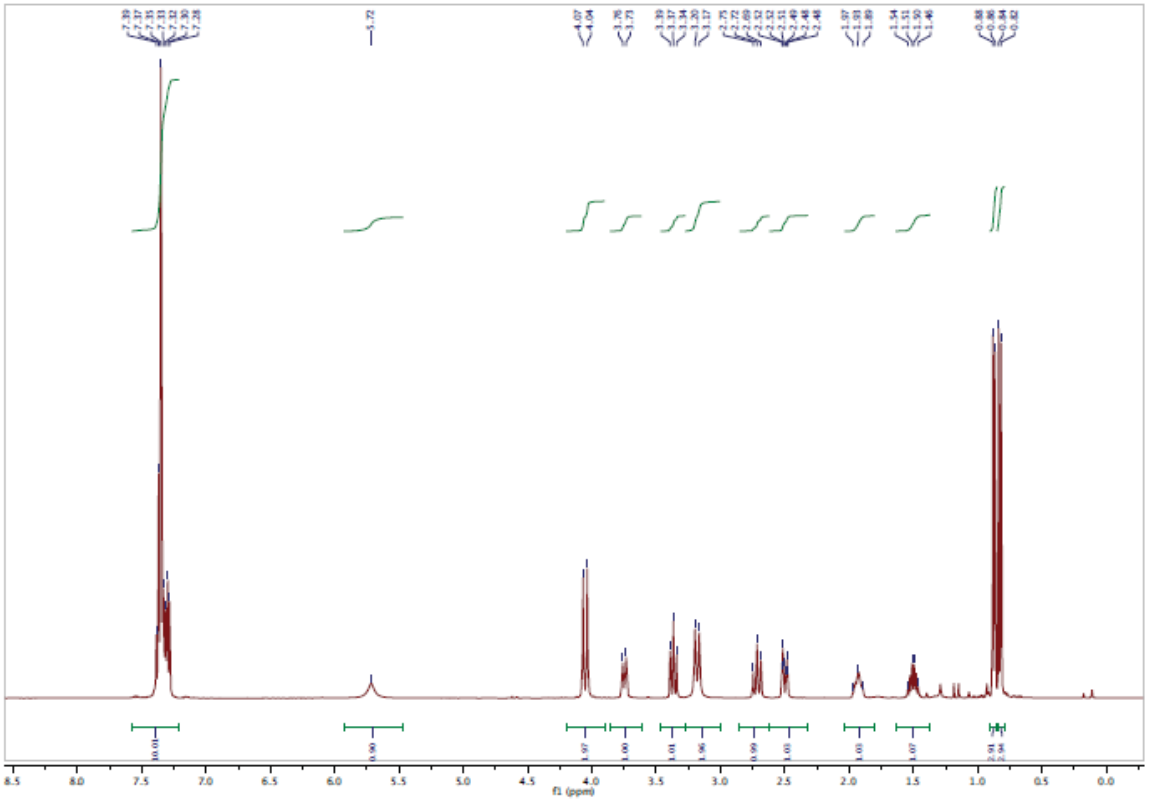
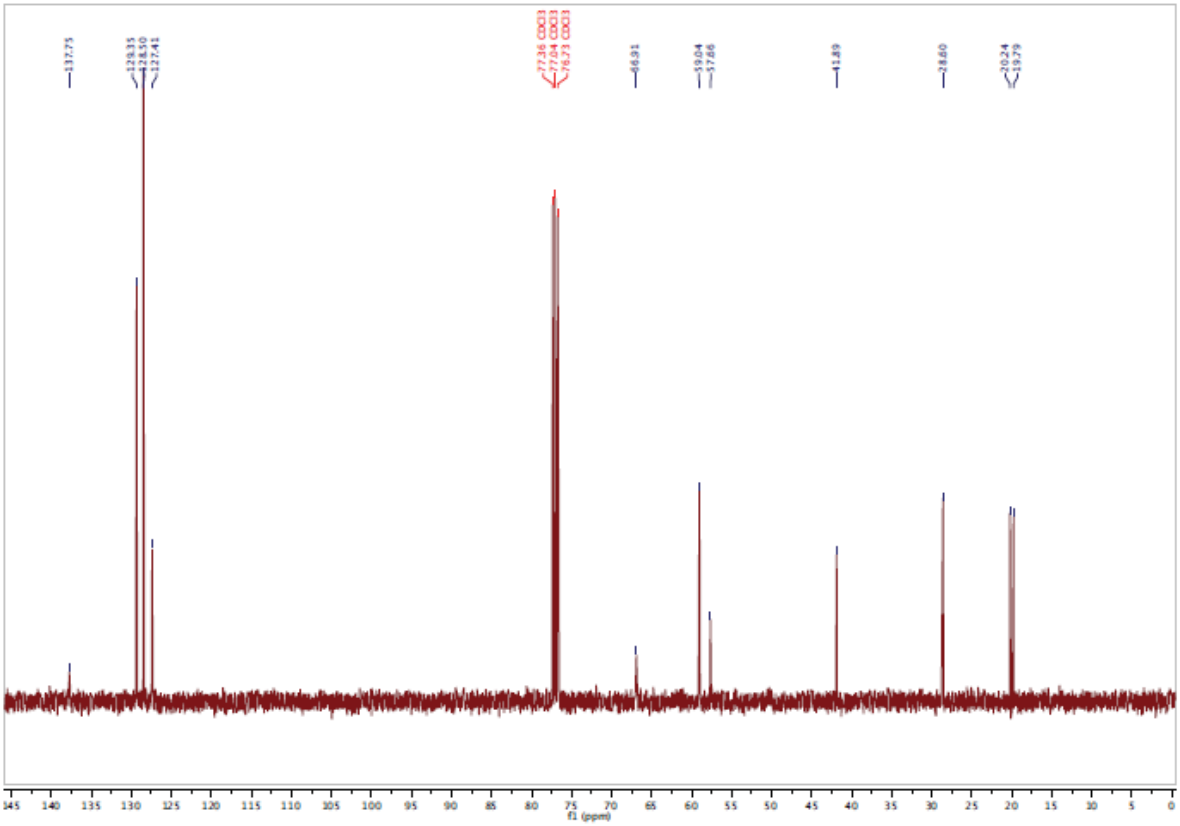
Assignment 2: ^{1}H and ^{13}C Spectra





Assignment 3: ^{1}H and ^{13}C Spectra

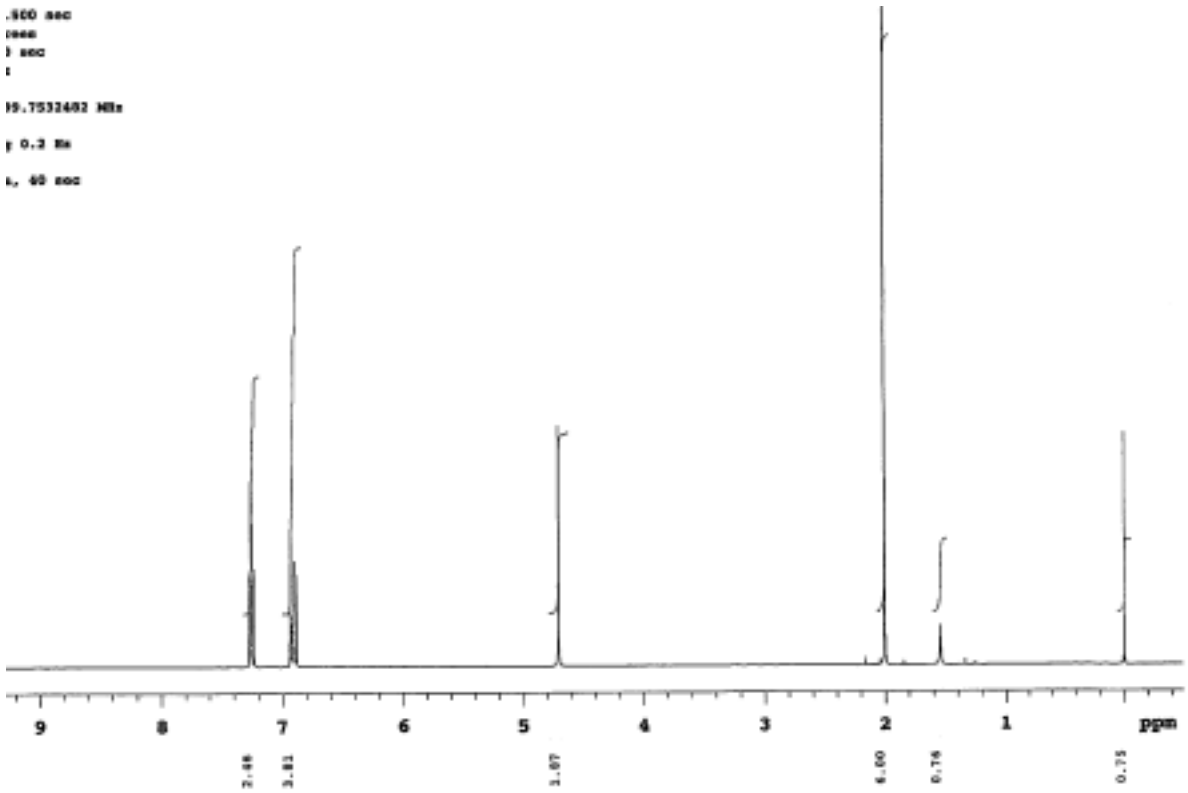


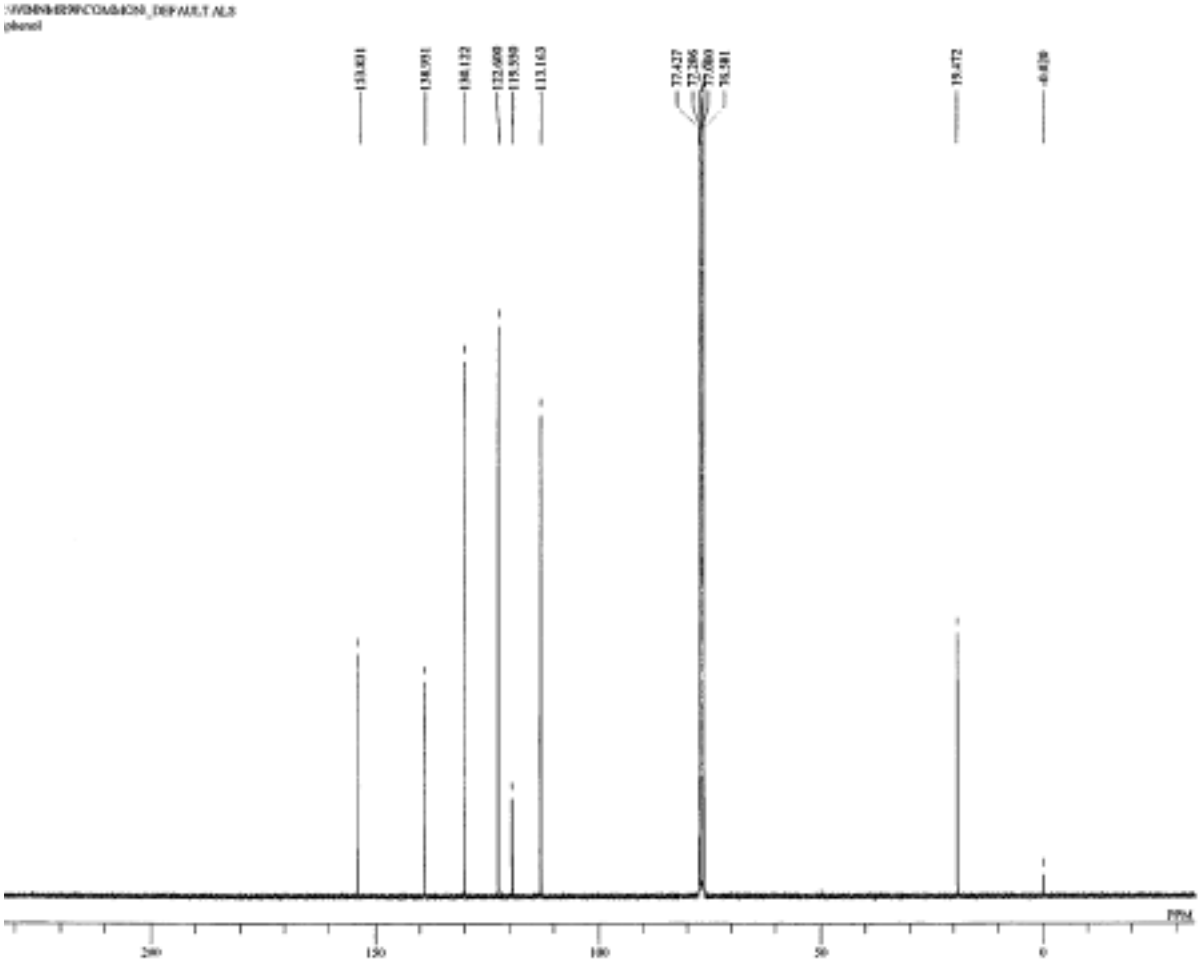


Assignment 4:

Analytical data: A white solid; $[\alpha]_D$ = –76.2 (c 0.99, $CHCl_3$); **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.25 (dd, 2H, *J* = 7.9, 7.9 Hz), 6.92 (d, 2H, *J* = 7.9 Hz), 6.90 (d, 2H, *J* = 7.9 Hz), 4.71 (s, 2H), 2.01 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 153.8, 139.0, 130.1, 122.6, 119.6, 113.2, 19.5; IR ($CHCl_3$) 3537, 3317, 2924, 1609, 1578, 1462, 1327, 1281, 1261, 1177, 1080, 1022, 1007, 949 cm^{-1}; MS (EI) *m/z* 214 (M+, 96), 199 (100), 181 (31), 171 (20), 152 (16); Calcd for $C_{14}H_{14}O_2$: C, 78.48; H, 6.59%. Found: C, 78.25; H, 6.46%.

Assignment 4: ^{1}H and ^{13}C Spectra

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PPM
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100
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