

Supporting Information

Silver-Catalyzed Aldehyde Olefination Using Siloxy Alkynes

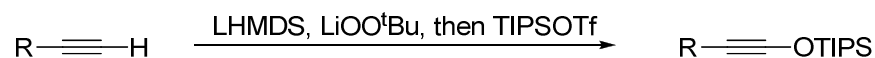
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5735 South Ellis Ave., Chicago, IL 60637

General. Ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. Anhydrous dichloromethane (HPLC grade) was purified by distillation over calcium hydride. Anhydrous tetrahydrofuran was freshly distilled from sodium-benzophenone. Triisopropylsilyl trifluoromethanesulfonate (TIPSOTf) was distilled under reduced pressure over calcium hydride. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using Whatman precoated silica gel plates. Flash column chromatography was performed over Silicycle silica gel (230-400 mesh). ^1H NMR and ^{13}C NMR spectra were recorded on Bruker DRX-400 or DMX-500 spectrometers using residual solvent peaks as an internal standard. Infrared spectra were recorded with a Nicolet FTIR spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with an Agilent 1100 LCMS using the following conditions unless otherwise noted; APCI, POS, SCAN, 70, with methanol or dichloromethane as the eluting solvent.

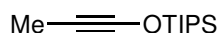
General Procedure A: Preparation of Siloxy Alkynes



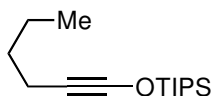
Anhydrous *tert*-butyl hydroperoxide (TBHP) was prepared following a detailed literature procedure.¹ CAUTION: SOLUTIONS OF OXIDANTS AND OXIDIZABLE SUBSTRATES ARE POTENTIALLY HAZARDOUS AND POSSIBLY SUBJECT TO VIOLENT DECOMPOSITION BY ADVENTITIOUS CATALYSTS. Safety considerations related to handling solutions of TBHP have been previously discussed. See reference 1 and further references cited therein.

A solution of alkyne (2 mmol) in THF (10 mL) was treated at -78 °C with freshly prepared 1.0 M solution of LiHMDS in THF (2.4 mL). At the same time, a solution of lithium *t*-butyl peroxide was generated through treating a solution of anhydrous *t*-butyl hydrogen peroxide (3.7 M in toluene, 2.4 mmol, 0.65 mL) in THF (10 mL) with 1.0 M LiHMDS (2.6 mL) at -78 °C. Lithium *t*-butyl peroxide solution was

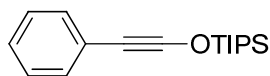
transferred to the alkynyllithium solution via cannula and the resulting mixture was allowed to warm to 0 °C over 0.5 h, stirred at the same temperature for 2 h and cooled to -78 °C before the drop-wise addition of triisopropylsilyl trifluoromethanesulfonate (2.6 mmol, 0.7 mL). The resulting reaction mixture was allowed to warm up to 0 °C, stirred for 0.5 h and diluted with hexanes (50 mL). The organic layer was washed with saturated aqueous NaHCO₃ (40 mL), H₂O (40 mL), brine (30 mL), dried (Na₂SO₄), filtered and concentrated. The residue was subjected to purification via Kugelrohr distillation.



The above siloxy alkyne was prepared in 80% yield according to the general procedure A except that the product was purified by silica gel column (pretreated with Et₃N) chromatography. ¹H NMR (500 Hz, CDCl₃) δ 1.66 (s, 3H), 1.27-1.20 (m, 3H), 1.10 (d, 18H, *J* = 7.5 Hz); ¹³C NMR (125 Hz, CDCl₃) δ 85.4, 25.5, 17.3, 11.8, 1.51; IR (neat, cm⁻¹) 2947, 2869, 2289, 1464; MS(APCI) Calculated for [C₁₂H₂₄OSi]⁺: 212.16; [M⁺ + MeOH + H]: 245.19; Found: 245.1.

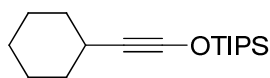


The above siloxy alkyne was prepared in 95% yield according to the general procedure A. ¹H NMR (500 MHz, CDCl₃) δ 2.05 (t, 2H, *J* = 6.3 Hz), 1.41-1.35 (m, 4H), 1.27-1.20 (m, 3H), 1.11 (d, 18H, *J* = 7.5 Hz), 0.87 (t, 3H, *J* = 6.8 Hz); ¹³C NMR (125 MHz, CDCl₃) δ 86.7, 32.1, 30.4, 21.9, 17.3, 16.9, 13.6, 11.8; IR (neat, cm⁻¹) 2946, 2868, 2278; MS (APCI) Calculated for [C₁₅H₃₁OSi]⁺: 255.48; Found: 255.0.



The above siloxy alkyne was prepared in 85% yield according to the general procedure A. ¹H NMR (500 MHz, CDCl₃) δ 7.32-7.30 (m, 2H), 7.25-7.22 (m, 2H), 7.19-7.15 (m, 1H), 1.38-1.32 (m, 3H), 1.18 (d, 18H, *J* = 7.5 Hz); ¹³C NMR (125 MHz, CDCl₃) δ 131.4, 128.1, 125.9, 125.2, 96.8, 33.5, 17.3, 11.9; IR (neat, cm⁻¹)

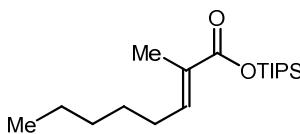
2946, 2868, 2266; MS (APCI) Calculated for $[C_{18}H_{31}OSi]^+$ 307.52; $[M^+ + MeOH + H]$: 307.52; Found: 307.2.



The above siloxy alkyne was prepared in 91% yield according to the general procedure A. 1H NMR (500 MHz, $CDCl_3$) δ 2.28-2.24 (m, 1H), 1.74-1.67 (m, 2H), 1.67-1.64 (m, 2H), 1.47 (m, 1H), 1.34-1.21 (m, 8H), 1.12 (d, 18H, $J = 7.0$ Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 87.2, 35.1, 34.0, 28.0, 26.1, 25.1, 17.4, 11.8; IR (neat, cm^{-1}) 2293, 2868, 2274, 2076, 1464; MS (APCI) Calculated for $[C_{17}H_{33}OSi]^+$: 281.23; Found: 281.1.

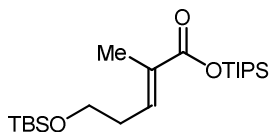
General Procedure B: AgNTf₂-Catalyzed Aldehyde Olefination

A solution of siloxy alkyne (0.20 mmol) and aldehyde (0.22 mmol) in CH_2Cl_2 (4 mL) was cooled to -78 °C under inert nitrogen atmosphere and treated with AgNTf₂ (3.9 mg, 0.01 mmol). The reaction mixture was stirred at the same temperature for 30 min. The reaction was allowed to warm to room temperature and stirred for another 30 min. The solvent was removed under reduced pressure. Crude product was purified directly by silica gel column chromatography to afford the requisite olefination product.



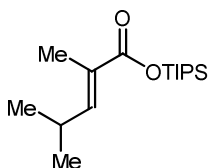
6

Ester 6 was prepared in 87% yield according to the general procedure B. 1H NMR (500 Hz, $CDCl_3$) δ 6.81 (t, 1H, $J = 7.5$ Hz), 2.17 (m, 2H), 1.82 (s, 3H), 1.45-1.25 (m, 9H), 1.08 (d, 18H, $J = 7.5$ Hz), 0.89 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, $CDCl_3$) δ 168.1, 143.4, 128.6, 31.5, 28.8, 28.3, 22.5, 17.8, 14.0, 12.6, 12.0; IR (neat, cm^{-1}) 2945, 2868, 1691, 1646, 1465; MS (EI) Found: 313.2.



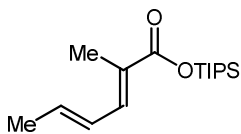
7

Ester 7 was prepared in 75% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 6.84 (t, 1H, $J = 7.5$ Hz), 3.71 (t, 2H, $J = 6.3$ Hz), 2.40 (m, 2H), 1.84 (s, 3H), 1.32 (m, 3H), 1.09 (d, 18H, $J = 7.5$ Hz), 0.88 (s, 9H), 0.04 (s, 6H); ^{13}C NMR (100 Hz, CDCl_3) δ 167.9, 139.6, 130.3, 61.7, 32.5, 25.9, 18.3, 17.9, 12.8, 12.0, -5.4; IR (neat, cm^{-1}) 2948, 1692, 1650, 1464; MS (EI) Found: 401.2.



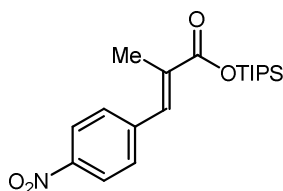
8

Ester 8 was prepared in 87% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 6.61 (d, 1H, $J = 9.5$ Hz), 2.62 (m, 1H), 1.84 (d, 3H, $J = 4.5$ Hz), 1.30 (m, 3H), 1.09 (d, 3H, $J = 7.5$ Hz), 1.02 (d, 6H, $J = 6.5$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 168.4, 149.7, 126.6, 28.0, 22.0, 17.8, 12.5, 12.0; IR (neat, cm^{-1}) 2961, 2869, 1693, 1646, 1465; MS (EI) Found: 285.1.



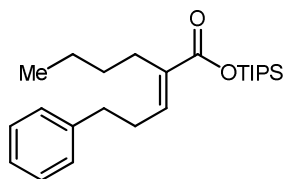
9

Ester 9 was prepared in 75% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 7.19 (d, 1H, $J = 11.5$ Hz), 6.37 (m, 1H), 6.08 (m, 1H), 1.92 (s, 3H), 1.87 (d, 3H, $J = 6.5$ Hz), 1.35 (m, 3H), 1.09 (d, 18H, $J = 7.5$ Hz); ^{13}C NMR (100 Hz, CDCl_3) δ 168.5, 139.2, 137.7, 127.6, 126.0, 18.9, 17.8, 12.8, 12.0; IR (neat, cm^{-1}) 3033, 2945, 2868, 1685, 1644, 1610; MS (EI) Found: 283.1.



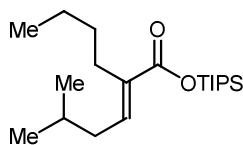
10

Ester 10 was prepared in 84% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 8.25 (d, 2H, $J = 8.5$ Hz), 7.72 (s, 1H), 7.54 (d, 2H, $J = 8.5$ Hz), 2.13 (d, 3H, $J = 1.5$ Hz), 1.39 (m, 3H), 1.13 (d, 18H, $J = 7.5$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 167.5, 147.1, 142.6, 136.5, 133.4, 130.2, 123.6, 17.8, 14.5, 12.0; IR (neat, cm^{-1}) 3080, 2946, 2868, 1692, 1597; MS (EI) Found: 364.1.



11

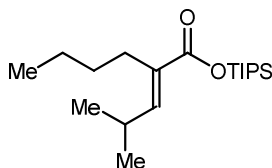
Ester 11 was prepared in 85% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 7.30-7.26 (m, 2H), 7.21-7.18 (m, 3H), 6.82 (t, 1H, $J = 7.5$ Hz), 2.76 (t, 2H, $J = 7.5$ Hz), 2.53-2.48 (m, 2H), 2.24 (t, 2H, $J = 7.5$ Hz), 1.36-1.26 (m, 7H), 1.09 (d, 18H, $J = 7.5$ Hz), 0.88 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 167.7, 141.8, 141.2, 134.2, 128.4, 126.1, 35.1, 31.5, 30.7, 26.8, 22.7, 17.8, 14.0, 12.0; IR (neat, cm^{-1}) 3064, 2956, 1693, 1642, 1604, 1496; MS (EI) Found: 389.2.



12

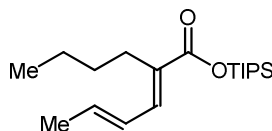
Ester 12 was prepared in 93% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 6.82 (t, 1H, $J = 7.5$ Hz), 2.28 (t, 2H, $J = 7.3$ Hz), 2.07 (t, 2H, $J = 7.3$ Hz), 1.77-1.71 (m, 1H), 1.38-1.30 (m, 7H), 1.09 (d, 18H, $J = 7.5$ Hz), 0.94 (d, 6H, $J = 7.0$ Hz), 0.90 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ

168.9, 142.2, 134.1, 37.6, 31.6, 28.4, 26.9, 22.8, 22.5, 17.9, 14.0, 12.0; IR (neat, cm^{-1}) 2956, 2869, 1692, 1641, 1465; MS (EI) Found: 341.3.



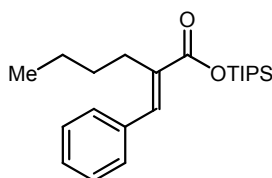
13

Ester 13 was prepared in 94% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 6.58 (d, 1H, $J = 10$ Hz), 2.65-2.61 (m, 1H), 2.28 (t, 2H, $J = 7.8$ Hz), 1.40-1.29 (m, 7H), 1.09 (d, 18H, $J = 7.5$ Hz), 1.02 (d, 6H, $J = 6.5$ Hz), 0.90 (t, 3H, $J = 7.3$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 168.2, 149.7, 131.3, 32.1, 27.9, 27.0, 22.8, 22.4, 17.9, 13.4, 12.0; IR (neat, cm^{-1}) 2959, 2869, 1692, 1642, 1465; MS (EI) Found: 327.2.



14

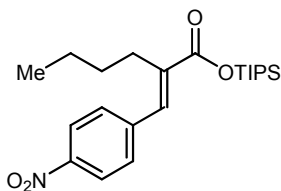
Ester 14 was prepared in 66% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 7.18 (d, 1H, $J = 11.5$ Hz), 6.39-6.33 (m, 1H), 6.12-6.05 (m, 1H), 2.38 (t, 2H, $J = 7.5$ Hz), 1.87 (dd, 3H, $J_1 = 7.0$ Hz, $J_2 = 1.5$ Hz), 1.44-1.25 (m, 7H), 1.09 (d, 18H, $J = 7.5$ Hz), 0.91 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 168.3, 139.3, 137.8, 131.1, 127.5, 32.0, 27.0, 22.7, 18.9, 17.9, 14.0, 12.0; IR (neat, cm^{-1}) 3032, 2946, 2868, 1685, 1642, 1605, 1465; MS (EI) Found: 325.2.



15

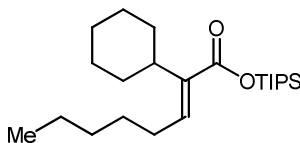
Ester 15 was prepared in 73% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 7.71 (s, 1H), 7.41-7.37 (m, 4H), 7.34-7.31 (m, 1H), 2.55-2.51 (m, 2H), 1.59-1.53 (m, 2H), 1.43-1.35 (m, 5H), 1.44 (d, 18H, $J = 7.5$ Hz),

0.92 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 168.3, 139.2, 136.0, 134.9, 129.3, 128.4, 128.2, 31.5, 27.6, 22.9, 17.9, 13.9, 12.0; IR (neat, cm^{-1}) 2946, 2868, 1690, 1627, 1465; MS (EI) Found: 361.1.



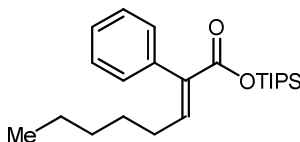
16

Ester 16 was prepared in 84% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 8.24 (d, 2H, $J = 8.5$ Hz), 7.68 (s, 1H), 7.49 (d, 2H, $J = 8.5$ Hz), 2.49 (t, 2H, $J = 8.0$ Hz), 1.55-1.51 (m, 2H), 1.42-1.34 (m, 5H), 1.12 (d, 18H, $J = 7.5$ Hz), 0.88 (t, 3H, $J = 7.3$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 167.4, 147.1, 142.7, 138.4, 136.3, 129.8, 123.7, 31.4, 27.7, 22.8, 17.8, 13.8, 12.0; IR (neat, cm^{-1}) 3079, 2947, 2868, 1694, 1597, 1522; MS (EI) Found: 406.1.



17

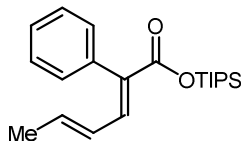
Ester 17 was prepared in 72% yield according to the general procedure B. ^1H NMR (400 Hz, CDCl_3) δ 6.69 (t, 1H, $J = 7.5$ Hz), 2.40-2.19 (m, 2H), 2.20 (m, 1H), 2.19 (m, 5H), 1.50-1.21 (m, 13H), 1.09 (d, 18H, $J = 7.5$ Hz), 0.88 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 168.7, 167.9, 142.7, 138.9, 138.0, 137.8, 41.3, 38.5, 32.8, 31.5, 30.5, 29.6, 29.5, 28.8, 28.2, 27.0, 26.8, 26.2, 25.9, 22.6, 22.5, 17.9, 14.0, 12.1; IR (neat, cm^{-1}) 2927, 2867, 1691, 1465; MS (EI) Found: 381.2.



18

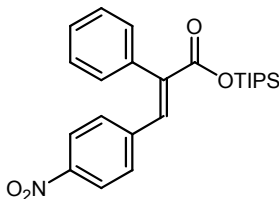
Ester 18 was prepared in 76% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 7.35-7.32 (m, 2H), 7.28-7.25 (m, 1H), 7.15-7.13 (m, 2H), 7.09 (t, 1H, $J = 7.5$ Hz), 2.07 (m, 2H), 1.42-1.21 (m, 9H), 1.02 (d, 18H, $J = 7.5$

Hz), 0.84 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 166.8, 145.8, 136.1, 135.0, 129.6, 127.8, 127.1, 31.4, 29.6, 28.5, 22.4, 17.7, 13.9, 11.9; IR (neat, cm^{-1}) 2945, 2868, 1697, 1637, 1465; MS (EI) Found: 375.2.



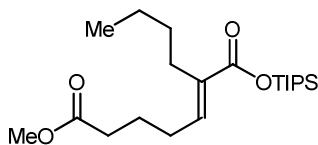
19

Ester 19 was prepared in 76% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 7.46 (d, 1H, $J = 10.0$ Hz), 7.38-7.35 (m, 2H), 7.31-7.30 (m, 1H), 7.22-7.20 (m, 2H), 6.19-6.12 (m, 2H), 1.79 (d, 3H, $J = 6.5$ Hz), 1.31-1.25 (m, 3H), 1.05 (d, 18H, $J = 7.5$ Hz); ^{13}C NMR (100 Hz, CDCl_3) δ 167.2, 141.3, 139.6, 135.9, 131.7, 130.1, 128.4, 127.8, 127.2, 18.8, 17.7, 11.9; IR (neat, cm^{-1}) 2945, 2867, 1690, 1637, 1465; MS (EI) Found: 345.2.



20

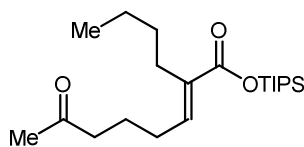
Ester 20 was prepared in 69% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 8.01 (d, 2H, $J = 9.0$ Hz), 7.87 (s, 1H), 7.37-7.35 (m, 3H), 7.21-7.17 (m, 4H), 1.35-1.29 (m, 3H), 1.04 (d, 18H, $J = 7.5$ Hz); ^{13}C NMR (100 Hz, CDCl_3) δ 166.6, 147.3, 141.3, 137.5, 135.4, 131.0, 129.3, 128.8, 128.2, 123.3, 17.7, 11.8; IR (neat, cm^{-1}) 3060, 2945, 2867, 1695, 1595, 1522; MS (EI) Found: 426.1.



23

Diester 23 was prepared in 80% yield according to the general procedure B. ^1H NMR (500 Hz, CDCl_3) δ 6.73 (t, 1H, $J = 7.5$ Hz), 3.67 (s, 3H), 2.34 (t, 2H, $J = 7.5$ Hz), 2.28-2.20 (m, 4H), 1.79-1.76 (m, 2H), 1.36-1.29 (m, 7H), 1.07 (d, 18H, $J =$

7.5 Hz), 0.88 (t, 3H, $J = 7.0$ Hz); ^{13}C NMR (125 Hz, CDCl_3) δ 173.6, 167.7, 141.5, 134.6, 51.5, 33.5, 31.6, 27.9, 26.9, 24.1, 22.8, 17.9, 14.0, 12.0; IR (neat, cm^{-1}) 2956, 2868, 1743, 1693, 1642; MS (EI) Found: 385.6.



24

Ester 24 was prepared in 76% yield according to the general procedure B. ^1H NMR (400 Hz, CDCl_3) δ 6.75 (t, 1H, $J = 7.5$ Hz), 2.44 (t, 2H, $J = 9.2$ Hz), 2.27 (t, 2H, $J = 9.2$ Hz), 2.21-2.15 (m, 2H), 2.13 (s, 3H), 1.63-1.57 (m, 2H), 1.47-1.28 (m, 9H), 1.07 (d, 18H, $J = 7.5$ Hz), 0.89 (t, 3H, $J = 8.7$ Hz); ^{13}C NMR (100 Hz, CDCl_3) δ 208.8, 167.8, 142.5, 133.9, 43.5, 31.6, 28.5, 28.4, 26.9, 23.5, 22.8, 17.8, 17.7, 14.0, 12.0; IR (neat, cm^{-1}) 2945, 2867, 1719, 1690, 1641, 1465; MS (EI) Found: 383.3.

ppm

Integral



OTPS
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- 1.660
- 1.652
- 1.272
- 1.256
- 1.241
- 1.230
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- 1.218
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- 1.109
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- 1.046

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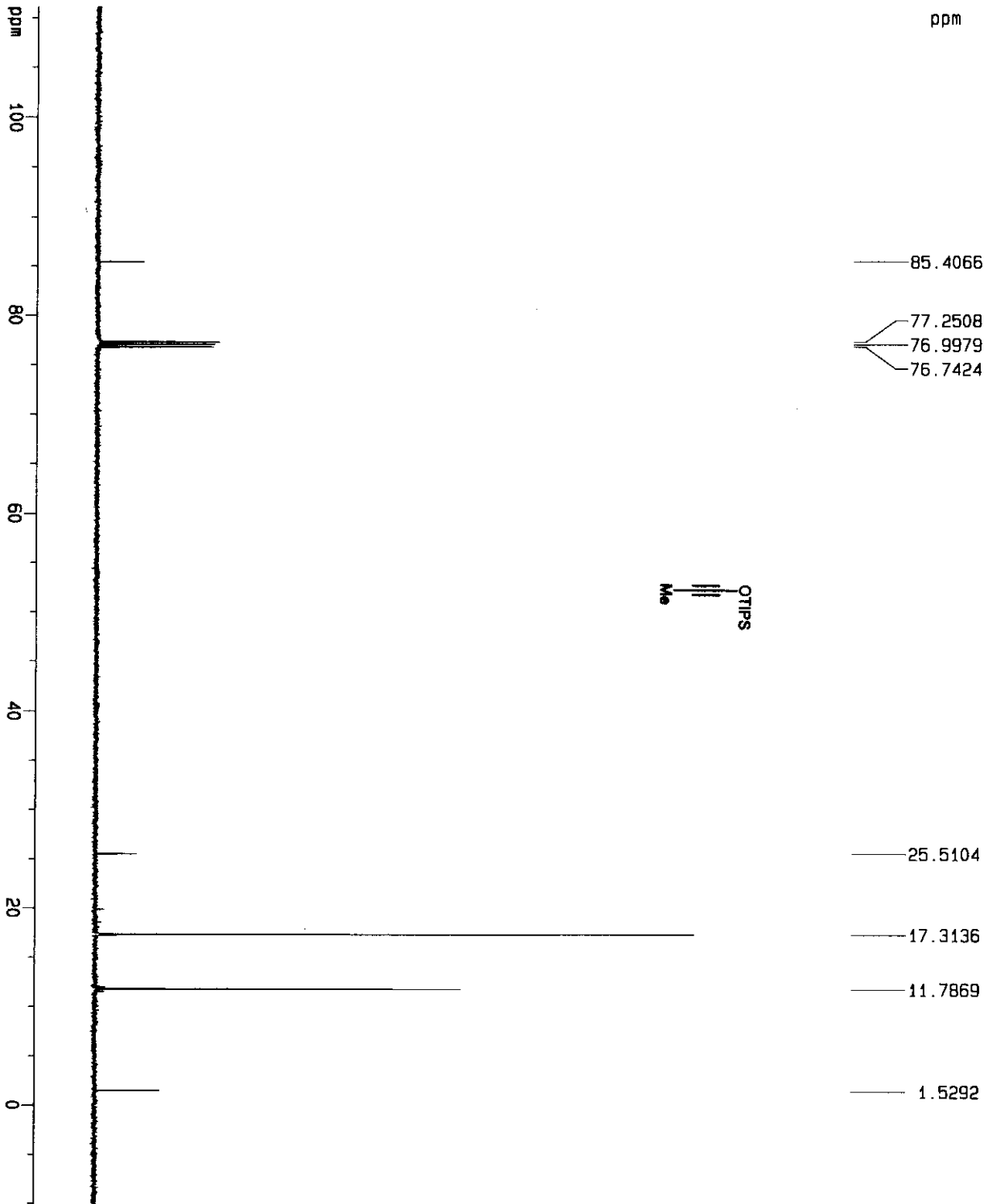
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DE 4.50 usec
TE 300.0 K
D1 10.00000000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SF01 500.1320118 MHz

F2 - Processing parameters
SI 16384
SF 500.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 7.756 ppm
F1 3879.05 Hz
F2P 0.455 ppm
F2 227.56 Hz
PPMCH 0.36505 ppm/cm
HZCH 182.57472 Hz/cm

ppm



Current Data Parameters
 NAME TIP50-propyne
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051220
 Time 10.52
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgdc
 TD 238090
 SOLVENT Aceton
 NS 12
 DS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 8192
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.1338000 MHz

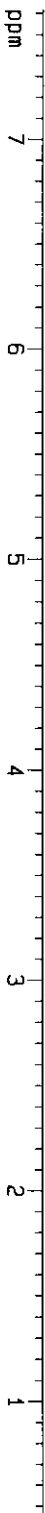
F2 - Processing parameters
 SI 32768
 SF 125.7577982 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CK 20.00 cm
 F1P 111.123 ppm
 F1 13974.52 Hz
 F2P -10.295 ppm
 F2 -1294.63 Hz
 PPKCM 5.07086 ppm/cm
 HZCM 763.45758 Hz/cm

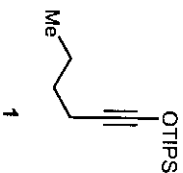
ppm

ppm

Integral



- 2.061
- 2.050
- 2.036
- 1.398
- 1.394
- 1.386
- 1.381
- 1.374
- 1.256
- 1.241
- 1.226
- 1.117
- 1.102
- 0.885
- 0.873
- 0.871
- 0.858



Current Data Parameters
 NAME TIPSO-hexy-924
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050925
 Time 20.43

INSTRUM spect

PROBHD 5 mm QNP 1H

PULPROG zg

TD 32768

SOLVENT CDCl3

NS 4

DS 0

SMH 5208.333 Hz

FIDRES 0.158946 Hz

AQ 3.1457779 sec

RG 8

DW 96.000 usec

DE 4.50 usec

TE 300.0 K

D1 2.00000000 sec

==== CHANNEL f1 =====

NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters

SI 16384
 SF 500.1300132 MHz
 NDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 7.620 ppm
 F1 3810.89 Hz
 F2P 0.450 ppm
 F2 225.28 Hz
 PPMCM 0.35847 ppm/cm
 HZCM 179.28041 Hz/cm

ppm

ppm

100

80

60

40

20

86.6584

77.2592

77.0044

76.7501

32.0854

30.4279

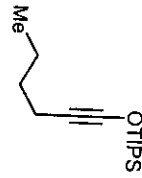
21.8715

17.3151

16.8630

13.5902

11.8160



Current Data Parameters
 NAME TIPSD-hexy-924
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

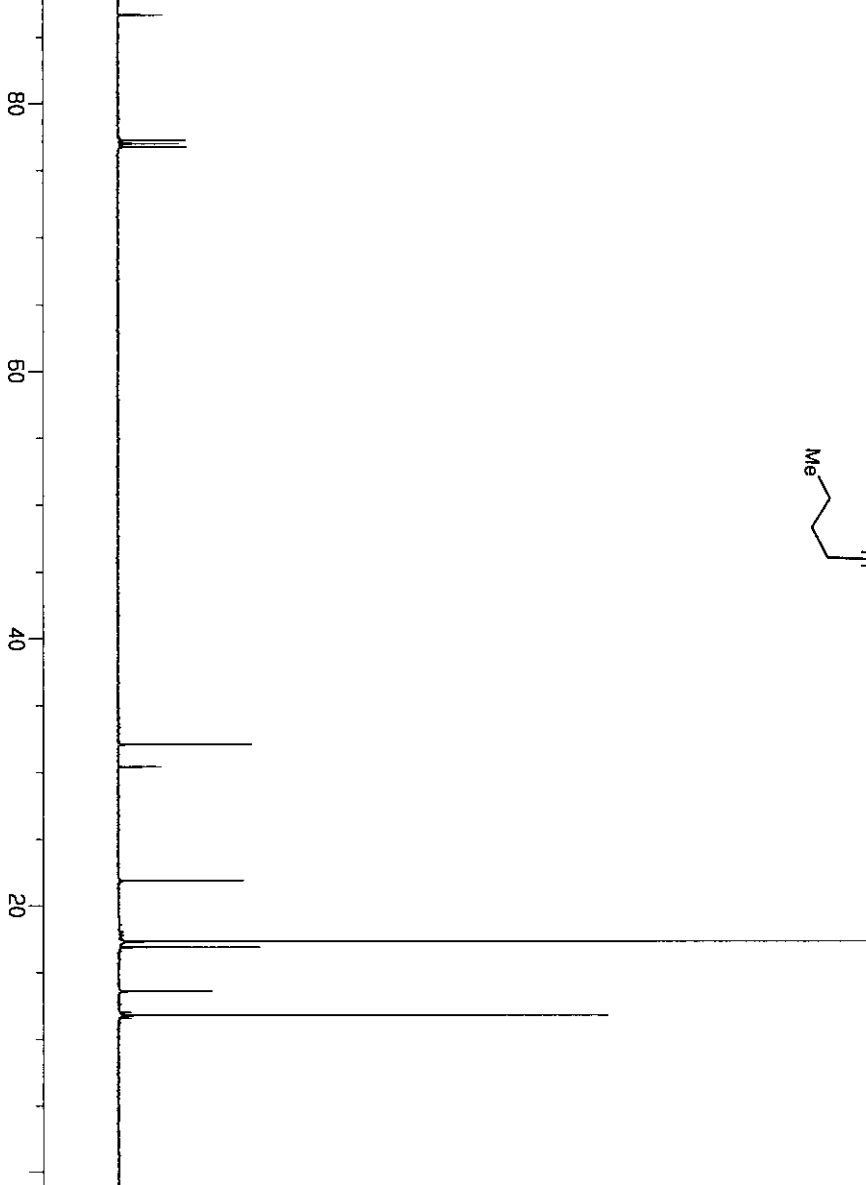
Date_ 20050925
 Time 20.46
 INSTRUM spect
 PROHD 5 mm QNP 1H
 PULPROG zgdc
 T0 238090
 SOLVENT Aceton
 NS 18
 DS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 4096
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

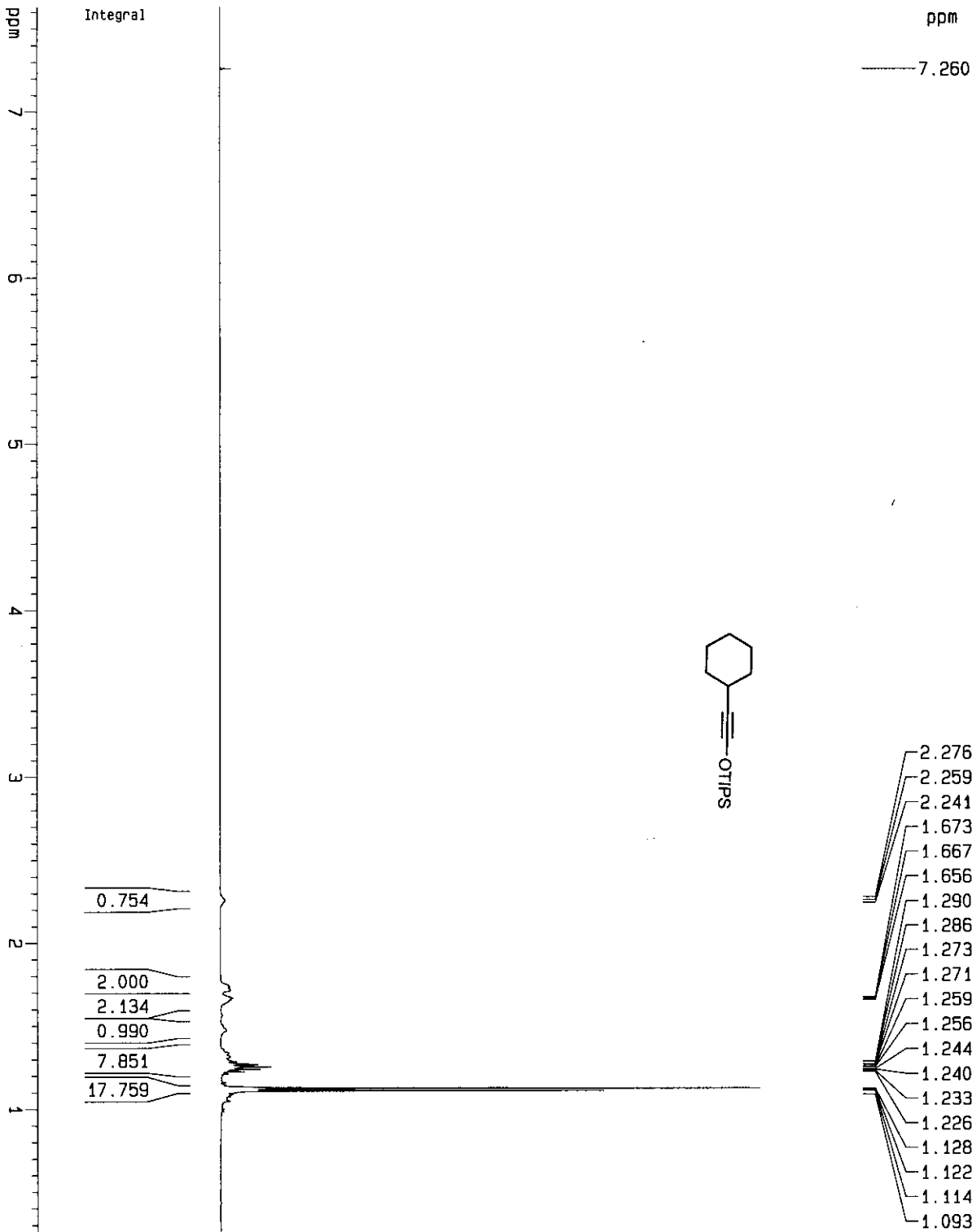
***** CHANNEL f1 *****
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 P2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 500.1339800 MHz

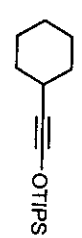
F2 - Processing parameters
 SI 32768
 SF 125.7577898 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 111.701 ppm
 F1 14047.23 Hz
 F2P -1.140 ppm
 F2 -143.31 Hz
 PPMCM 5.64201 ppm/cm
 HZCM 709.52722 Hz/cm





ppm
7.260



- 2.276
- 2.259
- 2.241
- 1.673
- 1.667
- 1.656
- 1.290
- 1.286
- 1.273
- 1.271
- 1.259
- 1.256
- 1.244
- 1.240
- 1.233
- 1.226
- 1.128
- 1.122
- 1.114
- 1.093

- 0.754
- 2.000
- 2.134
- 0.990
- 7.851
- 17.759

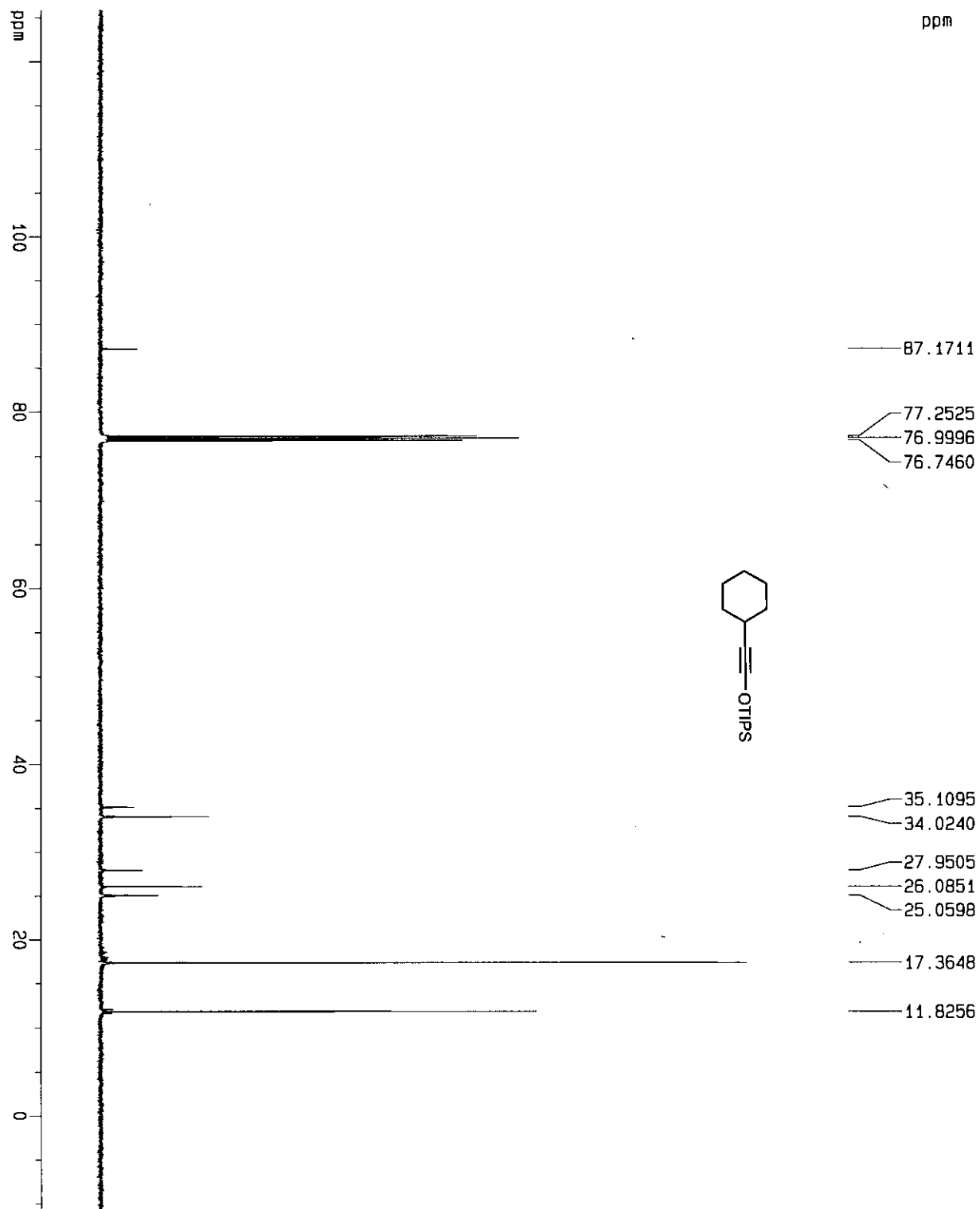
Current Data Parameters
NAME TIPSD-Cy
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050923
Time 23.26
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SMH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 32
DM 96.000 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SF01 500.1320118 MHz

F2 - Processing parameters
S1 16384
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 7.632 ppm
F1 3816.79 Hz
F2P 0.290 ppm
F2 125.23 Hz
PPMCM 0.36906 ppm/cm
HZCM 184.57797 Hz/cm



Current Data Parameters
 NAME TIPSD-Cy
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050923
 Time 23.31

INSTRUM spect
 PROBD 5 mm GNP 1H
 PULPROG zgpg30

TD 238090
 SOLVENT Aceton
 NS 203

DS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz

AQ 2.9999840 sec
 RG 8192

DE 12.600 usec
 TE 7.50 usec
 D1 300.0 K

D1 4.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB

SFO1 125.7736214 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec

PL2 120.00 dB
 PL12 19.00 dB
 SF02 500.1338000 MHz

F2 - Processing Parameters
 SI 32768
 SF 125.7577922 MHz

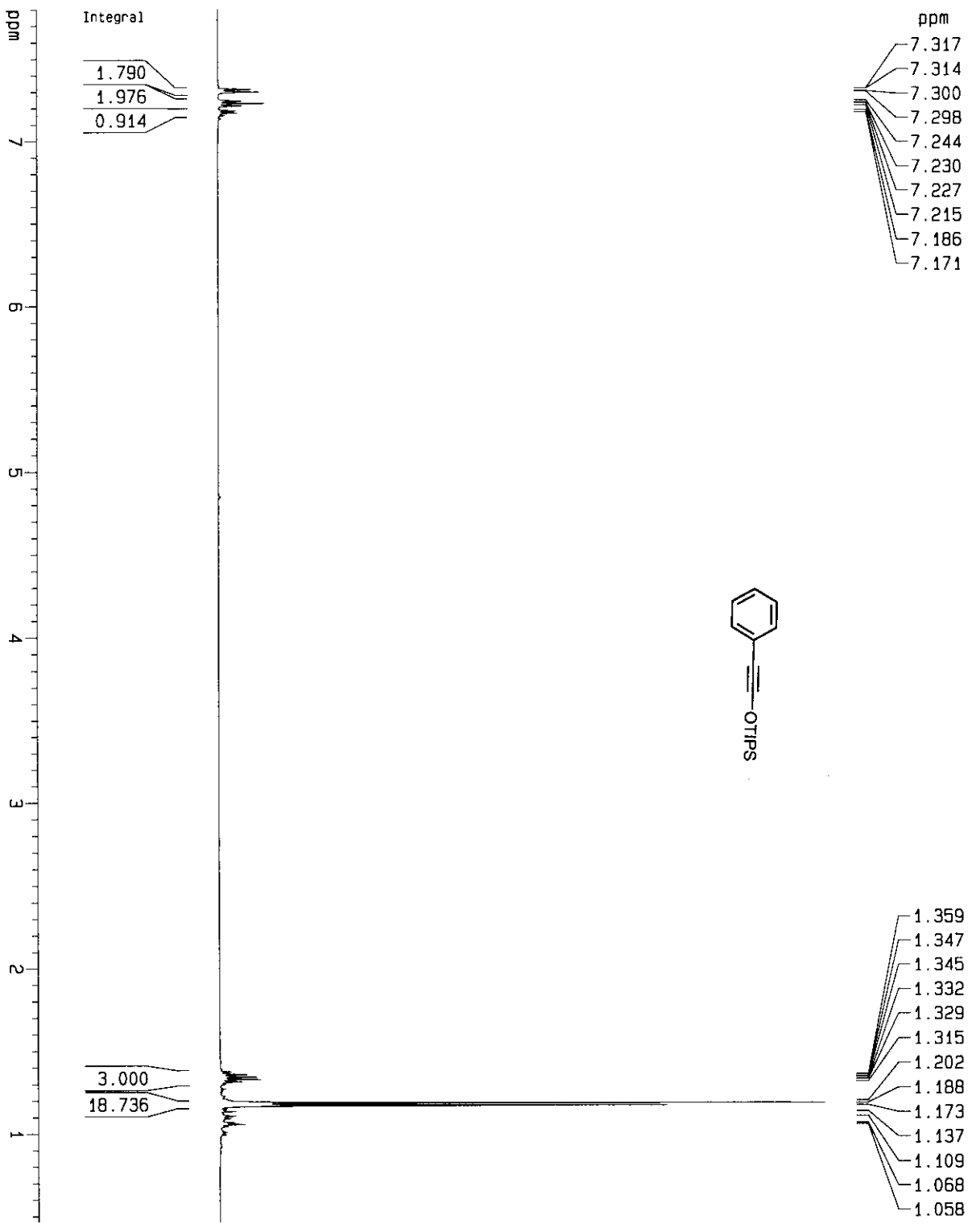
WDW EM
 SSB 0
 LB 1.00 Hz

GB 0
 PC 1.40

1D NMR plot parameters
 CK 20.00 cm
 F1P 125.871 dpm

F1 15829.25 Hz
 F2P -10.519 ppm
 F2 -1335.36 Hz

PPMCM 6.82447 dpm/cm
 HZCM 856.23053 Hz/cm



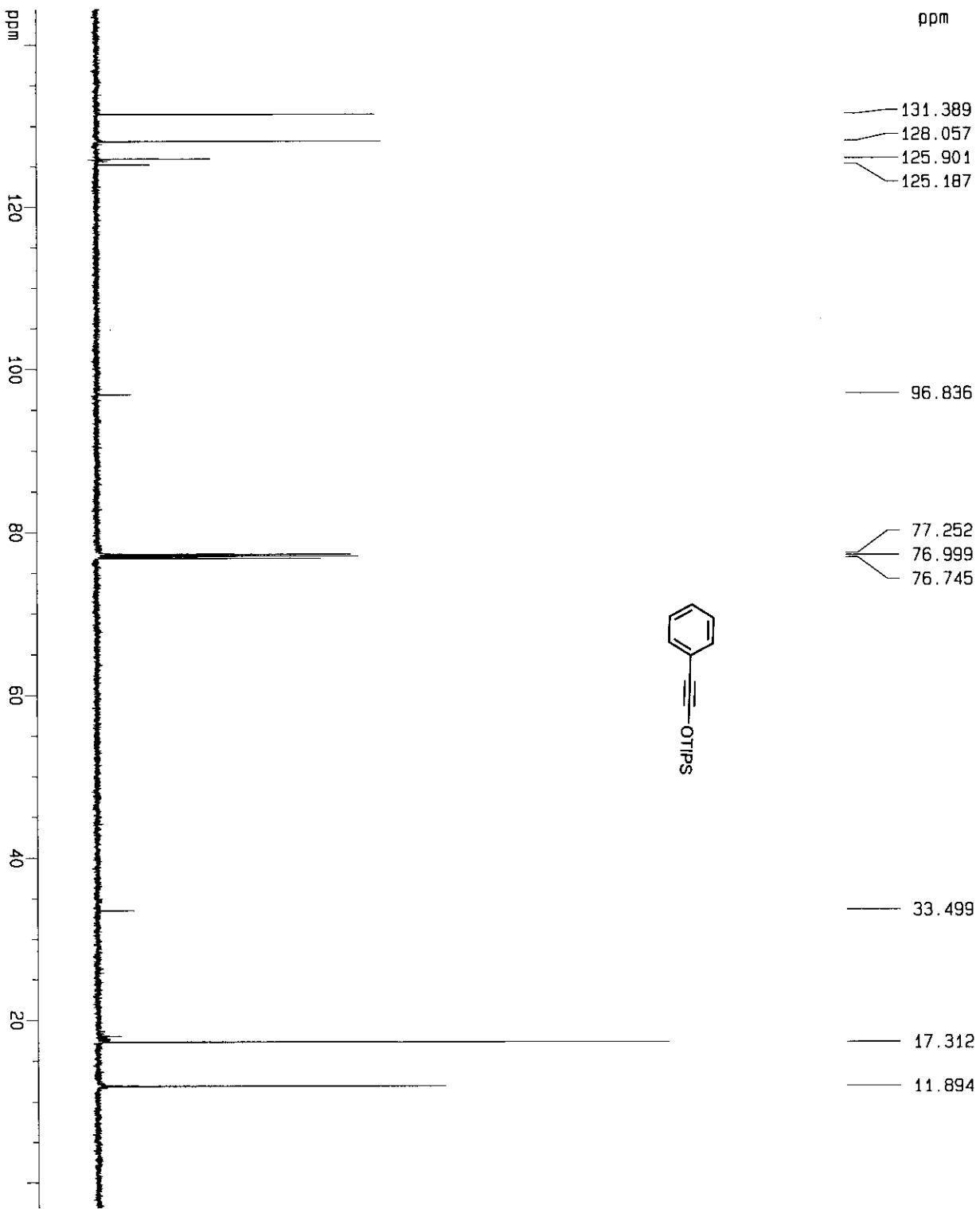
Current Data Parameters
 NAME TIPSOpheacety1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050808
 Time 22.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 32
 DM 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300181 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 F1P 7.801 ppm
 F1 3901.56 Hz
 F2P 0.466 ppm
 F2 233.08 Hz
 PPMQCM 0.36675 ppm/cm
 HZCM 183.42390 Hz/cm



Current Data Parameters
 NAME TIPSophaecety1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050808
 Time 22.56

INSTRUM spect
 PROBDI 5 mm QNP 1H
 PULPROG zgpg30

TD 238090
 SOLVENT Aceton
 NS 35

OS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz

AQ 2.9999840 sec
 RG 2048

DE 12.600 usec
 TE 7.50 usec
 D1 300.0 K

D1 4.00000000 sec
 D11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB

SF01 125.7736214 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec

PL2 120.00 dB
 PL12 19.00 dB

SF02 500.1338000 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577946 MHz

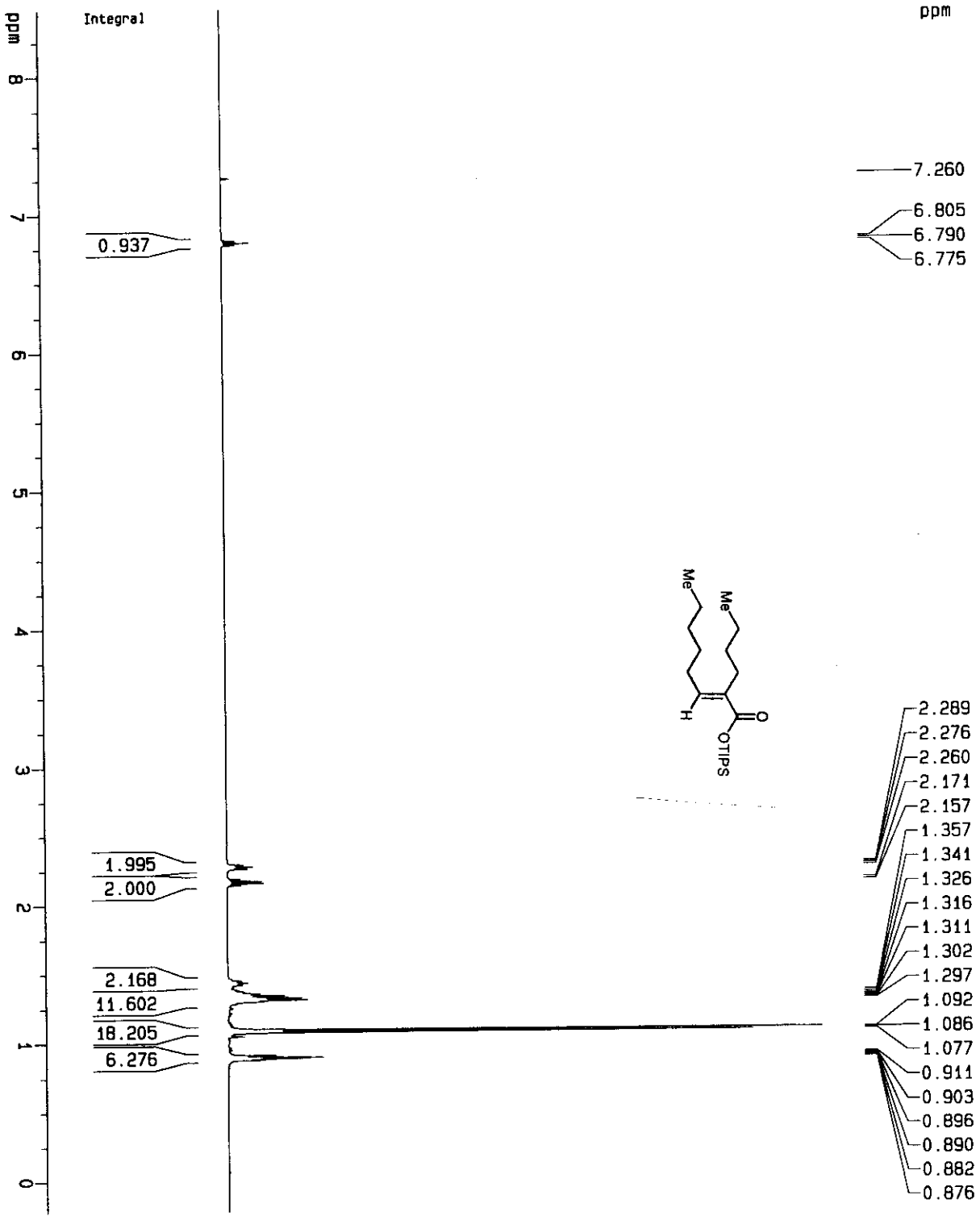
WDW EM
 SSB 0
 LB 1.00 Hz

GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 144.373 ppm

F1 18156.03 Hz
 F2P -3.111 ppm

F2 -391.24 Hz
 PPMCM 7.37420 ppm/cm
 HZCM 927.36371 Hz/cm



Current Data Parameters
 NAME hexnal_pdt
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051215
 Time 12.42
 INSTRUM spect
 PROBHID 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 16
 DM 62.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1337510 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300129 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.484 ppm
 F1 4243.21 Hz
 F2P -0.223 ppm
 F2 -111.58 Hz
 PPMCM 0.43537 ppm/cm
 HZCM 217.73967 Hz/cm

ppm

167.934

143.444

133.490

77.259

77.003

76.750

31.635

31.587

28.613

28.564

26.802

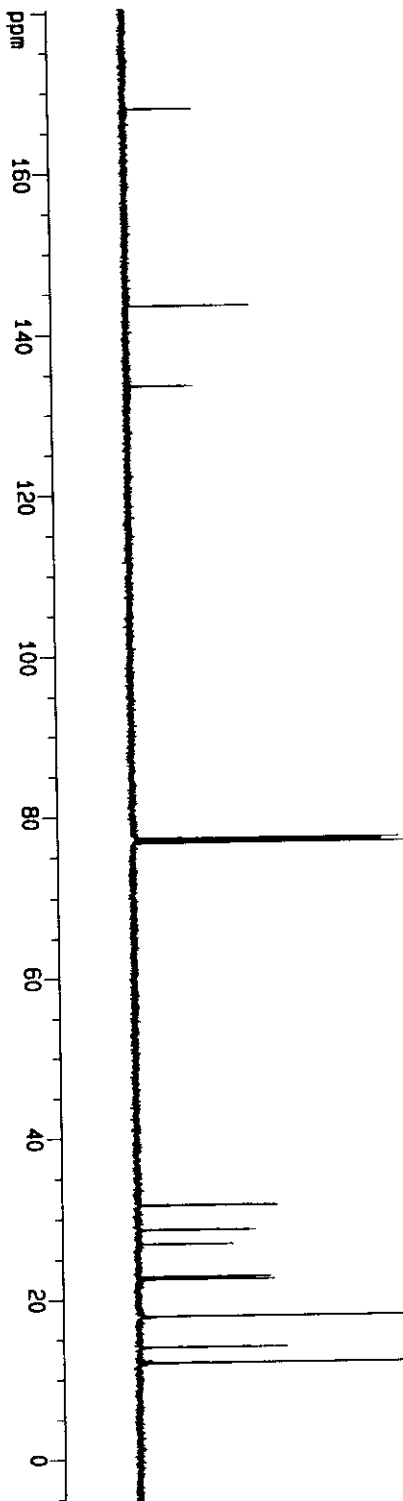
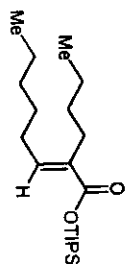
22.784

22.476

17.854

13.979

12.025



Current Data Parameters
 NAME hexnal_jdt
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051215
 Time 12.48
 INSTRUM spect
 PROBDW 5 mm QNP 1H
 PULPROG zgpg
 TD 238090
 SOLVENT Acetone
 NS 40
 DS 0
 SMH 39682.539 HZ
 FIDRES 0.166670 HZ
 AQ 2.9999840 sec
 RG 8192
 DW 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 D11 0.03000000 sec

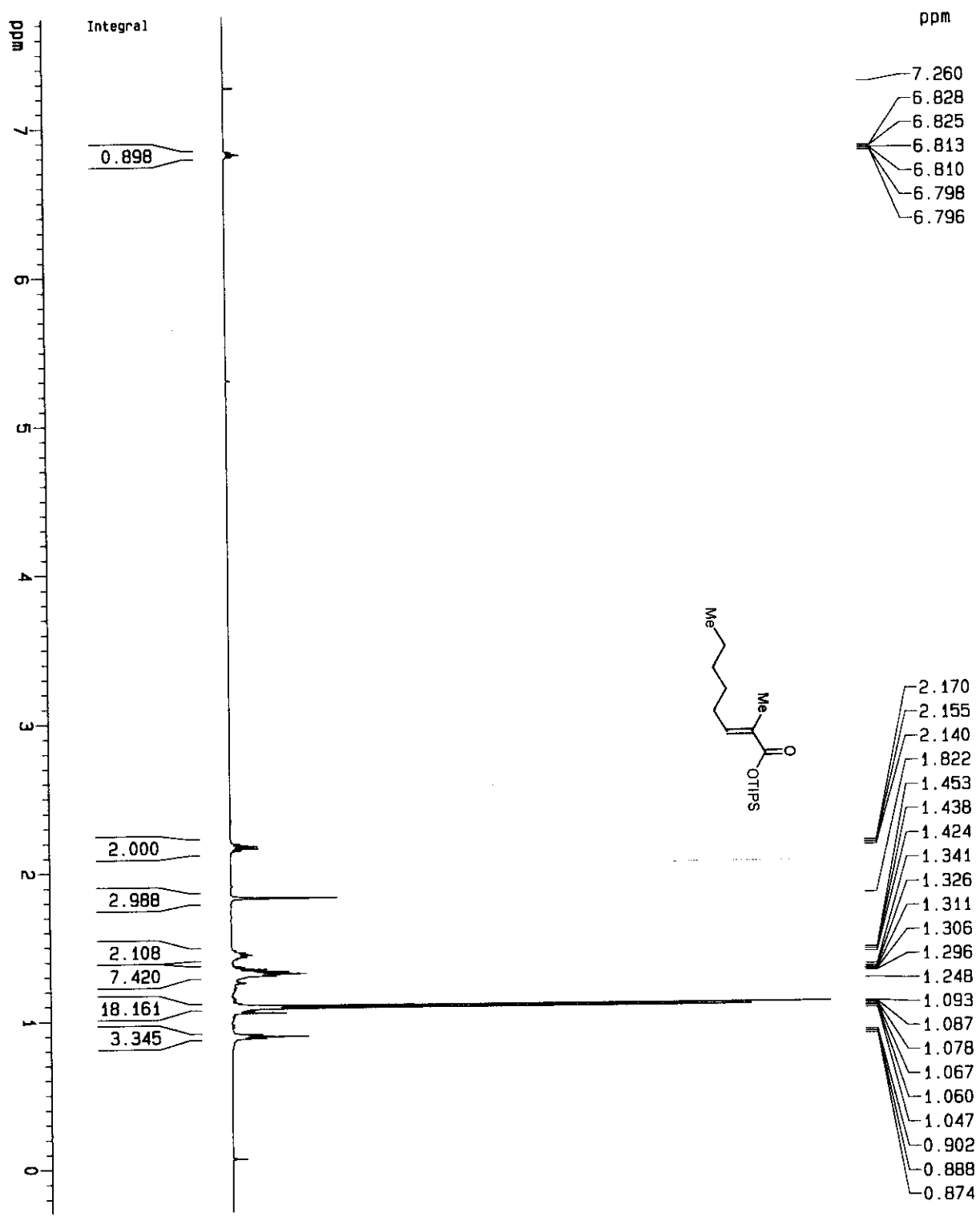
CHANNEL f1
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

CHANNEL f2
 waitz16

QPPRG2 waitz16
 NUC2 1H
 PCPG2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 500.1338000 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577910 MHz
 KDM EM
 SSB 0
 LB 1.00 HZ
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 180.435 ppm
 F1 22686.63 Hz
 F2P -5.140 ppm
 F2 -646.42 Hz
 PPMCM 9.27778 ppm/cm
 HZCM 1165.75293 Hz/cm



ppm
 7.260
 6.828
 6.825
 6.813
 6.810
 6.798
 6.796

2.170
 2.155
 2.140
 1.822
 1.453
 1.438
 1.424
 1.341
 1.326
 1.311
 1.306
 1.296
 1.248
 1.093
 1.087
 1.078
 1.067
 1.060
 1.047
 0.902
 0.888
 0.874

Integral
 0.898

2.000
 2.988
 2.108
 7.420
 18.161
 3.345

Current Data Parameters
 NAME propylsilyl.pdt1
 EXPNO 3
 PROCNO 1

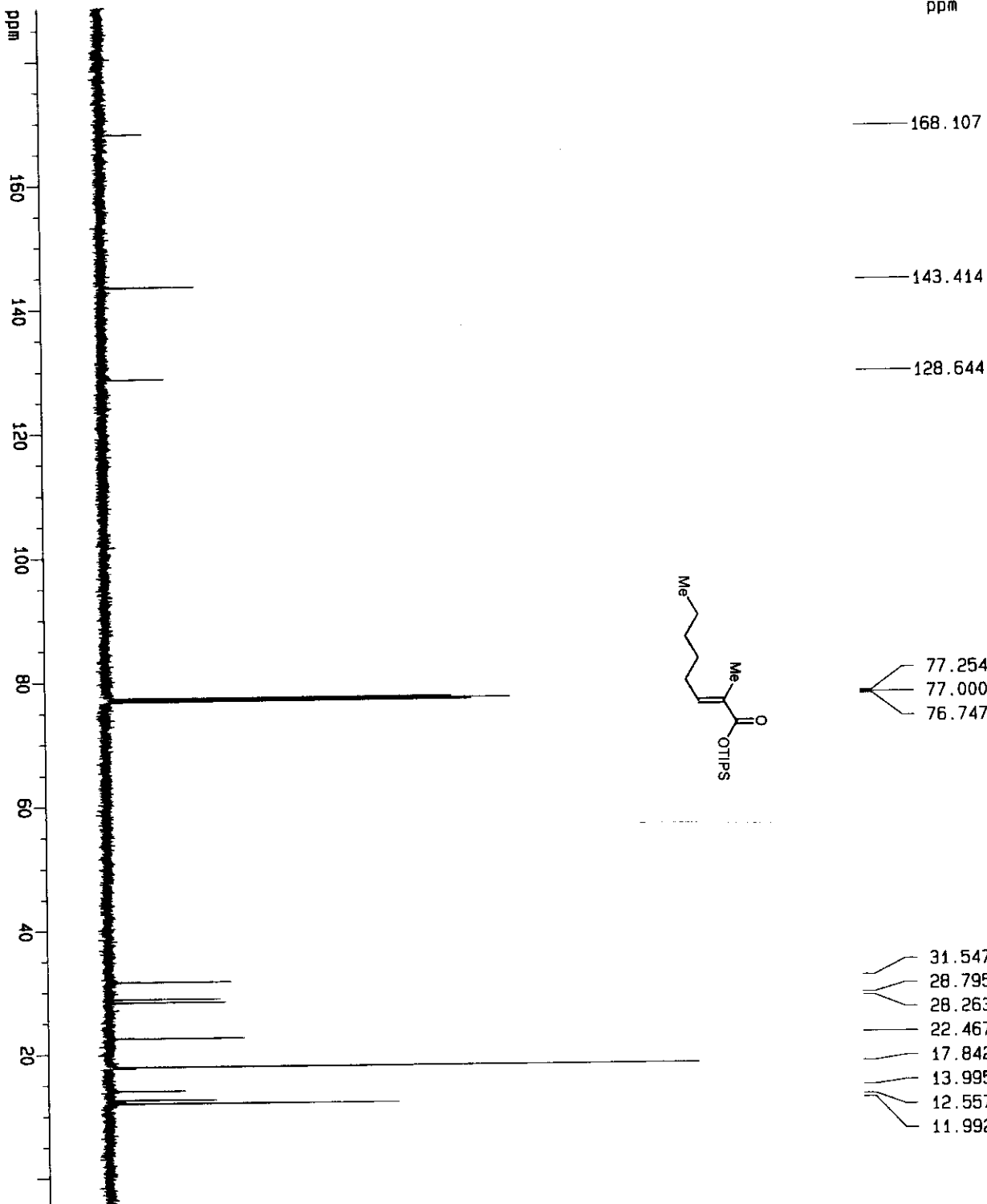
F2 - Acquisition Parameters
 Date_ 20051220
 Time 19.28
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 32
 DK 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 500.1320118 MHz

F2 - Processing parameters
 SI 46384
 SF 500.1300123 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

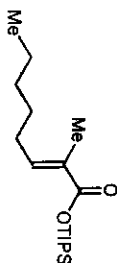
1D NMR plot parameters
 CX 20.00 cm
 F1P 7.745 DDM
 F1 3873.39 Hz
 F2P -0.292 DDM
 F2 -146.08 Hz
 PPMCM 0.40184 DDM/cm
 HZCM 200.97372 Hz/cm

ppm



168.107
143.414
128.644
77.254
77.000
76.747

31.547
28.795
28.263
22.467
17.842
13.995
12.557
11.992



Current Data Parameters
NAME propyns11_pdt1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051220
Time 19.32

INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 238090

SOLVENT Aceton
NS 28
DS 0

SWH 39682.539 HZ
FIDRES 0.166670 HZ
AQ 2.9999840 sec

RG 8192
DM 12.600 usec
DE 7.50 usec

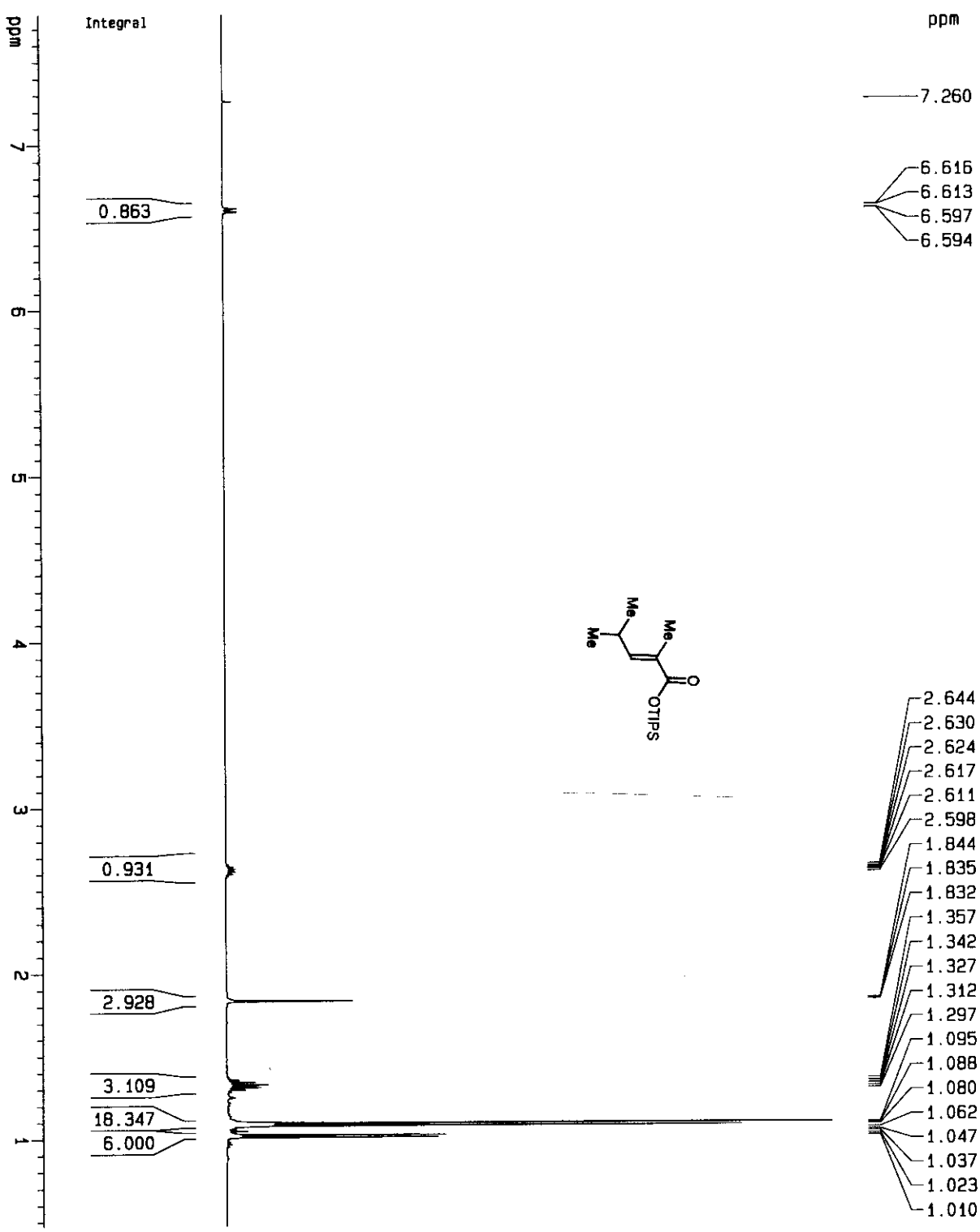
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 8.20 usec
PL1 0.00 dB
SF01 125.7736214 MHz

***** CHANNEL f2 *****
CPOPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 120.00 dB
PL12 19.00 dB
SF02 500.1338000 MHz

F2 - Processing parameters
SI 32768
SF 125.7577982 MHz
WDW EM
SSB 0
LB 1.00 HZ
GB 0
PC 1.40

ID NMR plot parameters
CX 20.00 cm
F1P 188.637 ppm
F1 23722.62 Hz
F2P -4.121 ppm
F2 -518.23 Hz
PPMCH 9.63791 ppm/cm
HZCM 1212.04285 Hz/cm



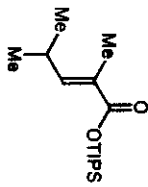
Current Data Parameters
 NAME proyn_1sobuly
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051221
 Time 23.37
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 32
 DW 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300151 MHz
 MDW EM
 SSB 0
 LB 0.30 HZ
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.785 ppm
 F1 3893.74 Hz
 F2P 0.475 ppm
 F2 237.56 Hz
 PPMCH 0.36552 ppm/cm
 HZCM 182.80905 Hz/cm



ppm

168.367

149.734

126.600

77.255

77.000

76.748

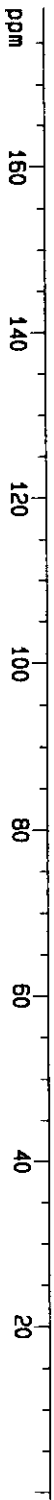
28.005

21.984

17.844

12.540

12.003



Current Data Parameters
 NAME proyn_1sduuty
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20051221
 Time 23.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TD 238090
 SOLVENT Aceton
 NS 57
 DS 0
 SMH 39682.538 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 6192
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****

NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

***** CHANNEL f2 *****

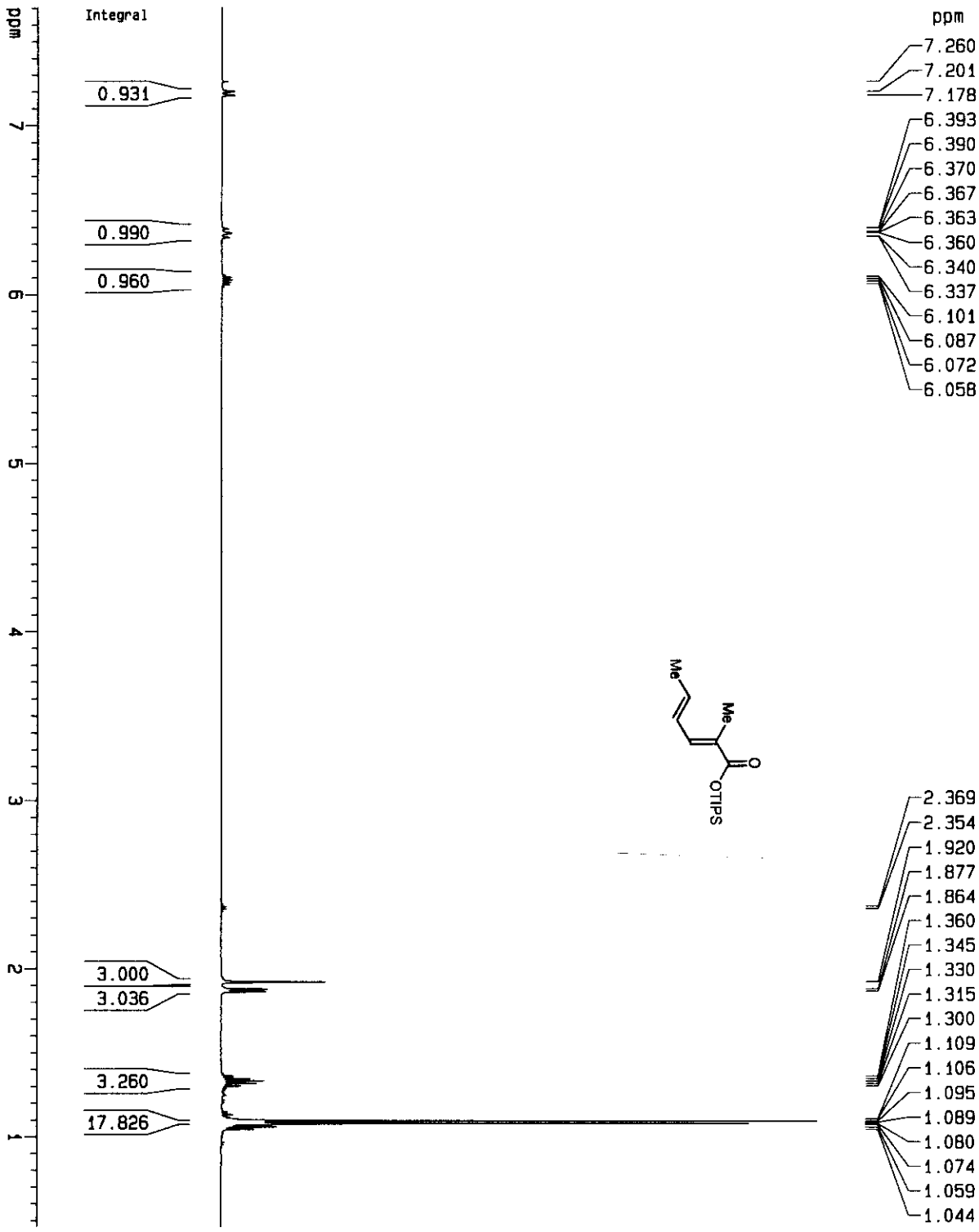
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 500.1338000 MHz

F2 - Processing parameters

SI 32768
 SF 125.7577922 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 F1P 179.159 ppm
 F1 22530.61 Hz
 F2P -0.905 ppm
 F2 -113.85 Hz
 PPGCM 9.00320 ppm/cm
 HZCM 1132.22266 Hz/cm



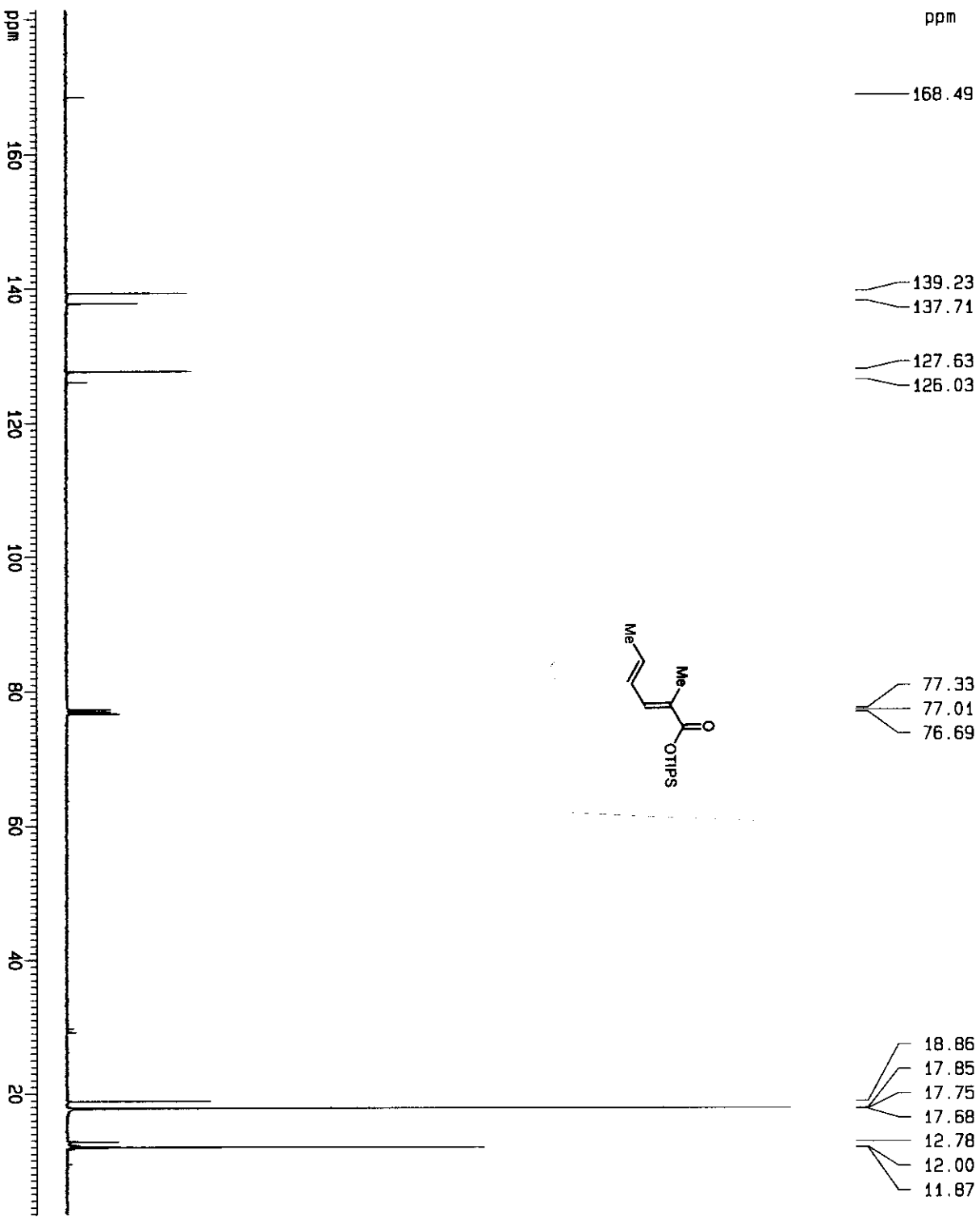
Current Data Parameters
 NAME propylsilyl_proto
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051224
 Time 21.46
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 32
 DM 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300155 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.704 ppm
 F1 3853.18 Hz
 F2P 0.463 ppm
 F2 231.49 Hz
 PPMCM 0.36207 ppm/cm
 HZCM 181.08444 Hz/cm



ppm

168.49

139.23

137.71

127.63

126.03

77.33

77.01

76.69

18.86

17.85

17.75

17.68

12.78

12.00

11.87

Current Data Parameters

NAME pros1_croton.d

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20051225

Time 13.56

INSTRUM spect

PROBHD 5 mm QNP 1H

PULPROG zgdc

TD 121208

SOLVENT CDCl3

NS 342

DS 0

SWH 30303.031 Hz

FIDRES 0.250008 Hz

AQ 1.9999820 sec

RG 2048

DW 16.500 usec

DE 7.50 usec

TE 300.0 K

D1 3.00000000 sec

d11 0.03000000 sec

***** CHANNEL f1 *****

NUC1 13C

P1 11.00 usec

PL1 -2.00 dB

SFO1 100.6258087 MHz

***** CHANNEL f2 *****

CPDPRG2 waltz16

NUC2 1H

PCPD2 101.00 usec

PL2 120.00 dB

PL12 19.00 dB

SFO2 400.1324710 MHz

F2 - Processing parameters

SI 46384

SF 100.6127717 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 181.436 ppm

F1 18254.73 Hz

F2P 1.921 ppm

F2 193.33 Hz

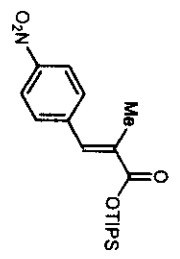
PRMCH 8.97570 ppm/cm

HZCH 903.07043 Hz/cm

ppm
8
7
6
5
4
3
2
1

Integral
1.964
0.944
2.010
3.000
3.064
17.720

ppm
8.261
8.258
8.248
8.244
7.720
7.547
7.530
7.260



2.127
2.124
1.418
1.403
1.388
1.372
1.358
1.141
1.135
1.129
1.126
1.120

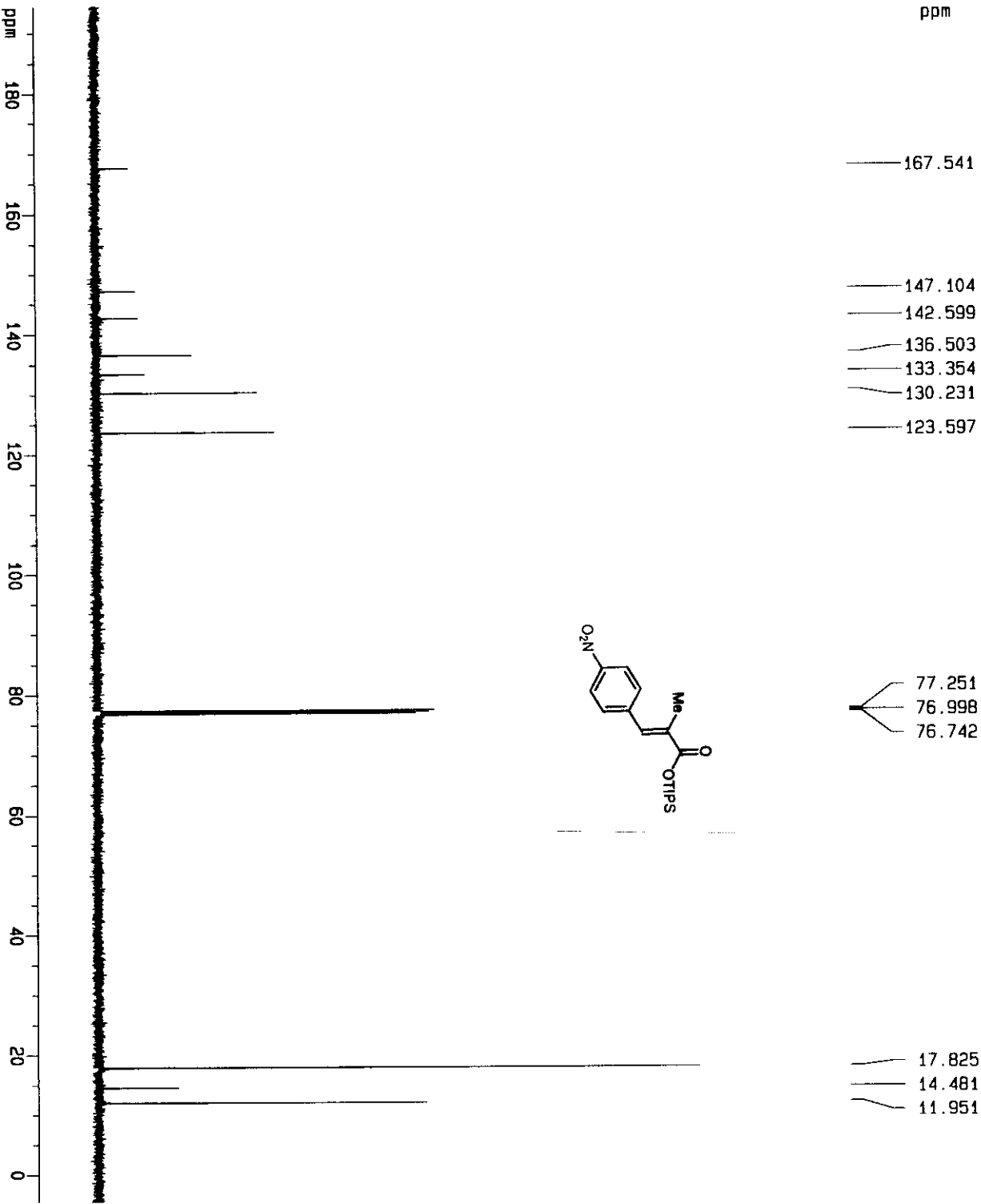
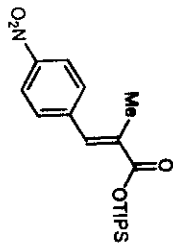
Current Data Parameters
 NAME Propynsil_dpt2
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051220
 Time 19.49
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.145779 sec
 RG 32
 DM 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300123 MHz
 MDH EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.696 ppm
 F1 4348.94 Hz
 F2P 0.625 ppm
 F2 312.48 Hz
 PPGCM 0.40354 ppm/cm
 HZCM 201.82294 Hz/cm



Current Data Parameters
 NAME propylsulf1.Dtz2
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20051220
 Time 19.53
 INSTNUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TD 288090
 SOLVENT Aceton
 NS 31
 DS 0
 SMH 39582.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 8192
 DW 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****

NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

***** CHANNEL f2 *****

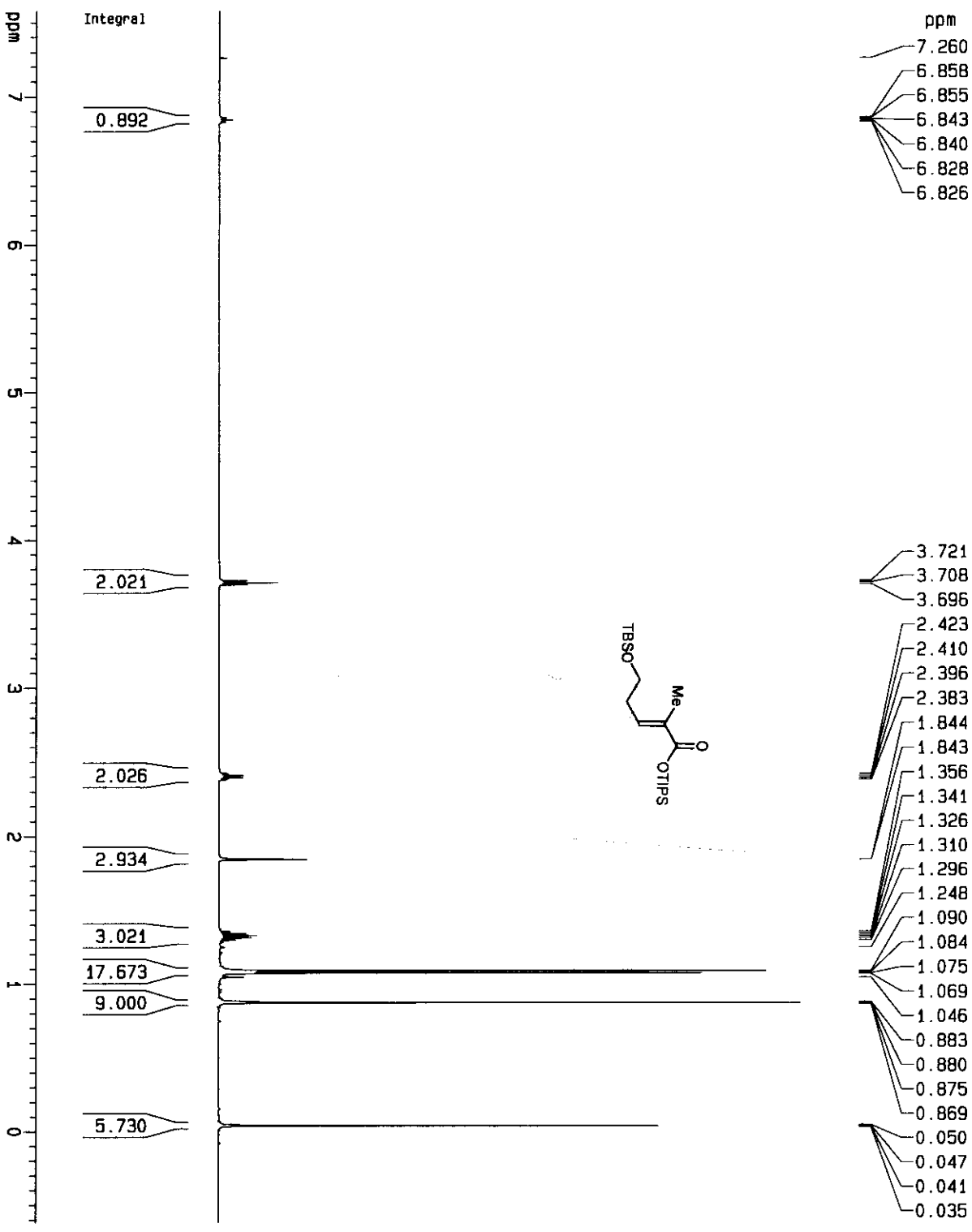
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 500.1338000 MHz

F2 - Processing parameters

SI 32768
 SF 125.7577946 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 F1P 194.449 ppm
 F1 24453.46 Hz
 F2P -4.483 ppm
 F2 -563.79 Hz
 PPMQCM 9.94660 ppm/cm
 HZCM 1250.86267 Hz/cm



Current Data Parameters
 NAME propyls1_OTBS
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051224
 Time 20.52

INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg

TD 32768
 SOLVENT CDCl3
 NS 4

DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz

AQ 3.1457779 sec
 RG 32
 DW 96.000 usec
 DE 4.50 usec

TE 300.0 K
 D1 5.00000000 sec

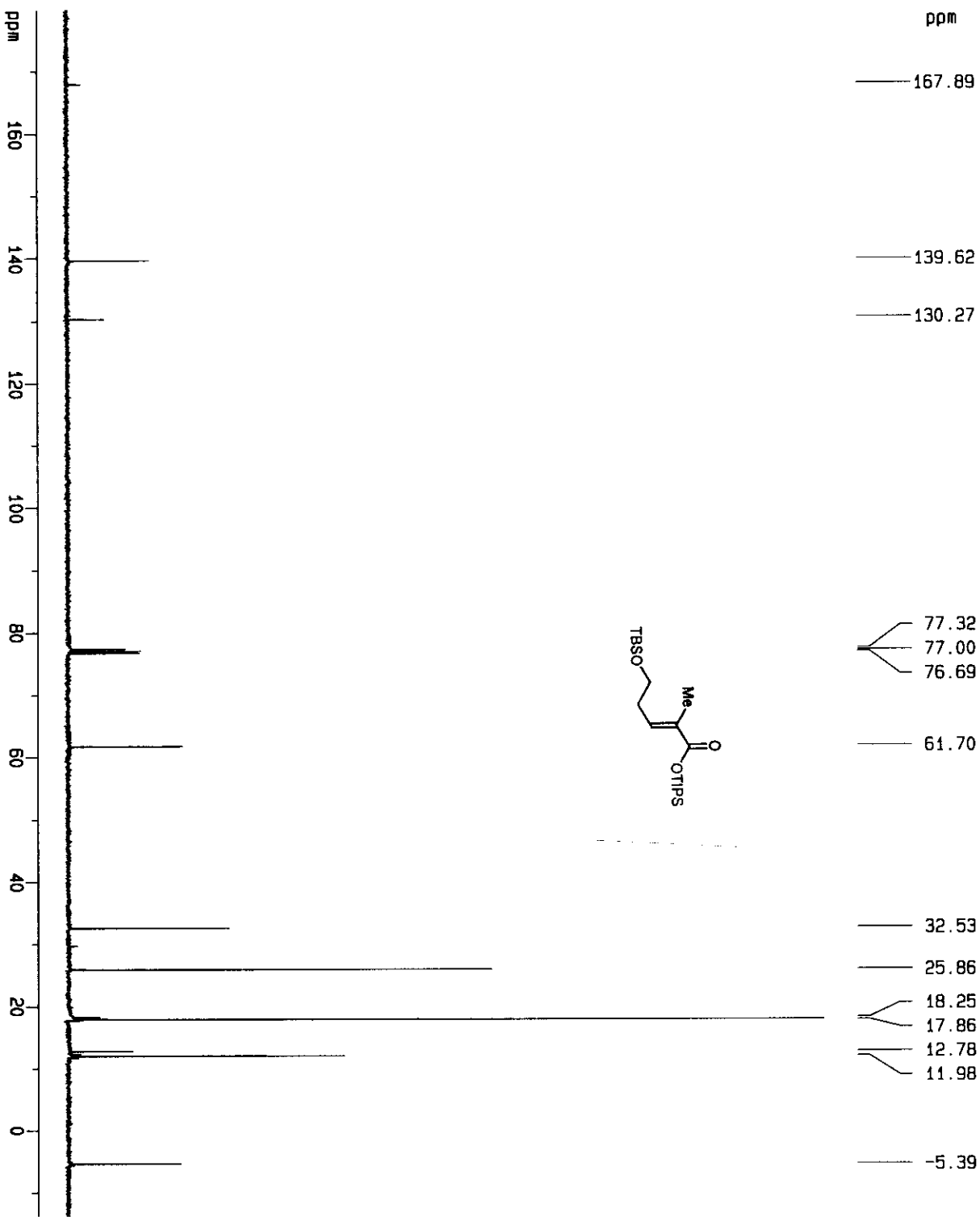
***** CHANNEL f1 *****
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300155 MHz
 WDW EM
 SSB 0

LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.578 ppm
 F1 3769.94 Hz

F2P -0.618 ppm
 F2 -308.89 Hz
 PPMCM 0.40978 ppm/cm
 HZCM 204.94159 Hz/cm



Current Data Parameters
 NAME TBSO.gdt
 EXPNO 1
 PROCNO 1

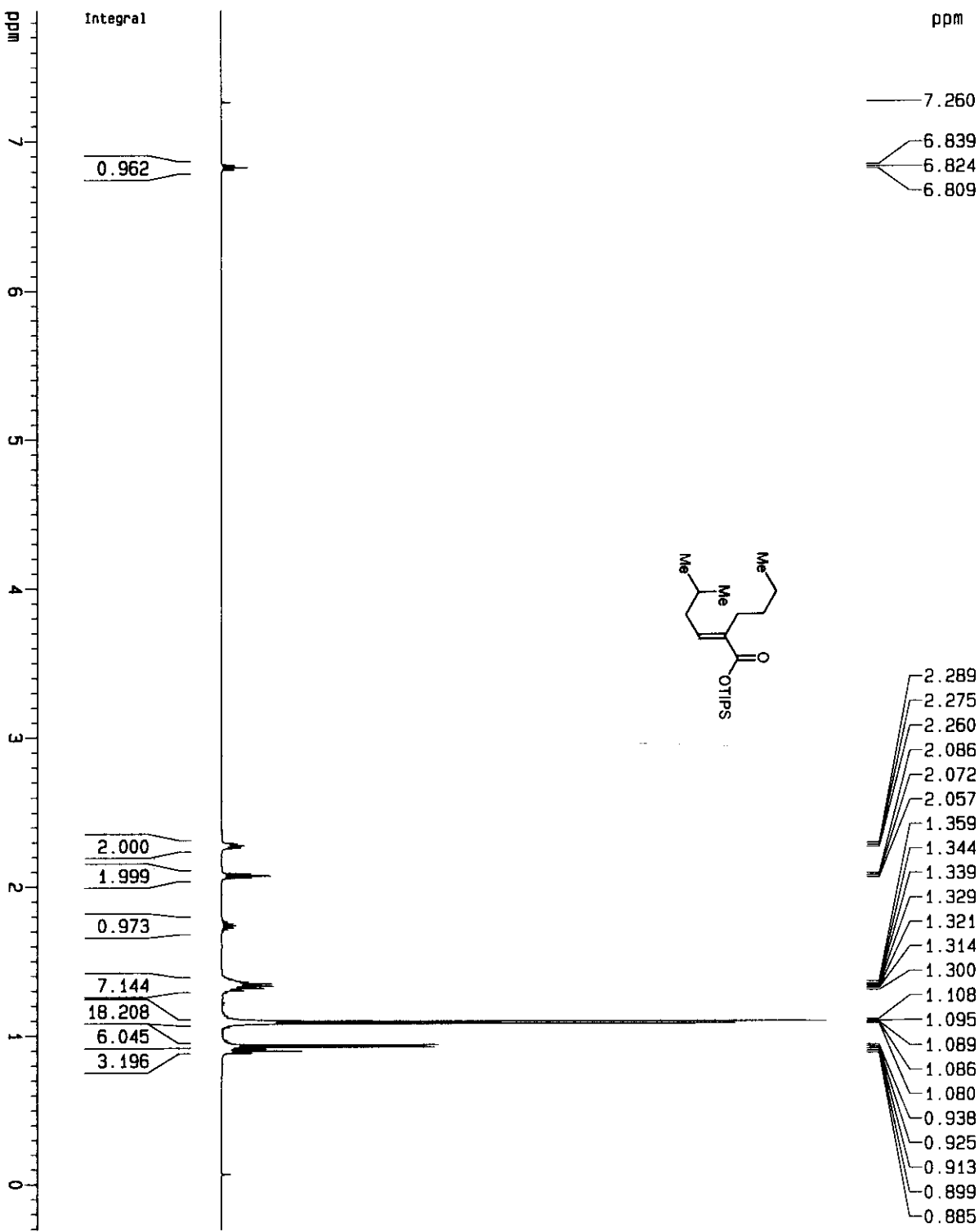
F2 - Acquisition Parameters
 Date_ 20051224
 Time 21.26
 INSTNUM spect
 PROBNM 5 mm QNP 1H
 PULPROG zgdc
 TD 121208
 SOLVENT CDCl3
 NS 235
 DS 0
 SMH 30303.031 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999820 sec
 RG 4096
 DW 16.500 usec
 DE 7.50 usec
 TE 300.0 K
 D1 3.00000000 sec
 D11 0.03000000 sec

CHANNEL f1
 NUC1 13C
 P1 11.00 usec
 PL1 -2.00 dB
 SFO1 100.6258087 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 101.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 400.1324710 MHz

F2 - Processing parameters
 SI 16384
 SF 100.6127717 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 F1P 179.773 ppm
 F1 18087.50 Hz
 F2P -13.703 ppm
 F2 -1378.69 Hz
 PPMCM 9.67381 ppm/cm
 HZCM 973.30927 Hz/cm



Current Data Parameters
 NAME 1svaler_dot
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051215
 Time 20.08
 INSTNUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 32
 DW 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300129 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1p 7.879 ppm
 F1 3940.69 Hz
 F2p -0.305 ppm
 F2 -152.38 Hz
 PPMCM 0.40920 ppm/cm
 HZCM 204.65353 Hz/cm

ppm

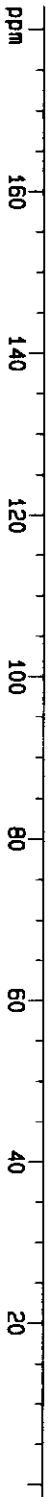
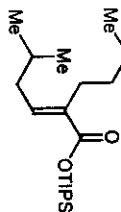
167.866

142.222

134.115

77.259
77.004
76.750

37.631
31.558
28.381
26.850
22.821
22.494
17.862
14.002
12.031



Current Data Parameters
 NAME Isovalter_dpt
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051215
 Time 20.23

INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TD 238090
 SOLVENT Aceton
 NS 111
 DS 0

SMH 39682.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec

RG 8192
 DW 12.600 usec
 DE 7.50 usec
 TE 300.0 K

D1 4.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****

NUC1 ¹³C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

***** CHANNEL f2 *****

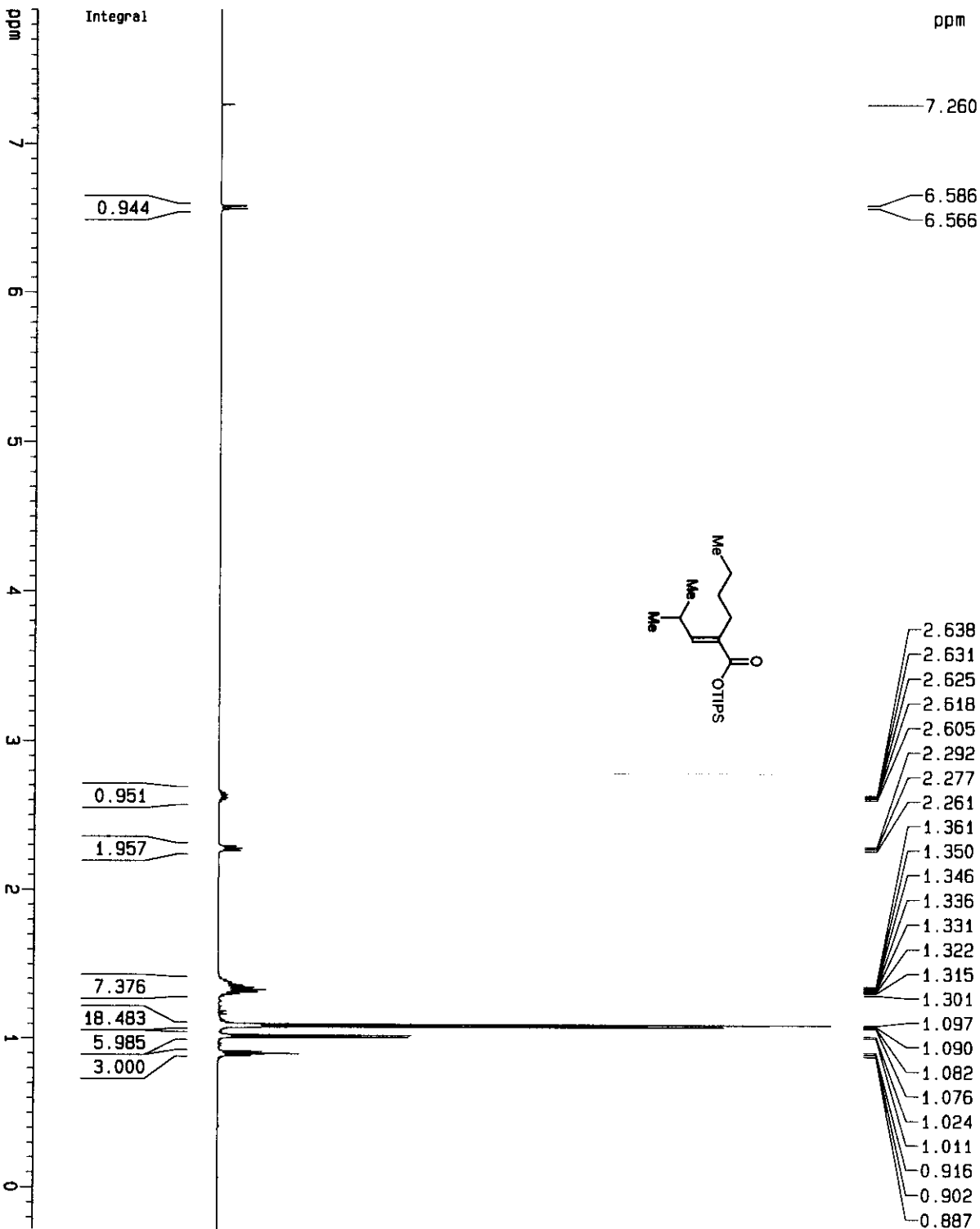
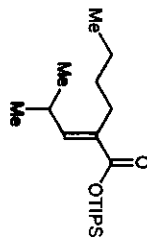
CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.1338000 MHz

F2 - Processing parameters

SI 32768
 SF 125.7577898 MHz
 KW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 F1P 182.826 ppm
 F1 22991.79 Hz
 F2P -1.701 ppm
 F2 -213.87 Hz
 PPMCM 9.22653 ppm/cm
 HZCM 1160.28296 Hz/cm



Current Data Parameters
 NAME 1sobutyl1.pdt
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051215
 Time 18.35
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 64
 DW 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300129 MHz
 KW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.902 ppm
 F1 3952.01 Hz
 F2P -0.282 ppm
 F2 -141.06 Hz
 PPMCH 0.40920 ppm/cm
 HZCH 204.65353 Hz/cm

ppm

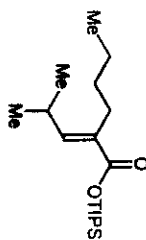
168.232

149.740

131.294

77.251
76.998
76.742

32.086
27.908
26.970
22.826
22.388
17.861
13.984
12.047



ppm
160
140
120
100
80
60
40
20
0

Current Data Parameters
 NAME Isobuty1_ddt
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20051215
 Time 18.40
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgdc
 TD 238090
 SOLVENT Aceton
 NS 34
 DS 0
 SMH 39882.539 Hz
 FIDRES 0.166570 Hz
 AQ 2.9999840 sec
 RG 8192
 DW 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.1338000 MHz

F2 - Processing parameters

SI 32768
 SF 125.7577898 MHz
 WDW EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 F1P 181.797 ppm
 F1 22882.38 Hz
 F2P -5.474 ppm
 F2 -688.34 Hz
 PPMCH 9.36382 ppm/cm
 HZCM 1177.53613 Hz/cm

ppm

Integral

0.944
4.082
0.979

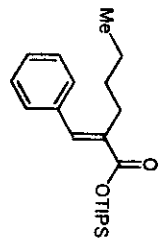
2.000

2.080
5.136
17.969
3.240

ppm

7.714
7.413
7.401
7.397
7.384
7.371
7.340
7.336
7.329
7.323
7.316
7.311
7.260

2.546
2.530
2.513
2.049
1.575
1.558
1.550
1.543
1.419
1.404
1.389
1.374
1.360
1.143
1.128
1.057
1.003
0.988
0.937
0.923
0.908



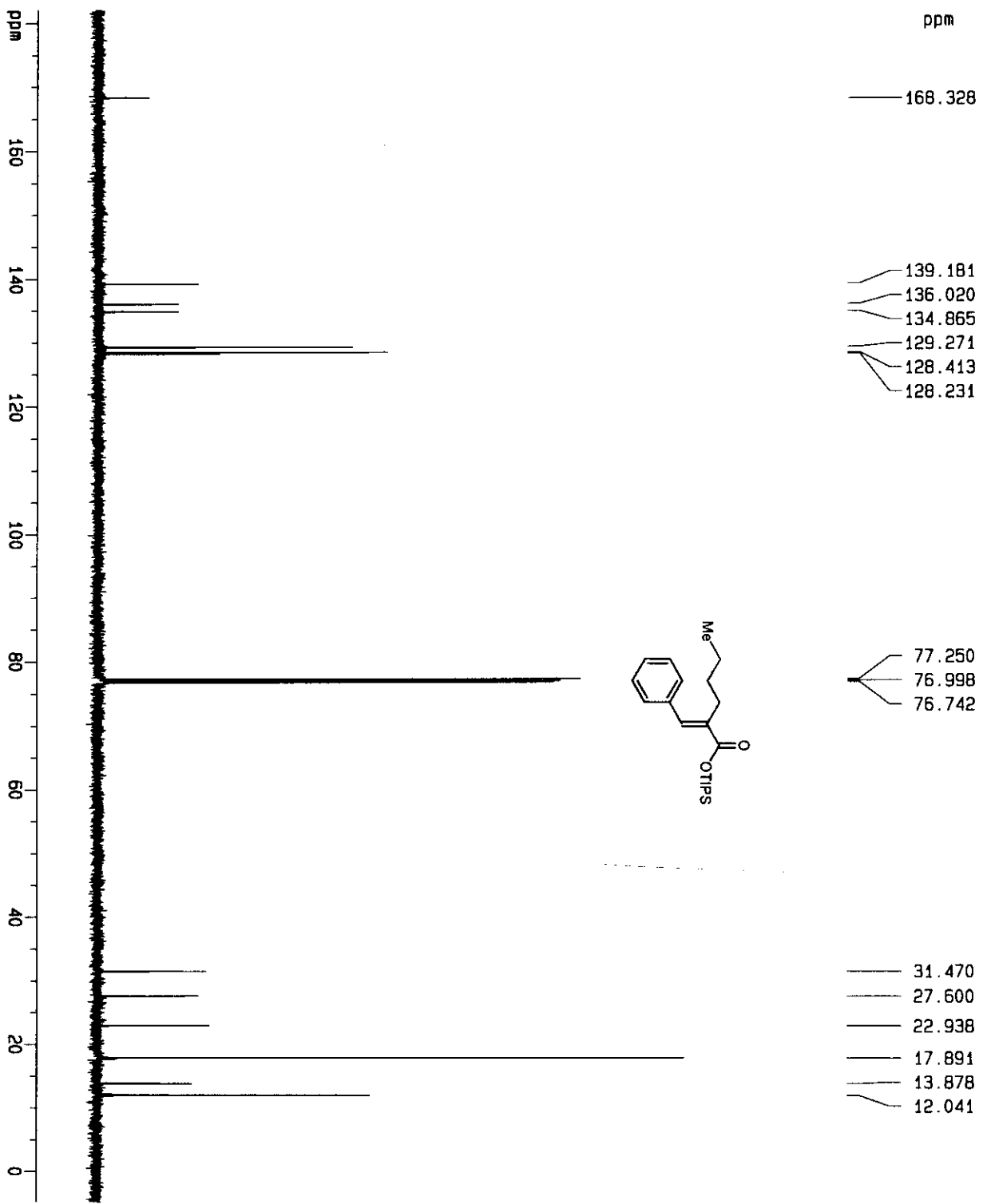
Current Data Parameters
 NAME benzald_pdt
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051214
 Time 18.59
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.044731 sec
 RG 64
 DM 62.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

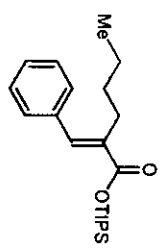
===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1337510 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300129 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.972 ppm
 F1 4487.07 Hz
 F2P -0.293 ppm
 F2 -146.43 Hz
 PPMCM 0.46323 ppm/cm
 HZCM 231.67503 Hz/cm



- 168.328
- 139.181
- 136.020
- 134.865
- 129.271
- 128.413
- 128.231
- 77.250
- 76.998
- 76.742
- 31.470
- 27.600
- 22.938
- 17.891
- 13.878
- 12.041



Current Data Parameters
 NAME benzal_dct
 EXPNO 4
 PROCNO 1

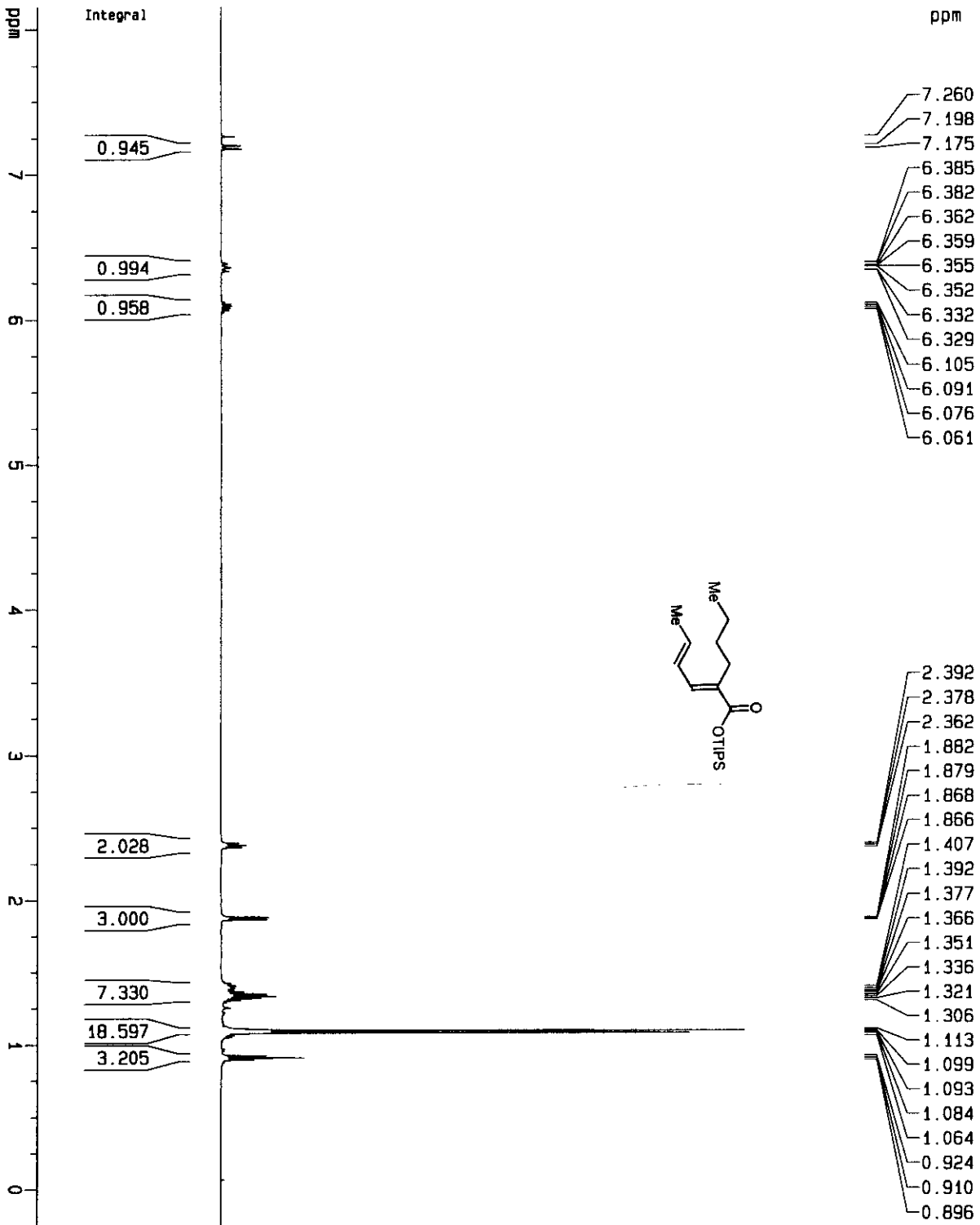
F2 - Acquisition Parameters
 Date_ 20051214
 Time 19.04
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgdc
 TD 238090
 SOLVENT Aceton
 NS 48
 DS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 8192
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

CHANNEL f1
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.1388000 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577934 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 182.111 ppm
 F1 22501.88 Hz
 F2P -4.816 ppm
 F2 -605.71 Hz
 PPMCM 9.34638 ppm/cm
 HZCM 1175.37964 Hz/cm



Current Data Parameters
 NAME crotonal_d14.pdt
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051214
 Time 22.32
 INSTRUM spect
 PROBH0 5 mm GNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0

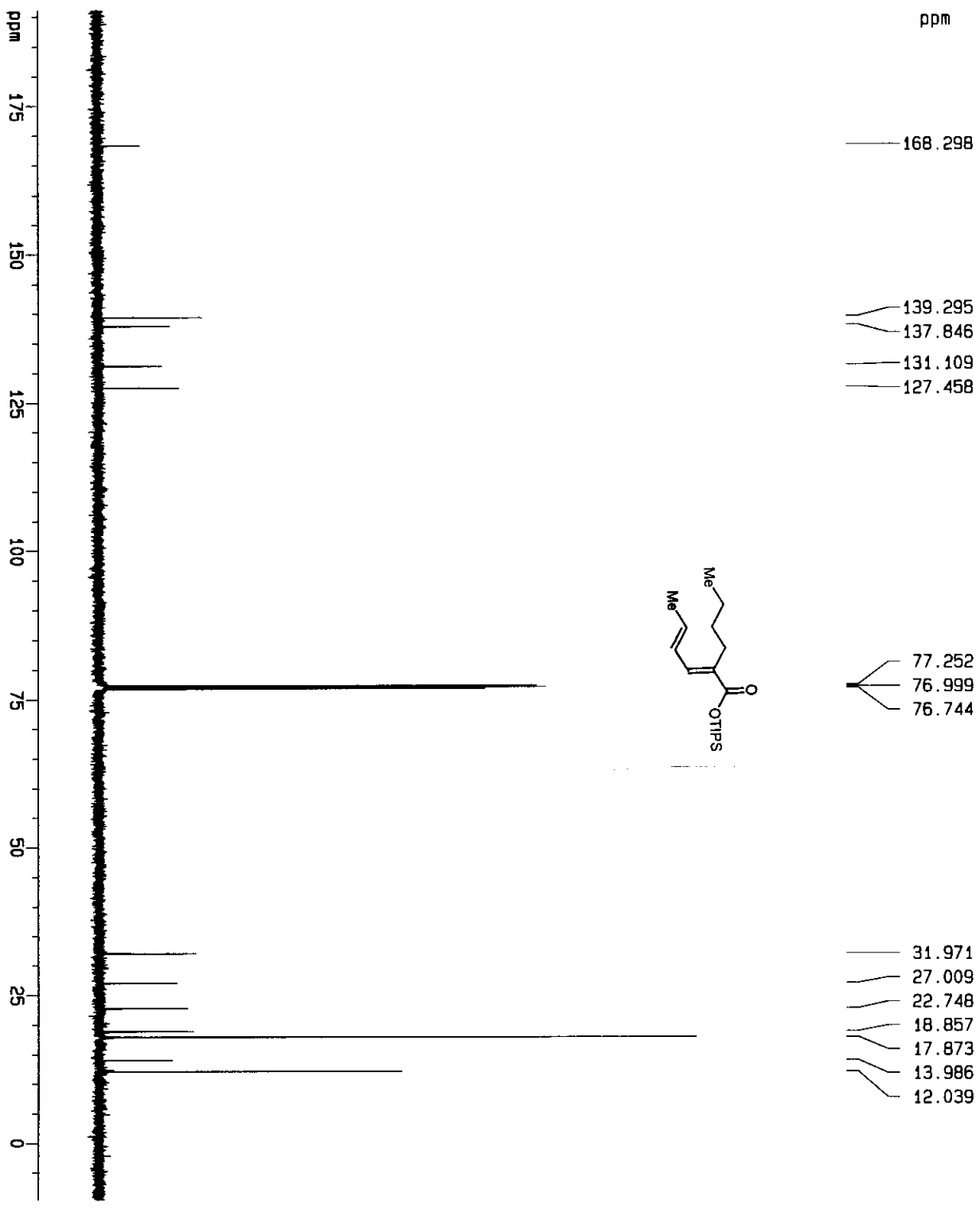
SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 64
 DW 62.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1337510 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300129 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.153 ppm
 F1 4077.73 Hz
 F2P -0.241 ppm
 F2 -120.29 Hz
 PPMCM 0.41969 ppm/cm
 HZCM 209.90106 Hz/cm

ppm



Current Data Parameters
 NAME crotonalid_pdt
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20051214
 Time 22.38
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 238090
 SOLVENT Aceton
 NS 48
 DS 0
 SMI 39582.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 8192
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

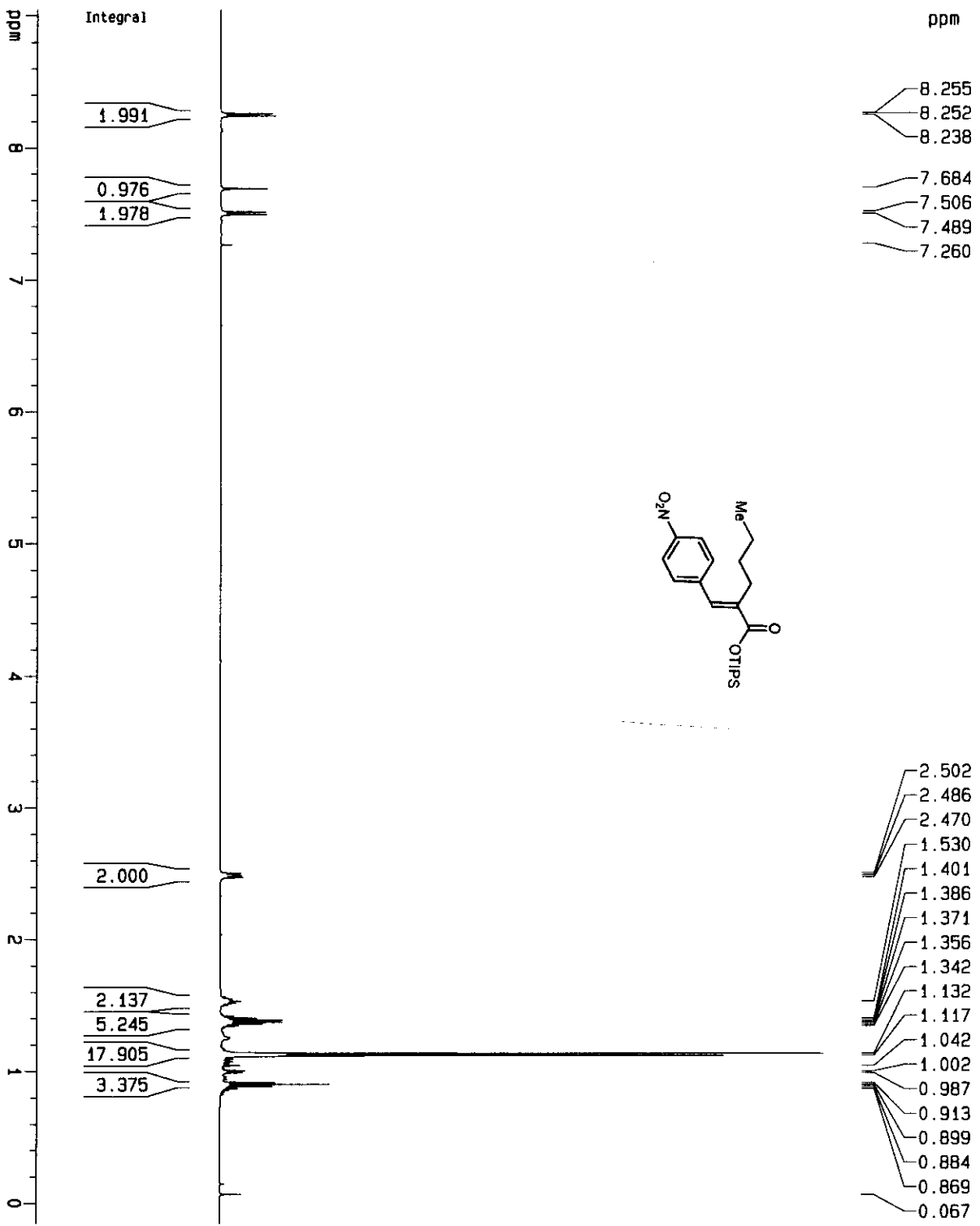
***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 P2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.1338000 MHz

F2 - Processing parameters

SI 32768
 SF 125.7577910 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 F1P 191.048 ppm
 F1 24025.77 Hz
 F2P -9.599 ppm
 F2 -1207.15 Hz
 PPMCM 10.03235 ppm/cm
 HZCM 1261.64600 Hz/cm



Current Data Parameters
 NAME Nitrobenz_pdt
 EXPNO 2
 PROCNO 1

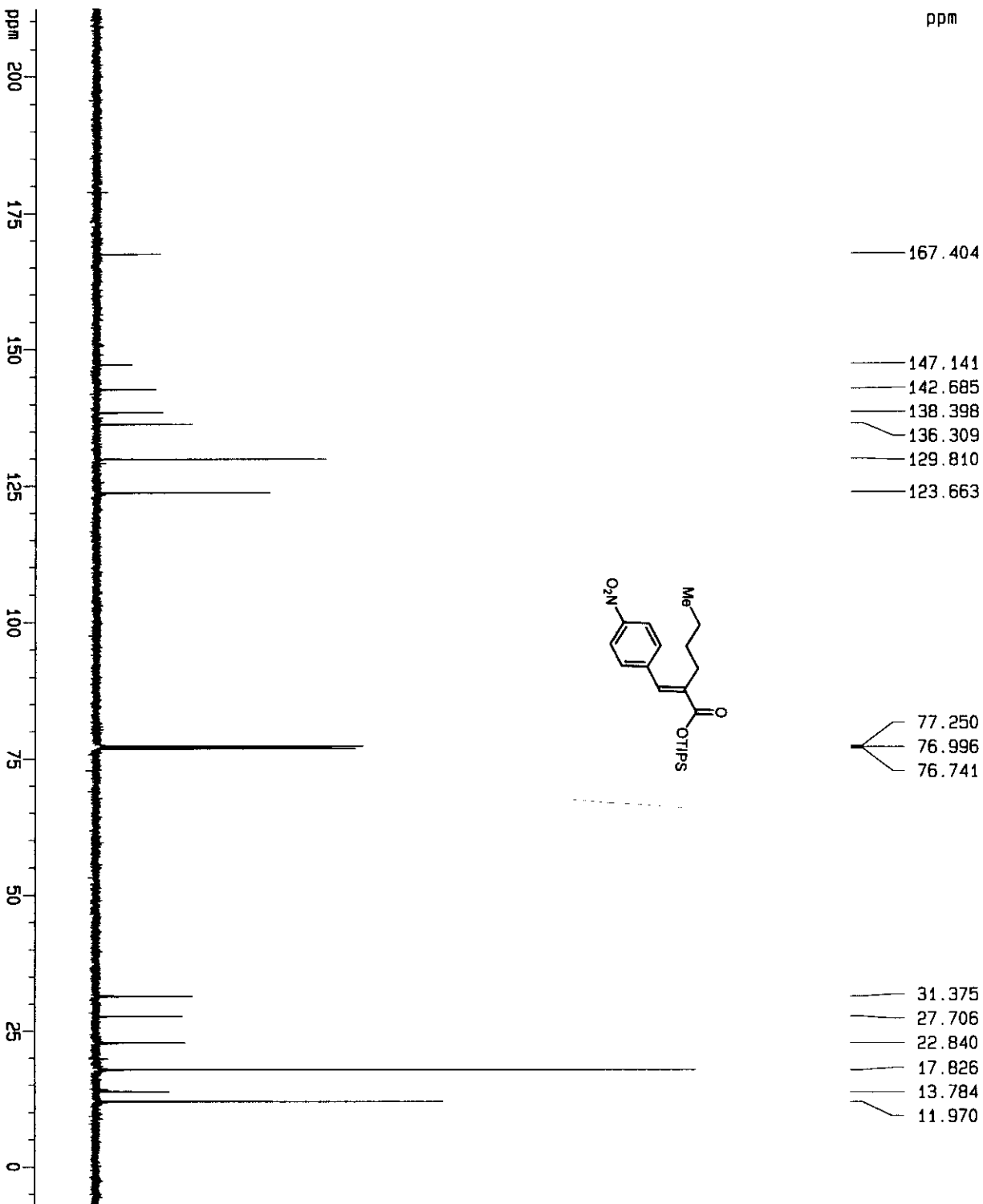
F2 - Acquisition Parameters
 Date_ 20051213
 Time 16.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.044731 sec
 RG 32
 DW 62.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 30.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1337510 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300129 MHz
 MDH EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 9.041 ppm
 F1 4521.91 Hz
 F2P -0.153 ppm
 F2 -76.75 Hz
 PPMCM 0.45975 ppm/cm
 HZCM 229.93309 Hz/cm

ppm



Current Data Parameters
 NAME nitrobenz_pdt
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20051213
 Time 16:57
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgdc
 TD 238090
 SOLVENT Aceton
 NS 31
 DS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999840 sec
 RG 8192
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

CHANNEL f1 -----

NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

CHANNEL f2 -----

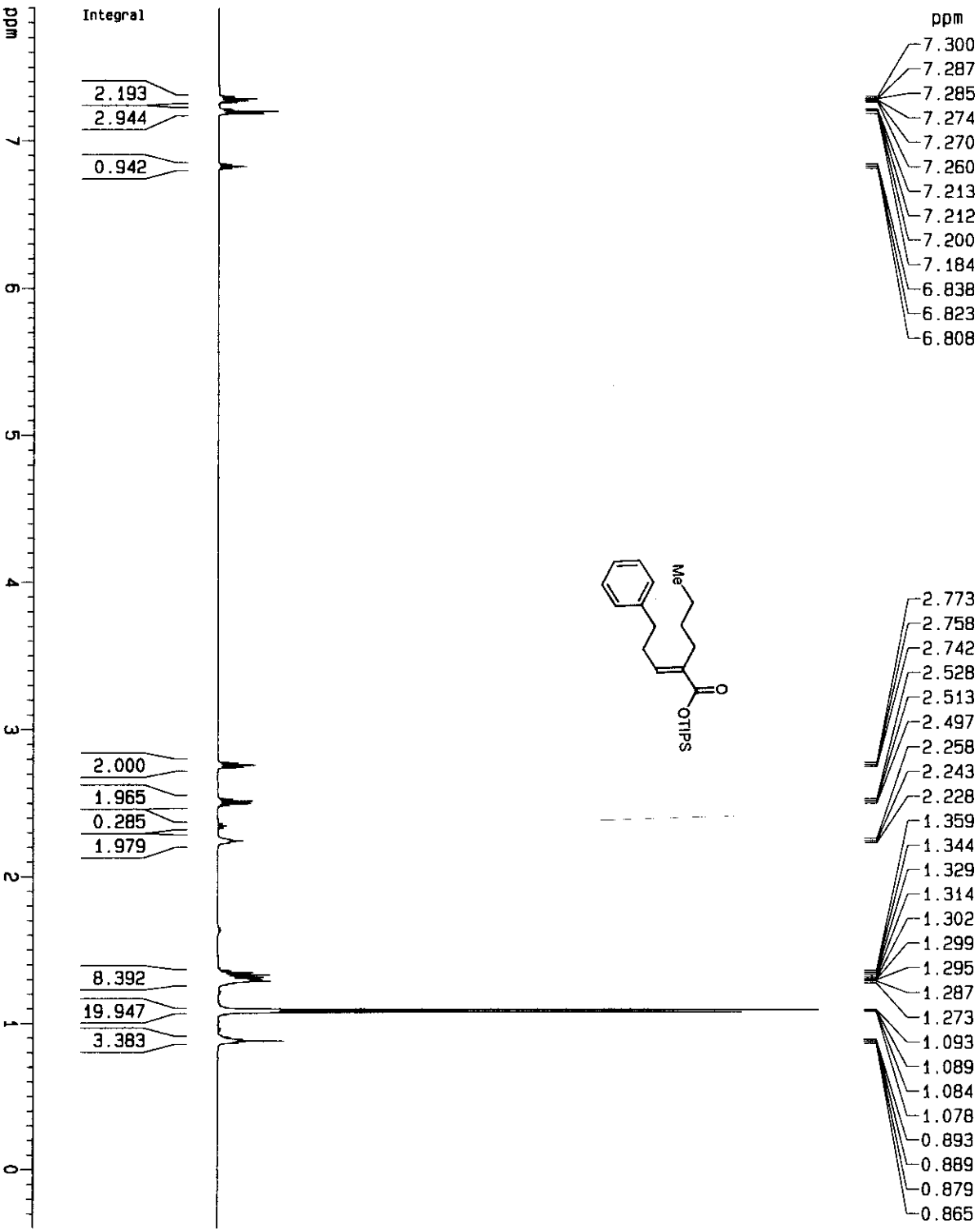
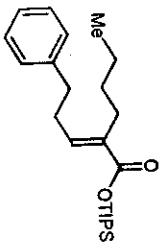
CPDPRG2 waltz16
 NUC2 1H
 P2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.1338000 MHz

F2 - Processing parameters

SI 32768
 SF 125.7577946 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 F1P 212.284 ppm
 F1 26696.39 Hz
 F2P -7.227 ppm
 F2 -908.85 Hz
 PPMCH 10.97556 ppm/cm
 HZCM 1390.26233 Hz/cm



Current Data Parameters
 NAME cinnam_pdt
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051216
 Time 19.54

INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg

TD 32768
 SOLVENT CDCl3
 NS 4

DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz

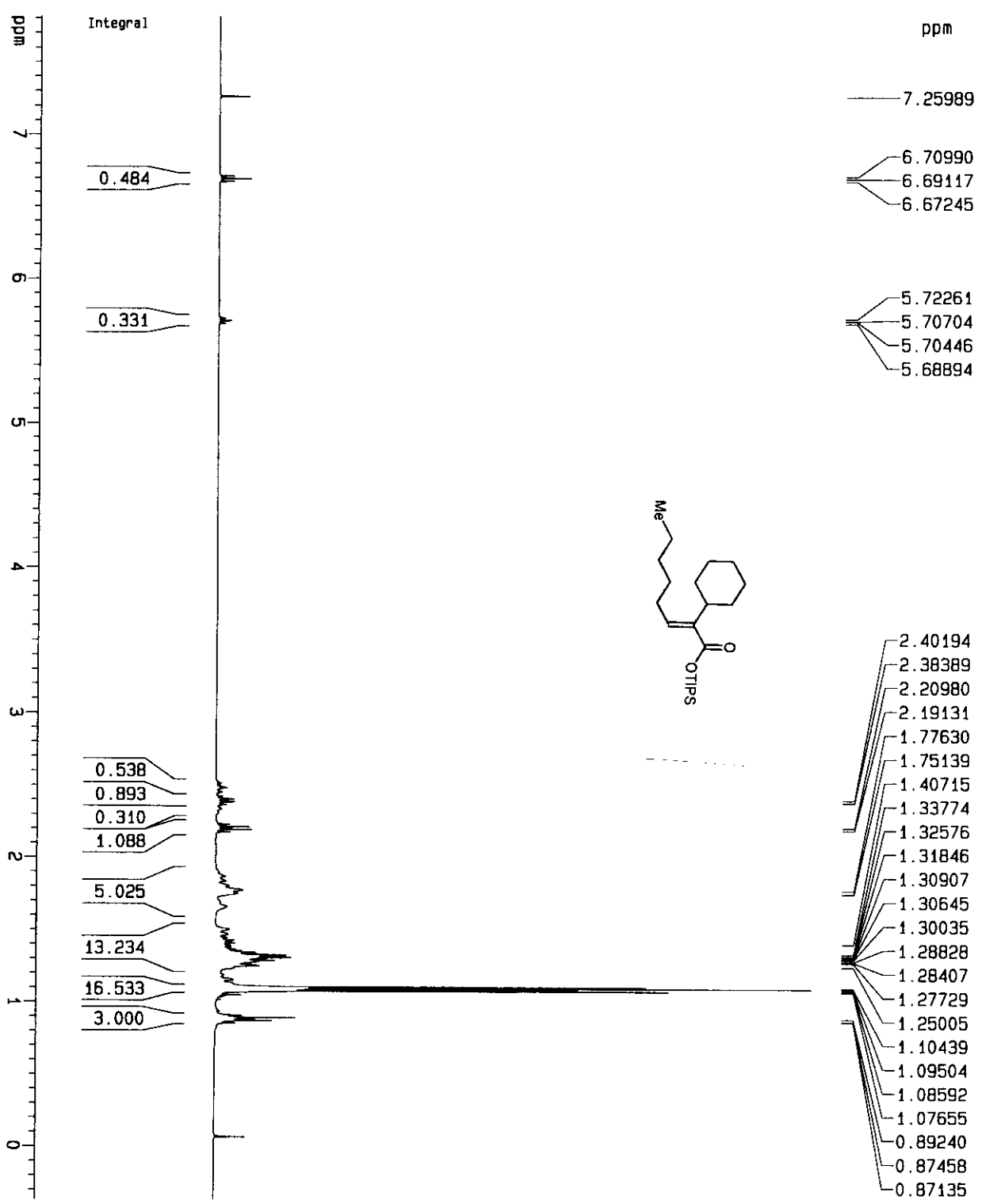
AG 3.1457779 sec
 RG 32
 DW 96.000 usec

DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing Parameters
 SI 16384
 SF 500.1300129 MHz
 KW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F4P 7.902 ppm
 F1 3952.01 Hz
 F2P -0.395 ppm
 F2 -197.67 Hz
 PPMCM 0.41486 ppm/cm
 HZCM 207.48415 Hz/cm



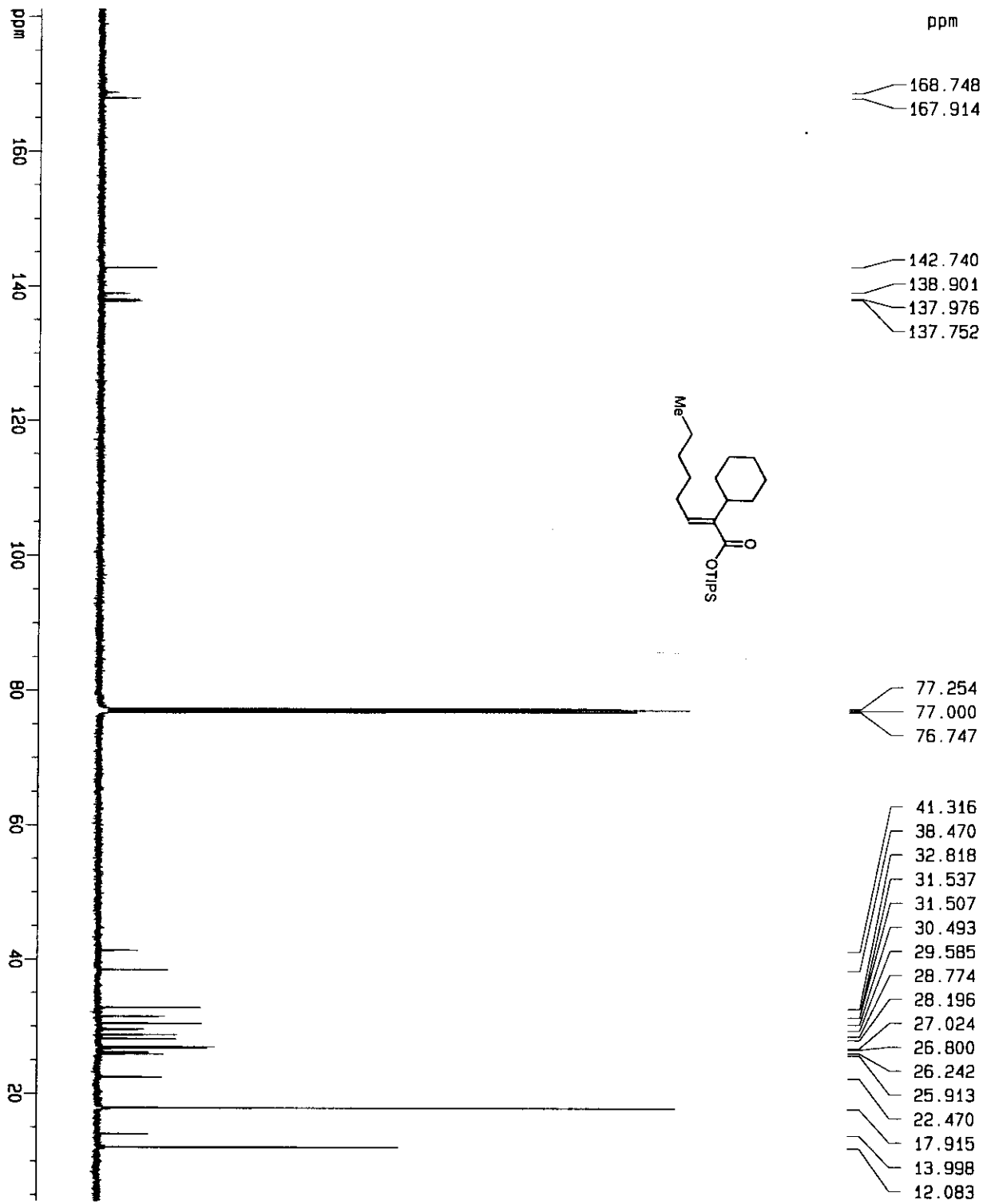
Current Data Parameters
 NAME phenyl1_crude
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051219
 Time 11.45
 INSTRUM spect
 PROBD 5 mm QNP 1H
 PULPROG zg
 TD 16384
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 4807.692 Hz
 FIDRES 0.293438 Hz
 AQ 1.7039860 sec
 RG 32
 DW 104.000 usec
 DE 5.00 usec
 TE 300.0 K
 D1 10.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300099 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.813 ppm
 F1 3126.33 Hz
 F2P -0.369 ppm
 F2 -147.78 Hz
 PPMCM 0.40913 ppm/cm
 HZCM 163.70564 Hz/cm



Current Data Parameters

NAME	Cy_01e1n_jdt
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20051219
Time	21.29
INSTRUM	spect
PROBHD	5 mm QNP 1H
PULPROG	zgdc
TD	238090
SOLVENT	Aceton
NS	302
DS	0
SMH	39682.539 Hz
FIDRES	0.166670 Hz
AQ	2.9999940 sec
RG	8192
DM	12.600 usec
DE	7.50 usec
TE	300.0 K
D1	4.00000000 sec
d11	0.03000000 sec

CHANNEL f1

NUC1	13C
P1	8.20 usec
PL1	0.00 dB
SFO1	125.7736214 MHz

CHANNEL f2

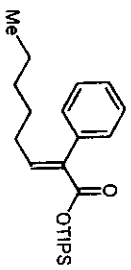
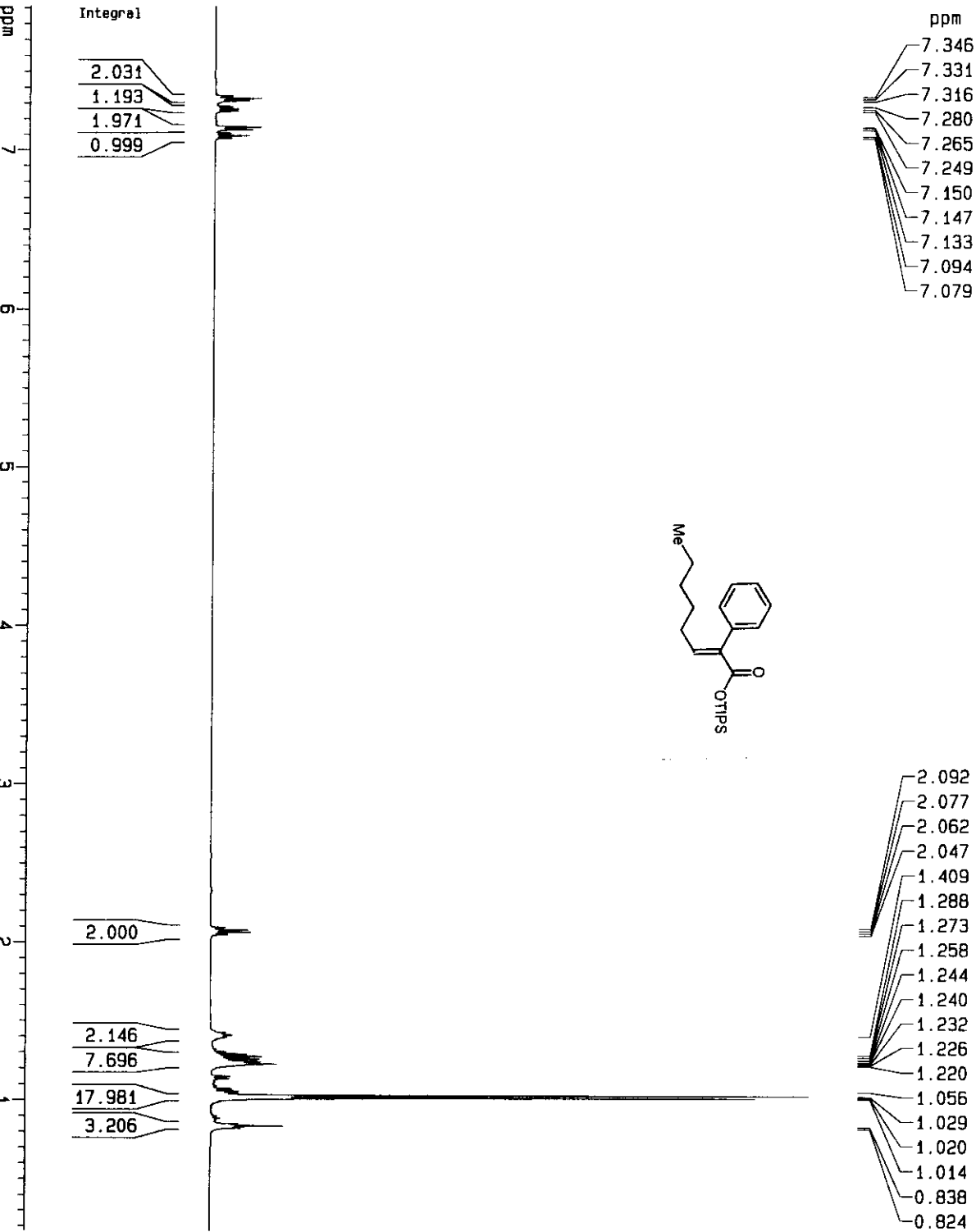
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	120.00 dB
PL12	19.00 dB
SFO2	500.1338000 MHz

F2 - Processing parameters

SI	32768
SF	125.7577922 MHz
WDM	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	181.092 ppm
F1	22773.70 Hz
F2P	4.111 ppm
F2	516.96 Hz
PPMCM	8.84905 ppm/cm
HZCM	1112.83655 Hz/cm



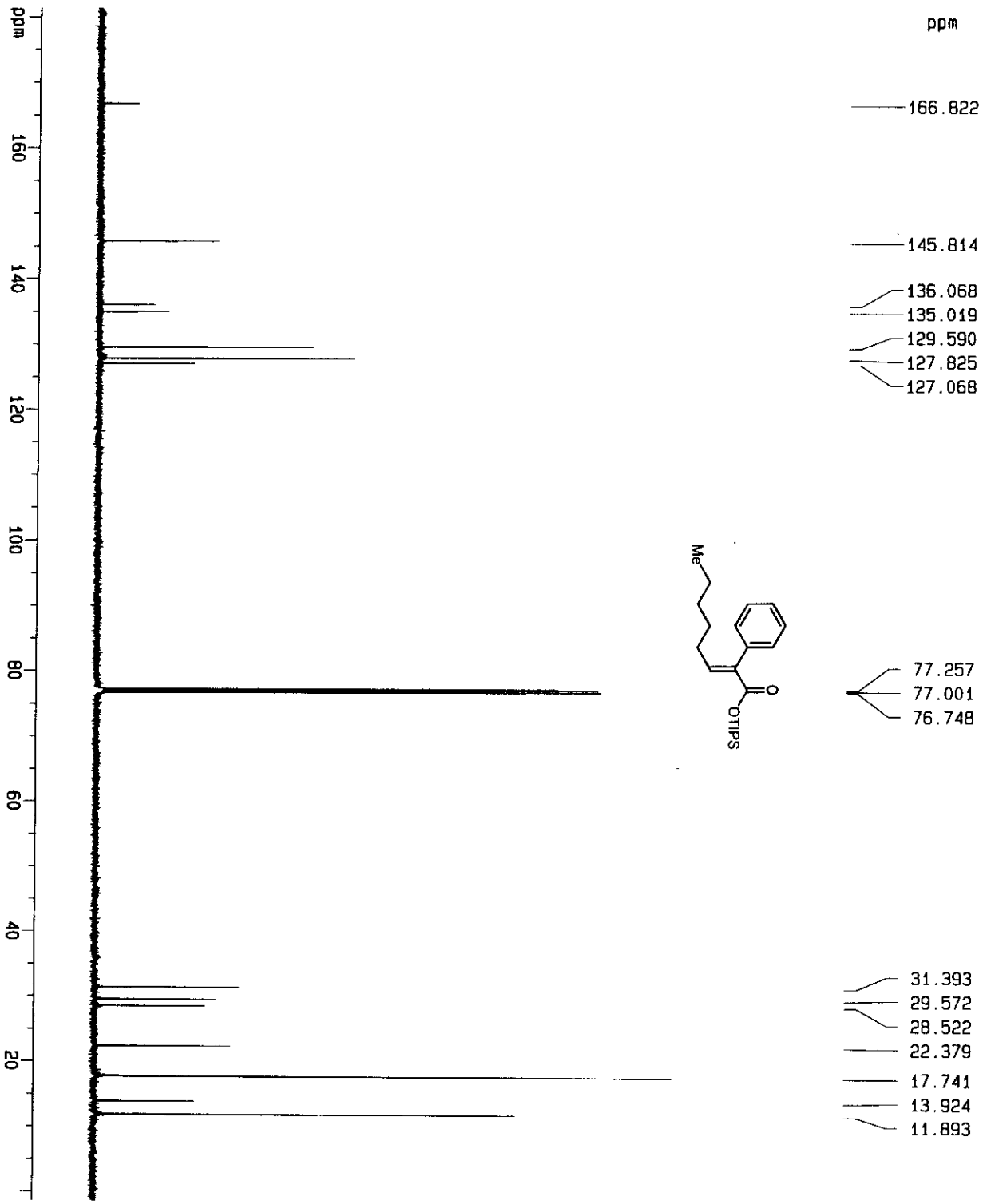
Current Data Parameters
 NAME phenyl1_dft
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051219
 Time 20.57
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 32
 DW 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300181 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.914 ppm
 F1 3958.17 Hz
 F2P 0.172 ppm
 F2 85.89 Hz
 PPM/CW 0.38713 ppm/cm
 HZ/CW 193.61412 Hz/cm



Current Data Parameters
 NAME phenyl1.pdt
 EXPNO 2
 PROCNO 1

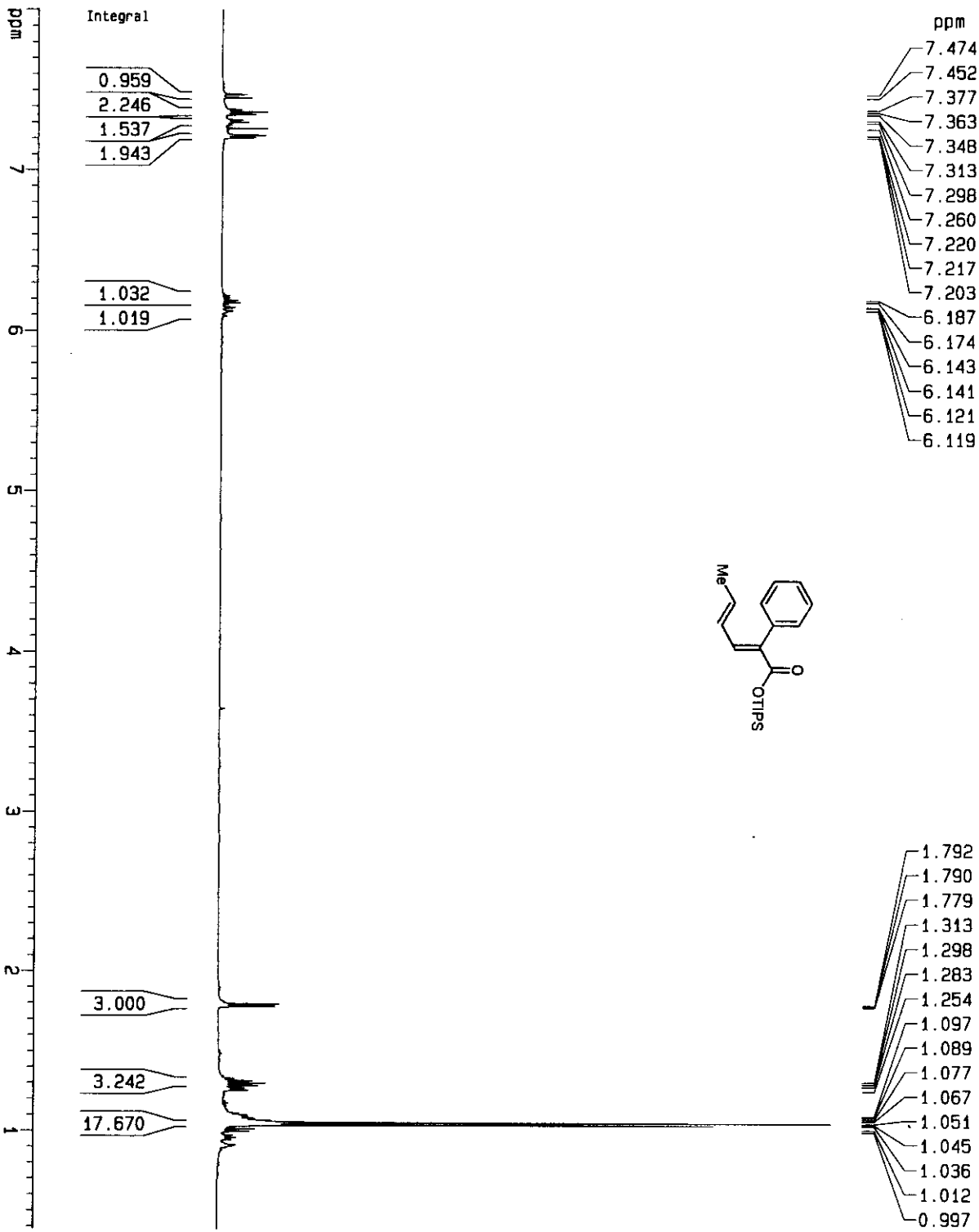
F2 - Acquisition Parameters
 Date_ 20051219
 Time 20.32
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 238090
 SOLVENT Acetone
 NS 185
 DS 0
 SMH 39682.539 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999640 sec
 RG 8192
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec

CHANNEL f1
 NUC1 13C
 P1 8.20 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

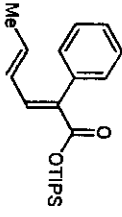
CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 500.1338000 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577934 MHz
 MIDW EH
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 181.425 ppm
 F1 22815.62 Hz
 F2P -1.387 ppm
 F2 -174.38 Hz
 PPMCH 9.14058 ppm/cm
 HZCM 1149.49663 Hz/cm



ppm
 7.474
 7.452
 7.377
 7.363
 7.348
 7.313
 7.298
 7.260
 7.220
 7.217
 7.203
 6.187
 6.174
 6.143
 6.141
 6.121
 6.119



1.792
 1.790
 1.779
 1.313
 1.298
 1.283
 1.254
 1.097
 1.089
 1.077
 1.067
 1.051
 1.045
 1.036
 1.012
 0.997

Current Data Parameters
 NAME phesi_croton1
 EXRNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051230
 Time 18.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 128
 DM 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing Parameters
 SI 16384
 SF 500.1300151 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.004 ppm
 F1 4002.96 Hz
 F2P 0.383 ppm
 F2 191.57 Hz
 PPMCM 0.38104 ppm/cm
 HZCM 190.56982 Hz/cm

ppm

167.22

141.28

139.61

135.88

131.67

130.11

128.42

128.05

127.83

127.23

77.33

77.00

76.69

29.70

18.84

17.79

17.73

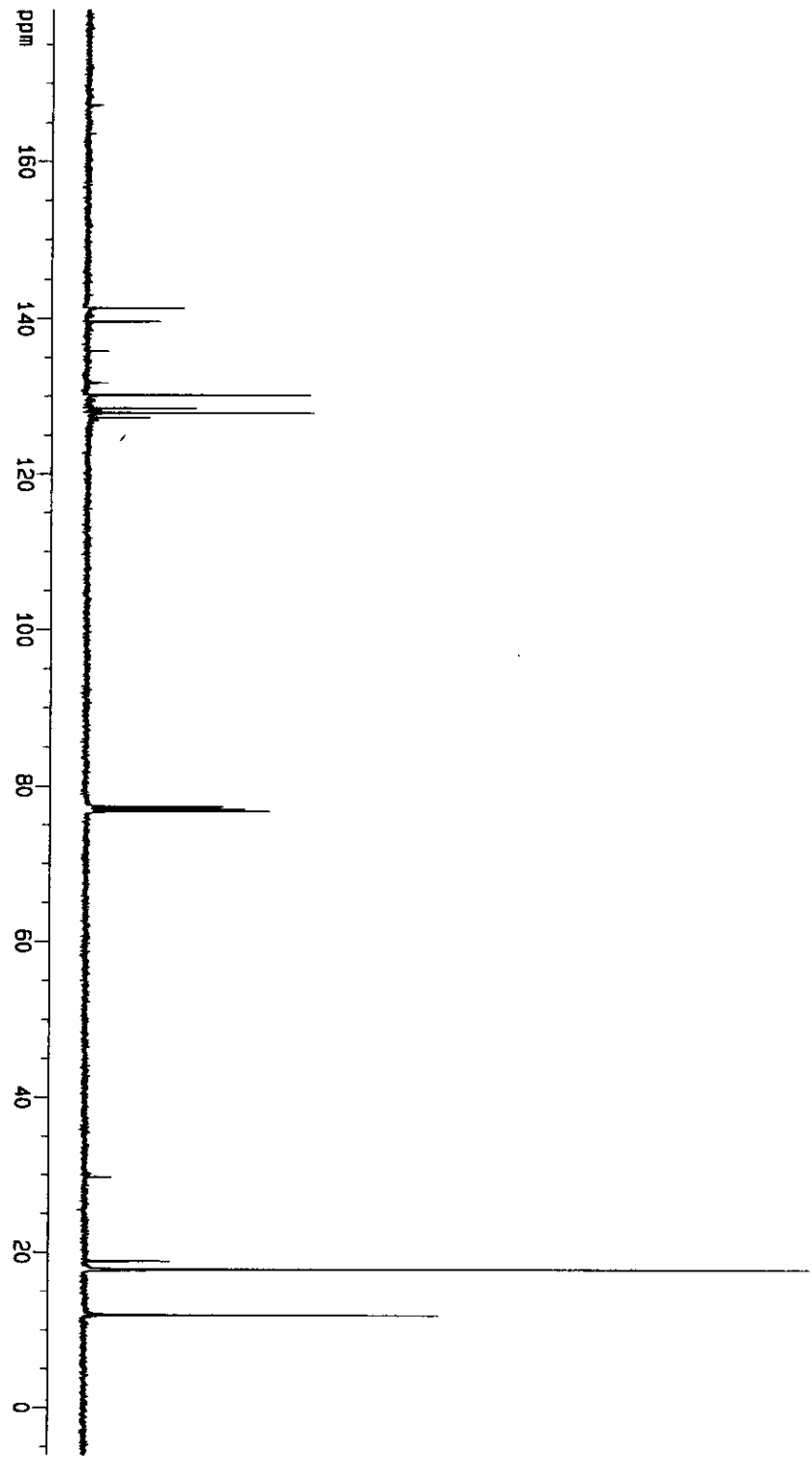
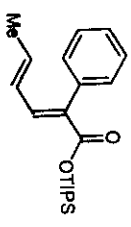
17.64

12.07

11.93

11.82

11.76



Current Data Parameters

NAME phesi_cproton1

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20051230

Time 19.09

INSTRUM spect

PROBHD 5 mm QNP 1H

PULPROG zgpg

TD 121208

SOLVENT CDCl3

NS 1024

DS 0

SMH 30303.031 HZ

FIDRES 0.250008 HZ

AQ 1.9999820 sec

RG 2048

DW 16.500 usec

DE 7.50 usec

TE 300.0 K

D1 3.00000000 sec

d11 0.03000000 sec

***** CHANNEL f1 *****

NUC1 13C

P1 11.00 usec

PL1 -2.00 dB

SFO1 100.6258087 MHz

***** CHANNEL f2 *****

CPDPRG2 waltz16

NUC2 1H

PCPD2 101.00 usec

PL2 120.00 dB

PL12 19.00 dB

SFO2 400.1324710 MHz

F2 - Processing parameters

SI 16384

SF 100.6127718 MHz

MOM EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 179.422 ppm

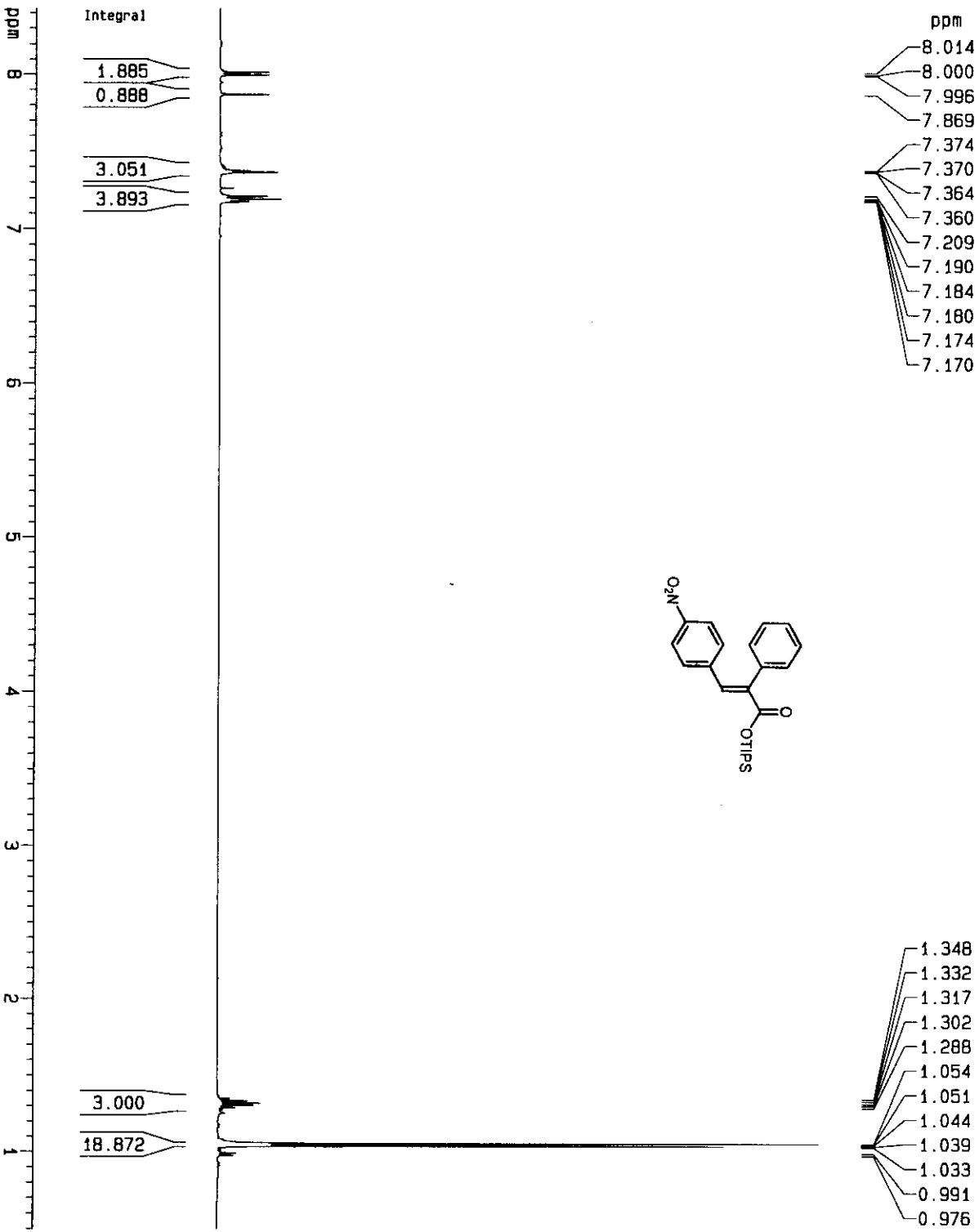
F1 18052.11 Hz

F2P -6.076 ppm

F2 -611.35 Hz

PPMCK 9.27489 ppm/cm

HZCK 933.17279 Hz/cm



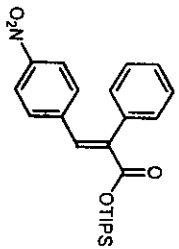
ppm

- 8.014
- 8.000
- 7.996
- 7.869
- 7.374
- 7.370
- 7.364
- 7.360
- 7.209
- 7.190
- 7.184
- 7.180
- 7.174
- 7.170

Integral

- 1.885
- 0.888
- 3.051
- 3.893

- 1.348
- 1.332
- 1.317
- 1.302
- 1.288
- 1.054
- 1.051
- 1.044
- 1.039
- 1.033
- 0.991
- 0.976



Current Data Parameters

NAME phesi_NO2benz

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20051230

Time 16.22

INSTRUM spect

PROBHD 5 mm QNP 1H

PULPROG zg

TD 32768

SOLVENT CDCl3

NS 4

DS 0

SMH 5208.333 Hz

FIDRES 0.158946 Hz

AQ 3.1457779 sec

RG 32

DM 96.000 usec

DE 4.50 usec

TE 300.0 K

D1 10.00000000 sec

***** CHANNEL f1 *****

NUC1 1H

P1 10.00 usec

PL1 0.00 dB

SFO1 500.1320118 MHz

F2 - Processing parameters

SI 16384

SF 500.1300151 MHz

MDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 8.429 ppm

F1 4215.67 Hz

F2P 0.498 ppm

F2 249.06 Hz

PPMCM 0.39656 ppm/cm

HZCM 198.33058 Hz/cm

ppm

166.55

141.32

137.47

135.35

131.16

131.03

129.27

128.80

128.24

123.40

123.33

77.33

77.00

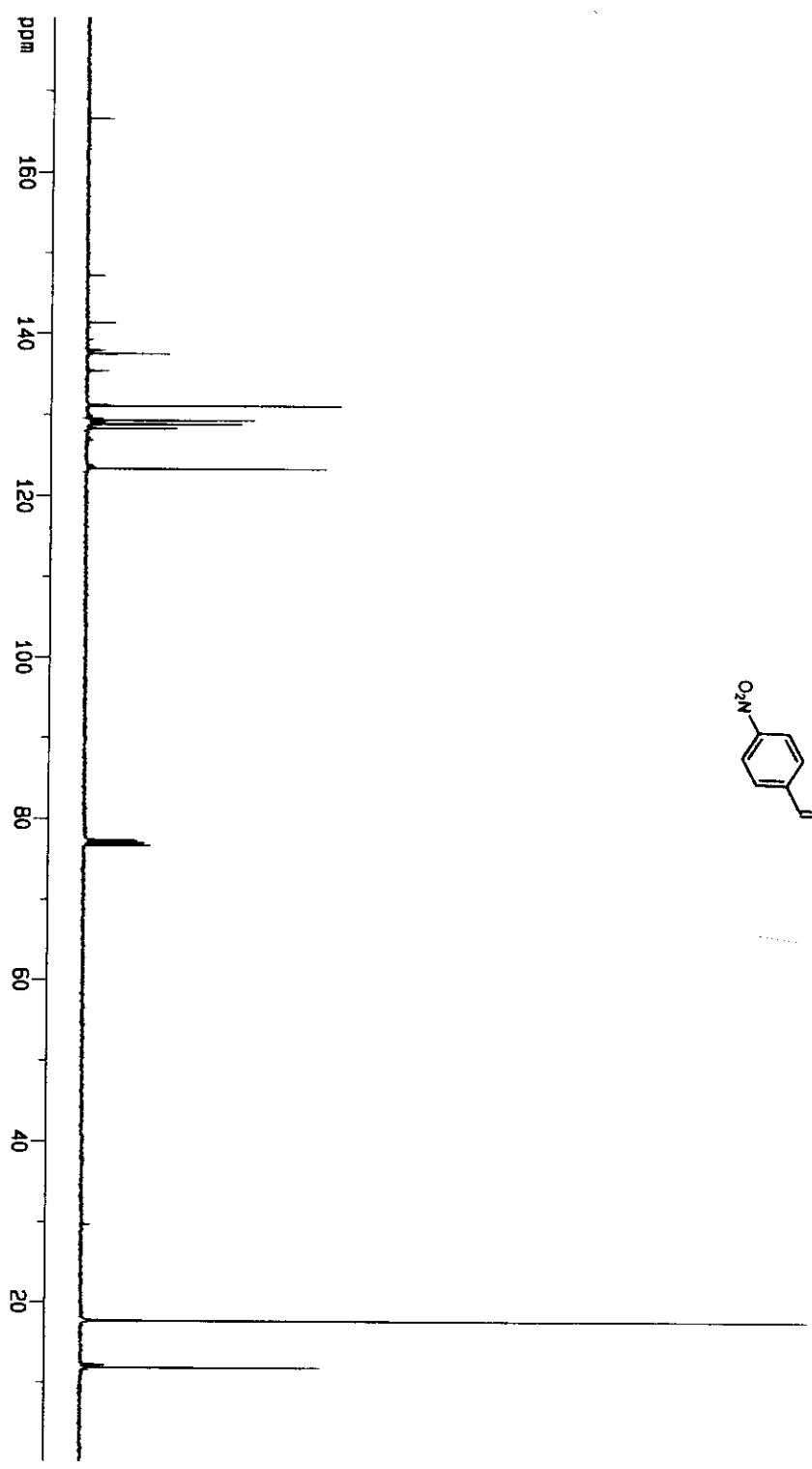
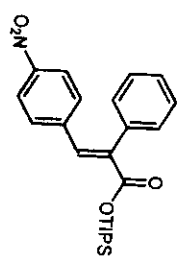
76.69

17.70

17.61

12.22

11.85



Current Data Parameters

NAME phesi_NO2benz

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20051230

Time 16.38

INSTRUM spect

PROBHD 5 mm QNP 1H

PULPROG zgpg

TD 121208

SOLVENT CDCl3

NS 622

DS 0

SMH 30303.031 Hz

FTDRES 0.250008 Hz

AQ 1.9999820 sec

RG 2048

DM 16.500 usec

DE 7.50 usec

TE 300.0 K

D1 3.00000000 sec

d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1 13C

P1 11.00 usec

PL1 -2.00 dB

SF01 100.6258087 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 101.00 usec

PL2 120.00 dB

PL12 19.00 dB

SF02 400.1324710 MHz

F2 - Processing parameters

SI 16384

SF 100.6127736 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 179.089 ppm

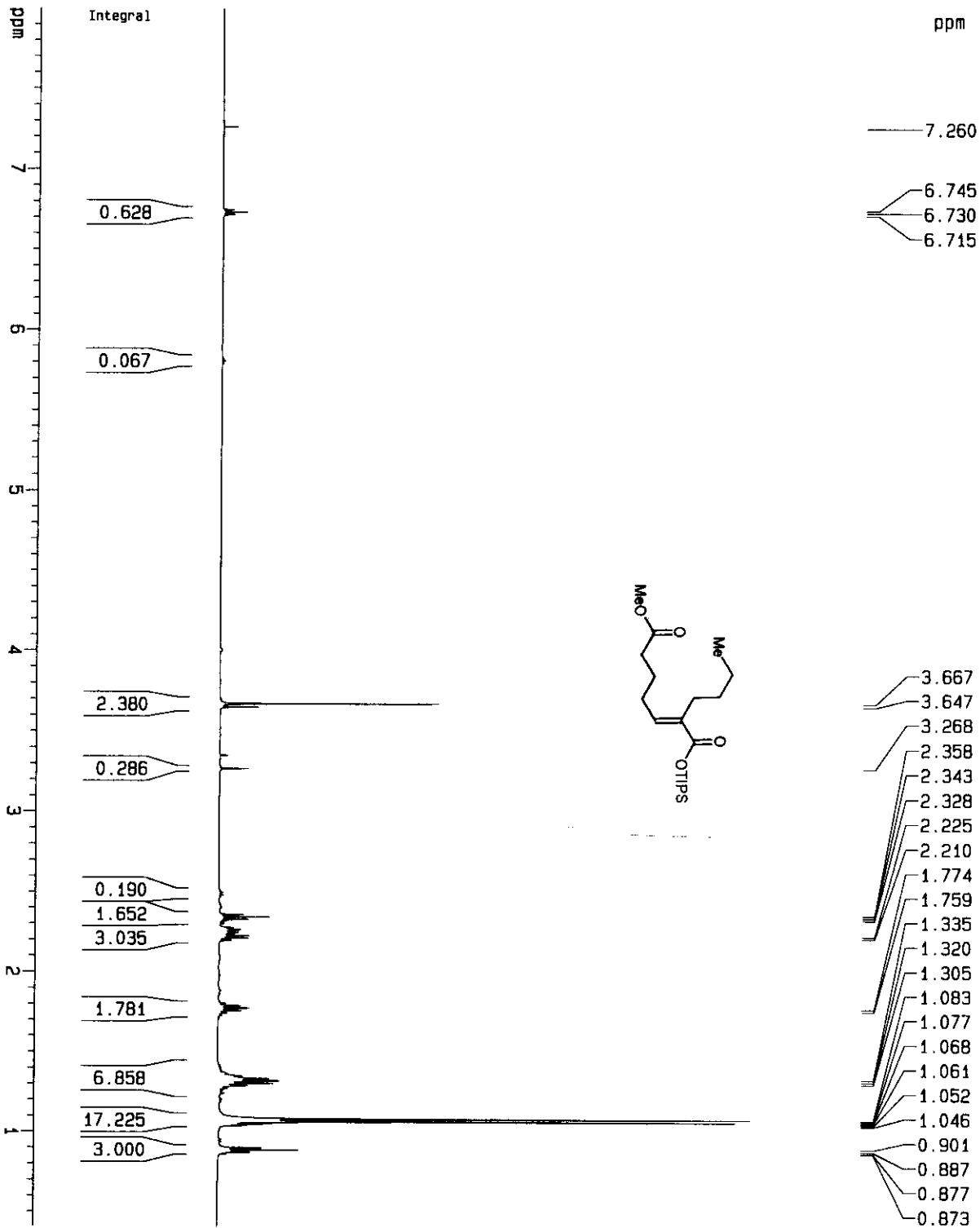
F1 18018.66 Hz

F2P 0.240 ppm

F2 24.15 Hz

PPKCH 8.94246 ppm/cm

HZCH 899.72571 Hz/cm



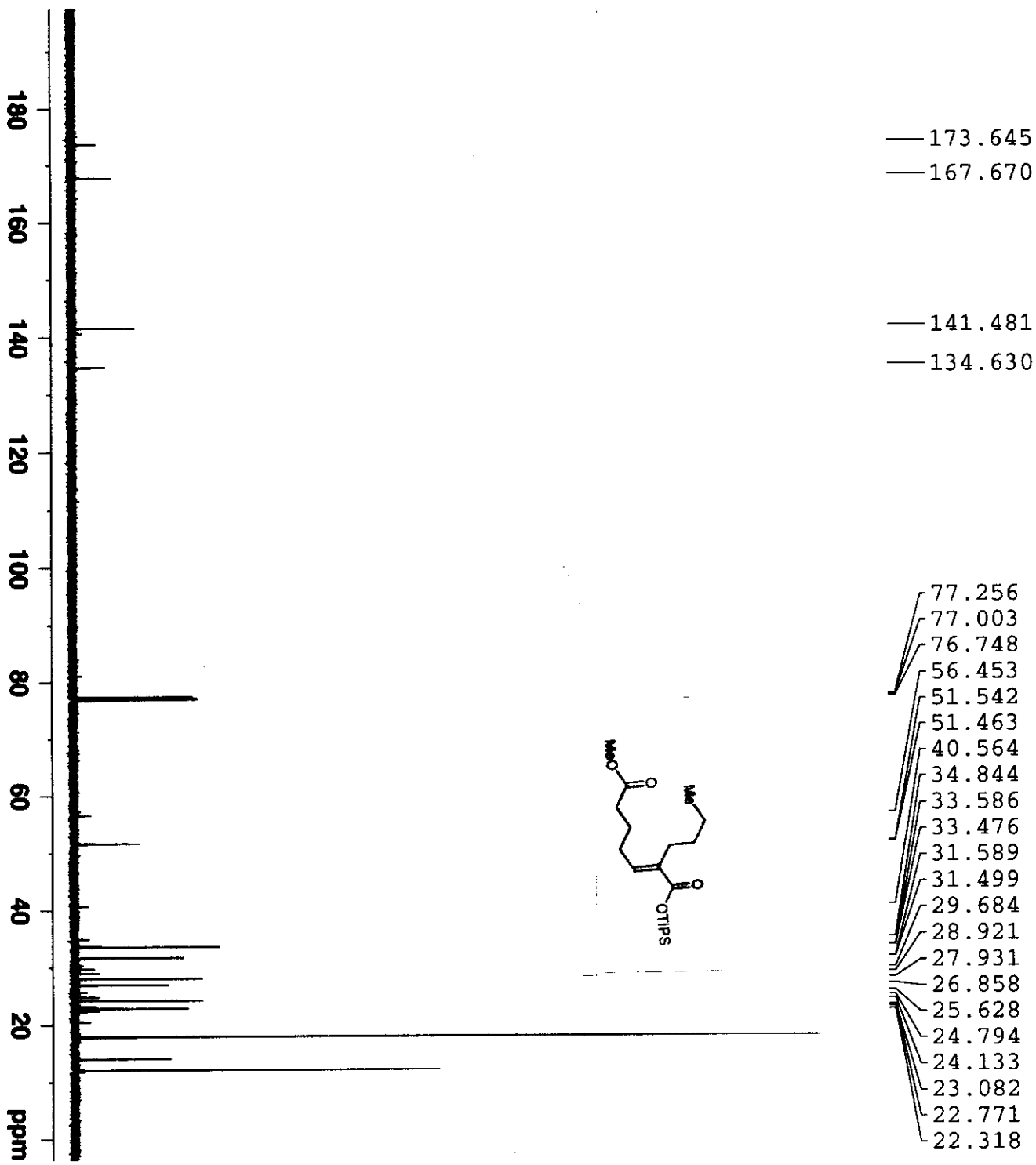
Current Data Parameters
 NAME ester_jd011229
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051229
 Time 21.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 7507.507 Hz
 FIDRES 0.229111 Hz
 AQ 2.1823988 sec
 RG 32
 DW 66.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 10.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 500.1335009 MHz

F2 - Processing parameters
 S1 16384
 SF 500.1300152 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 7.997 ppm
 F1 3999.44 Hz
 F2P 0.408 ppm
 F2 204.26 Hz
 PPMCM 0.37942 ppm/cm
 HZCM 189.75929 Hz/cm

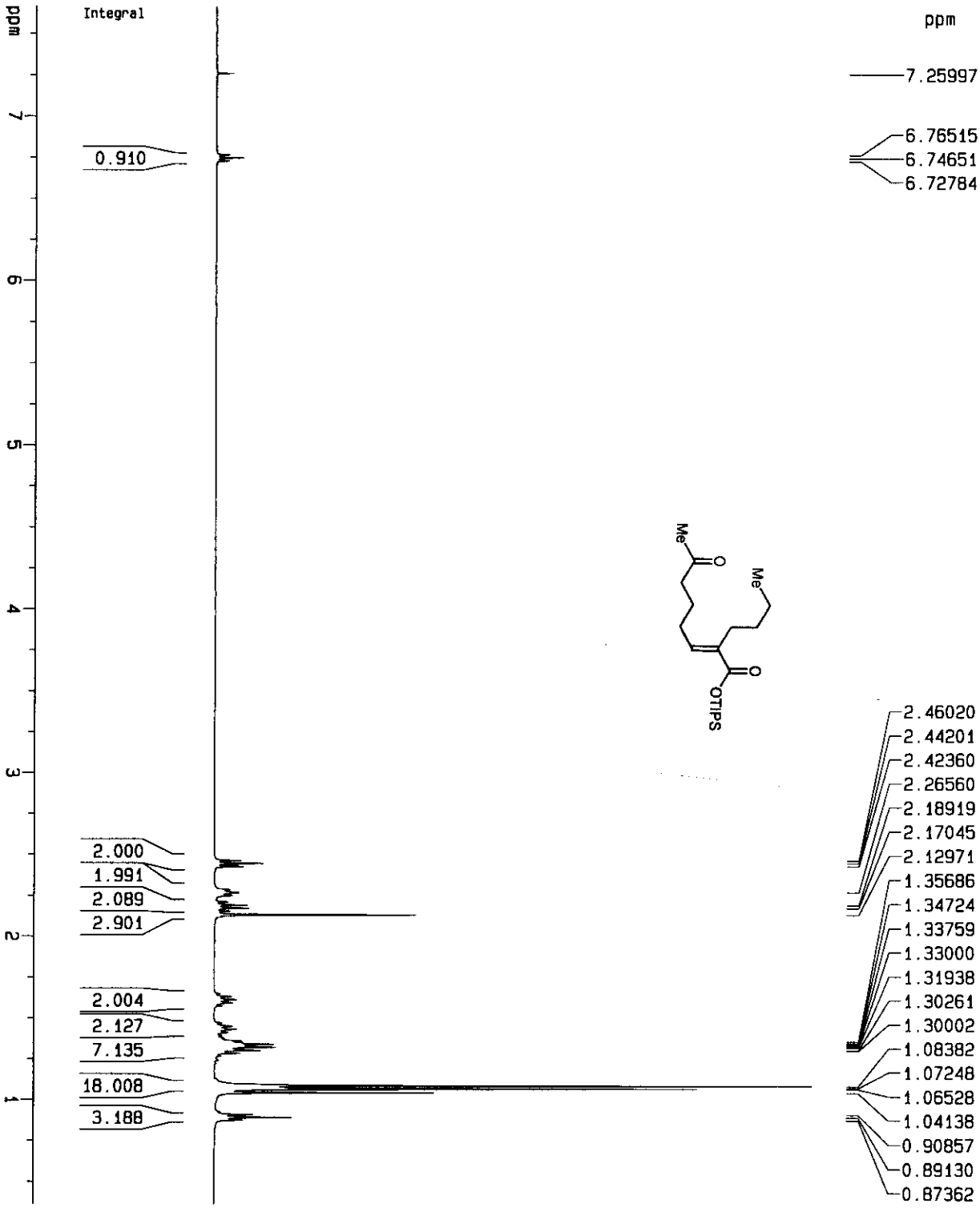


```

NAME          c:\name1.pdt
EXPNO         2
PROCNO        1
Date_         20080326
Time         17.52
INSTRUM       spect
PROBHD        5 mm PAQNP 1H/
PULPROG       zgpg
TD            197364
SOLVENT       CDCl3
NS            81
DS            0
SWH           29761.904 Hz
FIDRES        0.150797 Hz
AQ            3.3157651 se
RG            2050
DE            16.800 use
TE            296.1 K
D1            4.00000000 se
D11           0.03000000 se
TDO           1

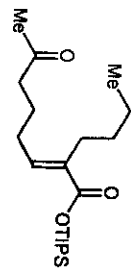
===== CHANNEL f1 =====
NUC1          13C
P1            8.00 use
PL1           1.00 de
PL1W          72.42802429 W
SFO1          125.7716224 MH

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 use
PL2           0.00 de
PL2W         16.50 de
PL13         17.00 de
PL2W         24.54113007 W
PL12W        0.54940748 W
PL13W        0.48965994 W
SFO2         500.1325006 MH
SI           131072
SF           125.7577890 MH
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.40
  
```



ppm

7.25997
6.76515
6.74651
6.72784



2.46020
2.44201
2.42360
2.26560
2.18919
2.17045
2.12971
1.35686
1.34724
1.33759
1.33000
1.31938
1.30261
1.30002
1.08382
1.07248
1.06528
1.04138
0.90857
0.89130
0.87362

2.000
1.991
2.089
2.901
2.004
2.127
7.135
18.008
3.188

Current Data Parameters
NAME ketolide.pdt
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060102
Time 20.04
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 16384
SOLVENT CDCl3
DS 4
NS 0
SMH 4807.692 Hz
FIDRES 0.293438 Hz
AQ 1.7039860 sec
RG 35.9
DM 104.000 usec
DE 6.00 usec
TE 300.0 K
D1 10.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.50 usec
PL1 0.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 7.667 ppm
F1 3057.81 Hz
F2P 0.360 ppm
F2 143.93 Hz
PPMCM 0.36537 ppm/cm
HZCM 146.19418 Hz/cm

ppm

208.75

167.81

142.50

133.94

77.33

77.01

76.69

43.45

31.60

29.88

28.49

28.43

26.85

23.55

22.77

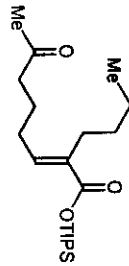
17.85

17.68

13.98

12.26

11.99



ppm

Current Data Parameters
 NAME KetoIaIe.pdt
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060102
 Time 20.08
 INSTRUM spect
 PROBDW 5 mm QNP 1H
 PULPROG zgdc
 TO 121208
 SOLVENT CDCl3
 NS 299
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999820 sec
 RG 4597.6
 DW 16.500 usec
 DE 7.50 usec
 TE 300.0 K
 D1 3.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 11.00 usec
 PL1 -2.00 dB
 SFO1 100.6258087 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 101.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 400.1324710 MHz

F2 - Processing Parameters
 SI 16384
 SF 100.6127718 MHz
 KW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 226.646 ppm
 F1 22803.44 Hz
 F2P -7.055 ppm
 F2 -709.84 Hz
 PPMCM 11.68504 ppm/cm
 HZCM 1175.66394 Hz/cm

200

150

100

50

0