Supporting Information

Acylation of Alkenes with the aid of $AlCl_3$ and 2,6-Dibromopyridine

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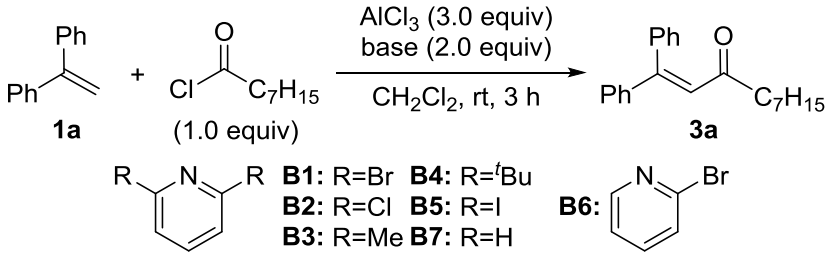
1. Supplemental Tables and Figures

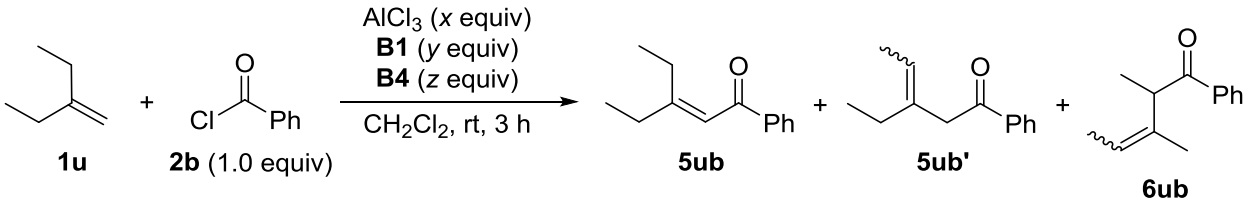
Table S1. Acylation of 1,1-Diphenylethylene (**1a**) with Octyanoyl Chloride in the Presence of Various Bases.[a]



entry	base	p*K*a[b]	**3a** (%)[c]	**1a** (%)[c]
1	**B1**	−2.2	quant	n.d.
2	**B2**	−2.8	59	trace
3	**B5**	−1.9	68	20
4	**B6**	0.9	35	trace
5	**B4**	5.5	8	14
6	**B3**	6.5	n.d.	n.d.
7	**B7**	5.2	16	2
8	Et_3N	10.8	5	n.d.
9	iPr_2NEt	10.8	5	n.d.
10	none	–	14	9

[a] Reaction conditions: **1a** (0.40 mmol), **2a** (0.40 mmol), $AlCl_3$ (1.20 mmol), base (0.80 mmol), CH_2Cl_2 (1.0 mL), rt, 3 h. [b] Calculated value for the conjugate acid. [c] Determined by ^1H NMR analysis using CH_2Br_2 as the internal standard.

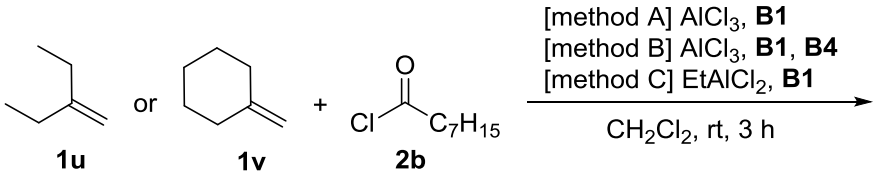
Table S2. Optimization of Molar Equivalences of $AlCl_3$/**B1**/**B4** in the Acylation of 2-Ethylbut-1-ene (**1s**) with Benzoyl Chloride (**2b**).[a]



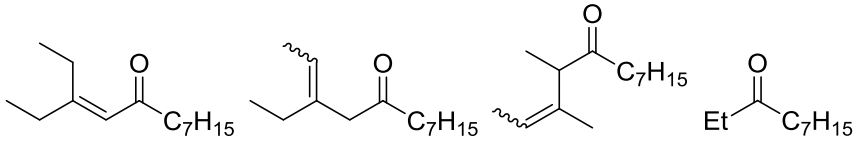
entry	*x*	*y*	*z*	**5ub** (%)[b]	**5ub'** (%)[b]	**6ub** (%)[b]
1	1.0	0.5	1.0	5	trace	trace
2	1.0	1.0	1.0	2	n.d.	n.d.
3	2.0	0.5	1.0	trace	5	10
4	2.0	0.5	1.5	33	6	10
5	2.0	1.0	1.0	2	2	trace
6	3.0	0.5	1.0	28	9	23
7	3.0	0.5	1.5	28	6	6
8	3.0	1.0	1.0	29	n.d.	12
9	3.0	1.0	1.5	35	trace	trace
10	3.0	2.0	1.0	42	3	9
11	3.0	2.0	1.5	28	trace	trace

[a] Reaction conditions: **1** (0.40 mmol), **2b** (0.40 mmol), $AlCl_3$ (0.40*x* mmol), **B1** (0.40*y* mmol), **B4** (0.40*z* mmol), CH_2Cl_2 (1.0 mL), rt, 3 h. [b] Determined by ^1H NMR analysis.

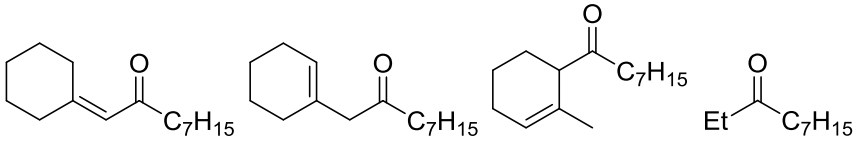
Scheme S1. Acylation of Terminal Alkenes with Octanoyl Chloride.[a,b]



1u **1v** **2b**



	3ua	**3ua'**	**6ua**	**4a**
method A	3%	trace	46%[c]	--
method B	11%	n.d.	n.d.	--
method C	55%	4%[d]	4%[d]	-[e]



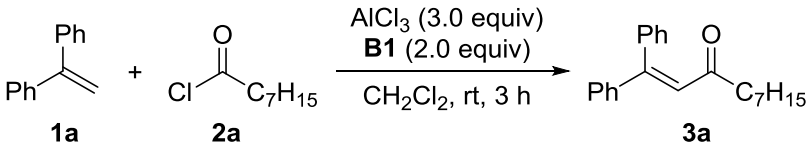
	3va	**3va'**	**3la**	**4a**
method A	n.d.	n.d.	83%	--
method B	6%	25%	4%	--
method C	65%	trace	9%	21%

[a] Reaction conditions: **1** (0.40 mmol), **2** (0.40 mmol), $AlCl_3$ (1.20 mmol), **B1** (0.80 mmol) for method A, **1** (0.40 mmol), **2** (0.40 mmol), $AlCl_3$ (1.20 mmol), **B1** (0.40 mmol), **B4** (0.60 mmol) for method B, **1** (0.40 mmol), **2** (0.50 mmol), $EtAlCl_2$ (0.40 mmol), **B1** (0.40 mmol) for method C. [b] The products could not be separated by column chromatography. The yields are those calculated by ^1H NMR analysis of the mixture. [c] *E*/*Z* = 78/22. [d] *E*/*Z* could not be determined. [e] Yield could not be determined because of the signal overlap.

2. General Information

Melting points were taken with a micro melting point apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra were measured with tetramethylsilane as an internal standard and $CDCl_3$ as a solvent unless otherwise noted. Silica gel $60GF_{254}$ was used for TLC. Silica gel columns were prepared by use of Silica gel 60 (63–200 μm). Water- and air-sensitive reactions were routinely carried out under nitrogen. Toluene was distilled from sodium diphenyl ketyl. Dichloromethane was distilled from calcium hydride.

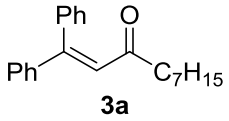
3. Typical Procedure for the Acylation



To a suspension of 2,6-dibromoropyridine (**B1**) (190 mg, 0.80 mmol) and $AlCl_3$ (160 mg, 1.20 mmol) in dichloromethane (1.0 mL) were added ethene-1,1-diyldibenzene (**1a**) (*d* = 1.03; 70.0 μL, 0.40 mmol), and octanoyl chloride (*d* = 0.95; 68.5 μL, 0.40 mmol) under nitrogen, and the mixture was stirred at room temperature for 3 h. The reaction was quenched with 2 M HCl, and the mixture was extracted with chloroform. The extract was dried over $MgSO_4$, and evaporated to leave a residue, which was purified by column chromatography on silica gel with hexane/ethyl acetate (7:1) as the eluent to give **3a** (117.3 mg, 96%).

A large scale reaction (1.0 mmol) was carried out in a 10 mL flask using ethene-1,1-diyldibenzene (**1a**) (*d* = 1.03; 176 μL, 1.00 mmol), octanoyl chloride (*d* = 0.95; 171 μL, 1.00 mmol), $AlCl_3$ (400 mg, 3.00 mmol), 2,6-dibromoropyridine (**B1**) (474 mg, 2.00 mmol), dichloromethane (2.5 mL) to give **3a** (259 mg, 85%).

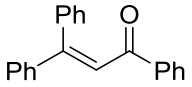
1,1-Diphenyldec-1-en-3-one (3a)



3a

Purified by column chromatography with hexane/ethyl acetate (7:1) as the eluent to give **3a** (117 mg, 96%). A yellow oil, **^{1}H NMR** (400 MHz) δ 0.86 (t, *J* = 7.1 Hz, 3H), 1.09–1.30 (m, 8H), 1.48 (quint, *J* = 7.0 Hz, 2H), 2.22 (t, *J* = 7.5 Hz, 2H), 6.56–6.59 (s, 1H), 7.17–7.23 (m, 2H), 7.27–7.42 (m, 8H); **^{13}C NMR** (100 MHz) δ 14.1, 22.6, 24.4, 29.0, 29.2, 31.7, 43.3, 126.8, 128.3, 128.4, 128.6, 129.3, 129.6, 139.1, 141.1, 153.1, 202.7 (one signal is missing); **IR** (ATR) 696, 767, 1446, 1572, 1591, 1691, 2856, 2929, 2655, 3023 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{22}H_{26}O$ (M), 306.1984, found 306.1983.

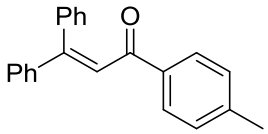
1,3,3-Triphenylprop-2-en-1-one (3b)[1,2]



3b

Purified by column chromatography with chloroform as the eluent to give **3b** (91 mg, 80%). A colorless oil, **^{1}H NMR** (400 MHz) δ 7.11 (s, 1H), 7.14–7.20 (m, 2H), 7.21–7.28 (m, 3H), 7.32–7.41 (m, 7H), 7.43–7.48 (m, 1H), 7.87–7.93 (m, 2H); **^{13}C NMR** (100 MHz) δ 124.1, 128.1, 128.4, 128.5, 128.7, 128.8, 129.4, 129.8, 132.7, 138.3, 139.1, 141.4, 154.7, 192.7 (one signal is missing); **IR** (ATR) 695, 762, 1213, 1269, 1448, 1491, 1598, 1661, 3058, 3440 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{21}H_{16}O$ (M), 284.1201, found 284.1205.

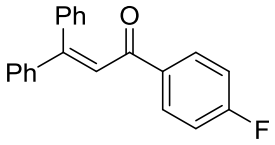
3,3-Diphenyl-1-(*p*-tolyl)prop-2-en-1-one (3c)



3c

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3c** (104 mg, 87%). A yellow powder, **^{1}H NMR** (400 MHz) δ 2.35 (s, 3H), 7.10 (s, 1H), 7.14–7.21 (m, 4H), 7.22–7.30 (m, 3H), 7.31–7.40 (m, 5H), 7.80–7.82 (m, 2H); **^{13}C NMR** (100 MHz) δ 21.7, 124.3, 128.1, 128.3, 128.5, 128.6, 129.0, 129.2, 129.3, 139.8, 135.8, 139.2, 141.6, 143.6, 154.2, 192.3; **IR** (ATR) 697, 754, 1034, 1137, 1209, 1220, 1270, 1446, 1606, 1659, 2922, 3027, 3058 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{22}H_{18}O$ (M), 298.1358, found 298.1353.

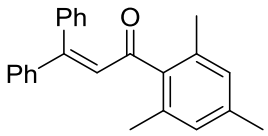
1-(4-Fluorophenyl)-3,3-diphenylprop-2-en-1-one (3d)



3d

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3d** (116 mg, 96%). A yellow powder, **^{1}H NMR** (400 MHz) δ 7.01 (t, J = 8.7 Hz), 7.04 (s, 1H Hz), 7.13–7.18 (m, 2H), 7.22–7.28 (m, 3H), 7.33–7.40 (m, 5H), 7.86–7.93 (m, 2H); **^{13}C NMR** (100 MHz) δ 115.5 ($^2J_{C–F}$ = 22.0 Hz), 123.9, 128.2, 128.57, 128.59, 128.7, 129.5, 129.9, 131.5 ($^3J_{C–F}$ = 9.5 Hz), 134.6 ($^4J_{C–F}$ = 2.9 Hz), 139.0, 141.3, 154.9, 165.5 ($^1J_{C–F}$ = 252.9 Hz), 191.5; **IR** (ATR) 699, 764, 845, 1032, 1153, 1213, 1505, 1598, 1662, 3027, 3060 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{21}H_{15}FO$ (M), 302.1107, found 302.1109.

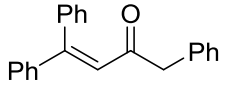
1-Mesityl-3,3-diphenylprop-2-en-1-one (3e)



3e

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3e** (109 mg, 83%). A yellow paste, **^{1}H NMR** (400 MHz) δ 2.16 (s, 3H), 2.20 (s, 6H), 6.61 (s, 2H), 6.86 (s, 1H), 7.06–7.09 (m, 2H), 7.14–7.21 (m, 3H), 7.28–7.36 (m, 5H); **^{13}C NMR** (100 MHz) δ 20.1, 21.0, 127.4, 127.6, 128.0, 128.5, 128.6, 129.0, 129.7, 133.9, 138.2, 138.3, 139.0, 141.2, 155.2, 199.3 (one signal is missing); **IR** (ATR) 699, 759, 1063, 1216, 1285, 1446, 1567, 1629, 2922, 3012 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{24}H_{22}O$ (M), 326.1671, found 326.1670.

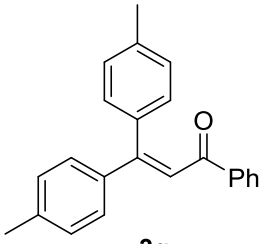
1,4,4-Triphenylbut-3-en-2-one (3f)



3f

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3f** (47 mg, 40%). A yellow paste, **^{1}H NMR** (400 MHz) δ 3.56 (s, 2H), 6.60 (s, 1H), 7.08–7.11 (m, 2H), 7.16–7.41 (m, 13H); **^{13}C NMR** (100 MHz) δ 50.3, 125.9, 127.1, 128.46, 128.51, 128.6, 128.7, 128.8, 129.6, 129.68, 129.74, 134.7, 139.0, 141.1, 154.2, 199.1; **IR** (ATR) 698, 756, 1077, 1446, 1494, 1570, 1589, 1686, 2924, 3028, 3059 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{22}H_{16}O$ (M−2H), 296.1201, found 296.1203.

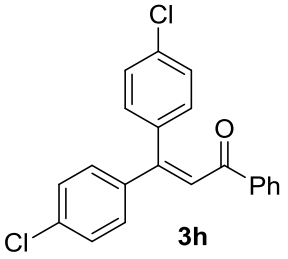
1-Phenyl-3,3-di-*p*-tolylprop-2-en-1-one (3g)



3g

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3g** (106 mg, 85%). A yellow powder, **^{1}H NMR** (400 MHz) δ 2.31 (s, 3H), 2.37 (s, 3H), 7.06–7.09 (m, 5H), 7.14–7.18 (m, 2H), 7.26–7.30 (m, 2H), 7.34–7.39 (m, 2H), 7.44–7.49 (m, 1H), 7.89–7.93 (m, 2H); **^{13}C NMR** (100 MHz) δ 21.39, 21.43, 122.8, 128.4, 128.74, 128.78, 128.84, 129.2, 129.8, 132.6, 136.3, 138.3, 138.6, 138.9, 139.7, 155.4, 192.6; **IR** (ATR) 758, 1018, 1209, 1448, 1508, 1598, 1658, 2921, 3026 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{23}H_{20}O$ (M), 312.1514, found 312.1520.

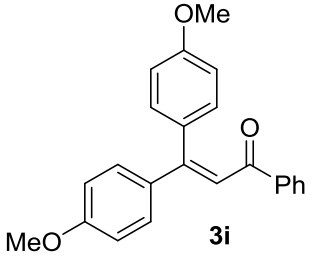
3,3-Bis(4-chlorophenyl)-1-phenylprop-2-en-1-one (3h)



3h

Purified by column chromatography with chloroform/hexane (1:1) as the eluent to give **3h** (130 mg, 92%). A yellow powder, **^{1}H NMR** (400 MHz) δ 7.08–7.12 (m, 2H), 7.12 (s, 1H), 7.24–7.30 (m, 4H), 7.33–7.37 (m, 2H), 7.38–7.43 (m, 2H), 7.50–7.54 (m, 1H), 7.88–7.92 (m, 2H); **^{13}C NMR** (100 MHz) δ 124.6, 128.6, 128.7, 128.8, 128.9, 129.9, 131.1, 133.2, 134.7, 135.8, 137.1, 138.0, 139.5, 152.4, 192.1; **IR** (ATR) 692, 758, 831, 1014, 1091, 1214, 1448, 1492, 1582, 1661, 3028, 3062 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{21}H_{14}Cl_2O$ (M), 352.0422, found 352.0422.

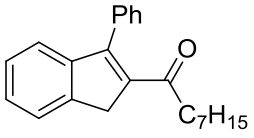
3,3-Bis(4-methoxyphenyl)-1-phenylprop-2-en-1-one (3i)[3]



3i

Purified by column chromatography with chloroform as the eluent to give **3i** (76 mg, 55%). A yellow paste, **^{1}H NMR** (400 MHz) δ 3.78 (s, 3H,), 3.84 (s, 3H), 6.76–6.82 (m, 2H), 6.86–6.91 (m, 2H), 7.00 (s, 1H), 7.10–7.15 (m, 2H), 7.31–7.40 (m, 4H), 7.44–7.50 (m, 1H), 7.88–7.93 (m, 2H); **^{13}C NMR** (100 MHz) δ 55.3, 55.5, 113.6, 113.9, 121.6, 128.4, 128.8, 130.4, 131.6, 132.5, 134.4, 138.9, 155.2, 160.0, 160.9, 192.7 (one signal is missing); **IR** (ATR) 761, 834, 1035, 1174, 1214, 1250, 1511, 1605, 1654, 2838, 3012 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{23}H_{20}O_3$ (M), 344.1412, found 344.1411.

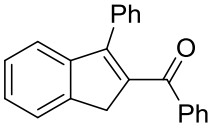
1-(3-Phenyl-1*H*-inden-2-yl)octan-1-one (3ja)



3ja

Purified by column chromatography with hexane/ethyl acetate (7:1) as the eluent to give **3ja** (106 mg, 83%). A yellow oil, **^{1}H NMR** (400 MHz) δ 0.84 (t, J = 7.3 Hz, 3H), 1.00–1.27 (m, 8H, CH_2), 1.46 (quint, J = 7.4 Hz), 2.28 (t, J = 7.6 Hz, 2H), 3.86 (s, 2H), 7.17 (d, J = 7.6 Hz, 1H), 7.29 (t, J = 7.3 Hz, 1H), 7.34–7.39 (m, 3H), 7.44–7.57 (m, 4H); **^{13}C NMR** (100 MHz) δ 14.1, 22.6, 24.6, 29.0, 29.1, 31.7, 39.3, 41.7, 123.1, 124.2, 126.9, 128.0, 128.5, 128.7, 128.7, 135.3, 141.1, 143.3, 145.8, 151.1, 200.4; **IR** (ATR) 726, 758, 1377, 1462, 1650, 2856, 2927, 3024, 3062 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{23}H_{26}O$ (M), 318.1984, found 318.1983.

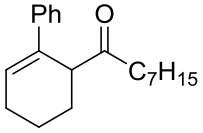
Phenyl(3-phenyl-1*H*-inden-2-yl)methanone (3jb)



3jb

Purified by column chromatography with chloroform as the eluent to give **3jb** (115 mg, 96%). A orange paste, **^{1}H NMR** (400 MHz) δ 4.03 (s, 2H), 7.06–7.12 (m, 2H), 7.12–7.19 (m, 3H), 7.20–7.27 (m, 3H), 7.33–7.42 (m, 2H), 7.47–7.51 (m, 1H), 7.53–7.58 (m, 2H), 7.58–7.63 (m, 1H); **^{13}C NMR** (100 MHz) δ 40.7, 122.7, 124.4, 127.0, 127.6, 127.8, 128.2, 129.3, 129.4, 131.9, 134.1, 138.0, 140.3, 143.7, 144.3, 149.9, 195.7 (one signal is missing); **IR** (ATR) 726, 747, 1214, 1628, 1712, 2401, 3017, 3682 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{22}H_{16}O$ (M), 296.1201, found 296.1196.

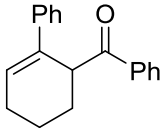
1-(2-Phenyl-2-cyclohexen-1-yl)octan-1-one (3ka)



3ka

Purified by column chromatography with hexane/ethyl acetate (8:1) as the eluent to give **3ka** (115 mg, 100%). A yellow oil, **^{1}H NMR** (400 MHz) δ 0.85 (t, *J* = 7.3 Hz, 3H), 1.02–1.45 (m, 10H), 1.60–1.76 (m, 2H), 1.85–2.01 (m, 2H), 2.20–2.38 (m, 4H), 3.73–3.79 (m, 1H), 6.22 (td, *J* = 4.0, 1.3 Hz, 1H), 7.17–7.30 (m, 5H); **^{13}C NMR** (100 MHz) δ 14.1, 19.5, 22.6, 23.7, 25.7, 26.5, 29.1, 31.7, 40.5, 51.3, 125.7, 126.9, 128.5, 128.8, 135.4, 142.0, 212.9 (one signal is missing); **IR** (ATR) 697, 758, 1355, 1445, 1494, 1708, 2857, 2928, 3024, 3058 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{20}H_{28}O$ (M), 284.2140, found 284.2142.

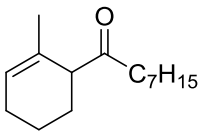
Phenyl(2-pheylcyclohex-2-en-1-yl)methanone (3kb)



3kb

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3kb** (83 mg, 79%). A white powder, **^{1}H NMR** (400 MHz) δ 1.63–1.66 (m, 2H), 1.98–2.18 (m, 2H), 2.20–2.41 (m, 2H), 4.68–4.76 (m, 1H), 6.36–6.41 (m, 1H), 7.10–7.16 (m, 1H), 7.17–7.22 (m, 2H), 7.25–7.30 (m, 2H), 7.42–7.48 (m, 2H), 7.52–7.57 (m, 1H), 7.98–8.03 (m, 2H); **^{13}C NMR** (100 MHz) δ 18.8, 25.7, 27.4, 45.3, 125.5, 126.8, 128.4, 128.6, 128.8, 129.0, 133.0, 135.3, 136.2, 141.8, 201.2; **IR** (ATR) 699, 747, 901, 976, 1209, 1338, 1447, 1597, 1681, 2937, 3011 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{19}H_{18}O$ (M), 262.1358, found 262.1358.

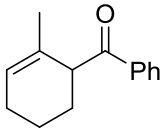
1-(2-Methyl-2-cyclohexen-1-yl)octan-1-one (3la)



3la

Purified by column chromatography with hexane/ethyl acetate (7:1) as the eluent to give **3la** (85.2 mg, 96%). A yellow oil, **^{1}H NMR** (400 MHz) δ 0.88 (t, *J* = 7.1 Hz, 3H), 1.22–1.34 (m, 8H), 1.46–1.65 (m, 7H), 1.68–1.88 (m, 2H), 1.94–2.11 (m, 2H), 2.39–2.53 (m, 2H), 3.06–3.12 (brt, *J* = 6.2 Hz, 1H), 5.62–5.67 (m, 1H); **^{13}C NMR** (100 MHz) δ 14.1, 19.7, 22.7, 22.7, 24.0, 25.1, 26.3, 29.2, 29.3, 31.7, 41.4, 53.2, 125.4, 130.9, 213.4; **IR** (ATR) 754, 1094, 1130, 1377, 1407, 1455, 1708, 2857, 2926, 3403 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{15}H_{26}O$ (M), 222.1984, found 222.1985.

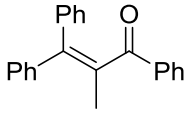
(2-Methylcyclohex-2-en-1-yl)(phenyl)methanone (3lb)



3lb

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3lb** (69 mg, 85%). A dark brown paste, **^{1}H NMR** (400 MHz) δ 1.50–1.68 (m, 2H), 1.63 (d, *J* = 1.8 Hz, 3H), 1.81–1.90 (m, 1H), 1.93–2.18 (m, 3H), 4.00 (t, *J* = 5.8 Hz, 1H), 5.74 (m, 1H), 7.45–7.50 (m, 2H), 7.53–7.58 (m, 1H), 7.98–8.03 (m, 2H); **^{13}C NMR** (100 MHz) δ 19.6, 22.9, 25.2, 27.5, 47.9, 125.8, 128.6, 128.8, 131.3, 133.0, 136.8, 202.3; **IR** (ATR) 702, 753, 1210, 1448, 1580, 1597, 1676, 2934, 3011 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{14}H_{16}O$ (M), 200.1201, found 200.1199.

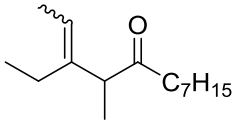
2-Mehtyl-1,3,3-triphenylprop-2-en-1-one (3mb)



3mb

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3mb** (77 mg, 64%). A white powder, **^{1}H NMR** (400 MHz) δ 2.15 (s, 3H), 6.95–7.03 (m, 5H), 7.22–7.42 (m, 8H), 7.76–7.82 (m, 2H); **^{13}C NMR** (100 MHz) δ 20.0, 127.6, 127.7, 127.9, 128.2, 128.4, 129.3, 129.97, 130.03, 132.7, 134.9, 136.9, 141.0, 141.4, 143.8, 201.3; **IR** (ATR) 701, 753, 1216, 1261, 1325, 1448, 1492, 1597, 1653, 2919, 3022, 3059 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{22}H_{18}O$ (M), 298.1358, found 298.1353.

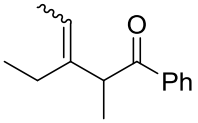
3-Ethyl-4-methyldodec-2-en-5-one (3na)



3na

Purified by column chromatography with hexane/ethyl acetate (10:1) as the eluent to give **3na** (67 mg, 51%, *E*/*Z* = 76:24). A brown oil, **^{1}H NMR** (400 MHz) δ for the *E* isomer 0.87 (t, *J* = 7.1 Hz, 3H), 0.94–0.99 (t, *J* = 7.6 Hz, 3H), 1.13 (d, *J* = 6.8 Hz, 3H), 1.19–1.36 (m, 10H), 1.63 (d, *J* = 6.8 Hz, 3H), 2.20–2.07 (q, 2H), 2.27–2.51 (m, 2H), 3.13 (q, *J* = 6.9 Hz, 1H), 5.29 (q, *J* = 6.9 Hz, 1H); **^{13}C NMR** (100 MHz) δ for the *E* isomer 13.4, 14.2, 15.7, 22.7, 22.8, 24.2, 29.2, 29.3, 31.8, 40.5, 53.9, 120.2, 121.9, 141.3, 212.5; **IR** (ATR) 1016, 1068, 1135, 1375, 1410, 1459, 1713, 2857, 2928, 2961, 3411 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{15}H_{28}O$ (M), 224.2140, found 224.2137.

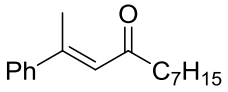
3-Ethyl-2-methyl-1-phenylpent-3-en-1-one (3nb)



3nb

Purified by column chromatography with hexane/ethyl acetate (20:1) as the eluent to give **3nb** (42 mg, 52%, *E*/*Z* = 92:8). A colorless oil, **^{1}H NMR** (400 MHz) δ for the *E* isomer 0.97 (t, *J* = 7.6 Hz, 3H), 1.31 (d, *J* = 6.8 Hz, 3H), 1.58 (d, *J* = 6.8 Hz, 3H), 2.03–2.21 (m, 2H), 4.09 (q, *J* = 6.8 Hz, 1H), 5.35 (q, *J* = 6.8 Hz, 1H), 7.38–7.45 (m, 2H), 7.48–7.55 (m, 1H), 7.94–7.99 (m, 2H); **^{13}C NMR** (100 MHz) δ for the *E* isomer 13.6, 17.1, 22.5, 48.7, 122.4, 128.5, 128.6, 132.7, 137.3, 141.7, 201.9 (1 signal is missing); **IR** (ATR) 693, 758, 977, 1220, 1449, 1597, 1682, 1726, 2935, 2970 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{14}H_{18}O$ (M), 202.1358, found 202.1358.

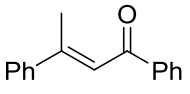
(*E*)-2-Phenylundec-2-en-4-one (3oa)



3oa

Purified by column chromatography with hexane/ethyl acetate (7:1) as the eluent to give **3oa** (52 mg, 53%). A colorless oil, **^{1}H NMR** (400 MHz) δ 0.88 (t, *J* = 7.0 Hz, 3H), 1.13–1.38 (m, 10H), 2.53 (t, *J* = 7.6 Hz, 2H), 2.54 (s, 3H), 6.50 (s, 1H), 7.34–7.41 (m, 3H), 7.45–7.51 (m, 2H); **^{13}C NMR** (100 MHz) δ 14.1, 18.4, 22.7, 24.4, 29.2, 29.3, 31.8, 45.0, 124.3, 126.5, 128.6, 129.0, 142.7, 153.6, 201.8; **IR** (ATR) 694, 726, 755, 1446, 1574, 1600, 1683, 2855, 2926, 3024 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{17}H_{24}O$ (M), 244.1827, found 244.1825.

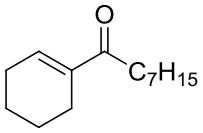
(*E*)-1,3-Diphenylbut-2-en-1-one (3ob)[4]



3ob

Purified by column chromatography with chloroform as the eluent to give **3ob** (32 mg, 35%). A yellow oil, **^{1}H NMR** (400 MHz) δ 2.60 (d, *J* = 1.4 Hz, 3H), 7.17 (q, *J* = 1.4 Hz, 1H), 7.38–7.50 (m, 5H), 7.52–7.61 (m, 3H), 7.97–8.02 (m, 2H); **^{13}C NMR** (100 MHz) δ 19.0, 122.3, 126.6, 128.4, 128.7, 128.8, 129.3, 132.7, 139.5, 142.9, 155.3, 192.0; **IR** (ATR) 695, 751, 1048, 1215, 1276, 1448, 1493, 1600, 1655, 2926, 3019 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{16}H_{14}O$ (M), 222.1045, found 222.1047.

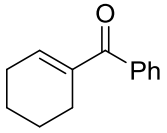
1-(Cyclohex-1-en-1-yl)octan-1-one (3pa)



3pa

The reaction was conducted in 1,2-dichlroethane at 60 °C for 3 h. Purified by column chromatography with hexane/ethyl acetate (7:1) as the eluent. **3pa** (50%) was obtained as a mixture containing **3pa′** and **3pa″** (see, Table 3). A yellow oil, **^{1}H NMR** (400 MHz) δ 0.88 (t, 3H, *J* = 7.0 Hz), 1.20–1.36(m, 8H), 1.52–1.66(m, 6H), 2.19–2.28 (m, 4H), 2.61 (t, *J* = 7.7 Hz, 2H), 6.89 (brs, 1H); **^{13}C NMR** (100 MHz) δ 14.1, 21.6, 22.0, 22.6, 23.2, 24.9, 26.1, 29.2, 29.4, 31.7, 37.1, 139.3, 139.4, 201.9; **IR** (ATR) 760, 1216, 1458, 1668, 1713, 2859, 2931, 3462, 3506, 3538 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{14}H_{24}O$ (M), 208.1827, found 208.1826.

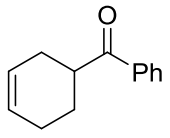
Cyclohex-1-en-1-yl(phenyl)methanone (3pb)[5]



3pb

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3pb** (17 mg, 22%). A colorless oil, **^{1}H NMR** (400 MHz) δ 1.64–1.80 (m, 4H), 2.23–2.31 (m, 2H), 2.39–2.46 (m, 2H), 6.58–6.64 (m, 1H), 7.37–7.53 (m, 3H), 7.60–7.66 (m, 2H); **^{13}C NMR** (100 MHz) δ 21.8, 22.2, 24.1, 26.3, 128.1, 129.3, 131.4, 138.9, 144.2, 198.4; **IR** (ATR) 706, 757, 1217, 1258, 1380, 1447, 1578, 1644, 2863, 2938, 3019, 3394 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{13}H_{14}O$ (M), 186.1045, found 186.1044.

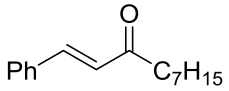
Cyclohex-3-en-1-yl(phenyl)methanone (3pb″)



3pb"

Purified by column chromatography with chloroform/hexane (4:1) as the eluent to give **3pb″** (22 mg, 30%). A light yellow oil, **^{1}H NMR** (400 MHz) δ 1.66–1.79 (m, 1H), 1.94–2.05 (m, 1H), 2.11–2.29 (m, 3H), 2.30–2.42 (m, 1H), 3.48–3.59 (m, 1H), 5.71–5.82 (m, 2H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.53–7.60 (m, 1H), 7.92–8.01 (m, 2H); **^{13}C NMR** (100 MHz) δ 25.0, 25.9, 28.0, 41.7, 125.9, 126.7, 128.4, 128.8, 133.0, 136.4, 203.6; **IR** (ATR) 699, 755, 1231, 1448, 1597, 1681, 2840, 2928, 3026 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{13}H_{14}O$ (M), 186.1045, found 186.1045.

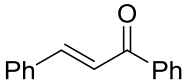
(*E*)-1-Phenyldec-1-en-3-one (3qa)



3qa

Purified by column chromatography with chloroform as the eluent to give **3qa** (36 mg, 39%). A orange paste, **^{1}H NMR** (400 MHz) δ 0.86–0.91 (m, 3H), 1.23–1.38 (m, 8H), 1.68 (quint, *J* = 7.3 Hz, 2H), 2.66 (t, *J* = 7.3 Hz, 2H), 6.74 (d, *J* = 16.1 Hz, 1H,), 7.36–7.41 (m, 3H), 7.50–7.61 (m, 3H); **^{13}C NMR** (100 MHz) δ 14.1, 22.7, 24.4, 29.2, 29.3, 31.7, 41.0, 126.3, 128.3, 129.0, 130.4, 134.6, 142.3, 200.7;**IR** (ATR) 688, 747, 1175, 1450, 1611, 1651, 1690, 2854, 2926, 3019, 3063 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{16}H_{22}O$ (M), 230.1671, found 230.1671.

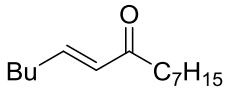
(*E*)-1,3-Diphenyl-2-propen-1-one (3qb)[6–8]



3qb

Purified by column chromatography with chloroform as the eluent to give **3qb** (21 mg, 25%). A orange paste, **^{1}H NMR** (400 MHz) δ 7.40–7.45 (m, 3H), 7.48–7.68 (m, 6H), 7.82 (d, *J* = 15.5 Hz, 1H), 8.00–8.05 (m, 2H); **^{13}C NMR** (100 MHz) δ 122.3, 128.6, 128.7, 128.8, 129.1, 130.7, 132.9, 135.0, 138.4, 145.0, 190.7; **IR** (ATR) 689, 747, 1017, 1215, 1335, 1450, 1605, 1663, 2922, 3026, 3060 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{15}H_{12}O$ (M), 208.0888, found 208.0891.

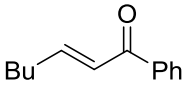
(*E*)-Tetradec-5-en-7-one (3ra)



3ra

Purified by column chromatography with chloroform as the eluent to give **3ra** (31 mg, 37%). A yellow oil, **^{1}H NMR** (400 MHz) δ 0.82–0.95 (m, 6H), 1.18–1.38 (m, 10H), 1.40–1.49 (m, 2H), 1.56–1.63 (m, 2H), 2.21 (qd, *J* = 7.0, 1.5 Hz, 2H), 2.52 (t, *J* = 7.5 Hz, 2H), 6.09 (dt, *J* = 15.8, 1.5 Hz, 1H), 6.83 (dt, *J* = 15.8, 7.0 Hz, 1H); **^{13}C NMR** (100 MHz) δ 13.8, 14.1, 22.3, 22.6, 24.4, 29.1, 29.3, 30.2, 31.7, 32.1, 40.1, 130.3, 147.3, 201.1; **IR** (ATR) 981, 1288, 1378, 1409, 1466, 1631, 1675, 1699, 2858, 2928, 2958 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{14}H_{26}O$ (M), 210.1984, found 210.1985.

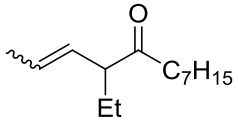
(*E*)-1-Phenylhept-2-en-1-one (3rb)



3rb

Purified by column chromatography with chloroform as the eluent to give **3rb** (15 mg, 20%). A colorless oil, **^{1}H NMR** (400 MHz) δ 0.94 (t, *J* = 7.3 Hz, 3H), 1.39 (sixt, *J* = 7.3 Hz, 2H), 1.52 (quint, *J* = 7.3 Hz, 2H), 2.33 (qd, *J* = 7.0, 1.4 Hz, 2H), 6.88 (dt, *J* = 15.5, 1.5 Hz, 1H), 7.07 (dt, *J* = 15.5, 7.0 Hz, 1H), 7.43–7.50 (m, 2H), 7.52–7.58 (m, 1H), 7.90–7.95 (m, 2H); **^{13}C NMR** (100 MHz) δ 14.0, 22.5, 30.4, 32.7, 126.0, 128.6, 128.7, 132.7, 138.2, 150.3, 191.1; **IR** (ATR) 755, 1005, 1218, 1448, 1621, 1670, 2873, 2930, 2960, 3015 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{13}H_{16}O$ (M), 188.1201, found 188.1198.

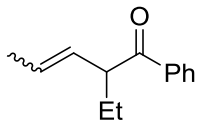
4-Ethyldodec-2-en-5-one (3ta)



3ta

Purified by column chromatography with hexane/ethyl acetate (5:1) as the eluent to give **3ta** (38 mg, 12%, *E*:*Z* = 71:29). Obtained as a hardly separable mixture with byproducts. The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ for the *E* isomer 0.81–0.90 (m, 6H), 1.21–1.32 (m, 8H), 1.43 (quint, *J* = 7.2 Hz , 2H), 1.51–1.60 (m, 2H), 1.69 (d, *J* = 6.5 Hz, 3H), 2.38 (t, *J* = 7.5 Hz, 2H), 2.93 (q, *J* = 8.1 Hz, 1H), 5.30 (ddq, *J* = 15.2, 9.0, 1.6 Hz, 1H), 5.56 (dqd, *J* = 15.2, 6.5, 0.5 Hz, 1H); **^{13}C NMR** (100 MHz) δ for the *E* isomer 11.9, 14.2, 22.7, 23.7, 24.4, 29.2, 29.3, 29.4, 31.8, 41.6, 43.0, 128.7, 129.4, 212.4; **IR** (ATR) 968, 1378, 1408, 1460, 1669, 1713, 1769, 2857, 2926, 2958 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{14}H_{26}O$ (M), 210.1984, found 210.1984.

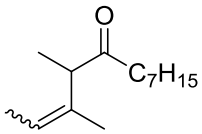
2-Ethyl-1-phenyl-pent-3-en-1-one (3tb)



3tb

Purified by column chromatography with hexane/ethyl acetate (10:1) as the eluent to give **3tb** (26 mg, 15%, *E*:*Z* = 70:30). Obtained as a hardly separable mixture with byproducts. The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ for the *E* isomer 0.91 (t, *J* = 7.1 Hz, 3H), 1.59–1.66 (m, 2H), 1.67 (d, *J* = 6.2 Hz, 3H), 3.89 (q, *J* = 7.2 Hz, 1H), 5.50 (ddq, *J* = 15.3, 8.4, 1.2 Hz, 1H), 5.59 (q, *J* = 15.3, 6.2, 1.1 Hz), 7.52–7.57 (m, 1H) , 7.42–7.49 (m, 2H)7.95–7.99 (m, 2H); **^{13}C NMR** (100 MHz) δ for the *E* isomer 12.0, 18.2, 25.7, 52.5, 128.56, 128.60, 128.65, 128.7, 129.8, 132.9, 201.8; **IR** (ATR) 700, 1204, 1262, 1447, 1580, 1597, 1682, 2875, 2964, 3346, 3519 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{13}H_{16}O$ (M), 188.1201, found 188.1203.

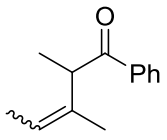
3,4-Dimethyldodec-2-en-5-one (6ua)



6ua

Purified by column chromatography with hexane/ethyl acetate (8:1) as the eluent. Obtained as a hardly separable mixture with byproducts (**6ua**, 46%, *E*/*Z* = 78/22, see Scheme S1). The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ for the *E* isomer 0.87 (t, *J* = 7.9 Hz, 3H), 1.11 (d, *J* = 6.8 Hz, 3H), 1.19–1.32 (m, 8H), 1.47–1.57 (m, 5H), 1.62 (dq, *J* = 6.8, 1.0 Hz, 3H), 2.27–2.49 (m, 2H), 3.16 (q, *J* = 6.8 Hz, 1H), 5.38–5.47 (m, 1H); **^{13}C NMR** (100 MHz) δ for the *E* isomer 13.4, 13.7, 14.2, 14.5, 22.7, 24.1, 29.2, 29.3, 31.8, 40.4, 56.1, 122.6, 135.1, 212.5; **IR** (ATR) 1133, 1376, 1409, 1463, 1617, 1688, 1714, 2857, 2928, 2959, 3494 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{14}H_{26}O$ (M), 210.1984, found 210.1985.

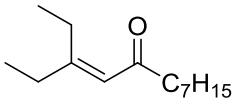
2,3-Dimethyl-1-phenylpent-3-en-1-one (6ub)



6ub

Purified by column chromatography with hexane/ethyl acetate (10:1) as the eluent. Obtained as a hardly separable mixture with byproducts (**6ub**, 46%, *E*/*Z* = 81/19, see Scheme 2). The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ 1.29 (d, *J* = 7.0 Hz, 3H, 1.55–1.58 (m, 3H), 1.59–1.61 (m, 3H), 4.07 (q, *J* = 7.0 Hz, 1H), 5.40–5.48 (m, 1H), 7.38–7.45 (m, 2H), 7.48–7.55 (m, 1H), 7.94–8.00 (m, 2H); **^{13}C NMR** (100 MHz) δ for the mixture 12.2, 12.4, 13.2, 13.5, 13.76, 13.79, 14.5, 16.1, 16.8, 19.6, 26.4, 27.3, 31.3, 43.9, 48.5, 50.7, 111.0, 118.9, 121.2, 122.6, 128.1, 128.3, 128.50, 128.52, 128.6, 132.4, 132.7, 132.87, 132.90, 135.8, 136.2, 136.9, 137.0, 150.9, 201.2, 201.5, 202.0; **IR** (ATR) 691, 743, 963, 1179, 1372, 1448, 1682, 2935, 2972, 3349 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{13}H_{16}O$ (M), 188.1201, found 188.1200.

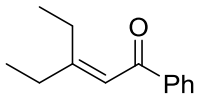
3-Ethyldodec-3-en-5-one (3ua)



3ua

The reaction was conducted using **2a** (*d* = 0.95; 81.9 μL, 0.48 mmol), $EtAlCl_2$ (1.0 M solution in hexane; 0.38 mL, 0.40 mmol) and **B1** (95 mg, 0.40 mmol). Purified by column chromatography with chloroform as the eluent. Obtained as a hardly separable mixture with byproducts (**3ua**, 55%, see Scheme S1). The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ 0.88 (t, *J* = 7.0 Hz, 3H), 1.05 (t, *J* = 7.5 Hz, 3H), 1.07 (t, *J* = 7.5 Hz, 3H), 1.21–1.34 (m, 8H), 1.54–1.64 (m, 2H), 2.17 (qd, *J* = 7.5, 1.2 Hz, 2H), 2.42 (t, *J* = 7.5 Hz, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 5.99 (s, 1H); **^{13}C NMR** (100 MHz) δ 12.3, 13.1, 14.2, 22.8, 24.4, 25.9, 29.3, 29.4, 31.1, 31.8, 44.6, 121.4, 165.7, 201.3; **IR** (ATR) 759, 1216, 1372, 1456, 1713, 2858, 2928, 2957 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{14}H_{26}O$ (M), 210.1984, found 210.1984.

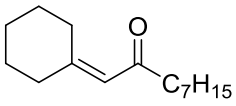
3-Ethyl-1-phenylpent-2-en-1-one (3ub)



3ub

The reaction was conducted using **2b** (d = 0.69; 49 μL, 0.40 mmol), $EtAlCl_2$ (1.0 M solution in hexane; 0.77 mL, 0.80 mmol) and **B1** (95 mg, 0.40 mmol). Purified by column chromatography with hexane/ethyl acetate (10:1) as the eluent. Obtained as a hardly separable mixture with byproducts (**3ub**, 64%, see Scheme 2). The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ 1.13 (t, J = 7.6 Hz, 3H), 1.17 (t, J = 7.6 Hz, 3H), 2.31 (qd, J = 7.6, 1.2 Hz, 2H), 2.62 (q, J = 7.6 Hz, 2H), 6.67 (s, 1H), 7.38–7.45 (m, 2H), 7.48–7.55 (m, 1H), 7.91–7.95 (m, 2H); **^{13}C NMR** (100 MHz) δ 12.4, 13.2, 26.4, 31.3, 119.0, 128.3, 128.6, 132.4, 139.6, 167.3, 191.7; **IR** (ATR) 692, 757, 871, 1231, 1273, 1448, 1609, 1662, 2936, 2971 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{13}H_{16}O$ (M), 188.1201, found 188.1202.

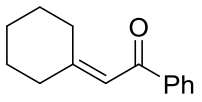
1-Cyclohexylidenenonan-2-one (3va)



3va

The reaction was conducted using **2a** (d = 0.95; 81.9 μL, 0.48 mmol), $EtAlCl_2$ (1.0 M solution in hexane; 0.38 mL, 0.40 mmol) and **B1** (95 mg,0.40 mmol). Purified by column chromatography with chloroform as the eluent. Obtained as a hardly separable mixture with byproducts (**3va**, 68%, see Scheme S1). The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ 0.88 (t, J = 6.8 Hz, 3H), 1.21–1.36 (m, 8H), 1.53–1.70 (m, 8H), 2.13–2.19 (m, 2H), 2.40 (t, J = 7.4 Hz, 2H), 2.60–2.82 (m, 2H), 5.97 (s, 1H); **^{13}C NMR** (100 MHz) δ 14.2, 22.7, 24.4, 26.4, 28.0, 28.9, 29.3, 29.4, 30.0, 31.8, 38.2, 44.6, 121.1, 161.6, 202.3; **IR** (ATR) 761, 1217, 1378, 1457, 1621, 1710, 2858, 2929, 3446 cm^{-1}; **HR-MS** (EI-magnetic sector) calcd for $C_{15}H_{26}O$ (M), 222.1984, found 222.1984.

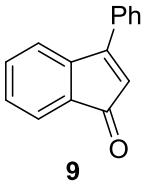
2-Cyclohexylidene-1-phenylethanone (3vb)[9,10]



3vb

The reaction was conducted using **2b** (d = 0.95; 48.1 μL, 0.40 mmol), $EtAlCl_2$ (1.0 M solution in hexane; 0.58 mL, 0.60 mmol) and **B1** (95mg, 0.40 mmol). Purified by column chromatography with hexane/ethyl acetate (10:1) as the eluent. Obtained as a hardly separable mixture with byproducts (**3vb**, 63%, see Scheme S1). The yield was calculated by ^{1}H NMR analysis of the mixture. A yellow oil, **^{1}H NMR** (400 MHz) δ 1.59–1.75 (m, 6H), 2.27–2.34 (m, 2H), 2.74–2.81 (m, 2H), 6.60 (s, 1H), 7.42–7.55 (m, 3H), 7.92–7.96 (m, 2H); **^{13}C NMR** (100 MHz) δ 26.4, 28.1, 29.0, 30.8, 38.5, 118.8, 128.4, 128.5, 132.4, 139.4, 162.9, 192.5; **IR** (ATR) 699, 979, 1448, 1610, 1656, 1817, 1963, 2586, 2933, 3510cm^{-1}; **HR-MS** (EI-magnetic sector) calculated for $C_{14}H_{16}O$ (M), 200.1201, found 200.1202.

3-Phenyl-1*H*-inden-1-one (9)[11]



9

The reaction was conducted using **7b** (120 mg, 0.40 mmol), $AlCl_3$ (160mg, 0.60 mmol) and **B1** (190mg, 0.80 mmol). Purified by column chromatography with chloroform/hexane (2:1) as the eluent to give **9** (55.8 mg, 68%). A brown oil, **^{1}H NMR** (400 MHz) δ 6.01 (s, 1H), 7.28–7.42 (m, 3H), 7.48–7.59 (m, 2H), 7.63–7.74 (m, 2H); **^{13}C NMR** (100 MHz) δ 121.7, 122.8, 123.1, 127.5, 129.1, 129.4, 130.6, 132.5, 133.0, 133.2, 144.1, 163.0, 197.2.

4. References

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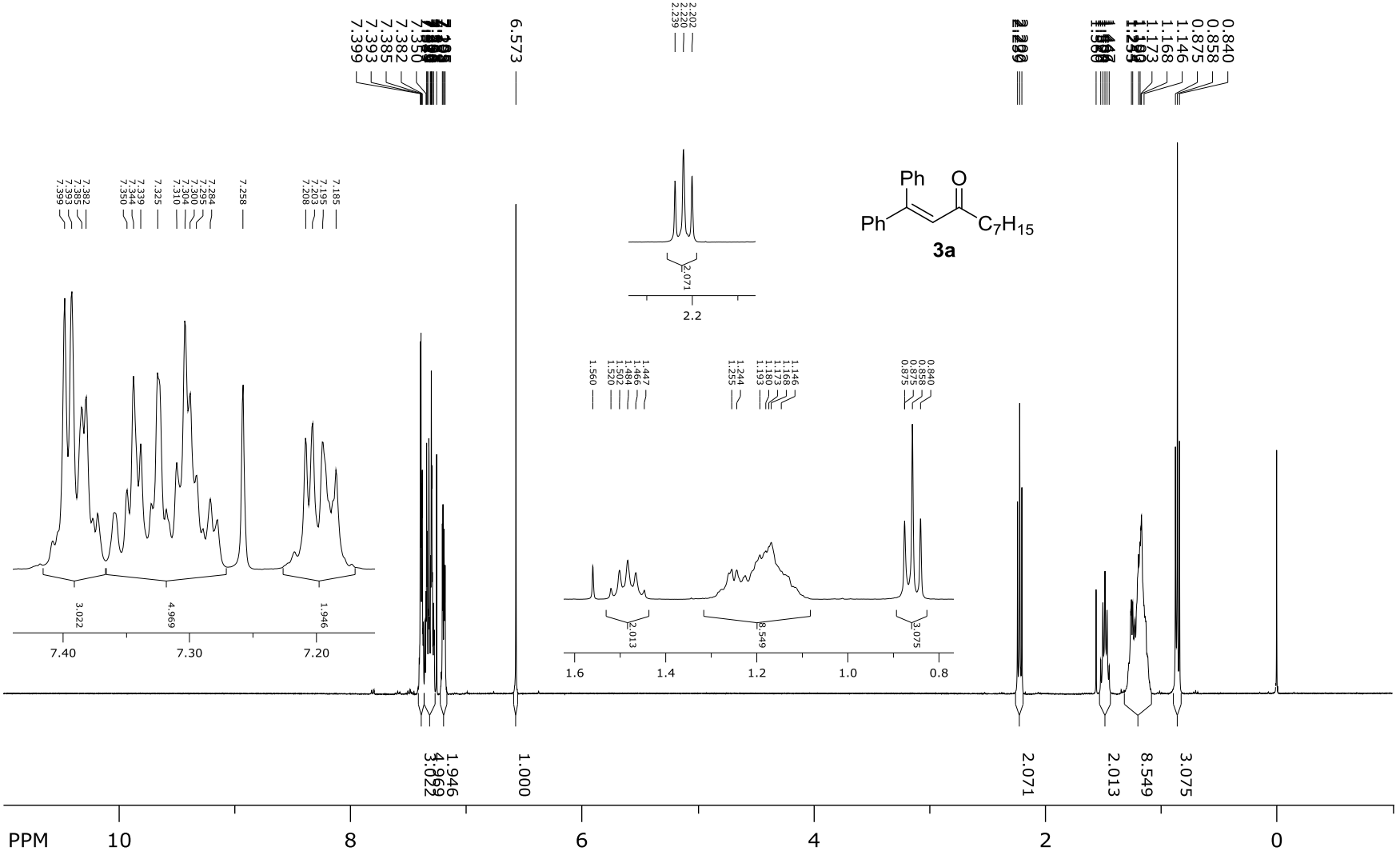
5. ^{1}H and ^{13}C NMR Spectral Charts for Compounds Synthesized

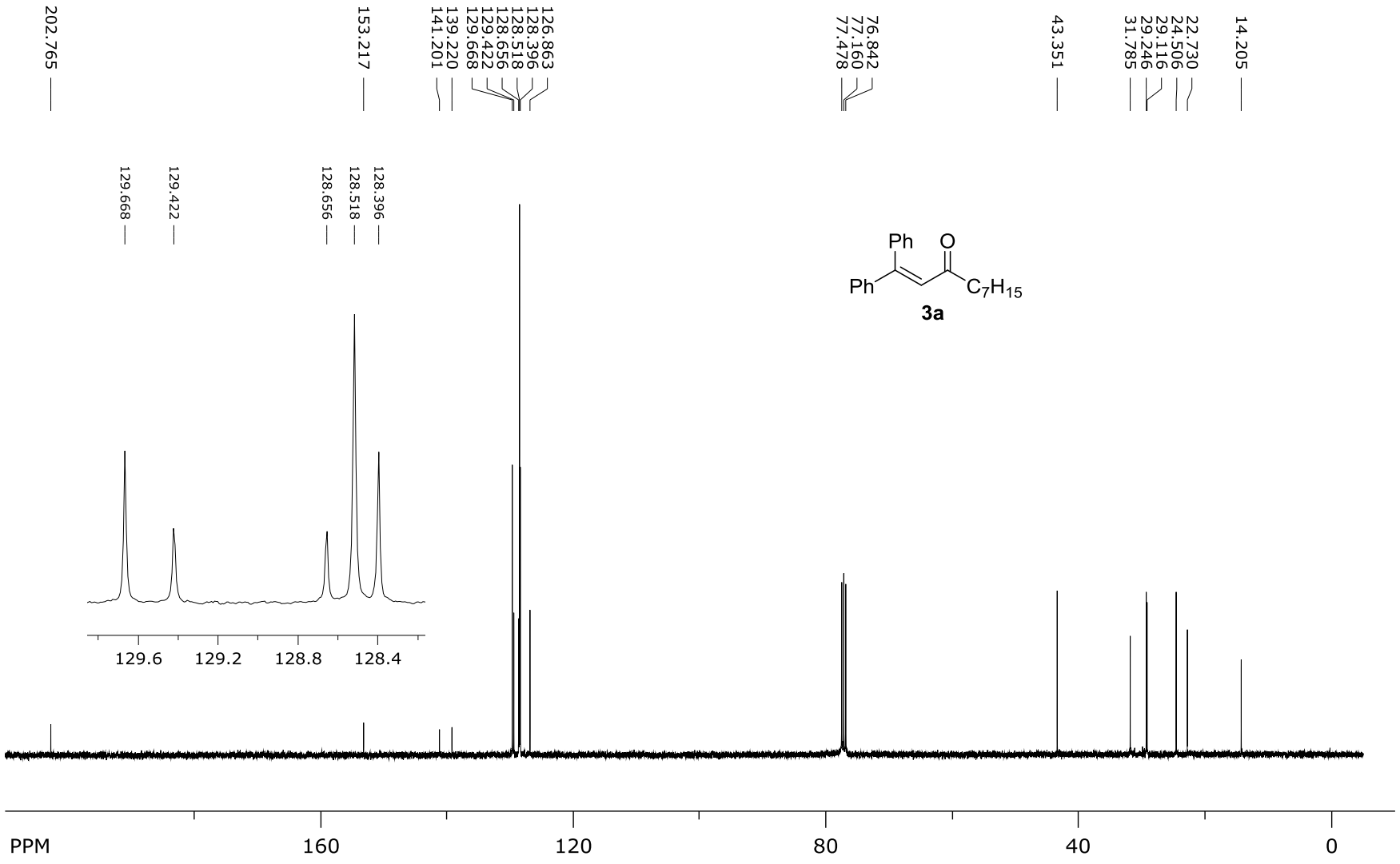
5.1. 1,1-diphenyldec-1-en-3-one (3a)

^{1}H NMR (400 MHz)



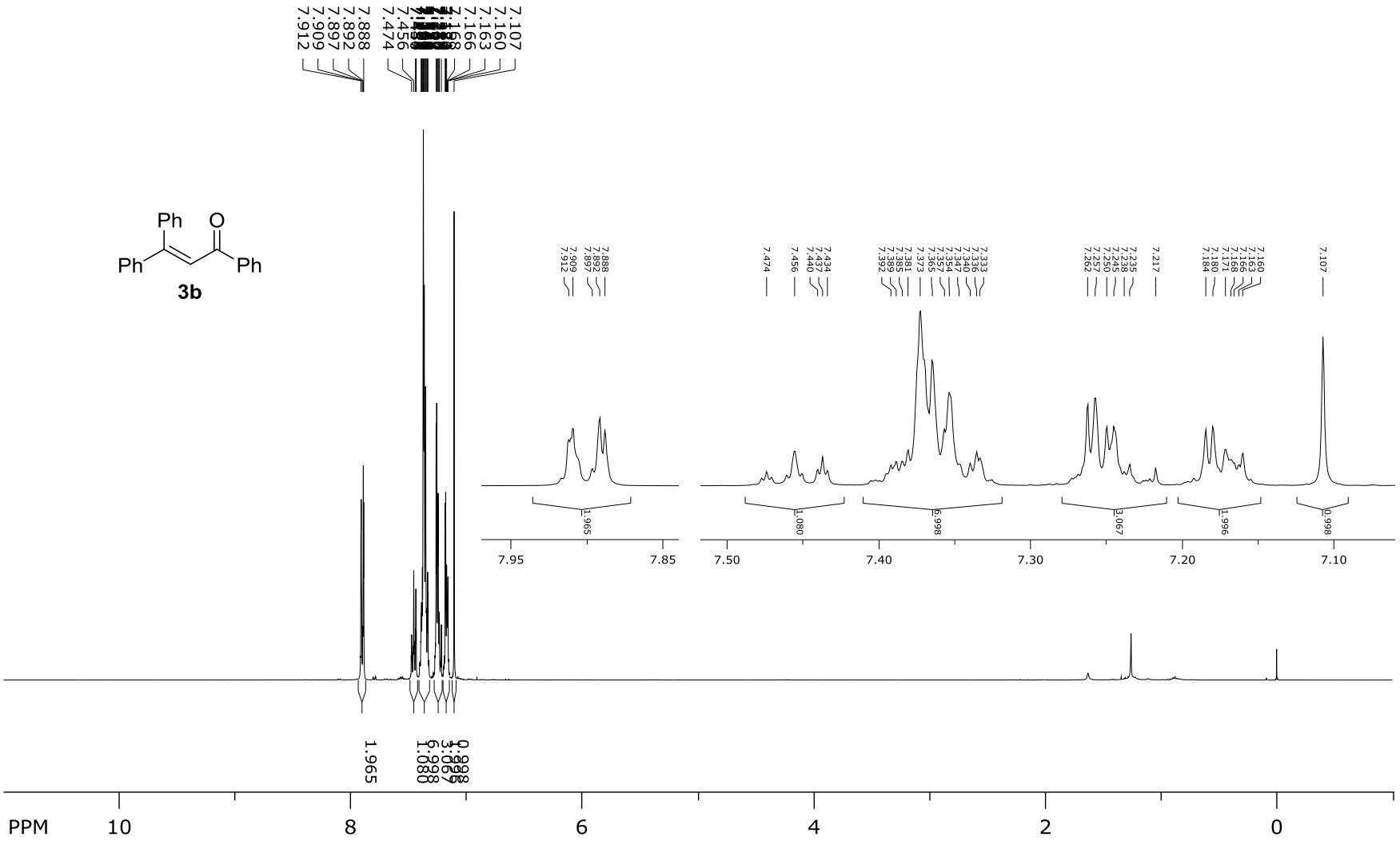
1,1-diphenyldec-1-en-3-one (3a)

^{13}C NMR (100 MHz)



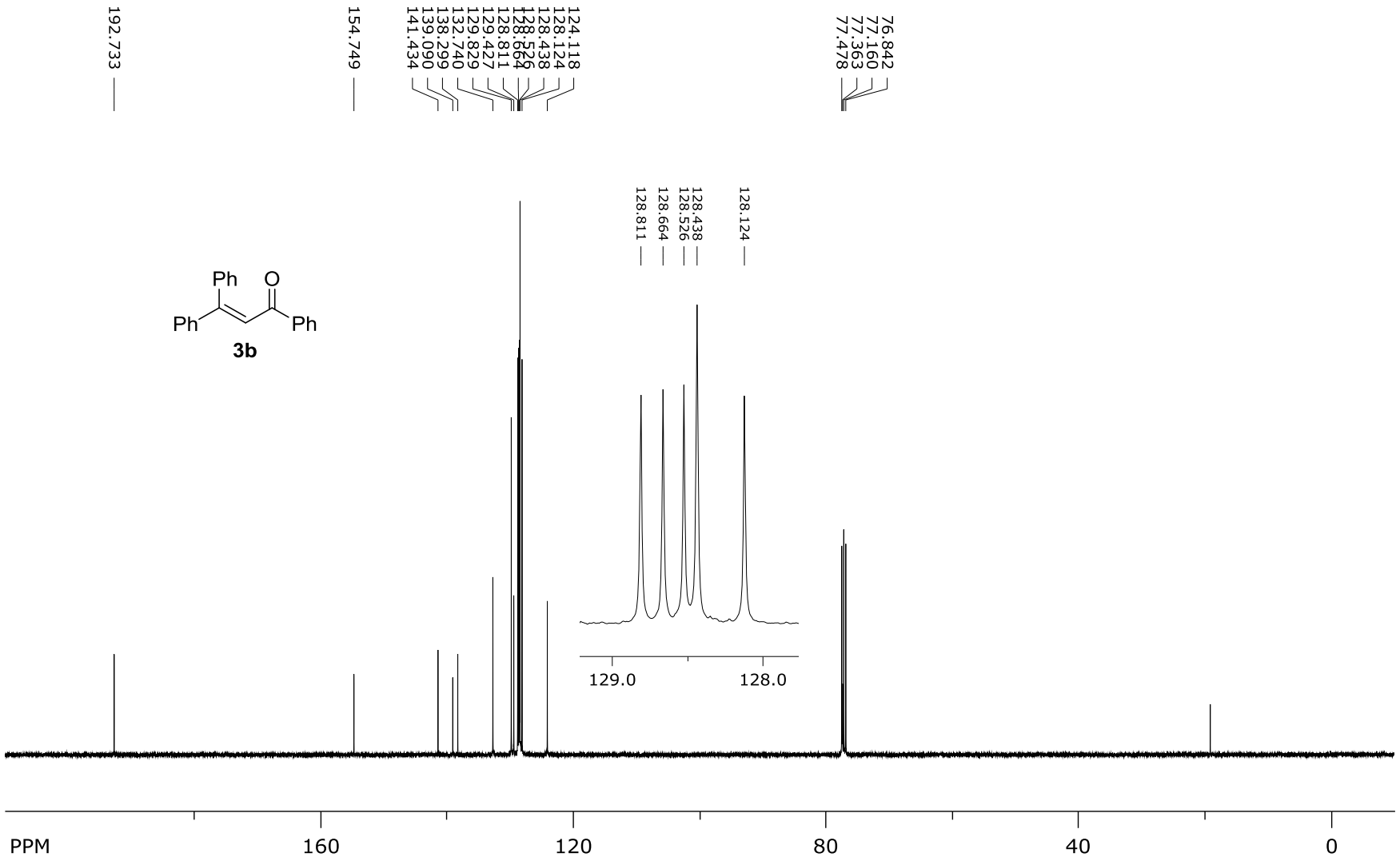
5.2. 1,3,3-Triphenylprop-2-en-1-one (3b)

^{1}H NMR (400 MHz)



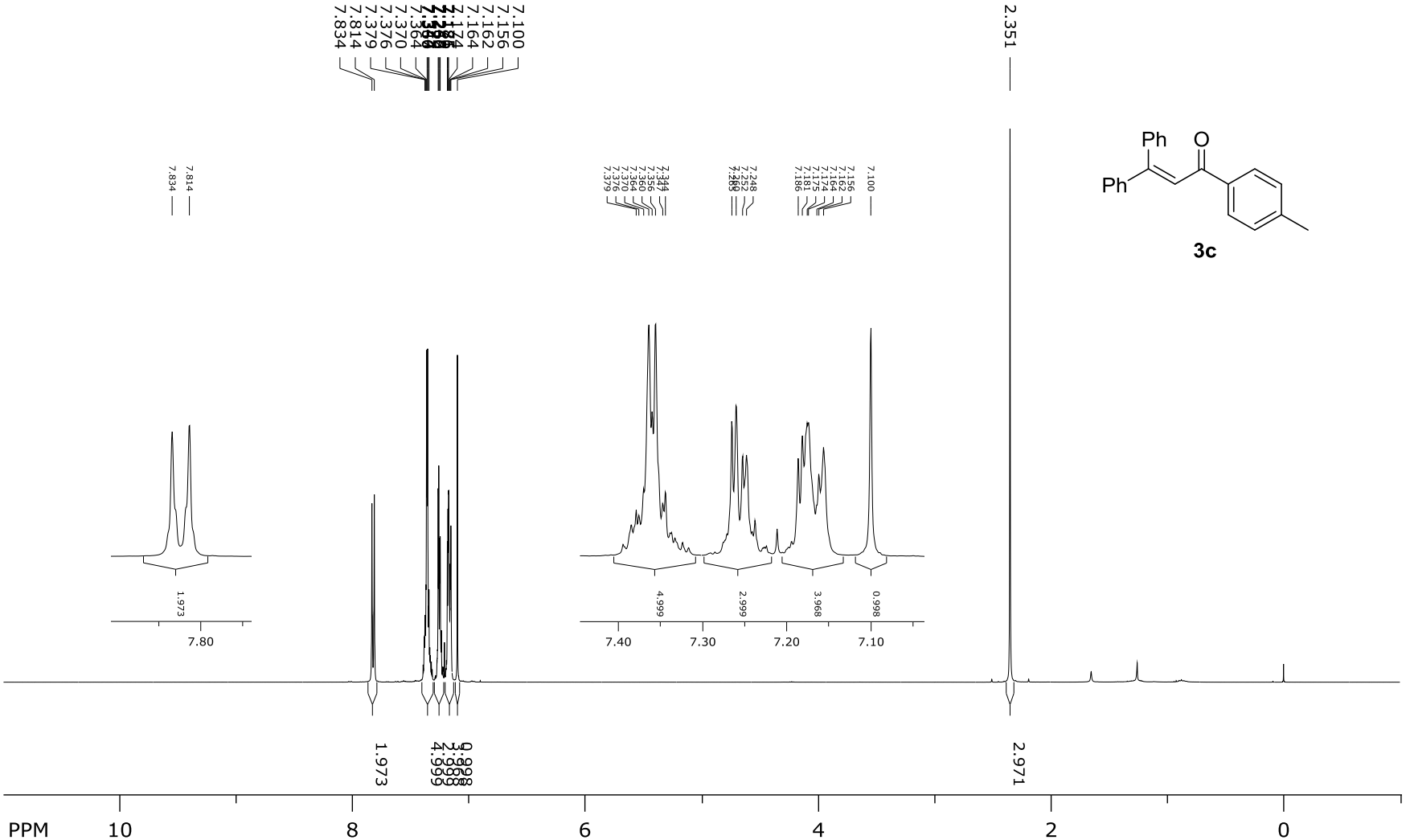
1,3,3-Triphenylprop-2-en-1-one (3b)

^{13}C NMR (100 MHz)



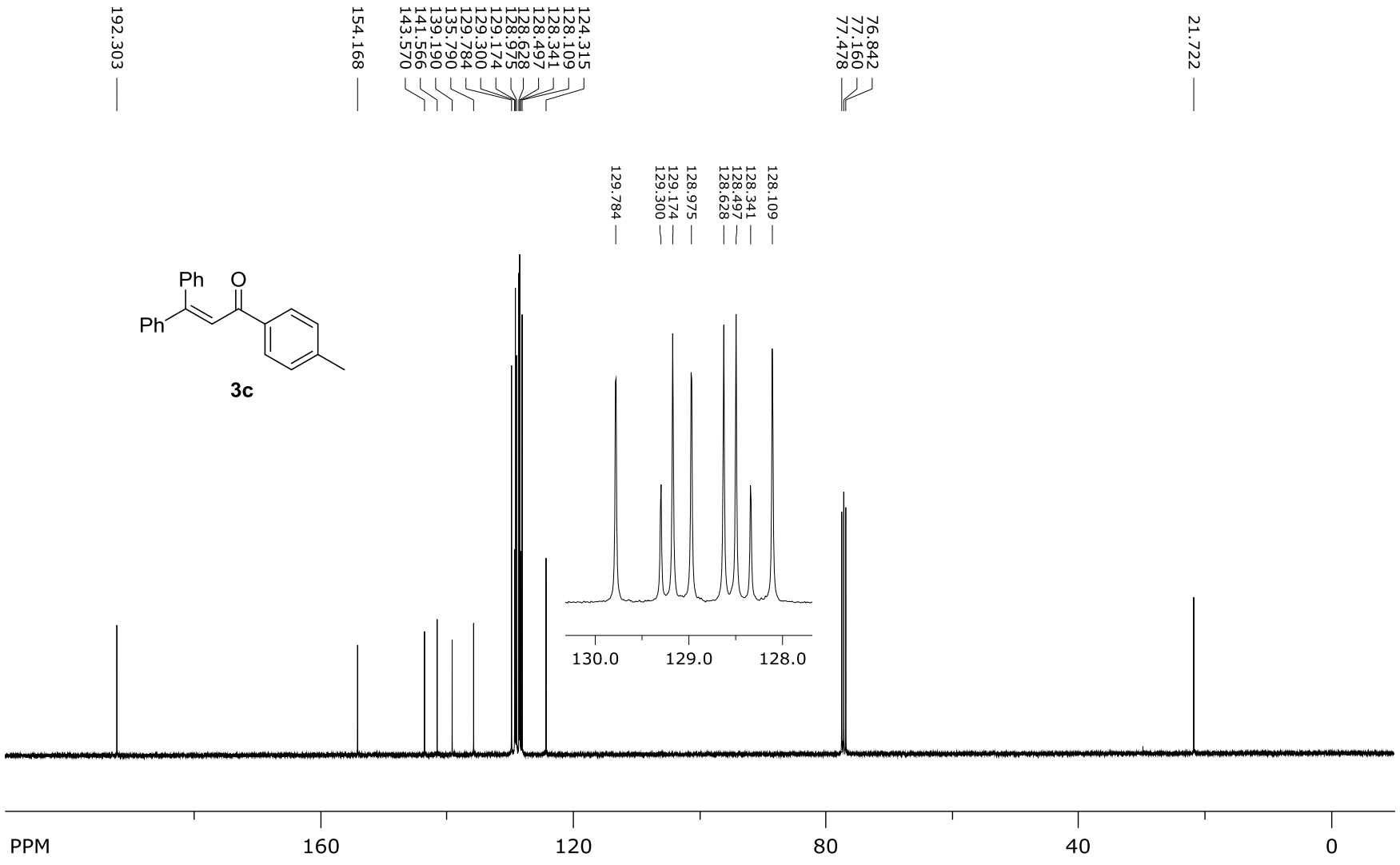
5.3. 3,3-Diphenyl-1-(*p*-tolyl)prop-2-en-1-one (3c)

^{1}H NMR (400 MHz)



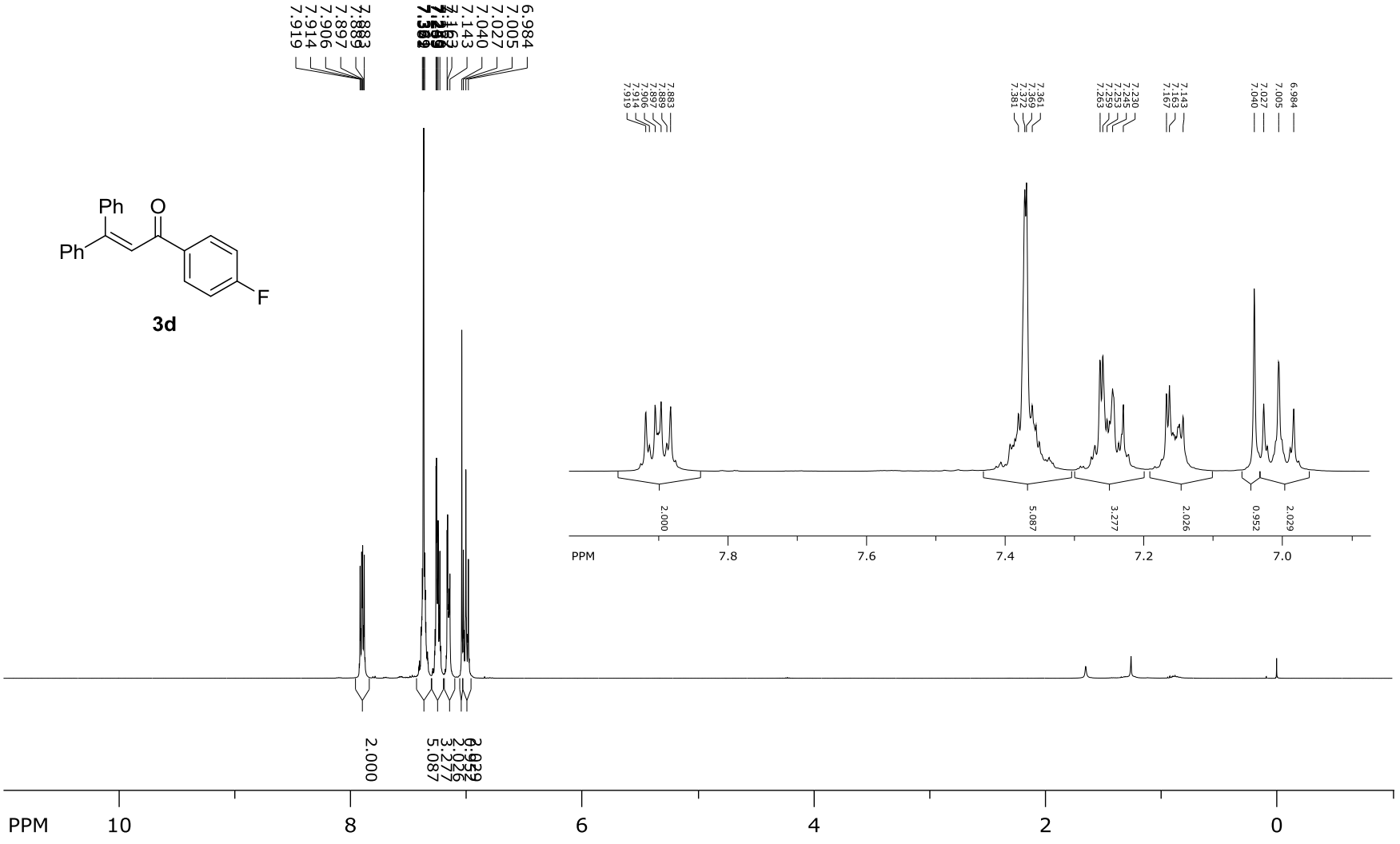
3,3-Diphenyl-1-(*p*-tolyl)prop-2-en-1-one (3c)

^{13}C NMR (100 MHz)



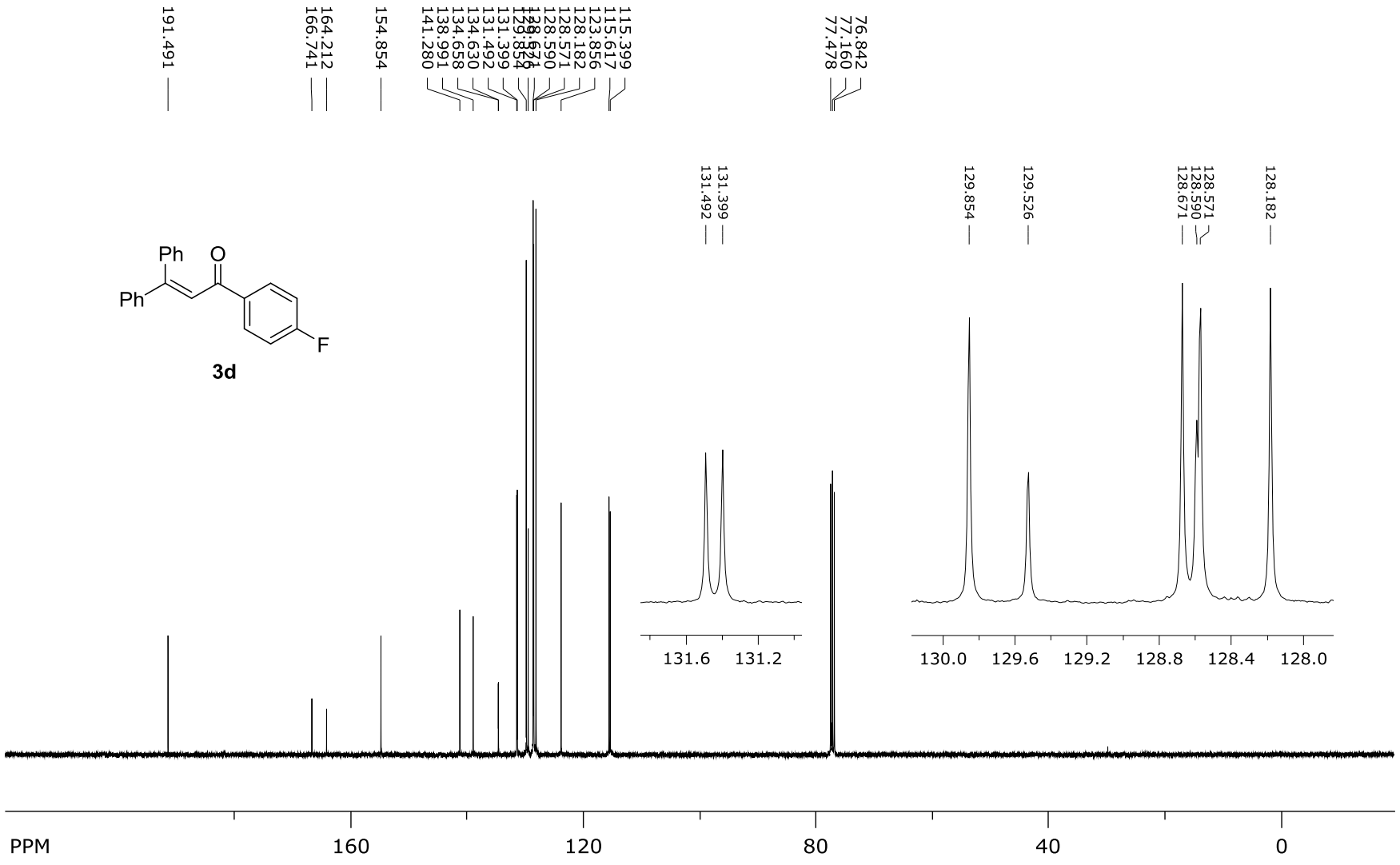
5.4. 1-(4-Fluorophenyl)-3,3-diphenylprop-2-en-1-one (3d)

^{1}H NMR (400 MHz)



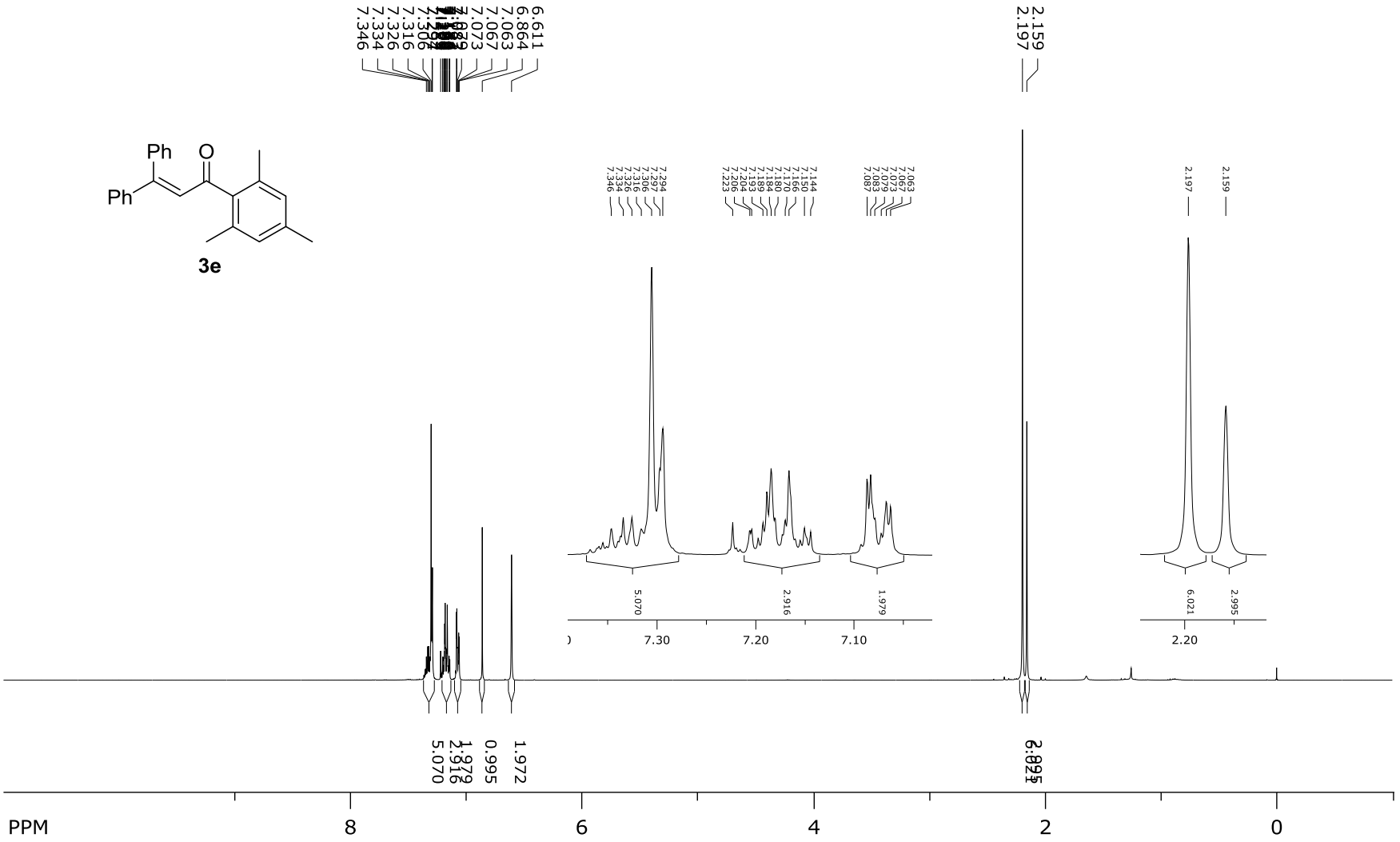
1-(4-Fluorophenyl)-3,3-diphenylprop-2-en-1-one (3d)

^{13}C NMR (100 MHz)



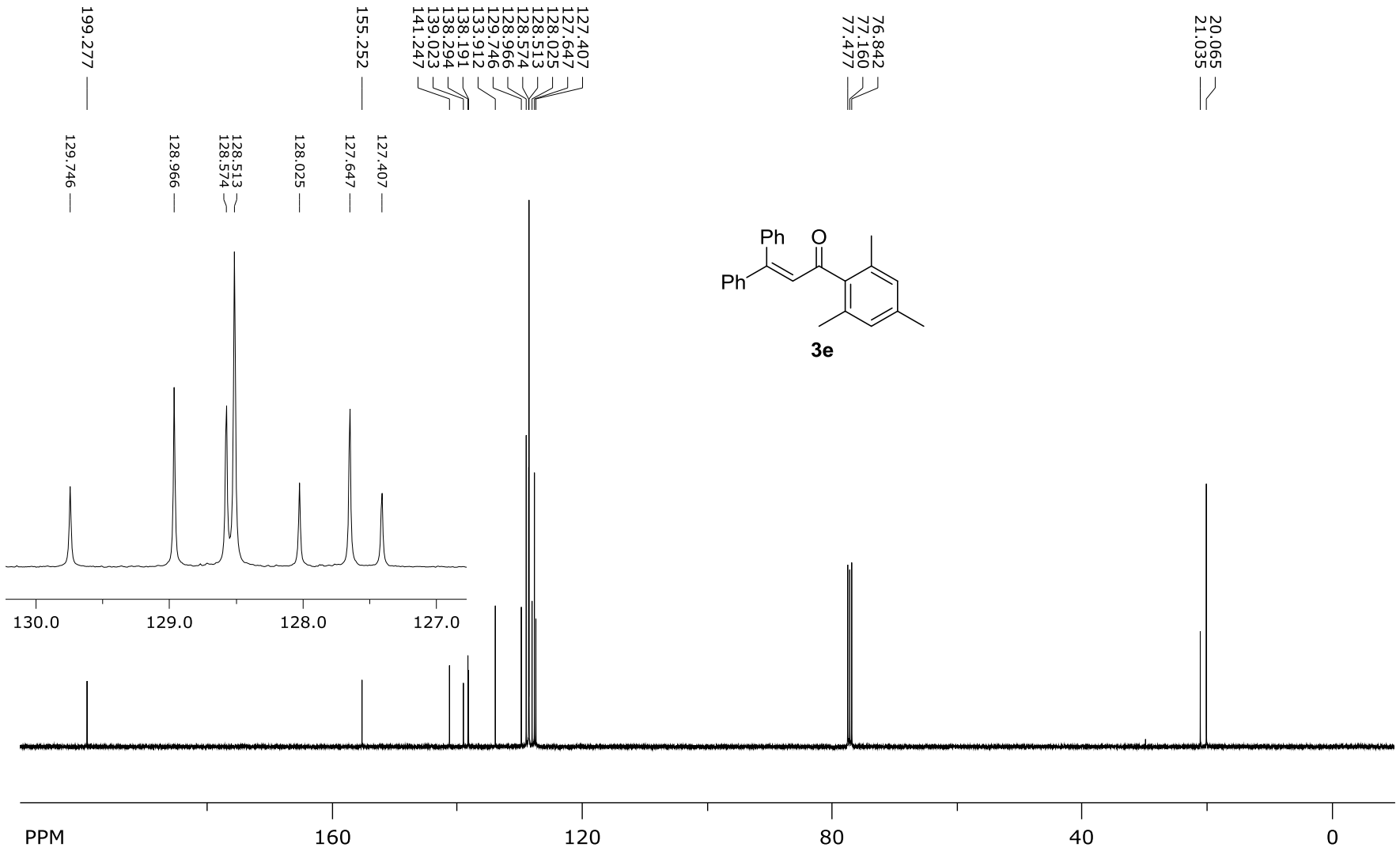
5.5. 1-Mesityl-3,3-diphenylprop-2-en-1-one (3e)

^{1}H NMR (400 MHz)



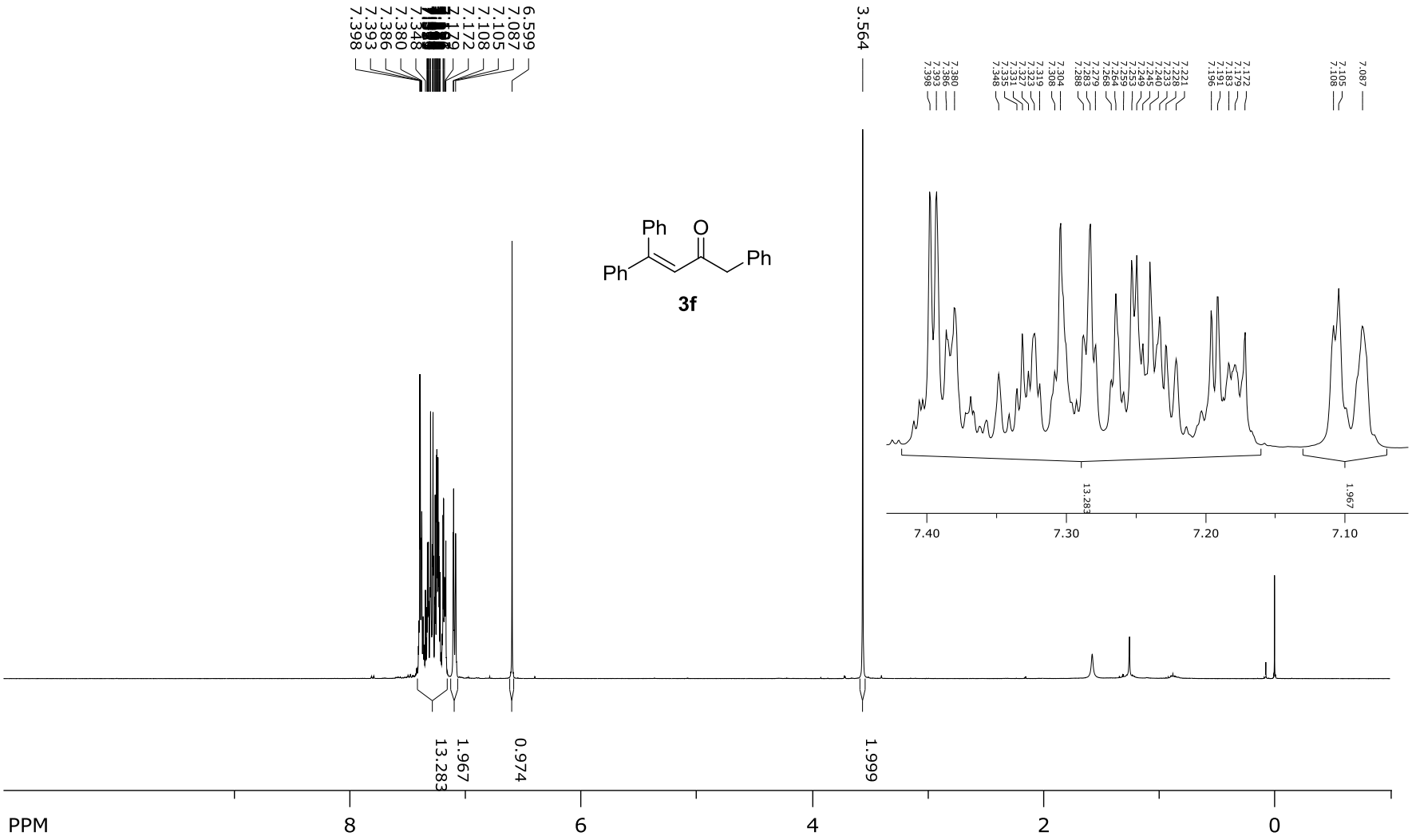
1-Mesityl-3,3-diphenylprop-2-en-1-one (3e)

^{13}C NMR (100 MHz)



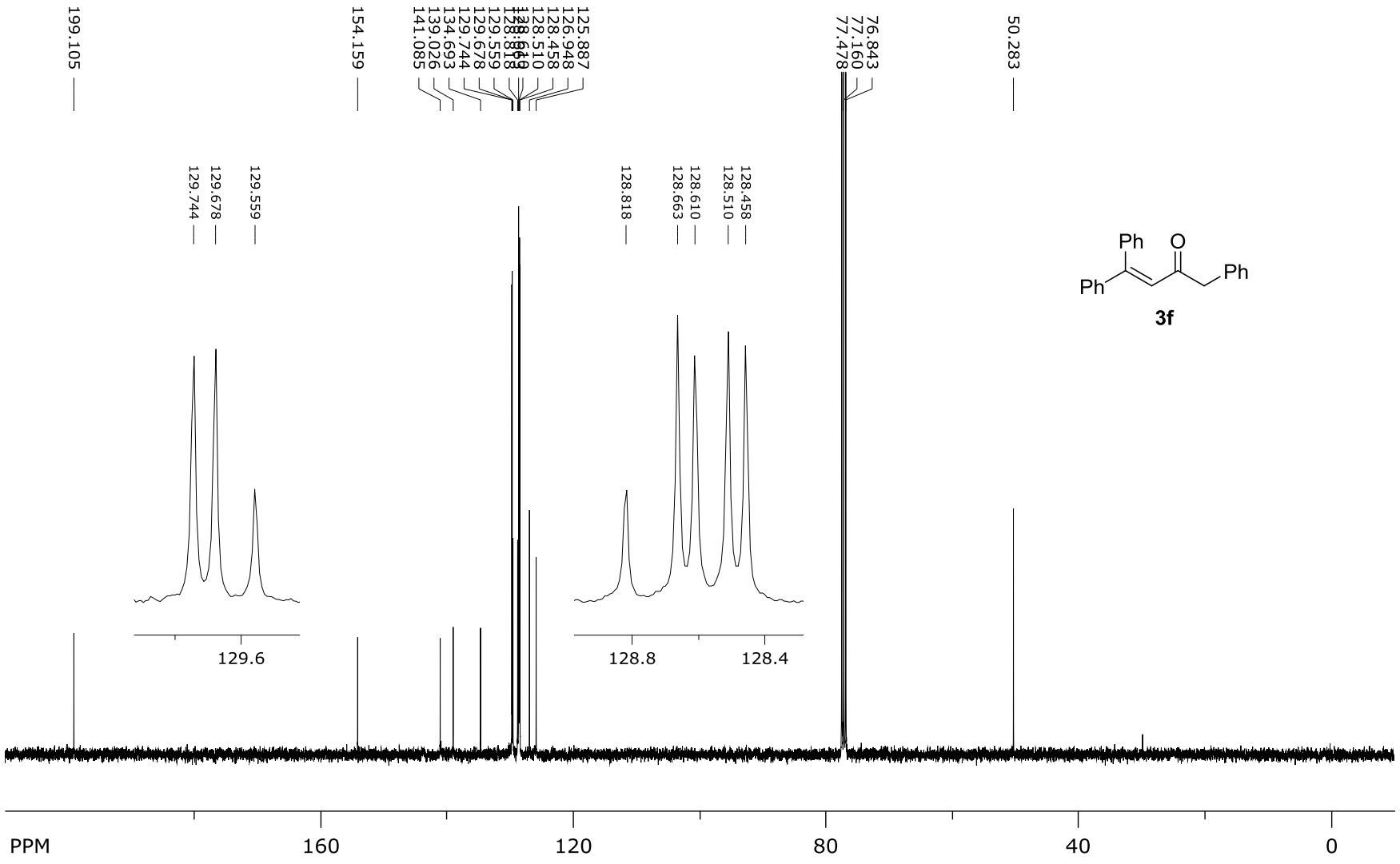
5.6. 1,4,4-Triphenylbut-3-en-2-one (3f)

^{1}H NMR (400 MHz)



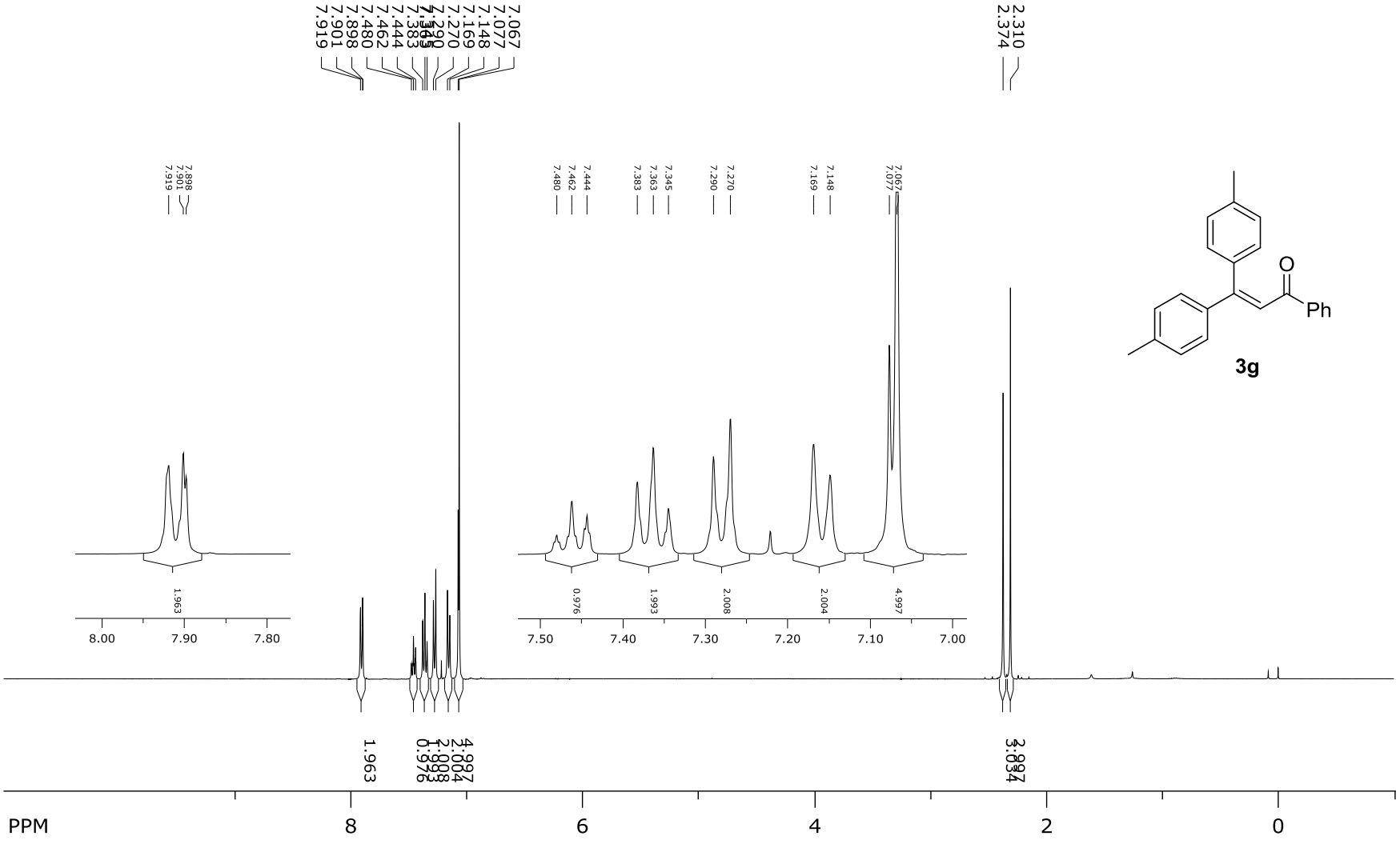
1,4,4-Triphenylbut-3-en-2-one (3f)

^{13}C NMR (100 MHz)



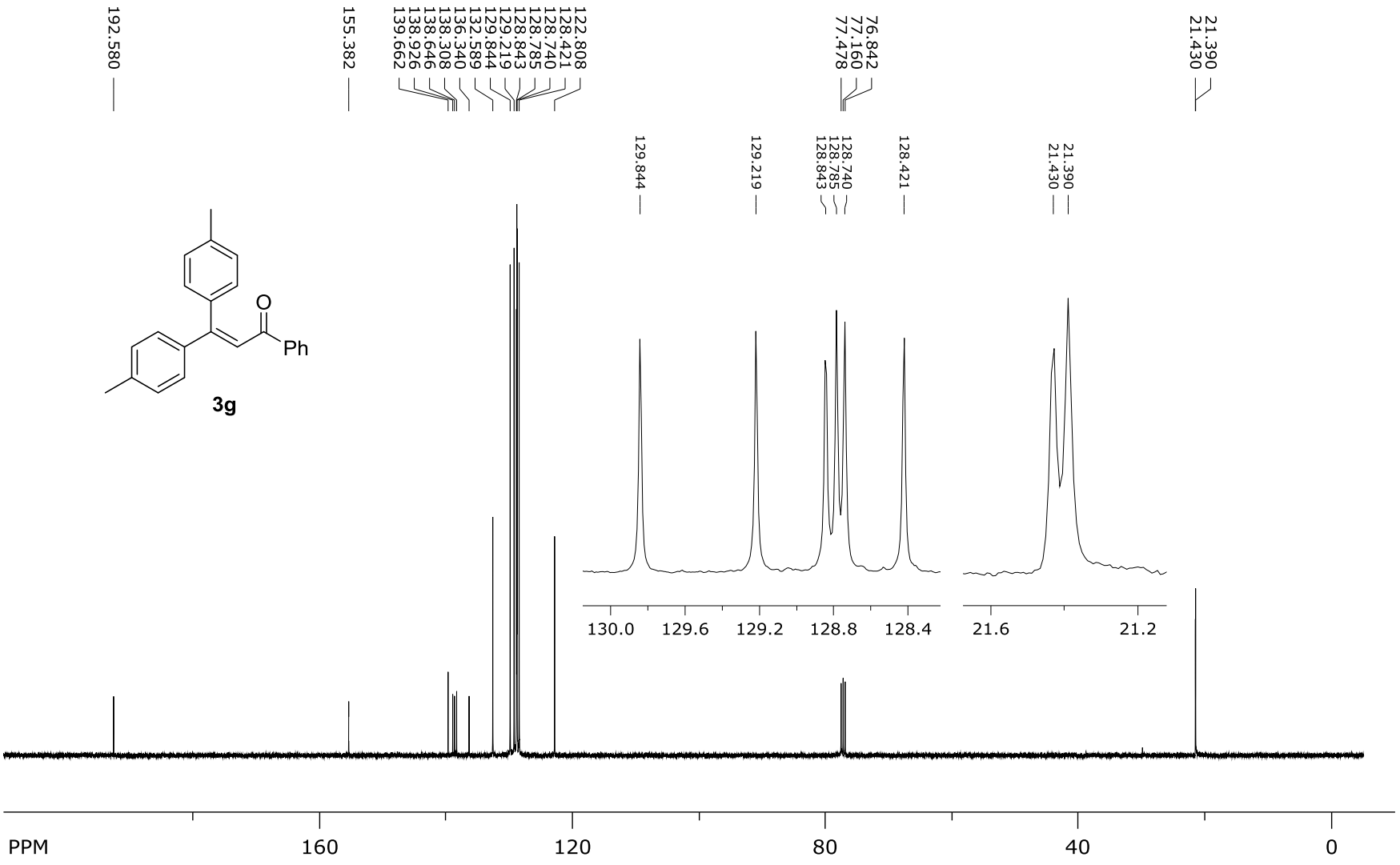
5.7. 1-Phenyl-3,3-di-*p*-tolylprop-2-en-1-one (3g)

^{1}H NMR (400 MHz)



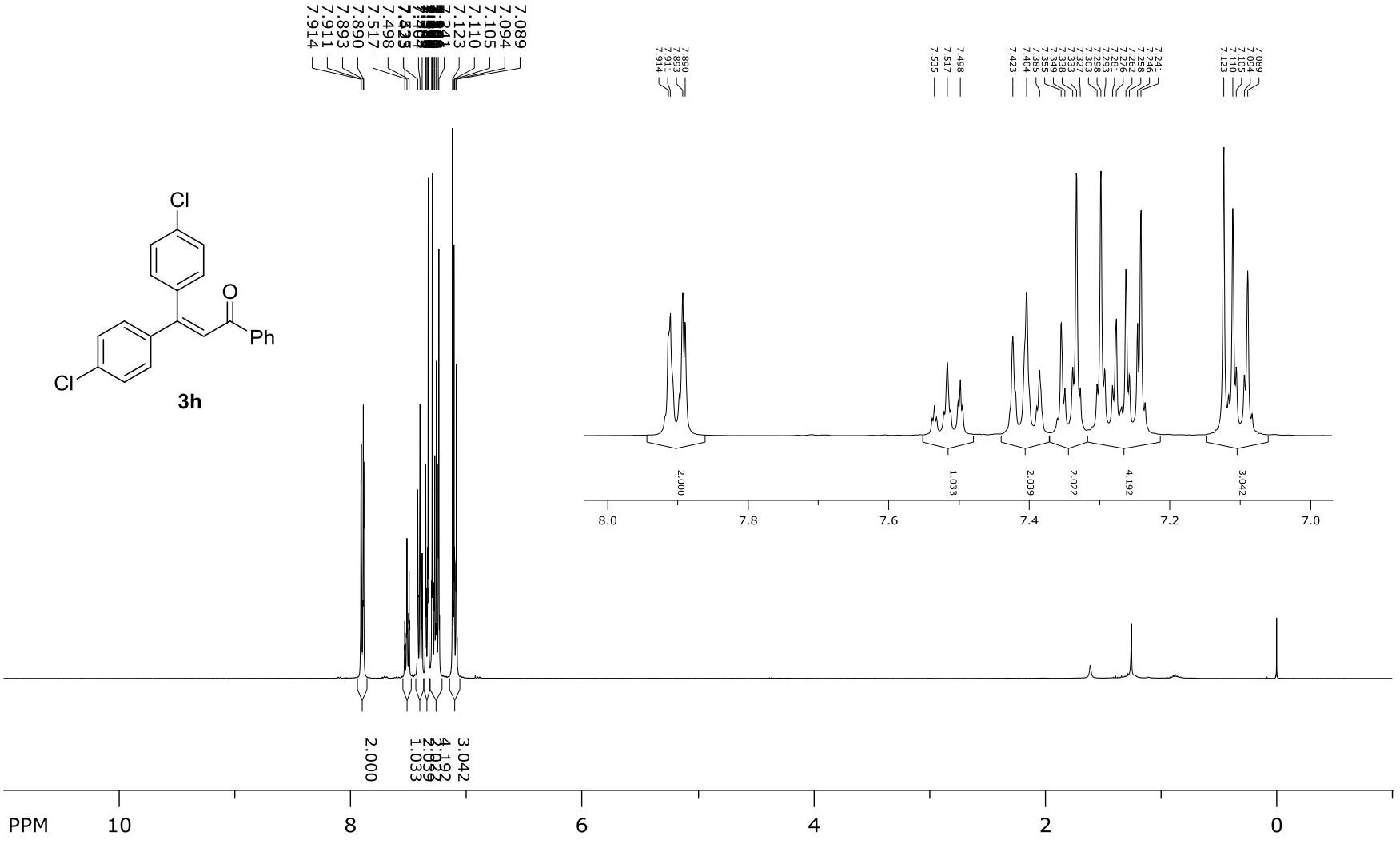
1-Phenyl-3,3-di-*p*-tolylprop-2-en-1-one (3g)

^{13}C NMR (100 MHz)



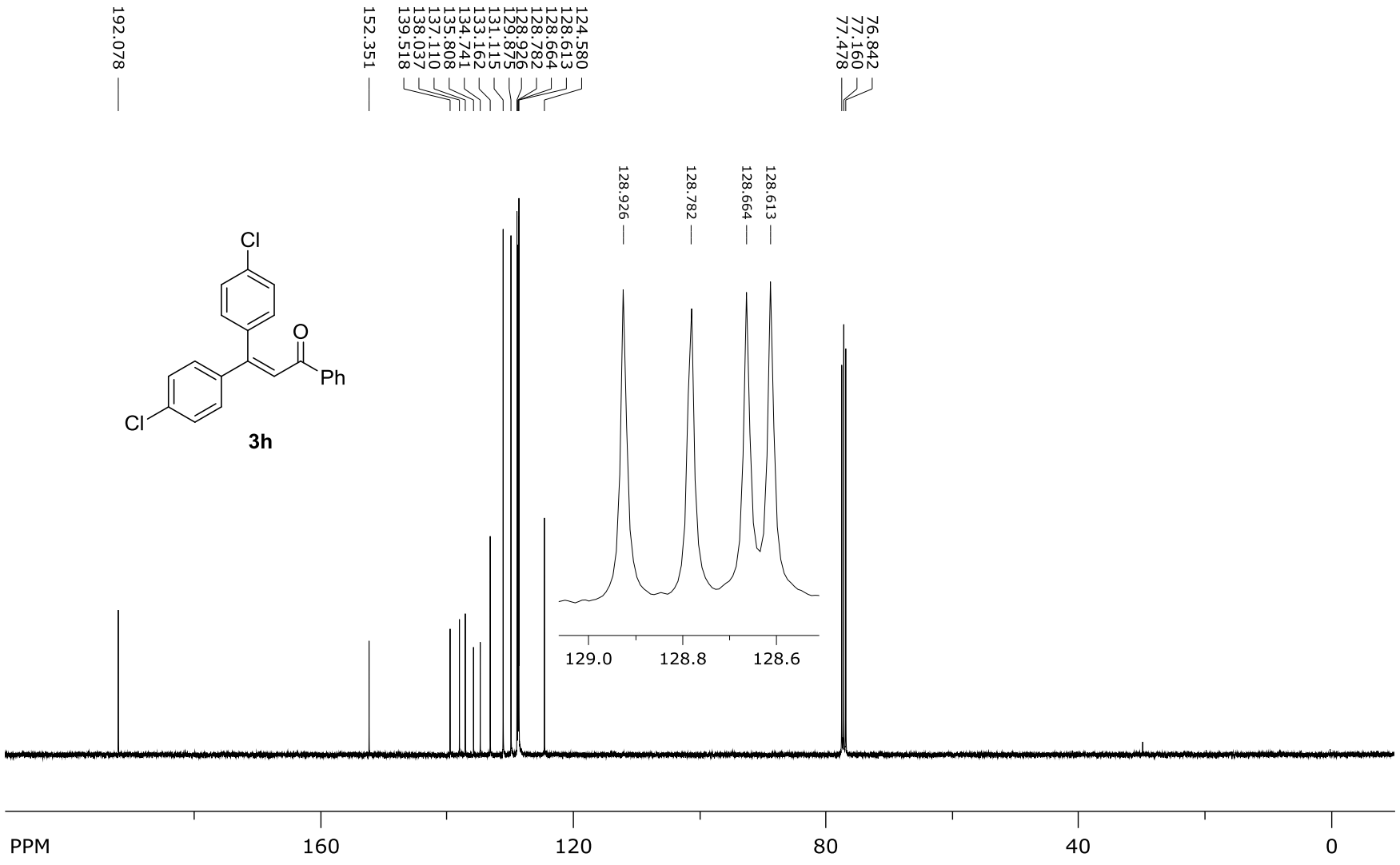
5.8. 3,3-Bis(4-chlorophenyl)-1-phenylprop-2-en-1-one (3h)

^{1}H NMR (400 MHz)



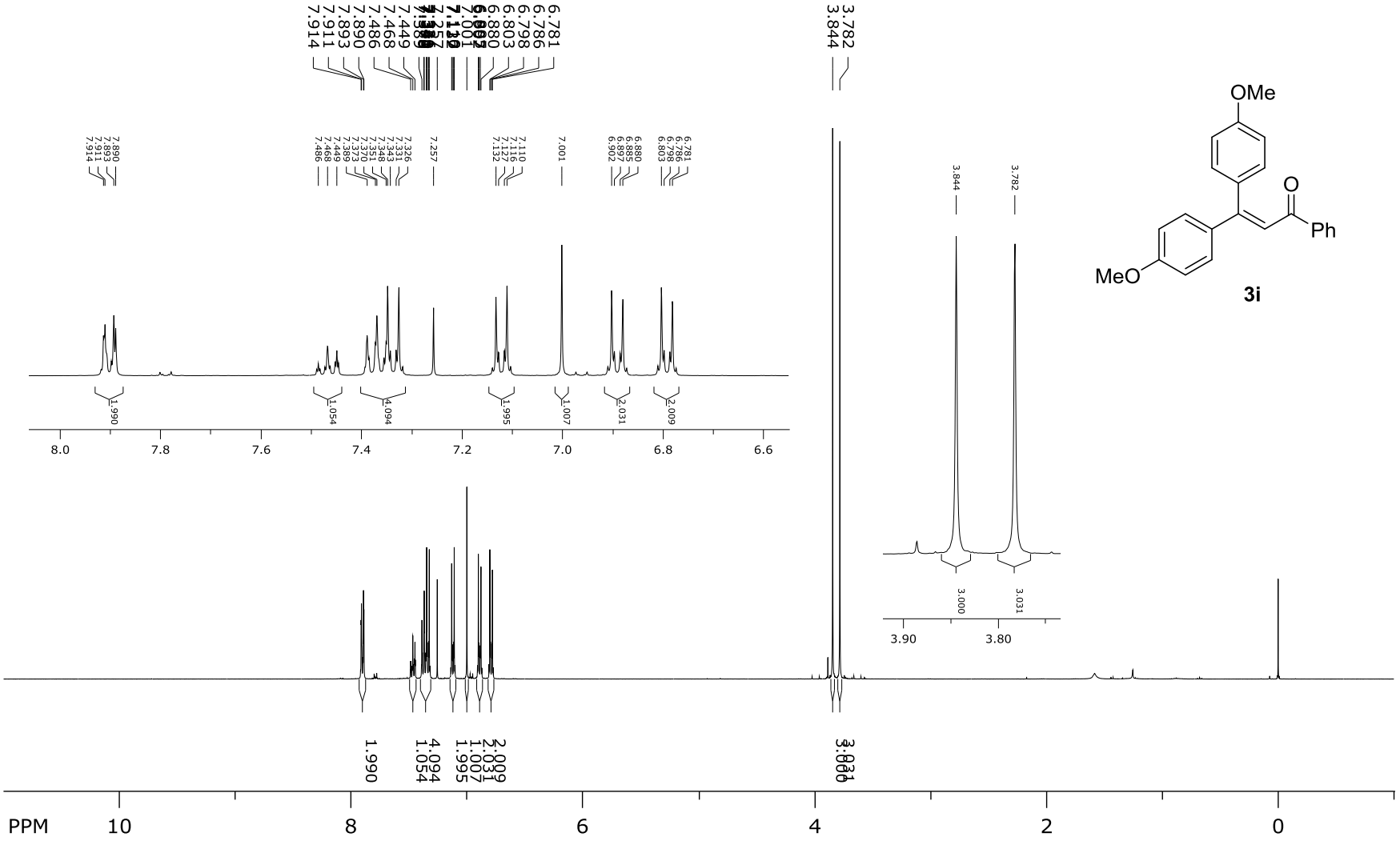
3,3-Bis(4-chlorophenyl)-1-phenylprop-2-en-1-one (3h)

^{13}C NMR (100 MHz)



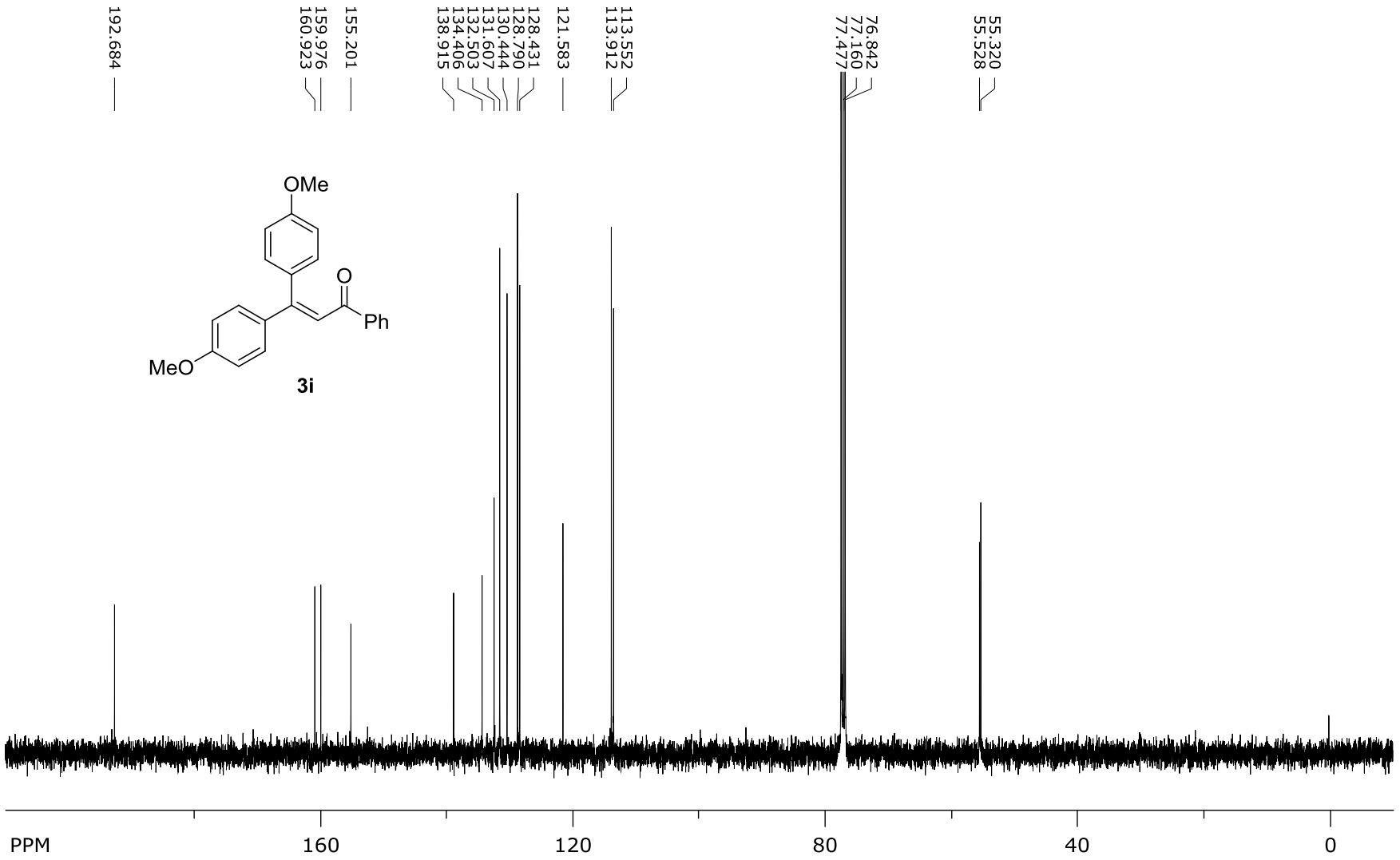
5.9. 3,3-Bis(4-methoxyphenyl)-1-phenylprop-2-en-1-one (3i)

^{1}H NMR (400 MHz)



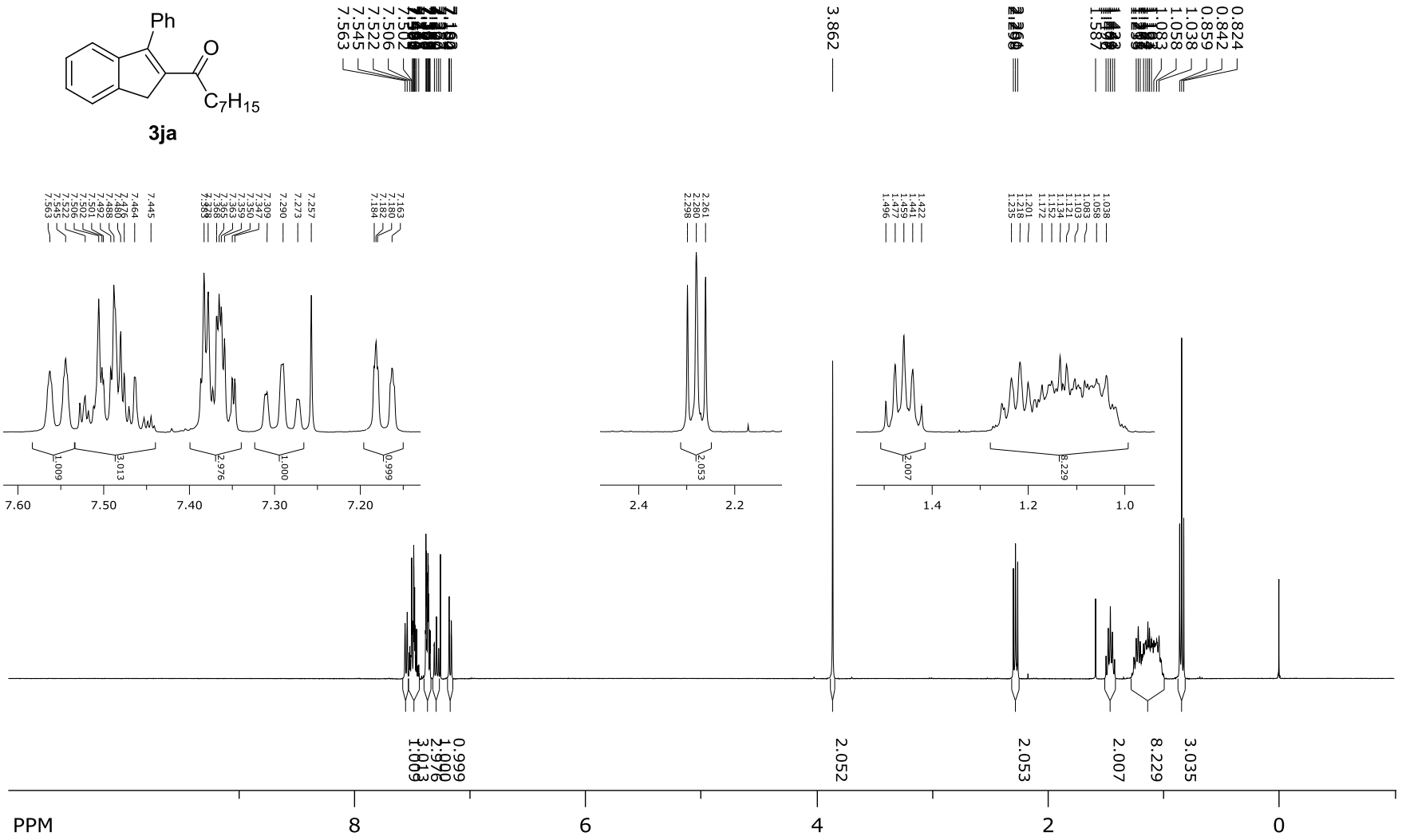
3,3-Bis(4-methoxyphenyl)-1-phenylprop-2-en-1-one (3i)

^{13}C NMR (100 MHz)



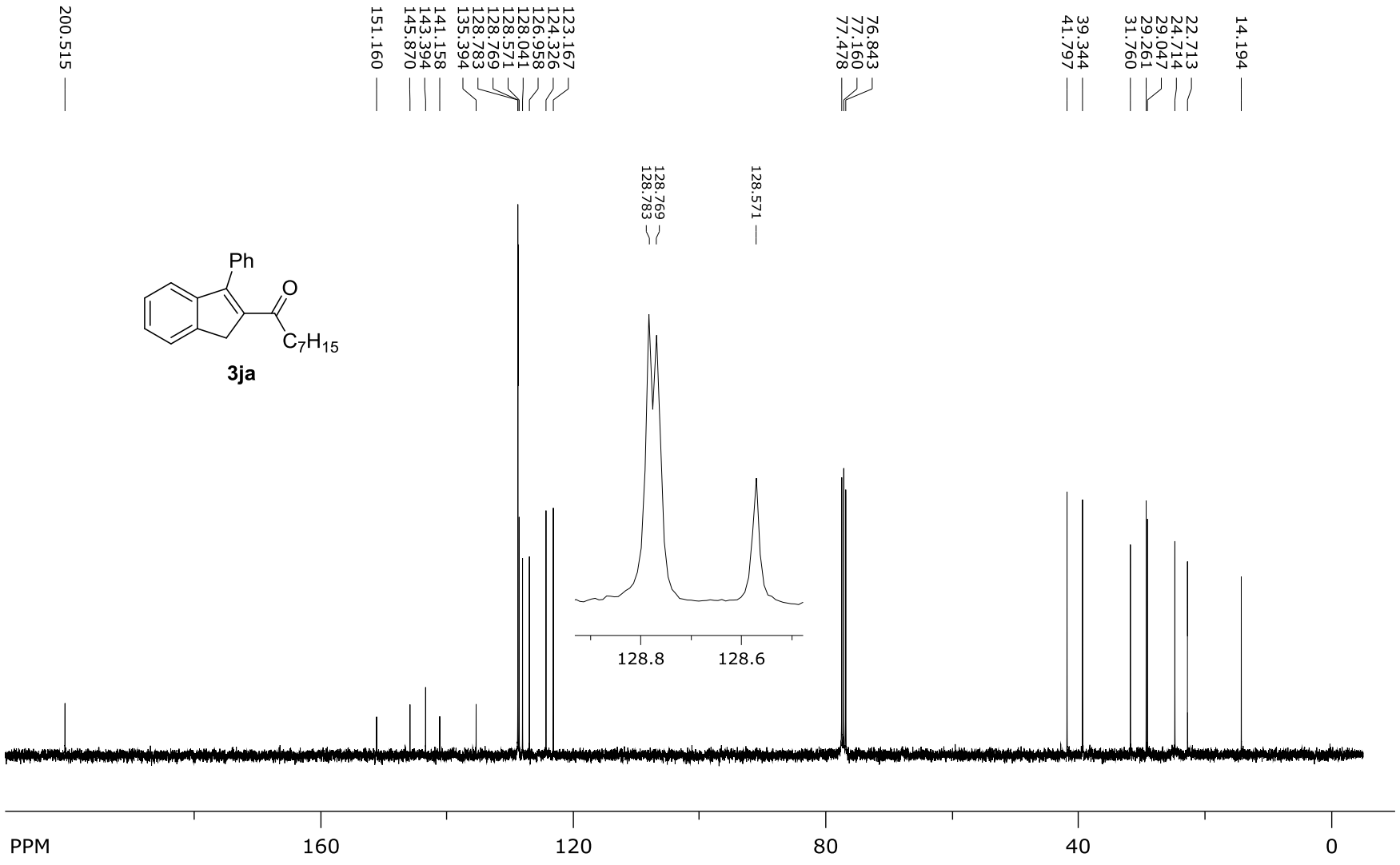
5.10. 1-(3-Phenyl-1*H*-inden-2-yl)octan-1-one (3ja)

^{1}H NMR (400 MHz)



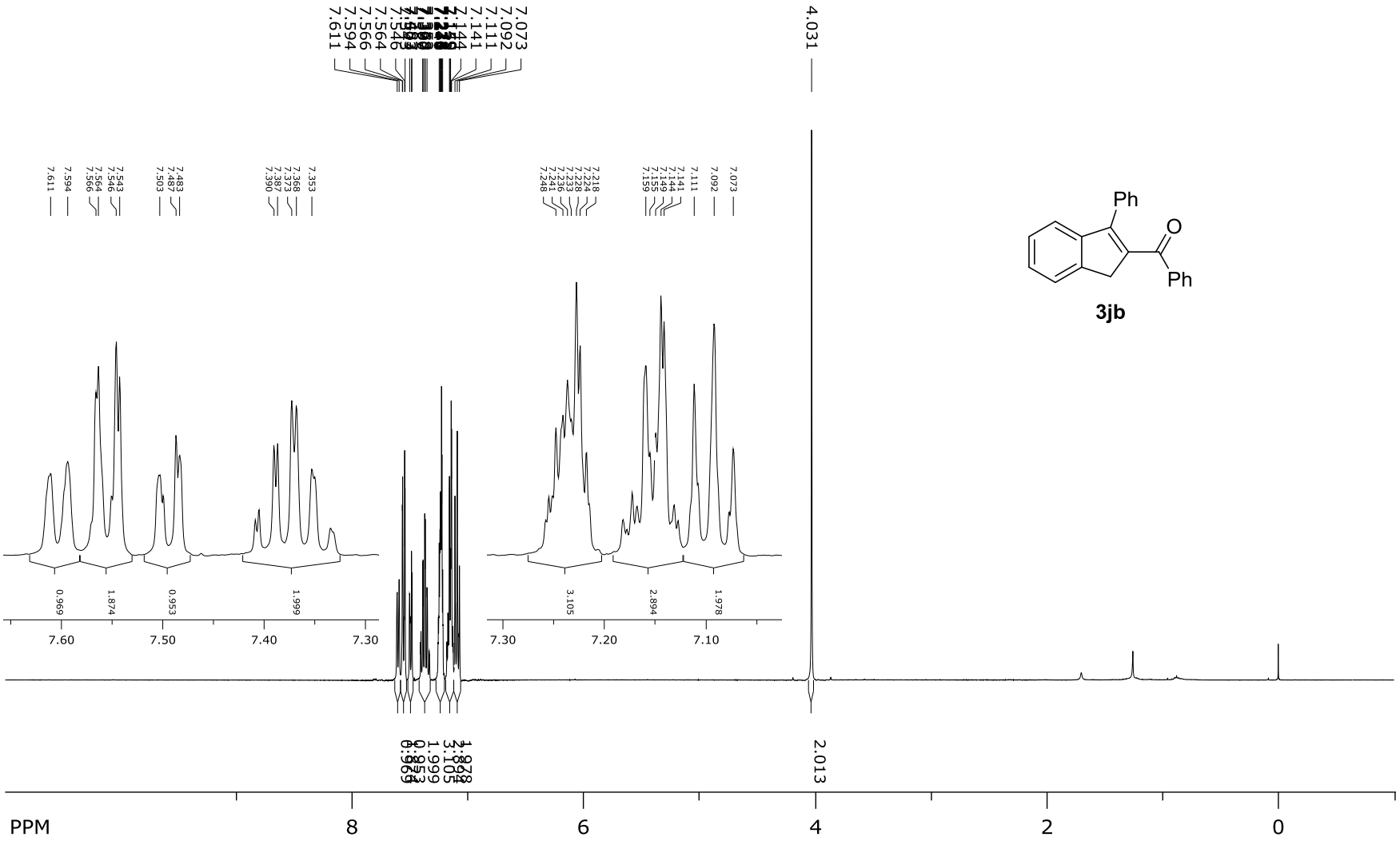
1-(3-Phenyl-1*H*-inden-2-yl)octan-1-one (3ja)

^{13}C NMR (100 MHz)



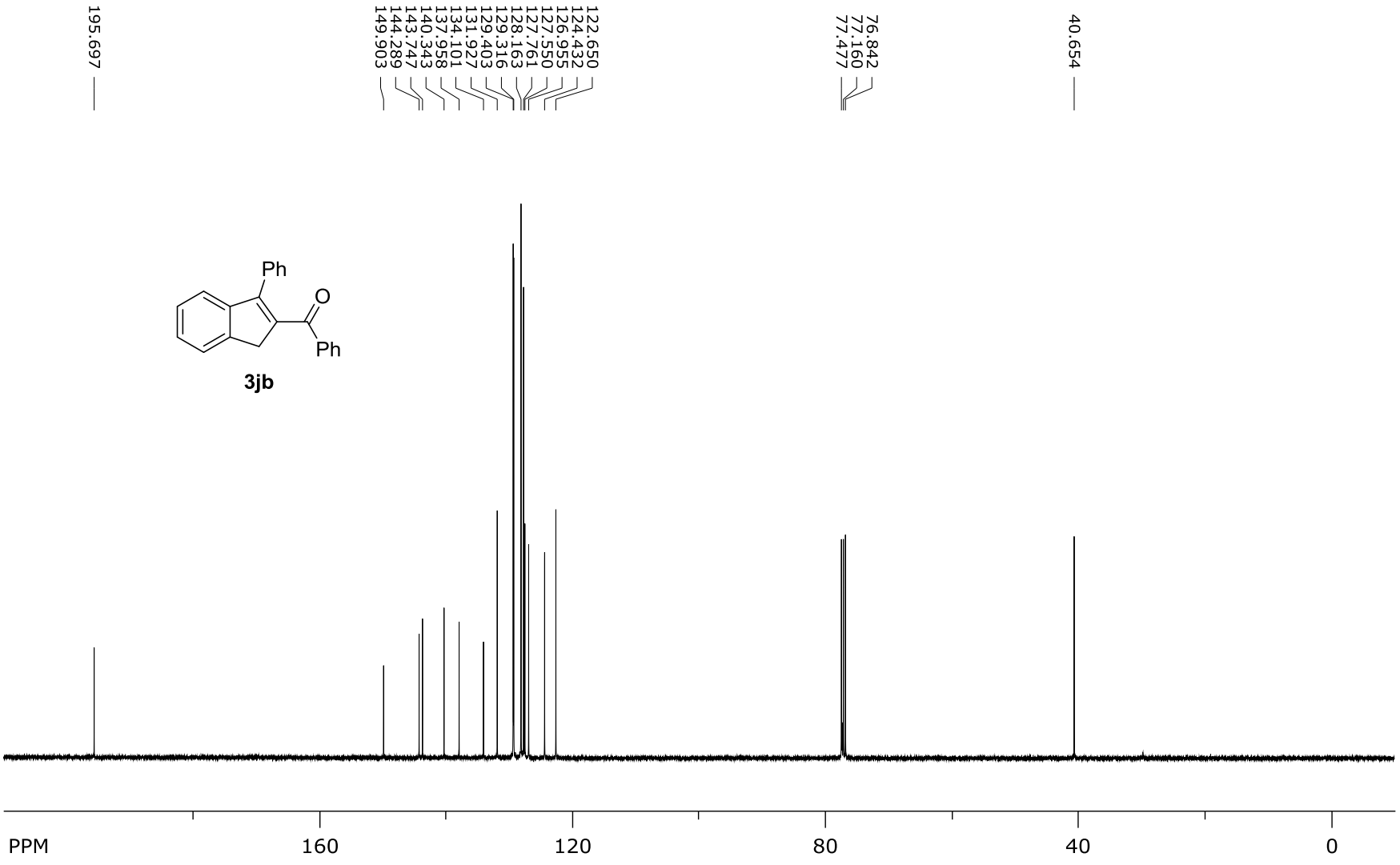
5.11. Phenyl(3-phenyl-1*H*-inden-2-yl)methanone (3jb)

^{1}H NMR (400 MHz)



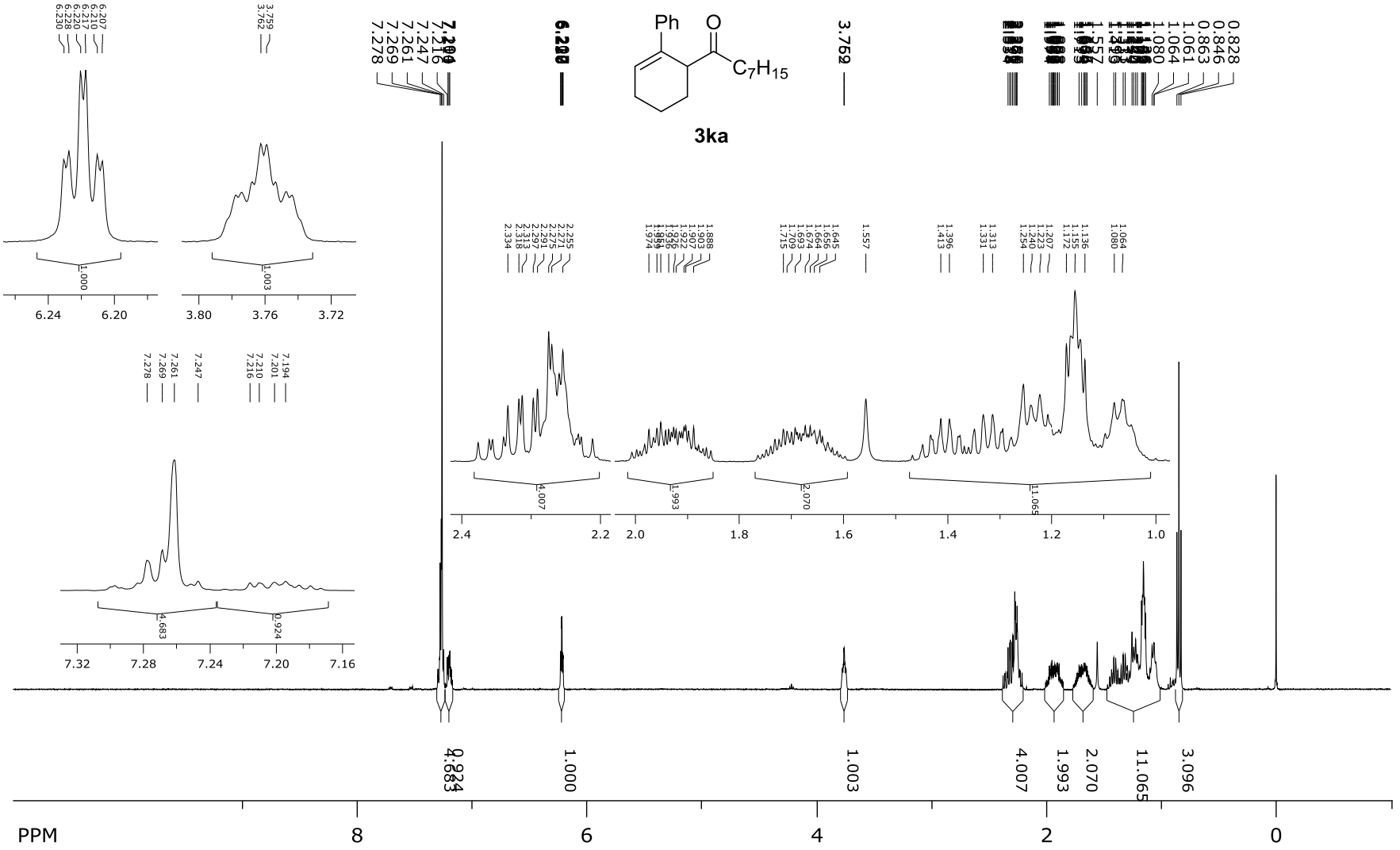
Phenyl(3-phenyl-1*H*-inden-2-yl)methanone (3jb)

^{13}C NMR (100 MHz)



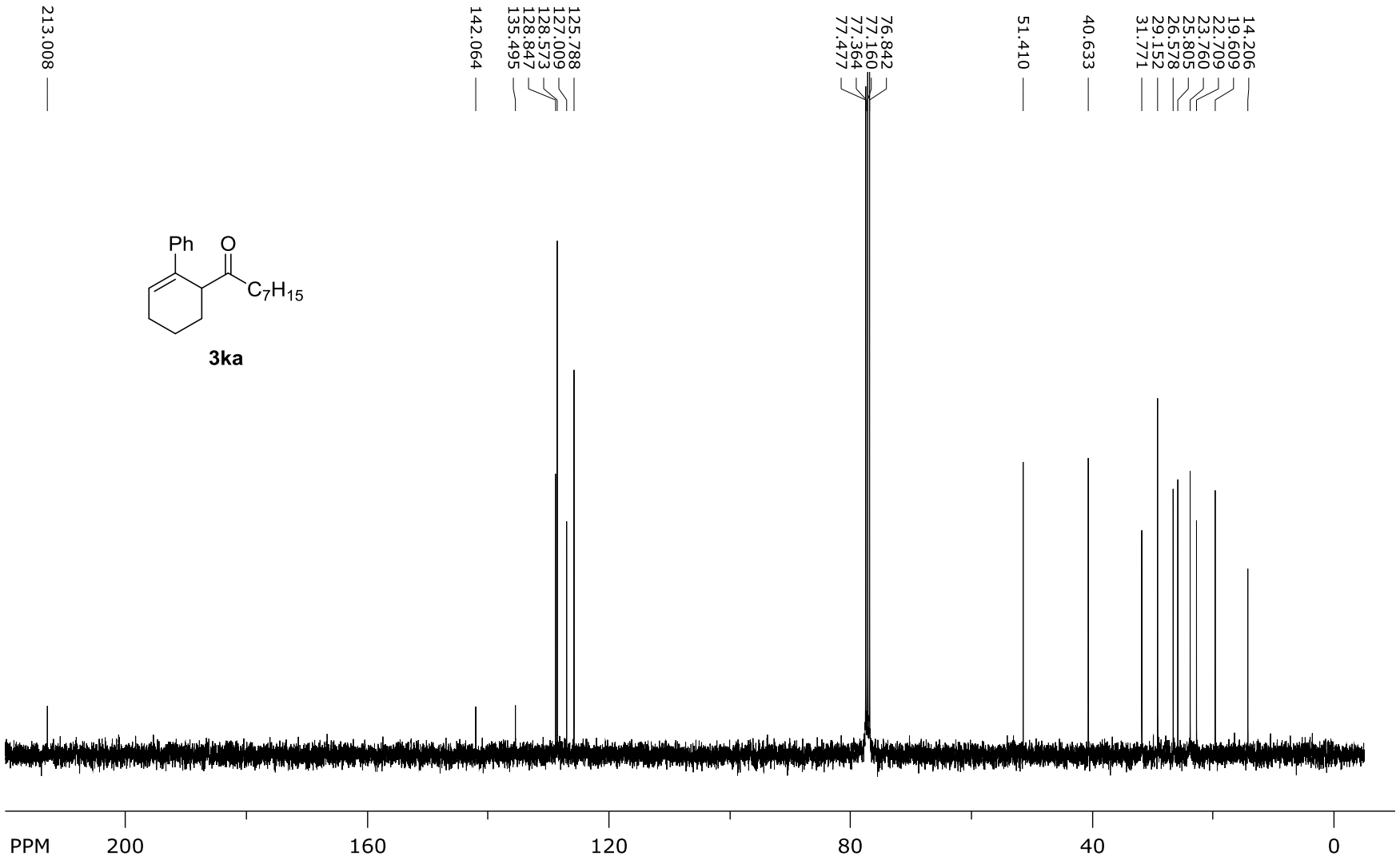
5.12. 1-(2-Phenyl-2-cyclohexen-1-yl)octan-1-one (3ka)

^{1}H NMR (400 MHz)



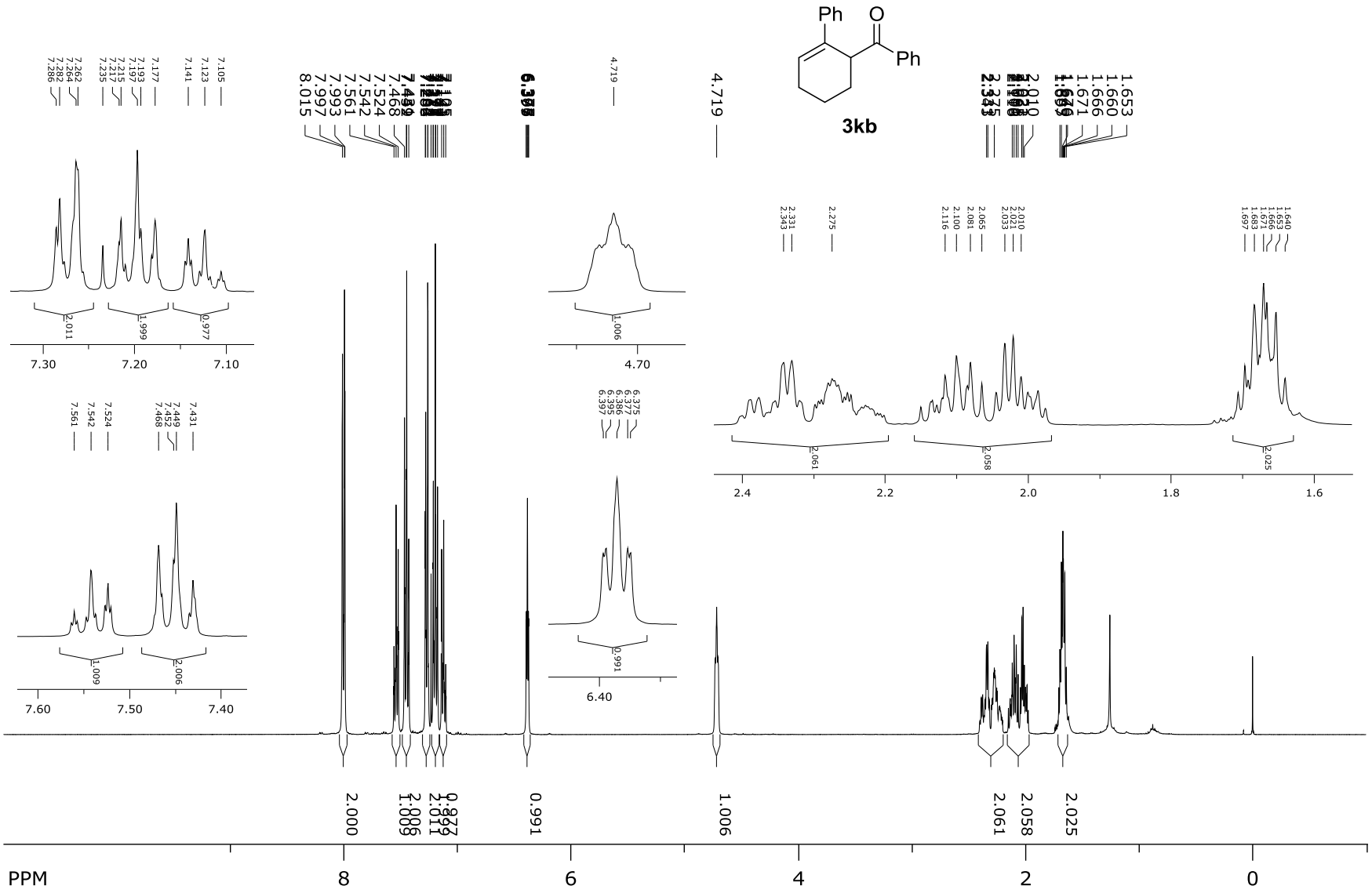
1-(2-Phenyl-2-cyclohexen-1-yl)octan-1-one (3ka)

^{13}C NMR (100 MHz)



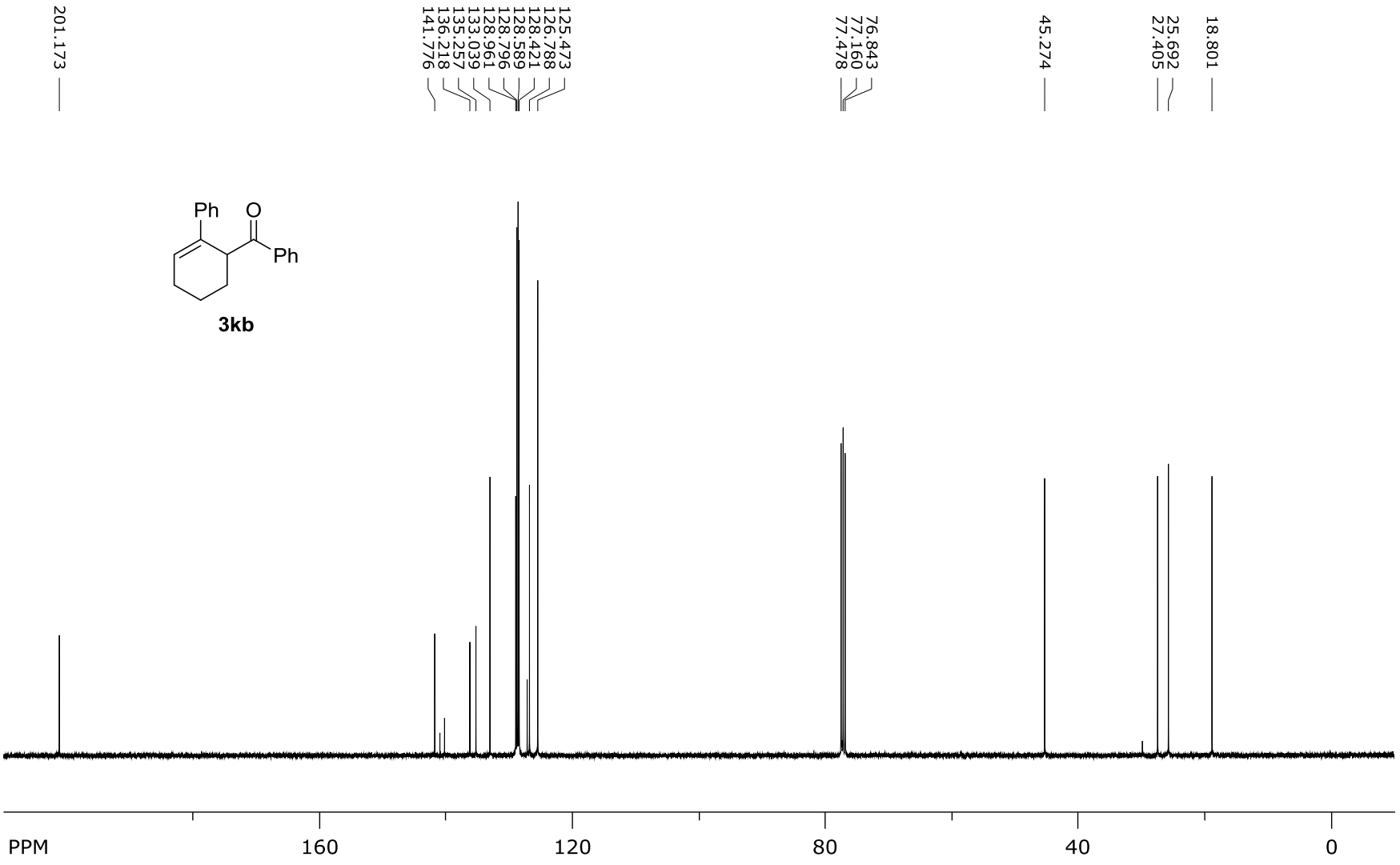
5.13. (2-Pheylcyclohex-2-en-1-yl)(phenyl)methanone (3kb)

^{1}H NMR (400 MHz)



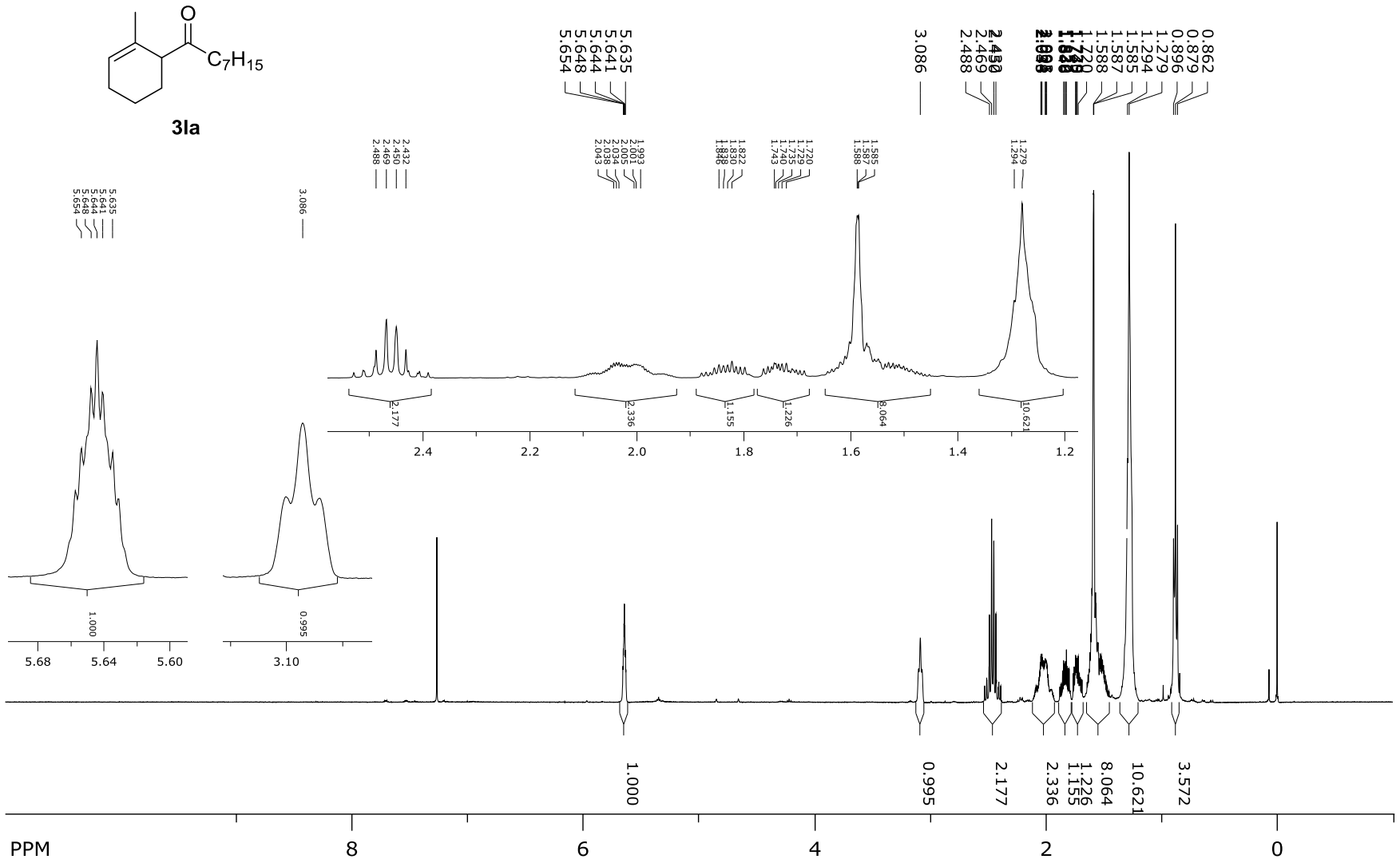
(2-Pheylcyclohex-2-en-1-yl)(phenyl)methanone (3kb)

^{13}C NMR (100 MHz)



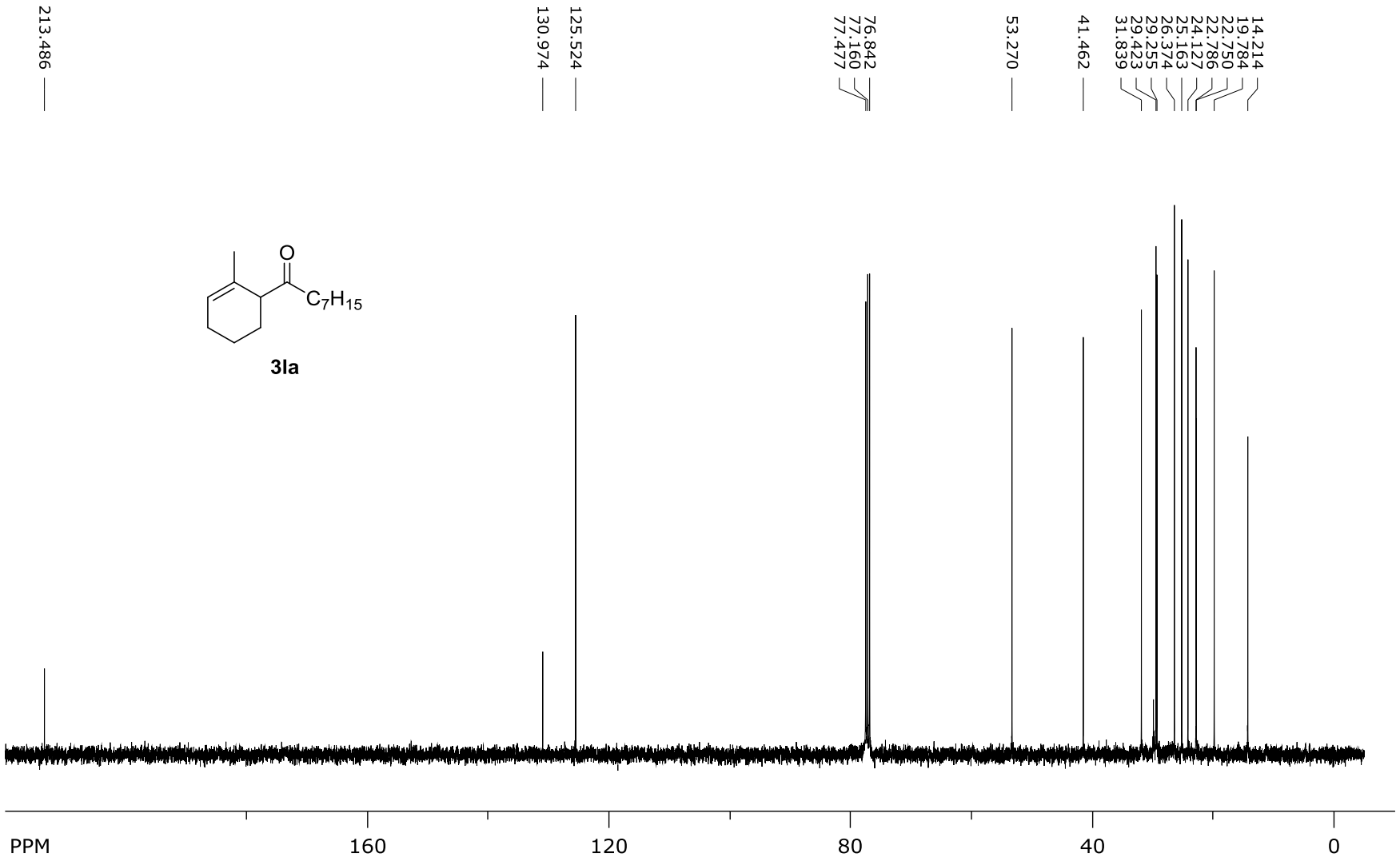
5.14. 1-(2-Methyl-2-cyclohexen-1-yl)octan-1-one (3la)

^{1}H NMR (400 MHz)



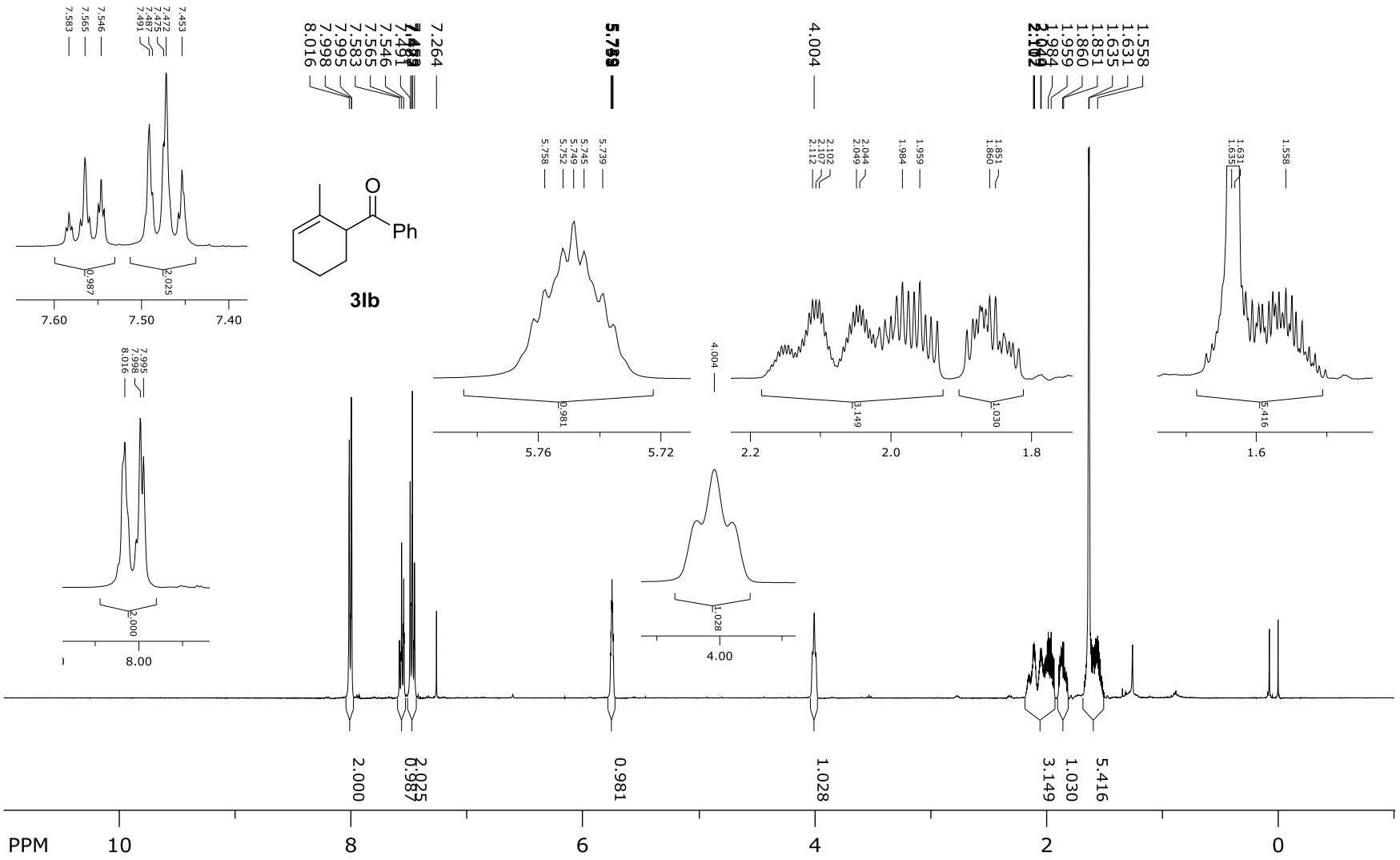
1-(2-Methyl-2-cyclohexen-1-yl)octan-1-one (3la)

^{13}C NMR (100 MHz)



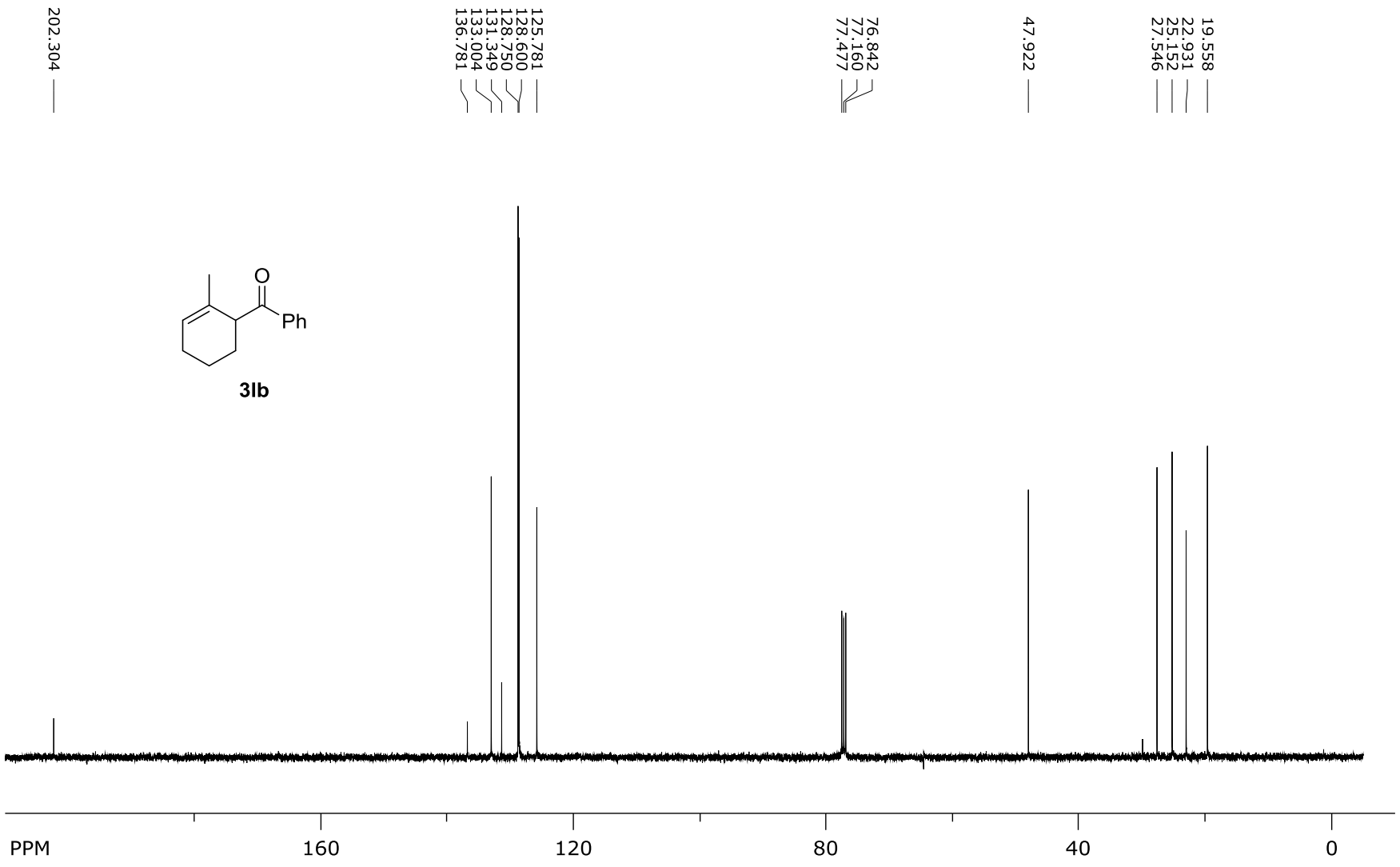
5.15. (2-Methylcyclohex-2-en-1-yl)(phenyl)methanone (3lb)

^{1}H NMR (400 MHz)



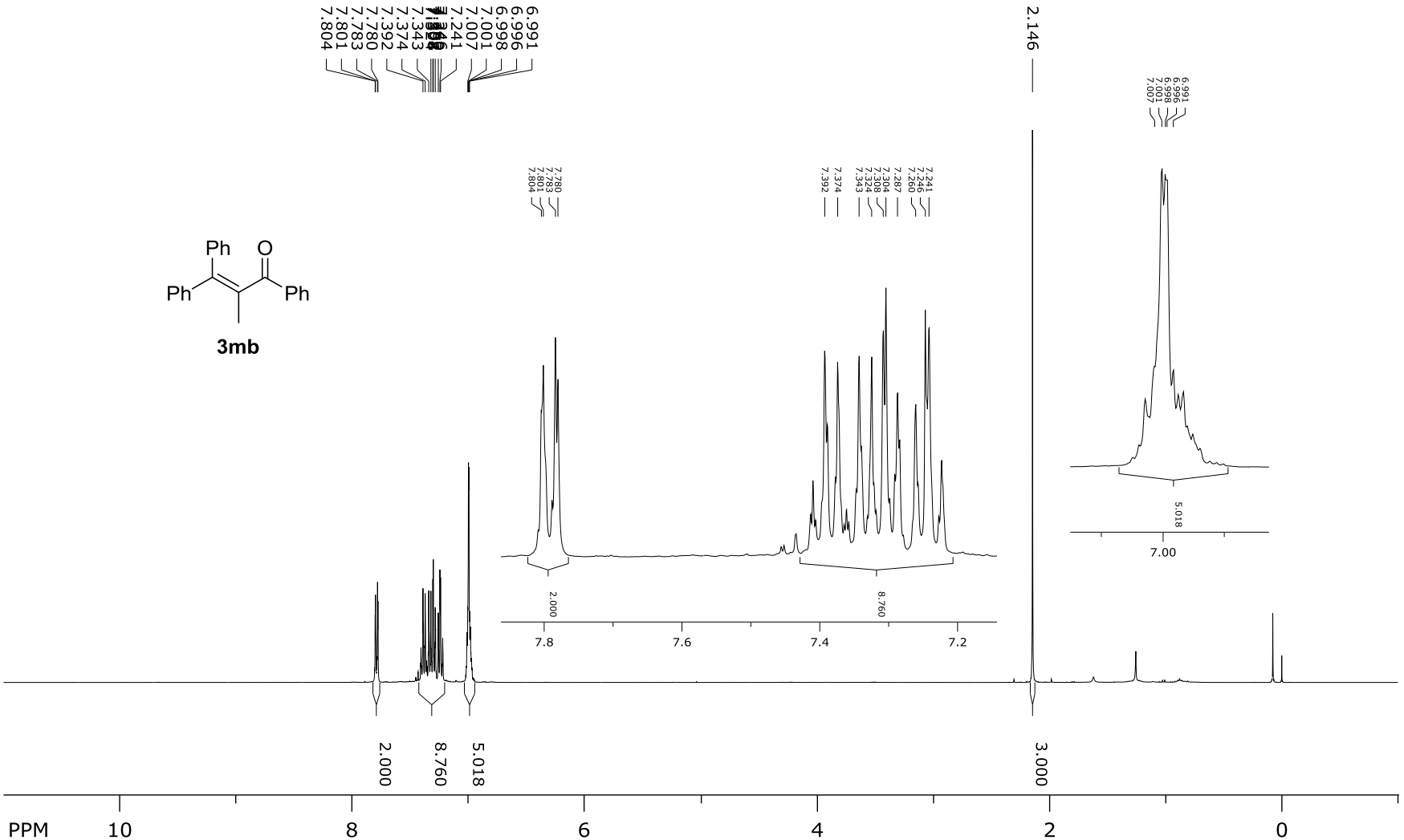
(2-Methylcyclohex-2-en-1-yl)(phenyl)methanone (3lb)

^{13}C NMR (100 MHz)



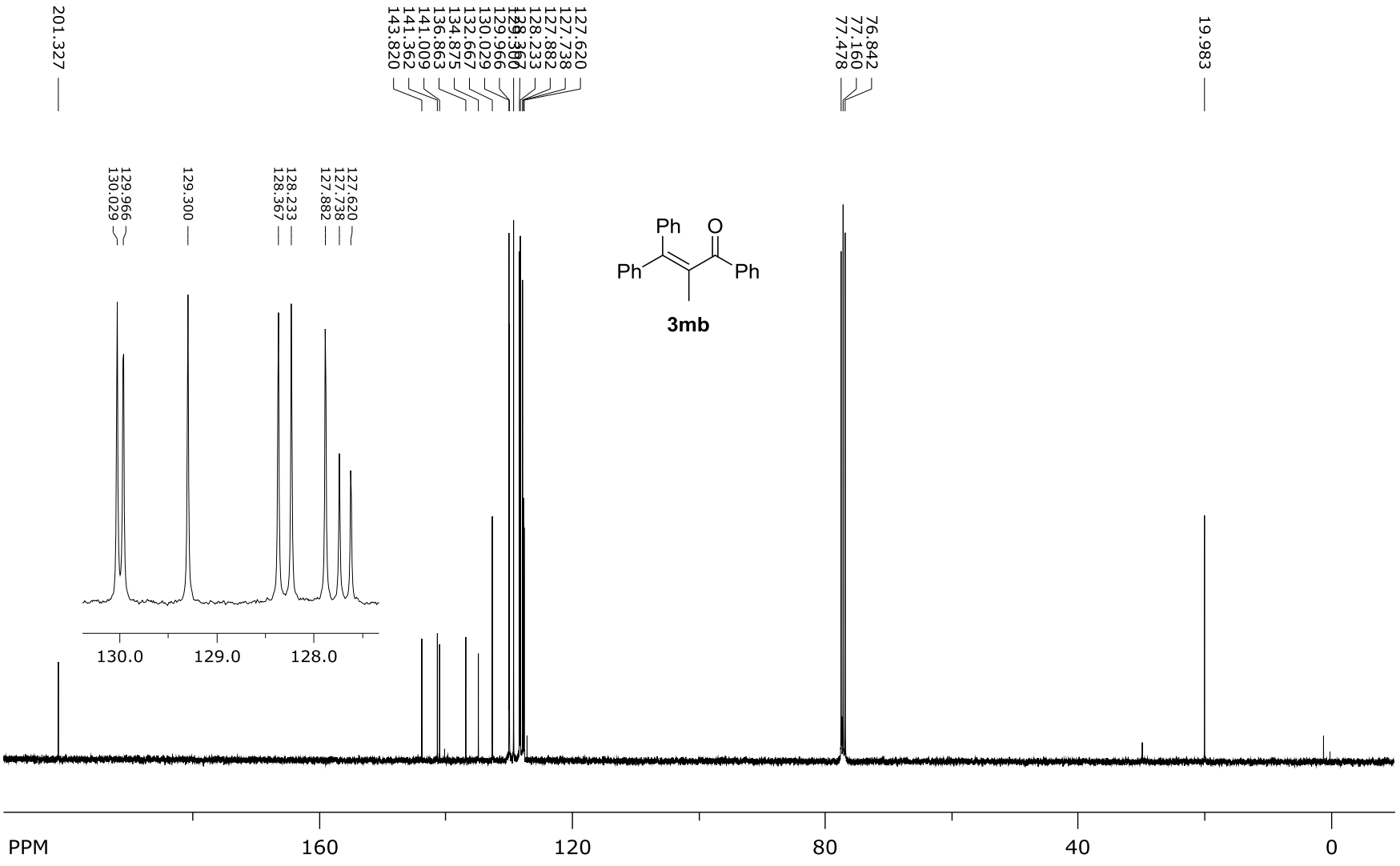
5.16. 2-Mehtyl-1,3,3-triphenylprop-2-en-1-one (3mb)

^{1}H NMR (400 MHz)



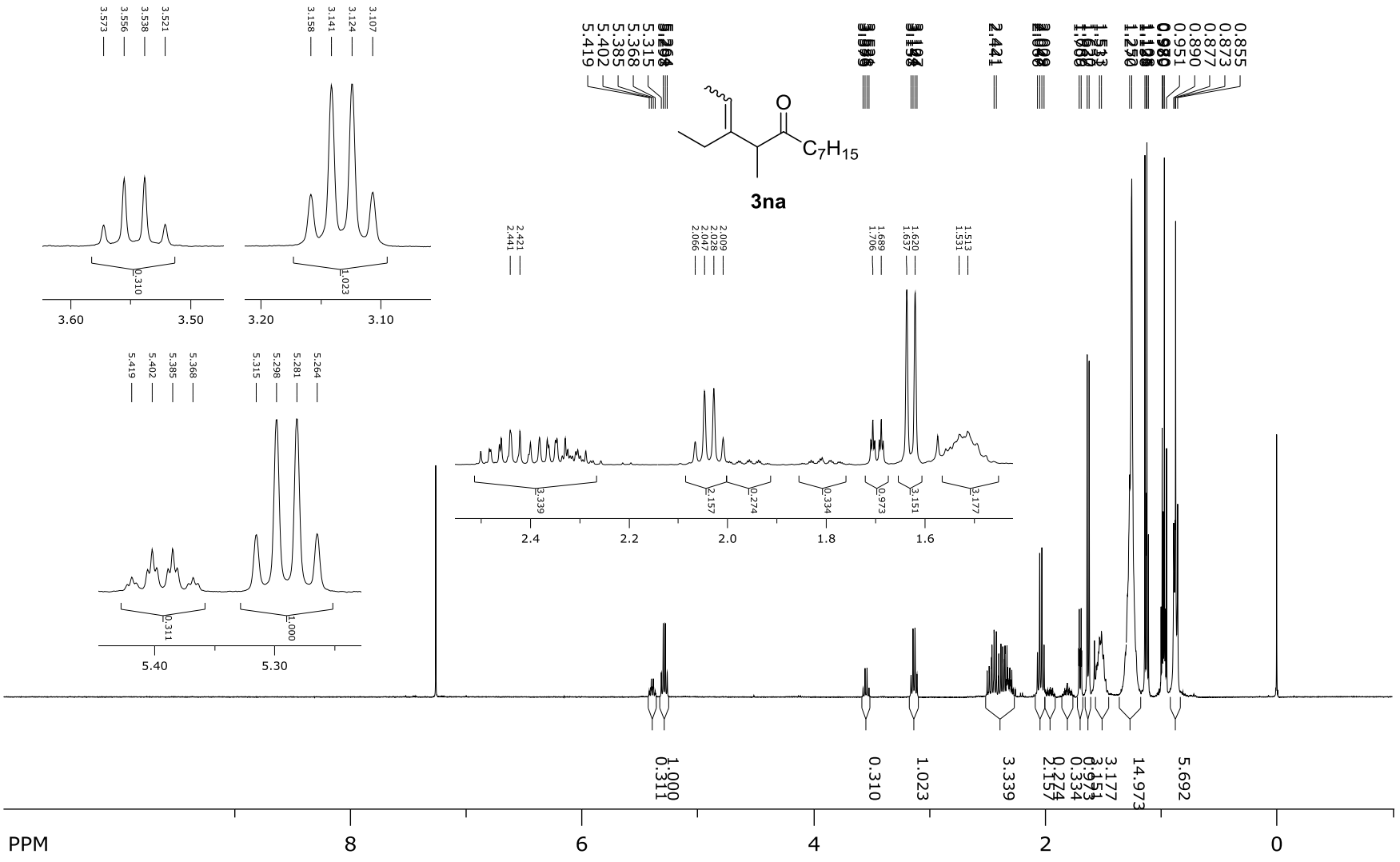
2-Mehtyl-1,3,3-triphenylprop-2-en-1-one (3mb)

^{13}C NMR (100 MHz)



5.17. 3-Ethyl-4-methyldodec-2-en-5-one (3na)

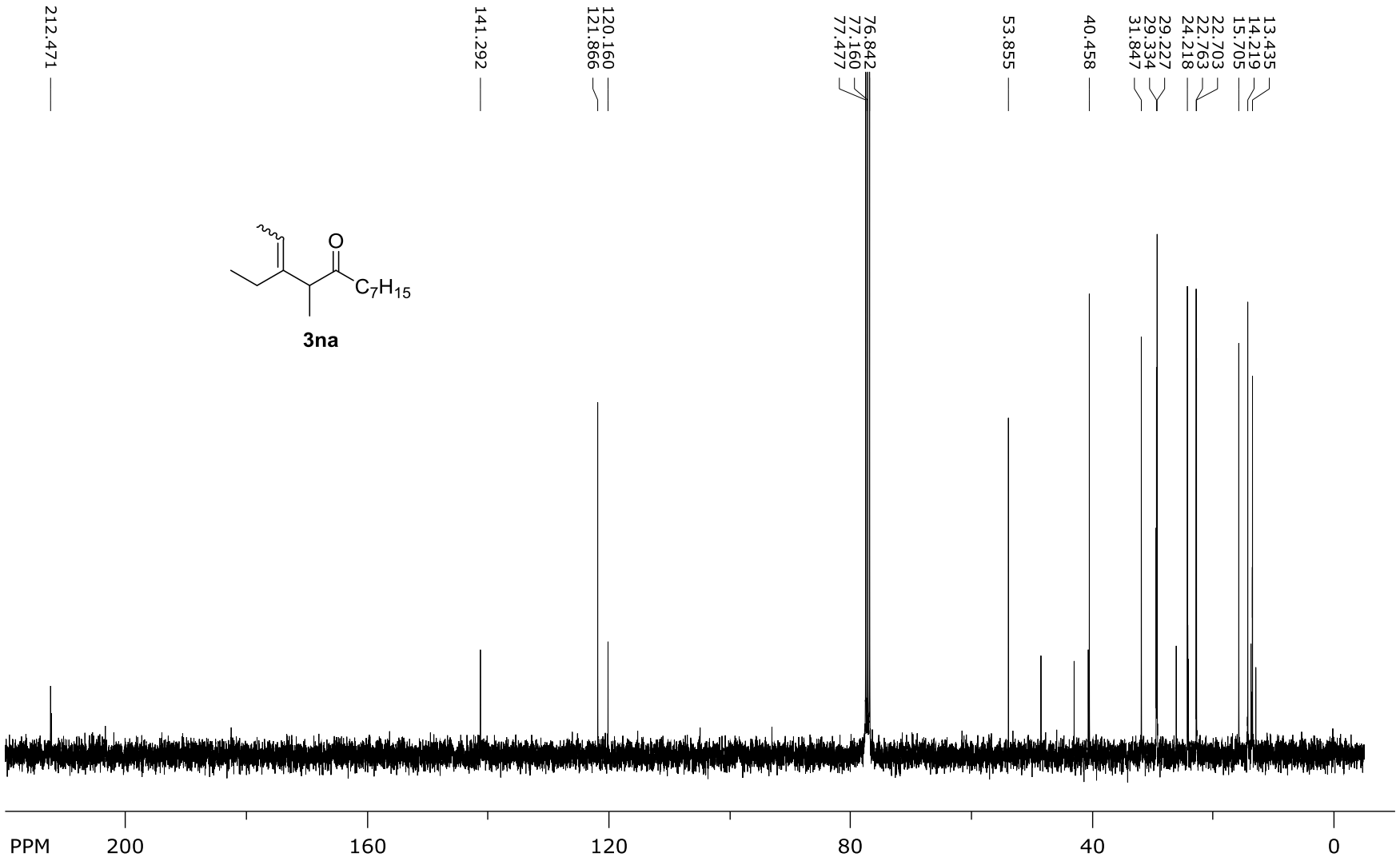
^{1}H NMR (400 MHz)



3-Ethyl-4-methyldodec-2-en-5-one (3na)

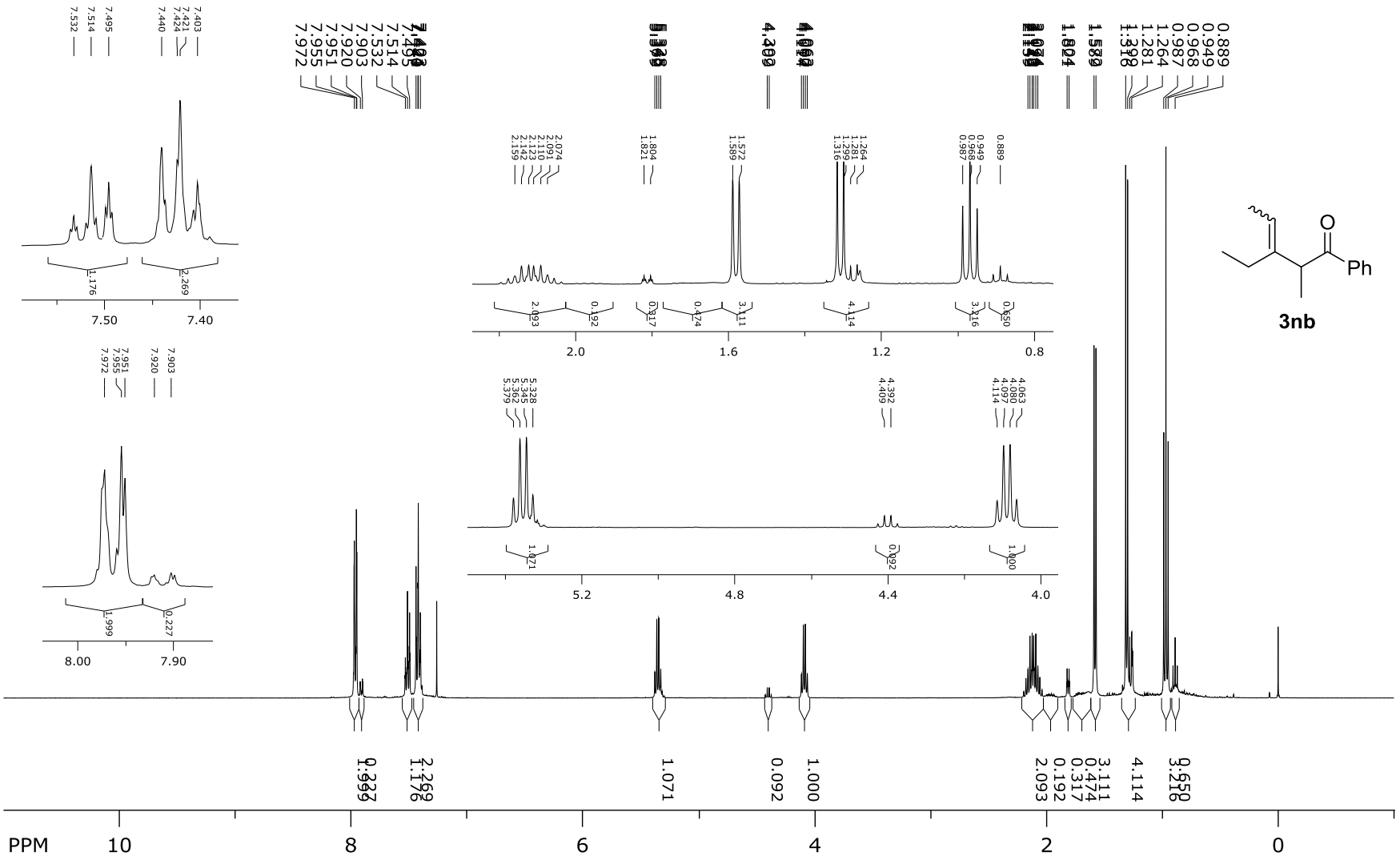
^{13}C NMR (100 MHz)

Only signals of the *E* isomer were picked up.



5.18. 3-Ethyl-2-methyl-1-phenylpent-3-en-1-one (3nb)

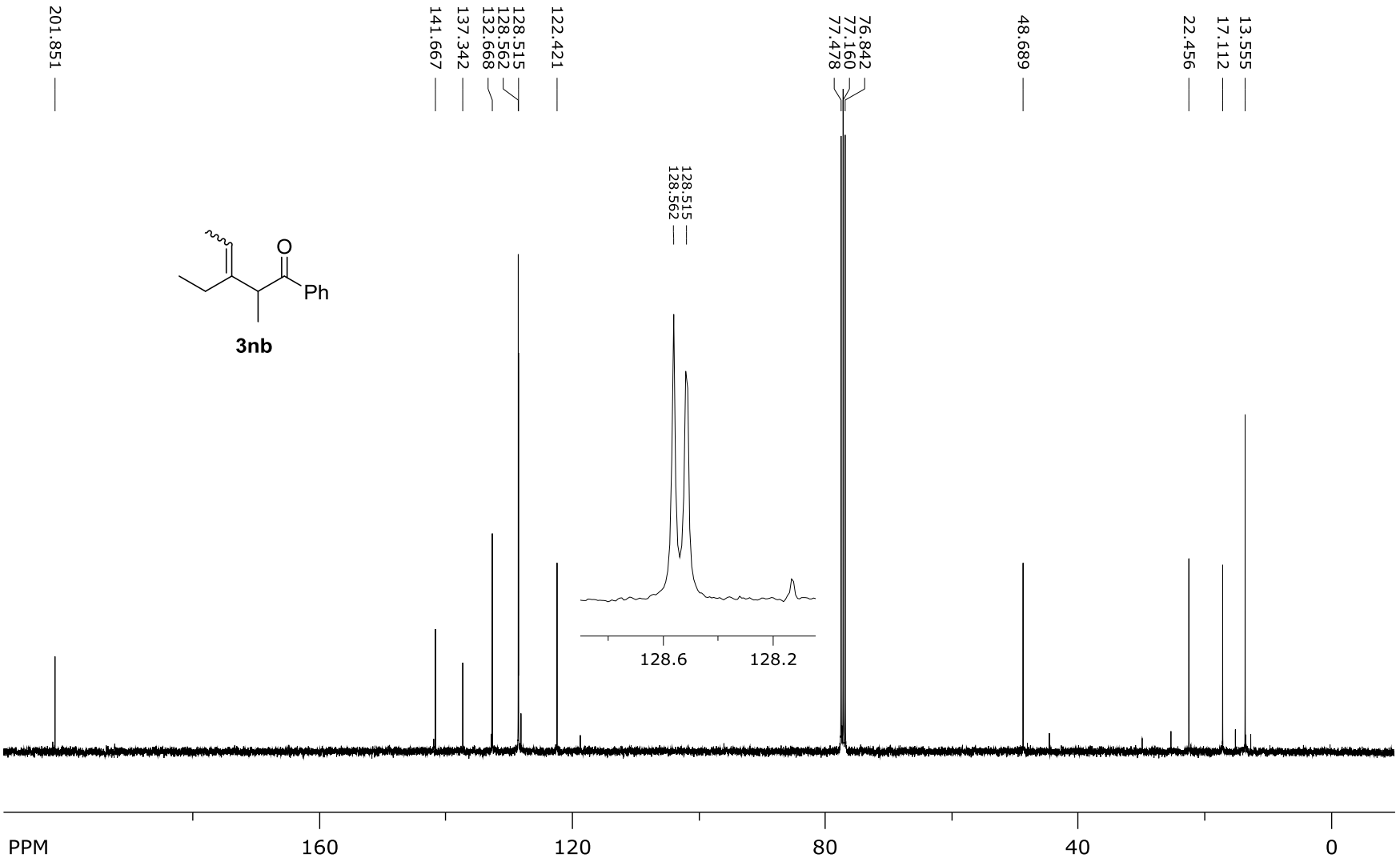
^{1}H NMR (400 MHz)



3-Ethyl-2-methyl-1-phenylpent-3-en-1-one (3nb)

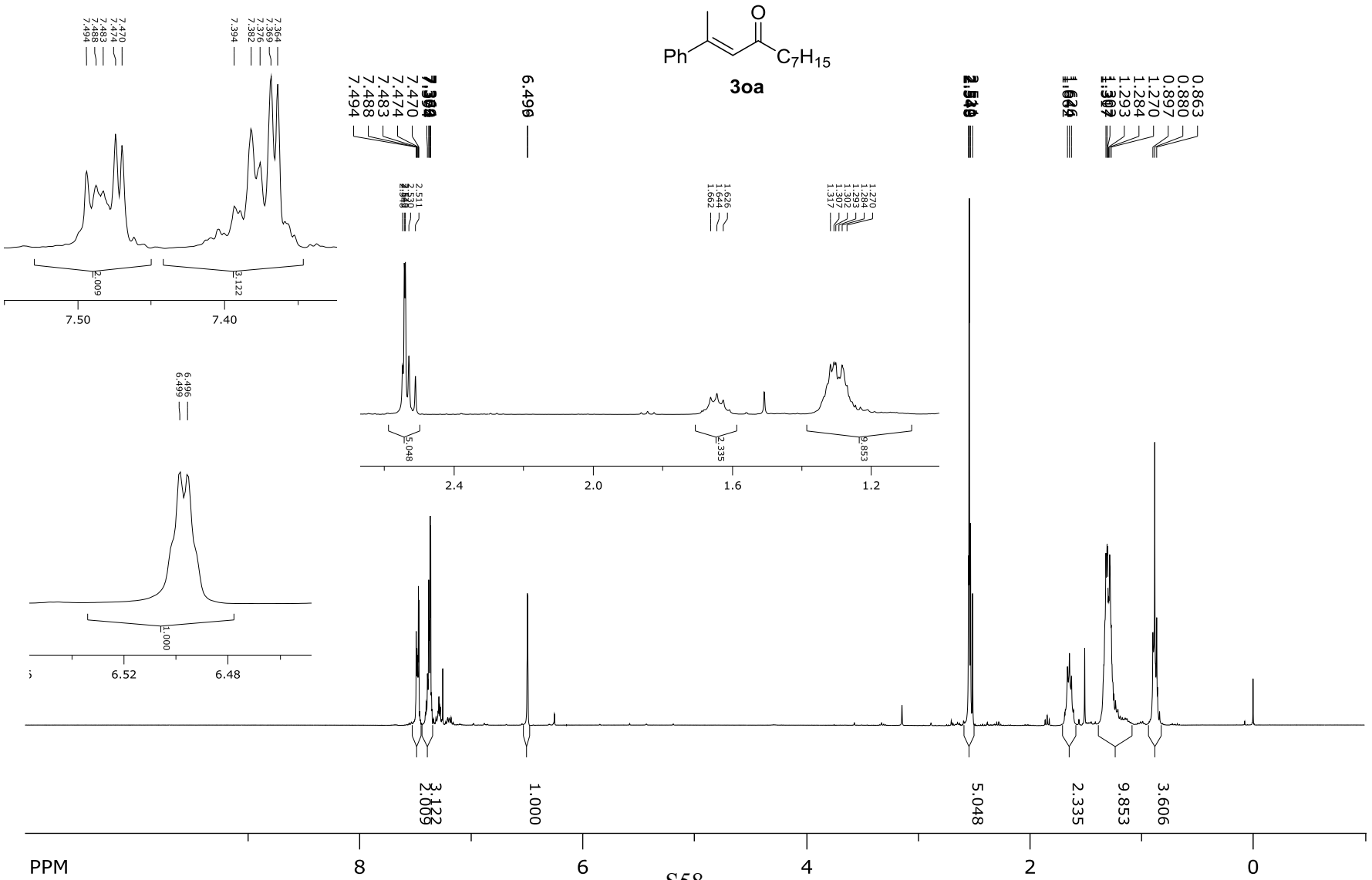
^{13}C NMR (100 MHz)

Only signals of the *E* isomer were picked up.



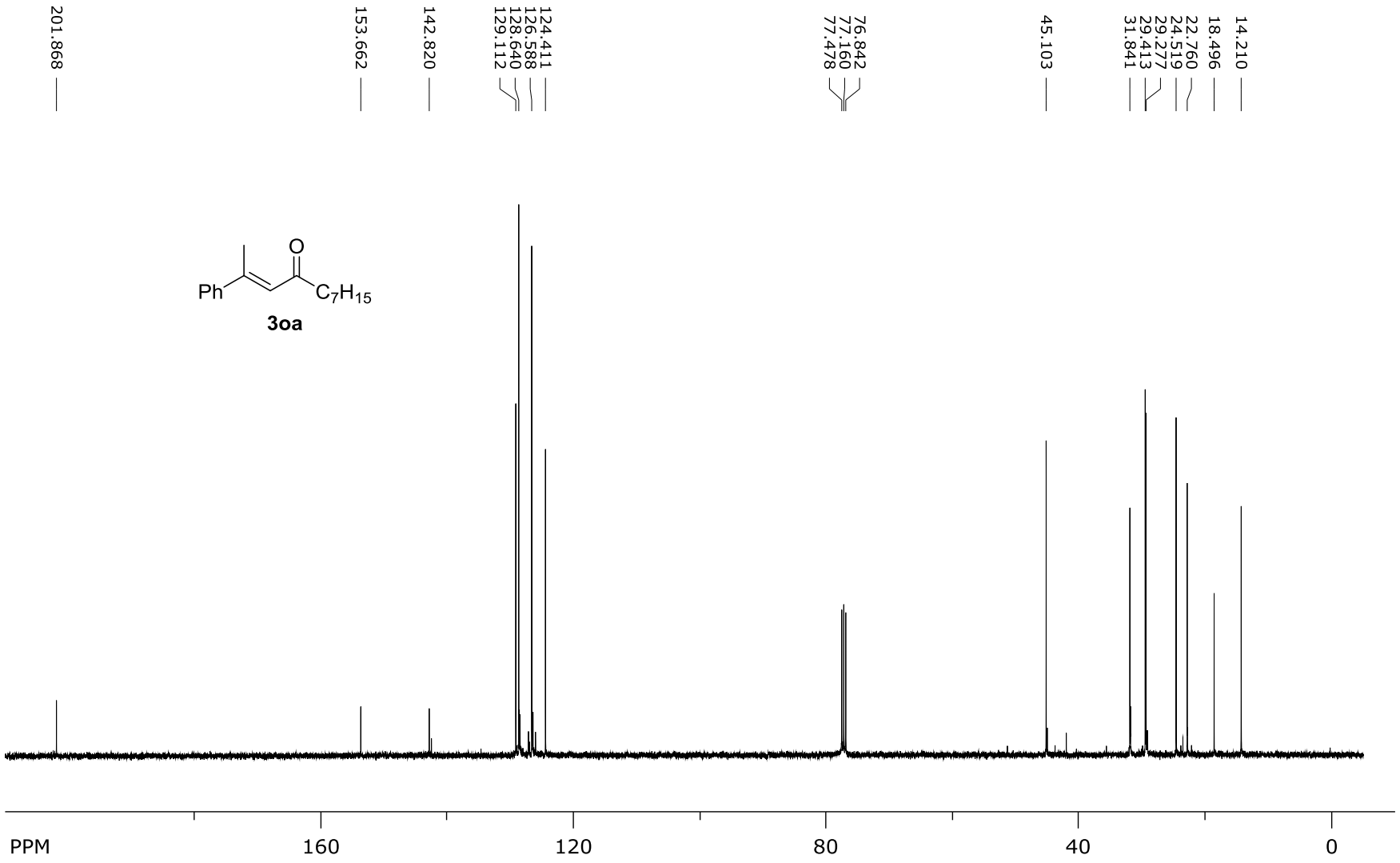
5.19. (*E*)-2-Phenylundec-2-en-4-one (3oa)

^{1}H NMR (400 MHz)



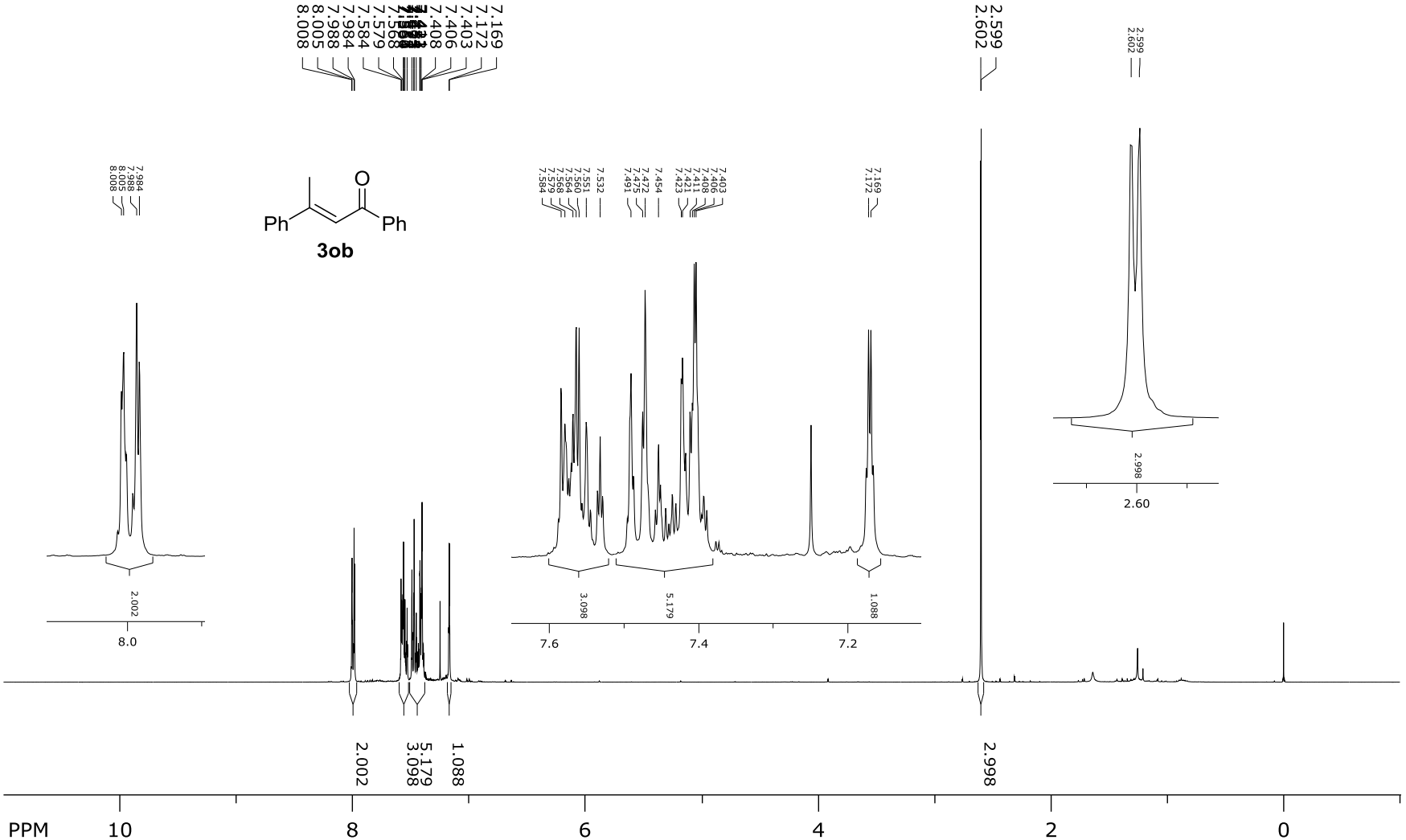
(*E*)-2-Phenylundec-2-en-4-one (3oa)

^{13}C NMR (100 MHz)



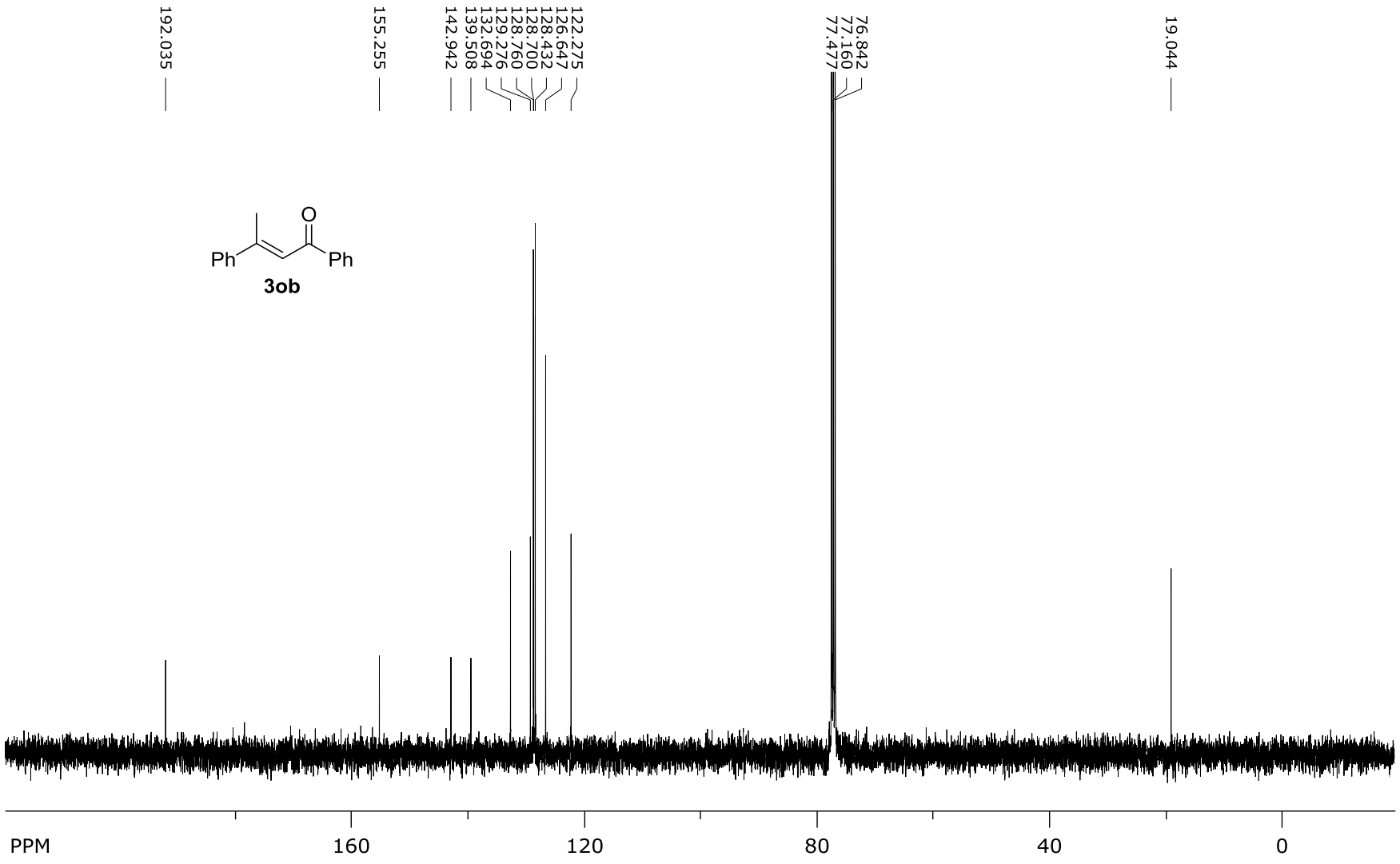
5.20. (*E*)-1,3-Diphenylbut-2-en-1-one (3ob)

^{1}H NMR (400 MHz)



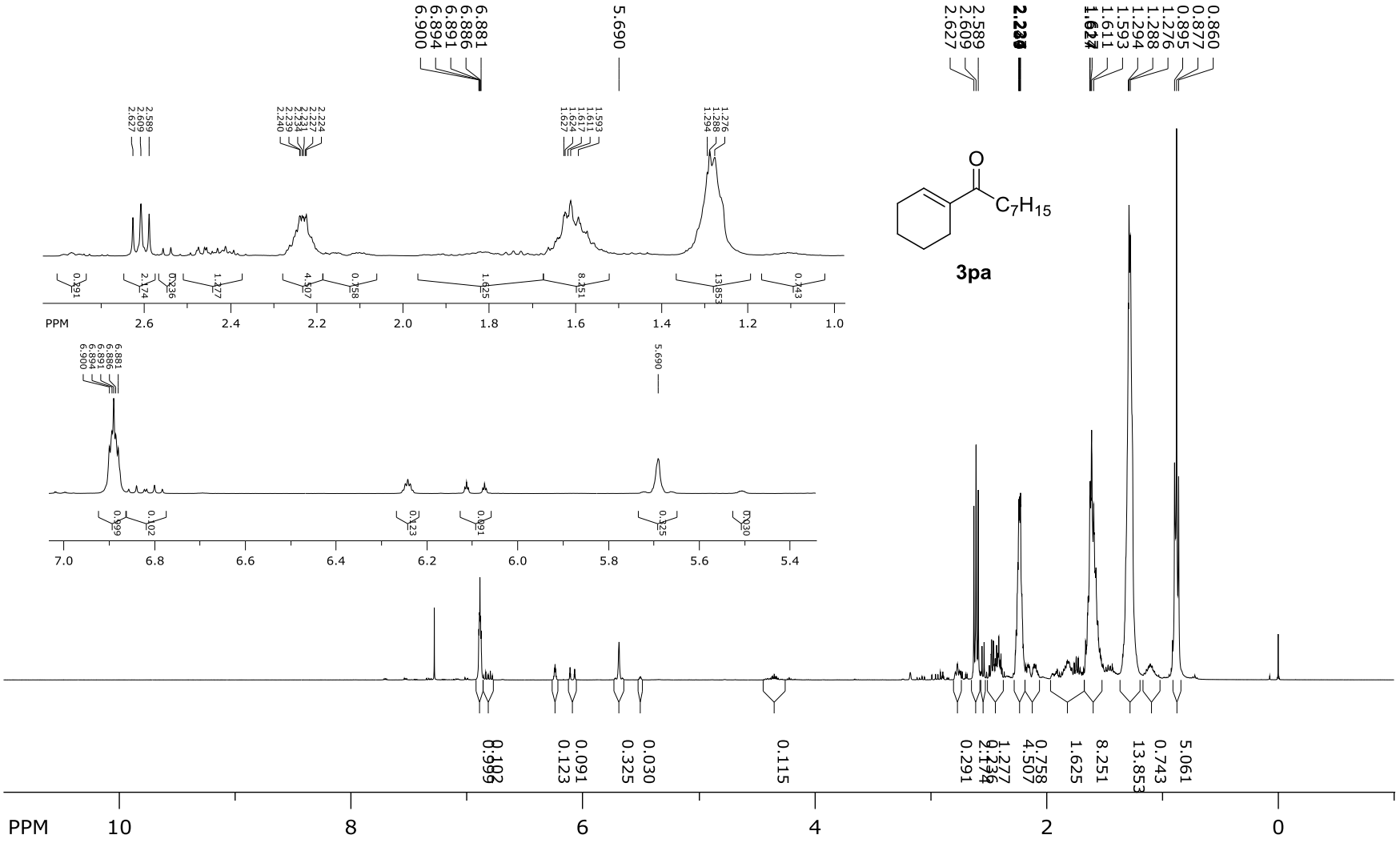
(*E*)-1,3-Diphenylbut-2-en-1-one (3ob)

^{13}C NMR (100 MHz)



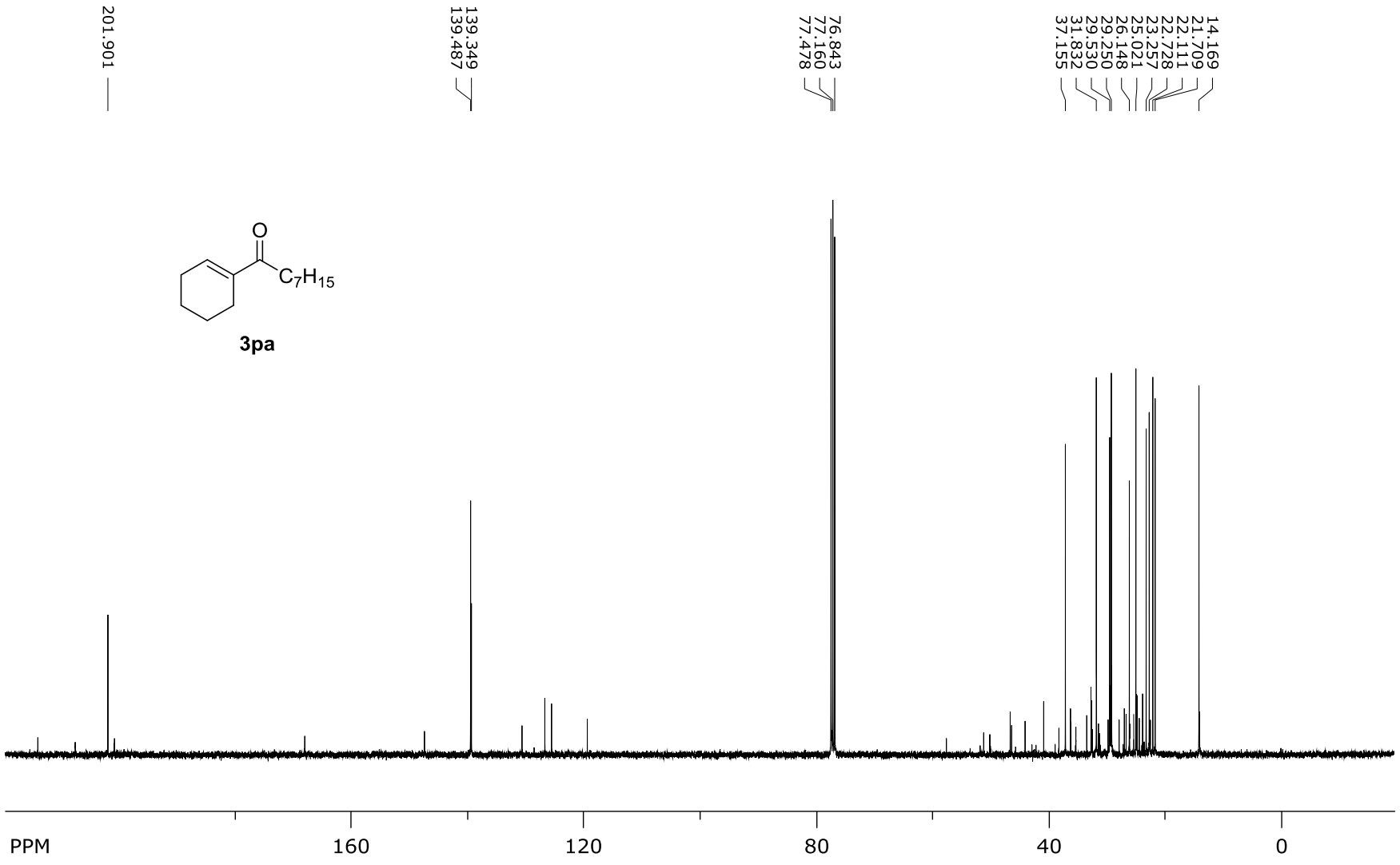
5.21. 1-(Cyclohex-1-en-1-yl)octan-1-one (3pa)

^{1}H NMR (400 MHz)



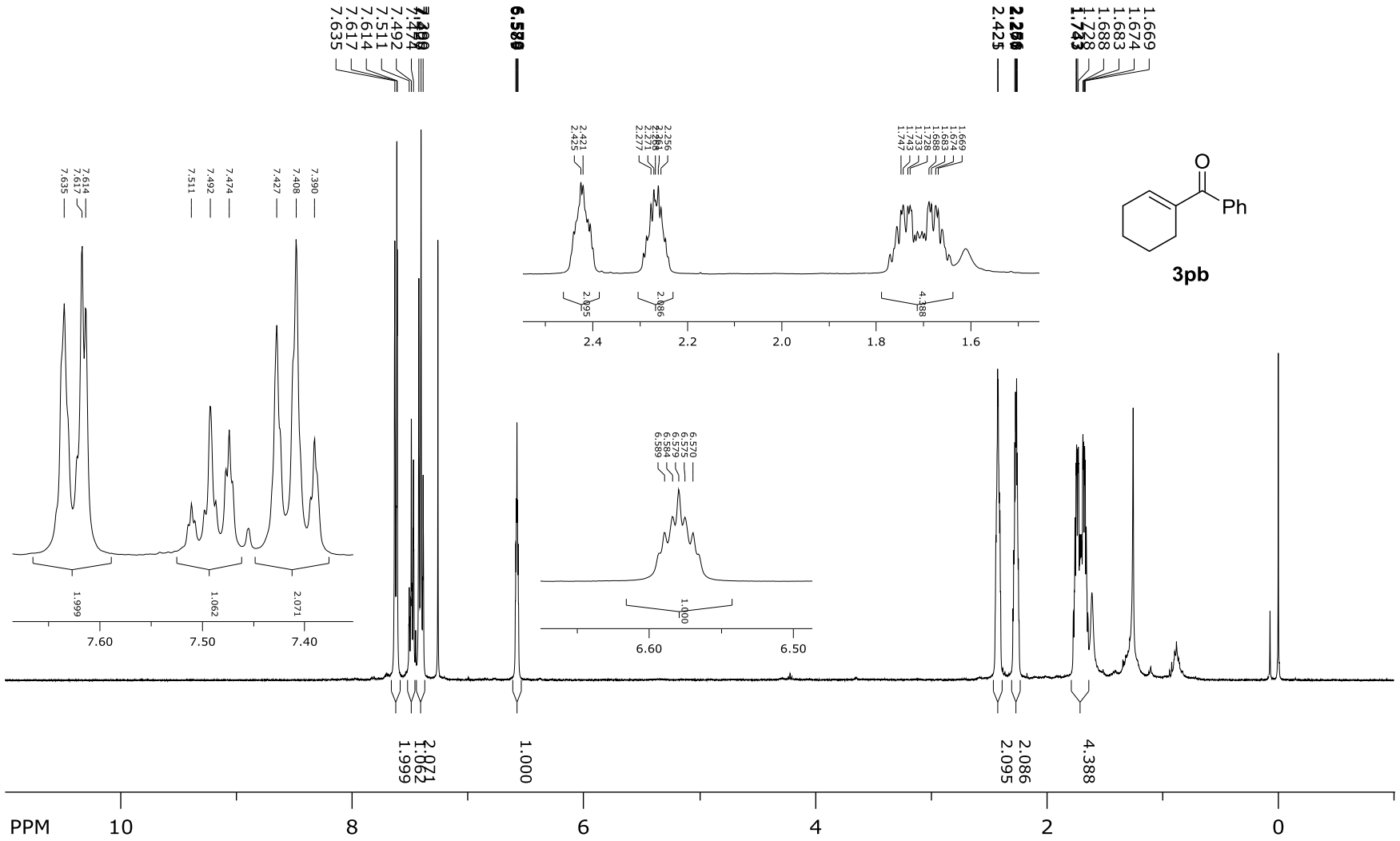
1-(Cyclohex-1-en-1-yl)octan-1-one (3pa)

^{13}C NMR (100 MHz)



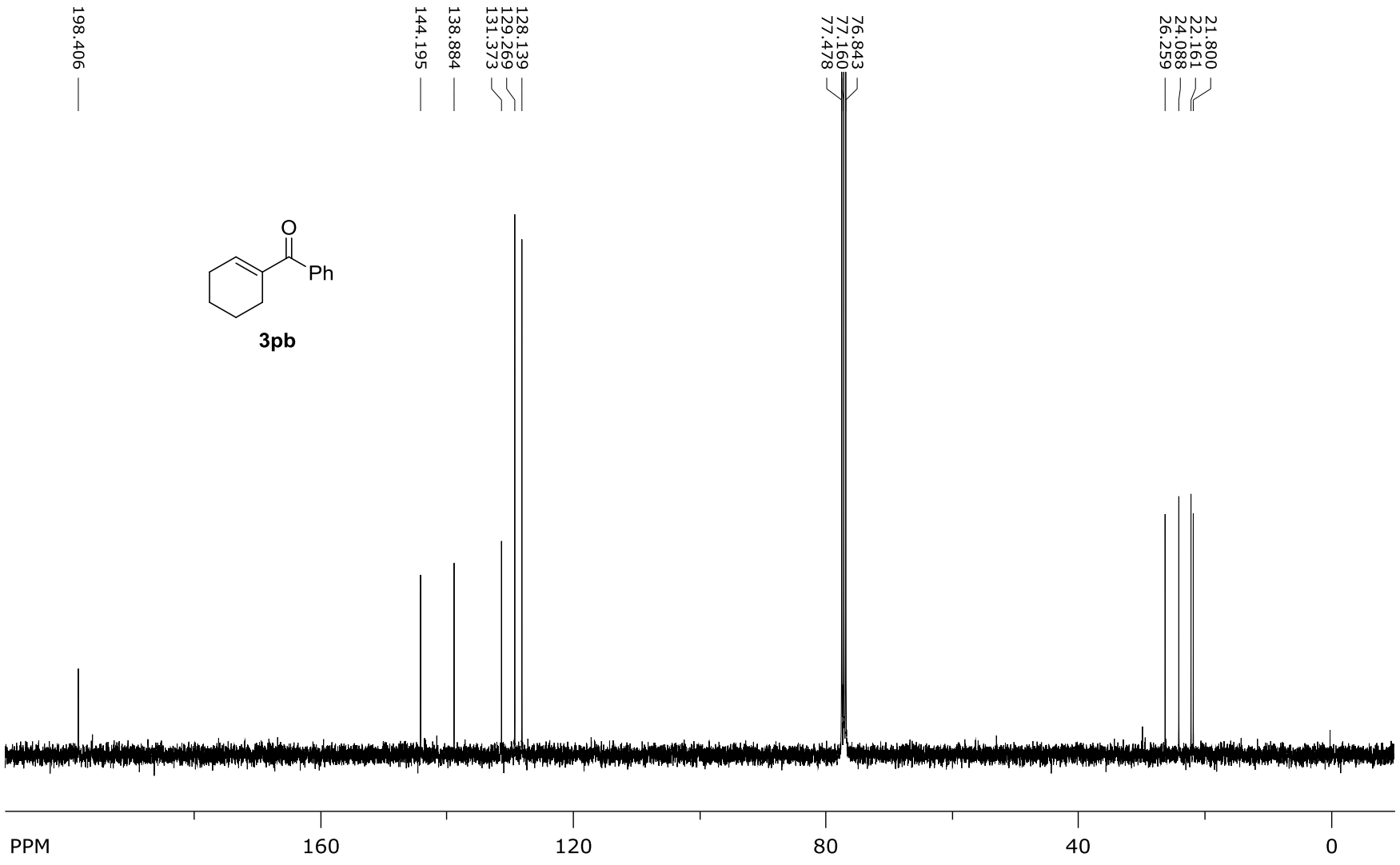
5.22. Cyclohex-1-en-1-yl(phenyl)methanone (3pb)

^{1}H NMR (400 MHz)



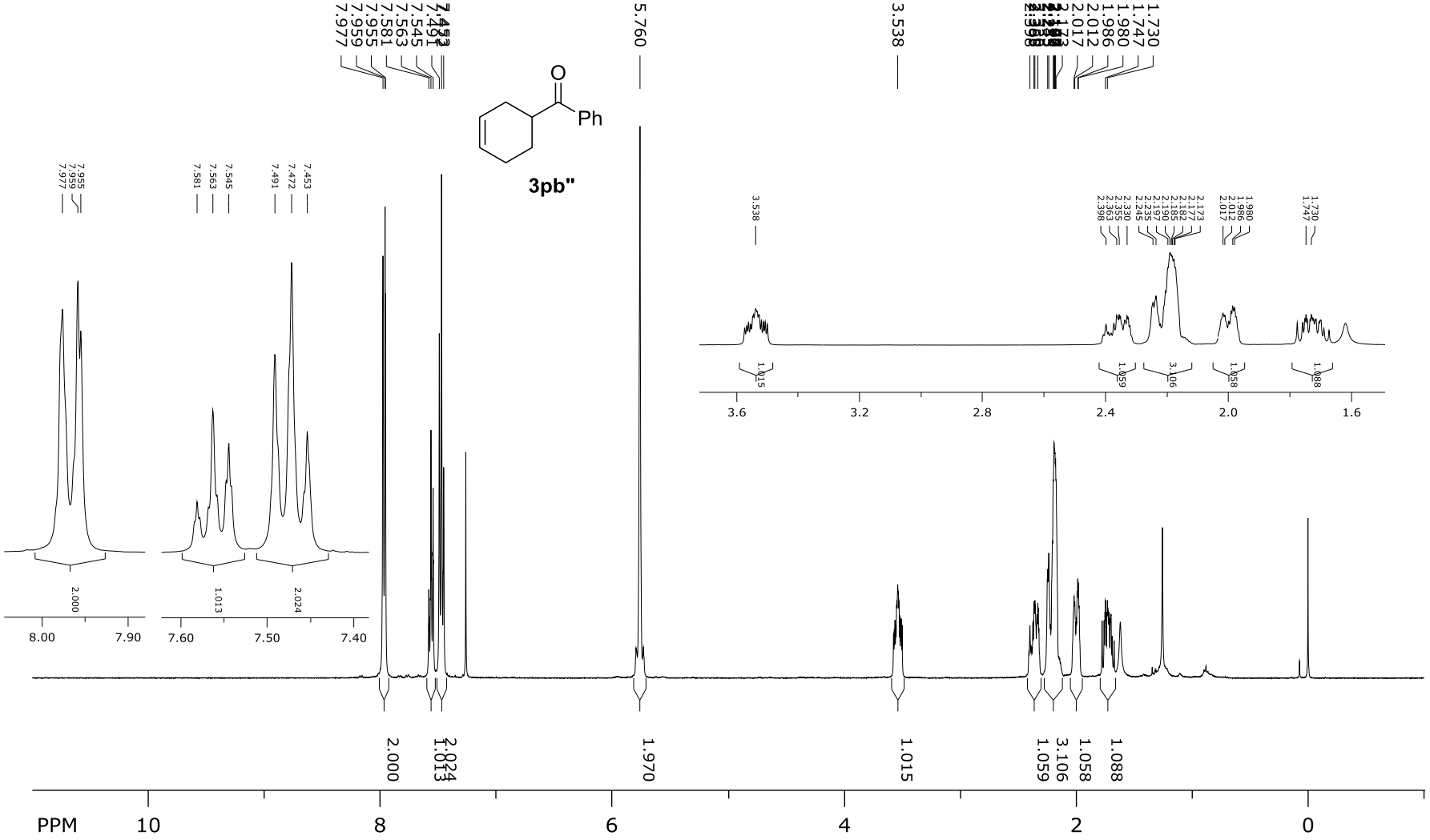
Cyclohex-1-en-1-yl(phenyl)methanone (3pb)

^{13}C NMR (100 MHz)



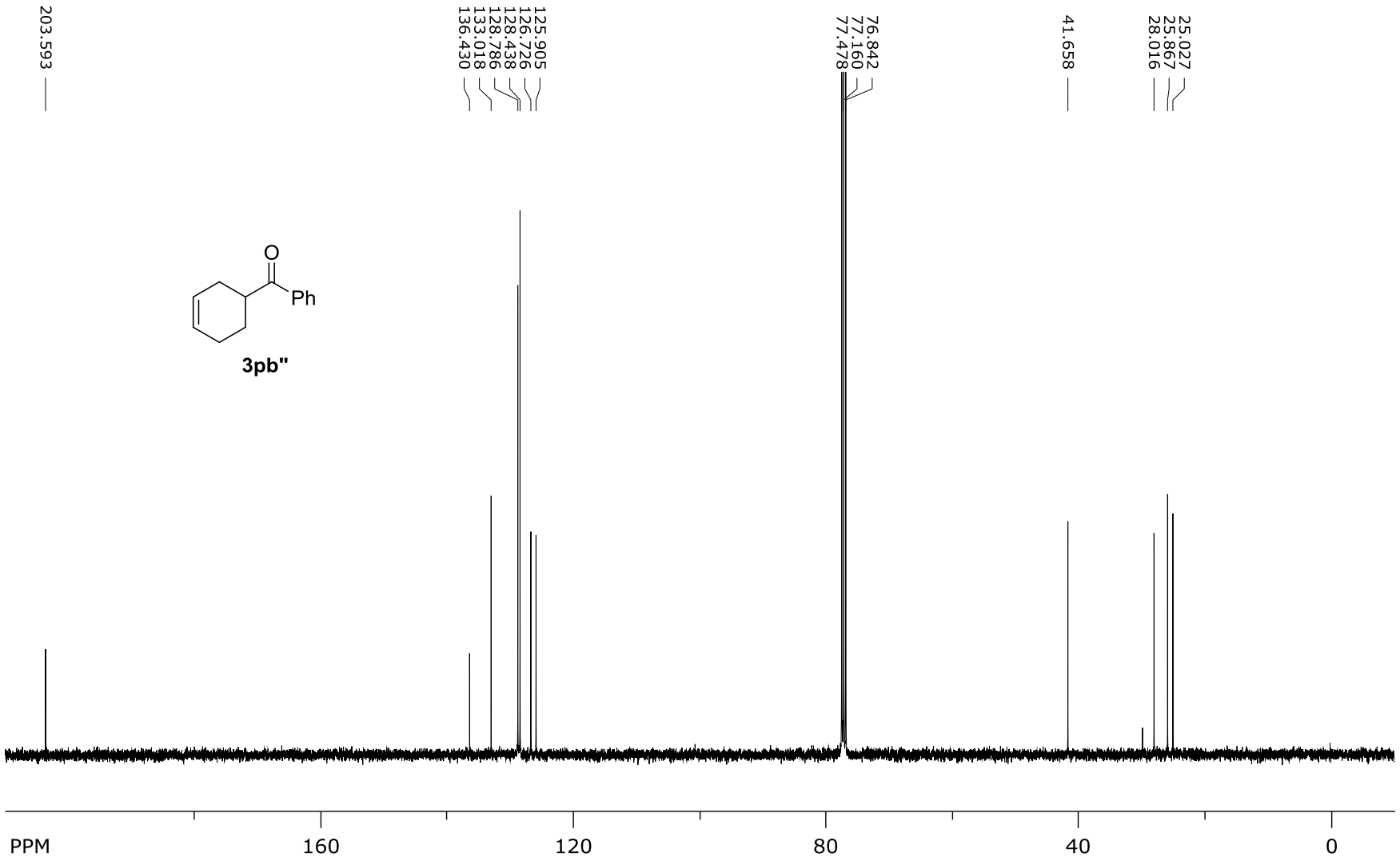
5.23. Cyclohex-3-en-1-yl(phenyl)methanone (3pb″)

^{1}H NMR (400 MHz)



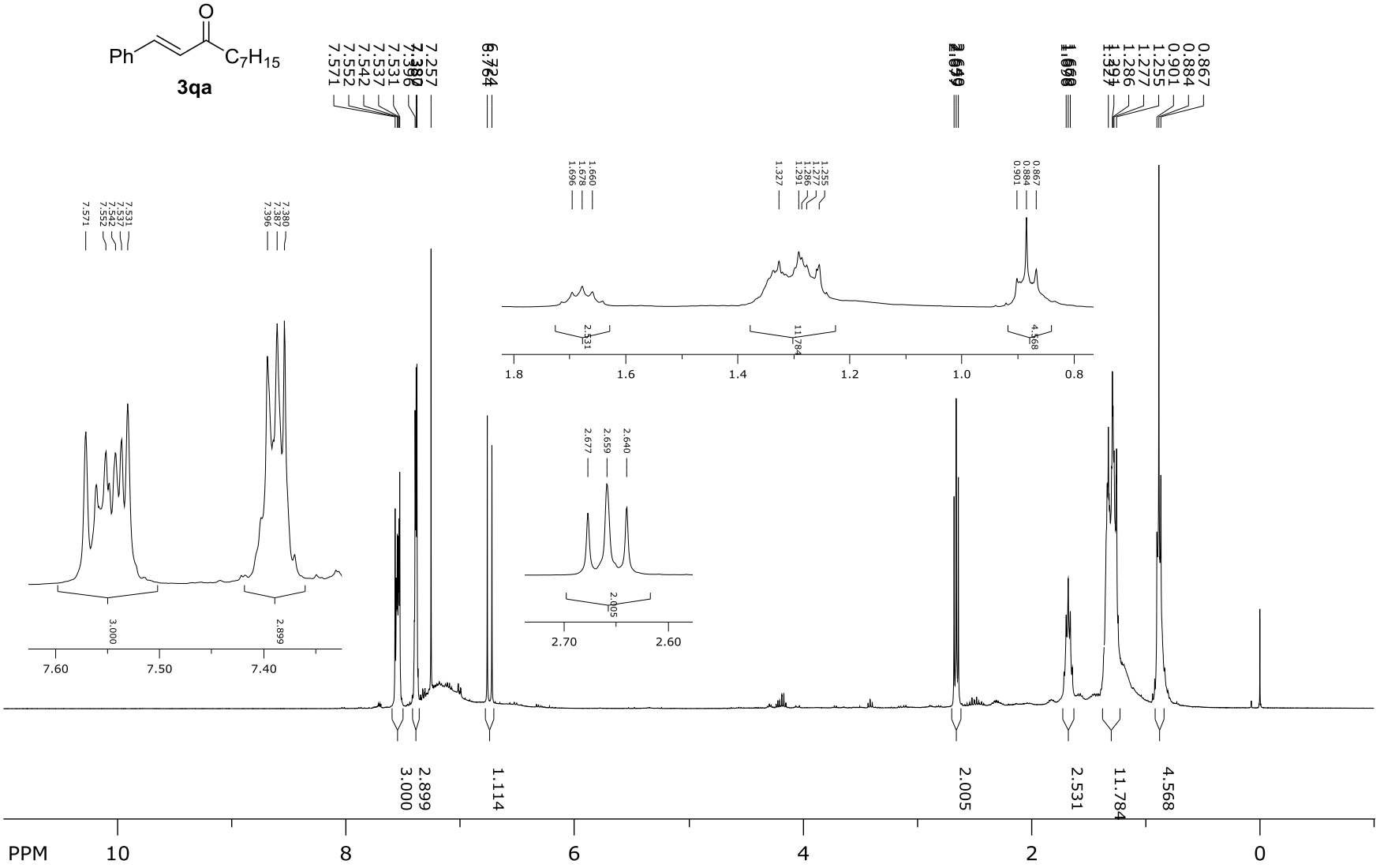
Cyclohex-3-en-1-yl(phenyl)methanone (3pb″)

^{13}C NMR (100 MHz)



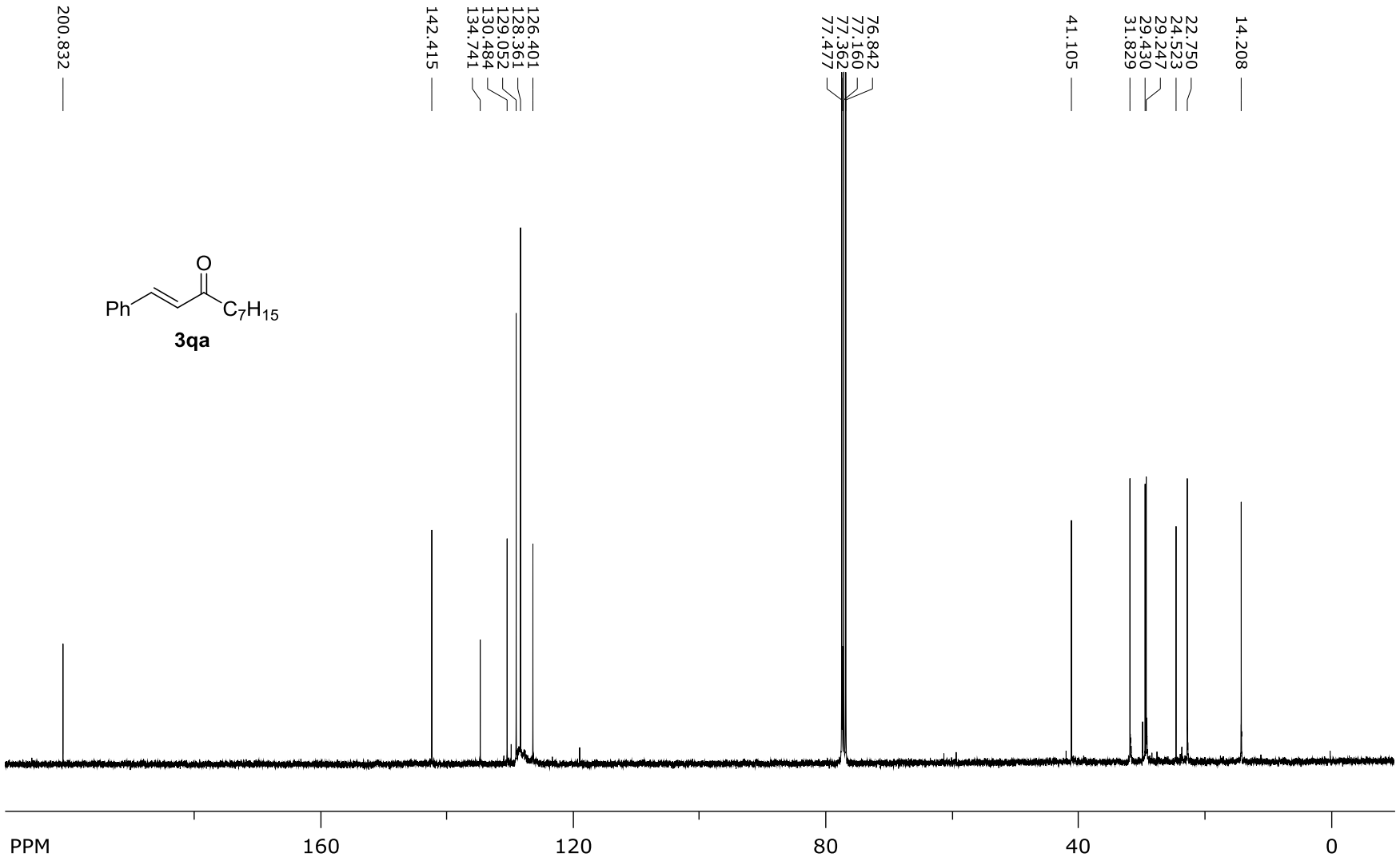
5.24. (*E*)-1-Phenyldec-1-en-3-one (3qa)

^{1}H NMR (400 MHz)



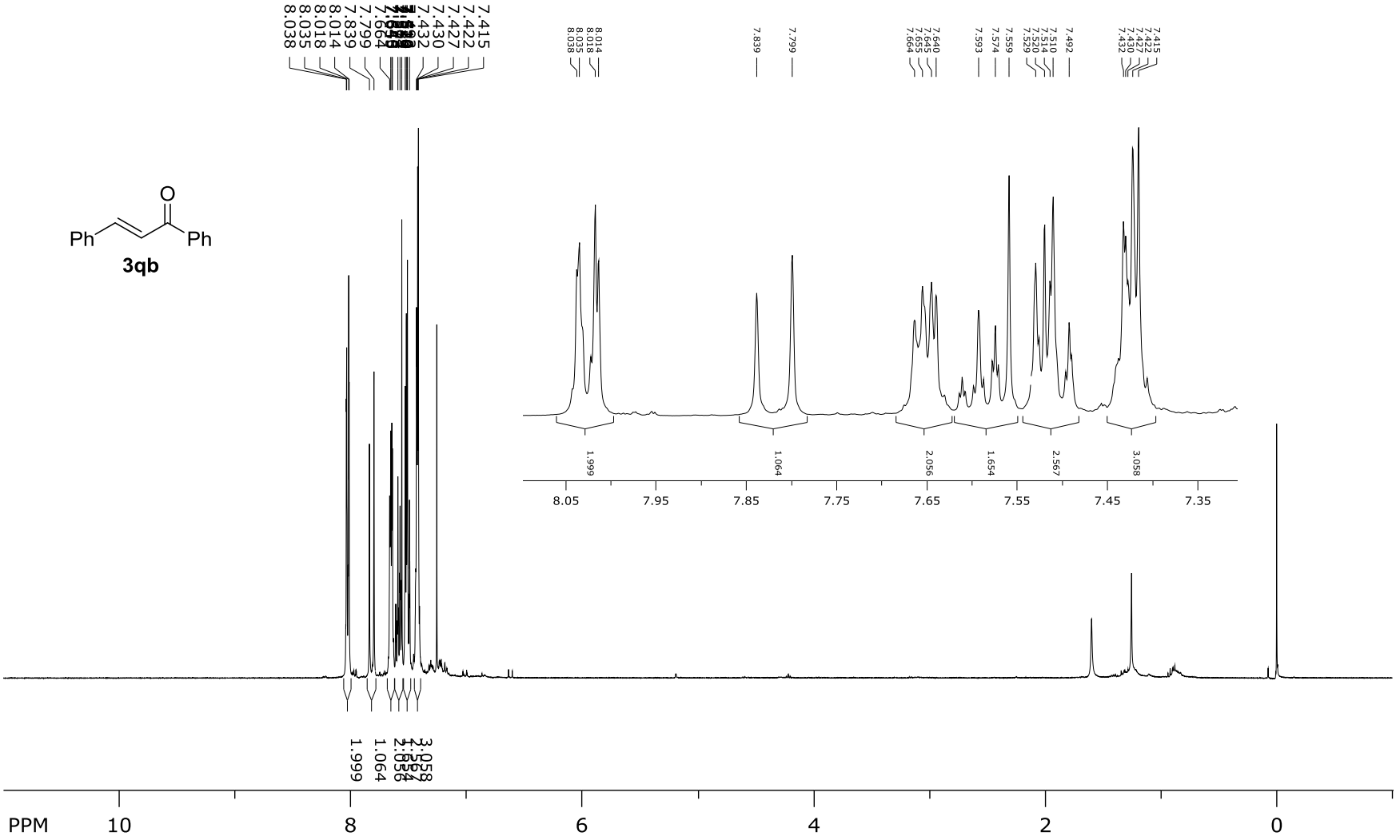
(*E*)-1-Phenyldec-1-en-3-one (3qa)

^{13}C NMR (100 MHz)



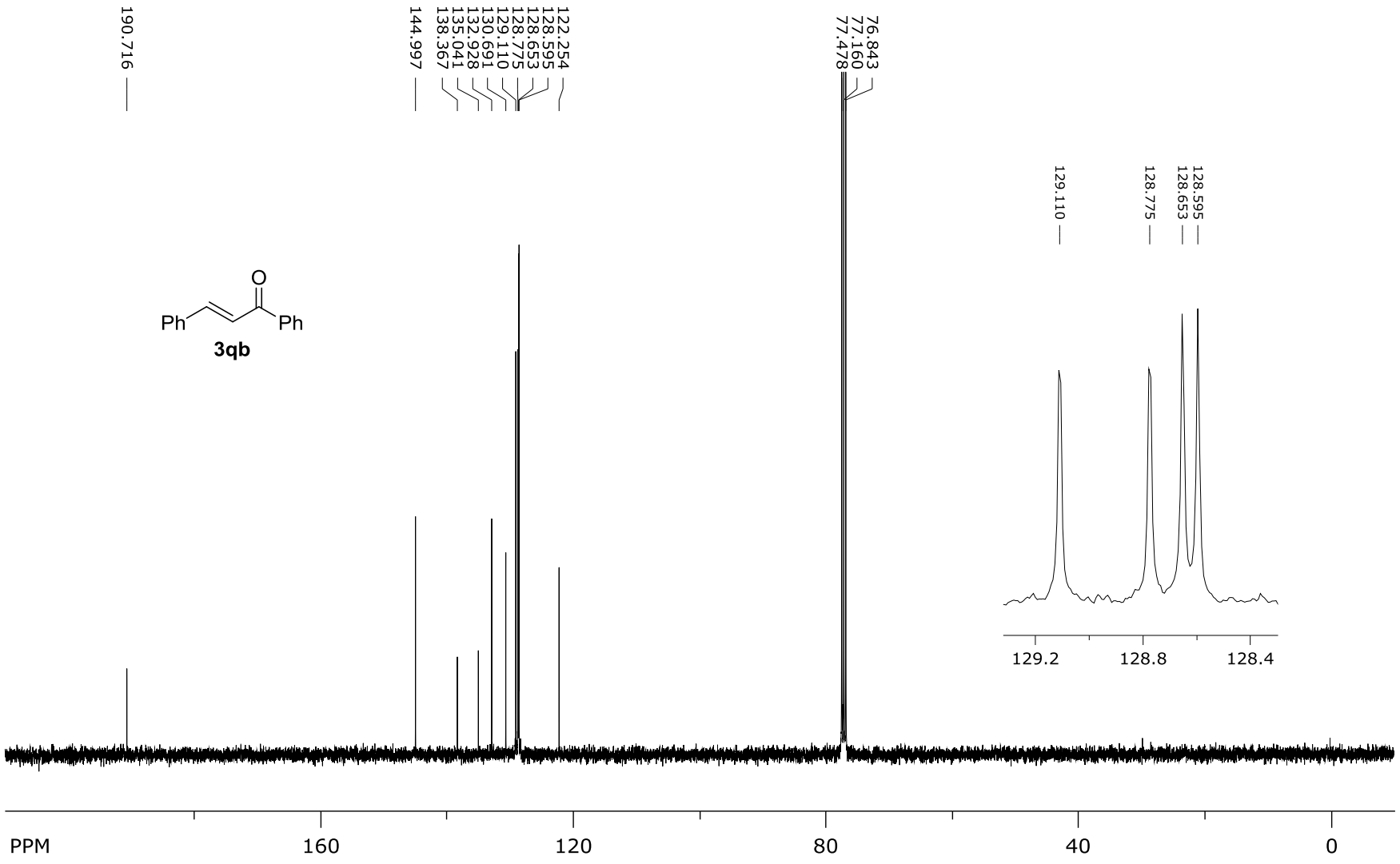
5.25. (*E*)-1,3-Diphenyl-2-propen-1-one (3qb)

^{1}H NMR (400 MHz)



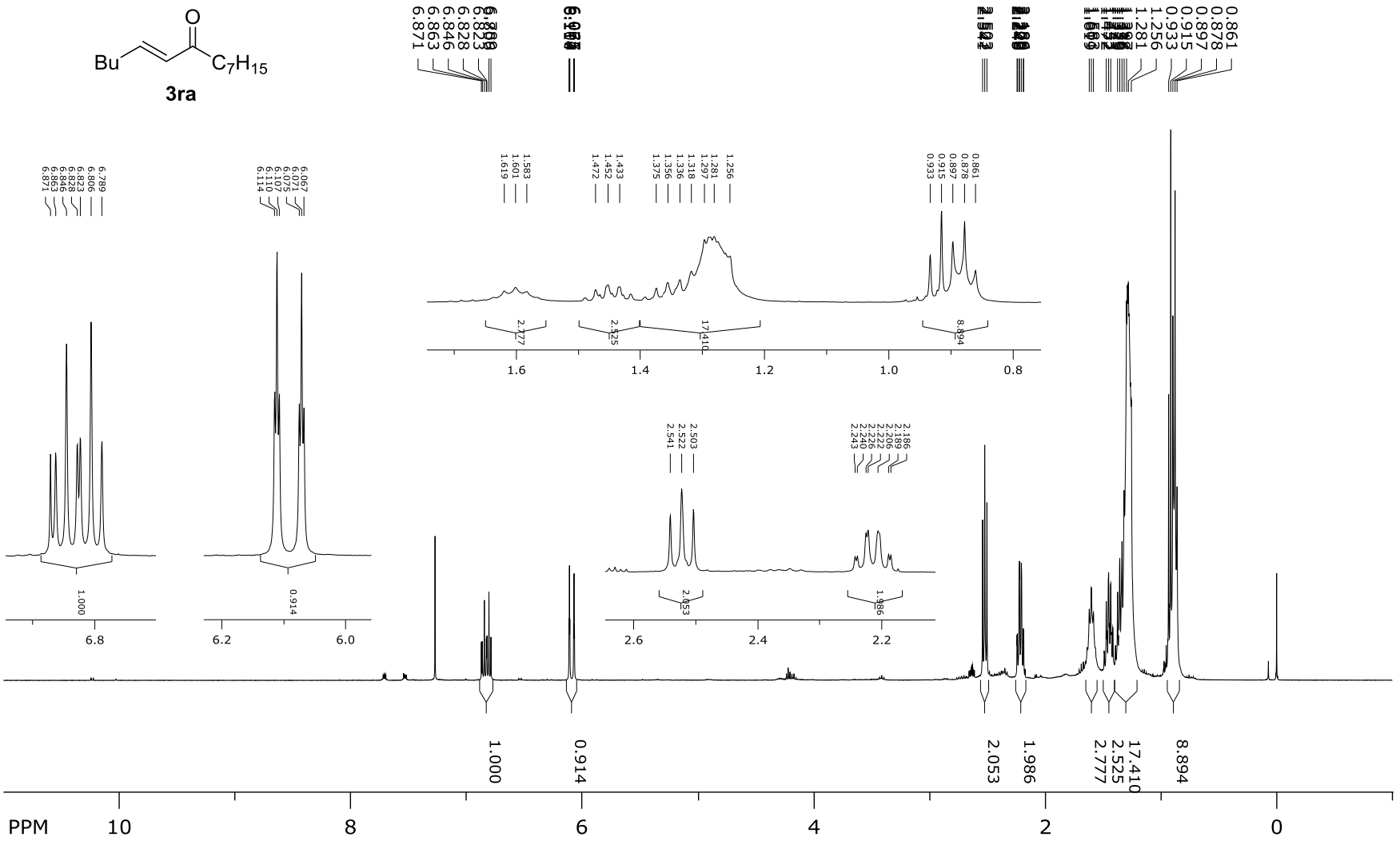
(*E*)-1,3-Diphenyl-2-propen-1-one (3qb)

^{13}C NMR (100 MHz)



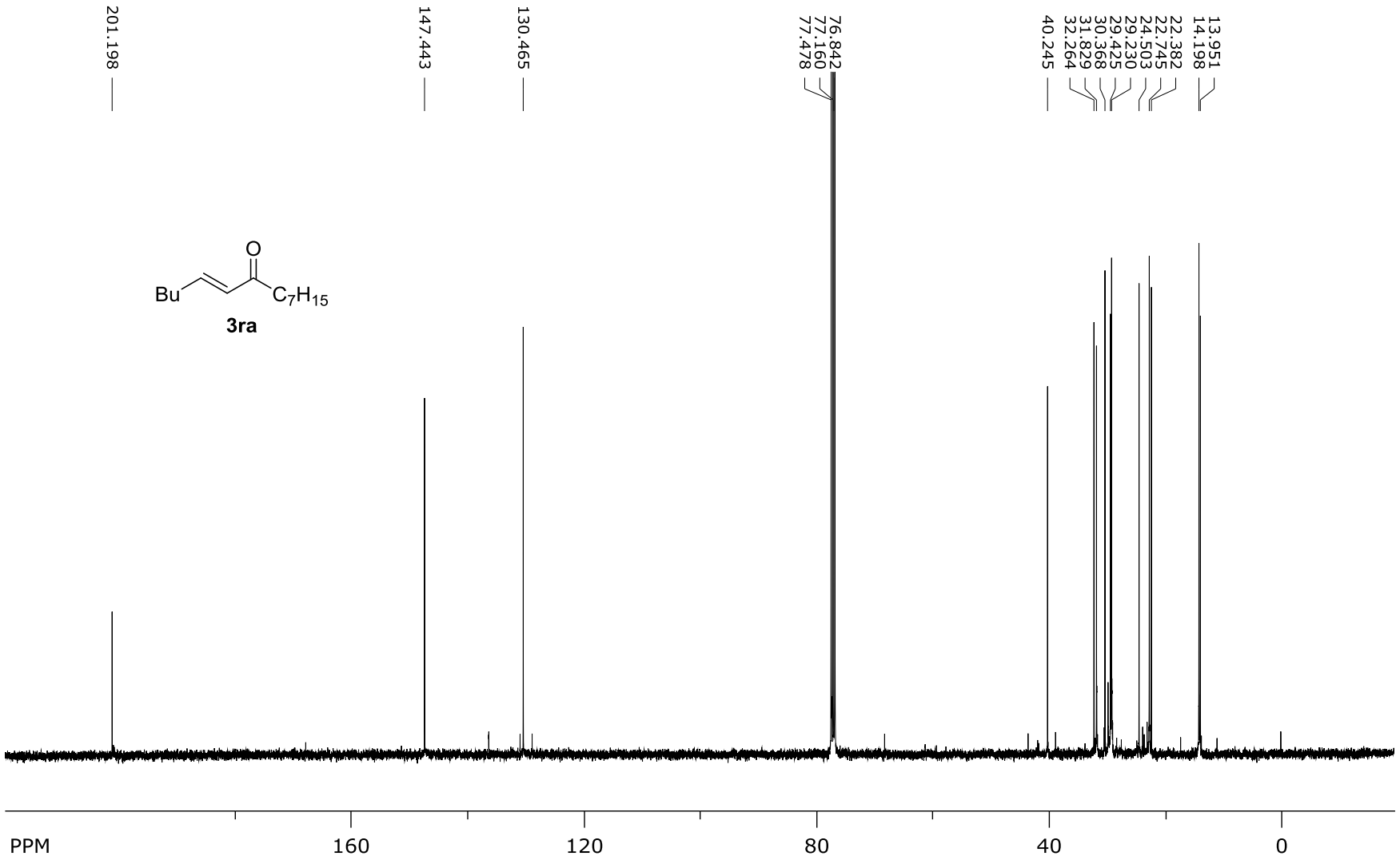
5.26. (*E*)-Tetradec-5-en-7-one (3ra)

^{1}H NMR (400 MHz)



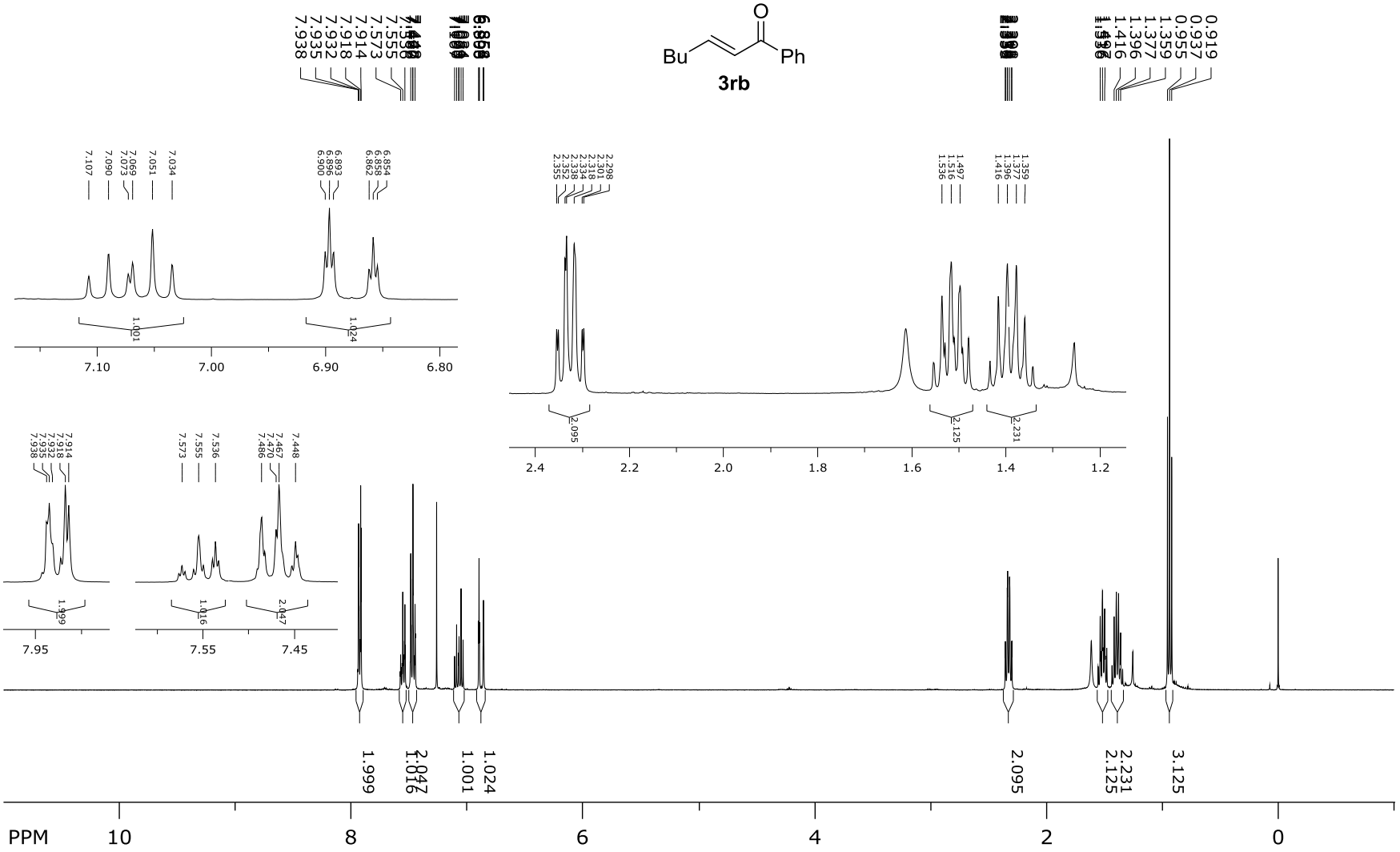
(*E*)-Tetradec-5-en-7-one (3ra)

^{13}C NMR (100 MHz)



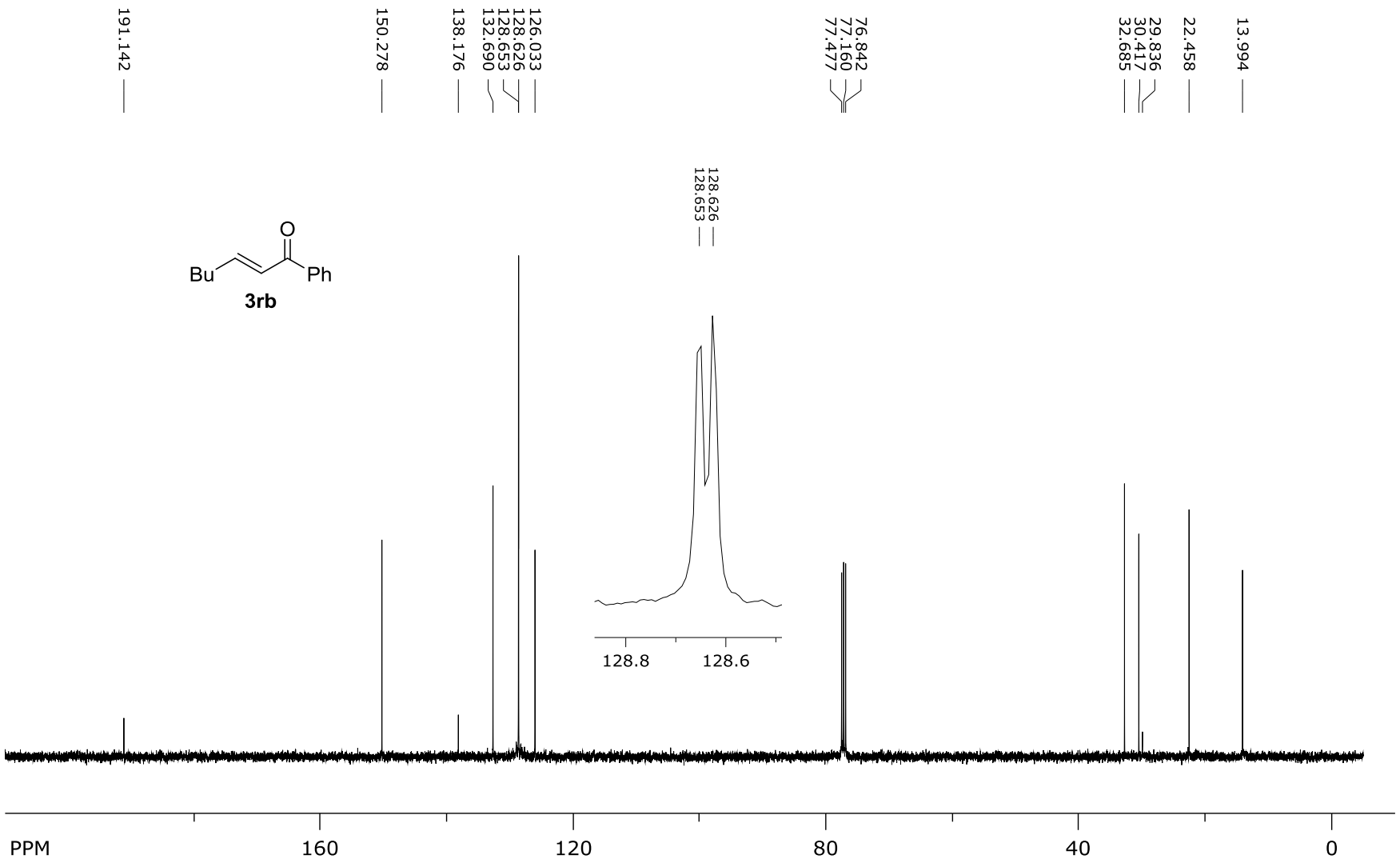
5.27. (*E*)-1-Phenylhept-2-en-1-one (3rb)

^{1}H NMR (400 MHz)



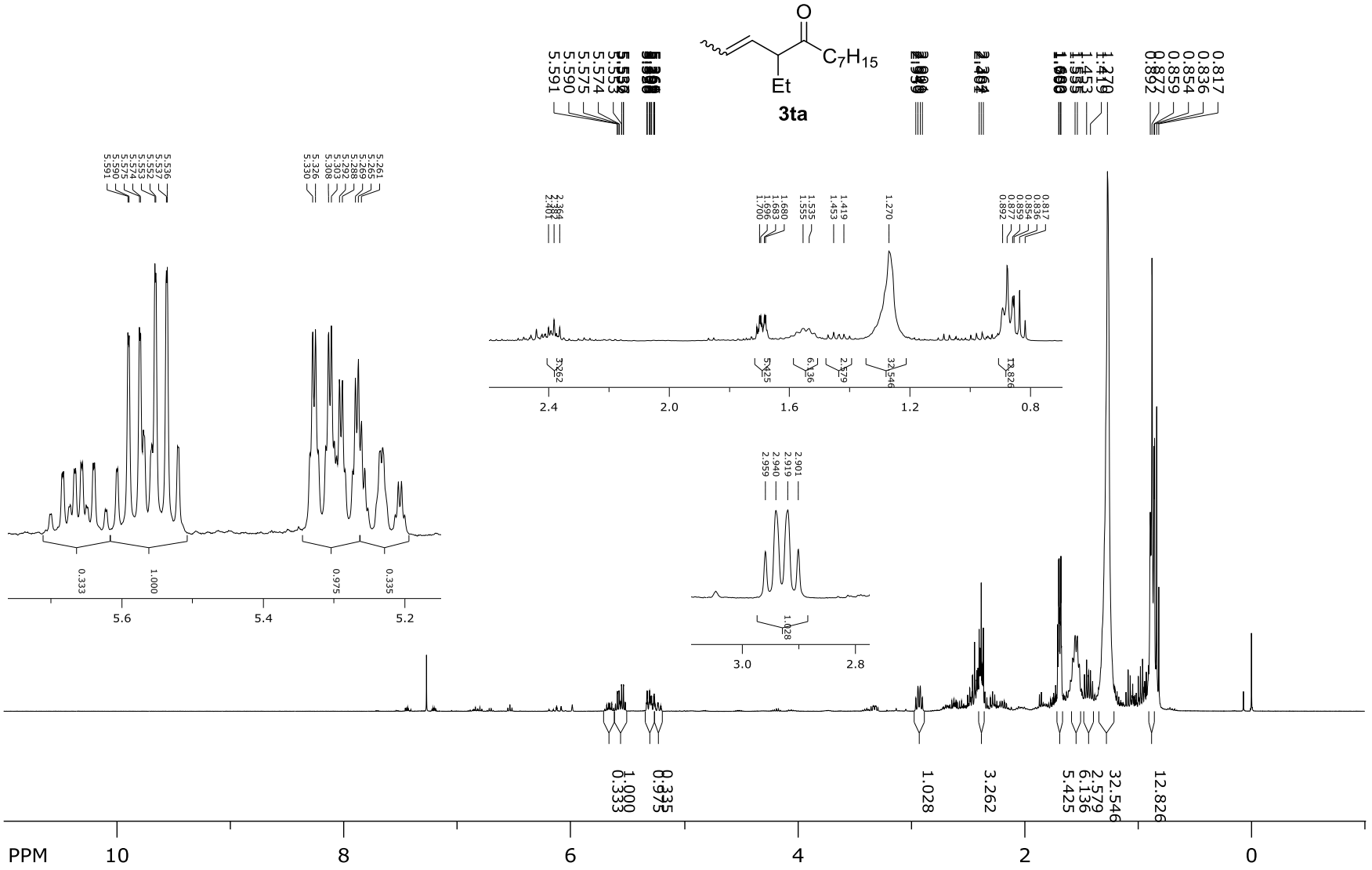
(*E*)-1-Phenylhept-2-en-1-one (3rb)

^{13}C NMR (100 MHz)



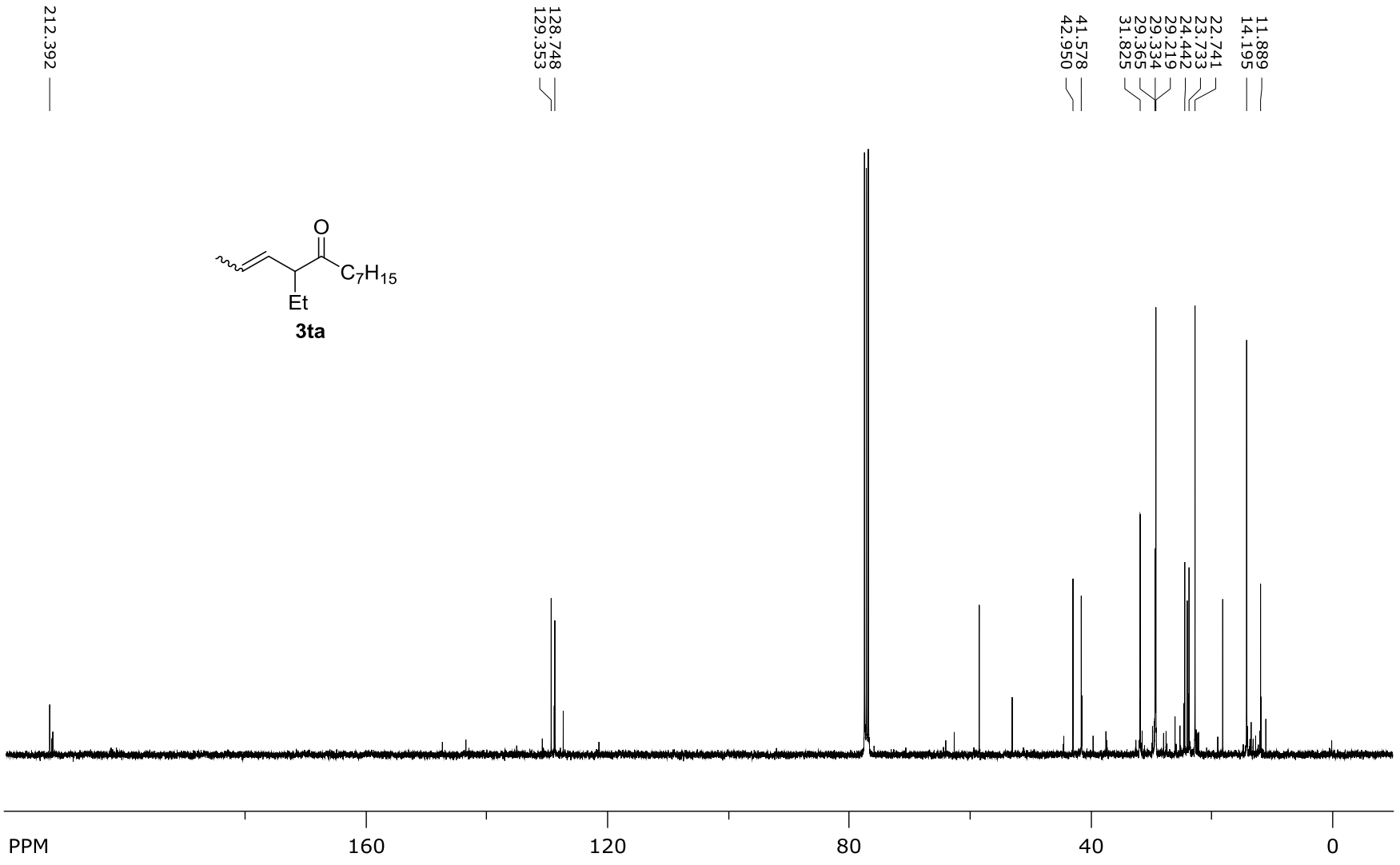
5.28. 4-Ethyldodec-2-en-5-one (3ta)

^{1}H NMR (400 MHz)



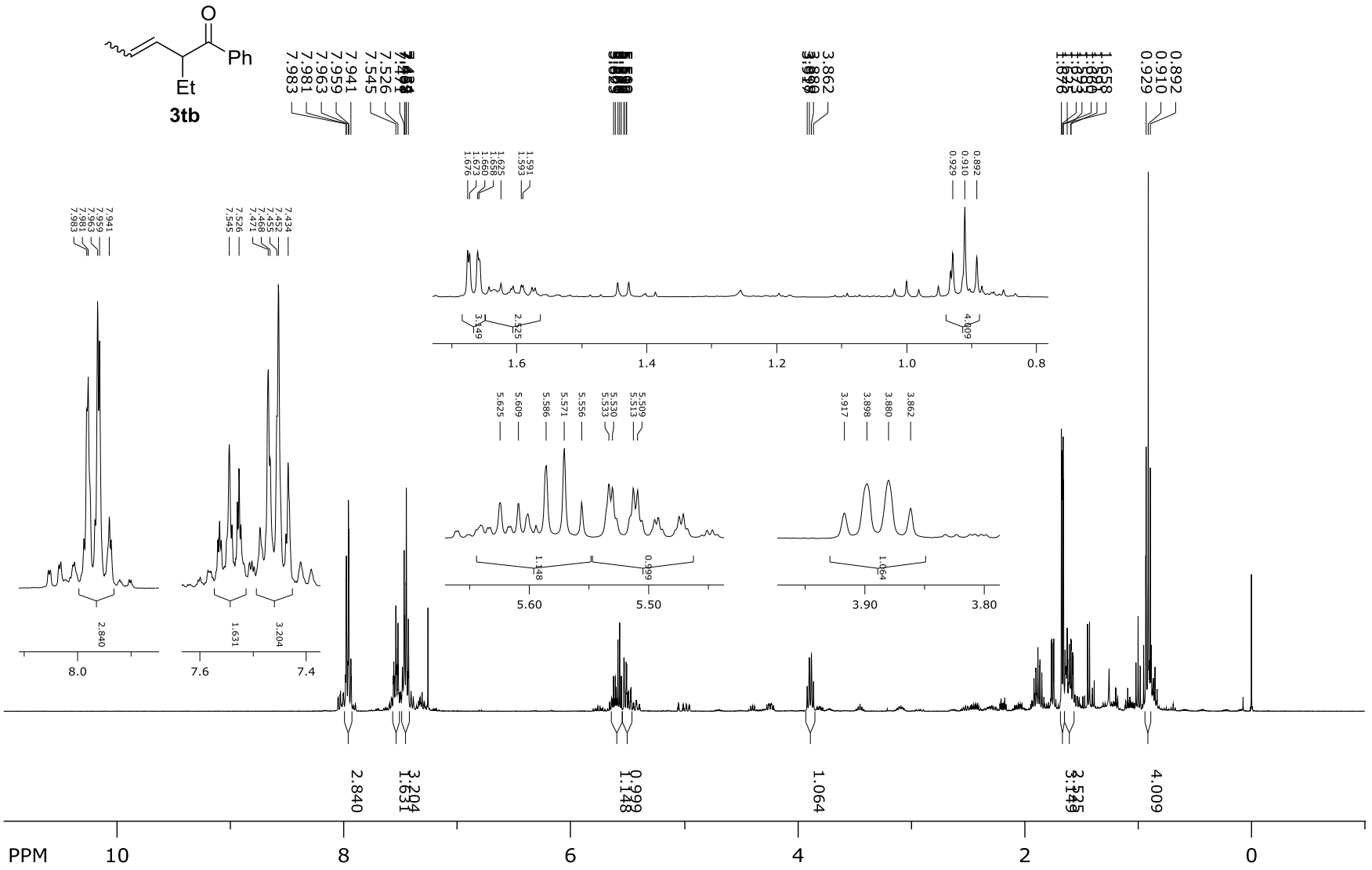
4-Ethyldodec-2-en-5-one (3ta)

^{13}C NMR (100 MHz)



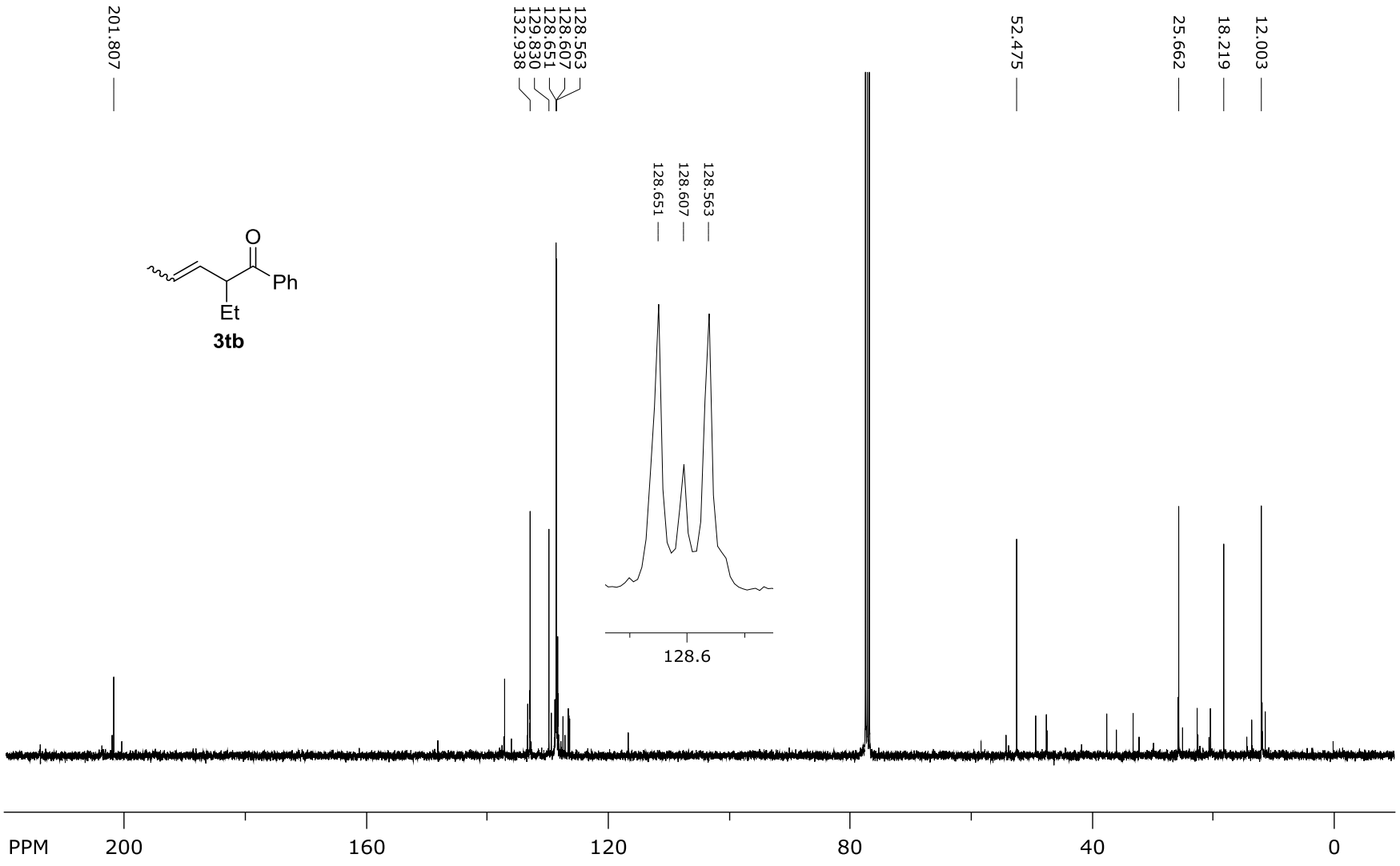
5.29. 2-Ethyl-1-phenyl-pent-3-en-1-one (3tb)

^{1}H NMR (400 MHz)



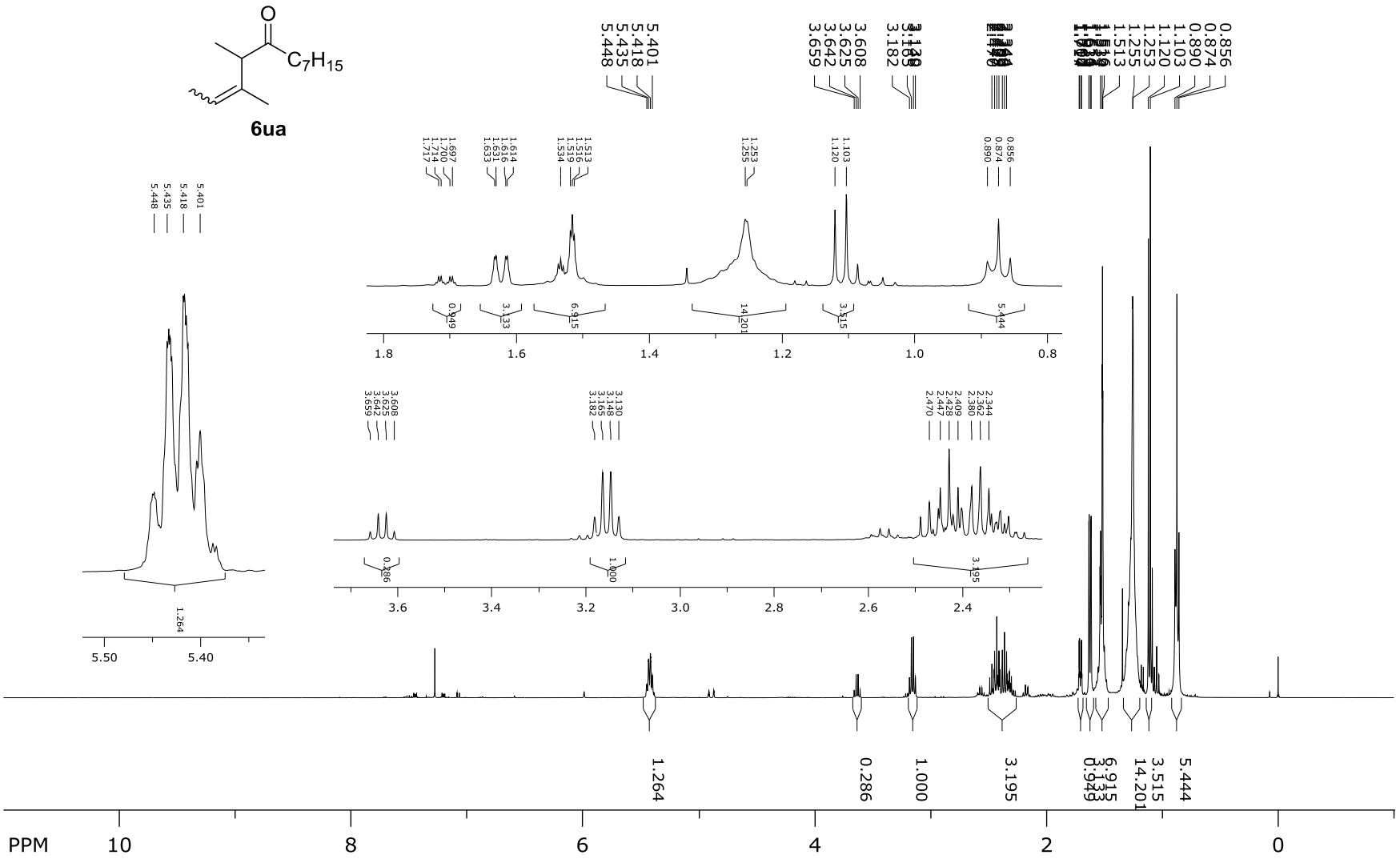
2-Ethyl-1-phenyl-pent-3-en-1-one (3tb)

^{13}C NMR (100 MHz)



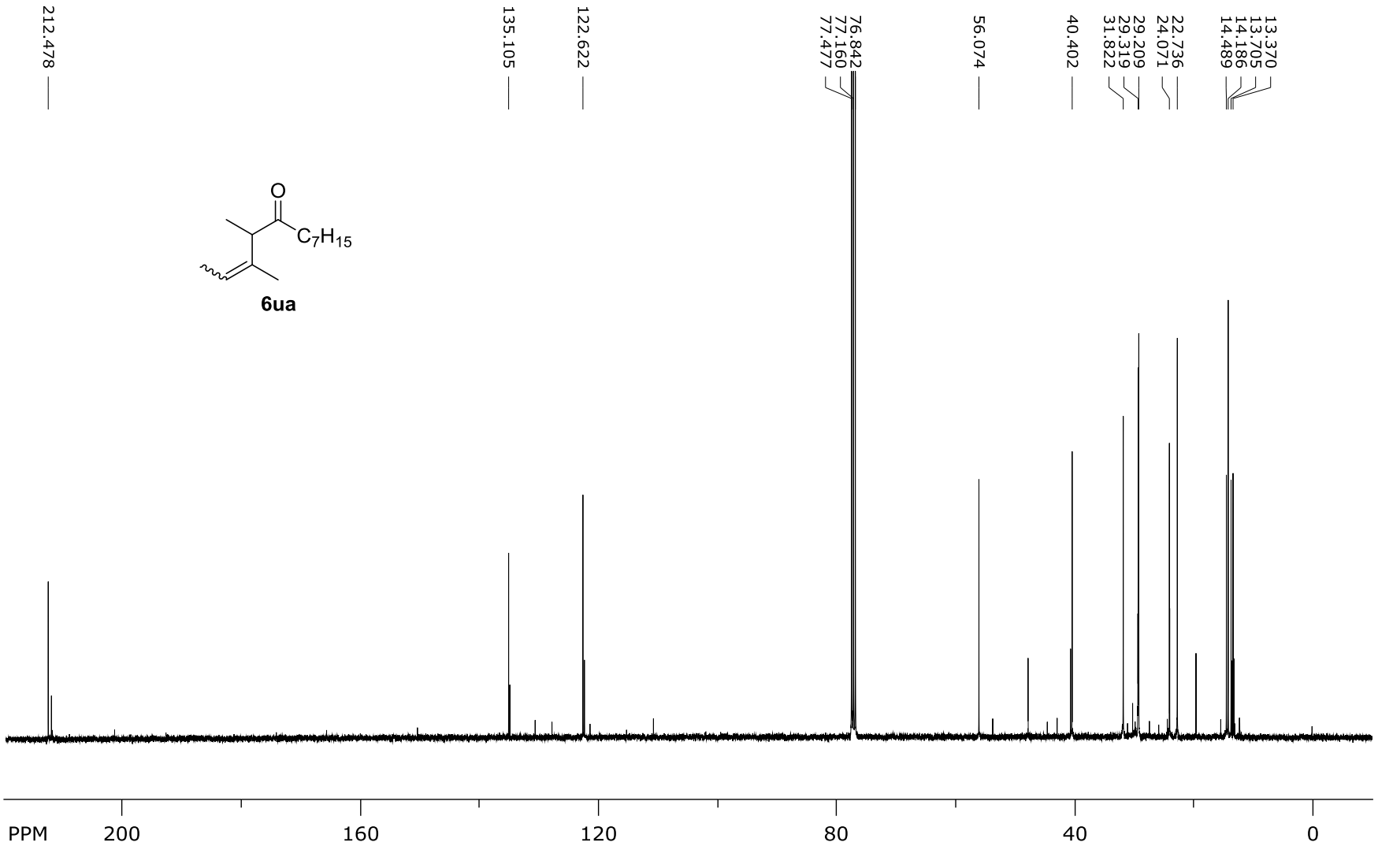
5.30. 3,4-Dimethyldodec-2-en-5-one (6ua)

^{1}H NMR (400 MHz)



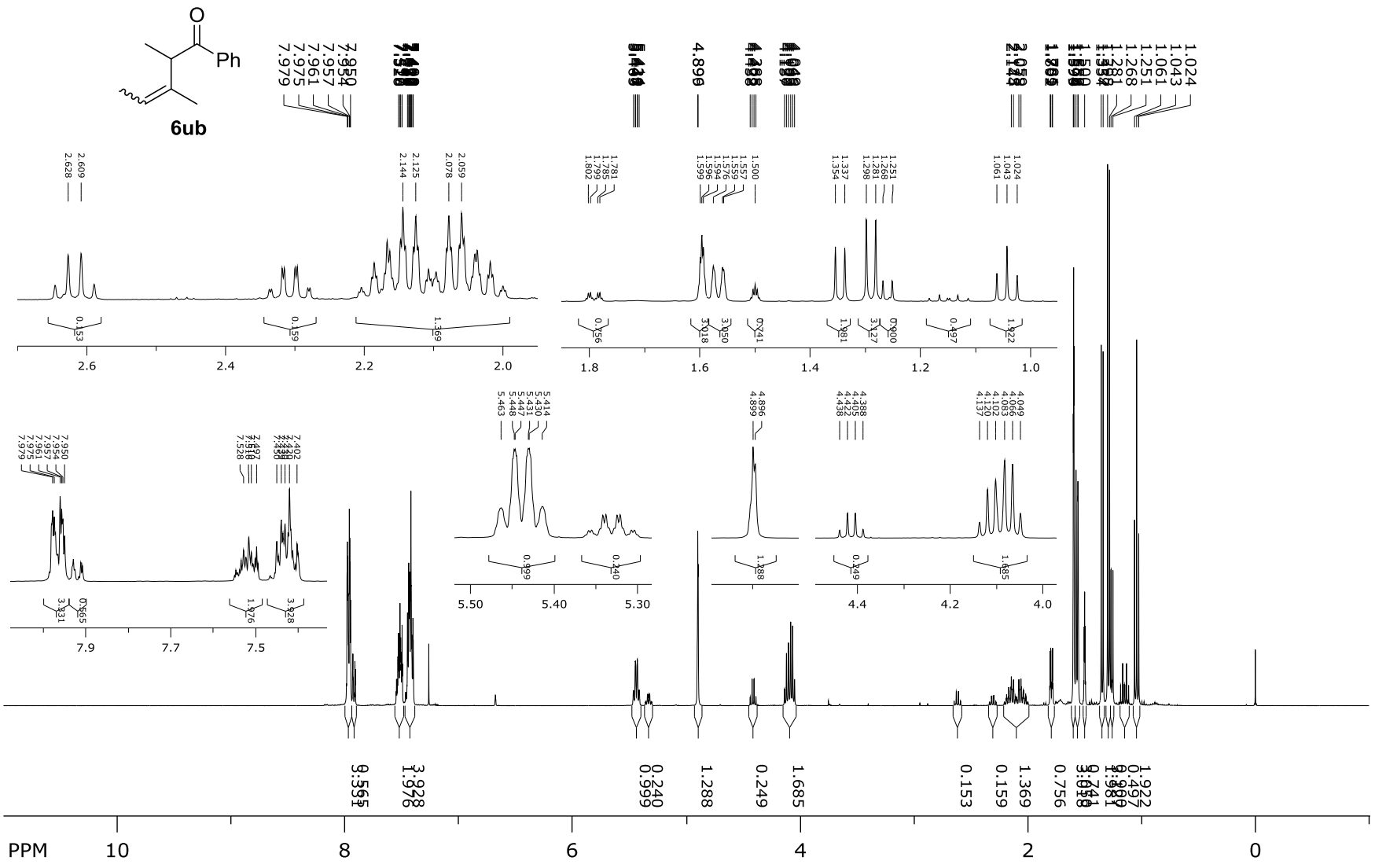
3,4-Dimethyldodec-2-en-5-one (6ua)

^{13}C NMR (100 MHz)



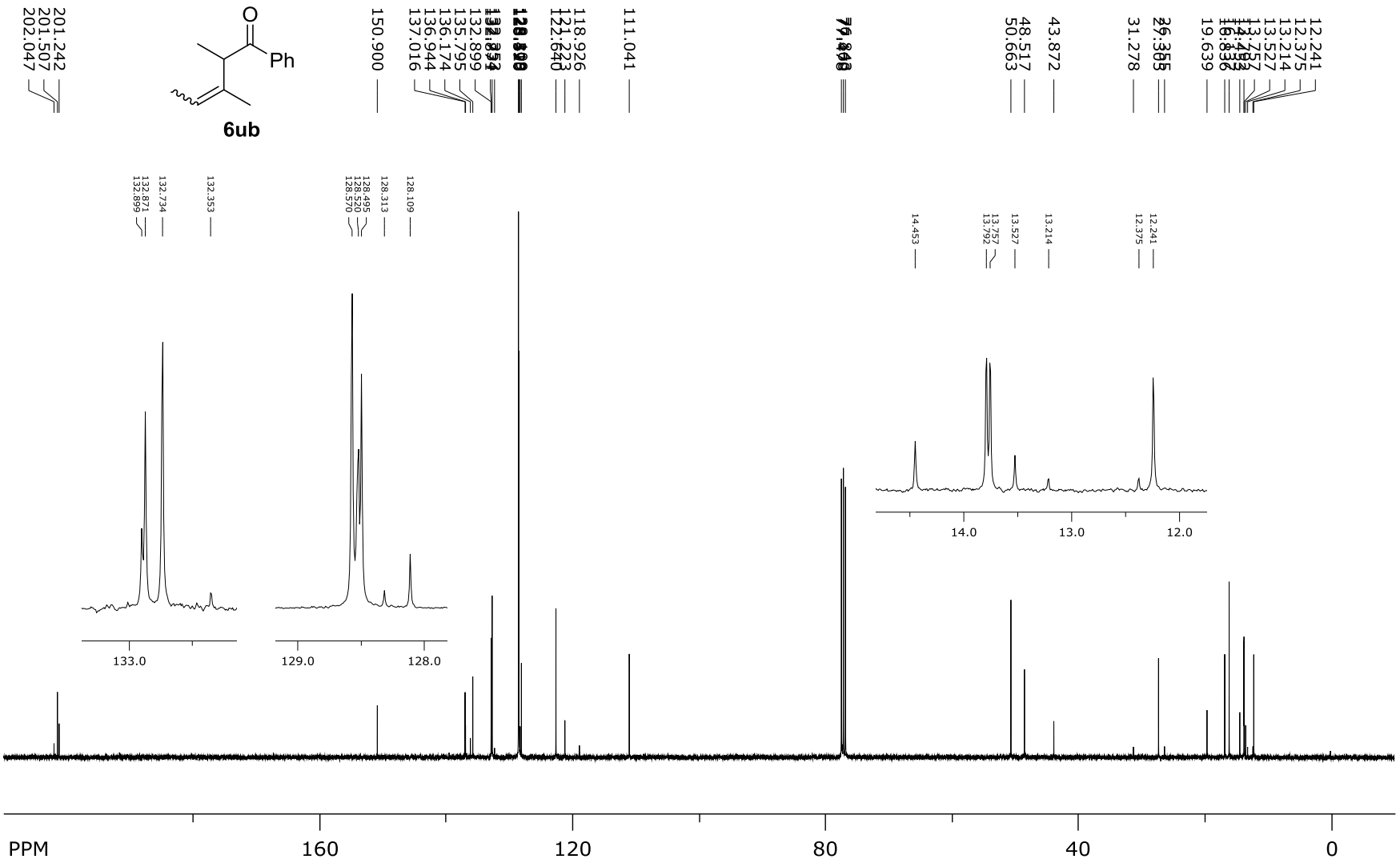
5.31. 2,3-Dimethyl-1-phenylpent-3-en-1-one (6ub)

^{1}H NMR (400 MHz)



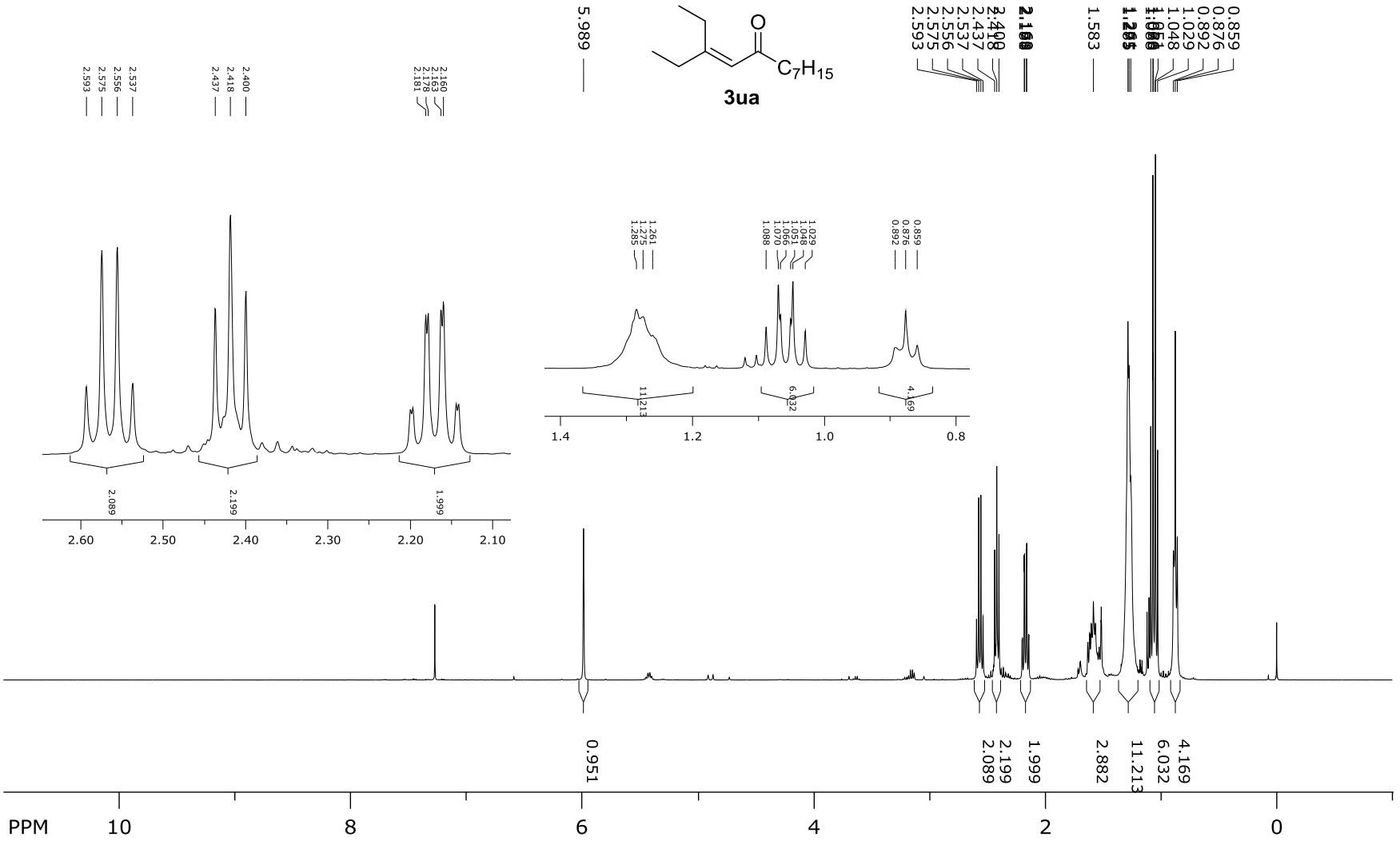
2,3-Dimethyl-1-phenylpent-3-en-1-one (6ub)

^{13}C NMR (100 MHz)



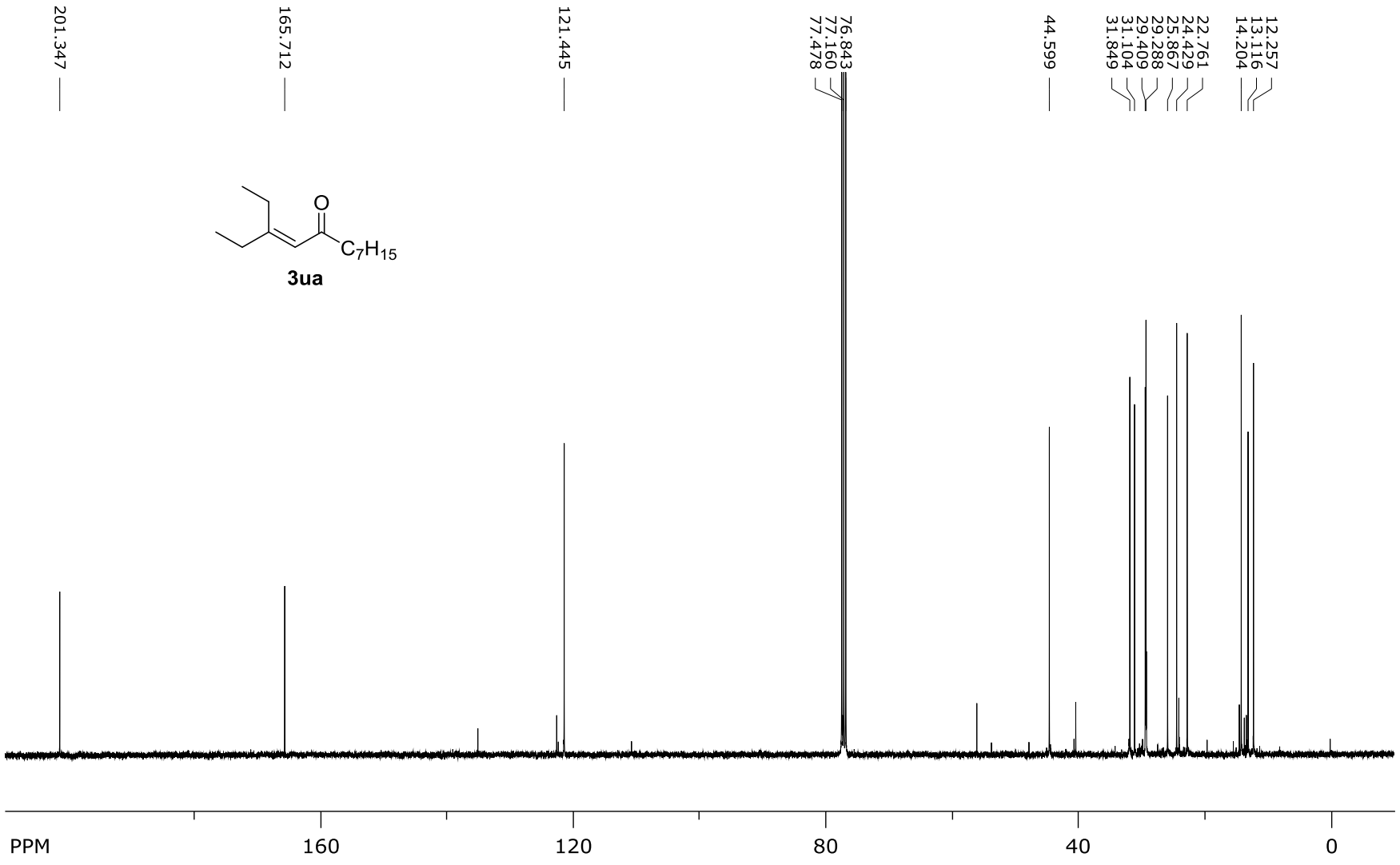
5.32. 3-Ethyldodec-3-en-5-one (3ua)

^{1}H NMR (400 MHz)



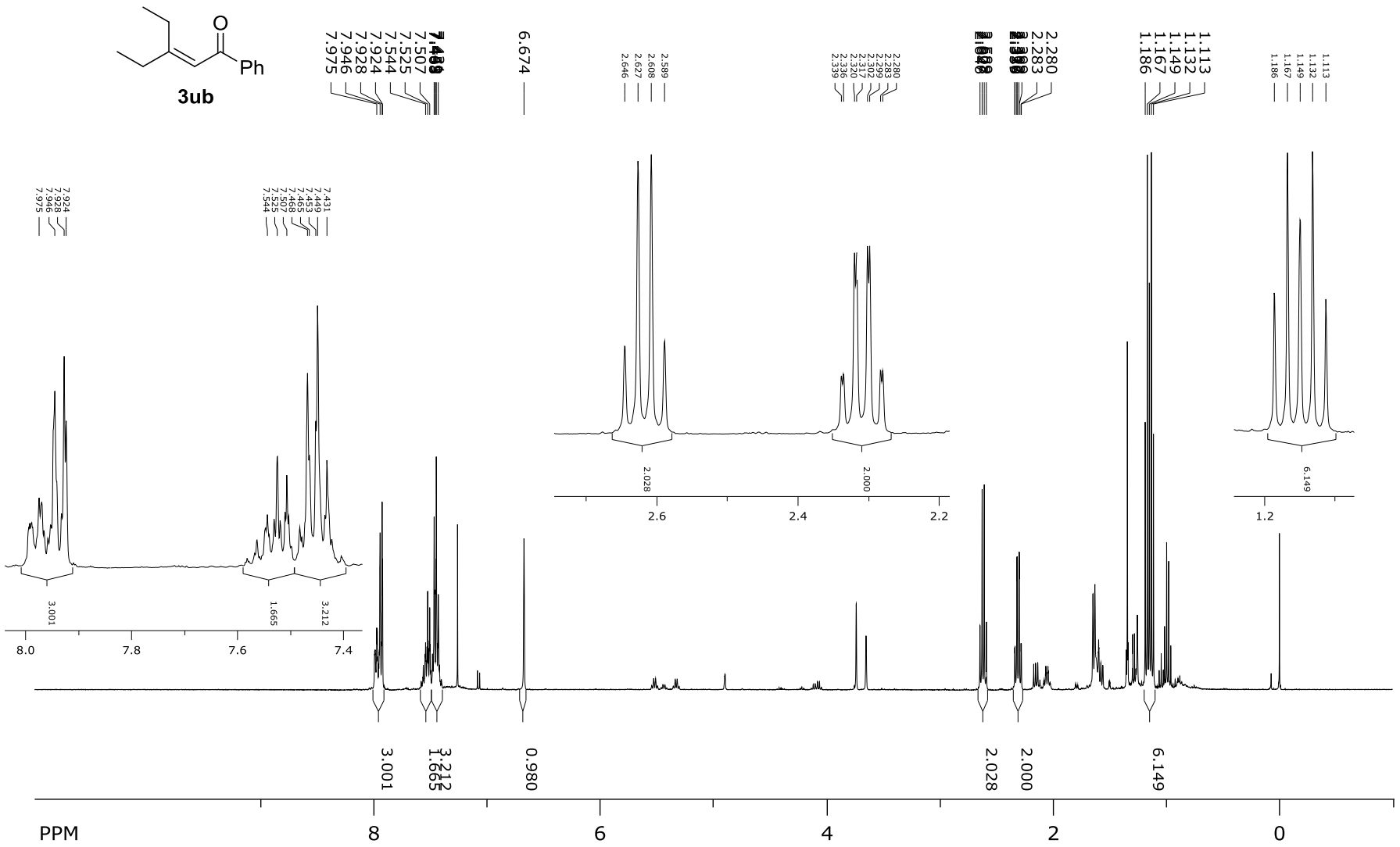
3-Ethyldodec-3-en-5-one (3ua)

^{13}C NMR (100 MHz)



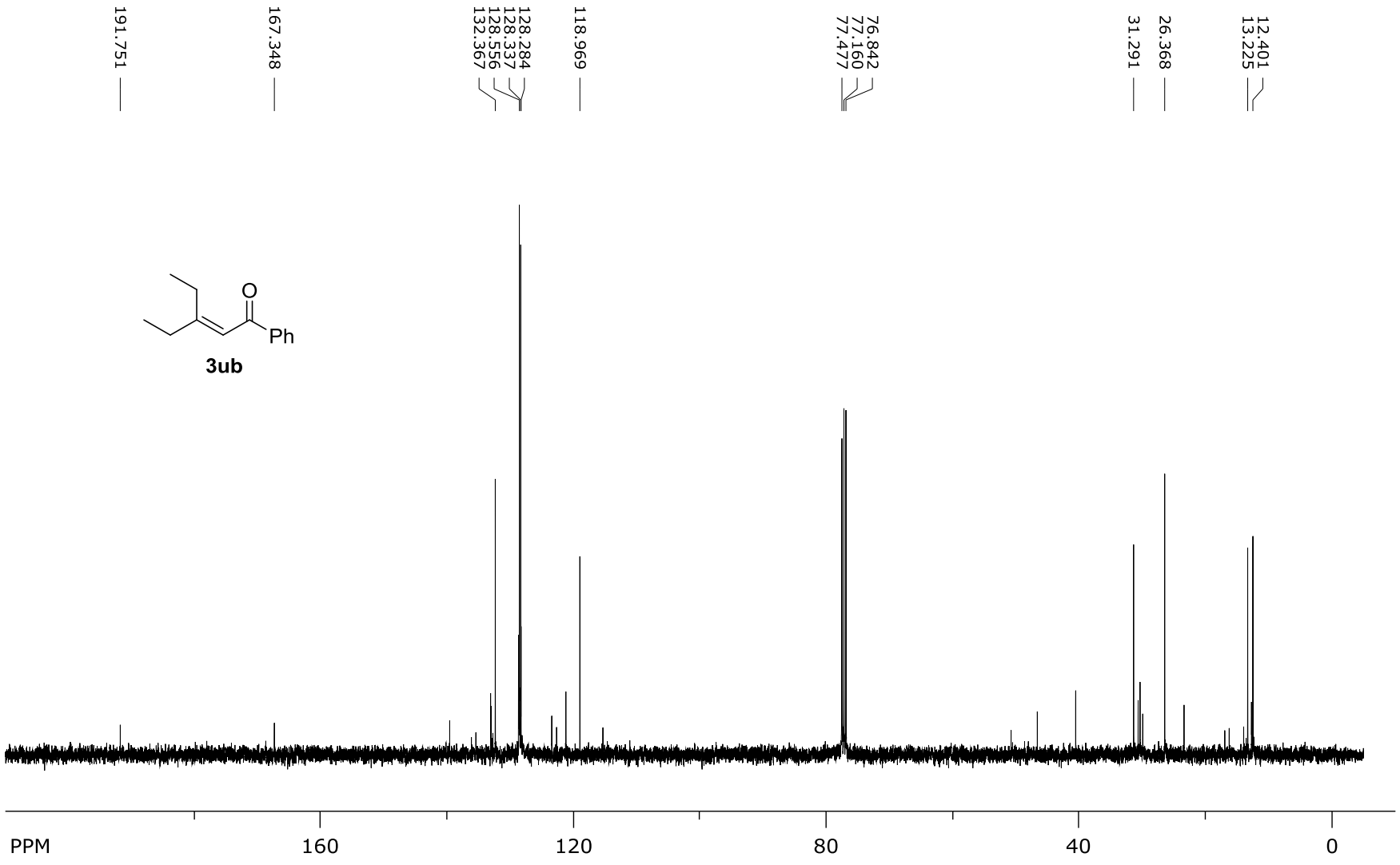
5.33. 3-Ethyl-1-phenylpent-2-en-1-one (3ub)

^{1}H NMR (400 MHz)



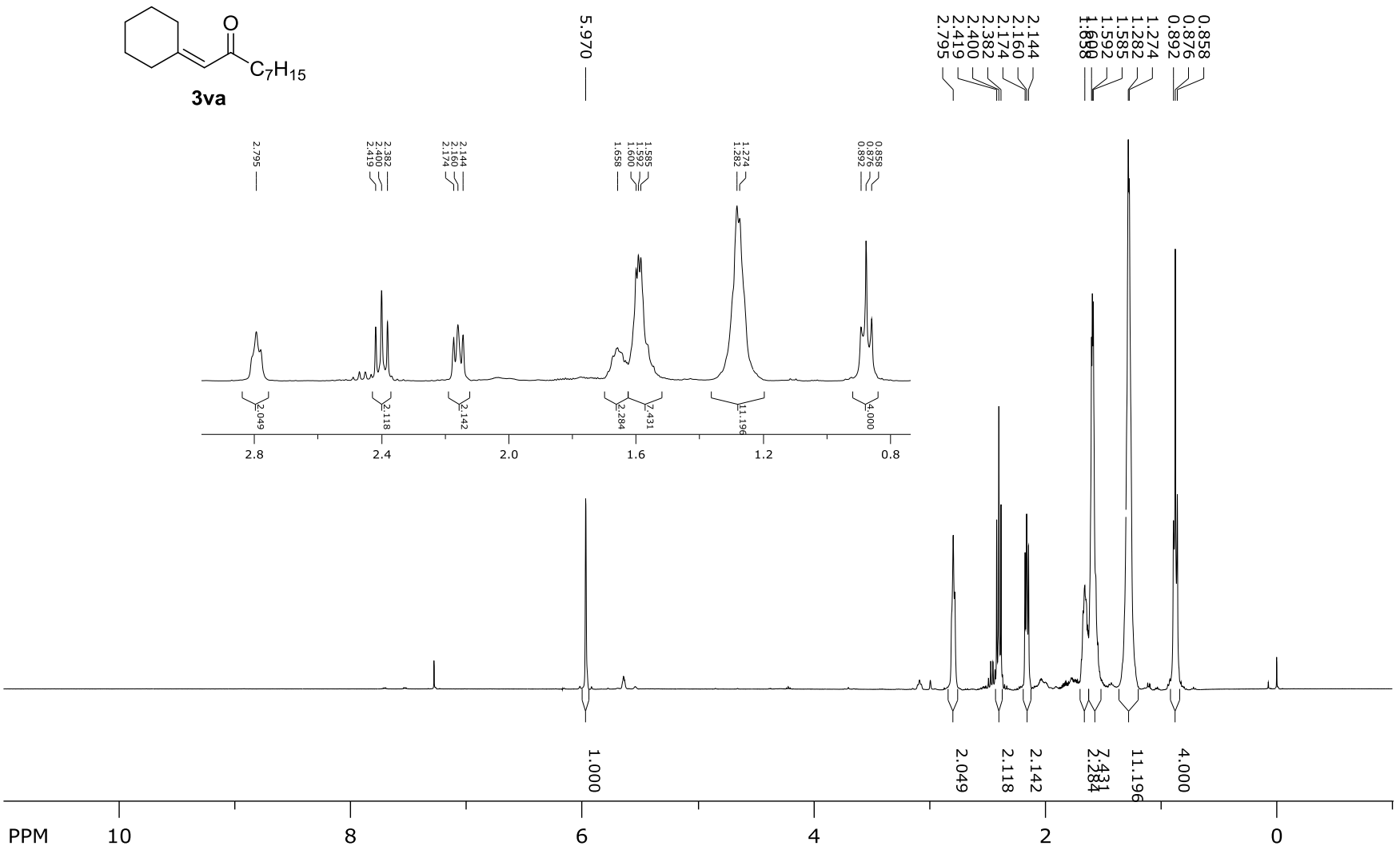
3-Ethyl-1-phenylpent-2-en-1-one (3ub)

^{13}C NMR (100 MHz)



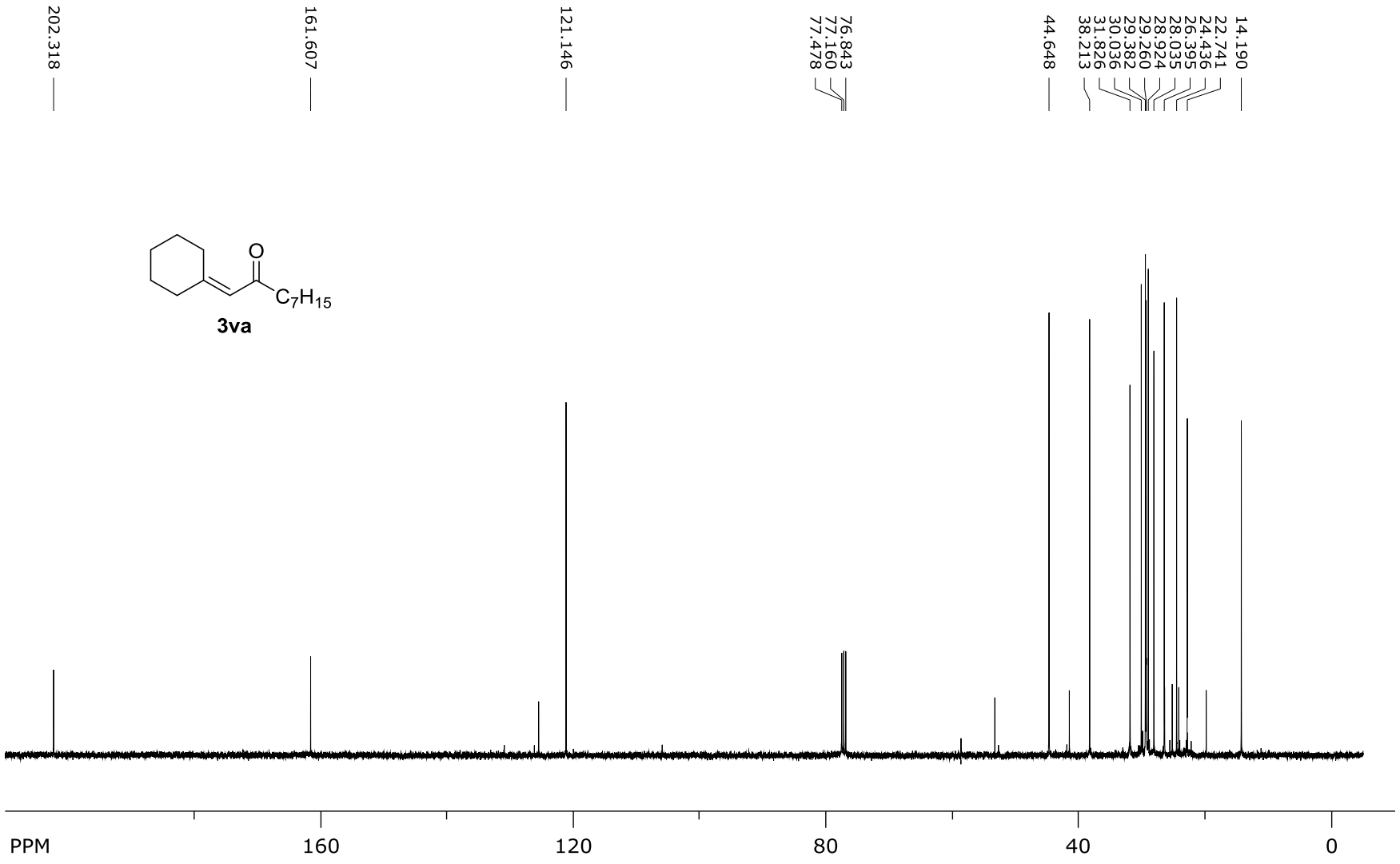
5.34. 1-Cyclohexylidenenonan-2-one (3va)

^{1}H NMR (400 MHz)



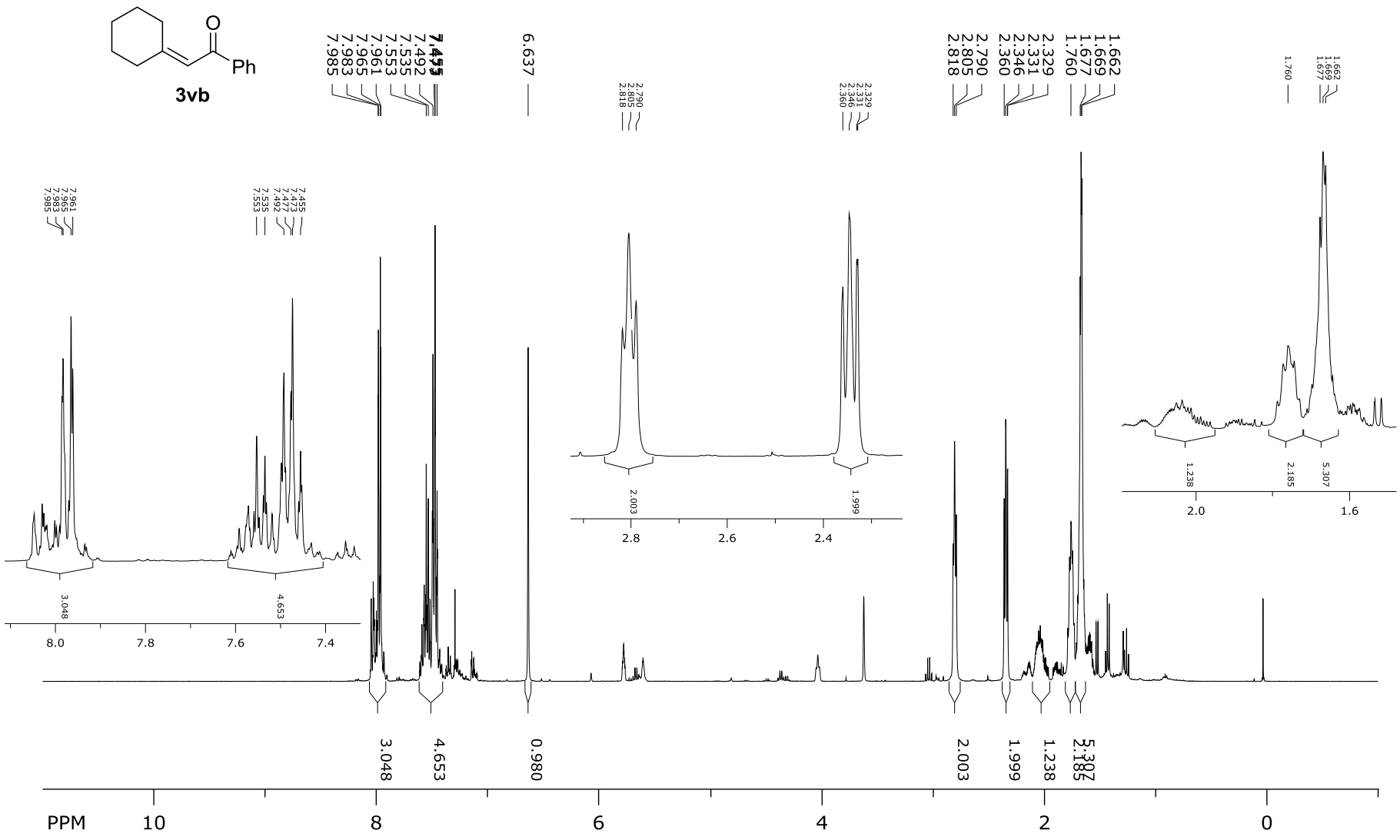
1-Cyclohexylidenenonan-2-one (3va)

^{13}C NMR (100 MHz)



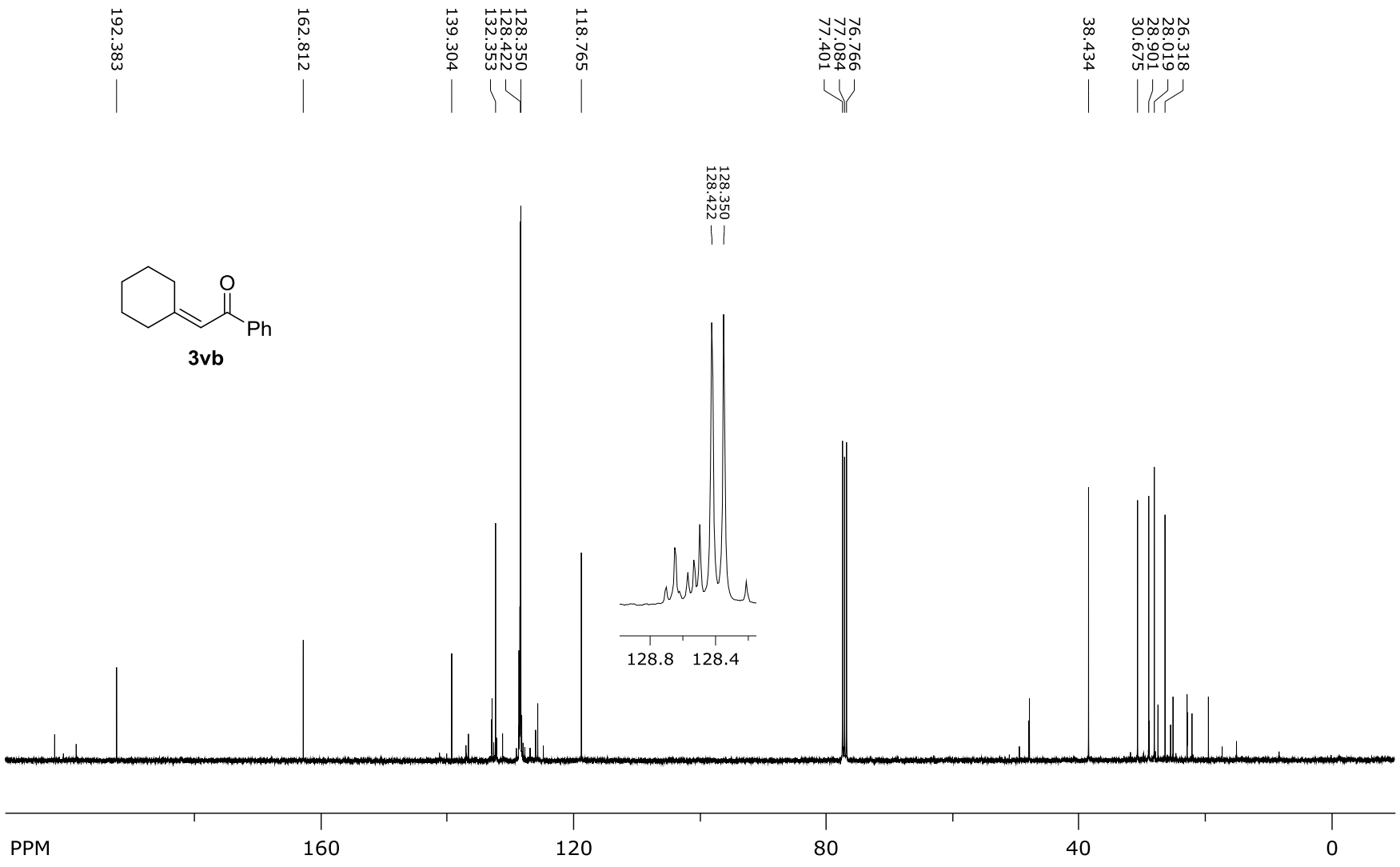
5.35. 2-Cyclohexylidene-1-phenylethanone (3vb)

^{1}H NMR (400 MHz)



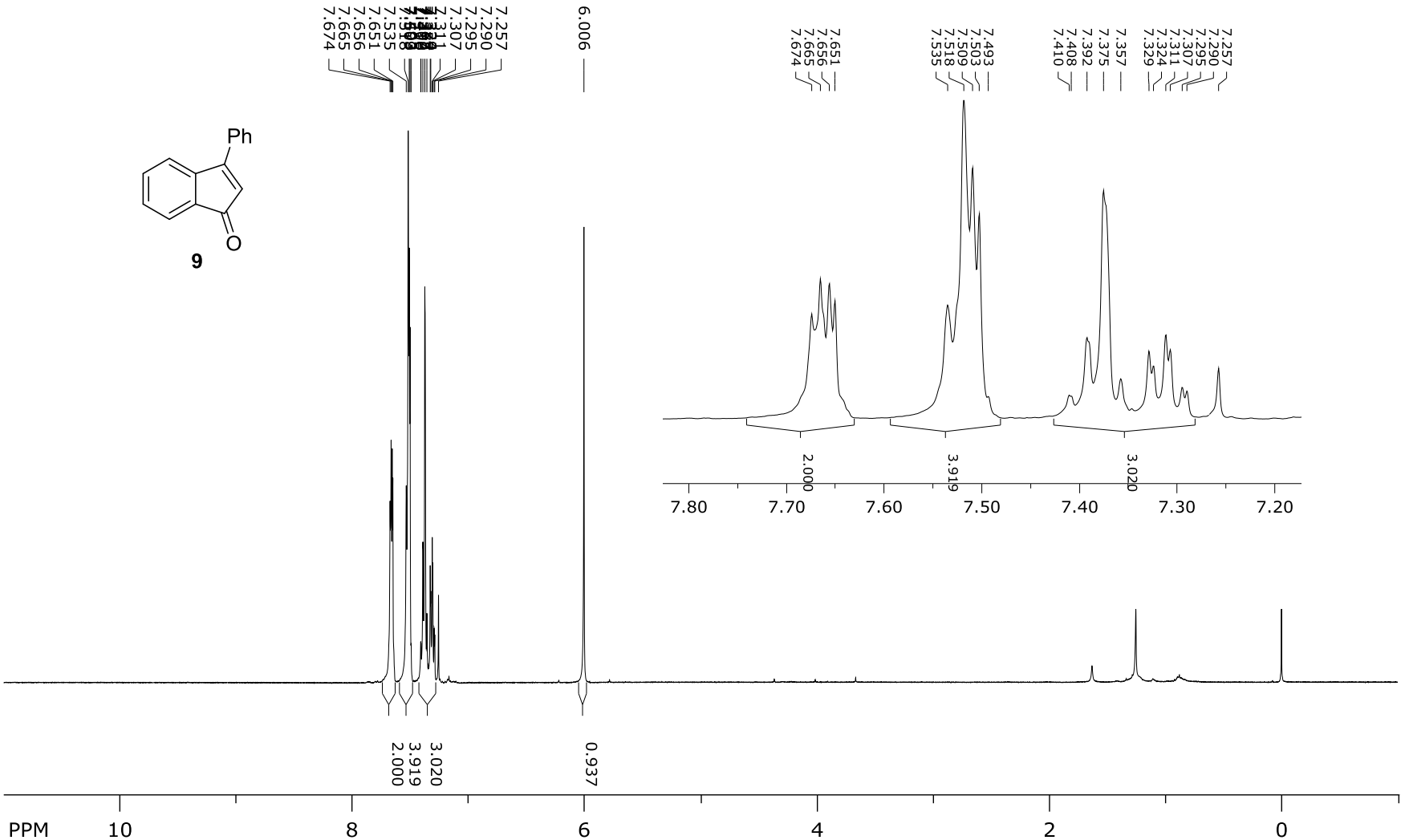
2-Cyclohexylidene-1-phenylethanone (3vb)

^{13}C NMR (100 MHz)



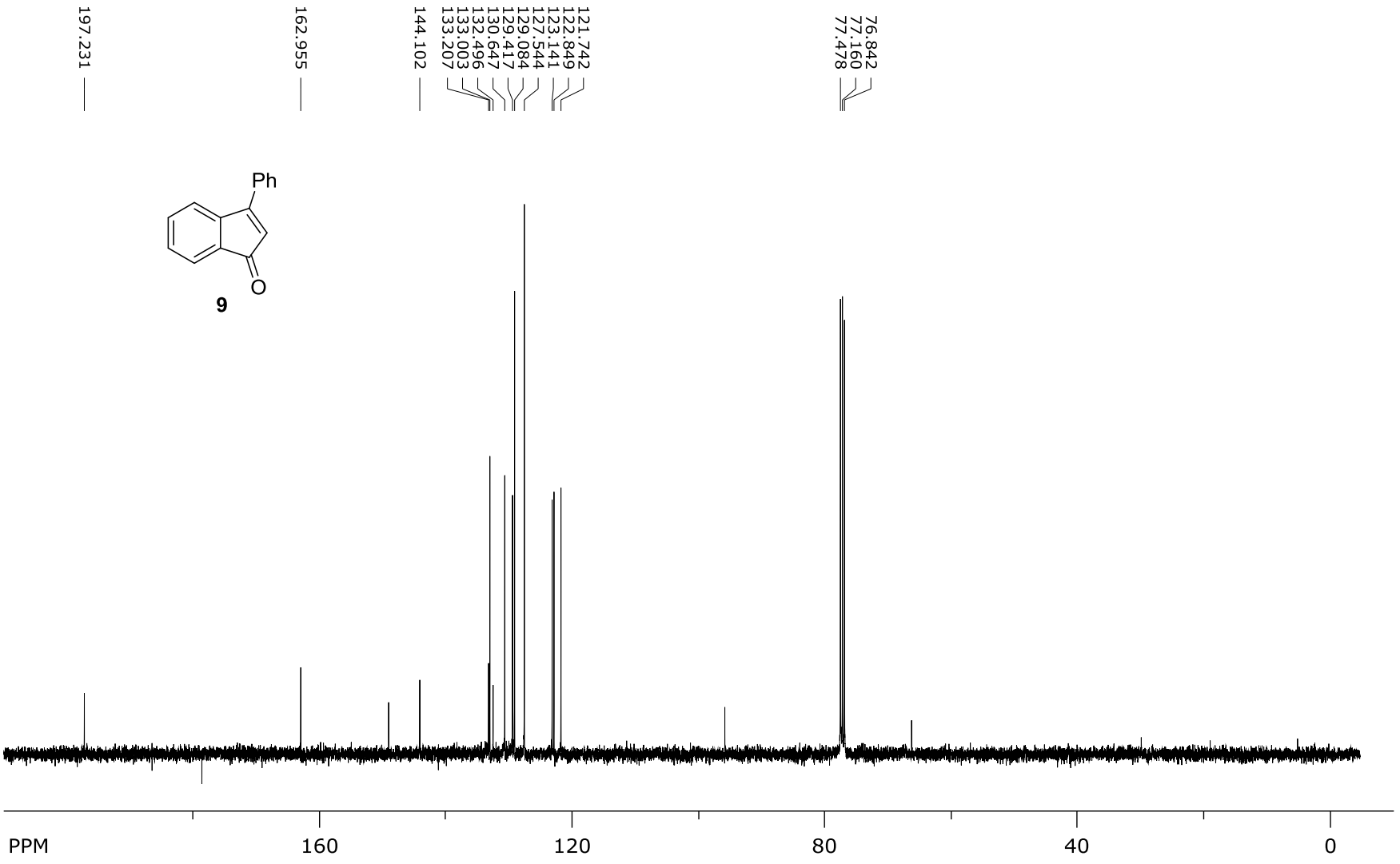
5.36. 3-Phenyl-1*H*-inden-1-one (9)

^{1}H NMR (400 MHz)



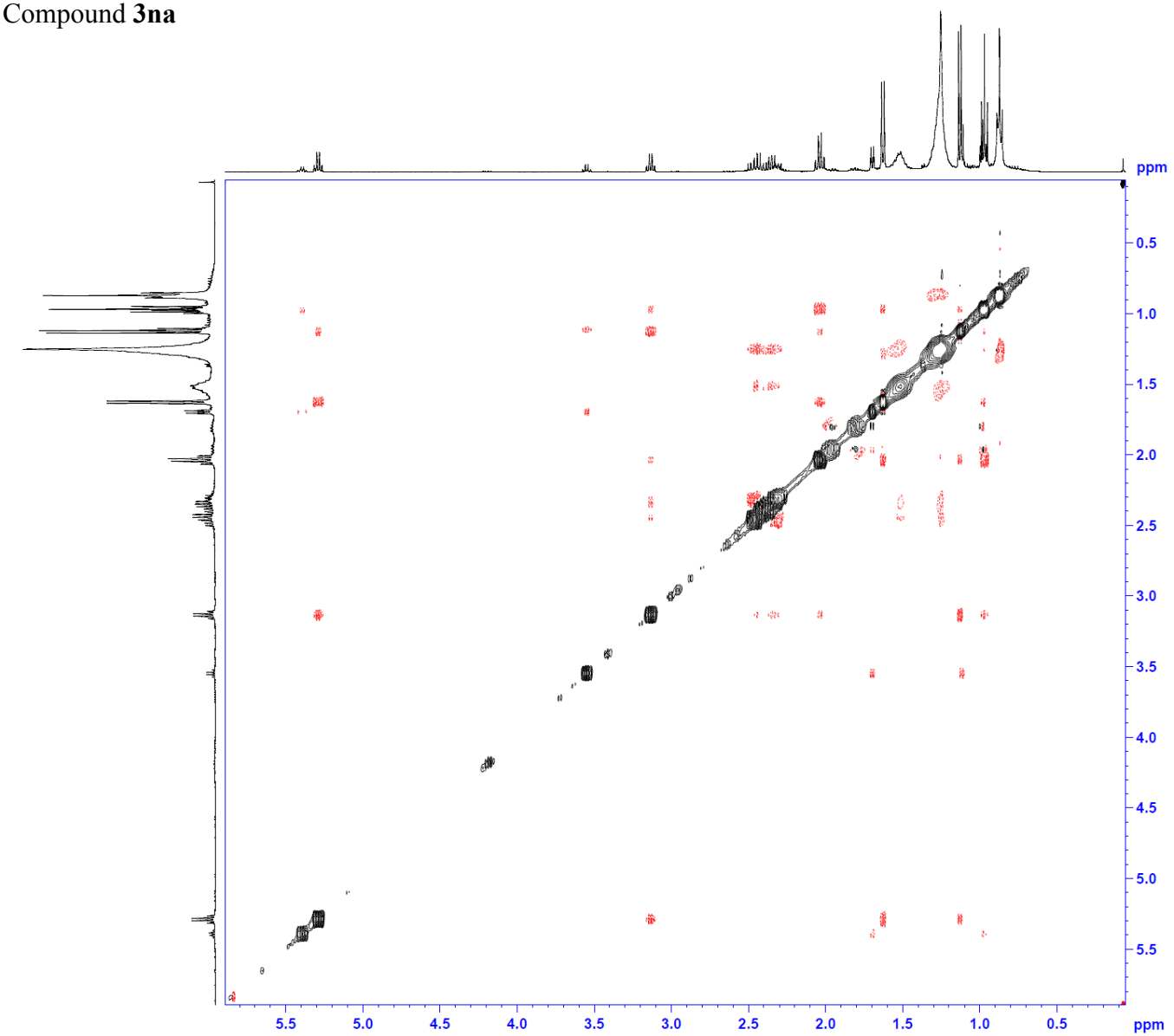
3-Phenyl-1*H*-inden-1-one (9)

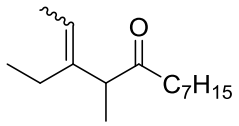
^{13}C NMR (100 MHz)



6. NOESY Spectral Charts

6.1. Compound **3na**





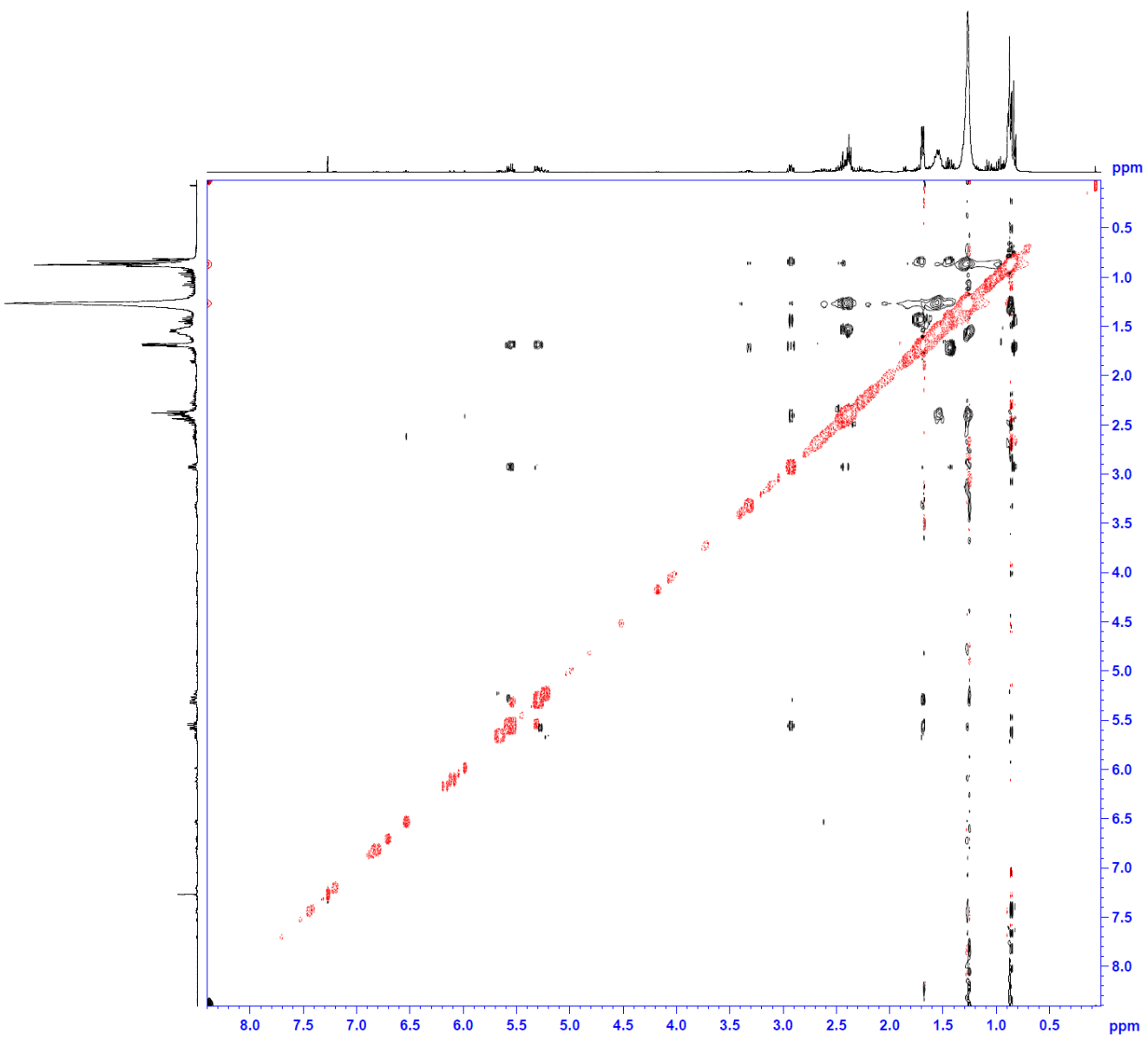
3na

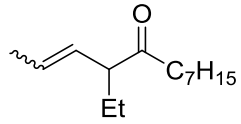
```
NAME                 esp6-6
EXPNO                     3
PROCNO                    1
Date_              20181107
Time                 22.13
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG          noesygpph
TD                     4096
SOLVENT              CDCl3
NS                        16
DS                         4
SWH                2336.448 Hz
FIDRES             0.570422 Hz
AQ                 0.8765940 sec
RG                        64
DW                  214.000 usec
DE                    6.50 usec
TE                  296.0 K
D0                 0.00019490 sec
D1                 6.00000000 sec
D8                 2.50000000 sec
D16                0.00020000 sec
IN0                0.00042800 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
P2                    30.00 usec
PL1                   -0.50 dB
PL1W              13.47187042 W
SFO1              400.0311982 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPZ1                  40.00 %
P16                 1000.00 usec
ND0                       1
TD                      256
SFO1              400.0312 MHz
FIDRES            9.126752 Hz
SW                    5.841 ppm
FnMODE            States-TPPI
SI                      1024
SF                400.0300082 MHz
WDW                    QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
PC                     1.00
SI                      1024
MC2               States-TPPI
SF                400.0300082 MHz
WDW                    QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
```

6.2. Compound 3ta





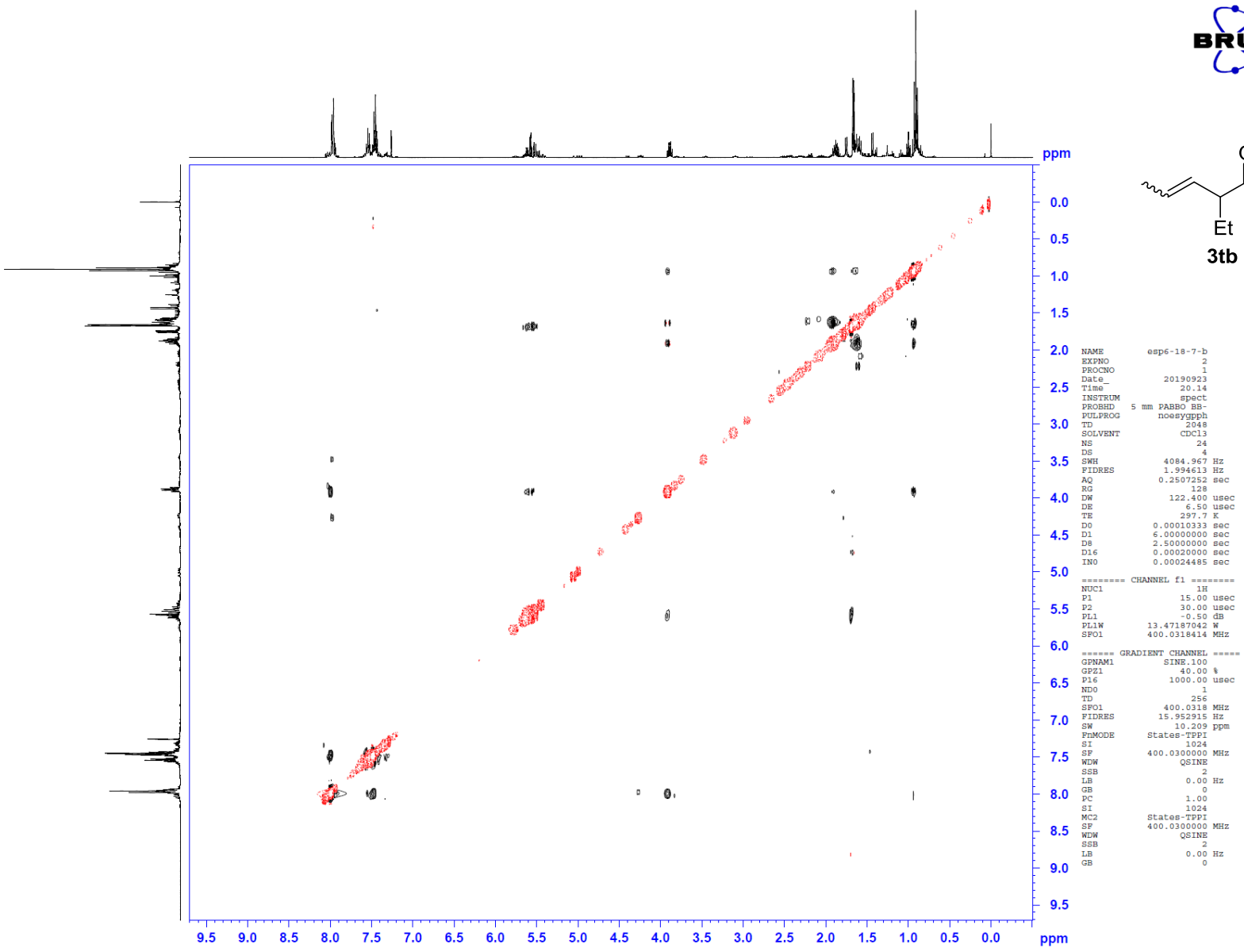
3ta

```
NAME          esp6-18-6-a
EXPNO                   2
PROCNO                  1
Date_            20190922
Time                20.14
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG         noesygpph
TD                   2048
SOLVENT             CDCl3
NS                     24
DS                      4
SWH               3355.705 Hz
FIDRES            1.638528 Hz
AQ                0.3052020 sec
RG                     64
DW                 149.000 usec
DE                   6.50 usec
TE                 298.0 K
D0                0.00012990 sec
D1                6.00000000 sec
D8                2.50000000 sec
D16               0.00020000 sec
IN0               0.00029800 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
P2                  30.00 usec
PL1                 -0.50 dB
PL1W           13.47187042 W
SFO1          400.0316919 MHz

====== GRADIENT CHANNEL =====
GPNAM1            SINE.100
GPZ1                40.00 %
P16               1000.00 usec
ND0                     1
TD                    256
SFO1            400.0317 MHz
FIDRES          13.108221 Hz
SW                  8.389 ppm
FnMODE         States-TPPI
SI                   1024
SF            400.0300075 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.00
SI                   1024
MC2            States-TPPI
SF            400.0300075 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

6.2. Compound 3tb



3tb

```
NAME          esp6-18-7-b
EXPNO                   2
PROCNO                  1
Date_            20190923
Time                20.14
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG         noesygpph
TD                   2048
SOLVENT             CDCl3
NS                     24
DS                      4
SWH              4084.967 Hz
FIDRES           1.994613 Hz
AQ               0.2507252 sec
RG                    128
DW                122.400 usec
DE                  6.50 usec
TE                297.7 K
D0             0.00010333 sec
D1             6.00000000 sec
D8             2.50000000 sec
D16            0.00020000 sec
IN0            0.00024485 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
P2                 30.00 usec
PL1                -0.50 dB
PL1W          13.47187042 W
SFO1         400.0318414 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPZ1                40.00 %
P16               1000.00 usec
NDO                    1
TD                   256
SFO1           400.0318 MHz
FIDRES         15.952915 Hz
SW                10.209 ppm
FnMODE        States-TPPI
SI                  1024
SF           400.0300000 MHz
WDW                QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
PC                  1.00
SI                  1024
MC2           States-TPPI
SF           400.0300000 MHz
WDW                QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
```