Supporting Information

***Org. Commun*. 9:4 (2016) 102-107**

Oxidation reaction of 4-allyl-4-hydroperoxy-2-methoxycyclohexa-2,5-dienone in the presence of potassium permanganate absent co-oxidant

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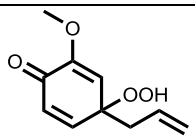
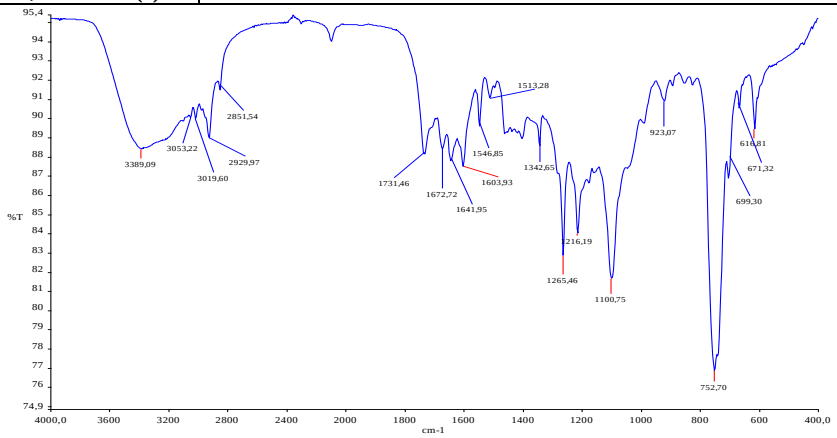
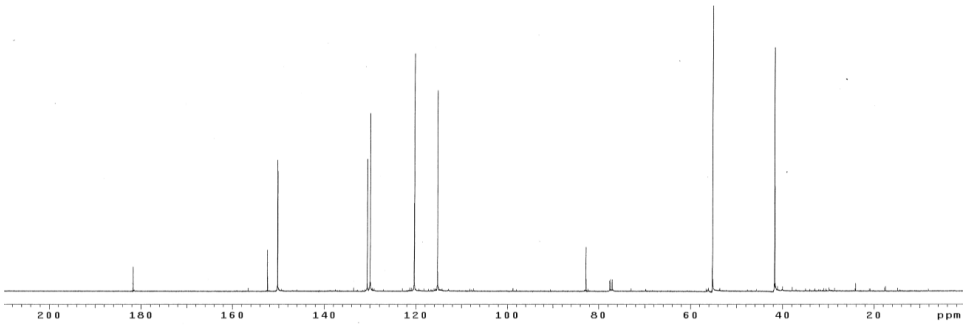
S1: Spectral data of reported compounds

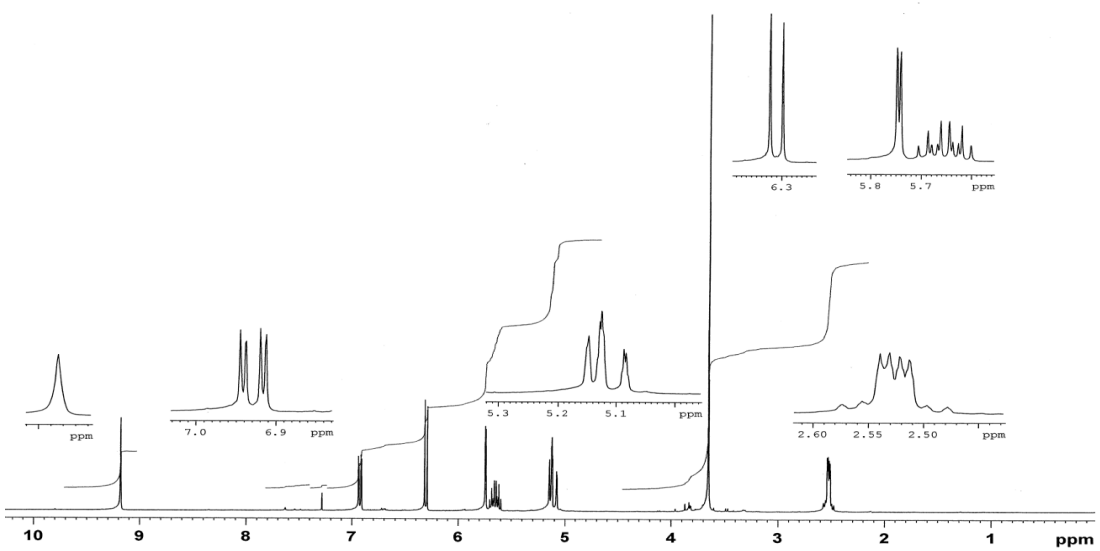


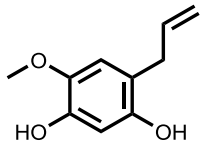
4-allyl-4-hydroperoxy-2-methoxycyclohexa-2,5-dienone (5)

^{1}H-NMR (400 MHz, $CDCl_3$, ppm): δ 9.49 (bs, 1H), 6.88 (dd, 1H, *J* = *9.8*, *2.9* Hz), 6.25 (d, 1H, *J* = *9.8* Hz), 5.71 (d, 1H, *J* = *2.9* Hz), 5.60 (m, 1H), 5.03 (m, 2H), 3.59 (s, 3H), 2.46 (m, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 181.7, 152.4, 150.2, 130.6, 129.9, 120.3, 115.2, 82.7, 55.2, 41.6. IR (KBr, cm^{-1}): 3389.1, 2929.9, 1731.5, 1672.7, 1265.5, 1216.2, 1100.7, 752.9



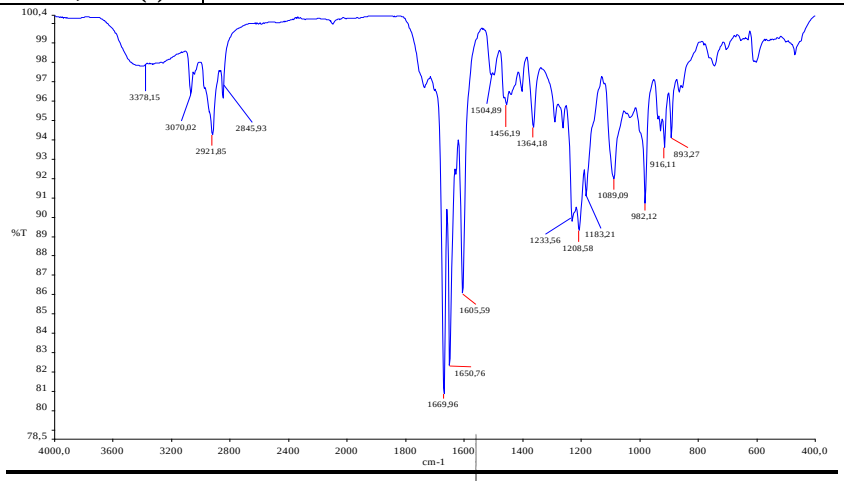


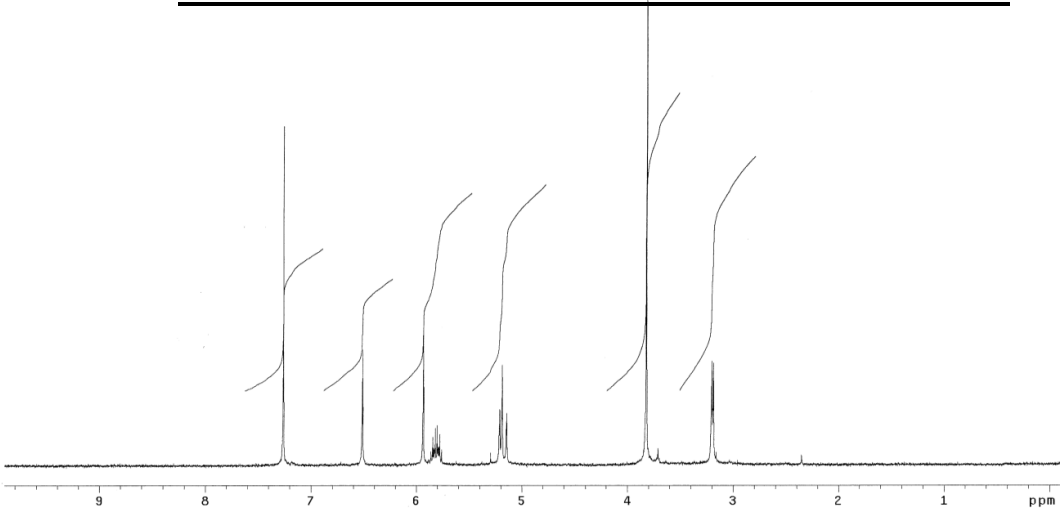


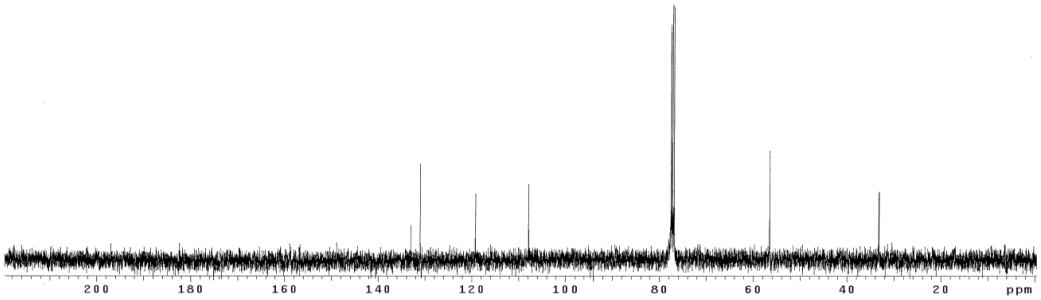


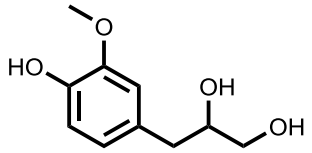
4-allyl-6-methoxybenzene-1,3-diol (6)

^{1}H-NMR (400 MHz, $CDCl_3$, ppm): δ 6.52 (s, 1H), 5.93 (s, 1H), 5.80 (m, 1H), 5.18 (m, 2H), 3.82 (s, 3H), 3.19 (m, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 132.9, 131.1, 107.8, 119.3, 33.1. IR (KBr, cm^{-1}): 3378.1, 2921.8, 1669.9, 1605.6, 1208.6, 1089.1.



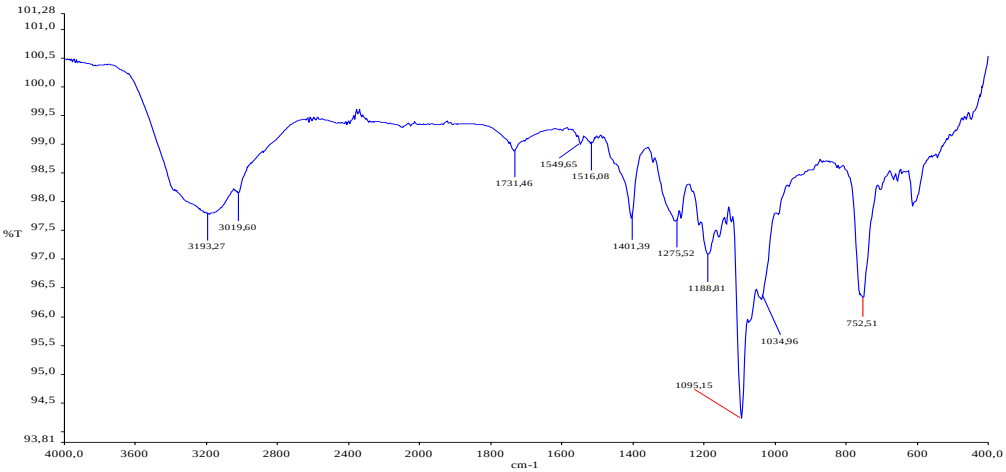


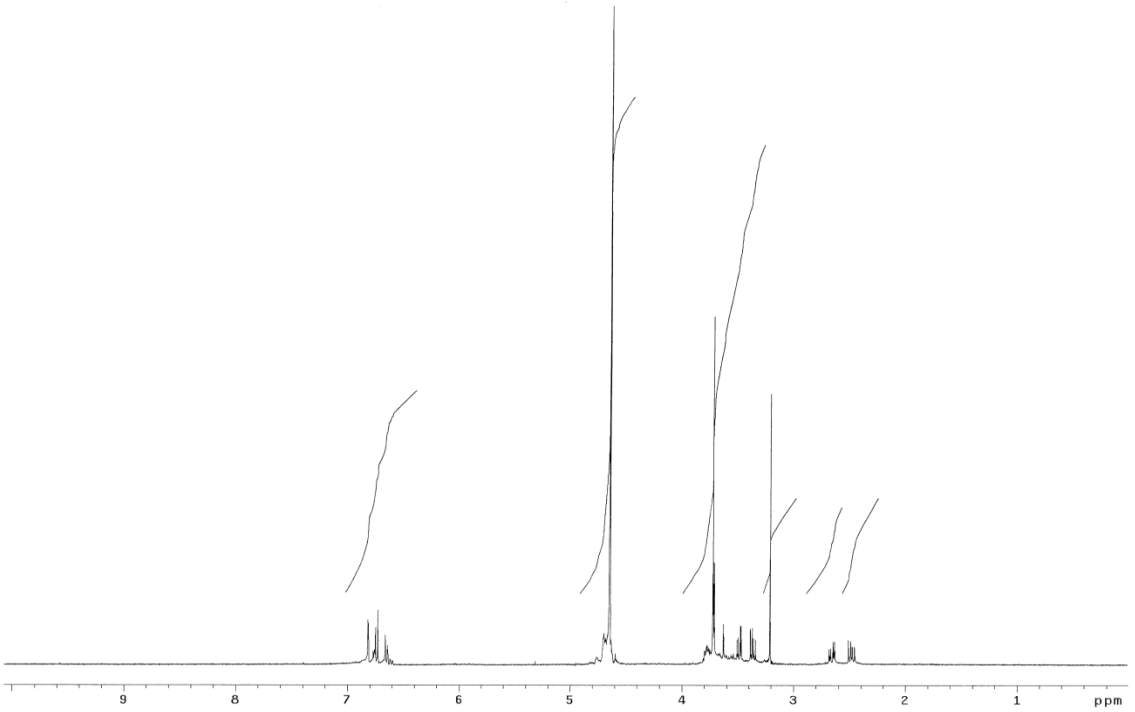


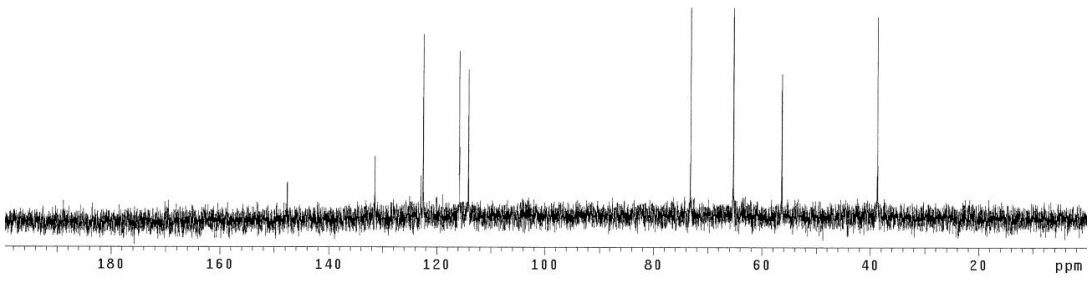


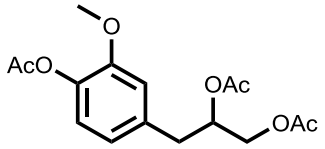
3-(4-hydroxy-3-methoxyphenyl)propane-1,2-diol (7)

^{1}H-NMR (400 MHz, D_2O, ppm): δ 6.80 (d, 1H, *J* = 1,8 Hz), δ 6.73 (d, 1H, *J* = 8,0 Hz), 6.65 (dd, 1H, *J* = 8.0, 1.8 Hz), 3.75 (m, 1H), 3.72 (s, 3H), 3.48 (dd, 1H, *J* = 11.7, 3.9 Hz), 3.35 (dd, 1H, *J* = 11.7, 6.6 Hz), 2.65 (dd, 1H, *J* = 13.9, 5.1 Hz), 2.48 (dd, 1H, *J* = 13.9, 8.4 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 147.5, 131.4, 122.9, 122.5, 115.8, 114.1, 73.1, 65.2, 56.3, 38.6. IR (KBr, cm^{-1}): 3193.3, 3019.6, 1401.4, 1275.5, 1188.8, 1095.1.



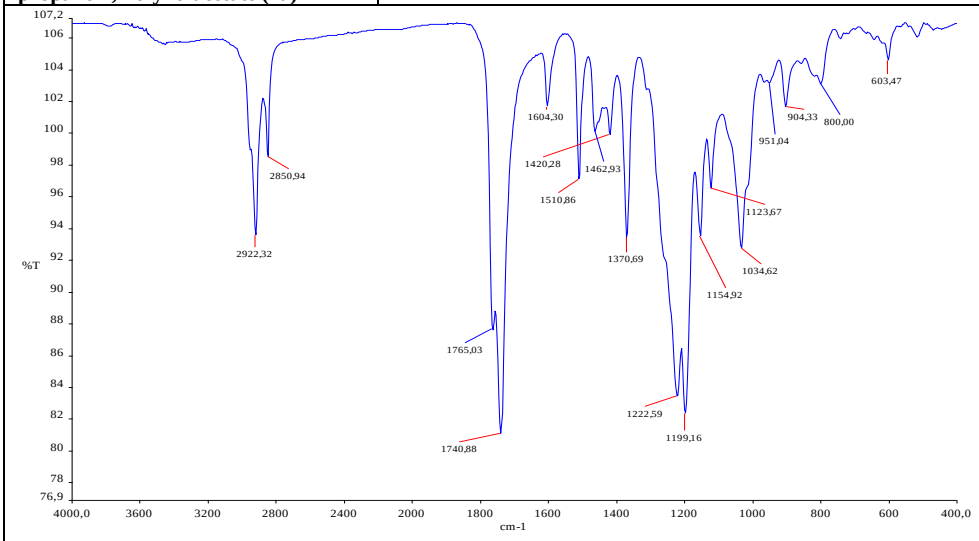


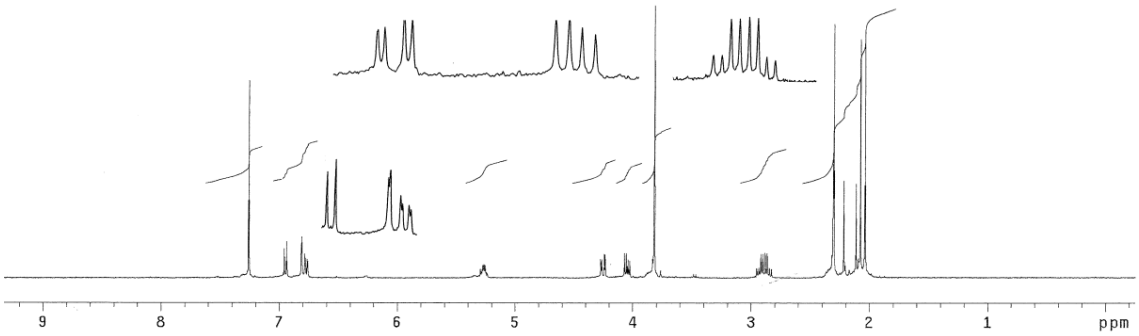


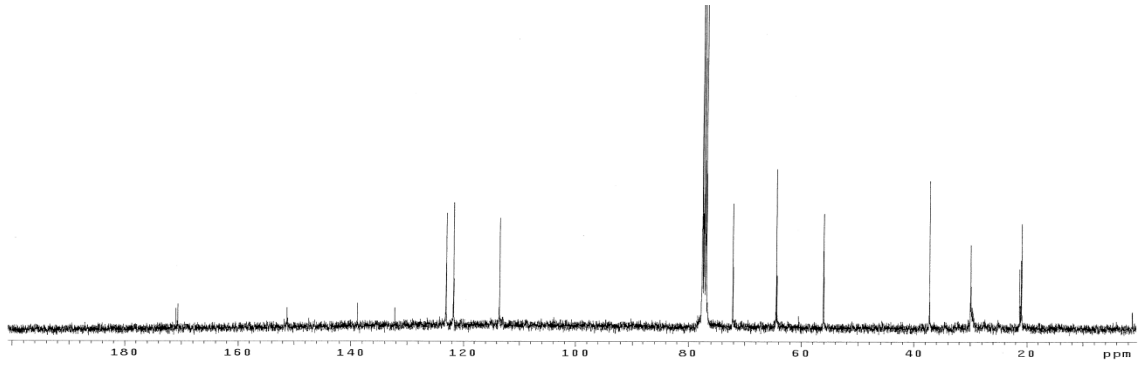


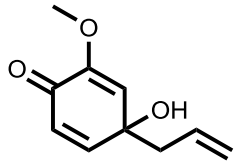
3-(4-acetoxy-3-methoxyphenyl) propane-1,2-diyl diacetate (7a)

^{1}H-NMR (400 MHz, $CDCl_3$, ppm): δ 6.95 (d, 1H, *J* = 8.0 Hz), δ 6.81 (d, 1H, *J* = 1.8 Hz), 6.77 (dd, 1H, *J* = 8.0, 1.8 Hz), 5.26, (m, 1H), 4.25 (dd, 1H, *J* = 11.9, 3.3 Hz), 4.04 (dd, 1H, *J* = 11.9, 6.2 Hz), 3.82 (s, 3H), 2.93 (dd, 1H, *J* = 13.9, 6.8 Hz), 2.85 (dd, 1H, *J* = 13.9, 6.8 Hz), 2.30 (s, 3H), 2.09 (s, 3H), 2.04 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 170.9, 170.6, 151.2, 138.8, 132.2, 122.9, 121.7, 113.5, 72.1, 64.4, 56.1, 37.2, 29.9, 21.0, 20.9. IR (KBr, cm^{-1}): 2922.3, 1765.0, 1510.9, 1370.7, 1199.2, 1034.6.



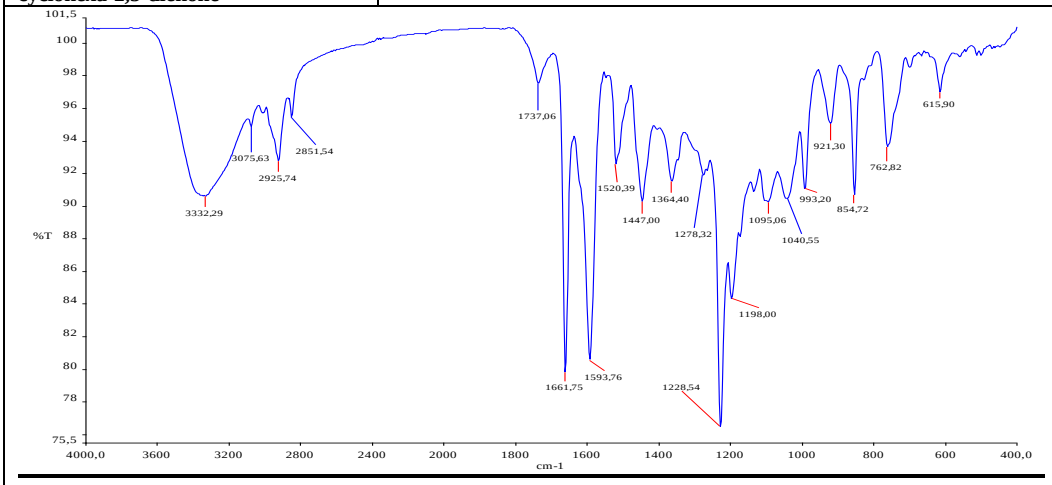


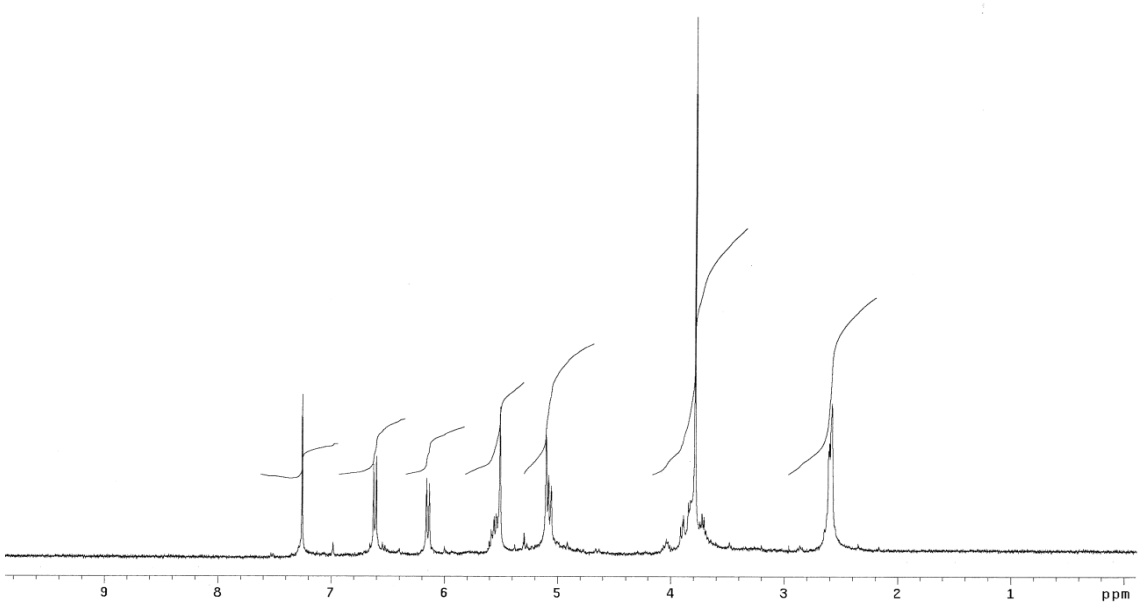


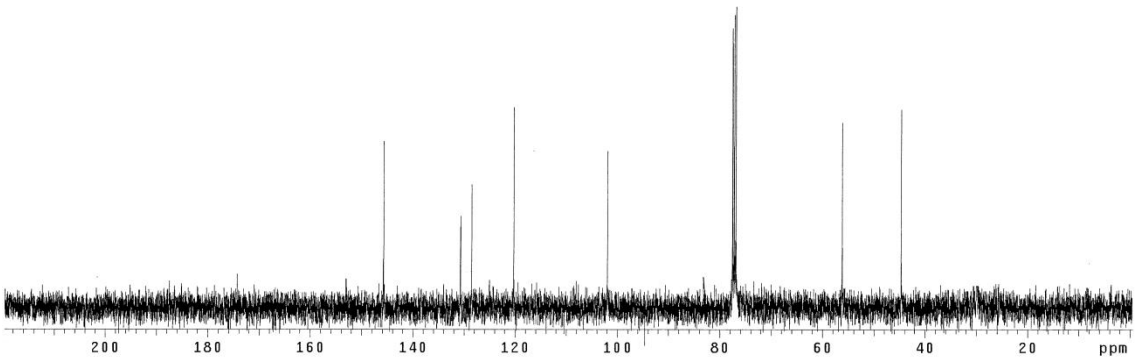


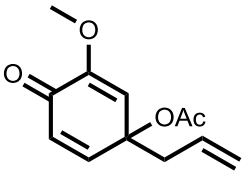
4-allyl-4-hydroxy-2-methoxy cyclohexa-2,5-dienone

^{1}H-NMR (400 MHz, $CDCl_3$, ppm): δ 6.61 (d, 1H, *J* = 10.1 Hz), 6.15 (d, 1H, *J* = 10.1 Hz), 5.52, (s, 1H), 5.51 (m, 1H), 5.08 (m, 2H), 3.79 (s, 3H), 2.59 (m, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 174.1, 154.2, 145.7, 130.8, 128.5, 120.3, 101.9, 82.3, 56.2, 44.6. IR (KBr, cm^{-1}): 3332.3, 2925.7, 1737.1, 1661.7, 1593.8, 1228.5, 1095.1.



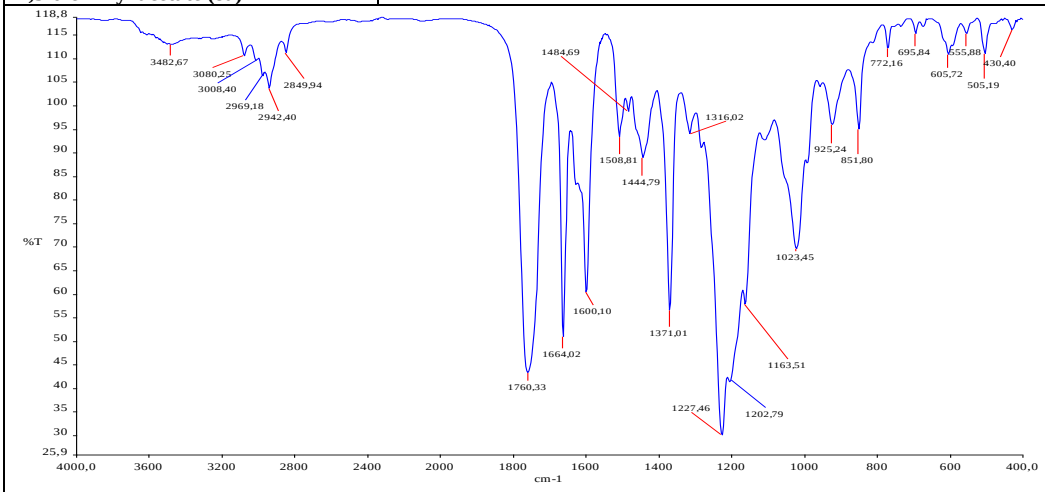


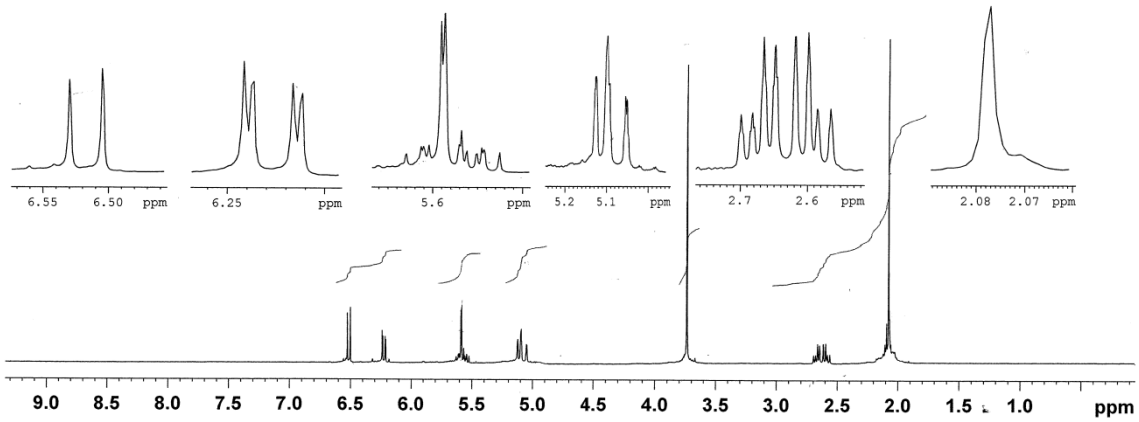


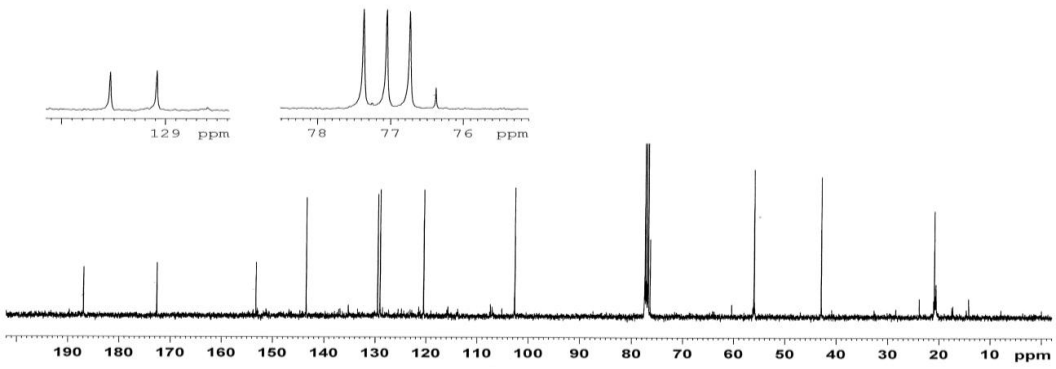


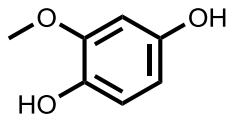
1-allyl-3-methoxy-4-oxocyclohexa-2,5-dien-1-yl acetate (8a)

^{1}H-NMR (400 MHz, $CDCl_3$, ppm): δ 6.52 (d, 1H, *J* = 10.1 Hz), δ 6.22 (dd, 1H, *J* = 10.1, 1.8 Hz), 5.59, (d, 1H, *J* = 1.8 Hz), 5.57 (m, 1H), 5.09 (m, 2H), 3.73 (s, 3H), 2.66 (dd, 1H, *J* = 13.5, 6.8 Hz), 2.58 (dd, 1H, *J* = 13.5, 7.9 Hz), 2.08 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 186.8, 172.6, 156.1, 143.4, 129.5, 129.1, 120.4, 102.6, 76.4, 56.0, 42.9. IR (KBr, cm^{-1}): 2942.4, 1760.3, 1664.0, 1371.0, 1227.5, 1023.4.



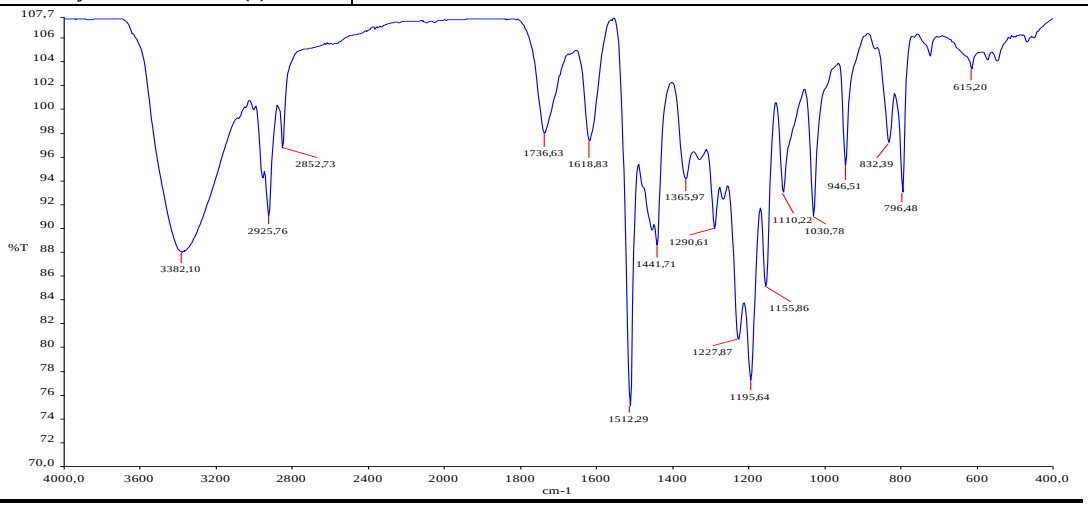


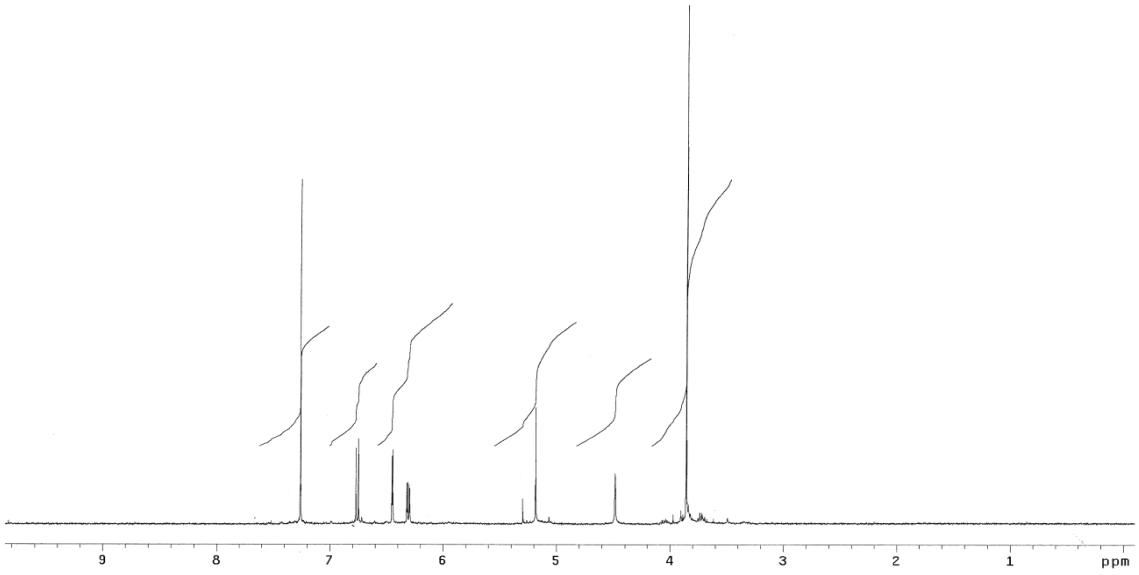


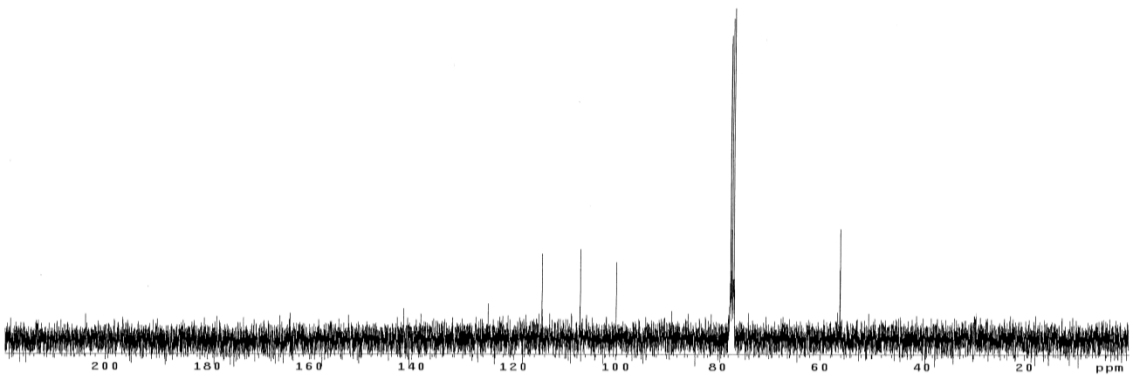


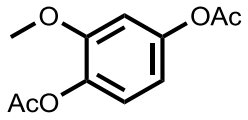
2-methoxybenzene-1,4-diol (9)

^{1}H-NMR (400 MHz, $CDCl_3$, ppm): δ 6.76 (d, 1H, *J* = 8.4 Hz), 6.44 (d, 1H, *J* = 2.8 Hz), 6.31 (dd, ??, *J* = 8.4, 2.8 Hz), 5.18 (bs, 1H), 4.48 (bs, 1H), 3.86 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 140.5, 124.9, 114.5, 107.0, 99.8, 56.4. IR (KBr, cm^{-1}): 3382.1, 2925.8, 1736.6, 1618.8, 1582.3, 1227.9, 1195.6.









2-methoxy-1,4-phenylene diacetate (9a)

^{1}H-NMR (400 MHz, $CDCl_3$, ppm): δ 7.01 (d, 1H, J = 8.6 Hz), δ 6.73 (d, 1H, J = 2.5 Hz), 6.68 (dd,1H, J = 8.6, 2.5 Hz), 3.81 (s, 3H), 2.31 (s, 3H), 2.29 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, ppm): δ 169.3, 168.9, 151.6, 148.9, 137.3, 122.9, 113.3, 106.5, 56.0, 21.1, 20.6. IR (KBr, cm^{-1}): 2938.9, 1765.7, 1604.8, 1509.3, 1268.9, 1216.8, 1197.5, 1035.2.