Supporting Information For:

Indium or Zinc-Mediated One-Pot Synthesis of Homoallylamines, β-Amino Esters, and β-Amino Nitriles

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General. Reagents were obtained from commercial sources. Indium powder was purchased from Aldrich (99.99%, stabilized with 1% MgO). Particularly oxidizable aldehydes such as benzaldehyde and isobutyraldehyde were distilled from time to time. All liquid aldehydes were stored under nitrogen in the cold. Allyl bromide was stored in the cold and sometimes redistilled over P_4O_{10} when its water content became too high (decreased reactivity with indium under the employed reaction conditions). Tetrahydrofuran (THF) was distilled from sodium and benzophenone. All reactions were run in flamed-dried glassware under nitrogen and magnetic stirring. Column chromatography of all amines was performed on basic alumina (Acros organics, 50-200 μm). Thin layer chromatography (TLC) was carried out on aluminium sheets precoated with silica gel 60 F_{254} (E. Merck). The plates were inspected by UV light followed by development with iodine vapor. Melting points were determined with a Kofler bench or an heating microscope. IR spectra were recorded on a Nicolet 205 FT-IR spectrometer and are reported in wavenumbers (cm^{-1}). NMR spectra were measured using dilute solutions on a Brucker ARX 400 (^1H at 400.13 MHz, ^{13}C at 100.61 MHz) spectrometer. Chemical shifts are reported in ppm on the δ scale from tetramethylsilane (TMS) which is used as an internal standard. Elemental analyses were performed by ICSN (Gif sur Yvette). High-resolution mass spectra (HRMS) were obtained under electronic impact at 70 eV from a Varian MAT 311 spectrometer at the Centre Régional de Mesures Physiques de l'Ouest (Rennes).

Representative procedures.

Synthesis of homoallylamines: In a two-necked reaction flask equipped with a condenser (in all these expeiments, air cooling was sufficient and no circulation of tap water was used) connected to an oil bubbler, benzaldehyde (102 μl, 1 mmole) was injected through a septum followed by dibenzylamine (202 μl, 1.05 mmole) and titanium(IV) isopropoxide (342 μl, 1.15 mmole). This reaction mixture was smoothly stirred at 40 °C for 2 hours and then allowed to cool at rt. Vacuum was cautiously applied to remove 2-propanol formed as visualized by foaming. As viscosity increased, removal of 2-propanol

was completed by applying vacuum while heating at 40 °C under stirring for *ca.* 40 min. After cooling at rt, anhydrous THF (1 mL) was introduced under nitrogen followed by indium powder (92 mg, 0.8 mmole) or zinc dust (82 mg, 1.25 mmole) and allyl bromide (130 μl, 1.5 mmole). The resulting mixture was smoothly stirred at 30 °C for 4 hours and then allowed to cool at rt. Saturated aqueous sodium carbonate (5 mL) was added during which indium or zinc hydroxide and titanium dioxide precipitated. This resulting mixture was extracted and the settled minerals were washed with ether (4 x *ca.* 10 mL). After drying of the organic extracts (Na_2SO_4), filtration of suspended minerals over a short pad of celite, and concentration, the remaining residue was purified by chromatography on basic alumina (4 g) with elution by petroleum ether. The homoallylamine **2** (R = Ph, R' = Bn) [1-dibenzylamino-1-phenylbut-3-ene] eluted rapidly as showed by TLC and was isolated after removal of solvent.

Synthesis of β-amino esters: The same procedure as previously described for the synthesis of **2** (R = Ph, R' = Bn) was followed except that allyl bromide was replaced by isopropyl bromoacetate (162 μl, 1.25 mmole) with further reaction at 40 °C for 40 h in darkness (wrapping with an aluminium foil). Additionaly to prevent any leak of solvent as reaction time was far longer, hermetic sealing was realized by putting a second reversed septum on the lateral neck and by tight stoppering of the top of the condenser. Work-up was performed by addition of 5% aqueous sodium bicarbonate (5 mL) instead of aqueous Na_2CO_3 (to prevent a possible saponification). After the same extractive procedures, another difference was that the crude product needed to be dissolved in hot petroleum ether before its deposit on basic alumina. Elution with petroleum ether afforded a small amount of isopropyl dibenzylaminoacetate (a few %, R_f = 0.37 (ethyl acetate / petroleum ether 1:9)) followed by more polar β-amino ester **3** (R = Ph) [isopropyl 3-dibenzylamino-3-phenylpropanoate].

Synthesis of β-amino nitriles: The same procedure as previously described for the synthesis of **3** was followed using iodoacetonitrile (87 μl, 1.2 mmole) as a reactive halide with further reaction at 40 °C for 18 h in darkness (aluminium foil). Addition of saturated aqueous sodium carbonate (5 mL) followed by the same extractive procedure with ether afforded an oily colored residue. Chromatography on basic alumina (8 g) with transfer using petroleum ether plus a minimum amount of toluene, and gradient elution from petroleum ether to petroleum ether+3% ethyl acetate afforded solid β-amino nitrile **4** (R = Ph, R' = Bn) which still contained yellow impurities. Purification was completed by recristallization in petroleum ether+10% ethyl acetate to afford white crystals melting at 109 °C.

In all the described reactions with diallylamine, 157 μl *e.g.* 1.25 mmole was used starting from 1 mmole of aldehyde.

PHYSICAL DATA OF THE COMPOUNDS

1-Dibenzylamino-1-phenylbut-3-ene (**2**: R = Ph, R' = Bn): Colorless oil which readily cristallized yielding white crystals, m.p. 61-63 °C (petroleum ether); R_f = 0.54 (ethyl acetate / petroleum ether 1:9); IR (CCl_4, KBr) ν 3085, 3064, 3029, 2930, 2835, 2803, (1947, 1882, 1873, and 1810: small, aromatic harmonics), 1641, 1603, 1494, 1455, 1120, 1073, 1029, 971, 912, 699 cm^{-1}; ^1H NMR (400 MHz,

$CDCl_3$): δ = 7.41-7.32 (m, 6H aromatic), 7.32-7.24 (m, 5H aromatic), 7.24-7.17 (m, 4H aromatic), 5.79 (dddd, 1H, *J* = 17.2, 10.1, 7.2, 6.3 Hz, H-C_3), 5.04 (ddt, 1H, *J* = 17.1, 1.9, 1.5 Hz, H-C_4), 4.99 (ddt, 1H, *J* = 10.1, 2.0, 1.2 Hz, H-C_4), 3.81 (dd, 1H, *J* = 7.9, 7.5 Hz, H-C_1), 3.79 (d, 2H, *J* = 13.9 Hz, C$\underline{H}_2$Ph), 3.18 (d, 2H, *J* = 13.9 Hz, C$\underline{H}_2$Ph), 2.84 (dddt, 1H, *J* = 14.7, 7.5, 7.2, 1.3 Hz, H-C_2), 2.55 (dddt, 1H, *J* = 14.5, 7.9, 6.3, 1.5 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.17 (2 C_{ipso} of Bn), 138.51 (C_{ipso} of Ph), 136.63 (dtddd, *J* = 153.1, 6.4, 3.3, 2.5, 0.9 Hz, C_3 *e.g.* $\underline{C}$H=CH_2), 128.93 (dm, *J* = 157.1 Hz, 2 $\underline{C}H_{ortho}$ of Ph), 128.75 (dm, *J* = 158.1 Hz, 4 $\underline{C}H_{ortho}$ of Bn), 128.17 (broad dd, *J* = 159.3, 7.6 Hz, 4 $\underline{C}H_{meta}$ of Bn), 127.89 (ddm, *J* = 159.6, 7.6 Hz, 2 $\underline{C}H_{meta}$ of Ph), 127.04 (dddd, *J* = 160.1, 7.8, 7.1, 1.1 Hz, $\underline{C}H_{para}$ of Ph), 126.76 (broad dt, *J* = 160.0, 7.5 Hz, 2 $\underline{C}H_{para}$ of Bn), 116.07 (ddt, *J* = 157.5, 153.5, 6.0 Hz, C_4), 61.48 (dm, *J* = 134.9 Hz, C_1), 53.47 (tttd, *J* = 131.9, 4.3, 4.2, 3.7 Hz, 2 $\underline{C}H_2$Ph), 35.29 (tddt, *J* = 126.0, 11.5, 7.0, 4.5 Hz, C_2); elemental analysis calcd for $C_{24}H_{25}N$ (327.47): C 88.03, H 7.69, N 4.28; found: C 88.25, H 7.61, N 4.28.

1-(4-Bromophenyl)-1-dibenzylaminobut-3-ene (**2**: R = *p* -Br-C_6H_4, R' = Bn): White crystals melting at 99 °C (petroleum ether); R_f = 0.54 (ethyl acetate / petroleum ether 1:19); IR (CCl_4, KBr) ν 3086, 3066, 3029, 2931, 2835, 2803, 1641, 1603, 1588, 1494, 1455, 1074, 1012, 913, 699, 539 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d pseudo t, 2H, *J* = 8.8, 2.6-1.9 Hz), 7.36 (pseudo dm, 4H, *J* ≈ 8 Hz, H_{ortho} of Bn), 7.30 (t pseudo t, 4H, *J* ≈ 7.5, 1.5 Hz, H_{meta} of Bn), 7.22 (ddt, 2H, *J* = 8.1, 6.3, 1.4 Hz, H_{para} of Bn), 7.10 (d pseudo t, 2H, *J* = 8.8, 2.6-1.9 Hz), 5.74 (dddd, 1H, *J* = 17.1, 10.2, 6.9, 6.7 Hz, H-C_3), 5.04 (ddt, 1H, *J* = 17.1, 1.9, 1.5 Hz, H-C_4), 5.00 (ddt, 1H, *J* = 10.2, 1.9, 1.2 Hz, H-C_4), 3.77 (dd, 1H, *J* = 7.9, 7.6 Hz, H-C_1), 3.77 (d, 2H, *J* = 13.8 Hz, C$\underline{H}_2$Ph), 3.18 (d, 2H, *J* = 13.7 Hz, C$\underline{H}_2$Ph), 2.82 (dddt, 1H, *J* = 14.5, 7.6, 6.9, 1.3 Hz, H-C_2), 2.53 (dddt, 1H, *J* = 14.5, 7.9, 6.7, 1.4 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.83 (2 C_{ipso} of Bn), 137.72 (C_{ipso} δ to Br), 136.13 (C_3), 131.05 (2 $\underline{C}$H β to Br), 130.58 (2 $\underline{C}$H γ to Br), 128.70 (4 $\underline{C}H_{ortho}$ of Bn), 128.26 (4 $\underline{C}H_{meta}$ of Bn), 126.90 (2 $\underline{C}H_{para}$ of Bn), 120.94 (C_{ipso} α to Br), 116.47 (C_4), 60.92 (C_1), 53.45 (2 $\underline{C}H_2$Ph), 34.88 (C_2).

1-Dibenzylamino-1-(4-methoxyphenyl)but-3-ene (**2**: R = *p*-MeO-C_6H_4, R' = Bn): White crystals melting at 93 °C; R_f = 0.39 (ethyl acetate / petroleum ether 1:9); IR (CCl_4, KBr) ν 3085, 3064, 3028, 3004, 2932, 2835, 2802, (2062, 1948, 1885, 1873, and 1812: small, aromatic harmonics), 1640, 1609, 1583, 1512, 1494, 1455, 1305, 1250, 1179, 1100, 1072, 1038, 1029, 971, 911, 862, 832, 699, 549 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (pseudo dm, 4H, *J* ≈ 7.5 Hz, H_{ortho} of Bn), 7.30 (psreudo tt, 4H, *J* = 7.5, 1.5 Hz, H_{meta} of Bn), 7.21 (ddt, 2H, *J* = 8.1, 6.4, 1.3 Hz, H_{para} of Bn), 7.15 (d pseudo t, 2H, *J* = 8.7, 2.5 Hz), 6.90 (d pseudo t, 2H, *J* = 8.7, 2.5 Hz), 5.78 (dddd, 1H, *J* = 17.2, 10.2, 7.1, 6.5 Hz, H-C_3), 5.03 (ddt, 1H, *J* = 17.2, 1.9, 1.5 Hz, H-C_4), 4.99 (ddt, 1H, *J* = 10.2, 1.9, 1.2 Hz, H-C_4), 3.82 (s, 3H, OMe), 3.78 (d, 2H, *J* = 13.8 Hz, C$\underline{H}_2$Ph), 3.77 (dd, 1H, *J* = 7.9, 7.6 Hz, H-C_1), 3.18 (d, 2H, *J* = 13.8 Hz, C$\underline{H}_2$Ph), 2.83 (dddt, 1H, *J* = 14.5, 7.6, 7.1, 1.2 Hz, H-C_2), 2.54 (dddt, 1H, *J* = 14.5, 7.9, 6.5, 1.4 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.53 (C_{ipso} α to OMe), 140.28 (2 C_{ipso} of Bn), 136.79 (C_3), 130.62 (C_{ipso} δ to OMe), 129.95 (2 $\underline{C}$H γ to OMe), 128.75 (4 $\underline{C}H_{ortho}$ of Bn), 128.17 (4 $\underline{C}H_{meta}$ of Bn), 126.73 (2 $\underline{C}H_{para}$ of Bn), 115.96 (C_4), 113.22 (2 $\underline{C}$H β to OMe), 60.79 (C_1), 55.19 (OMe), 53.43 (2 $\underline{C}H_2$Ph), 35.46 (C_2); HRMS (EI, 70 eV) *m/z* (%): calcd for $C_{22}H_{22}NO$ 316.1701 [M – $CH_2CH=CH_2$]$^+$, found 316.1698 (45), 224 (5.5) [$PhCH_2$-N=C-C_6H_4-OMe]$^+$, 121 (7.3) [*p*-MeO-

$C_6H_4CH_2]^+$, 107 (1.0) [*p*-MeO-$C_6H_4]^+$, 91 (100), $[C_7H_7]^+$, 65 (3.5), $[C_5H_5]^+$.

1-Cyclohexyl-1-dibenzylaminobut-3-ene (**2**: R = *c*-C_6H_{11}, R' = Bn): Colorless oil; R_f = 0.60 (ethyl acetate/petroleum ether 1:19); IR (neat, KBr) ν 3084, 3063, 3027, 2924, 2851, 2798, (1945, 1869, and 1807: small, aromatic harmonics), 1637, 1603, 1494, 1452, 1028, 980, 906, 745, 698 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36 (pseudo dm, 4H, *J* ≈ 8 Hz, H_{ortho}), 7.28 (pseudo tt, 4H, *J* = 7.4, 1.5 Hz, H_{meta}), 7.20 (ddt, 2H, *J* = 8.1, 6.4, 1.4 Hz, H_{para}), 5.84 (dddd, 1H, *J* = 17.1, 10.1, 7.0, 6.9 Hz, H-C_3), 5.04 (ddt, 1H, *J* = 17.1, 1.9, 1.6 Hz, H-C_4), 4.98 (ddt, 1H, *J* = 10.1, 1.9, 1.3 Hz, H-C_4), 3.75 (d, 2H, *J* = 13.8 Hz, C$\underline{H}_2$Ph), 3.52 (d, 2H, *J* = 13.8 Hz, C$\underline{H}_2$Ph), 2.46 (dddt, 1H, *J* = 14.3, 7.0, 5.6, 1.4 Hz, H-C_2), 2.40 (ddd, 1H, *J* = 7.2, 5.7, 5.6 Hz, H-C_1), 2.18 (dddt, 1H, *J* = 14.3, 6.9, 5.7, 1.3 Hz, H-C_2), 2.09 (dm, 1H, *J* = 13.0 Hz, H equatorial which correlates with C at 31.12 ppm), 1.73-1.47 (m, 5H, 4H equatorial β and γ to C_1 at 1.73-1.56 ppm, and H α to C_1 at 1.54 ppm), 1.25-1.00 (m, 3H axial with 1H δ to C_1 tdt at 1.07 ppm, 2 J_{aa} = 12.4 Hz, J_{gem} = 12.0 Hz, 2 J_{ae} = 3.2 Hz), 0.98-0.78 (m, 2H axial β to C_1 which correlates with C at 31.02 and 31.12 ppm); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.53 (2 C_{ipso}), 139.04 (C_3), 128.93 (4 $\underline{C}H_{ortho}$), 128.04 (4 $\underline{C}H_{meta}$), 126.62 (2 $\underline{C}H_{para}$), 115.14 (C_4), 62.05 (C_1), 54.35 (2 $\underline{C}H_2$Ph), 40.23 ($\underline{C}$H α to C_1), 31.45 (C_2), 31.12 and 31.02 (2 $\underline{C}H_2$ β to C_1), 26.66, 26.64, and 26.62 (2 $\underline{C}H_2$ γ to C_1 and $\underline{C}H_2$ δ to C_1); HRMS (EI, 70 eV) *m/z* (%): calcd for $C_{21}H_{26}N$ 292.2065 $[M - CH_2CH{=}CH_2]^+$, found 292.2071 (67), 250 (13) $[M - C_6H_{11}]^+$, 91 (100), $[C_7H_7]^+$, 65 (1.9) $[C_5H_5]^+$.

3-Dibenzylamino-2-methylhex-5-ene (**2**: R = *i*-Pr, R' = Bn): See compound **22** in L. Tussa, C. Lebreton, P. Mosset, *Chem. Eur. J.* **1997**, *3*, 1064-1070.

3-Dibenzylamino-1-phenylhex-5-ene (**2**: R = $PhCH_2CH_2$, R' = Bn): Slightly yellow oil; R_f = 0.55 (ethyl acetate/petroleum ether 1:9); IR (neat, KBr) ν 3084, 3062, 3026, 2930, 2800, 1946 and 1870 and 1807 (harmonics of Ph), 1639, 1602, 1494, 1454, 1363, 1073, 1029, 909, 746 with a shoulder at 730, 698, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36 (pseudo dm, 4H, *J* = 8.2 Hz, H_{ortho} of Bn), 7.29 (pseudo tt, 4H, *J* = 7.4, 1.6 Hz, H_{meta} of Bn), 7.25-7.18 (m, 4H, 2H_{meta} of Ph and 2H_{para} of Bn), 7.13 (ddt, 1H, *J* = 8.2, 6.5, 1.4 Hz, H_{para} of Ph), 7.06 (dm, 2H, *J* = 6.8 Hz, H_{ortho} of Ph), 5.72 (dddd, 1H, *J* = 17.0, 10.2, 7.5, 6.5 Hz, H-C_5), 5.00 (ddt, 1H, *J* = 17.0, 2.1, 1.4 Hz, H-C_6), 4.97 (ddt, 1H, *J* = 10.2, 2.1, 1.1 Hz, H-C_6), 3.70 (d, 2H, *J* = 13.7 Hz, C$\underline{H}_2$Ph), 3.51 (d, 2H, *J* = 13.7 Hz, C$\underline{H}_2$Ph), 2.84 (ddd, 1H, *J* = 13.7, 10.5, 5.5 Hz, H-C_1), 2.66 (dddd, 1H, *J* = 8.2, 8.2, 5.7, 5.1 Hz, H-C_3), 2.51 (dddt, 1H, *J* = 14.0, 6.5, 5.1, 1.4 Hz, H-C_4), 2.41 (ddd, 1H, *J* = 13.7, 10.5, 5.7 Hz, H-C_1), 2.03 (dddt, 1H, *J* = 14.0, 8.2, 7.5, 1.2 Hz, H-C_4), 1.82 (dddd, 1H, *J* = 13.9, 10.5, 8.2, 5.7 Hz, H-C_2), 1.63 (dddd, 1H, *J* = 13.9, 10.5, 5.7, 5.5 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.91 (C_{ipso} of Ph), 140.34 (2 C_{ipso} of Bn), 137.29 (C_5 *e.g.* $\underline{C}H{=}CH_2$), 128.91 (4 $\underline{C}H_{ortho}$ of Bn), 128.35 (2 $\underline{C}H_{ortho}$ of Ph), 128.26 (2 $\underline{C}H_{meta}$ of Ph), 128.15 (4 $\underline{C}H_{meta}$ of Bn), 126.75 (2 $\underline{C}H_{para}$ of Bn), 125.55 ($\underline{C}H_{para}$ of Ph), 115.96 (C_6), 57.15 (C_3), 53.42 (2 $\underline{C}H_2$Ph), 33.64 (C_4), 33.48 (C_1), 32.56 (C_2); HRMS (EI, 70 eV) *m/z* (%): calcd for $C_{26}H_{29}N$ 355.2300 $[M]^+$, found 355.2317 (0.3), calcd for $C_{23}H_{24}N$ 314.1909 $[M - CH_2CH{=}CH_2]^+$, found 314.1910 (71), 250 (2.1) $[M - CH_2CH_2Ph]^+$, 91 (100), $[C_7H_7]^+$, 65 (4.4), $[C_5H_5]^+$.

1-Diallylamino-1-phenylbut-3-ene (**2**: R = Ph, R' = allyl): Colorless liquid; R_f = 0.54 (ethyl acetate / petroleum ether 1:9); IR (neat, KBr) ν 3077, 3028, 3006, 2977, 2927, 2812, 1641, 1601, 1493, 1452, 1417, 995, 916, 758, 746, 702, 649, 543 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.29 (m, 2H, H_{meta} of Ph), 7.27-7.22 (m, 3H, H_{ortho} and H_{para} of Ph), 5.82 (dddd, 2H, *J* = 17.3, 10.1, 7.2, 5.3 Hz, $N(CH_2C\underline{H}=CH_2)_2$), 5.70 (dddd, 1H, *J* = 17.1, 10.2, 6.9, 6.9 Hz, H-C_3 *e.g.* $CH_2C\underline{H}=CH_2$), 5.16 (dddd, 2H, *J* = 17.3, 2.0, 1.7, 1.4 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 5.11 (dddd, 2H, *J* = 10.1, 2.0, 1.7, 0.9 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 4.99 (ddt, 1H, *J* = 17.1, 2.0, 1.5 Hz, H-C_4), 4.93 (ddt, 1H, *J* = 10.2, 2.0, 1.2 Hz, H-C_4), 3.82 (dd, 1H, *J* = 8.5, 6.4 Hz, H-C_1), 3.26 (dddd, 2H, *J* = 14.4, 5.2, 1.7, 1.7 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.83 (dddd, 2H, *J* = 14.4, 7.3, 1.4, 0.9 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.68 (ddddd, 1H, *J* = 14.2, 6.9, 6.4, 1.5, 1.2 Hz, H-C_2), 2.52 (ddddd, 1H, *J* = 14.2, 8.5, 6.9, 1.5, 1.2 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.83 (C_{ipso} of Ph), 136.84 (2C, $N(CH_2\underline{C}H=CH_2)_2$), 136.37 ($C_3$), 128.72 (2C, $\underline{C}H_{ortho}$ of Ph), 127.92 (2C, $\underline{C}H_{meta}$ of Ph), 126.93 ($\underline{C}H_{para}$ of Ph), 116.86 (2C, $N(CH_2CH=\underline{C}H_2)_2$), 116.04 ($C_4$), 63.29 ($C_1$), 52.61 (2C, $N(\underline{C}H_2CH=CH_2)_2$), 36.50 ($C_2$).

4-Diallylamino-3-ethylhept-6-ene (**2**: R = $CHEt_2$, R' = allyl): Colorless liquid; R_f = 0.55 (ethyl acetate / petroleum ether 1:19); IR (neat, KBr) ν 3078, 3007, 2965, 2933, 2876, 2806, 1640, 1460, 1450, 1417, 1379, 1264, 1159, 1101, 995, 915 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 5.86 (dddd, 1H, *J* = 17.1, 10.1, 7.2, 6.9 Hz, H-C_6 *e.g.* $CH_2C\underline{H}=CH_2$), 5.77 (dddd, 2H, *J* = 17.2, 10.0, 7.3, 5.1 Hz, $N(CH_2C\underline{H}=CH_2)_2$), 5.12 (dddd, 2H, *J* = 17.2, 2.0, 1.8, 1.4 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 5.04 (dddd, 2H, *J* = 10.0, 2.0, 1.7, 1.1 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 5.02 (ddt, 1H, *J* = 17.1, 2.0, 1.6 Hz, H-C_7), 4.95 (ddt, 1H, *J* = 10.1, 2.0, 1.2 Hz, H-C_7), 3.20 (dddd, 2H, *J* = 14.4, 5.1, 1.8, 1.7 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 3.01 (dddd, 2H, *J* = 14.4, 7.3, 1.4, 1.1 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.66 (ddd, 1H, *J* = 7.0, 6.4, 5.8 Hz, H-C_4), 2.28 (dddt, 1H, *J* = 14.7, 6.9, 6.4, 1.4 Hz, H-C_5), 2.11 (dddt, 1H, *J* = 14.7, 7.2, 5.8, 1.4 Hz, H-C_5), 1.55-1.42 (m, 2H, $C\underline{H}_2CH_3$), 1.39-1.27 (m, 2H, $C\underline{H}_2CH_3$), 1.25-1.13 (m, 1H, H-C_3), 0.83 (t, 3H, *J* = 7.4 Hz, $C\underline{H}_3$), 0.81 (t, 3H, *J* = 7.2 Hz, $C\underline{H}_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.90 (C_6), 138.06 (2C, $N(CH_2\underline{C}H=CH_2)_2$), 115.85 (2C, $N(CH_2CH=\underline{C}H_2)_2$), 115.02 ($C_7$), 59.71 ($C_4$ *e.g.* $\underline{C}$H-N), 53.53 (2C, $N(\underline{C}H_2CH=CH_2)_2$), 43.02 ($C_3$ *e.g.* $\underline{C}HEt_2$), 32.34 (C_5), 21.80 ($\underline{C}H_2CH_3$), 21.74 ($\underline{C}H_2CH_3$), 11.23 ($\underline{C}H_3$), 10.80 ($\underline{C}H_3$).

Isopropyl 3-dibenzylamino-3-phenylpropanoate (**3**: R = Ph, R' = Bn): White crystals melting at 62 °C (petroleum ether); R_f = 0.32 (ethyl acetate / petroleum ether 1:9); IR (CCl_4, KBr) ν 3444 (very small, overtone of C=O), 3086, 3063, 3029, 2980, 2934, 2836, 2805, (1948, 1876, and 1809: small, aromatic harmonics), 1732 (C=O), 1603, 1585 (small), 1494, 1454, 1374, 1258, 1170, 1108, 1082, 1074, 1029, 975, 908, 699 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39-7.32 (m, 6H aromatic), 7.32-7.25 (m, 7H aromatic), 7.21 (ddt, 2H, *J* = 8.1, 6.3, 1.3 Hz, H_{para} of Bn), 4.93 (septet, 1H, *J* = 6.3 Hz, $OC\underline{H}(CH_3)_2$), 4.31 (dd, 1H, *J* = 8.2, 7.3 Hz, H-C_3 e.g. $C\underline{H}$-N), 3.72 (d, 2H, *J* = 13.7 Hz, $C\underline{H}_2Ph$), 3.27 (d, 2H, *J* = 13.7 Hz, $C\underline{H}_2Ph$), 3.05 (dd, 1H, *J* = 14.5, 7.3 Hz, H-C_2), 2.75 (dd, 1H, *J* = 14.5, 8.2 Hz, H-C_2), 1.15 (d, 3H, *J* = 6.3 Hz, $C\underline{H}_3$), 1.10 (d, 3H, *J* = 6.3 Hz, $C\underline{H}_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.26 (C_1), 139.68 (2 C_{ipso} of Bn), 138.14 (C_{ipso} of Ph), 128.78 (4 $\underline{C}H_{ortho}$ of Bn), 128.57 (2 $\underline{C}H_{ortho}$ of Ph), 128.18 (4 $\underline{C}H_{meta}$ of Bn), 128.02 (2 $\underline{C}H_{meta}$ of Ph), 127.33 ($\underline{C}H_{para}$ of Ph), 126.90 (2

$\underline{C}H_{para}$ of Bn), 67.80 ($O\underline{C}H(CH_3)_2$), 59.07 (C_3), 53.83 (2 $\underline{C}H_2Ph$), 36.50 (C_2), 21.72 ($\underline{C}H_3$), 21.71 ($\underline{C}H_3$); HRMS (EI, 70 eV) *m/z* (%): calcd for $C_{26}H_{29}NO_2$ 387.2198 $[M]^+$, found 387.2181 (2.8), 310 (1.3) $[M-Ph]^+$, 296 (8.5) $[M-CH_2Ph]^+$, 286 (80) $[M-CH_2CO_2i\text{-}Pr]^+$, 196 (22) $[(PhCH_2)_2N]^+$, 91 (100), $[C_7H_7]^+$, 77 (0.9) $[C_6H_5]^+$, 65 (3.1), $[C_5H_5]^+$; elemental analysis calcd for $C_{26}H_{29}NO_2$ (387.52): C 80.59, H 7.54, N 3.61; found: C 80.15, H 7.91, N 3.54.

Isopropyl 3-dibenzylamino-3-(4-fluorophenyl)propanoate (**3**: R = *p*-F-C_6H_4, R' = Bn): White crystals melting at 85 °C (petroleum ether); R_f = 0.30 (ethyl acetate / petroleum ether 1:9); IR (CCl_4, KBr) ν 3429 (very small, overtone of C=O), 3086, 3064, 3029, 2981, 2935, 2836, 2825, 2806, (1954, 1894, and 1811: small, aromatic harmonics), 1728 (C=O), 1603, 1585 (small), 1509, 1495, 1454, 1373, 1355, 1307, 1278, 1256, 1224, 1170, 1161, 1109 (with a shoulder at 1098), 1075, 1046, 1030, 983, 973, 910, 873, 839, 826, 736, 700, 560, 533, 515 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 (pseudo dm, 4H, $J \approx 7.5$ Hz, H_{ortho} of Bn), 7.30 (pseudo tt, 4H, $J \approx 7.5$, 1.5 Hz, H_{meta} of Bn), 7.24 (dd pseudo t, 2H, J_{HF} = 5.0 Hz, J_{HH} = 9.0, 3.1-2.1 Hz, H γ to F), 7.22 (ddt, 2H, J = 7.9, 6.1, 1.6 Hz, H_{para} of Bn), 7.04 (dd pseudo t, 2H, J_{HF} = 8.4 Hz, J_{HH} = 9.0, 3.1-2.1 Hz, H β to F), 4.92 (qq, 1H, J = 6.3, 6.3 Hz, $C\underline{H}Me_2$), 4.29 (dd, 1H, J = 8.6, 6.8 Hz, H-C_3), 3.68 (d, 2H, J = 13.7 Hz, $C\underline{H}_2Ph$), 3.27 (d, 2H, J = 13.7 Hz, $C\underline{H}_2Ph$), 3.03 (dd, 1H, J = 14.5, 6.8 Hz, H-C_2), 2.73 (dd, 1H, J = 14.5, 8.6 Hz, H-C_2), 1.14 (d, 3H, J = 6.3 Hz, $C\underline{H}_3$), 1.11 (d, 3H, J = 6.3 Hz, $C\underline{H}_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.15 (C_1), 162.04 (C_{ipso} α to F, d, J_{CF} = 245.7 Hz), 139.47 (2 C_{ipso} of Bn), 134.18 (C_{ipso} δ to F, d, J_{CF} = 3.3 Hz), 130.02 (2 $\underline{C}H$ γ to F, d, J_{CF} = 7.9 Hz), 128.74 (4 $\underline{C}H_{ortho}$ of Bn), 128.26 (4 $\underline{C}H_{meta}$ of Bn), 127.01 (2 $\underline{C}H_{para}$ of Bn), 114.87 (2 $\underline{C}H$ β to F, d, J_{CF} = 21.1 Hz), 67.92 ($O\underline{C}H(CH_3)_2$), 58.38 (C_3), 53.79 (2 $\underline{C}H_2Ph$), 36.19 (C_2), 21.71 (2 $\underline{C}H_3$).

Isopropyl 3-(4-chlorophenyl)-3-dibenzylaminopropanoate (**3**: R = *p*-Cl-C_6H_4, R' = Bn): White crystals melting at 84-85 °C (petroleum ether); R_f = 0.33 (ethyl acetate / petroleum ether 1:9); IR (CCl_4, KBr) ν 3444 (very small, overtone of C=O), 3087, 3064, 3029, 2981, 2936, 2835, 2805, (1947, 1900, 1870, 1809: small, aromatic harmonics), 1732 (C=O), 1602 (with a shoulder at 1596), 1494, 1454, 1374, 1309, 1254, 1170, 1107, 1074, 1030, 1015, 975, 908, 824, 726, 699, 539 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.27 (m, 10H, $4H_{ortho}$ of Bn + $4H_{meta}$ of Bn + 2H γ to Cl), 7.25-7.19 (m, 4H, $2H_{para}$ of Bn + 2H β to Cl), 4.92 (qq, 1H, J = 6.3, 6.3 Hz, $C\underline{H}Me_2$), 4.28 (dd, 1H, J = 8.6, 6.8 Hz, H-C_3), 3.67 (d, 2H, J = 13.7 Hz, $C\underline{H}_2Ph$), 3.27 (d, 2H, J = 13.7 Hz, $C\underline{H}_2Ph$), 3.02 (dd, 1H, J = 14.6, 6.8 Hz, H-C_2), 2.73 (dd, 1H, J = 14.6, 8.6 Hz, H-C_2), 1.15 (d, 3H, J = 6.3 Hz, $C\underline{H}_3$), 1.12 (d, 3H, J = 6.3 Hz, $C\underline{H}_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.05 (C_1), 139.35 (2 C_{ipso} of Bn), 136.96 (C_{ipso} δ to Cl), 133.09 (C_{ipso} α to Cl), 129.81 (2 $\underline{C}H$ γ to Cl), 128.73 (4 $\underline{C}H_{ortho}$ of Bn), 128.27 (4 $\underline{C}H_{meta}$ of Bn), 128.21 (2 $\underline{C}H$ β to Cl), 127.04 (2 $\underline{C}H_{para}$ of Bn), 67.98 ($O\underline{C}H(CH_3)_2$), 58.37 (C_3), 53.78 (2 $\underline{C}H_2Ph$), 35.91 (C_2), 21.72 (2 $\underline{C}H_3$).

Isopropyl 3-dibenzylamino-3-(4-methoxyphenyl)propanoate (**3**: R = *p*-MeO-C_6H_4, R' = Bn): White crystals melting at 99.5-100.5 °C (petroleum ether); R_f = 0.30 (ethyl acetate / petroleum ether 1:9); IR (CCl_4, KBr) ν 3442 (very small, overtone of C=O), 3086, 3064, 3029, 2980, 2935, 2836, 2804, (2061, 1948, 1885, 1809: small, aromatic harmonics), 1731 (C=O), 1610, 1584, 1513, 1495, 1455,

1374, 1306, 1251, 1180, 1108, 1073, 1036, 1030, 975, 909, 835, 828, 699 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35 (broad pseudo dm, 4H, $J \approx 8$ Hz, H_{ortho} of Bn), 7.29 (pseudo tt, 4H, $J \approx 7.5$, 1.5 Hz, H_{meta} of Bn), 7.21 (ddt, 2H, J = 8.1, 6.3, 1.4 Hz, H_{para} of Bn), 7.19 (d pseudo t, 2H, J = 8.7, 3.0-2.1 Hz, H arom. γ to OMe), 6.89 (d pseudo t, 2H, J = 8.7, 3.0-2.1 Hz, H arom. β to OMe), 4.93 (qq, 1H, J = 6.3, 6.2 Hz, C<u>H</u>Me_2), 4.26 (dd, 1H, J = 8.2, 7.4 Hz, H-C_3), 3.81 (s, 3H, OMe), 3.71 (d, 2H, J = 13.8 Hz, C<u>H</u>$_2$Ph), 3.25 (d, 2H, J = 13.8 Hz, C<u>H</u>$_2$Ph), 3.03 (dd, 1H, J = 14.4, 7.4 Hz, H-C_2), 2.72 (dd, 1H, J = 14.4, 8.2 Hz, H-C_2), 1.15 (d, 3H, J = 6.2 Hz, C<u>H</u>$_3$), 1.12 (d, 3H, J = 6.3 Hz, C<u>H</u>$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.33 (C_1), 158.74 (C_{ipso} α to OMe), 139.77 (2 C_{ipso} of Bn), 130.19 (C_{ipso} δ to OMe), 129.64 (2 <u>C</u>H γ to OMe), 128.78 (4 <u>C</u>H_{ortho} of Bn), 128.17 (4 <u>C</u>H_{meta} of Bn), 126.87 (2 <u>C</u>H_{para} of Bn), 113.33 (2 <u>C</u>H β to OMe), 67.78 (O<u>C</u>H$(CH_3)_2$), 58.43 (C_3), 55.21 (OMe), 53.77 (2 <u>C</u>H_2Ph), 36.72 (C_2), 21.752 (<u>C</u>H_3), 21.746 (<u>C</u>H_3).

Isopropyl 3-diallylamino-3-phenylpropanoate (**3**: R = Ph, R' = allyl): Colorless liquid; R_f = 0.35 (ethyl acetate/petroleum ether 1:9); IR (neat, KBr) ν 3442 (small, overtone of C=O), 3079, 3030, 2980, 2933, 2880, 2814, 1732 (C=O), 1642, 1602, 1583 (small), 1494, 1468, 1453, 1418, 1374, 1313, 1305, 1282, 1258, 1195, 1175, 1145, 1109, 1081, 995, 987, 968, 918, 861, 824, 764, 752, 703 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.29 (m, 2H, H_{meta} of Ph), 7.28-7.22 (m, 3H, H_{ortho} and H_{para} of Ph), 5.80 (dddd, 2H, J = 17.3, 10.2, 7.3, 5.1 Hz, N(CH_2C<u>H</u>=$CH_2)_2$), 5.16 (dddd, 2H, J = 17.3, 1.9, 1.7, 1.4 Hz, N(CH_2CH=C<u>H</u>$_2)_2$), 5.12 (dddd, 2H, J = 10.2, 1.9, 1.7, 1.0 Hz, N(CH_2CH=C<u>H</u>$_2)_2$), 4.94 (1H, qq, J = 6.3, 6.3 Hz, C<u>H</u>$(CH_3)_2$), 4.37 (dd, 1H, J = 8.1, 7.6 Hz, H-C_3), 3.23 (dddd, 2H, J = 14.3, 5.1, 1.7, 1.7 Hz, N(C<u>H</u>$_2$CH=$CH_2)_2$), 2.76 (dddd, 2H, J = 14.3, 7.3, 1.4, 1.0 Hz, N(C<u>H</u>$_2$CH=$CH_2)_2$), 2.95 (dd, 1H, J = 14.4, 8.1 Hz, H-C_2), 2.64 (dd, 1H, J = 14.4, 7.6 Hz, H-C_2), 1.17 (d, 3H, J = 6.3 Hz, C<u>H</u>$_3$), 1.14 (d, 3H, J = 6.3 Hz, C<u>H</u>$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.36 (C_1), 138.30 (C_{ipso}), 136.89 (2C, N(CH_2<u>C</u>H=$CH_2)_2$), 128.47 (2 <u>C</u>H_{ortho}), 128.01 (2 <u>C</u>H_{meta}), 127.27 (<u>C</u>H_{para}), 116.92 (2C, N(CH_2CH=<u>C</u>$H_2)_2$), 67.61 (O<u>C</u>H$(CH_3)_2$), 59.78 (C_3), 52.74 (2C, N(<u>C</u>H_2CH=$CH_2)_2$), 37.87 (C_2), 21.80 (<u>C</u>H_3), 21.72 (<u>C</u>H_3).

Isopropyl 3-(4-chlorophenyl)-3-diallylaminopropanoate (**3**: R = *p* -Cl-C_6H_4, R' = allyl): Colorless oil; R_f = 0.34 (ethyl acetate/petroleum ether 1:9); IR (neat, KBr) ν 3442 (small, overtone of C=O), 3079, 2980, 2935, 2881, 2814, 1902 and 1844 (small, aromatic harmonics), 1733 (C=O), 1643, 1594, 1492, 1468, 1451, 1417, 1374, 1310, 1255, 1174, 1146, 1108, 1094, 1015, 920, 864, 830, 540 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.29 (d pseudo t, 2H, J = 8.5, 2.5-2.0 Hz, H γ to Cl), 7.19 (d pseudo t, 2H, J = 8.5, 2.5-2.0 Hz, H β to Cl), 5.79 (dddd, 2H, J = 17.3, 10.2, 7.2, 5.3 Hz, N(CH_2C<u>H</u>=$CH_2)_2$), 5.16 (dddd, 2H, J = 17.3, 1.9, 1.7, 1.4 Hz, N(CH_2CH=C<u>H</u>$_2)_2$), 5.13 (dddd, 2H, J = 10.2, 1.9, 1.7, 1.0 Hz, N(CH_2CH=C<u>H</u>$_2)_2$), 4.94 (1H, qq, J = 6.3, 6.3 Hz, C<u>H</u>$(CH_3)_2$), 4.34 (dd, 1H, J = 8.1, 7.6 Hz, H-C_3), 3.19 (dddd, 2H, J = 14.3, 5.3, 1.7, 1.7 Hz, N(C<u>H</u>$_2$CH=$CH_2)_2$), 2.76 (dddd, 2H, J = 14.3, 7.2, 1.4, 1.0 Hz, N(C<u>H</u>$_2$CH=$CH_2)_2$), 2.92 (dd, 1H, J = 14.5, 7.6 Hz, H-C_2), 2.62 (dd, 1H, J = 14.5, 8.1 Hz, H-C_2), 1.17 (d, 3H, J = 6.3 Hz, C<u>H</u>$_3$), 1.14 (d, 3H, J = 6.3 Hz, C<u>H</u>$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.11 (C_1), 137.11 (C_{ipso} δ to Cl), 136.53 (2C, N(CH_2<u>C</u>H=$CH_2)_2$), 133.00 (C_{ipso} α to Cl), 129.73 (2 <u>C</u>H γ to Cl), 128.20 (2 <u>C</u>H β to Cl), 117.17 (2C, N(CH_2CH=<u>C</u>$H_2)_2$), 67.78 (O<u>C</u>H$(CH_3)_2$), 59.17 (C_3), 52.69 (2C, N(<u>C</u>H_2CH=$CH_2)_2$), 37.52 (C_2), 21.78 (<u>C</u>H_3), 21.71 (<u>C</u>H_3).

Isopropyl 3-cyclohexyl-3-diallylaminopropanoate (**3**: R = *c*-C_6H_{11}, R' = allyl): Colorless liquid; R_f = 0.52 (ethyl acetate/petroleum ether 1:9); IR (neat, KBr) ν 3440 (small, overtone of C=O), 3078, 3006, 2979, 2925, 2853, 2805, 1731 (C=O), 1643, 1468, 1449, 1419, 1373, 1312, 1278, 1258, 1224, 1177, 1110, 995, 962, 917, 850, 822 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 5.76 (dddd, 2H, *J* = 17.2, 10.1, 7.3, 5.0 Hz, $N(CH_2C\underline{H}=CH_2)_2$), 5.15 (dddd, 2H, *J* = 17.2, 1.9, 1.7, 1.4 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 5.06 (dddd, 2H, *J* = 10.1, 1.9, 1.7, 0.8 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 4.99 (1H, qq, *J* = 6.3, 6.3 Hz, $C\underline{H}(CH_3)_2$), 3.17 (dddd, 2H, *J* = 14.3, 5.0, 1.7, 1.7 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.96 (ddd, 1H, *J* = 8.7, 7.0, 5.2 Hz, H-C_3), 2.90 (dddd, 2H, *J* = 14.3, 7.3, 1.4, 0.8 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.44 (dd, 1H, *J* = 14.9, 5.2 Hz, H-C_2), 2.19 (dd, 1H, *J* = 14.9, 7.0 Hz, H-C_2), 2.02 (dm, 1H, *J* = 13.2 Hz), 1.76-1.65 (m, 2H), 1.65-1.56 (m, 2H), 1.38 (dddt, 1H, *J* = 11.6, 11.2, 8.4, 3.3 Hz), 1.28-1.19 (m, 1H), 1.23 (d, 3H, *J* = 6.3 Hz, $C\underline{H}_3$), 1.22 (d, 3H, *J* = 6.3 Hz, $C\underline{H}_3$), 1.19-1.07 (m, 2H), 0.97-0.83 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.30 (C_1), 137.48 (2C, $N(CH_2\underline{C}H=CH_2)_2$), 116.28 (2C, $N(CH_2CH=\underline{C}H_2)_2$), 67.47 ($O\underline{C}H(CH_3)_2$), 61.17 ($C_3$), 53.10 (2C, $N(\underline{C}H_2CH=CH_2)_2$), 41.24 ($\underline{C}H$ α to C_3), 33.83 ($\underline{C}H_2$, C_2), 30.96 and 30.35 (2 $\underline{C}H_2$ β to C_3), 26.54 and 26.45 and 26.32 (2 $\underline{C}H_2$ γ to C_3 and $\underline{C}H_2$ δ to C_3), 21.85 ($\underline{C}H_3$), 21.75 ($\underline{C}H_3$).

Isopropyl 3-diallylamino-4-ethylhexanoate (**3**: R = $CHEt_2$, R' = allyl): Colorless liquid; R_f = 0.54 (ethyl acetate/petroleum ether 1:9); IR (neat, KBr) ν 3441 (small, overtone of C=O), 3079, 2978, 2966, 2936, 2877, 2807, 1731 (C=O), 1642, 1467, 1452, 1420, 1374, 1308, 1260, 1180, 1145, 1110, 994, 963, 918, 860 (small), 823 (small) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 5.78 (dddd, 2H, *J* = 17.2, 10.1, 7.3, 5.1 Hz, $N(CH_2C\underline{H}=CH_2)_2$), 5.15 (dddd, 2H, *J* = 17.2, 2.0, 1.7, 1.4 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 5.07 (dddd, 2H, *J* = 10.1, 2.0, 1.7, 1.0 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 4.99 (1H, qq, *J* = 6.3, 6.3 Hz, $C\underline{H}(CH_3)_2$), 3.16 (dddd, 2H, *J* = 14.3, 5.1, 1.7, 1.7 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 3.14 (overlapped ddd, 1H, *J* = 7.9, 6.6, 5.5 Hz, H-C_3), 2.92 (dddd, 2H, *J* = 14.3, 7.3, 1.4, 1.0 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.46 (dd, 1H, *J* = 14.9, 5.5 Hz, H-C_2), 2.17 (dd, 1H, *J* = 14.9, 6.6 Hz, H-C_2), 1.55-1.31 (m, 4H, $(C\underline{H}_2CH_3)_2$), 1.24 (d, 3H, *J* = 6.3 Hz, $CH(C\underline{H}_3)_2$), 1.23 (d, 3H, *J* = 6.3 Hz, $CH(C\underline{H}_3)_2$), 1.20-1.06 (m, 1H, H-C_4 *e.g.* $C\underline{H}Et_2$), 0.83 (pseudo t, 3H, *J* = 7.3 Hz, $CH(CH_2C\underline{H}_3)_2$), 0.81 (pseudo t, 3H, *J* = 7.3 Hz, $CH(CH_2C\underline{H}_3)_2$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.22 (C_1), 137.39 (2C, $N(CH_2\underline{C}H=CH_2)_2$), 116.35 (2C, $N(CH_2CH=\underline{C}H_2)_2$), 67.48 ($O\underline{C}HMe_2$), 57.93 ($C_3$ *e.g.* $\underline{C}H$-N), 53.14 (2C, $N(\underline{C}H_2CH=CH_2)_2$), 43.35 ($C_4$ *e.g.* $\underline{C}HEt_2$), 33.93 (C_2), 21.85 (CH-$\underline{C}H_3$), 21.79 (CH-$\underline{C}H_3$), 21.47 ($\underline{C}H_2CH_3$), 21.44 ($\underline{C}H_2CH_3$), 11.10 ($CH_2\underline{C}H_3$), 10.20 ($CH_2\underline{C}H_3$).

3-Dibenzylamino-3-phenylpropionitrile (**4**; R = Ph, R' = Bn): White crystals melting at 109 °C (petroleum ether + 10% EtOAc); R_f = 0.30 (ether/petroleum ether 1:4); IR (CCl_4, KBr) ν 3087, 3065, 3030, 2933, 2838, 2807, 2251 (C≡N), (1948, 1875, and 1811: small, aromatic harmonics), 1602, 1495, 1455, 1124, 1075, 1029, 976, 699, 534 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.46 (broad dm, 4H, *J* = 7.3 Hz, H_{ortho} of Bn), 7.42 (pseudo tt, 2H, *J* = 8.0, 1.8 Hz, H_{meta} of Ph), 7.39-7.32 (m, 5H, $1H_{para}$ of Ph at 7.36 ppm and $4H_{meta}$ of Bn psreudo tt at 7.35 ppm, *J* = 7.5, 1.5 Hz), 7.26 (ddt, 2H, *J* = 8.1, 6.5, 1.3 Hz, H_{para} of Bn), 7.22 (pseudo dm, 2H, $J \approx 7$ Hz, H_{ortho} of Ph), 4.20 (dd, 1H, *J* = 9.3, 6.5 Hz, H-C_3), 3.79 (d, 2H, *J* = 13.8 Hz, $C\underline{H}_2Ph$), 3.23 (d, 2H, *J* = 13.8 Hz, $C\underline{H}_2Ph$), 3.10 (dd, 1H, *J* = 16.9, 9.3

Hz, H-C_2), 2.72 (dd, 1H, *J* = 16.9, 6.5 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.75 (2 C_{ipso} of Bn), 135.49 (C_{ipso} of Ph), 128.77 (dm, *J* = 158.5 Hz, 4 $\underline{C}H_{ortho}$ of Bn), 128.53 (4 $\underline{C}H_{meta}$ of Bn, dd, *J* = 159.9, 7.7 Hz and 2 $\underline{C}H_{ortho}$ of Ph)*, 128.26 (d pseudo t, *J* = 161.0, 7.7 Hz, $\underline{C}H_{para}$ of Ph), 128.15 (2 $\underline{C}H_{meta}$ of Ph), 127.30 (dt, *J* = 160.3, 7.5 Hz, 2 $\underline{C}H_{para}$ of Bn), 118.31 (C_1 e.g. $\underline{C}N$), 58.39 (dm, *J* = 139.3 Hz, C_3), 53.67 (tttd, *J* = 132.7, 4.5, 4.0, 4.0 Hz, 2 $\underline{C}H_2Ph$), 20.25 (td, *J* = 134.6, 5.1 Hz, C_2); elemental analysis calcd for $C_{23}H_{22}N_2$ (326.44): C 84.63, H 6.79, N 8.58; found: C 84.45, H 6.83, N 8.59.

*Whereas these carbons superimpose in dilute $CDCl_3$ solution, they split when concentration increases. For instance, in a 0.59 M solution in $CDCl_3$, the 4 $\underline{C}H_{meta}$ of Bn were recorded at 128.48 ppm while the 2 $\underline{C}H_{ortho}$ of Ph were recorded at 128.46 ppm.

3-(4-Chlorophenyl)-3-dibenzylaminopropionitrile (**4**: R = *p*-Cl-C_6H_4, R' = Bn): Slightly yellow crystals melting at 151 °C (petroleum ether + 15% EtOAc); R_f = 0.20 (ethyl acetate / petroleum ether 1:9); IR (Nujol, KBr) ν 3083, 3027, 2251 (small, C≡N), 2240 (very small), (1955, 1914, 1878, and 1819: small, aromatic harmonics), 1600, 1493, 1486, 1412, 1241, 1125, 1110, 1095, 1085, 1075, 1031, 1013, 977, 912, 907, 861, 836, 830, 786, 747, 731, 726, 702, 544, 498, 488, 468 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (broad pseudo dm, 4H, *J* = 7.5 Hz, H_{ortho} of Bn), 7.40 (d pseudo t, 2H, *J* = 8.5, 2.6-1.9 Hz, H γ to Cl), 7.35 (psreudo tt, 4H, *J* = 7.4, 1.8-1.4 Hz, H_{meta} of Bn), 7.27 (ddt, 2H, *J* = 8.1, 6.4, 1.3 Hz, H_{para} of Bn), 7.17 (d pseudo t, 2H, *J* = 8.5, 2.6-1.9 Hz, H β to Cl), 4.19 (dd, 1H, *J* = 8.8, 6.9 Hz, H-C_3), 3.76 (d, 2H, *J* = 13.8 Hz, $C\underline{H}_2Ph$), 3.23 (d, 2H, *J* = 13.8 Hz, $C\underline{H}_2Ph$), 3.06 (dd, 1H, *J* = 16.9, 8.8 Hz, H-C_2), 2.72 (dd, 1H, *J* = 16.9, 6.9 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.42 (2 C_{ipso} of Bn), 134.20 (C_{ipso}), 134.15 (C_{ipso}), 129.41 (2 $\underline{C}H$ γ to Cl), 128.77 (2 $\underline{C}H$ β to Cl), 128.70 (4 $\underline{C}H_{ortho}$ of Bn), 128.61 (4 $\underline{C}H_{meta}$ of Bn), 127.44 (2 $\underline{C}H_{para}$ of Bn), 118.00 (C_1 e.g. $\underline{C}N$), 57.87 (C_3), 53.65 (2 $\underline{C}H_2Ph$), 19.96 (C_2); elemental analysis calcd for $C_{23}H_{21}N_2Cl$ (360.89): C 76.55, H 5.87, N 7.76; found: C 76.69, H 5.91, N 7.47.

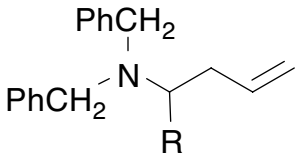
3-Diallylamino-3-phenylpropionitrile (**4**; R = Ph, R' = allyl): Yellow oil; R_f = 0.21 (ethyl acetate / petroleum ether 1:9); IR (neat, KBr) ν 3078, 3070, 3031, 3007, 2978, 2928, 2818, 2248 (C≡N), 1642, 1602, 1495, 1453, 1420, 1356, 1266, 1122, 1082, 997, 981, 923, 783, 759, 744, 703 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (pseudo ddt, 2H, H_{meta} of Ph, *J* ≈ 7.5, 6.5, 1.6 Hz), 7.32 (pseudo ddt, 1H, H_{para} of Ph, *J* = 8.5, 5.9, 1.5 Hz), 7.27 (pseudo dm, 2H, H_{ortho} of Ph, *J* ≈ 6.5 Hz), 5.84 (dddd, 2H, *J* = 17.2, 10.2, 7.0, 5.5 Hz, $N(CH_2C\underline{H}{=}CH_2)_2$), 5.22 (dddd, 2H, *J* = 17.2, 1.8, 1.6, 1.5 Hz, $N(CH_2CH{=}C\underline{H}_2)_2$), 5.17 (dddd, 2H, *J* = 10.2, 1.8, 1.6, 1.1 Hz, $N(CH_2CH{=}C\underline{H}_2)_2$), 4.20 (dd, 1H, *J* = 7.2, 7.1 Hz, H-C_3), 3.22 (dddd, 2H, *J* = 14.5, 5.5, 1.6, 1.6 Hz, $N(C\underline{H}_2CH{=}CH_2)_2$), 2.92 (dddd, 2H, *J* = 14.5, 7.0, 1.5, 1.1 Hz, $N(C\underline{H}_2CH{=}CH_2)_2$), 2.91 (dd, 1H, *J* = 16.8, 7.1 Hz, H-C_2), 2.77 (dd, 1H, *J* = 16.8, 7.2 Hz, H-C_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.46 (C_{ipso} of Ph), 135.82 (2C, $N(CH_2\underline{C}H{=}CH_2)_2$), 128.56 (2C, $\underline{C}H_{ortho}$ of Ph), 128.10 ($\underline{C}H_{para}$ of Ph), 127.83 (2C, $\underline{C}H_{meta}$ of Ph), 118.30 (C_1 *e.g.* $\underline{C}N$), 117.72 (2C, $N(CH_2CH{=}\underline{C}H_2)_2$), 59.72 ($C_3$), 52.73 (2C, $N(\underline{C}H_2CH{=}CH_2)_2$), 21.43 ($C_2$).

3-Cyclohexyl-3-diallylaminopropionitrile (**4**; R = *c*-C_6H_{11}, R' = allyl): Slightly yellow oil with a small bug-like smell; R_f = 0.34 (ethyl acetate/petroleum ether 1:9); IR (neat, KBr) ν 3079, 3007, 2927, 2853, 2810, 2241 (C≡N), 1642, 1449, 1419, 1266, 1115, 997, 920 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 5.75 (dddd, 2H, *J* = 17.2, 10.1, 7.7, 4.6 Hz, $N(CH_2C\underline{H}=CH_2)_2$), 5.19 (dddd, 2H, *J* = 17.2, 1.9, 1.9, 1.2 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 5.10 (dddd, 2H, *J* = 10.1, 1.9, 1.9, 0.8 Hz, $N(CH_2CH=C\underline{H}_2)_2$), 3.35 (dddd, 2H, *J* = 14.3, 4.6, 1.9, 1.9 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.96 (dddd, 2H, *J* = 14.3, 7.7, 1.2, 0.8 Hz, $N(C\underline{H}_2CH=CH_2)_2$), 2.77 (ddd, 1H, *J* = 9.6, 6.2, 4.3 Hz [apparent ddd, *J* = 9.6, 6.1, 4.4 Hz], H-C_3), 2.43 (dd, 1H, *J* = 17.2, 4.3 Hz [apparent dd, *J* = 17.2, 4.4 Hz], H-C_2)*, 2.36 (dd, 1H, *J* = 17.2, 6.2 Hz [apparent dd, *J* = 17.2, 6.1 Hz], H-C_2)*, 2.07 (dm, 1H, *J* = 13.2 Hz), 1.80-1.55 (m, 5H), 1.34-1.07 (m, 3H), 1.03-0.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.72 (2C, $N(CH_2\underline{C}H=CH_2)_2$), 119.58 ($C_1$ *e.g.* $\underline{C}N$), 117.00 (2C, $N(CH_2CH=\underline{C}H_2)_2$), 60.17 ($C_3$), 52.74 (2C, $N(\underline{C}H_2CH=CH_2)_2$), 39.63 ($\underline{C}H$ α to C_3, correlates with protons at 1.61 ppm), 30.65 and 30.54 (2 $\underline{C}H_2$ β to C_3, correlates with protons at 2.07, 1.74, and 1.03-0.80 ppm), 26.36 and 26.10 and 25.99 (2 $\underline{C}H_2$ γ to C_3 and $\underline{C}H_2$ δ to C_3, correlates with protons at 1.80-1.61 and 1.34-1.07 ppm), 14.72 (C_2).

*These two protons are the AB part of an ABX system which was analyzed by computer. That explains the small differences between the observed and the real coupling constants.

REPRESENTATIVE SPECTRA

^{1}H and ^{13}C NMR spectra are given for 10 compounds (successively for each of them, the full proton spectrum, expanded extracts, the full carbon ^{1}H-decoupled spectrum with expanded extracts and DEPT 135).



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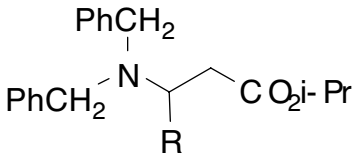

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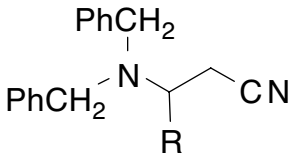
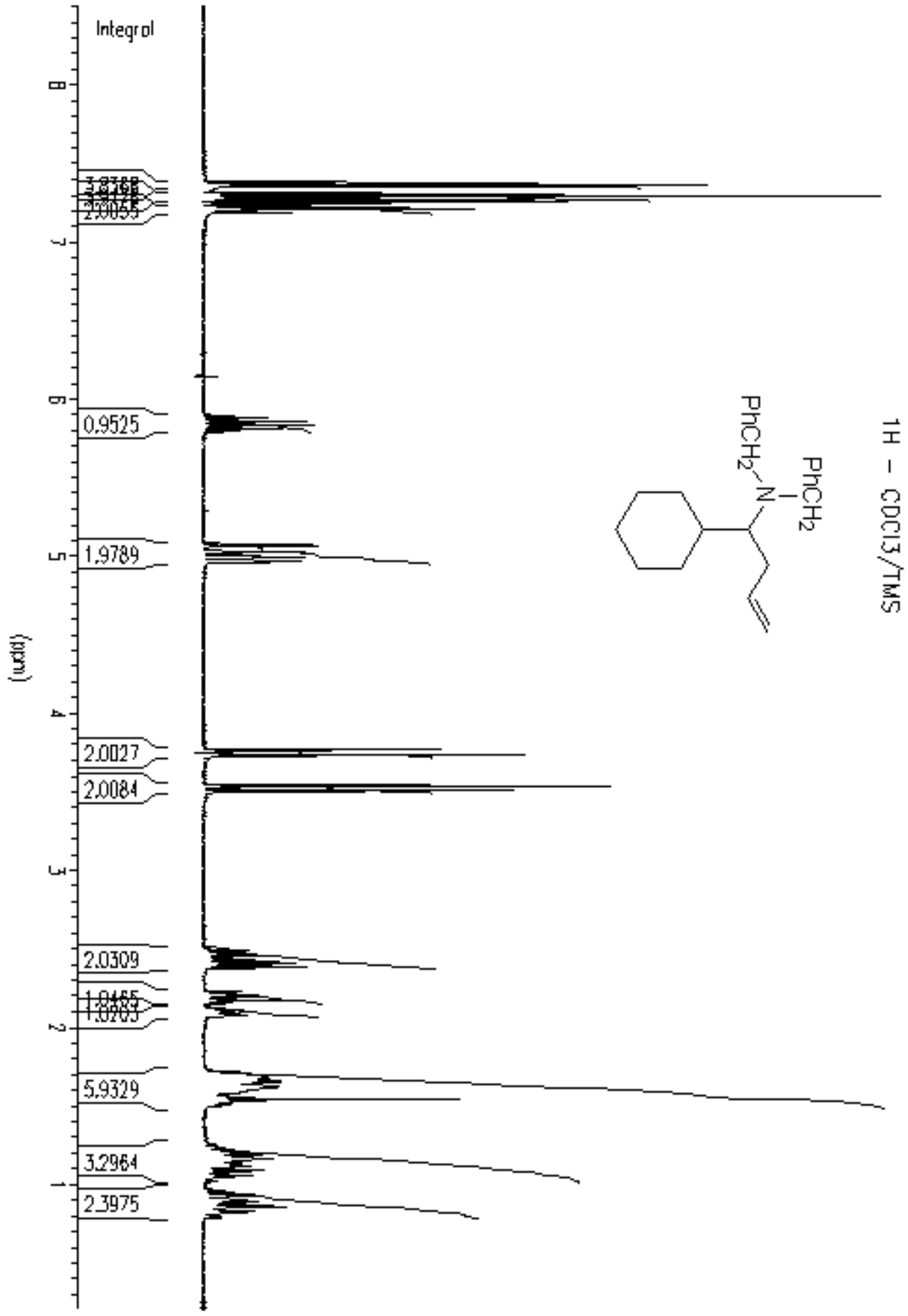


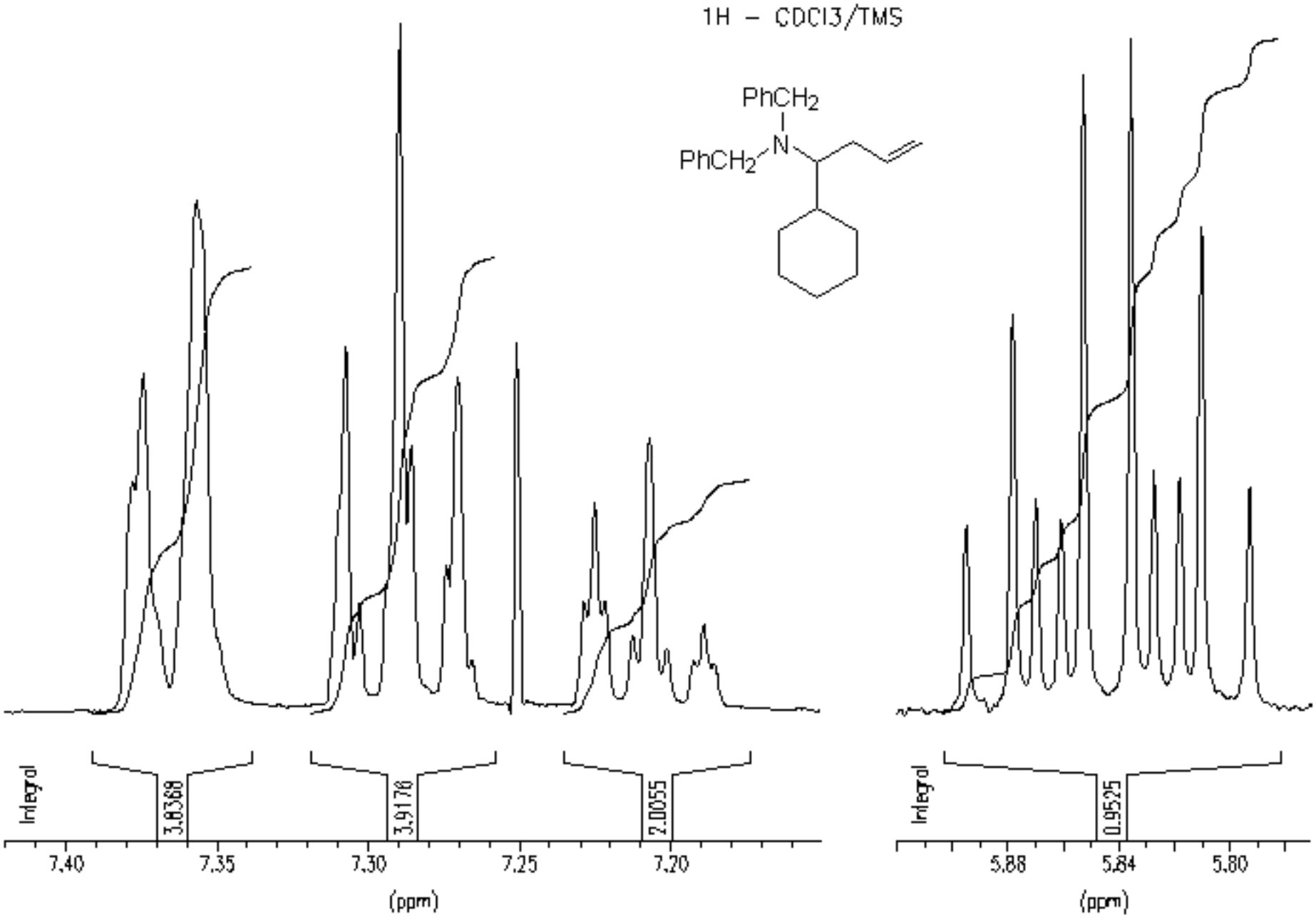
4

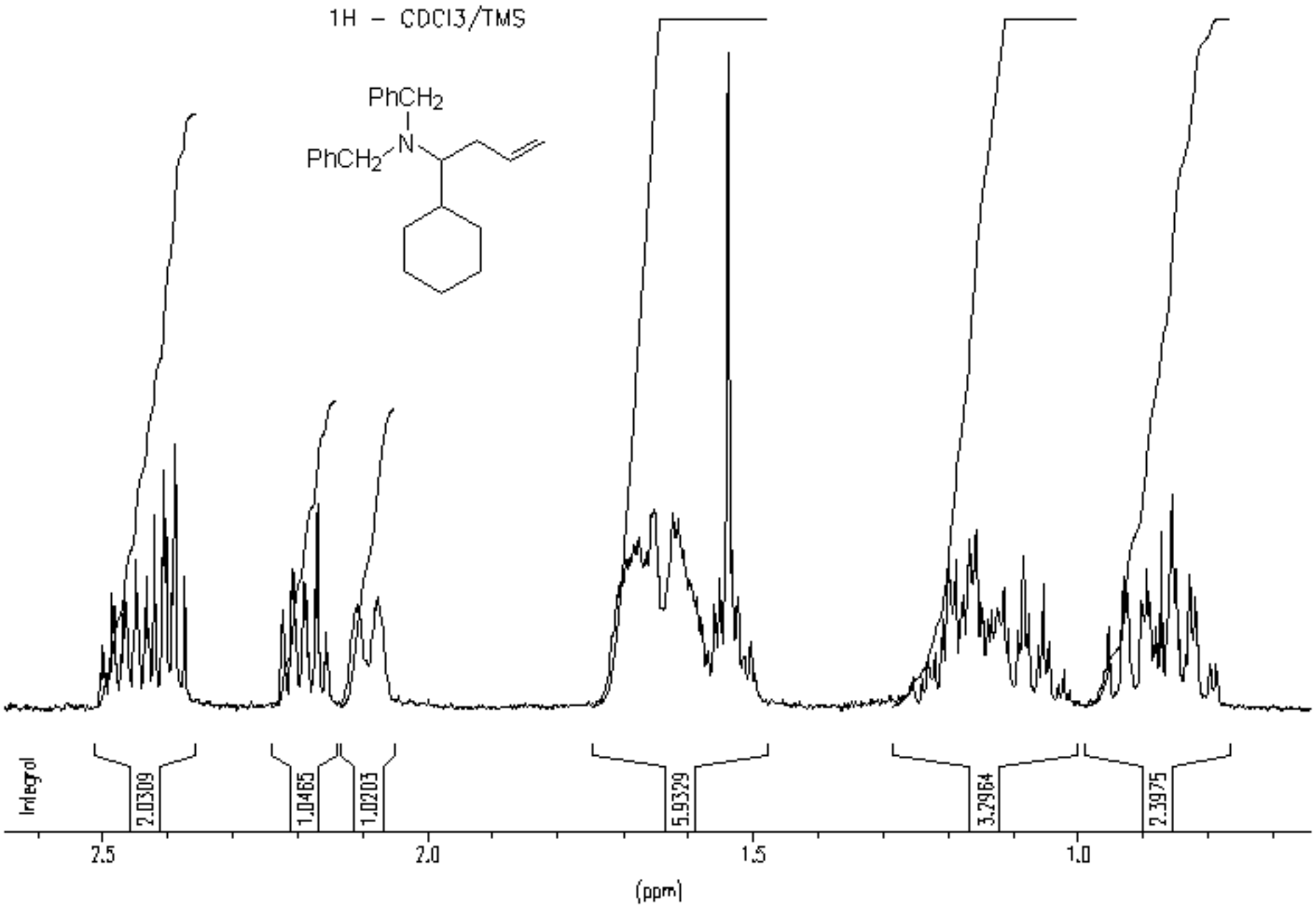
Compound **2** (R = Ph, R' = Bn):

129.0
128.0
127.0
(ppm)
128.9601
128.7696
128.1886
127.9165
127.0615
126.7677
200
150
100
50
(ppm)
140.1971
138.5393
136.6672
128.9601
128.7696
128.1886
127.9165
127.0615
126.7677
116.0890
13C - 1H decoupled
CDCl3/TMS
77.3270
77.0104
76.6929
61.5024
53.4796
35.2967
PhCH2
N
Ph
PhCH2
0.0001

Compound **2** (R = *c*-C_6H_{11}, R' = Bn):

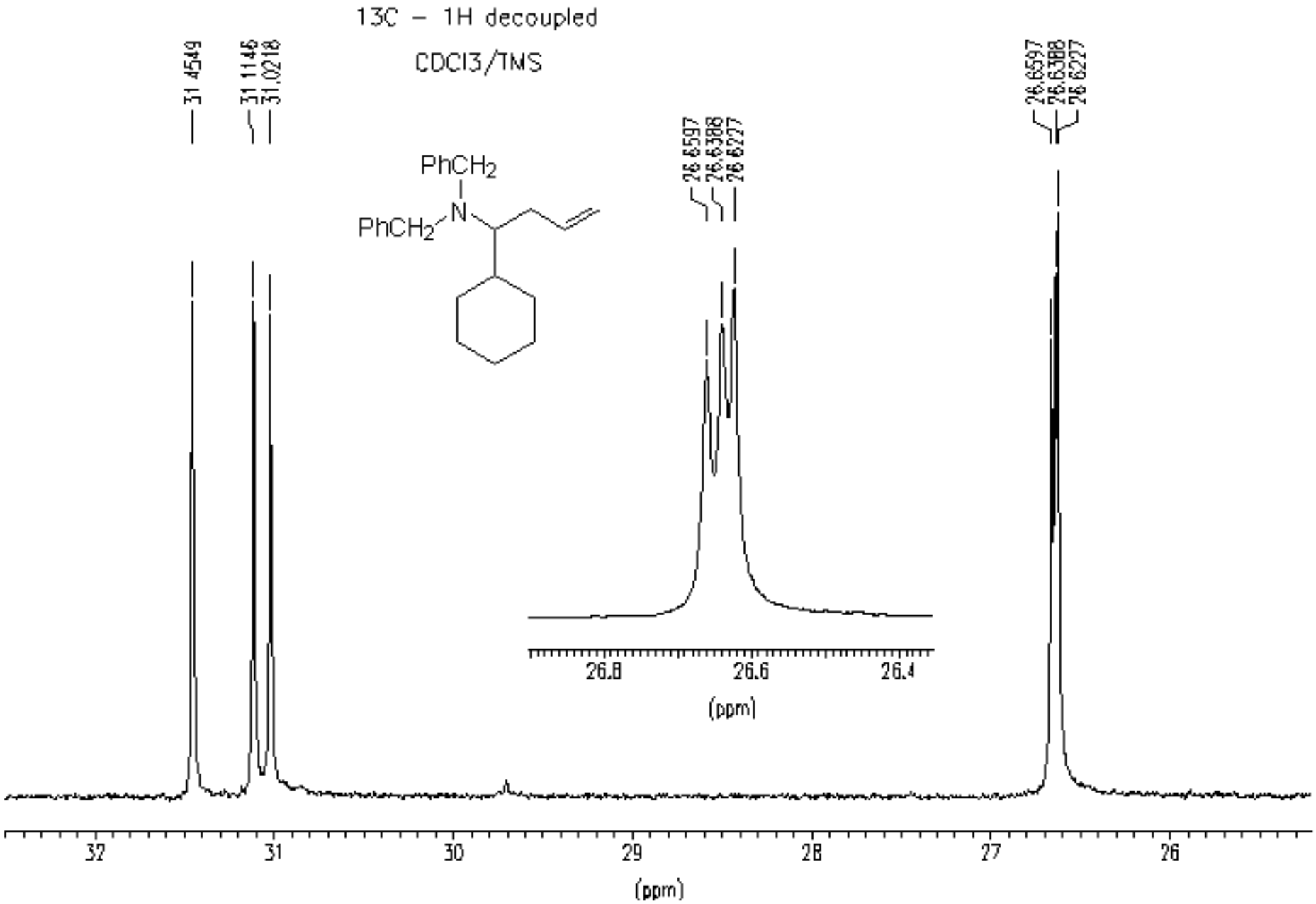



1H – CDCl3/TMS
PhCH2
N
PhCH2
Integral
3.8368
3.9178
2.0055
7.40
7.35
7.30
7.25
7.20
(ppm)
Integral
0.9525
5.88
5.84
5.80
(ppm)


1H – CDCl3/TMS
PhCH2
N
PhCH2
Integrol
2.0309
1.0465
1.0203
5.9329
3.2964
2.3975
2.5
2.0
1.5
1.0
(ppm)

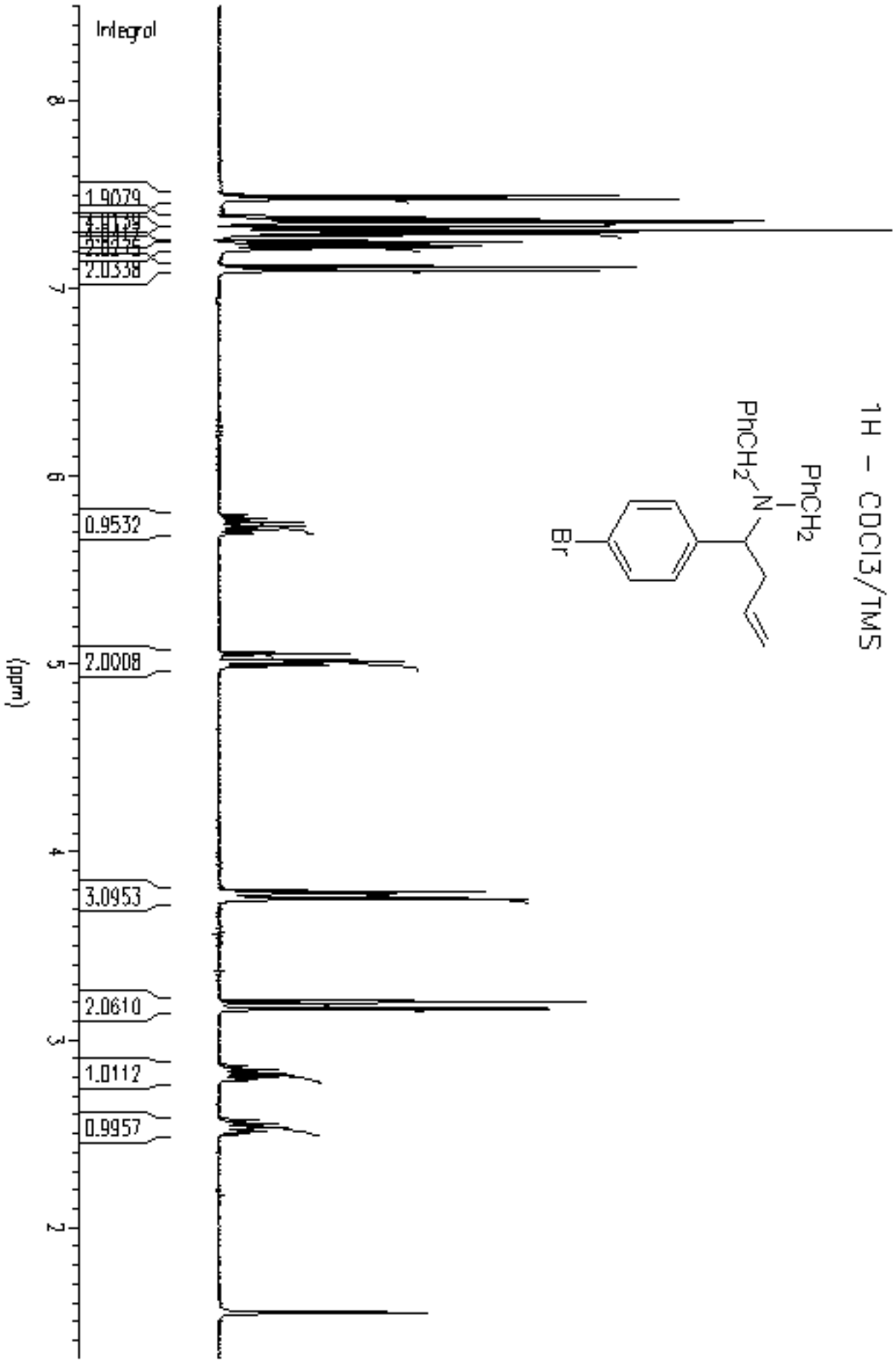
140.5183
139.0320
128.9249
128.0349
126.6207
115.1325
77.3250
77.0075
76.6899
62.0454
54.3525
40.2341
31.4549
31.1146
31.0218
26.6597
26.6388
26.6227
0.0000
PhCH2
N
PhCH2
13C - 1H decoupled
CDCl3/TMS
(ppm)
200
150
100
50
0
140
130
120

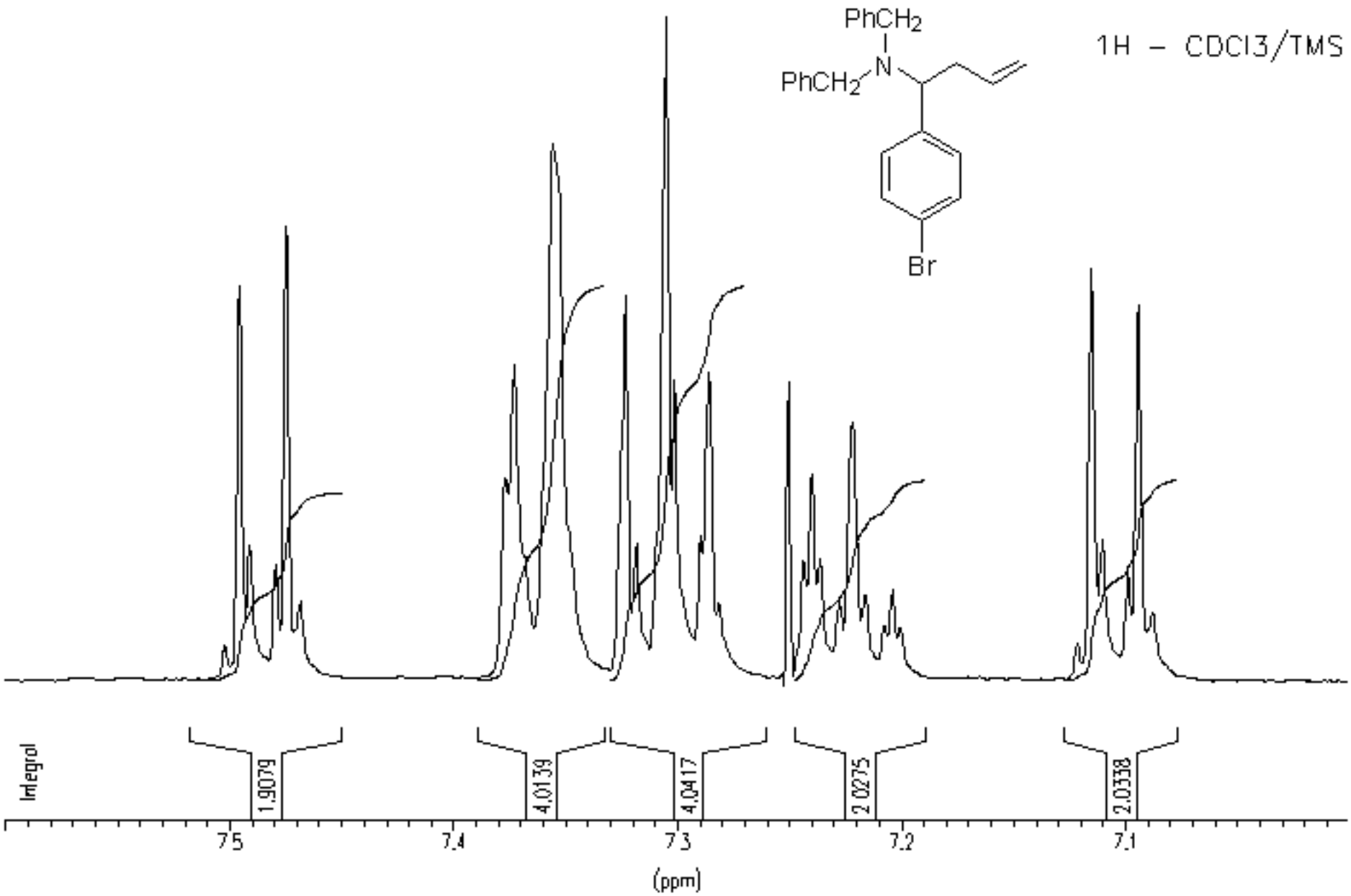
62.0454
54.3525
40.2341
31.4549
31.1146
31.0218
26.6597
26.6388
26.6227
13C - 1H decoupled
CDCl3/TMS
PhCH2
N
PhCH2
65
60
55
50
45
40
35
30
25
(ppm)

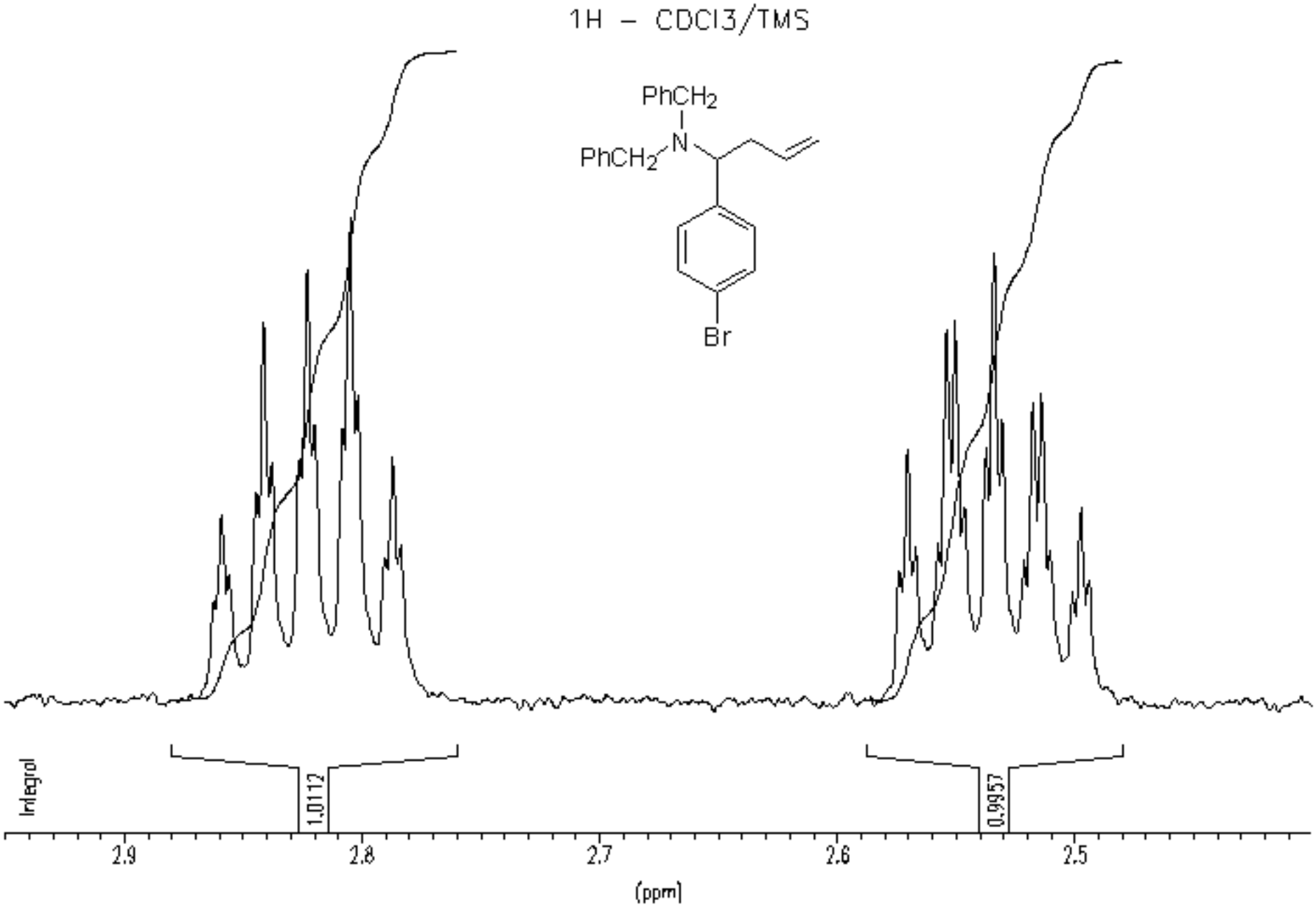

13C – 1H decoupled
CDCl3/TMS
31.4549
31.1146
31.0218
26.6597
26.6388
26.6227
PhCH2
N
PhCH2
26.8
26.6
26.4
(ppm)
32
31
30
29
28
27
26
(ppm)

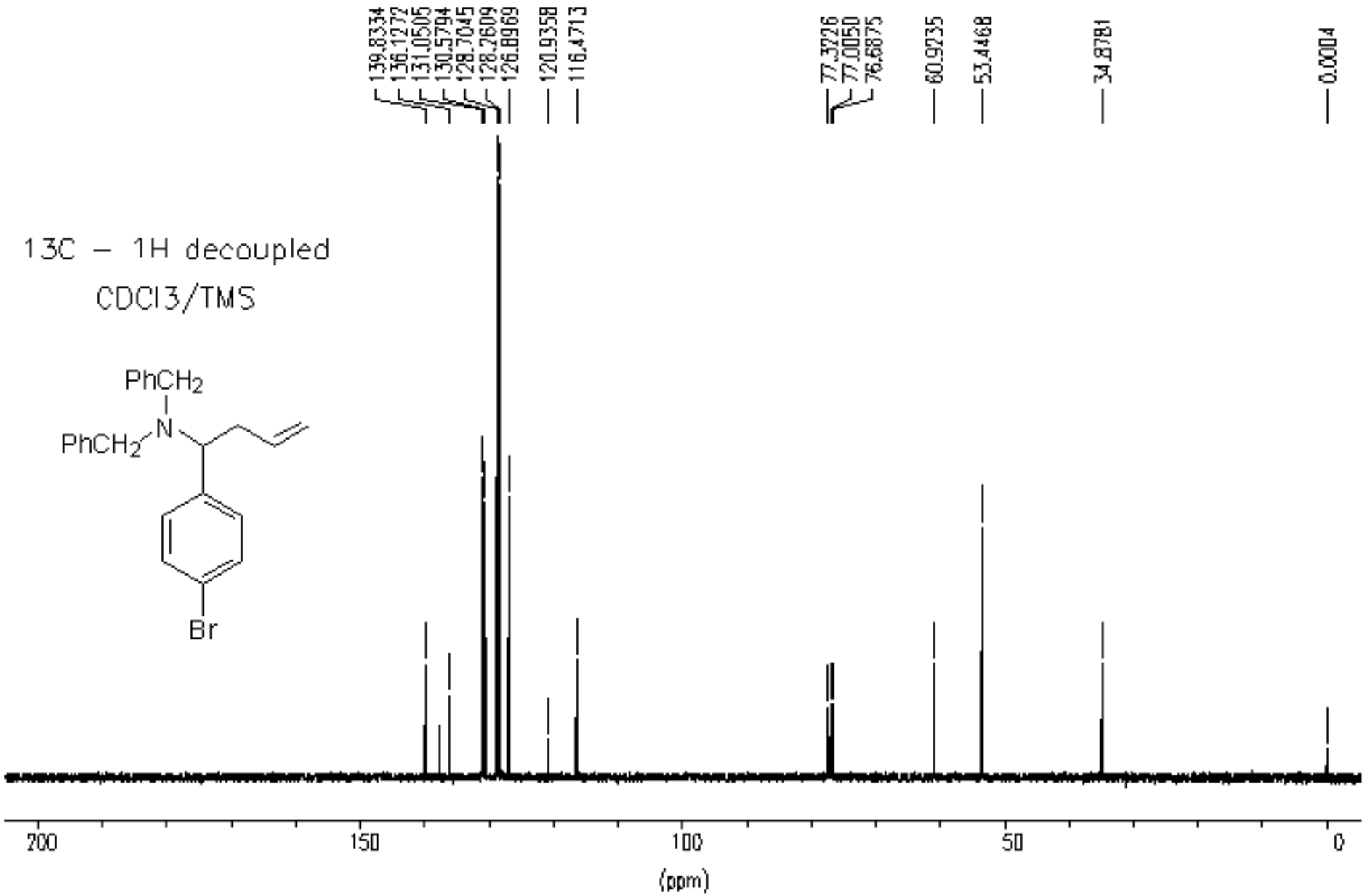
13C - DEPT 135
CDCl3/TMS
PhCH2
N
PhCH2
150
100
50
0
(ppm)
139.0444
128.9275
128.0390
126.6223
115.1341
62.0448
54.3469
40.2312
31.4527
31.1153
31.0243
26.6629
26.6414
26.6237
0.0000

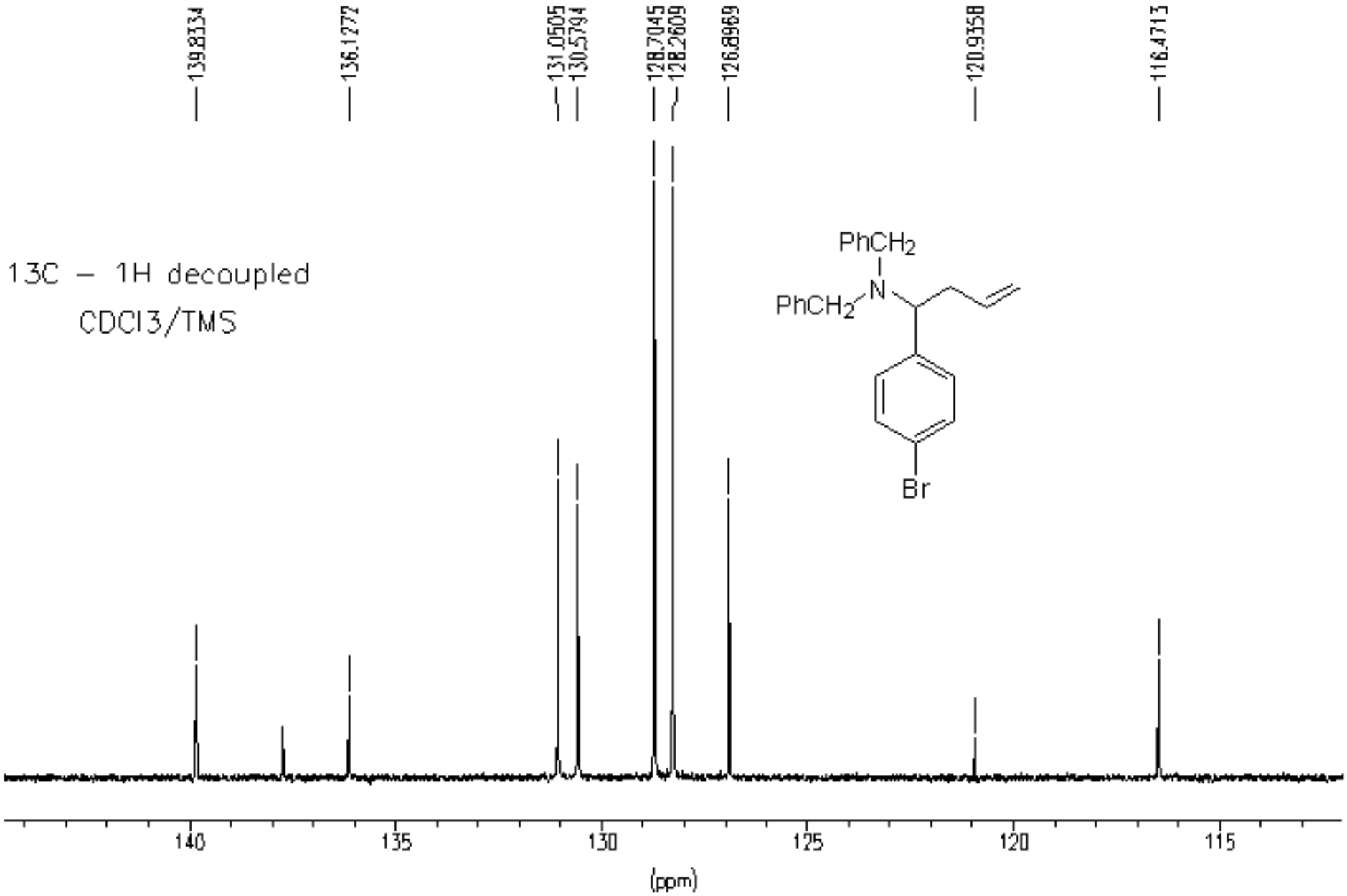
Compound **2** (R = *p*-Br-C_6H_4, R' = Bn):

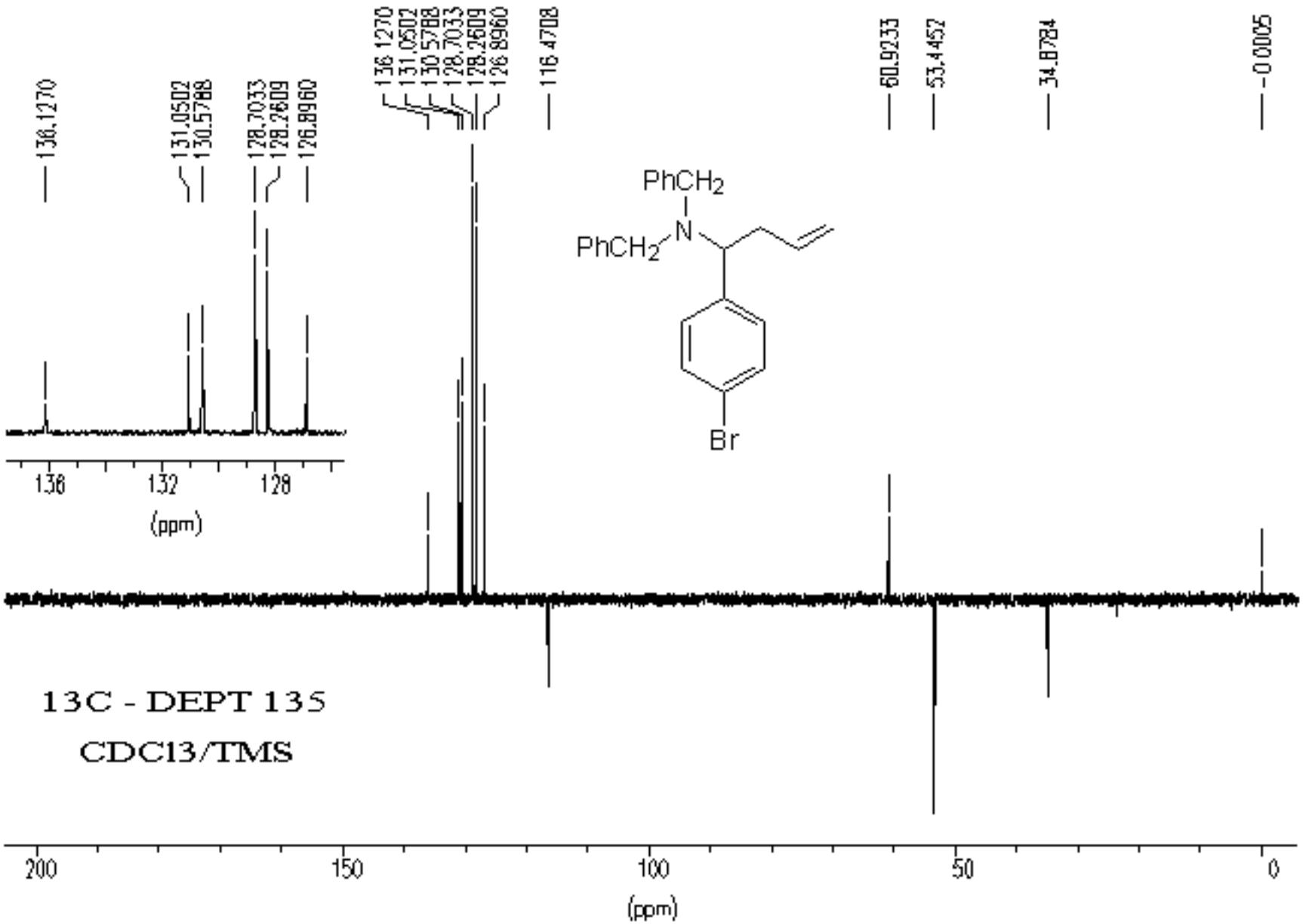



PhCH2
N
PhCH2
Br
1H – CDCl3/TMS
Integrol
1,9079
4,0139
4,0417
2,0275
2,0338
7.5
7.4
7.3
7.2
7.1
(ppm)

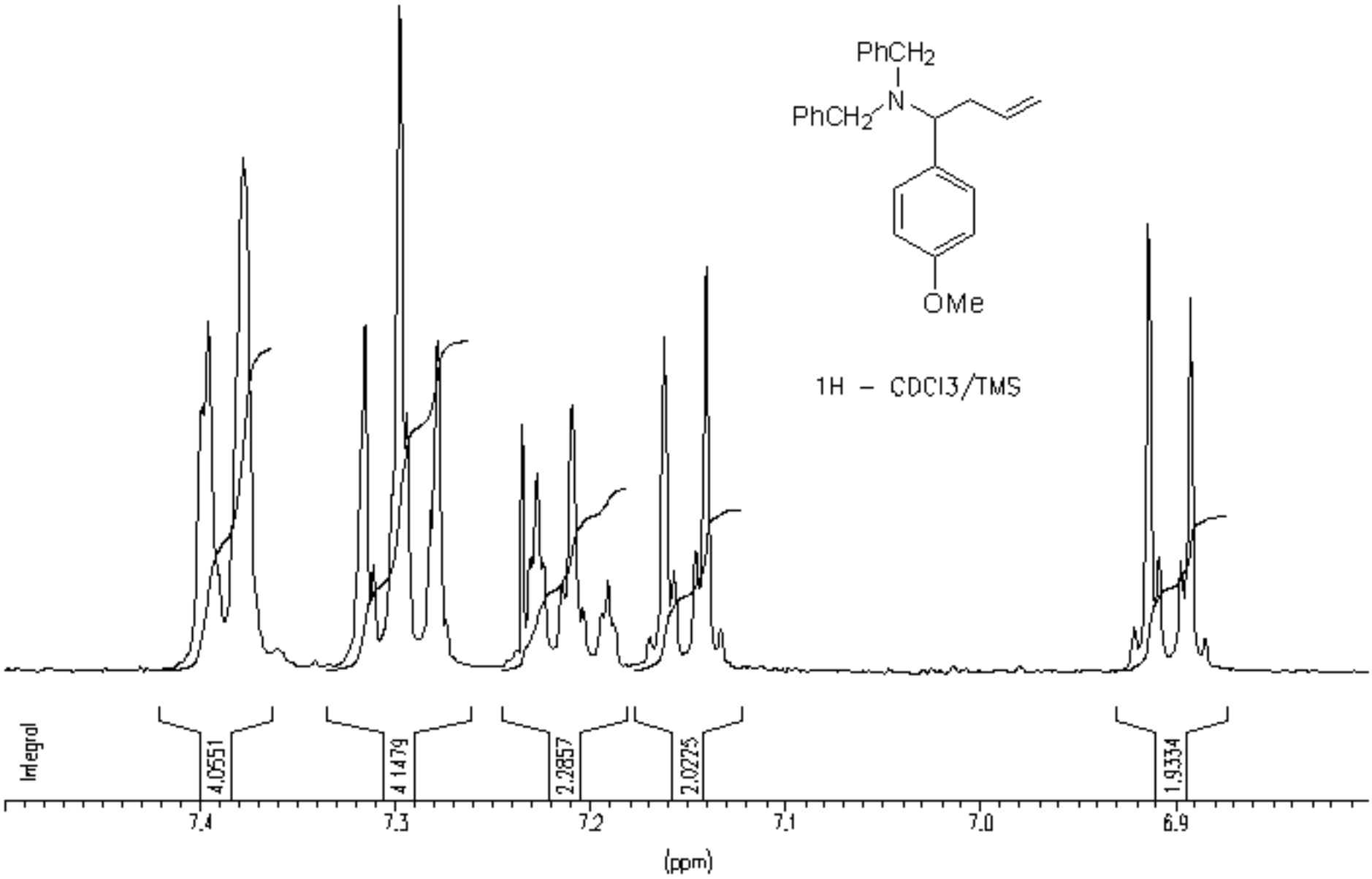

1H – CDCl3/TMS
PhCH2
N
PhCH2
Br
Integral
1,0112
0,9957
2.9
2.8
2.7
2.6
2.5
(ppm)

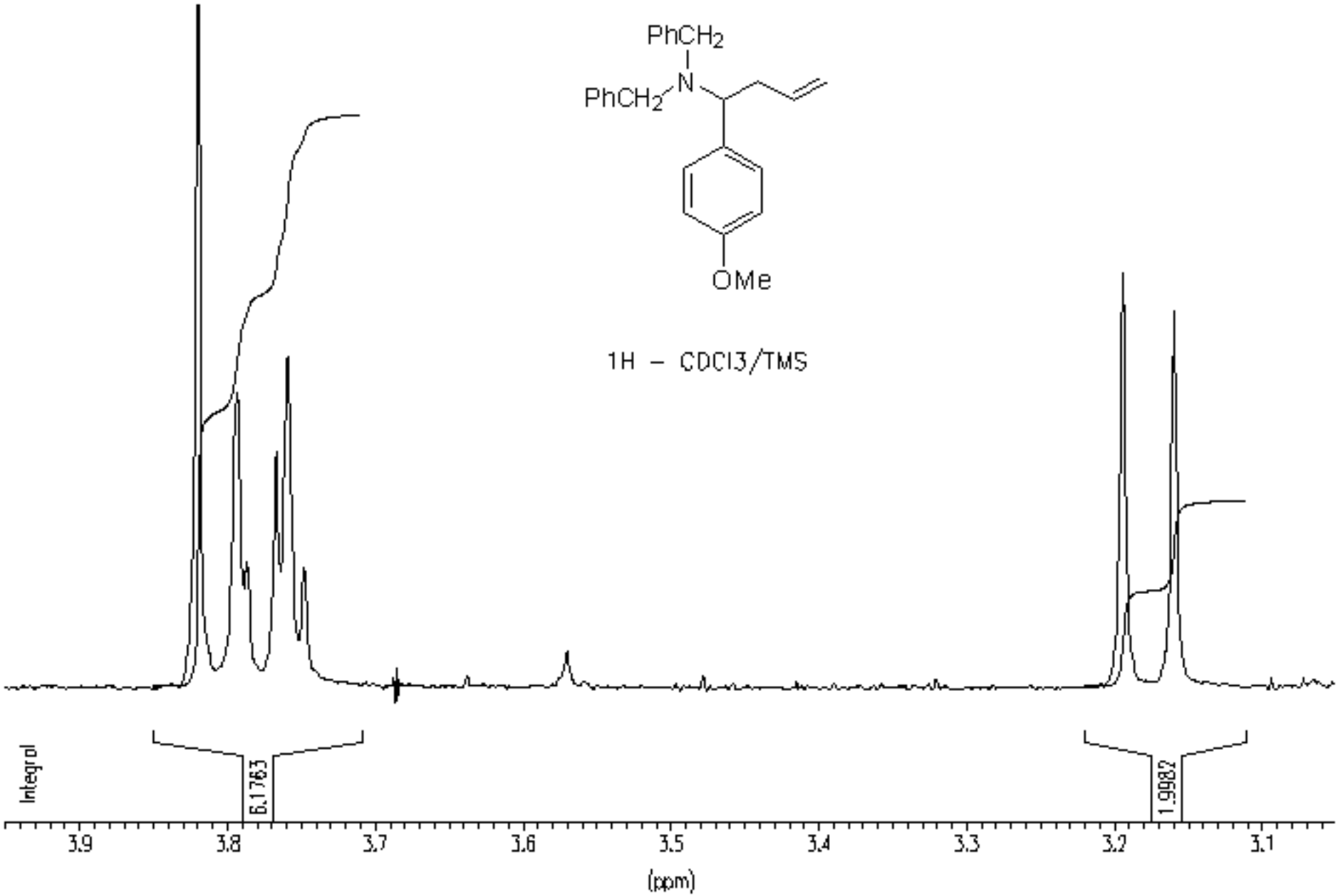

139.8334
136.1272
131.0505
130.5794
128.7045
128.2609
126.8969
120.9358
116.4713
77.3226
77.0050
76.6875
60.9235
53.4468
34.8781
0.0004
13C – 1H decoupled
CDCl3/TMS
PhCH2
N
PhCH2
Br
200
150
100
50
0
(ppm)


139.8334
136.1272
131.0505
130.5794
128.7045
128.2609
126.8969
120.9358
116.4713
13C – 1H decoupled
CDCl3/TMS
PhCH2
N
PhCH2
Br
140
135
130
125
120
115
(ppm)

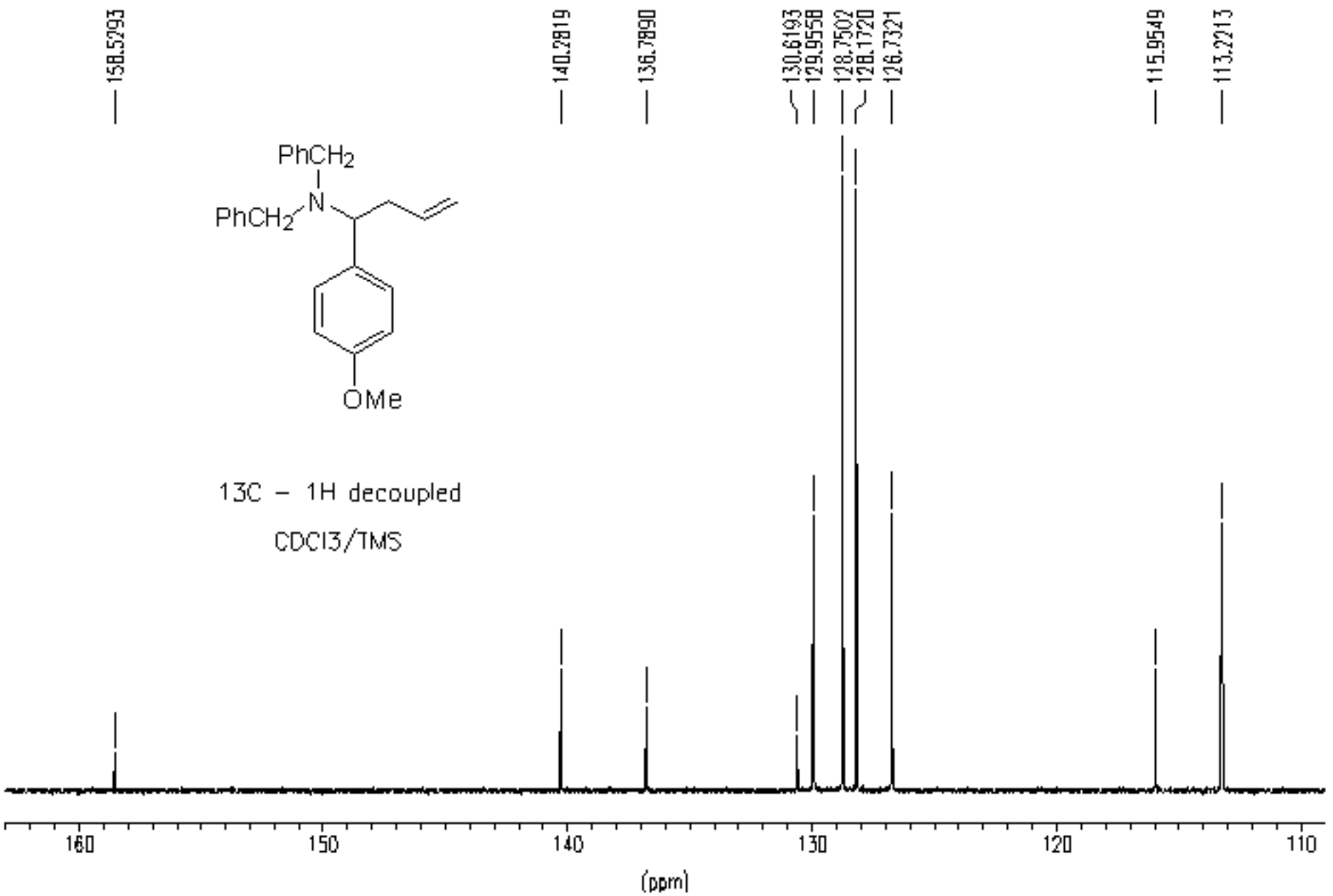

136.1270
131.0502
130.5788
128.7033
128.2609
126.8960
116.4708
60.9233
53.4452
34.8784
-0.0005
PhCH2
N
PhCH2
Br
136
132
128
(ppm)
13C - DEPT 135
CDCl3/TMS
200
150
100
50
0
(ppm)

Compound **2** (R = *p*-MeO-C_6H_4, R' = Bn):

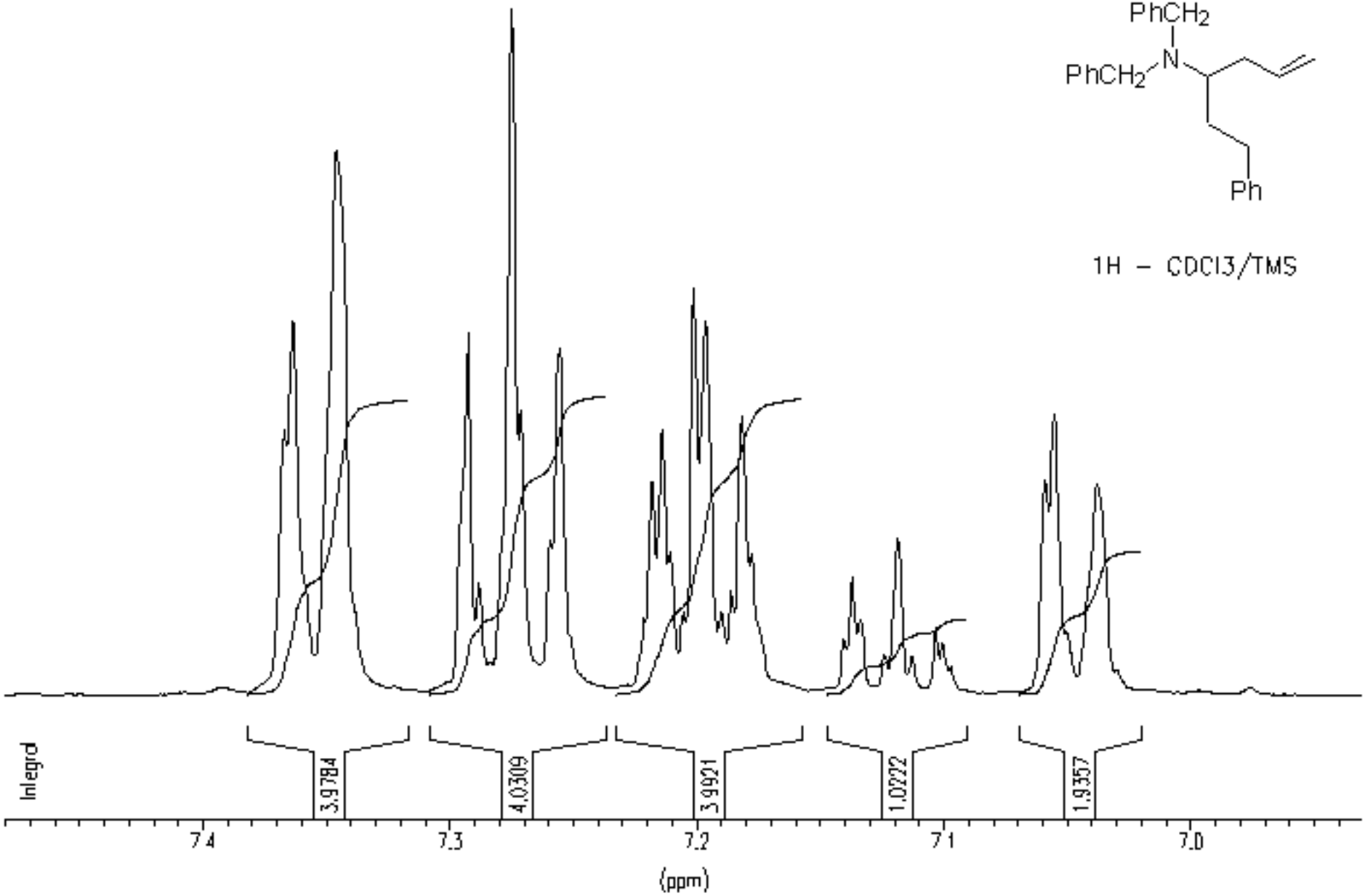

PhCH2
N
PhCH2
OMe
1H – CDCl3/TMS
Integrol
4.0551
4.1479
2.2857
2.0225
1.9334
7.4
7.3
7.2
7.1
7.0
6.9
(ppm)

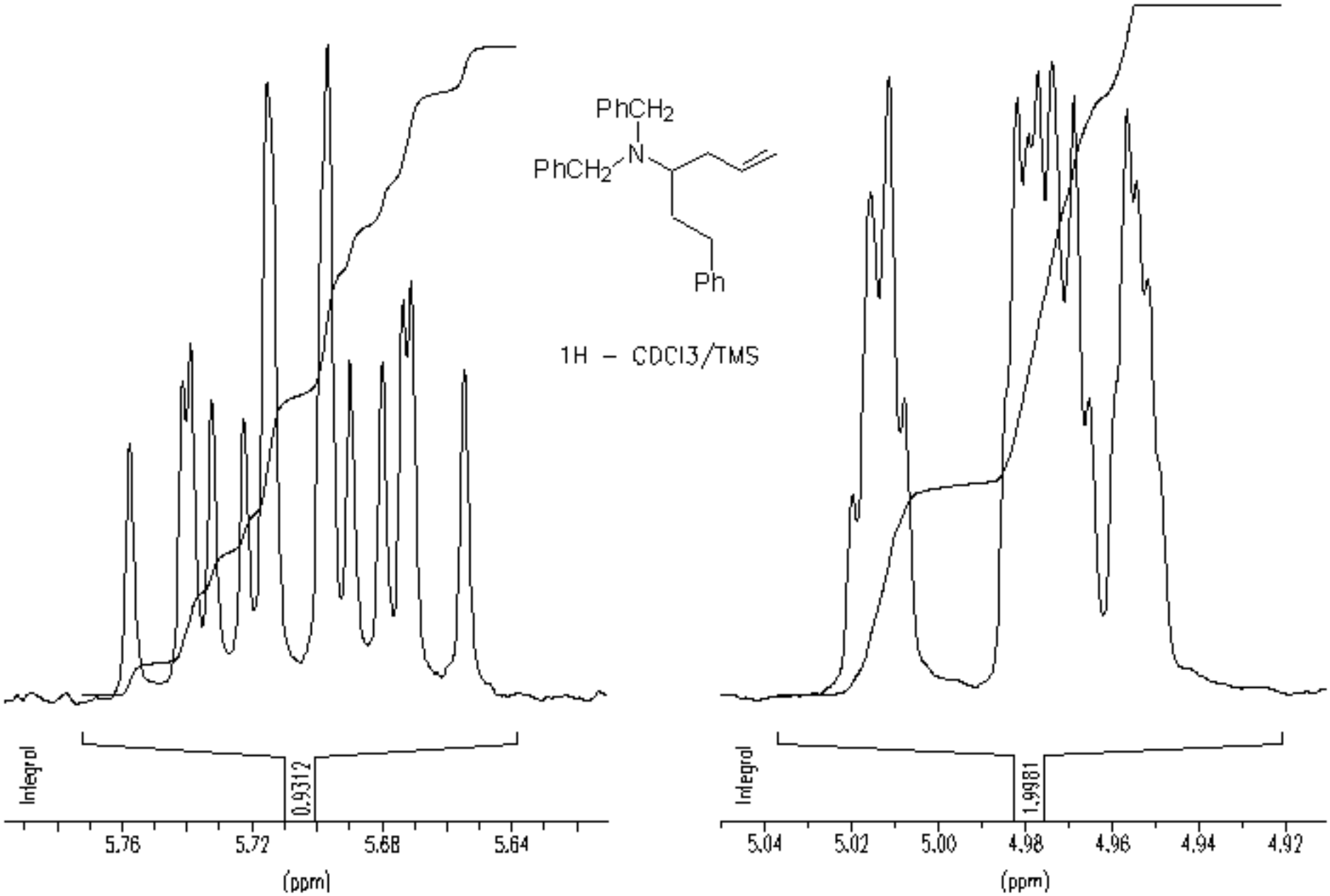

PhCH2
N
PhCH2
OMe
1H – CDCl3/TMS
Integral
6.1763
1.9982
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
(ppm)

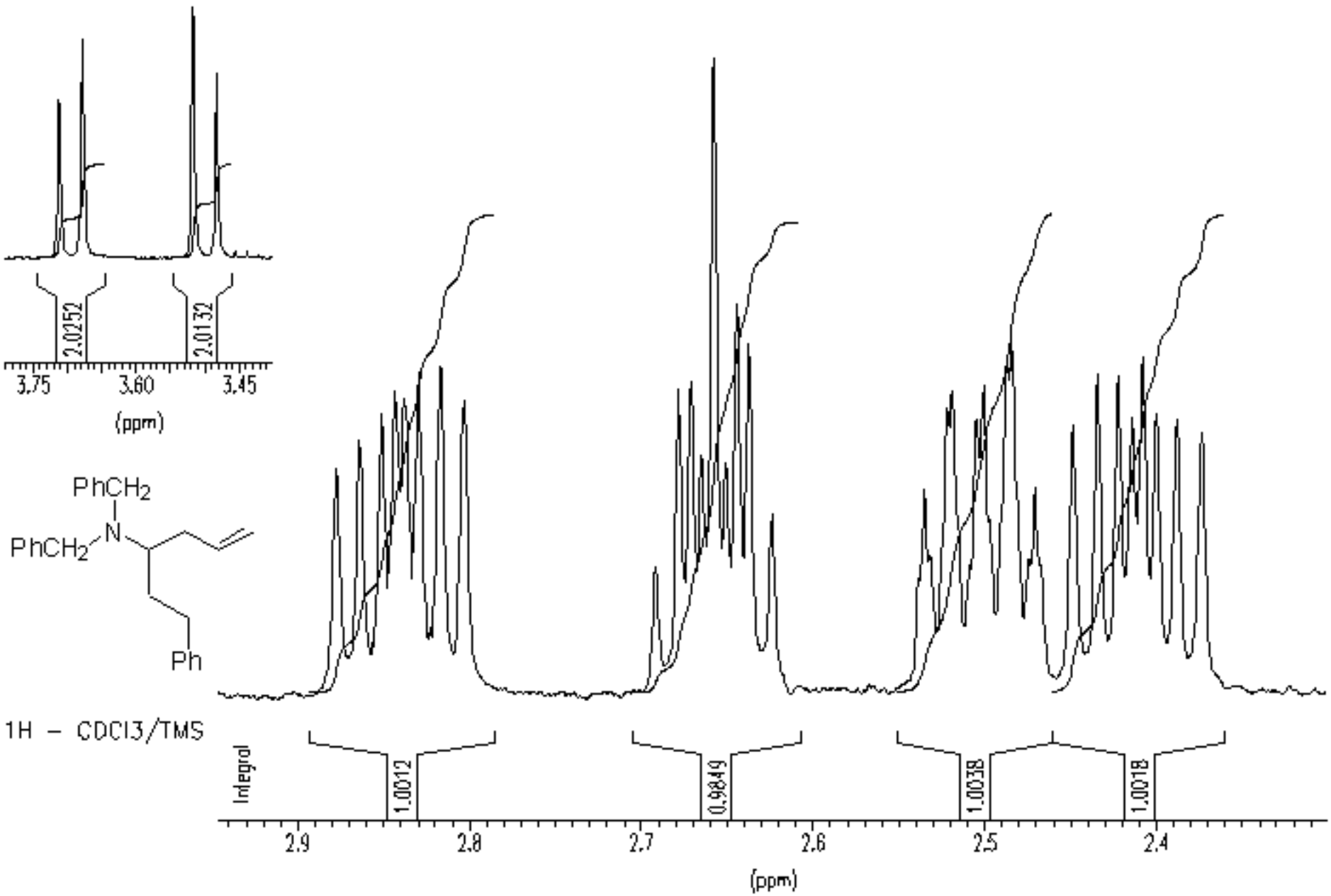
13C - 1H decoupled
CDCl3/TMS
PhCH2
N
PhCH2
OMe
158.5293
140.2819
136.7890
130.6193
129.9558
128.7502
128.1720
126.7321
115.9549
113.2213
77.3294
77.0128
76.6952
60.7948
55.1853
53.4299
35.4612
-0.0004
200
150
100
50
0
(ppm)

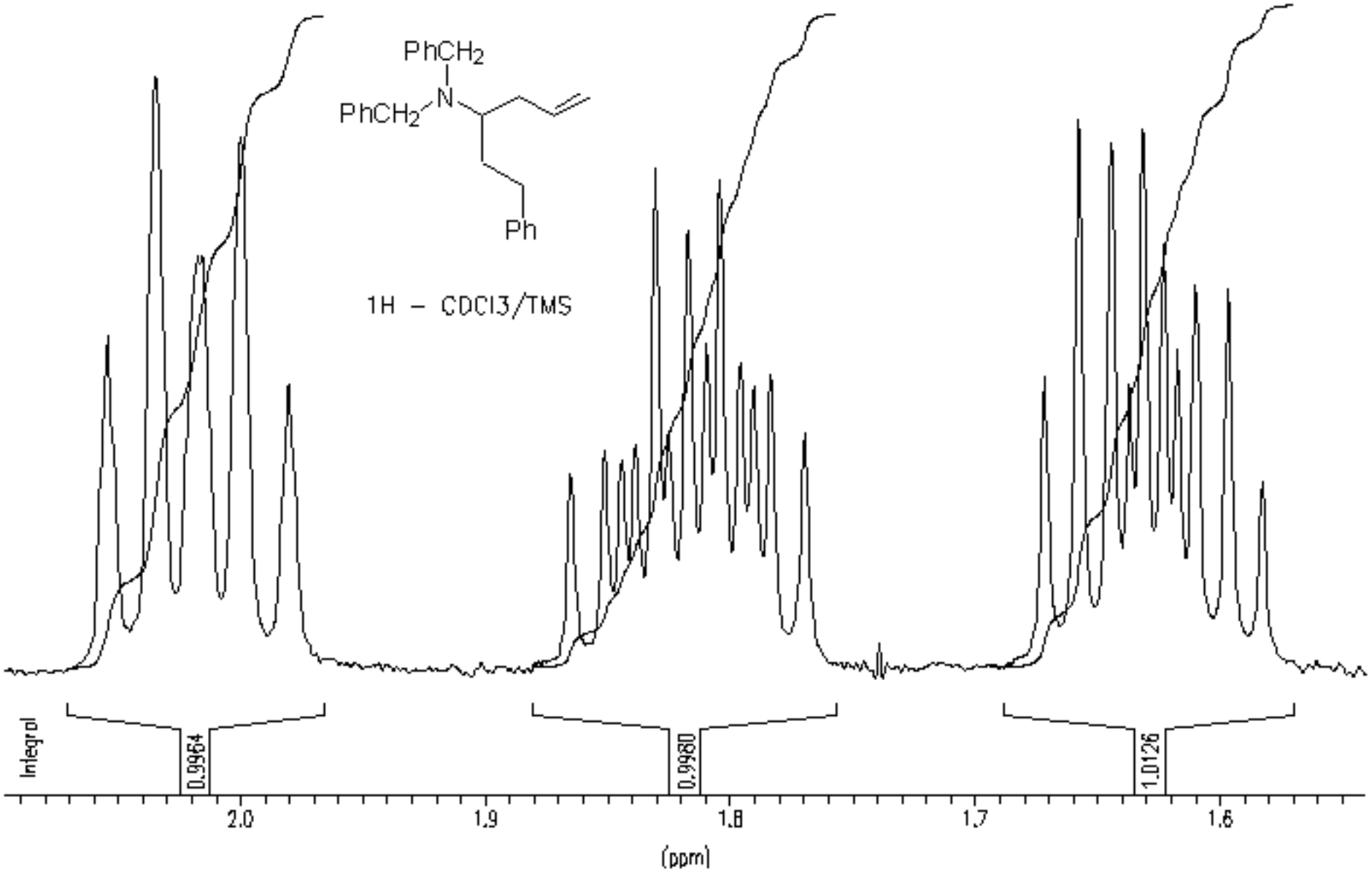

158.5293
140.2819
136.7890
130.6193
129.9558
128.7502
128.1720
126.7321
115.9549
113.2213
PhCH2
N
PhCH2
OMe
13C – 1H decoupled
CDCl3/TMS
160
150
140
130
120
110
(ppm)

Compound **2** (R = CH_2CH_2Ph, R' = Bn):


PhCH2
N
PhCH2
Ph
1H – CDCl3/TMS
Inlegrd
3.9784
4.0309
3.9921
1.0222
1.9357
7.4
7.3
7.2
7.1
7.0
(ppm)


PhCH2
N
PhCH2
Ph
1H – CDCl3/TMS
Integral
0.9312
5.76
5.72
5.68
5.64
(ppm)
Integral
1.9981
5.04
5.02
5.00
4.98
4.96
4.94
4.92
(ppm)


2.0252
2.0132
3.75
3.60
3.45
(ppm)
PhCH2
PhCH2
N
Ph
1H – CDCl3/TMS
Integral
1.0012
0.9849
1.0038
1.0018
2.9
2.8
2.7
2.6
2.5
2.4
(ppm)

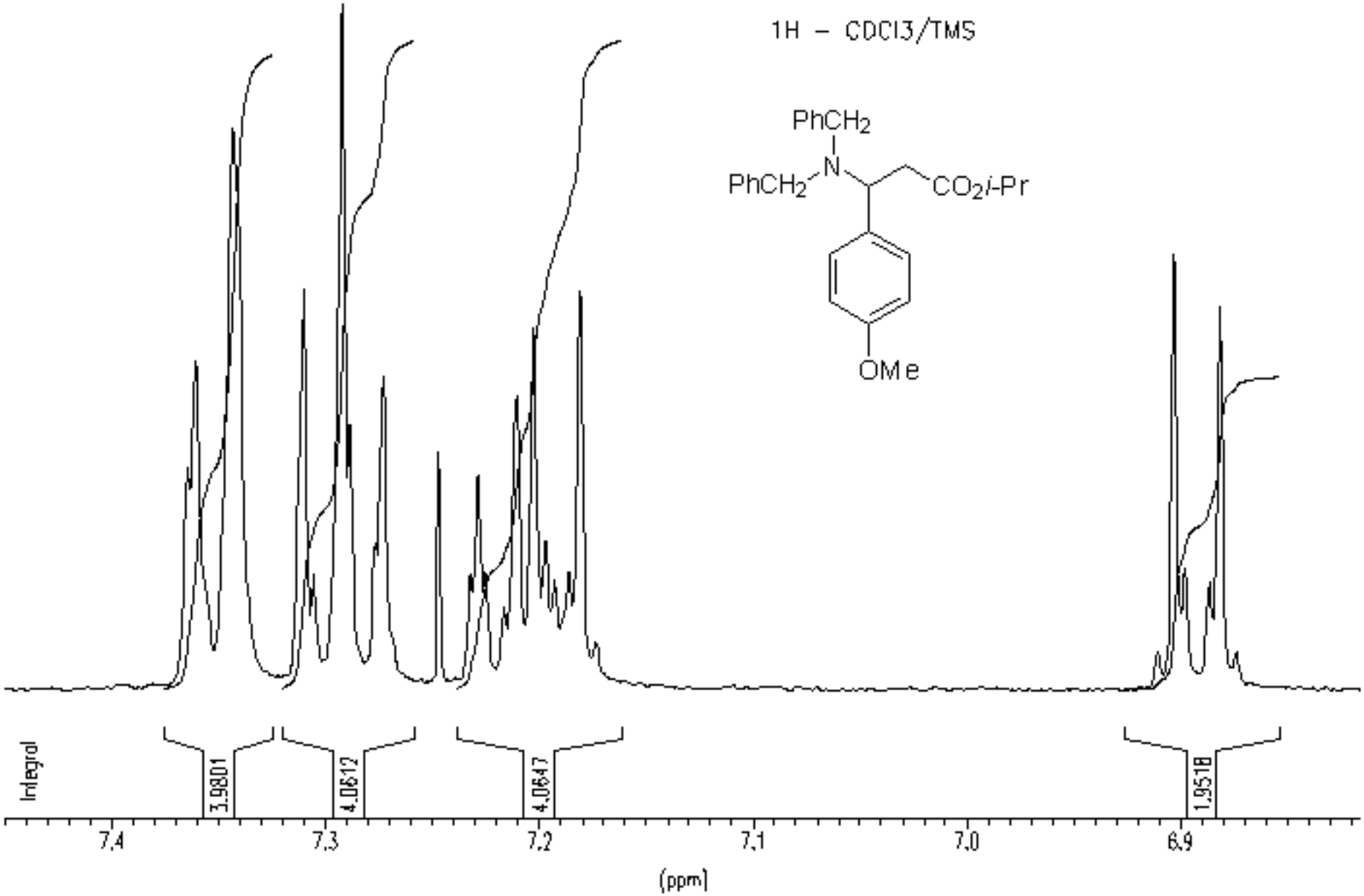

PhCH2
N
PhCH2
Ph
1H – CDCl3/TMS
Integral
0.9964
0.9980
1.0126
2.0
1.9
1.8
1.7
1.6
(ppm)

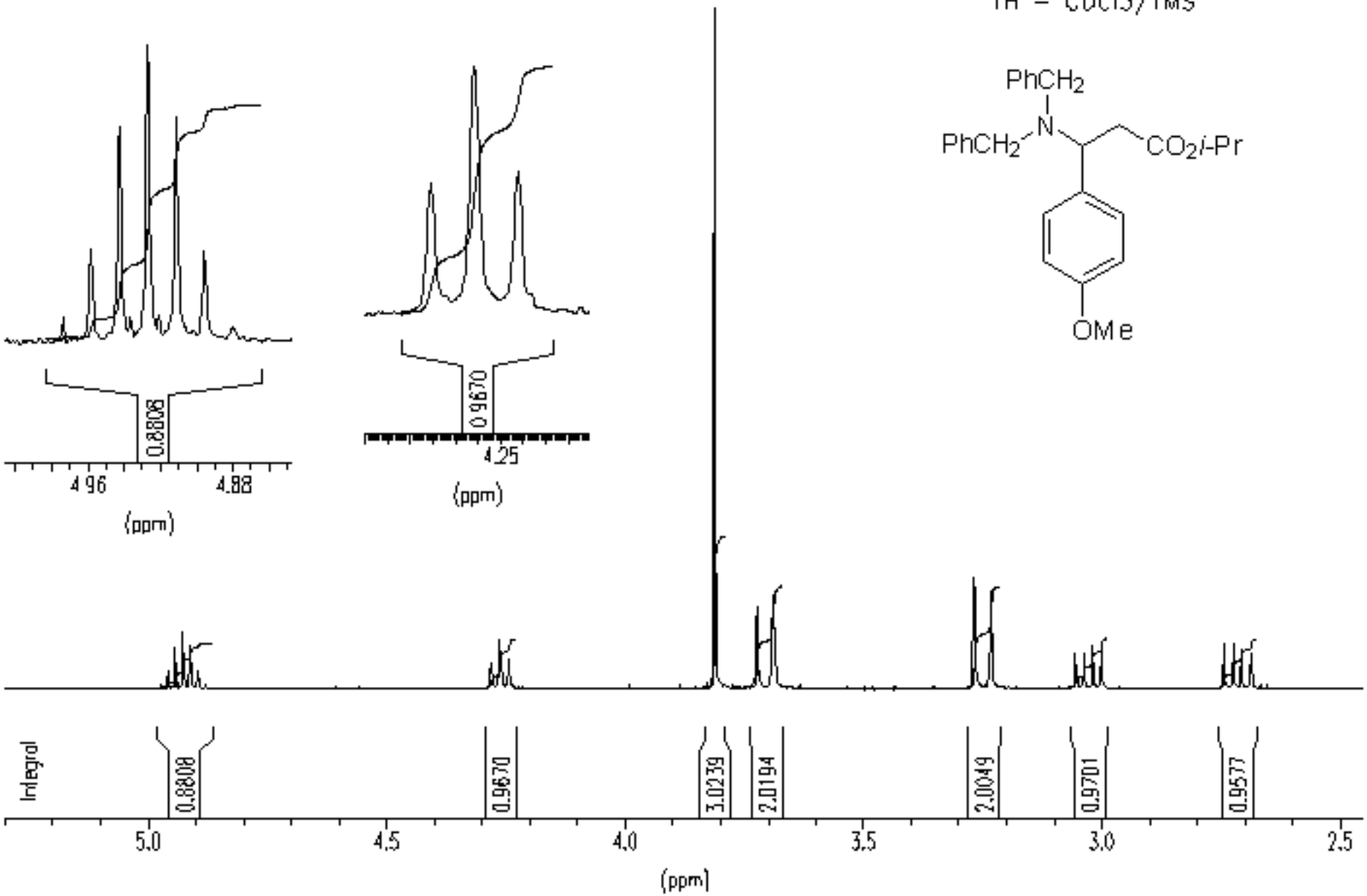
13C - 1H decoupled
CDCl3/TMS
PhCH2
N
PhCH2
Ph
200
150
100
50
0
(ppm)
142.9060
140.3382
137.2946
128.9060
128.3543
128.2605
128.1467
126.7477
125.5515
115.9629
77.3335
77.0160
76.6975
57.1516
53.4198
33.6369
33.4767
32.5620
-0.0000

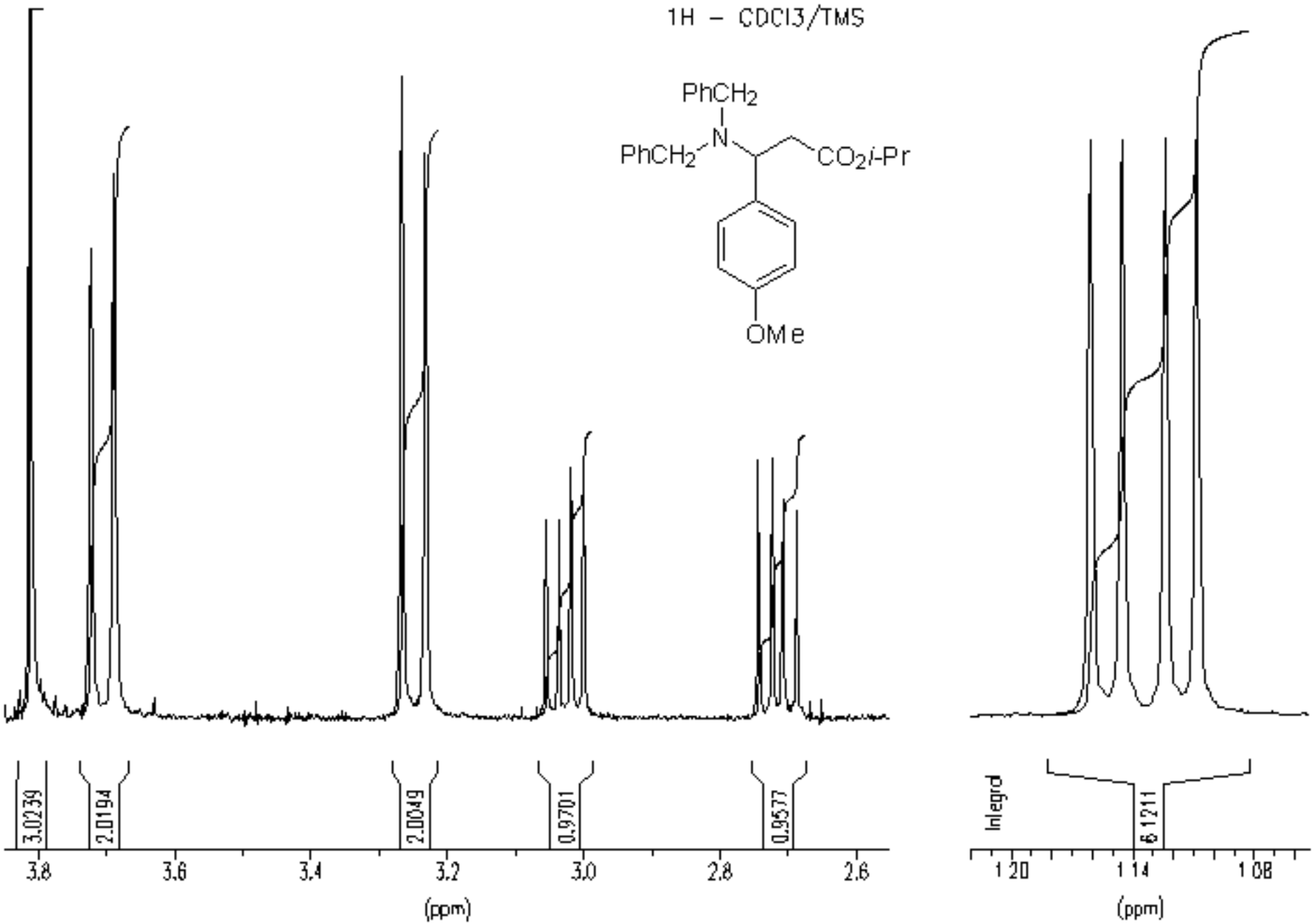
Compound **3** (R = Ph, R' = Bn):

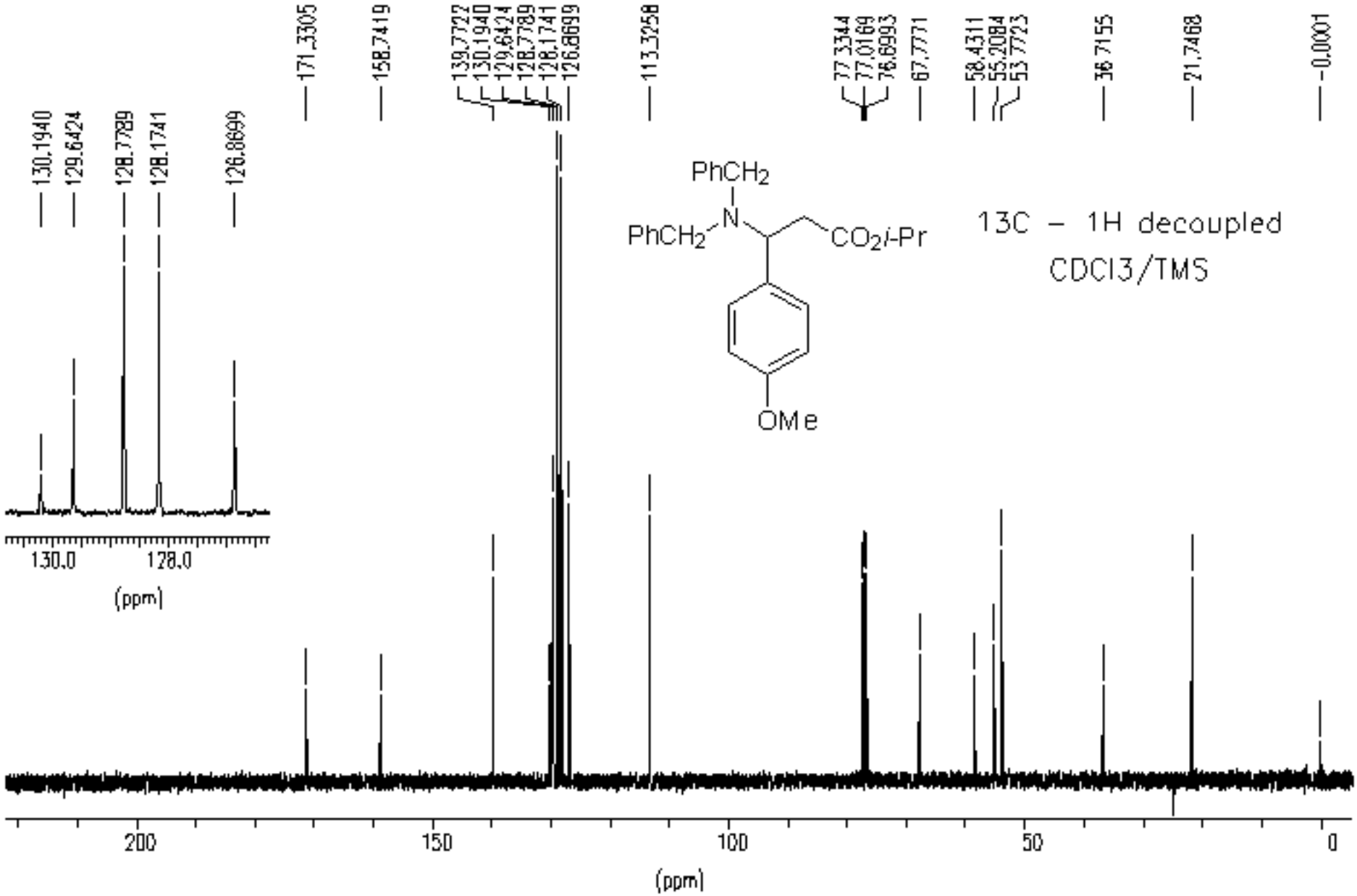
Compound **3** (R = *p*-Cl-C_6H_4, R' = Bn):

Compound **3** (R = *p*-MeO-C_6H_4, R' = Bn):

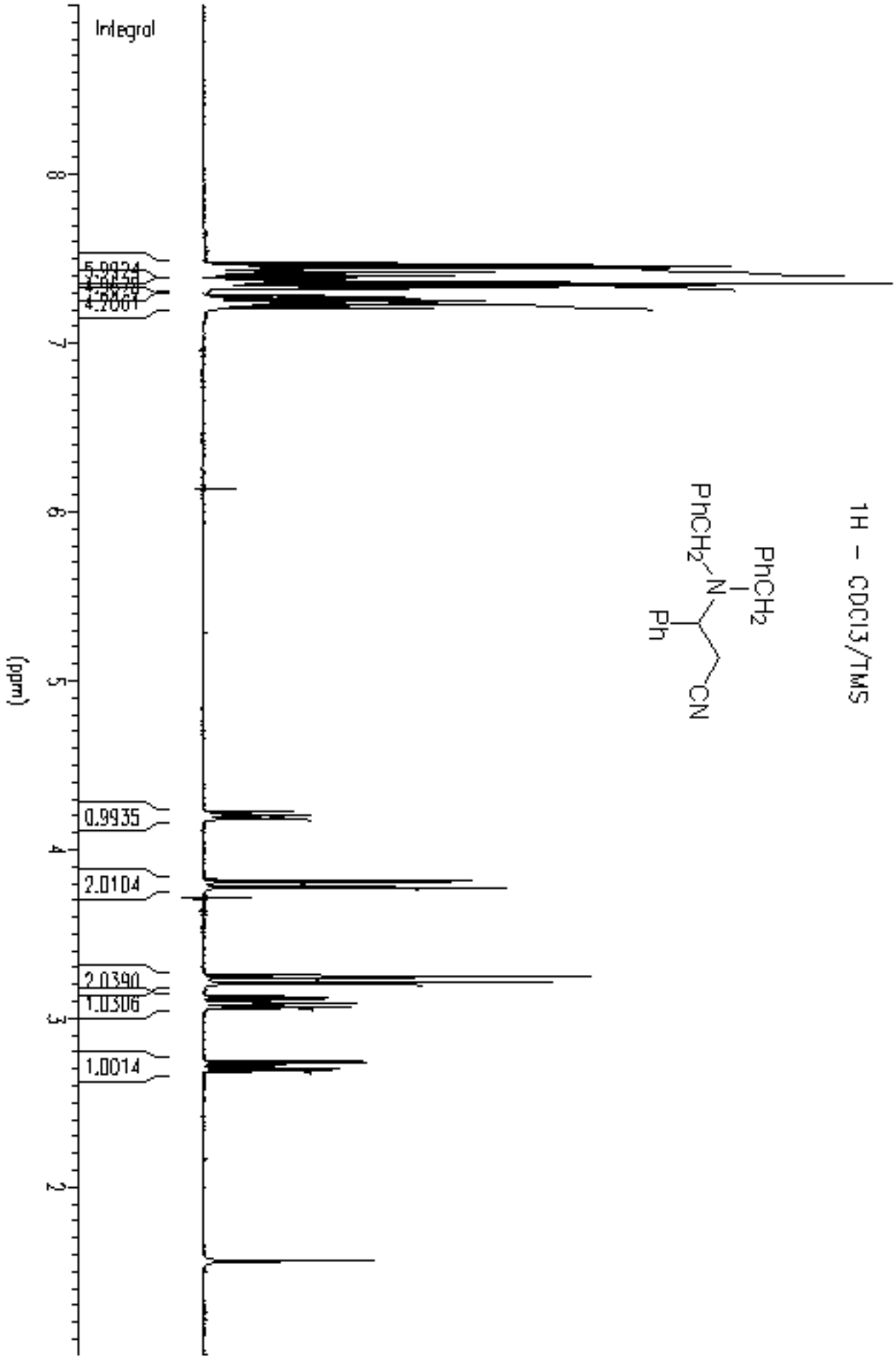

1H – CDCl3/TMS
PhCH2
N
PhCH2
CO2i-Pr
OMe
Integral
3.9801
4.0612
4.0647
1.9518
7.4
7.3
7.2
7.1
7.0
6.9
(ppm)

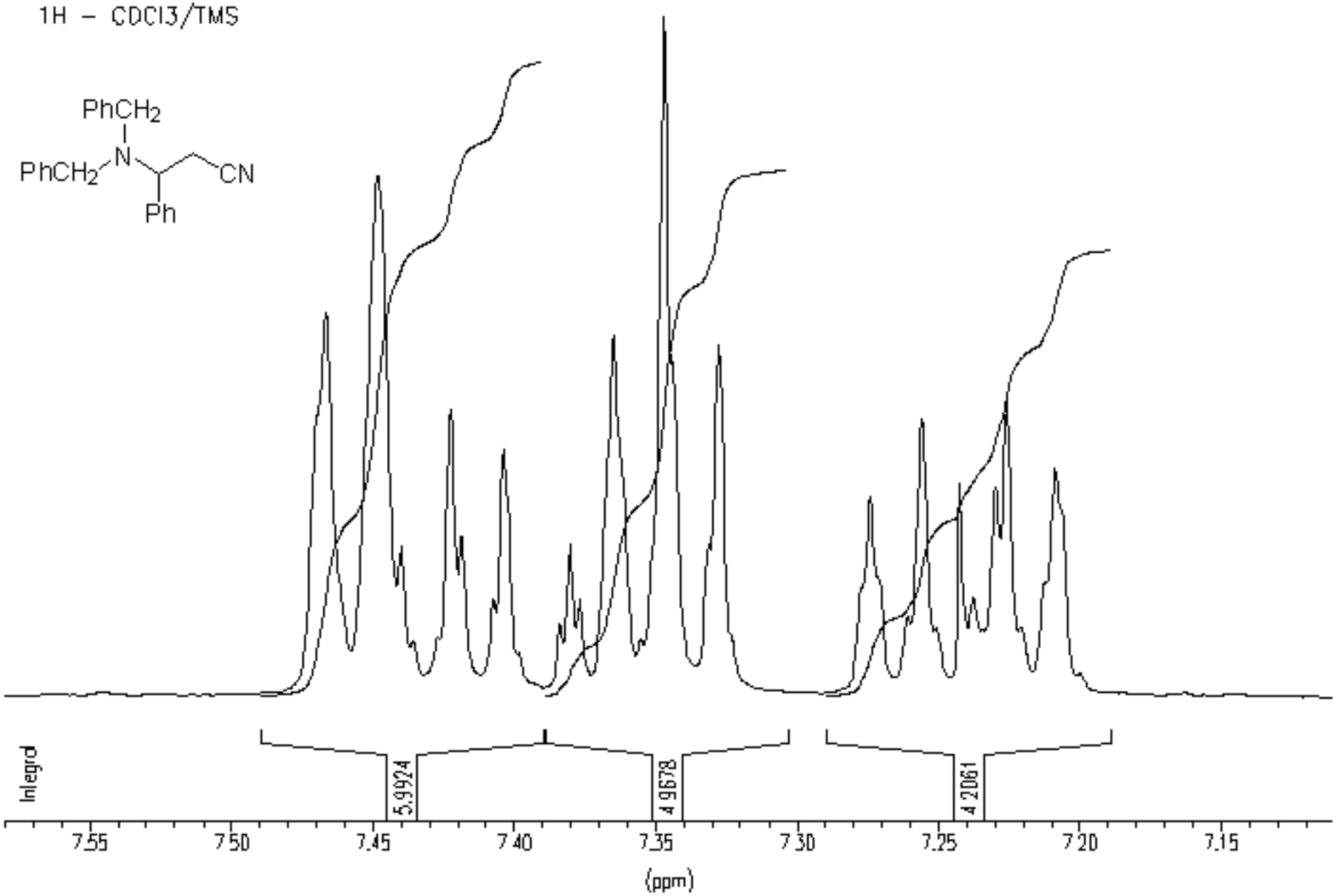

1H – CDCl3/TMS
PhCH2
N
PhCH2
CO2i-Pr
OMe
0.8808
4.96
4.88
(ppm)
0.9670
4.25
(ppm)
Integral
0.8808
0.9670
3.0239
2.0194
2.0049
0.9701
0.9577
5.0
4.5
4.0
3.5
3.0
2.5
(ppm)

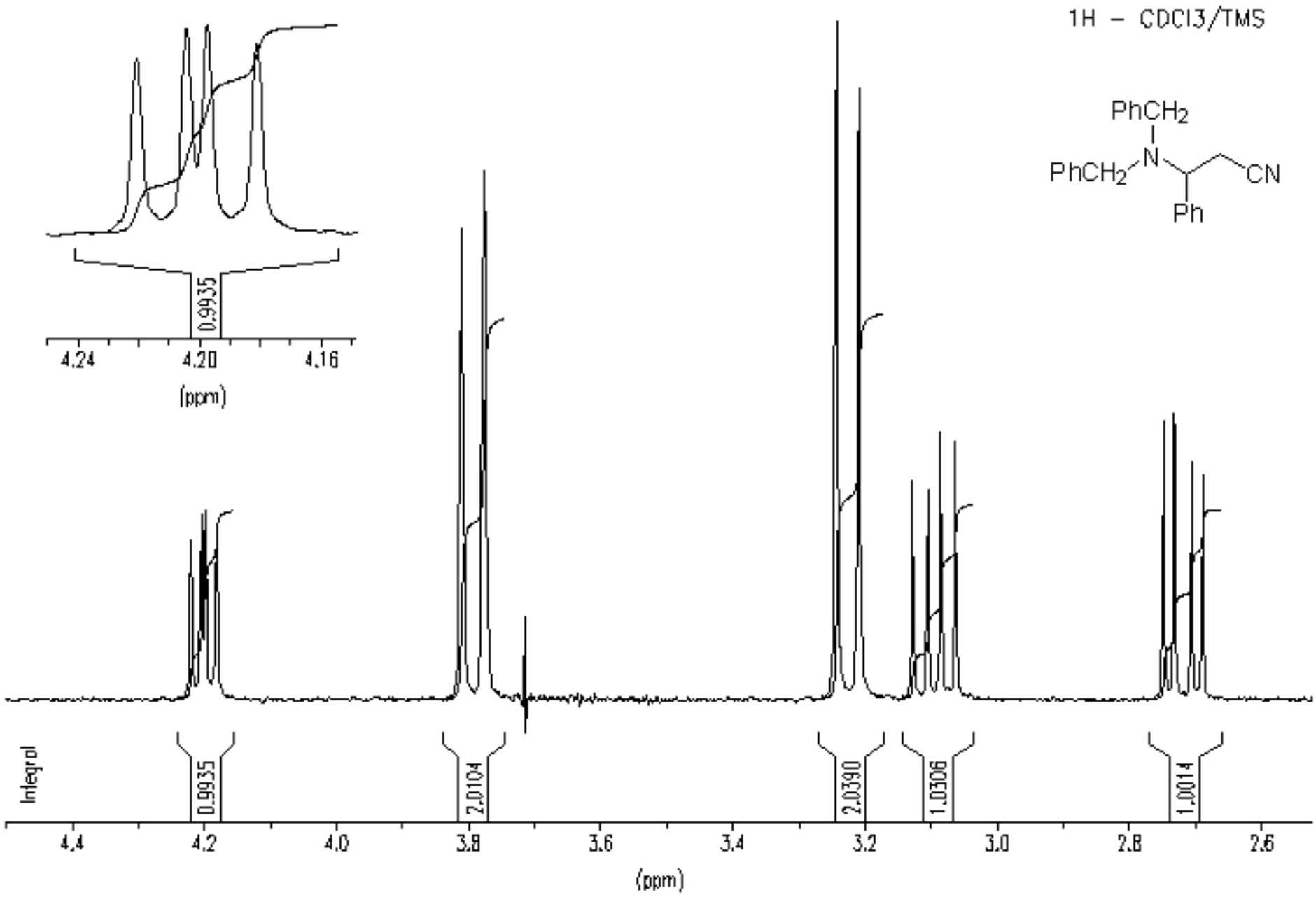

1H – CDCl3/TMS
PhCH2
N
PhCH2
CO2i-Pr
OMe
3.0239
2.0194
2.0049
0.9701
0.9577
3.8
3.6
3.4
3.2
3.0
2.8
2.6
(ppm)
Integrd
6.1211
1.20
1.14
1.08
(ppm)

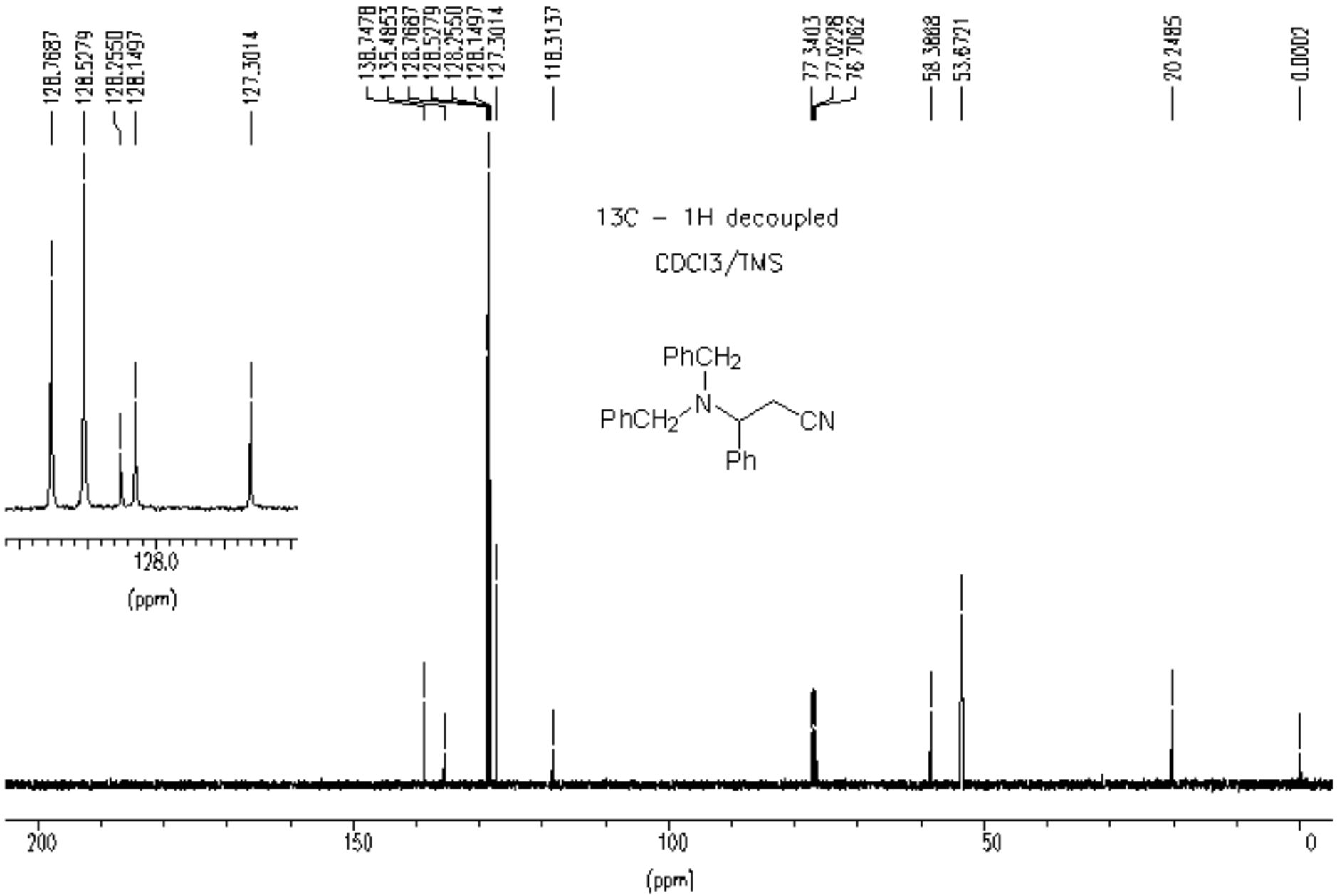

171.3305
158.7419
139.7722
130.1940
129.6424
128.7789
128.1741
126.8699
113.3258
77.3344
77.0169
76.6993
67.7771
58.4311
55.2084
53.7723
36.7155
21.7468
-0.0001
130.1940
129.6424
128.7789
128.1741
126.8699
130.0
128.0
(ppm)
PhCH2
N
PhCH2
CO2i-Pr
OMe
13C – 1H decoupled
CDCl3/TMS
200
150
100
50
0
(ppm)

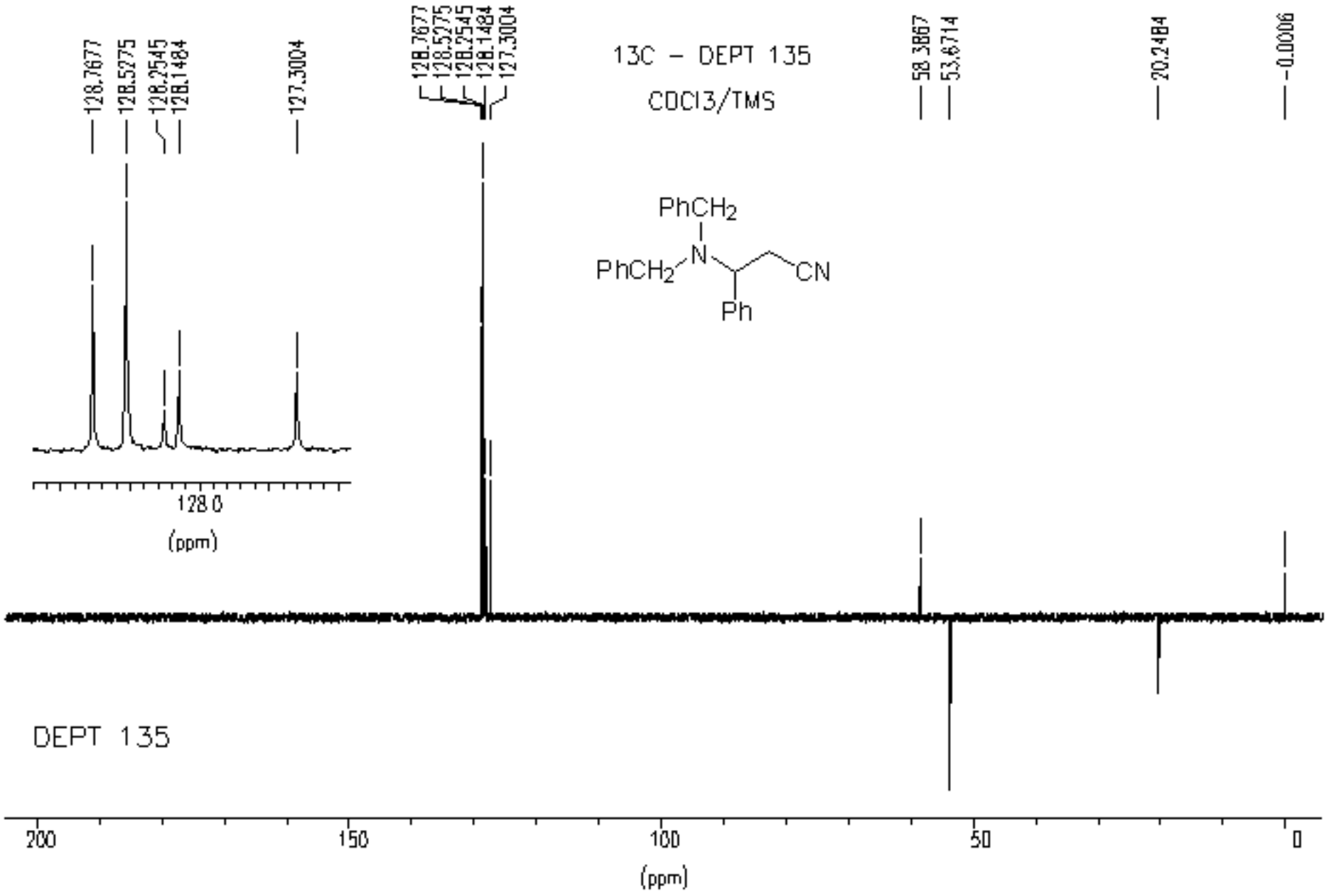
Compound **4** (R = Ph, R' = Bn):



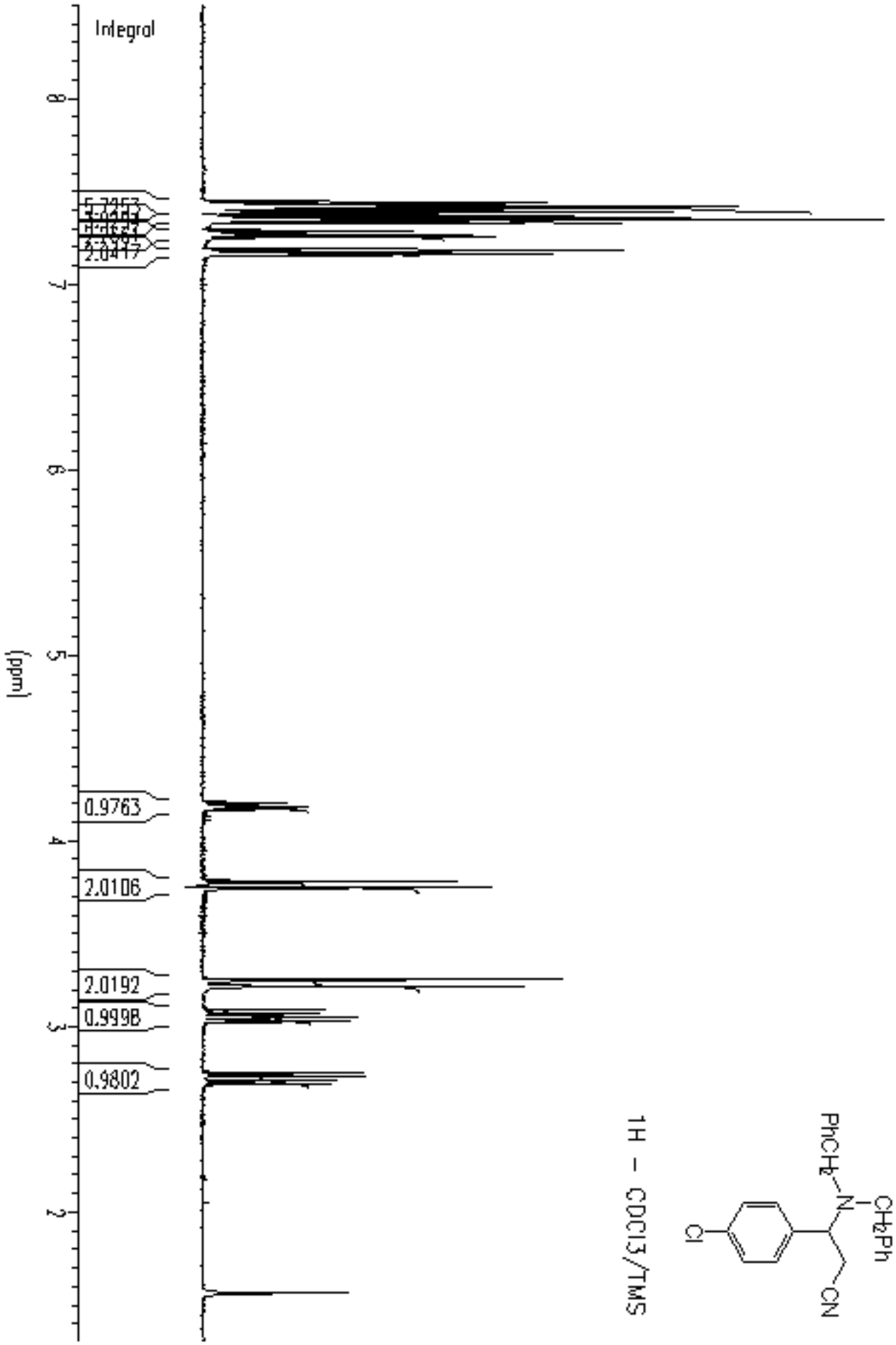

1H – CDCl3/TMS
PhCH2
N
PhCH2
CN
Ph
Integrd
5.9924
4.9678
4.2061
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
(ppm)


1H – CDCl3/TMS
PhCH2
PhCH2
N
CN
Ph
0.9935
4.24
4.20
4.16
(ppm)
Integral
0.9935
2.0104
2.0390
1.0306
1.0014
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
(ppm)


128.7687
128.5279
128.2550
128.1497
127.3014
138.7478
135.4853
128.7687
128.5279
128.2550
128.1497
127.3014
118.3137
77.3403
77.0228
76.7062
58.3868
53.6721
20.2485
0.0002
13C – 1H decoupled
CDCl3/TMS
PhCH2
N
PhCH2
CN
Ph
128.0
(ppm)
200
150
100
50
0
(ppm)


128.7677
128.5275
128.2545
128.1484
127.3004
128.7677
128.5275
128.2545
128.1484
127.3004
13C - DEPT 135
CDCl3/TMS
58.3867
53.6714
20.2484
-0.0006
PhCH2
PhCH2
N
CN
Ph
128.0
(ppm)
DEPT 135
200
150
100
50
0
(ppm)

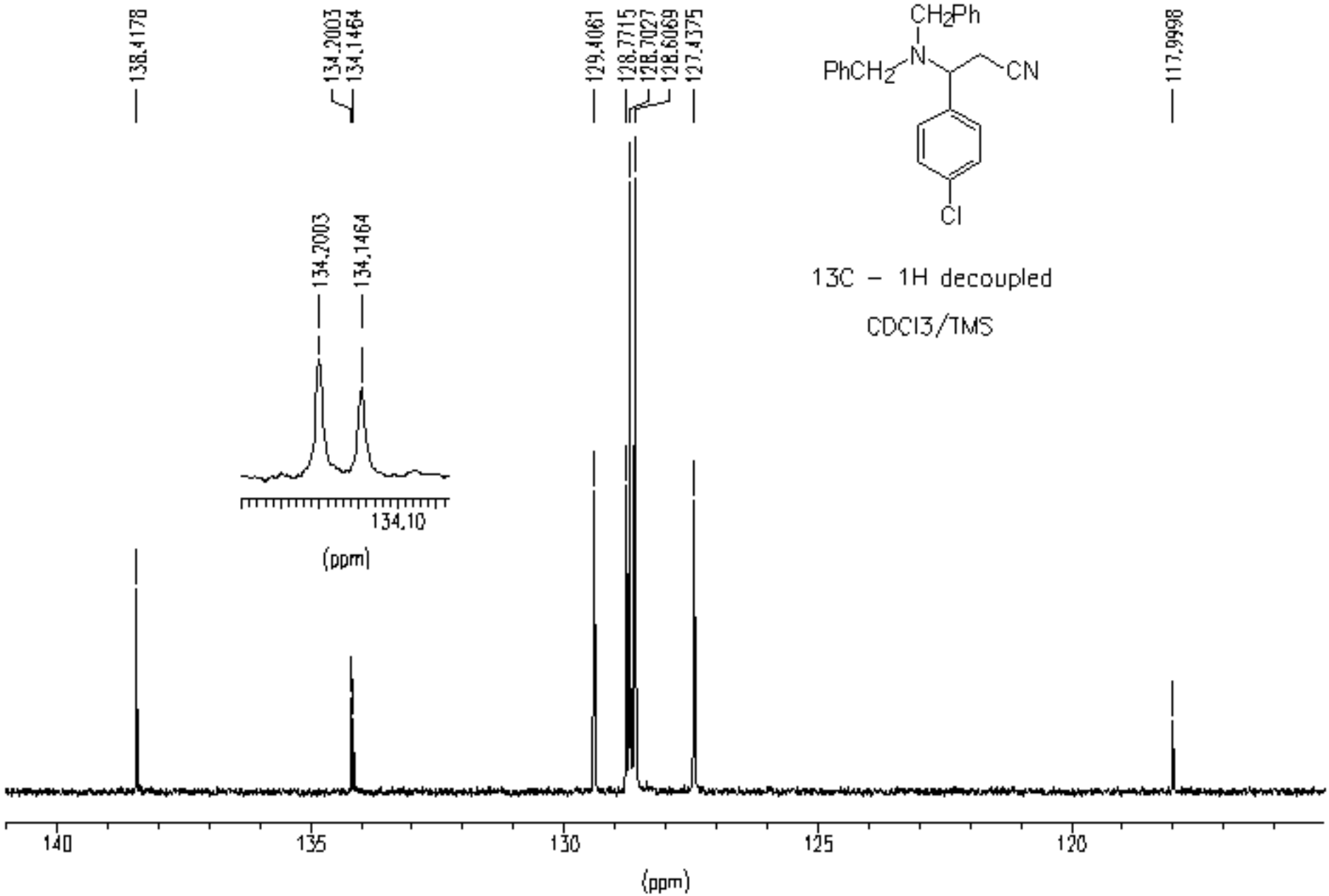
Compound **4** (R = *p*-Cl-C_6H_4, R' = Bn):

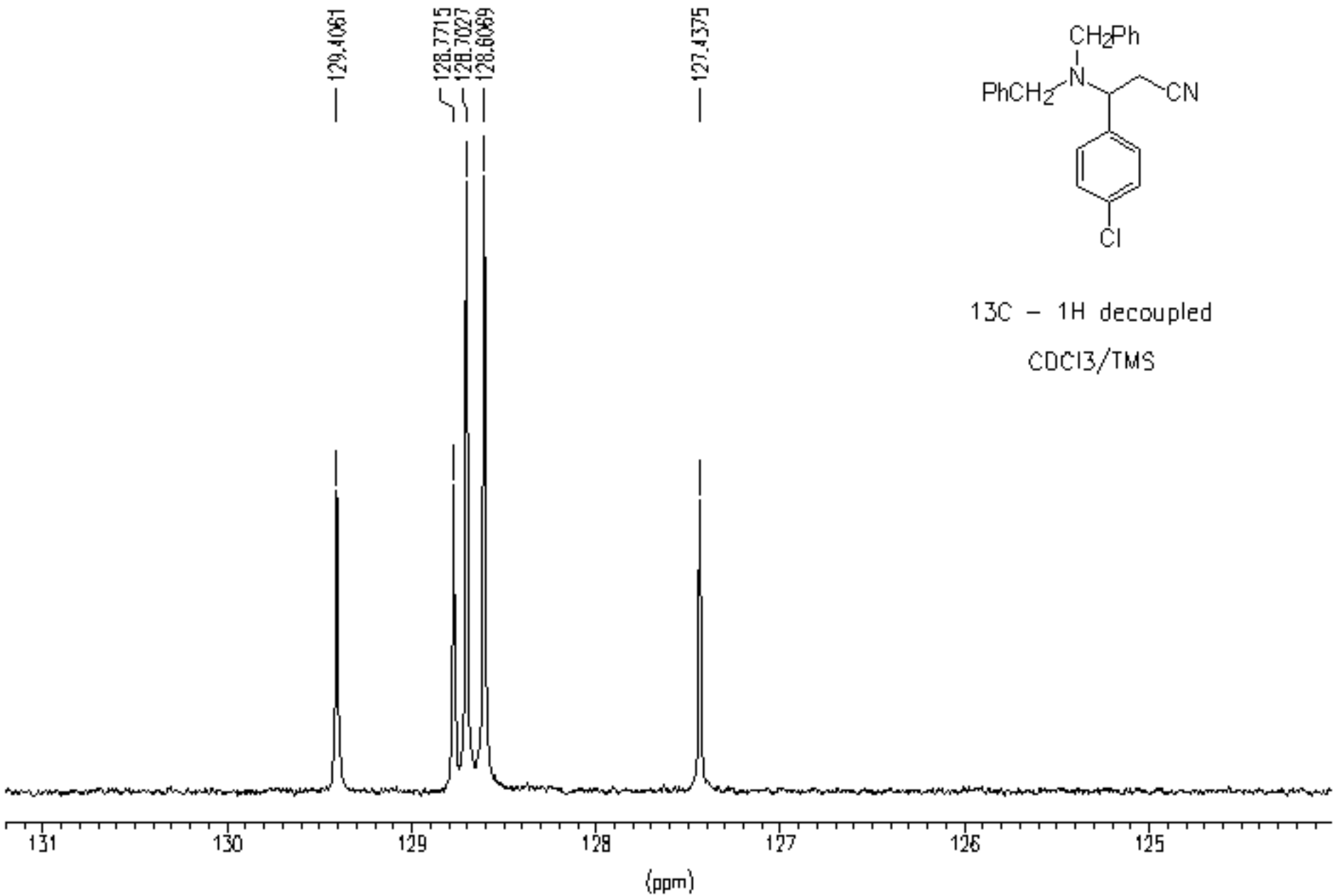


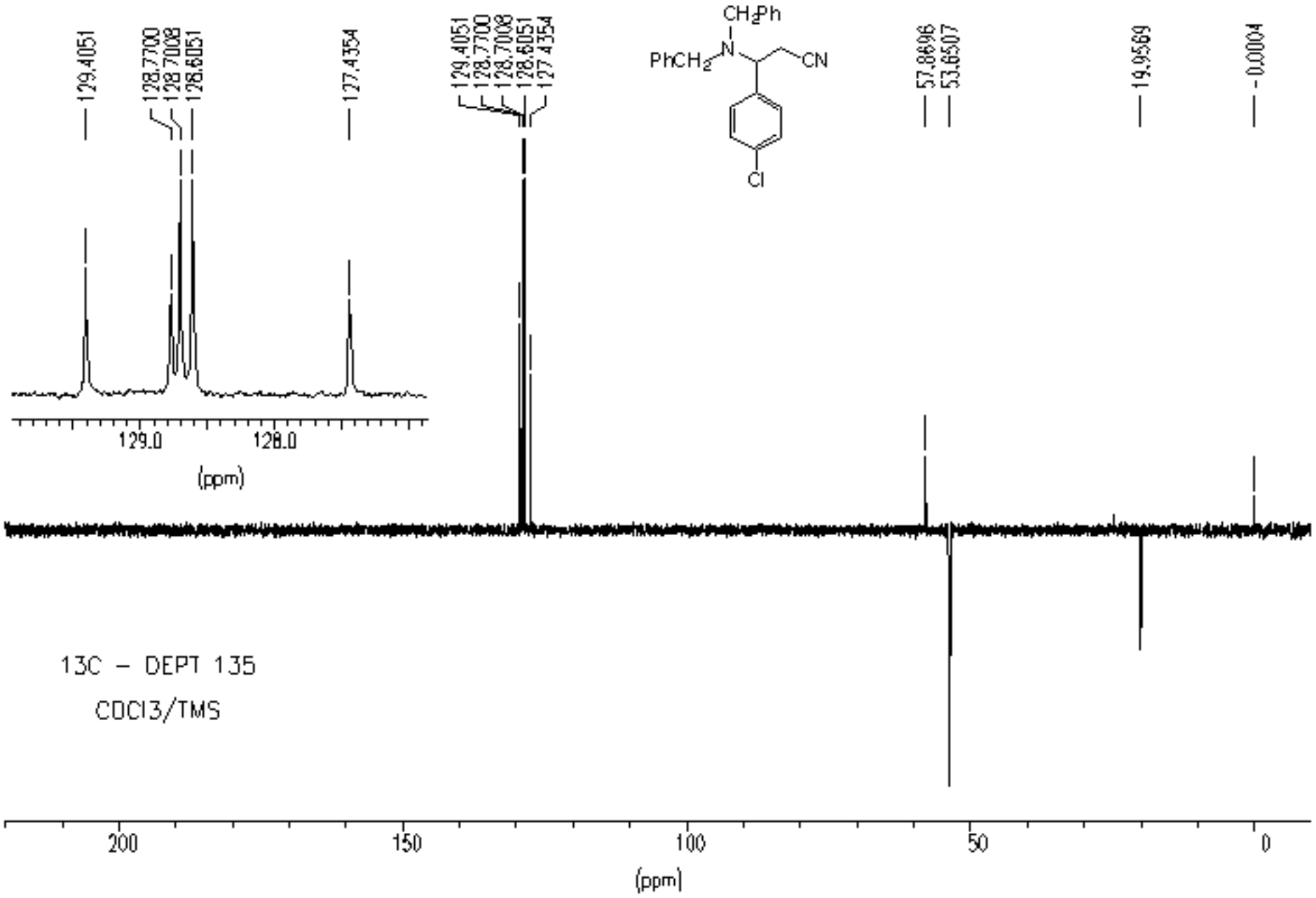
Integral
5.7253
3.9294
2.2661
2.0417
7.5
7.4
7.3
7.2
7.1
(ppm)
2976.94
2975.48
2968.01
2965.28
2956.79
2954.21
2948.40
2946.58
2941.18
2939.78
2935.05
2933.52
2931.74
2915.81
2914.45
2913.11
2909.33
2907.13
2904.91
2902.30
2901.25
2899.92
2898.58
2875.85
2873.28
2871.37
2866.76
2864.85
2862.25
1H - CDCl3/TMS
PhCH2
N
CH2Ph
CN
Cl

4.20
(ppm)
0.9763
4.18
Integral
0.9763
2.0106
2.0192
0.9998
0.9802
4.0
3.5
3.0
2.5
(ppm)
1682.78
1675.81
1674.03
1667.07
1512.86
1499.10
1300.29
1286.49
1236.20
1227.40
1219.29
1210.52
1099.00
1092.07
1082.12
1075.19
1H - CDCl3/TMS
PhCH2
N
CH2Ph
CN
Cl

13C - 1H decoupled
CDCl3/TMS
PhCH2
N
CH2Ph
CN
Cl
200
150
100
50
0
(ppm)
138.4178
134.2003
134.1464
129.4061
128.7715
128.7027
128.6069
127.4375
117.9998
77.3323
77.0150
76.6967
57.8711
53.6516
19.9575
0.0004


138.4178
134.2003
134.1464
129.4061
128.7715
128.7027
128.6069
127.4375
117.9998
CH2Ph
PhCH2
N
CN
Cl
13C – 1H decoupled
CDCl3/TMS
134.10
(ppm)
140
135
130
125
120
(ppm)


129.4061
128.7715
128.7027
128.6069
127.4375
CH2Ph
N
PhCH2
CN
Cl
13C – 1H decoupled
CDCl3/TMS
131
130
129
128
127
126
125
(ppm)


129.4051
128.7700
128.7008
128.6051
127.4354
129.4051
128.7700
128.7008
128.6051
127.4354
CH2Ph
PhCH2
N
CN
Cl
57.8696
53.6507
19.9569
0.0004
129.0
128.0
(ppm)
13C - DEPT 135
CDCl3/TMS
200
150
100
50
0
(ppm)