Supporting Information

Palladium-Catalyzed Decarboxylation of Allenyl 3-Oxoalkanoates: An Efficient Synthesis of 3,4-Allenyl Ketones

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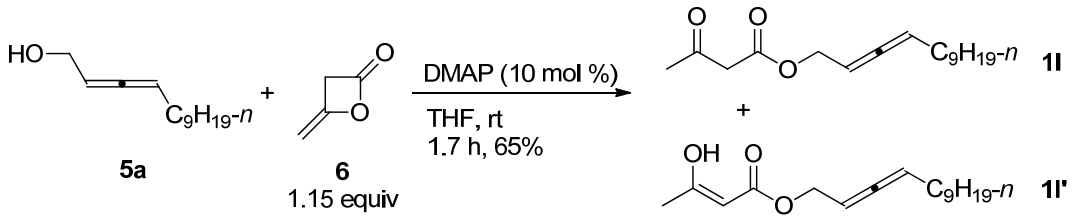
General Information. All reactions were carried out in oven-dried Schlenk tubes. DPEphos was purchased from Acros. *t*-BuOH was distilled over magnesium turnings with I_2. THF and DME were distilled over sodium wire with diphenyl ketone as the indicator. All the temperatures are referred to the oil baths used. Aged starting materials may cause a lower yield of the products, thus, fresh starting materials are recommended. For the synthesis of the ketoesters **1**, the data of ^{1}H NMR with * indicate the peaks of the enol form.

1. Synthesis of starting materials 1

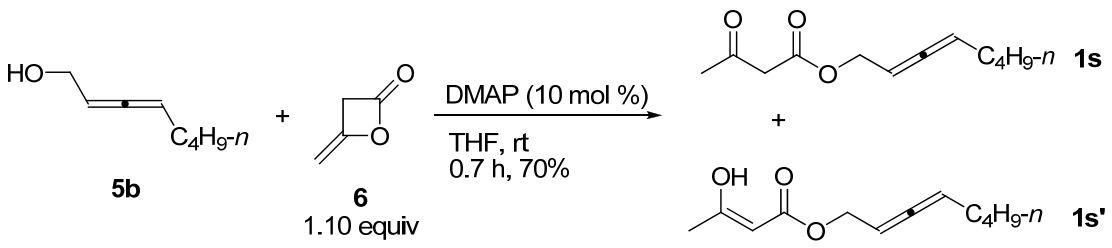
(1) Trideca-2,3-dienyl 3-oxobutanoate (1l)



Typical Procedure I: To a round-bottomed flask were added sequentially **5a** (1.9600 g, 10.0 mmol), THF (30 mL), **6** (950.0 mg, 11.5 mol), and DMAP (119.1 mg, 1.0 mmol). The resulting mixture was stirred at room temperature. Upon completion as monitored by TLC, the reaction was quenched with saturated aqueous $NaHCO_3$, extracted with Et_2O, and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20/1) afforded **1l** and **1l'** (1.8154 g, 65%, ketone : enol = 7.7:1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.30-5.16 (m, 2 H, HC=C=CH), 4.65-4.51 (m, 2 H, OCH_2), 3.43 (s, 2 H, $COCH_2$), 2.25 (s, 3 H, $COCH_3$), 2.06-1.90 (m, 2 H, $C=CCH_2$), 1.47-1.10 (m,

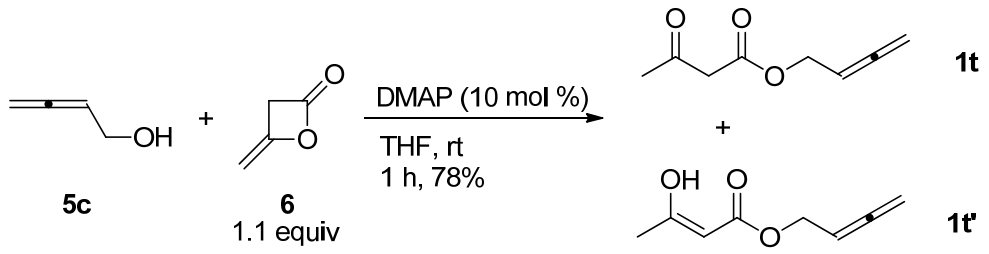
14 H，C_7H_{14}), 0.85 (t, J = 6.6 Hz, 3 H, CH_3). The following signals are discernible for **1l'**: δ 12.00* (s, 1 H, OH), 4.97* (s, 1 H, C=CH); IR (neat, cm^{-1}): 2926, 2855, 1967, 1747, 1721, 1653, 1456, 1361, 1228, 1151, 1029; MS (70 ev, EI) *m/z* (%): 280 (M^+, 0.80), 43 (100); Anal. Calcd. for $C_{17}H_{28}O_3$ (%): C 72.82, H 10.06; Found: C 72.83, H 10.19.

(2) Octa-2,3-dienyl 3-oxobutanoate (1s)



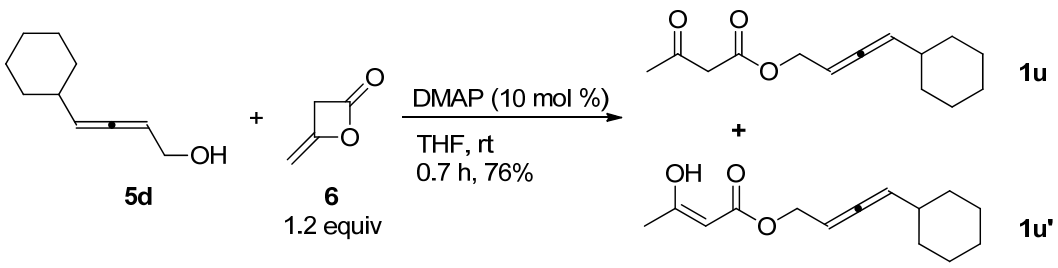
Following the procedure for the preparation of **1l**, the reaction of **5b** (379.3 mg, 3.0 mmol), THF (16 mL), **6** (273.1 mg, 3.3 mol), and DMAP (36.7 mg, 0.3 mmol) afforded **1s** and **1s'** (441.3 mg, 70%, ketone : enol = 9.1:1) (eluent: petroleum ether/ethyl acetate = 15/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.33-5.16 (m, 2 H, HC=C=CH), 4.67-4.53 (m, 2 H, OCH_2), 3.45 (s, 2 H, $COCH_2$), 2.27 (s, 3 H, $COCH_3$), 2.07-1.93 (m, 2 H, $C=CCH_2$), 1.45-1.19 (m, 4 H, C_2H_4), 0.89 (t, J = 6.9 Hz, 3 H, CH_3). The following signals are discernible for **1s'**: δ 12.01* (s, 1 H, OH), 4.99* (s, 1 H, C=CH); IR (neat, cm^{-1}): 2959, 2931, 2867, 1966, 1747, 1720, 1651, 1451, 1412, 1363, 1315, 1233, 1149, 1028; MS (70 ev, EI) *m/z* (%): 192 (M^+-H_2O, 0.64), 83 (100); Anal. Calcd. for $C_{12}H_{18}O_3$ (%): C 68.54, H 8.63; Found: C 68.47, H 8.53.

(3) Buta-2,3-dienyl 3-oxobutanoate (1t)



Following the procedure for the preparation of **1l**, the reaction of **5c** (1.0524 g, 15.0 mmol), THF (40 mL), **6** (1.3550 g, 16.5 mol), and DMAP (182.1 mg, 1.5 mmol) afforded **1t** and **1t'** (1.8017 g, 78%, ketone : enol = 10:1) (eluent: petroleum ether/ethyl acetate = 10/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.35-5.22 (m, 1 H, CH=C=C), 4.89-4.80 (m, 2 H, C=C=CH_2), 4.67-4.56 (m, 2 H, OCH_2), 3.45 (s, 2 H, $COCH_2$), 2.25 (s, 3 H, CH_3). The following signals are discernible for **1t'**: δ 11.96* (s, 1 H, OH), 4.98* (s, 1 H, C=CH), 1.94* (s, 3 H, CH_3); IR (neat, cm^{-1}): 2956, 1958, 1746, 1721, 1652, 1440, 1411, 1361, 1313, 1269, 1150, 1030; MS (70 ev, EI) *m/z* (%): 111 (M^+-$COCH_3$, 1.18), 43 (100); Anal. Calcd. for $C_8H_{10}O_3$ (%): C 62.33, H 6.54; Found: C 62.12, H 6.61.

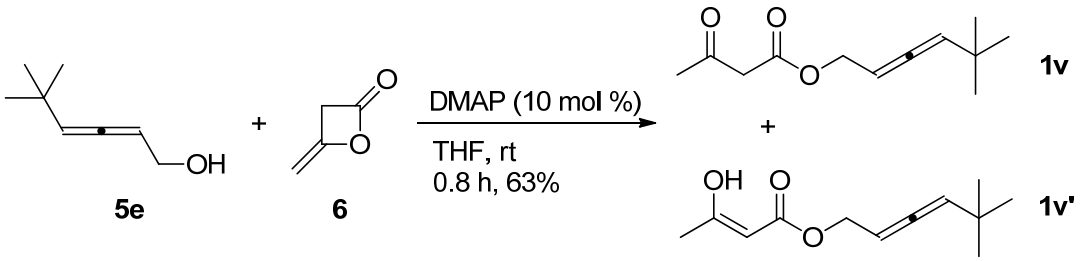
(4) 4-Cyclohexylbuta-2,3-dienyl 3-oxobutanoate (1u)



Following the procedure for the preparation of **1l**, the reaction of **5d** (2.7050 g, 17.7 mmol), THF (50 mL), **6** (1.7541 g, 21.3 mol), and DMAP (216.7 mg, 1.77 mmol) afforded **1u** and **1u'** (3.1713 g, 76%, ketone : enol = 10:1) (eluent: petroleum

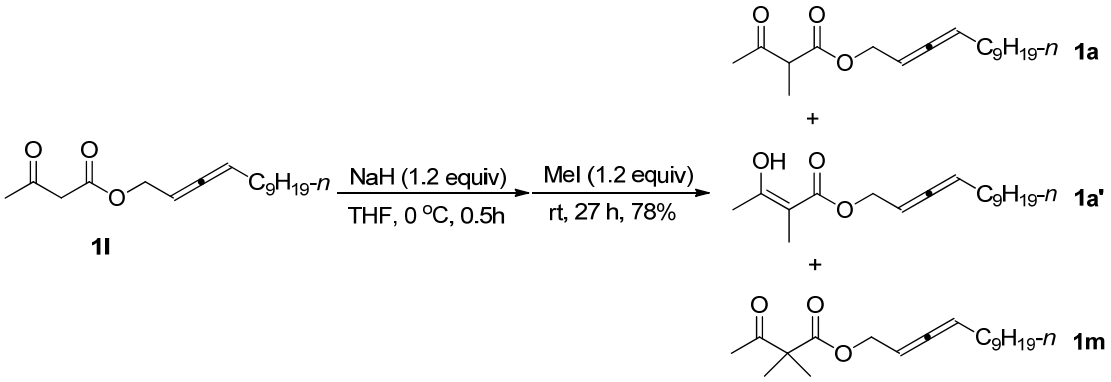
ether/ethyl ether = 10/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.34-5.20 (m, 2 H, HC=C=CH), 4.67-4.53 (m, 2 H, OCH_2), 3.45 (s, 2 H, CH_2), 2.26 (s, 3 H, CH_3), 2.06-1.92 (m, 1 H, C=CCH), 1.80-1.55 (m, 5 H), 1.35-0.98 (m, 5 H). The following signals are discernible for **1u'**: δ 12.02* (s, 1 H, OH), 4.99* (s, 1 H, C=CH); IR (neat, cm^{-1}): 2926, 2852, 1963, 1745, 1720, 1651, 1448, 1411, 1362, 1314, 1267, 1230, 1149, 1028; MS (70 ev, EI) *m/z* (%): 151 (M^+-$C_4H_5O_2$, 10.24), 43 (100); Anal. Calcd. for $C_{14}H_{20}O_3$ (%): C 71.16, H 8.53; Found: C 71.37, H 8.72.

(5) 5,5-Dimethylhexa-2,3-dienyl 3-oxobutanoate (1v)



Following the procedure for the preparation of **1l**, the reaction of **5e** (2.0462 g, 16.2 mmol), THF (50 mL), **6** (1.4625 g, 17.8 mol), and DMAP (198.1 mg, 1.62 mmol) afforded **1v** and **1v'** (2.1488 g, 63%, ketone : enol = 8.3:1) (eluent: petroleum ether/ethyl ether = 10/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.34-5.21 (m, 2 H, HC=C=CH), 4.67-4.52 (m, 2 H, OCH_2), 3.45 (s, 2 H, $COCH_2$), 2.26 (s, 3 H, $COCH_3$), 1.03 (s, 9 H, 3×CH_3). The following signals are discernible for **1v'**: δ 12.02* (s, 1 H, OH), 4.99* (s, 1 H, C=CH), 1.94* (s, 3 H, $C=CCH_3$); IR (neat, cm^{-1}): 2961, 2905, 2868, 1964, 1746, 1721, 1651, 1457, 1412, 1362, 1315, 1255, 1149, 1028; MS (70 ev, EI) *m/z* (%): 210 (M^+, 1.52), 43 (100); HRMS Calcd for $C_{12}H_{18}O_3$ (M^+): 210.1256; Found: 210.1257.

(6) Trideca-2,3-dienyl 2-methyl-3-oxobutanoate (1a) and trideca-2,3-dienyl 2,2-dimethyl-3-oxobutanoate (1m)



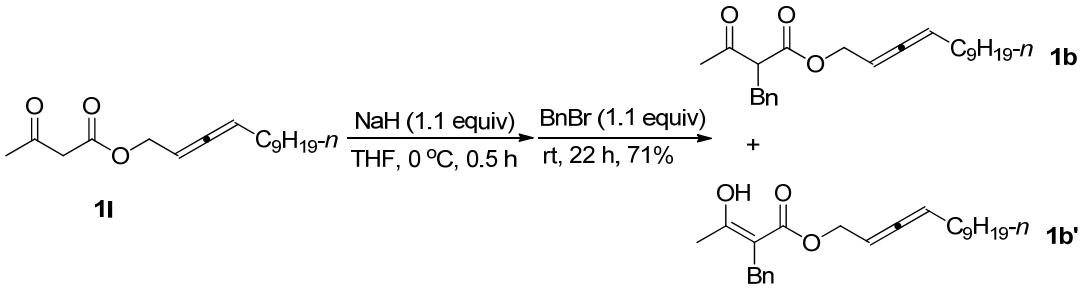
Typical Procedure II: To a suspension of NaH (60% in mineral oil, 145.0 mg, 3.6 mol) in THF (4 mL) was added **1l** (836.3 mg, 3.0 mmol) at 0 °C and the reaction mixture was stirred for 30 min at 0 °C. To the resulting mixture was added MeI (0.23 mL, d = 2.28 g/mL, 524.4 mg, 3.6 mol). The reaction mixture was allowed to warm up to room temperature and stirred for 27 h. The reaction was quenched with saturated NaCl, extracted with Et_2O, and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and chromatography on silica gel (eluent: petroleum ether/ethyl ether = 50/1) afforded **1a**/**1a'** (681.5 mg, 78%, ketone : enol = 10.7:1) and **1m** (155.8 mg, 17%).

1a and **1a'**: liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.32-5.16 (m, 2 H, HC=C=CH), 4.67-4.52 (m, 2 H, OCH_2), 3.51 (q, *J* = 7.2 Hz, 1 H, CH), 2.24 (s, 3 H, CH_3), 2.06-1.93 (m, 2 H, $C=CCH_2$), 1.47-1.17 (m, 17 H, CH_3 and C_7H_{14}), 0.87 (t, *J* = 6.6 Hz, 3 H, CH_3). The following signals are discernible for **1a'**: δ 12.61* (s, 1 H, OH), 1.75* (s, 3 H, CH_3); IR (neat, cm^{-1}): 2926, 2855, 1963, 1746, 1720, 1457, 1377, 1359, 1325, 1239, 1194, 1153; MS (70 ev, EI) *m/z* (%): 195 (M^+-$C_5H_7O_2$, 5.31), 43 (100); Anal.

Calcd. for $C_{18}H_{30}O_3$ (%): C 73.43, H 10.27; Found: C 73.60, H 10.35.

1m: liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.33-5.17 (m, 2 H, HC=C=CH), 4.66-4.53 (m, 2 H, OCH_2), 2.16 (s, 3 H, $COCH_3$), 2.05-1.94 (m, 2 H, $C=CCH_2$), 1.45-1.20 (m, 20 H, 2×CH_3 and C_7H_{14}), 0.88 (t, J = 6.6 Hz, 3 H, CH_3); ^{13}C NMR (300 MHz, $CDCl_3$) δ 205.62, 205.56, 173.2, 93.1, 86.3, 63.6, 55.6, 31.8, 29.5, 29.4, 29.2, 29.0, 28.8, 28.2, 25.7, 22.6, 21.78, 21.76, 14.0; IR (neat, cm^{-1}): 2926, 2855, 1965, 1717, 1466, 1264, 1152, 1116; MS (70 ev, EI) *m/z* (%): 195 (M^+-$C_6H_9O_2$, 12.21), 85 (100); Anal. Calcd. for $C_{19}H_{32}O_3$ (%): C 73.98, H 10.46; Found: C 74.29, H 10.41.

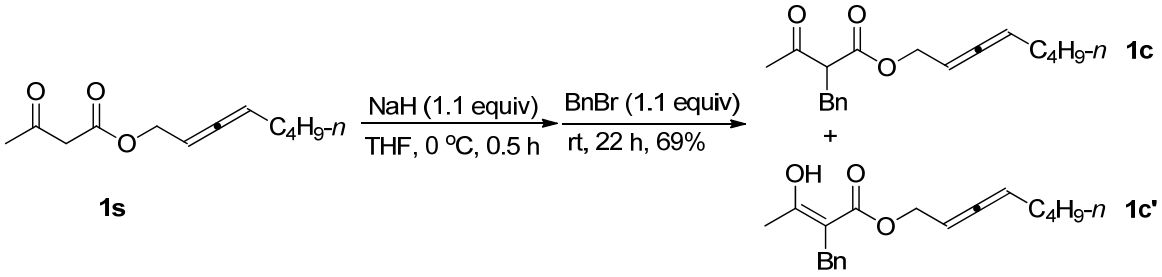
(7) Trideca-2,3-dienyl 2-benzyl-3-oxobutanoate (1b)



Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 88.1 mg, 2.2 mol), THF (4 mL), **1l** (561.3 mg, 2.0 mmol), and BnBr (376.4 mg, 2.2 mol, ketone : enol = 10.3:1) afforded **1b** and **1b'** (531.3 mg, 71%) (eluent: petroleum ether/ethyl acetate = 50/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33-7.12 (m, 5 H, Ar-H), 5.32-5.11 (m, 2 H, HC=C=CH), 4.63-4.48 (m, 2 H, OCH_2), 3.79 (t, J = 7.7 Hz, 1 H, CH), 3.17 (d, J = 7.5 Hz, 2 H, CH_2 of Bn), 2.19 (s, 3 H, $COCH_3$), 2.07-1.93 (m, 2 H, $C=CCH_2$), 1.48-1.17 (m, 14 H, C_7H_{14}), 0.88 (t, J = 6.6 Hz, 3 H, CH_3). The following signals are discernible for **1b'**: δ 12.89* (s, 1 H, OH), 3.59* (s, 2 H, CH_2); IR (neat, cm^{-1}): 2926, 2854, 1965, 1745, 1719, 1456, 1361, 1207, 1143; MS (70 ev, EI) *m/z* (%): 370 (M^+, 0.50), 195 (M^+-$C_{11}H_{11}O_2$, 1.73), 175 (100);

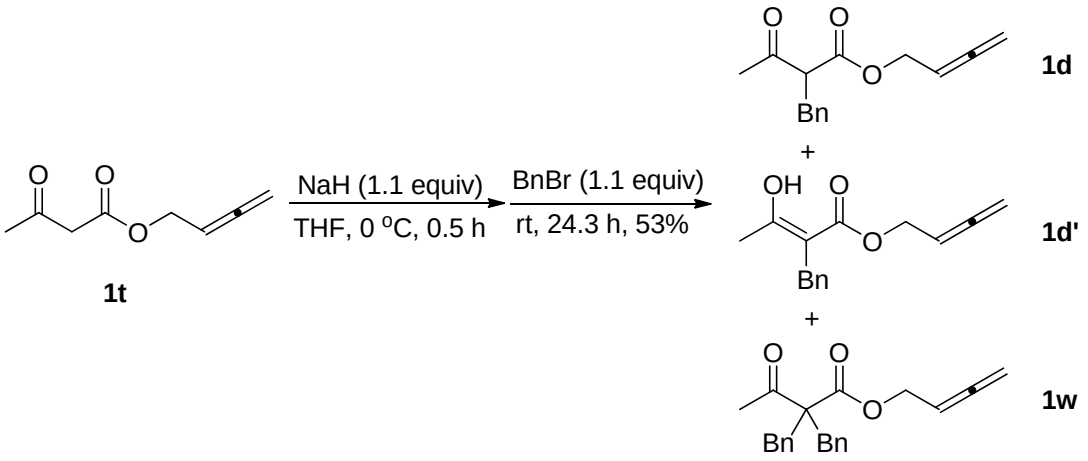
HRMS Calcd for $C_{24}H_{34}O_3$ (M^+): 370.2508, Found: 370.2498. Anal. Calcd. for $C_{24}H_{34}O_3$ (%): C 77.80, H 9.25; Found: C 77.37, H 9.37.

(8) Octa-2,3-dienyl 2-benzyl-3-oxobutanoate (1c)



Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 88.6 mg, 2.2 mol), THF (4 mL), **1s** (418.7 mg, 2.0 mmol), and BnBr (377.2 mg, 2.2 mol) afforded **1c** and **1c'** (412.7 mg, 69%, ketone : enol = 13.3:1) (eluent: petroleum ether/ethyl acetate = 50/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33-7.13 (m, 5 H, Ar-H), 5.32-5.11 (m, 2 H, HC=C=CH), 4.63-4.48 (m, 2 H, OCH_2), 3.80 (t, *J* = 7.7 Hz, 1 H, CH), 3.17 (d, *J* = 7.8 Hz, 2 H, CH_2), 2.19 (s, 3 H, $COCH_3$), 2.07-1.93 (m, 2 H, $C=CCH_2$), 1.45-1.23 (m, 4 H, C_2H_4), 0.90 (t, *J* = 7.1 Hz, 3 H, CH_3). The following signals are discernible for **1c'**: δ 12.90* (s, 1 H, OH), 3.59* (s, 2 H, CH_2); IR (neat, cm^{-1}): 2958, 2930, 2865, 1965, 1744, 1719, 1645, 1607, 1496, 1451, 1361, 1243, 1210, 1143; MS (70 ev, EI) *m/z* (%): 300 (M^+, 1.20), 43 (100); HRMS Calcd for $C_{19}H_{24}O_3$ (M^+): 300.1725; Found: 300.1729.

(9) Buta-2,3-dienyl 2-benzyl-3-oxobutanoate (1d) and buta-2,3-dienyl 2,2-dibenzyl-3-oxobutanoate (1w)



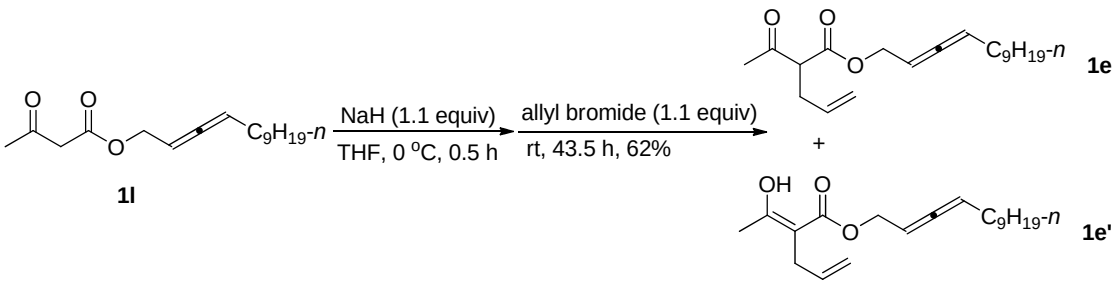
Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 236.1 mg, 5.87 mol), THF (4 mL), **1t** (754.1 mg, 4.89 mmol) and BnBr (915.0 mg, 5.38 mol) afforded **1d** and **1d'** (627.8 mg, 53%, ketone : enol = 16.7:1) (eluent: petroleum ether/ethyl acetate = 50/1) and **1w** (306.7 mg, 19%).

1d and **1d'**: liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.12 (m, 5 H, Ar-H), 5.30-5.12 (m, 1 H, HC=C=C), 4.89-4.77 (m, 2 H, C=C=CH_2), 4.67-4.49 (m, 2 H, OCH_2), 3.80 (t, *J* = 7.7 Hz, 1 H, CH), 3.17 (d, *J* = 7.7 Hz, 2 H, CH_2 of Bn), 2.19 (s, 3 H, CH_3). The following signals are discernible for **1d'**: δ 12.86* (s, 1 H, OH), 3.59* (s, 2 H, CH_2), 2.04* (s, 3 H, CH_3); IR (neat, cm^{-1}): 2936, 1958, 1743, 1717, 1645, 1606, 1496, 1448, 1358, 1209, 1145; MS (70 ev, EI) *m/z* (%): 244 (M^+, 3.26), 131 (100); HRMS Calcd for $C_{15}H_{16}O_3$ (M^+): 244.1099; Found: 244.1100.

1w: liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.18 (m, 6 H, Ar-H), 7.18-7.09 (m, 4 H, Ar-H), 5.23-5.12 (m, 1 H, HC=C=C), 4.87-4.82 (m, 2 H, C=C=CH_2), 4.58-4.52 (m, 2 H, OCH_2), 3.22 (s, 4 H, 2×CH_2), 1.96 (s, 3 H, CH_3); ^{13}C NMR (300 MHz, $CDCl_3$) δ 210.1, 205.5, 171.4, 136.2, 130.1, 128.3, 126.9, 85.5, 76.7, 66.1, 63.0, 39.8, 29.2; IR (neat, cm^{-1}): 3063, 3031, 2932, 1957, 1740, 1710, 1603, 1495, 1449, 1355, 1265, 1229, 1182, 1085; MS (70 ev, EI) *m/z* (%): 334 (M^+, 1.96), 91 (100); HRMS

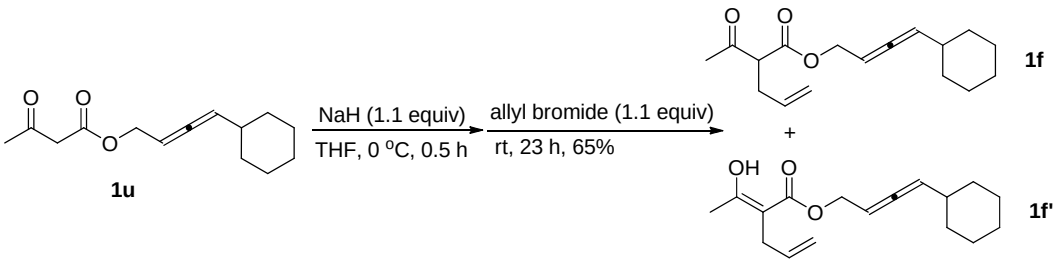
Calcd for $C_{22}H_{22}O_3$ (M^+): 334.1569; Found: 334.1567.

(10) Trideca-2,3-dienyl 2-acetylpent-4-enoate (1e)



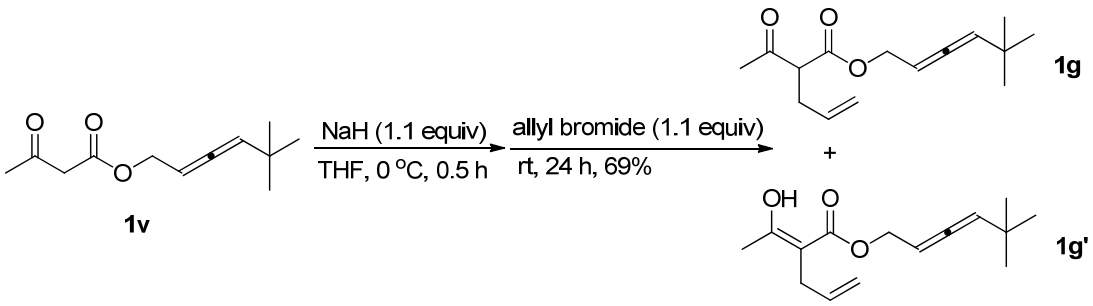
Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 88.7 mg, 2.2 mol), THF (4 mL), **1l** (562.2 mg, 2.0 mmol), and allyl bromide (266.7 mg, 2.2 mol) afforded **1e** and **1e'** (399.6 mg, 62%, ketone : enol = 9.6:1) (eluent: petroleum ether/ethyl acetate = 50/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.87-5.67 (m, 1 H), 5.32-5.17 (m, 2 H), 5.15-4.92 (m, 2 H), 4.67-4.52 (m, 2 H, OCH_2), 3.52 (t, *J* = 7.2 Hz, 1 H, CH), 2.58 (t, *J* = 6.9 Hz, 2 H, CH_2), 2.22 (s, 3 H, CH_3), 2.08-1.91 (m, 2 H, C=C=CCH_2), 1.48-1.13 (m, 14 H, C_7H_{14}), 0.86 (t, *J* = 6.3 Hz, 3 H, CH_3). The following signals are discernible for **1e'**: δ 12.74* (s, 1 H, OH), 2.92* (d, *J* = 5.7 Hz, 2 H, CH_2 of allyl); IR (neat, cm^{-1}): 2927, 2855, 1966, 1745, 1720, 1644, 1443, 1361, 1239, 1147; MS (70 ev, EI) *m/z* (%): 195 (M^+-$C_7H_9O_2$, 3.10), 43 (100); Anal. Calcd. for $C_{20}H_{32}O_3$ (%): C 74.96, H 10.06; Found: C 75.02, H 10.24.

(11) 4-Cyclohexylbuta-2,3-dienyl 2-acetylpent-4-enoate (1f)



Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 132.5 mg, 3.3 mol), THF (6 mL), **1u** (708.5 mg, 3.0 mmol), and allyl bromide (399.7 mg, 3.3 mol) afforded **1f** and **1f'** (538.6 mg, 65%, ketone : enol = 13.8:1) (eluent: petroleum ether/ethyl acetate = 60/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.85-5.65 (m, 1 H), 5.32-5.20 (m, 2 H), 5.13-4.91 (m, 2 H), 4.66-4.52 (m, 2 H, OCH_2), 3.52 (t, *J* = 7.4 Hz, 1 H, CH), 2.58 (t, *J* = 7.2 Hz, 2 H, CH_2 of allyl), 2.22 (s, 3 H, CH_3), 2.05-1.90 (m, 1 H, C=C=CCH), 1.79-1.55 (m, 5 H), 1.35-0.98 (m, 5 H). The following signals are discernible for **1f'**: δ 12.75* (s, 1 H, OH), 2.93* (d, *J* = 6.0 Hz, 2 H, CH_2 of allyl); IR (neat, cm^{-1}): 2926, 2852, 1964, 1744, 1718, 1643, 1446, 1360, 1330, 1229, 1183, 1149; MS (70 ev, EI) *m/z* (%): 151 (M^+-$C_7H_9O_2$, 5.67), 43 (100); Anal. Calcd. for $C_{17}H_{24}O_3$ (%): C 73.88, H 8.75; Found: C 74.18, H 8.80.

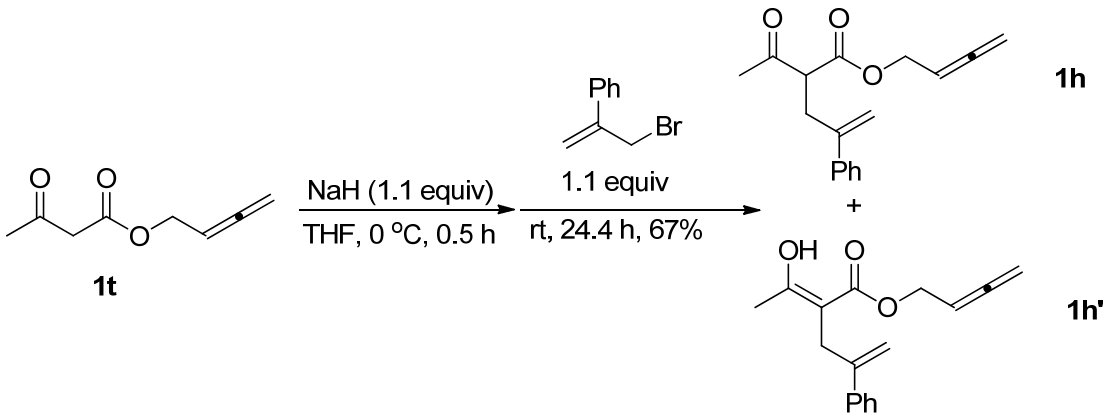
(12) 5,5-Dimethylhexa-2,3-dienyl 2-acetylpent-4-enoate (1g)



Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 132.7 mg, 3.3 mol), THF (6 mL), **1v** (630.2 mg, 3.0 mmol), and allyl bromide (399.8 mg, 3.3 mol) afforded **1g** and **1g'** (517.3 mg, 69%, ketone : enol =

11.7:1) (eluent: petroleum ether/ethyl acetate = 50/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.83-5.65 (m, 1 H), 5.33-5.20 (m, 2 H), 5.13-4.89 (m, 2 H), 4.66-4.50 (m, 2 H, OCH_2), 3.51 (t, *J* = 7.2 Hz, 1 H, CH), 2.58 (t, *J* = 7.2 Hz, 2 H, CH_2 of allyl), 2.22 (s, 3 H, $COCH_3$), 1.02 (s, 9 H, 3×CH_3). The following signals are discernible for **1g'**: δ 12.74* (s, 1 H, OH), 2.92* (d, *J* = 6.0 Hz, 2 H, CH_2), 1.97* (s, 3 H, CH_3); IR (neat, cm^{-1}): 3076, 2961, 2868, 1964, 1744, 1719 1644, 1441, 1362, 1329, 1244, 1185, 1151; MS (70 ev, EI) *m/z* (%): 250 (M^+, 1.80), 43 (100); HRMS Calcd for $C_{15}H_{22}O_3$ (M^+): 250.1569; Found: 250.1571.

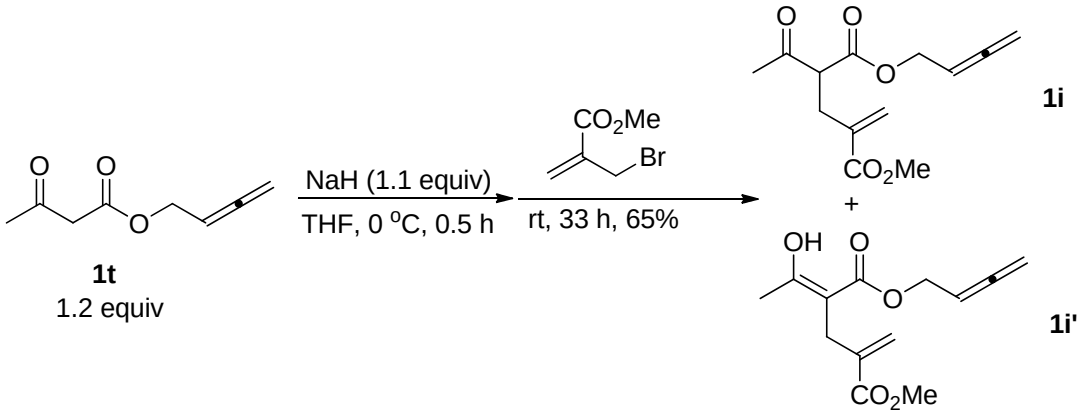
(13) Buta-2,3-dienyl 2-acetyl-4-phenylpent-4-enoate (1h)



Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 132.3 mg, 3.3 mol), THF (15 mL), **1t** (462.7 mg, 3.0 mmol), and 2-phenylallyl bromide (650.0 mg, 3.3 mol) afforded **1h** and **1h'** (540.1 mg, 67%, ketone : enol = 15.4:1) (eluent: petroleum ether/ethyl acetate = 50/1) as a liquid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.24 (m, 5 H, Ar-H), 5.30 (s, 1 H, one proton of $C=CCH_2$), 5.28-5.18 (m, 2 H), 5.11 (s, 1 H, one proton of $C=CCH_2$), 4.95-4.79 (m, 2 H, $C=C=CH_2$), 4.67-4.52 (m, 2 H, OCH_2), 3.62 (t, *J* = 7.2 Hz, 1 H, CH), 3.15-3.02 (m, 2 H, CH_2), 2.18 (s, 3 H, CH_3). The following signals are discernible for **1h'**: 12.89* (s,

1 H, OH), 3.35* (s, 2 H, CH_2), 1.98* (s, 3 H, CH_3); IR (neat, cm^{-1}): 1957, 1740, 1715, 1630, 1574, 1494, 1443, 1358, 1262, 1244, 1212, 1145, 1064, 1027; MS (70 ev, EI) *m/z* (%): 270 (M^+, 0.58), 43 (100); Anal. Calcd. for $C_{17}H_{18}O_3$ (%): C 75.53, H 6.71; Found: C 75.75, H 6.88.

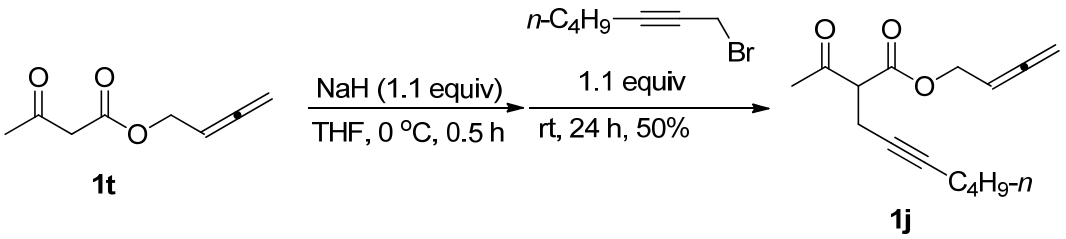
(14) Buta-2,3-dienyl 2-acetyl-4-(methoxycarbonyl)pent-4-enoate (1i)



Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 176.2 mg, 4.4 mol), THF (20 mL), **1t** (738.2 mg, 4.8 mmol), and methyl 2-(bromomethyl)acrylate (715.7 mg, 4.0 mol) afforded **1i** and **1i'** (655.6 mg, 65%, ketone : enol = 18.2:1) (eluent: petroleum ether/ethyl acetate = 25/1) as a liquid: ^1H NMR (400 MHz, $CDCl_3$) δ 6.18 (s, 1 H, one proton of CH_2), 5.63 (s, 1 H, one proton of CH_2), 5.27-5.18 (m, 1 H, HC=C=C), 4.85-4.77 (m, 2 H, C=C=CH_2), 4.63-4.50 (m, 2 H, OCH_2), 3.81 (t, *J* = 7.2 Hz, 1 H, CH), 3.73 (s, 3 H, CH_3), 2.87-2.73 (m, 2 H, CH_2), 2.22 (s, 3 H, CH_3). The following signals are discernible for **1i'**: δ 12.83* (s, 1 H, OH), 6.14* (s, 1 H, one proton of CH_2), 5.40* (m, 1 H, one proton of CH_2), 3.17* (s, 2 H, CH_2), 1.95* (s, 3 H, CH_3); IR (neat, cm^{-1}): 2954, 1958, 1714, 1632, 1440, 1359, 1342, 1263, 1221, 1195, 1138, 1070; MS (70 ev, EI) *m/z* (%): 183 (M^+-C_4H_5O, 16.69), 43 (100); Anal. Calcd. for $C_{13}H_{16}O_5$ (%): C 61.90, H 6.39; Found: C 62.08, H

6.31.

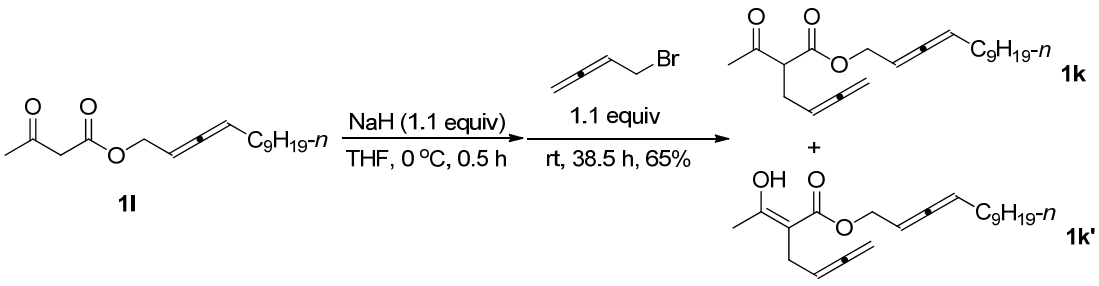
(15) Buta-2,3-dienyl 2-acetylnon-4-ynoate (1j)



1t **1j**

Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 354.0 mg, 8.8 mol), THF (40 mL), **1t** (1.2336 g, 8.0 mmol), and 1-bromohept-2-yne (1.5409 g, 8.8 mol) afforded **1j** (999.6 mg, 50%) (eluent: petroleum ether/ethyl acetate = 50/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.35-5.22 (m, 1 H), 4.89-4.80 (m, 2 H), 4.68-4.55 (m, 2 H), 3.64 (t, *J* = 7.5 Hz, 1 H), 2.73-2.63 (m, 2 H), 2.28 (s, 3 H), 2.15-2.02 (m, 2 H), 1.50-1.27 (m, 4 H), 0.87 (t, *J* = 6.9 Hz, 3 H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 209.9, 201.5, 168.2, 85.8, 82.6, 76.9, 75.7, 63.1, 58.8, 30.8, 29.5, 21.8, 18.2, 18.0, 13.5; IR (neat, cm^{-1}): 2958, 2933, 2873, 2237, 1959, 1744, 1719, 1643, 1618, 1462, 1434, 1358, 1268, 1221, 1140, 1070; MS (70 ev, EI) *m/z* (%): 249 (M^++1, 0.73), 43 (100); Anal. Calcd. for $C_{15}H_{20}O_3$ (%): C 72.55, H 8.12; Found: C 72.30, H 8.24.

(16) Trideca-2,3-dienyl 2-acetylhexa-4,5-dienoate (1k)

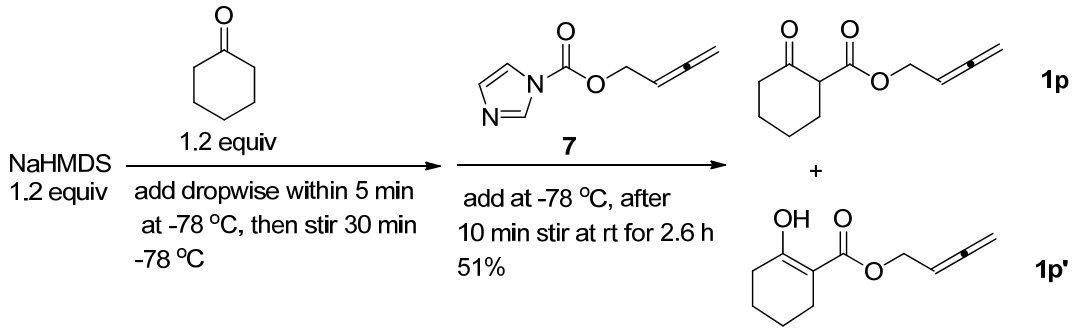


1l

Following the procedure for the preparation of **1a**, the reaction of NaH (60% in mineral oil, 110.2 mg, 2.75 mol), THF (5 mL), **1l** (702.3 mg, 2.50 mmol), and

4-bromobuta-1,2-diene (366.8 mg, 2.75 mol) afforded **1k** and **1k'** (541.3 mg, 65%, ketone : enol = 8.8:1) (eluent: petroleum ether/ethyl acetate = 50/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.32-5.05 (m, 3 H), 4.67-4.52 (m, 4 H), 3.60 (t, *J* = 7.4 Hz, 1 H, COCH), 2.61-2.46 (m, 2 H, CH_2), 2.25 (s, 3 H, $COCH_3$), 2.05-1.92 (m, 2 H, CH_2), 1.48-1.13 (m, 14 H, C_7H_{14}), 0.86 (t, *J* = 6.3 Hz, 3 H, CH_3). The following signals are discernible for **1k'**: δ 12.70* (s, 1 H, OH), 2.92-2.86* (m, 2 H, CH_2); IR (neat, cm^{-1}): 2926, 2855, 1958, 1745, 1720, 1647, 1616, 1442, 1359, 1329, 1242, 1217, 1150, 1077, 1033; MS (70 ev, EI) *m/z* (%): 332 (M^+, 0.19), 205 (M^+-C_9H_{19}, 1.38), 43 (100); Anal. Calcd. for $C_{21}H_{32}O_3$ (%): C 75.86, H 9.70; Found: C 75.88, H 9.52.

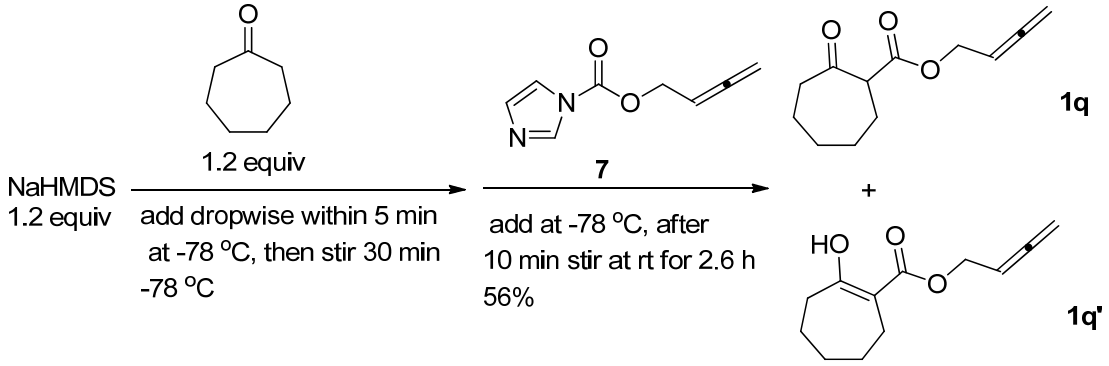
(17) Buta-2,3-dienyl 2-oxocyclohexanecarboxylate (1p)[1]



Typical Procedure III: To a solution of NaHMDS (1.3232 g, 7.2 mmol) in DME (25 mL) was added cyclohexanone (706.9 mg, 7.2 mmol) in 5 mL of DME at -78 °C within 5 min. The reaction mixture was stirred for 30 min at -78 °C. Then to the resulting mixture was added **7** (987.0 mg, 6.0 mmol). After 10 min the cooling bath was removed and the reaction was allowed to warm up to room temperature and stirred at room temperature for 2.6 h. The resulting mixture was quenched with an

aqueous solution of saturated NH_4Cl (30 mL), extracted with Et_2O (3×30 mL), and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and chromatography on silica gel (eluent: petroleum ether/dichloromethane = 2/1) afforded **1p** and **1p'** (593.8 mg, 52%, ketone : enol = 1:3.5) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.12* (s, 1 H, OH), 5.38-5.24* (m, 1 H, HC=C=C), 4.92-4.78* (m, 2 H, C=C=CH_2), 4.73-4.55* (m, 2 H, OCH_2), 2.59-1.52* (m, 8 H, 4×CH_2). The following signals are discernible for **1p**: δ 3.39 (dd, J_1 = 9.8 Hz, J_2 = 6.5 Hz, 1 H, COCH); IR (neat, cm^{-1}): 2939, 2860, 1958, 1745, 1715, 1653, 1612, 1446, 1422, 1396, 1357, 1333, 1319, 1294, 1256, 1212, 1174, 1078, 1052; MS (70 ev, EI) *m/z* (%): 194 (M^+, 2.13), 125 (100); HRMS Calcd for $C_{11}H_{14}O_3$ (M^+): 194.0943; Found: 194.0942.

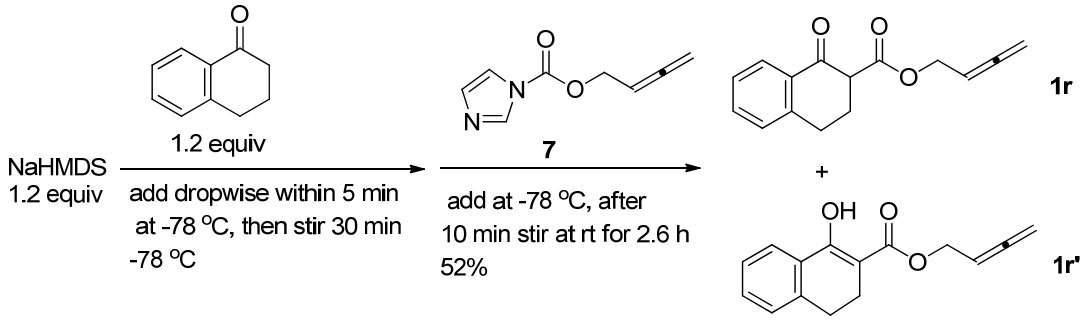
(18) Buta-2,3-dienyl 2-oxocycloheptanecarboxylate (1q)



Following the procedure for the preparation of **1p**, the reaction of NaHMDS (1.8542 g, 10.1 mmol), DME (30 mL), cycloheptanone (1.1340 g, 10.1 mmol), and **7** (1.3791 g, 8.4 mmol) afforded **1q** and **1q'** (979.7 mg, 56%, ketone : enol = 8.1:1) (eluent: petroleum ether/ethyl ether = 20/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.36-5.20 (m, 1 H, HC=C=C), 4.88-4.78 (m, 2 H, C=C=CH_2), 4.70-4.51 (m, 2 H, OCH_2), 3.60-3.48 (m, 1 H, CH), 2.69-2.35 (m, 2 H), 2.16-1.34 (m, 8 H). The following signals are discernible for **1q'**: δ 12.60* (s, 1 H, OH); IR (neat, cm^{-1}): 2929,

2855, 1958, 1741, 1704, 1638, 1610, 1454, 1395, 1376, 1354, 1307, 1262, 1238, 1212, 1181, 1154, 1123, 1040, 1010; MS (70 ev, EI) *m/z* (%): 208 (M^+, 1.45), 55 (100); HRMS Calcd for $C_{12}H_{16}O_3$ (M^+): 208.1099; Found: 208.1093.

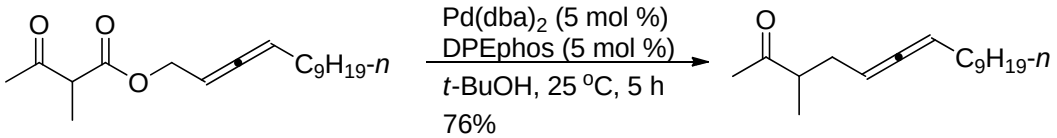
(19) Buta-2,3-dienyl 1-oxo-1,2,3,4-tetrahydronaphthalene-2-carboxylate (1r)



Following the procedure for the preparation of **1p**, the reaction of NaHMDS (1.3241 g, 7.2 mmol), DME (30 mL), 3,4-dihydronaphthalen-1(2*H*)-one (1.0525 g, 7.2 mmol), and **7** (986.9 mg, 6.0 mmol) afforded **1r** and **1r'** (750.7 mg, 52%, ketone : enol = 1:1.5) (eluent: petroleum ether/dichloromethane = 2/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.37* (s, 1 H, OH), 7.85-7.77* (m, 1 H, Ar-H), 7.37-7.23* (m, 2 H, Ar-H), 7.17* (d, *J* = 6.9 Hz, 1 H, Ar-H), 5.43-5.27* (m, 1 H, HC=C=C), 4.92-4.79* (m, 2 H, C=C=CH_2), 4.79-4.63* (m, 2 H, OCH_2), 2.82* (t, *J* = 7.2 Hz, 2 H, CH_2), 2.65-2.44* (m, 2 H, CH_2). The following signals are discernible for **1r**: δ 8.05 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.53-7.45 (m, 1 H, Ar-H), 3.63 (dd, J_1 = 10.2 Hz, J_2 = 5.1 Hz, 1 H), 3.14-2.93 (m, 2 H, CH_2), 2.43-2.32 (m, 1 H, one proton of CH_2); IR (neat, cm^{-1}): 2945, 1957, 1740, 1686, 1645, 1616, 1597, 1569, 1490, 1452, 1390, 1353, 1324, 1295, 1260, 1209, 1197, 1167, 1130, 1083, 1024; MS (70 ev, EI) *m/z* (%): 242 (M^+, 7.20), 115 (100); HRMS Calcd for $C_{15}H_{14}O_3$ (M^+): 242.0943; Found: 242.0943.

2. Palladium-Catalyzed decarboxylation of allenyl 3-oxoalkanoates

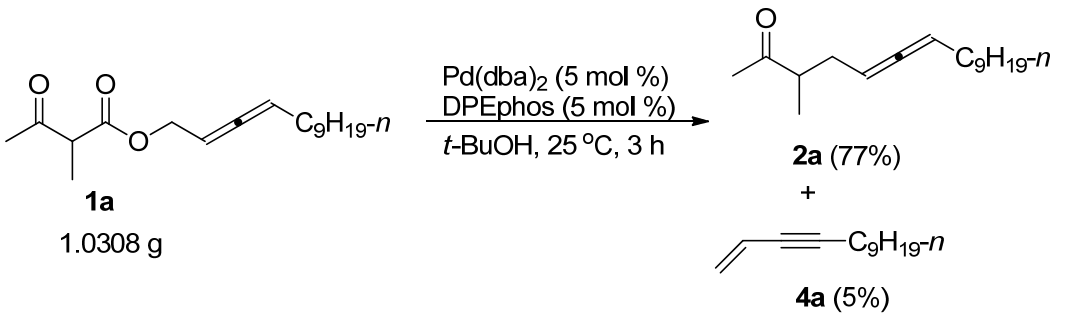
(1) 3-Methyl-5,6-hexadecadien-2-one (2a)



1a **2a**

Typical Procedure IV: To a flame-dried Schlenk tube were added $Pd(dba)_2$ (11.5 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), *t*-BuOH (1 mL), **1a** (115.9 mg, 0.40 mmol), and 1 mL of *t*-BuOH sequentially under argon. The mixture was stirred at 25 ^{o}C with a preheated oil bath and monitored by TLC. Upon completion, the resulting mixture was concentrated and purified by chromatography on silica gel (eluent: petroleum ether/ethyl ether = 50/1) to afford **2a** (74.7 mg, 76%) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.12-4.93 (m, 2 H, HC=C=CH), 2.67-2.52 (m, 1 H, COCH), 2.40-2.23 (m, 1 H, one proton of CH_2), 2.12 (s, 3 H, $COCH_3$), 2.07-1.87 (m, 3 H, CH_2 and one proton of CH_2), 1.43-1.16 (m, 14 H, $CC_7H_{14}C$), 1.09 (d, J = 3.6 Hz, 3 H, $COCCH_3$), 0.85 (t, J = 6.3 Hz, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.8, 211.7, 204.40, 204.36, 91.8, 91.6, 88.1, 46.7, 32.2, 32.1, 31.9, 29.5, 29.4, 29.3, 29.2, 29.12, 29.08, 28.9, 28.8, 28.19, 28.17, 22.6, 16.1, 14.0; IR (neat, cm^{-1}): 2958, 2925, 2854, 1962, 1716, 1459, 1375, 1358, 1166; MS (70 ev, EI) *m/z* (%): 250 (M^+, 8.29), 95 (100); HRMS Calcd for $C_{17}H_{30}O$ (M^+): 250.2297; Found: 250.2295.

(2) Synthesis of 3-methyl-5,6-hexadecadien-2-one 2a in one gram scale



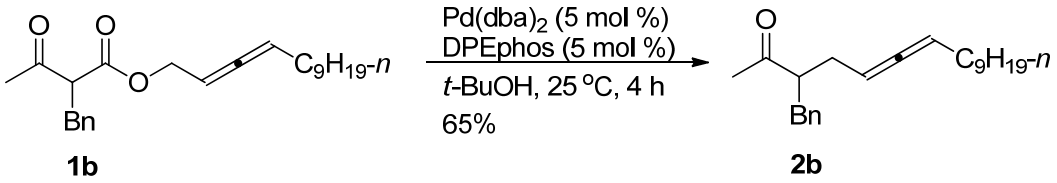
To a flame-dried round-flask were added $Pd(dba)_2$ (100.2 mg, 0.175 mmol), DPEphos (94.1 mg, 0.175 mmol), *t*-BuOH (15 mL), and **1a** (1.0308 g, 3.50 mmol) sequentially under argon. The mixture was stirred at 25 °C with a preheated oil bath and monitored by TLC. Upon completion, the resulting mixture was concentrated and purified by chromatography on silica gel (eluent: petroleum ether/ethyl ether = 50/1) to afford **2a** (677.8 mg, 77%) and **4a** (31.3 mg, 5%).

2a: liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.12-4.94 (m, 2 H, HC=C=CH), 2.67-2.53 (m, 1 H, COCH), 2.40-2.25 (m, 1 H, one proton of CH_2), 2.13 (s, 3 H, $COCH_3$), 2.07-1.87 (m, 3 H, CH_2 and one proton of CH_2), 1.43-1.16 (m, 14 H, $CC_7H_{14}C$), 1.10 (d, J = 3.6 Hz, 3 H, $COCCH_3$), 0.86 (t, J = 6.3 Hz, 3 H, CH_3).

4a: liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.78 (ddt, J_1 = 17.4 Hz, J_2 = 10.8 Hz, J_3 = 2.1 Hz, 1 H, C=CHC), 5.54 (dd, J_1 = 17.4 Hz, J_2 = 2.4 Hz, 1 H, one proton of H_2C=C), 5.36 (dd, J_1 = 10.8 Hz, J_2 = 2.1 Hz, 1 H, one proton of H_2C=C), 2.29 (td, J_1 = 6.8 Hz, J_2 = 2.0 Hz, 2 H, CH_2), 1.63-1.45 (m, 2 H, CH_2), 1.45-1.15 (m, 12 H, 6×CH_2), 0.88 (t, 3 H, J_2 = 6.8 Hz, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 125.4, 117.7, 91.2, 79.3, 31.9, 29.5, 29.3, 29.2, 28.9, 28.7, 22.7, 19.3, 14.1; IR (neat, cm^{-1}): 2925, 2855, 2228, 1609, 1465, 1412, 1260, 1096, 1018; MS (70 ev, EI) *m/z* (%): 178 (M^+, 1.01), 79 (100); HRMS Calcd for $C_{13}H_{22}$ (M^+): 178.1722; Found: 178.1721.

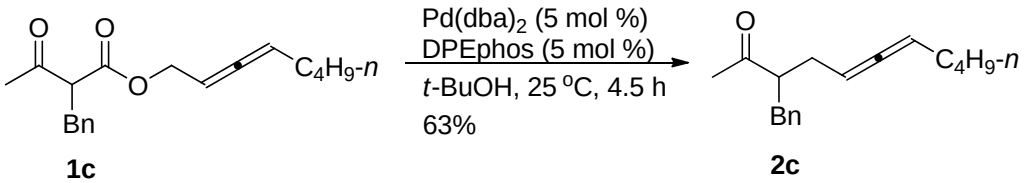
The following compounds were prepared according to Typical Procedure IV.

(3) 3-Benzyl-5,6-hexadecadien-2-one (2b)



The reaction of $Pd(dba)_2$ (11.3 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), and **1b** (147.4 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2b** (84.6 mg, 65%) (eluent: petroleum ether/ethyl ether = 60/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.22 (m, 2 H, Ar-H), 7.22-7.11 (m, 3 H, Ar-H), 5.17-4.97 (m, 2 H, HC=C=CH), 2.97-2.83 (m, 2 H, CH_2), 2.81-2.67 (m, 1 H, one proton of CH_2), 2.39-2.24 (m, 1 H, one proton of CH_2), 2.20-2.06 (m, 1 H, one proton of CH_2), 2.05-1.90 (m, 5 H, CH_3 and CH_2), 1.43-1.19 (m, 14 H, $CC_7H_{14}C$), 0.88 (t, J = 6.5 Hz, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.3, 211.2, 204.42, 204.37, 139.4, 139.3, 128.85, 128.82, 128.4, 126.3, 92.05, 91.95, 87.90, 87.88, 53.96, 53.93, 37.42, 37.36, 31.8, 30.59, 30.57, 30.3, 30.2, 29.5, 29.4, 29.3, 29.13, 29.07, 29.05, 28.8, 22.6, 14.1; IR (neat, cm^{-1}): 2925, 2854, 1961, 1714, 1496, 1458, 1358, 1212, 1160; MS (70 ev, EI) *m/z* (%): 326 (M^+, 4.94), 91 (100); HRMS Calcd for $C_{23}H_{34}O$ (M^+): 326.2610; Found: 326.2609.

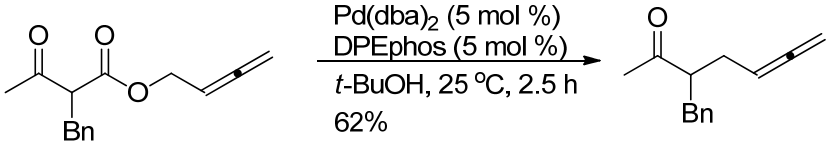
(4) 3-Benzyl-5,6-undecadien-2-one (2c)



The reaction of $Pd(dba)_2$ (11.7 mg, 0.020 mmol), DPEphos (11.1 mg, 0.020 mmol),

and **1c** (120.1 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2c** (64.6 mg, 63%) (eluent: petroleum ether/ethyl ether = 60/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.23 (m, 2 H, Ar-H), 7.23-7.11 (m, 3 H, Ar-H), 5.17-4.97 (m, 2 H, HC=C=CH), 2.97-2.83 (m, 2 H, one proton of CH_2), 2.81-2.67 (m, 1 H, one proton of CH_2), 2.39-2.24 (m, 1 H, COCH and one proton of CH_2), 2.20-2.06 (m, 1 H, one proton of CH_2), 2.05-1.90 (m, 5 H, $COCH_3$ and CH_2), 1.44-1.27 (m, 4 H, CC_2H_4C), 0.94-0.84 (m, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.4, 211.3, 204.41, 204.38, 139.4, 139.3, 128.85, 128.83, 128.4, 126.3, 92.0, 91.9, 87.90, 87.87, 53.96, 53.94, 37.4, 37.3, 31.25, 31.19, 30.60, 30.55, 30.4, 30.2, 28.5, 22.10, 22.07, 13.8; IR (neat, cm^{-1}): 2957, 2927, 2858, 1961, 1713, 1496, 1450, 1358, 1161; MS (70 ev, EI) *m/z* (%): 256 (M^+, 0.98), 91 (100); HRMS Calcd for $C_{18}H_{24}O$ (M^+): 256.1827; Found: 256.1825.

(5) 3-Benzyl-5,6-heptadien-2-one (2d)

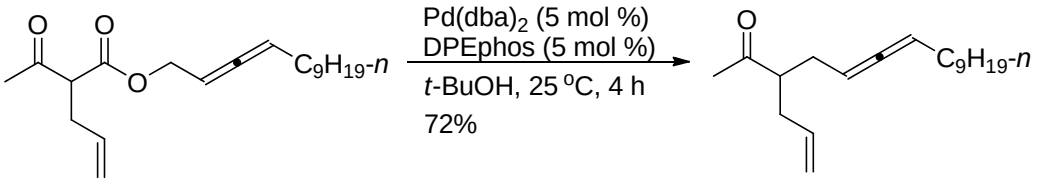


1d **2d**

The reaction of $Pd(dba)_2$ (11.6 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), and **1d** (97.9 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2d** (49.9 mg, 62%) [eluent: petroleum ether (b.p. 30-60 °C)/ethyl ether = 50/1] as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.23 (m, 2 H, Ar-H), 7.23-7.11 (m, 3 H, Ar-H), 5.11-5.00 (m, 1 H, CCH=C=C), 4.77-4.63 (m, 2 H, C=C=CH_2), 3.00-2.83 (m, 2 H, COCH and one proton of CH_2), 2.80-2.67 (m, 1 H, one proton of CH_2), 2.39-2.25 (m, 1 H, one proton of CH_2), 2.20-2.05 (m, 1 H, one proton of CH_2), 2.01 (s, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.2, 208.8, 139.2, 128.8, 128.4, 126.3, 87.3, 75.6, 53.7, 37.4, 30.3,

29.6; IR (neat, cm^{-1}): 3063, 3028, 2921, 2854, 1955, 1710, 1603, 1496, 1453, 1440, 1352, 1213, 1161, 1081, 1030; MS (70 ev, EI) *m/z* (%): 200 (M^+, 1.11), 91 (100); HRMS Calcd for $C_{14}H_{16}O$ (M^+): 200.1201; Found: 200.1203.

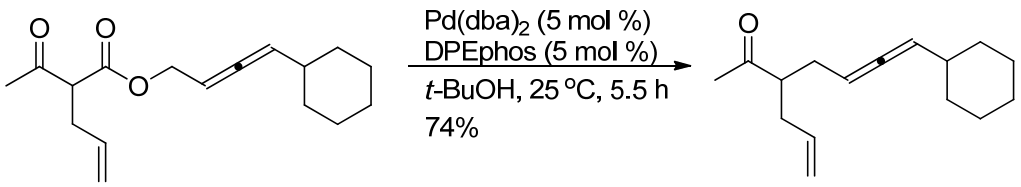
(6) 3-Allyl-5,6-hexadecadien-2-one (2e)



1e **2e**

The reaction of $Pd(dba)_2$ (11.6 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), and **1e** (127.4 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2e** (79.3 mg, 72%) (eluent: petroleum ether/ethyl ether = 80/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.78-5.62 (m, 1 H, C=CHC), 5.12-4.93 (m, 4 H, CH_2=C and HC=C=CH), 2.71-2.59 (m, 1 H, COCH), 2.40-2.18 (m, 3 H, CH_2 and one proton of CH_2), 2.18-2.04 (m, 4 H, $COCH_3$ and one proton of CH_2), 2.00-1.88 (m, 2 H, CH_2), 1.42-1.16 (m, 14 H, $CC_7H_{14}C$), 0.86 (t, *J* = 6.8 Hz, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.0, 210.9, 204.4, 204.3, 135.3, 116.9, 92.0, 91.8, 88.0, 87.9, 51.93, 51.90, 35.29, 35.27, 31.9, 30.20, 30.18, 29.54, 29.48, 29.4, 29.3, 29.2, 29.1, 28.8, 22.6, 14.1; IR (neat, cm^{-1}): 3078, 2926, 2854, 1962, 1714, 1641, 1441, 1358, 1163; MS (70 ev, EI) *m/z* (%): 276 (M^+, 1.48), 43 (100); HRMS Calcd for $C_{19}H_{32}O$ (M^+): 276.2453; Found: 276.2455.

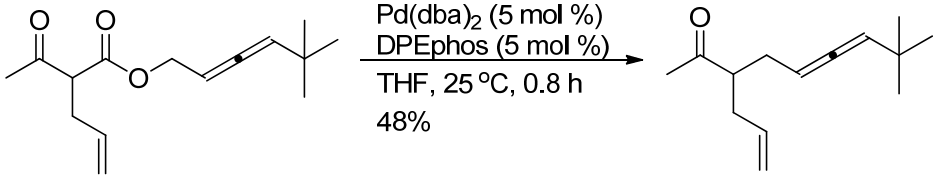
(7) 3-Allyl-7-cyclohexyl-5,6-heptadien-2-one (2f)



1f **2f**

The reaction of $Pd(dba)_2$ (11.3 mg, 0.020 mmol), DPEphos (10.7 mg, 0.020 mmol), and **1f** (110.7 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2f** (68.8 mg, 74%) (eluent: petroleum ether/ethyl ether = 50/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.78-5.62 (m, 1 H, C=CHC), 5.13-4.97 (m, 4 H, CH_2=C and HC=C=CH), 2.72-2.59 (m, 1 H, COCH), 2.41-2.04 (m, 7 H), 2.01-1.86 (m, 1 H), 1.77-1.56 (m, 5 H), 1.35-0.97 (m, 5 H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.1, 211.0, 203.2, 203.1, 135.3, 117.0, 98.0, 97.8, 89.0, 88.9, 52.1, 51.9, 37.20, 37.17, 35.4, 35.3, 33.03, 33.00, 32.9, 30.34, 30.27, 29.6, 29.5, 26.1, 26.0; IR (neat, cm^{-1}): 3077, 2925, 2851, 1960, 1713, 1641, 1445, 1357, 1222, 1163; MS (70 ev, EI) *m/z* (%): 232 (M^+, 2.23), 43 (100); HRMS Calcd for $C_{16}H_{24}O$ (M^+): 232.1827; Found: 232.1828.

(8) 3-Allyl-8,8-dimethyl-5,6-nonadien-2-one (2g)

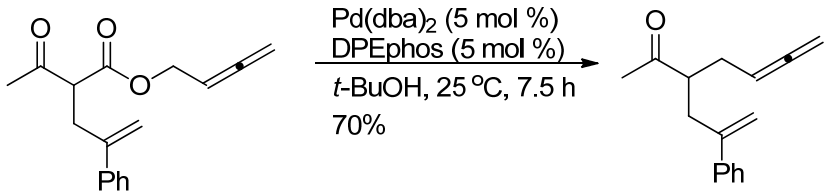


1g **2g**

The reaction of $Pd(dba)_2$ (11.6 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), and **1g** (100.2 mg, 0.40 mmol) in 2 mL of THF afforded **2f** (39.6 mg, 48%) [eluent: petroleum ether (b.p. 30-60 °C)/ethyl ether = 60/1] as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.78-5.62 (m, 1 H, C=CH), 5.13-4.97 (m, 4 H, CH_2=C and HC=C=CH), 2.73-2.59 (m, 1 H, COCH), 2.41-2.18 (m, 3 H, CH_2 and one proton of CH_2),

2.18-2.03 (m, 4 H, $COCH_3$ and one proton of CH_2), 1.00 (s, 9 H, $C(CH_3)_3$); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.0, 210.9, 201.6, 201.5, 135.3, 117.00, 116.98, 103.9, 103.7, 90.0, 89.8, 52.2, 51.8, 35.4, 35.3, 31.7, 30.5, 30.4, 30.1, 29.7, 29.5; IR (neat, cm^{-1}): 3079, 2961, 2865, 1960, 1715, 1641, 1475, 1461, 1441, 1362, 1258, 1192, 1163; MS (70 ev, EI) *m/z* (%): 206 (M^+, 0.58), 205 206 (M^+-1, 2.46), 191 (100); HRMS Calcd for $C_{14}H_{22}O$ (M^+): 206.1671; Found: 206.1673.

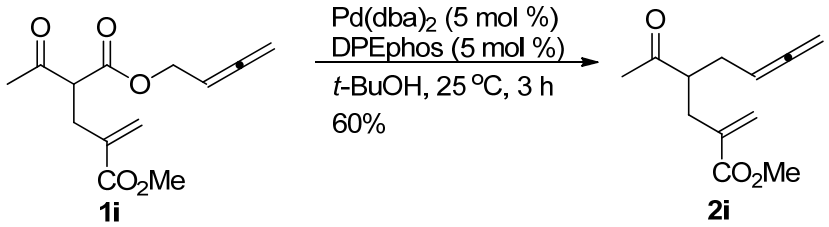
(9) 3-(2-Phenylallyl)-5,6-heptadien-2-one (2h)



The reaction of $Pd(dba)_2$ (11.2 mg, 0.020 mmol), DPEphos (10.6 mg, 0.020 mmol), and **1h** (108.1 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2h** (63.1 mg, 70%) (eluent: petroleum ether/ethyl ether = 40/1) as a liquid: ^1H NMR (400 MHz, $CDCl_3$) δ 7.41-7.24 (m, 5 H, Ar-H), 5.30 (s, 1 H, one proton of CH_2=C), 5.07 (s, 1 H, one proton of CH_2=C), 5.04-4.95 (m, 1 H, HC=C=C), 4.69-4.61 (m, 2 H, C=C=CH_2), 2.83 (dd, J_1 = 13.6 Hz, J_2 = 7.2 Hz, 1 H, one proton of C=CCH_2), 2.76-2.67 (quint, J_1 = 5.2 Hz, 1 H, COCH), 2.64 (dd, J_1 = 13.6 Hz, J_2 = 6.4 Hz, 1 H, one proton of C=CCH_2), 2.35-2.24 (m, 1 H, one proton of C=C=CCH_2), 2.21-2.12 (m, 1 H, one proton of C=C=CCH_2), 2.07 (s, 3 H, $COCH_3$); ^{13}C NMR (100.5 MHz, $CDCl_3$) δ 211.1, 208.9, 145.7, 140.2, 128.4, 127.6, 126.1, 114.9, 87.0, 75.4, 50.2, 36.9, 29.9, 29.7; IR (neat, cm^{-1}): 2986, 2919, 2852, 1955, 1711, 1627, 1600, 1574, 1494, 1442, 1353, 1305, 1214, 1161, 1107, 1076, 1028; MS (70 ev, EI) *m/z* (%): 226 (M^+, 1.46), 43 (100); HRMS

Calcd for $C_{16}H_{18}O$ (M^+): 226.1358; Found: 226.1359.

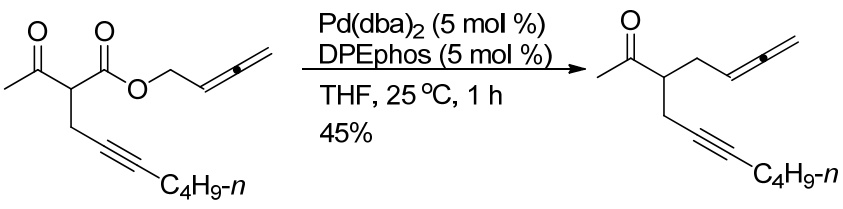
(10) Methyl 4-acetyl-2-methylene-6,7-octadienoate (2i)



1i **2i**

The reaction of $Pd(dba)_2$ (11.5 mg, 0.020 mmol), DPEphos (10.9 mg, 0.020 mmol), and **1i** (101.2 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2i** (50.1 mg, 60%) [eluent: petroleum ether (b.p. 30-60 °C)/ethyl ether = 25/1] as a liquid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.18 (s, 1 H, one proton of CH_2=C), 5.55 (s, 1 H, one proton of CH_2=C), 5.05-4.95 (m, 1 H, HC=C=C), 4.71-4.61 (m, 2 H, C=C=CH_2), 3.73 (s, 3 H, CO_2CH_3), 2.91-2.82 (m, 1 H, COCH), 2.60 (dd, J_1 = 14.0 Hz, J_2 = 7.2 Hz, 1 H, one proton of C=CCH_2), 2.37 (dd, J_1 = 13.6 Hz, J_2 = 6.4 Hz, 1 H, one proton of C=CCH_2), 2.35-2.21 (m, 1 H, one proton of CH_2), 2.20-2.06 (m, 4 H, $COCH_3$ and one proton of CH_2); ^{13}C NMR (100.5 MHz, $CDCl_3$) δ 210.6, 208.9, 167.1, 137.4, 127.5, 86.9, 75.5, 51.9, 50.4, 33.5, 29.7, 29.4; IR (neat, cm^{-1}): 2995, 2953, 2927, 2849, 1955, 1713, 1631, 1439, 1352, 1333, 1308, 1279, 1198, 1140; MS (70 ev, EI) *m/z* (%): 207 (M^+-1, 1.65), 193 (M^+-CH_3, 4.59), 43 (100); HRMS Calcd for $C_{12}H_{16}O_3$ (M^+): 208.1099; Found: 208.1102.

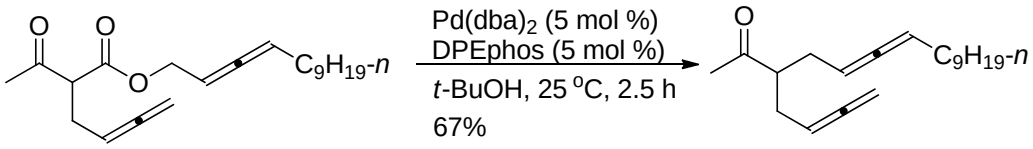
(11) 3-(2,3-Butadienyl)-5-decyn-2-one (2j)



1j **2j**

The reaction of $Pd(dba)_2$ (11.6 mg, 0.020 mmol), DPEphos (10.9 mg, 0.020 mmol), and **1j** (99.9 mg, 0.40 mmol) in 2 mL of THF afforded **2j** (36.7 mg, 45%) (eluent: petroleum ether/ethyl ether = 60/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.11-4.98 (m, 1 H, HC=C=C), 4.75-4.62 (m, 2 H, C=C=CH_2), 2.79-2.67 (m, 1 H, COCH), 2.47-2.29 (m, 3 H, CH_2 and one proton of CH_2), 2.28-2.07 (m, 6 H, $COCH_3$, CH_2, and one proton of CH_2), 1.53-1.28 (m, 4 H, CC_2H_4C), 0.88 (t, J = 7.1 Hz, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 210.1, 208.9, 87.0, 82.4, 76.7, 75.5, 51.2, 31.0, 29.7, 29.1, 21.9, 20.6, 18.3, 13.6; IR (neat, cm^{-1}): 2958, 2932, 2873, 1956, 1715, 1434, 1364, 1162; MS (70 ev, EI) *m/z* (%): 205 (M^++1, 1.10), 189 (M^+-CH_3, 1.10), 43 (100); HRMS Calcd for $C_{14}H_{20}O$ (M^+): 204.1514; Found: 204.1514.

(12) 3-(2,3-Butadienyl)-5,6-hexadecadien-2-one (2k)

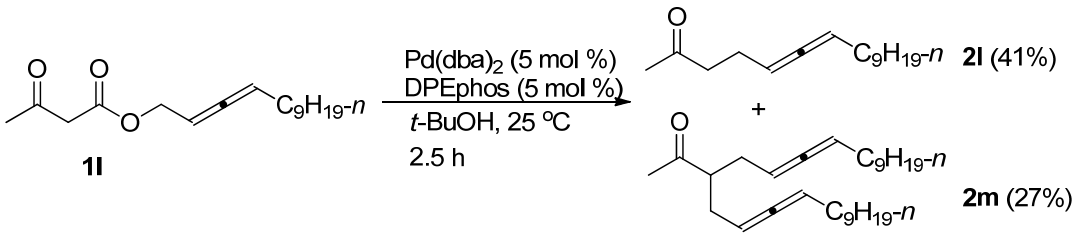


1k **2k**

The reaction of $Pd(dba)_2$ (11.6 mg, 0.020 mmol), DPEphos (10.9 mg, 0.020 mmol), and **1k** (133.6 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2k** (77.1 mg, 67%) (eluent: petroleum ether/ethyl ether = 80/1) as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.12-4.93 (m, 3 H, C=C=CH and HC=C=CH), 4.74-4.59 (m, 2 H, C=C=CH_2), 2.73-2.62 (quintet, J = 6.6 Hz, 1 H, COCH), 2.37-2.21 (m, 2 H), 2.21-2.05 (m, 5 H), 2.01-1.87 (m, 2 H, CH_2), 1.42-1.16 (m, 14 H, $CC_7H_{14}C$), 0.85 (t, J = 6.5 Hz, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 210.6, 210.5, 208.9, 204.44, 204.38, 91.9, 91.8,

87.79, 87.76, 87.3, 75.3, 51.73, 51.66, 31.8, 30.42, 30.39, 29.5, 29.39, 29.35, 29.3, 29.2, 29.12, 29.10, 29.06, 29.05, 28.8, 22.6, 14.0; IR (neat, cm^{-1}): 2956, 2925, 2854, 1957, 1716, 1466, 1440, 1352, 1161; MS (70 ev, EI) *m/z* (%): 288 (M^+, 1.78), 43 (100); HRMS Calcd for $C_{20}H_{32}O$ (M^+): 288.2453; Found: 288.2453.

(13) 5,6-Hexadecadien-2-one (2l) and 3-(2,3-tridecadienyl)-5,6-hexadecadien-2-one (2m)



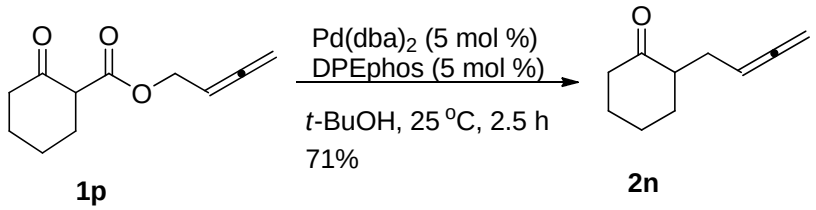
The reaction of $Pd(dba)_2$ (11.5 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), and **1l** (111.5 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2l** (38.9 mg, 41%) and **2m** (44.5 mg, 27%) (eluent: petroleum ether/ethyl ether = 50/1).

2l: liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.16-5.04 (m, 2 H, HC=C=CH), 2.52 (t, *J* = 7.2 Hz, 2 H, $COCH_2$), 2.28-2.17 (m, 2 H, CH_2), 2.13 (s, 3 H, $COCH_3$), 2.00-1.87 (m, 2 H, CH_2), 1.42-1.15 (m, 14 H, $CC_7H_{14}C$), 0.86 (t, *J* = 6.6 Hz, 3 H, CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 208.1, 203.6, 92.5, 89.6, 42.4, 31.8, 29.9, 29.5, 29.4, 29.3, 29.14, 29.10, 28.9, 22.7, 22.6, 14.0; IR (neat, cm^{-1}): 2956, 2924, 2854, 1963, 1720, 1465, 1442, 1363, 1260, 1225, 1160, 1018; MS (70 ev, EI) *m/z* (%): 236 (M^+, 2.07), 43 (100); HRMS Calcd for $C_{16}H_{28}O$ (M^+): 236.2140; Found: 236.2139.

2m: liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.16-4.94 (m, 4 H, two HC=C=CH), 2.73-2.62 (m, 1 H, COCH), 2.39- 2.22 (m, 2 H), 2.22-2.06 (m, 5 H), 2.02-1.88 (m, 4

H, two CH_2),1.42-1.15 (m, 28 H, two $CC_7H_{14}C$), 0.87 (t, J = 6.8 Hz, 6 H, two CH_3); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 211.0, 210.9, 210.8, 204.40, 204.36, 204.3, 91.92, 91.88, 91.8, 88.01, 87.98, 87.96, 52.0, 51.93, 51.86, 31.9, 30.4, 29.6, 29.5, 29.4, 29.3, 29.2, 29.15, 29.11, 28.9, 22.7, 14.1; IR (neat, cm^{-1}): 2955, 2923, 2853, 1963, 1715, 1465, 1441, 1362, 1160, 1058; MS (70 ev, EI) *m/z* (%): 414 (M^+, 2.52), 43 (100); HRMS Calcd for $C_{29}H_{50}O$ (M^+): 414.3862; Found: 414.3863.

(14) 2-(2,3-Butadienyl)cyclohexanone (2n)

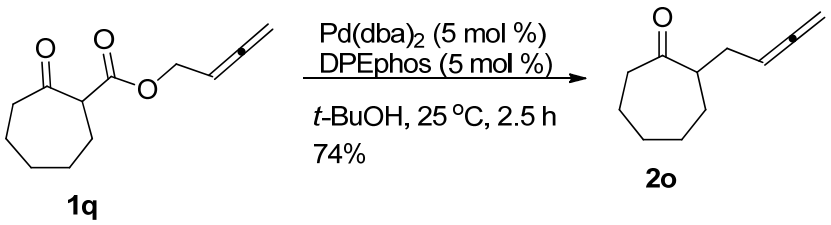


1p **2n**

The reaction of $Pd(dba)_2$ (11.6 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), and **1p** (79.0 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2n**[2] (43.3 mg, 71%) [eluent: petroleum ether (b.p. 30-60 °C)/ethyl ether = 40/1] as a liquid: ^1H NMR (300 MHz, $CDCl_3$) δ 5.14-5.02 (m, 1 H, CH=C=C), 4.68- 4.56 (m, 2 H, C=C=CH_2), 2.50-2.22 (m, 4 H), 2.22-2.10 (m, 1 H), 2.10-1.96 (m, 1 H), 1.96-1.76 (m, 2 H), 1.73-1.54 (m, 2 H), 1.46-1.25 (m, 1 H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 212.2, 208.8, 87.9, 74.7, 50.3, 42.0, 33.5, 28.2, 27.9, 25.0; IR (neat, cm^{-1}): 2934, 2860, 1955, 1707, 1448, 1431, 1367, 1340, 1314, 1223, 1181, 1128, 1071, 1035; MS (70 ev, EI) *m/z* (%): 150 (M^+, 7.06), 41 (100); HRMS Calcd for $C_{10}H_{14}O$ (M^+): 150.1045; Found: 150.1046.

No data was reported in the reference 2.

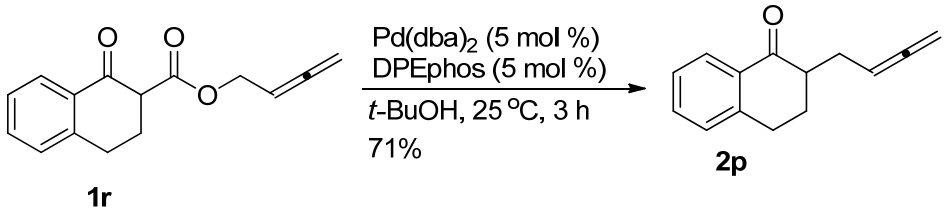
(15) 2-(2,3-Butadienyl)cycloheptanone (2o)



1q **2o**

The reaction of $Pd(dba)_2$ (11.4 mg, 0.020 mmol), DPEphos (10.9 mg, 0.020 mmol), and **1q** (83.7 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2o** (48.9 mg, 74%) [eluent: petroleum ether (b.p. 30-60 °C)/ethyl ether = 50/1] as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.09-4.97 (m, 1 H, H=C=C), 4.68- 4.55 (m, 2 H, C=C=CH_2), 2.70-2.56 (m, 1 H), 2.53-2.30 (m, 3 H), 2.05-1.72 (m, 5 H), 1.72-1.52 (m, 1 H), 1.52-1.16 (m, 3 H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 215.1, 208.8, 87.9, 75.0, 51.1, 43.2, 30.9, 30.4, 29.2, 28.8, 23.9; IR (neat, cm^{-1}): 2926, 2854, 1955, 1699, 1453, 1374, 1344, 1260, 1219, 1163, 1130, 1102, 1031; MS (70 ev, EI) *m/z* (%): 164 (M^+, 3.59), 41 (100); HRMS Calcd for $C_{11}H_{16}O$ (M^+): 164.1201; Found: 164.1203.

(16) 2-(2,3-Butadienyl)-3,4-dihydronaphthalen-1(*2H*)-one (2p)



1r **2p**

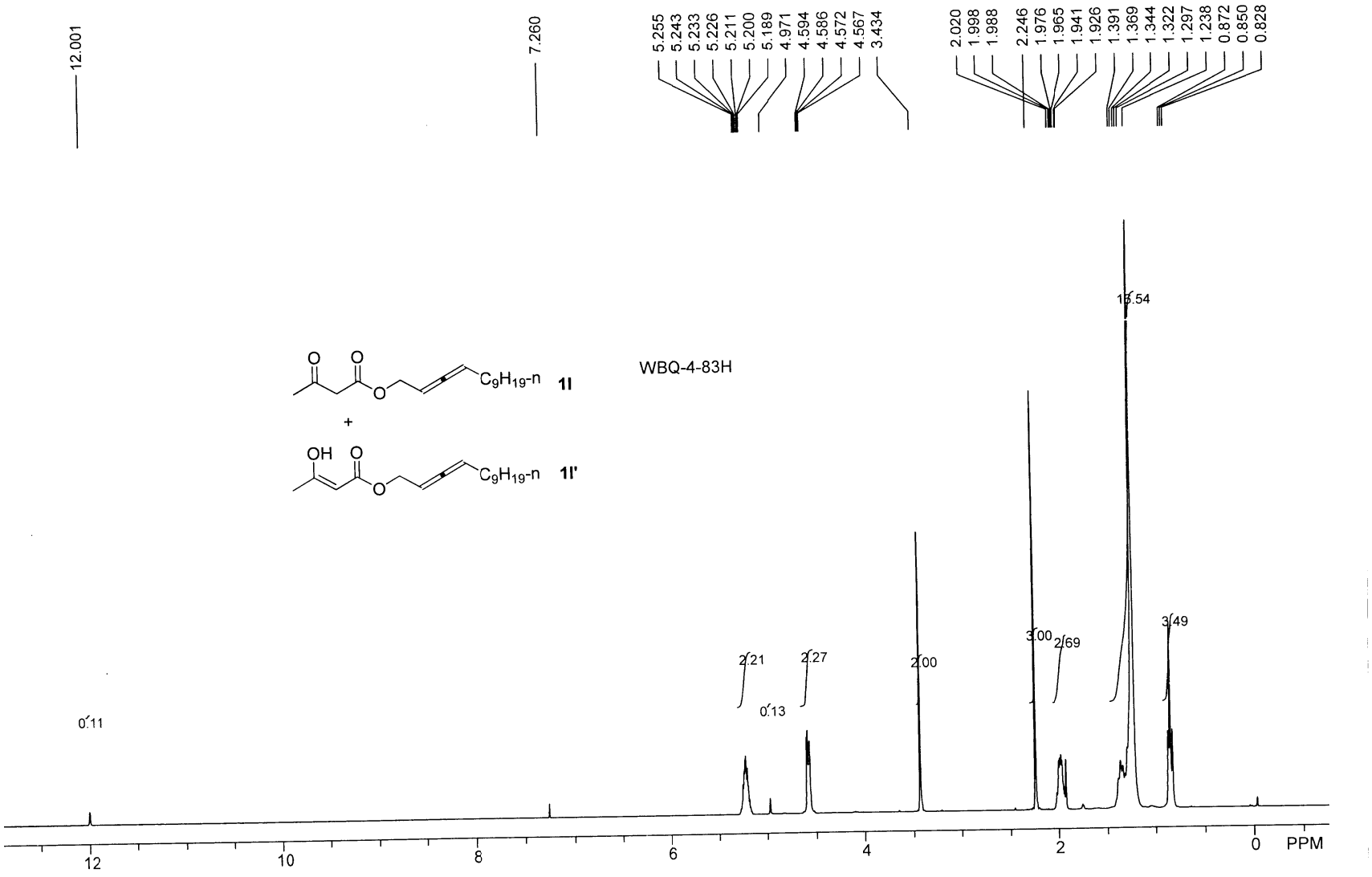
The reaction of $Pd(dba)_2$ (11.7 mg, 0.020 mmol), DPEphos (11.0 mg, 0.020 mmol), and **1r** (96.6 mg, 0.40 mmol) in 2 mL of *t*-BuOH afforded **2p** (55.9 mg, 71%) [eluent: petroleum ether (b.p. 30-60 °C)/ethyl ether = 60/1] as a liquid: ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.1 Hz, 1 H, Ar-H), 7.45 (t, *J* = 7.4 Hz, 1 H, Ar-H), 7.29 (t, *J* = 7.8 Hz, 1 H, Ar-H), 7.23 (d, *J* = 7.5 Hz, 1 H, Ar-H), 5.23-5.11 (m, 1 H, HC=C=C),

4.73- 4.65 (m, 2 H, C=C=CH_2), 3.10-2.93 (m, 2 H), 2.77-2.53 (m, 2 H), 2.35-2.15 (m, 2 H), 2.01-1.84 (m, 1 H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 209.1, 199.3, 144.0, 133.2, 132.5, 128.7, 127.4, 126.5, 87.6, 74.9, 47.4, 28.7, 28.6, 28.1; IR (neat, cm^{-1}): 2927, 2861, 1955, 1680, 1600, 1482, 1454, 1433, 1361, 1325, 1279, 1231, 1217, 1156, 1113, 1086, 1030, 1001; MS (70 ev, EI) *m/z* (%): 198 (M^+, 28.41), 90 (100); HRMS Calcd for $C_{14}H_{14}O$ (M^+): 198.1045; Found: 198.1044.

References:

1. Trost, B. M.; Xu, J. Y. *J. Org. Chem.* **2007**, *72*, 9372.

2. Pattenden, G.; Robertson, G. M. *Tetrahedron Lett.* **1983**, *24*, 4617.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5.243
5.233
5.226
5.211
5.200
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4.971
4.594
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4.572
4.567
3.434
2.020
1.998
1.988
2.246
1.976
1.965
1.941
1.926
1.391
1.369
1.344
1.322
1.297
1.238
0.872
0.850
0.828
WBQ-4-83H
1l
1l'
0.11
2.21
0.13
2.27
2.00
3.00
2.69
15.54
3.49
12
10
8
6
4
2
0
PPM

WBQ-4-83C
1l
1l'
+
205.592
200.271
166.740
93.115
86.285
77.430
77.000
76.578
63.769
49.942
31.815
30.030
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29.240
28.967
28.885
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14.032
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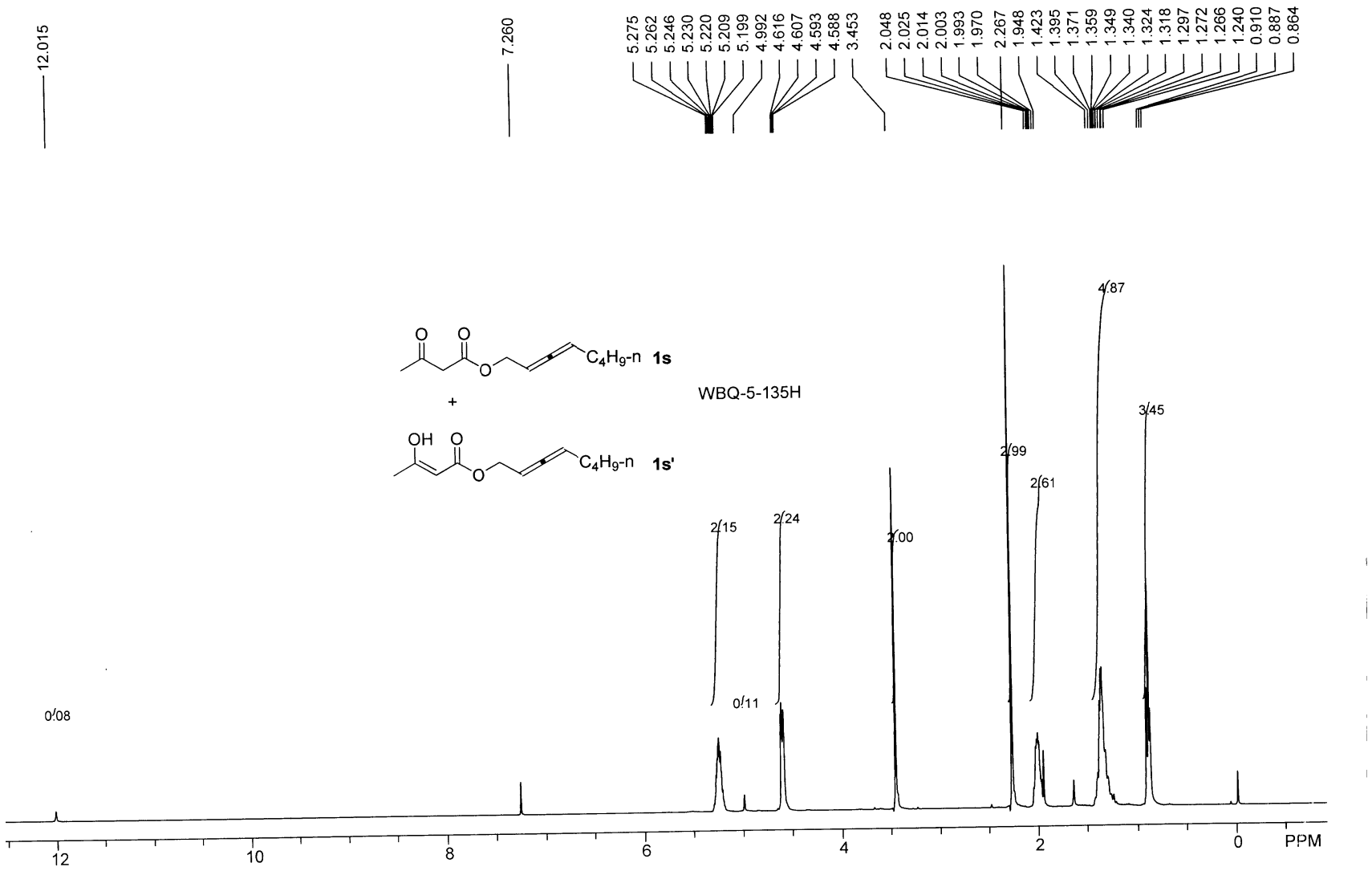
50
100
150
200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5.275
5.262
5.246
5.230
5.220
5.209
5.199
4.992
4.616
4.607
4.593
4.588
3.453
2.048
2.025
2.014
2.003
1.993
1.970
2.267
1.948
1.423
1.395
1.371
1.359
1.349
1.340
1.324
1.318
1.297
1.272
1.266
1.240
0.910
0.887
0.864
C4H9-n 1s
+
C4H9-n 1s'
WBQ-5-135H
0.08
2.15
0.11
2.24
2.00
2.99
2.61
4.87
3.45
12
10
8
6
4
2
0
PPM

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1s
1s'
+
205.671
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166.816
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77.430
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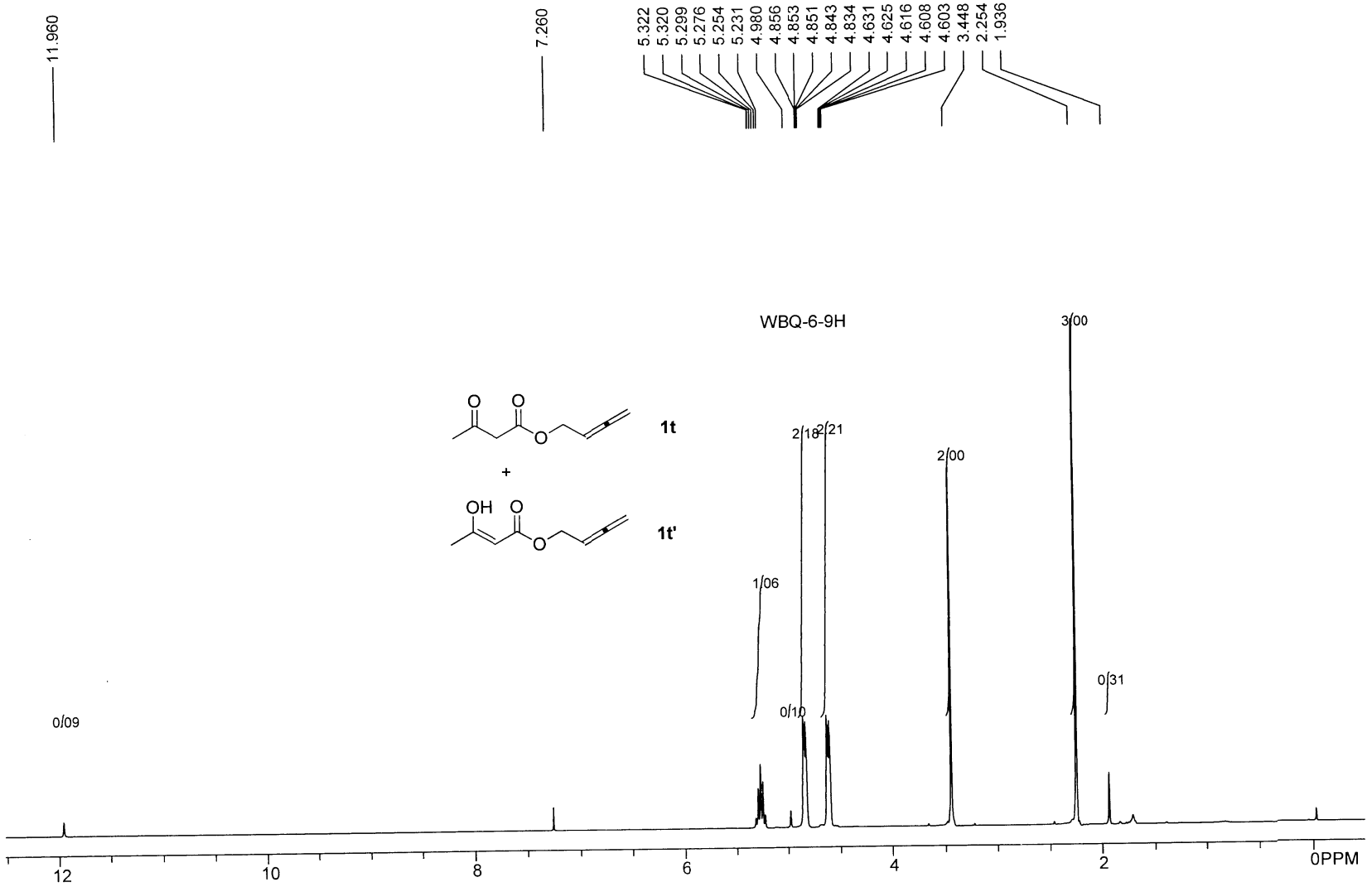
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5.299
5.276
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5.231
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4.851
4.843
4.834
4.631
4.625
4.616
4.608
4.603
3.448
2.254
1.936
WBQ-6-9H
1t
+
1t'
OH
O
0.09
1.06
2.18
2.21
0.10
2.00
3.00
0.31
12
10
8
6
4
2
0PPM

WBQ--6-9C
1t
1t'
209.812
200.247
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76.770
76.574
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30.090
200
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100
50
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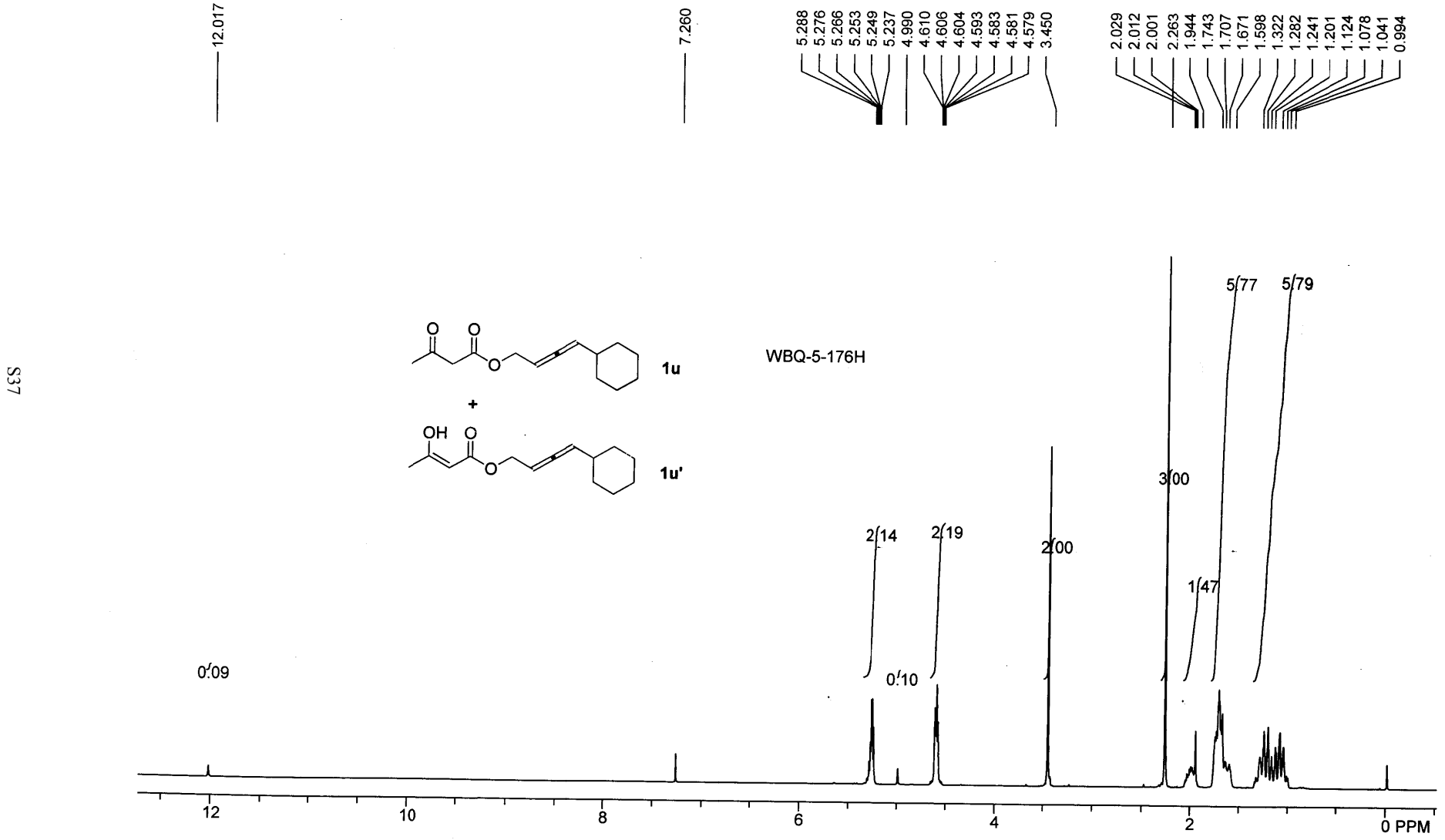
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4.604
4.593
4.583
4.581
4.579
3.450
2.029
2.012
2.001
2.263
1.944
1.743
1.707
1.671
1.598
1.322
1.282
1.241
1.201
1.124
1.078
1.041
0.994
1u
+
1u'
WBQ-5-176H
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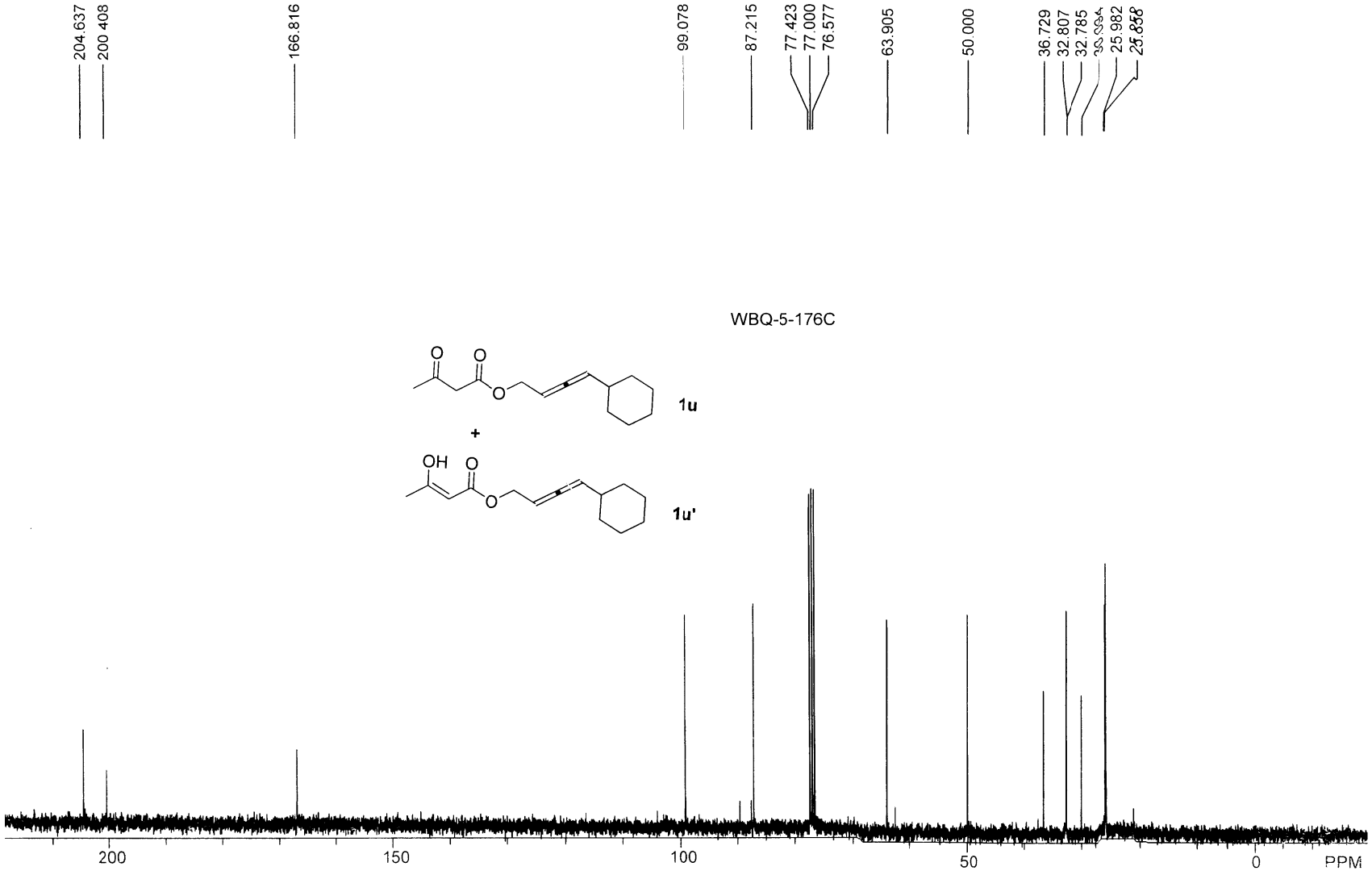
10
8
6
4
2
0 PPM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50.000
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25.858
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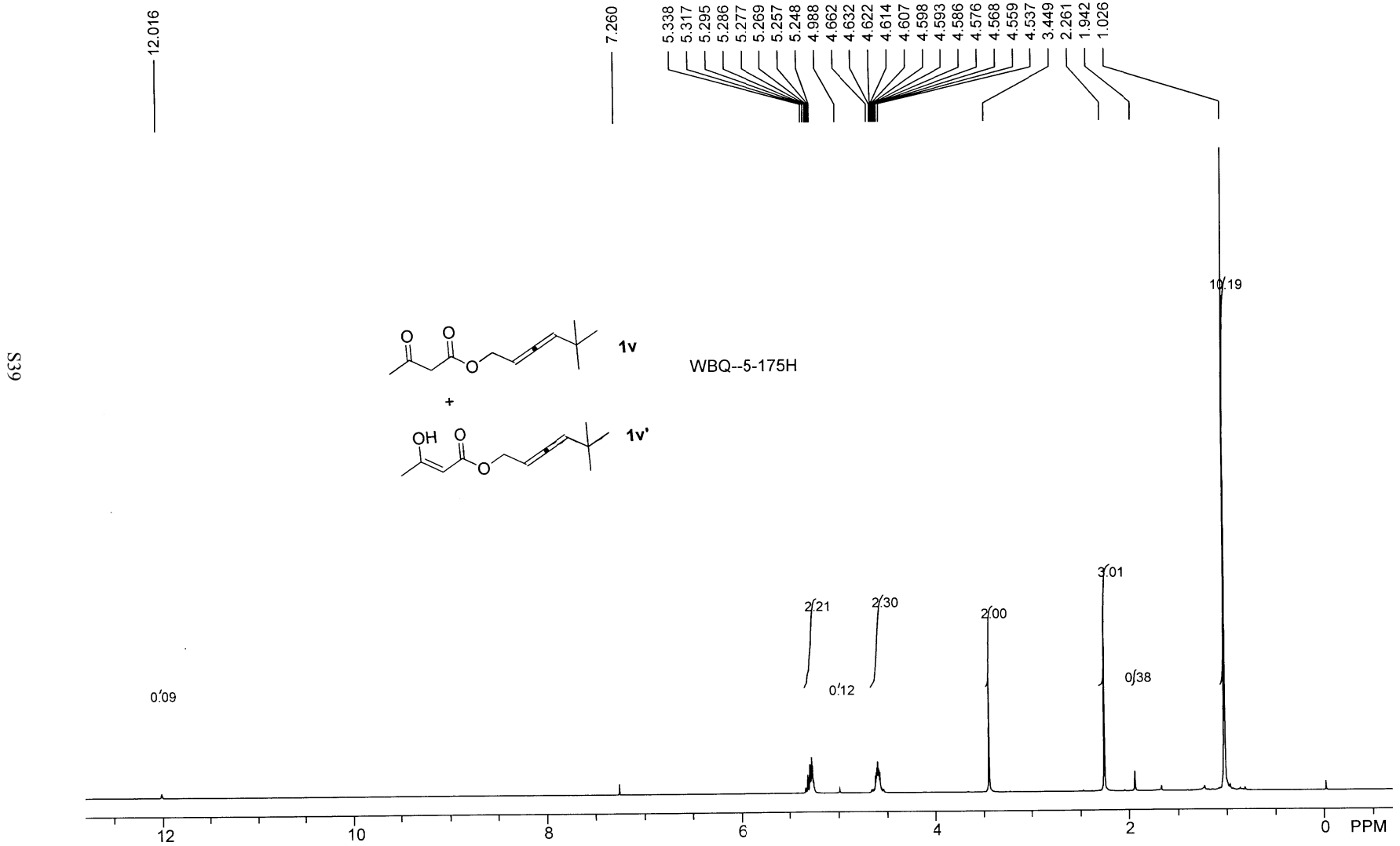
+
1u'
200
150
100
50
0
PPM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5.248
4.988
4.662
4.632
4.622
4.614
4.607
4.598
4.593
4.586
4.576
4.568
4.559
4.537
3.449
2.261
1.942
1.026
1v
+
1v'
WBQ--5-175H
10.19
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2.30
2.00
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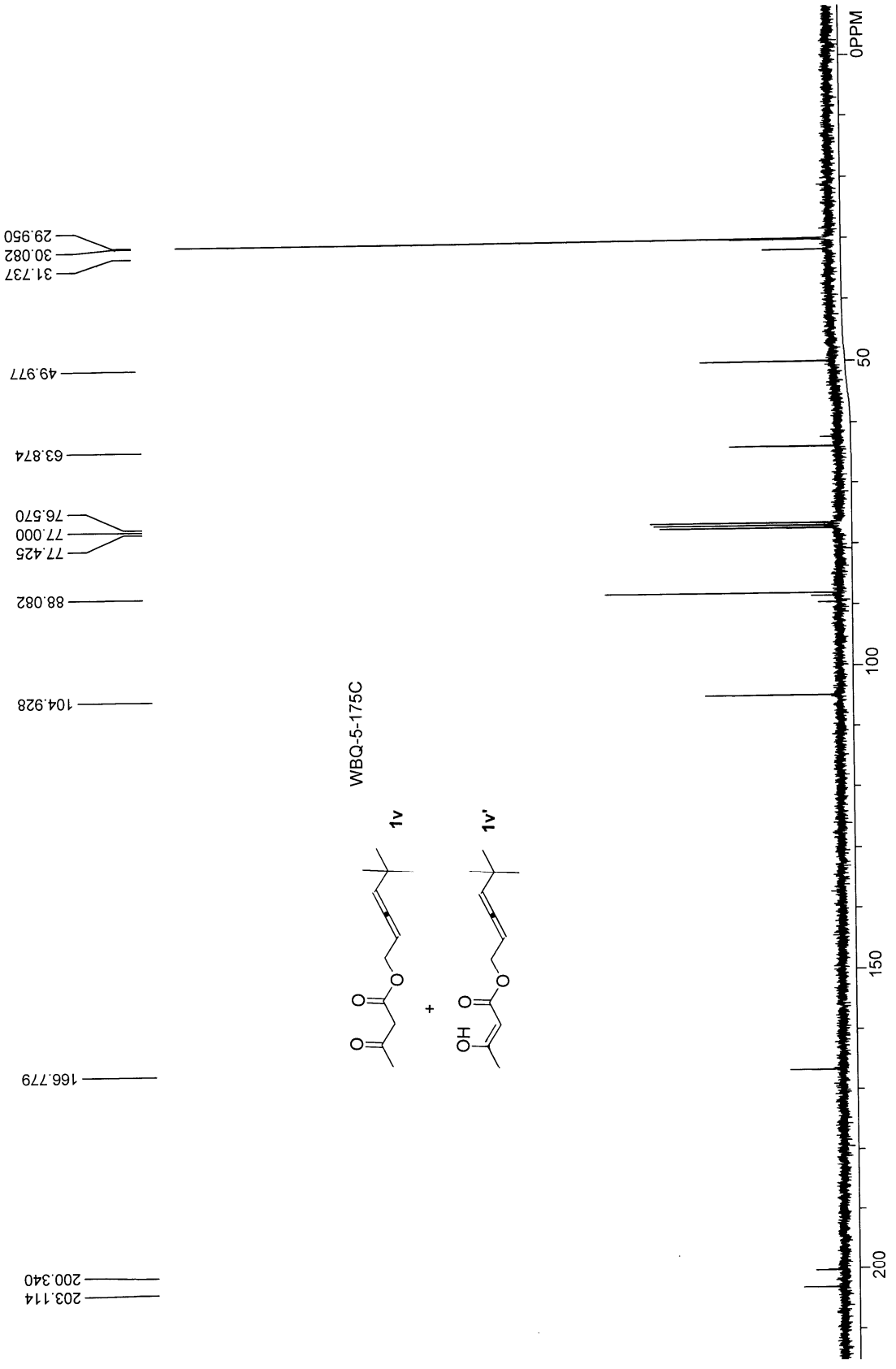
0.12
0.09
12
10
8
6
4
2
0
PPM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1v'
+
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O
O
O
O
O
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50
100
150
200
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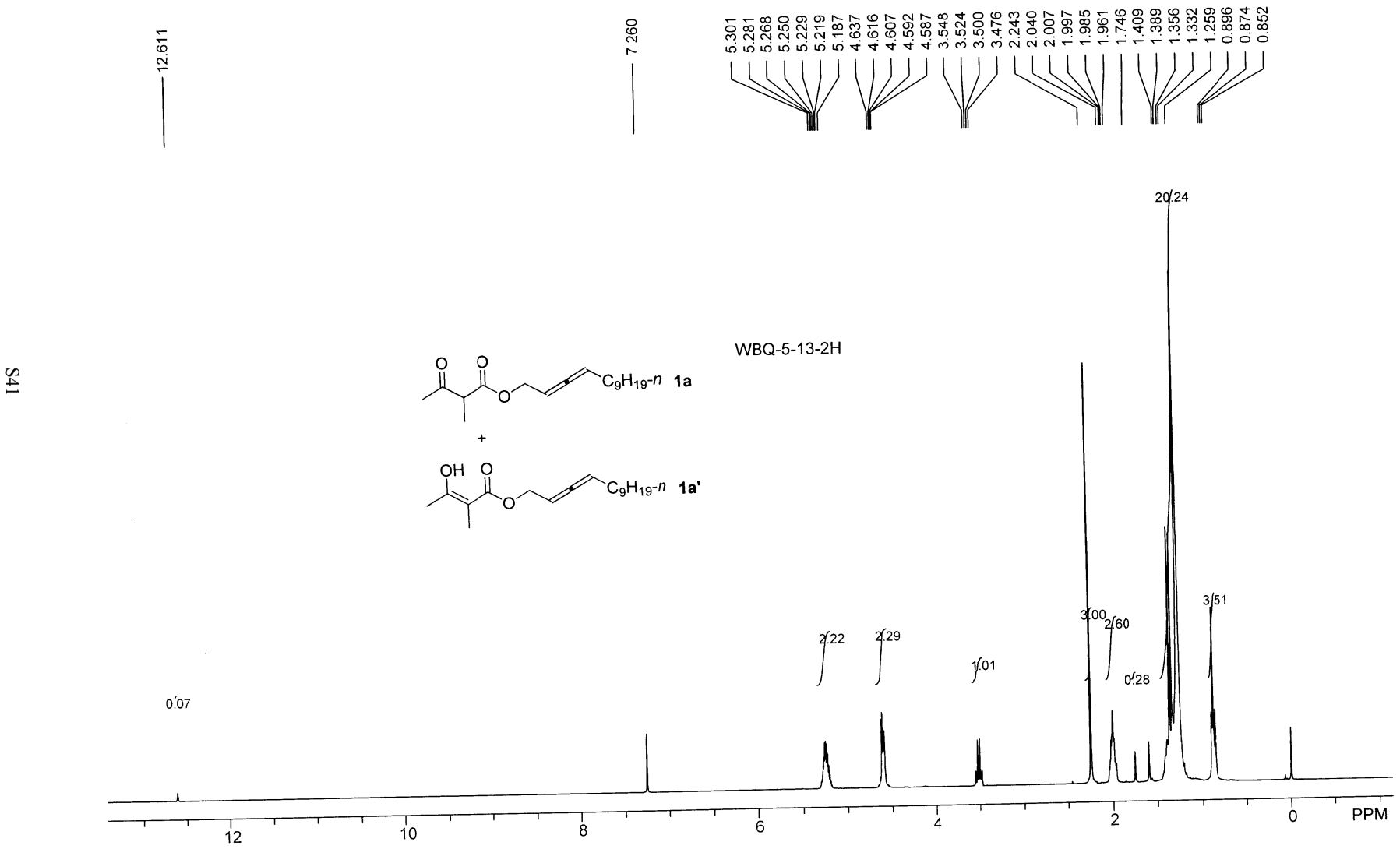
200.340
203.114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4.616
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4.592
4.587
3.548
3.524
3.500
3.476
2.243
2.040
2.007
1.997
1.985
1.961
1.746
1.409
1.389
1.356
1.332
1.259
0.896
0.874
0.852
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C9H19-n 1a
+
OH
C9H19-n 1a'
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2.29
1.01
3.00
2.60
0.28
20.24
3.51
12
10
8
6
4
2
0
PPM

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77.000
76.574
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29.459
29.319
29.215
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28.802
28.365
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1a'
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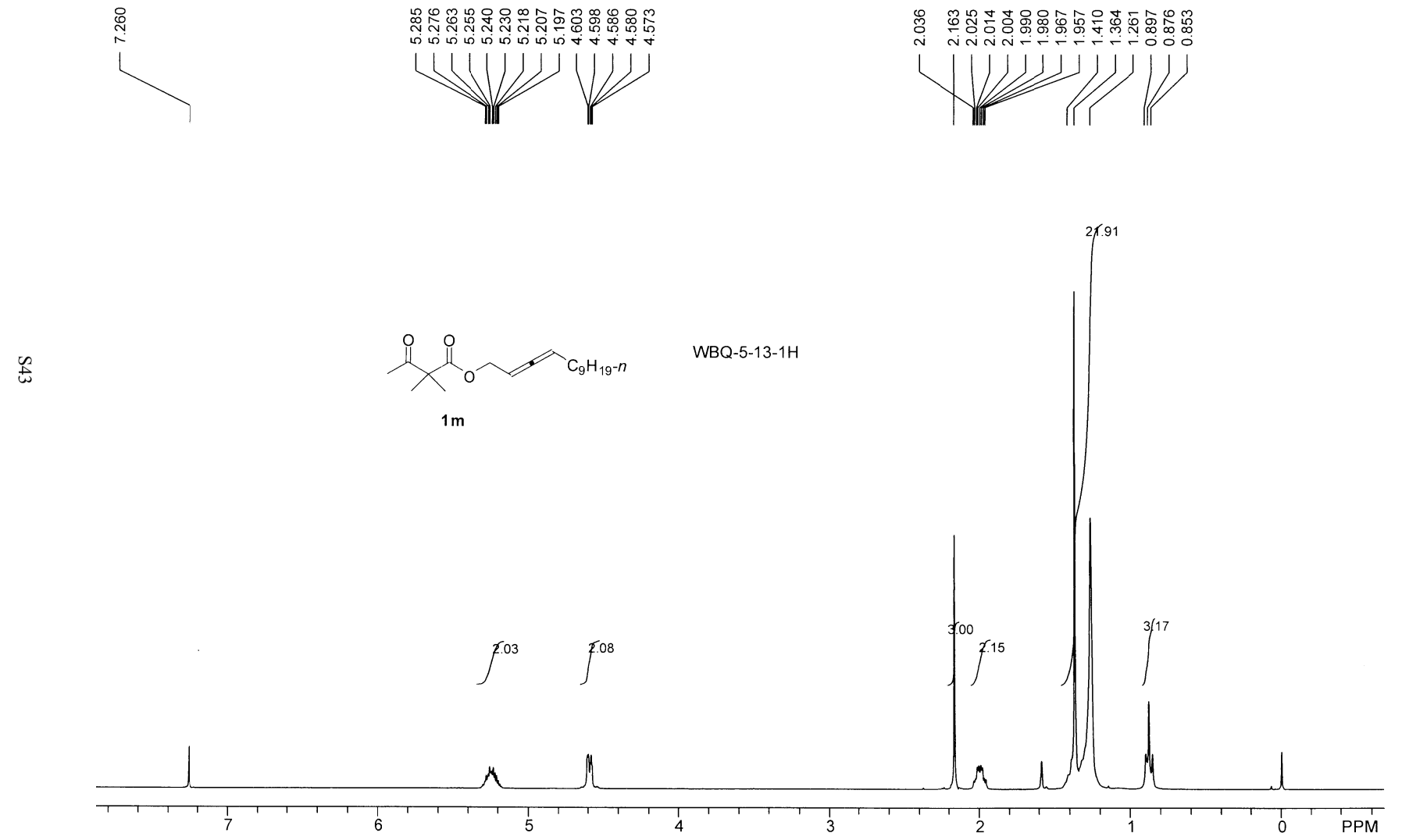
50
100
150
200
PPM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4.580
4.573
2.036
2.163
2.025
2.014
2.004
1.990
1.980
1.967
1.957
1.410
1.364
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0.897
0.876
0.853
O
O
O
C9H19-n
1m
WBQ-5-13-1H
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3.00
3.17
2.15
2.08
2.03
7
6
5
4
3
2
1
0
PPM


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173.218
93.132
86.278
77.420
77.000
76.580
63.552
55.644
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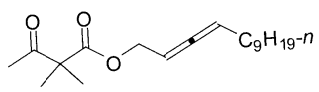
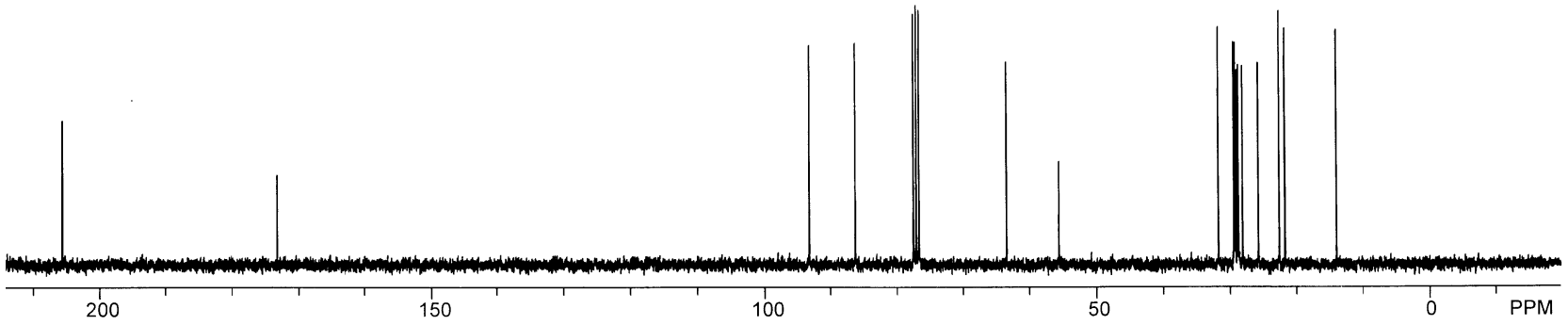

O
O
O
C_9H_{19}-*n*

1m

WBQ-5-13-1C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50
0
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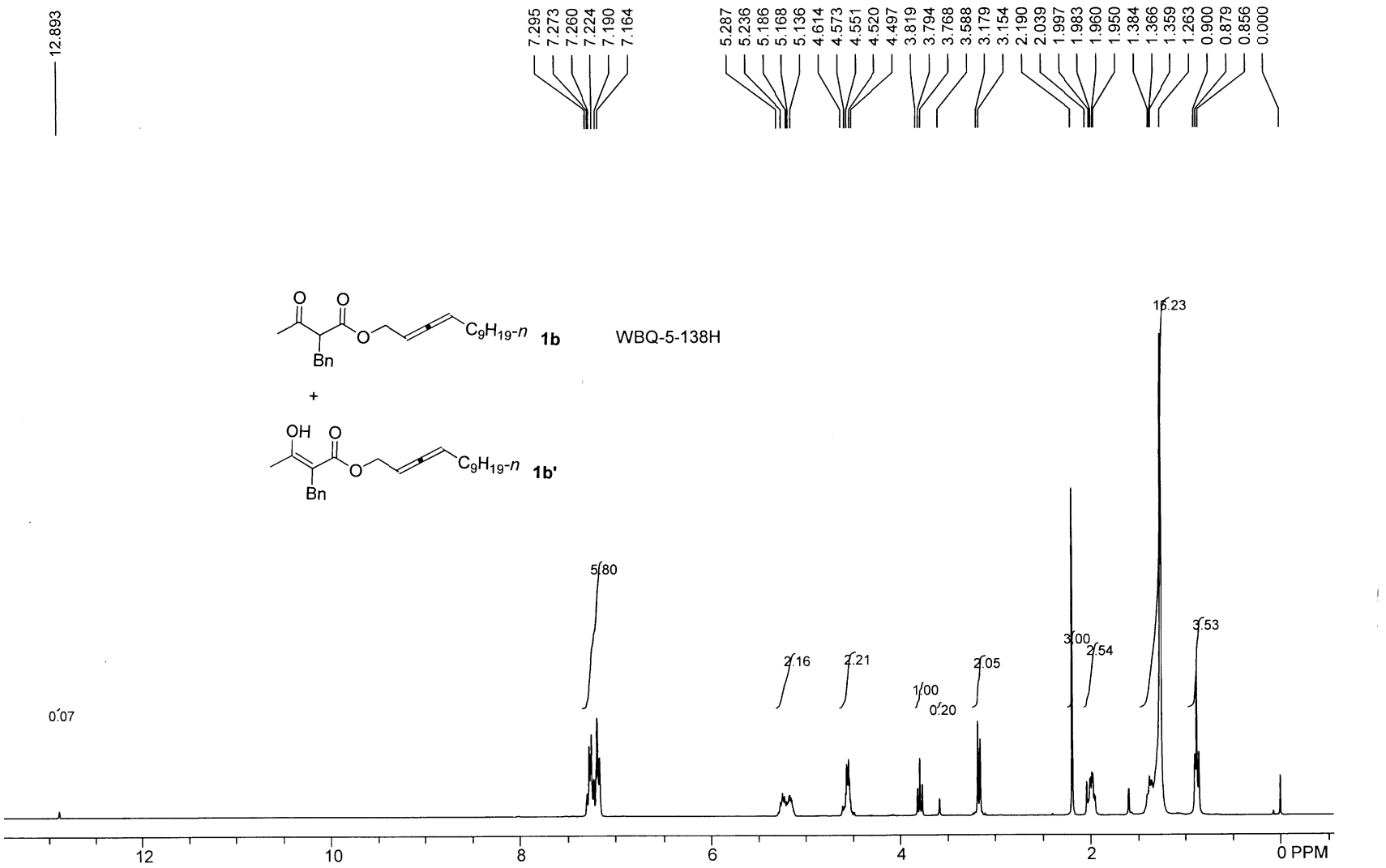
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4.573
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O
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1b
Bn
+
OH
O
O
C9H19-n
1b'
Bn
WBQ-5-138H
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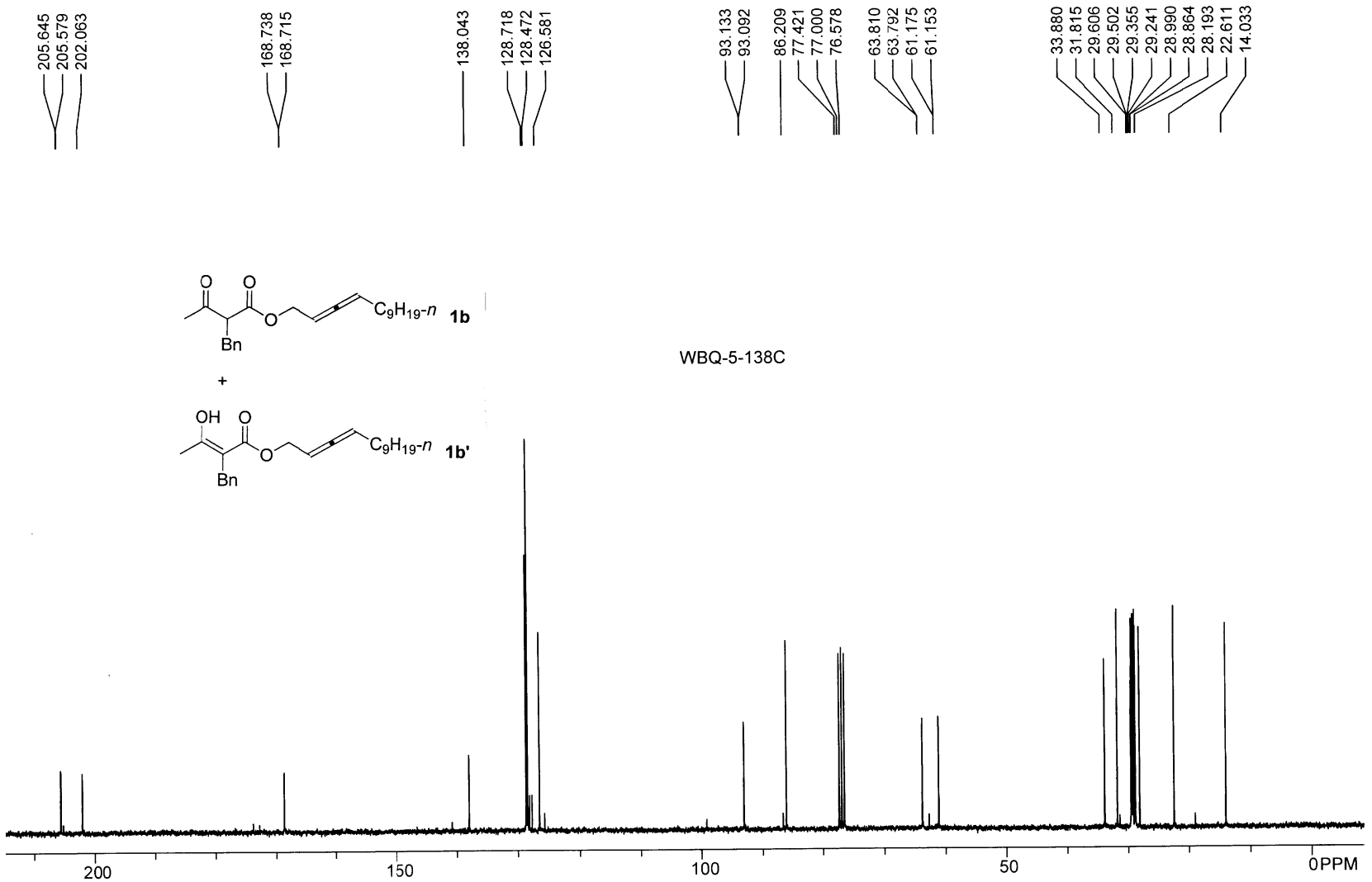
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63.792
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33.880
31.815
29.606
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29.355
29.241
28.990
28.864
28.193
22.611
14.033
O
O
O
Bn
C9H19-n
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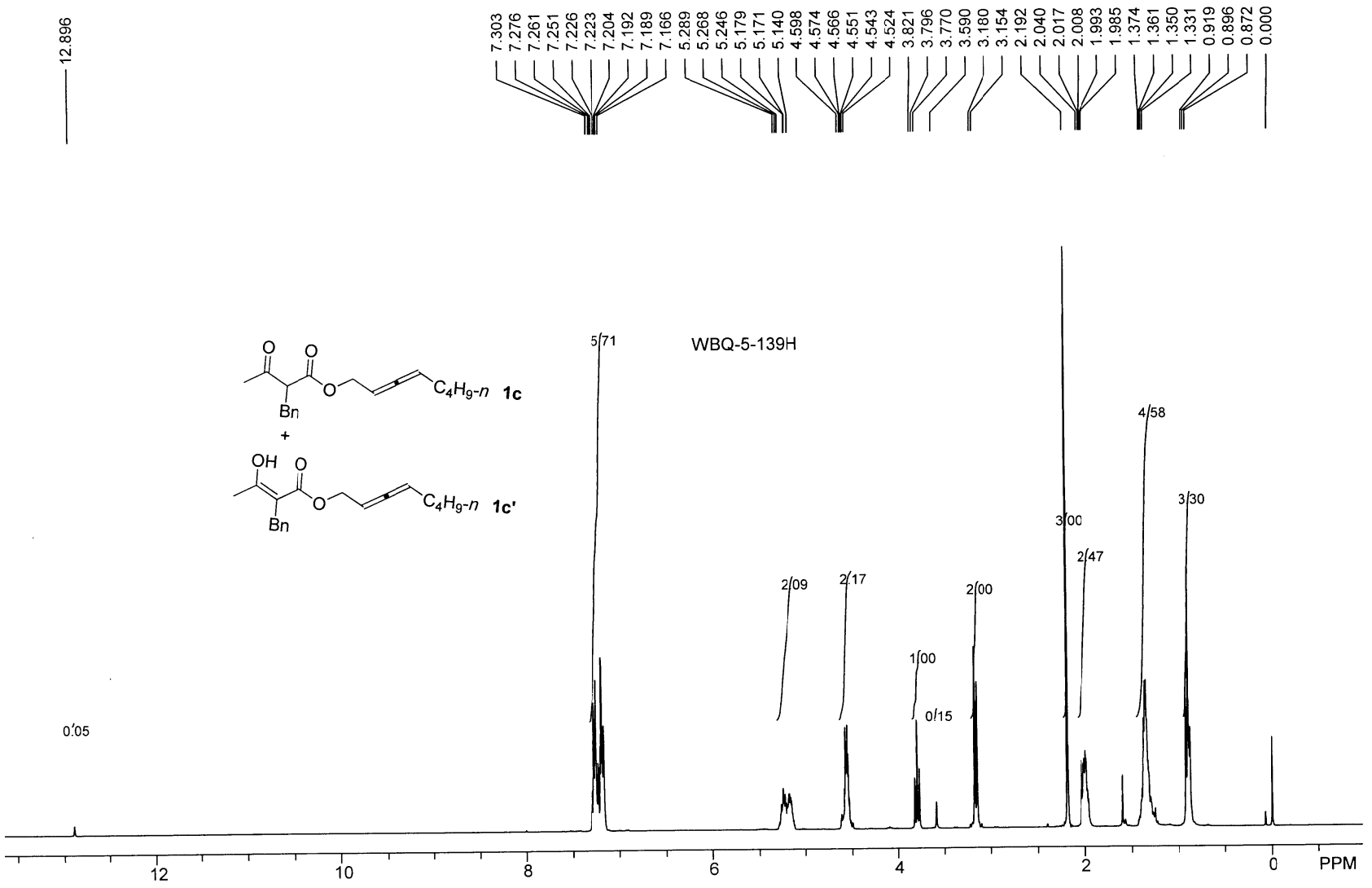
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5.140
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4.574
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4.551
4.543
4.524
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3.590
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1.985
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1.361
1.350
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0.872
0.000
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3.30
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2.47
2.09
2.17
2.00
1.00
0.15
0.05
Bn
C4H9-n 1c
+
OH
Bn
C4H9-n 1c'
12
10
8
6
4
2
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PPM

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33.844
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C4H9-n
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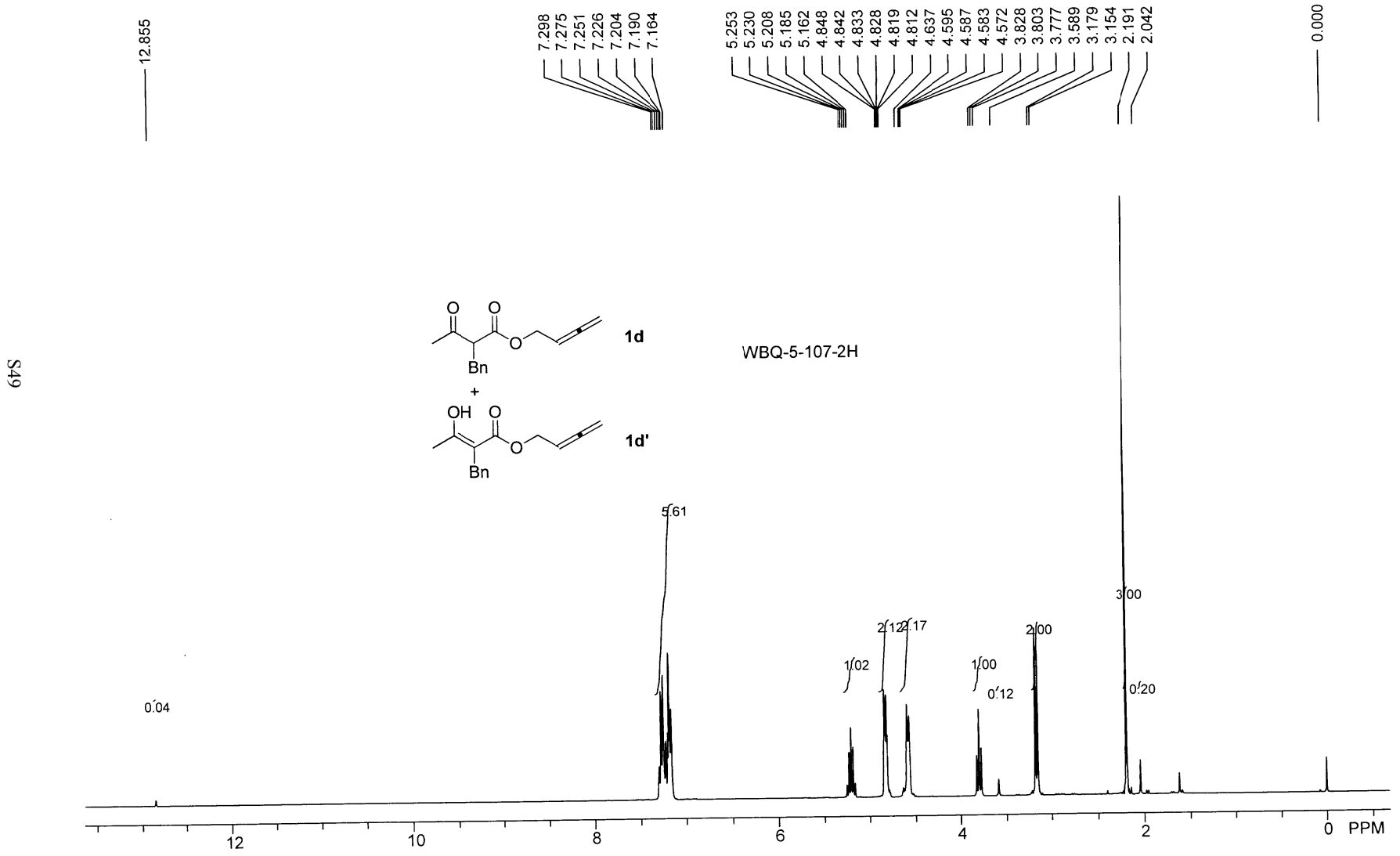
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4.583
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3.154
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10
8
6
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2
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PPM

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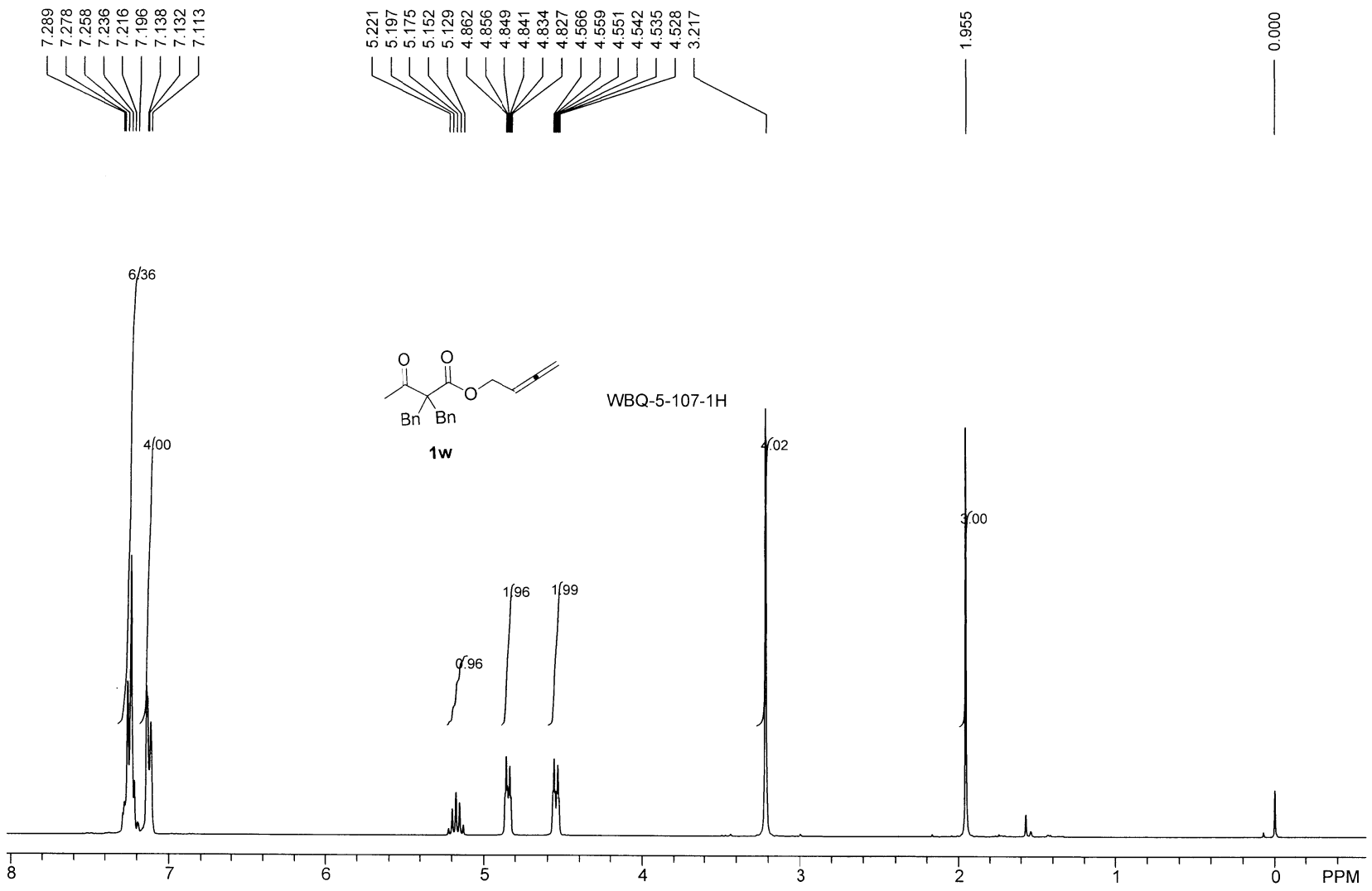
200
PPM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4.542
4.535
4.528
3.217
1.955
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4.00
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1.99
4.02
3.00
O
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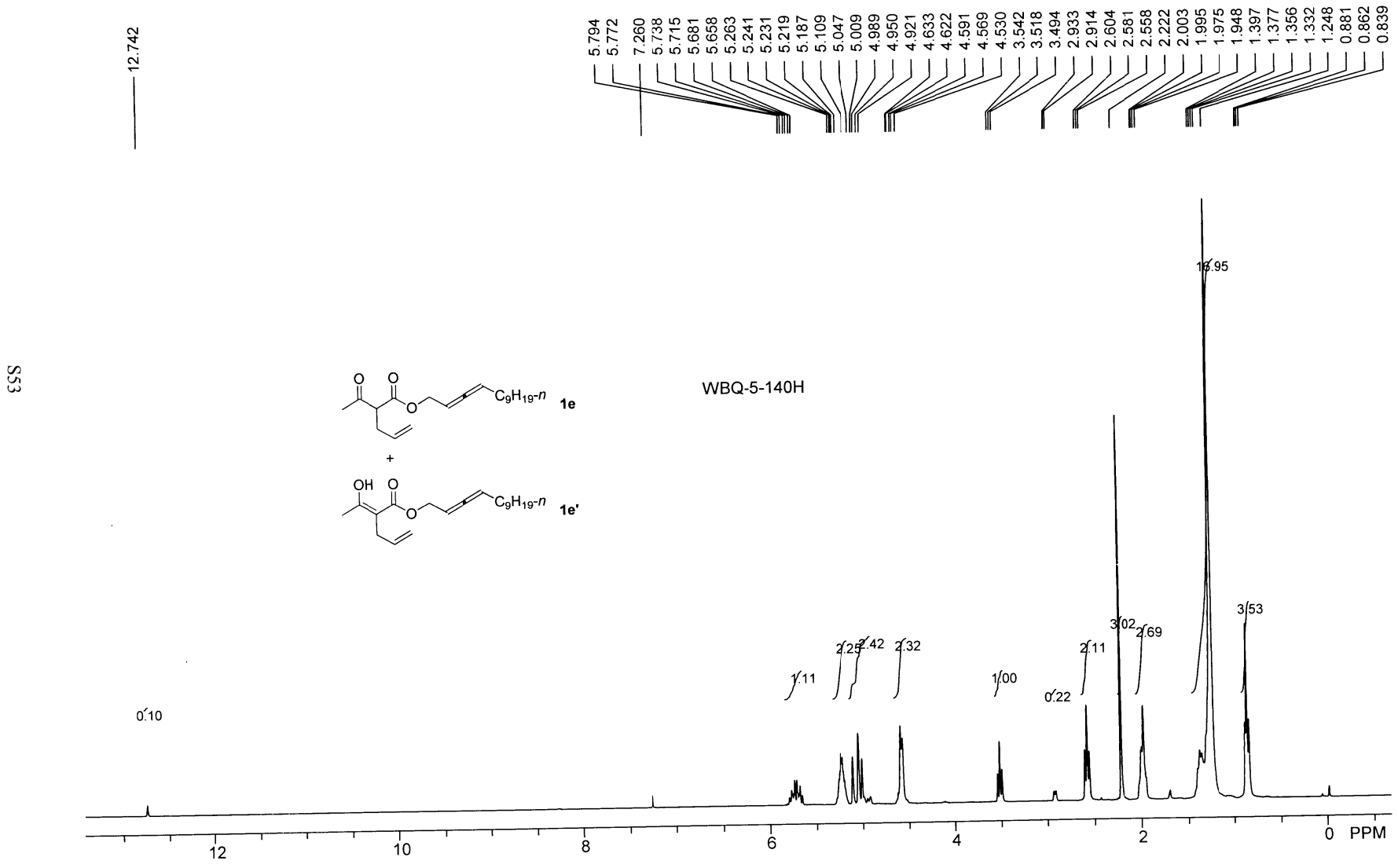
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4.569
4.530
3.542
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0.839
WBQ-5-140H
1e
1e'
0.10
1.11
2.25
2.42
2.32
1.00
0.22
2.11
3.02
2.69
16.95
3.53
12
10
8
6
4
2
0
PPM

PPM
0
50
100
150
200
WBQ-5-140C
1e
1e'
C_9H_{19}-n
14.038
22.613
28.206
28.862
28.993
29.103
29.256
29.365
29.511
31.830
32.099
59.129
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77.000
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93.172
117.438
134.136
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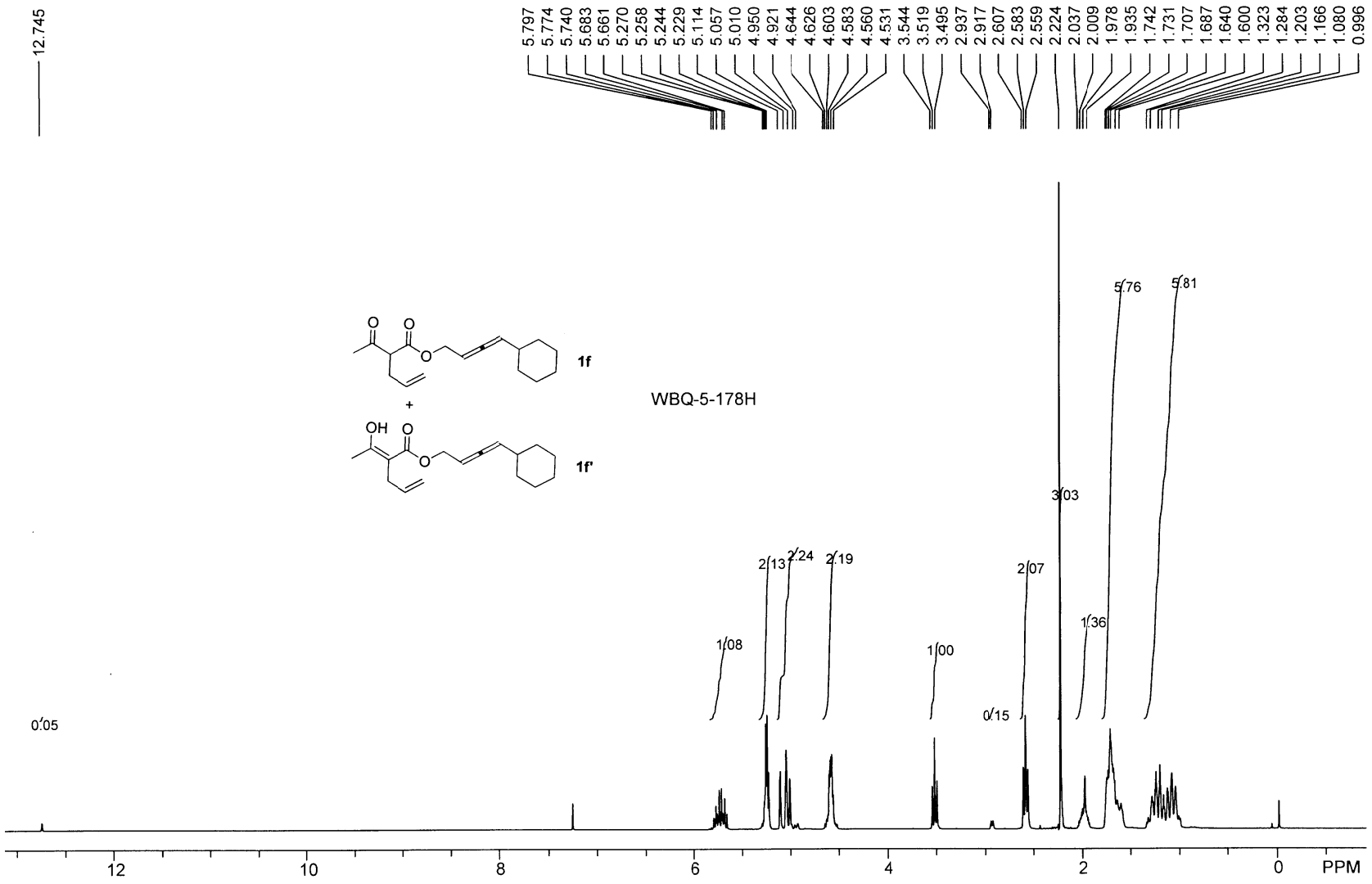
205.694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5.229
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5.057
5.010
4.950
4.921
4.644
4.626
4.603
4.583
4.560
4.531
3.544
3.519
3.495
2.937
2.917
2.607
2.583
2.559
2.224
2.037
2.009
1.978
1.935
1.742
1.731
1.707
1.687
1.640
1.600
1.323
1.284
1.203
1.166
1.080
0.996
1f
+
1f'
WBQ-5-178H
0.05
1.08
2.13
2.24
2.19
1.00
0.15
2.07
3.03
1.36
5.76
5.81
12
10
8
6
4
2
0
PPM

WBQ-5-178C
1f
1f'
+
204.742
202.153
168.914
134.126
117.431
99.042
87.189
77.421
77.000
76.576
63.913
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29.107
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25.861
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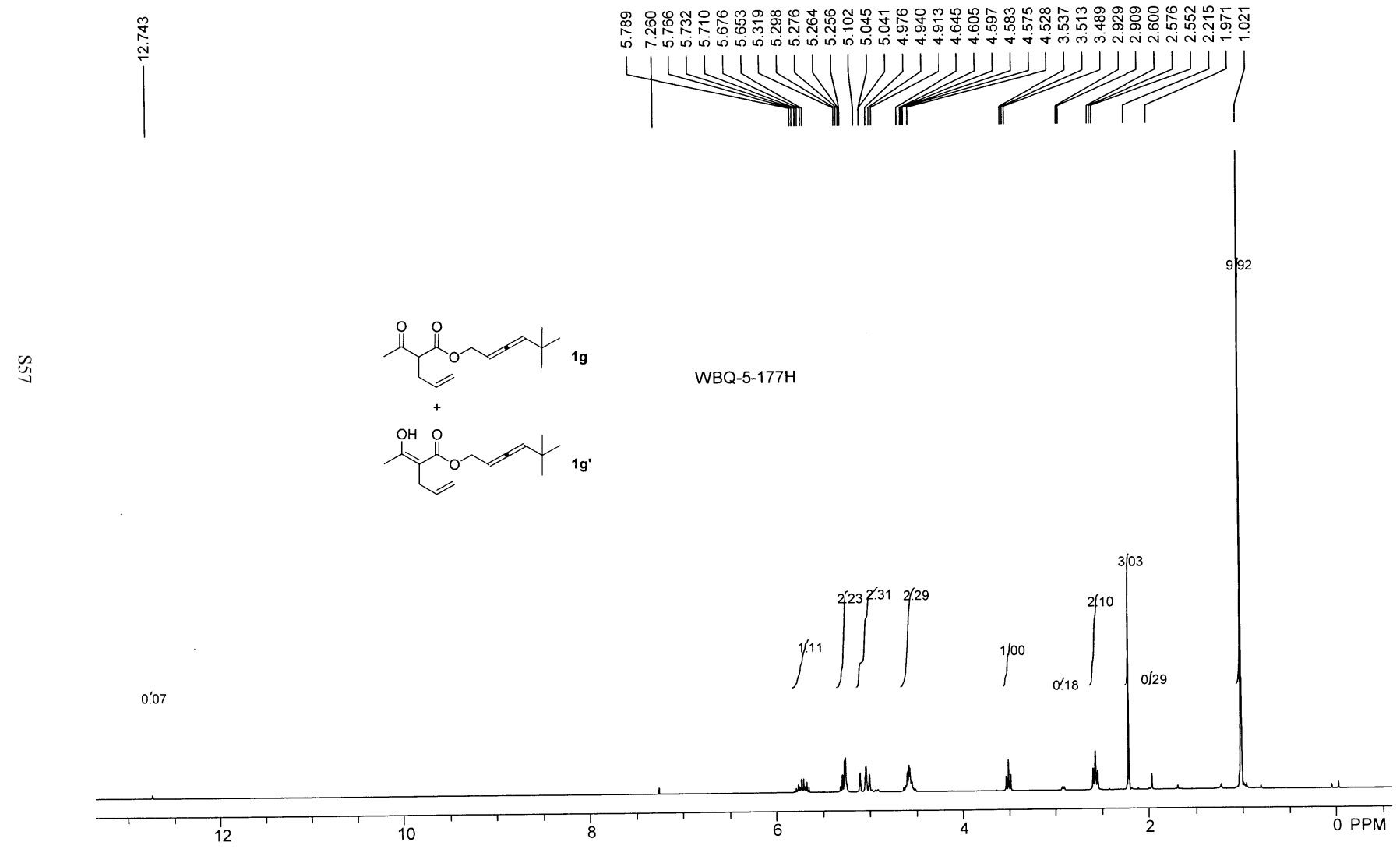
100
150
200
PPM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5.710
5.676
5.653
5.319
5.298
5.276
5.264
5.256
5.102
5.045
5.041
4.976
4.940
4.913
4.645
4.605
4.597
4.583
4.575
4.528
3.537
3.513
3.489
2.929
2.909
2.600
2.576
2.552
2.215
1.971
1.021
1g
+
1g'
WBQ-5-177H
9.92
3.03
2.23
2.31
2.29
2.10
1.11
1.00
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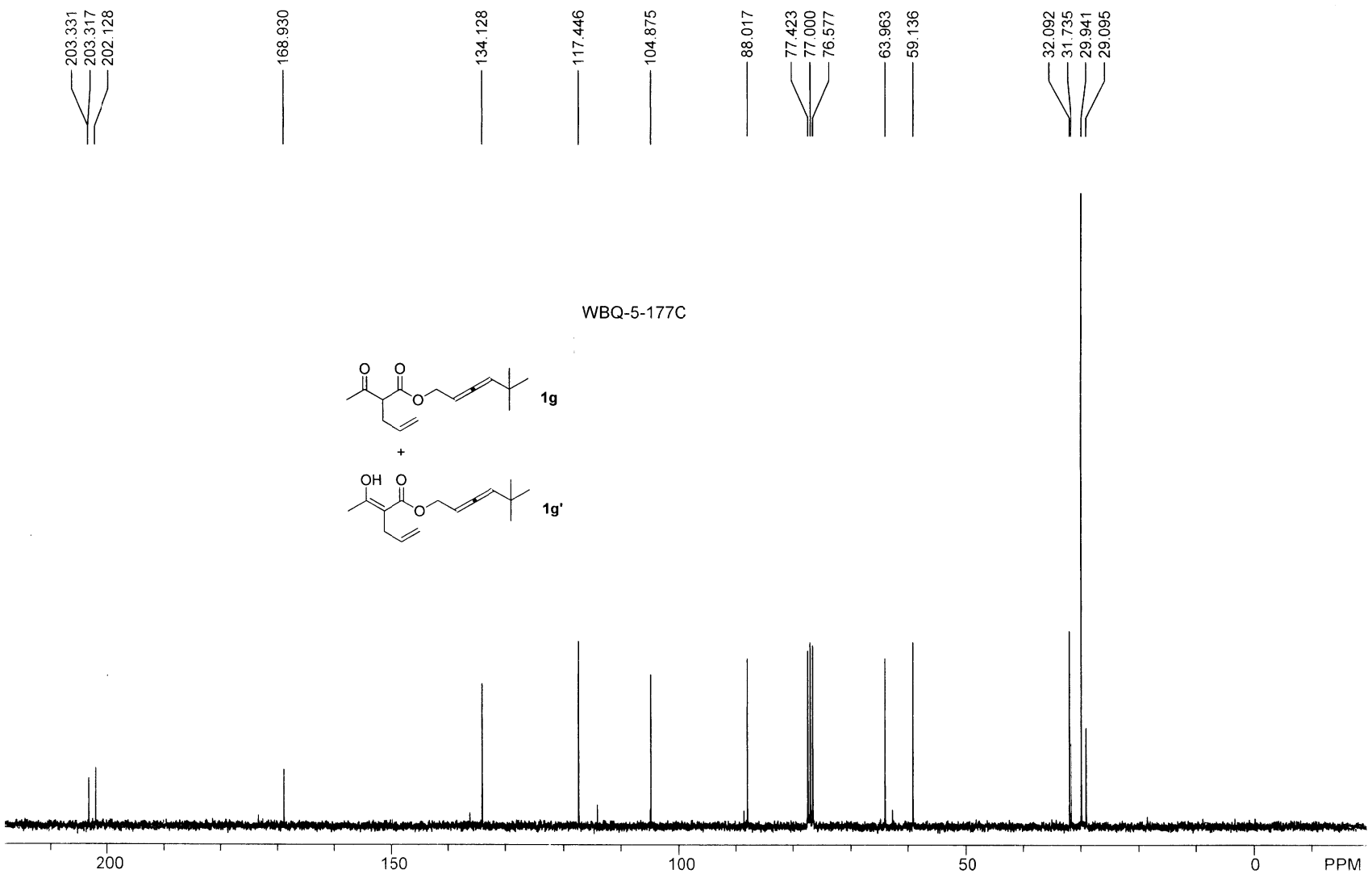
4
2
0 PPM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104.875
88.017
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77.000
76.577
63.963
59.136
32.092
31.735
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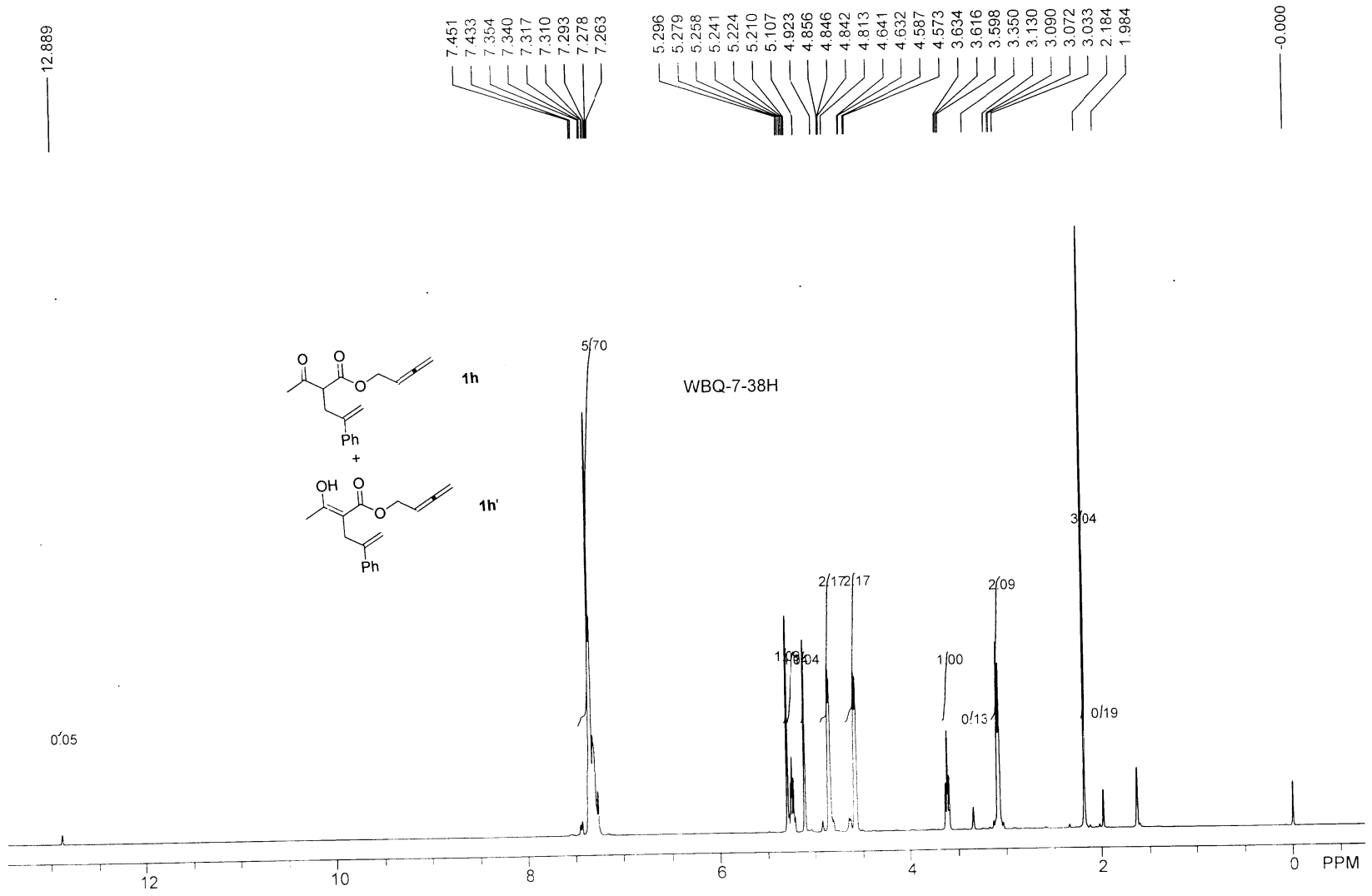
29.095
WBQ-5-177C
1g
+
1g'
200
150
100
50
0
PPM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7.451
7.433
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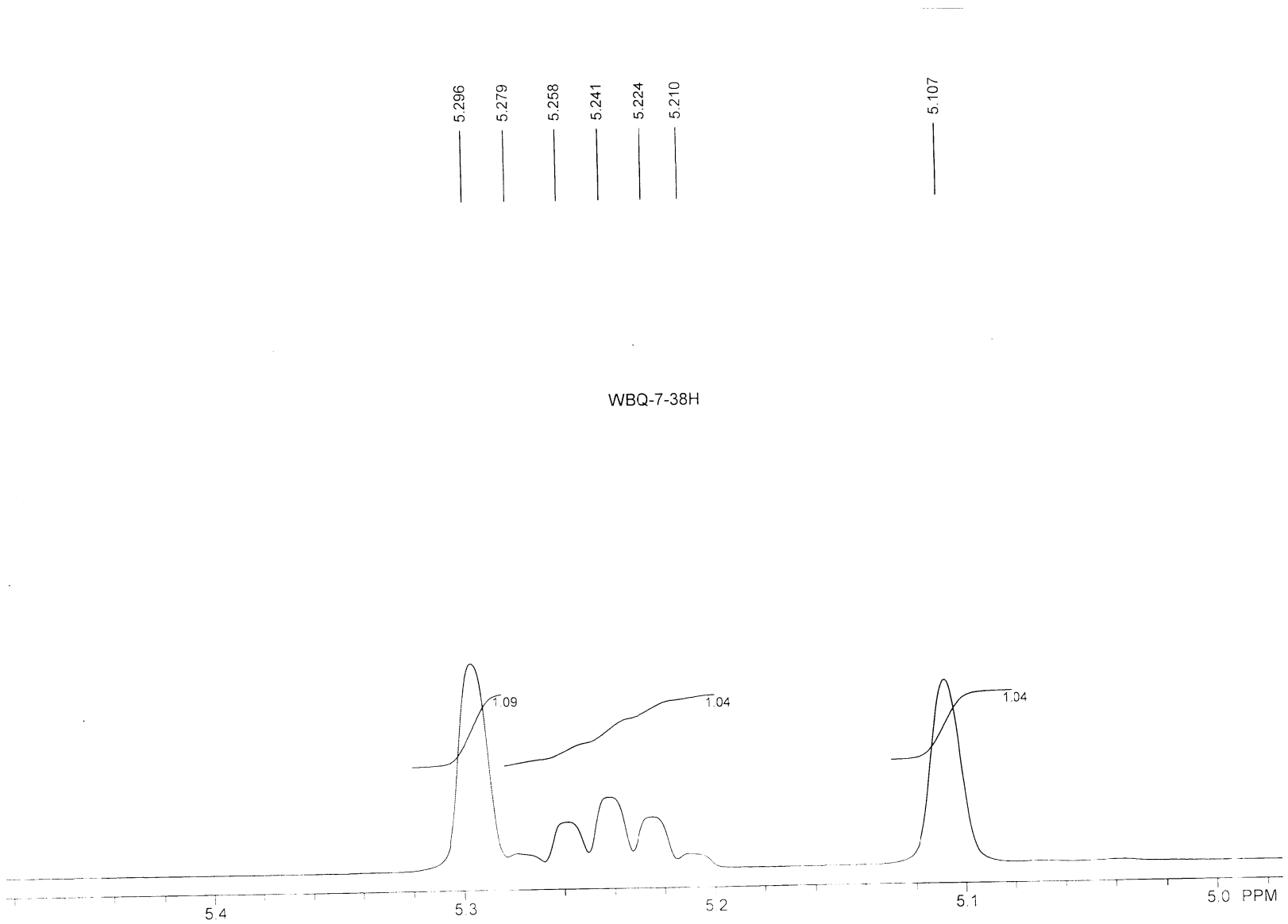
7.317
7.310
7.293
7.278
7.263
5.296
5.279
5.258
5.241
5.224
5.210
5.107
4.923
4.856
4.846
4.842
4.813
4.641
4.632
4.587
4.573
3.634
3.616
3.598
3.350
3.130
3.090
3.072
3.033
2.184
1.984
-0.000
1h
1h'
Ph
OH
WBQ-7-38H
5.70
2.17
2.17
2.09
3.04
1.00
0.13
0.19
0.05
PPM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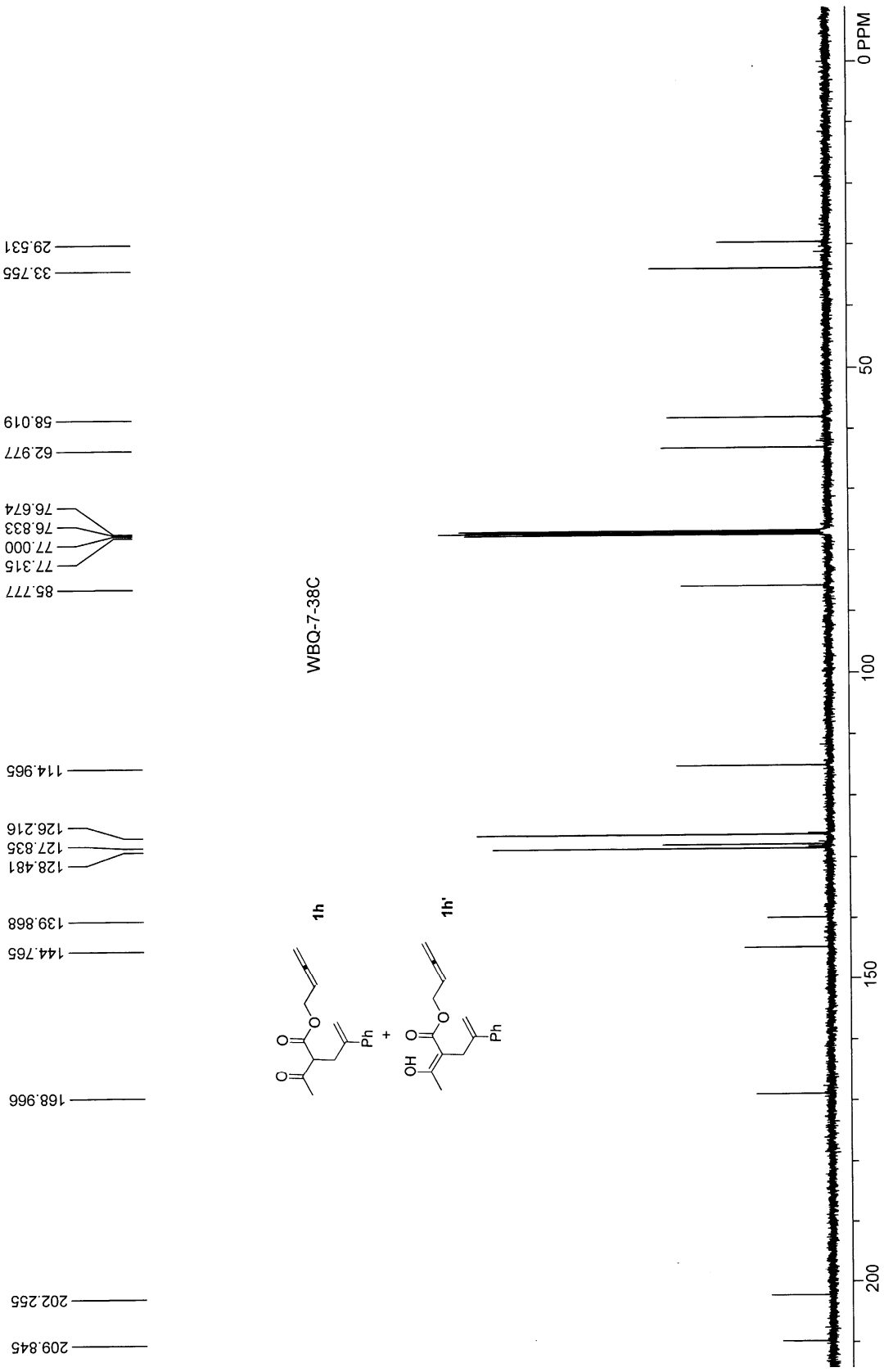
5.279
5.258
5.241
5.224
5.210
5.107
WBQ-7-38H
1.09
1.04
1.04
5.4
5.3
5.2
5.1
5.0 PPM


WBQ-7-38C
1h
1h'
Ph
OH
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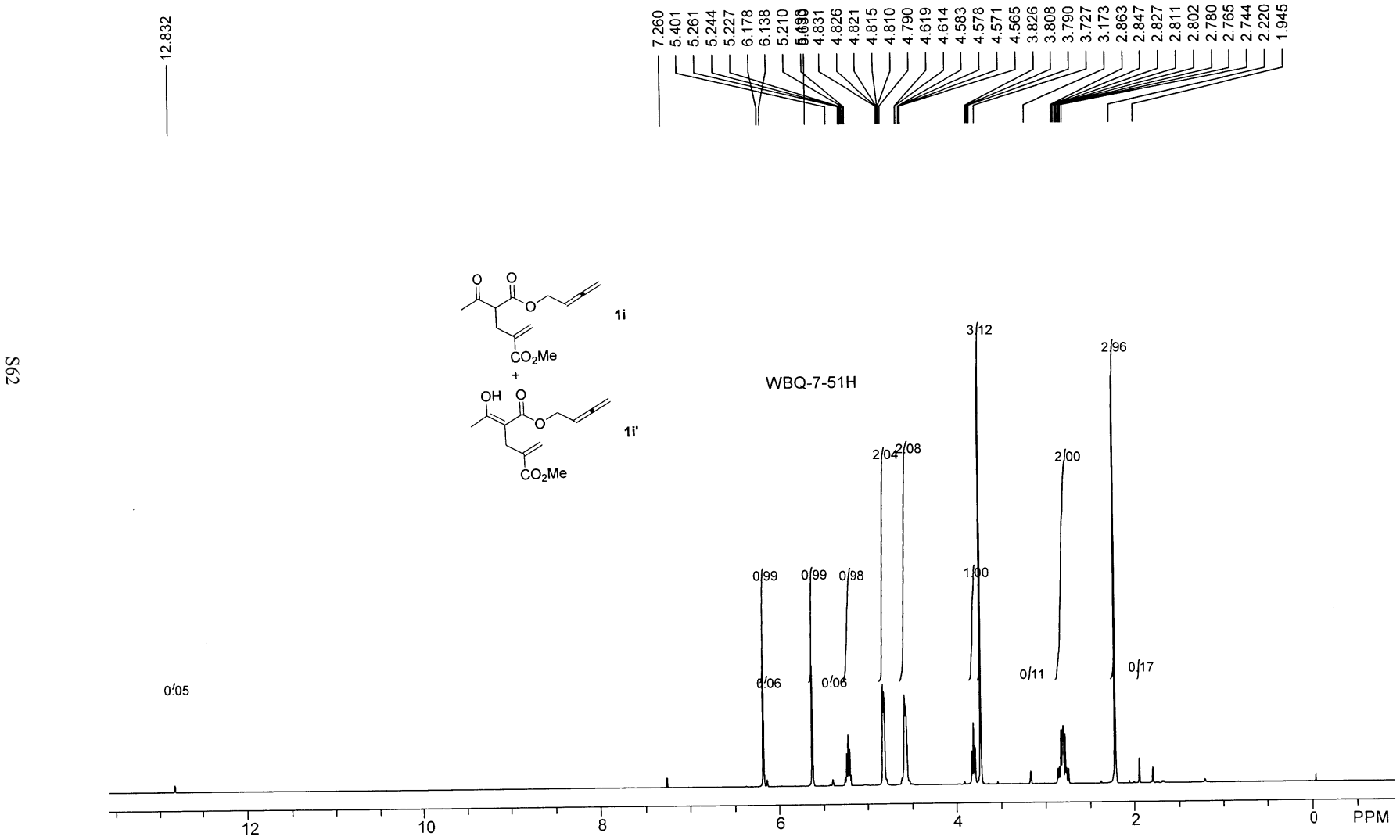
127.835
126.216
114.965
85.777
77.315
77.000
76.833
76.674
62.977
58.019
33.755
29.531
200
150
100
50
0 PPM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6.138
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4.826
4.821
4.815
4.810
4.790
4.619
4.614
4.583
4.578
4.571
4.565
3.826
3.808
3.790
3.727
3.173
2.863
2.847
2.827
2.811
2.802
2.780
2.765
2.744
2.220
1.945
1i
1i'
WBQ-7-51H
0.05
0.99
0.99
0.98
0.06
0.06
0.06
2.04
2.08
3.12
1.00
0.11
2.00
2.96
0.17
12
10
8
6
4
2
0
PPM

WBQ--7-51C
1i
1i'
CO2Me
OH
PPM
200
150
100
50
209.794
201.720
168.549
166.715
136.326
128.191
85.711
77.315
77.000
76.791
76.673
62.944
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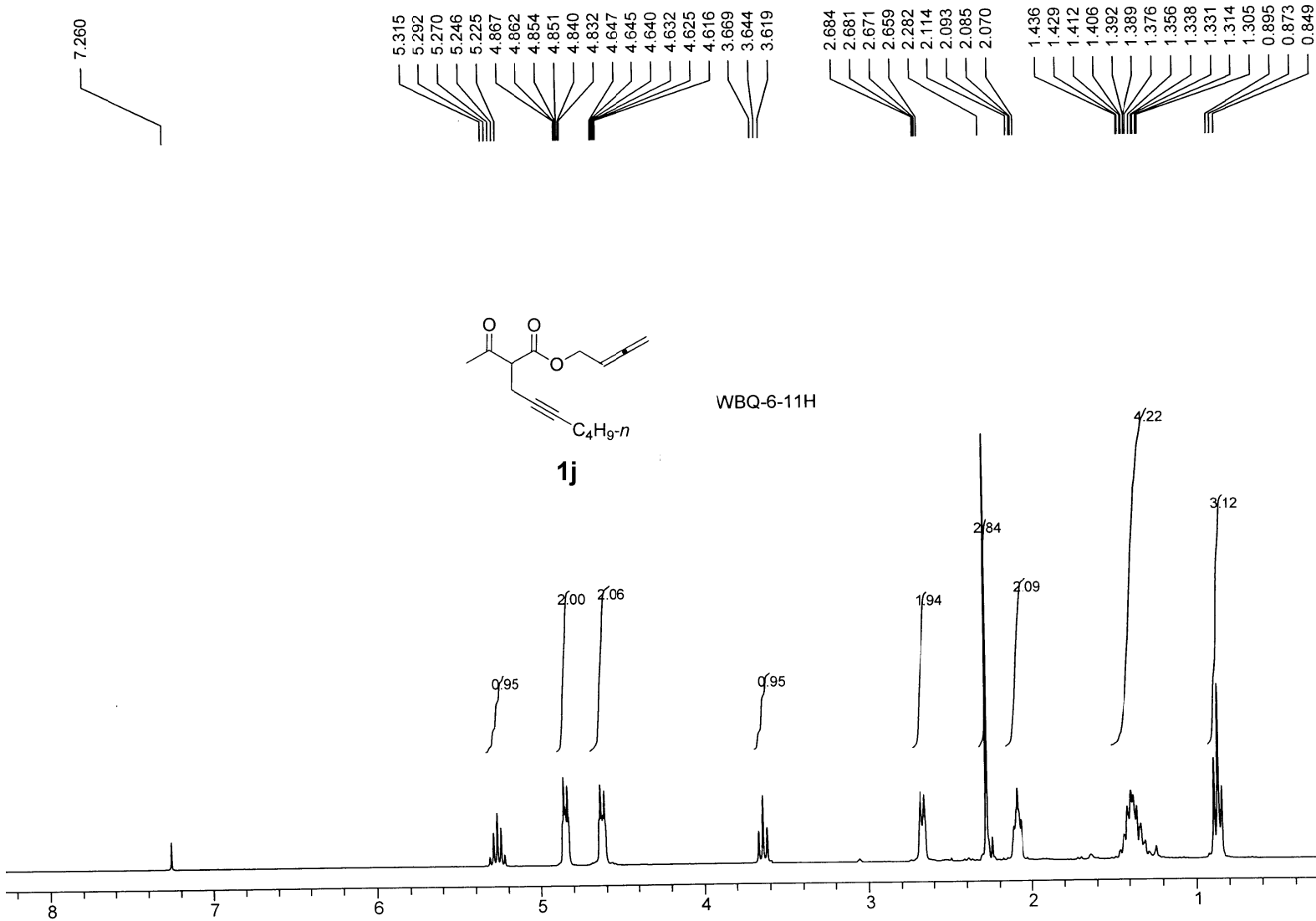
51.915
30.474
29.324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5.246
5.225
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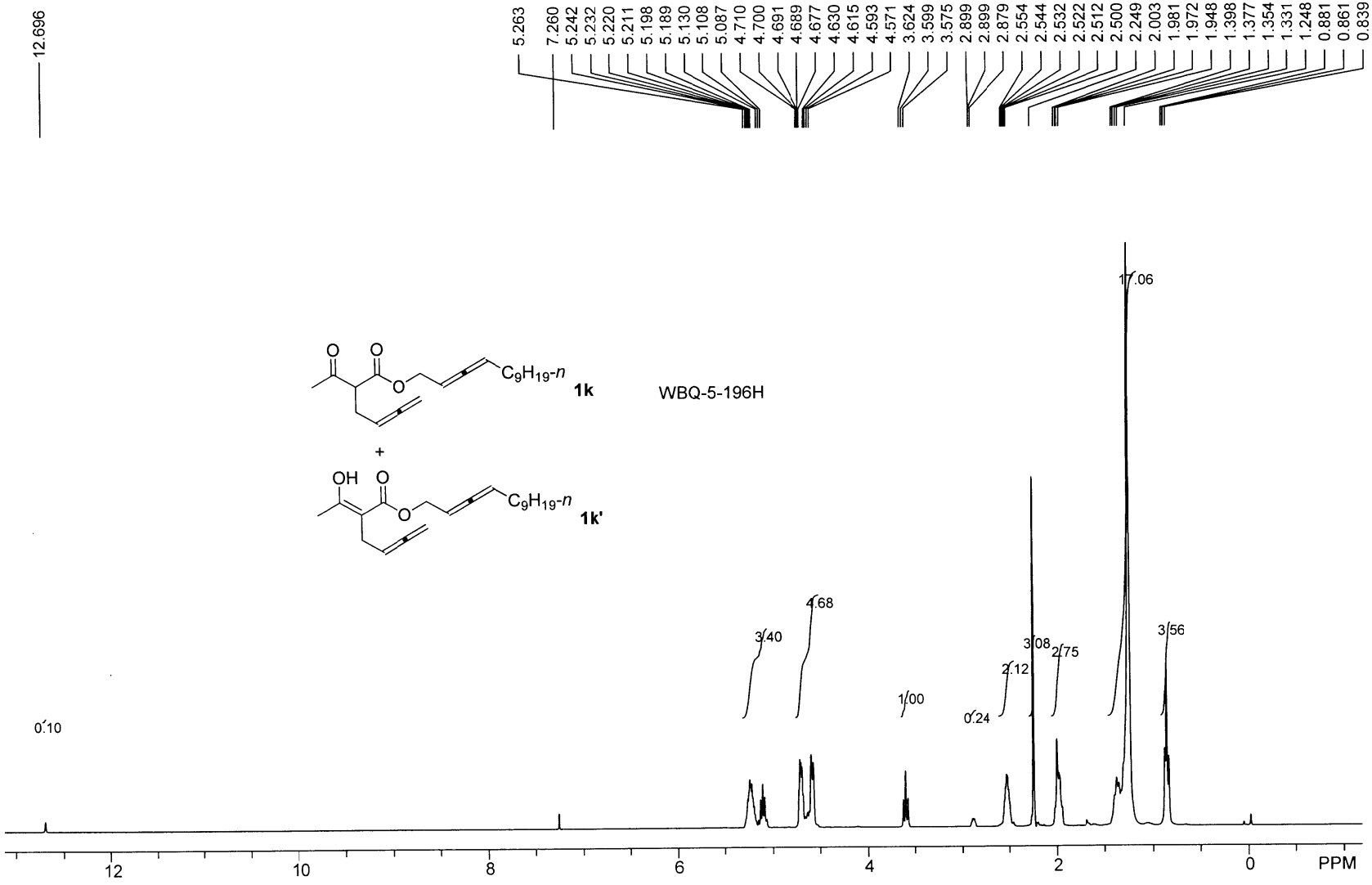
4.851
4.840
4.832
4.647
4.645
4.640
4.632
4.625
4.616
3.669
3.644
3.619
2.684
2.681
2.671
2.659
2.282
2.114
2.093
2.085
2.070
1.436
1.429
1.412
1.406
1.392
1.389
1.376
1.356
1.338
1.331
1.314
1.305
0.895
0.873
0.849
O
O
O
C_4H_9-*n*
1j
WBQ-6-11H
0.95
2.00
2.06
0.95
1.94
2.84
2.09
4.22
3.12
8
7
6
5
4
3
2
1
0PPM

209.850
201.516
168.172
85.793
82.600
77.423
77.000
76.869
76.577
75.658
63.088
58.764
30.823
29.533
21.782
18.246
17.976
13.506
WBQ-6-11C
1j
C4H9-n
O
O
O
PPM
200
150
100
50
0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5.242
5.232
5.220
5.211
5.198
5.189
5.130
5.108
5.087
4.710
4.700
4.691
4.689
4.677
4.630
4.615
4.593
4.571
3.624
3.599
3.575
2.899
2.899
2.879
2.554
2.544
2.532
2.522
2.512
2.500
2.249
2.003
1.981
1.972
1.948
1.398
1.377
1.354
1.331
1.248
0.881
0.861
0.839
O
O
O
C9H19-n
1k
+
OH
O
O
C9H19-n
1k'
WBQ-5-196H
17.06
4.68
3.40
3.56
3.08
2.75
2.12
1.00
0.24
0.10
12
10
8
6
4
2
0
PPM

208.485
205.645
202.042
168.755
93.190
86.917
86.271
77.424
77.000
76.576
76.357
63.827
58.666
31.839
29.520
29.373
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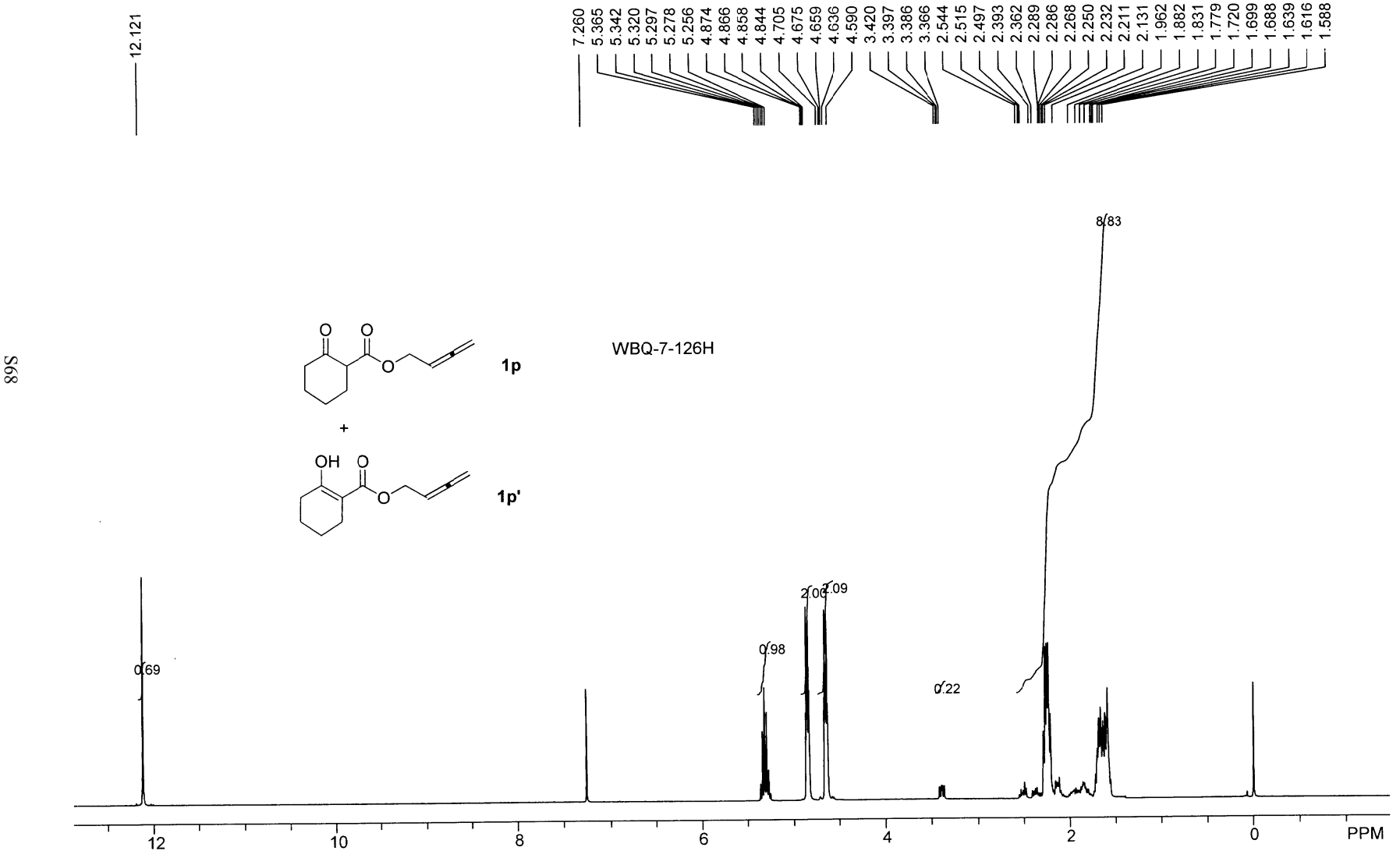
28.876
28.223
26.342
22.628
14.046
WBQ-5-196C
1k
1k'
PPM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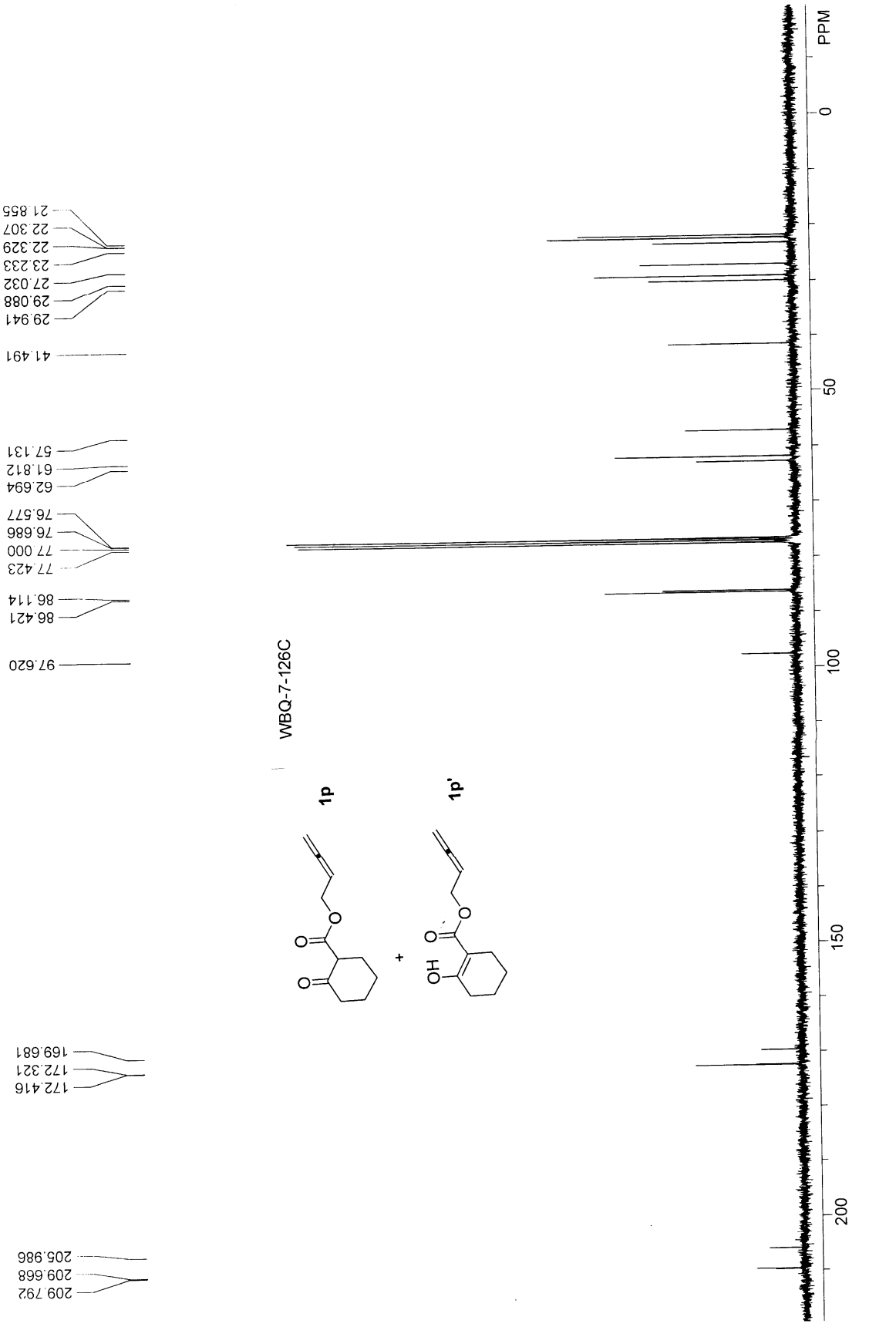
5.365
5.342
5.320
5.297
5.278
5.256
4.874
4.866
4.858
4.844
4.705
4.675
4.659
4.636
4.590
3.420
3.397
3.386
3.366
2.544
2.515
2.497
2.393
2.362
2.289
2.286
2.268
2.250
2.232
2.211
2.131
1.962
1.882
1.831
1.779
1.720
1.699
1.688
1.639
1.616
1.588
WBQ-7-126H
1p
+
1p'
8.83
2.09
2.06
0.98
0.69
0.22
12
10
8
6
4
2
0
PPM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1p
1p'
PPM
0
50
100
150
200
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172.321
169.681
97.620
86.421
86.114
77.423
77.000
76.686
76.577
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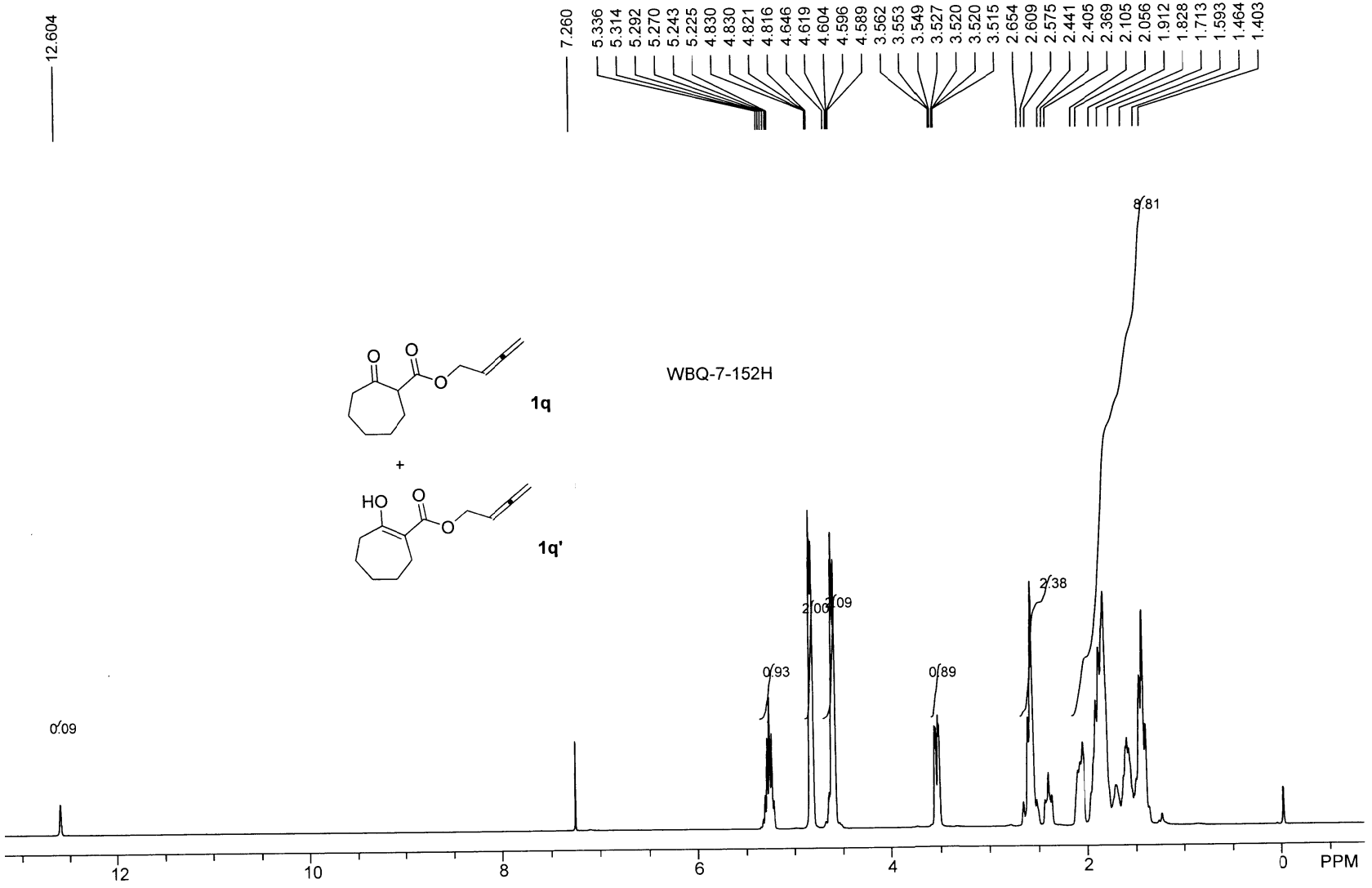
29.088
27.032
23.233
22.329
22.307
21.855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5.243
5.225
4.830
4.821
4.816
4.646
4.619
4.604
4.596
4.589
3.562
3.553
3.549
3.527
3.520
3.520
3.515
2.654
2.609
2.575
2.441
2.405
2.369
2.105
2.056
1.912
1.828
1.713
1.593
1.464
1.403
WBQ-7-152H
1q
+
1q'
0.09
0.93
2.00
2.09
0.89
2.38
8.81
12
10
8
6
4
2
0
PPM

209.718
208.650
170.184
86.038
77.424
77.000
76.646
76.575
62.642
58.836
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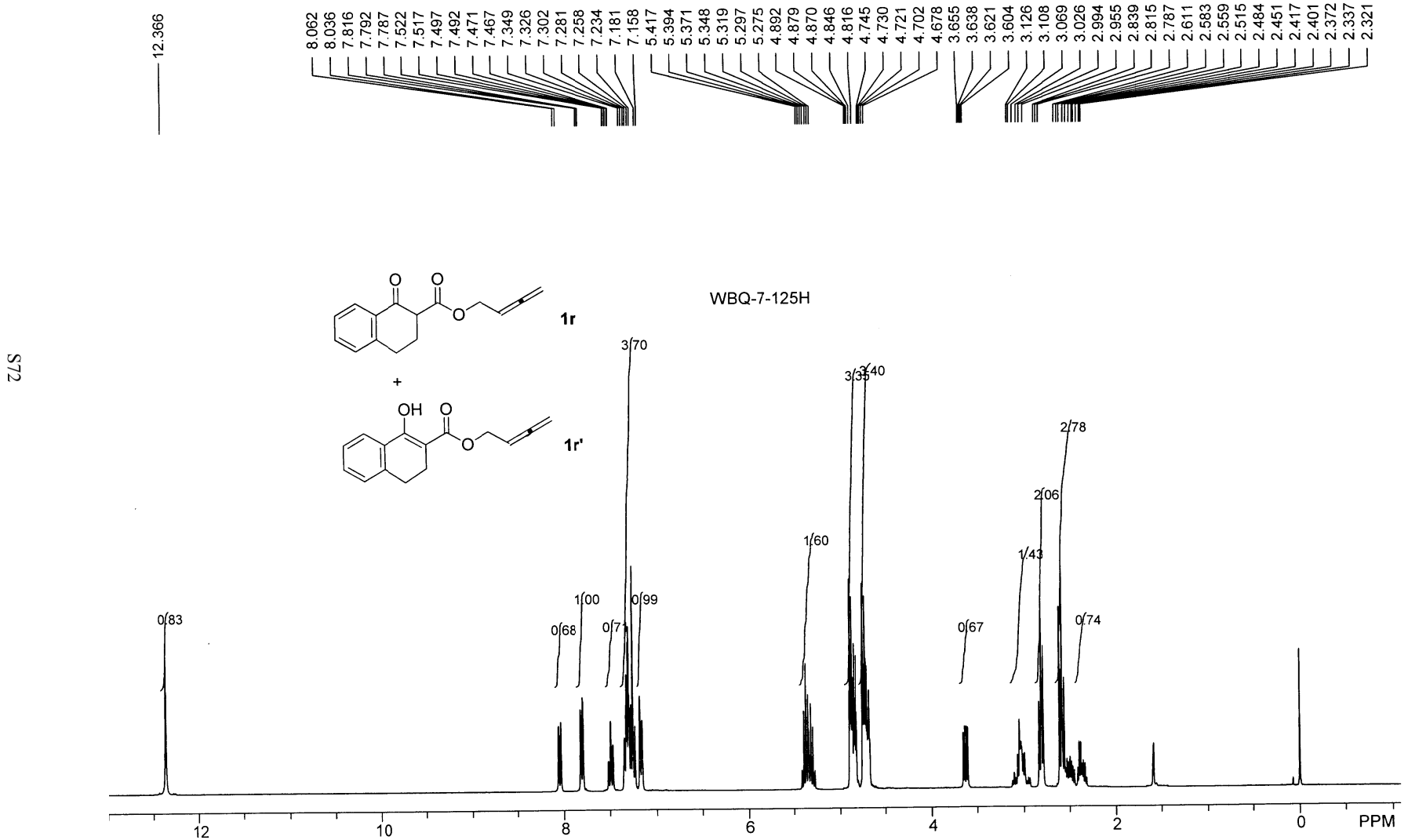
27.543
24.320
WBQ-7-152C
1q
1q'
0 PPM
50
100
150
200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7.517
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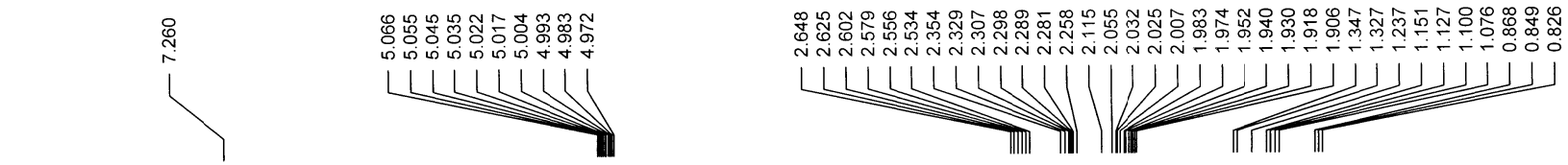
7.467
7.349
7.326
7.302
7.281
7.258
7.234
7.181
7.158
5.417
5.394
5.371
5.348
5.319
5.297
5.275
4.892
4.879
4.870
4.846
4.816
4.745
4.730
4.721
4.702
4.678
3.655
3.638
3.621
3.604
3.126
3.108
3.069
3.026
2.994
2.955
2.839
2.815
2.787
2.611
2.583
2.559
2.515
2.484
2.451
2.417
2.401
2.372
2.337
2.321
WBQ-7-125H
1r
+
1r'
OH
3.70
3.34
3.31
2.78
2.06
1.60
1.43
1.00
0.99
0.83
0.74
0.68
0.67
0.7
12
10
8
6
4
2
0
PPM

209.722
192.976
172.311
169.891
165.339
143.607
139.442
133.873
131.714
130.562
129.920
128.767
127.748
127.397
126.886
126.554
124.344
96.813
86.376
86.121
77.422
77.000
76.729
76.578
62.854
62.210
54.494
27.726
27.597
26.368
20.458
WBQ-7-125C
1r
1r'
O
O
O
O
OH
+
PPM
0
50
100
150
200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5.004
4.993
4.983
4.972
2.648
2.625
2.602
2.579
2.556
2.534
2.354
2.329
2.307
2.298
2.289
2.281
2.258
2.115
2.055
2.032
2.025
2.007
1.983
1.974
1.952
1.940
1.930
1.918
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1.327
1.237
1.151
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1.100
1.076
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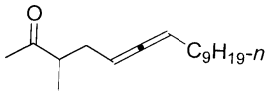
0.849
0.826


O
C9H19-n

2a

WBQ-7-133H
1.98
1.00
1.05
3.02
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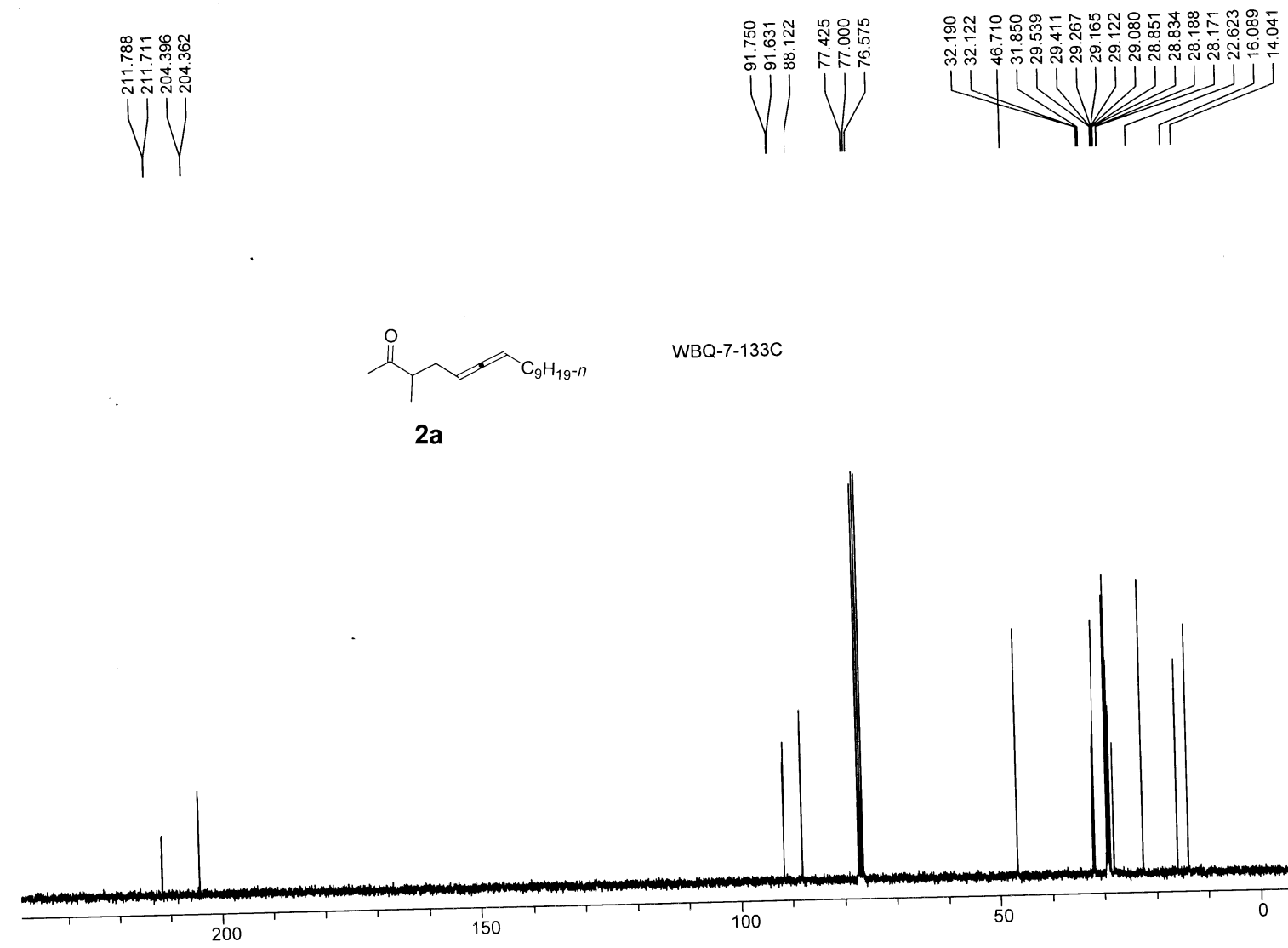
14.86
3.01
3.15
8
7
6
5
4
3
2
1
0
PPM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77.425
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76.575
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32.122
46.710
31.850
29.539
29.411
29.267
29.165
29.122
29.080
28.851
28.834
28.188
28.171
22.623
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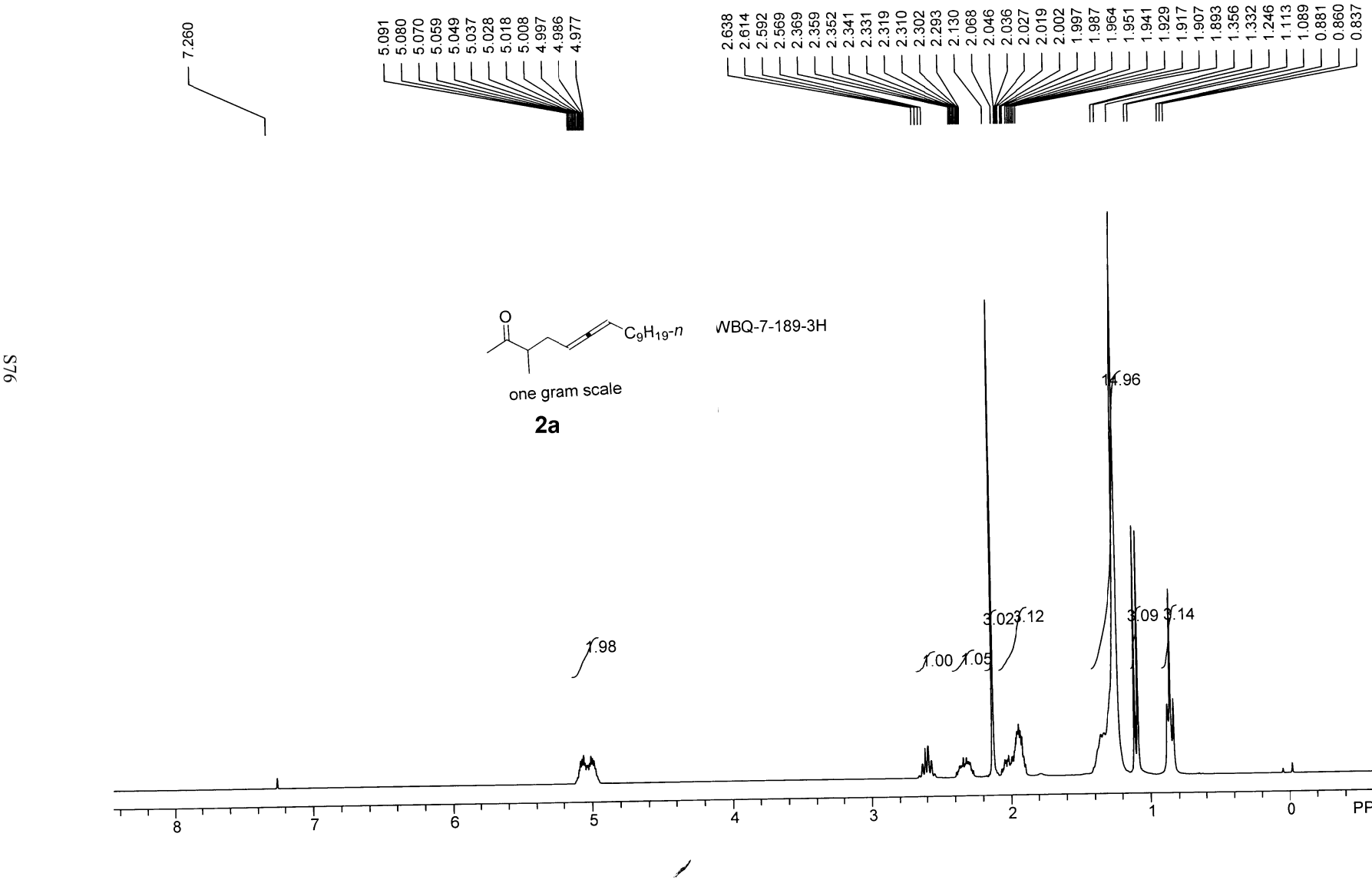
O
C_9H_{19}-*n*
WBQ-7-133C
200
150
100
50
0
PPM

2a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5.059
5.049
5.037
5.028
5.018
5.008
4.997
4.986
4.977
2.638
2.614
2.592
2.569
2.369
2.359
2.352
2.341
2.331
2.319
2.310
2.302
2.293
2.130
2.068
2.046
2.036
2.027
2.019
2.002
1.997
1.987
1.964
1.951
1.941
1.929
1.917
1.907
1.893
1.356
1.332
1.246
1.113
1.089
0.881
0.860
0.837
O
C_9H_{19}-*n*
one gram scale
2a
WBQ-7-189-3H
1.98
1.00
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14.96
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6
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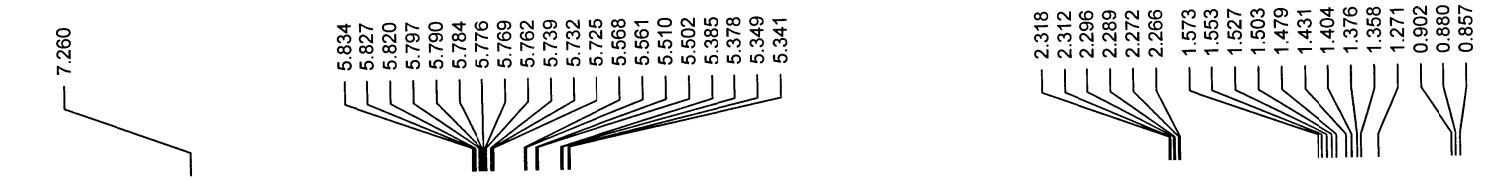
1
0
PPM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5.784
5.776
5.769
5.762
5.739
5.732
5.725
5.568
5.561
5.510
5.502
5.385
5.378
5.349
5.341
2.318
2.312
2.296
2.289
2.272
2.266
1.573
1.553
1.527
1.503
1.479
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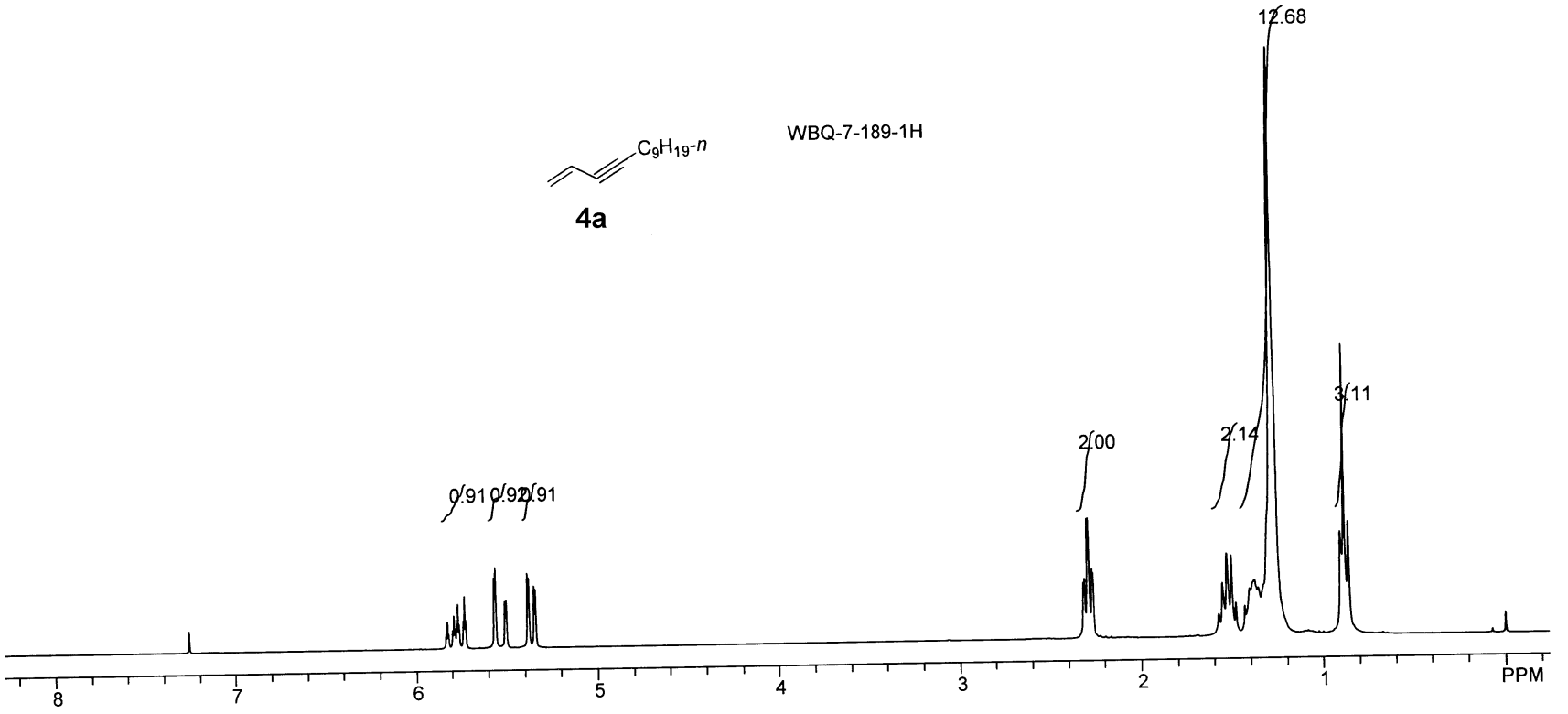
0.857


WBQ-7-189-1H
C_9H_{19}-*n*
4a
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0.91
0.92
0.91
8
7
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4
3
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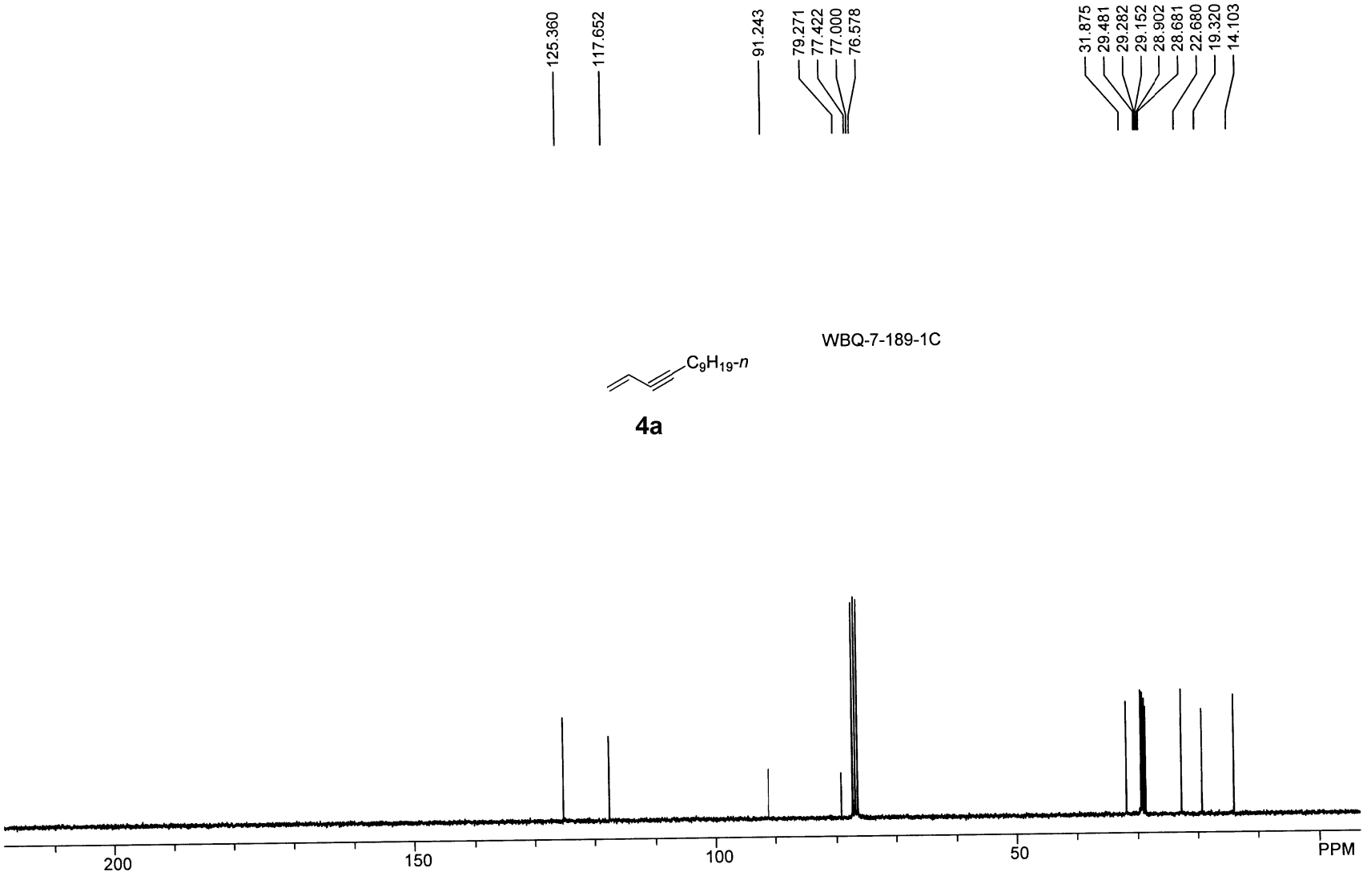
1
PPM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91.243
79.271
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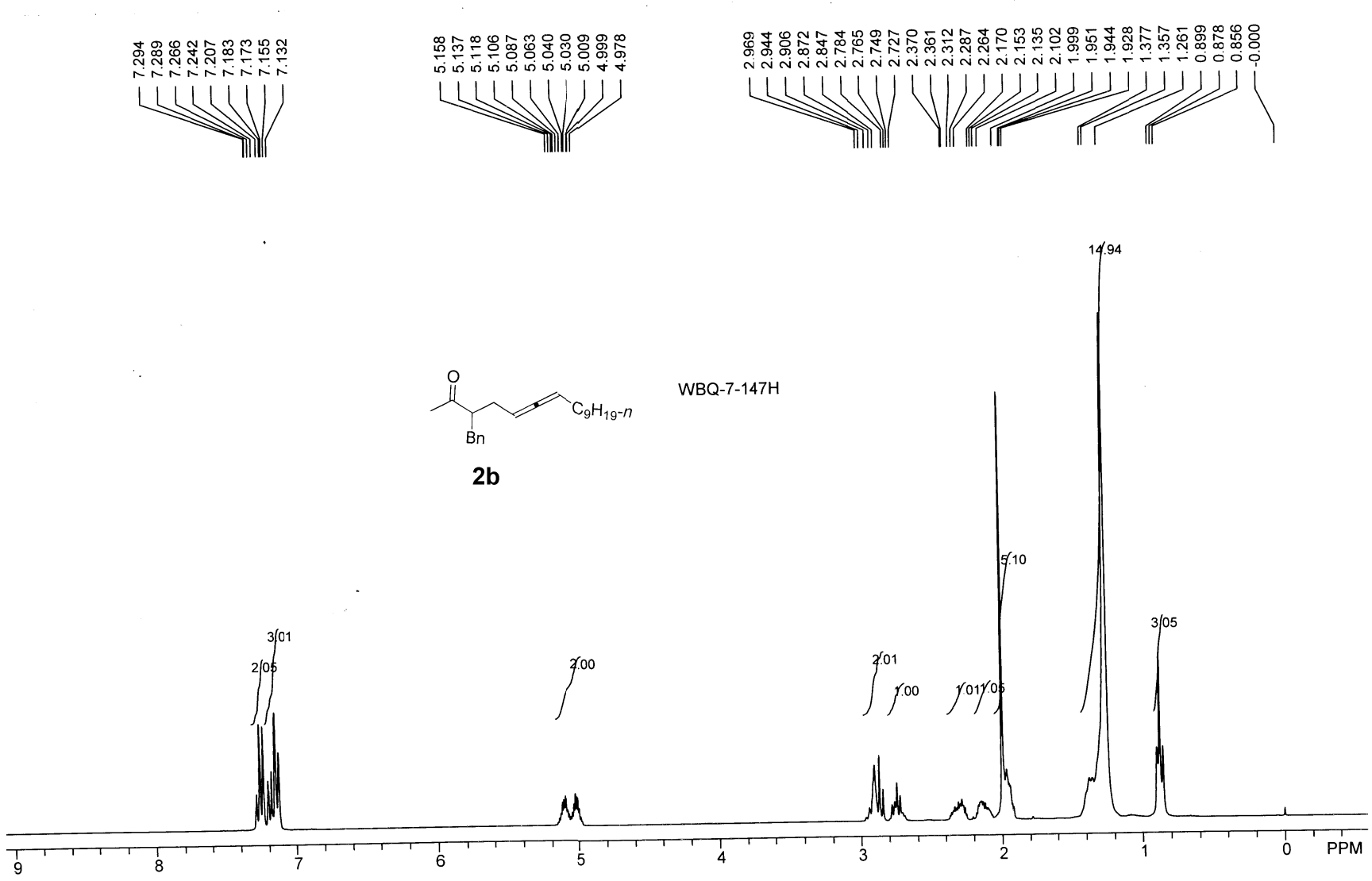
77.000
76.578
31.875
29.481
29.282
29.152
28.902
28.681
22.680
19.320
14.103
WBQ-7-189-1C
C_9H_{19}-*n*
200
150
100
50
PPM

4a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7.173
7.155
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5.158
5.137
5.118
5.106
5.087
5.063
5.040
5.030
5.009
4.999
4.978
2.969
2.944
2.906
2.872
2.847
2.784
2.765
2.749
2.727
2.370
2.361
2.312
2.287
2.264
2.170
2.153
2.135
2.102
1.999
1.951
1.944
1.928
1.377
1.357
1.261
0.899
0.878
0.856
-0.000
O
Bn
C_9H_{19}-*n*
2b
WBQ-7-147H
14.94
5.10
3.05
3.01
2.05
2.00
2.01
1.00
1.01
1.05
9
8
7
6
5
4
3
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0
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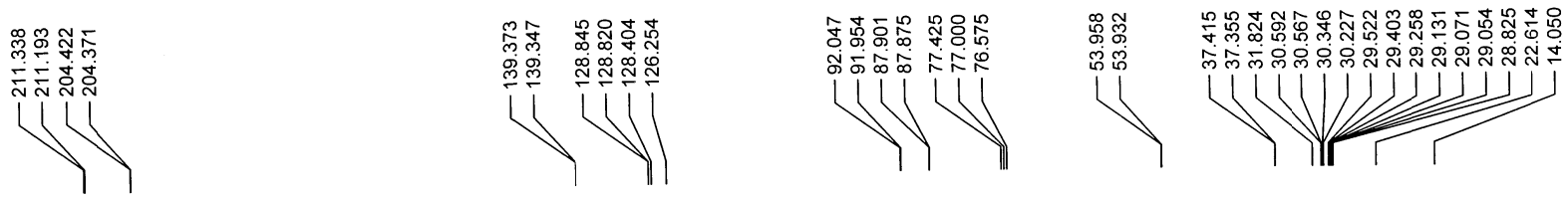
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204.371
139.373
139.347
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128.820
128.404
126.254
92.047
91.954
87.901
87.875
77.425
77.000
76.575
53.958
53.932
37.415
37.355
31.824
30.592
30.567
30.346
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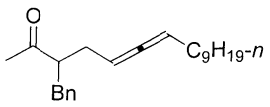
29.403
29.258
29.131
29.071
29.054
28.825
22.614
14.050

WBQ-7-147C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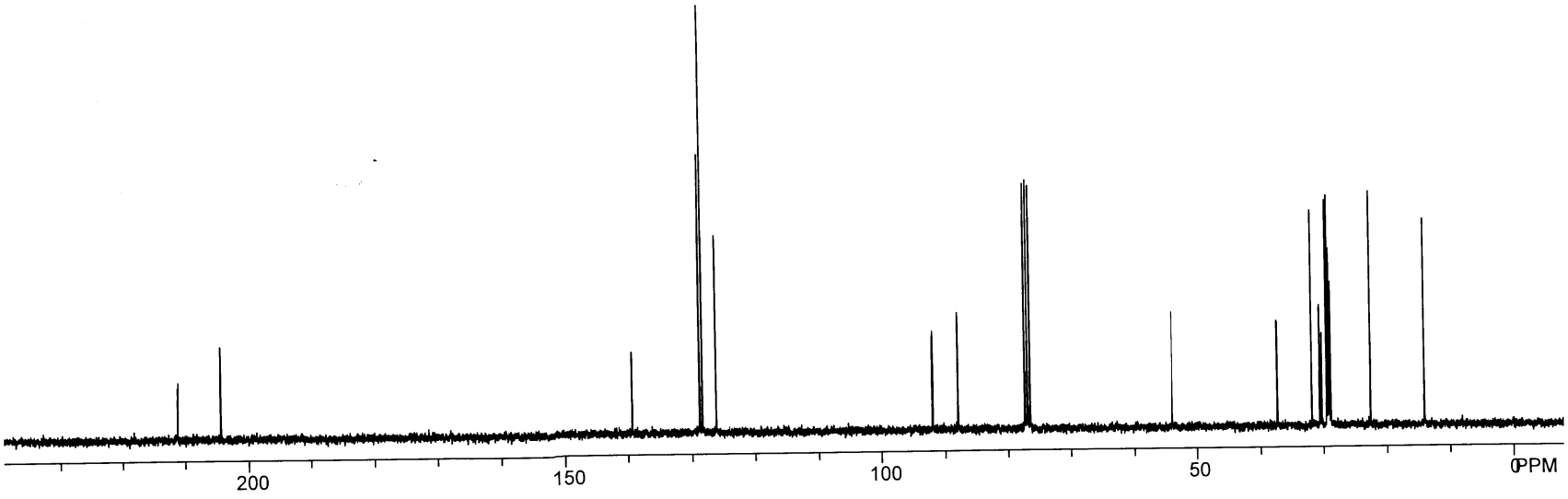
C_9H_{19}-*n*
Bn

2b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150
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50
0
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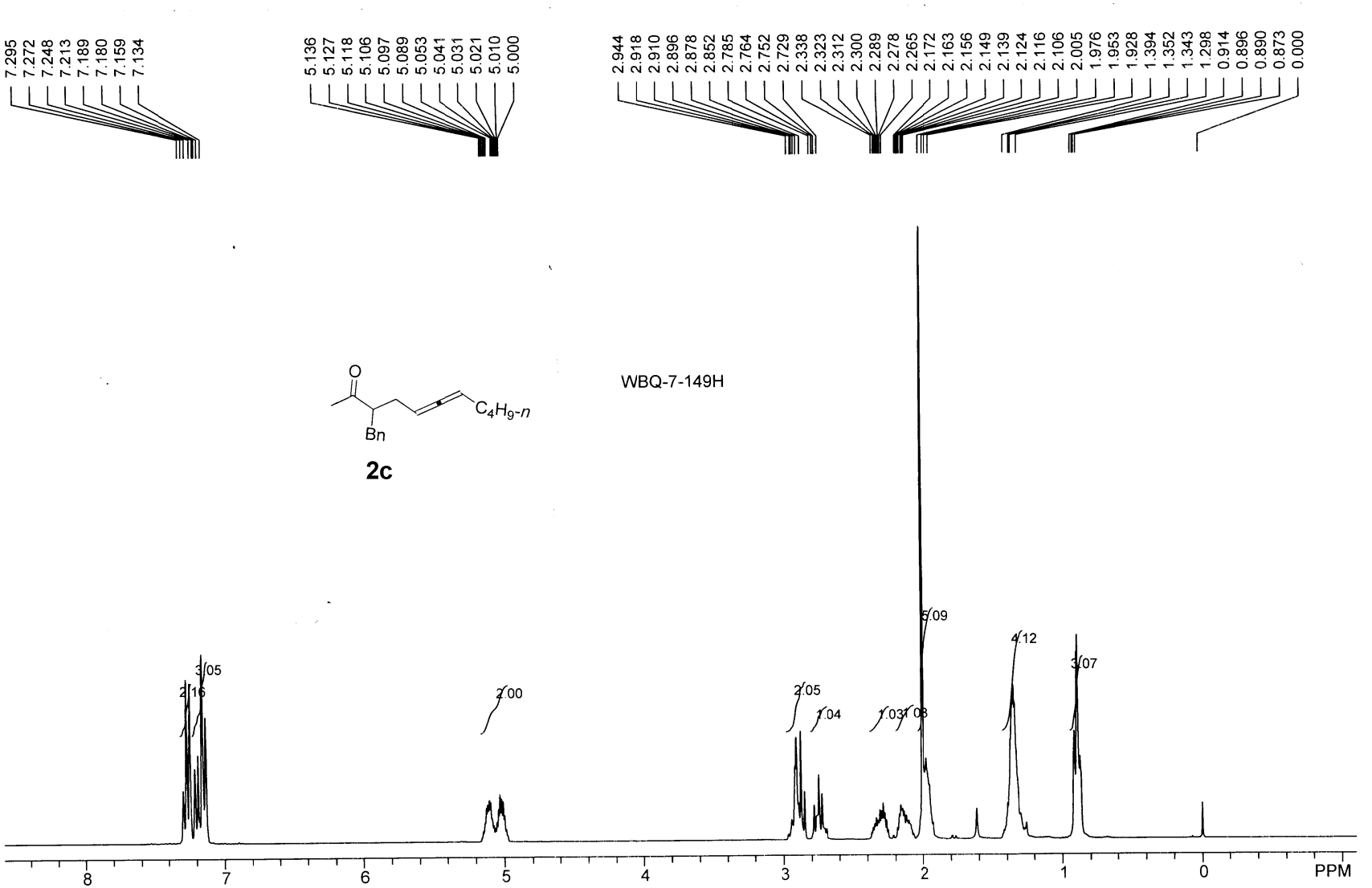
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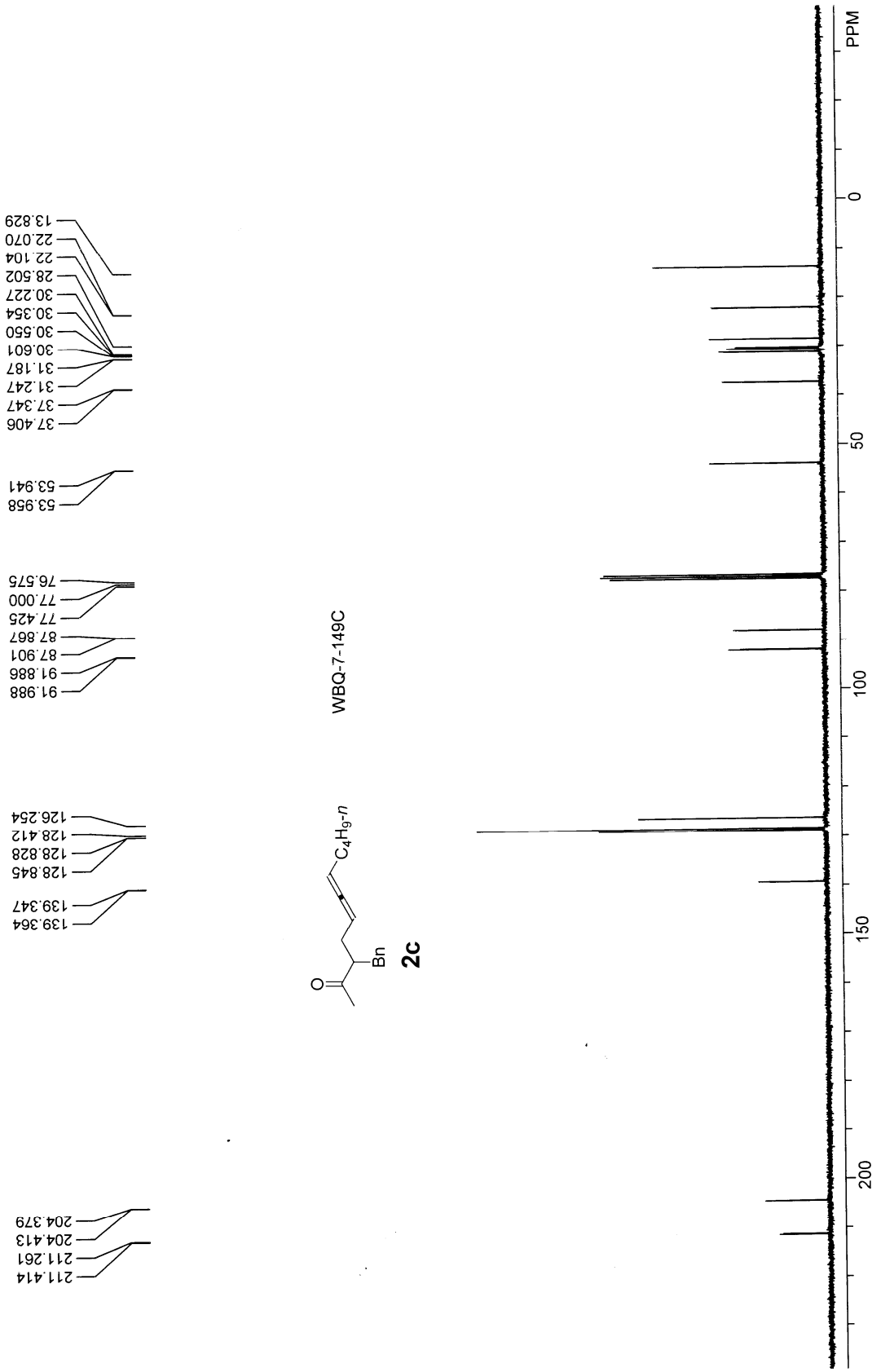
5.127
5.118
5.106
5.097
5.089
5.053
5.041
5.031
5.021
5.010
5.000
2.944
2.918
2.910
2.896
2.878
2.852
2.785
2.764
2.752
2.729
2.338
2.323
2.312
2.300
2.289
2.278
2.265
2.172
2.163
2.156
2.149
2.139
2.124
2.116
2.106
2.005
1.976
1.953
1.928
1.394
1.352
1.343
1.298
0.914
0.896
0.890
0.873
0.000
O
Bn
C_4H_{9}-*n*
2c
WBQ-7-149H
3.05
2.16
2.00
2.05
1.04
1.03
1.08
5.09
4.12
3.07
8
7
6
5
4
3
2
1
0
PPM


WBQ-7-149C
2c
Bn
O
C_4H_{9}-n
PPM
0
50
100
150
200
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22.104
28.502
30.227
30.354
30.550
30.601
31.187
31.247
37.347
37.406
53.941
53.958
76.575
77.000
77.425
87.867
87.901
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128.828
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139.364
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204.413
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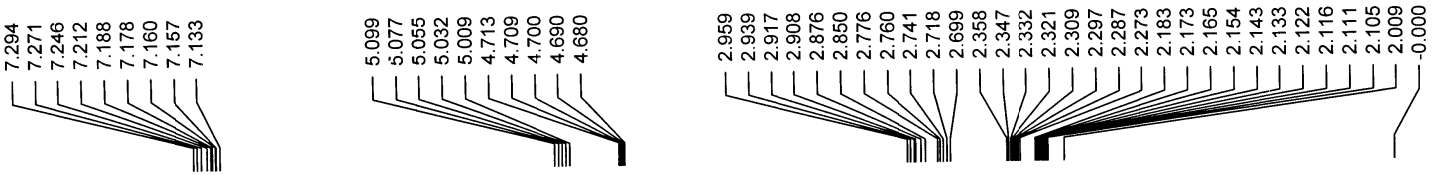
211.414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7.246
7.212
7.188
7.178
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7.157
7.133
5.099
5.077
5.055
5.032
5.009
4.713
4.709
4.700
4.690
4.680
2.959
2.939
2.917
2.908
2.876
2.850
2.776
2.760
2.741
2.718
2.699
2.358
2.347
2.332
2.321
2.309
2.297
2.287
2.273
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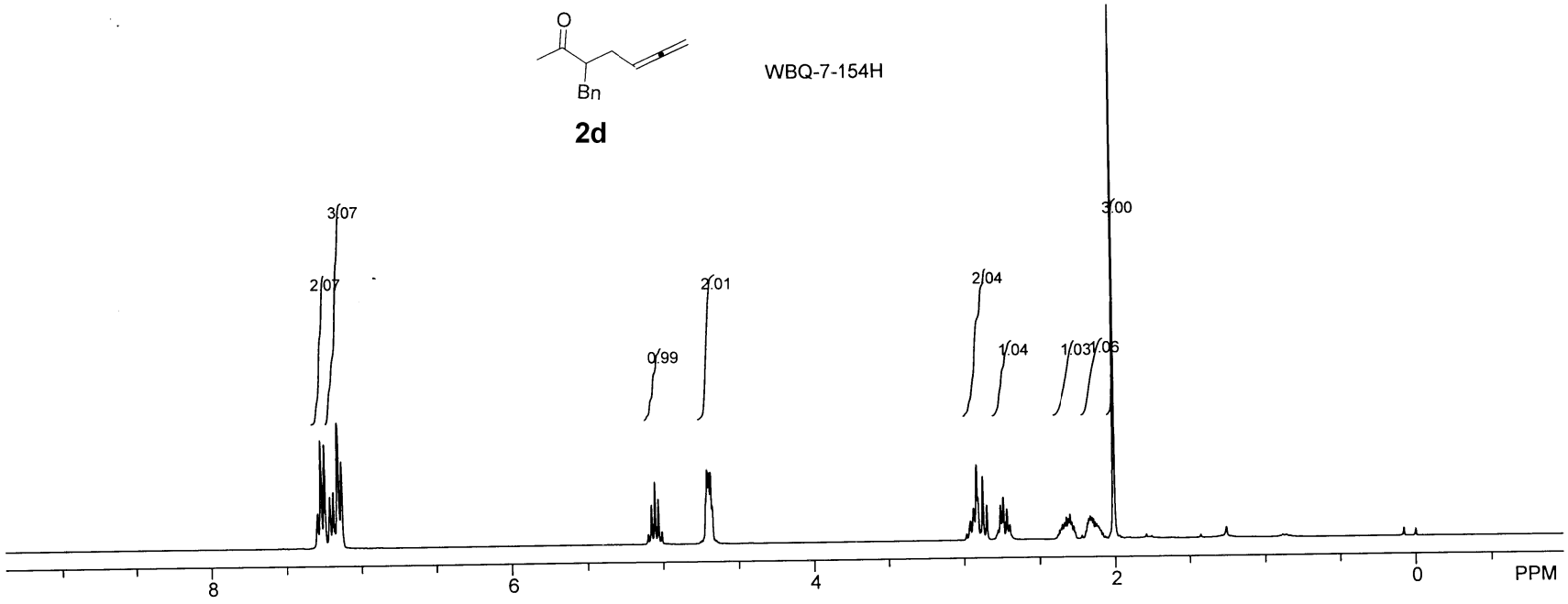
2.173
2.165
2.154
2.143
2.133
2.122
2.116
2.111
2.105
2.009
-0.000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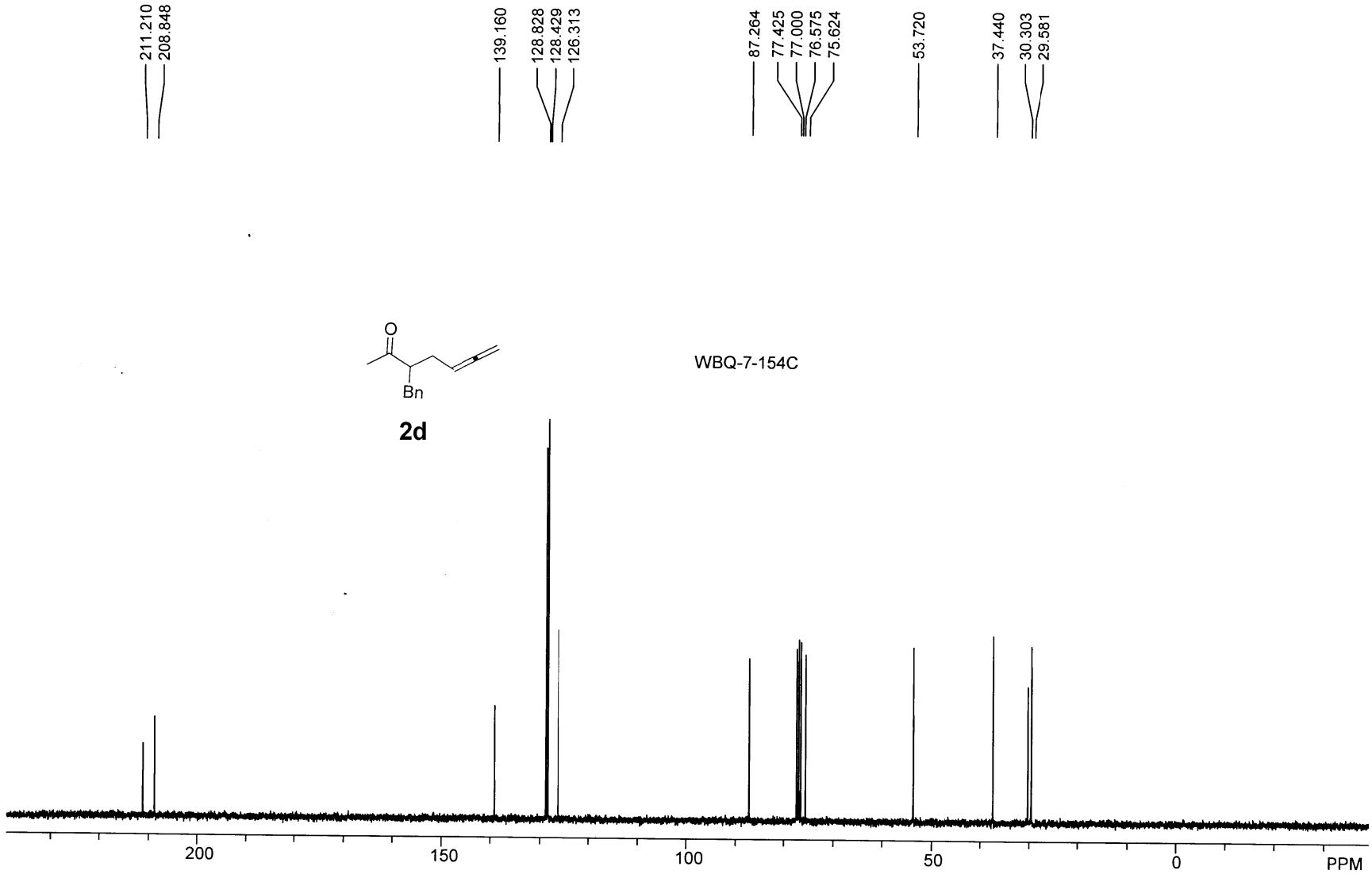
Bn
WBQ-7-154H
2d
3.07
2.07
0.99
2.01
2.04
1.04
1.03
1.06
3.00
8
6
4
2
0
PPM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208.848
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128.828
128.429
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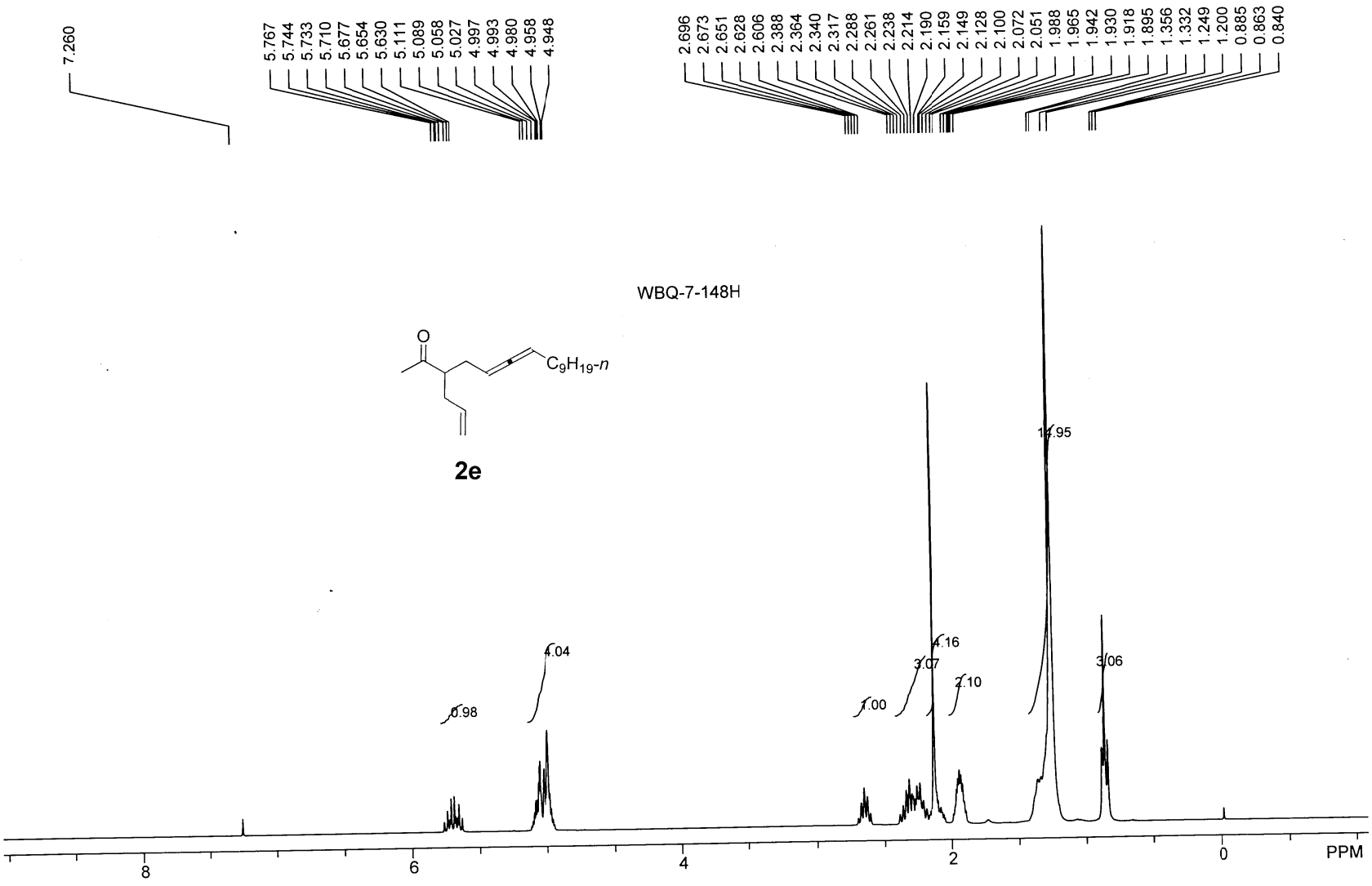
87.264
77.425
77.000
76.575
75.624
53.720
37.440
30.303
29.581
O
Bn
2d
WBQ-7-154C
200
150
100
50
0
PPM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5.710
5.677
5.654
5.630
5.111
5.089
5.058
5.027
4.997
4.993
4.980
4.958
4.948
2.696
2.673
2.651
2.628
2.606
2.388
2.364
2.340
2.317
2.288
2.261
2.238
2.214
2.190
2.159
2.149
2.128
2.100
2.072
2.051
1.988
1.965
1.942
1.930
1.918
1.895
1.356
1.332
1.249
1.200
0.885
0.863
0.840
WBQ-7-148H
O
C9H19-n
2e
0.98
4.04
1.00
3.07
4.16
2.10
14.95
3.06
8
6
4
2
0
PPM

210.972
210.862
204.388
204.328
135.260
116.942
91.954
91.818
87.969
87.935
77.425
77.000
76.575
51.927
51.901
35.291
35.274
31.850
30.201
30.176
29.539
29.479
29.420
29.275
29.156
29.097
28.834
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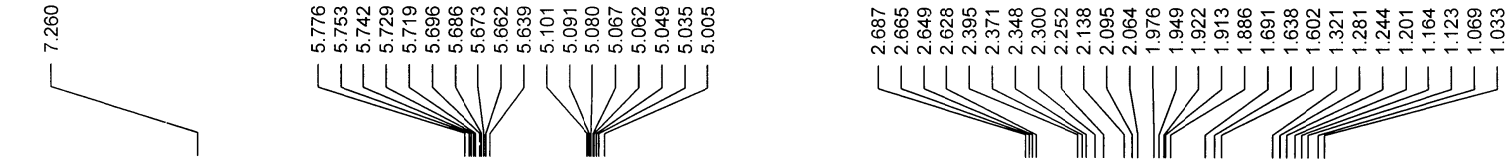
WBQ-7-148C
C_9H_{19}-*n*
O
2e
PPM
0
50
100
150
200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5.673
5.662
5.639
5.101
5.091
5.080
5.067
5.062
5.049
5.035
5.005
2.687
2.665
2.649
2.628
2.395
2.371
2.348
2.300
2.252
2.138
2.095
2.064
1.976
1.949
1.922
1.913
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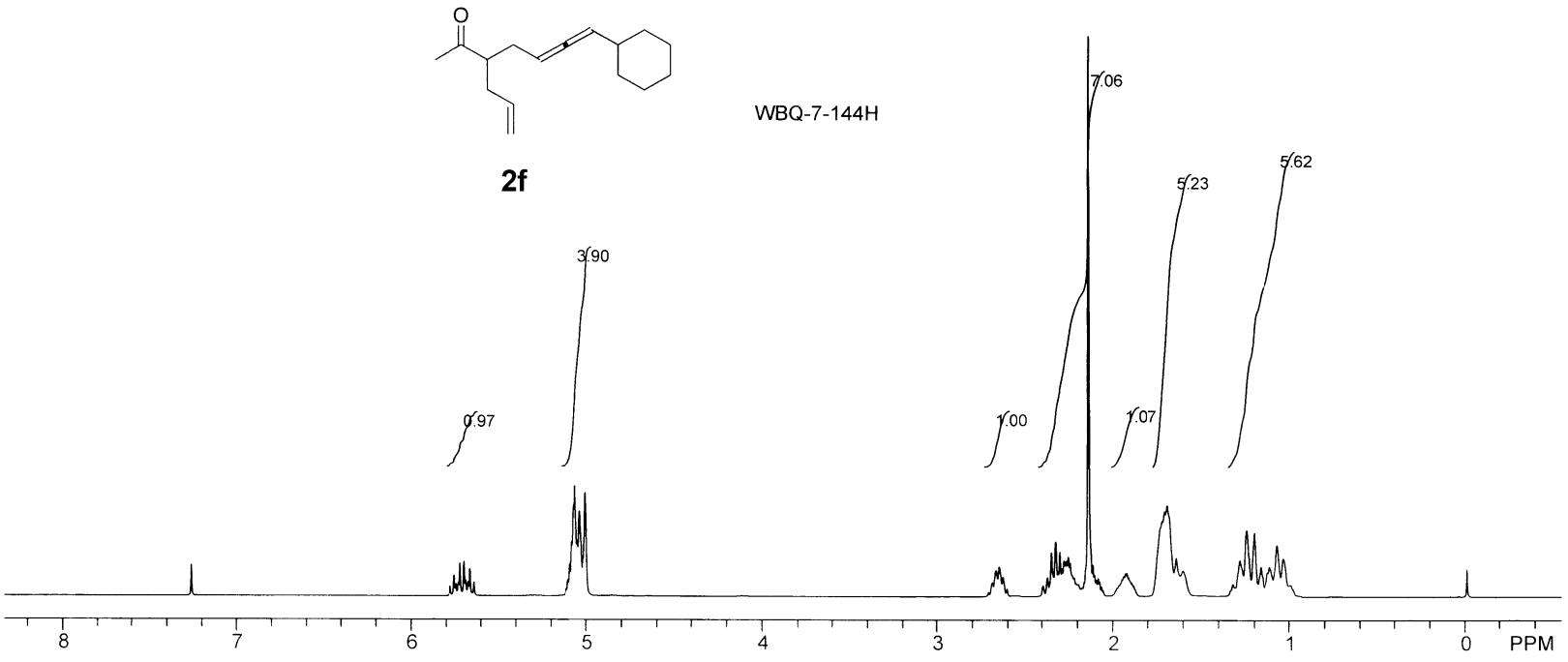
1.033


O
2f
WBQ-7-144H
7.06
5.62
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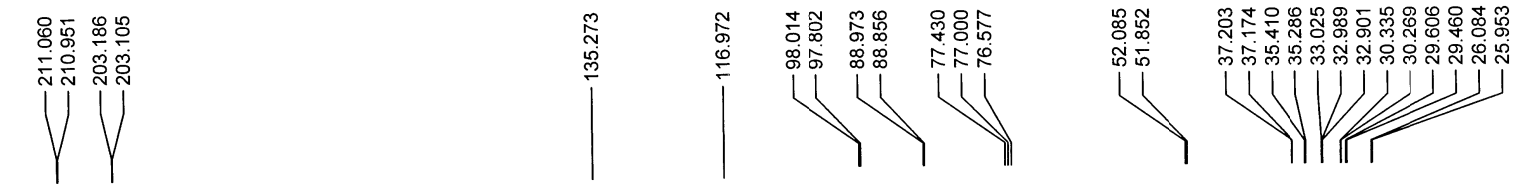
3.90
0.97
1.00
1.07
8
7
6
5
4
3
2
1
0
PPM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88.856
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77.000
76.577
52.085
51.852
37.203
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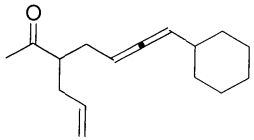
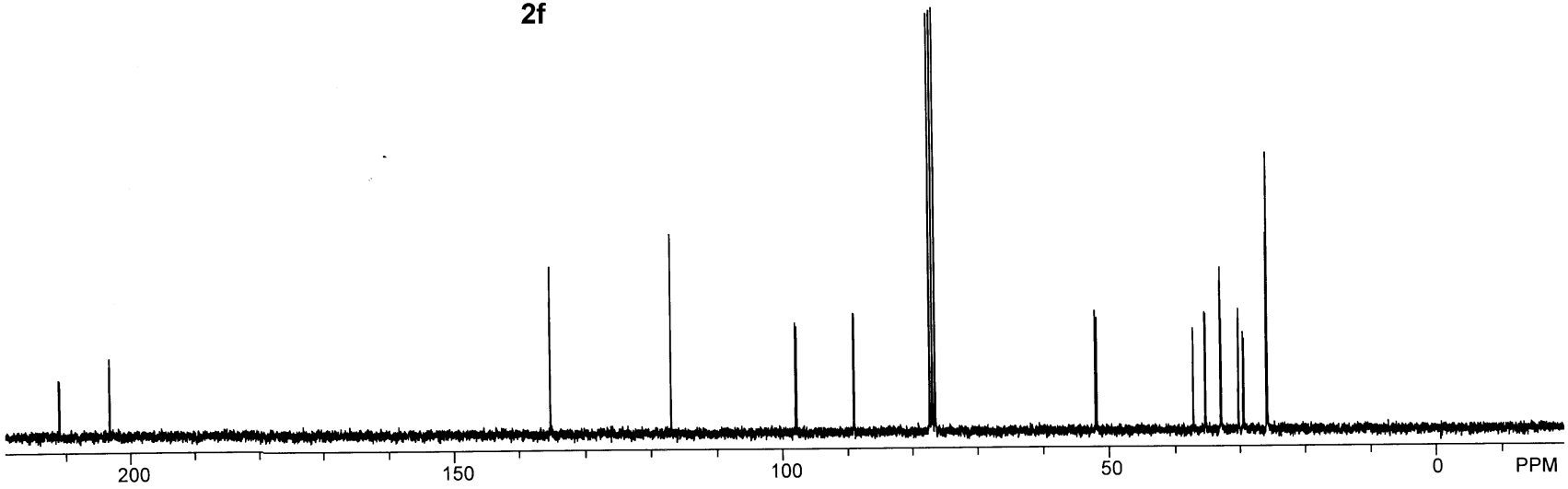
25.953


O

2f

WBQ-7-144C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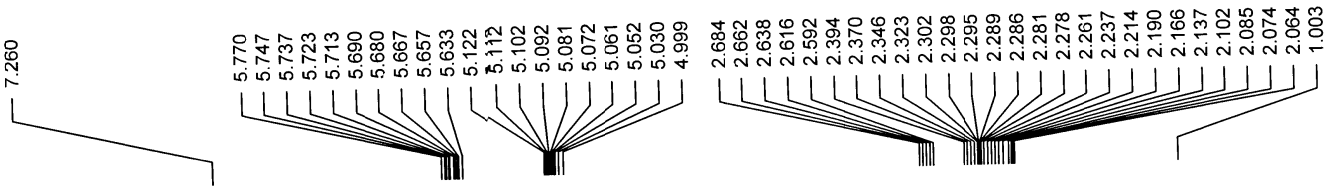
100
50
0
PPM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5.680
5.667
5.657
5.633
5.122
5.112
5.102
5.092
5.081
5.072
5.061
5.052
5.030
4.999
2.684
2.662
2.638
2.616
2.592
2.394
2.370
2.346
2.323
2.302
2.298
2.295
2.289
2.286
2.281
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2.102
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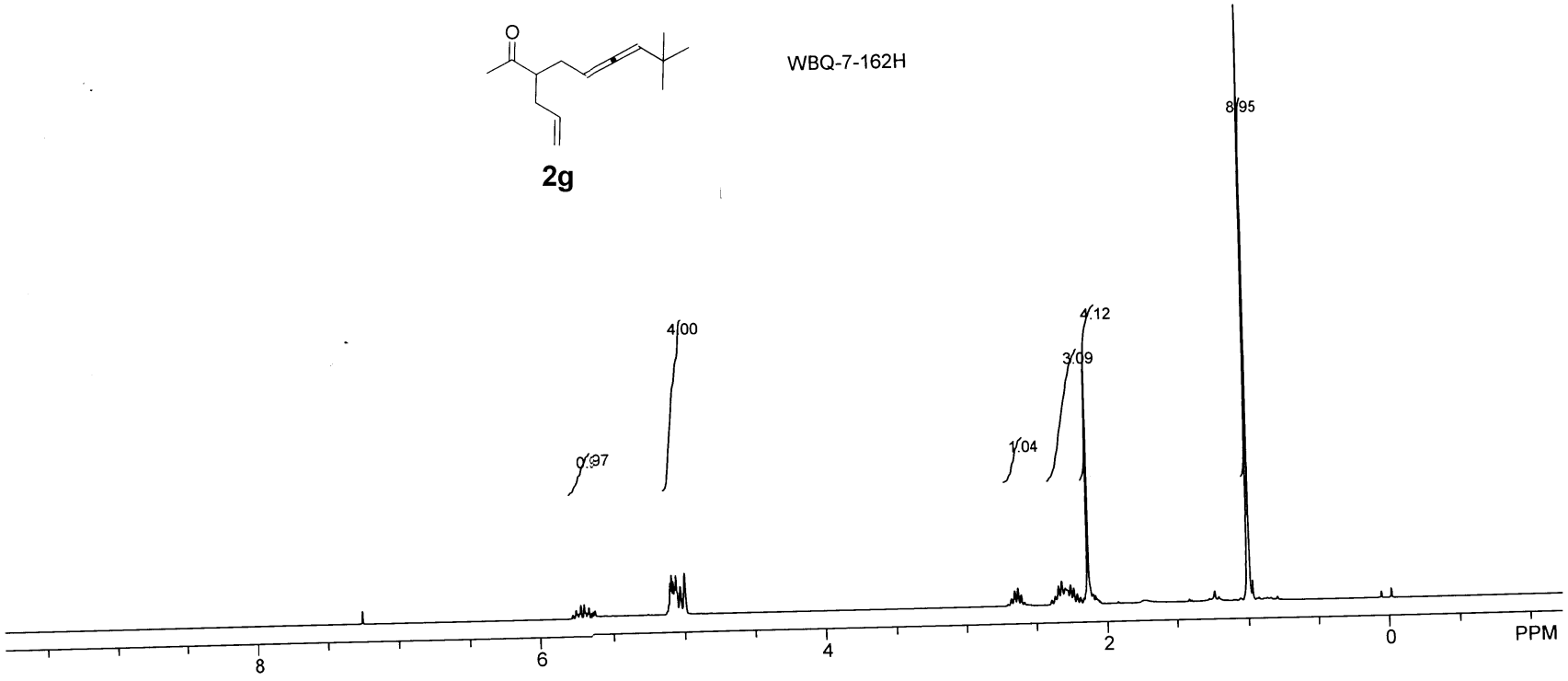
2.074
2.064
1.003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2g
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8
6
4
2
0
PPM

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77.425
77.000
76.575
52.233
51.808
35.444
35.274
31.697
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WBQ-7-162C
2g
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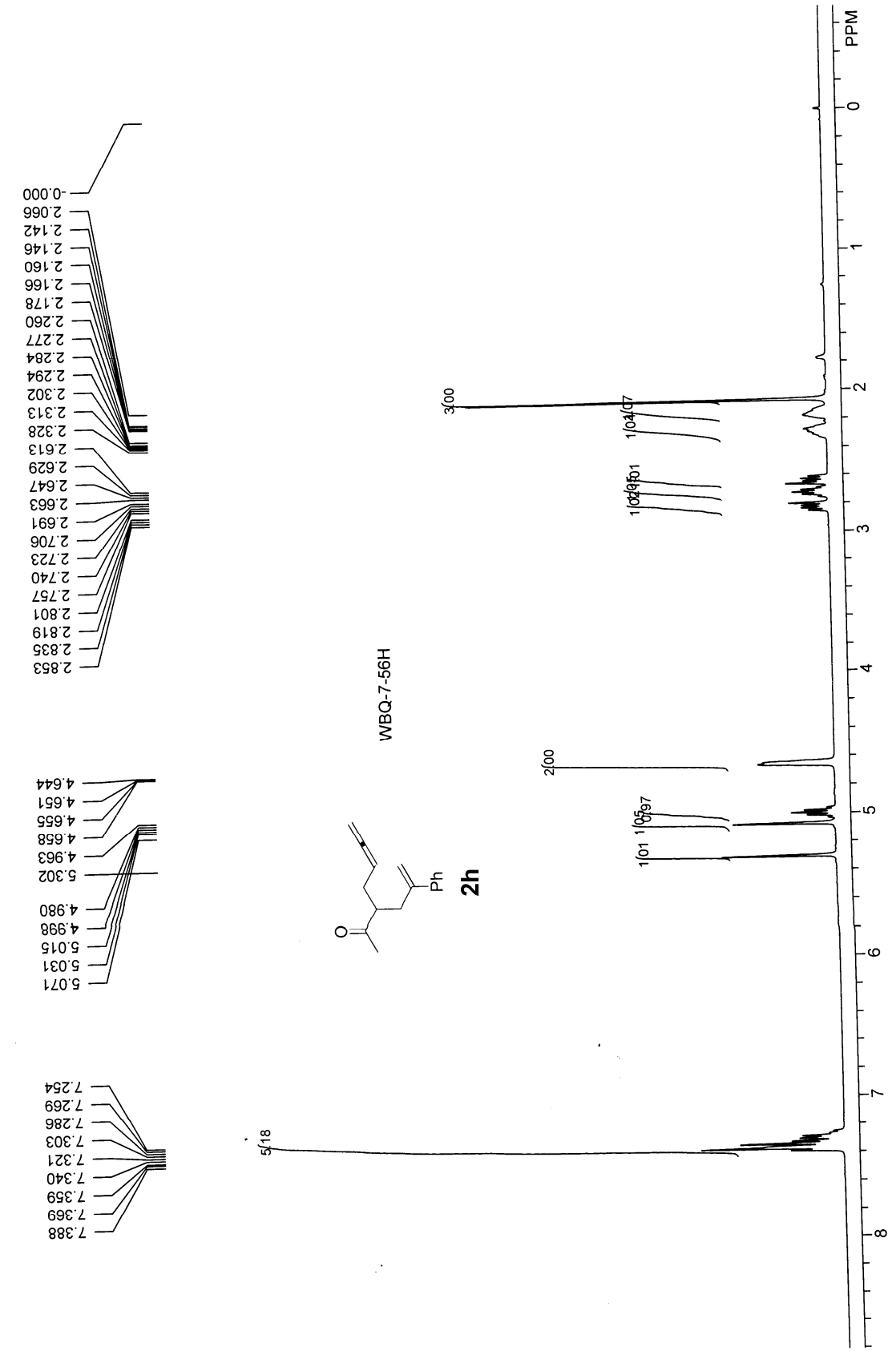
100
150
200


WBQ-7-56H
2h
Ph
O
PPM
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2
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5
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7
8
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2.00
1.04
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1.01
1.05
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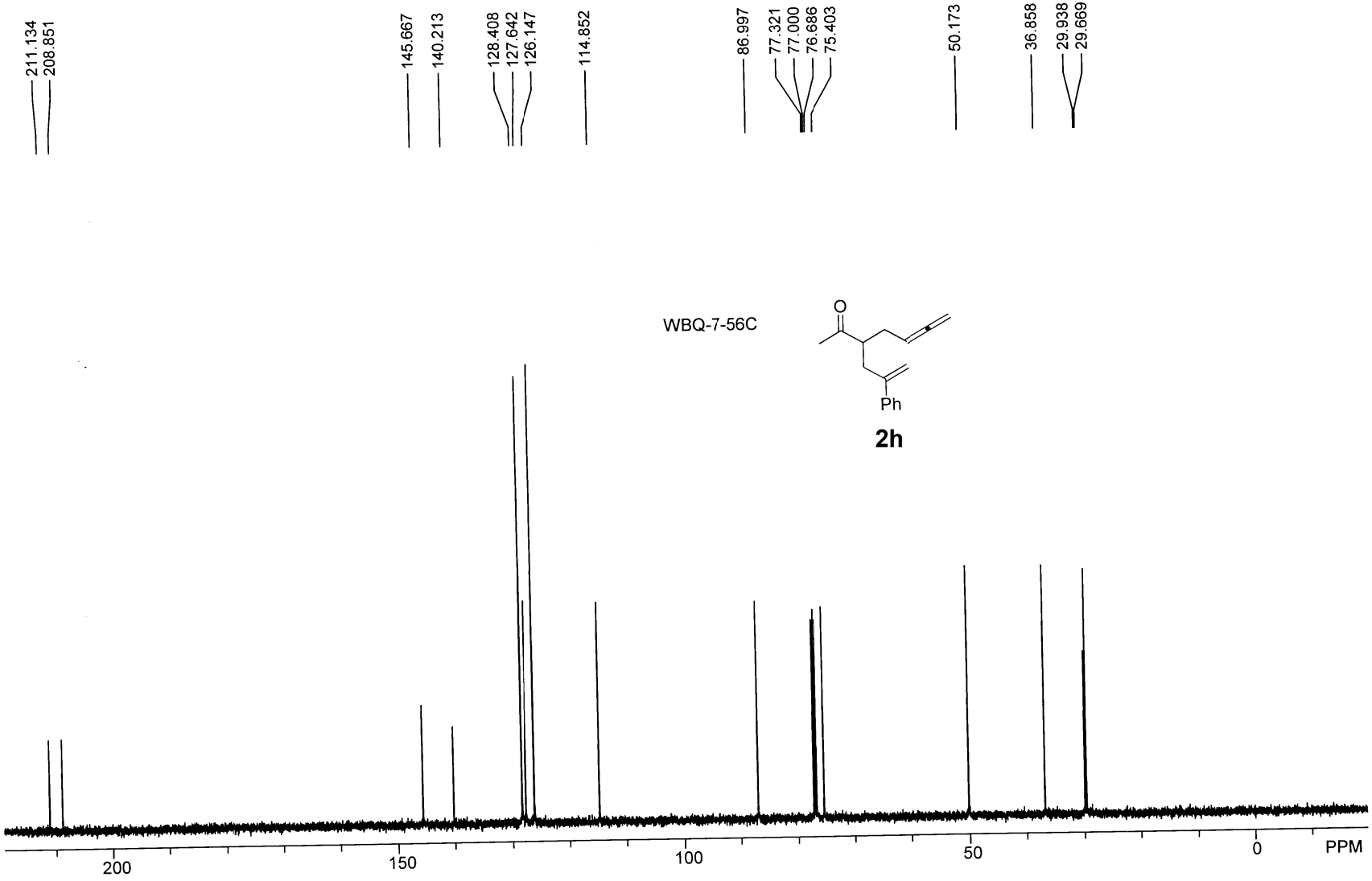
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77.000
76.686
75.403
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36.858
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29.669
WBQ-7-56C
O
Ph
2h
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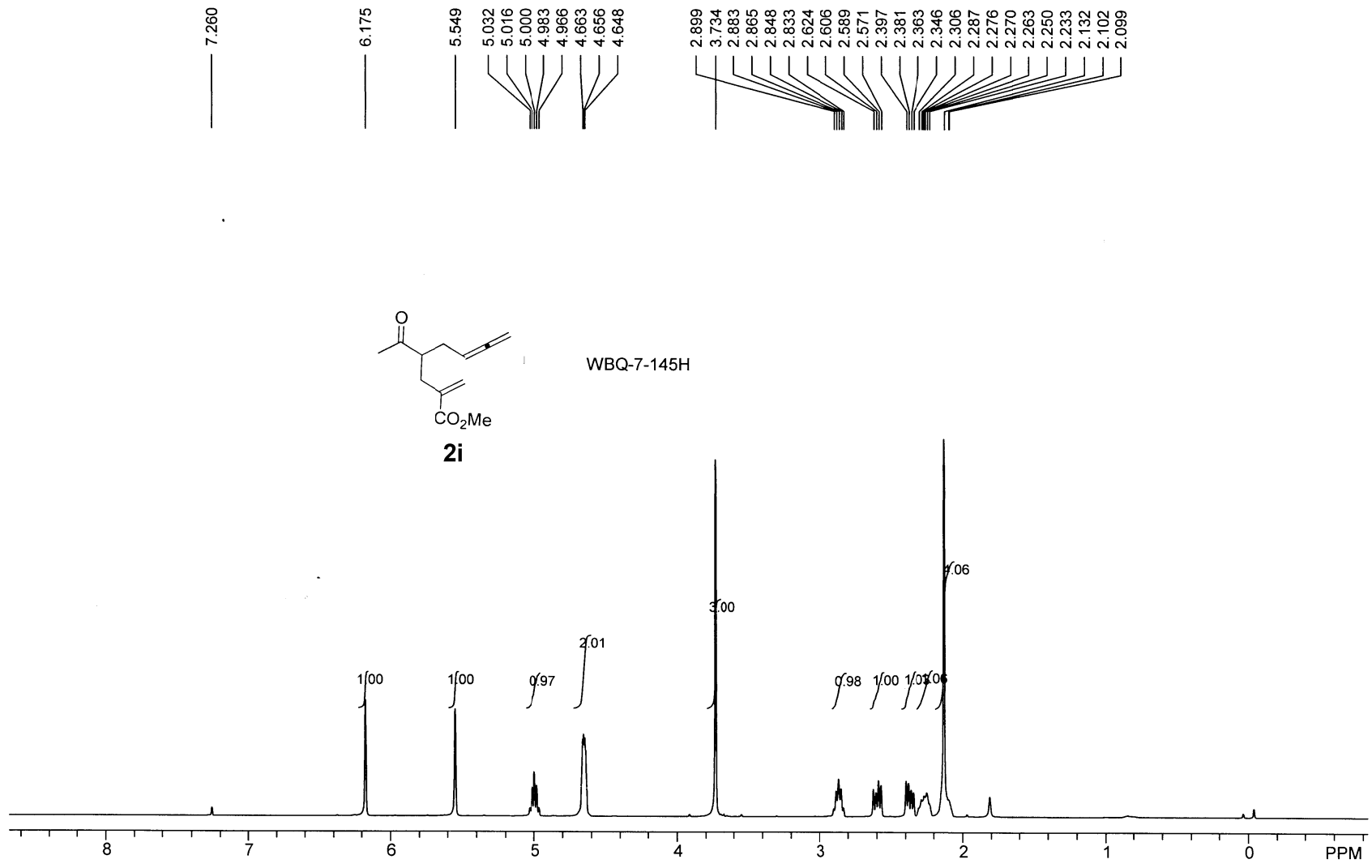
150
100
50
0
PPM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4.663
4.656
4.648
2.899
3.734
2.883
2.865
2.848
2.833
2.624
2.606
2.589
2.571
2.397
2.381
2.363
2.346
2.306
2.287
2.276
2.270
2.263
2.250
2.233
2.132
2.102
2.099
O
CO2Me
2i
WBQ-7-145H
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1.00
0.97
2.01
3.00
0.98
1.00
1.03
4.06
8
7
6
5
4
3
2
1
0
PPM


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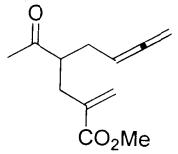
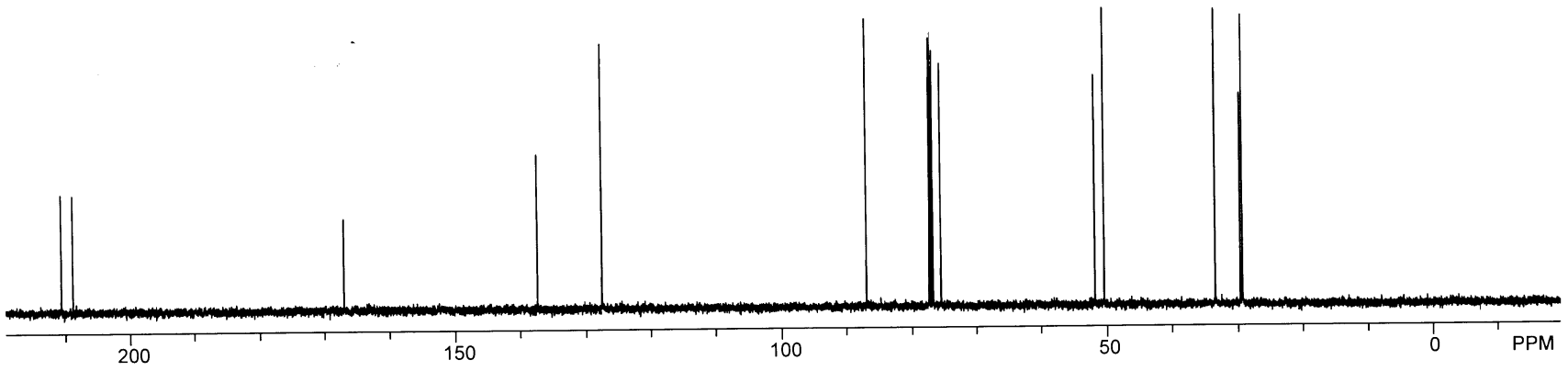
WBQ-7-145C


O
CO2Me

2i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50
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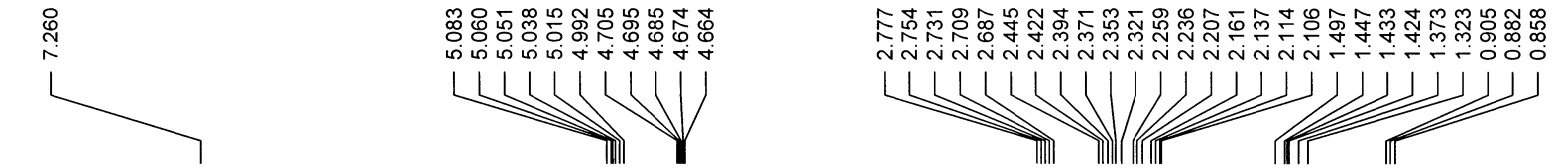
PPM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5.015
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4.674
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2.777
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2.687
2.445
2.422
2.394
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2.353
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2.161
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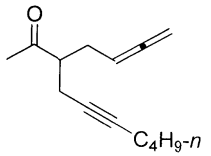
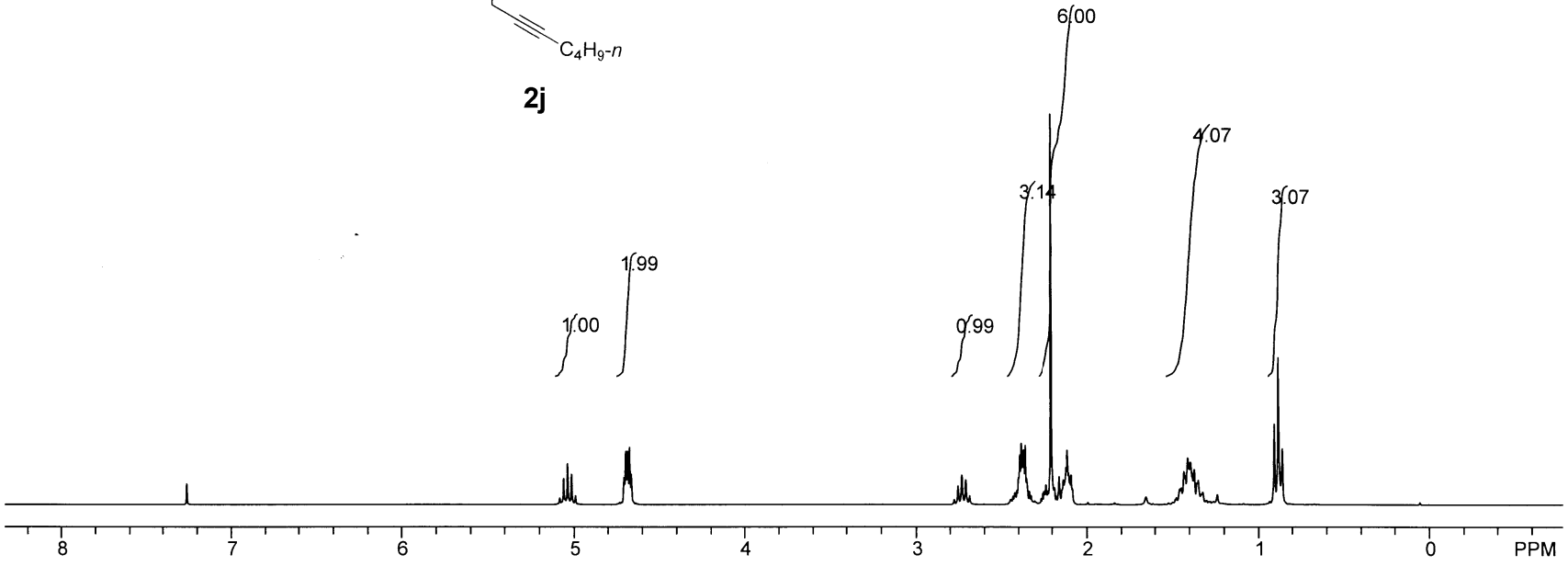

O
C_4H_9-*n*

2j


WBQ-7-156H
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5
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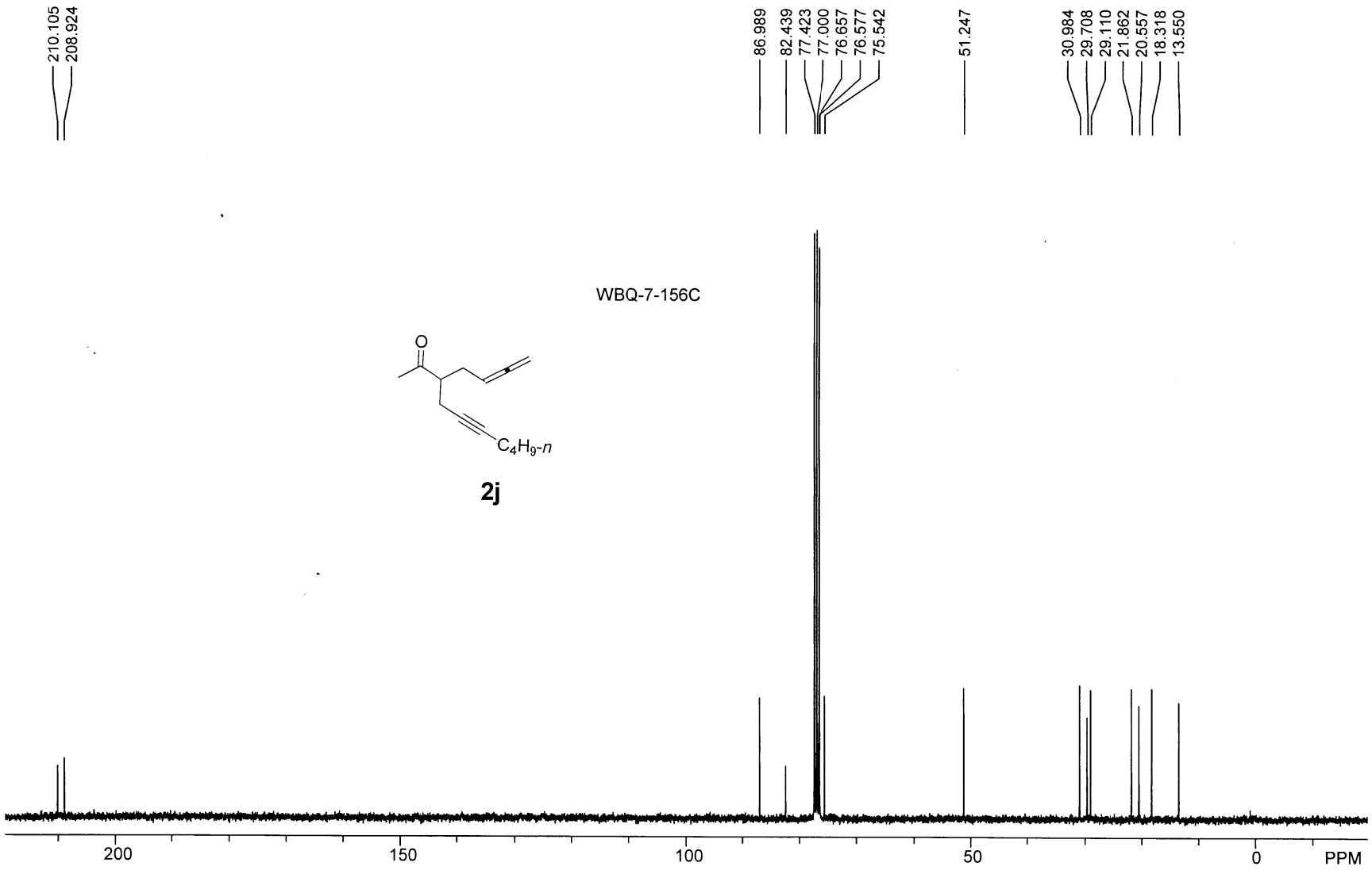
1
0
PPM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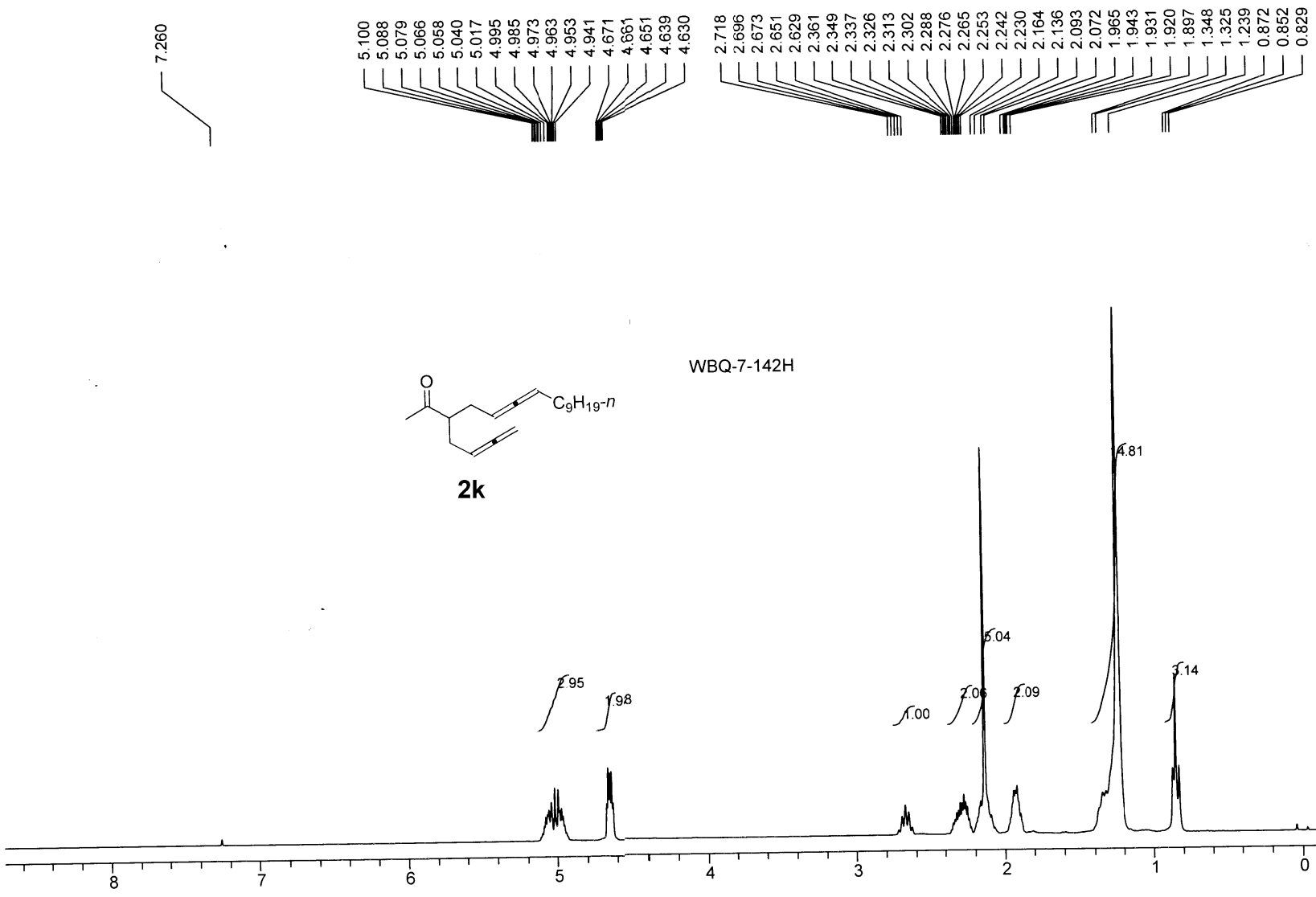
2j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5.017
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4.953
4.941
4.671
4.661
4.651
4.639
4.630
2.718
2.696
2.673
2.651
2.629
2.361
2.349
2.337
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2.302
2.288
2.276
2.265
2.253
2.242
2.230
2.164
2.136
2.093
2.072
1.965
1.943
1.931
1.920
1.897
1.348
1.325
1.239
0.872
0.852
0.829
WBQ-7-142H
O
C9H19-n
2k
2.95
1.98
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2.09
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3.14
8
7
6
5
4
3
2
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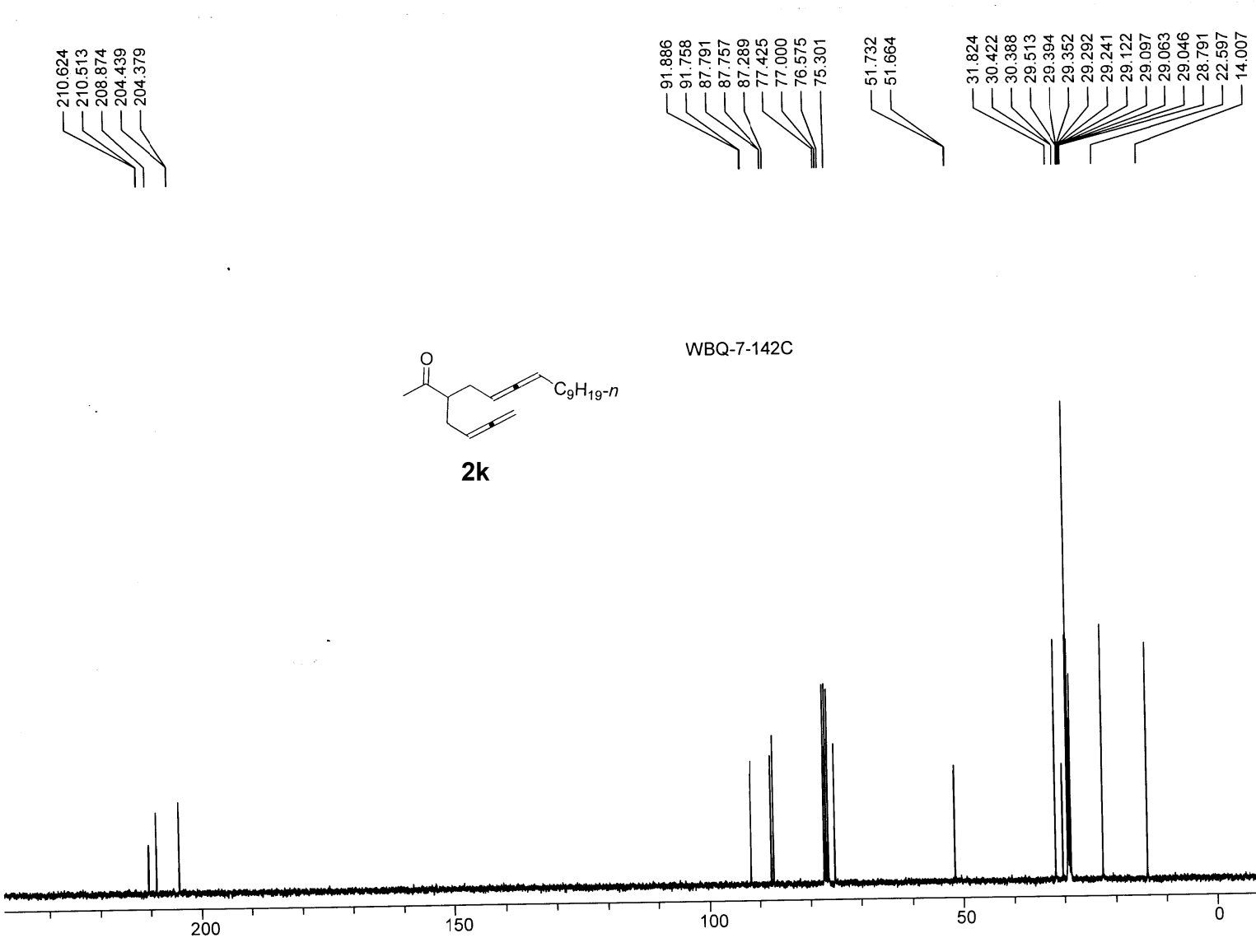
PPM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77.000
76.575
75.301
51.732
51.664
31.824
30.422
30.388
29.513
29.394
29.352
29.292
29.241
29.122
29.097
29.063
29.046
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WBQ-7-142C
O
C_9H_{19}-*n*
2k
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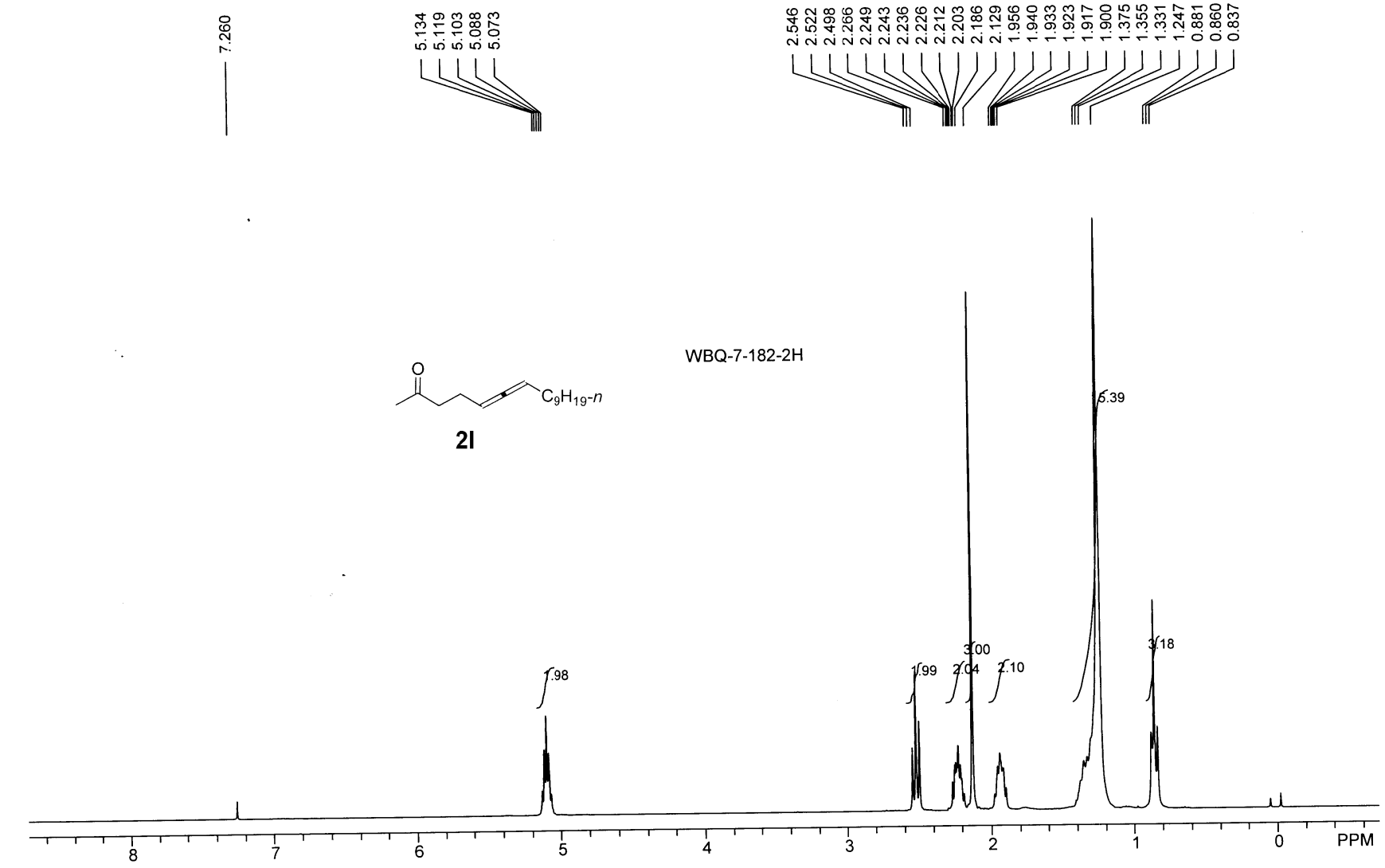
150
100
50
0
PPM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2.236
2.226
2.212
2.203
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2.129
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1.940
1.933
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1.917
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1.375
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1.331
1.247
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C9H19-n
2l
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1.99
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3.00
2.10
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3.18
8
7
6
5
4
3
2
1
0
PPM

208.117
203.597

92.455
89.634

77.416
77.000
76.575

31.841
42.360
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22.623
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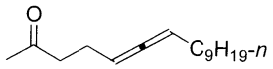
WBQ-7-182-2C



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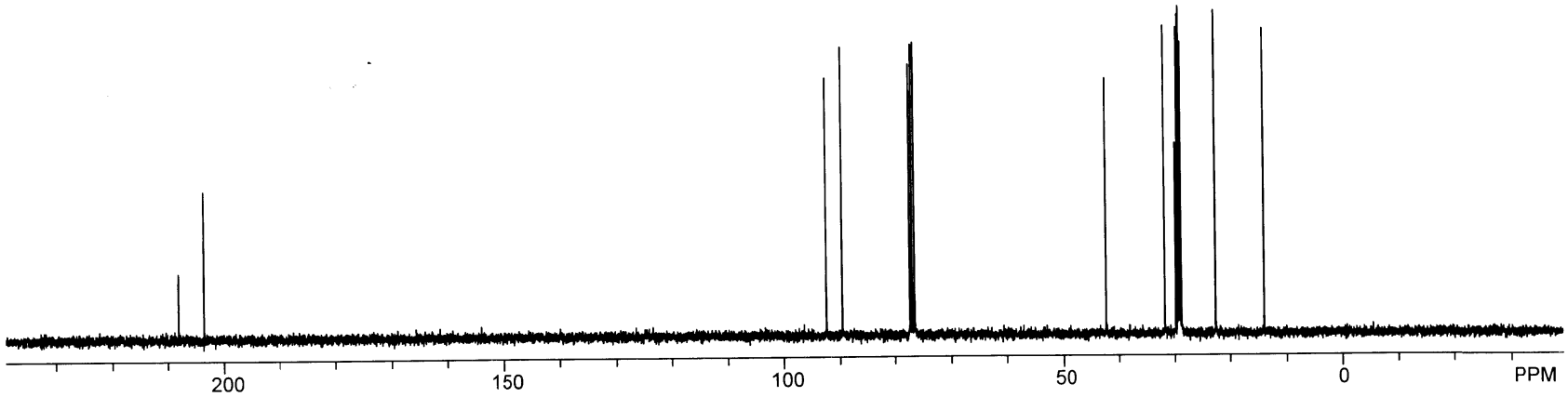

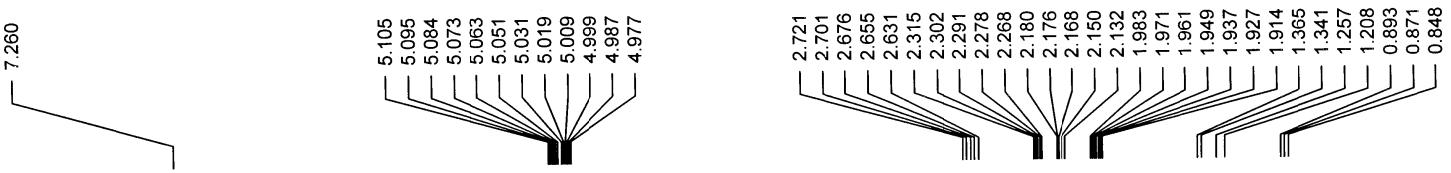

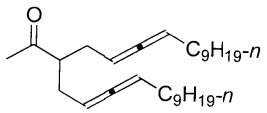

2m

WBQ-7-182-1H

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204.320

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91.877
91.775
88.011
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87.960
77.425
77.000
76.575

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51.927
51.859

31.875
30.388
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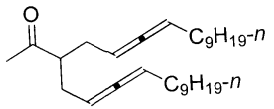
14.075

WBQ-7-182-1C



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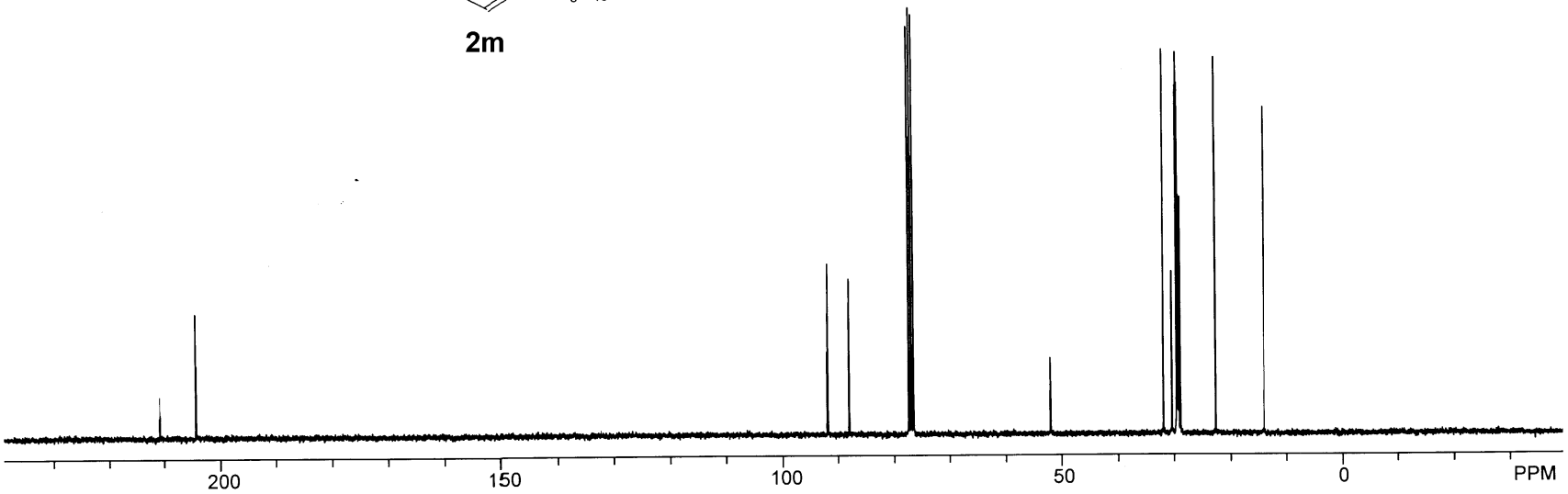

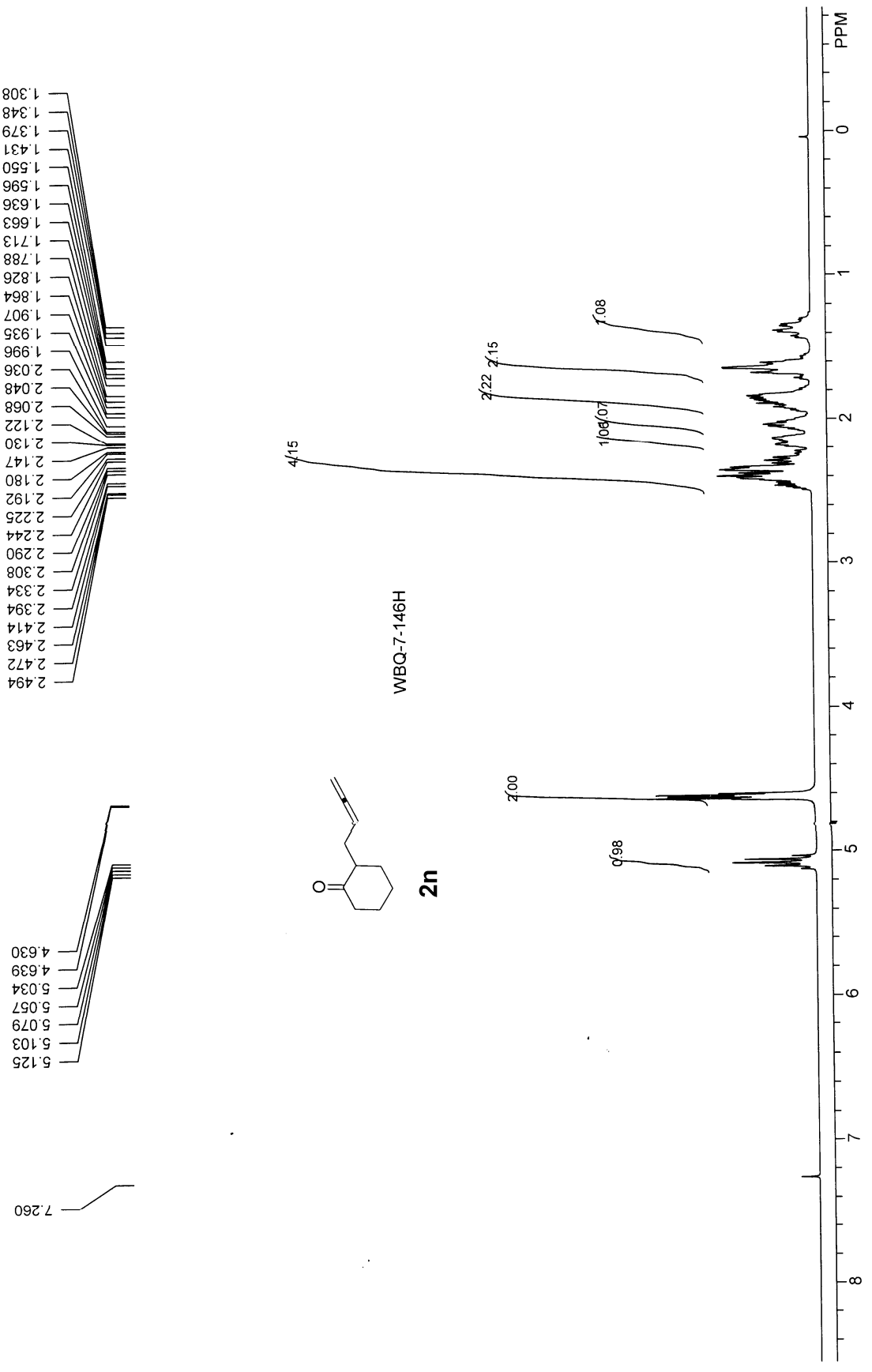
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2.394
2.334
2.308
2.290
2.244
2.225
2.192
2.180
2.147
2.130
2.122
2.068
2.048
2.036
1.996
1.935
1.907
1.864
1.826
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1.636
1.596
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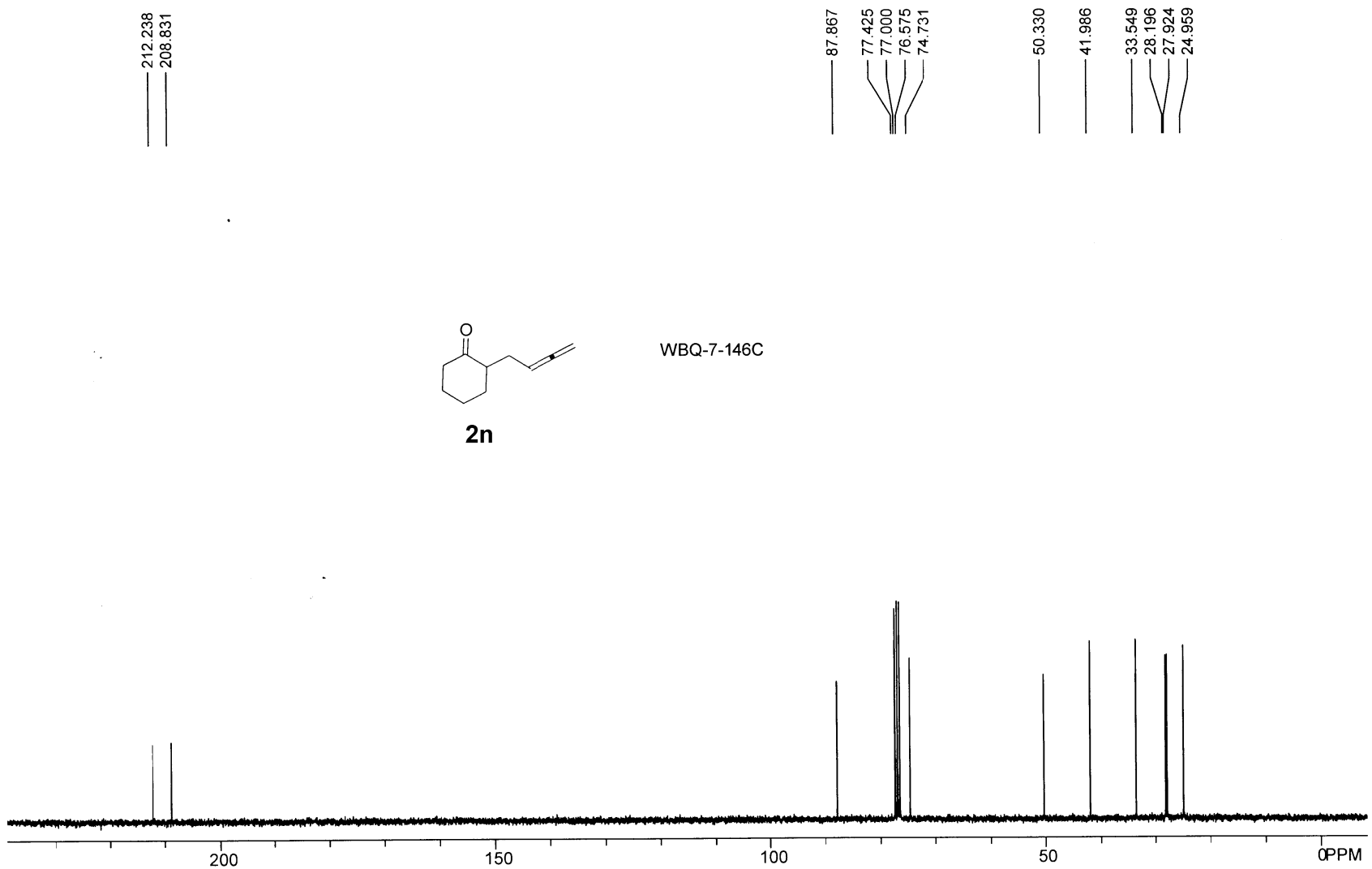
PPM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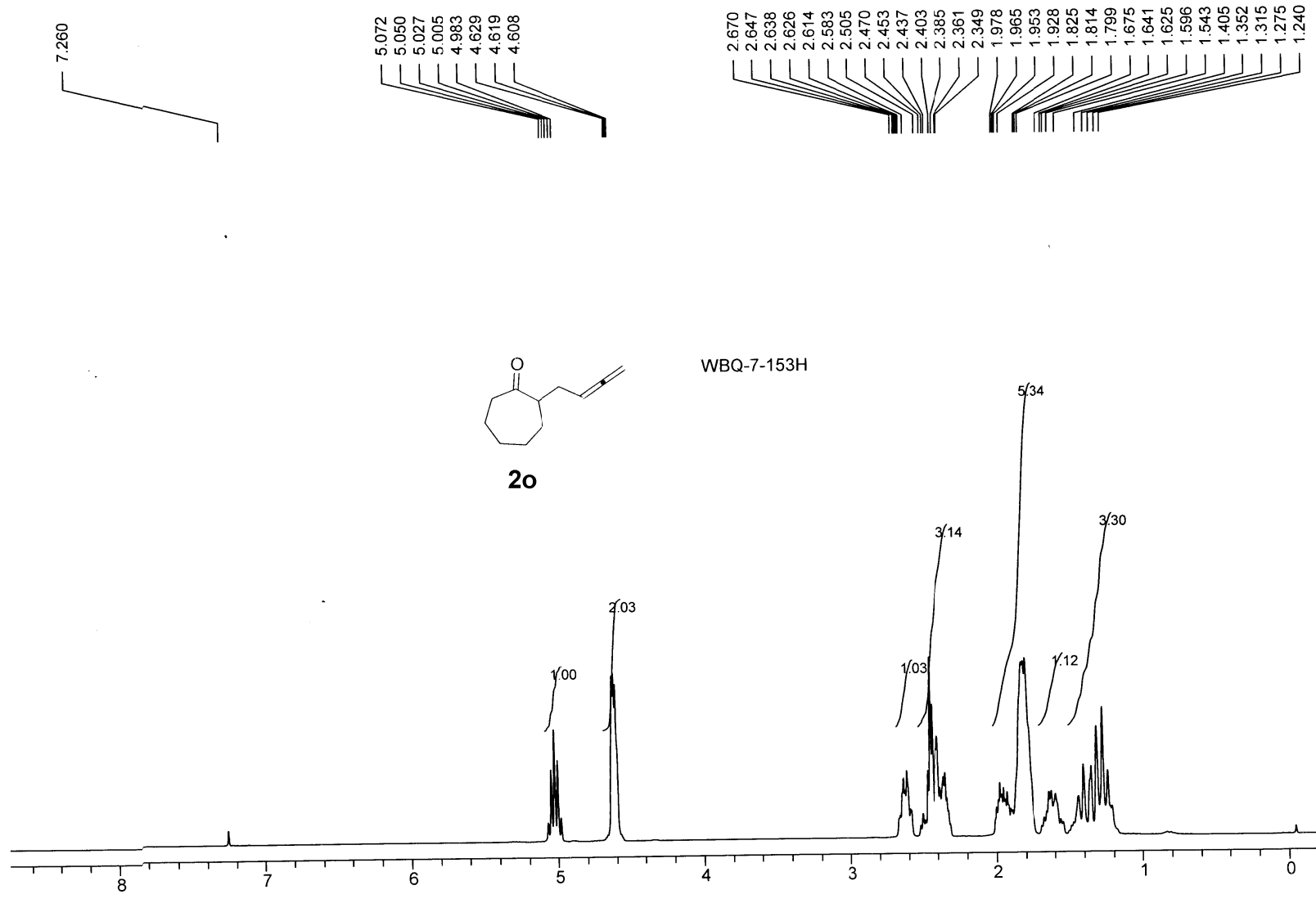
27.924
24.959
O
WBQ-7-146C
200
150
100
50
0PPM

2n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4.619
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2.614
2.583
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2.453
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2.403
2.385
2.361
2.349
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1.953
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1.825
1.814
1.799
1.675
1.641
1.625
1.596
1.543
1.405
1.352
1.315
1.275
1.240
O
2o
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7
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5
4
3
2
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0
PPM


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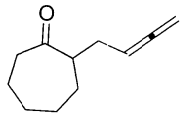
WBQ-7-153C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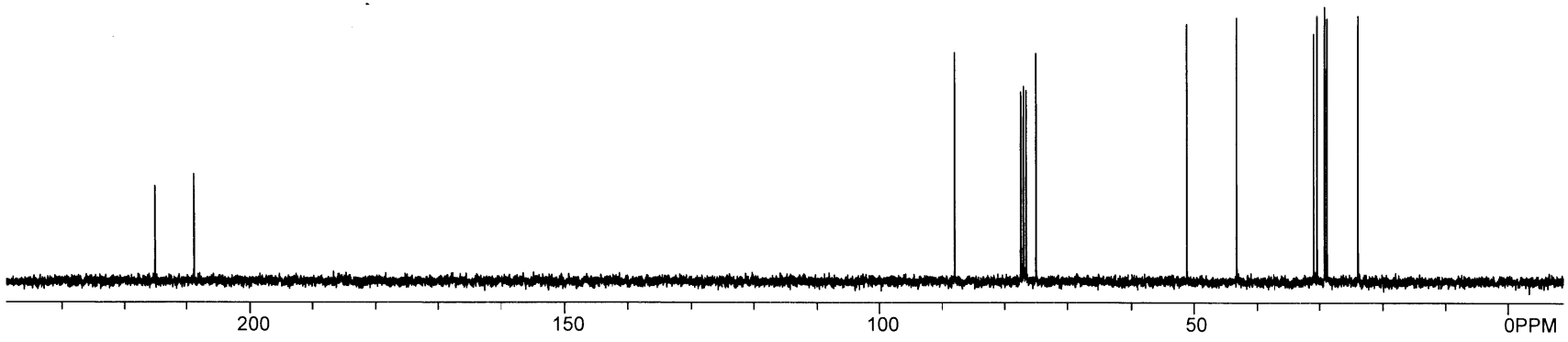
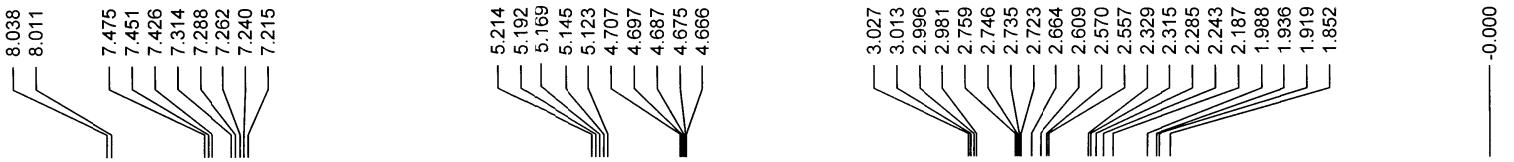

200
150
100
50
0PPM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4.666
3.027
3.013
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2.723
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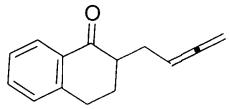
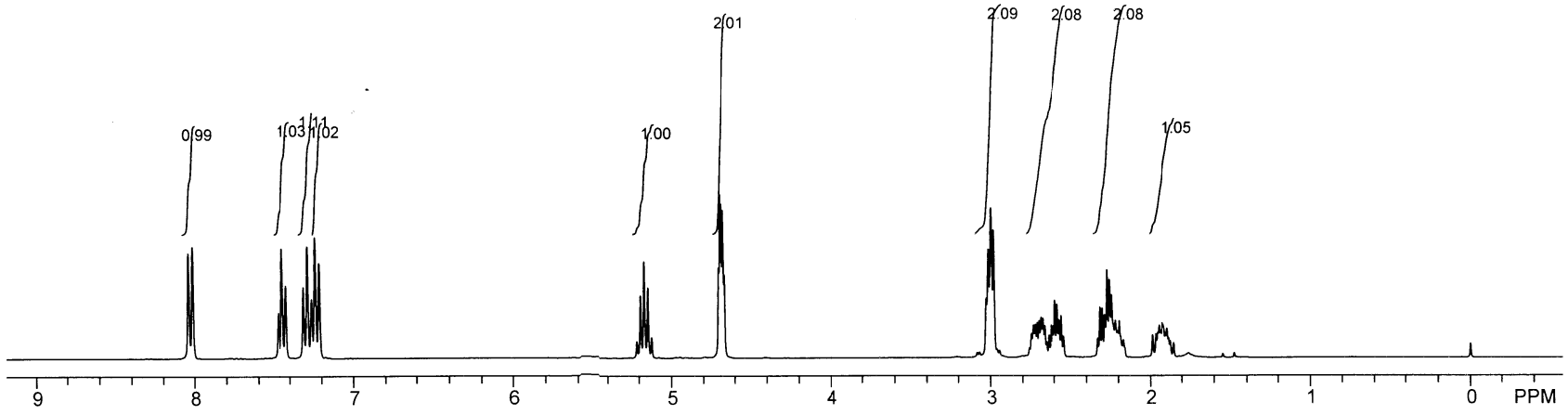
-0.000

WBQ-7-143H


O

2p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1.02
1.00
2.01
2.09
2.08
2.08
1.05
9
8
7
6
5
4
3
2
1
0
PPM

PPM
0
50
100
150
200
WBQ-7-143C
2p
O
28.118
28.621
28.658
47.389
74.893
76.577
77.000
77.423
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126.516
127.369
128.667
132.488
133.151
144.008
199.292
209.106