Generation of α-phosphonovinyl radicals and development of a new route to highly functionalized vinylphosphonates and vinylphosphonate-incorporated carbocyclic or heterocyclic compounds via a radical trapping sequence[†]

Takafumi Ageno[a], Tatsuo Okauchi[a], Toru Minami[a*] and Masaru Ishida[b*]

[a]Department of Applied Chemistry, Kyushu Institute of Technology, Sensui-cho, Tobata, Kitakyushu 804-8550, Japan, [b]Department of Chemistry, Faculty of Engineering, Gifu University, Yanagido, Gifu, 501-1193, Japan. E-mail: minami@che.kyutech.ac.jp and ishidam@apchem.gifu-u.ac.jp

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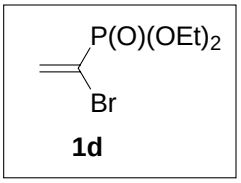
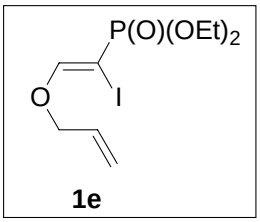
Materials. Benzene was distilled from CaH_2, and acetonitrile was distilled from P_2O_5 and redistilled from CaH_2. THF was distilled from sodium benzophenone ketyl in a recycling still. Diisopropylamine (DIA) was refluxed with CaH_2 and then distilled. A commercial solution of *n*-BuLi (1.47 M, 1.57 M, 1.59 M in hexane) were used. The starting materials **1a-c** and diethyl phosphonoacetaldehyde diethyl acetal were prepared according to the established procedures.[1]



1d

Diethyl 1-bromovinylphosphonate[2] (1d): To a solution of $Pd(PPh_3)_4$, generated in situ from $Pd(OAc)_2$ (17.7 mg, 0.08 mmol) and PPh_3 (83 mg, 0.32 mmol) in benzene (30 mL) at room temperature for 15 min, was added a solution of diethyl ethynylphosphonate (644 mg, 3.97 mmol) and Bu_3SnH (1.4 mL, 5.16 mmol) in benzene (10 mL). The reaction mixture was stirred for 10 min. The mixture was quenched by addition of phosphate buffer (pH = 7), and the organic layer was extracted with AcOEt, washed with brine, dried over Na_2SO_4, and concentrated *in vacuo*. The residue was chromatographed on silica gel (AcOEt : hexane = 1:1) to give diethyl 1-(tributylstannyl)vinylphosphonate (1.48 g, 82 %); IR (neat) 1241, 1058, 1024, 964, 815 cm^{-1}; ^1H NMR δ 1.00 (9H, t, J = 7.2 Hz), 1.12 (6H, t, J = 8.0 Hz), 1.38-1.44 (12H, m), 1.58-1.65 (6H, m), 4.10-4.18 (4H, m), 6.34 (1H, dd, J = 3.3 Hz, $^3J_{P\text{-}H}$ = 61.2 Hz), 7.00 (1H, dd, $^3J_{P\text{-}H}$ = 34.5 Hz); ^{13}C NMR δ 10.3, 13.6, 16.4 (d, $^3J_{P\text{-}C}$ = 6.0 Hz), 27.3, 28.2, 61.3 (d, $^2J_{P\text{-}C}$ = 6.0 Hz), 142.7 (d, $^1J_{P\text{-}C}$ = 131.0 Hz), 144.2 (d, $^2J_{P\text{-}C}$ = 2.0 Hz); ^{119}Sn NMR (186 MHz) δ -30.5 - -29.9 (d, $J_{P\text{-}Sn}$ = 111.6 Hz); Anal. Calcd for $C_{18}H_{39}O_3PSn$: C, 47.71; H, 8.67. Found: C, 47.44; H, 8.54. To a cooled solution of diethyl 1-(tributylstannyl)vinylphosphonate (1.04 g, 2.29 mmol) in CCl_4 (10 mL) at - 5 ℃ was added dropwise over 10 min a solution of Br_2 (0.13 mL, 2.52 mmol) in CCl_4 (10 mL), and then the mixture was stirred at this temperature for 45 min. The reaction was quenched by the addition of aqueous $Na_2S_2O_3$ and organic layer was extracted with CH_2Cl_2, washed with a saturated water solution of NaCl, dried over Na_2SO_4, and concentrated *in vacuo*. The residue was chromatographed on silica gel (AcOEt : hexane = 1:1) to give **1d** as colorless oil. Yield 512 mg (92%). ^1H-NMR δ 1.36-1.40 (6H, m), 4.14-4.20 (4H, m), 6.46

(1H, dd, $^{3}J_{P\text{-}H}$ = 37.2 Hz), 6.91 (1H, dd, $^{3}J_{P\text{-}H}$ = 14.4 Hz); ^{13}C-NMR δ 16.0 (d, $^{3}J_{P\text{-}C}$ = 6.2 Hz), 63.2 (d, $^{2}J_{P\text{-}C}$ = 5.4 Hz), 119.2 (d, $^{1}J_{P\text{-}C}$ = 200.0Hz), 135.3 (d, $^{2}J_{P\text{-}C}$ = 13.9 Hz).

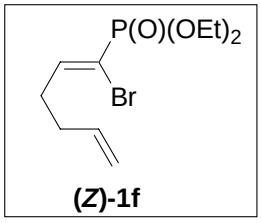


1e

Diethyl (*Z*)-2-allyloxy-1-(iodo)-vinylphosphonate (1e): To a solution of diethyl phosphonoacetaldehyde diethyl acetal (6.65 g, 26.16 mmol) in benzene (10 mL) was added allyl alcohol (3.9 mL, 57.55 mmol) and TsOH (450 mg, 0.26 mmol), and the reaction mixture was heated at reflux with stirring until benzene-ethanol azeotrope was completely removed (34.5h). The reaction mixture was cooled to room temperature, and then distilled under reduced pressure to give diethyl phosphonoacetaldehyde diallyl acetal as colorless oil. Yield 5.62 g (77 %). Bp 120 ℃ / 4 mmHg; ^{1}H-NMR δ 1.18 (6H, t, *J* = 7.1 Hz), 2.10 (2H, dd, $^{2}J_{P\text{-}H}$ = 18.7 Hz, *J* = 5.8 Hz), 3.93-4.00 {[(OC*H*$_2$CHCH$_2$)$_2$, 4H, m], [P(OC*H*$_2$CH$_3$)$_2$, 4H, m]}, 4.88 (1H, m), 5.02-5.05 (2H, m), 5.14-5.19 (2H, m), 5.74-5.81 (2H, m); ^{13}C-NMR δ 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz), 31.4 (d, $^{1}J_{P\text{-}C}$ = 139.5 Hz), 61.5 (d, $^{2}J_{P\text{-}C}$ = 6.2 Hz), 97.4, 116.8, 133.9. To a solution of diethylphosphonoacetaldehyde diallyl acetal (139 mg, 0.5 mmol) in THF (1.0 mL) at -78 ℃ was added *n*-BuLi (1.59 M in hexane, 0.31 mL, 0.5 mmol). The reaction mixture was stirred at -78 ℃ for 1.0 h, and at room temperature overnight. The reaction was quenched by the addition of phosphate buffer (pH = 7). After similar workup, the residue was chromatographed on silica gel (AcOEt : hexane = 1:1) to give (*E*)-2-allyloxy-vinylphosphonate. Yield 110 mg (quant. yield). ^{1}H-NMR δ 1.33 (6H, t, *J* = 7.1 Hz), 4.02-4.10 (4H, m), 4.38 (2H, d, *J* = 5.5 Hz), 4.77 (1H, dd, $^{2}J_{P\text{-}H}$ = 9.7 Hz, *J* = 13.6 Hz), 5.28-5.32 (1H, m), 5.34-5.38 (1H, m), 5.90-5.94 (1H, m), 7.21 (1H, dd, $^{3}J_{P\text{-}H}$ = 11.5 Hz, *J* = 13.5 Hz); ^{13}C-NMR δ 16.3 (d, $^{3}J_{P\text{-}C}$ = 6.7 Hz), 61.4 (d, $^{2}J_{P\text{-}C}$ = 5.2 Hz), 71.1, 88.9 (d, $^{1}J_{P\text{-}C}$ = 199.2 Hz), 118.8, 131.6, 162.7 (d, $^{2}J_{P\text{-}C}$ = 21.2 Hz); Anal. Calcd for $C_9H_{17}O_4P$: C, 49.09; H, 7.78. Found: C, 48.86; H, 7.87. To a solution of LDA (0.72 mmol) in THF (2.5 mL) at -78 ℃ was added dropwise a solution of (*E*)-2-allyloxy-vinylphosphonate (132 mg, 0.6 mmol) in THF (0.5 mL), and the mixture was stirred for 50 min. Then, $CuBrSMe_2$ (62 mg, 0.3 mmol) was added to the mixture. After stirring for 45 min at -78 ℃, a solution of I_2 (168 mg, 0.66 mmol) in THF (1.5 mL) was added dropwise to the mixture and the reaction mixture

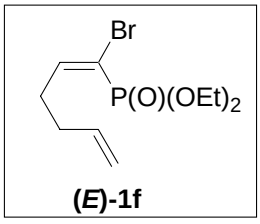
was stirred for 3 h. The reaction was quenched by the addition of aqueous $Na_2S_2O_3$. After similar workup, the residue was chromatographed on silica gel (AcOEt) to give **1e** as yellow oil. Yield 153 mg (74 %). ^{1}H-NMR δ 1.33-1.39 (6H, m), 4.04-4.12 (4H, m), 4.62-4.65 (2H, m), 5.32-5.41 (2H, m), 5.91-5.96 (1H, m), 7.38 (1H, d, $^3J_{P\text{-}H}$ = 7.6 Hz); ^{13}C-NMR δ 16.0 (d, $^3J_{P\text{-}C}$ = 6.6 Hz), 56.1 (d, $^1J_{P\text{-}C}$ = 204.4 Hz), 62.4 (d, $^2J_{P\text{-}C}$ = 4.7 Hz), 74.8, 119.4, 131.7, 163.6 (d, $^2J_{P\text{-}C}$ = 31.3 Hz); MS *m/z* 346 (M^+); HRMS(M^+) Calcd for $C_9H_{16}IO_4P$ 345.9831, Found 345.9835.

Diethyl 1-bromo-hexa-1,5-dienylphosphonate (1f): To a solution of LDA (6.27 mmol) in THF (15 mL) at -78 ℃ was added dropwise a solution of tetraethyl methylenediphosphonate (821 mg, 2.85 mmol) in THF (3 mL), and the mixture was warmed to room temperature. *N*-bromosuccinimide (559 mg, 3.14 mmol) was added to the deep yellow mixture at room temperature, and the mixture was stirred for 15 min. After the mixture was cooled to -78 ℃, a solution of 4-pentenal (239 mg, 2.85 mmol) in THF (3 mL) was added to the mixture. The reaction mixture was immediately warmed to room temperature with protecting from light and was stirred for 20 h. The reaction was quenched by the addition of sat. aqueous NH_4Cl. After similar workup, the residue was chromatographed on silica gel (AcOEt : hexane = 1:1) to give (*Z*)-**1f** (444 mg, 53 %) and (*E*)-**1f** (148 mg, 17 %) as pale yellow oil.



(*Z*)-1f

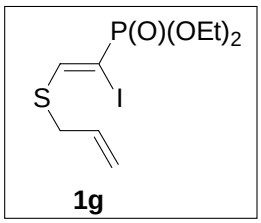
(*Z*)-1f: R_f0.48 (AcOEt : hexane = 1:1); ^{1}H-NMR δ 1.33 (6H, t, *J* = 7.1 Hz), 2.20-2.25 (2H, m), 2.39-2.45 (2H, m), 4.03-4.15 (4H, m), 4.98-5.06 (2H, m), 5.72-5.81 (1H, m), 7.10 (1H, td, $^3J_{P\text{-}H}$ = 14.2 Hz); ^{13}C-NMR δ 16.2 (d, $^3J_{P\text{-}C}$ = 6.5 Hz), 31.2 (d, $^3J_{P\text{-}C}$ = 13.3 Hz), 31.4, 64.0 (d, $^2J_{P\text{-}C}$ = 5.2 Hz), 113.0 (d, $^1J_{P\text{-}C}$ = 205.5 Hz), 115.8, 136.7, 149.6 (d, $^2J_{P\text{-}C}$ = 14.4 Hz); HRMS(M^+) Calcd for $C_{10}H_{18}BrO_3P$ 296.0177, Found 296.0029.



(*E*)-1f

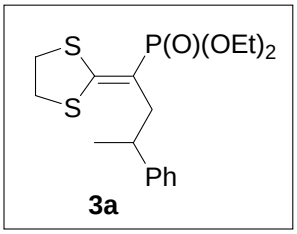
(*E*)-1f: R_f0.67 (AcOEt : Hexane = 1:1); ^{1}H-NMR δ 1.33-1.36 (6H, m), 2.14-2.21 (2H, m), 2.66-2.73 (2H, m), 4.08-4.15 (4H, m), 4.98-5.06 (2H, m), 5.74-5.78 (1H, m), 6.90 (1H, td, $^3J_{P\text{-}H}$ = 39.5 Hz); ^{13}C-NMR δ 16.2 (d, $^3J_{P\text{-}C}$ = 6.7 Hz), 30.6 (d, $^3J_{P\text{-}C}$ = 3.2 Hz), 32.8 (d, $^4J_{P\text{-}C}$ = 1.4 Hz), 62.9 (d, $^2J_{P\text{-}C}$ = 5.4 Hz), 109.3 (d, $^1J_{P\text{-}C}$

= 197.7 Hz), 115.9, 136.8, 153.9 (d, $^2J_{P\text{-}C}$ = 16.2 Hz); HRMS(M^+) Calcd for $C_{10}H_{18}BrO_3P$ 296.0177, Found 296.0141.



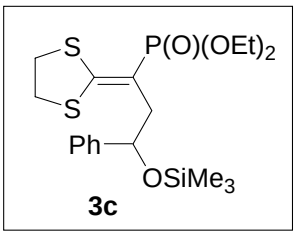
1g

Synthesis of Diethyl (*Z*)-2-allylthio-1-iodovinylphosphonate (1g) from Diethyl (*E*)-2-ethoxy-1-(trimethylsilyl)vinylphosphonate. A solution of lithium allylthiolate, generated in situ from allylthiol (381 mg, 3.6 mmol) in THF (18 mL) and *n*-BuLi (3.6 mmol) at -78 ^oC, was added dropwise to a solution of diethyl (*E*)-2-ethoxy-1-(trimethylsilyl)vinylphosphonate (841 mg, 3.0 mmol) in THF (12 mL) *via cannula*. After being stirred for 10 min at this temperature, the mixture was then warmed to room temperature and stirred for 7.0 h. After similar workup, the residue was chromatographed on silica gel (AcOEt : hexane = 1:1) to give (*E*)- and (*Z*)-2-allylthio-1-(trimethylsilyl)vinylphosphonates in 438 mg (47 %) and 122 mg (13 %) yields, respectively, as colorless oil. **(*E*)-isomer**: R_f0.53 (AcOEt); ^{1}H-NMR δ 0.27 (9H, s) 1.30 (6H, t, *J* = 7.0 Hz), 3.47 (2H, d, *J* = 7.0 Hz), 3.99-4.01 (4H, m), 5.17-5.29 (2H, m), 5.82-5.90 (1H, m), 8.02 (1H, d, $^3J_{P\text{-}H}$ = 31.7 Hz); ^{13}C-NMR δ -0.7, 16.3, 37.8, 61.1 (d, $^2J_{P\text{-}C}$ = 5.3 Hz), 118.5, 122.7 (d, $^1J_{P\text{-}C}$ = 139.0 Hz), 133.1, 160.4 (d, $^2J_{P\text{-}C}$ = 15.9 Hz. **(*Z*)-isomer**: R_f0.67 (AcOEt); ^{1}H-NMR δ 0.17 (9H, s), 1.31-1.35 (6H, m), 3.39 (2H, d, *J* = 7.1 Hz), 4.03-4.13 (4H, m), 5.17-5.23 (2H, m), 5.82-5.88 (1H, m), 7.34 (1H, d, $^3J_{P\text{-}H}$ = 56.0 Hz); ^{13}C-NMR δ -0.6, 16.4, 37.8, 61.1 (d, $^2J_{P\text{-}C}$ = 5.4 Hz), 118.1, 124.4 (d, $^1J_{P\text{-}C}$ = 143.8 Hz), 133.9, 156.3. To a solution of **(*E*)-isomer** (438 mg, 1.42 mmol) in MeCN (10 mL) at room temperature was added NaI (319 mg, 2.13 mmol) and *N*-chlorosuccinimide (284 mg, 2.13 mmol). The mixture was stirred for 2 days at this temperature. The reaction was quenched by the addition of aqueous $Na_2S_2O_3$. After similar workup, the residue was chromatographed on silica gel (AcOEt) to give **1g** as yellow crystal. Yield 413 mg (80 %). ^{1}H-NMR δ 1.33-1.37 (6H, m), 3.55 (2H, d, *J* = 7.0 Hz), 4.04-4.12 (4H, m), 5.19-5.30 (2H, m), 5.81-5.93 (1H, m), 8.09 (1H, d, $^3J_{P\text{-}H}$ = 14.7 Hz); ^{13}C-NMR δ 16.2, 36.3, 62.8 (d, $^2J_{P\text{-}C}$ = 5.1 Hz), 78.8 (d, $^1J_{P\text{-}C}$ = 197.6 Hz), 119.1, 133.0, 155.8 (d, $^2J_{P\text{-}C}$ = 18.5 Hz); MS *m/z* 362 (M^+); HRMS(M^+) Calcd for $C_9H_{16}IO_3PS$ 361.9602, Found 361.9604.



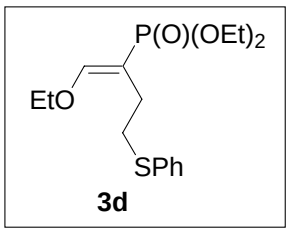
3a

Diethyl 3-phenyl-1-(1,3-dithiolan-2-ylidene)butylphosphonate (3a): IR (neat) 798, 1024, 1240, 1529, 2977, 3448 cm^{-1}; ^{1}H-NMR δ 1.29-1.34 (9H, m), 2.58-2.72 (2H, m), 3.18-3.22 (1H, m), 3.30-3.36 (2H, m), 3.40-3.42 (2H, m), 3.99-4.13 (4H, m), 7.16-7.20 (1H, m), 7.29-7.31 (4H, m); ^{13}C-NMR δ 16.3 (d, $^{3}J_{P\text{-}C}$ = 6.2 Hz), 20.4, 27.8, 36.8, 39.0, 45.2 (d, $^{2}J_{P\text{-}C}$ = 8.7 Hz), 61.6 (d, $^{2}J_{P\text{-}C}$ = 4.1 Hz), 112.0 (d, $^{1}J_{P\text{-}C}$ = 187.3 Hz), 125.9, 127.0, 128.2, 147.1, 158.6 (d, $^{2}J_{P\text{-}C}$ = 14.7 Hz); MS m/z 372 (M^{+}); HRMS(M^{+}) Calcd for $C_{17}H_{25}O_3PS_2$ 372.0983, Found 372.0981.



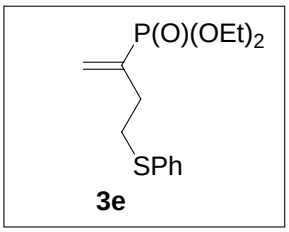
3c

Diethyl 3-(trimethylsiloxy)-3-phenyl-1-(1,3-dithiolan-2-ylidene)propylphosphonate (3c): IR (neat) 750, 840, 964, 1054, 1247, 1529, 2981, 3430 cm^{-1}; ^{1}H-NMR δ 0.02 (9H, s), 1.32-1.36 (6H, m), 2.61-2.87 (2H, m), 3.16-3.28 (1H, m), 3.27-3.31 (1H, m), 3.36-3.39(2H, m), 4.05-4.15 (4H, m), 4.99 (1H, m), 7.19-7.22 (m, 1H), 7.27-7.30 (2H, m), 7.36-7.38 (2H, m); ^{13}C-NMR δ 0.02, 16.4 (d, $^{3}J_{P\text{-}C}$ = 4.3 Hz), 36.7, 38.9, 47.2 (d, $^{2}J_{P\text{-}C}$ = 8.7 Hz), 61.6 (d, $^{2}J_{P\text{-}C}$ = 5.7 Hz), 73.7, 109.8 (d, $^{1}J_{P\text{-}C}$ = 189.8 Hz), 125.8, 126.8, 127.9, 145.0, 160.5 (d, $^{2}J_{P\text{-}C}$ = 14.8 Hz); HRMS(M^{+}- $C_{10}H_{15}OSi$) Calcd for $C_9H_{16}O_3PS_2$ 267.0278, Found 267.0319; (M^{+}- $C_9H_{16}O_3PS_2$) Calcd for $C_{10}H_{15}OSi$ 179.0892, Found 179.0875.



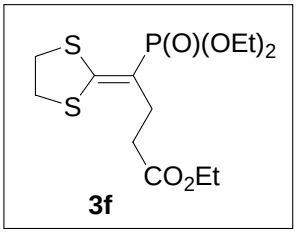
3d

Diethyl (*E*)-2-ethoxy-1-(2'-phenylthioethyl)-vinylphosphonate (3d): IR (neat) 742, 794, 1024, 1637, 2981, 3448 cm^{-1}; ^{1}H-NMR δ 1.29-1.33 (9H, m), 2.42-2.51 (2H, m), 2.99-3.03 (2H, m), 4.00-4.10 (6H, m), 7.04 (1H, m, $^{3}J_{P\text{-}H}$ = 10.5 Hz), 7.15 (1H, t, J = 7.5 Hz), 7.25-7.29 (2H, t, J = 8.4 Hz), 7.35-7.37 (2H, d, J = 7.9 Hz); ^{13}C-NMR δ 15.3, 16.3 (d, $^{3}J_{P\text{-}C}$ = 6.5 Hz), 24.5, 30.9, 61.3 (d, $^{2}J_{P\text{-}C}$ = 5.2 Hz), 69.8, 101.8 (d, $^{1}J_{P\text{-}C}$ = 194.6 Hz), 125.3, 128.1, 128.7, 136.6, 159.6 (d, $^{2}J_{P\text{-}C}$ = 28.8 Hz); HRMS(M^{+}) Calcd for $C_{16}H_{25}O_4PS$ 344.1211, Found 344.1198.



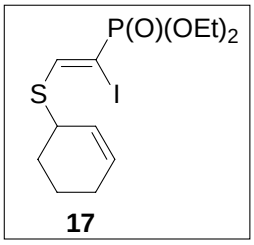
3e

Diethyl 1-(2'-phenylthioethyl)-vinylphosphonate (3e): IR (neat) 798, 1022, 1259, 1438, 1583, 2967, 3455 cm^{-1}; ^{1}H-NMR δ 1.31 (6H, t), 2.54-2.61 (2H, m), 3.10-3.14 (2H, m), 4.03-4.12 (4H, m), 5.82 (1H, dd, $^{3}J_{H-P}$ = 47.9 Hz, J = 1.4 Hz), 6.11 (1H, dd, $^{3}J_{H-P}$ = 22.5 Hz, J = 0.5 Hz), 7.19 (1H, m), 7.27-7.31 (4H, m); ^{13}C-NMR δ 16.3 (d, $^{3}J_{P-C}$ = 6.4 Hz), 32.1 (d, $^{3}J_{P-C}$ = 4.5 Hz), 32.5 (d, $^{2}J_{P-C}$ = 11.3 Hz), 62.0 (d, $^{2}J_{P-C}$ = 5.8 Hz), 126.0, 128.4 (d, $^{1}J_{P-C}$ = 164.5 Hz), 128.9, 129.2, 131.0 (d, $^{2}J_{P-C}$ = 9.3 Hz), 133.0; HRMS(M^{+}) Calcd for $C_{14}H_{21}O_3PS$ 300.0949, Found 300.0950.



3f

Ethyl 4-(diethylphosphono)-4-(1,3-dithiolan-2-ylidene)butyrate (3f): ^{1}H-NMR δ 1.21-1.26 (3H, m), 1.30 (6H, t, J = 7.2 Hz), 2.48-2.53 (2H, m), 2.63-2.71 (2H, m), 3.34-3.36 (2H, m), 3.38-3.39 (2H, m), 4.01-4.13 [(P(O)(OCH_2CH$_3$)$_2$, 4H, m), (CO_2CH_2CH$_3$, 2H, m)]; ^{13}C-NMR δ 14.2, 16.3 (d, $^{3}J_{P-C}$ = 6.5 Hz), 30.7 (d, $^{2}J_{P-C}$ = 8.1 Hz), 32.3, 36.9, 39.1, 60.4, 61.7 (d, $^{2}J_{P-C}$ = 5.2 Hz), 110.3 (d, $^{1}J_{P-C}$ = 189.2 Hz), 159.2 (d, $^{2}J_{P-C}$ = 15.2 Hz), 172.8; HRMS(M^{+}) Calcd for $C_{13}H_{23}O_5PS_2$ 354.0725, Found 354.0738.

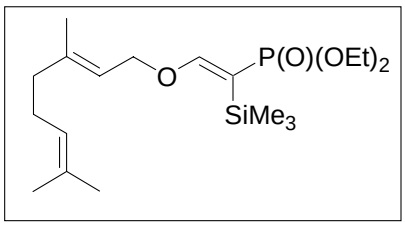


17

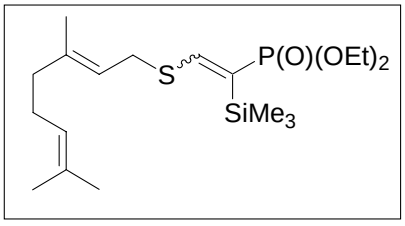
Diethyl (*Z*)-2-cyclohexenylthio-1-iodovinylphosphonate (17): The reaction of lithium 2-cyclohexene-1-thiolate (4.46 mmol) with diethyl (*E*)-2-ethoxy-1-(trimethylsilyl)vinylphosphonate (1.04 g, 3.72 mmol) was carried out following procedures described above to give (*E*)- and (*Z*)-2-cyclohexenylthio-1-(trimethylsilyl)vinylphosphonates in 596 mg (46 %) and 216 mg (17 %) yields, respectively, as colorless oil. **(*E*)-isomer:** R_f0.53 (AcOEt); ^{1}H-NMR δ 0.27 (9H, s) 1.31 (6H, t, J = 7.1 Hz), 1.50-1.59 (1H, m), 1.75-1.90 (2H, m), 2.02-2.07 (3H, m), 3.74-3.75 (1H, m), 3.99-4.06 (4H, m), 5.69-5.73 (1H, m), 5.88-5.92 (1H, m), 8.22 (1H, d, $^{3}J_{P-H}$ = 31.7 Hz); ^{13}C-NMR δ -0.7, 16.3, 19.1, 24.6, 30.3, 45.1, 61.1 (d, $^{2}J_{P-C}$ = 5.1 Hz), 121.9 (d, $^{1}J_{P-C}$ = 138.6 Hz), 126.0, 131.6, 160.9; **(*Z*)-isomer:** R_f0.65 (AcOEt): The **(*E*)-isomer** (552 mg, 1.58 mmol) was treated with NaI (355 mg, 2.37 mmol) and *N*-chlorosuccinimide (317 mg, 2.37 mmol) according to similar procedures described for **1g** to give **17** as yellow crystals. Yield

595 mg (94 %). ^{1}H-NMR δ 1.37 (6H, t, J = 7.1 Hz), 1.60-1.71 (1H, m), 1.83-1.89 (3H, m), 2.05-2.11 (2H, m), 3.89-3.90 (1H, m), 4.05-4.15 (4H, m), 5.71-5.74 (1H, m), 5.92-5.95 (1H, m), 8.22 (1H, d, $^{3}J_{P-H}$ = 14.7 Hz); ^{13}C-NMR δ 16.2 (d, $^{3}J_{P-C}$ = 7.9 Hz), 19.2, 24.5, 30.6, 43.6, 62.7, 77.8 (d, $^{1}J_{P-C}$ = 197.9 Hz), 125.8, 132.3, 156.1; HRMS(M^{+}) Calcd for $C_{12}H_{20}IO_3PS$ 401.9915, Found 401.9912.

General procedure for the synthesis of diethyl 2-geranyloxy-1-(trimethylsilyl)-vinylphosphonate and diethyl 2-geranylthio-1-(trimethylsilyl)-vinylphosphonate: A solution of RLi, generated in situ from RH (R = geranyloxy or geranylthio, 3.6 mmol) in THF (18 mL) and *n*-BuLi (3.6 mmol) at –78 ^{o}C for 1.0 h, was added dropwise *via cannula* to a solution of diethyl (*E*)-2-ethoxy-1-(trimethylsilyl)vinylphosphonate (841 mg, 3.0 mmol) in THF (12 mL). After similar workup, the residue was chromatographed on silica gel (AcOEt : hexane = 1:1) to give (*E*)-2-geranyloxy-1-(trimethylsilyl)-vinylphosphonate and a mixture of (*E*)- and (*Z*)-2-geranylthio-1-(trimethylsilyl)-vinylphosphonates, respectively, as colorless oil.



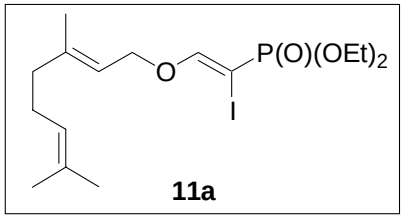
Diethyl (*E*)-2-geranyloxy-1-(trimethylsilyl)-vinylphosphonate : Yield 40 %. ^{1}H-NMR δ 0.17 (9H, s), 1.23 (6H, t, J = 7.1 Hz), 1.60 (3H, s), 1.68 (6H, s), 2.03-2.11 (4H, m), 3.95-4.08 (4H, m), 4.48 (2H, d, J = 6.9 Hz), 5.06-5.09 (1H, m), 5.32-5.36 (1H, m), 7.49 (1H, d, $^{3}J_{P-H}$ = 16.4 Hz); ^{13}C-NMR δ -0.38, 16.2, 16.3 (d, $^{3}J_{P-C}$ = 7.8 Hz), 16.5, 25.6, 26.1, 39.4, 60.7 (d, $^{2}J_{P-C}$ = 5.1 Hz), 70.3, 98.7 (d, $^{1}J_{P-C}$ = 155.3 Hz), 118.8, 123.5 (d, $^{2}J_{P-C}$ = 13.9 Hz), 131.8, 142.4, 170.5; HRMS(M^{+}) Calcd for $C_{19}H_{37}O_4PSi$ 388.2199, Found 388.2183.



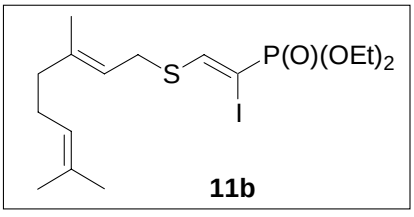
The mixture of diethyl (*E*)- and (*Z*)- 2-geranylthio-1-(trimethylsilyl)-vinylphosphonate: Yield 56 % (*E*/*Z* = 74/26). ^{1}H-NMR δ 0.16 (33/100 × 9H, s, for ***Z* isomer**), 0.26 (9H, s, for ***E* isomer**), 1.26-1.34 [(6 + 33/100 × 6) H, m, for ***Z* isomer** and ***E* isomer**], 1.60 [(3 + 33/100 × 3) H, s, for ***Z* isomer** and ***E* isomer**], 1.67 [(3 + 33/100 × 3) H, s, for ***Z***

isomer and ***E* isomer**], 1.71 [(3 + 33/100 × 3) H, s, for ***Z* isomer** and ***E* isomer**], 2.04-2.08 [(4 + 33/100 × 4) H, s, for ***Z* isomer** and ***E* isomer**], 3.43 (33/100 × 2H, d, J = 7.9 Hz, for ***Z* isomer**), 3.52 (2H, d, J = 7.8 Hz, for ***E* isomer**), 3.97-4.09 [(4 + 33/100 × 4) H, m, for ***Z* isomer** and ***E* isomer**], 5.07 [(1 + 33/100) H, t, for ***Z* isomer** and ***E* isomer**], 5.29 [(1 + 33/100) H, t, for ***Z* isomer** and ***E* isomer**], 7.36 (33/100 × 1H, d, $^{3}J_{P\text{-}H}$ = 56.3 Hz, ***Z* isomer**), 8.08 (1H, dd, $^{3}J_{P\text{-}H}$ = 31.8 Hz, for ***E* isomer**); ^{13}C-NMR δ -0.75, 16.3, 17.7 (d, $^{3}J_{P\text{-}C}$ = 5.3 Hz), 25.6, 26.4, 26.5, 32.5, 33.0, 39.5, 61.2 (d, $^{2}J_{P\text{-}C}$ = 5.5 Hz), 61.5, 118.6, 118.7, 119.6, 121.7 (d, $^{1}J_{P\text{-}C}$ = 141.4 Hz), 123.7, 131.7, 131.8, 140.2, 140.9; HRMS(M^{+}) Calcd for $C_{19}H_{37}O_3PSSi$ 404.1970, Found 404.1946.

General procedure for the synthesis of diethyl 2-geranyloxy-1-iodovinylphosphonate (11a) and diethyl 2-geranylthio-1-iodovinylphosphonate (11b): To a solution of the vinylsilanes (1.16 mmol) prepared above in MeCN (8 mL) at room temperature was added NaI (1.74 mmol) and *N*-chlorosuccinimide (1.74 mmol). The mixture was stirred for 2 days at this temperature. After similar workup, the residue was chromatographed on silica gel (AcOEt) to give **11a,b** and recovered starting materials.



11a



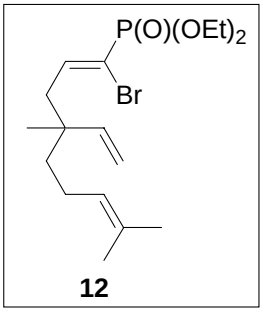
11b

Diethyl 2-geranyloxy-1-iodovinylphosphonate (11a): Yield 16 %. ^{1}H-NMR δ 1.20-1.23 (6H, m), 1.47 (3H, s), 1.55 (3H, s), 1.59 (3H, s), 1.91-1.98 (4H, m), 3.88-4.00 (4H, m), 4.52 (d, J = 7.0 Hz), 4.94 (1H, t, J = 1.4 Hz), 5.26 (1H, t, J = 1.1 Hz), 7.25 (1H, d, $^{3}J_{P\text{-}H}$ = 7.6 Hz); ^{13}C-NMR δ 16.2, 16.7, 17.5, 25.6, 26.1, 55.3 (d, $^{1}J_{P\text{-}C}$ = 205.9 Hz), 62.3 (d, $^{2}J_{P\text{-}C}$ = 4.8 Hz), 71.0, 118.1, 123.4, 132.0, 143.7, 163.8; HRMS(M^{+}) Calcd for $C_{16}H_{28}IO_4P$ 442.0770, Found 442.0820.

Diethyl 2-geranylthio-1-iodovinylphosphonate (11b): Yield 23 %. ^{1}H-NMR δ 1.32-1.36 (6H, m), 1.60 (3H, s), 1.68 (3H, s), 1.72 (3H, s), 2.06-2.10 (4H, m), 3.59 (d, J = 7.9 Hz), 4.03-4.12 (4H, m), 5.07 (1H, t), 5.31 (1H, t), 8.13 (1H, d, $^{3}J_{P\text{-}H}$ = 14.7 Hz); ^{13}C-NMR δ 16.2 (d, $^{3}J_{P\text{-}C}$ = 5.0 Hz), 17.7, 25.6, 26.4,

31.4, 39.5, 62.7 (d, $^{2}J_{P\text{-}C}$ = 4.9 Hz), 77.9 (d, $^{1}J_{P\text{-}C}$ = 196.8 Hz), 118.5, 123.4, 131.9, 141.6, 156.7 (d, $^{2}J_{P\text{-}C}$ = 17.4 Hz); HRMS(M^{+}) Calcd for $C_{16}H_{28}IO_3PS$ 458.0542, Found 458.0558.

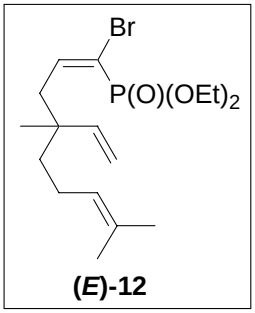
Diethyl 1-bromo-4,8-dimethyl-4-vinyl-nona-1,7-dienylphosphonate (12): This derivative was prepared following similar procedures described for **1f** by using tetraethyl methylenediphosphonate (493 mg, 1.71 mmol), NBS (335 mg, 1.88 mmol) and 3,7-dimethyl-3-vinyl-6-octenal[3] (309 mg, 1.71 mmol) in 224 mg (33 %) yield together with (*E*)-**12** (256 mg, 38 %).



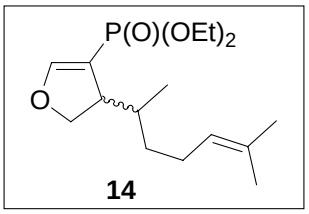
12

Diethyl 1-bromo-4,8-dimethyl-4-vinyl-nona-1,7-dienylphosphonate (12): ^{1}H-NMR δ 1.03 (3H, s), 1.31-1.37 (8H, m), 1.56 (3H, s), 1.65 (3H, s), 1.80-1.92 (2H, m), 2.34-2.37 (2H, ddd, $^{4}J_{P\text{-}H}$ = 6.9 Hz, *J* = 3.0 Hz), 4.04-4.12 (4H, m), 4.94 (1H, dd, *J* = 17.5 Hz), 5.02-5.05 (2H, m), 5.71 (1H, dd, *J* = 17.5 Hz), 7.08 (1H, td, $^{3}J_{P\text{-}H}$ = 14.4 Hz); ^{13}C-NMR δ 16.2 (d, $^{3}J_{P\text{-}C}$ = 6.5 Hz), 17.6, 22.8, 25.6, 40.0, 40.8, 42.8 (d, $^{3}J_{P\text{-}C}$ = 12.9 Hz), 62.9 (d, $^{2}J_{P\text{-}C}$ = 5.3 Hz), 112.9, 114.0 (d, $^{1}J_{P\text{-}C}$ = 204.9 Hz), 124.3, 131.4, 145.3, 147.4 (d, $^{2}J_{P\text{-}C}$ = 15.0 Hz); HRMS(M^{+}) Calcd for $C_{17}H_{30}BrO_3P$ 392.1116, Found 392.1077, 394.1048.

Diethyl (*E*)-1-bromo-4,8-dimethyl-4-vinyl-nona-1,7-dienylphosphonate ((*E*)-12): ^{1}H-NMR δ 1.00 (3H, s), 1.31-1.36 (8H, m), 1.55 (3H, s), 1.64 (3H, m), 1.86-1.89 (2H, m), 2.56-2.59 (1H, m), 2.72-2.78 (1H, m), 4.07-4.15 (4H, m), 4.94 (1H, dd, *J* = 17.5 Hz), 5.03-5.08 (2H, m), 5.70 (1H, dd, *J* = 17.6 Hz), 6.88 (1H, td, $^{3}J_{P\text{-}H}$ = 39.9 Hz); ^{13}C-NMR δ 16.2 (d, $^{3}J_{P\text{-}C}$ = 6.6 Hz), 17.6, 22.2, 22.7, 25.7, 40.0, 40.9, 41.9, 62.8 (d, $^{2}J_{P\text{-}C}$ = 3.8 Hz), 112.0 (d, $^{1}J_{P\text{-}C}$ = 243.6 Hz), 113.2, 124.5, 131.4, 145.3, 152.2 (d, $^{2}J_{P\text{-}C}$ = 16.3 Hz); HRMS(M^{+}) Calcd for $C_{17}H_{30}BrO_3P$ 392.1116, Found 392.1095, 394.1121.

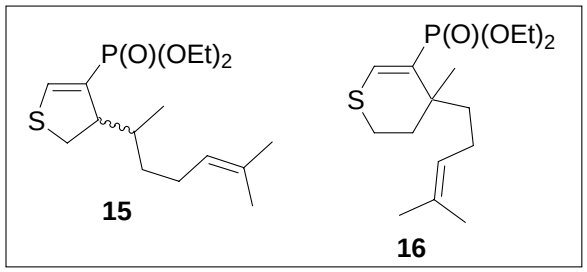


(*E*)-12



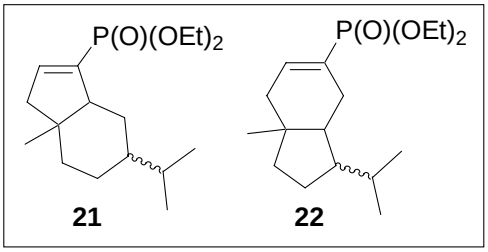
14

The mixture of 3-diethylphosphono-4α-and-4β-(6'-methyl-5'-hepten-2'-yl)-4,5-dihydrofurans (14): ^{13}C-NMR (125.65 MHz) δ 13.1, 13.6, 16.3 (d, $^{3}J_{P\text{-}C}$ = 5.0 Hz), 16.4 (d, $^{3}J_{P\text{-}C}$ = 3.8 Hz), 17.5, 17.6, 17.6, 17.7, 25.7, 25.9, 26.1, 26.9, 27.9, 30.2, 33.0, 34.0, 35.4, 47.2 (d, $^{2}J_{P\text{-}C}$ = 11.3 Hz), 48.8 (d, $^{2}J_{P\text{-}C}$ = 8.8 Hz), 61.4 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 61.6 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 73.1 (d, $^{3}J_{P\text{-}C}$ = 12.6 Hz), 74.4 (d, $^{3}J_{P\text{-}C}$ = 12.6 Hz), 103.4 (d, $^{1}J_{P\text{-}C}$ = 213.6 Hz), 103.8 (d, $^{1}J_{P\text{-}C}$ = 213.6 Hz), 124.2, 124.6, 131.2, 131.6, 159.1 (d, $^{2}J_{P\text{-}C}$ = 27.6 Hz), 159.7 (d, $^{2}J_{P\text{-}C}$ = 28.9 Hz); HRMS(M^{+}) Calcd for $C_{16}H_{29}O_4P$ 316.1804, Found 316.1765.



15 **16**

The mixture of 3-diethylphosphono-4α-and-4β-(6'-methyl-5'-hepten-2'-yl)-4,5-dihydrothiophenes (15) and 3-diethylphosphono-4-methyl-4-(4'-methyl-3'-penten-1'-yl)-4,5-dihydro-2*H*-thiopyran (16): 4:1 mixture of **15** and **16**. ^{13}C-NMR (125.65 MHz) δ 13.5, 13.6, 16.3 (d, $^{3}J_{P\text{-}C}$ = 5.0 Hz), 16.4 (d, $^{2}J_{P\text{-}C}$ = 7.5 Hz), 17.7, 18.1, 21.8, 21.9, 22.0, 23.7, 23.9, 25.4, 25.6, 25.7, 25.9, 26.4, 26.9, 27.8, 27.9, 29.4, 29.9, 30.5, 33.0 (d, $^{3}J_{P\text{-}C}$ = 16.3 Hz), 33.9 (d, $^{3}J_{P\text{-}C}$ = 13.8 Hz), 34.5, 35.2, 35.7, 36.9, 38.0, 45.4, 47.7, 47.8, 49.6, 53.3 (d, $^{2}J_{P\text{-}C}$ = 15.1 Hz), 55.4 (d, $^{2}J_{P\text{-}C}$ = 15.1 Hz), 61.6 (d, $^{2}J_{P\text{-}C}$ = 6.3 Hz), 61.9 (d, $^{2}J_{P\text{-}C}$ = 6.3 Hz), 123.7, 124.3, 124.7, 125.3 (d, $^{1}J_{P\text{-}C}$ = 191.0 Hz), 125.4 (d, $^{1}J_{P\text{-}C}$ = 191.0 Hz), 131.1, 131.6, 137.4 (d, $^{2}J_{P\text{-}C}$ = 15.1 Hz), 145.7 (d, $^{2}J_{P\text{-}C}$ = 17.6 Hz), 146.1 (d, $^{2}J_{P\text{-}C}$ = 18.8 Hz): HRMS(M^{+}) Calcd for $C_{16}H_{29}O_3PS$ 332.1575, Found 332.1554.



21 **22**

The mixture of 7-diethylphosphono-4-isopropyl-1-methyl-bicyclo[4.3.0]non-7-ene (21) and 4-diethylphosphono-7-isopropyl-1-methyl-bicyclo[4.3.0]non-3-ene (22): A solution of α-bromovinylphosphonate **12** (79 mg, 0.20 mmol), Bu_3SnH (90 mg, 0.3 mmol) and AIBN (3.3 mg, 0.02 mmol) in benzene (4 mL) was heated under reflux for 2.5 h, until starting **12** was consumed completely. After removal of the solvent, the residue was chromatographed on preparative TLC (silica gel; AcOEt : hexane = 1 : 1) to give a difficultly separable

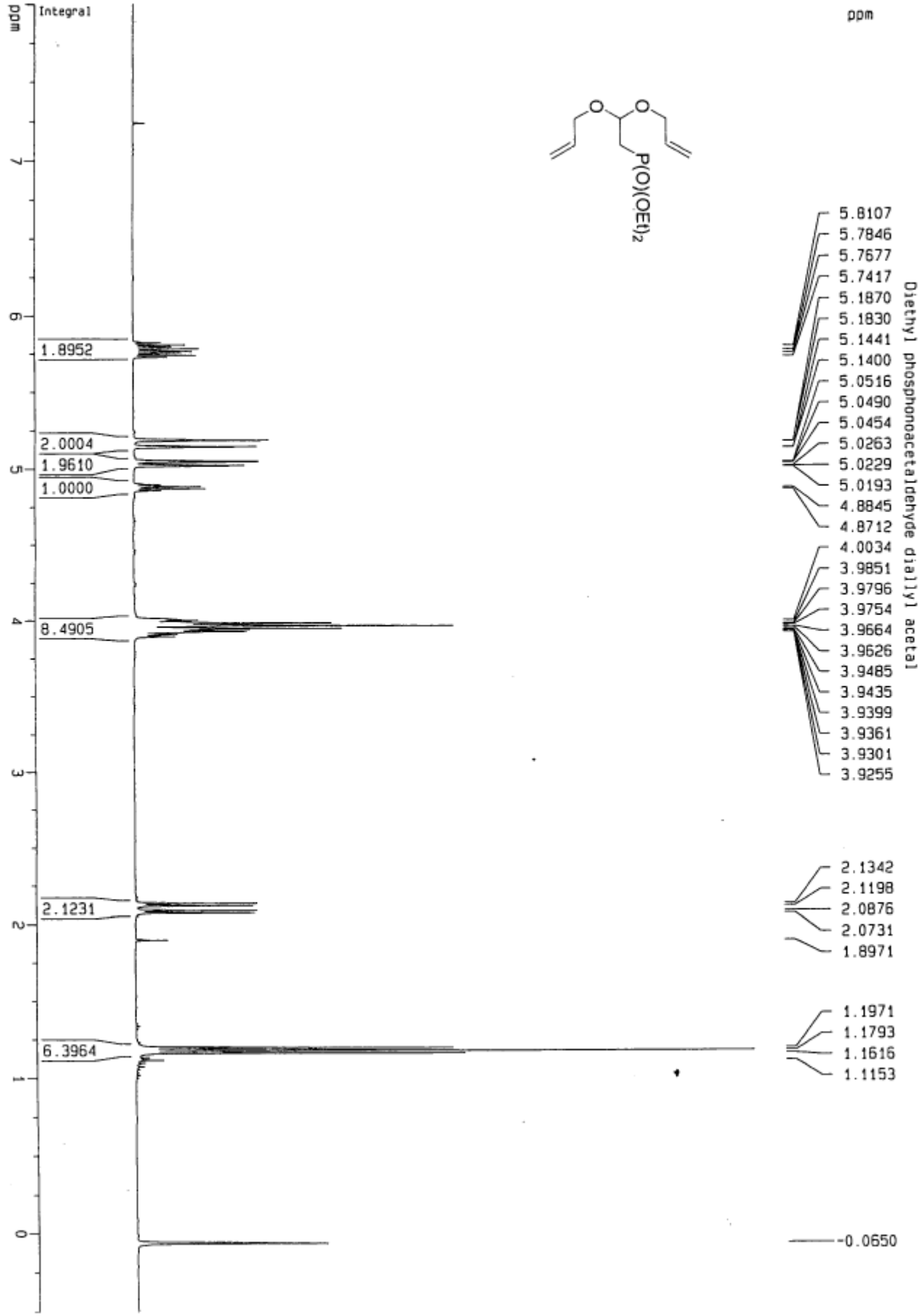
18:82 mixture of **21** and **22** in 58 mg (92 %) yield. colorless oil; ^{13}C-NMR (125.65 MHz, $CDCl_3$) δ 16.3 (d, $^3J_{P\text{-}C}$ = 4.1 Hz), 16.4 (d, $^3J_{P\text{-}C}$ = 4.0 Hz), 17.2, 17.9, 19.7, 19.8, 20.0, 22.0 (d, $^3J_{P\text{-}C}$ = 9.3 Hz), 22.0, 22.2, 22.3, 22.8, 23.9 (d, $^3J_{P\text{-}C}$ = 9.3 Hz), 24.8, 25.5, 25.9, 26.3, 26.5, 29.1, 29.4, 29.5, 30.3, 32.6, 32.8, 34.3, 34.9 (d, $^2J_{P\text{-}C}$ = 17.6 Hz), 35.4, 35.6, 36.5, 37.3 (d, $^2J_{P\text{-}C}$ = 17.6 Hz), 39.3, 39.4, 39.9, 41.4, 42.4 (d, $^3J_{P\text{-}C}$ = 18.6Hz), 43.0 (d, $^3J_{P\text{-}C}$ = 8.3 Hz), 47.3 (d, $^3J_{P\text{-}C}$ = 17.6 Hz), 48.0, 49.8, 52.3 (d, $^2J_{P\text{-}C}$ = 12.4 Hz), 54.8 (d, $^2J_{P\text{-}C}$ = 12.4 Hz), 61.4 (d, $^2J_{P\text{-}C}$ = 5.2 Hz), 61.4 (d, $^2J_{P\text{-}C}$ = 5.2 Hz), 125.0 (d, $^1J_{P\text{-}C}$ = 181.9 Hz), 126.1 (d, $^1J_{P\text{-}C}$ = 181.9 Hz), 142.1 (d, $^2J_{P\text{-}C}$ = 9.3 Hz), 142.7 (d, $^2J_{P\text{-}C}$ = 10.3 Hz), 146.2 (d, $^2J_{P\text{-}C}$ = 13.4 Hz), 148.5 (d, $^2J_{P\text{-}C}$ = 13.4 Hz); HRMS(M^+) Calcd for $C_{17}H_{31}O_3P$ 314.2011, Found 314.2037.

References

(1) Kouno, R.; Okauchi, T.; Nakamura, M.; Ichikawa, J.; Minami, T. *J. Org. Chem*. **1998**, *63*, 6239.

(2) Rengaraju, S.; Berlin, K. D., *J. Org. Chem*. **1972**, *37*, 3304.

(3) 3,7-dimethyl-3-vinyl-6-octenal was prepared in 57 % yield from methyl 3,7-dimethyl-3-vinyl-6-octenylcarboxylate and DIBAL-H in CH_2Cl_2 at -78 ℃ for 2h.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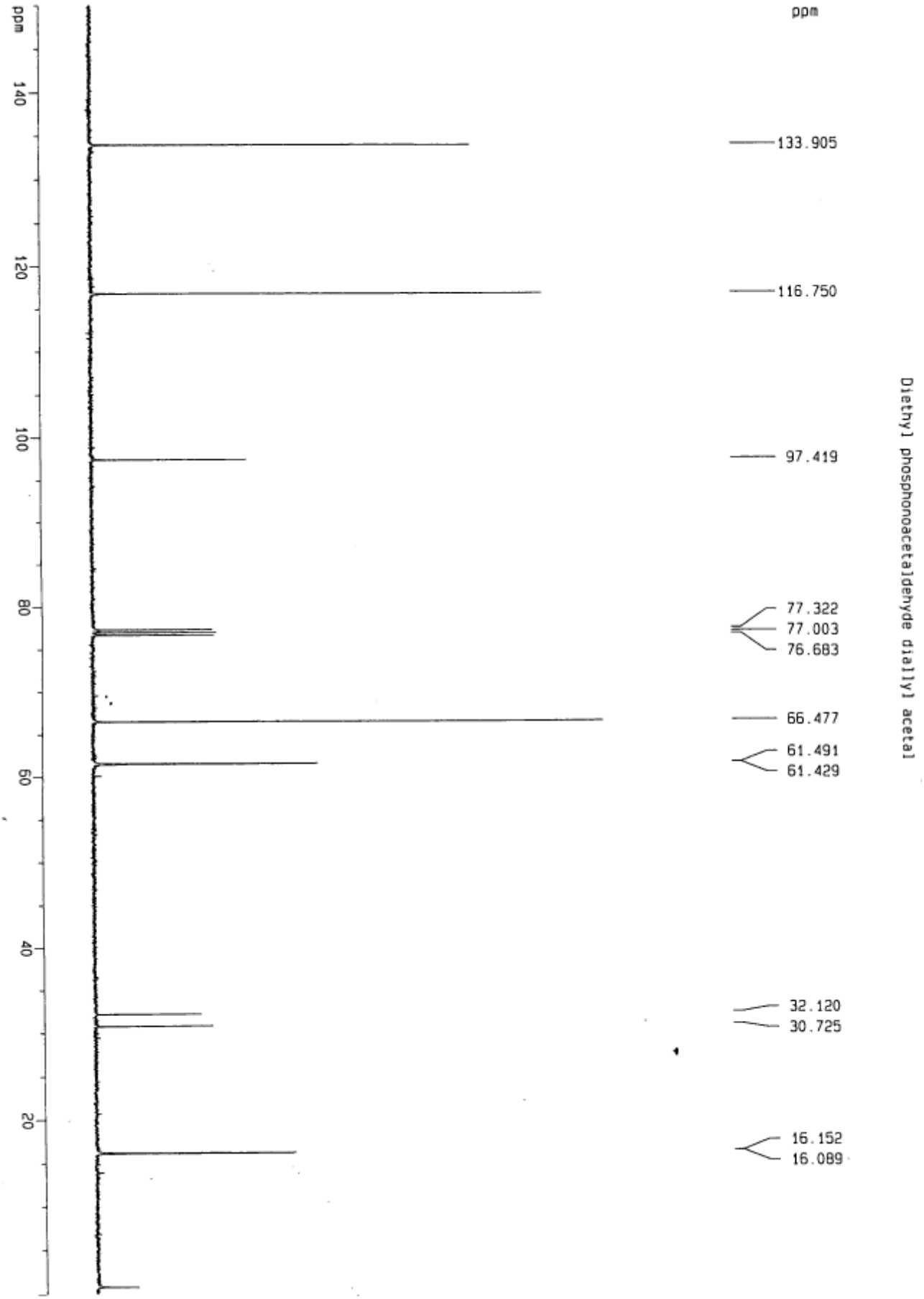
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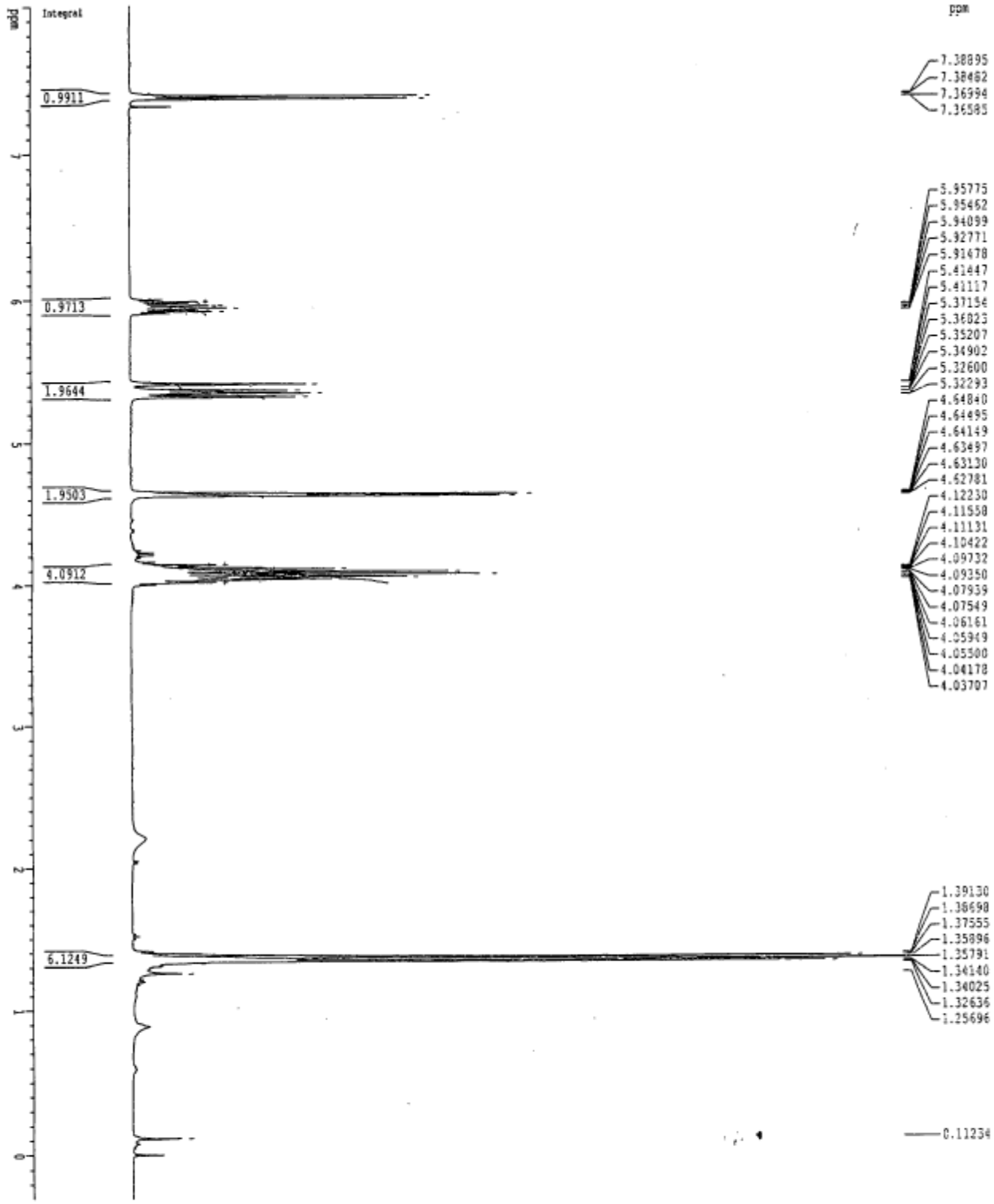
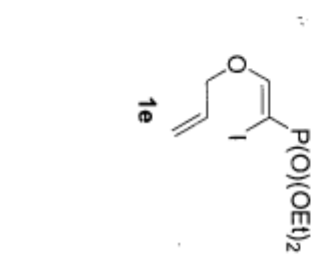
Diethyl phosphonoacetaldehyde diallyl acetal





1e

Current Data Parameters
NAME 03ppmo
EXPNO 254
PROCNO 1

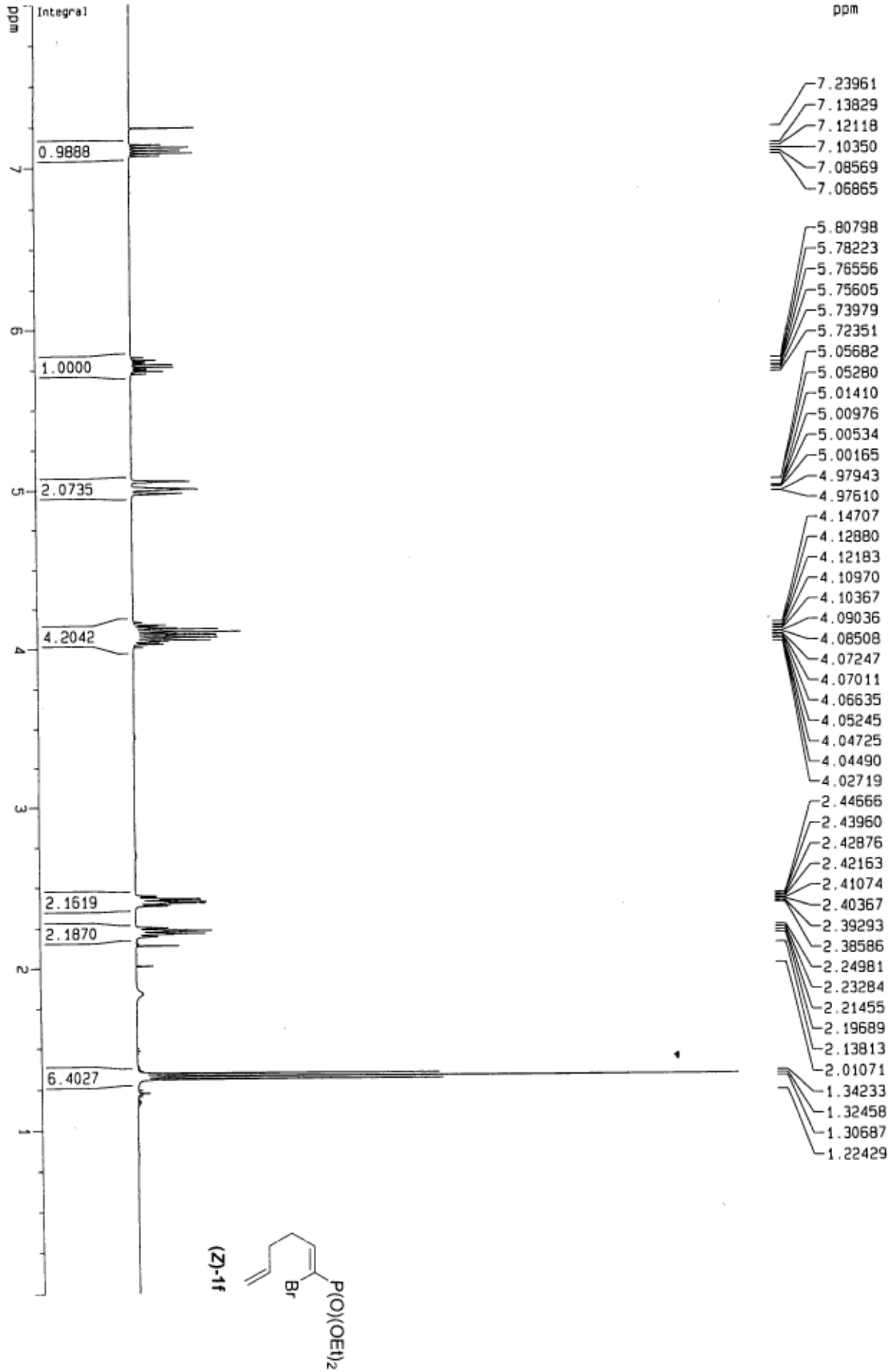
F2 - Acquisition Parameters
Date_ 20020515
Time / 1.48
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 64
DW 60.600 usec
DE 6.00 usec
TE 100.0 K
D1 1.00000000 sec

---------- CHANNEL f1 ----------
NUC1 1H
P1 7.90 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299878 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 8.000 ppm
F1P 3201.04 Hz
F1 -0.369 ppm
F2P -126.84 Hz
F2 0.27467 ppm/cm
PPMCM 110.70263 Hz/cm

```
Current Data Parameters
NAME                  03agenno
EXPNO                   2541
PROCNO                     1

F2 - Acquisition Parameters
Date_              20020515
Time                   2.07
INSTRUM              dpx400
PROBHD     5 mm BBO BB-
PULPROG              zgpdc30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        2
SWH               25062.656 Hz
FIDRES                0.382426 Hz
AQ                1.3074932 sec
RG                     6502
DW                   19.950 usec
DE                    6.00 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec

========== CHANNEL f1 ========
NUC1                    13C
P1                     7.90 usec
PL1                   -2.00 dB
SFO1          100.6237959 MHz

========== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   -6.00 dB
PL12                  15.50 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF            100.6127798 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
F1P                  234.041 ppm
F1                 23547.49 Hz
F2P                 -15.059 ppm
F2                 -1515.17 Hz
PPMCM                 8.30334 ppm/cm
HZCM               835.42188 Hz/cm
```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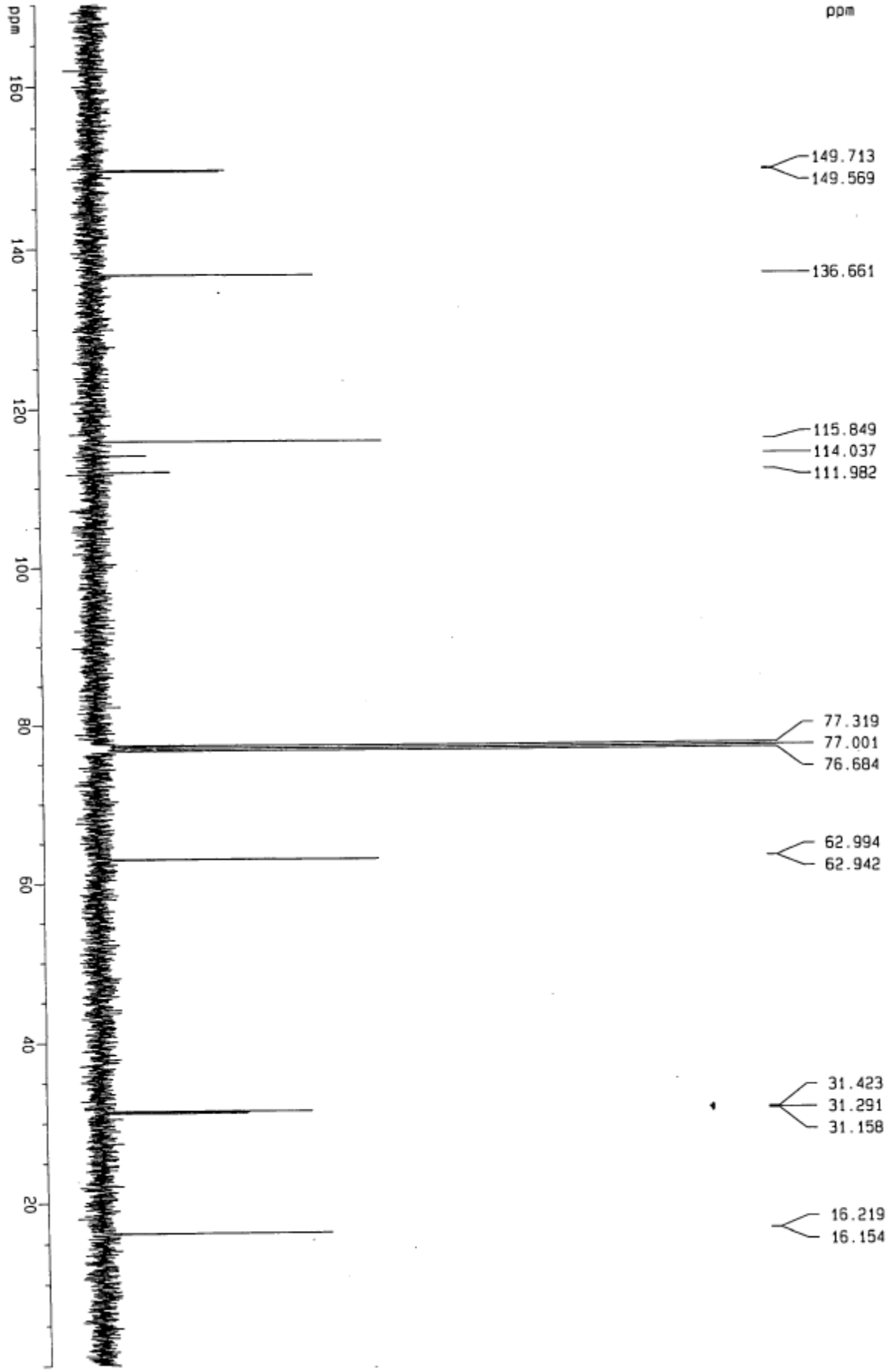
2.0735
4.2042
2.1619
2.1870
6.4027
ppm
7.23961
7.13829
7.12118
7.10350
7.08569
7.06865
5.80798
5.78223
5.76556
5.75605
5.73979
5.72351
5.05682
5.05280
5.01410
5.00976
5.00534
5.00165
4.97943
4.97610
4.14707
4.12880
4.12183
4.10970
4.10367
4.09036
4.08508
4.07247
4.07011
4.06635
4.05245
4.04725
4.04490
4.02719
2.44666
2.43960
2.42876
2.42163
2.41074
2.40367
2.39293
2.38586
2.24981
2.23284
2.21455
2.19689
2.13813
2.01071
1.34233
1.32458
1.30687
1.22429
(Z)-1f
Br
P(O)(OEt)2


ppm
160
140
120
100
80
60
40
20
ppm
149.713
149.569
136.661
115.849
114.037
111.982
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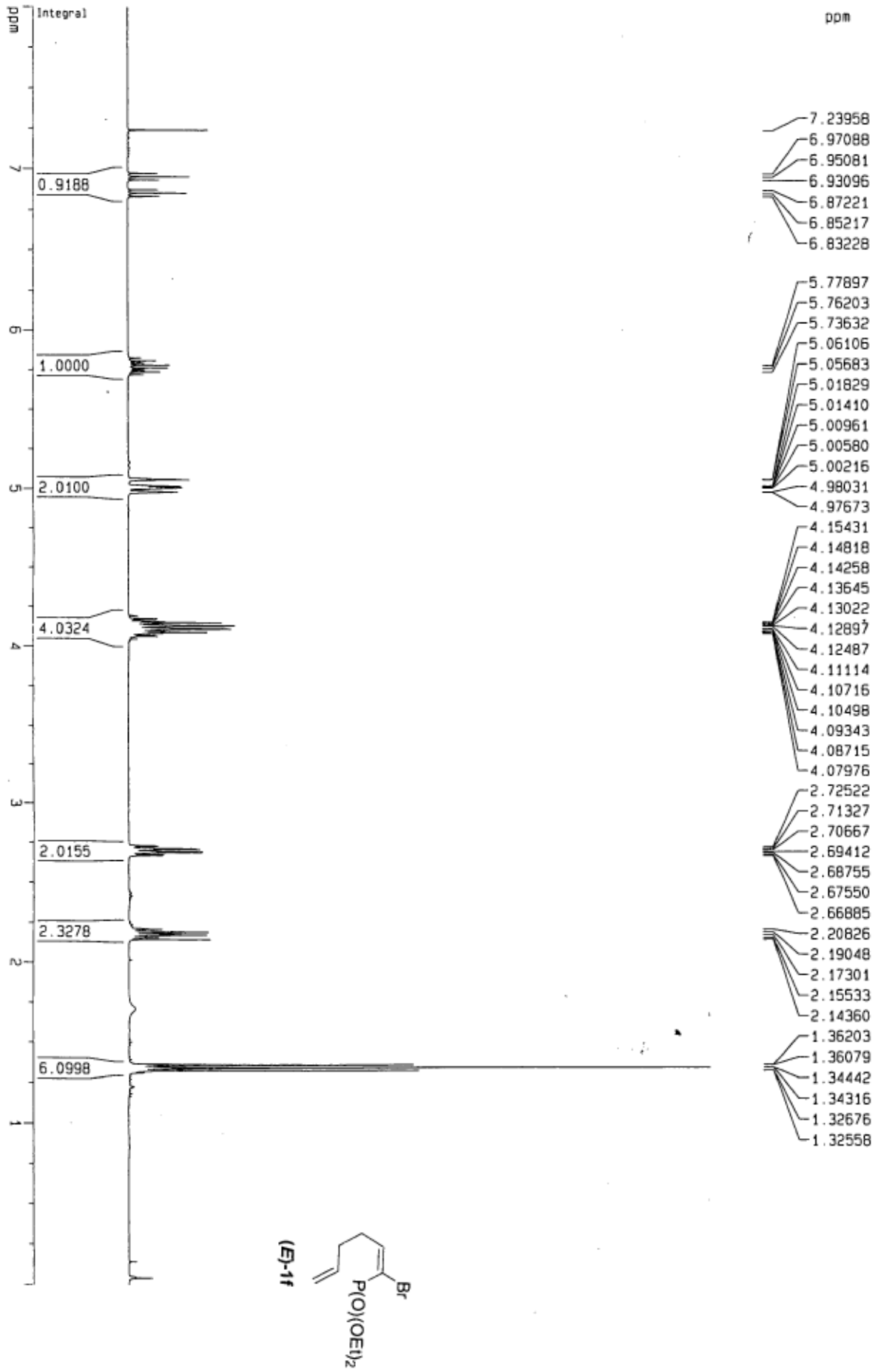
77.001
76.684
62.994
62.942
31.423
31.291
31.158
16.219
16.154


ppm
Integral
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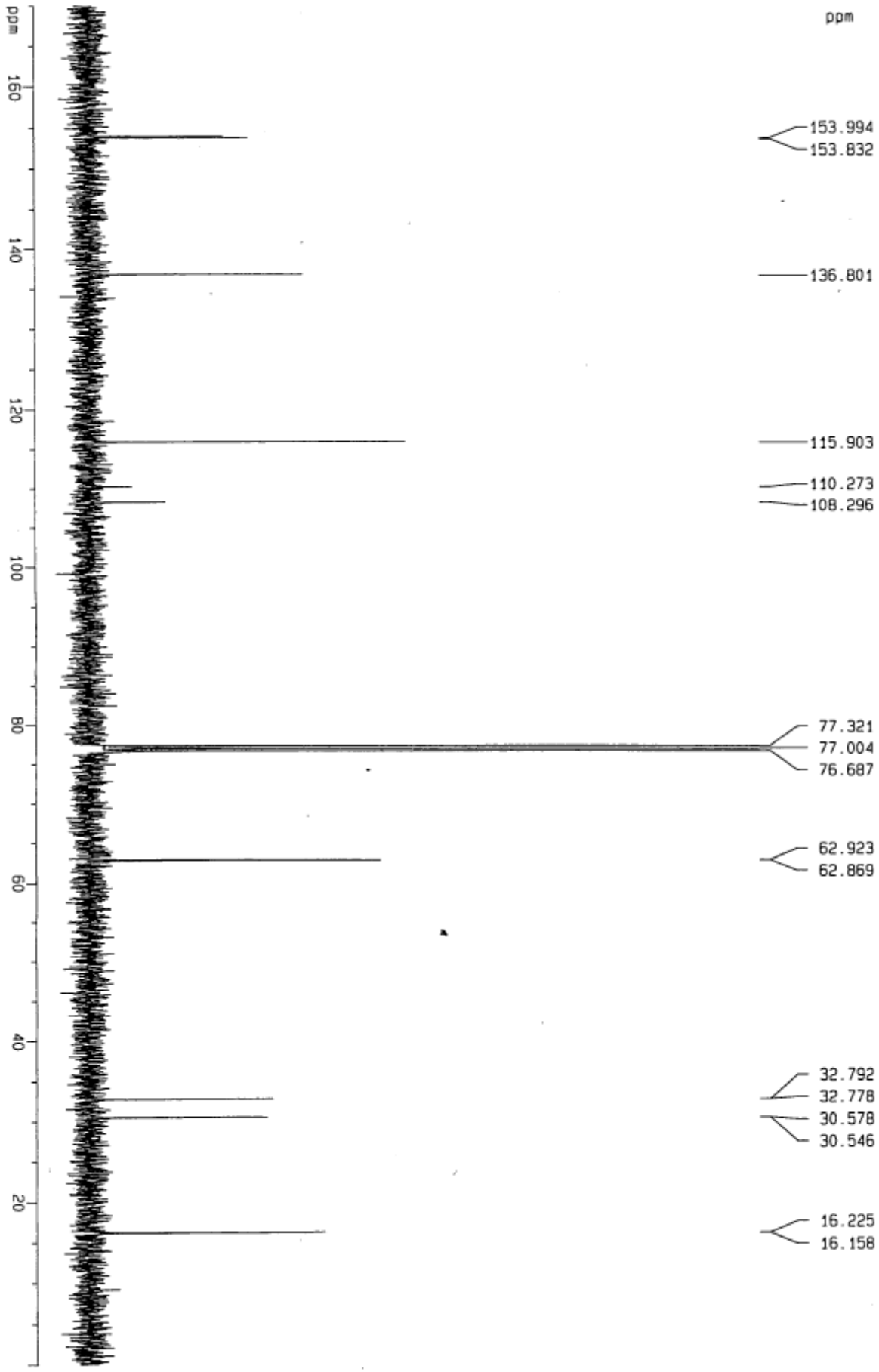
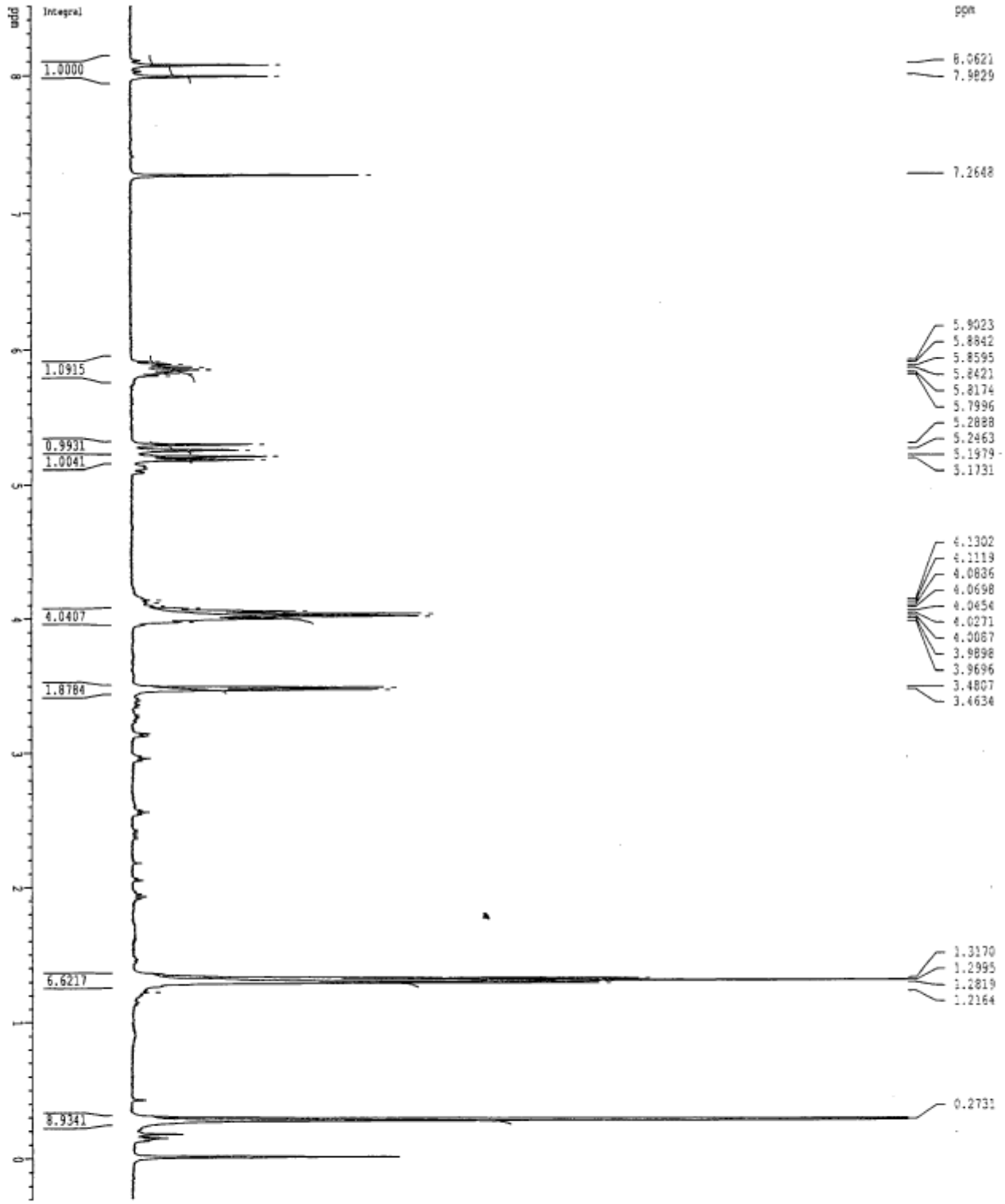
1.0000
2.0100
4.0324
2.0155
2.3278
6.0998
ppm
7.23958
6.97088
6.95081
6.93096
6.87221
6.85217
6.83228
5.77897
5.76203
5.73632
5.06106
5.05683
5.01829
5.01410
5.00961
5.00580
5.00216
4.98031
4.97673
4.15431
4.14818
4.14258
4.13645
4.13022
4.12897
4.12487
4.11114
4.10716
4.10498
4.09343
4.08715
4.07976
2.72522
2.71327
2.70667
2.69412
2.68755
2.67550
2.66885
2.20826
2.19048
2.17301
2.15533
2.14360
1.36203
1.36079
1.34442
1.34316
1.32676
1.32558
(E)-1f
Br
P(O)(OEt)2


ppm
160
140
120
100
80
60
40
20
ppm
153.994
153.832
136.801
115.903
110.273
108.296
77.321
77.004
76.687
62.923
62.869
32.792
32.778
30.578
30.546
16.225
16.158


Integral
ppm
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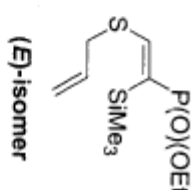
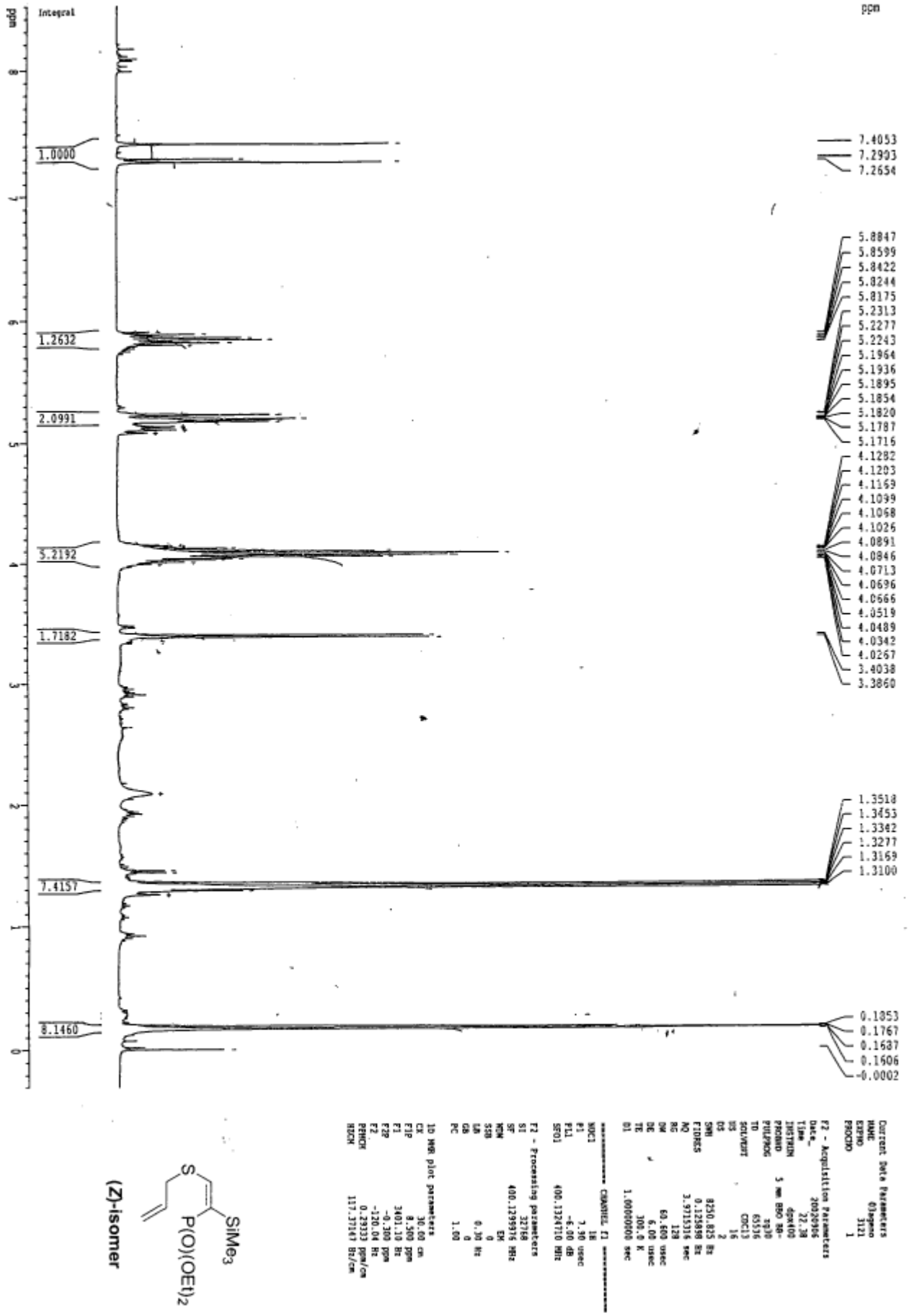
1.0915
0.9931
1.0041
4.0407
1.8784
6.6217
8.9341
8.0621
7.9829
7.2648
5.9023
5.8842
5.8595
5.8421
5.8174
5.7996
5.2888
5.2463
5.1979
5.1731
4.1302
4.1119
4.0836
4.0698
4.0454
4.0271
4.0087
3.9898
3.9696
3.4807
3.4634
1.3170
1.2995
1.2819
1.2164
0.2731
Current Data Parameters
NAME 03agemo
EXPNO 3491
PROCNO 1
F2 - Acquisition Parameters
Date_ 20021011
Time 11.13
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125899 Hz
AQ 3.9715316 sec
RG 512
DW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 7.90 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.23933 ppm/cm
HZCM 117.37147 Hz/cm

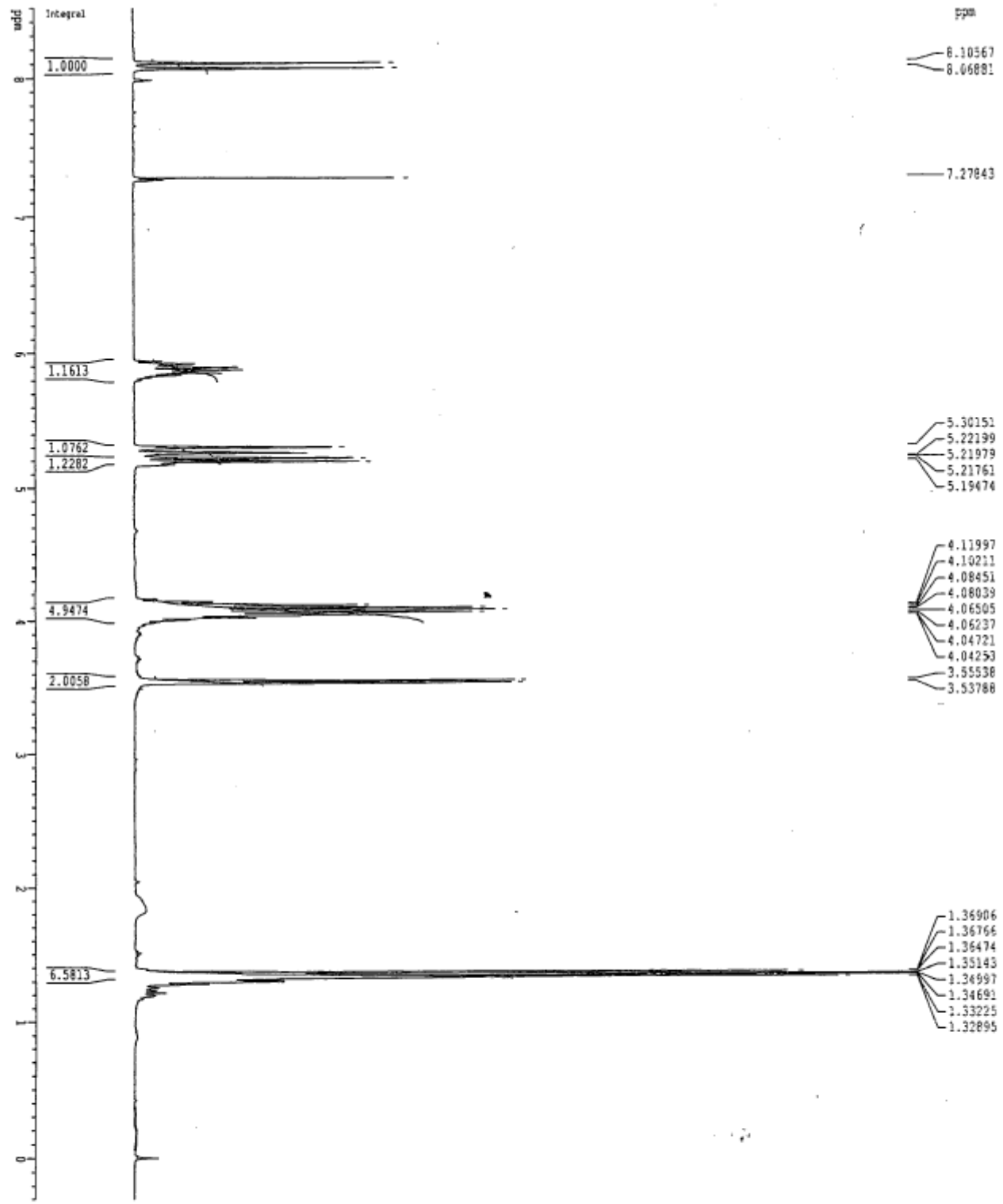

P(O)(OEt)2
S
SiMe3

(*E*)-isomer

```
Current Data Parameters
NAME                  03agono
EXPNO                    3123
PROCNO                      1

F2 - Acquisition Parameters
Date_              20020906
Time                   23.18
INSTRUM                dpx400
PROBHD     5 mm BBO BB-
PULPROG                zgdc30
TD                      65536
SOLVENT                 CDCl3
NS                        512
DS                          2
SWH                 25062.656 Hz
FIDRES                0.382426 Hz
AQ                    1.3074932 sec
RG                       6502
DW                     19.950 usec
DE                      6.00 usec
TE                     300.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                       7.90 usec
PL1                     -2.00 dB
SFO1          100.6237959 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                     -6.00 dB
PL12                    15.50 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF              100.6127752 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       30.00 cm
F1P                    234.086 ppm
F1                   23552.07 Hz
F2P                    -15.014 ppm
F2                   -1510.58 Hz
PPMCM                  8.30334 ppm/cm
HZCM                 835.42188 Hz/cm
```


ppm
Integral
1.0000
1.2632
2.0991
5.2192
1.7182
7.4157
8.1460
7.4053
7.2903
7.2654
5.8847
5.8599
5.8422
5.8244
5.8175
5.2313
5.2277
5.2243
5.1964
5.1936
5.1895
5.1854
5.1820
5.1787
5.1716
4.1282
4.1203
4.1169
4.1099
4.1068
4.1026
4.0891
4.0846
4.0713
4.0696
4.0666
4.0519
4.0489
4.0342
4.0267
3.4038
3.3860
1.3518
1.3453
1.3342
1.3277
1.3169
1.3100
0.1053
0.1767
0.1687
0.1606
-0.0002
Current Data Parameters
NAME 03sgmon
EXPNO 3121
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020906
Time 22.38
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 128
DW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299976 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.29333 ppm/cm
HZCM 117.37147 Hz/cm
SiMe3
P(O)(OEt)2
S
(Z)-isomer

```
Current Data Parameters
NAME                  03aqeno
EXPNO                    3403
PROCNO                      1

F2 - Acquisition Parameters
Date_              20021002
Time               13.32
INSTRUM                 dpx400
PROBHD     5 mm BBO BB-
PULPROG                 zgpdc30
TD                      65536
SOLVENT                 CDCl3
NS                        768
DS                          2
SWH                 25062.656 Hz
FIDRES                0.382426 Hz
AQ                    1.3074932 sec
RG                       6502
DW                    19.950 usec
DE                     6.00 usec
TE                     300.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     7.90 usec
PL1                   -2.00 dB
SFO1           100.6237959 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                       1H
PCPD2                 80.00 usec
PL2                   -6.00 dB
PL12                  15.50 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF             100.6127729 MHz
WDW                        EM
SSB                         0
LB                     1.00 Hz
GB                          0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
F1P                 234.109 ppm
F1                  23554.37 Hz
F2P                 -14.991 ppm
F2                  -1508.28 Hz
PPMCM                 8.30334 ppm/cm
HZCM                835.42188 Hz/cm
```


ppm
Integral
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1.2282
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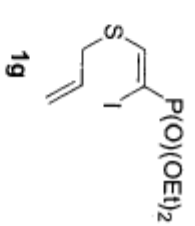
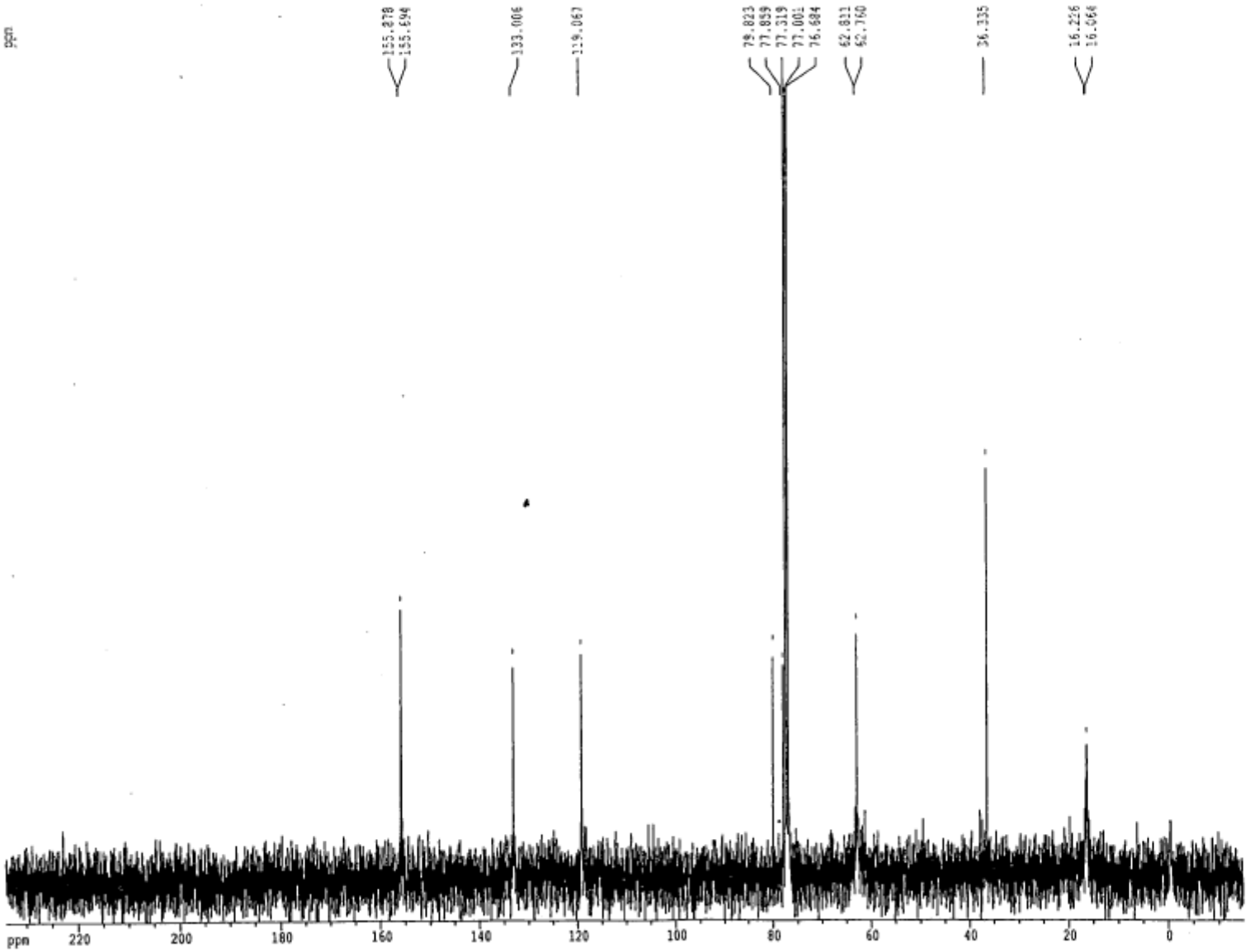
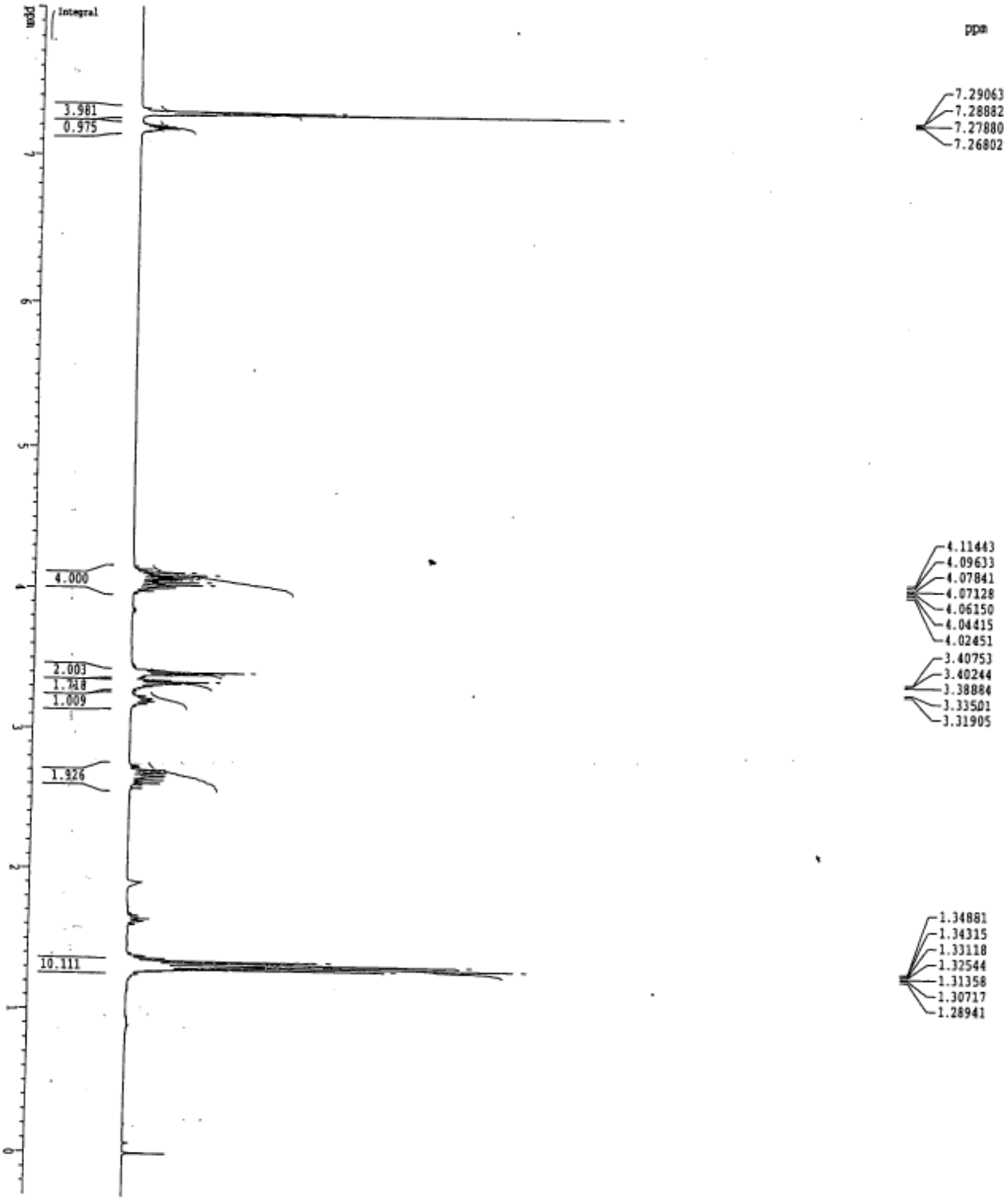
2.0058
6.5813
8.10567
8.06881
7.27843
5.30151
5.22199
5.21979
5.21761
5.19474
4.11997
4.10211
4.08451
4.08039
4.06505
4.06237
4.04721
4.04253
3.55538
3.53788
1.36906
1.36766
1.36474
1.35143
1.34997
1.34691
1.33225
1.32895


S
I
P(O)(OEt)2

1g




```
Current Data Parameters
NAME                  03ageno
EXPNO                    3411
PROCNO                      1

F2 - Acquisition Parameters
Date_              20021005
Time                   1.33
INSTRUM               dpx400
PROBHD      5 mm BBO BB-
PULPROG               zgdc30
TD                     65536
SOLVENT                CDCl3
NS                       512
DS                         2
SWH                25062.656 Hz
FIDRES             0.382426 Hz
AQ                 1.3074932 sec
RG                      3251
DW                    19.950 usec
DE                     6.00 usec
TE                    300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec

---------- CHANNEL f1 ---------
NUC1                      13C
P1                       7.90 usec
PL1                     -2.00 dB
SFO1               100.6237959 MHz

---------- CHANNEL f2 ---------
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -6.00 dB
PL12                    15.50 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                 100.6127729 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       30.00 cm
F1P                     234.109 ppm
F1                    23554.37 Hz
F2P                     -14.991 ppm
F2                    -1508.29 Hz
PPMCM                  8.30334 ppm/cm
HZCM                 835.42188 Hz/cm
```




```
Current Data Parameters
NAME                  Diagnos
EXPNO                    1311
PROCNO                      1

F2 - Acquisition Parameters
Date_              20111022
Time                   11.20
INSTRUM              dpx400
PROBHD     5 mm BBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      16
DS                       2
SWH                8250.825 Hz
FIDRES             0.125898 Hz
AQ                 3.9715116 sec
RG                     128
DW                  60.600 usec
DE                   6.00 usec
TE                 300.0 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.90 usec
PL1                 -6.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF                400.1300086 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    30.00 cm
F1P                 8.000 ppm
F1                3201.04 Hz
F2P                -0.300 ppm
F2                -120.04 Hz
PPMCM              0.27647 ppm/cm
HZCM              110.70264 Hz/cm
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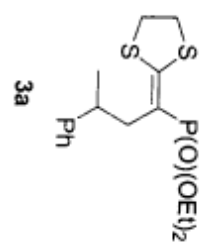
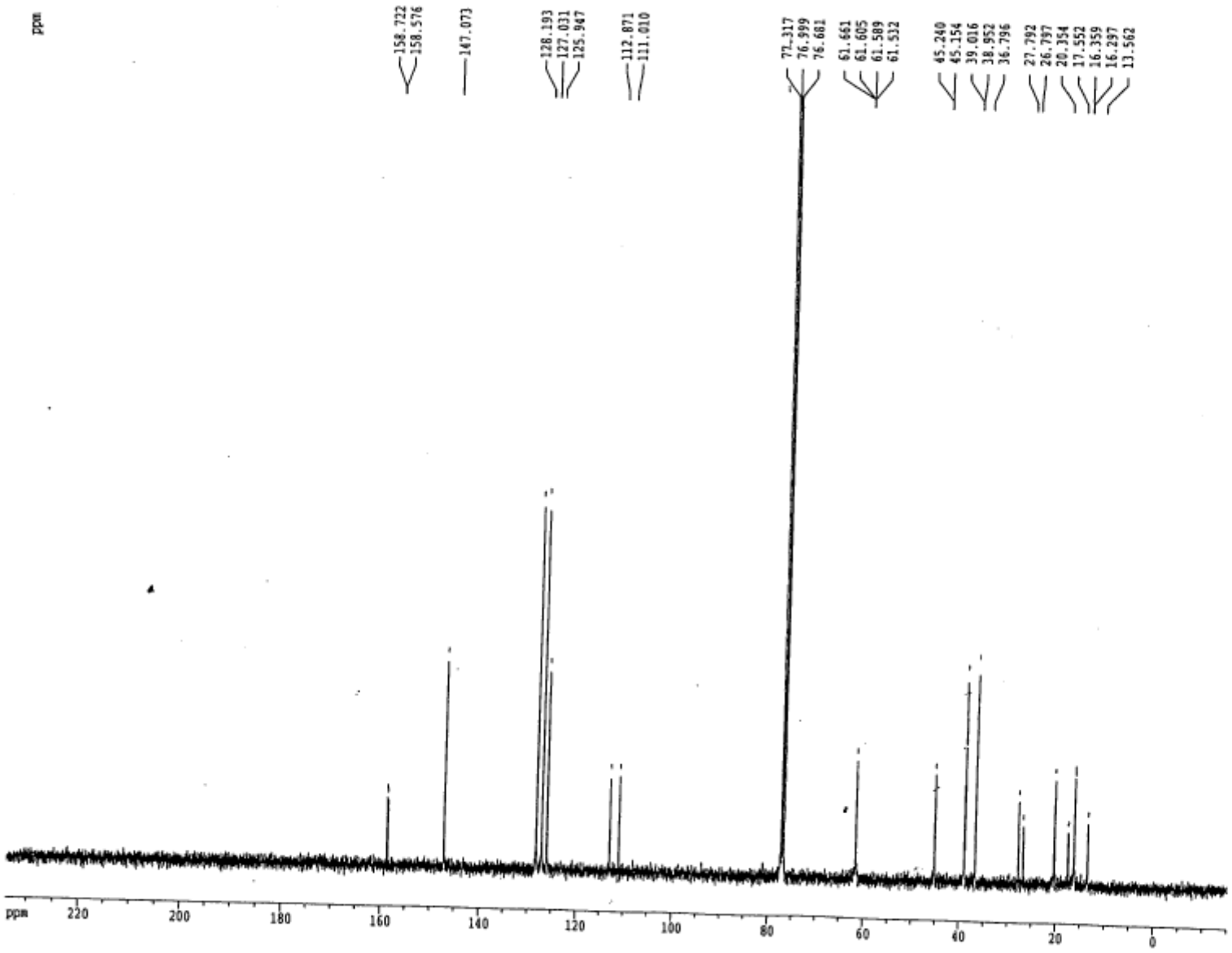


3a




```
Current Data Parameters
NAME                  03ageno
EXPNO                    1314
PROCNO                      1

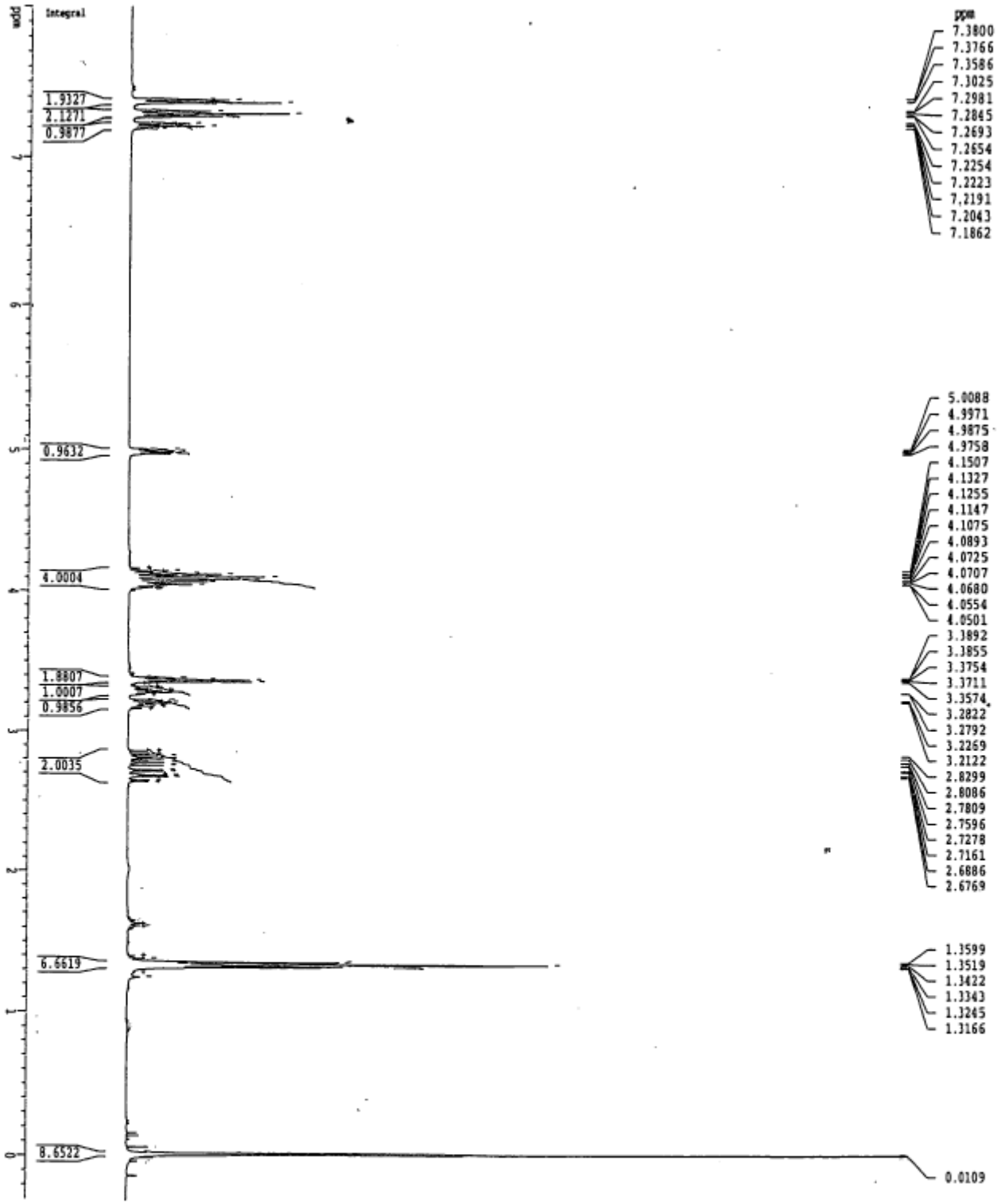
F2 - Acquisition Parameters
Date_                20011022
Time                    13.13
INSTRUM                dpx400
PROBHD      5 mm BBO BB-
PULPROG                zgdc30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          2
SWH                25062.656 Hz
FIDRES             0.382426 Hz
AQ                 1.3074932 sec
RG                       6502
DW                   19.950 usec
DE                    6.00 usec
TE                    300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec

========== CHANNEL f1 ======
NUC1                      13C
P1                    7.90 usec
PL1                  -2.00 dB
SFO1           100.6237959 MHz

========== CHANNEL f2 ======
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 80.00 usec
PL2                  -6.00 dB
PL12                  15.50 dB
SFO2           400.1316005 MHz

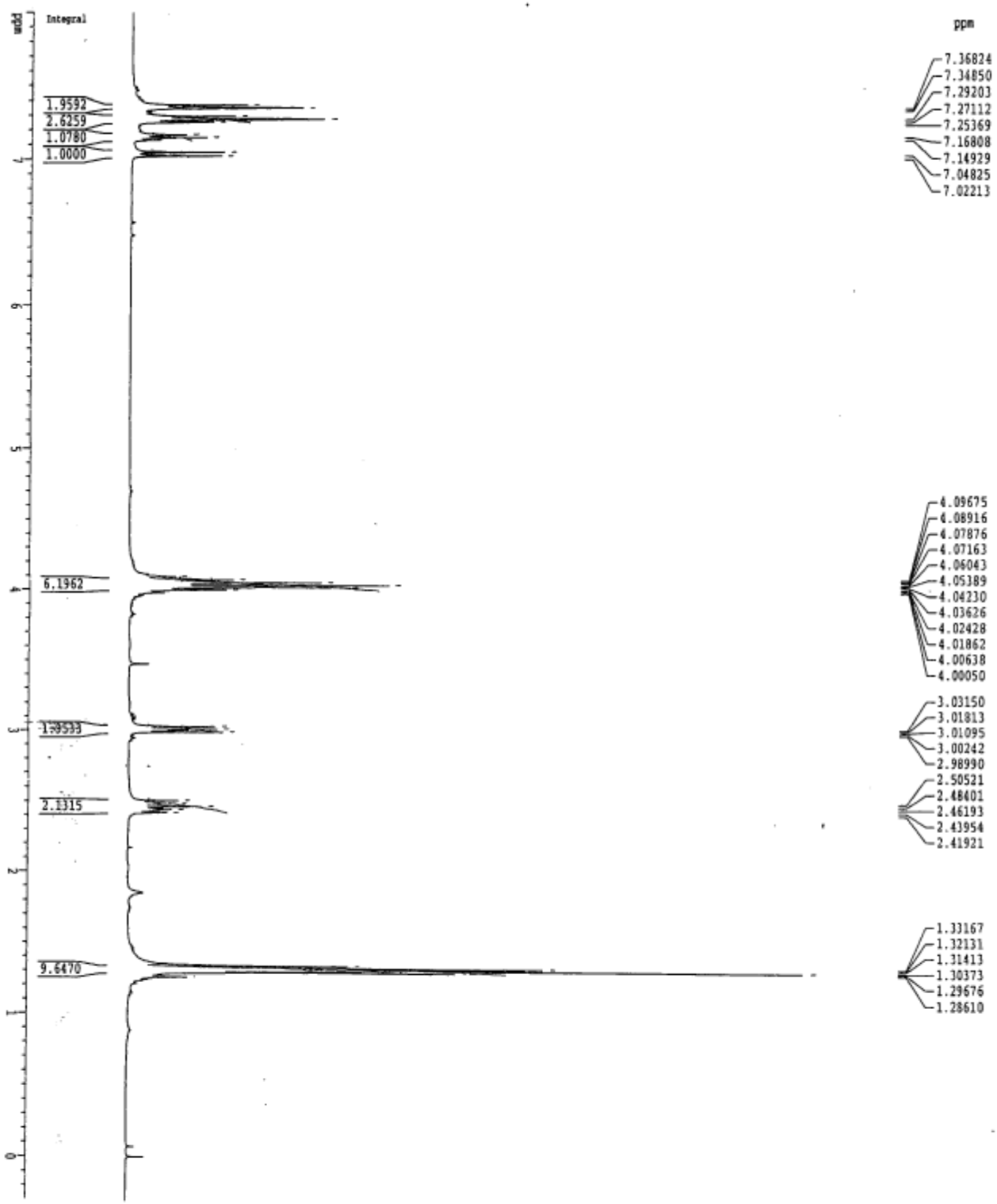
F2 - Processing parameters
SI                       32768
SF             100.6127759 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                    30.00 cm
F1P                 234.079 ppm
F1                  23551.31 Hz
F2P                 -15.021 ppm
F2                  -1511.34 Hz
PPMCM                8.30334 ppm/cm
HZCM               835.42188 Hz/cm
```


ppm
Integral
1.9327
2.1271
0.9877
0.9632
4.0004
1.8807
1.0007
0.9856
2.0035
6.6619
8.6522
0.0109
ppm
7.3800
7.3766
7.3586
7.3025
7.2981
7.2845
7.2693
7.2654
7.2254
7.2223
7.2191
7.2043
7.1862
5.0088
4.9971
4.9875
4.9758
4.1507
4.1327
4.1255
4.1147
4.1075
4.0893
4.0725
4.0707
4.0680
4.0554
4.0501
3.3892
3.3855
3.3754
3.3711
3.3574
3.2822
3.2792
3.2269
3.2122
2.8299
2.8086
2.7809
2.7596
2.7278
2.7161
2.6886
2.6769
1.3599
1.3519
1.3422
1.3343
1.3245
1.3166
Current Data Parameters
NAME 03agomo
EXPNO 2141
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020218
Time 12.24
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8350.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 90.5
DW 60.080 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.90 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 10.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.27667 ppm/cm
HZCM 110.76284 Hz/cm

3c

ppm
160.587
160.440
144.999
127.871
126.823
125.816
110.732
108.846
77.317
76.999
76.681
73.735
61.633
61.576
61.546
61.489
47.251
47.165
38.944
36.717
16.378
16.335
0.022
0.001
Current Data Parameters
NAME 03agemo
EXPNO 2146
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020218
Time 12.48
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3074932 sec
RG 6502
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ======
NUC1 13C
P1 7.90 usec
PL1 -2.00 dB
SFO1 100.6237959 MHz
========== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 15.50 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127767 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
FIP 234.071 ppm
FI 23550.55 Hz
F1P -15.029 ppm
F2P -1512.11 Hz
F2 8.30334 ppm/cm
PPMCM 835.42194 Hz/cm
HZCM



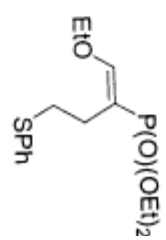
Current Data Parameters
NAME 01agomo
EXPNO 1747
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020119
Time 16.53
INSTRM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 1.9715316 sec
RG 203.2
DW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

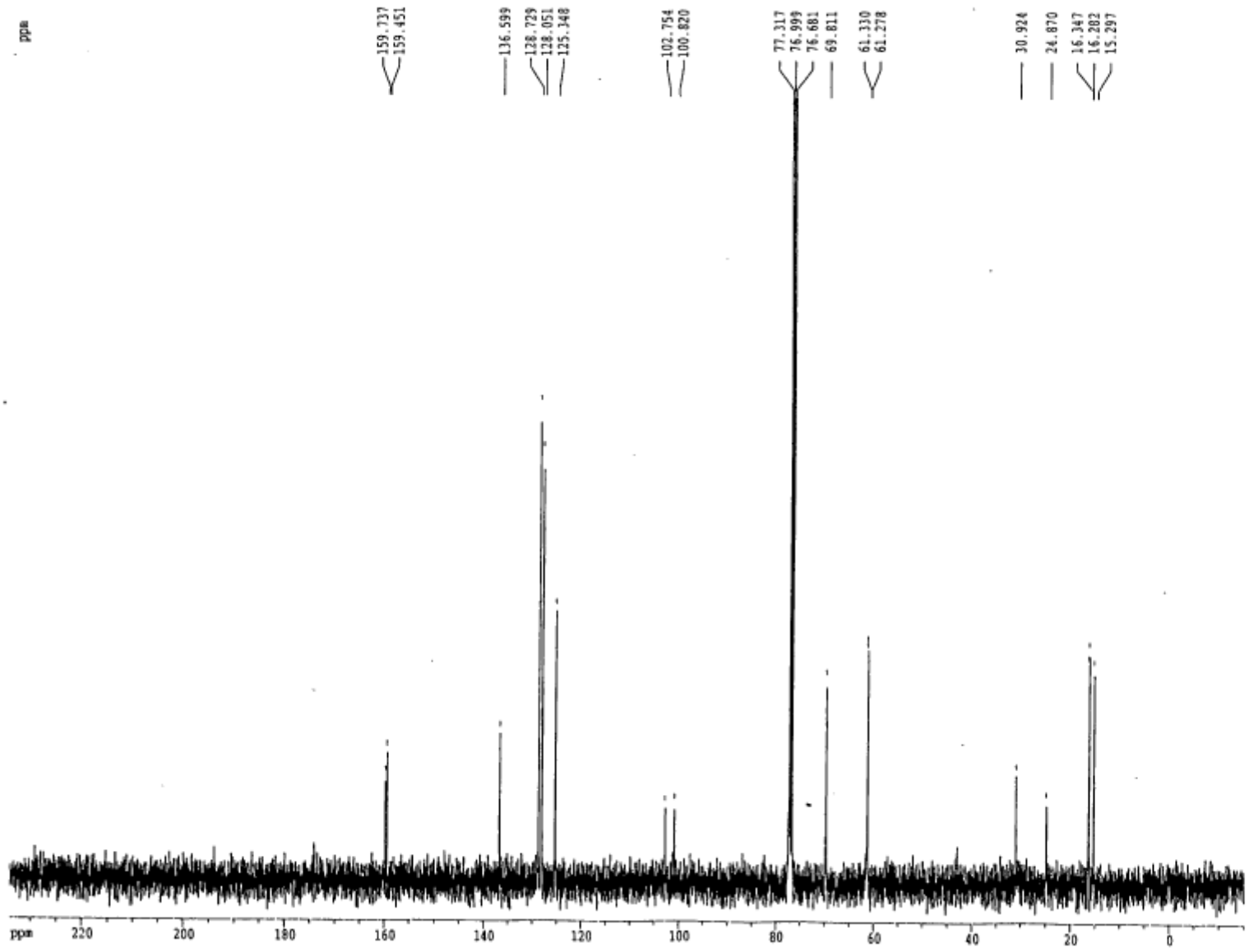
========== CHANNEL f1 ==========
NUC1 1H
P1 7.90 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300055 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 10.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.27667 ppm/cm
HZCM 110.70264 Hz/cm



3d



Current Data Parameters

NAME	03ageno
EXPNO	1748
PROCNO	1

F2 - Acquisition Parameters

Date_	20020119
Time	17.12
INSTRUM	dpx400
PROBHD	5 mm BBO BB-
PULPROG	zgdc30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	25062.656 Hz
FIDRES	0.382426 Hz
AQ	1.3074932 sec
RG	7298.2
DW	19.950 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec

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

NUC1	13C
P1	7.90 usec
PL1	-2.00 dB
SFO1	100.6237959 MHz

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

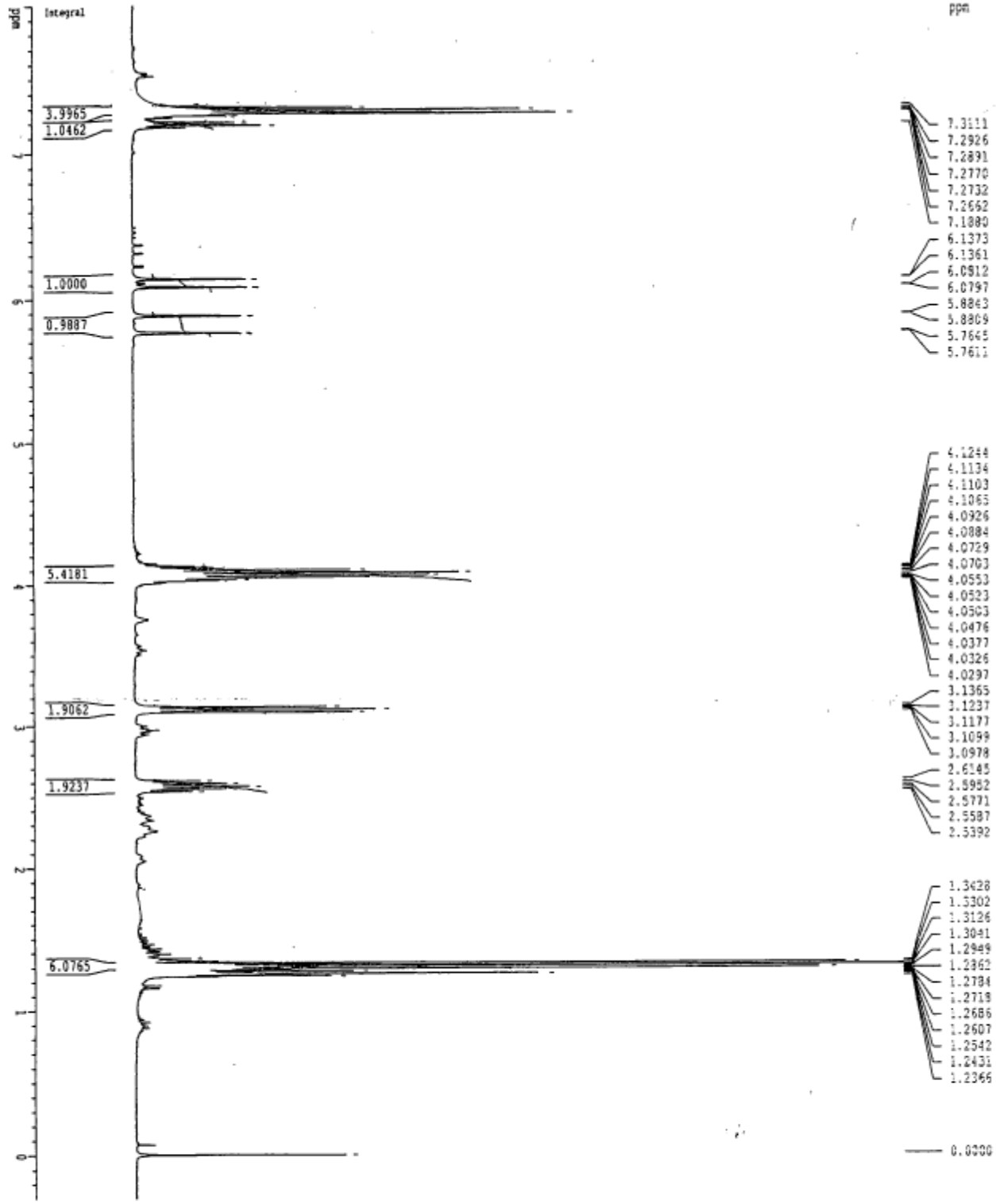
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-6.00 dB
PL12	15.50 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127744 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
F1P	234.094 ppm
F1	23552.84 Hz
F2P	-15.006 ppm
F2	-1509.81 Hz
PPMCM	8.30334 ppm/cm
HZCM	835.42188 Hz/cm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Integral
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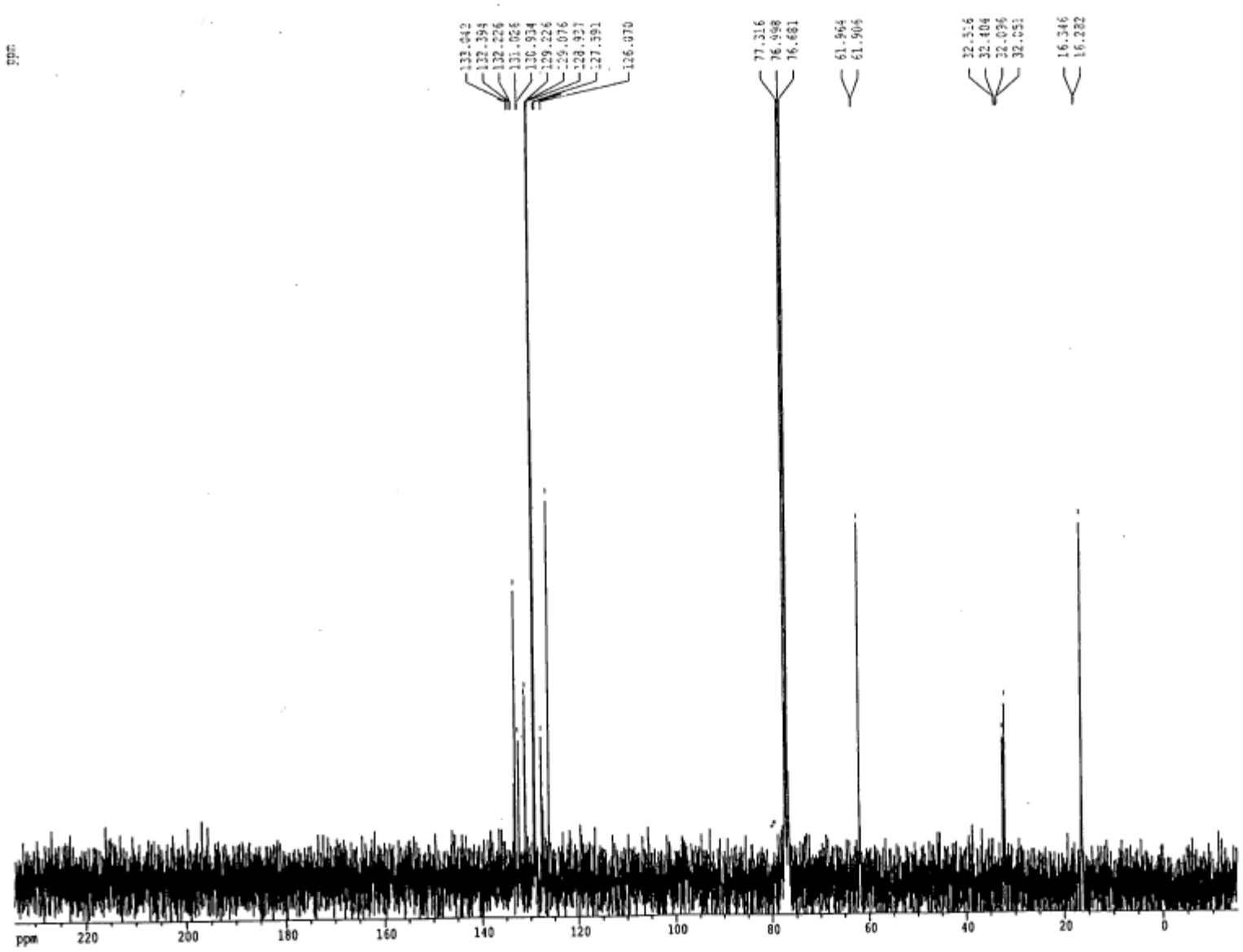
1.0000
0.9887
5.4181
1.9062
1.9237
6.0765
7.3111
7.2926
7.2891
7.2770
7.2732
7.2662
7.1880
6.1373
6.1361
6.0812
6.0797
5.8863
5.8809
5.7645
5.7611
4.1244
4.1134
4.1103
4.1065
4.0926
4.0884
4.0729
4.0703
4.0553
4.0523
4.0503
4.0476
4.0377
4.0326
4.0297
3.1365
3.1237
3.1177
3.1099
3.0978
2.6145
2.5952
2.5771
2.5587
2.5392
1.3428
1.3302
1.3126
1.3041
1.2949
1.2862
1.2784
1.2719
1.2686
1.2607
1.2542
1.2431
1.2366
0.0000
Current Data Parameters
NAME Diagano
EXPNO 483
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030619
Time 16.01
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 203.2
DW 60.560 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 8.000 ppm
F1P 3201.84 Hz
F1 -0.300 ppm
F2P -120.04 Hz
F2 0.27667 ppm/cm
PPMCM 110.70264 Hz/cm
P(O)(OEt)2
SPh
3e



Current Data Parameters

NAME	03ageno
EXPNO	4831
PROCNO	1

F2 - Acquisition Parameters

Date_	20030619
Time	16.33
INSTRUM	dpx400
PROBHD	5 mm BBO BB-
PULPROG	zgdc30
TD	65536
SOLVENT	CDCl3
NS	512
DS	2
SWH	25062.656 Hz
FIDRES	0.382426 Hz
AQ	1.3074932 sec
RG	6502
DW	19.950 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec

---------- CHANNEL f1 -------

NUC1	13C
P1	7.90 usec
PL1	-2.00 dB
SFO1	100.6237959 MHz

---------- CHANNEL f2 -------

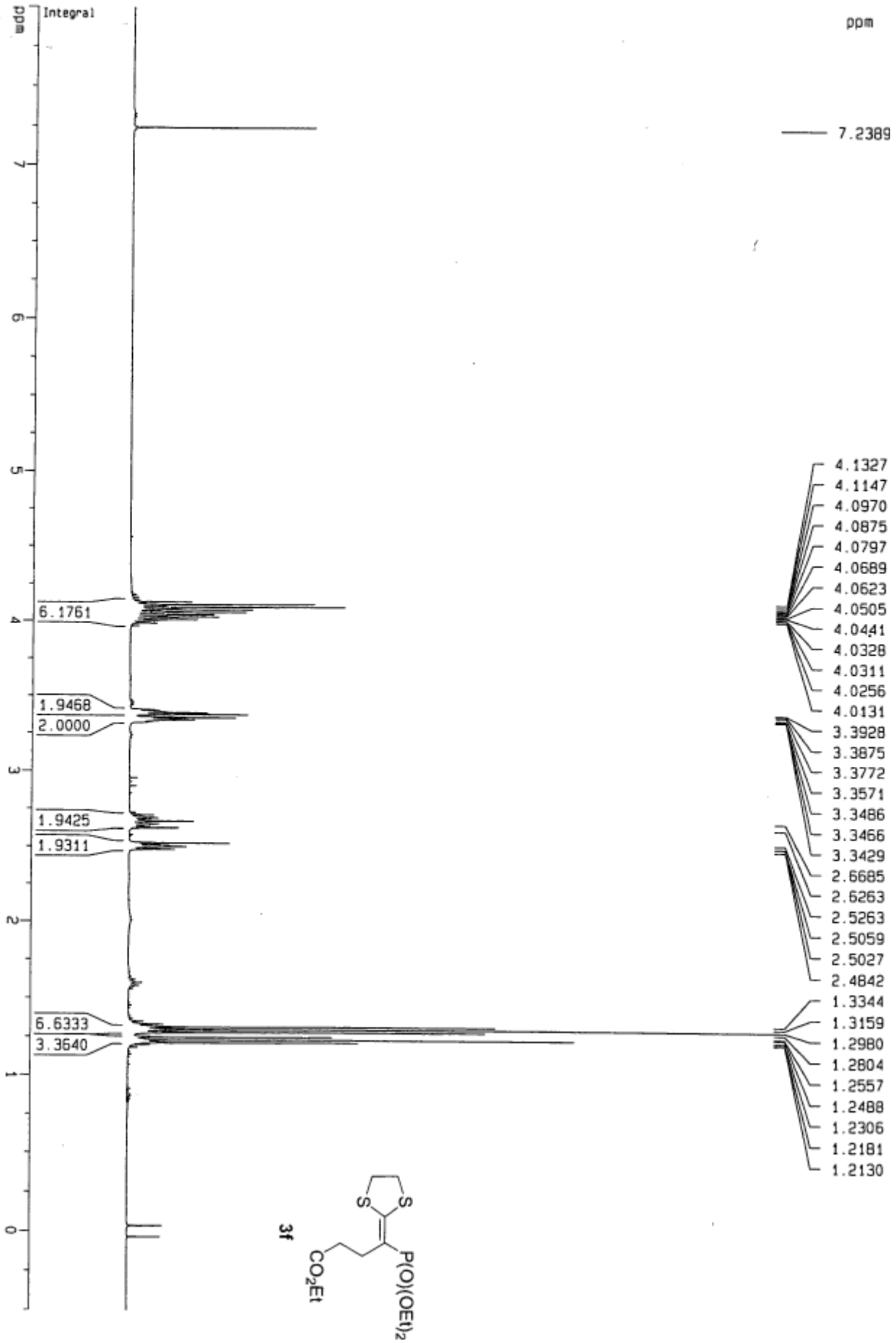
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-6.00 dB
PL12	10.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127721 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
F1P	234.117 ppm
F1	23555.14 Hz
F2P	-14.983 ppm
F2	-1507.52 Hz
PPMCM	8.30334 ppm/cm
HZCM	835.42188 Hz/cm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Integral
ppm
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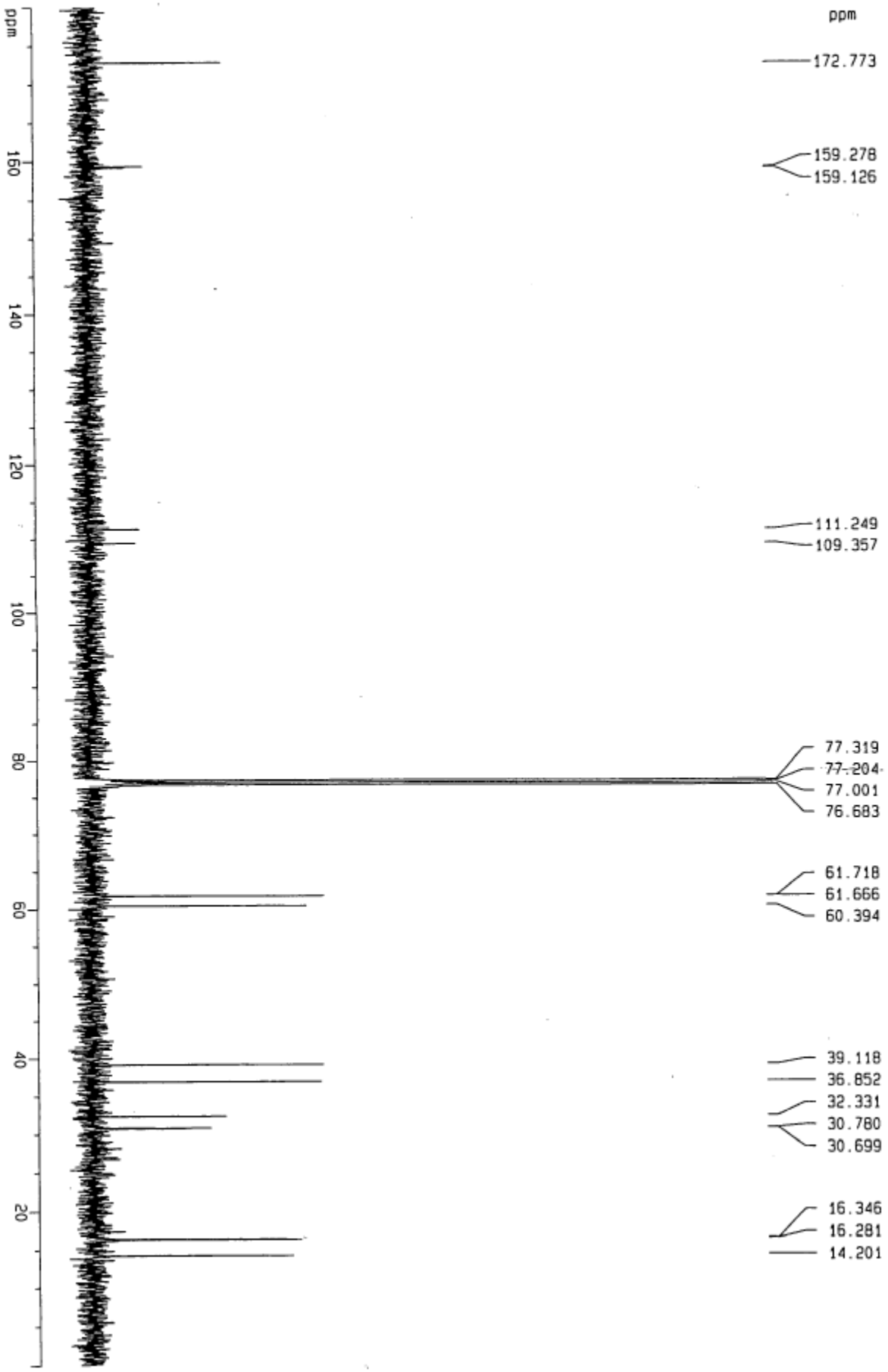
4.1327
4.1147
4.0970
4.0875
4.0797
4.0689
4.0623
4.0505
4.0441
4.0328
4.0311
4.0256
4.0131
3.3928
3.3875
3.3772
3.3571
3.3486
3.3466
3.3429
2.6685
2.6263
2.5263
2.5059
2.5027
2.4842
1.3344
1.3159
1.2980
1.2804
1.2557
1.2488
1.2306
1.2181
1.2130
6.1761
1.9468
2.0000
1.9425
1.9311
6.6333
3.3640
3f
S
S
P(O)(OEt)2
CO2Et


ppm
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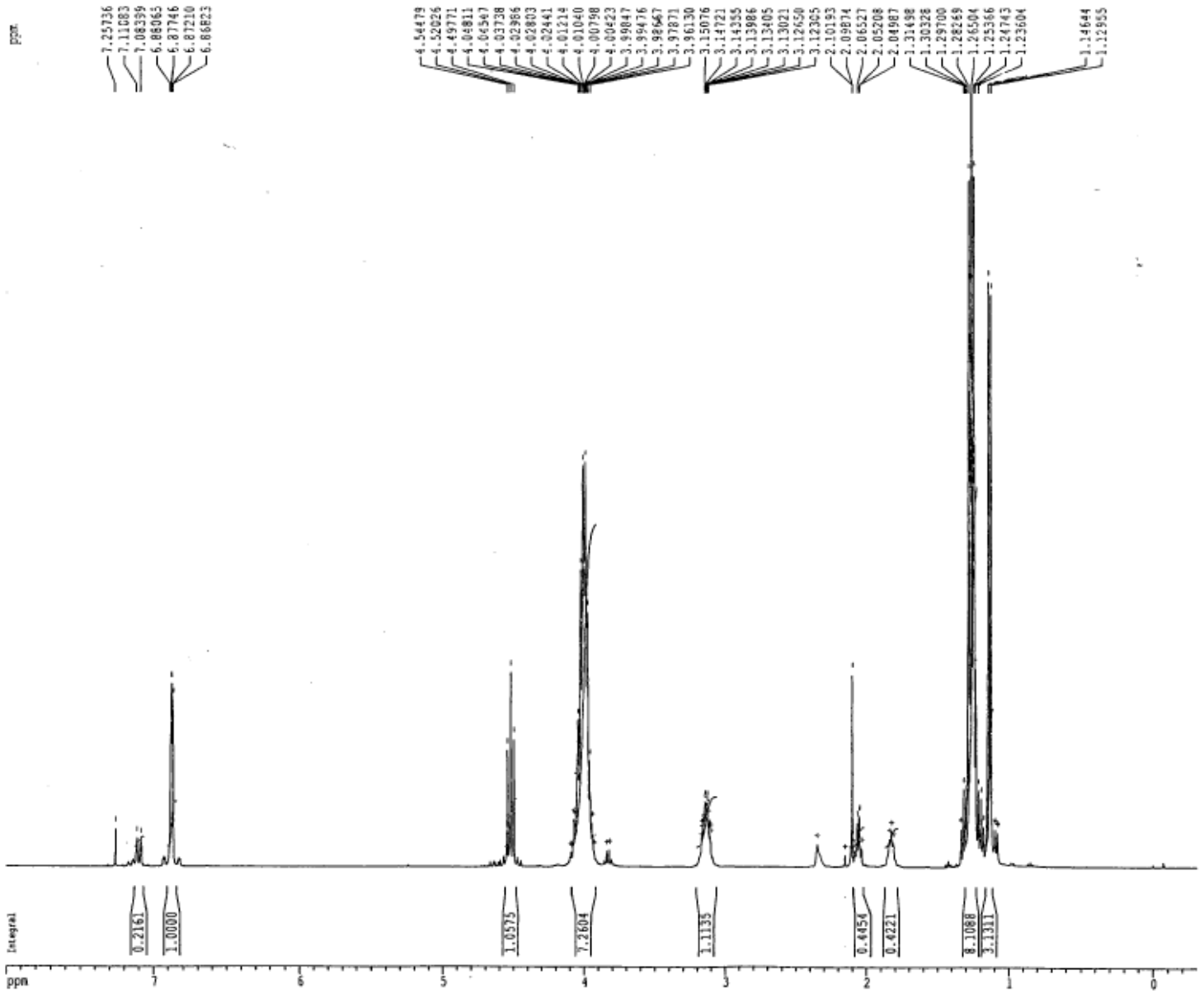
159.126
111.249
109.357
77.319
77.204
77.001
76.683
61.718
61.666
60.394
39.118
36.852
32.331
30.780
30.699
16.346
16.281
14.201
ppm
160
140
120
100
80
60
40
20



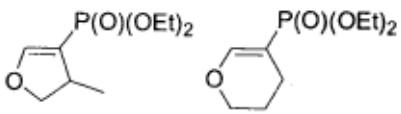

```
Current Data Parameters
NAME                  03agano
EXPNO                      433
PROCNO                       1

F2 - Acquisition Parameters
Date_               20030317
Time                    15.04
INSTRUM                 dpx400
PROBHD       5 mm BBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8250.825 Hz
FIDRES               0.125898 Hz
AQ                   3.9715316 sec
RG                         64
DW                    60.600 usec
DE                     6.00 usec
TE                     300.0 K
D1                  1.00000000 sec

========== CHANNEL f1 ==========
NUC1                       1H
P1                       7.90 usec
PL1                     -6.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                         32768
SF                  400.1300112 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00

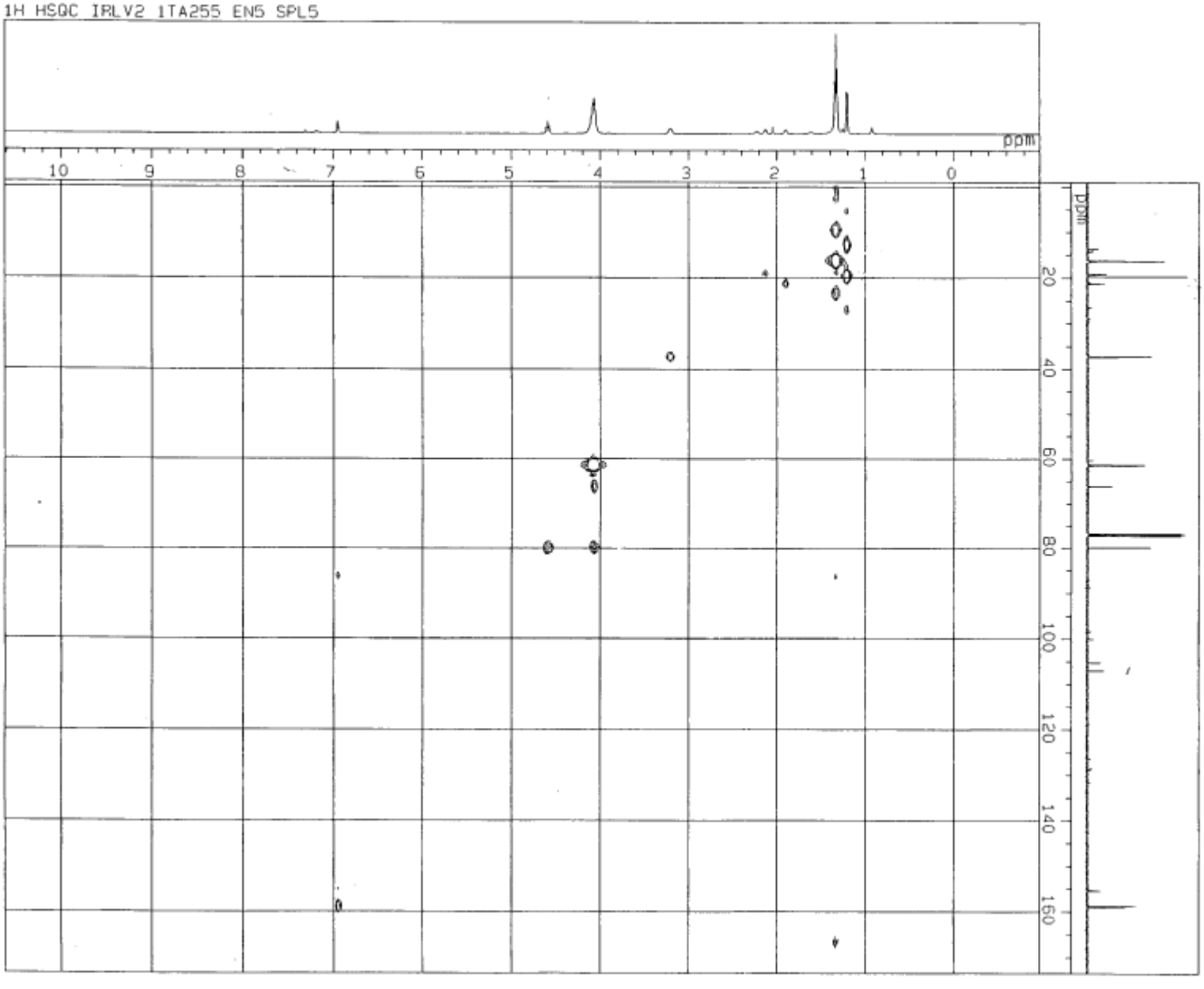
1D NMR plot parameters
CX                         30.00 cm
F1P                        8.000 ppm
F1                       3201.04 Hz
F2P                       -0.300 ppm
F2                       -120.04 Hz
PPMCM                    0.27667 ppm/cm
HZCM                   110.70264 Hz/cm
```



5e

6e

ppm
220
200
180
160
140
120
100
80
60
40
20
0
158.951
158.665
107.116
104.990
100.193
98.226
79.806
79.685
77.321
77.003
76.685
66.160
61.617
61.334
61.342
61.317
61.263
61.192
61.005
37.228
37.134
30.780
21.245
21.147
19.925
19.660
19.371
19.112
16.454
16.270
16.202
16.154
Current Data Parameters
NAME 03aqeno
EXPNO 4331
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030317
Time 15.36
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 512
DS 2
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3074932 sec
RG 6502
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.90 usec
PL1 -2.00 dB
SFO1 100.6237959 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 15.50 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127782 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
F1P 234.056 ppm
F1 23549.02 Hz
F2P -15.044 ppm
F2 -1513.64 Hz
PPMCM 8.30334 ppm/cm
HZCM 835.42188 Hz/cm



20-MAY-2002 18:04:33.17

DFILE : ALPHA
SFILE : 1TA2552HSQC_E5S5
HR2FILE: 1TA2550NON_E5S5
HR1FILE: 1TA2550BCM_E5S5

COMNT : 1H HSQC IRLV2 1T
EXMOD : HSQC
IRMOD : IRLV2
POINT : 512
FREQU : 5793.74 Hz
SCANS : 128
DUMMY : 32
ACQTM : 0.0884 sec
PD : 1.1116 sec
RGAIN : 10

CLFRQ : 21958.72 Hz
CLPNT : 256
TOSCN : 128
CINWT : 10.00 usec
CINT2 : 22.77 usec

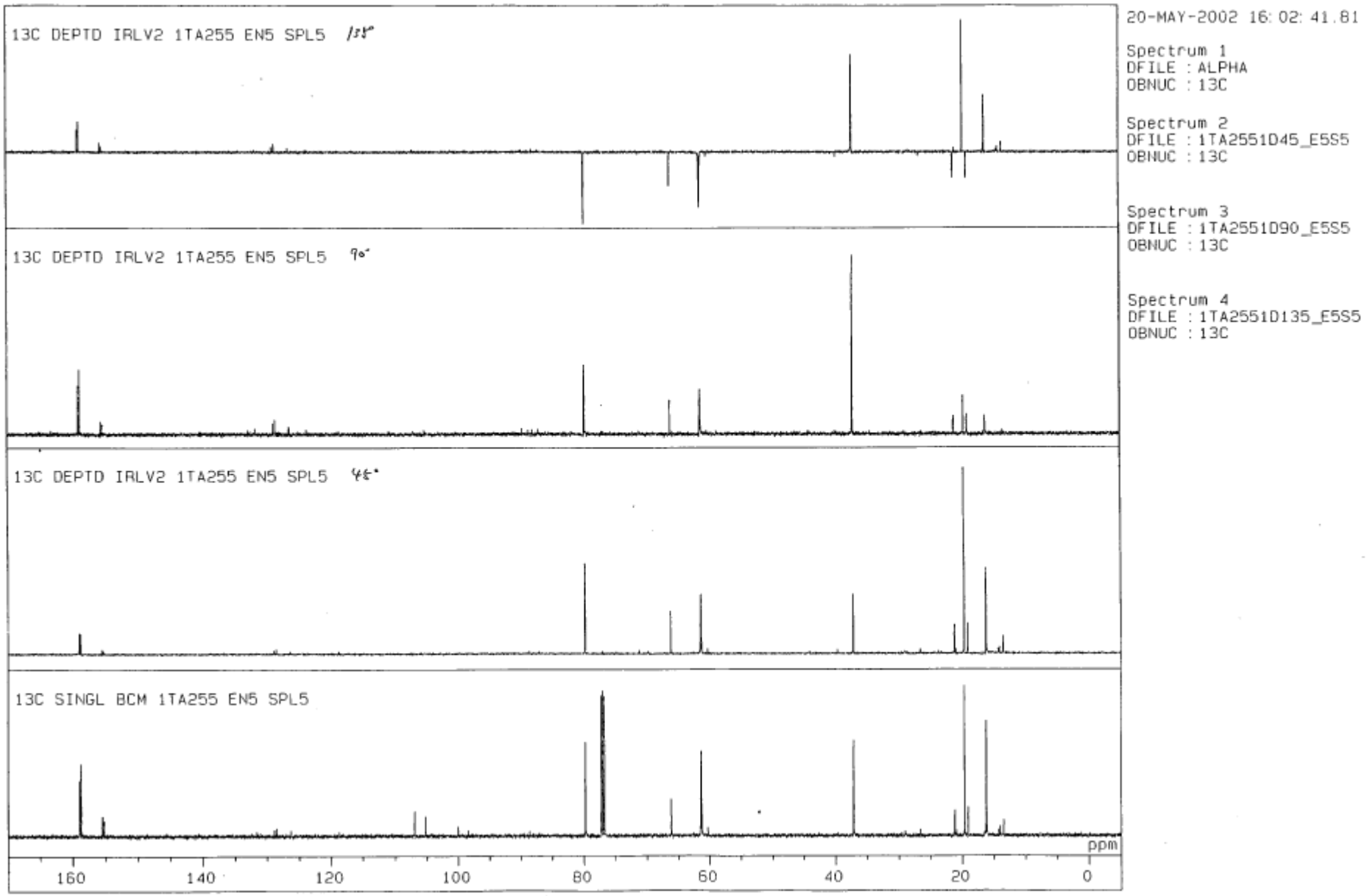
PW1 : 39.50 usec
PW3 : 9.00 usec
PI1 : 120.0000 msec
PI3 : 69.6800 msec
JCNST : 140.00 Hz

OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162308.99 Hz

IRNUC : 13C
IRFRQ : 125.65 MHz
IRSET : 126162.64 Hz
IRATN : 511
IRRPW : 1.5 usec
IRBP1 : 50
IRBP2 : 6
IRRNS : 4

ADBIT : 16
CTEMP : 23.2 c
CSPED : 0 Hz
SLVNT : CDCL3

RESOL : 11.32 Hz
CLRSO : 85.78 Hz
TLINE : 4
THTOP : 0.2462
THBTM : 0.0843
operator


13C DEPTD IRLV2 1TA255 EN5 SPL5
13C DEPTD IRLV2 1TA255 EN5 SPL5
13C DEPTD IRLV2 1TA255 EN5 SPL5
13C SINGL BCM 1TA255 EN5 SPL5
20-MAY-2002 16:02:41.81
Spectrum 1
DFILE : ALPHA
OBNUC : 13C
Spectrum 2
DFILE : 1TA2551D45_E5S5
OBNUC : 13C
Spectrum 3
DFILE : 1TA2551D90_E5S5
OBNUC : 13C
Spectrum 4
DFILE : 1TA2551D135_E5S5
OBNUC : 13C
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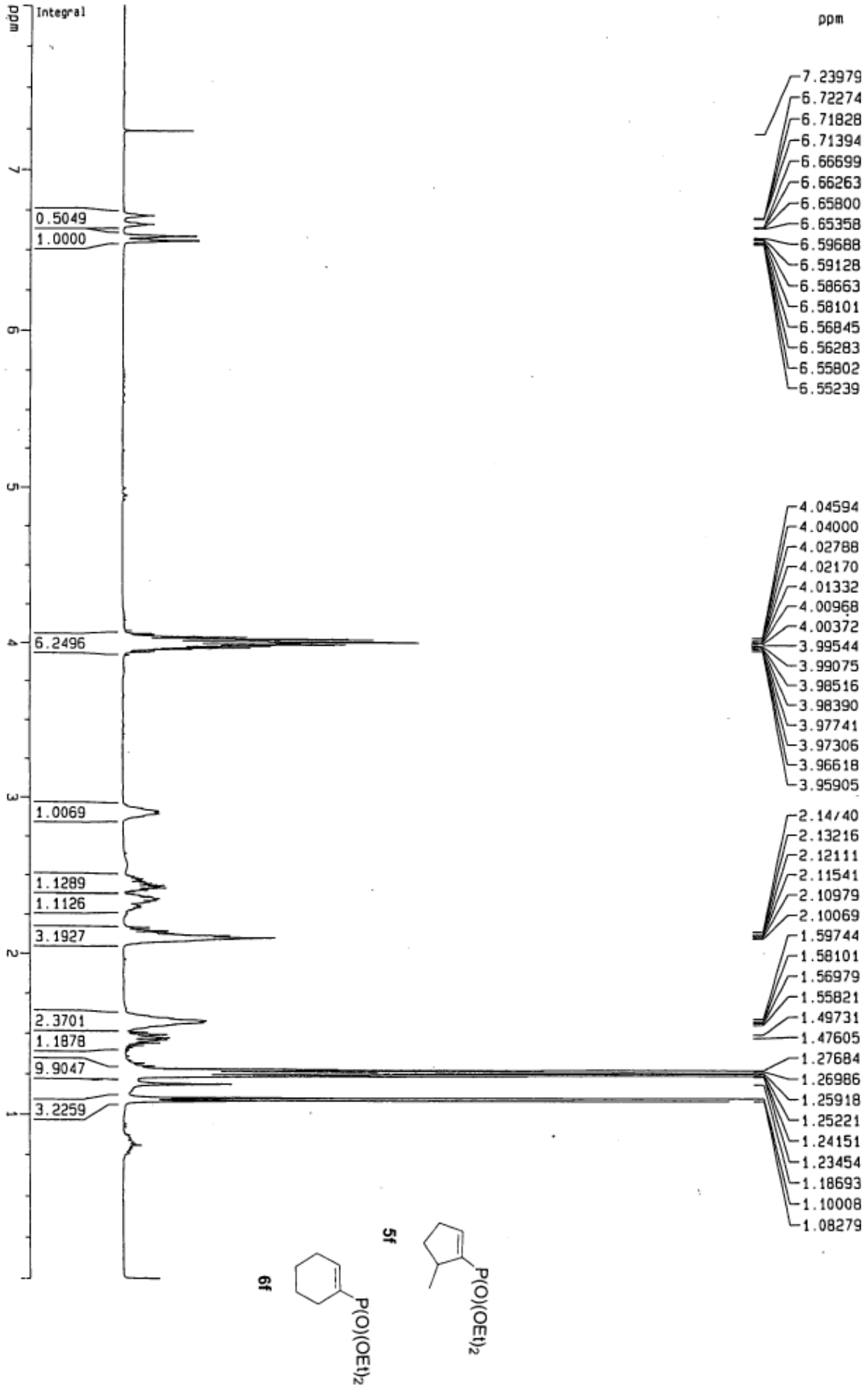
140
120
100
80
60
40
20
0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2.3701
1.1878
9.9047
3.2259
7.23979
6.72274
6.71828
6.71394
6.66699
6.66263
6.65800
6.65358
6.59688
6.59128
6.58663
6.58101
6.56845
6.56283
6.55802
6.55239
4.04594
4.04000
4.02788
4.02170
4.01332
4.00968
4.00372
3.99544
3.99075
3.98516
3.98390
3.97741
3.97306
3.96618
3.95905
2.14740
2.13216
2.12111
2.11541
2.10979
2.10069
1.59744
1.58101
1.56979
1.55821
1.49731
1.47605
1.27684
1.26986
1.25918
1.25221
1.24151
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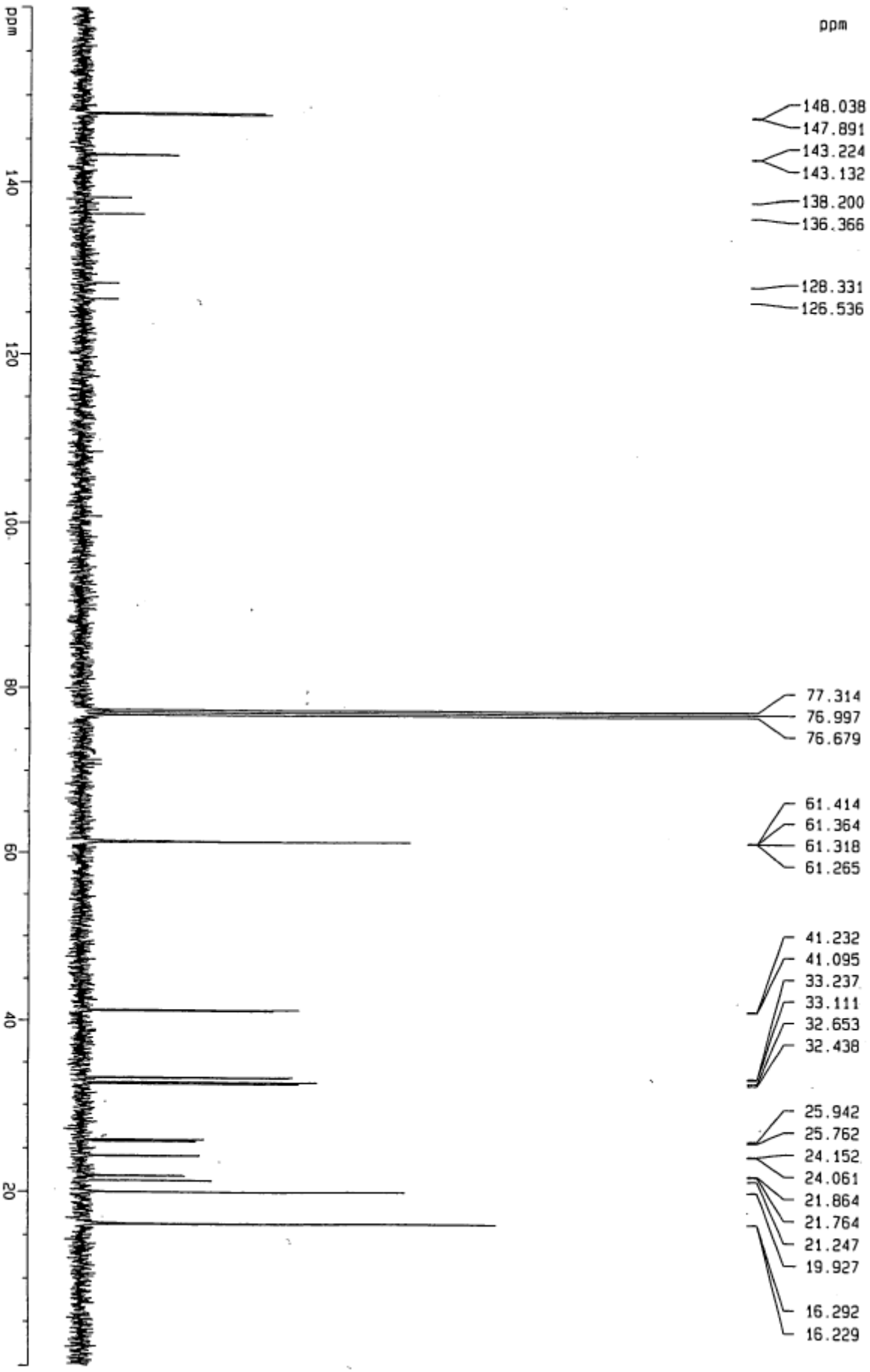
1.18693
1.10008
1.08279
6f
P(O)(OEt)2
5f
P(O)(OEt)2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120
100
80
60
40
20
ppm
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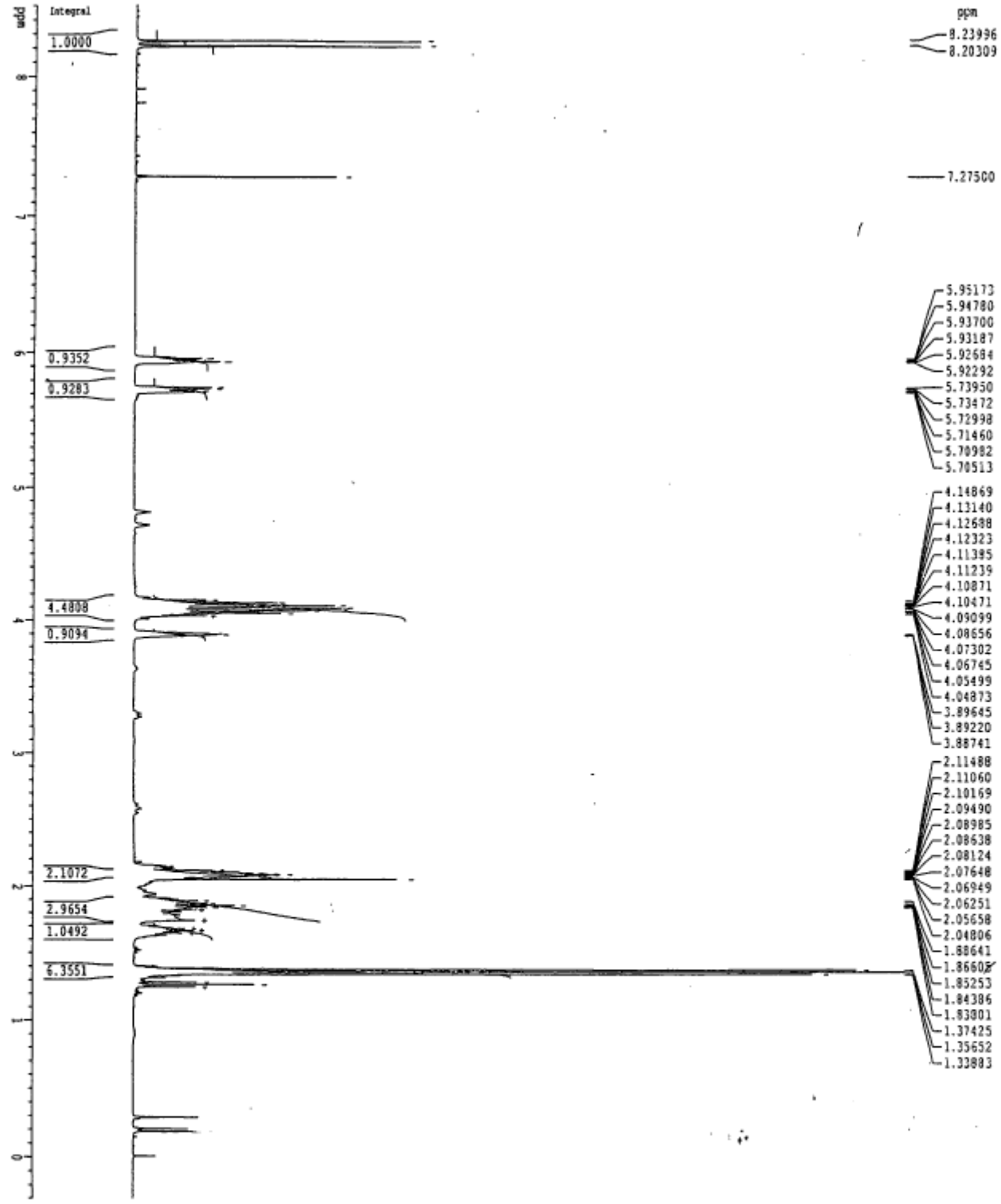
138.200
136.366
128.331
126.536
77.314
76.997
76.679
61.414
61.364
61.318
61.265
41.232
41.095
33.237
33.111
32.653
32.438
25.942
25.762
24.152
24.061
21.864
21.764
21.247
19.927
16.292
16.229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1.0492
6.3551
ppm
8.23996
8.20309
7.27500
5.95173
5.94780
5.93700
5.93187
5.92684
5.92292
5.73950
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5.72998
5.71460
5.70982
5.70513
4.14869
4.13140
4.12688
4.12323
4.11395
4.11239
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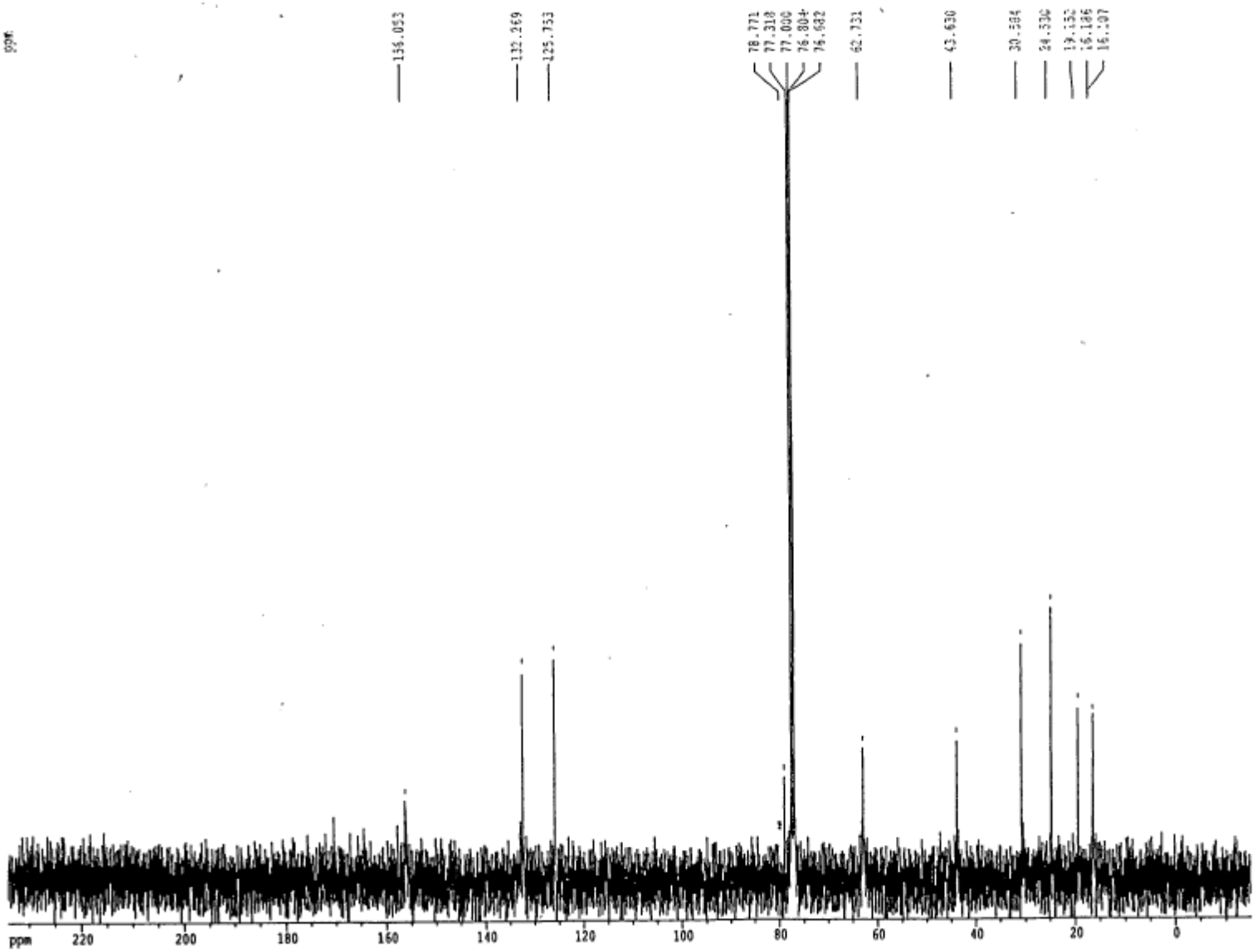
4.10471
4.09099
4.08656
4.07302
4.06745
4.05499
4.04873
3.89645
3.89220
3.88741
2.11488
2.11060
2.10169
2.09490
2.08985
2.08638
2.08124
2.07648
2.06949
2.06251
2.05658
2.04806
1.88641
1.86602
1.85253
1.84386
1.83801
1.37425
1.35652
1.33883
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
CHANNEL f1
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
IN
F1
F2P
F2
PPMCM
HZCM
S
I
P(O)(OEt)2

17



Current Data Parameters
NAME 03ageno
EXPNO 4501
PROCNO 1

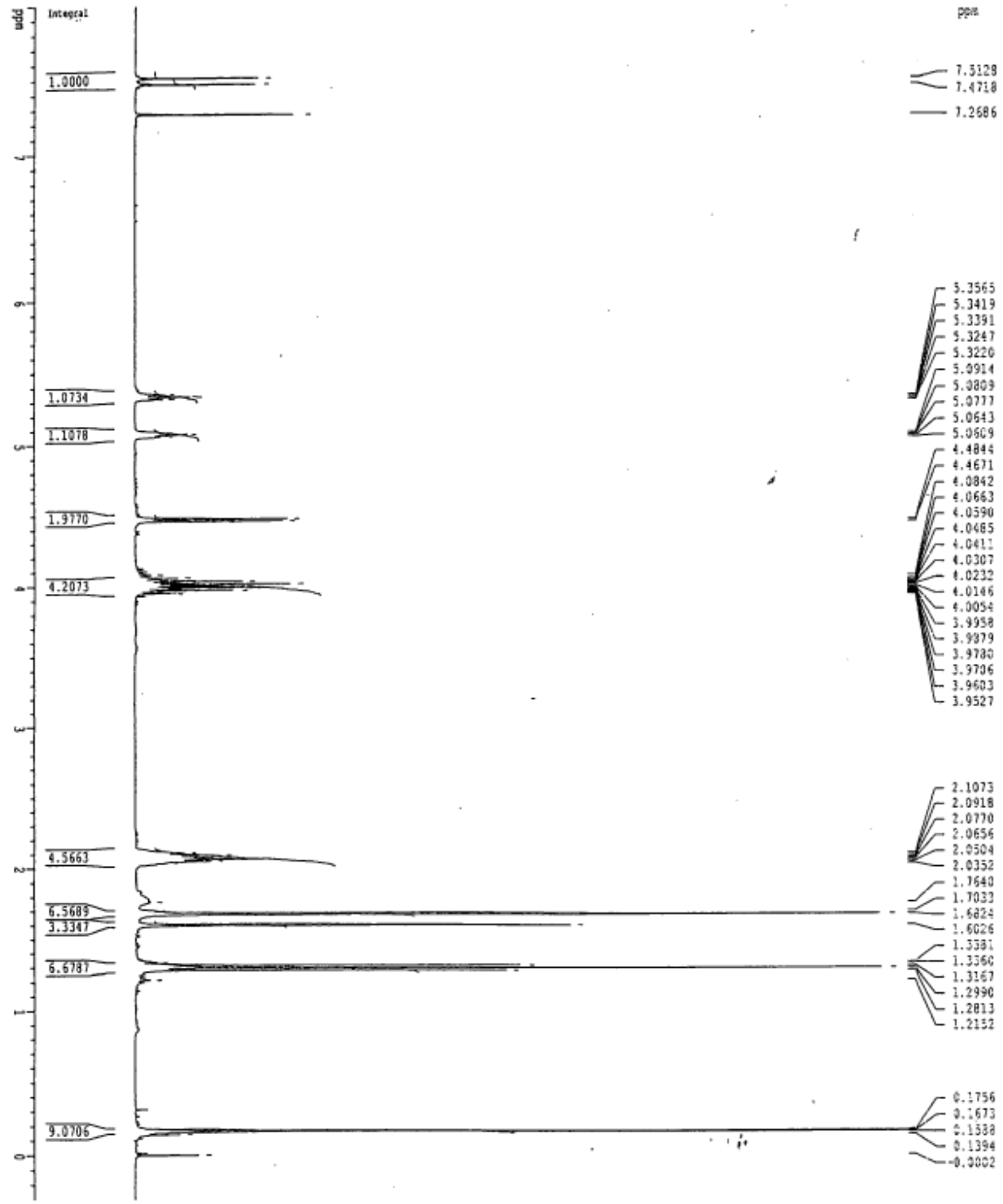
F2 - Acquisition Parameters
Date_ 20030424
Time 14.23
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 512
DS 2
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3074932 sec
RG 6502
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

---------- CHANNEL f1 ----------
NUC1 13C
P1 7.90 usec
PL1 -2.00 dB
SFO1 100.6237959 MHz

---------- CHANNEL f2 ----------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 15.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
F1P 234.102 ppm
F1 23553.60 Hz
F2P -14.999 ppm
F2 -1509.05 Hz
PPMCM 8.30334 ppm/cm
HZCM 835.42188 Hz/cm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1.1078
1.9770
4.2073
4.5663
6.5689
3.3347
6.6787
9.0706
7.5128
7.4718
7.2686
5.3565
5.3419
5.3391
5.3247
5.3220
5.0914
5.0809
5.0777
5.0643
5.0609
4.4844
4.4671
4.0842
4.0663
4.0590
4.0485
4.0411
4.0307
4.0232
4.0146
4.0054
3.9958
3.9879
3.9780
3.9706
3.9603
3.9527
2.1073
2.0918
2.0770
2.0656
2.0504
2.0352
1.7640
1.7033
1.6824
1.6026
1.3381
1.3360
1.3167
1.2990
1.2813
1.2152
0.1756
0.1673
0.1588
0.1394
-0.0002
Current Data Parameters
NAME 01sgeno
EXPNO 1211
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220314
Time 1.36
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8256.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 287.4
DW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 7.90 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.27667 ppm/cm
HZCM 110.70264 Hz/cm
O
P(O)(OEt)2
SiMe3

```
Current Data Parameters
NAME                  03apeno
EXPNO                    3253
PROCNO                      1

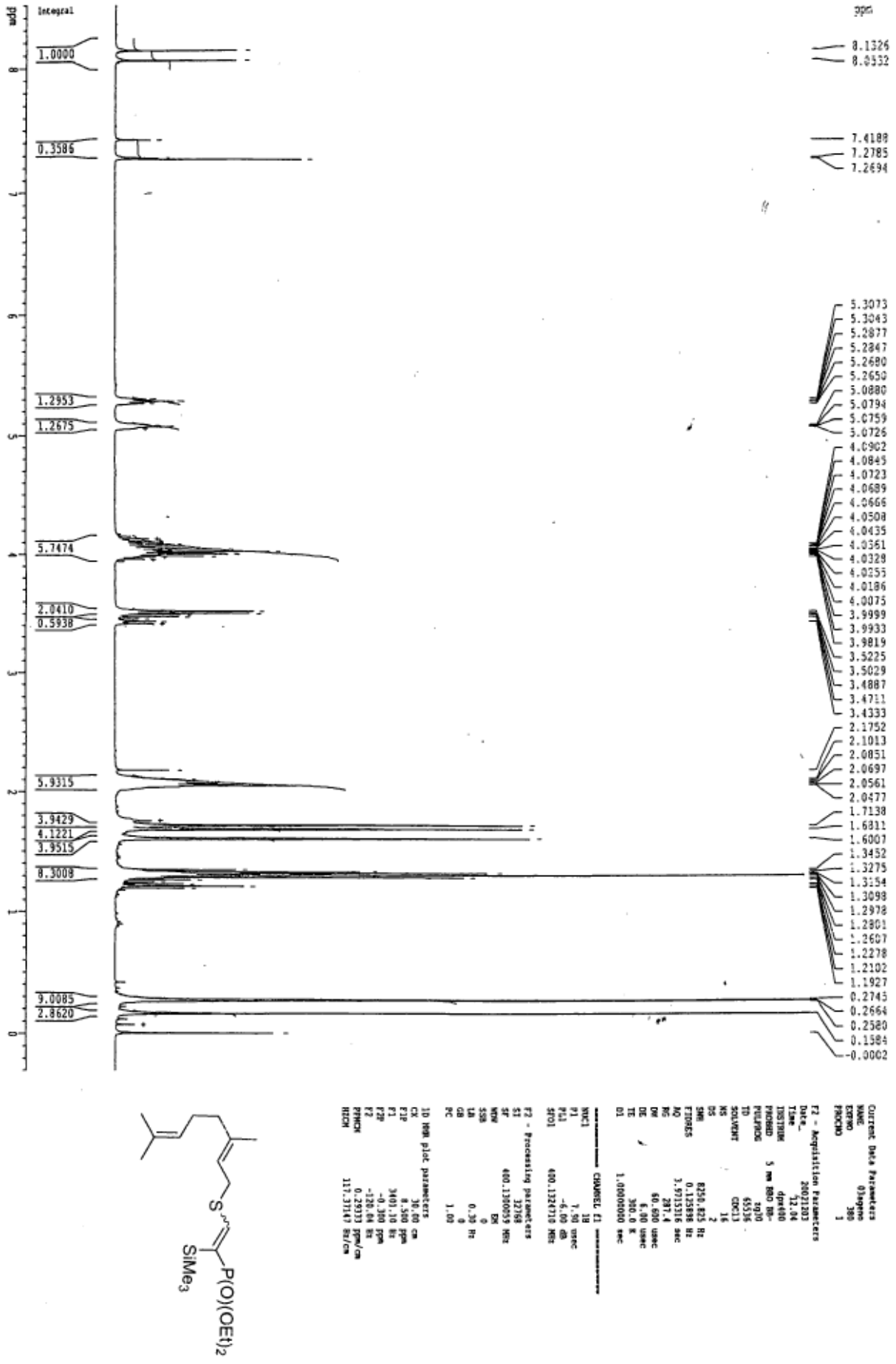
F2 - Acquisition Parameters
Date_              20020919
Time                   1.01
INSTRUM              dpx400
PROBHD     5 mm BBO BB-
PULPROG              zgdc30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        2
SWH               25062.656 Hz
FIDRES                0.382426 Hz
AQ                    1.3074932 sec
RG                       3251
DW                   19.950 usec
DE                    6.00 usec
TE                     300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     7.90 usec
PL1                    -2.00 dB
SFO1          100.6237959 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 80.00 usec
PL2                    -6.00 dB
PL12                   15.50 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF            100.6127736 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                      30.00 cm
F1P                    234.102 ppm
F1                   23553.60 Hz
F2P                   -14.999 ppm
F2                   -1509.05 Hz
PPMCM                 8.30334 ppm/cm
HZCM                835.42188 Hz/cm
```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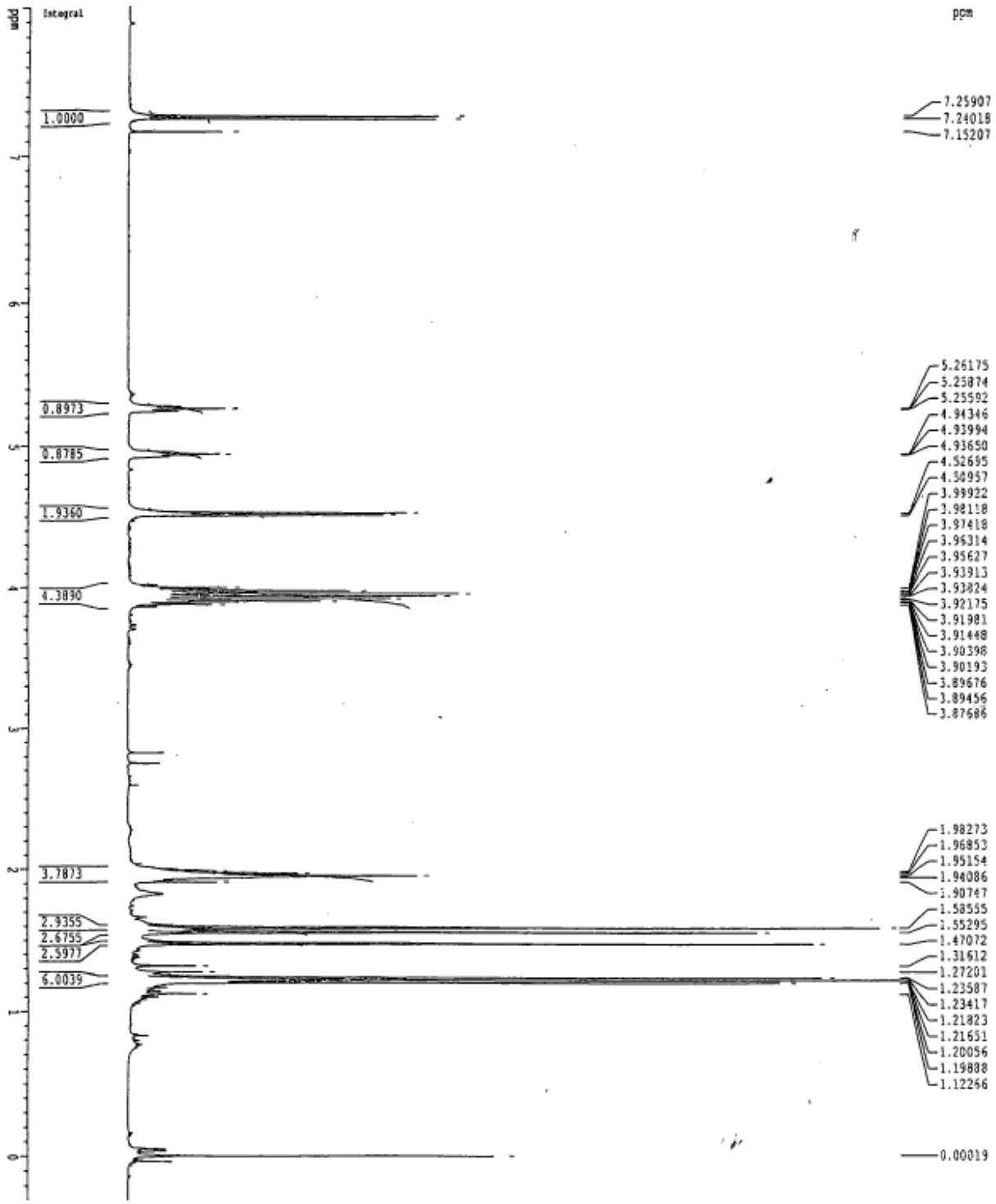
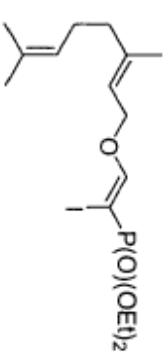
3.9429
4.1221
3.9515
8.3008
9.0085
2.8620
8.1326
8.0932
7.4188
7.2785
7.2694
5.3073
5.3043
5.2877
5.2847
5.2680
5.2650
5.0880
5.0794
5.0759
5.0726
4.0902
4.0845
4.0723
4.0689
4.0666
4.0508
4.0435
4.0361
4.0328
4.0255
4.0186
4.0075
3.9999
3.9933
3.9819
3.5225
3.5029
3.4887
3.4711
3.4333
2.1752
2.1013
2.0851
2.0697
2.0561
2.0477
1.7138
1.6811
1.6007
1.3452
1.3275
1.3154
1.3098
1.2978
1.2801
1.2607
1.2278
1.2102
1.1927
0.2745
0.2664
0.2580
0.1584
-0.0002
Current Data Parameters
NAME 01sgeno
EXPNO 380
PROCNO 1
F2 - Acquisition Parameters
Date_ 20021203
Time 12.04
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 287.4
DW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 7.50 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.25033 ppm/cm
HZCM 117.37147 Hz/cm
SiMe3
S
P(O)(OEt)2

ppm
220
200
180
160
140
120
100
80
60
40
20
0
161.754
140.863
140.240
131.830
131.756
123.712
122.390
120.985
119.552
118.732
118.699
77.320
77.002
76.684
61.494
61.189
61.054
30.525
32.998
32.467
26.454
26.370
25.630
17.683
17.630
16.260
-0.746
Current Data Parameters
NAME 01agemo
EXPNO 3761
PROCNO 1
F2 - Acquisition Parameters
Date_ 20021128
Time 15.05
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 512
DS 2
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3074932 sec
RG 6502
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.90 usec
PL1 -2.00 dB
SFO1 100.6237959 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 15.50 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
F1P 234.102 ppm
F1 23553.61 Hz
F2P -14.999 ppm
F2 -1509.05 Hz
PPMCM 8.30334 ppm/cm
HZCM 835.42188 Hz/cm





11a

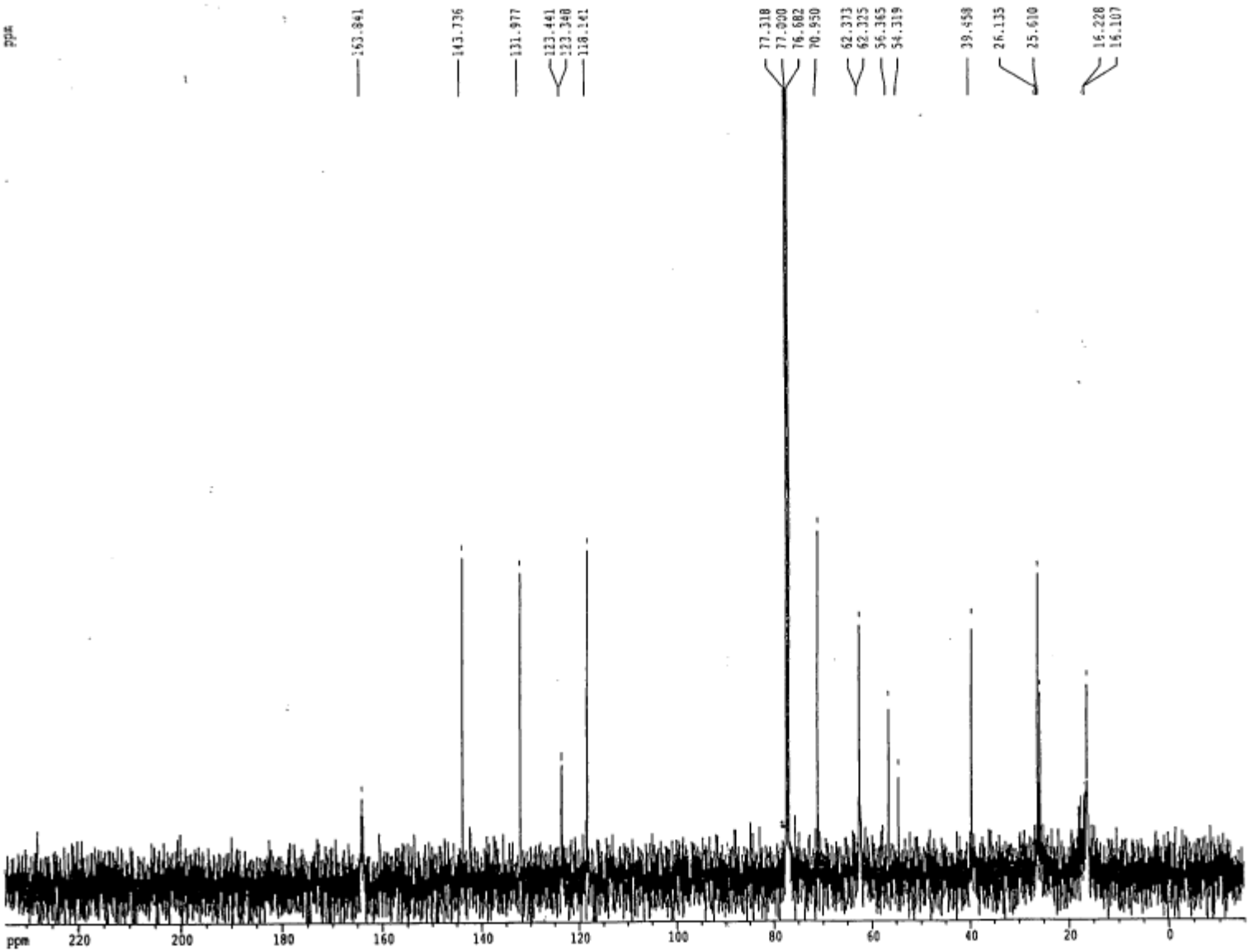
Current Data Parameters
NAME Diagnos
EXPNO 1361
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020926
Time 12.25
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 114
DW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300527 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.27467 ppm/cm
HZCM 110.70265 Hz/cm



Current Data Parameters

NAME	03ageno
EXPNO	3362
PROCNO	1

F2 - Acquisition Parameters

Date_	20020926
Time	12.42
INSTRUM	dpx400
PROBHD	5 mm BBO BB-
PULPROG	zgdc30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	25062.656 Hz
FIDRES	0.382426 Hz
AQ	1.3074932 sec
RG	3251
DW	19.950 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec

---------- CHANNEL f1 -------

NUC1	13C
P1	7.90 usec
PL1	-2.00 dB
SFO1	100.6237959 MHz

---------- CHANNEL f2 -------

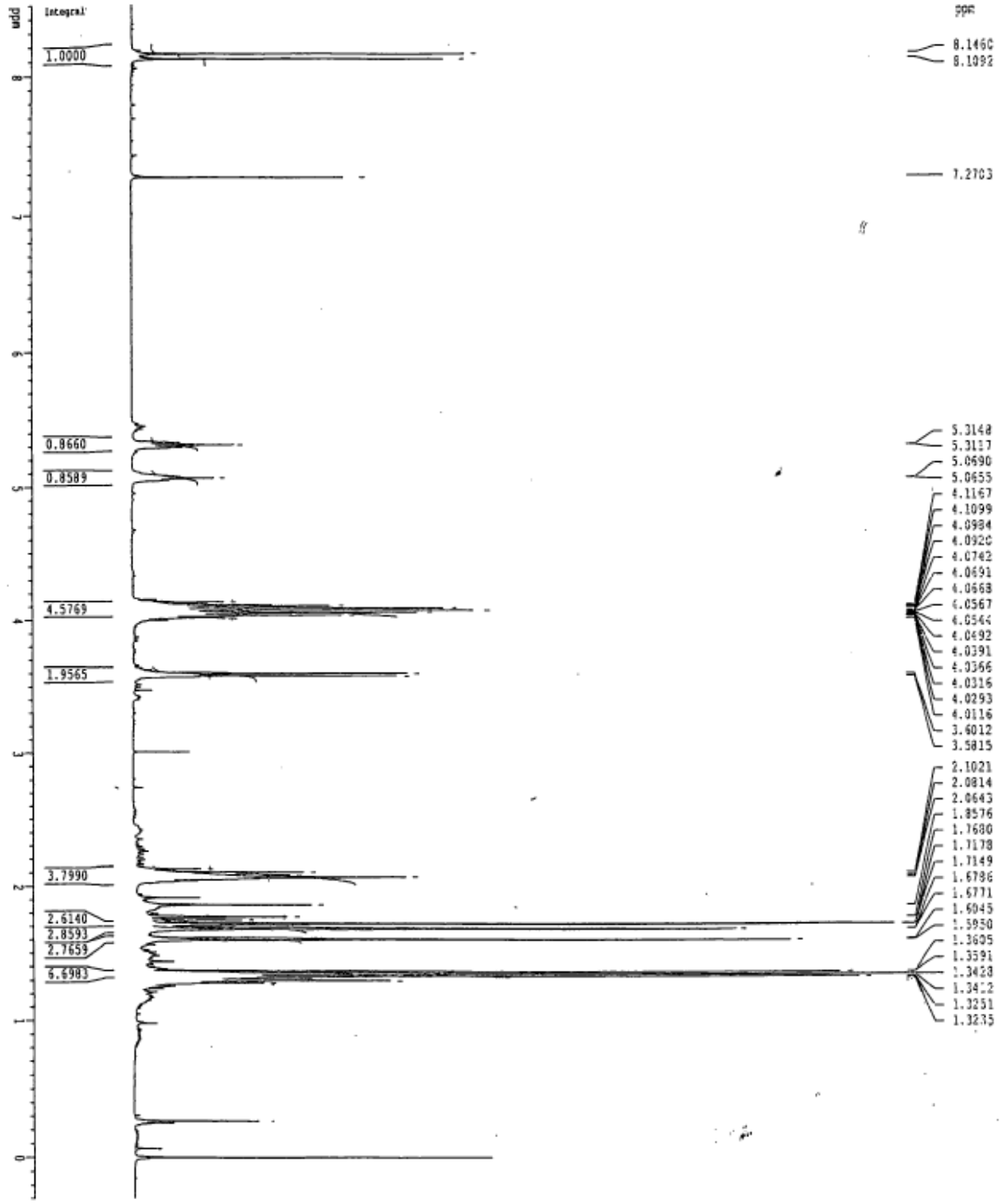
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-6.00 dB
PL12	15.50 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127752 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
F1P	234.086 ppm
F1	23552.08 Hz
F2P	-15.014 ppm
F2	-1510.58 Hz
PPMCM	8.30334 ppm/cm
HZCM	835.42194 Hz/cm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3.7990
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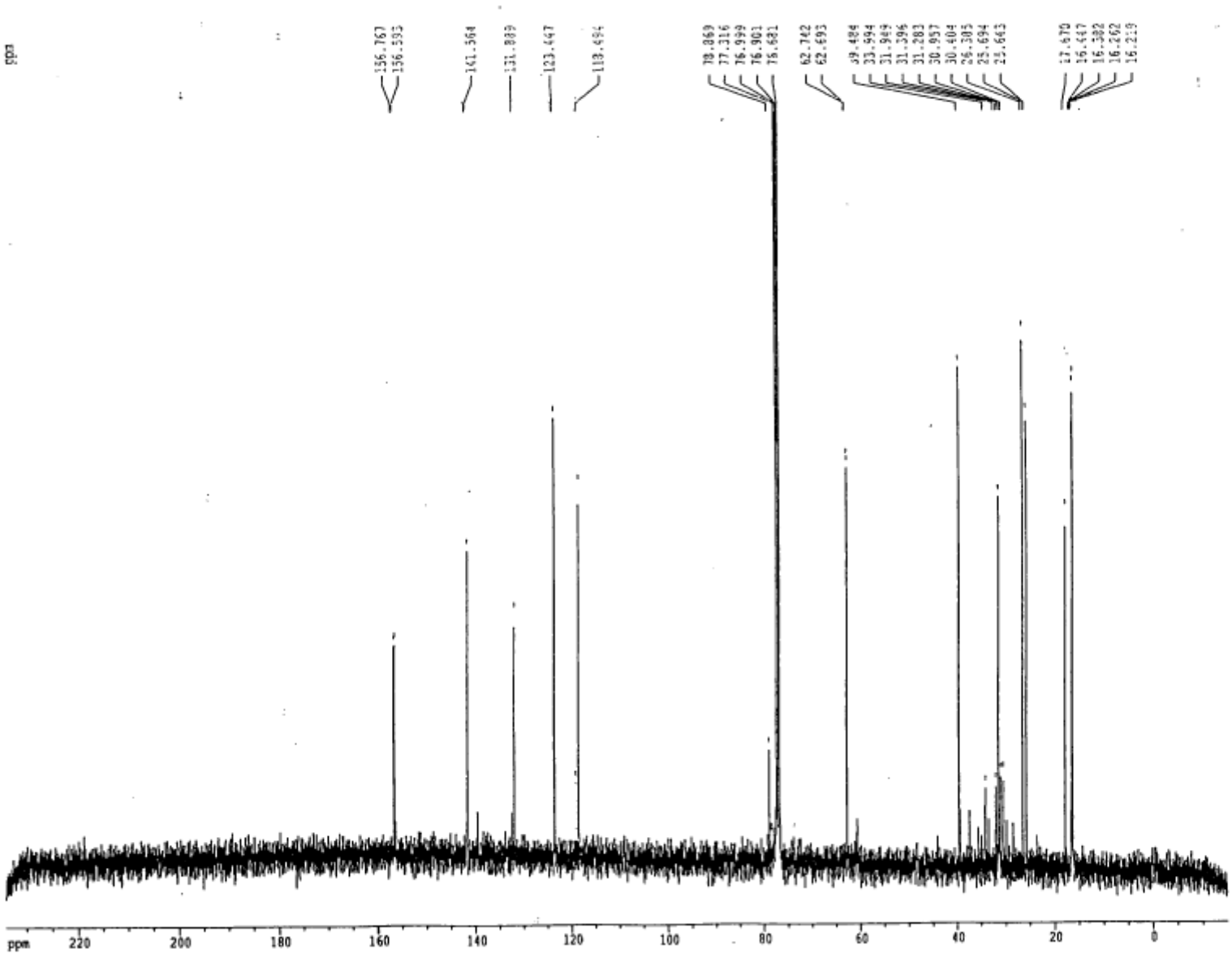
2.8593
2.7659
6.6983
8.1460
8.1092
7.2703
5.3148
5.3117
5.0690
5.0655
4.1167
4.1099
4.0984
4.0920
4.0742
4.0691
4.0668
4.0567
4.0544
4.0492
4.0391
4.0366
4.0316
4.0293
4.0116
3.6012
3.5815
2.1021
2.0814
2.0643
1.8576
1.7680
1.7178
1.7149
1.6786
1.6771
1.6045
1.5950
1.3605
1.3591
1.3428
1.3412
1.3251
1.3235
Current Data Parameters
NAME 03apono
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040216
Time 17.33
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125998 Hz
AQ 3.9715316 sec
RG 90.5
DW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
F2P 8.500 ppm
F1 3401.10 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.29333 ppm/cm
HZCM 117.37147 Hz/cm
S
I
P(O)(OEt)2
11b

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Current Data Parameters
NAME                  03ageno
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_              20040216
Time                  18.36
INSTRUM               dpx400
PROBHD     5 mm BBO BB-
PULPROG               zgdc30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         2
SWH               25062.656 Hz
FIDRES            0.382426 Hz
AQ                1.3074932 sec
RG                      6502
DW                   19.950 usec
DE                    6.00 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec

========== CHANNEL f1 ======
NUC1                     13C
P1                    7.90 usec
PL1                  -2.00 dB
SFO1           100.6237959 MHz

========== CHANNEL f2 ======
CPDPRG2              waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -6.00 dB
PL12                 10.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF             100.6127736 MHz
WDW                        EM
SSB                         0
LB                    1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                    30.00 cm
F1P                  234.102 ppm
F1                 23553.61 Hz
F2P                 -14.999 ppm
F2                -1509.05 Hz
PPMCM                8.30334 ppm/cm
HZCM               835.42188 Hz/cm
```

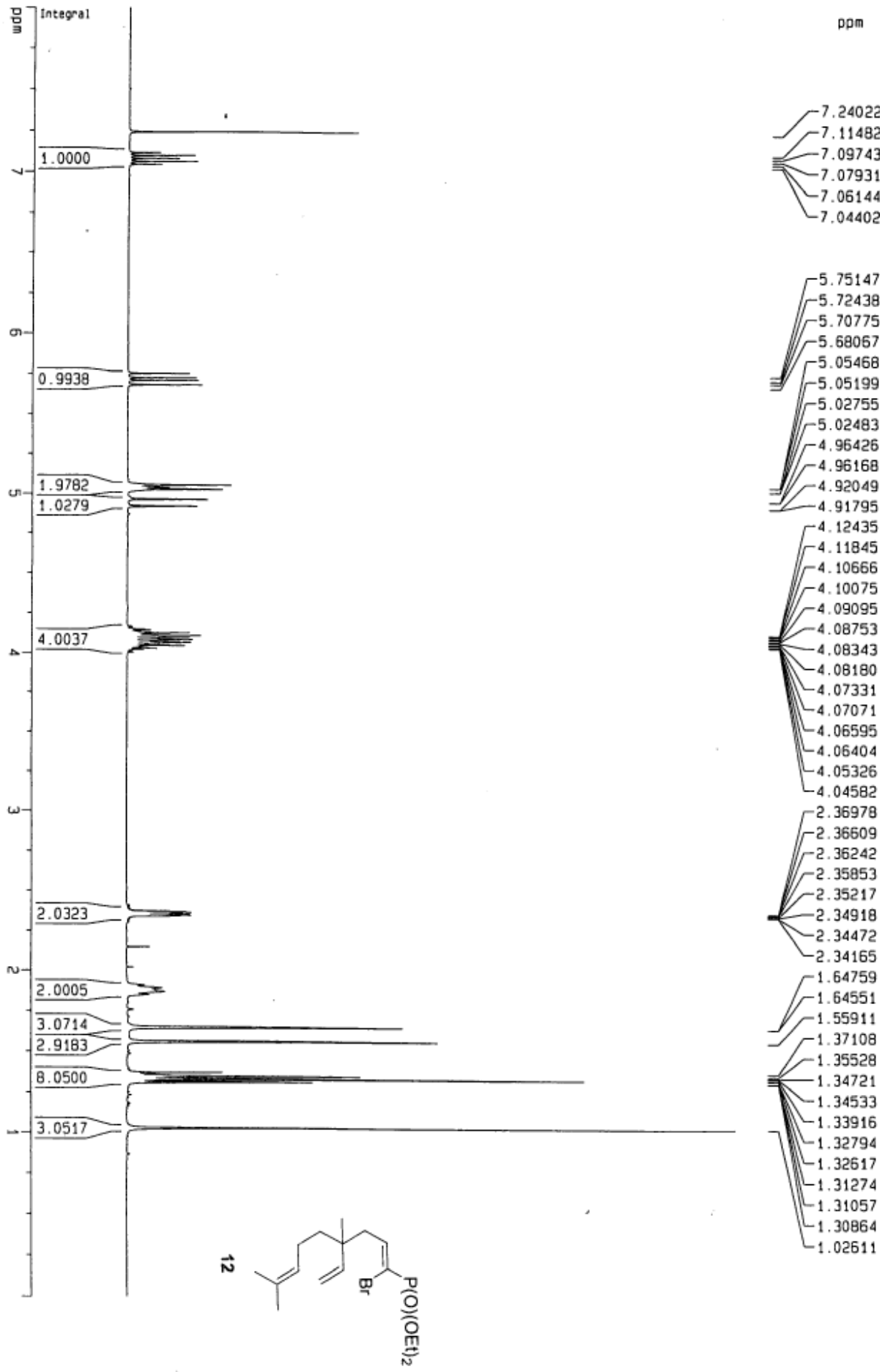
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3.0714
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8.0500
3.0517
ppm
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7.11482
7.09743
7.07931
7.06144
7.04402
5.75147
5.72438
5.70775
5.68067
5.05468
5.05199
5.02755
5.02483
4.96426
4.96168
4.92049
4.91795
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4.11845
4.10666
4.10075
4.09095
4.08753
4.08343
4.08180
4.07331
4.07071
4.06595
4.06404
4.05326
4.04582
2.36978
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2.34918
2.34472
2.34165
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1.37108
1.35528
1.34721
1.34533
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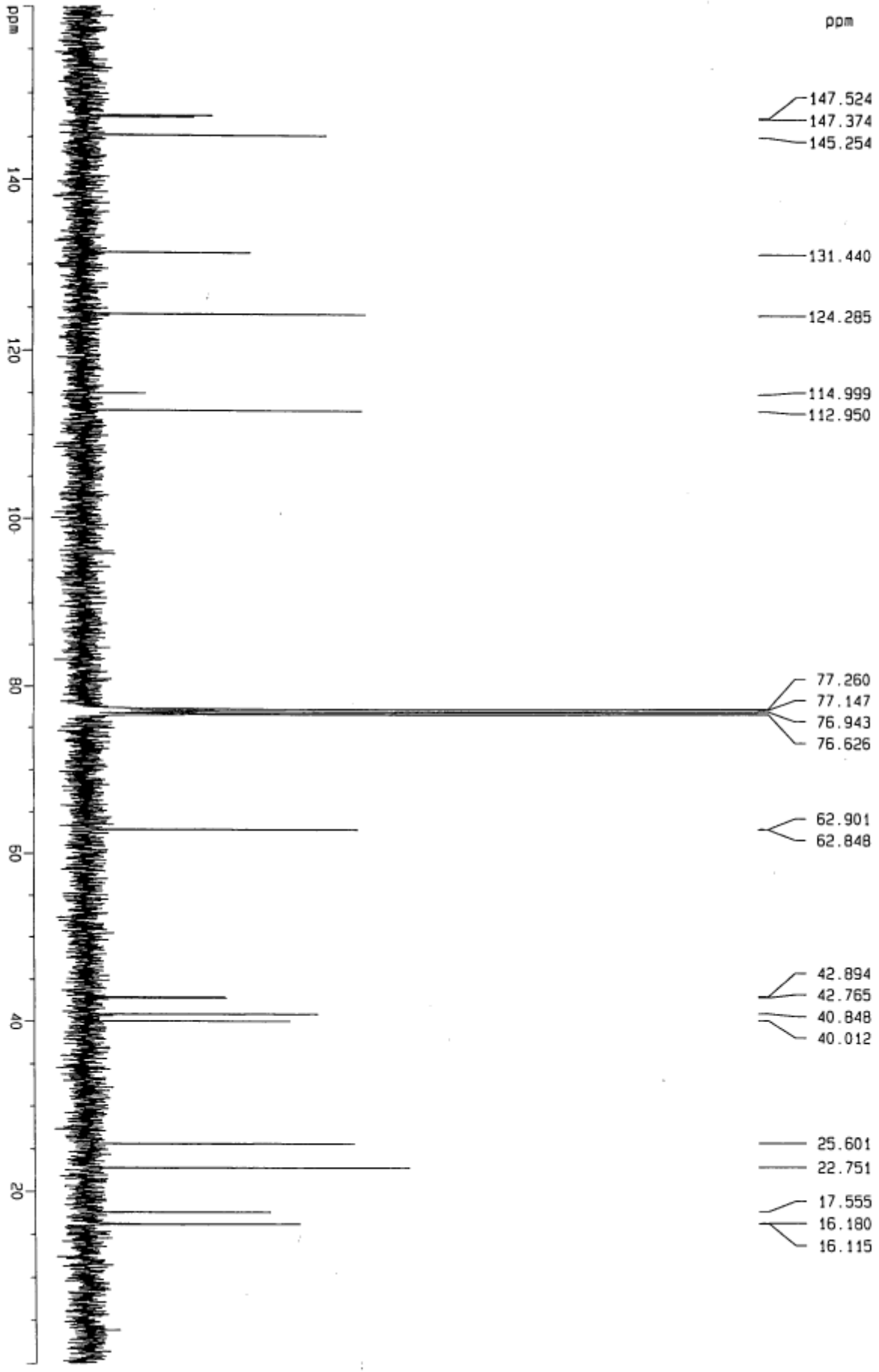
1.02611
12
Br
P(O)(OEt)2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80
60
40
20
ppm
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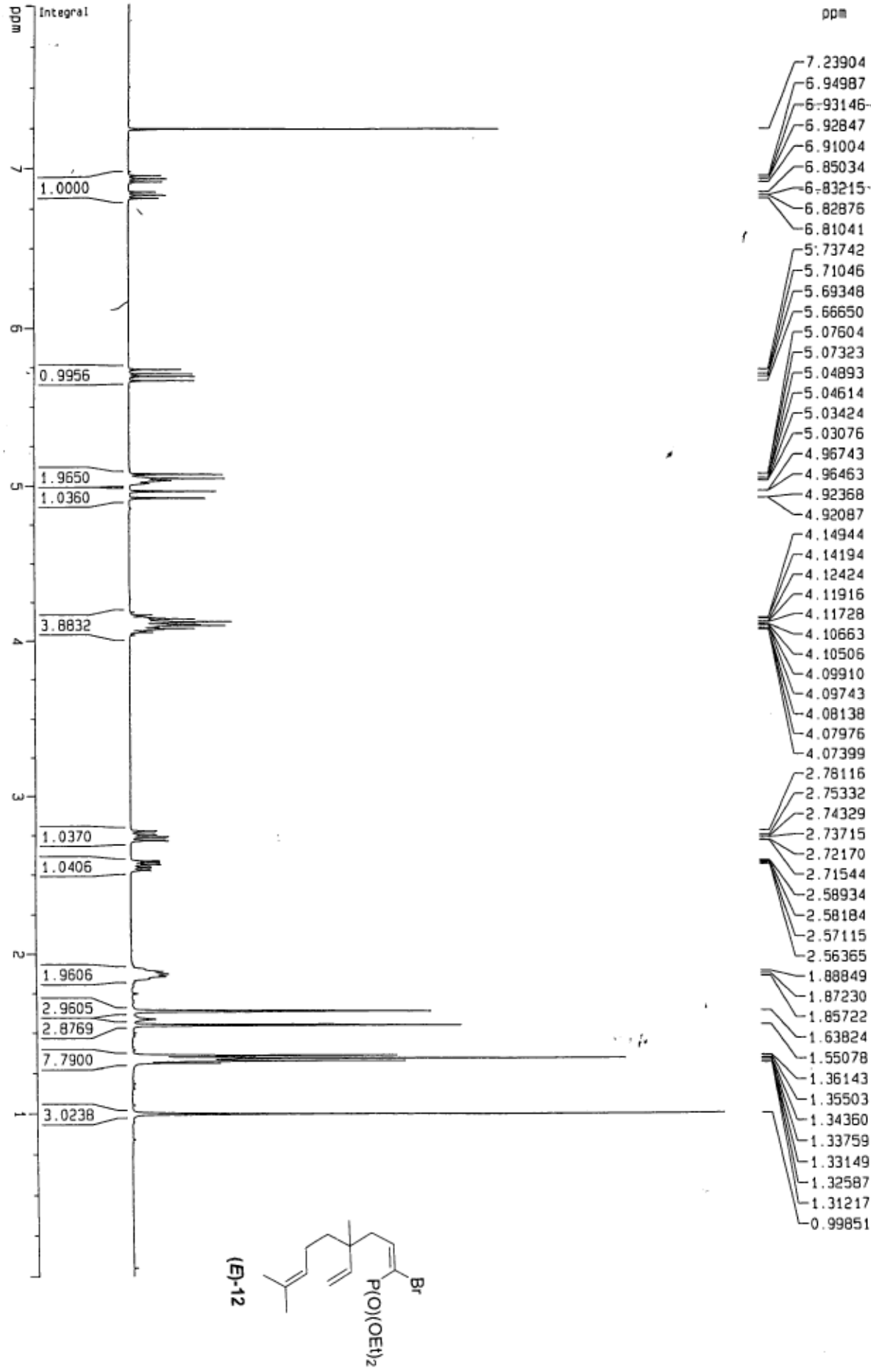
124.285
114.999
112.950
77.260
77.147
76.943
76.626
62.901
62.848
42.894
42.765
40.848
40.012
25.601
22.751
17.555
16.180
16.115


ppm
Integral
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1.0360
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1.0370
1.0406
1.9606
2.9605
2.8769
7.7900
3.0238
7.23904
6.94987
6.93146
6.92847
6.91004
6.85034
6.83215
6.82876
6.81041
5.73742
5.71046
5.69348
5.66650
5.07604
5.07323
5.04893
5.04614
5.03424
5.03076
4.96743
4.96463
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4.92087
4.14944
4.14194
4.12424
4.11916
4.11728
4.10663
4.10506
4.09910
4.09743
4.08138
4.07976
4.07399
2.78116
2.75332
2.74329
2.73715
2.72170
2.71544
2.58934
2.58184
2.57115
2.56365
1.88849
1.87230
1.85722
1.63824
1.55078
1.36143
1.35503
1.34360
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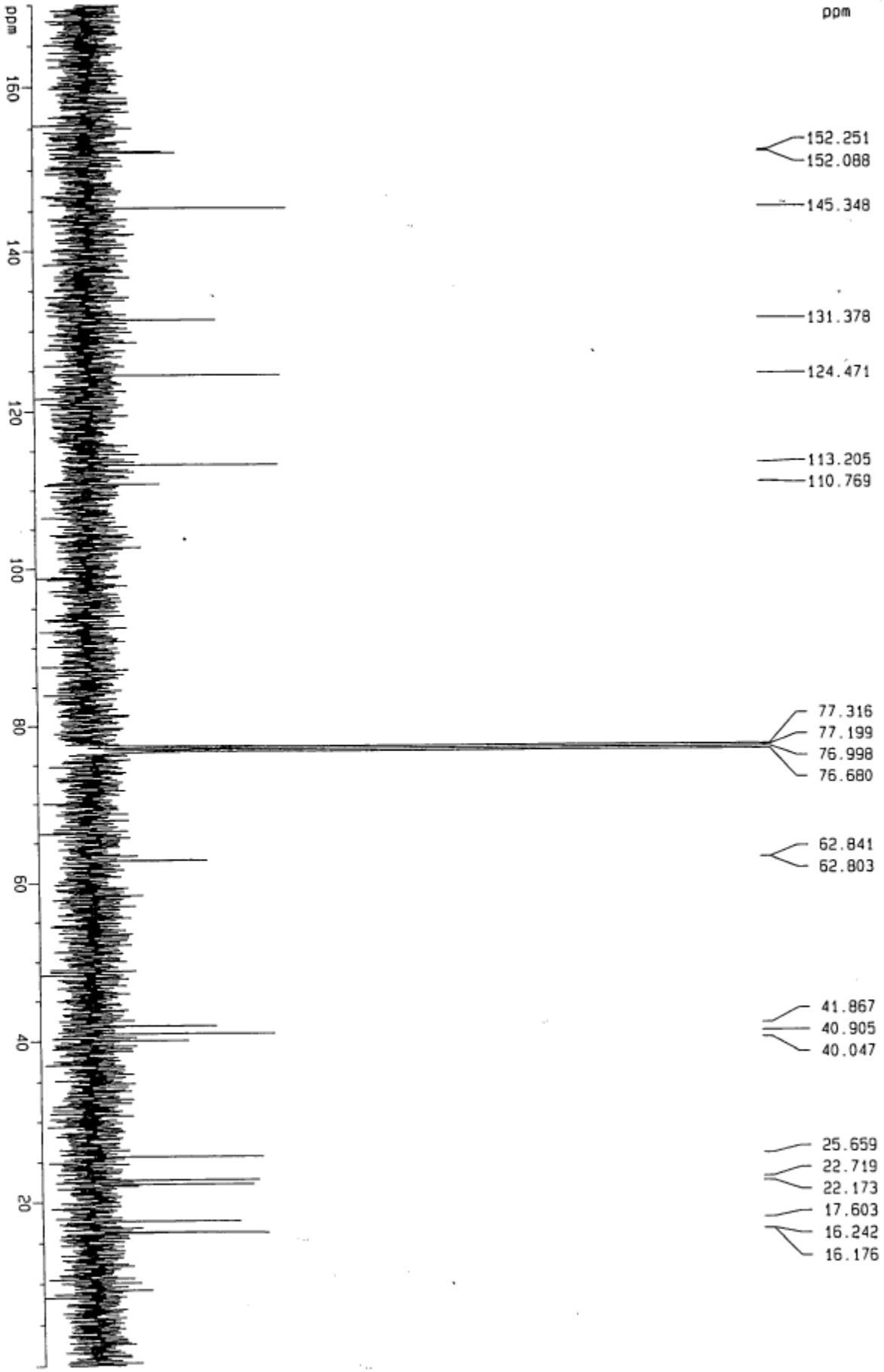
1.33149
1.32587
1.31217
0.99851
(E)-12
Br
P(O)(OEt)2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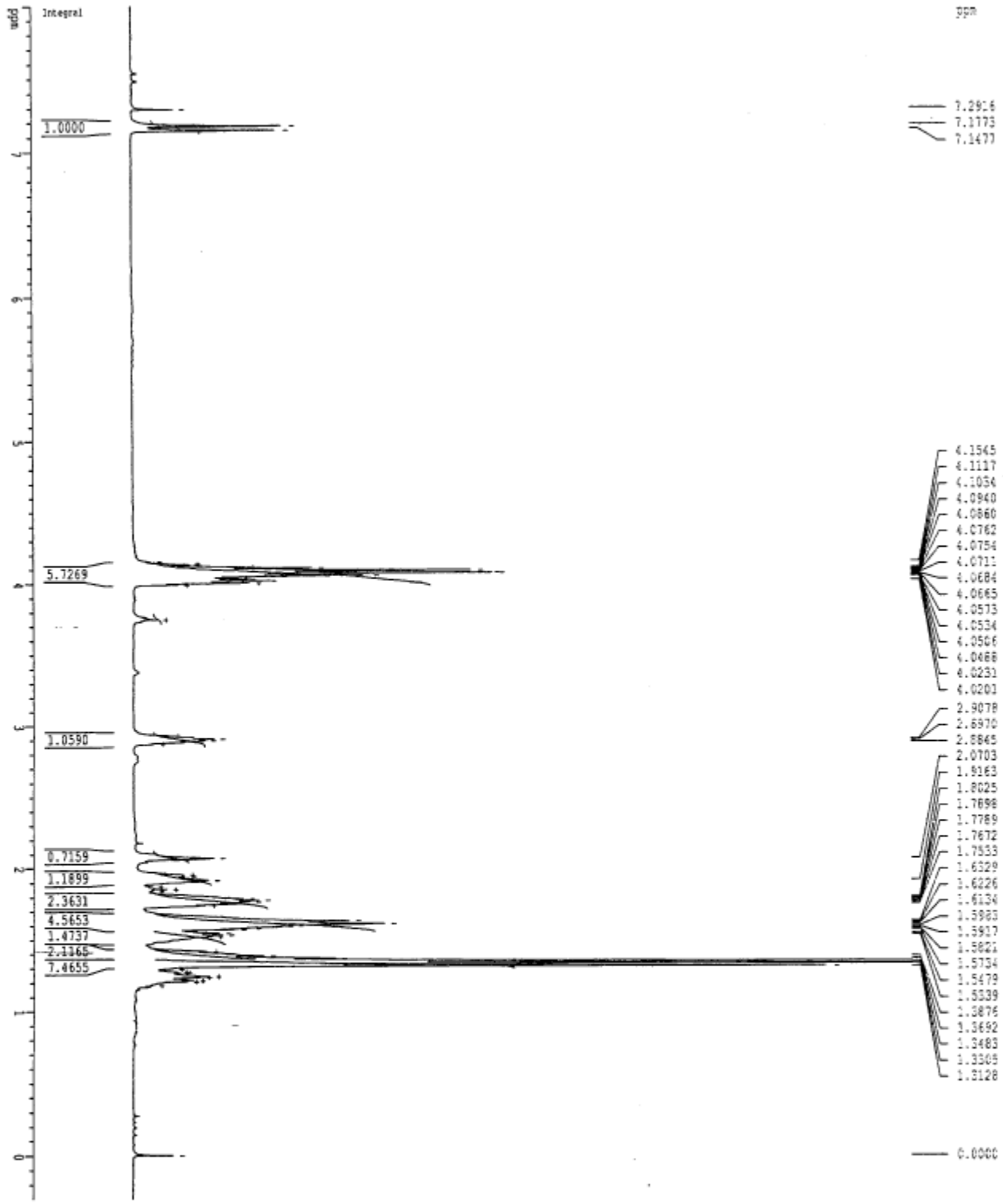
160
140
120
100
80
60
40
20
ppm
152.251
152.088
145.348
131.378
124.471
113.205
110.769
77.316
77.199
76.998
76.680
62.841
62.803
41.867
40.905
40.047
25.659
22.719
22.173
17.603
16.242
16.176


ppm
Integral
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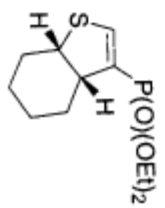
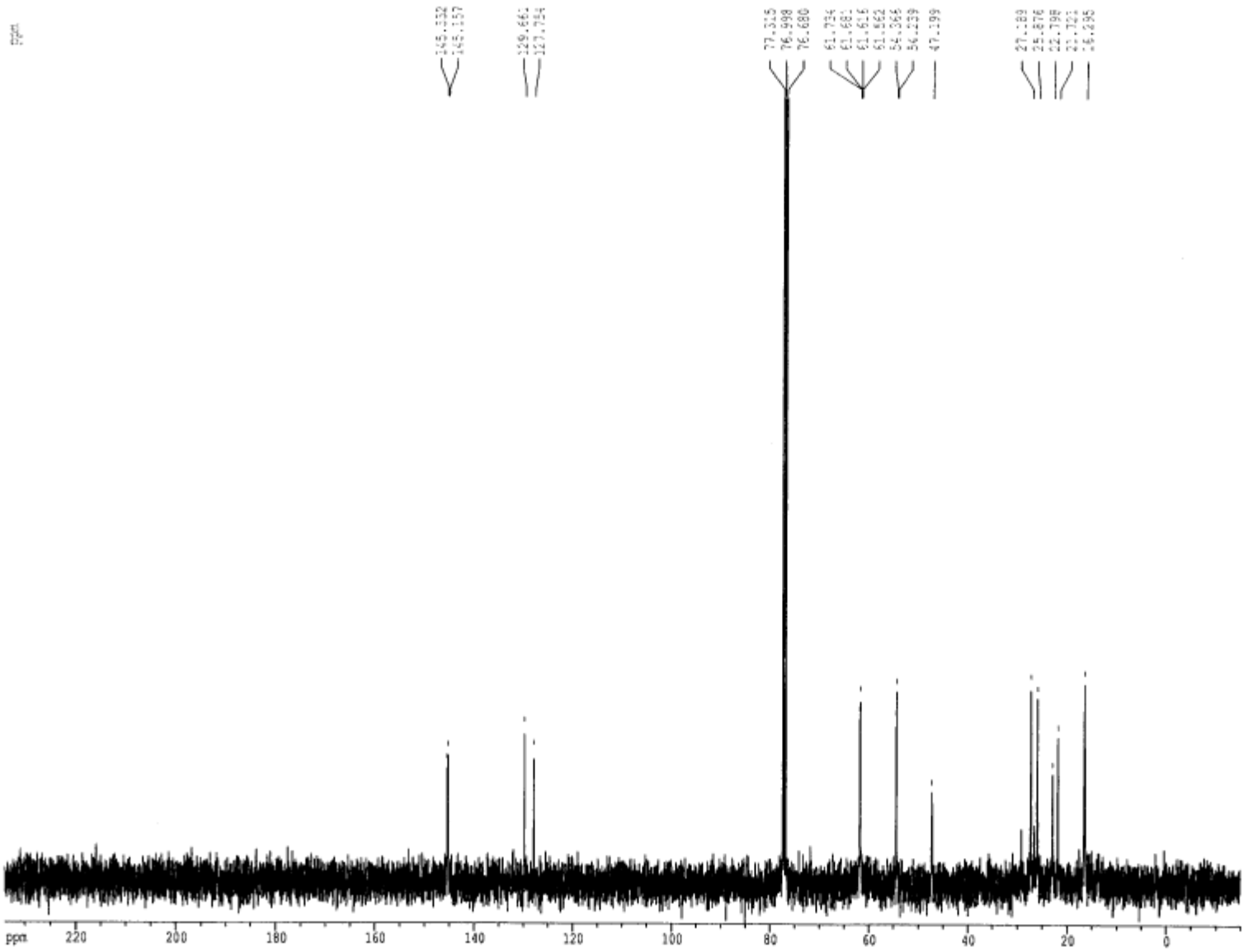
5.7269
1.0590
0.7159
1.1899
2.3631
4.5653
1.4737
2.1365
7.4655
ppm
7.2916
7.1773
7.1477
4.1545
4.1117
4.1034
4.0940
4.0860
4.0762
4.0754
4.0711
4.0684
4.0665
4.0573
4.0534
4.0506
4.0468
4.0231
4.0203
2.9078
2.6970
2.8845
2.0703
1.9163
1.8025
1.7698
1.7689
1.7672
1.7533
1.6329
1.6226
1.6134
1.5983
1.5917
1.5824
1.5734
1.5479
1.5339
1.3876
1.3692
1.3483
1.3305
1.3128
0.0000
Current Data Parameters
NAME 03agetno
EXPNO 4532
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030426
Time 19.35
INSTRUM dpx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 101.6
DW 60.600 usec
DE 4.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 2.90 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299976 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameter
CX 36.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.300 ppm
F2 -126.04 Hz
PPMCM 0.21667 ppm/cm
HZCM 110.76824 Hz/cm


S
H
H
P(O)(OEt)2

18



Current Data Parameters

NAME	03ageno
EXPNO	4533
PROCNO	1

F2 - Acquisition Parameters

Date_	20030426
Time	19.55
INSTRUM	dpx400
PROBHD	5 mm BBO BB-
PULPROG	zgdc30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	25062.656 Hz
FIDRES	0.382426 Hz
AQ	1.3074932 sec
RG	14596.5
DW	19.950 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec

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

NUC1	13C
P1	7.90 usec
PL1	-2.00 dB
SFO1	100.6237959 MHz

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

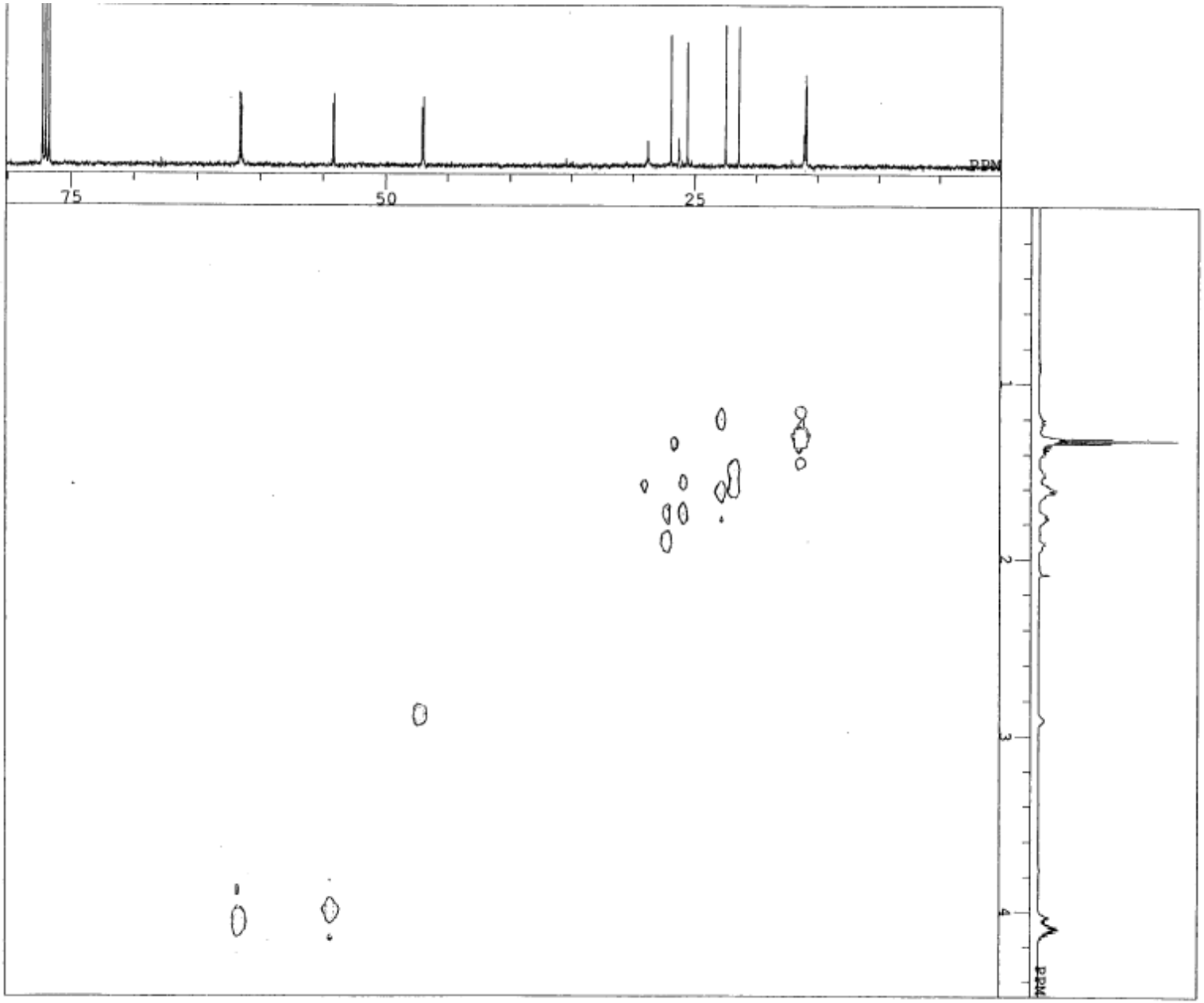
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-6.00 dB
PL12	15.50 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

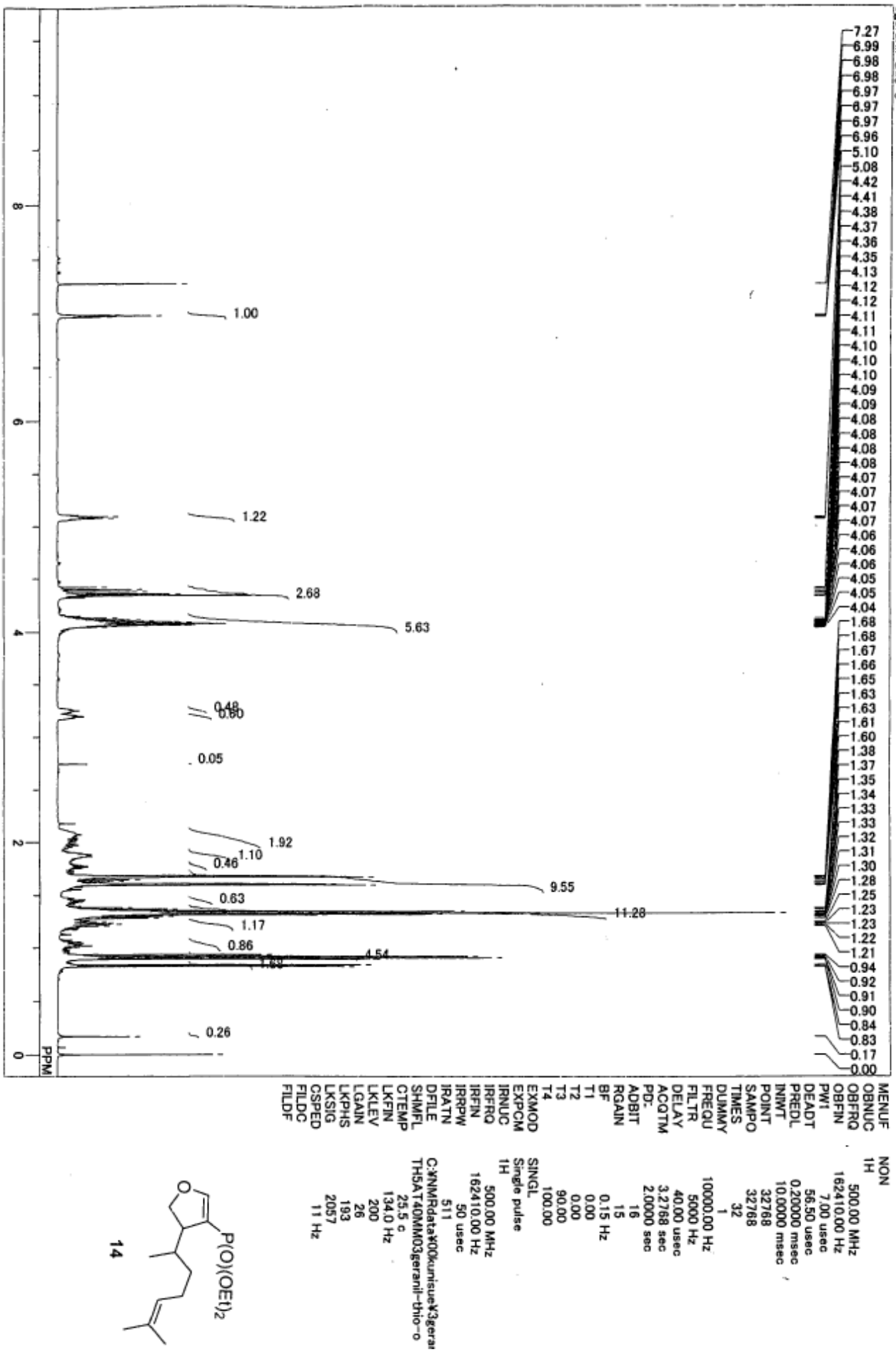
SI	32768
SF	100.6127759 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

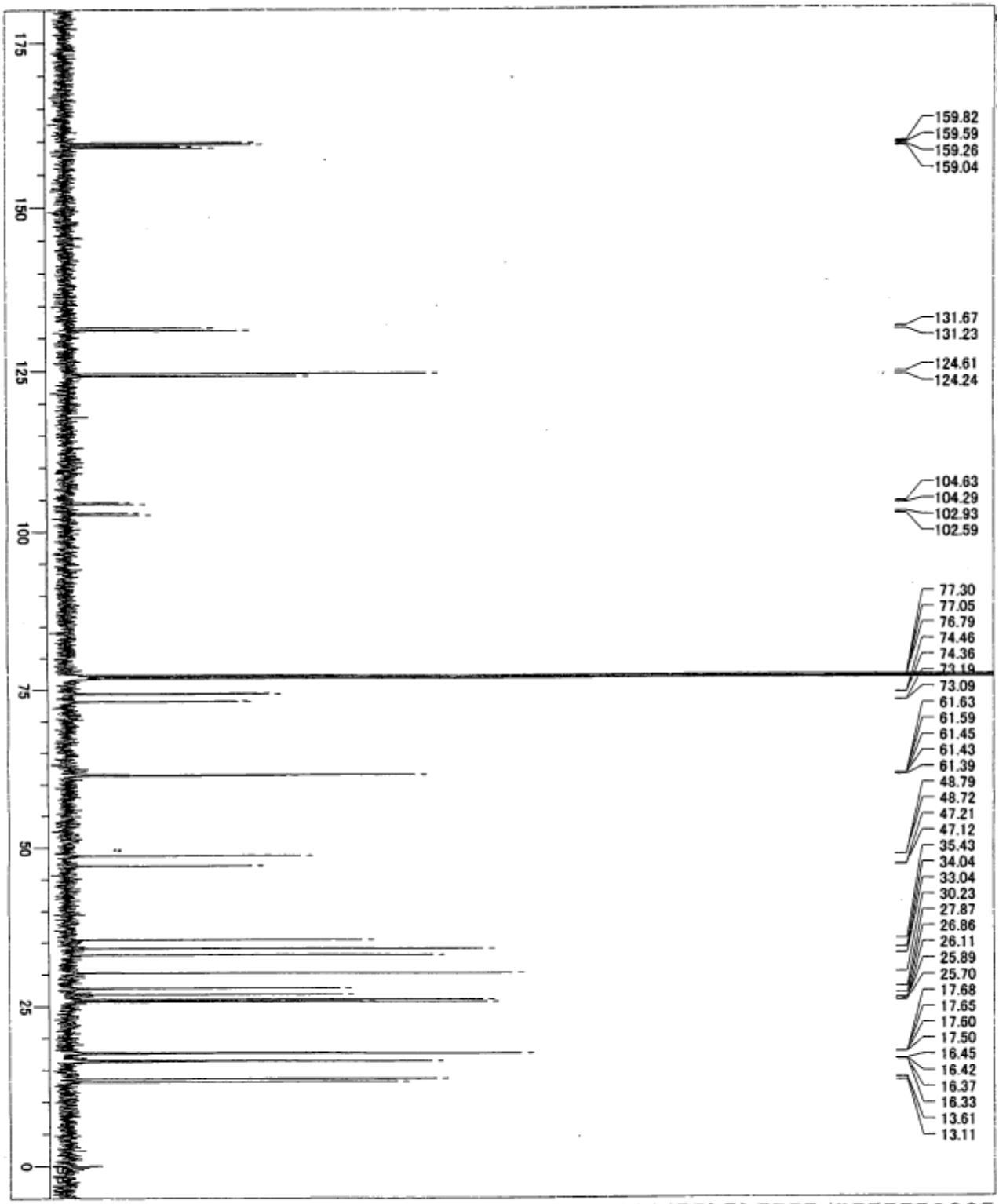
1D NMR plot parameters

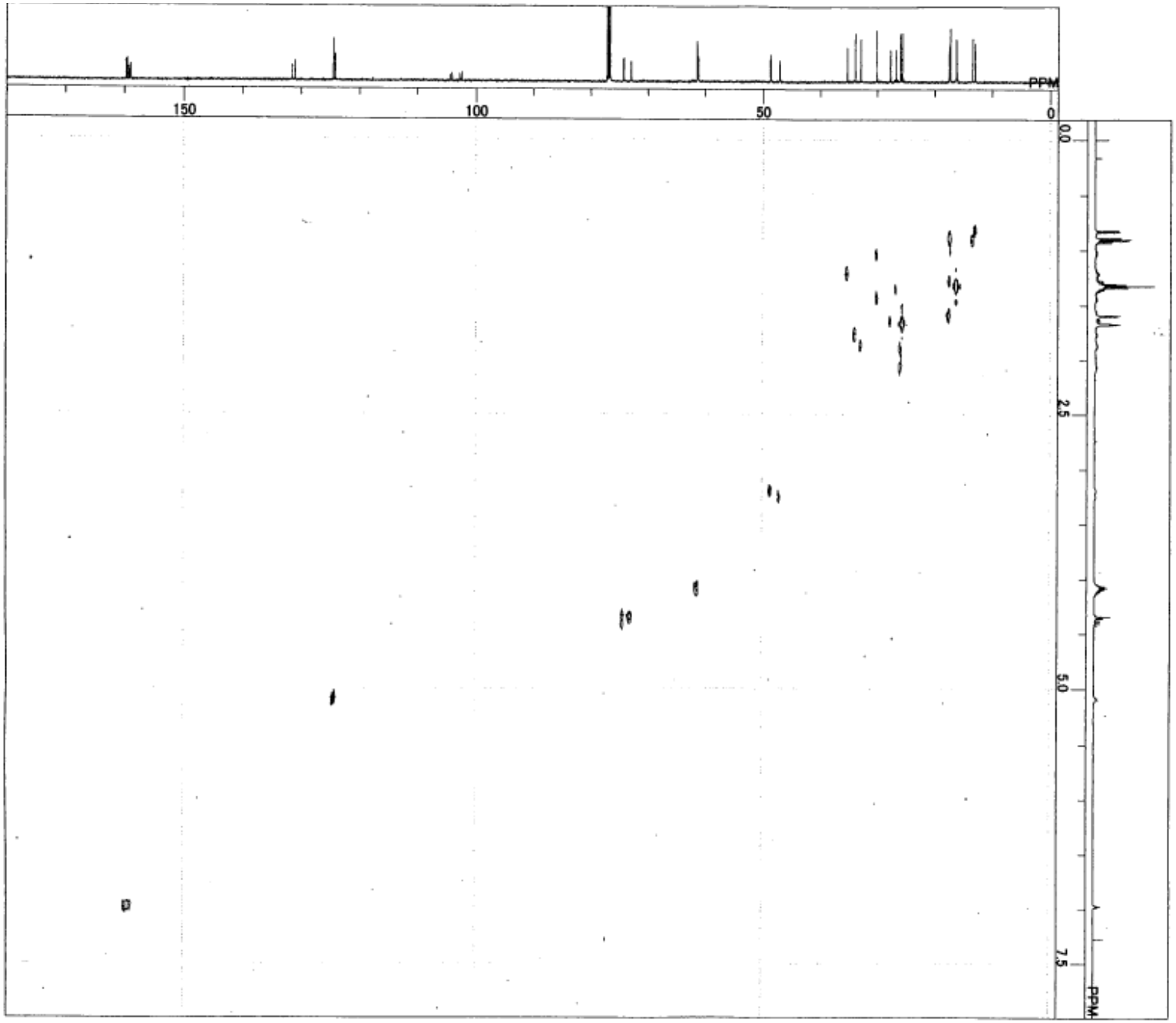
CX	30.00 cm
F1P	234.079 ppm
F1	23551.31 Hz
F2P	-15.021 ppm
F2	-1511.34 Hz
PPMCM	8.30334 ppm/cm
HZCM	835.42188 Hz/cm



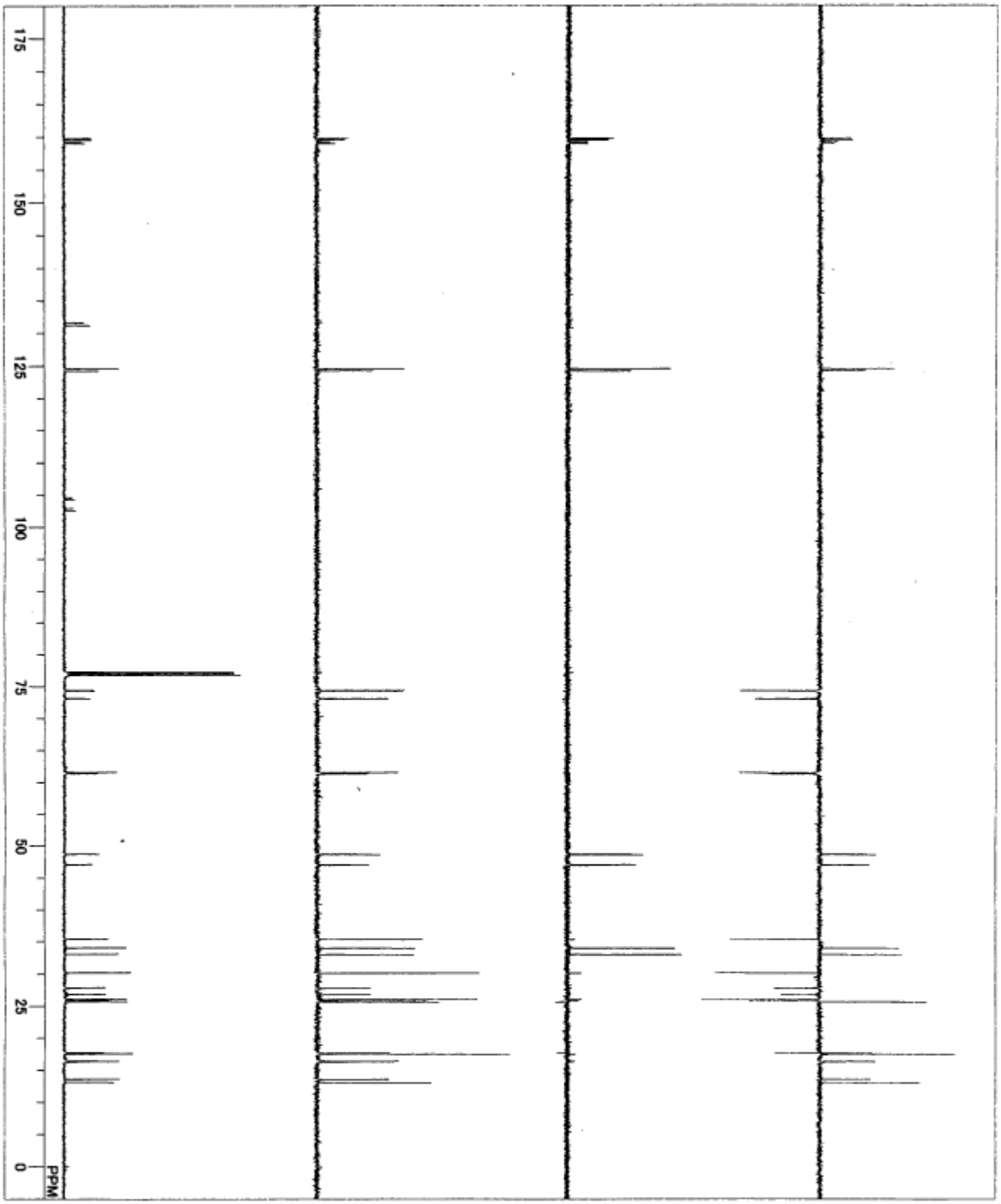
DFILE	C:\NMRdata\00kuni
COMNT	ta453
DATIM	Mon Apr 28 14:29:
EXMOD	CHSHF
OBNUC	13C
OBFRQ	125.65 MHz
OBSET	0.00 KHz
OBFIN	127892.80 Hz
POINT	512
FREQU	25125.63 Hz
CLPNT	256
TODAT	256
CLFRQ	5316.60 Hz
SCANS	32
ACQTM	0.0204 sec
PD	1.2000 sec
PW1	9.00 usec
PW2	26.00 usec
PW3	14.00 usec
PI1	80.0000 msec
PI2	1.0000 msec
PI3	20.0000 msec
IRNUC	1H
CTEMP	22.3 c
SLVNT	CDCL3
EXREF	77.00 ppm
CLEXR	0.00
RGAIN	30

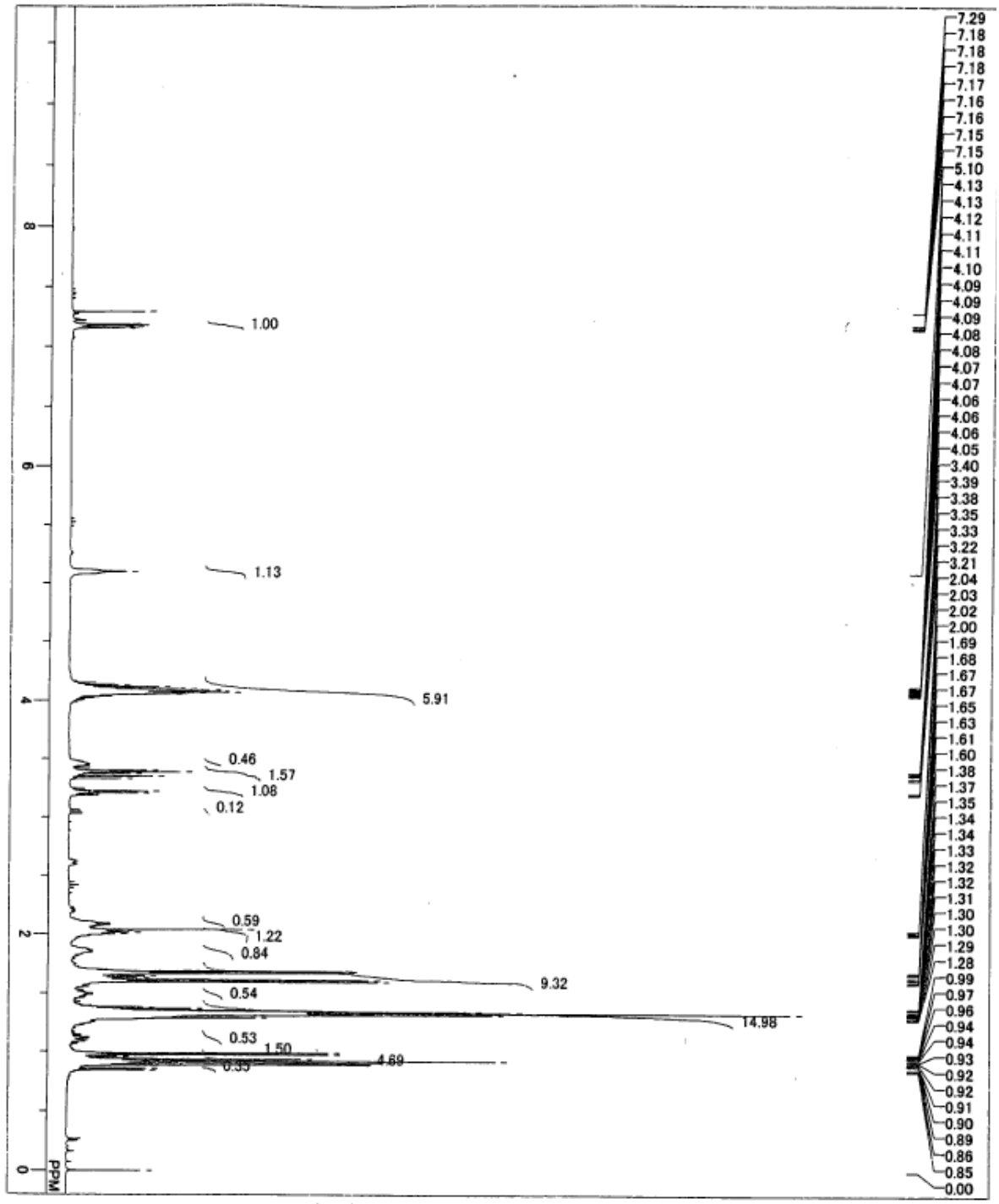

C:¥NMRdata¥00kunisue¥3geranil-thio-o1NON_E1.als
3geranil-thio-o
7.27
6.99
6.98
6.98
6.97
6.97
6.97
6.96
5.10
5.08
4.42
4.41
4.38
4.37
4.36
4.35
4.13
4.12
4.12
4.11
4.11
4.10
4.10
4.10
4.09
4.09
4.08
4.08
4.08
4.08
4.08
4.07
4.07
4.07
4.07
4.06
4.06
4.06
4.06
4.05
4.05
4.04
1.68
1.68
1.67
1.66
1.65
1.63
1.63
1.61
1.60
1.38
1.37
1.35
1.34
1.33
1.33
1.32
1.31
1.30
1.28
1.25
1.23
1.23
1.22
1.21
0.94
0.92
0.91
0.90
0.84
0.83
0.17
0.00
1.00
1.22
2.68
5.63
0.48
0.60
0.05
1.92
1.10
0.46
9.55
0.63
11.28
1.17
0.86
4.54
0.26
PPM
MENUF NON
OBNUC 1H
OBFRQ 500.00 MHz
OBFIN 162410.00 Hz
PW1 7.00 usec
DEADT 56.50 usec
PREDL 0.20000 msec
INWT 10.0000 msec
POINT 32768
SAMPO 32768
TIMES 32
DUMMY 1
FREQU 10000.00 Hz
FILTR 5000 Hz
DELAY 40.00 usec
ACQTM 3.2768 sec
PD- 2.0000 sec
ADBIT 16
RGAIN 15
BF 0.15 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD SINGL
EXPCM Single pulse
IRNUC 1H
IRFRQ 500.00 MHz
IRFIN 162410.00 Hz
IRRPW 50 usec
IRATN 511
DFILE C:¥NMRdata¥00kunisue¥3geran
SHMFL TH5AT40MM03geranil-thio-o
CTEMP 25.5 c
LKFIN 134.0 Hz
LKLEV 200
LGAIN 26
LKPHS 193
LKSIG 2057
GSPED 11 Hz
FILDC
FILDF
P(O)(OEt)2
14

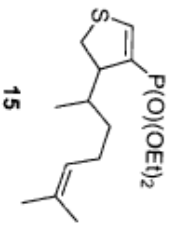

159.82
159.59
159.26
159.04
131.67
131.23
124.61
124.24
104.63
104.29
102.93
102.59
77.30
77.05
76.79
74.46
74.36
73.19
73.09
61.63
61.59
61.45
61.43
61.39
48.79
48.72
47.21
47.12
35.43
34.04
33.04
30.23
27.87
26.86
26.11
25.89
25.70
17.68
17.65
17.60
17.50
16.45
16.42
16.37
16.33
13.61
13.11
175
150
125
100
75
50
25
0
PPM
MENUF BCM
OBNUC 13C
OBFRQ 125.65 MHz
OBFIN 127958.00 Hz
PW1 4.50 usec
DEADT 15.45 usec
PREDL 0.20000 msec
INIWT 10.0000 msec
POINT 32768
SAMPO 32768
TIMES 1200
DUMMY 1
FREQU 33898.30 Hz
FILTR 16950 Hz
DELAY 11.80 usec
ACQTM 0.9667 sec
PD 2.0000 sec
ADBIT 16
RGAIN 29
BF 1.20 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD SINGL
EXPCM Single pulse
IRNUC 1H
IRFRQ 500.00 MHz
IRFIN 162410.00 Hz
IRRPW 50 usec
IRATN 511
DFILE C:¥NMRdata¥00k
SHMFL TH5AT40MM03g
CTEMP 25.9 c
LKFIN 134.0 Hz
LKLEV 200
LGAIN 26
LKPHS 193
LKSIG 2062
CSPED 11 Hz
FILDC
FILDF



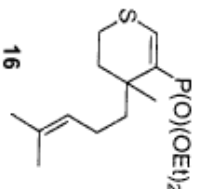
DFILE	C:¥NMRdata¥00k
EXMOD	CHSHF
IRMOD	IRLV2
COMNT	3geranil-thio-o
OBNUC	13C
OBSET	0.00 KHz
OBATN	511
FREQU	25380.71 Hz
POINT	1024
INTVL	39.4000 usec
CLFRQ	5316.32 Hz
CLPNT	256
CINTV	188.10 usec
TODAT	256
TIMES	32
SCANS	32
ACQTM	0.0403 sec
PD	1.2000 sec
PW1	9.00 usec
PW2	26.00 usec
PW3	14.60 usec
PI1	80.0000 msec
PI2	1.0000 msec
PI3	20.0000 msec
IRNUC	1H
IRSET	0.00 KHz
IRATN	511
IRRPW	50 usec
TRNUC	1H
TRSET	0.00 KHz
TRATN	511
TRRPW	0 usec
CTEMP	24.8 c
CSPED	14 Hz
SLVNT	CDCL3
LOOP1	1
XS	0.00 Hz
CXS	
XE	25380.71 Hz
CXE	
THTOP	
THBTM	
DEADT	5.00 usec
DELAY	15.36 usec
CINWT	10.00 usec


175
150
125
100
75
50
25
0
PPM
MENUF BCM
OBNUC 13C
OBFRQ 125.65 MHz
OBFIN 127958.00 Hz
PW1 4.50 usec
DEADT 15.45 usec
PREDL 0.20000 msec
INIWT 10.0000 msec
POINT 32768
SAMPO 32768
TIMES 1200
DUMMY 1
FREQU 33898.30 Hz
FILTR 16950 Hz
DELAY 11.80 usec
ACQTM 0.9667 sec
PD 2.0000 sec
ADBIT 16
RGAIN 29
BF 1.20 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD SINGL
EXPCM Single pulse
IRNUC 1H
IRFRQ 500.00 MHz
IRFIN 162410.00 Hz
IRPPW 50 usec
IRATN 511
DFILE C:¥NMRdata¥OOku
SHMFL TH5AT40MM03ger
CTEMP 25.9 c
LKFIN 134.0 Hz
LKLEV 200
LGAIN 26
LKPHS 193
LKSIG 2062
CSPED 11 Hz
FILDC
FILDF

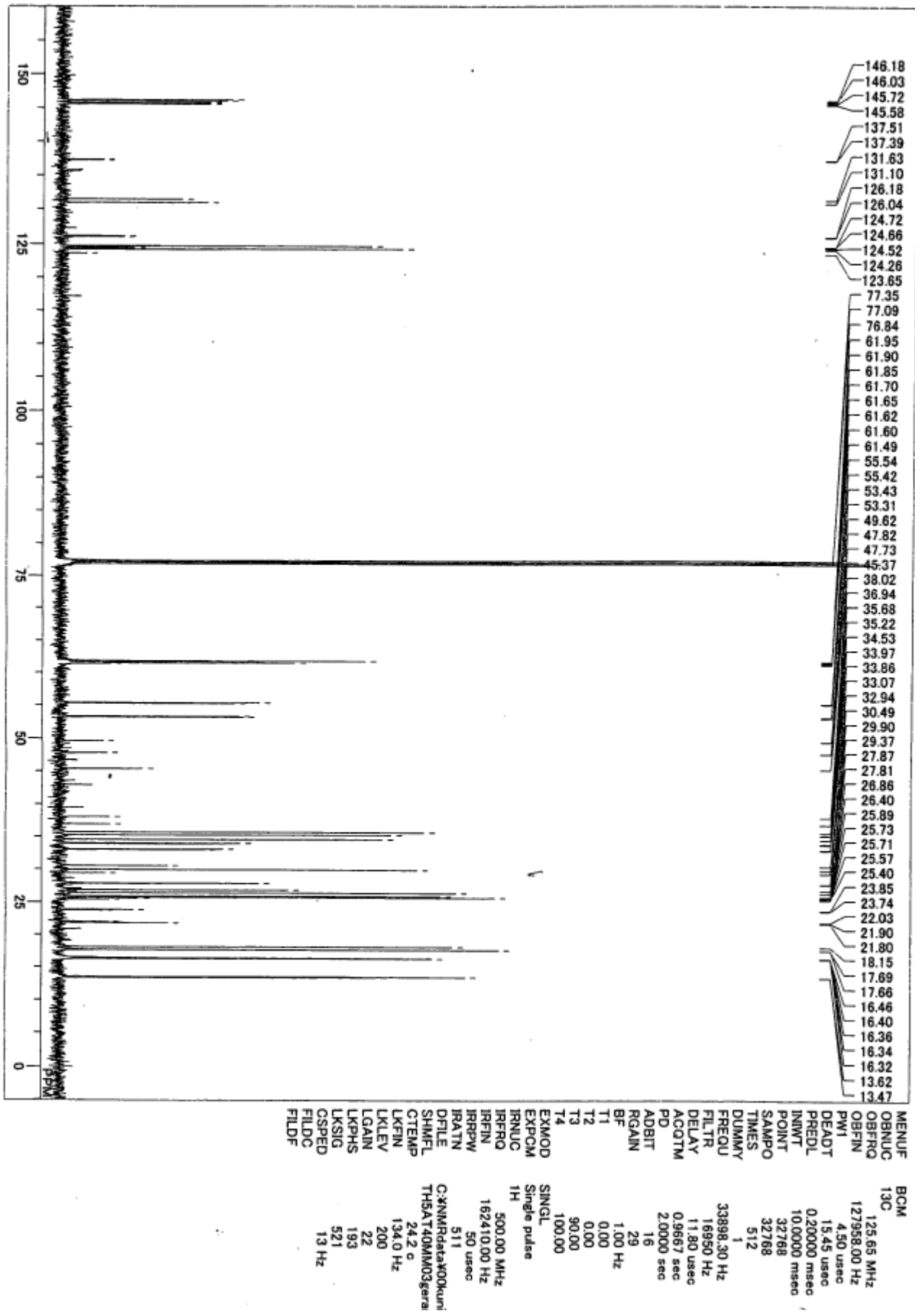

1.00
1.13
5.91
0.46
1.57
1.08
0.12
0.59
1.22
0.84
9.32
0.54
14.98
0.53
1.50
0.35
4.69
PPM
0
2
4
6
8

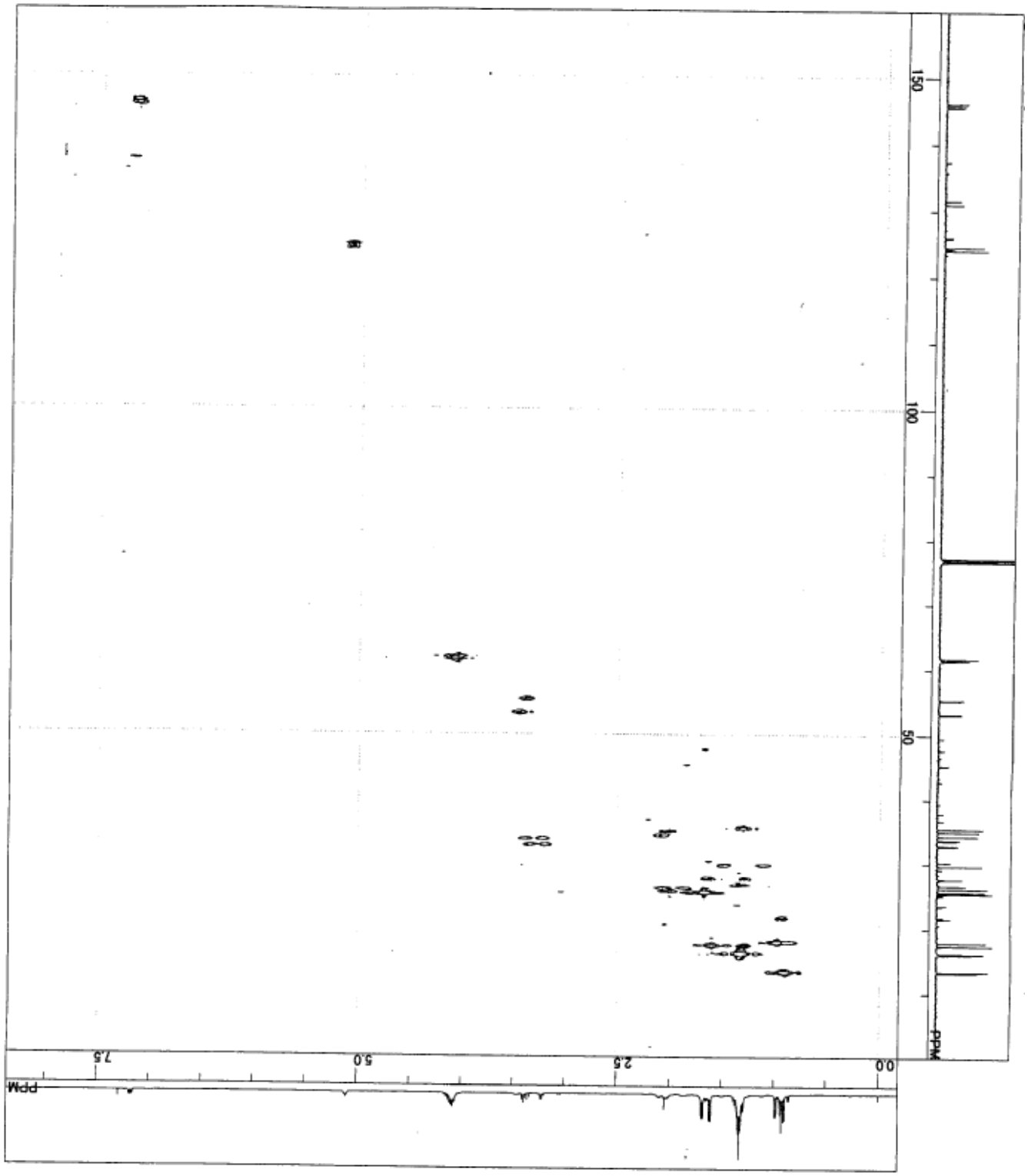

S
P(O)(OEt)2

15

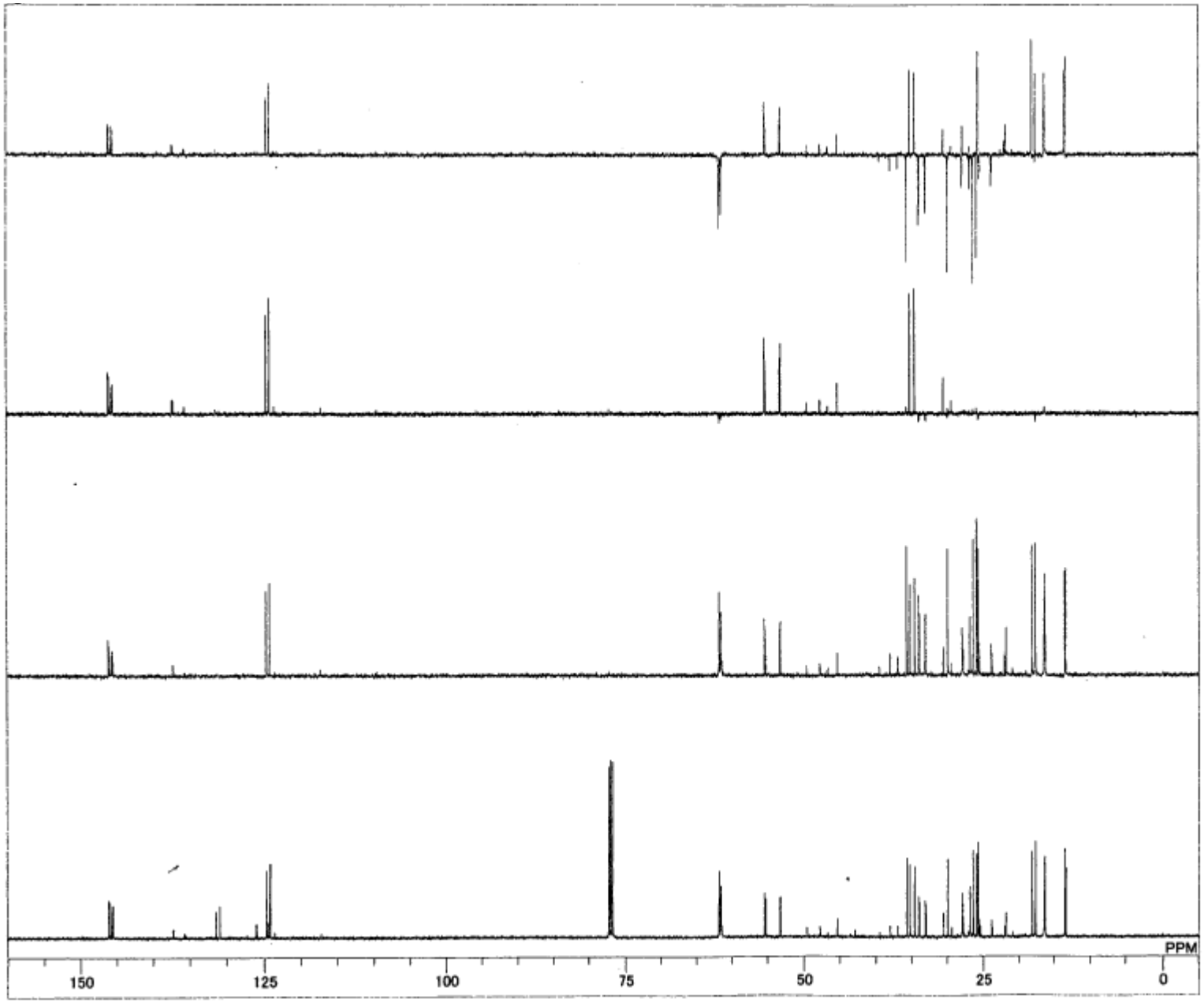

S
P(O)(OEt)2

16

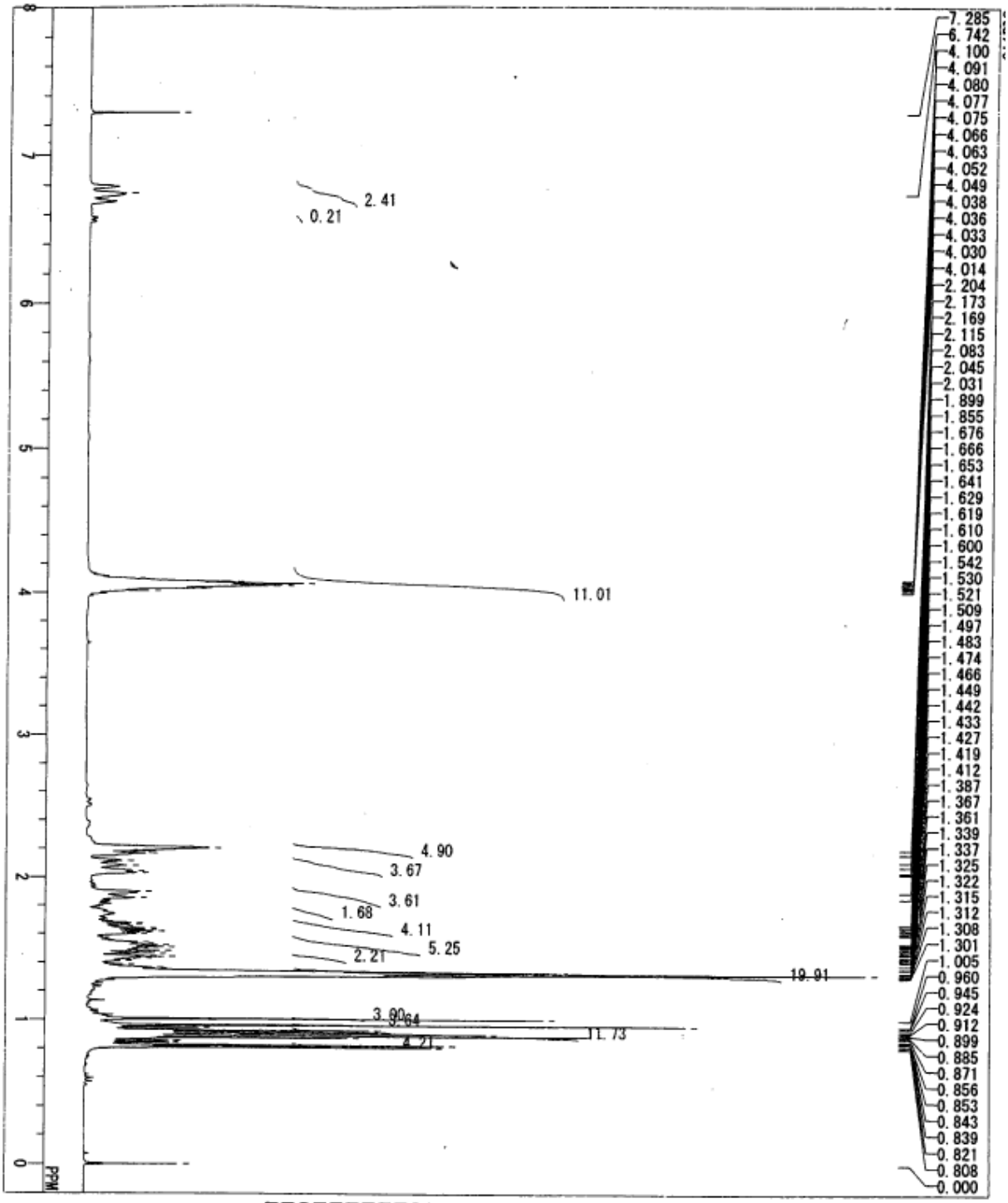

146.18
146.03
145.72
145.58
137.51
137.39
131.63
131.10
126.18
126.04
124.72
124.66
124.52
124.26
123.65
77.35
77.09
76.84
61.95
61.90
61.85
61.70
61.65
61.62
61.60
61.49
55.54
55.42
53.43
53.31
49.62
47.82
47.73
45.37
38.02
36.94
35.68
35.22
34.53
33.97
33.86
33.07
32.94
30.49
29.90
29.37
27.87
27.81
26.86
26.40
25.89
25.73
25.71
25.57
25.40
23.85
23.74
22.03
21.90
21.80
18.15
17.69
17.66
16.46
16.40
16.36
16.34
16.32
13.62
13.47
150
125
100
75
50
25
0
PPM
MENUF
OBNUC
OBFRQ
OBFIN
PW1
DEADT
PREDL
INIWT
POINT
SAMPO
TIMES
DUMMY
FREQU
FILTR
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IRFRQ
IRFIN
IRRPW
IRATN
DFILE
SHMFL
CTEMP
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
BCM
13C
125.65 MHz
127958.00 Hz
4.50 usec
15.45 usec
0.20000 msec
10.0000 msec
32768
32768
512
1
33898.30 Hz
16950 Hz
11.80 usec
0.9667 sec
2.0000 sec
16
29
1.00 Hz
0.00
0.00
90.00
100.00
SINGL
Single pulse
1H
500.00 MHz
162410.00 Hz
50 usec
511
C:¥NMRdata¥OOkuni
TH5AT40MM03gerai
24.2 c
134.0 Hz
200
22
193
521
13 Hz



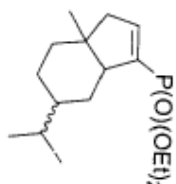
DFILE C:¥NMRdata¥00
EXMOD CHSHF
IRMOD IRLV2
COMNT 3geranil-thio-s
OBNUC 13C
OBSET 0.00 KHz
OBATN 511
FREQU 25125.63 Hz
POINT 1024
INTVL 39.8000 usec
CLFRQ 5316.32 Hz
CLPNT 256
CINTV 188.10 usec
TODAT 256
TIMES 32
SCANS 32
ACQTM 0.0408 sec
PD 1.2000 sec
PW1 9.00 usec
PW2 26.00 usec
PW3 14.60 usec
PI1 80.0000 msec
PI2 1.0000 msec
PI3 20.0000 msec
IRNUC 1H
IRSET 0.00 KHz
IRATN 511
IRRPW 50 usec
TRNUC 1H
TRSET 0.00 KHz
TRATN 511
TRRPW 0 usec
CTEMP 26.2 c
CSPED 10 Hz
SLVNT CDCL3
LOOP1 1
XS 0.00 Hz
CXS
XE 25125.63 Hz
CXE
THTOP
THBTM
DEADT 5.00 usec
DELAY 15.58 usec
CINWT 10.00 usec



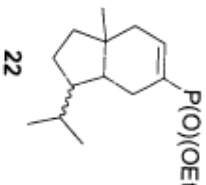
MENUF	BCM
OBNUC	13C
OBFRQ	125.65 MHz
OBFIN	127958.00 Hz
PW1	4.50 usec
DEADT	15.45 usec
PREDL	0.20000 msec
INIWT	10.0000 msec
POINT	32768
SAMPO	32768
TIMES	512
DUMMY	1
FREQU	33898.30 Hz
FILTR	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0000 sec
ADBIT	16
RGAIN	29
BF	1.00 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	SINGL
EXPCM	Single pulse
IRNUC	1H
IRFRQ	500.00 MHz
IRFIN	162410.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	C:¥NMRdata¥00ku
SHMFL	TH5AT40MM03ger
CTEMP	24.2 c
LKFIN	134.0 Hz
LKLEV	200
LGAIN	22
LKPHS	193
LKSIG	521
CSPED	13 Hz
FILDC	
FILDF	

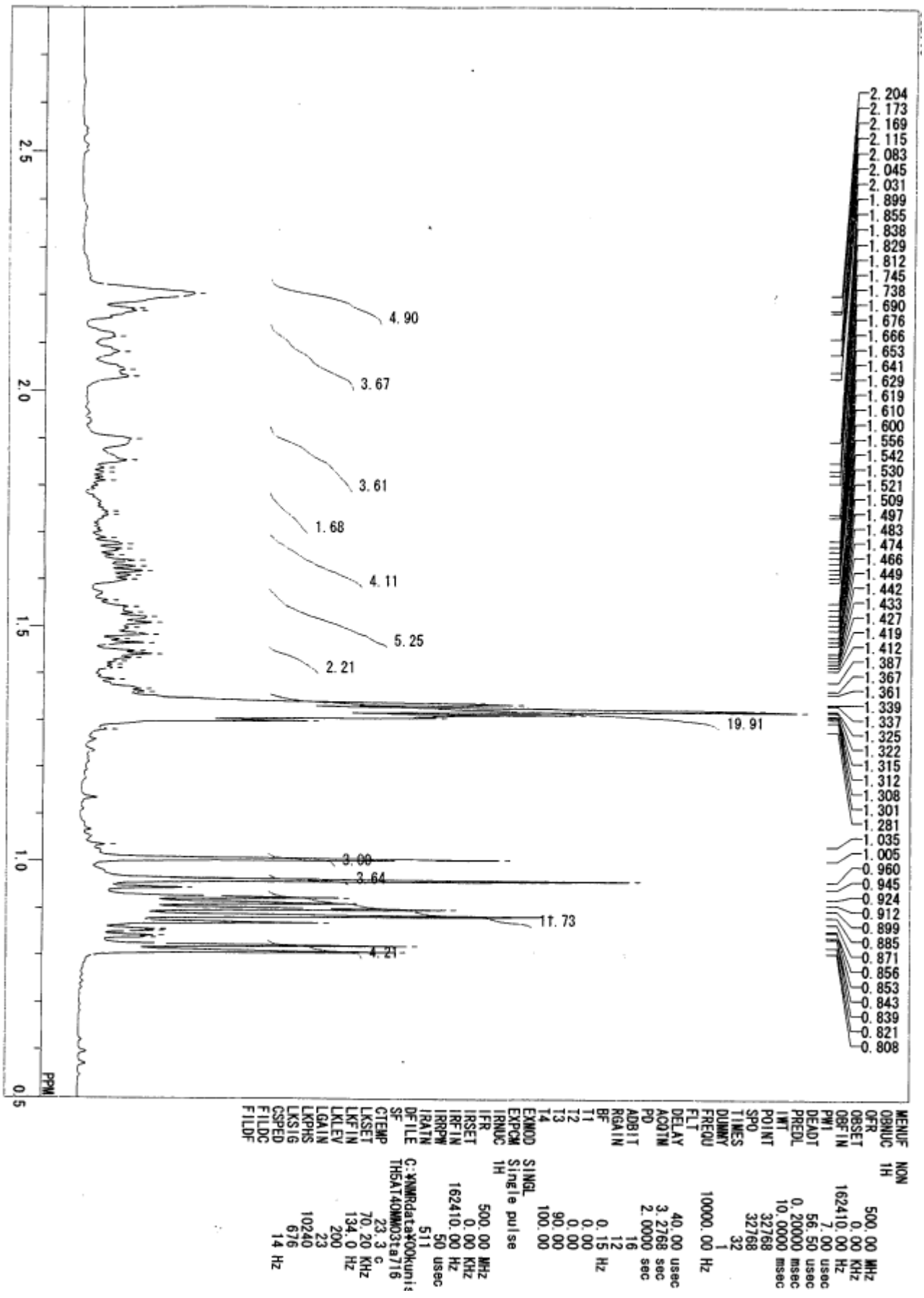

7.285
6.742
4.100
4.091
4.080
4.077
4.075
4.066
4.063
4.052
4.049
4.038
4.036
4.033
4.030
4.014
2.204
2.173
2.169
2.115
2.083
2.045
2.031
1.899
1.855
1.676
1.666
1.653
1.641
1.629
1.619
1.610
1.600
1.542
1.530
1.521
1.509
1.497
1.483
1.474
1.466
1.449
1.442
1.433
1.427
1.419
1.412
1.387
1.367
1.361
1.339
1.337
1.325
1.322
1.315
1.312
1.308
1.301
1.005
0.960
0.945
0.924
0.912
0.899
0.885
0.871
0.856
0.853
0.843
0.839
0.821
0.808
0.000
2.41
0.21
11.01
4.90
3.67
3.61
1.68
4.11
5.25
2.21
19.91
3.90
3.64
1.73
4.21
PPM
NON
1H
500.00 MHz
0.00 KHz
162410.00 Hz
7.00 usec
56.50 usec
0.20000 msec
10.0000 msec
32768
32768
32
1
10000.00 Hz
40.00 usec
3.2768 sec
2.0000 sec
16
12
0.15 Hz
0.00
0.00
90.00
100.00
SINGL
Single pulse
1H
500.00 MHz
0.00 KHz
162410.00 Hz
50 usec
511
C:¥NMRdata¥OOKkunisue¥3ta716¥NON_Eift.
TH5AT4OMMO3ta716
23.3 c
70.20 KHz
134.0 Hz
200
23
10240
676
14 Hz
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
OTEMP
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF

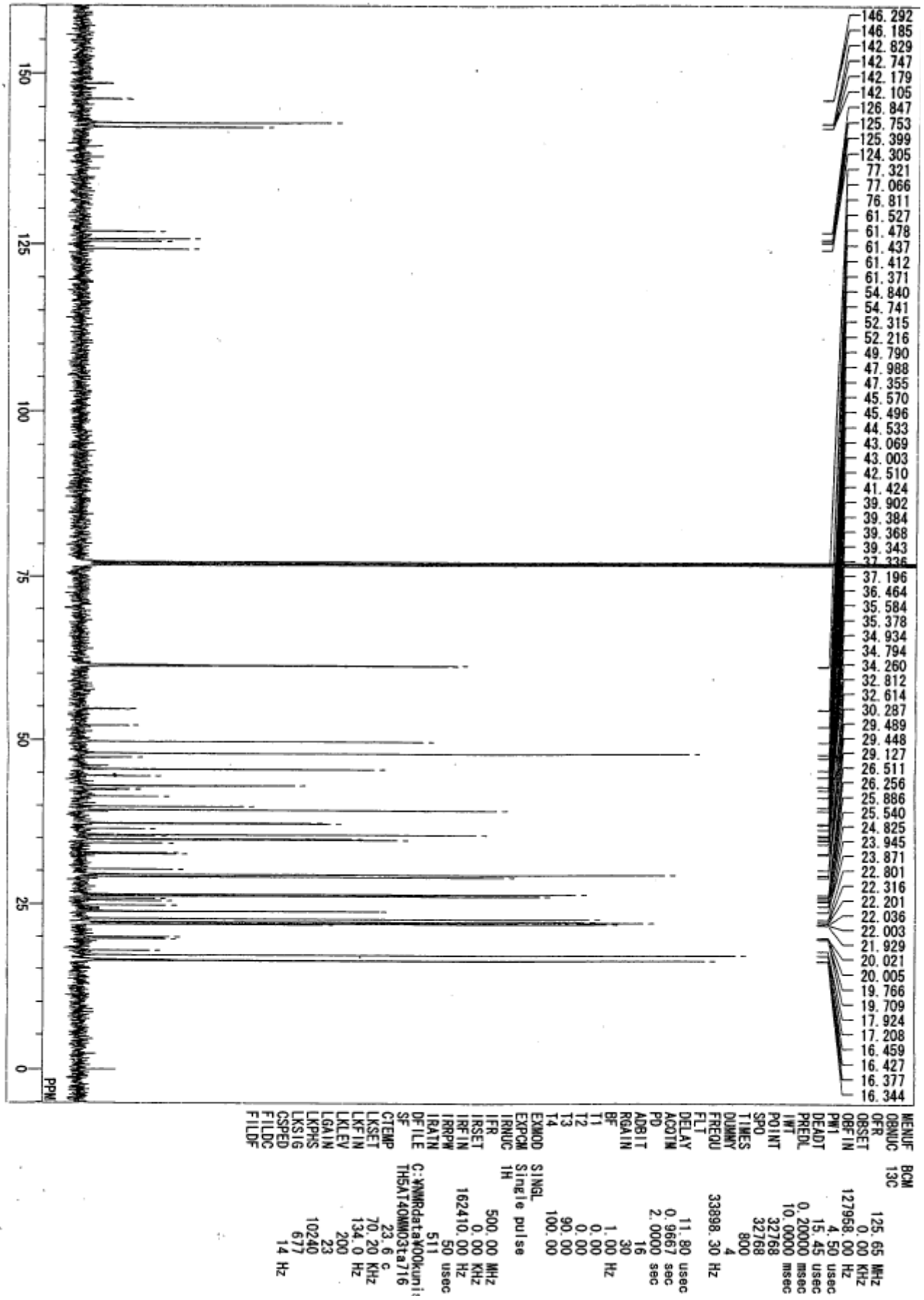
21


P(O)(OEt)2

22


P(O)(OEt)2


4.90
3.67
3.61
1.68
4.11
5.25
2.21
19.91
3.00
3.64
11.73
4.21
PPM
2.5
2.0
1.5
1.0
0.5
2.204
2.173
2.169
2.115
2.083
2.045
2.031
1.899
1.855
1.838
1.829
1.812
1.745
1.738
1.690
1.676
1.666
1.653
1.641
1.629
1.619
1.610
1.600
1.556
1.542
1.530
1.521
1.509
1.497
1.483
1.474
1.466
1.449
1.442
1.433
1.427
1.419
1.412
1.387
1.367
1.361
1.339
1.337
1.325
1.322
1.315
1.312
1.308
1.301
1.281
1.035
1.005
0.960
0.945
0.924
0.912
0.899
0.885
0.871
0.856
0.853
0.843
0.839
0.821
0.808
MENUF NON
OBNUC 1H
OFR 500.00 MHz
OBSET 0.00 KHz
OBFIN 162410.00 Hz
PW1 7.00 usec
DEADT 56.50 usec
PREDL 0.20000 msec
WT 10.0000 msec
POINT 32768
SPO 32768
TIMES 32
DUMMY 1
FREQU 10000.00 Hz
FLT
DELAY 40.00 usec
ACQTM 3.2768 sec
PD 2.0000 sec
ADBIT 16
RGAIN 12
BF 0.15 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD SINGL
EXPCM Single pulse
IRNUC 1H
IFR 500.00 MHz
IRSET 0.00 KHz
IRFIN 162410.00 Hz
IRRPW 50 usec
IRATN 511
DFILE C:¥NMRdata¥OOkuni¥
SF TH5AT4OMM03ta716
CTEMP 23.3 c
LKSET 70.20 KHz
LKFIN 134.0 Hz
LKLEV 200
LGAIN 23
LKPHS 10240
LKSIG 676
CSPED 14 Hz
FILDC
FILDF


146.292
146.185
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150
125
100
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25
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PPM
MENUF
OBNUC
OFR
OBSET
OBFIN
PW1
DEADT
PREDL
IWT
POINT
SPO
TIMES
DUMMY
FREQU
FLT
DELAY
ACQTM
PD
ADBIT
RGAIN
BF
T1
T2
T3
T4
EXMOD
EXPCM
IRNUC
IFR
IRSET
IRFIN
IRRPW
IRATN
DFILE
SF
CTEMP
LKSET
LKFIN
LKLEV
LGAIN
LKPHS
LKSIG
CSPED
FILDC
FILDF
BCM
13C
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0.00 KHz
127958.00 Hz
4.50 usec
15.45 usec
0.20000 msec
10.0000 msec
32768
32768
800
4
33898.30 Hz
11.80 usec
0.9667 sec
2.0000 sec
16
30
1.00 Hz
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SINGL
Single pulse
1H
500.00 MHz
0.00 KHz
162410.00 Hz
50 usec
511
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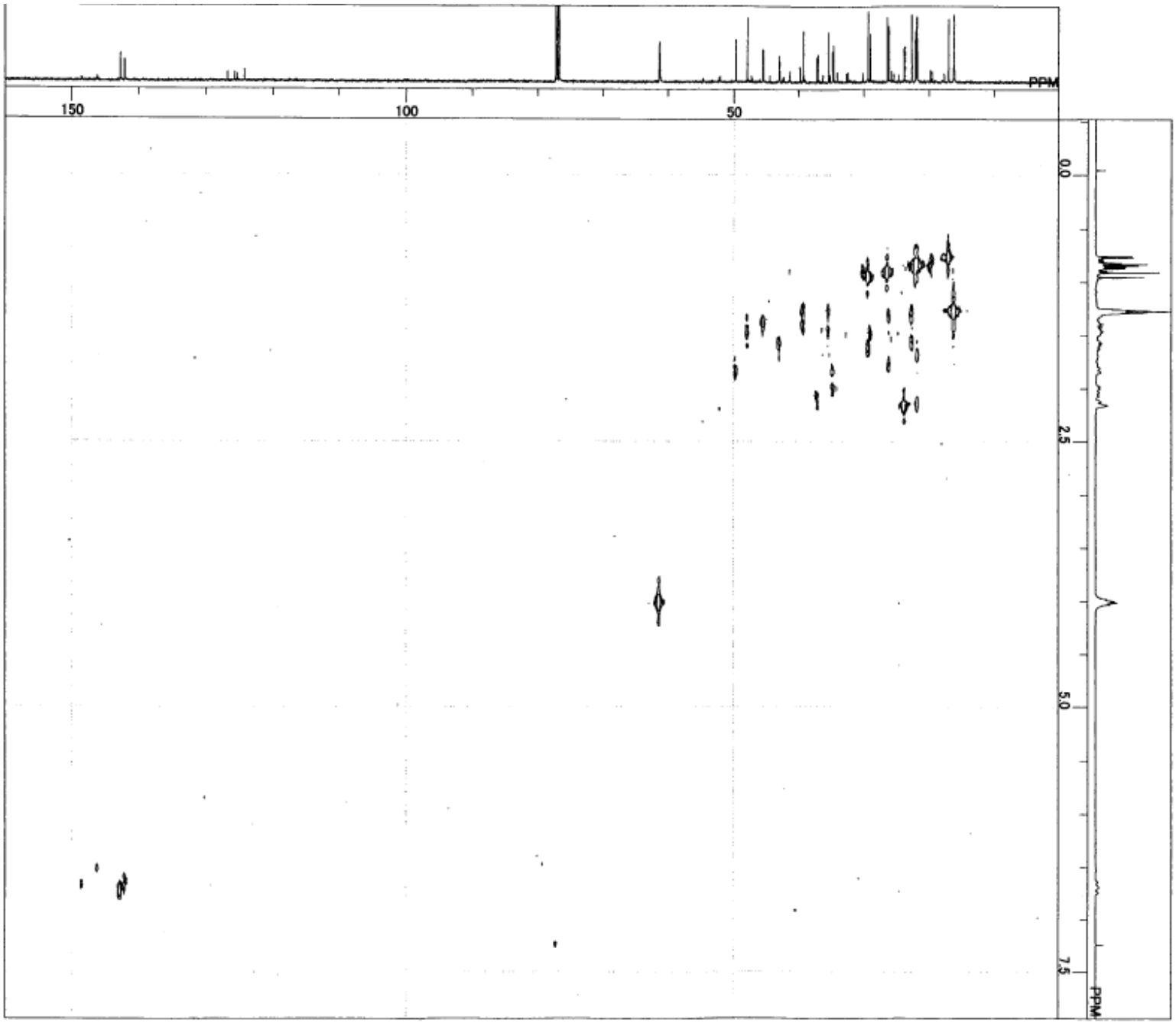
23.6 c
70.20 KHz
134.0 Hz
200
23
10240
677
14 Hz



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TIMES	64
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PW1	9.00 usec
PW2	26.00 usec
PW3	14.60 usec
PI1	80.0000 msec
PI2	1.0000 msec
PI3	20.0000 msec
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IRSET	0.00 KHz
IRATN	511
IRRPW	50 usec
TRNUC	1H
TRSET	0.00 KHz
TRATN	511
TRRPW	0 usec
CTEMP	25.1 c
CSPED	13 Hz
SLVNT	CDCL3
LOOP1	1
XS	0.00 Hz
CXS	
XE	25125.63 Hz
CXE	
THTOP	
THBTM	
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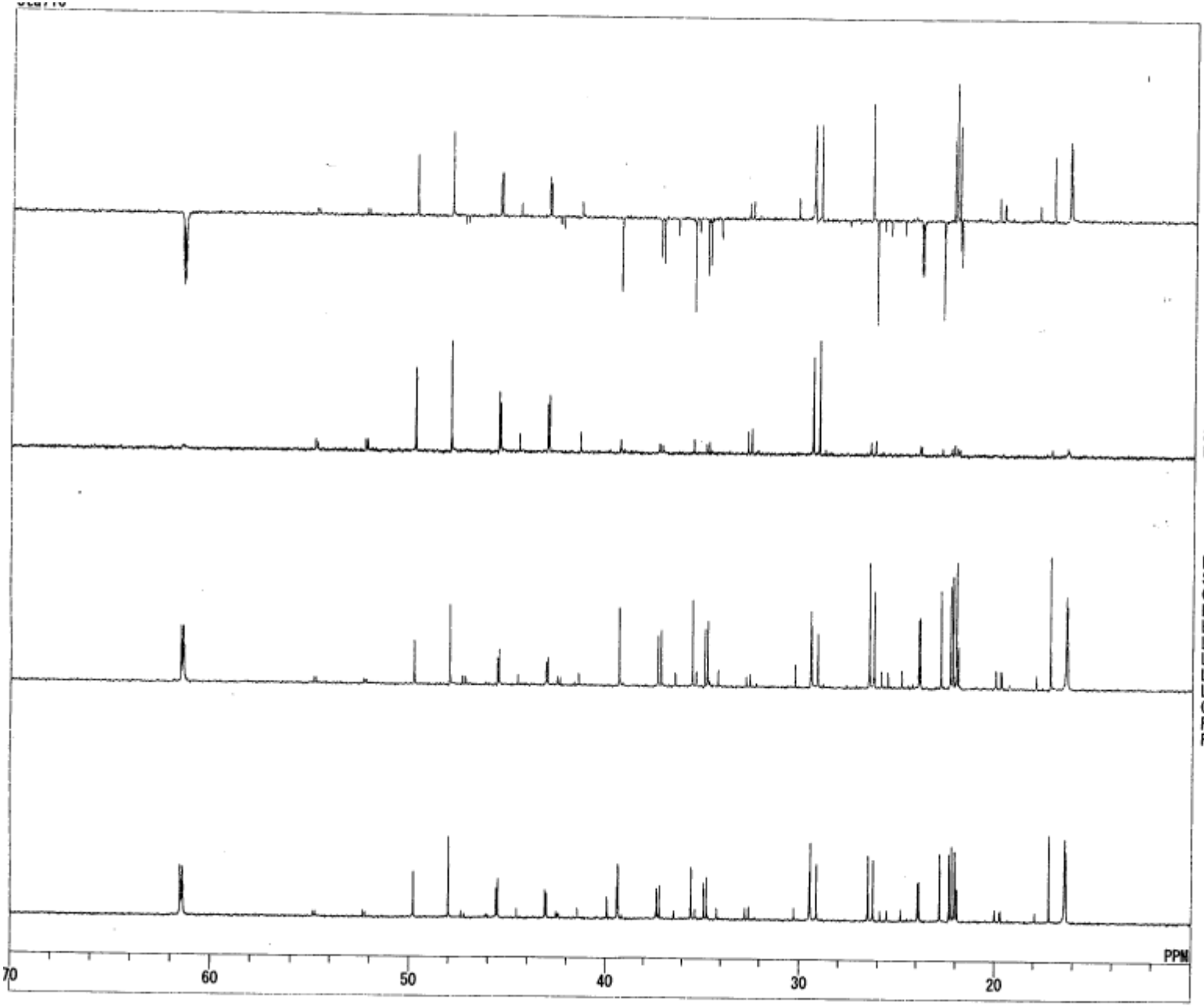
DELAY	15.58 usec
CINWT	10.00 usec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IWT 10.0000 msec
POINT 32768
SPO 32768
TIMES 800
DUMMY 4
FREQU 33898.30 Hz
FLT
DELAY 11.80 usec
ACQTM 0.9667 sec
PD 2.0000 sec
ADBIT 16
RGAIN 30
BF 1.00 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD SINGL
EXPCM Single pulse
IRNUC 1H
IFR 500.00 MHz
IRSET 0.00 KHz
IRFIN 162410.00 Hz
IRRPW 50 usec
IRATN 511
DFILE C:¥NMRdata¥00kuni
SF TH5AT40MN03ta716
CTEMP 23.6 c
LKSET 70.20 KHz
LKFIN 134.0 Hz
LKLEV 200
LGAIN 23
LKPHS 10240
LKSIG 677
CSPED 14 Hz
FILDC
FILDF
PPM
70
60
50
40
30
20

*Energies were given in hartrees.

---Cyclization and rearrangement reactions of **7'e** ----

Reactant 7'e (NIMAG=0), grand minimum

Sum of electronic and zero-point Energies (hartrees)= -269.710238

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-1.361734	1.449502	0.126437
C	-1.736153	0.229872	-0.198170
O	-1.038186	-0.952360	-0.106050
C	0.265722	-0.892432	0.479397
C	1.296639	-0.262342	-0.417733
C	2.244608	0.576164	0.000509
H	-2.728414	0.025140	-0.596867
H	-0.524390	2.020760	0.489531
H	1.257199	-0.575446	-1.460724
H	2.303672	0.902320	1.037537
H	3.004204	0.963578	-0.672625
H	0.221200	-0.377938	1.449719
H	0.517529	-1.944116	0.659191

Other minima (not appeared in the text)

Sum of electronic and zero-point Energies (hartrees)= -269.707960

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	2.677133	-0.686625	-0.022582
C	1.389863	-0.450391	0.113848
O	0.809428	0.770330	-0.154194
C	-0.541418	0.918921	0.311142
C	-1.517199	0.068755	-0.452593
C	-2.401380	-0.752079	0.115565
H	0.699811	-1.231909	0.435676
H	3.582932	-0.185540	-0.327803
H	-1.473769	0.167661	-1.536987
H	-2.458993	-0.869837	1.196134
H	-3.109320	-1.329199	-0.472943
H	-0.603152	0.712186	1.388907
H	-0.754928	1.982511	0.158287

Sum of electronic and zero-point Energies (hartrees)= -269.709306

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.676835	-0.989945	0.666715
C	1.579179	-0.174290	-0.361690
O	0.624081	0.781422	-0.627611
C	-0.343212	1.033087	0.387895
C	-1.504868	0.073961	0.406175
C	-1.746871	-0.869880	-0.500965
H	2.315843	-0.173140	-1.163039
H	1.170823	-1.295258	1.567738
H	-2.191478	0.221072	1.241109
H	-1.079895	-1.032343	-1.342179
H	-2.618406	-1.513795	-0.427937
H	0.151060	1.055814	1.370929
H	-0.706979	2.048677	0.185488

Sum of electronic and zero-point Energies (hartrees)= -269.707452

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.490180	0.628700	0.104218
C	-1.393948	-0.034373	0.403803
O	-0.543828	-0.573414	-0.536763
C	0.683672	-1.090648	-0.032581
C	1.749706	-0.051058	0.188982
C	1.638811	1.242271	-0.108669
H	-1.104500	-0.212556	1.441722
H	-3.054676	0.958005	-0.754239
H	2.673396	-0.438631	0.621250
H	0.731369	1.649567	-0.543352
H	2.454947	1.934939	0.075133
H	0.503068	-1.652243	0.898845
H	1.018652	-1.821128	-0.779769

Sum of electronic and zero-point Energies (hartrees)= -269.707447

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.488739	0.629929	0.104264
C	-1.394370	-0.036263	0.403725
O	-0.543723	-0.574230	-0.536981
C	0.684159	-1.090656	-0.032911
C	1.749435	-0.050364	0.188970
C	1.637523	1.243013	-0.108077
H	-1.107329	-0.218673	1.441596
H	-3.050879	0.963274	-0.754182
H	2.673471	-0.437446	0.620942
H	0.729703	1.649819	-0.542417
H	2.453159	1.936214	0.075939
H	0.503911	-1.652583	0.898398
H	1.019702	-1.820723	-0.780252

Sum of electronic and zero-point Energies (hartrees)= -269.709146

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.031150	1.047046	0.183942
C	-1.815565	-0.136743	-0.353915
O	-0.730479	-0.967506	-0.236837
C	0.344938	-0.519596	0.603974
C	1.267805	0.432615	-0.103146
C	2.582462	0.242782	-0.211451
H	-2.557191	-0.607440	-0.997451
H	-1.590859	1.802260	0.814037
H	0.806092	1.319870	-0.533361
H	3.069485	-0.638433	0.201929
H	3.225865	0.961253	-0.711981
H	-0.080939	-0.066063	1.511375
H	0.880440	-1.428025	0.893725

Sum of electronic and zero-point Energies (hartrees)= -269.706842

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	2.694825	-0.688651	-0.096389
C	1.678731	0.030728	0.330830
O	0.700383	0.539909	-0.490706
C	-0.550853	0.831030	0.150110
C	-1.419537	-0.386672	0.288469
C	-2.658069	-0.477873	-0.194585
H	1.575306	0.296402	1.386905
H	3.099430	-1.080164	-1.017145
H	-0.978844	-1.225167	0.827958
H	-3.118788	0.341000	-0.743887
H	-3.262821	-1.370191	-0.058217
H	-0.351985	1.282493	1.135777
H	-1.035949	1.584984	-0.476359

Transition structure 7'e/8'e (5-*exo*) (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -269.708766

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	1.246392	-0.880693	0.086702
C	1.594421	0.439520	-0.021910
C	0.719164	1.419385	-0.118062
C	-1.052734	-0.076362	0.441444
C	-2.204083	0.328766	-0.142956
C	-0.143441	-1.101832	-0.185210
H	2.678864	0.556497	0.010325
H	0.764856	2.494705	-0.192953
H	-0.892605	0.120911	1.499915
H	-2.429186	0.090288	-1.179929
H	-2.923655	0.947186	0.384817
H	-0.303052	-1.120738	-1.272956
H	-0.346324	-2.100175	0.217329

Other Transition structure (5-*exo*) (NIMAG=1)···higher energy

(not appeared in the text)

Sum of electronic and zero-point Energies (hartrees)= -269.705916

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	-0.948900	-0.913688	-0.415958
C	-1.489790	0.335930	-0.287055
C	-0.899448	1.320340	0.360514
C	1.140129	0.061538	0.483836
H	1.353961	0.490604	1.459894
C	0.175840	-1.106521	0.458973
H	-2.458277	0.394523	-0.785495
H	-1.098785	2.368064	0.525327
C	1.898792	0.418727	-0.578118
H	2.631553	1.217452	-0.510600
H	1.756315	-0.036594	-1.555297
H	-0.204832	-1.287654	1.472479
H	0.658123	-2.016979	0.092453

Transition structure 7'e/10'e (6-*endo*) (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -269.701246

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	1.084704	-0.910791	-0.117773
C	1.426295	0.415690	-0.110867
C	0.657385	1.473579	0.098348
C	-1.620501	0.771526	0.106804
C	-0.240948	-1.246636	0.344858
C	-1.270743	-0.440664	-0.384853
H	2.495221	0.504320	-0.324193
H	0.914869	2.524895	0.088190
H	-1.511159	1.004392	1.161916
H	-2.201021	1.479538	-0.479318
H	-1.466710	-0.694871	-1.424259
H	-0.323282	-2.322174	0.169369
H	-0.294479	-1.050739	1.424745

Product 8'e (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees)= -269.758279

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367567
C	1.203107	0.000000	1.943143
C	2.274353	0.038440	0.851598
C	3.365656	-0.968507	1.000144
C	1.375681	-0.210088	-0.402071
H	-0.987936	0.018579	1.813274
H	1.408458	0.020996	3.004761
H	2.720642	1.043222	0.808579
H	3.124648	-2.028002	1.007479
H	4.387404	-0.675292	1.216051
H	1.469152	-1.247715	-0.746674
H	1.590593	0.463005	-1.235183

Product 9'e (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees)= -269.756584

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.379499
C	1.384359	0.000000	1.888939
C	2.240365	0.336592	0.680388
C	2.335369	-1.036084	1.284529
C	1.262525	0.519852	-0.466360
H	-0.837968	-0.545815	1.802950
H	1.599804	0.396589	2.876959
H	3.081202	1.019777	0.754485
H	1.898593	-1.876430	0.749182
H	3.236224	-1.272087	1.845399
H	1.517893	-0.033676	-1.376261
H	1.149672	1.583205	-0.718921

Product 10'e (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees)= -269.768233

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	1.383416	0.369345	-0.166538
C	0.405368	1.312774	-0.051510
C	-0.904509	1.076105	0.082515
C	-1.477134	-0.318694	0.024791
C	0.990344	-0.963812	0.224090
C	-0.390644	-1.318387	-0.205282
H	0.829206	2.312448	-0.090686
H	-1.578121	1.921719	0.180957
H	-2.037796	-0.547831	0.953415
H	-2.230382	-0.387925	-0.776083
H	-0.620474	-2.336497	-0.503163
H	1.742345	-1.631543	-0.205169
H	1.087344	-1.013043	1.325410

Transition structure 8'e/9'e (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -269.741046

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	-1.410082	-0.126317	0.387631
C	-0.860645	1.078827	0.017503
C	0.420630	0.953770	-0.490402
C	0.772310	-0.507405	-0.489081
C	1.594552	-0.073977	0.664157
C	-0.571763	-1.168699	-0.169126
H	-1.414008	1.951110	0.337606
H	0.998985	1.731072	-0.968292
H	1.293097	-0.929402	-1.350290
H	1.195133	-0.116296	1.670068
H	2.633011	0.201994	0.525376
H	-0.508961	-1.973317	0.568912
H	-1.047108	-1.549733	-1.082731

Transition structure 9'e/10'e (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -269.739409

Cartesian Coordinates (Angstroms)

	X	Y	Z
O	-1.363223	0.204506	0.364898
C	-0.580141	1.222112	-0.088466
C	0.775141	0.947191	-0.246049
C	0.614963	-0.949627	-0.431721
C	1.416800	-0.159673	0.536983
C	-0.826790	-1.098691	-0.095479
H	-1.103093	2.064435	-0.531718
H	1.385472	1.559912	-0.904360
H	1.041781	-1.359772	-1.337443
H	1.119344	-0.240328	1.587311
H	2.499008	-0.219187	0.422183
H	-1.014665	-1.776493	0.747463
H	-1.421895	-1.432478	-0.954230

---Cyclization and rearrangement reactions of 7'f ----

Reactant 7'f (NIMAG=0), grand minimum

Sum of electronic and zero-point Energies (hartrees)= -233.796480

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.546162	-0.819074	0.057105
C	-2.061870	0.377613	-0.185208
C	-0.610328	0.796492	-0.110660
C	0.359514	-0.338187	0.261534
C	1.780335	0.136756	0.390346
C	2.803090	-0.283001	-0.355628
H	1.961841	0.892062	1.157964
H	-2.759837	1.176983	-0.472980
H	-3.517889	-1.296366	0.057747
H	3.810333	0.101124	-0.217140
H	2.672172	-1.033663	-1.132873
H	0.294640	-1.134052	-0.490149
H	0.025404	-0.778311	1.212369
H	-0.314138	1.230666	-1.076554

H	-0.520003	1.617962	0.616689

Other minima (not appeared in the text)

Sum of electronic and zero-point Energies (hartrees)= -233.795270

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.637892	-0.547567	-0.000621
C	-1.924845	0.555801	-0.000115
C	-0.416023	0.661451	0.001013
C	0.307392	-0.686202	0.000258
C	1.812736	-0.620365	0.000297
C	2.572554	0.476187	-0.000798
H	2.307538	-1.593025	0.000931
H	-2.454494	1.519334	-0.000417
H	-3.687652	-0.812406	-0.001323
H	3.657164	0.410033	-0.000818
H	2.153915	1.479147	-0.001585
H	-0.022702	-1.270943	-0.871233
H	-0.023143	-1.272189	0.870738
H	-0.106562	1.252933	-0.873175

H	-0.107592	1.251295	0.876678

Sum of electronic and zero-point Energies (hartrees)= -233.796278

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-3.047943	-0.255136	0.180409
C	-1.956054	0.372474	-0.191489
C	-0.619380	-0.273667	-0.479788
C	0.488760	0.212673	0.483534
C	1.820723	-0.426118	0.199532
C	2.926332	0.226781	-0.160508
H	1.853994	-1.513481	0.291601
H	-1.981812	1.467059	-0.295451
H	-4.069067	0.004734	0.430747
H	3.860440	-0.292286	-0.358501
H	2.941181	1.310028	-0.266532
H	0.175510	-0.019580	1.511596
H	0.579881	1.305102	0.420530
H	-0.315800	-0.040492	-1.509945
H	-0.718958	-1.363128	-0.414184

Sum of electronic and zero-point Energies (hartrees)= -233.795187

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	2.891994	-0.304107	-0.449172
C	1.905761	0.059865	0.337854
C	0.463200	-0.375689	0.208008
C	-0.479283	0.812427	-0.041682
C	-1.946212	0.477124	-0.133805
C	-2.501963	-0.731112	-0.032393
H	-2.597278	1.336069	-0.304908
H	2.116376	0.751614	1.166704
H	3.955518	-0.116261	-0.529735
H	-3.577035	-0.865192	-0.115861
H	-1.917750	-1.631830	0.135544
H	-0.173229	1.323824	-0.966646
H	-0.340991	1.561286	0.754387
H	0.159053	-0.886580	1.132825
H	0.374353	-1.103976	-0.605174

Sum of electronic and zero-point Energies (hartrees)= -233.796287

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	2.919661	0.645190	-0.163178
C	2.003214	-0.245337	0.138991
C	0.629640	-0.349922	-0.484834
C	-0.501807	-0.164849	0.552846
C	-1.869009	-0.361594	-0.042616
C	-2.828541	0.563269	-0.088110
H	-2.060632	-1.345579	-0.475584
H	2.220469	-0.985539	0.923191
H	3.927167	0.887990	0.151114
H	-3.797531	0.362858	-0.537647
H	-2.682468	1.558455	0.327686
H	-0.425147	0.833838	0.999515
H	-0.349136	-0.888274	1.368828
H	0.522691	-1.338971	-0.954903
H	0.525637	0.394682	-1.280801

Sum of electronic and zero-point Energies (hartrees)= -233.795173

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-1.979100	-1.097806	0.269812
C	-1.859676	0.049383	-0.358348
C	-0.730692	1.050887	-0.236981
C	0.461565	0.613108	0.636975
C	1.294913	-0.482402	0.027136
C	2.588297	-0.371886	-0.279080
H	0.777237	-1.420046	-0.173800
H	-2.664706	0.350763	-1.044489
H	-2.697650	-1.906412	0.313576
H	3.145038	-1.193853	-0.721714
H	3.144561	0.545738	-0.094342
H	0.070605	0.281594	1.609946
H	1.097180	1.486568	0.827947
H	-0.372947	1.305363	-1.244856
H	-1.151168	1.982580	0.170648

Sum of electronic and zero-point Energies (hartrees)= -233.792950

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.678738	-0.999442	-0.680551
C	1.641958	-0.142973	0.313963
C	0.627551	0.960239	0.534295
C	-0.521128	1.031319	-0.479843
C	-1.604271	-0.013382	-0.366583
C	-1.686327	-1.004852	0.520756
H	-2.404096	0.092124	-1.101766
H	2.435285	-0.191159	1.074194
H	2.307932	-1.822203	-0.995312
H	-2.527458	-1.692967	0.519692
H	-0.919173	-1.182475	1.269117
H	-0.104256	1.000097	-1.497150
H	-0.999064	2.018960	-0.393656
H	0.222217	0.874902	1.552805
H	1.169486	1.917263	0.519858

Sum of electronic and zero-point Energies (hartrees)= -233.794743

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.306310	1.461156	0.184777
C	1.750246	0.284441	-0.193356
C	1.019920	-1.037646	-0.102698
C	-0.399462	-0.972752	0.490151
C	-1.398065	-0.261874	-0.382928
C	-2.184345	0.744048	0.001773
H	-1.475164	-0.631486	-1.407827
H	2.763446	0.217448	-0.616078
H	1.677818	2.478230	0.187758
H	-2.899684	1.203166	-0.675542
H	-2.140097	1.149395	1.010519
H	-0.364176	-0.497716	1.477988
H	-0.739391	-2.007892	0.645492
H	0.980538	-1.486885	-1.107180
H	1.629090	-1.728503	0.498557

Sum of electronic and zero-point Energies (hartrees)= -233.795671

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.356295	-1.018915	-0.241612
C	-1.767824	0.046770	0.251547
C	-0.727405	0.894184	-0.447441
C	0.635415	0.910930	0.288056
C	1.337703	-0.419390	0.279489
C	2.564547	-0.631051	-0.198493
H	0.773842	-1.257251	0.690219
H	-2.029161	0.372587	1.269532
H	-3.101116	-1.736253	0.080280
H	3.023962	-1.615942	-0.182095
H	3.160411	0.174740	-0.623807
H	0.463447	1.230616	1.327951
H	1.280319	1.671400	-0.169839
H	-1.098581	1.927249	-0.507917
H	-0.589970	0.537678	-1.473599

Sum of electronic and zero-point Energies (hartrees)= -233.793616

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.262900	0.858226	0.038254
C	-1.512774	-0.148628	-0.345520
C	-0.531584	-0.913806	0.517958
C	0.856541	-1.100763	-0.119717
C	1.734528	0.120560	-0.234047
C	1.460310	1.356978	0.183551
H	2.702391	-0.067172	-0.702744
H	-1.598481	-0.506600	-1.382268
H	-3.013454	1.503587	-0.400763
H	2.181689	2.161078	0.063242
H	0.513530	1.621533	0.644238
H	0.736281	-1.544115	-1.121191
H	1.404276	-1.860599	0.458518
H	-0.949195	-1.914364	0.702040
H	-0.441764	-0.428745	1.496050

Sum of electronic and zero-point Energies (hartrees)= -233.795362

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.254714	-1.047625	-0.287014
C	-1.554391	-0.176102	0.401218
C	-0.834353	1.028011	-0.163502
C	0.675944	1.049878	0.169623
C	1.450064	-0.075129	-0.461619
C	2.218944	-0.944957	0.193590
H	1.356844	-0.162017	-1.545898
H	-1.463090	-0.309291	1.489215
H	-2.829323	-1.942983	-0.084619
H	2.760098	-1.733760	-0.322164
H	2.338743	-0.901229	1.274580
H	0.815383	1.030172	1.258757
H	1.080609	2.011558	-0.180260
H	-1.289708	1.941240	0.246206
H	-0.978524	1.061852	-1.249587

Sum of electronic and zero-point Energies (hartrees)= -233.794935

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.834943	-0.344389	0.210975
C	-1.612915	-0.400571	-0.267453
C	-0.682352	0.780531	-0.436916
C	0.561060	0.737968	0.488852
C	1.458021	-0.449324	0.263370
C	2.704990	-0.386454	-0.206152
H	1.036892	-1.425735	0.506721
H	-1.208997	-1.376500	-0.569898
H	-3.643435	-1.037249	0.409574
H	3.308824	-1.278081	-0.353536
H	3.173683	0.563407	-0.457505
H	0.210698	0.742602	1.530811
H	1.135420	1.660981	0.338991
H	-1.237531	1.704308	-0.241311
H	-0.338719	0.819695	-1.479898

Sum of electronic and zero-point Energies (hartrees)= -233.793560

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	2.698991	-0.342302	-0.280966
C	1.412342	-0.444516	-0.037280
C	0.567733	0.604891	0.655193
C	-0.620503	1.091050	-0.196028
C	-1.757213	0.119254	-0.402285
C	-1.948255	-1.049960	0.211397
H	-2.503038	0.447331	-1.128333
H	0.879309	-1.344560	-0.369578
H	3.467134	-0.946929	-0.747704
H	-2.820543	-1.661752	-0.001925
H	-1.255344	-1.445822	0.949461
H	-0.246328	1.411682	-1.179006
H	-1.034523	2.001994	0.264195
H	1.202893	1.461193	0.904297
H	0.191877	0.206363	1.608406

Sum of electronic and zero-point Energies (hartrees)= -233.795978

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.632653	-0.690262	0.217793
C	-1.451305	-0.398177	-0.275906
C	-0.781591	0.956084	-0.207652
C	0.610690	0.910804	0.468468
C	1.629807	0.127394	-0.313739
C	2.265131	-0.963496	0.117588
H	1.844320	0.501767	-1.317180
H	-0.869816	-1.186089	-0.773603
H	-3.274258	-1.561067	0.276242
H	2.994244	-1.483828	-0.498008
H	2.083692	-1.374711	1.108718
H	0.512614	0.495085	1.478684
H	0.962692	1.947001	0.580888
H	-1.428352	1.655297	0.332824
H	-0.665609	1.352470	-1.227868

Transition structure 7'f/8'f (5-*exo*) (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -233.790283

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.334724	-0.857163	0.085342
C	1.595442	0.623042	-0.090632
C	0.596174	1.477967	-0.048281
C	-1.077779	-0.126204	0.424024
C	-2.236084	0.276564	-0.157046
C	-0.151813	-1.156338	-0.181831
H	2.634928	0.947356	-0.217972
H	0.496116	2.554697	-0.116795
H	-0.932441	0.083914	1.483885
H	-2.471101	0.022986	-1.188255
H	-2.941458	0.918680	0.362507
H	-0.329223	-1.195608	-1.263591
H	-0.400371	-2.149433	0.219127
H	1.971915	-1.455639	-0.578669

H	1.607649	-1.154160	1.110303

Other Transition structure (5-*exo*) (NIMAG=1)···higher energy, (not appeared in the text)

Sum of electronic and zero-point Energies (hartrees)= -233.787149

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.042322	-0.931772	0.378426
C	1.556316	0.481351	0.216236
C	0.779265	1.410473	-0.297513
C	-1.154439	0.054934	-0.472079
H	-1.378238	0.530766	-1.424311
C	-0.202776	-1.130673	-0.509728
H	2.574133	0.698342	0.559592
H	0.862522	2.478029	-0.466074
C	-1.946511	0.349814	0.590108
H	-2.676958	1.152684	0.549047
H	-1.840394	-0.162509	1.544024
H	0.130994	-1.278251	-1.542697
H	-0.729903	-2.045211	-0.209587
H	1.813705	-1.669439	0.119863

H	0.799084	-1.109171	1.437445

Transition structure 7'f/10'f (6-*endo*) (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -233.785716

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.136698	-0.926371	-0.119393
C	1.457653	0.555410	-0.031874
C	0.605331	1.564063	0.006765
C	-1.654451	0.755364	0.135098
C	-0.295296	-1.309862	0.333594
C	-1.304971	-0.451658	-0.367114
H	2.533693	0.778920	-0.023942
H	0.785675	2.634678	0.050740
H	-1.524536	0.986440	1.188445
H	-2.257756	1.457399	-0.434741
H	-1.538577	-0.691680	-1.404121
H	-0.455142	-2.377646	0.136380
H	-0.370441	-1.160660	1.417873
H	1.293993	-1.260827	-1.156451

H	1.863312	-1.488296	0.483364

Product 8'f (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees)= -233.850204

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.425184	0.382812	-0.186330
C	0.324070	1.398650	-0.003623
C	-0.969609	1.075244	0.086153
C	-1.487438	-0.339419	-0.015411
C	0.987357	-1.028051	0.264222
C	-0.398819	-1.350488	-0.192678
H	0.618408	2.446236	0.049029
H	-1.714677	1.857922	0.223338
H	-2.093828	-0.565621	0.885404
H	-2.210872	-0.406899	-0.845262
H	-0.668169	-2.374648	-0.437279
H	1.702108	-1.781190	-0.088452
H	1.035725	-1.057259	1.369825
H	1.728785	0.357186	-1.244209

H	2.318051	0.691786	0.373601

Product 9'f (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees)= -233.835567

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-1.465046	0.143790	0.321851
C	-0.580504	1.252459	-0.174476
C	0.774353	0.754186	-0.436197
C	0.701042	-0.770193	-0.397133
C	1.442431	-0.054692	0.692093
C	-0.754606	-1.160162	-0.147207
H	-0.850891	2.302865	-0.145927
H	1.432766	1.280300	-1.123113
H	1.277572	-1.363243	-1.102735
H	1.011591	0.001635	1.689155
H	2.528585	-0.105497	0.676715
H	-0.858344	-1.974951	0.579447
H	-1.195254	-1.507583	-1.089626
H	-1.559197	0.160484	1.422032

H	-2.492851	0.213660	-0.059535

Product 10'f (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees)= -233.850204

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	1.425184	0.382812	-0.186330
C	0.324070	1.398650	-0.003623
C	-0.969609	1.075244	0.086153
C	-1.487438	-0.339419	-0.015411
C	0.987357	-1.028051	0.264222
C	-0.398819	-1.350488	-0.192678
H	0.618408	2.446236	0.049029
H	-1.714677	1.857922	0.223338
H	-2.093828	-0.565621	0.885404
H	-2.210872	-0.406899	-0.845262
H	-0.668169	-2.374648	-0.437279
H	1.702108	-1.781190	-0.088452
H	1.035725	-1.057259	1.369825
H	1.728785	0.357186	-1.244209

H	2.318051	0.691786	0.373601

Transition structure 8'f/9'f (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -233.822741

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-0.552469	-1.208351	-0.236631
C	-1.466630	-0.103400	0.368908
C	-0.793186	1.183289	-0.041630
C	0.497355	0.943898	-0.489738
C	0.806797	-0.528649	-0.477879
C	1.569898	-0.107337	0.720210
H	-1.217921	2.166103	0.135340
H	1.162833	1.683272	-0.919895
H	1.395065	-0.937826	-1.302069
H	1.125425	-0.152222	1.707265
H	2.616764	0.163822	0.643185
H	-0.471634	-2.093389	0.403591
H	-0.956001	-1.533244	-1.202609
H	-1.524065	-0.189698	1.466477

H	-2.501060	-0.183519	0.009279

Transition structure 9'f/10'f (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -233.820162

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	0.647489	-0.973228	-0.393487
C	1.399107	-0.162303	0.595955
C	0.835151	0.935005	-0.264184
C	-0.508051	1.295150	-0.171968
C	-1.390726	0.216324	0.394090
C	-0.837354	-1.127564	-0.195697
H	-0.913928	2.102772	-0.772891
H	1.519507	1.462467	-0.924163
H	2.484387	-0.251952	0.543814
H	1.055160	-0.198331	1.634525
H	1.164069	-1.448541	-1.219397
H	-1.077948	-1.970808	0.469703
H	-1.321067	-1.333977	-1.158310
H	-2.447401	0.360384	0.145663

H	-1.336476	0.177685	1.492806

---Cyclization and rearrangement reactions of 7'g ----

Reactant 7'g (NIMAG=0)

grand minimum

Sum of electronic and zero-point Energies (hartrees)= -592.697770

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.504770	1.194941	0.154011
C	-1.296802	0.790000	-0.153837
S	-0.832316	-0.950763	-0.182824
C	0.878456	-0.855906	0.533472
C	1.826763	-0.073169	-0.320019
C	2.415874	1.063312	0.060313
H	-0.504384	1.473994	-0.459117
H	-3.451318	0.766290	0.455006
H	2.010851	-0.474251	-1.316139
H	2.247291	1.492439	1.046016
H	3.097403	1.599643	-0.594171
H	0.820124	-0.453115	1.548841

H	1.179970	-1.907861	0.601091

other minima (not appeared in the text)

Sum of electronic and zero-point Energies (hartrees)= -592.697051

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-0.890399	1.904501	0.156262
C	-1.613866	0.859081	-0.156196
S	-1.175973	-0.885977	-0.105545
C	0.537942	-0.880115	0.568109
C	1.586832	-0.380513	-0.382574
C	2.500660	0.541940	-0.076932
H	-2.645266	0.963179	-0.495771
H	0.102898	2.173937	0.477736
H	1.582590	-0.835211	-1.372372
H	2.534309	1.014040	0.903422
H	3.257365	0.853327	-0.791426
H	0.550139	-0.324453	1.511671
H	0.706520	-1.938553	0.803443

Sum of electronic and zero-point Energies (hartrees)= -592.696747

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.168248	1.439232	-0.193381
C	-1.394775	0.631725	0.490483
S	-0.887659	-0.979890	-0.136460
C	0.915231	-0.964291	0.299367
C	1.711851	0.043142	-0.469427
C	2.373574	1.058612	0.087679
H	-1.061139	0.860869	1.503156
H	-2.650131	1.465097	-1.161650
H	1.717900	-0.081988	-1.551540
H	2.378803	1.217821	1.164185
H	2.937927	1.768444	-0.510470
H	1.017218	-0.814554	1.379685
H	1.236164	-1.987968	0.071663

Sum of electronic and zero-point Energies (hartrees)= -592.695413

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-1.265974	1.662540	0.506089
C	-1.670897	0.595040	-0.135812
S	-0.808673	-0.970992	-0.356367
C	0.616709	-0.806126	0.781665
C	1.780981	0.046723	0.342420
C	1.917402	0.699429	-0.810209
H	-2.644511	0.555648	-0.624797
H	-0.408971	2.035188	1.046357
H	2.580793	0.099154	1.083952
H	1.147091	0.675612	-1.575744
H	2.810443	1.280087	-1.022960
H	0.230640	-0.457000	1.748024
H	0.953956	-1.838451	0.942128

Sum of electronic and zero-point Energies (hartrees)= -592.694233

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.397620	1.087659	0.200308
C	-1.484432	0.237776	0.601310
S	-0.590018	-0.862362	-0.512112
C	1.027272	-0.974713	0.350933
C	1.946318	0.218310	0.282210
C	1.741698	1.361940	-0.368180
H	-1.243669	0.102489	1.656960
H	-2.856180	1.421501	-0.720218
H	2.872996	0.082551	0.843623
H	0.834204	1.545657	-0.934961
H	2.483255	2.155487	-0.349550
H	0.837191	-1.245536	1.398395
H	1.513079	-1.850191	-0.099943

Sum of electronic and zero-point Energies (hartrees)= -592.694509

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.680747	0.779503	0.392427
C	-1.384070	0.696770	0.222806
S	-0.597377	-0.726831	-0.561968
C	0.860381	-0.947634	0.538189
C	1.953918	0.088886	0.454336
C	2.091753	1.050532	-0.457528
H	-0.701473	1.499869	0.499774
H	-3.562871	0.183388	0.200715
H	2.701734	-0.004293	1.244228
H	1.376298	1.182142	-1.264600
H	2.935370	1.734063	-0.426397
H	0.503004	-1.039652	1.570401
H	1.258564	-1.934566	0.265993

Sum of electronic and zero-point Energies (hartrees)= -592.696248

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-1.806573	1.547741	0.158063
C	-1.938443	0.318783	-0.277954
S	-0.795672	-1.062598	-0.152766
C	0.629968	-0.310455	0.747536
C	1.529703	0.511264	-0.127338
C	2.829483	0.268092	-0.299448
H	-2.841122	0.002294	-0.802068
H	-1.112936	2.192510	0.676002
H	1.062712	1.348534	-0.643709
H	3.328033	-0.564406	0.193269
H	3.446100	0.892475	-0.939919
H	0.211623	0.274708	1.575214
H	1.171516	-1.157100	1.180312

Sum of electronic and zero-point Energies (hartrees)= -592.695878

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.489704	1.200234	-0.130585
C	-1.770004	0.292223	0.484101
S	-0.725821	-0.872723	-0.412212
C	0.857937	-0.688887	0.537753
C	1.606944	0.569811	0.223439
C	2.833330	0.604936	-0.299383
H	-1.804279	0.152169	1.565617
H	-2.666659	1.529526	-1.146078
H	1.084732	1.499843	0.445410
H	3.380902	-0.304261	-0.539928
H	3.337618	1.544443	-0.507741
H	0.602639	-0.752340	1.602806
H	1.447164	-1.575714	0.283354

Sum of electronic and zero-point Energies (hartrees)= -592.694734

Cartesian Coordinates (Angstroms)

	X	Y	Z
C	-2.886818	0.670863	0.236446
C	-1.653950	0.702646	-0.210033
S	-0.685470	-0.815395	-0.356349
C	0.779070	-0.418136	0.720745
C	1.727040	0.578614	0.127860
C	2.982063	0.302234	-0.229438
H	-1.182226	1.616580	-0.568781
H	-3.577677	-0.077039	0.604703
H	1.344017	1.590319	-0.003833
H	3.404178	-0.693885	-0.112477
H	3.635809	1.060138	-0.651928
H	0.386249	-0.083566	1.686799
H	1.272743	-1.383550	0.873628

Transition structure 7'g/8'g (5-*exo*) (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -592.691591

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	-1.449938	-0.652299	-0.073010
C	-1.243595	1.114322	0.070214
C	-0.060685	1.684225	0.095268
C	1.305314	-0.211857	-0.426948
C	2.531516	0.030764	0.096349
C	0.303006	-1.111646	0.249094
H	-2.193044	1.653743	0.115373
H	0.313258	2.695351	0.178617
H	1.122426	0.004609	-1.477862
H	2.779657	-0.243716	1.118779
H	3.293202	0.559450	-0.468913
H	0.476970	-1.131437	1.329845
H	0.393213	-2.136069	-0.131544

Other Transition structure (5-*exo*) (NIMAG=1)···higher energy

(not appeared in the text)

Sum of electronic and zero-point Energies (hartrees)= -592.689245

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	-1.214991	-0.734131	-0.287148
C	-1.213551	1.041299	-0.137909
C	-0.184723	1.700182	0.347857
C	1.435569	-0.069542	0.423665
H	1.899712	0.392572	1.292569
C	0.296564	-1.019248	0.728802
H	-2.136766	1.507129	-0.489581
H	0.065402	2.742661	0.493147
C	2.066075	0.006609	-0.772176
H	2.946782	0.627668	-0.904582
H	1.673872	-0.490557	-1.655575
H	0.008661	-0.930324	1.779674
H	0.582591	-2.058863	0.537286

Transition structure 7'g/10'g (6-*endo*) (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -592.689678

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	1.412024	-0.457534	-0.091702
C	0.921757	1.259483	-0.045533
C	-0.275751	1.784724	0.123110
C	-2.082180	0.165235	0.049451
C	-0.149343	-1.333686	0.403808
C	-1.293883	-0.833272	-0.408448
H	1.804160	1.890641	-0.196564
H	-0.601598	2.817970	0.154246
H	-2.128152	0.408836	1.106856
H	-2.833381	0.629719	-0.583215
H	-1.322193	-1.120547	-1.457381
H	0.076369	-2.391517	0.235767
H	-0.311187	-1.169457	1.473192

Product 8'g (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees)= -592.743268

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	1.600953	-0.440753	0.005209
C	0.929471	1.199674	-0.114441
C	-0.392385	1.288307	0.056525
C	-1.092749	-0.019954	0.391120
C	-2.452915	-0.179785	-0.201919
C	-0.115046	-1.135600	-0.095784
H	1.611785	2.024809	-0.287471
H	-0.936445	2.227778	0.037420
H	-1.172741	-0.092516	1.488463
H	-3.255878	-0.660250	0.347057
H	-2.623407	0.065217	-1.246348
H	-0.315597	-1.385313	-1.142227
H	-0.181229	-2.043523	0.506750

Product 9'g (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees) = -592.746952

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.749205
C	1.352359	0.000000	2.327168
C	2.388594	0.339387	1.265804
C	2.366040	-1.045738	1.848048
C	1.757857	0.601554	-0.091416
H	-0.899171	-0.306562	2.269963
H	1.469028	0.378576	3.340408
H	3.217759	0.991089	1.531153
H	1.992470	-1.865249	1.239740
H	3.167849	-1.312280	2.531767
H	2.253051	0.072148	-0.911179
H	1.754880	1.672111	-0.317999

Product 10'g (NIMAG=0)

Sum of electronic and zero-point Energies (hartrees) = -592.746952

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.749205
C	1.352359	0.000000	2.327168
C	2.388594	0.339387	1.265804
C	2.366040	-1.045738	1.848048
C	1.757857	0.601554	-0.091416
H	-0.899171	-0.306562	2.269963
H	1.469028	0.378576	3.340408
H	3.217759	0.991089	1.531153
H	1.992470	-1.865249	1.239740
H	3.167849	-1.312280	2.531767
H	2.253051	0.072148	-0.911179
H	1.754880	1.672111	-0.317999

Transition structure 8'g/9'g (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees) = -592.730692

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	-1.489826	-0.074872	0.264182
C	-0.469983	1.298821	-0.168050
C	0.829085	0.953184	-0.495218
C	1.111913	-0.519789	-0.431321
C	1.757638	-0.134227	0.846364
C	-0.218887	-1.277545	-0.367314
H	-0.857319	2.301836	-0.040934
H	1.554420	1.657996	-0.883596
H	1.784265	-0.922152	-1.192878
H	1.187328	-0.112344	1.766259
H	2.814567	0.101166	0.877160
H	-0.182009	-2.139186	0.303823
H	-0.522629	-1.612028	-1.363508

Transition structure 9'g/10'g (NIMAG=1)

Sum of electronic and zero-point Energies (hartrees)= -592.731784

Cartesian Coordinates (Angstroms)

	X	Y	Z
S	1.458804	-0.070282	0.248949
C	0.354216	-1.306411	-0.293142
C	-1.007926	-1.026409	-0.220124
C	-1.075645	0.891874	-0.374428
C	-1.596055	0.006496	0.694466
C	0.319592	1.383488	-0.273334
H	0.741236	-2.119099	-0.898719
H	-1.698344	-1.605995	-0.829004
H	-1.702885	1.175898	-1.210768
H	-1.110835	0.105970	1.668843
H	-2.680806	-0.048942	0.785699
H	0.455599	2.130803	0.517374
H	0.690085	1.791651	-1.217244

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