Supplementary Information

Ruthenium(IV) porphyrin catalyzed phosphoramidation of aldehyde with phosphoryl azide as nitrene source

Wenbo Xiao, Cong-Ying Zhou and Chi-Ming Che*

Department of Chemistry, State Key Laboratory of Synthetic Chemistry, and Open Laboratory of Chemical Biology of the Institute of Molecular Technology for Drug Discovery and Synthesis, The University of Hong Kong, Pokfulam Road, Hong Kong, China.

Fax: (852) 2857-1586 Tel: (852) 2859-2154 E-mail: cmche@hku.hk

I. General Information

Unless otherwise stated, all reactions were performed under argon atmosphere. DPPA and aldehydes were obtained commercially and used without further purification unless acid impurities were identified in aldehydes. Molecular sieves were dried at 400℃ for 3 h prior to use. All solvents were purified by distillation using standard methods. Metal porphyrins and organic azides were synthesized according to previously reported methods. All ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AV300 or AV400 NMR spectrometers with tetramethylsilane (TMS) as internal reference. ^{31}P NMR spectra were recorded on Bruker AV400 NMR spectrometer with 85% H_3PO_4 as external reference. Mass spectra were recorded on Finnigan MAT 95 mass spectrometer. Elemental analysis was conducted on Flash EA 1112 analyzer by Analysis & Test Center of Institute of Chemistry of Chinese Academy of Sciences. *Caution!* Organic azides are potentially explosive and should be handled with great care.

II. Synthesis of Ruthenium(IV) Porphyrins

Ruthenium(IV) porphyrins were synthesized according to the following references.

$[Ru^{IV}(TDCPP)Cl_2]$	J.-L. Zhang and C.-M. Che, *Chem. Eur. J.*, 2005, **11**, 3899.
$[Ru^{IV}(TTP)Cl_2]$	W.-H., Leung, T. S. M. Hun, H.-w. Hou, K.-Y. Wong, *J. Chem. Soc., Dalton Trans.* 1997, 237.

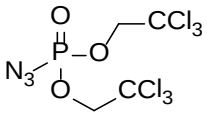
III. Synthesis of Phosphoryl Azides

Dimethyl phosphorazidate **3b**, diethyl phosphorazidate **3c** and bis(2, 2, 2-trichloroethyl) phosphorazidate **3d** were prepared according to the literature with minor modification.

General procedure for the synthesis of phosphoryl azides:

To a stirred solution of phosphorochloridate (3 mmol) in acetone (20 mL), was added sodium azide (4.5 mmol) in one portion at room temperature. The reaction mixture was stirred for 3h, during this period white solid precipitated. Then the mixture was filtered through a short celite, washed with 20ml of acetone. The filtrate was dried by a rotary evaporator at room temperature with a foil cover on the flask to prevent from light. The residue was purified by column chromatography (silica gel, DCM) to give pure product.

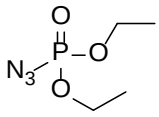
Bis(2, 2, 2-trichloroethyl) phosphorazidate 3d



White solid, 78% yield.

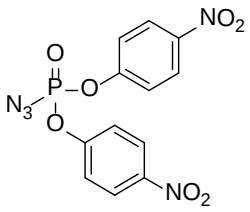
^{1}H NMR ($CDCl_3$,400MHz): δ4.71-4.65(m, 4H); ^{13}C NMR ($CDCl_3$,100MHz): δ94.2, 94.1, 77.5, 77.5; ^{31}P NMR ($CDCl_3$,162MHz): δ-2.3(s); HRMS(EI) m/z Calcd. for C4H4Cl6N3O3P $[M]^+$ 382.8121, found 382.8103.

References for the synthesis of phosphoryl azides:



3c

S. H. Kim, D. Y. Jung and S. Chang, *J. Org. Chem.*, 2007, **72**, 9769



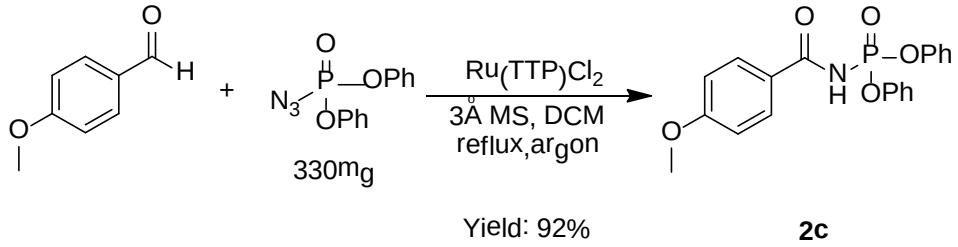
3e

T. Shioiri and S. Yamada, *Chem. Pharm. Bull.*,1974, **22**, 855

IV. General procedure for the phosphoramidation of aldehyde with phosphoryl azide catalyzed by [$Ru^{IV}(TTP)Cl_2$]

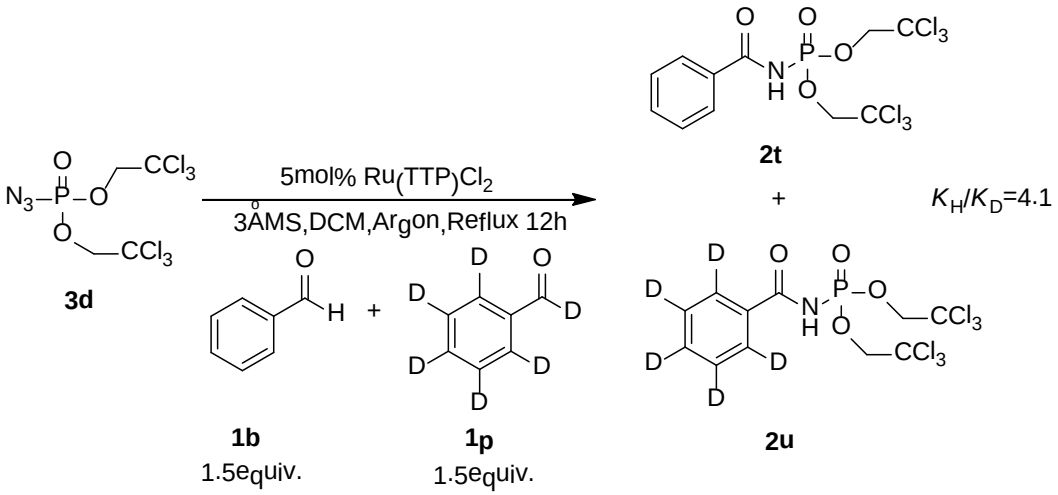
To an oven-dried schlenk flask with a rubber seal was added aldehyde (0.2mmol), DPPA (0.24 mmol), 3ÅMS (25 mg) and [$Ru^{IV}(TTP)Cl_2$] (5 mmol%). The flask was evacuated and backfilled with argon three times. Freshly distilled dichloromethane (1 mL) was added via syringe. The reaction mixture was stirred under reflux for 12h. After cooled down to room temperature, the reaction mixture was filtered through a short celite. The filtrate was concentrated by a rotary evaporator and purified by column chromatography (silica gel, DCM) to give pure product.

V. Procedure for the Scale-up Synthesis



To an oven-dried schlenk flask was added [$Ru^{IV}(TTP)Cl_2$] (42 mg, 0.05 mmol, 5 mol%) and 125 mg of 3Å molecular sieve. The sealed flask was degassed for 20min and backfilled with argon. The freshly distilled DCM (3 mL) and *p*-anisaldehyde (136 mg, 1 mmol, 1 equiv.) were added via syringe. The mixture was heated to reflux. A solution of DPPA (330 mg, 1.2 mmol, 1.2 equiv.) in 2.5 mL of DCM was added dropwise via syringe pump within 5h. After addition, the reaction mixture was stirred for another 7h. Then the reaction mixture was concentrated by a rotary evaporator and the residue was purified by column chromatography to give the pure product **2c** in 92% yield.

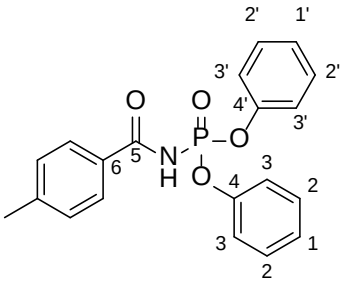
VI. Kinetic Isotope Effect Experiment



To an oven-dried schlenk flask with a rubber seal was added bis(2,2,2-trichloroethyl) phosphorazidate **3d** (77 mg, 0.2 mmol), [Ru^{IV}(TTP)Cl_2] (8.4 mg, 0.01 mmol, 5 mol%) and 50 mg of 3Å molecular sieve. The flask was evacuated and backfilled with argon three times. Then benzaldehyde **1b** (32 mg, 0.3 mmol) and benzaldehyde-*d*6 **1p** (34 mg, 0.3 mmol) were added. The reaction mixture was stirred under reflux for 12h. Upon the completion of the reaction, the mixture was allowed to cool and purified by a column chromatography (silica gel, hexane:EA=3:1) to give a mixture of bis(2,2,2-trichloroethyl) benzoylphosphoramidate **2t** and bis(2,2,2-trichloroethyl) benzoylphosphoramidate-*d*5 **2u** (the labile D of N-D was replaced by H during purification). The ratio of k_H/k_D was determined by ^{1}H NMR.

VII. Characterizations of Products

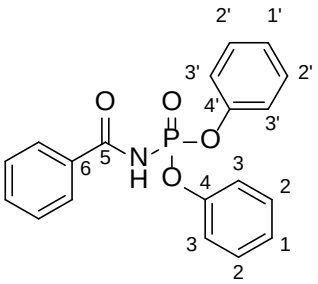
Diphenyl (4-methylbenzoyl)phosphoramidate 2a



^{1}H NMR ($CDCl_3$,400MHz): δ9.49(d, 1H, NH, $J_{H\text{-}P}$=10.3Hz), 7.86(d, 2H, J=7.8Hz), 7.25-7.22(m, 8H), 7.18(d, 2H, J=7.9Hz), 7.14-7.11(m, 2H), 2.38(s, 3H); ^{13}C NMR ($CDCl_3$,100MHz): δ167.5(d, C5, $J_{C\text{-}P}$=3.6Hz), 150.2(C4 or C4′), 150.1(C4 or C4′), 143.8, 129.8(C2 & C2′), 129.5(d, C6, $J_{C\text{-}P}$=11.4Hz), 129.3, 128.5, 125.6(C1 & C1′), 120.7(C3 or C3′), 120.6(C3 or C3′), 21.7; ^{31}P NMR ($CDCl_3$,162MHz): δ-9.1(d, $J_{P\text{-}H}$=10.3Hz).

HRMS(EI) m/z Calcd. for C20H18NO4P $[M]^+$ 367.0973, found 367.0957.

Diphenylbenzoylphosphoramidate 2b



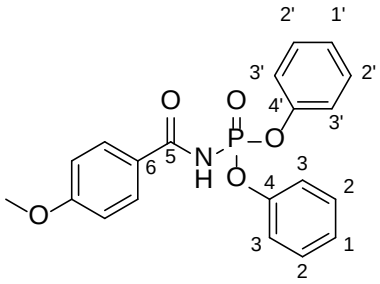
^{1}H NMR ($CDCl_3$,400MHz): δ9.62(d, 1H, NH, $J_{H\text{-}P}$=9.6Hz), 7.97(d, 2H, J=8.6Hz), 7.54(t, 1H, J=7.4Hz), 7.39(t, 2H, J=7.8Hz), 7.25(m, 8H), 7.17-7.11(m, 2H); ^{13}C NMR ($CDCl_3$,100MHz): δ167.6(d, C5, $J_{C\text{-}P}$=3.4Hz), 150.2(C4 or C4′), 150.1(C4 or C4′), 133.1, 132.3(d, C6, $J_{C\text{-}P}$=11.2Hz), 129.8(C2 & C2′), 128.6, 128.5,

125.7(C1 & C1′), 120.6(C3 or C3′), 120.6(C3 or C3′); ^{31}P NMR ($CDCl_3$,162MHz): δ-9.1(d, J_{P-H}=9.6Hz).

HRMS(EI) m/z Calcd. for C19H16NO4P $[M]^+$ 353.0817, found 353.0810.

Anal. Calcd. for C19H16NO4P: C, 64.59; H, 4.56; N, 3.96. Found: C, 64.59; H, 4.52; N, 3.92.

Diphenyl (4-methoxybenzoyl)phosphoramidate 2c

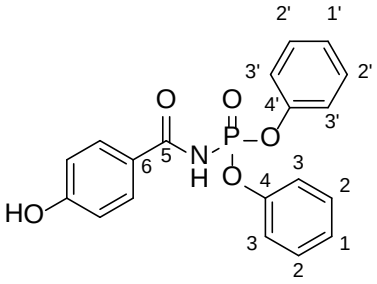


^{1}H NMR ($CDCl_3$,400MHz): δ8.79(d, 1H, NH, J_{H-P}=10.3Hz), 7.90(d, 2H, J=8.9Hz), 7.28-7.26(m, 8H), 7.17-7.13(m, 2H), 6.88(d, 2H, J=8.9Hz), 3.85(s, 3H); ^{13}C NMR ($CDCl_3$,100MHz): δ167.0(d, C5, J_{C-P}=3.2Hz), 163.5 (C-OMe), 150.3(C4 or C4′), 150.2(C4 or C4′), 131.1, 129.8(C2 & C2′), 125.6(C1 & C1′), 124.6(d, C6, J_{C-P}=11.3Hz), 120.7(C3 or C3′), 120.6(C3 or C3′), 113.8, 55.6; ^{31}P NMR ($CDCl_3$,162MHz): δ-8.8(d, J_{P-H}=10.3Hz).

HRMS(EI) m/z Calcd. for C20H18NO5P $[M]^+$ 383.0923, found 383.0912.

Anal. Calcd. for C20H18NO5P : C, 62.66; H, 4.73; N, 3.65. Found: C, 62.07; H, 4.71; N, 3.74.

Diphenyl (4-hydroxybenzoyl)phosphoramidate 2d

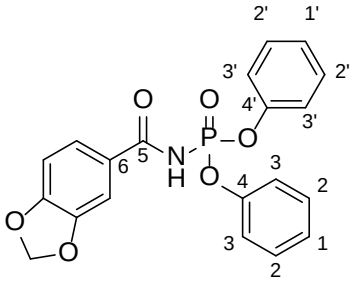


^{1}H NMR (*d*6-DMSO,400MHz): δ10.41(s, 1H), 10.37(s, 1H), 7.87(d, 2H, *J*=8.4Hz), 7.45(t, 4H, *J*=7.3Hz), 7.29-7.27(m, 6H), 6.85(d, 2H, *J*=7.9Hz); ^{13}C NMR (*d*6-Acetone,100MHz): δ167.5 (C5), 162.7 (C-OH), 151.5(C4 or C4′), 151.4(C4 or C4′), 131.4, 130.6(C2 & C2′), 126.2(C1 & C1′), 124.8(d, C6, $J_{C\text{-}P}$ =11.1Hz), 121.5(C3 or C3′), 121.4(C3 or C3′), 116.1; ^{31}P NMR ($CDCl_3$,162MHz): δ-9.7(s).

HRMS(EI) m/z Calcd. for C19H16NO5P $[M]^+$ 369.0766, found 369.0748.

Anal. Calcd. for C19H16NO5P: C, 61.79; H, 4.37; N, 3.79. Found: C, 61.78; H, 4.39; N, 3.73.

Diphenylbenzo[d][1,3]dioxole-5-carbonylphosphoramidate 2e

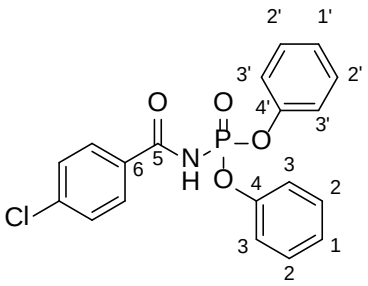


^{1}H NMR ($CDCl_3$,400MHz): δ9.58(d, 1H, NH, $J_{H\text{-}P}$=10.1Hz), 7.56(dd, 1H, *J*=8.2, 1.8Hz), 7.50(d, 1H, *J*=1.7Hz), 7.25-7.21(m, 8H), 7.15-7.13(m, 2H), 6.72(d, 1H, *J*=8.2Hz), 6.02(s, 2H); ^{13}C NMR ($CDCl_3$,100MHz): δ166.7(d, C5, $J_{C\text{-}P}$=3.1Hz), 151.7(C-O-dioxolane), 150.2(C4 or C4′), 150.1(C4 or C4′), 148.1(C-O-dioxolane), 129.8(C2 & C2′), 126.3(d, C6, $J_{C\text{-}P}$=11.3Hz), 125.7(C1 & C1′), 124.3,

120.6(C3 or C3′), 120.6(C3 or C3′), 108.8, 108.1, 101.9(O-CH_2-O); ^{31}P NMR ($CDCl_3$,162MHz): δ-9.0(d, J_{P-H}=9.9Hz).

HRMS(EI) m/z Calcd. for C20H16NO6P $[M]^+$ 397.0715, found 397.0708.

Diphenyl(4-chlorobenzoyl)phosphoramidate 2f

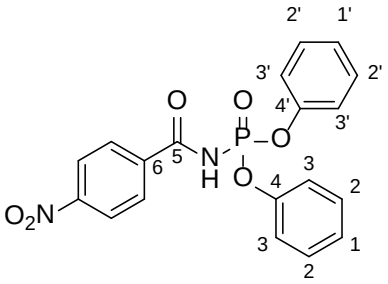


^{1}H NMR ($CDCl_3$,400MHz): δ9.65(d, 1H, NH, J_{H-P}=10.1Hz), 7.88(d, 2H, J=8.6Hz), 7.32(d, 2H, J=8.5Hz), 7.27-7.19(m, 8H), 7.15-7.13(m, 2H); ^{13}C NMR ($CDCl_3$,75MHz): δ166.6(d, C5, J_{C-P}=3.3Hz), 150.2(C4 or C4′), 150.1(C4 or C4′), 139.6(C-Cl), 130.6(d, C6, J_{C-P}=11.4Hz), 130.0, 129.9(C2 & C2′), 128.9, 125.8(C1 or C1′), 125.8(C1 or C1′), 120.6(C3 or C3′), 120.5(C3 or C3′); ^{31}P NMR ($CDCl_3$,162MHz): δ-9.2(d, J_{P-H}=9.9Hz).

HRMS(EI) m/z Calcd. for C19H15ClNO4P $[M]^+$ 387.0427 , found 387.0417.

Anal. Calcd. for C19H15ClNO4P: C, 58.85; H, 3.90; N, 3.61. Found: C, 58.38; H, 3.84; N, 3.68.

Diphenyl (4-nitrobenzoyl)phosphoramidate 2g

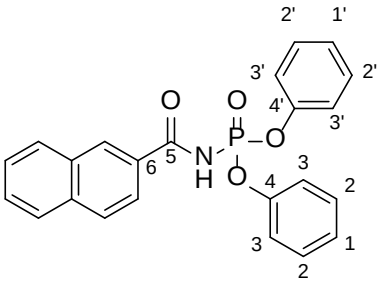


^{1}H NMR ($CDCl_3$,400MHz): δ10.22(d, 1H, NH, J_{H-P}=9.4Hz), 8.16(d, 2H, *J*=8.6Hz), 8.11(d, 2H, *J*=8.8Hz), 7.28(t, 4H, *J*=7.9Hz), 7.20-7.16(m,6H); ^{13}C NMR ($CDCl_3$, 75MHz): δ166.2 (d, C5, J_{C-P}=3.2Hz), 150.9(C-NO_2), 150.5(C4 or C4′), 150.4(C4 or C4′), 137.8(d, C6, J_{C-P}=11.7Hz), 130.4(C2 & C2′), 130.2, 126.5(C1 or C1′), 126.5(C1 or C1′), 124.2, 120.9(C3 or C3′), 120.9(C3 or C3′); ^{31}P NMR ($CDCl_3$,162MHz): δ-9.7(d, J_{P-H}=9.4Hz).

HRMS(EI) m/z Calcd. for C19H15N2O6P $[M]^+$ 398.0668 , found 398.0658.

Anal. Calcd. for C19H15N2O6P: C, 57.29; H, 3.80; N, 7.03. Found: C, 57.30; H, 3.87; N, 6.94.

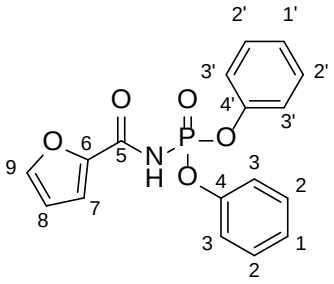
Diphenyl 2-naphthoylphosphoramidate 2h



^{1}H NMR ($CDCl_3$,400MHz): δ10.00(d, 1H, NH, J_{H-P}=10.2Hz), 8.61(s, 1H), 8.06(dd, 1H, *J*=8.6, 1.7Hz), 7.85(d, 1H, *J*=8.0Hz), 7.84(d, 1H, *J*=8.6Hz), 7.72(d, 1H, *J*=8.0Hz), 7.58(t, 1H, *J*=7.0Hz), 7.49(t, 1H, *J*=7.1Hz), 7.27-7.15(m, 8H), 7.08(t, 2H, *J*=7.1Hz); ^{13}C NMR ($CDCl_3$,100MHz): δ167.8(d, C5, J_{C-P}=3.4Hz), 150.2(C4 or C4′), 150.1(C4 or C4′), 135.5, 132.5, 129.9, 129.8(C2 & C2′), 129.6, 129.4(d, C6, J_{C-P}=11.2Hz), 128.5, 128.4, 127.7, 126.8, 125.6(C1 & C1′), 124.5, 120.7(C3 or C3′), 120.6(C3 or C3′); ^{31}P NMR ($CDCl_3$,162MHz): δ-8.8(d, J_{P-H} =9.9Hz).

HRMS(EI) m/z Calcd. for C23H18NO4P $[M]^+$ 403.0973 , found 403.0964.

Diphenyl furan-2-carbonylphosphoramidate 2i

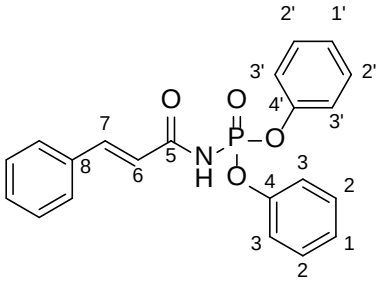


^{1}H NMR ($CDCl_3$,400MHz): δ8.71(d, 1H, NH, $J_{H\text{-}P}$=10.3Hz), 7.48(dd, 1H, H9, $J_{H9\text{-}H8}$=1.7Hz, $J_{H9\text{-}H7}$=0.7Hz), 7.31(d, 1H, H7, $J_{H7\text{-}H8}$=3.6Hz), 7.28-7.26(m, 8H), 7.18-7.15(m, 2H), 6.48(dd, 1H, H8, $J_{H8\text{-}H9}$=1.7Hz, $J_{H8\text{-}H7}$=3.6Hz); ^{13}C NMR ($CDCl_3$,100MHz): δ165.4 (C5), 157.4 (C6), 150.1(C4 or C4′), 150.0(C4 or C4′), 146.1(C9), 129.8(C2 & C2′), 125.7(C1 & C1′), 120.6(C3 or C3′), 120.6(C3 or C3′), 117.7(C7), 112.7(C8); ^{31}P NMR ($CDCl_3$,162MHz): δ-10.7(d, $J_{P\text{-}H}$=10.1Hz).

HRMS(EI) m/z Calcd. for C17H14NO5P $[M]^+$ 343.0610 , found 343.0599.

Anal. Calcd. for C17H14NO5P: C, 59.48; H, 4.11; N, 4.08. Found: C, 59.54; H, 4.12; N, 4.03.

Diphenylcinnamoylphosphoramidate 2j



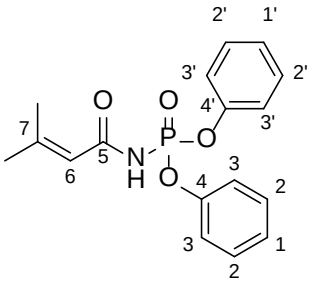
^{1}H NMR ($CDCl_3$,400MHz): δ9.21(d, 1H, NH, $J_{H\text{-}P}$=11.5Hz), 7.73(d, 1H, J_{trans}=15.8Hz), 7.46(d, 1H, J=7.12Hz), 7.45(d, 1H, J=7.64Hz), 7.39-7.36(m, 3H), 7.28-7.23(m, 8H), 7.15-7.14(m, 2H), 6.46(d, 1H, J_{trans}=15.7Hz); ^{13}C NMR ($CDCl_3$,100MHz): δ166.4 (C5), 150.1(C4 or C4′), 150.0(C4 or C4′), 144.8 (C7), 134.2(C8), 130.6, 129.9(C2 & C2′), 129.0, 128.4, 125.8(C1 & C1′), 120.6(C3 or

C3′), 120.6(C3 or C3′), 119.4(d, C6, $J_{C\text{-}P}$=12.9Hz); ^{31}P NMR ($CDCl_3$, 162MHz): δ-8.8(d, $J_{P\text{-}H}$=11.2Hz).

HRMS(EI) m/z Calcd. for C21H18NO4P $[M]^+$ 379.0973 , found 379.0956.

Anal. Calcd. for C21H18NO4P: C, 66.49; H, 4.78; N, 3.69. Found: C, 66.46; H, 4.76; N, 3.68.

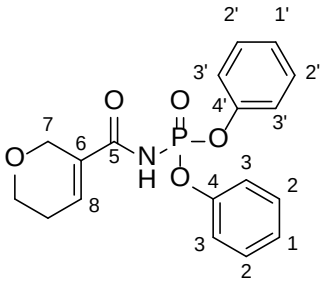
Diphenyl (3-methylbut-2-enoyl)phosphoramidate 2k



^{1}H NMR ($CDCl_3$,400MHz): δ8.66(d, 1H, NH, $J_{H\text{-}P}$=11.3Hz), 7.31-7.21(m,8H), 7.19-7.15(m,2H), 5.61(s, 1H), 2.17(s, 3H), 1.83(s, 3H); ^{13}C NMR ($CDCl_3$,100MHz): δ166.3(d, C5, $J_{C\text{-}P}$=2.6Hz), 158.4(d, C7, $J_{C\text{-}P}$=2.4Hz), 150.2(C4 or C4′), 150.1(C4 or C4′), 129.8(C2 & C2′), 125.6(C1 & C1′), 120.7(C3 or C3′), 120.6(C3 or C3′), 117.3(d, C6, $J_{C\text{-}P}$=12.9Hz), 27.7, 20.5; ^{31}P NMR ($CDCl_3$,162MHz): δ-9.1(d, $J_{P\text{-}H}$=11.8Hz).

HRMS(EI) m/z Calcd. for C17H18NO4P $[M]^+$ 331.0973, found 331.0964.

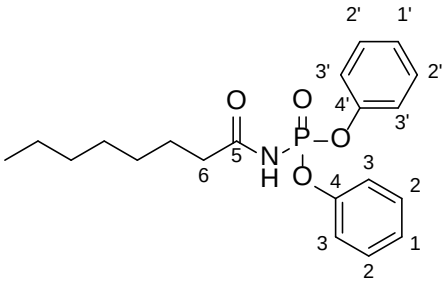
Diphenyl (5,6-dihydro-2H-pyran-3-carbonyl)phosphoramidate 2l



^{1}H NMR ($CDCl_3$,400MHz): δ9.34(d, 1H, NH, J_{H-P}=10.0Hz), 7.32-7.27(m, 4H), 7.22-7.16(m, 6H), 6.87-6.85(m, 1H), 4.30(dd, 2H, *J*=4.4, 2.5Hz), 3.68(t, 2H, *J*=5.5Hz), 2.17-2.11(m,2H); ^{13}C NMR ($CDCl_3$,100MHz): δ166.6(d, C5, J_{C-P} =3.3Hz), 150.6(C4 or C4′), 150.5(C4 or C4′), 135.9 (C8), 132.5(d, C6, J_{C-P} =10.4Hz), 130.2(C2 & C2′), 126.1(C1 & C1′), 120.9(C3 or C3′), 120.9(C3 or C3′), 64.8(C7), 63.6, 25.9; ^{31}P NMR ($CDCl_3$,162MHz): δ-9.1(d, J_{P-H}=9.9Hz).

HRMS(EI) m/z Calcd. for C18H18NO5P $[M]^+$ 359.0923 , found 359.0911.

Diphenyloctanoylphosphoramidate 2m

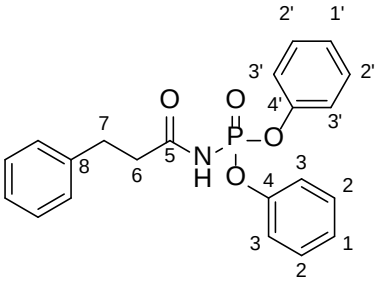


^{1}H NMR ($CDCl_3$,400MHz): δ9.06(d, 1H, NH, J_{H-P}=11.0Hz), 7.32-7.26(m,4H), 7.21-7.16(m, 6H), 2.19(t, 2H, *J*=7.3Hz), 1.50(m, 2H), 1.24(m, 8H), 0.88-0.84(m, 3H); ^{13}C NMR ($CDCl_3$,100MHz): δ174.6(d, C5, J_{C-P}=4.8Hz), 150.1(C4 or C4′), 150.0(C4 or C4′), 129.8(C2 & C2′), 125.7(C1 & C1′), 120.6(C3 or C3′), 120.5(C3 or C3′), 37.2(d, C6, J_{C-P}=9.5Hz), 31.7, 29.0, 28.9, 24.8, 22.7, 14.1; ^{31}P NMR ($CDCl_3$,162MHz): δ-10.4(d, J_{P-H}=11.1Hz)

HRMS(EI) m/z Calcd. for C20H26NO4P $[M]^+$ 375.1599, found 375.1593.

Anal. Calcd. for C20H26NO4P: C, 63.99; H, 6.98; N, 3.73. Found: C, 64.14; H, 7.07; N, 3.63.

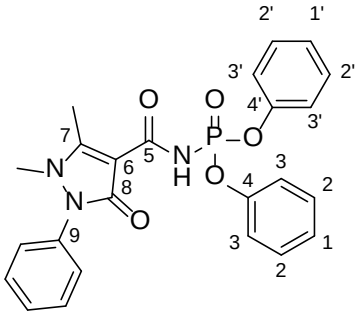
Diphenyl (3-phenylpropanoyl)phosphoramidate 2n



^{1}H NMR ($CDCl_3$,400MHz): δ9.15(d, 1H, NH, J_{H-P}=11.4Hz), 7.25-7.11(m, 15H), 2.84(t, 2H, J=7.7Hz), 2.50(t, 2H, J=7.7Hz); ^{13}C NMR ($CDCl_3$,100MHz): δ173.58(d, C5, J_{C-P}=4.8Hz), 150.0(C4 or C4′), 149.9(C4 or C4′), 140.3(C8), 129.8(C2 & C2′), 128.5, 128.5, 126.3, 125.7(C1 & C1′), 120.6(C3 or C3′), 120.5(C3 or C3′), 38.6(d, C6, J_{C-P}=9.9Hz), 30.5(C7); ^{31}P NMR ($CDCl_3$,162MHz): δ-9.8(d, J_{P-H}=11.6Hz).

HRMS(EI) m/z Calcd. for C21H20NO4P $[M]^+$ 381.1130 , found 381.1118.

Diphenyl (1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazole-4-carbonyl)-phosphoramidate 2o

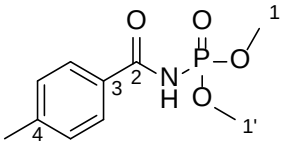


^{1}H NMR ($CDCl_3$,400MHz): δ10.30(d, 1H, NH, J_{H-P}=14.0Hz), 7.52(t, 2H, J=7.5Hz), 7.47(t, 1H, J=7.4Hz), 7.30-7.27(m, 10H), 7.16-7.13(m,2H), 3.33(s, 3H), 2.70(s, 3H); ^{13}C NMR ($CDCl_3$,100MHz): δ163.9(C5), 163.1(C8), 154.9(C7), 150.6(C4 or C4′), 150.5(C4 or C4′), 132.7(C9), 129.9, 129.7(C2 & C2′), 129.5, 127.0, 125.3(C1 & C1′), 120.8(C3 or C3′), 120.7(C3 or C3′), 98.3(d,

C6, J_{C-P} =12.5Hz), 33.4(N-CH_3), 12.1; ^{31}P NMR ($CDCl_3$,162MHz): δ-10.3(d, J_{P-H} =13.9Hz).

HRMS(EI) m/z Calcd. for C24H22N3O5P $[M]^+$ 463.1297 , found 463.1285.

Dimethyl (4-methylbenzoyl)phosphoramidate 2p

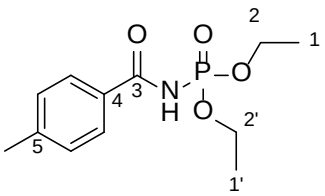


^{1}H NMR ($CDCl_3$,400MHz): δ9.01(d, 1H, NH, J_{H-P}=9.1Hz), 7.96(d, 2H, J=6.7Hz), 7.28(d, 2H, J=6.8Hz), 3.91(s, 3H), 3.88(s, 3H), 2.41(s, 3H); ^{13}C NMR ($CDCl_3$,100MHz): δ167.9(d, C2, J_{C-P}=2.0Hz), 143.8(C4), 129.6(d, C3, J_{C-P} =10.5Hz) 129.4, 128.4, 54.6(C1 or C1′), 54.5(C1 or C1′), 21.7; ^{31}P NMR ($CDCl_3$,162MHz): δ1.8(d, J_{P-H}=9.6Hz).

HRMS(EI) m/z Calcd. for C10H14NO4P $[M]^+$ 243.0660 , found 243.0649.

Anal. Calcd. for C10H14NO4P: C, 49.39; H, 5.80; N, 5.76. Found: C, 49.09; H, 5.78; N, 5.61.

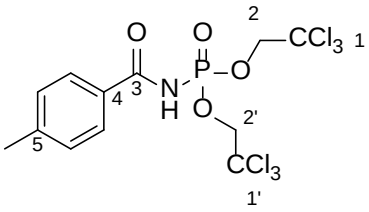
Diethyl (4-methylbenzoyl)phosphoramidate 2q



^{1}H NMR ($CDCl_3$,400MHz): δ8.83(d, 1H, NH, J_{H-P}=9.0Hz), 7.93(d, 2H, J=8.2Hz), 7.27(d, 2H, J=7.9Hz), 4.34-4.20(m, 4H), 2.41(s, 3H), 1.37(t, 6H, J=7.0Hz); ^{13}C NMR ($CDCl_3$,100MHz): δ167.4(C3), 143.3(C5), 129.6(d, C4, J_{C-P}=10.4Hz), 129.1, 128.0, 64.0(C2 or C2′), 63.9(C2 or C2′), 21.3, 15.9(C1 or C1′), 15.8(C1 or C1′); ^{31}P NMR ($CDCl_3$,162MHz): δ-1.5(q, J_{P-H}=8.0Hz).

HRMS(EI) m/z Calcd. for C12H18NO4P $[M]^+$ 271.0973 , found 271.0968.

Bis(2,2,2-trichloroethyl) (4-methylbenzoyl)phosphoramidate 2r

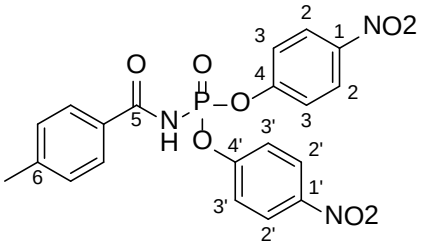


^{1}H NMR ($CDCl_3$,400MHz): δ9.46(d, 1H, NH, J_{H-P}=10.1Hz), 7.94(d, 2H, *J*=8.1Hz), 7.27(d, 2H, *J*=7.7Hz), 4.84(s, 2H), 4.82(s,2H), 2.42(s,3H); ^{13}C NMR ($CDCl_3$,75MHz): δ168.2(C3), 144.5(C5), 129.7, 128.8(d, C4, J_{C-P}=10.9Hz), 128.5, 94.8(C1 or C1′), 94.7(C1 or C1′), 77.9(C2 or C2′), 77.9(C2 or C2′), 21.8; ^{31}P NMR ($CDCl_3$,162MHz): δ-3.7(q, J_{P-H}= 7.9Hz).

HRMS(EI) m/z Calcd. for C12H12Cl6NO4P $[M]^+$ 474.8635 , found 474.8626.

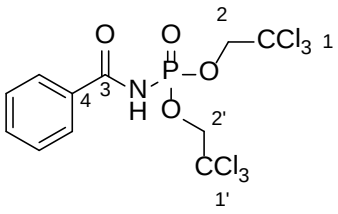
Anal. Calcd. for C12H12Cl6NO4P: C, 30.16; H, 2.53; N, 2.93. Found: C, 30.33; H, 2.59; N, 3.04.

Bis(4-nitrophenyl) (4-methylbenzoyl)phosphoramidate 2s



^{1}H NMR ($CDCl_3$,400MHz): δ8.97(s, 1H, NH), 8.18(d, 4H, *J*=8.4Hz), 7.81(d, 2H, *J*=7.9Hz), 7.42(d, 4H, *J*=8.7Hz), 7.25(d, 2H, *J*=7.5Hz), 2.43(s,3H); ^{13}C NMR ($CDCl_3$,100MHz): δ161.7 (C5), 154.2(C4 or C4′), 154.2(C4 or C4′), 145.6(C6), 145.3(C1 & C1′), 129.8, 128.3, 126.3, 125.9(C2 & C2′),, 121.4(C3 or C3′), 121.3(C3 or C3′), 115.8, 21.7; ^{31}P NMR ($CDCl_3$,162MHz): δ-10.4(s).

Bis(2,2,2-trichloroethyl) benzoylphosphoramidate 2t



^{1}H NMR ($CDCl_3$,400MHz): δ9.49(d, 1H, NH, J_{H-P}=8.6Hz), 8.05(d, 2H, *J*=7.5Hz), 7.60(t, 1H, *J*=7.4Hz), 7.48(t, 2H, *J*=7.6Hz), 4.85(s,2H), 4.83(s,2H); ^{13}C NMR ($CDCl_3$,100MHz):δ168.2(C3), 133.5, 131.5(d, C4, J_{C-P}=10.9Hz), 128.8, 128.3, 94.6(C1 or C1′), 94.5(C1 or C1′), 77.8(C2 or C2′), 77.8(C2 or C2′); ^{31}P NMR ($CDCl_3$,162MHz): δ-3.8(m).

HRMS(EI) m/z Calcd. for C11H10C6NO4P $[M]^+$ 460.8479 , found 460.8468.

X-Ray Data of Diphenyl(4-methylbenzoyl)phosphoramidate 2a

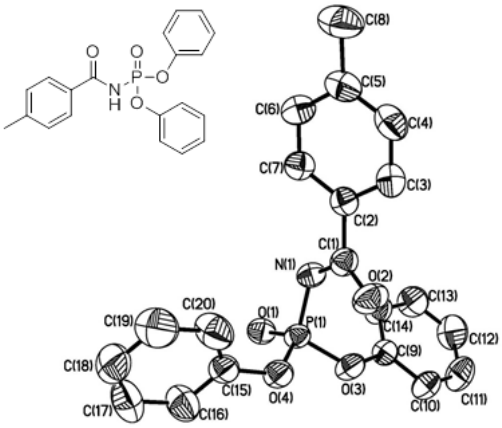


Fig. S1 X-ray crystal structure of **2a** (CCDC 862823 for **2a** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from

The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif).

Computing details

Program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008).

Crystal data

$C_{20}H_{18}NO_4P$	F(000) = 768
M_r = 367.32	D_x = 1.294 Mg m^{-3}
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation, λ = 1.54178 Å
a = 10.0023 (7) Å	Cell parameters from 216 reflections
b=10.6631(7)Å	θ=3–45°
c=17.6975(12)Å	μ=1.50mm^{-1}
β=92.303(2)°	T=296K
V=1886.0(2)$Å^3$	Block, Yellow
Z=4	0.04×0.04×0.03mm

Data collection

Radiation source: fine-focus sealed tube	3061reflectionswith$I>2\sigma(I)$
graphite	R_{int}=0.047
Absorption correction: Multi-scan	
SADABS	θ_{max}=65.9°,θ_{min}=4.8°
T_{min}=0.942,T_{max}=0.956	h=−11→10

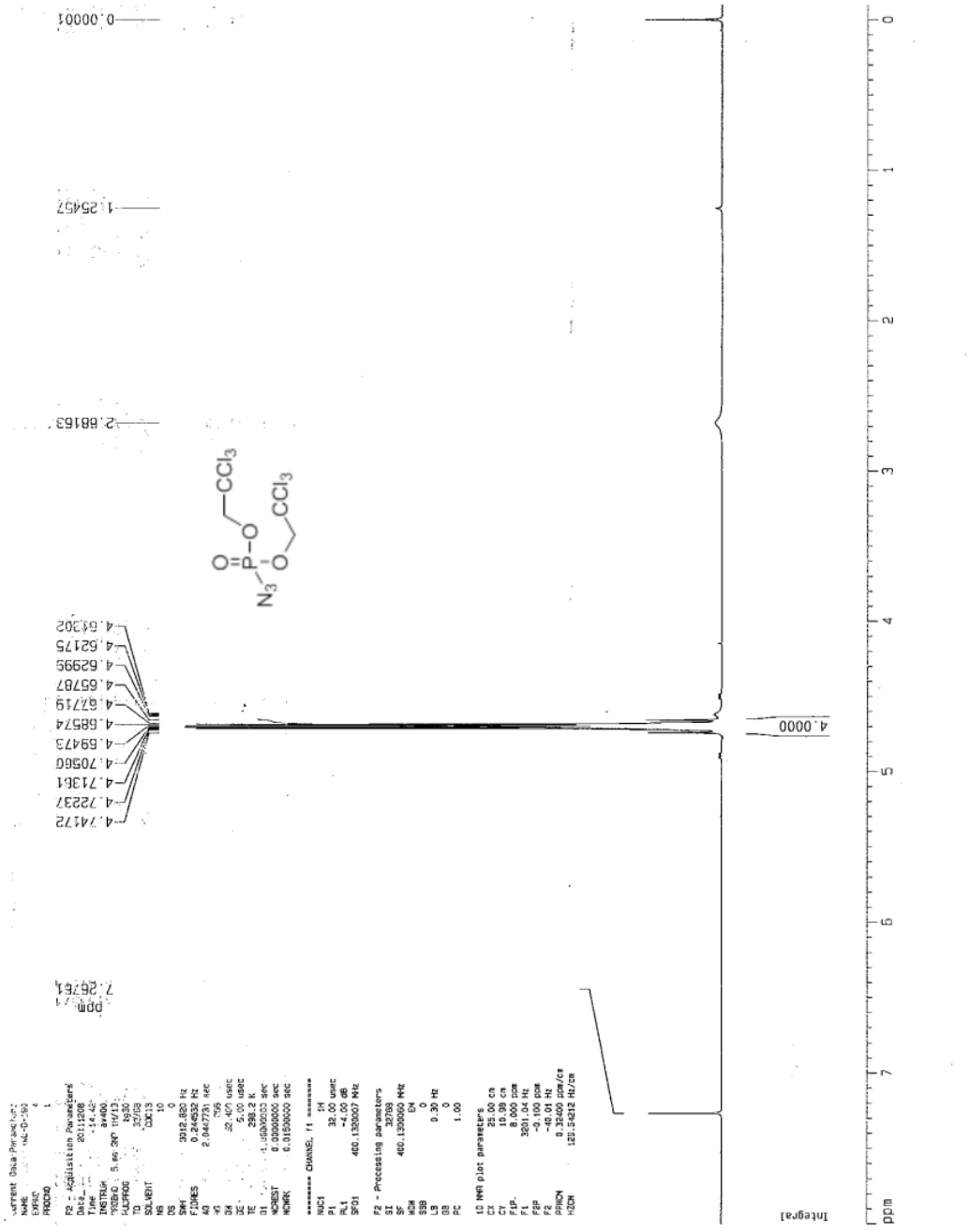
23806measuredreflections	k=−12→12
3232independentreflections	l=−20→20

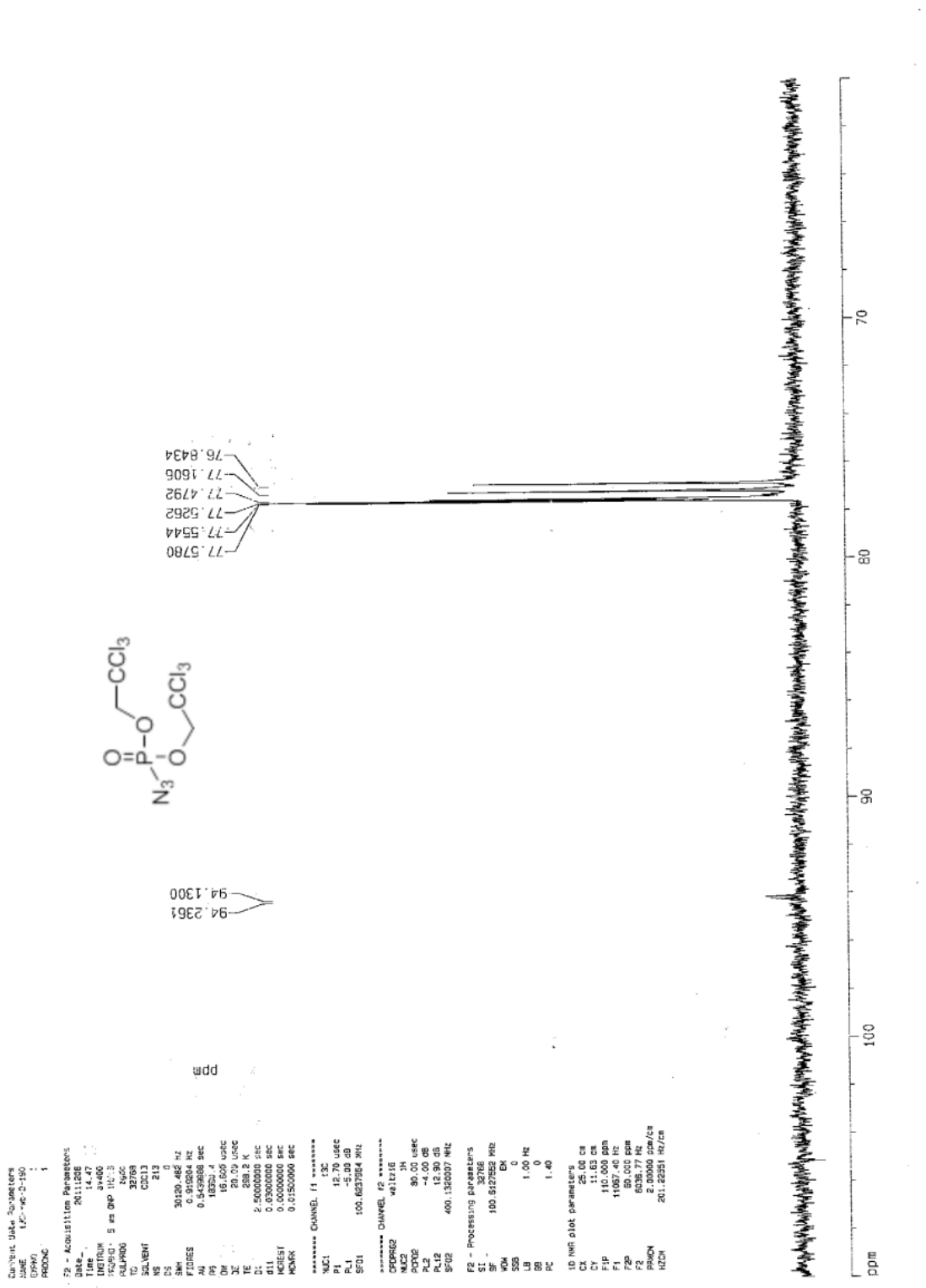
Refinement

Refinement on F^2	Primary atom site location: Structure-invariant direct methods
Least-square smatrix: Full	Secondary atom site location: Difference Fourier map
$R[F^2>2\sigma(F^2)]$=0.038	Hydrogen site location: Inferred from neighbouring sites
$wR(F^2)$=0.109	H-atom parameters constrained
S=1.04	$w=1/[\sigma^2(F_o^2)+(0.0697P)^2+0.352P]$ where $P = (F_o^2 + 2F_c^2)/3$
3232reflections	$(\Delta/\sigma)_{max}$=0.002
236parameters	$\Delta\rho_{max}$=0.18eÅ^{-3}
0restraints	$\Delta\rho_{min}$=−0.44eÅ^{-3}

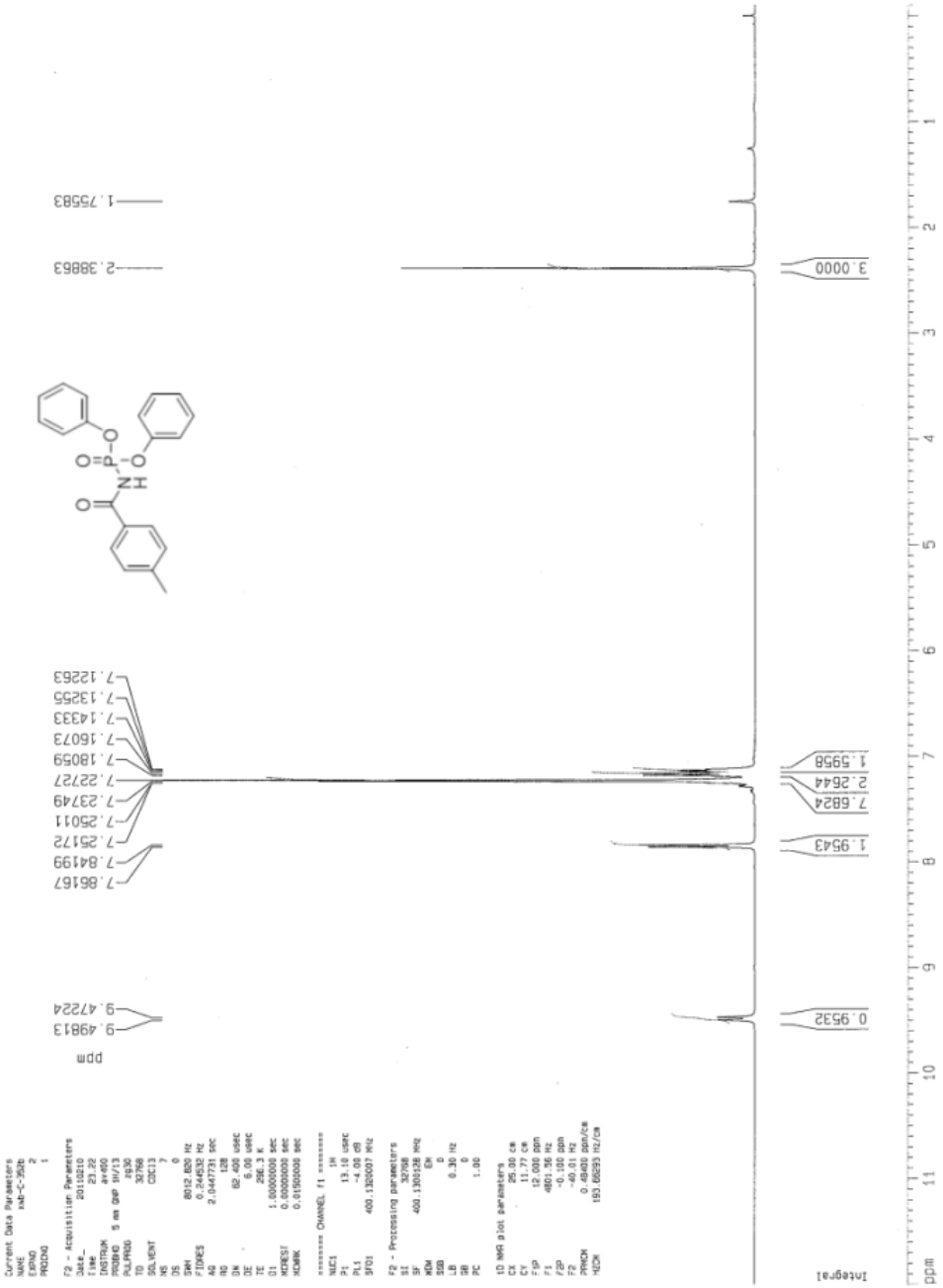
NMR Spectra

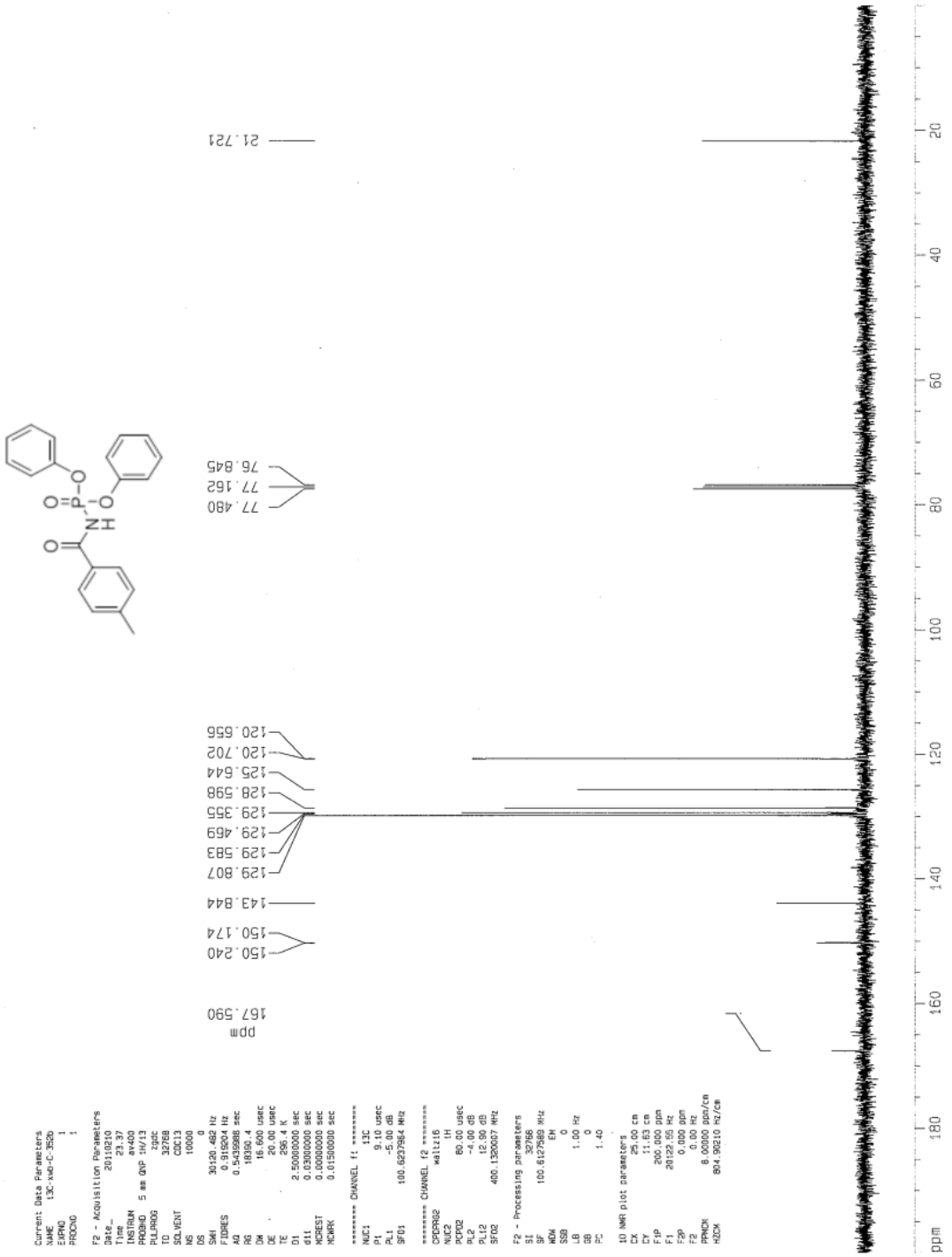
Bis(2,2,2-trichloroethyl)phosphorazidate3d

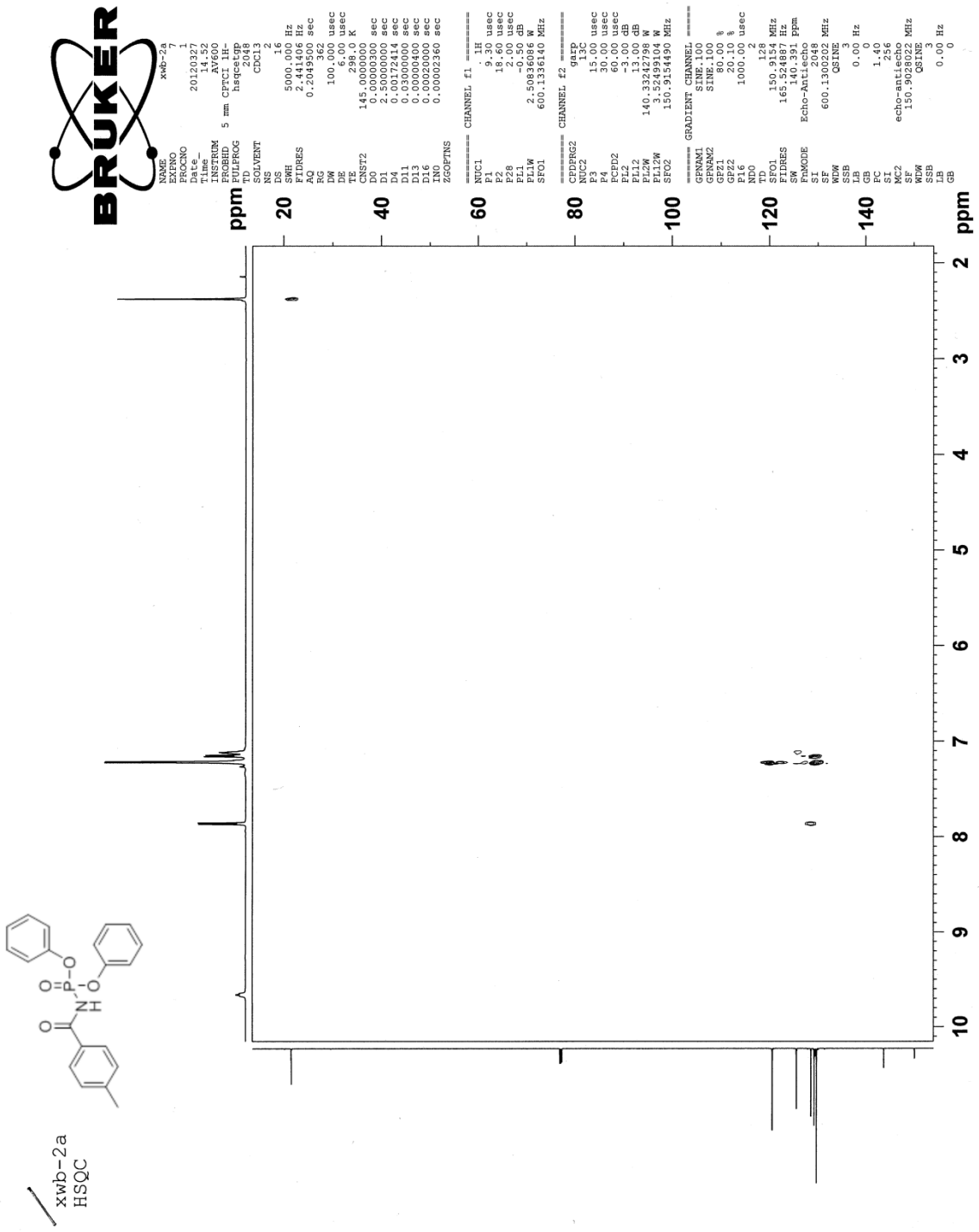



77.5780
77.5544
77.5262
77.4792
77.1606
76.8434
94.2361
94.1300
ppm
70
80
90
100

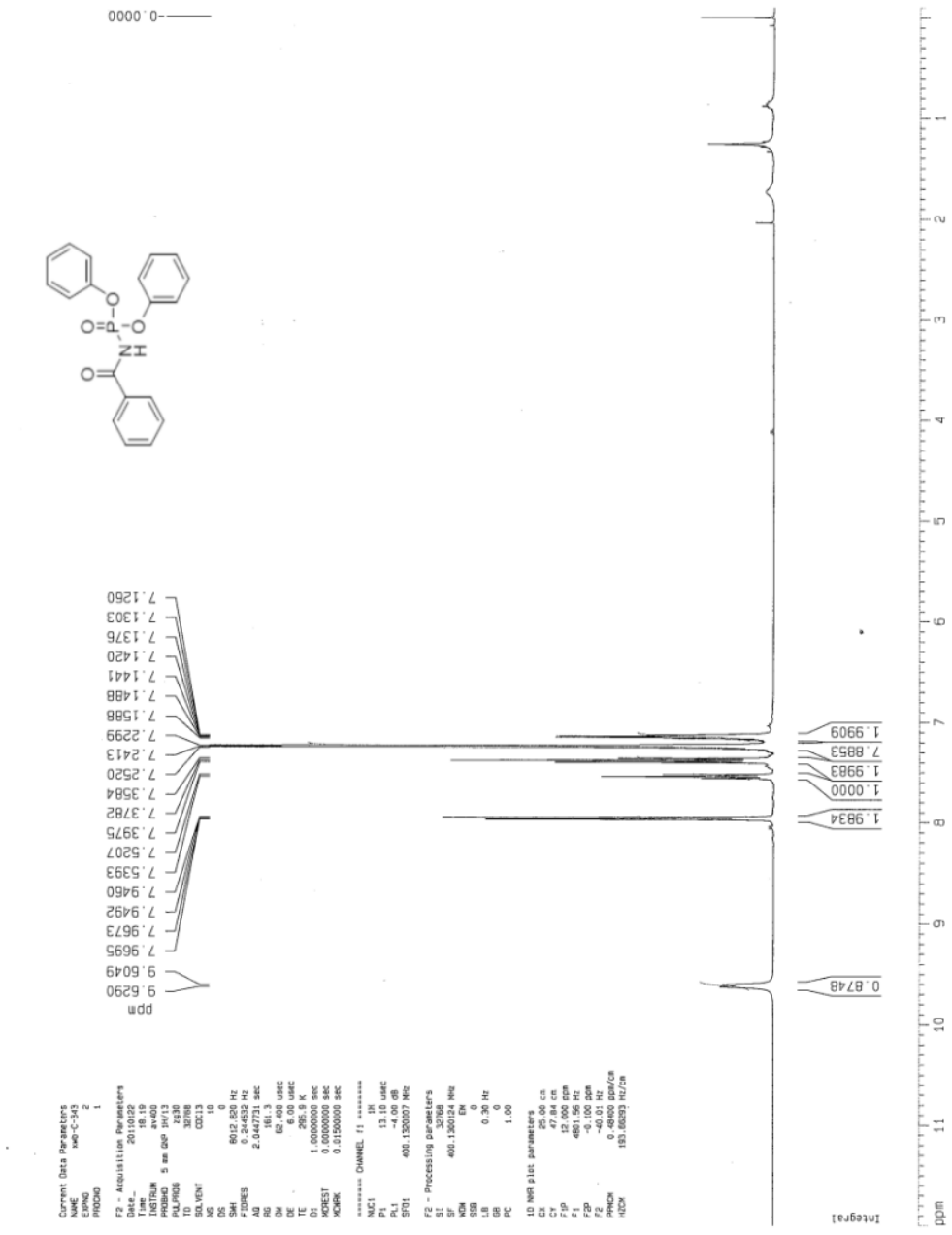
Diphenyl (4-methylbenzoyl)phosphoramidate 2a

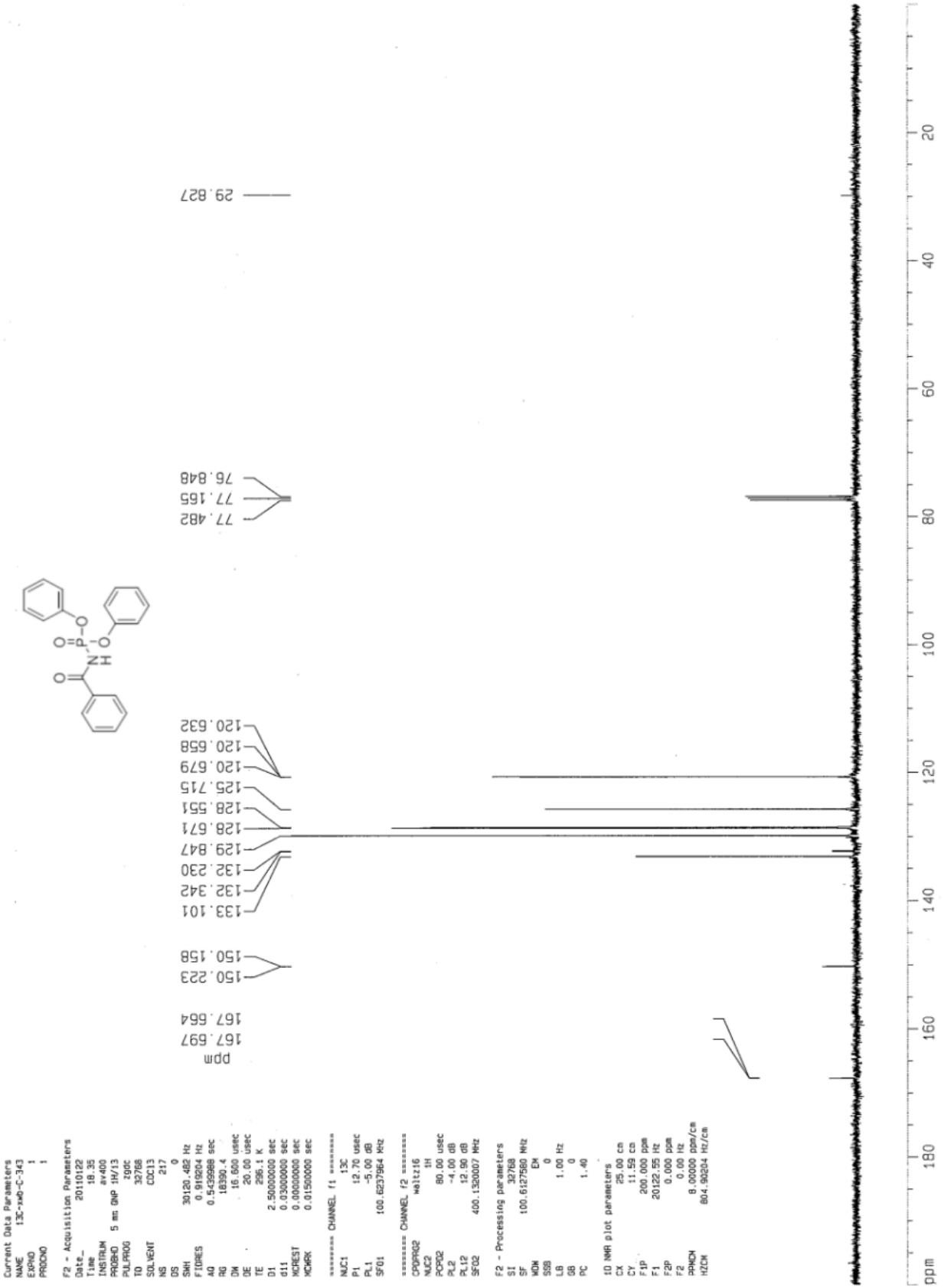


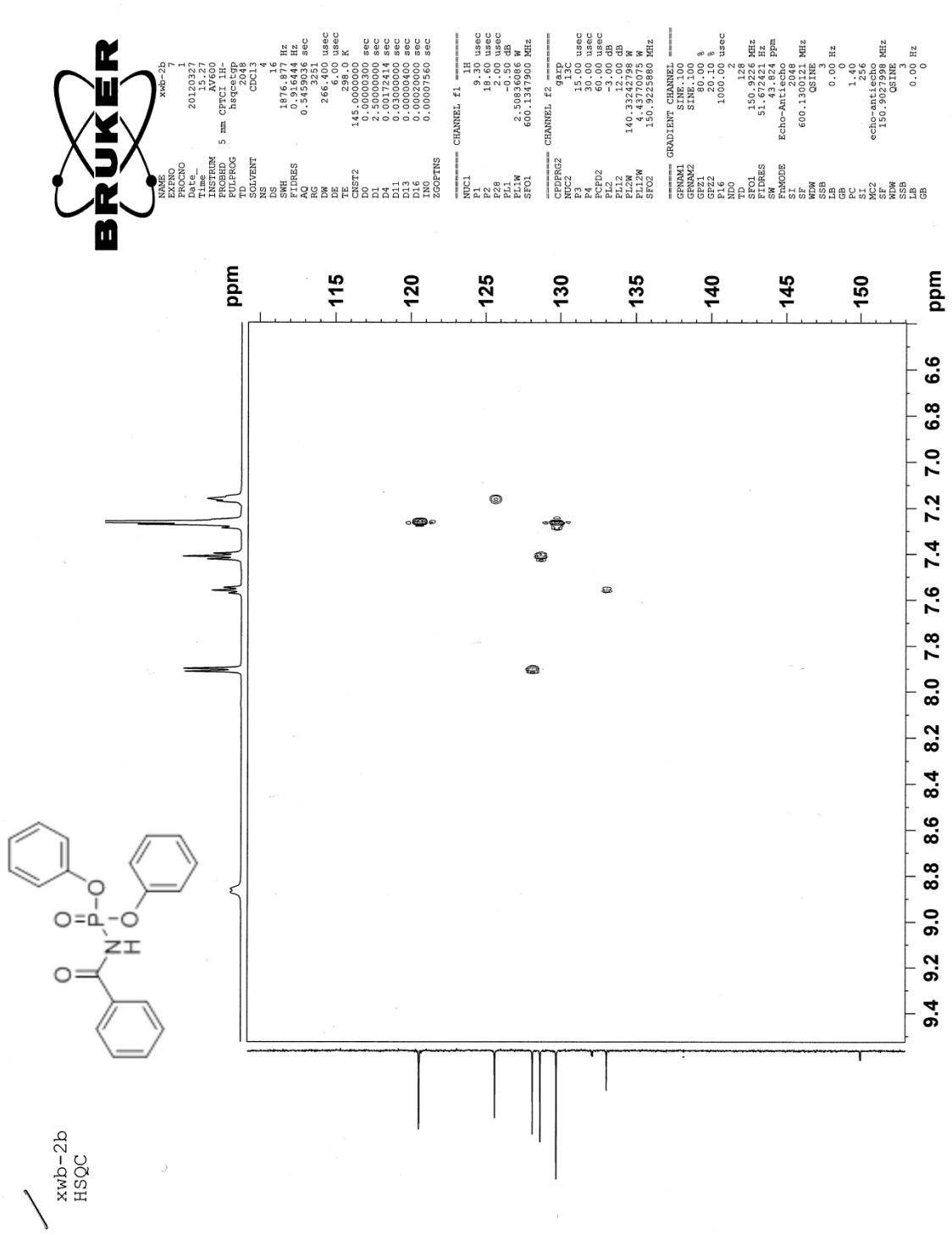

21.721
76.845
77.162
77.480
120.656
120.702
125.644
128.598
129.355
129.469
129.583
129.807
143.844
150.174
150.240
167.590
ppm
20
40
60
80
100
120
140
160
180
ppm


xwb-2a
HSQC
ppm
20
40
60
80
100
120
140
2
3
4
5
6
7
8
9
10

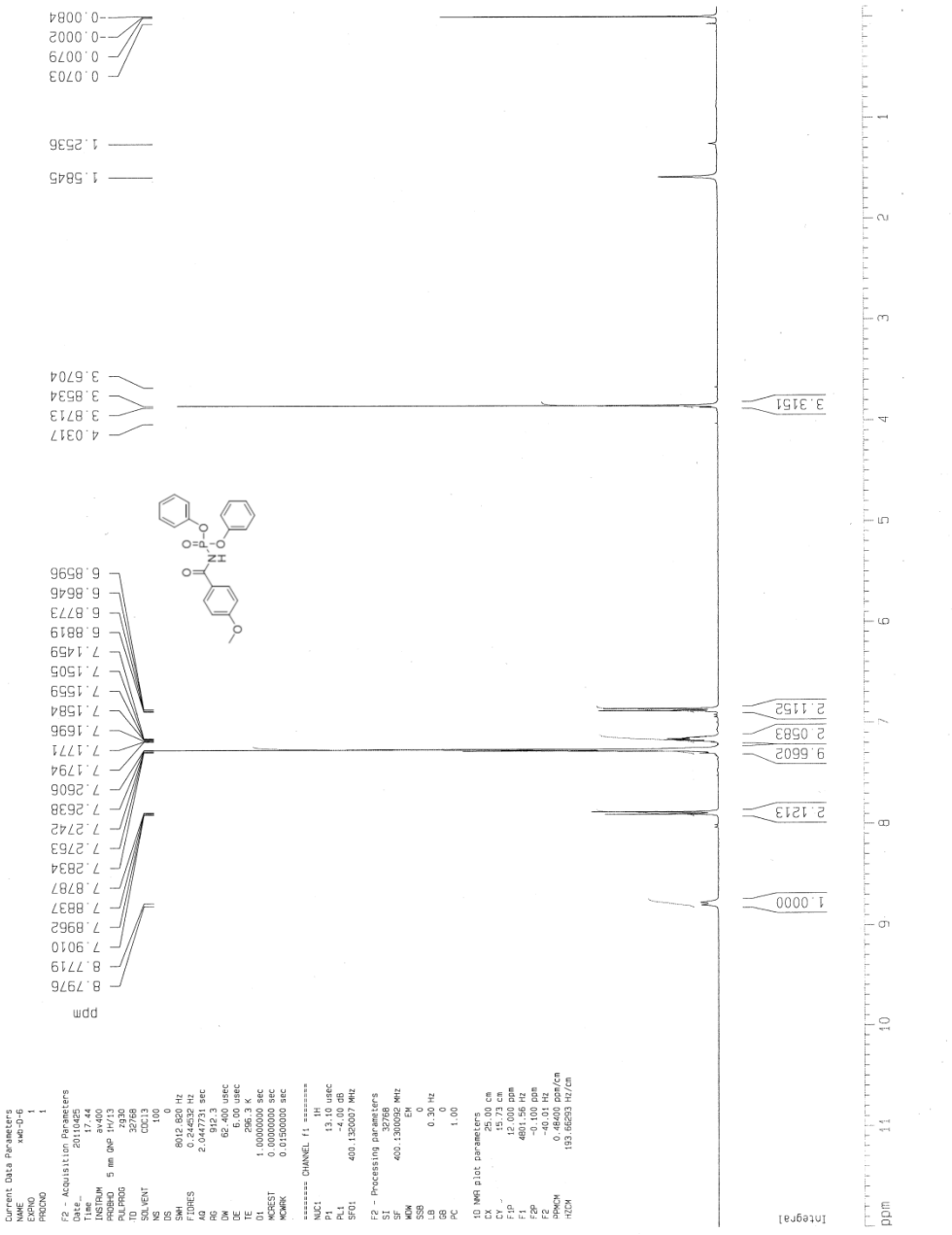
Diphenylbenzoylphosphoramidate 2b

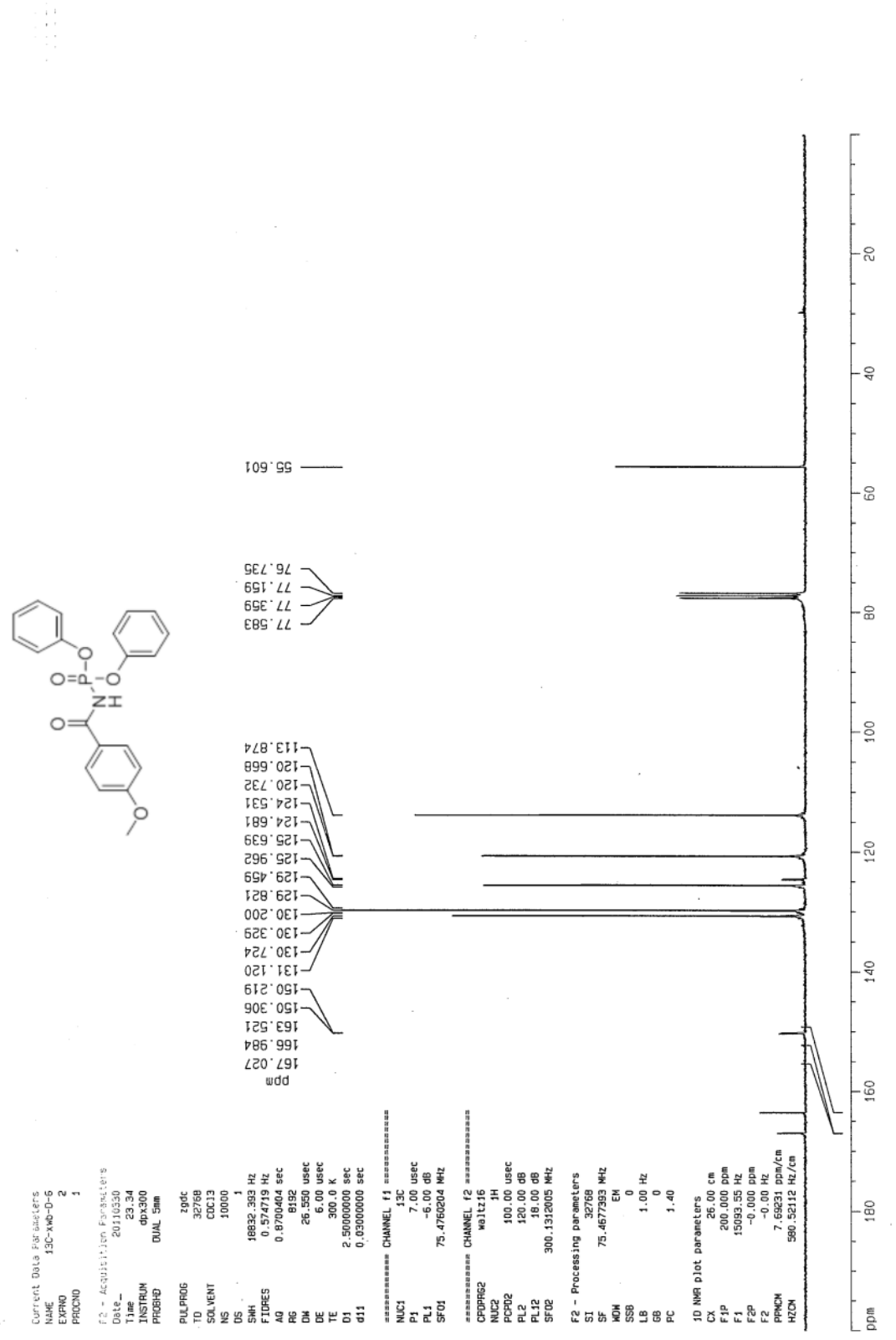



29.827
76.848
77.165
77.482
120.632
120.658
120.679
125.715
128.551
128.671
129.847
132.230
132.342
133.101
150.158
150.223
167.664
167.697
ppm
Current Data Parameters
NAME 13C-wxb-C-343
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110122
Time 18.35
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 217
DS 0
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 0.5439988 sec
RG 18390.4
DW 16.600 usec
DE 20.00 usec
TE 296.1 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 12.70 usec
PL1 -5.00 dB
SF01 100.6237964 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 12.90 dB
SF02 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 11.59 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90204 Hz/cm
ppm


xwb-2b
HSQC
ppm
115
120
125
130
135
140
145
150
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6

Diphenyl (4-methoxybenzoyl)phosphoramidate 2c




55.601
76.735
77.159
77.359
77.583
113.874
120.668
120.732
124.531
124.681
125.639
125.962
129.459
129.821
130.200
130.329
130.724
131.120
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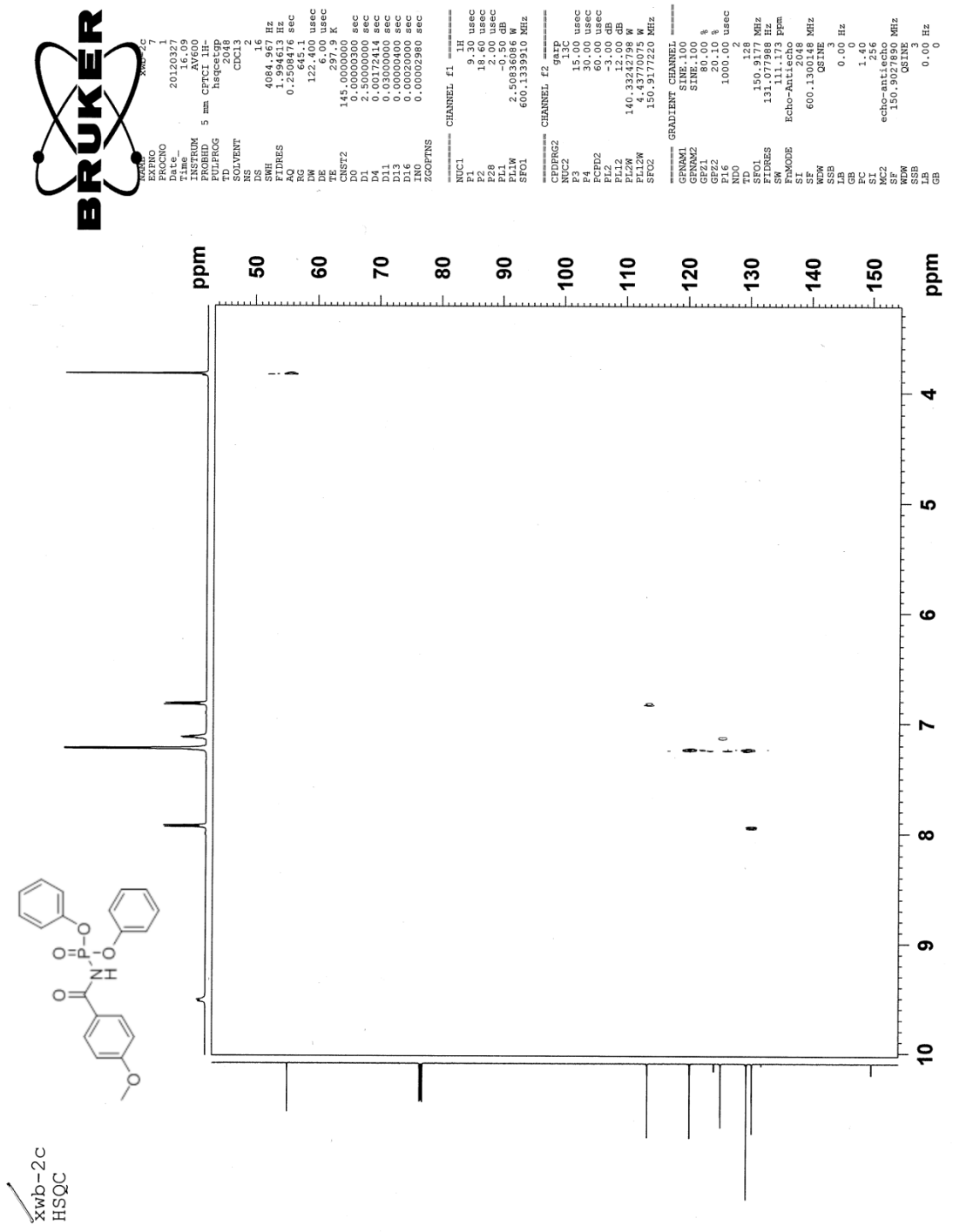
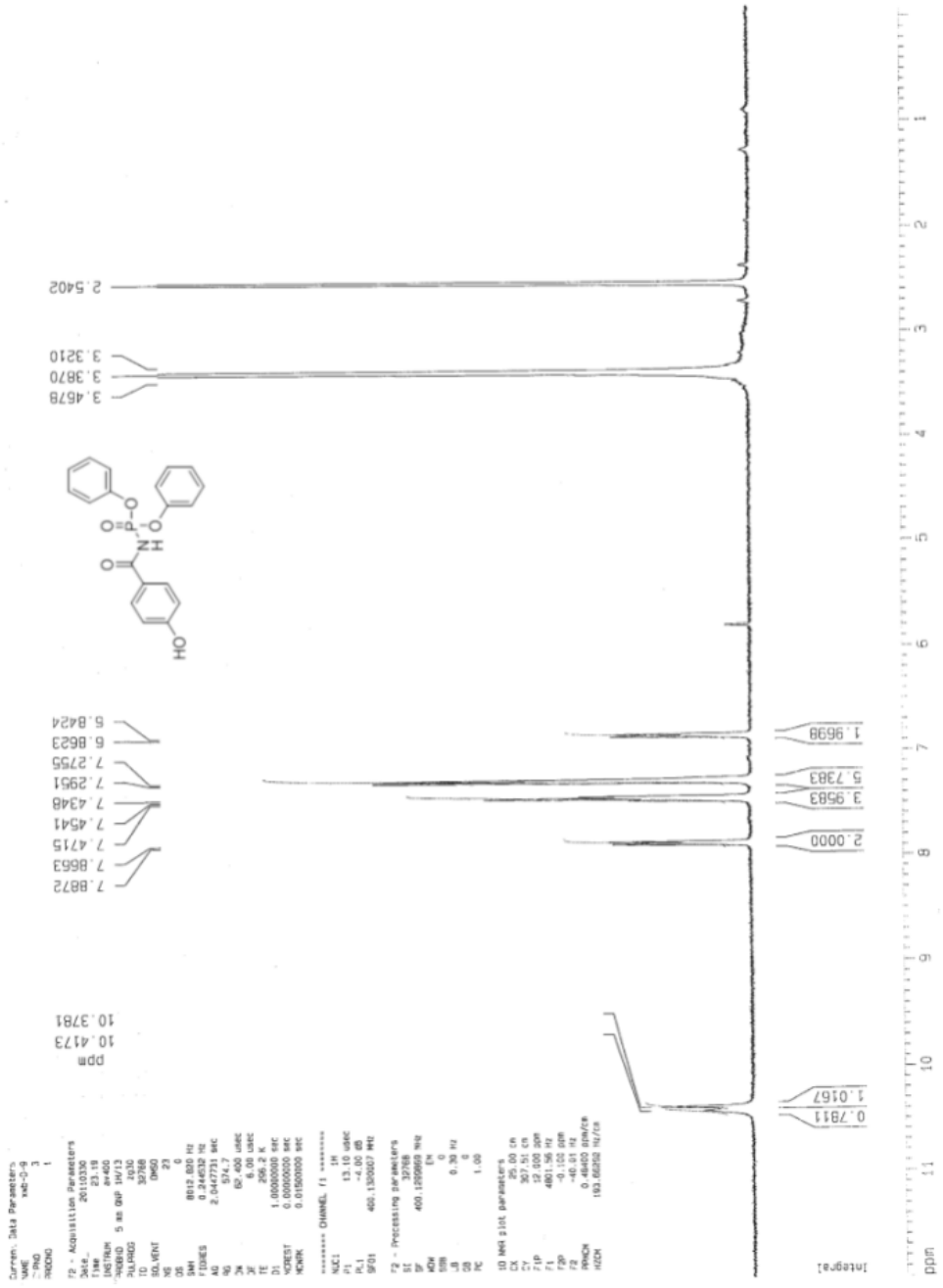
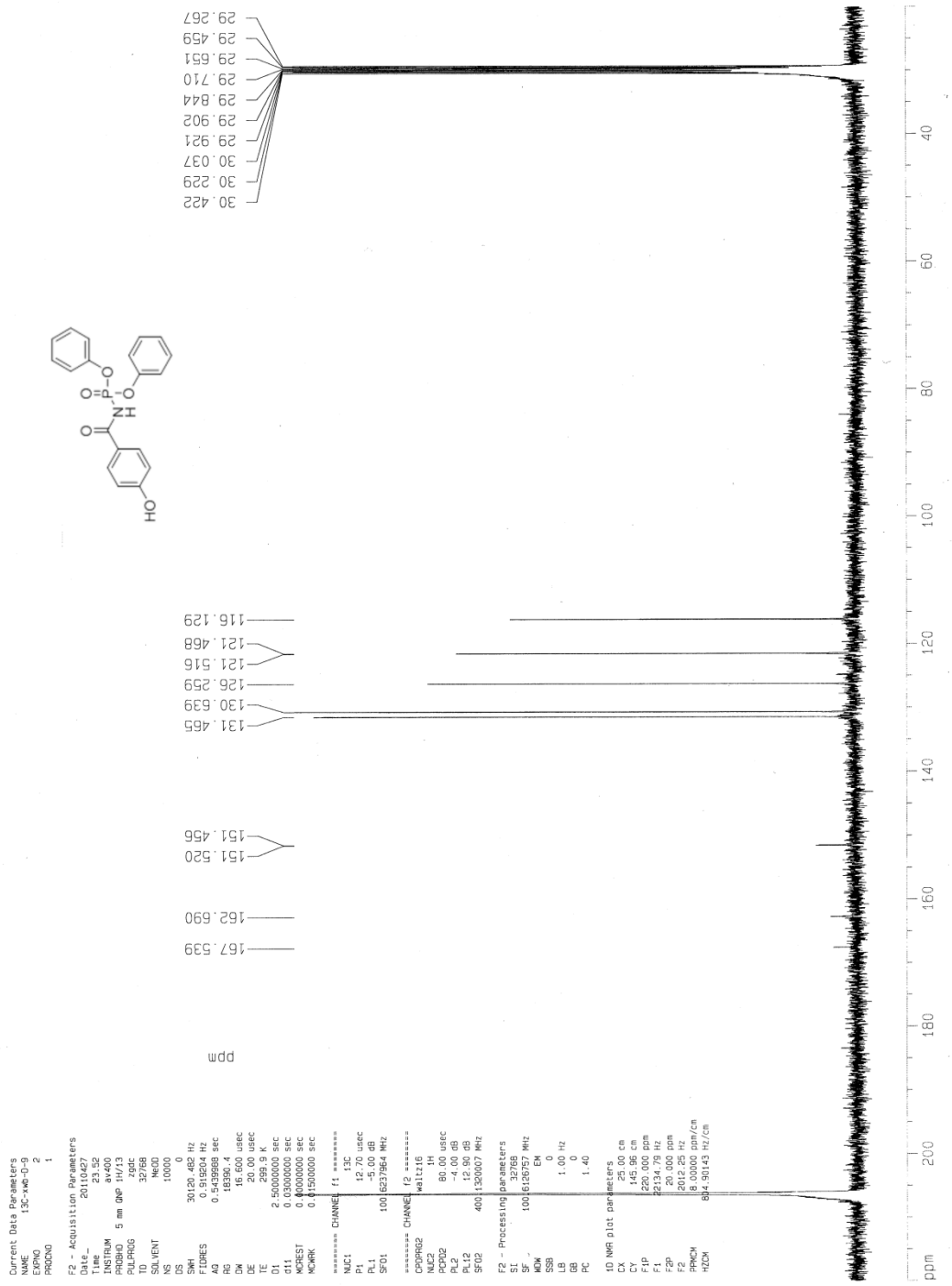
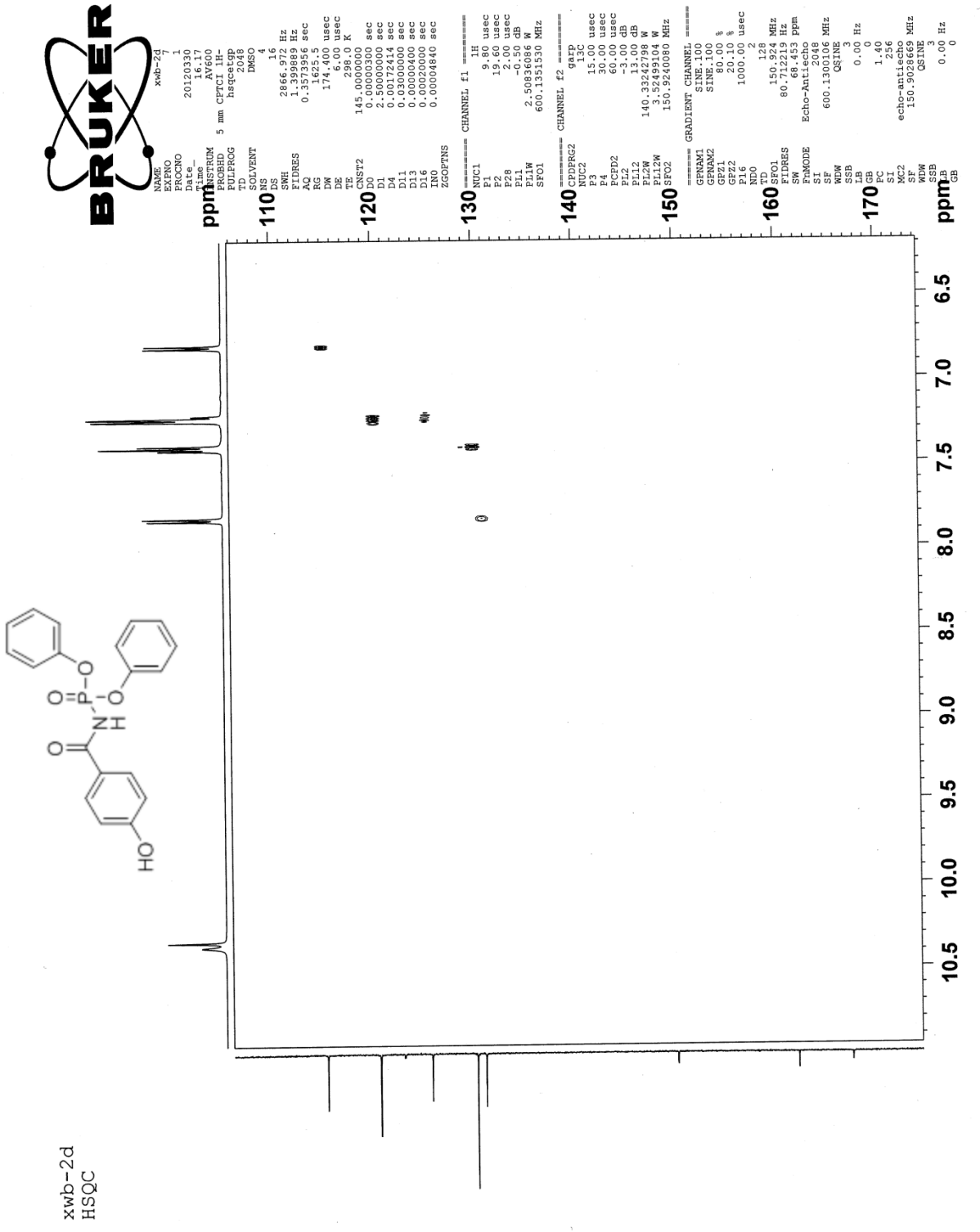
20
40
60
80
100
120
140
160
180
ppm


xwb-2c
HSQC
ppm
50
60
70
80
90
100
110
120
130
140
150
ppm
4
5
6
7
8
9
10

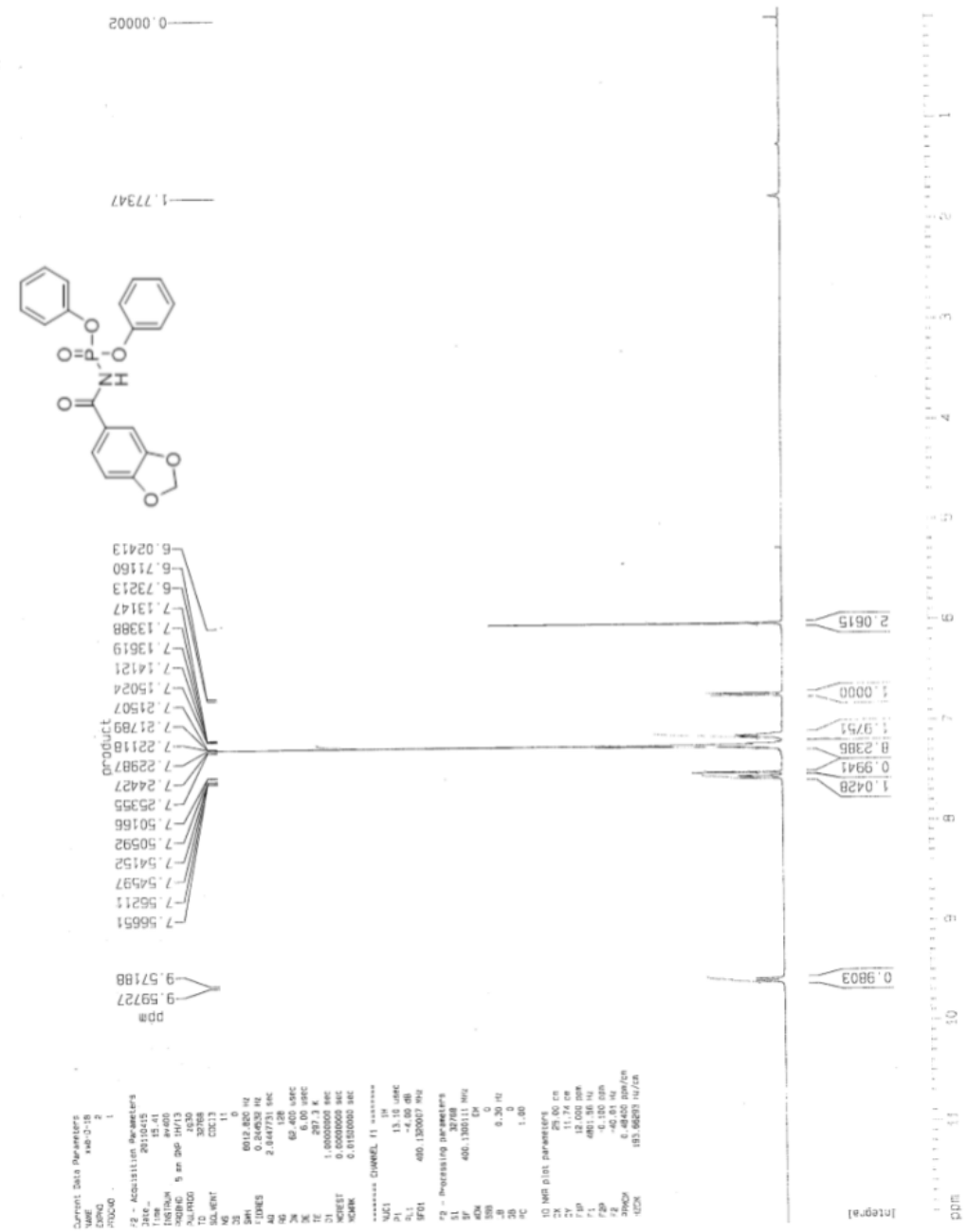
Diphenyl (4-hydroxybenzoyl)phosphoramidate 2d

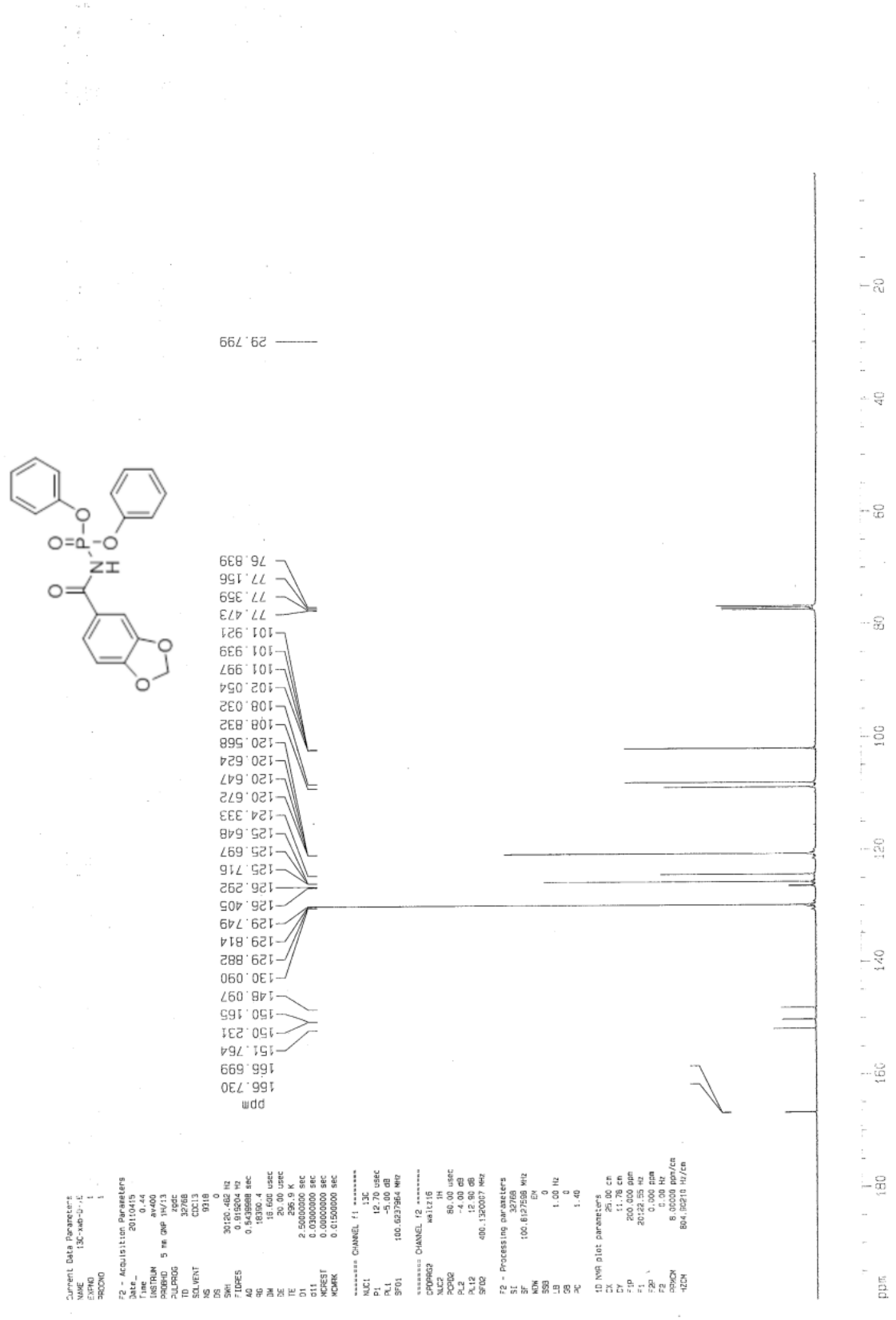


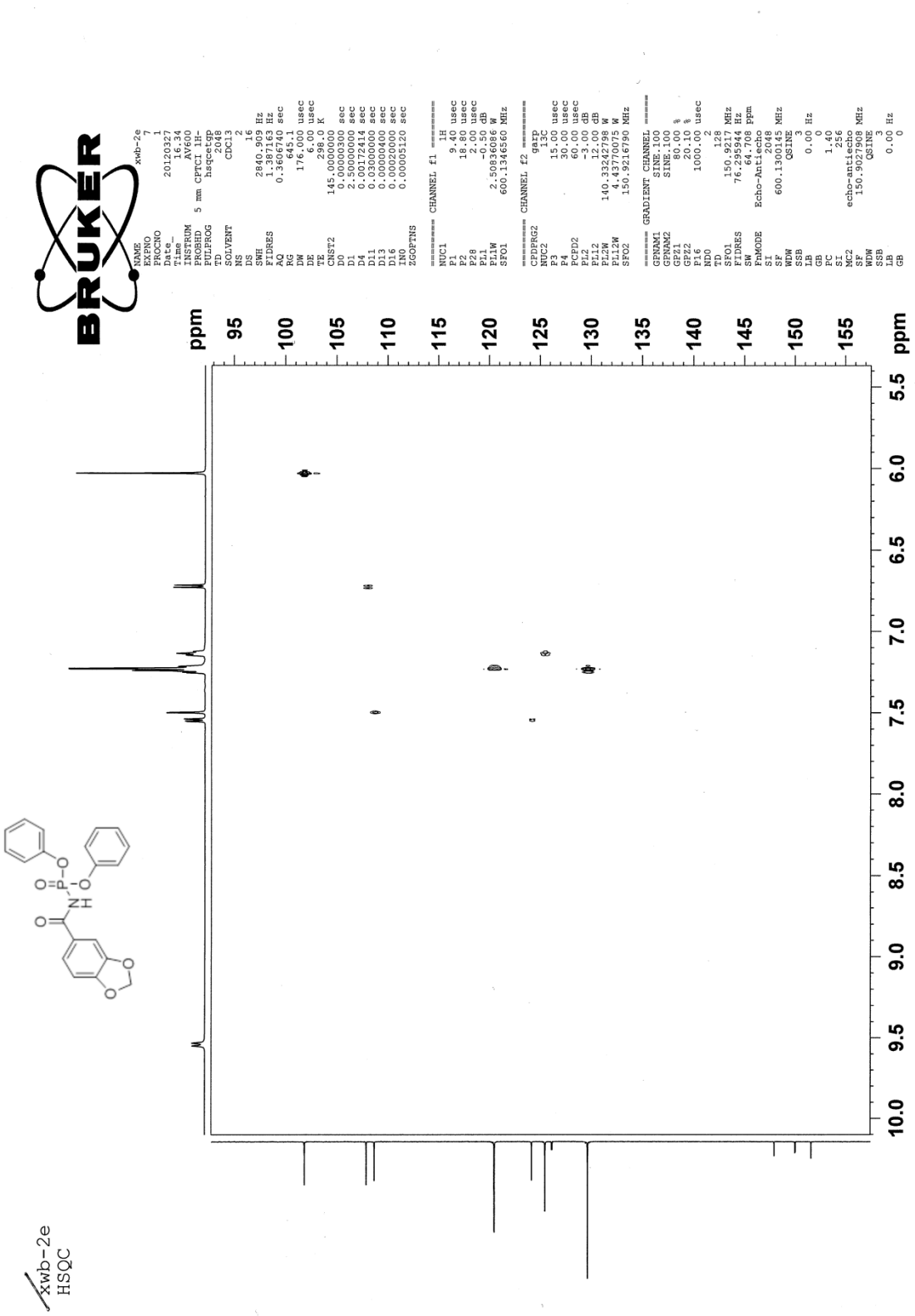

29.267
29.459
29.651
29.710
29.844
29.902
29.921
30.037
30.229
30.422
116.129
121.468
121.516
126.259
130.639
131.465
151.456
151.520
162.690
167.539
HO
ppm
ppm


xwb-2d
HSQC

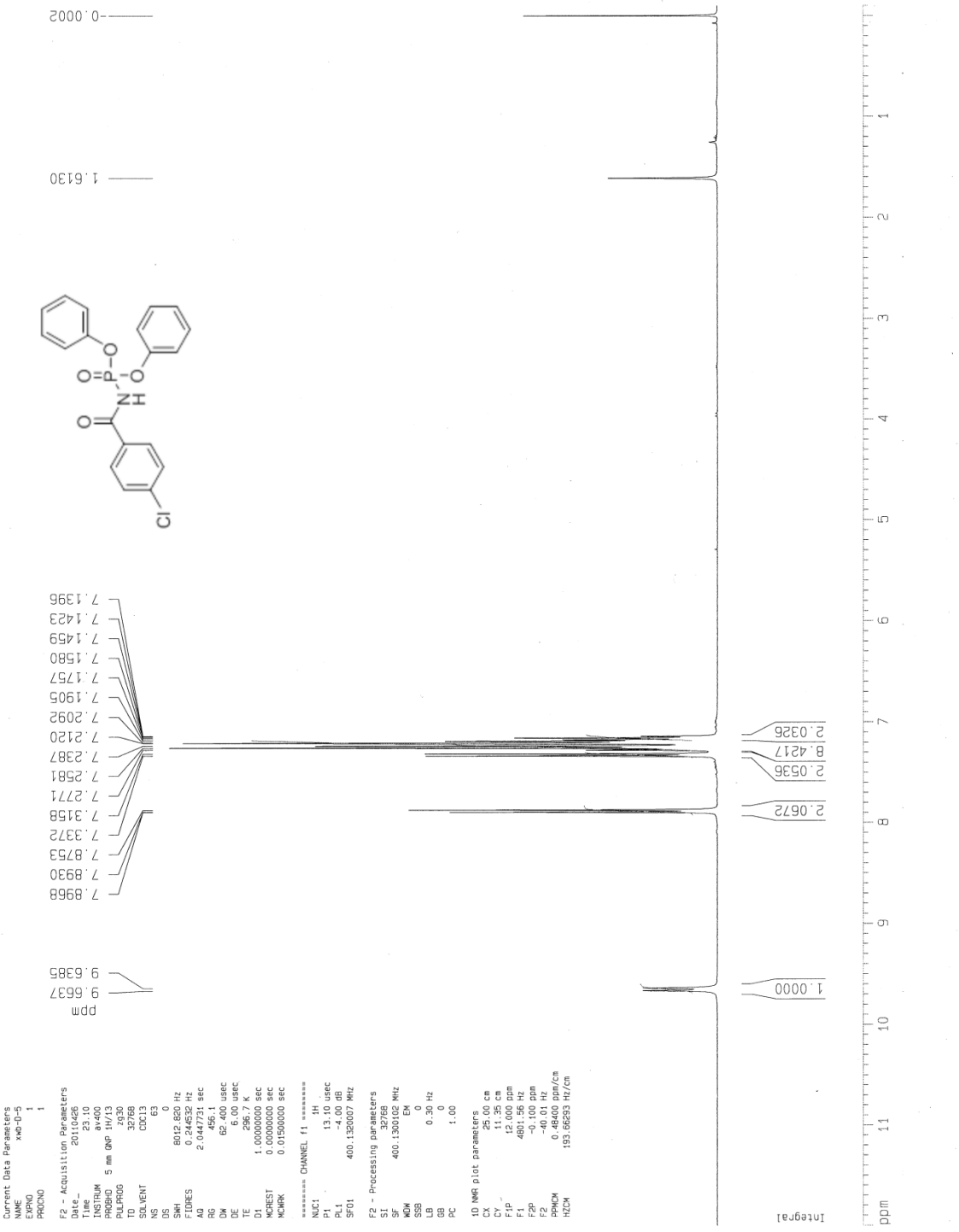
Diphenylbenzo[d][1,3]dioxole-5-carbonylphosphoramidate 2e

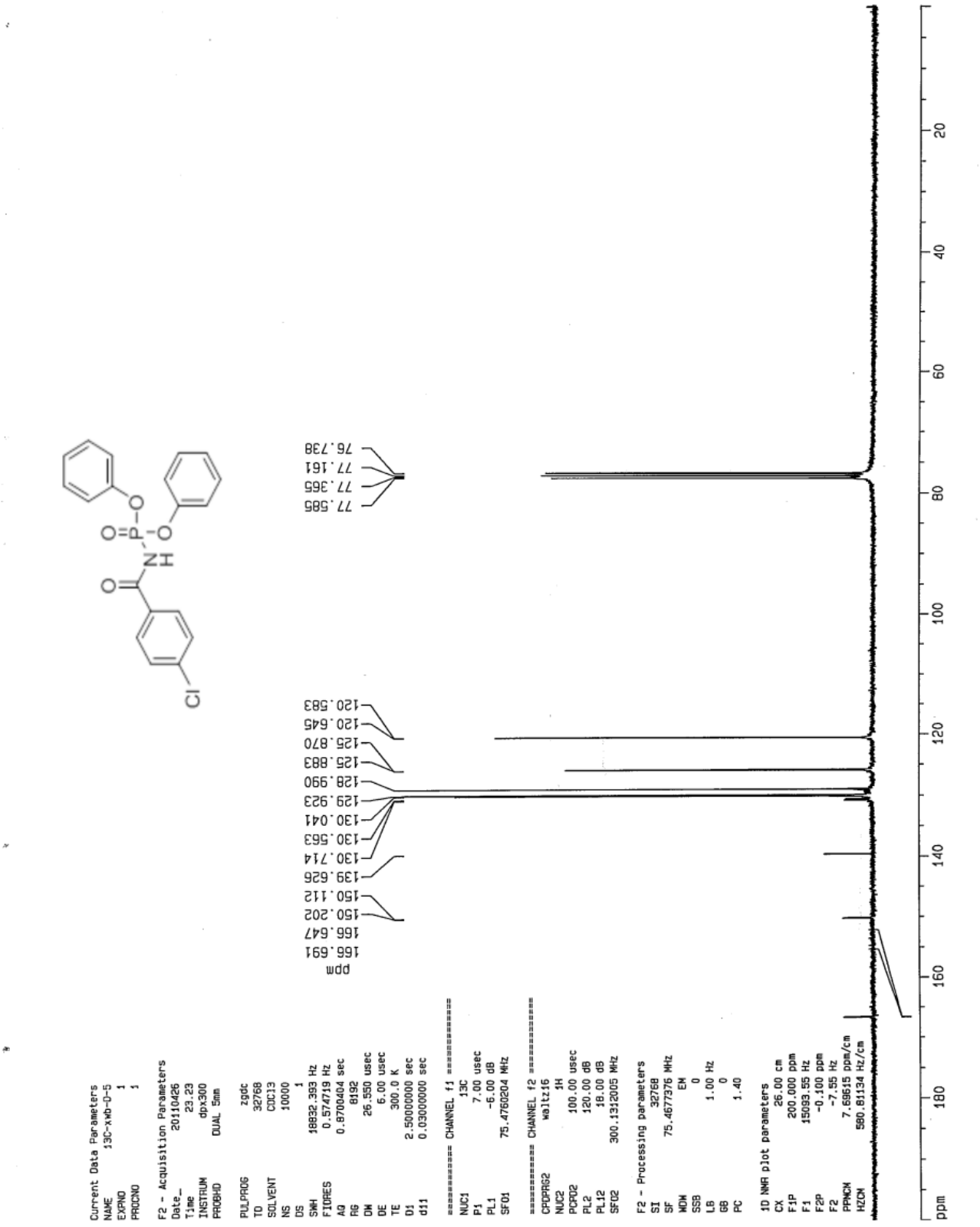


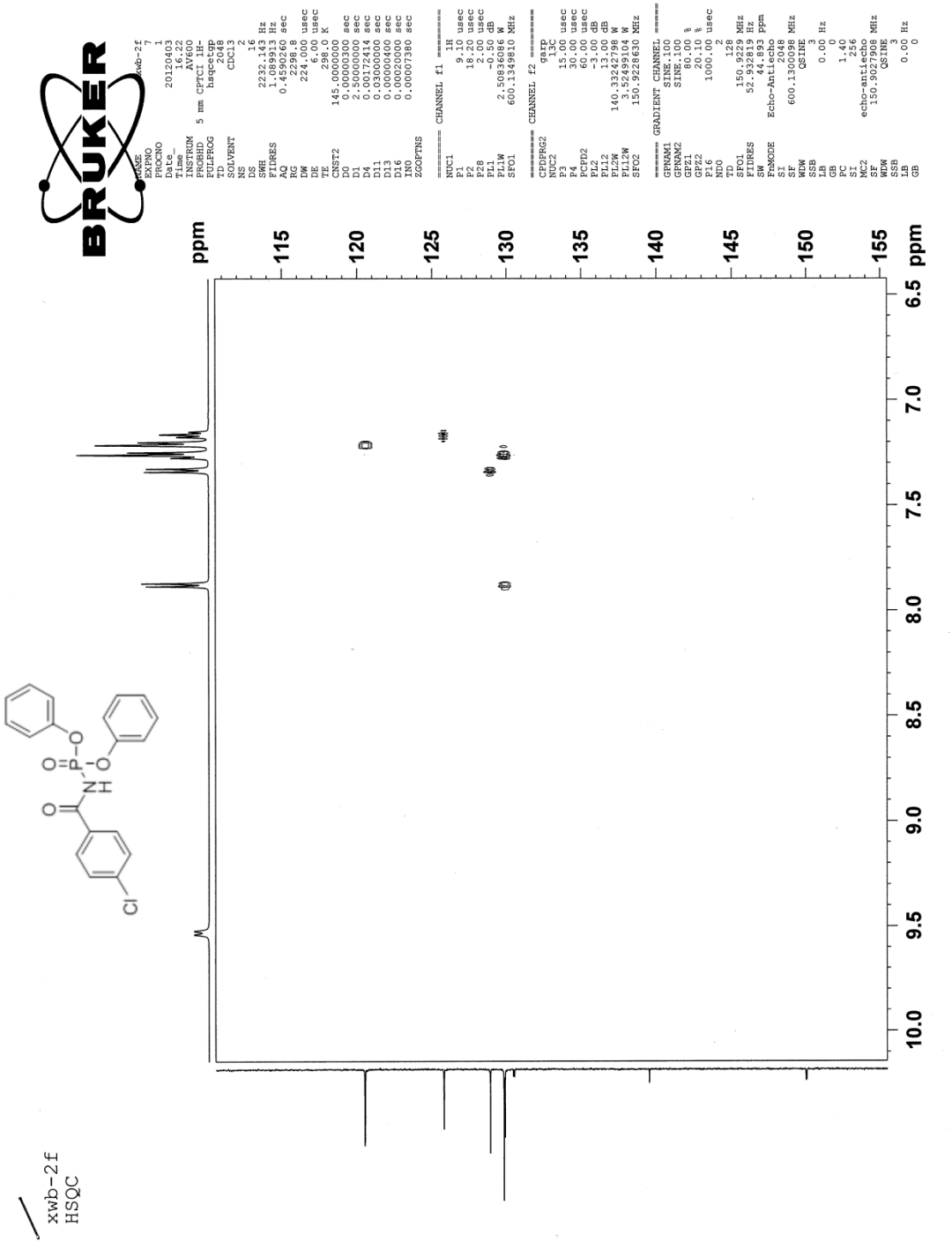

29.799
76.839
77.156
77.359
77.473
101.921
101.939
101.997
102.054
108.032
108.832
120.568
120.624
120.647
120.672
124.333
125.648
125.697
125.716
126.292
126.405
129.749
129.814
129.882
130.090
148.097
150.165
150.231
151.764
166.699
166.730
ppm
20
40
60
80
100
120
140
160
180
ppm


xwb-2e
HSQC
ppm
95
100
105
110
115
120
125
130
135
140
145
150
155
ppm
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.0

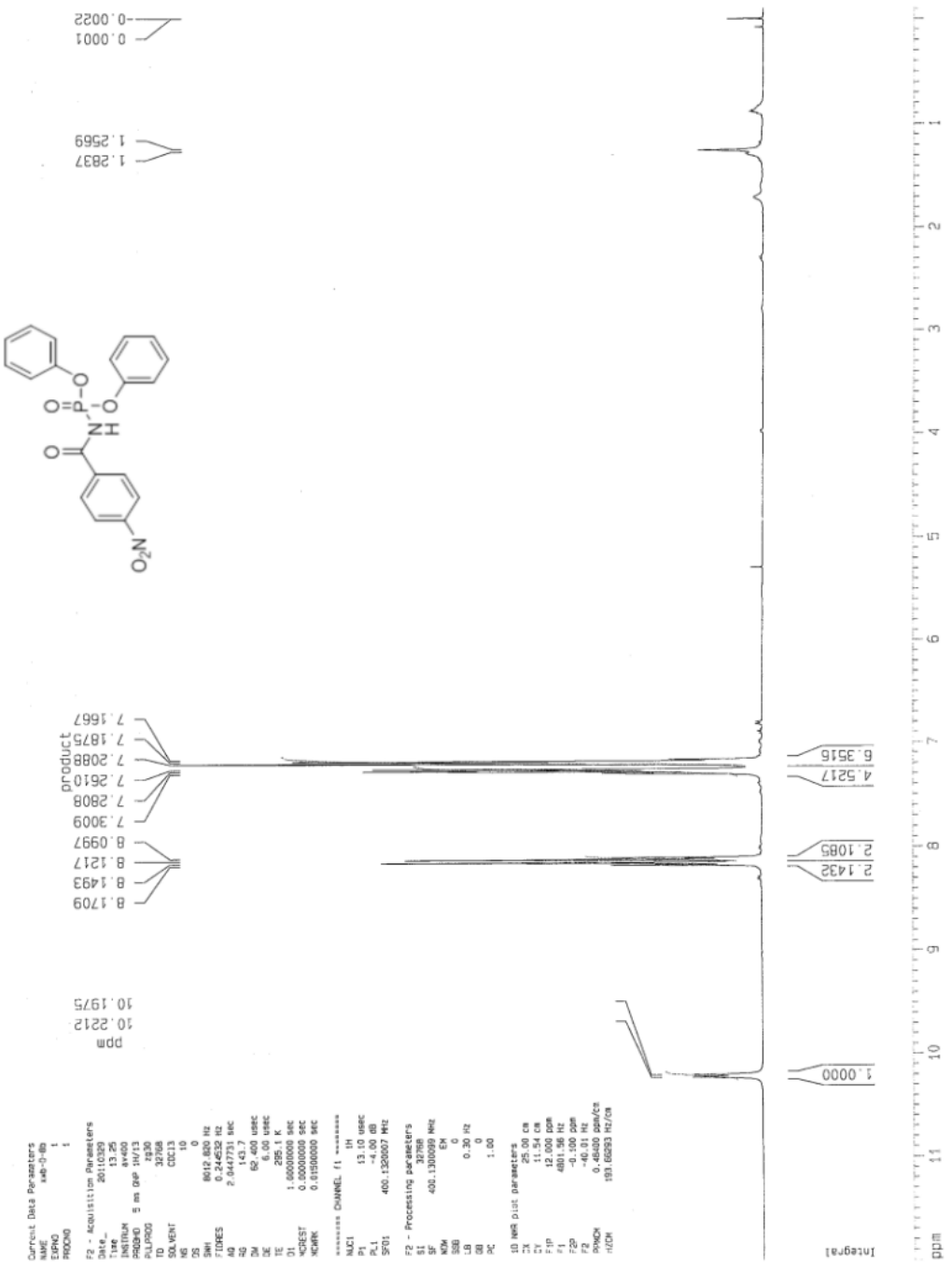
Diphenyl(4-chlorobenzoyl)phosphoramidate 2f

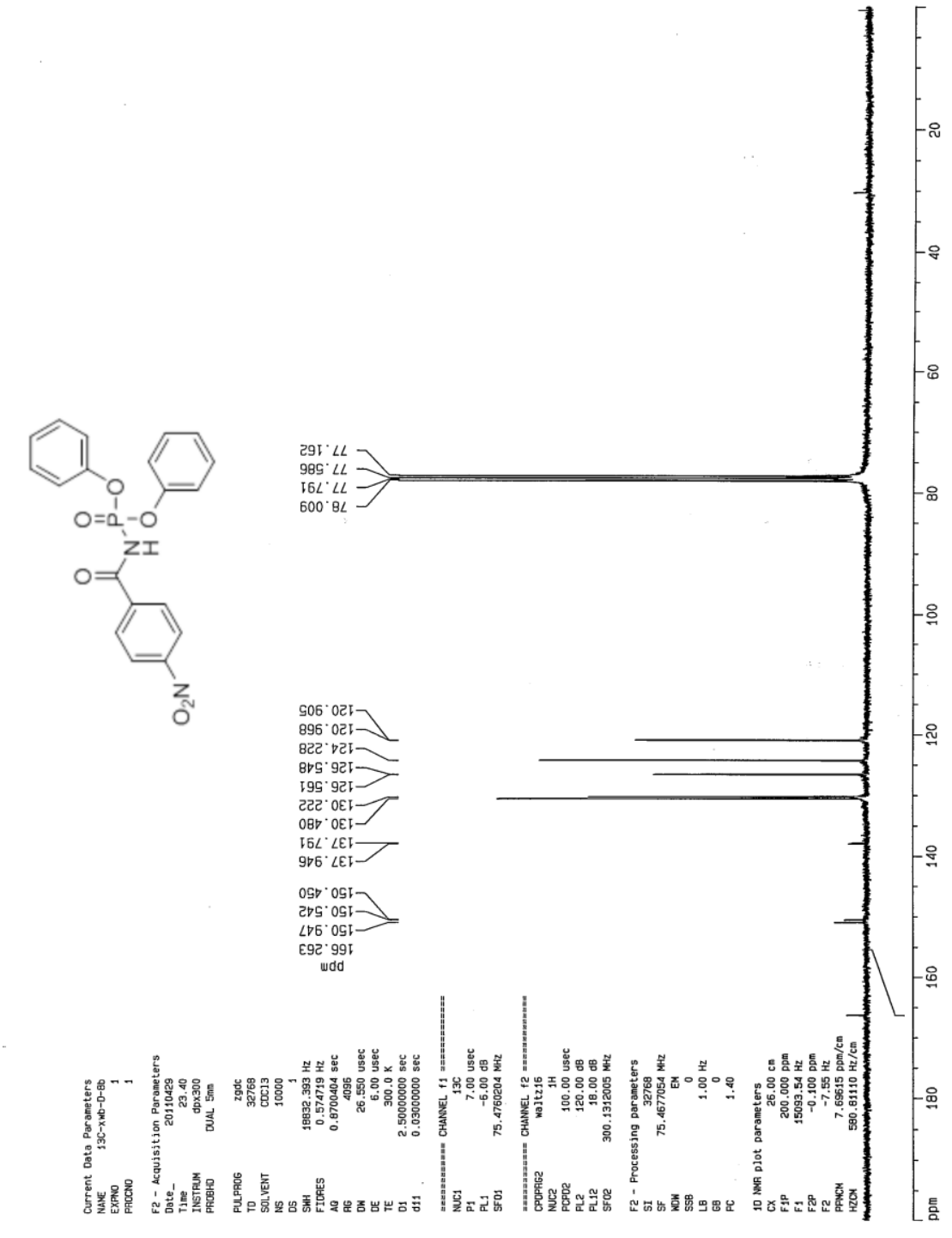


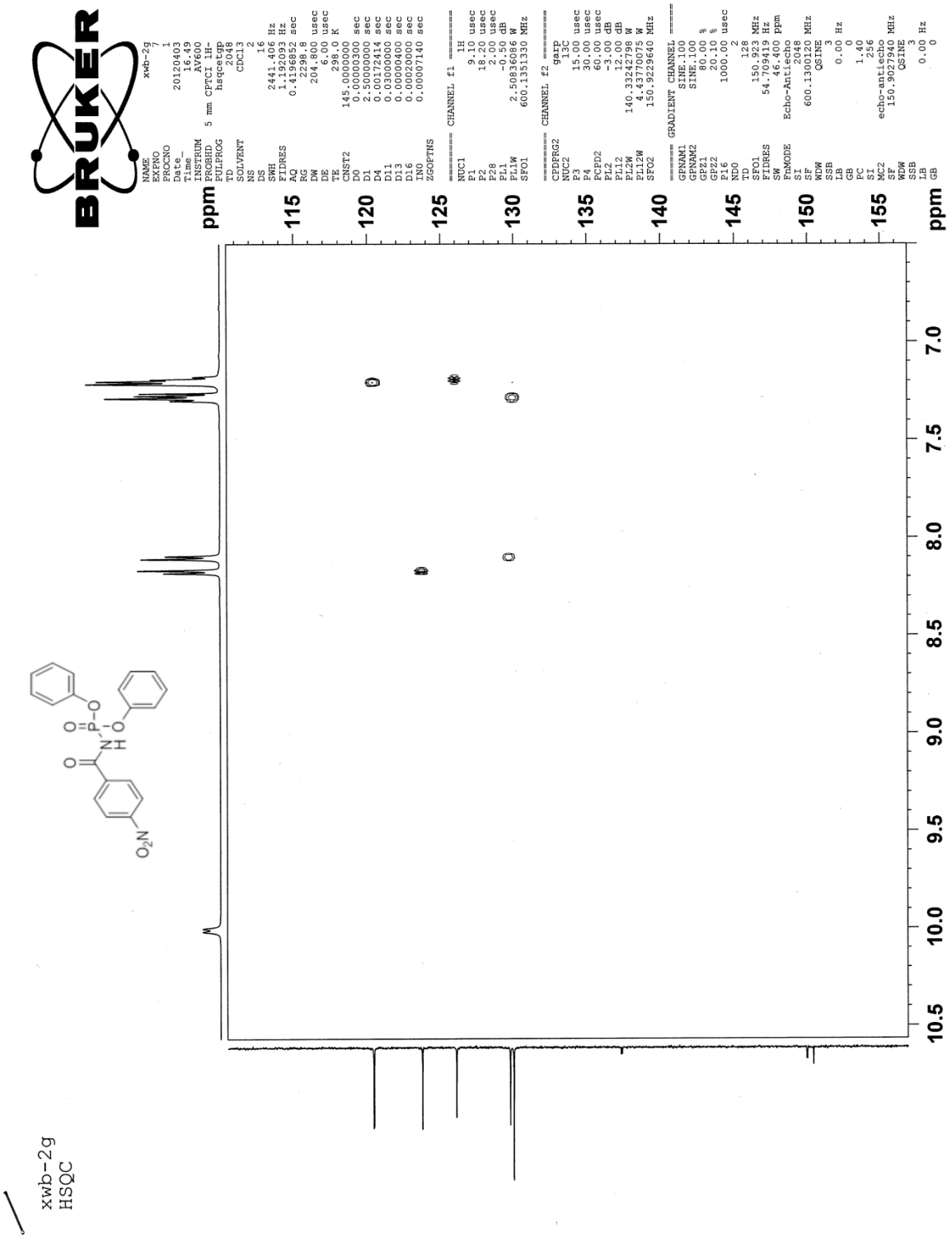

Current Data Parameters
NAME 13C-xwb-O-5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110426
Time 23.23
INSTRUM dpx300
PROBHD DUAL 5mm
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 10000
DS 1
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 8192
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.50000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 7.00 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677376 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 26.00 cm
F1P 200.000 ppm
F1 15093.55 Hz
F2P -0.100 ppm
F2 -7.55 Hz
PPMCM 7.69615 ppm/cm
HZCM 580.81134 Hz/cm
ppm
166.691
166.647
150.202
150.112
139.626
130.714
130.563
130.041
129.923
128.990
125.883
125.870
120.645
120.583
77.585
77.365
77.161
76.738
O
P
O
NH
O
Cl
ppm
20
40
60
80
100
120
140
160
180


xwb-2f
HSQC
ppm
115
120
125
130
135
140
145
150
155
6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.0
Cl

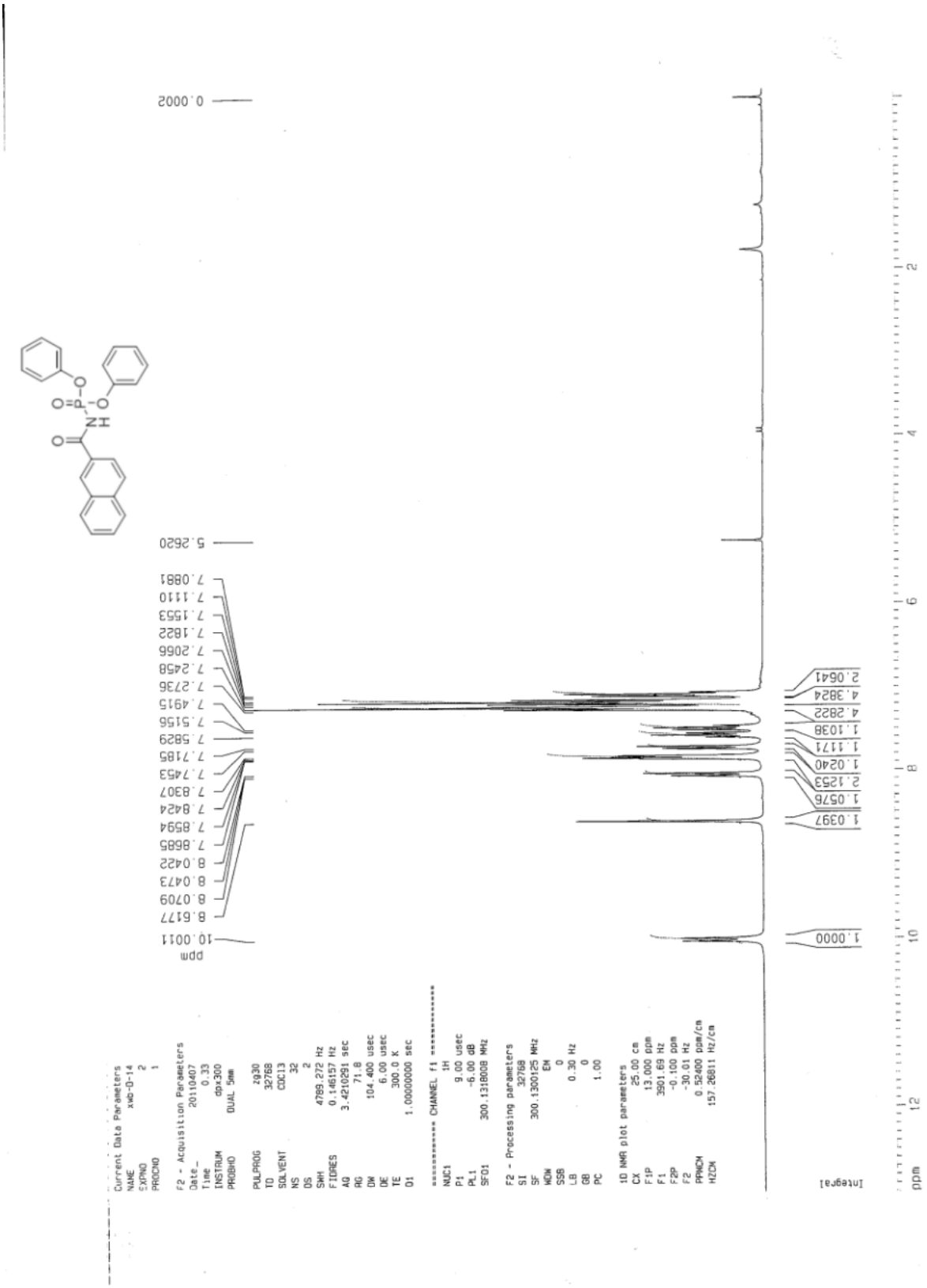
Diphenyl (4-nitrobenzoyl)phosphoramidate 2g

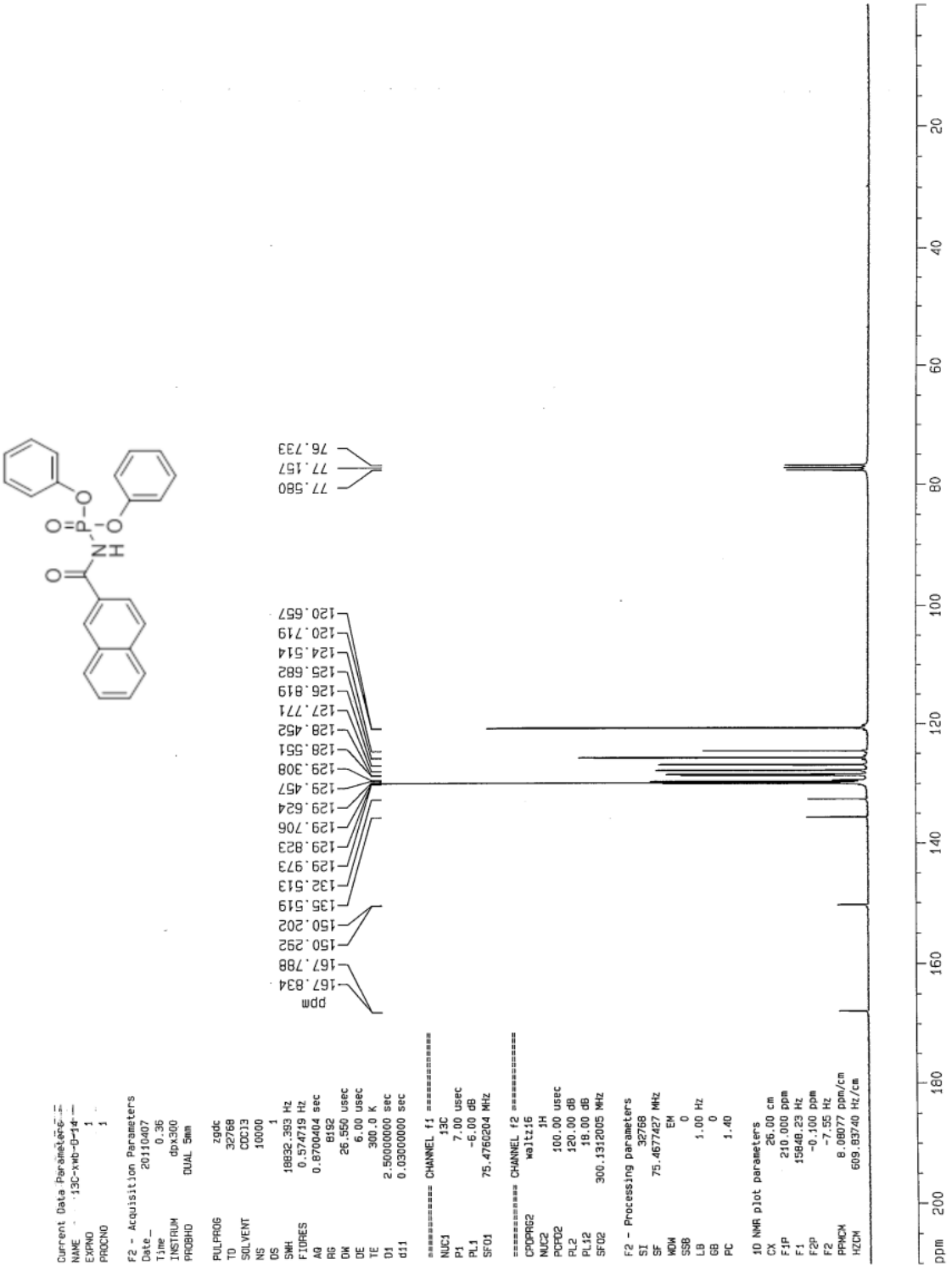


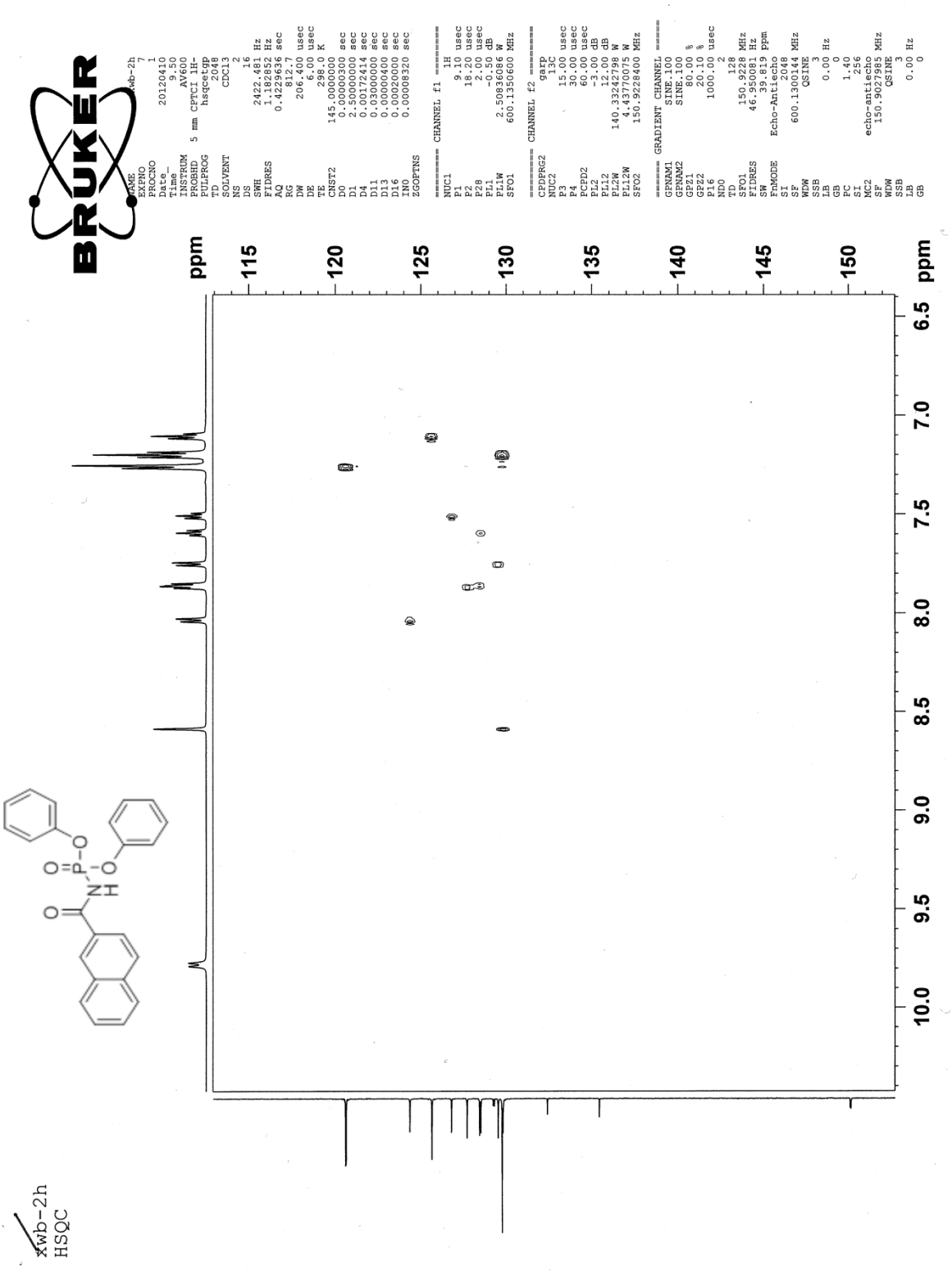

Current Data Parameters
NAME 13C-xwb-D-6b
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110429
Time 23.40
INSTRUM dpx300
PROBHD DUAL 5mm
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 10000
DS 1
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 4096
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.50000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 7.00 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677054 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 26.00 cm
F1P 200.000 ppm
F1 15093.54 Hz
F2P -0.100 ppm
F2 -7.55 Hz
PPMCM 7.69615 ppm/cm
HZCM 580.81110 Hz/cm
ppm
166.263
150.947
150.542
150.450
137.946
137.791
130.480
130.222
126.561
126.548
124.228
120.968
120.905
78.009
77.791
77.586
77.162
ppm
20
40
60
80
100
120
140
160
180
O
P
O
O
NH
O
O_2N


xwb-2g
HSQC
ppm
115
120
125
130
135
140
145
150
155
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5

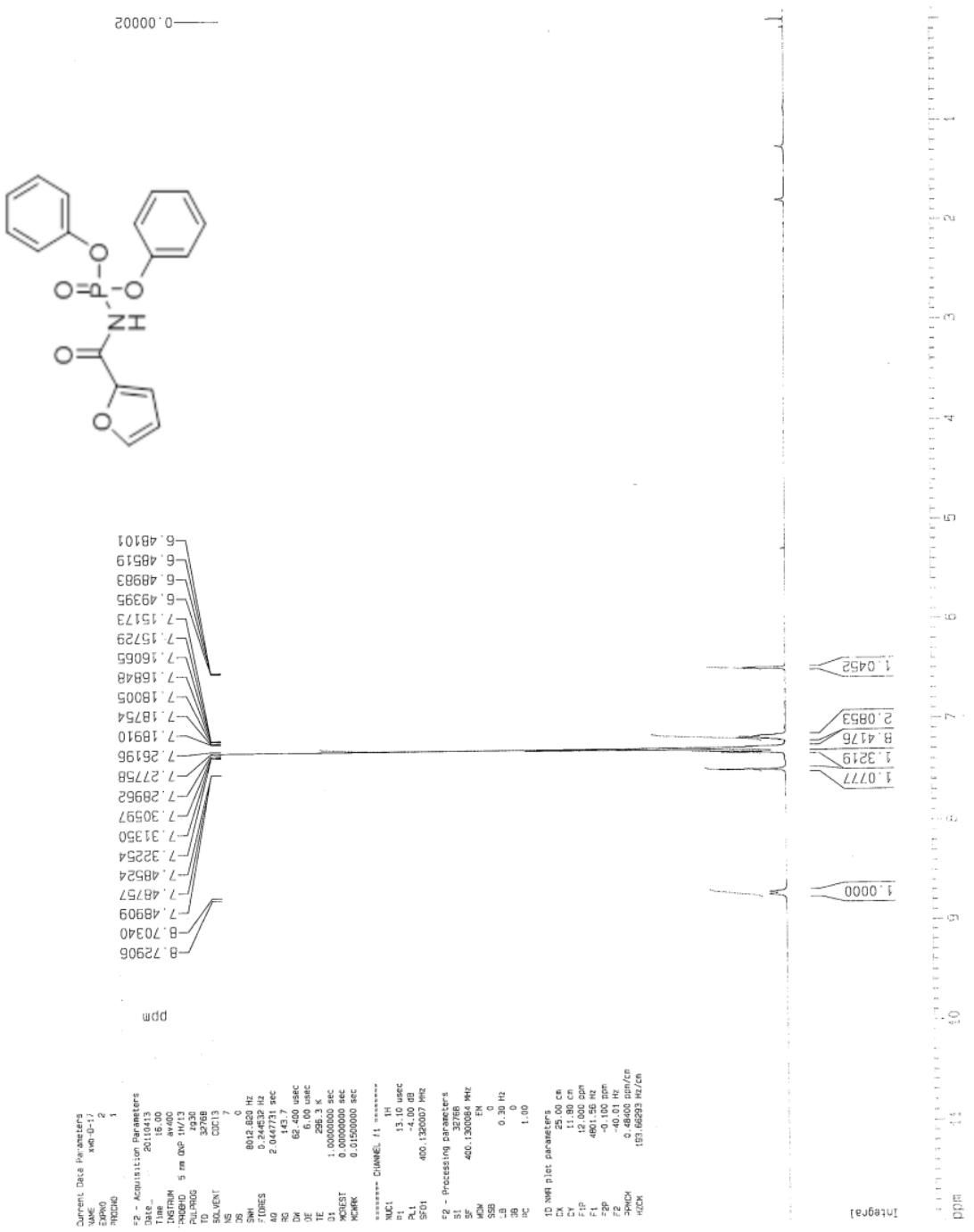
Diphenyl 2-naphthoylphosphoramidate 2h

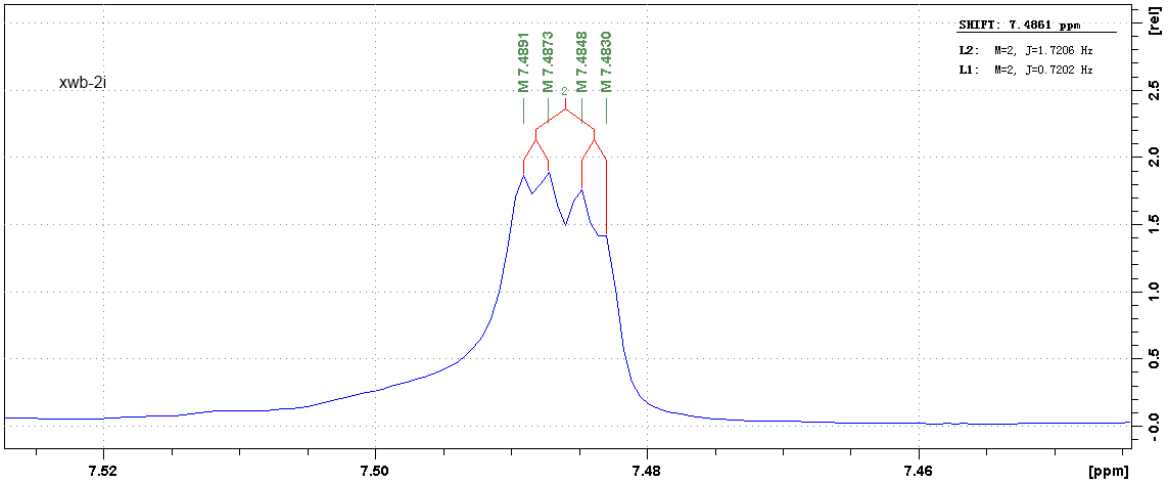


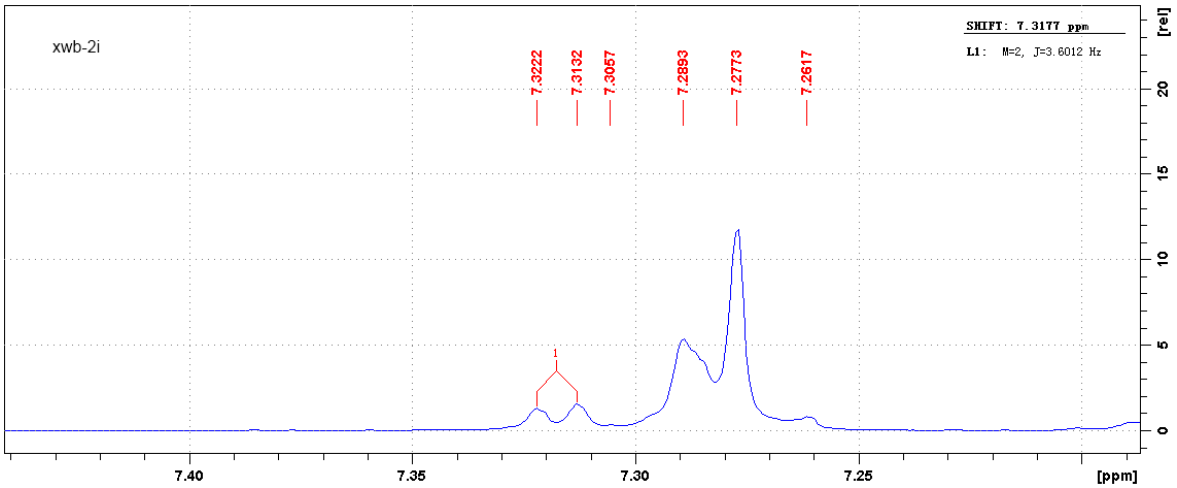

Current Data Parameters
NAME 13C-xwb-D-14
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110407
Time 0.36
INSTRUM dpx300
PROBHD DUAL 5mm
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 10000
DS 1
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 8192
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.50000000 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 7.00 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677427 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 26.00 cm
F1P 210.000 ppm
F1 15848.23 Hz
F2P -0.100 ppm
F2 -7.55 Hz
PPMCM 8.08077 ppm/cm
HZCM 609.83740 Hz/cm
ppm
167.834
167.788
150.292
150.202
135.519
132.513
129.973
129.823
129.706
129.624
129.457
129.308
128.551
128.452
127.771
126.819
125.682
124.514
120.719
120.657
77.580
77.157
76.733
ppm

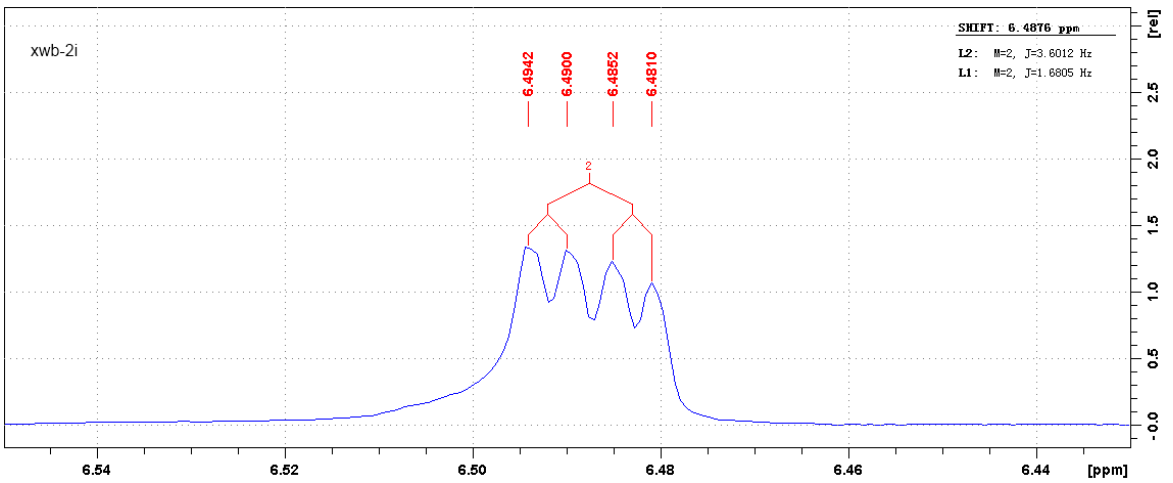

BRUKER
ppm
115
120
125
130
135
140
145
150
6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.0
xwb-2h
HSQC

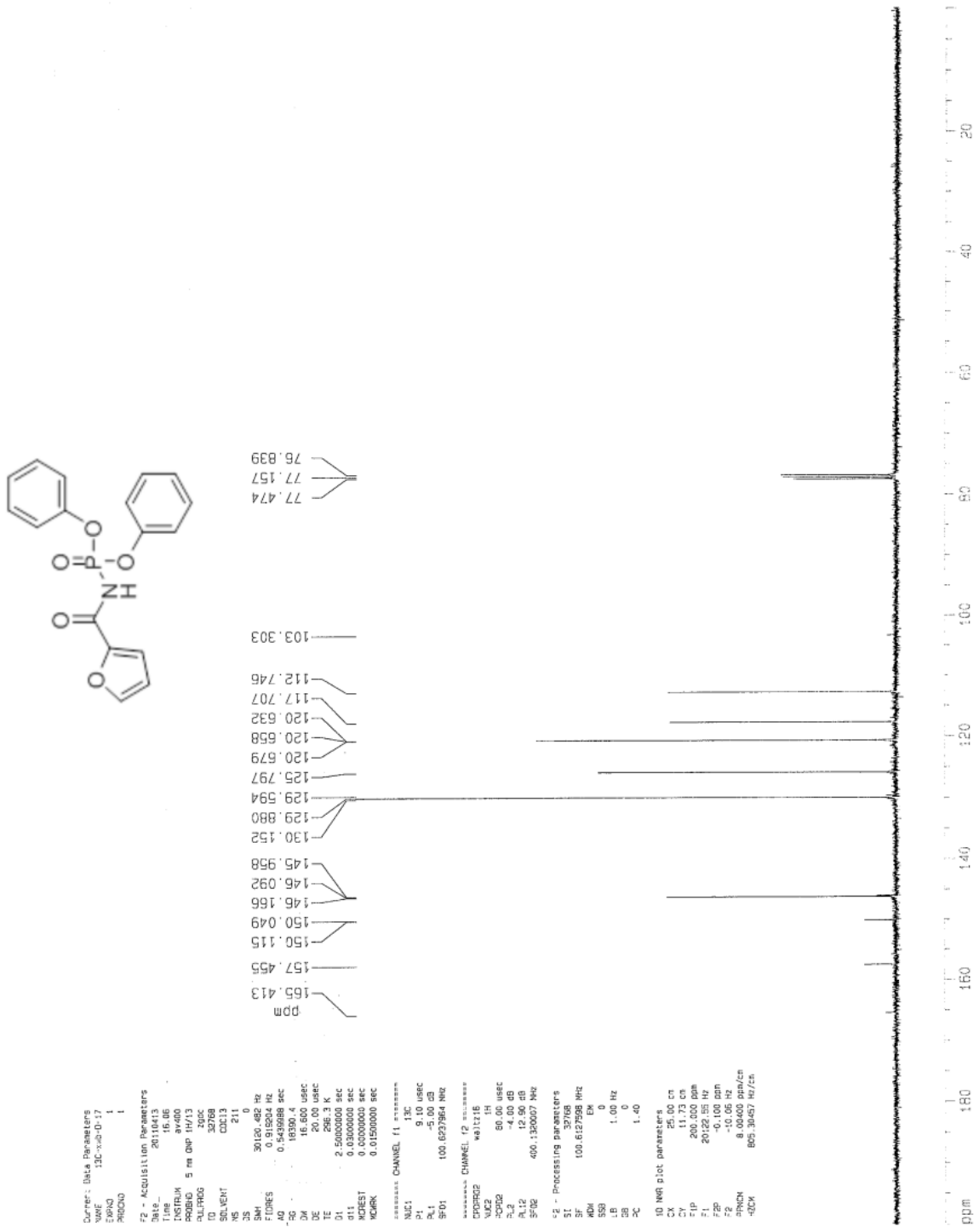
Diphenyl furan-2-carbonylphosphoramidate 2i

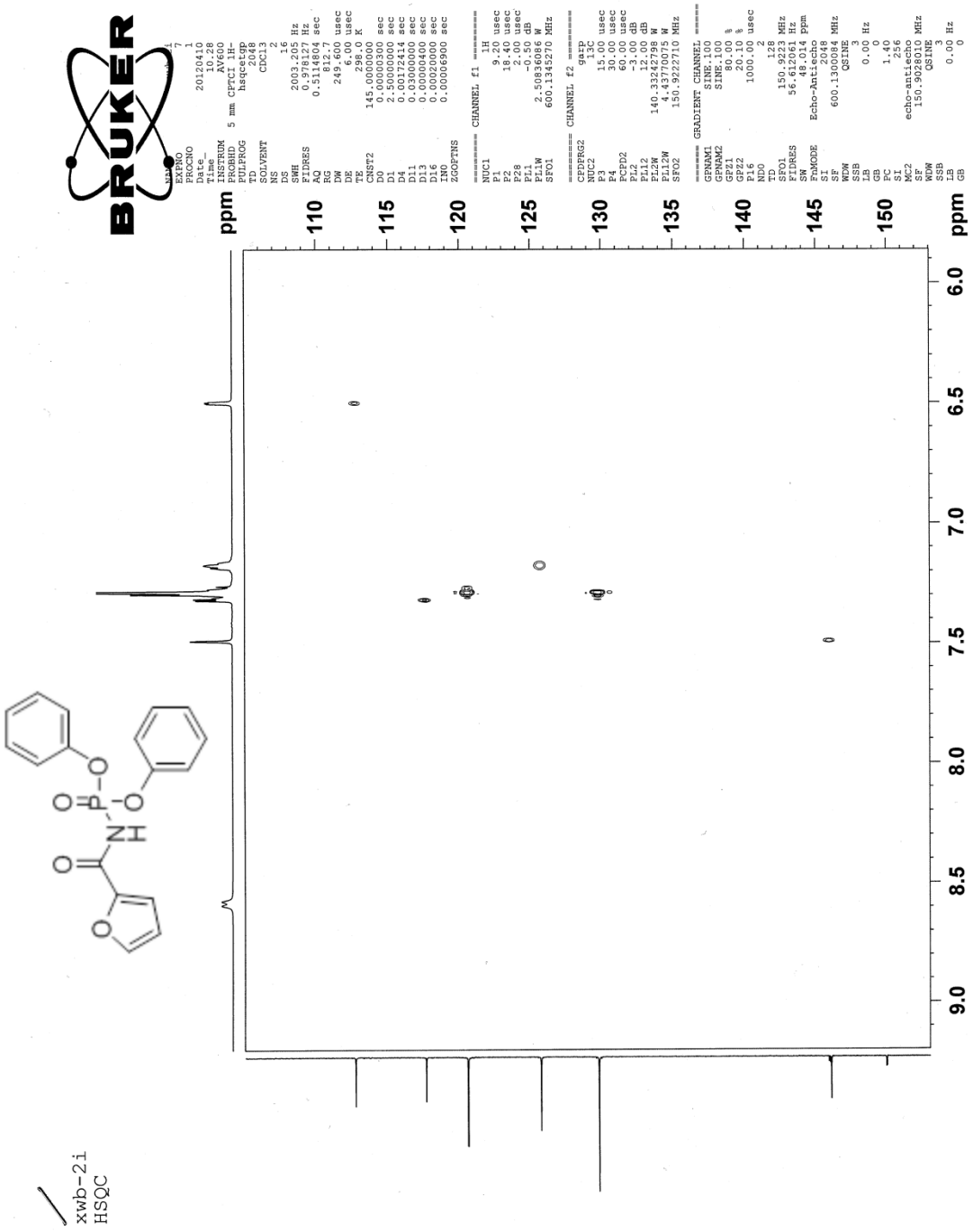



xwb-2i
M 7.4891
M 7.4873
M 7.4848
M 7.4830
SHIFT: 7.4861 ppm
L2: M=2, J=1.7206 Hz
L1: M=2, J=0.7202 Hz
[rel]
7.52
7.50
7.48
7.46
[ppm]

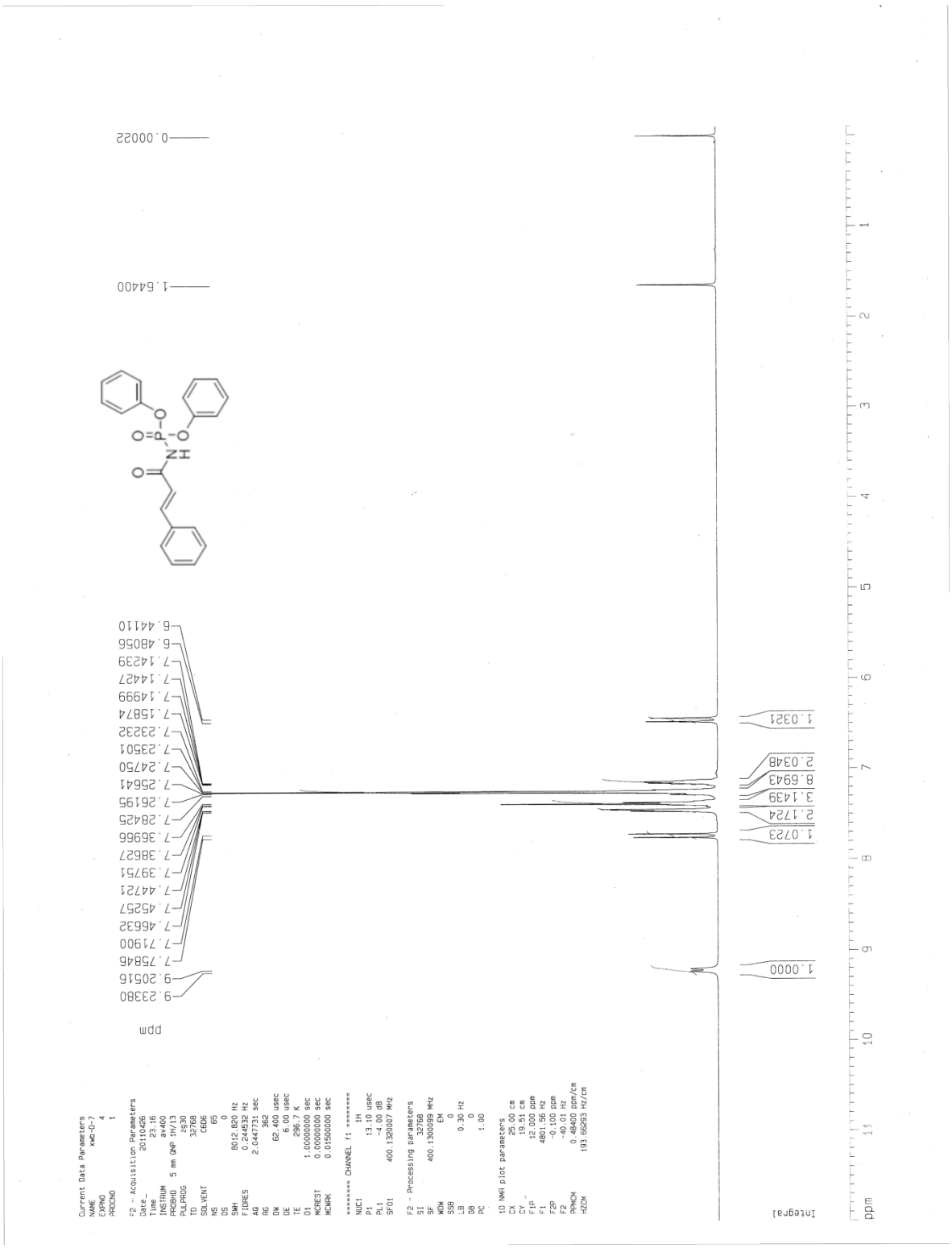

xwb-2i
7.3222
7.3132
7.3057
7.2893
7.2773
7.2617
SHIFT: 7.3177 ppm
L1: M=2, J=3.6012 Hz
[rel]
7.40
7.35
7.30
7.25
[ppm]

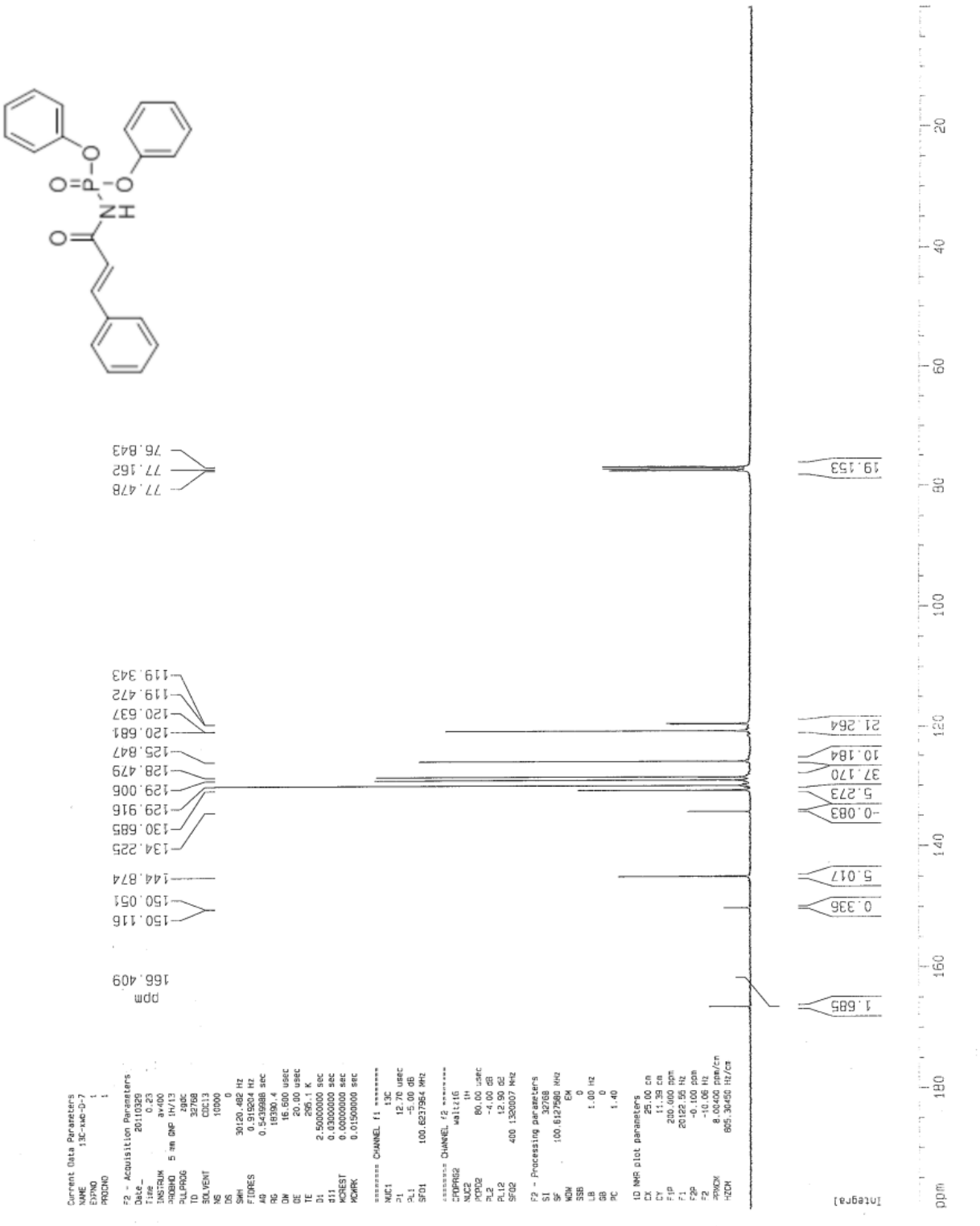

xwb-2i
6.4942
6.4900
6.4852
6.4810
SHIFT: 6.4876 ppm
L2: M=2, J=3.6012 Hz
L1: M=2, J=1.6805 Hz
[rel]
6.54
6.52
6.50
6.48
6.46
6.44
[ppm]

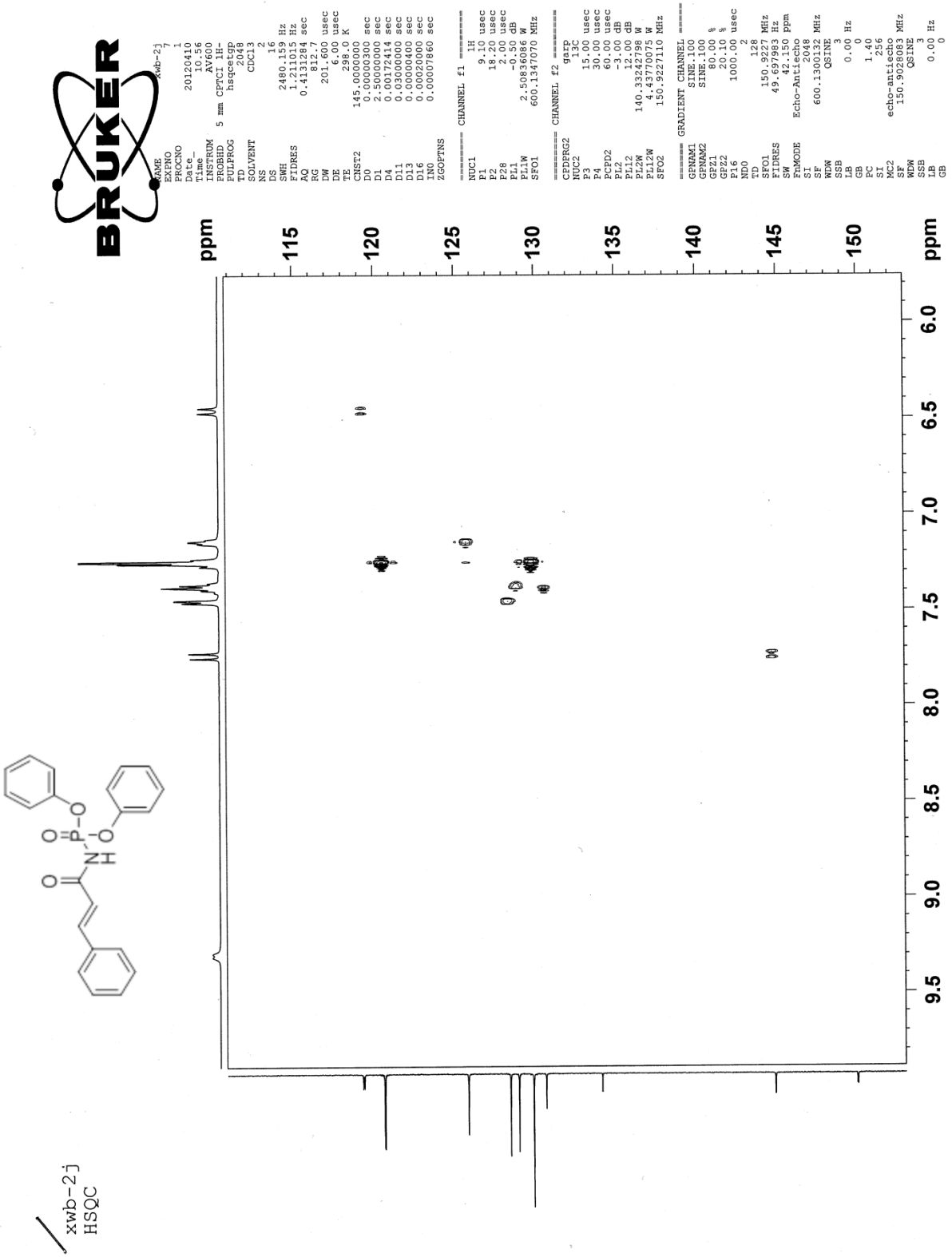

76.839
77.157
77.474
103.303
112.746
117.707
120.632
120.658
120.679
125.797
129.594
129.880
130.152
145.958
146.092
146.166
150.049
150.115
157.455
165.413
ppm
ppm


xwb-2i
HSQC
ppm
110
115
120
125
130
135
140
145
150
9.0
8.5
8.0
7.5
7.0
6.5
6.0

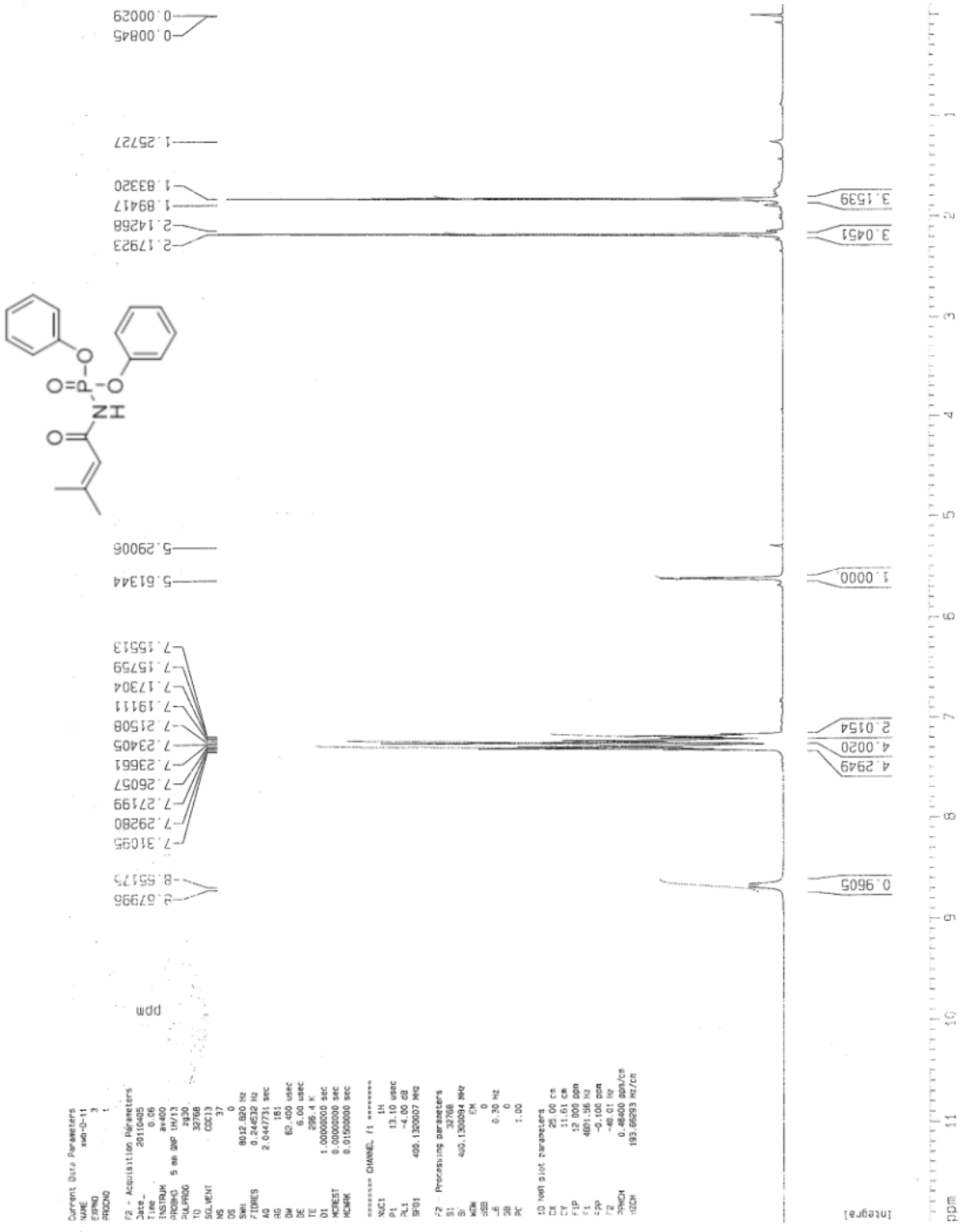
Diphenylcinnamoylphosphoramidate 2j

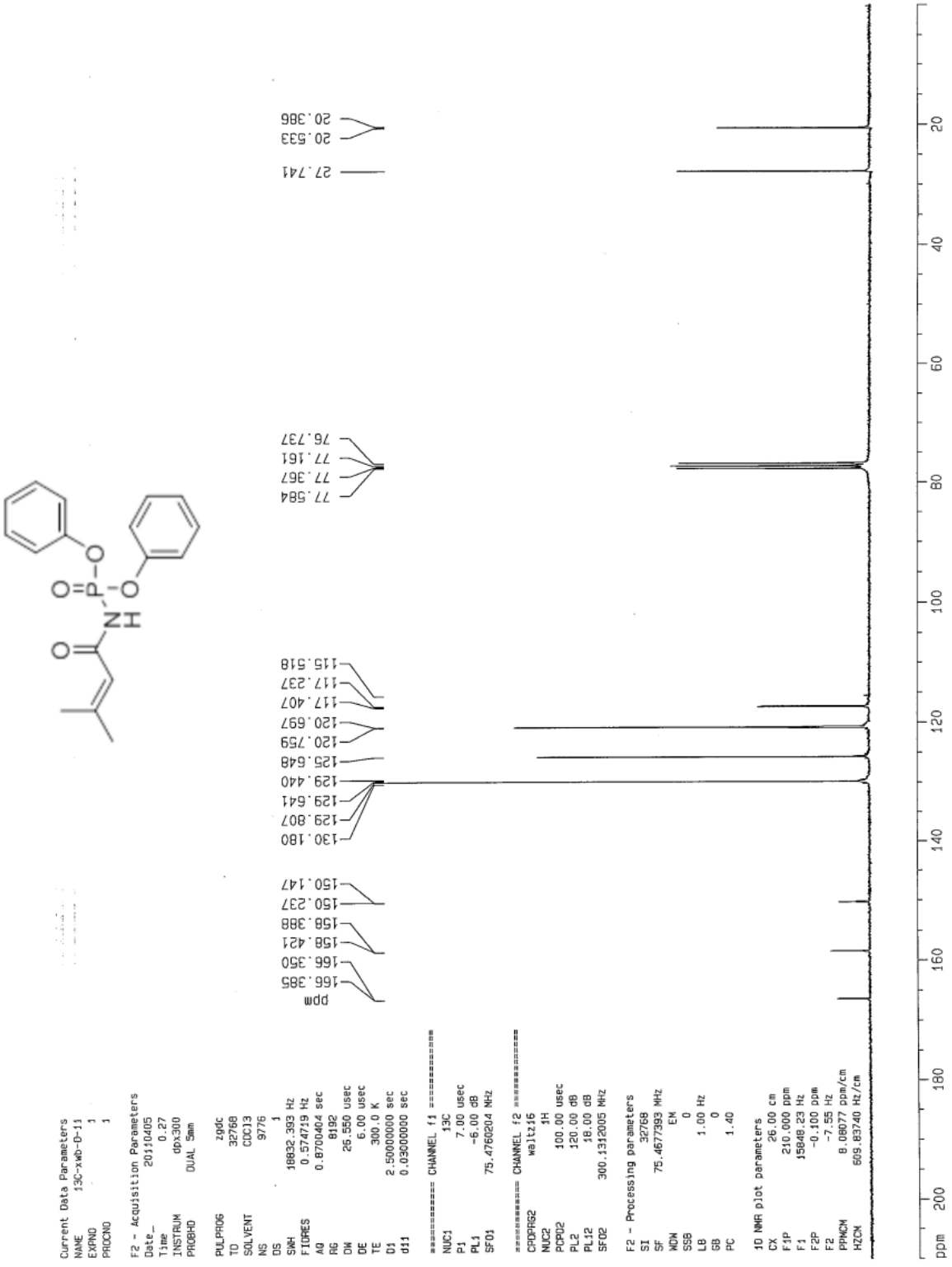


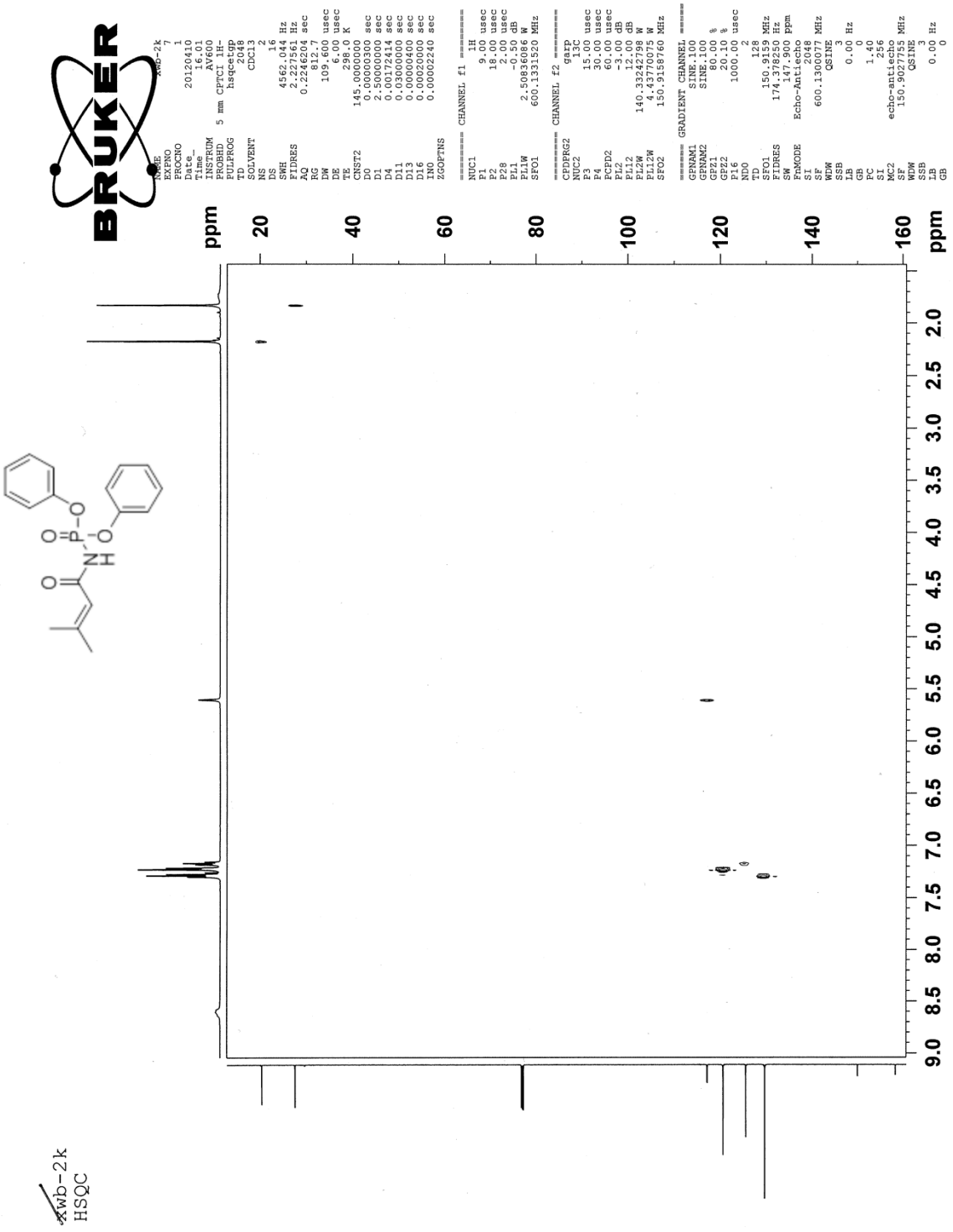

166.409
150.116
150.051
144.874
134.225
130.685
129.916
129.006
128.479
125.847
120.681
120.637
119.472
119.343
77.478
77.162
76.843
19.153
21.264
10.184
37.170
5.273
-0.083
5.017
0.336
1.685
Integral
ppm


xwb-2j
HSQC
ppm
115
120
125
130
135
140
145
150
6.0
6.5
7.0
7.5
8.0
8.5
9.0
9.5

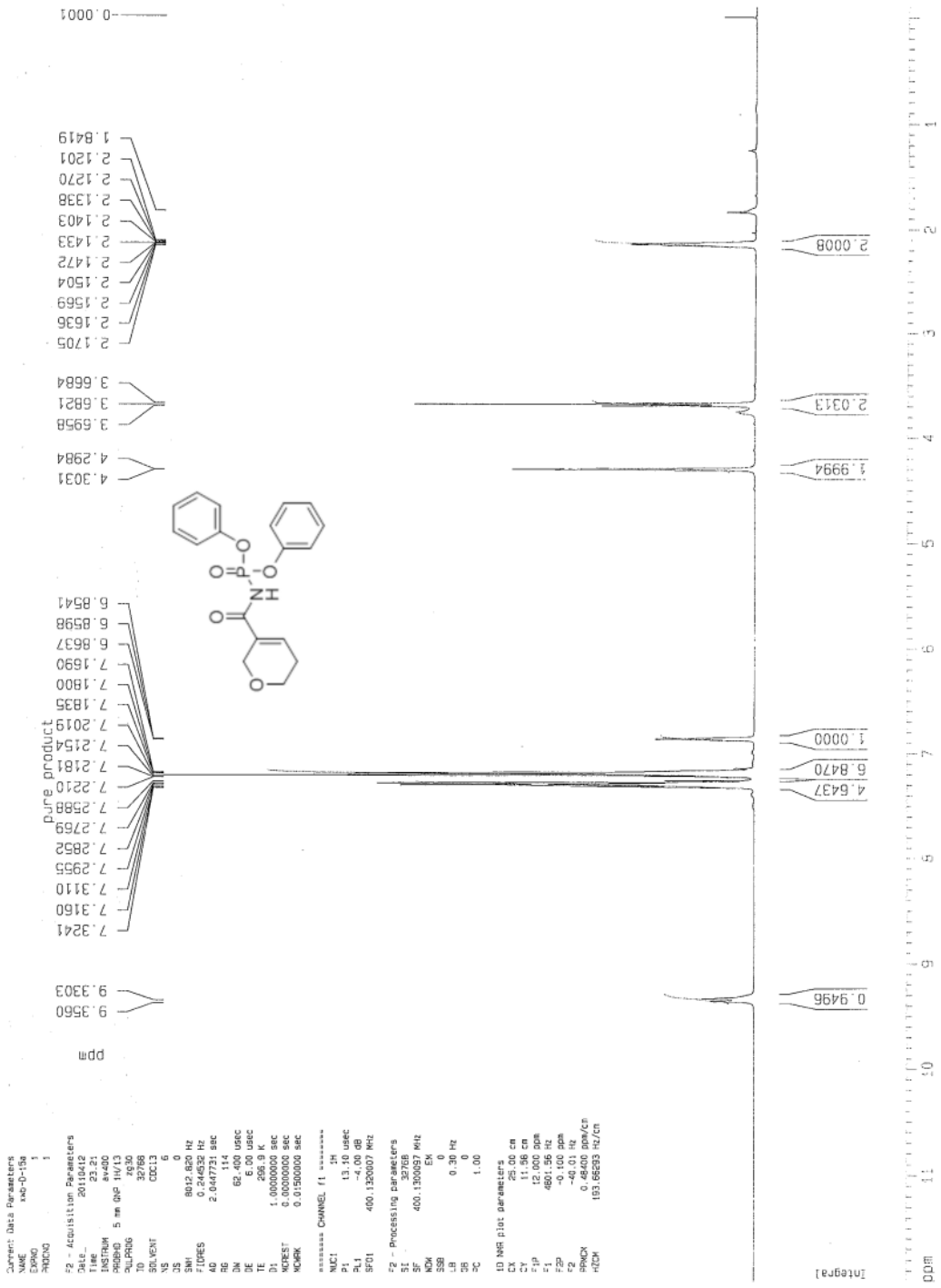
Diphenyl (3-methylbut-2-enoyl)phosphoramidate 2k

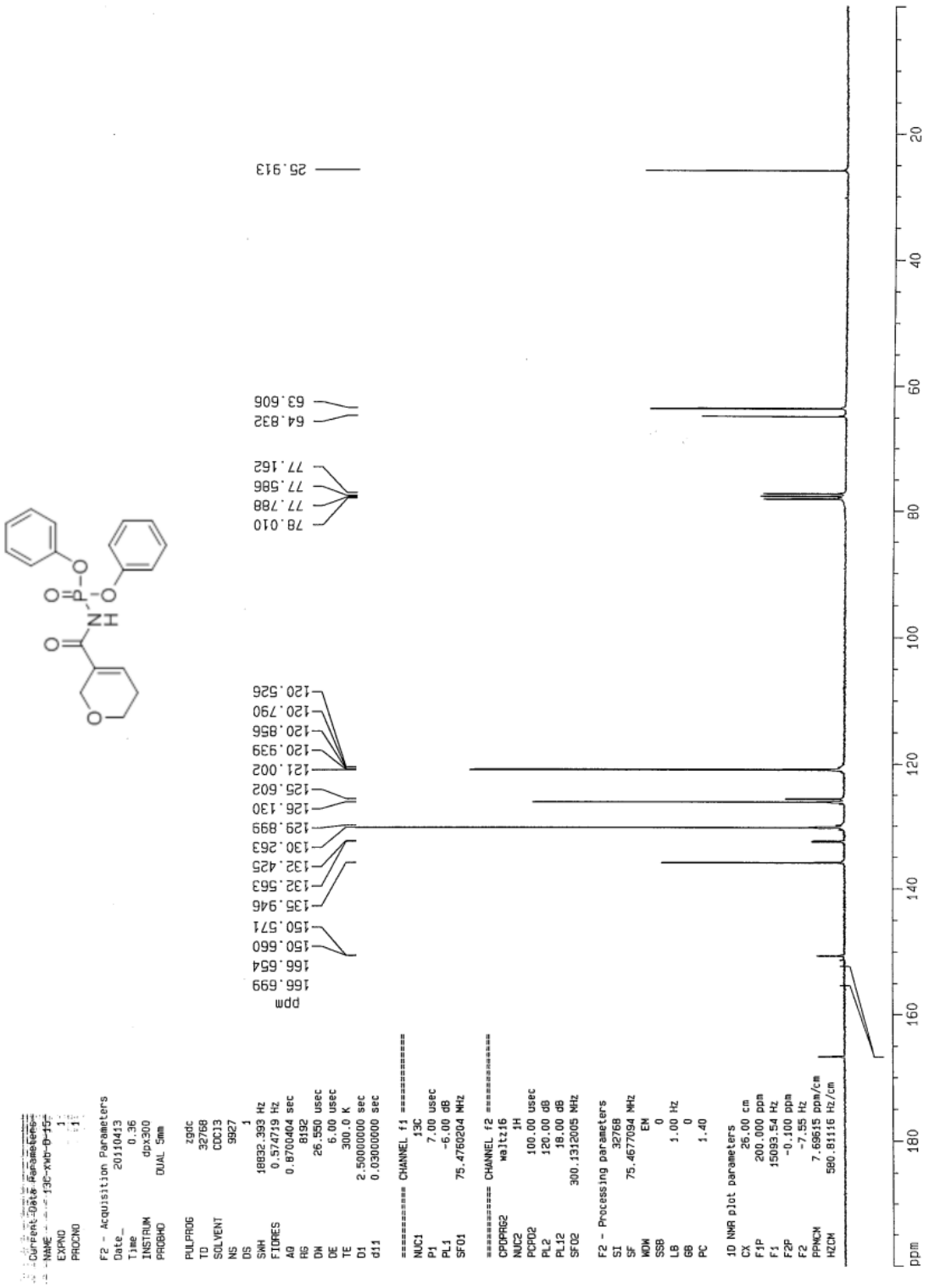


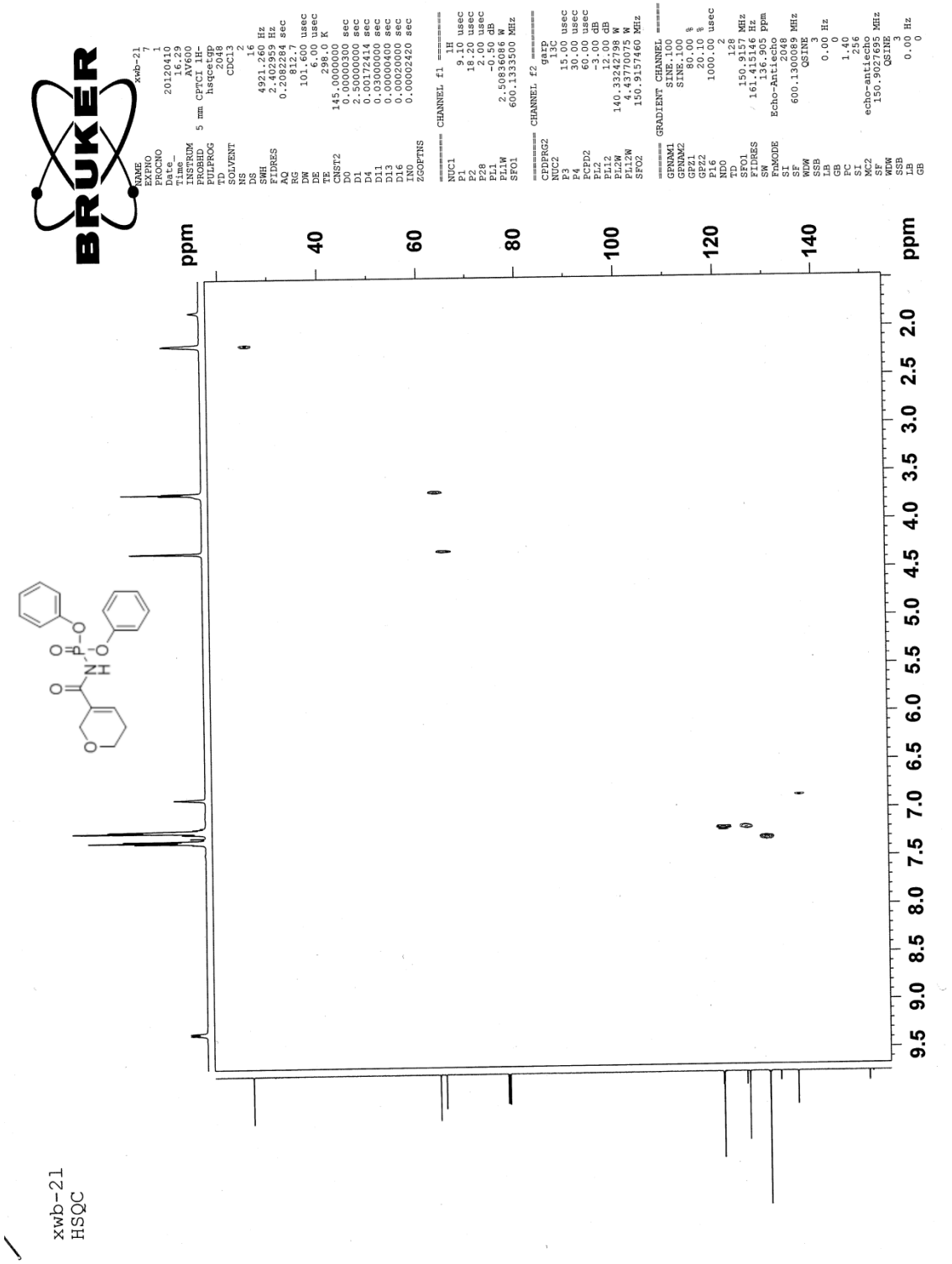

Current Data Parameters
NAME 13C-xwb-D-11
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110405
Time 0.27
INSTRUM dpx300
PROBHD DUAL 5mm
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 9776
DS 1
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 8192
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.50000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.00 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 26.00 cm
F1P 210.000 ppm
F1 15848.23 Hz
F2P -0.100 ppm
F2 -7.55 Hz
PPMCM 8.08077 ppm/cm
HZCM 609.83740 Hz/cm
ppm
166.385
166.350
158.421
158.388
150.237
150.147
130.180
129.807
129.641
129.440
125.648
120.759
120.697
117.407
117.237
115.518
77.584
77.367
77.161
76.737
27.741
20.533
20.386
O
O=P
O
NH
O
ppm
200
180
160
140
120
100
80
60
40
20


BRUKER
ppm
20
40
60
80
100
120
140
160
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9.0
xwb-2k
HSQC

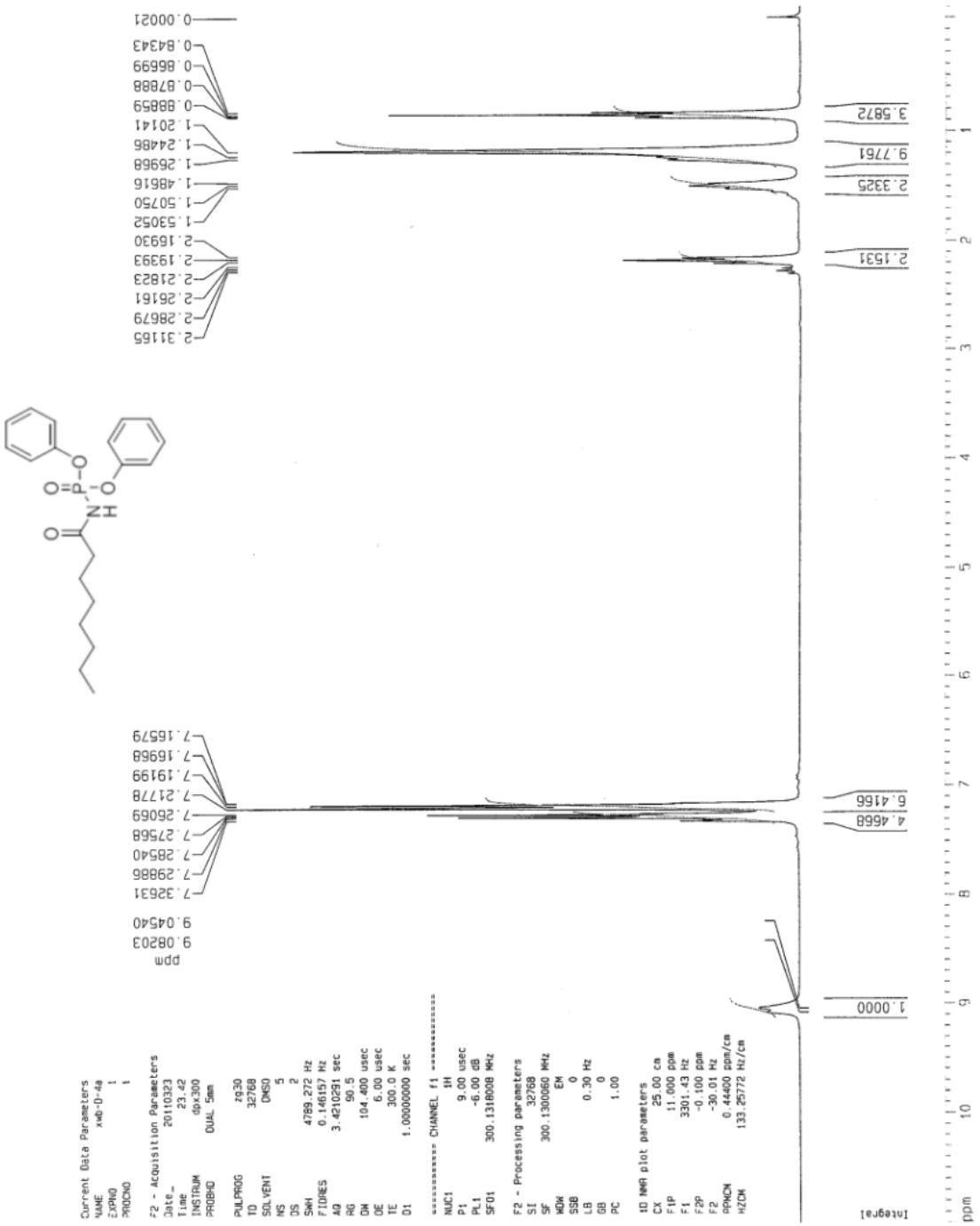
Diphenyl (5,6-dihydro-2H-pyran-3-carbonyl)phosphoramidate 2l

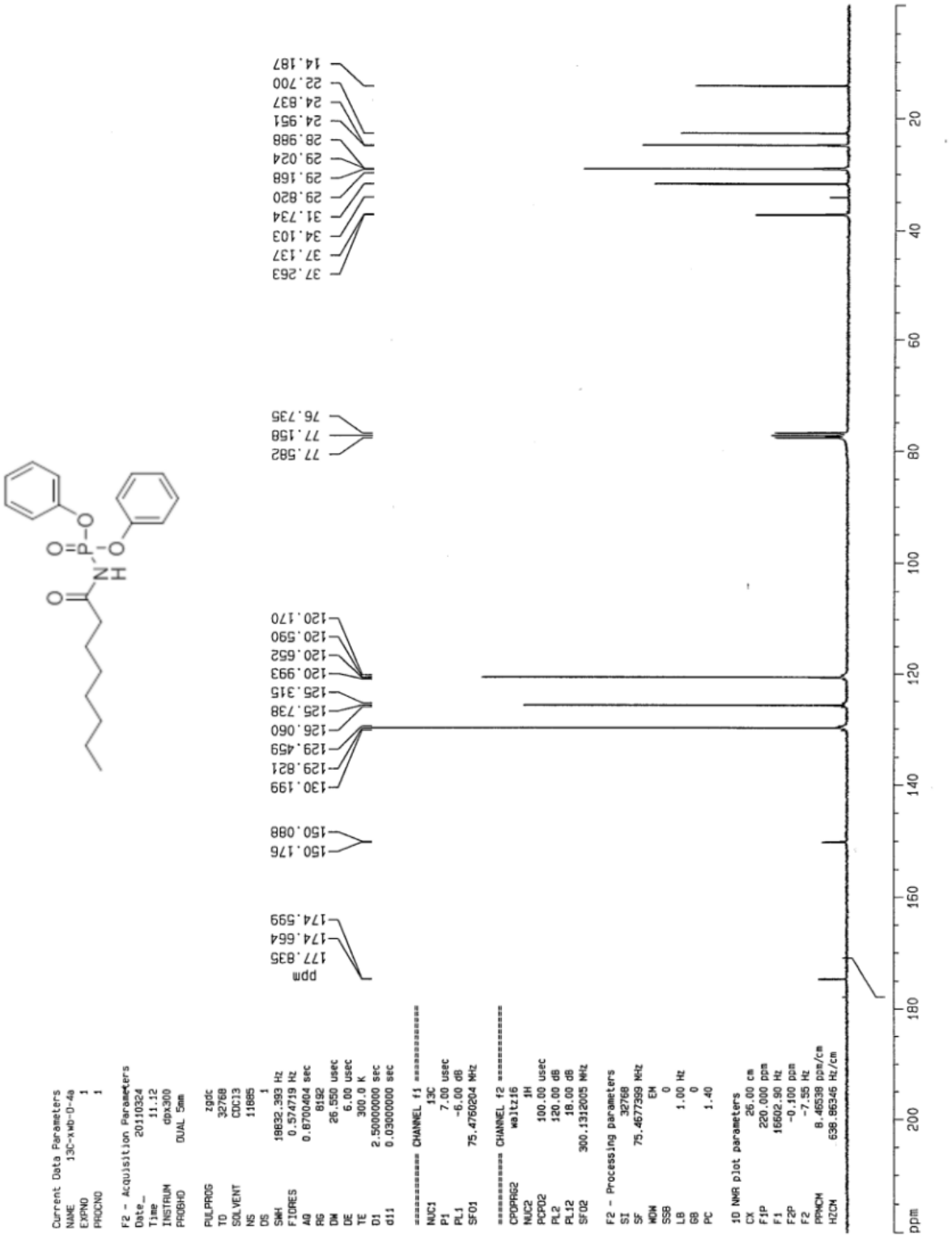


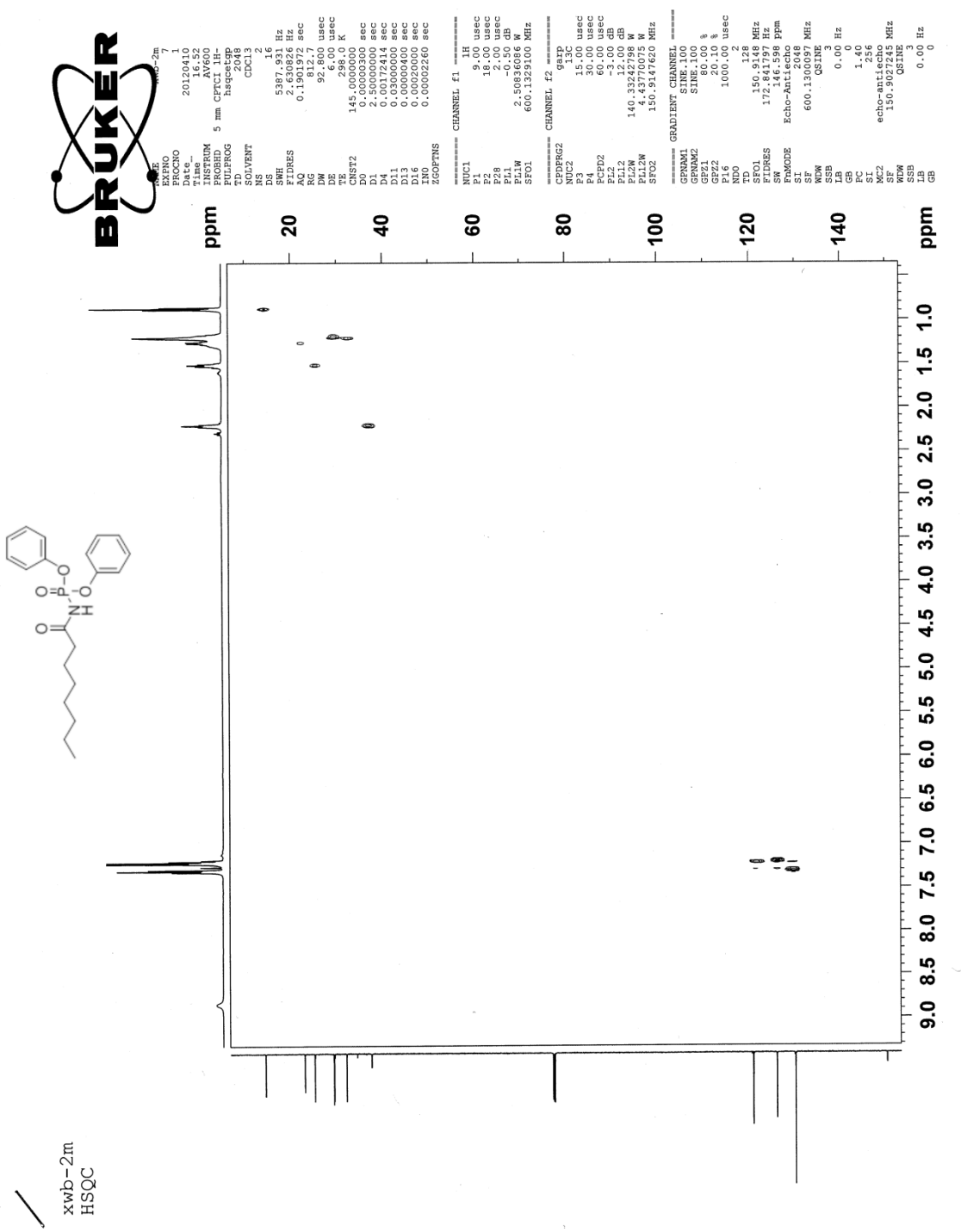

25.913
63.606
64.832
77.162
77.586
77.788
78.010
120.526
120.790
120.856
120.939
121.002
125.602
126.130
129.899
130.263
132.425
132.563
135.946
150.571
150.660
166.654
166.699
ppm
20
40
60
80
100
120
140
160
180
ppm
NH
O
P
O
O
O
O
O
Current Data Parameters
NAME 13C-xwb-D-15
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110413
Time 0.36
INSTRUM dpx300
PROBHD DUAL 5mm
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 9927
DS 1
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 8192
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.50000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 7.00 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677094 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 26.00 cm
F1P 200.000 ppm
F1 15093.54 Hz
F2P -0.100 ppm
F2 -7.55 Hz
PPMCM 7.69615 ppm/cm
HZCM 580.81116 Hz/cm


xwb-21
HSQC
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
40
60
80
100
120
140

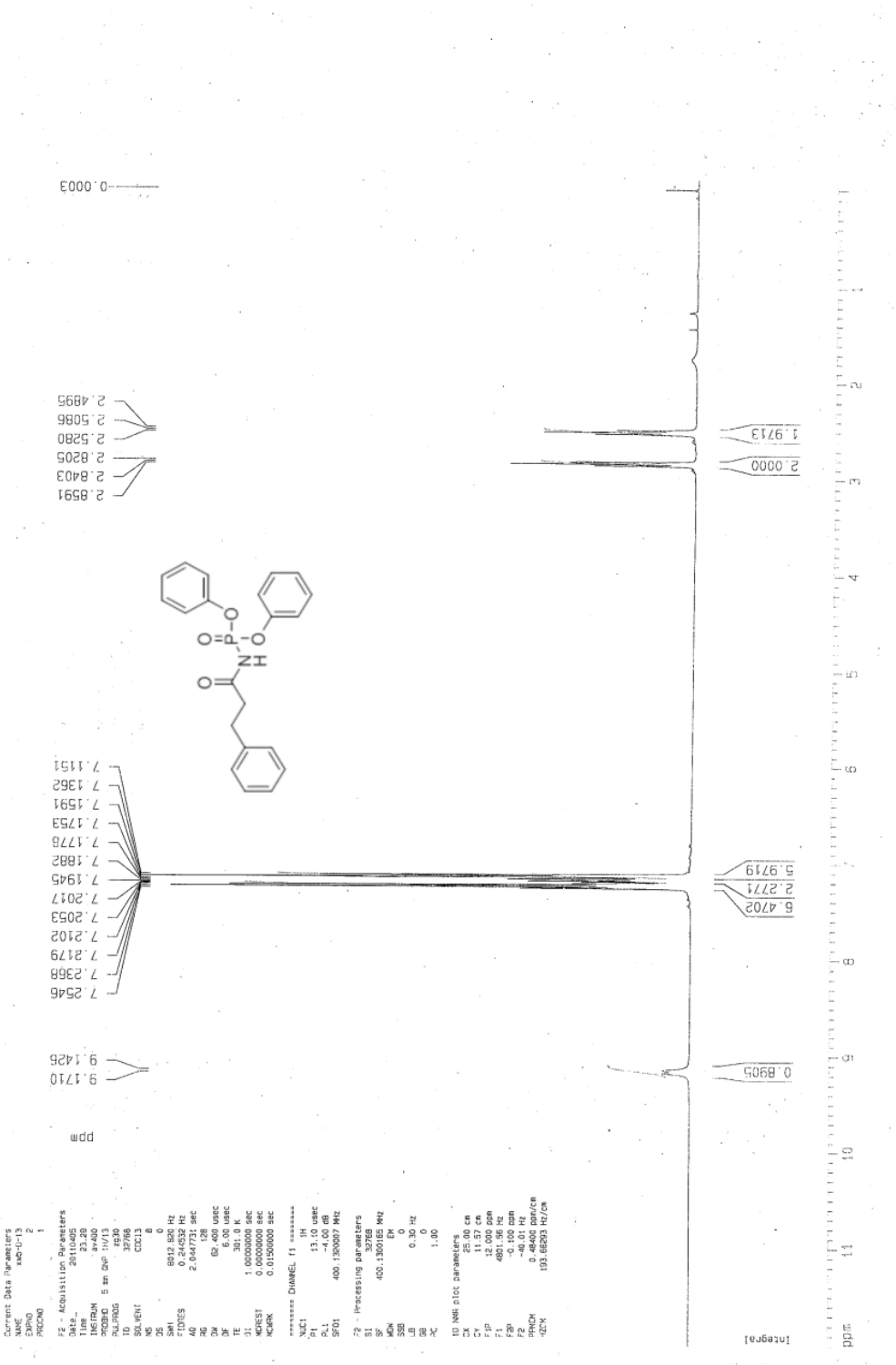
Diphenyloctanoylphosphoramidate 2m

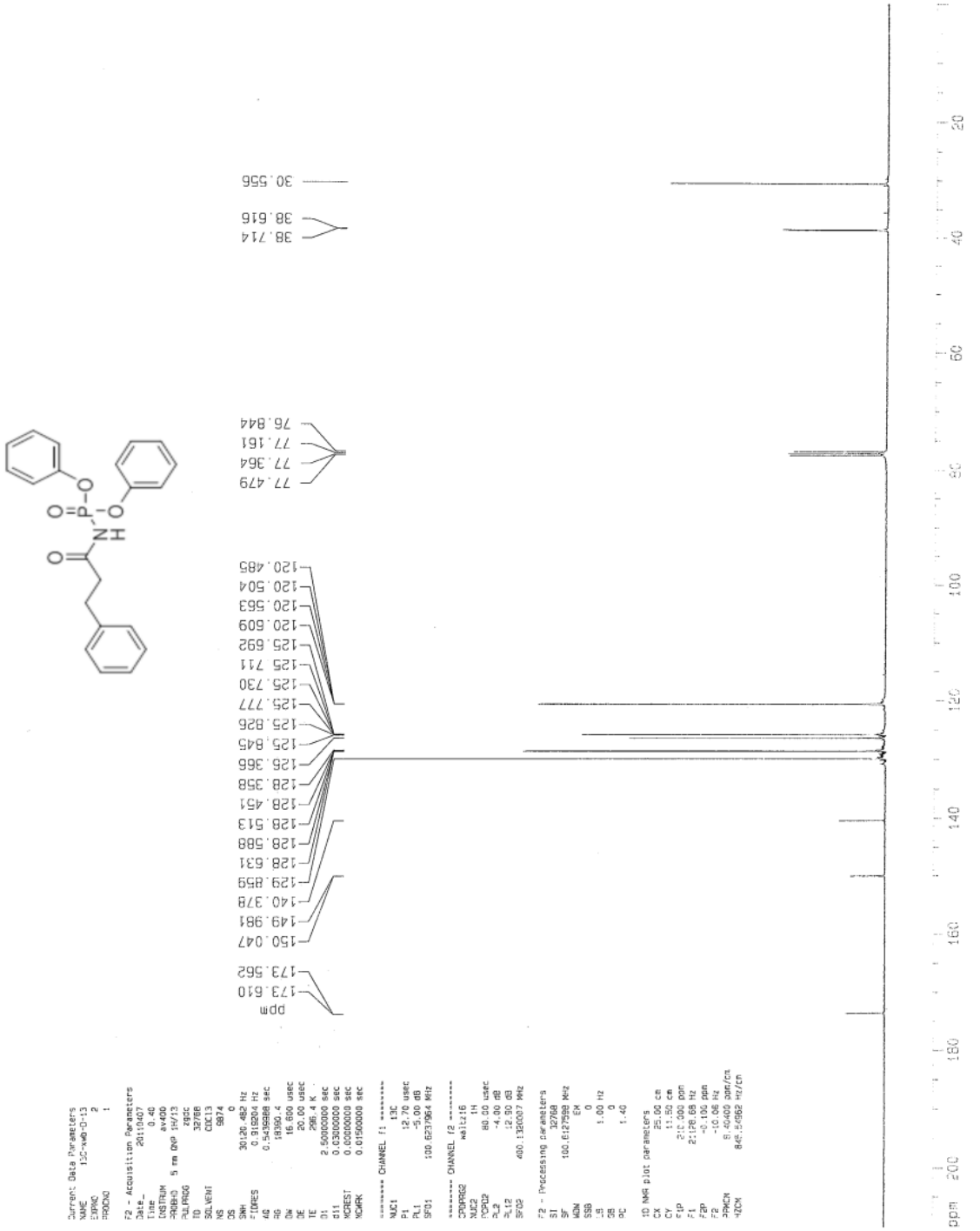


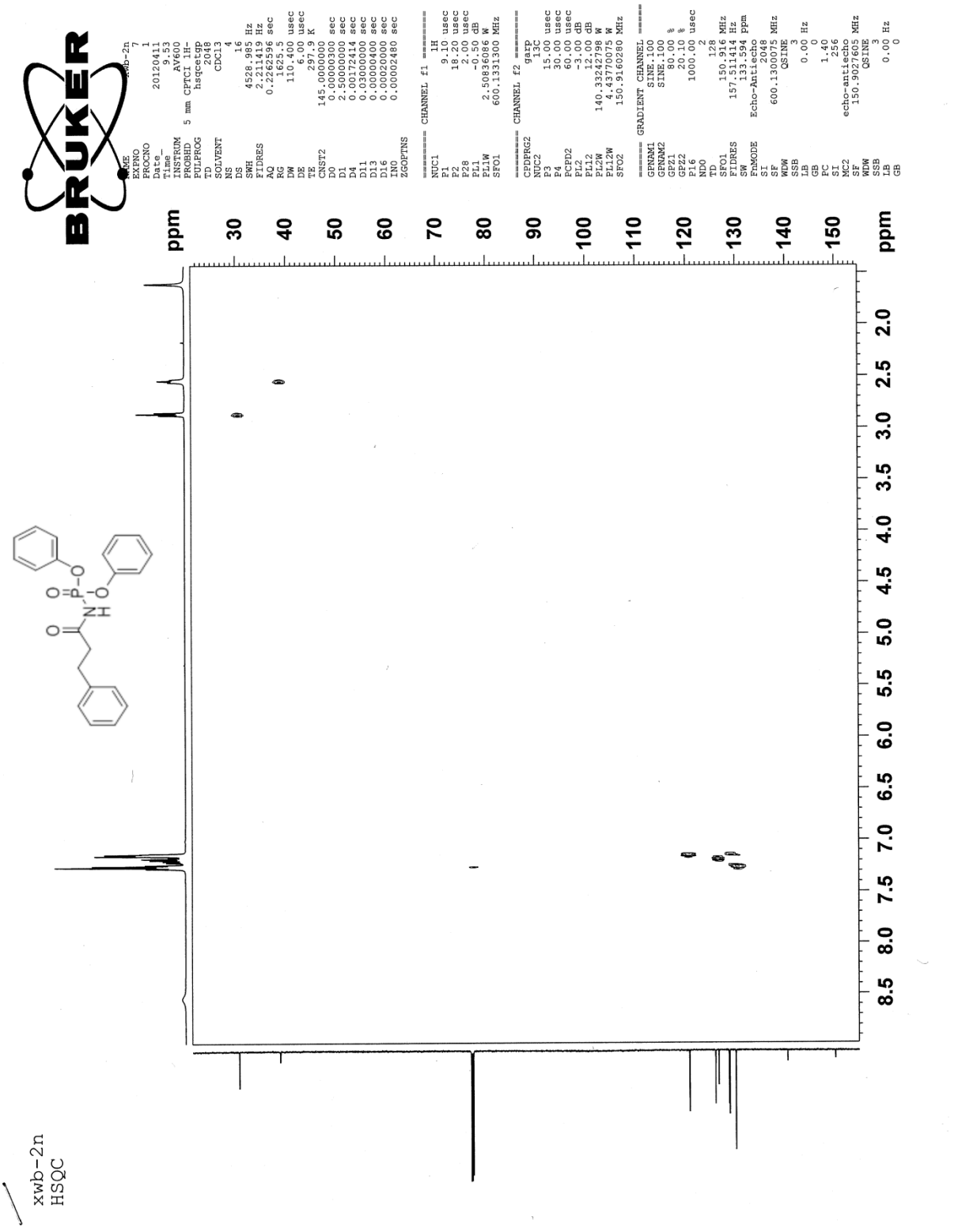

Current Data Parameters
NAME 13C-xwb-0-4a
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110324
Time 11.12
INSTRUM dpx300
PROBHD DUAL 5mm
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 11885
DS 1
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.87004404 sec
RG 8192
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.50000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 7.00 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4577399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 26.00 cm
F1P 220.000 ppm
F1 16602.90 Hz
F2P -0.100 ppm
F2 -7.55 Hz
PPMCM 8.46539 ppm/cm
HZCM 638.86345 Hz/cm
ppm
177.835
174.664
174.599
150.176
150.088
130.199
129.821
129.459
126.060
125.738
125.315
120.993
120.652
120.590
120.170
77.582
77.158
76.735
37.263
37.137
34.103
31.734
29.820
29.168
29.024
28.988
24.951
24.837
22.700
14.187
ppm


xwb-2m
HSQC
ppm

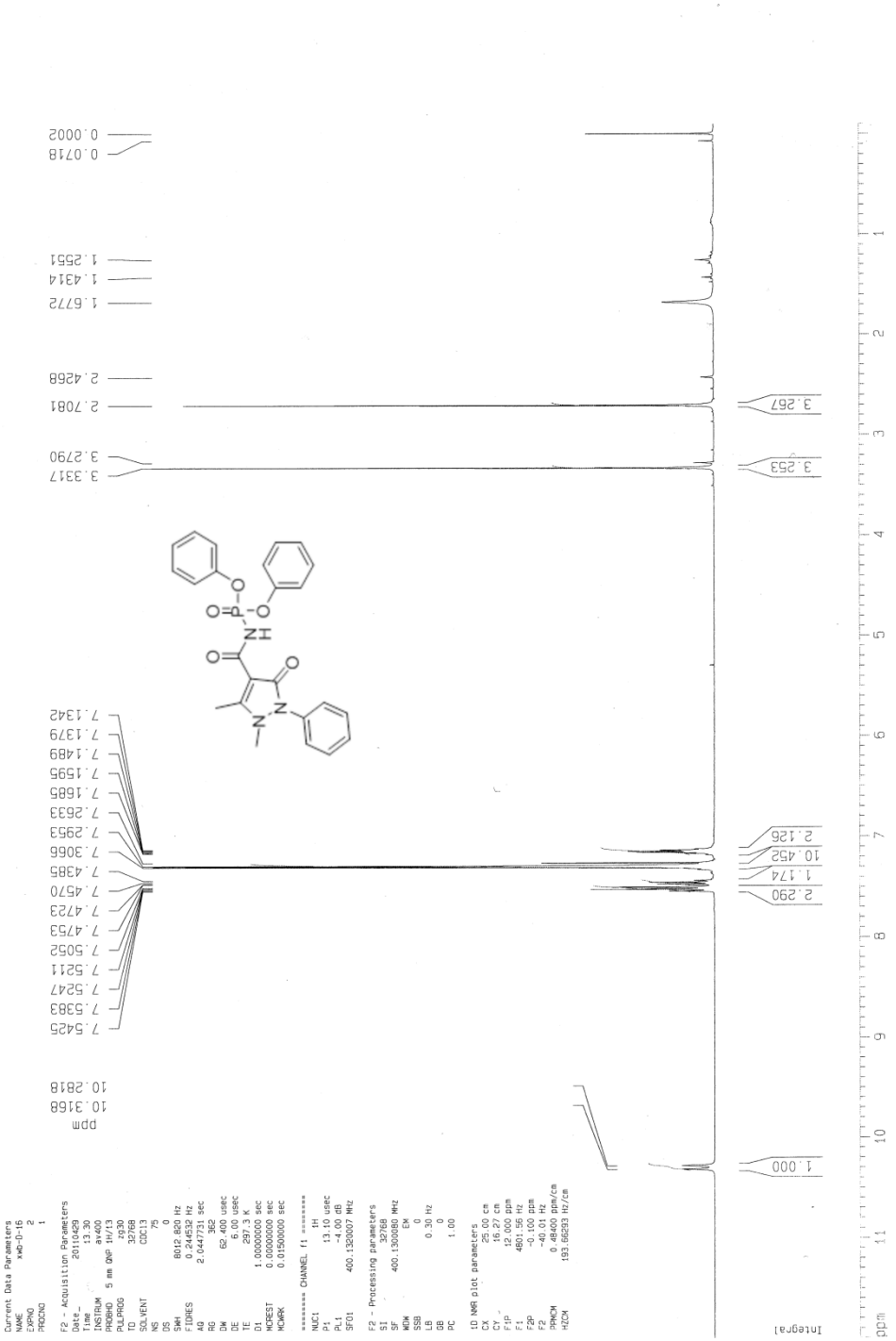
Diphenyl (3-phenylpropanoyl)phosphoramidate 2n

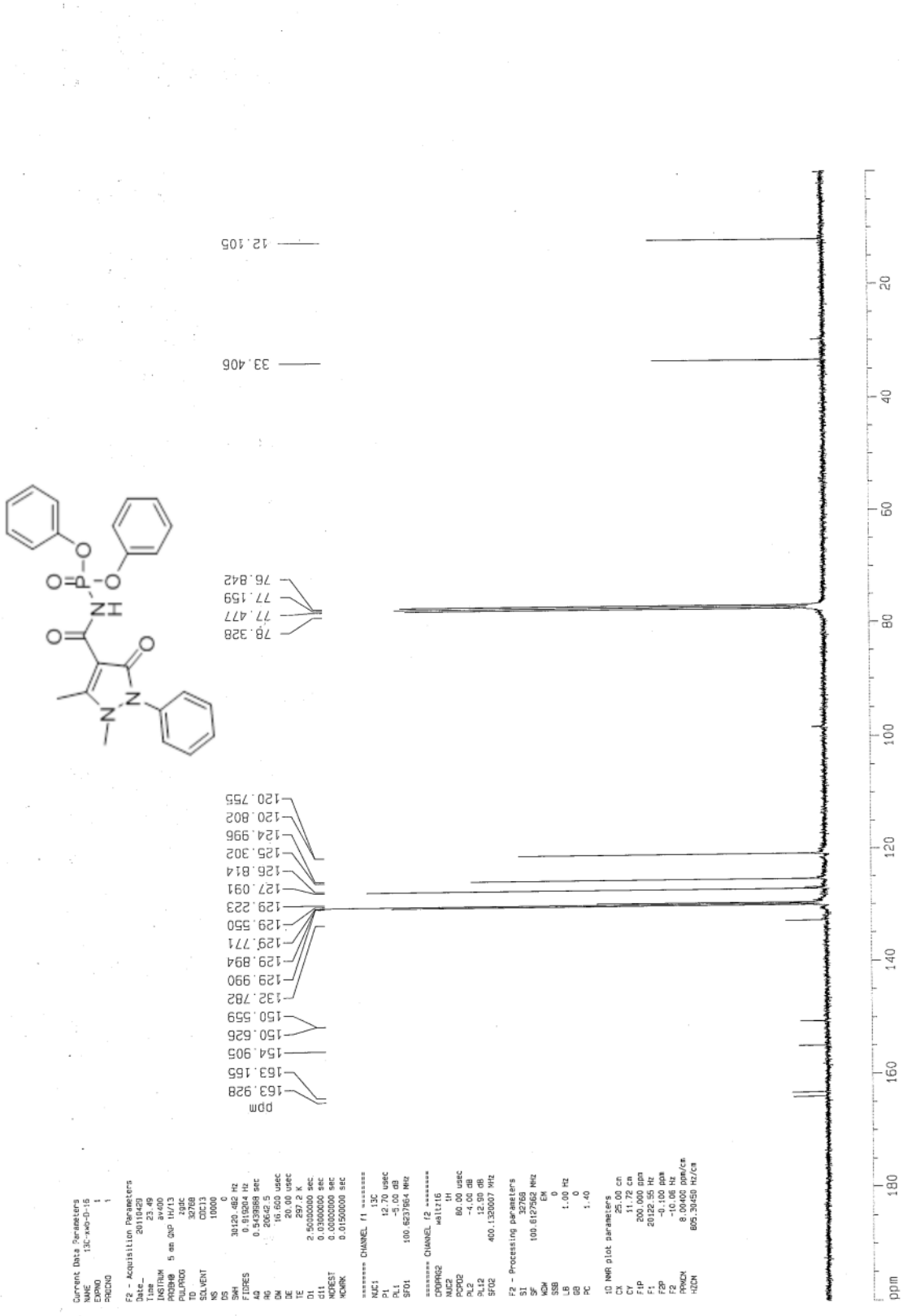


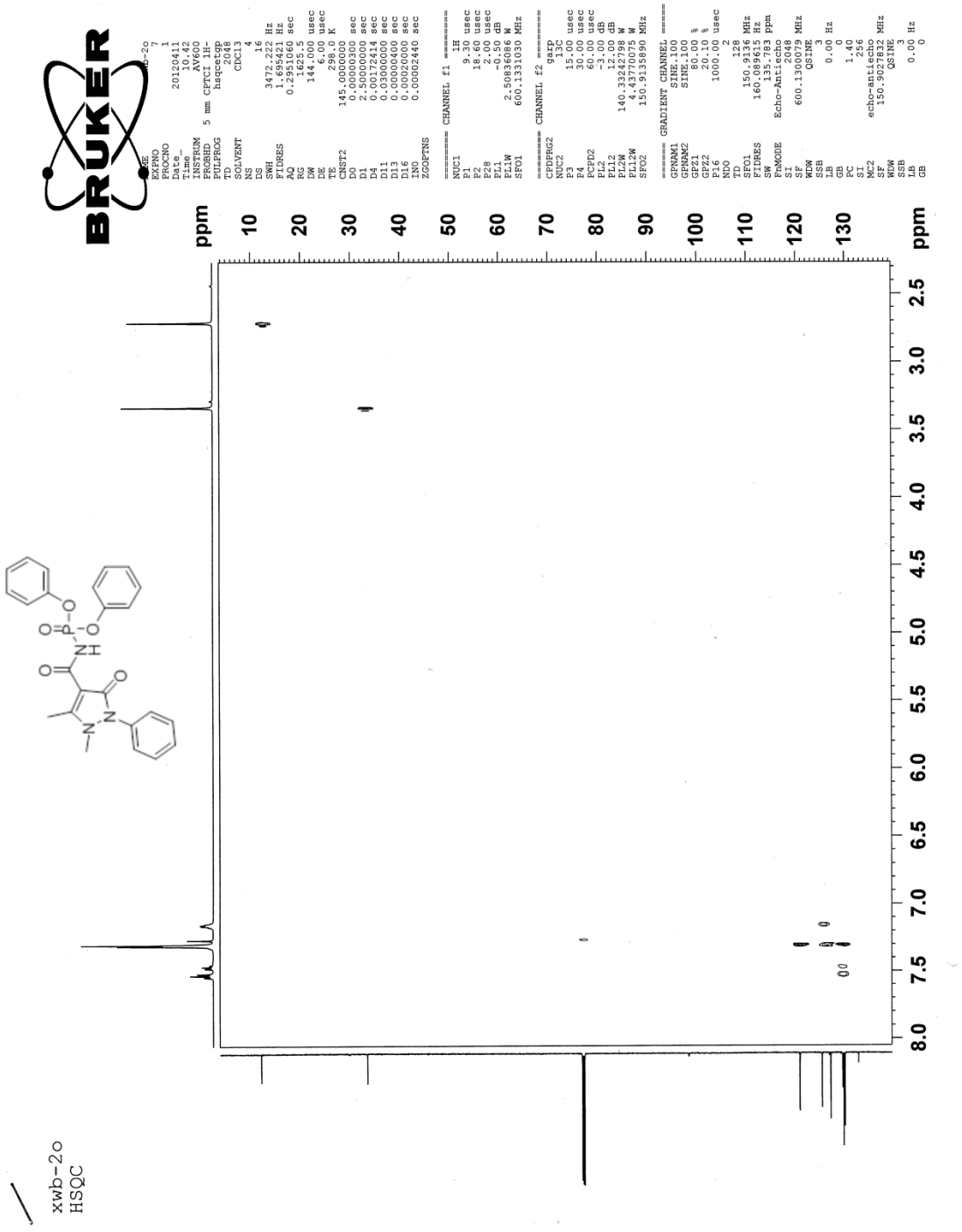

30.556
38.616
38.714
76.844
77.161
77.364
77.479
120.485
120.504
120.563
120.609
125.692
125.711
125.730
125.777
125.826
125.845
126.366
128.358
128.451
128.513
128.588
128.631
129.859
140.378
149.981
150.047
173.562
173.610
ppm
200
180
160
140
120
100
80
60
40
20


xwb-2n
HSQC
ppm

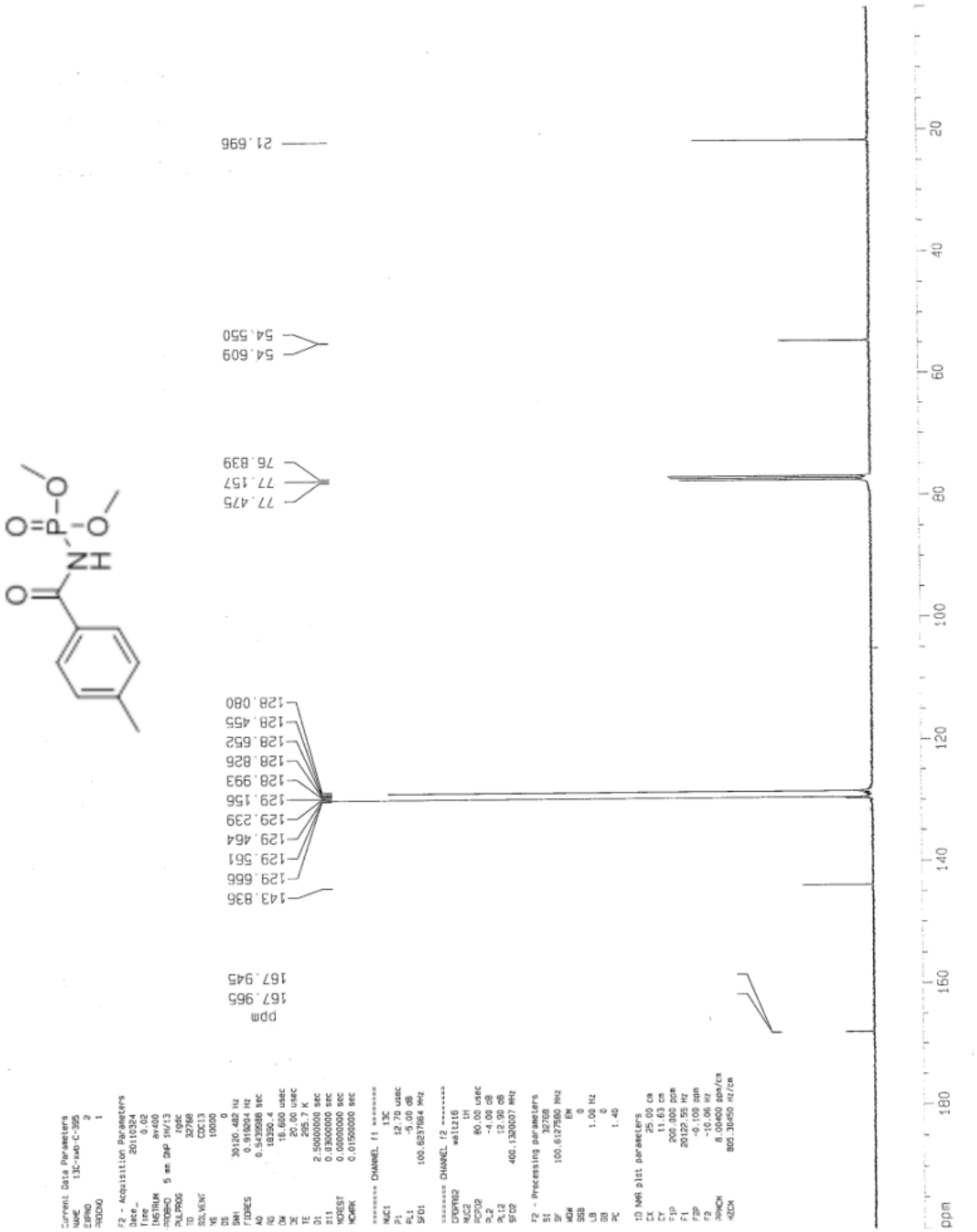
Diphenyl (1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazole-4-carbonyl)-phosphoramidate 2o

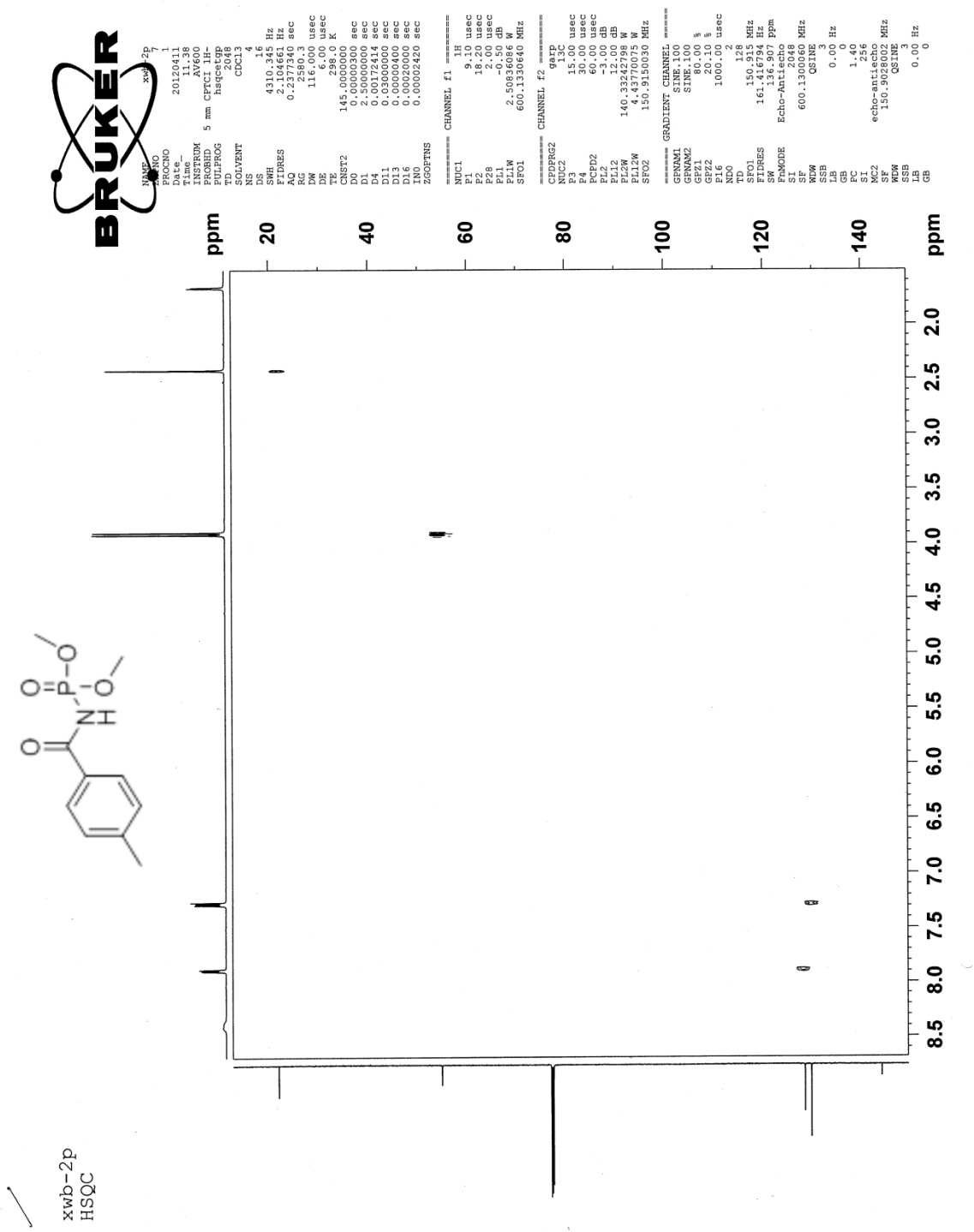



12.105
33.406
76.842
77.159
77.477
78.328
120.755
120.802
124.996
125.302
126.814
127.091
129.223
129.550
129.771
129.894
129.990
132.782
150.559
150.626
154.905
163.155
163.928
ppm
ppm

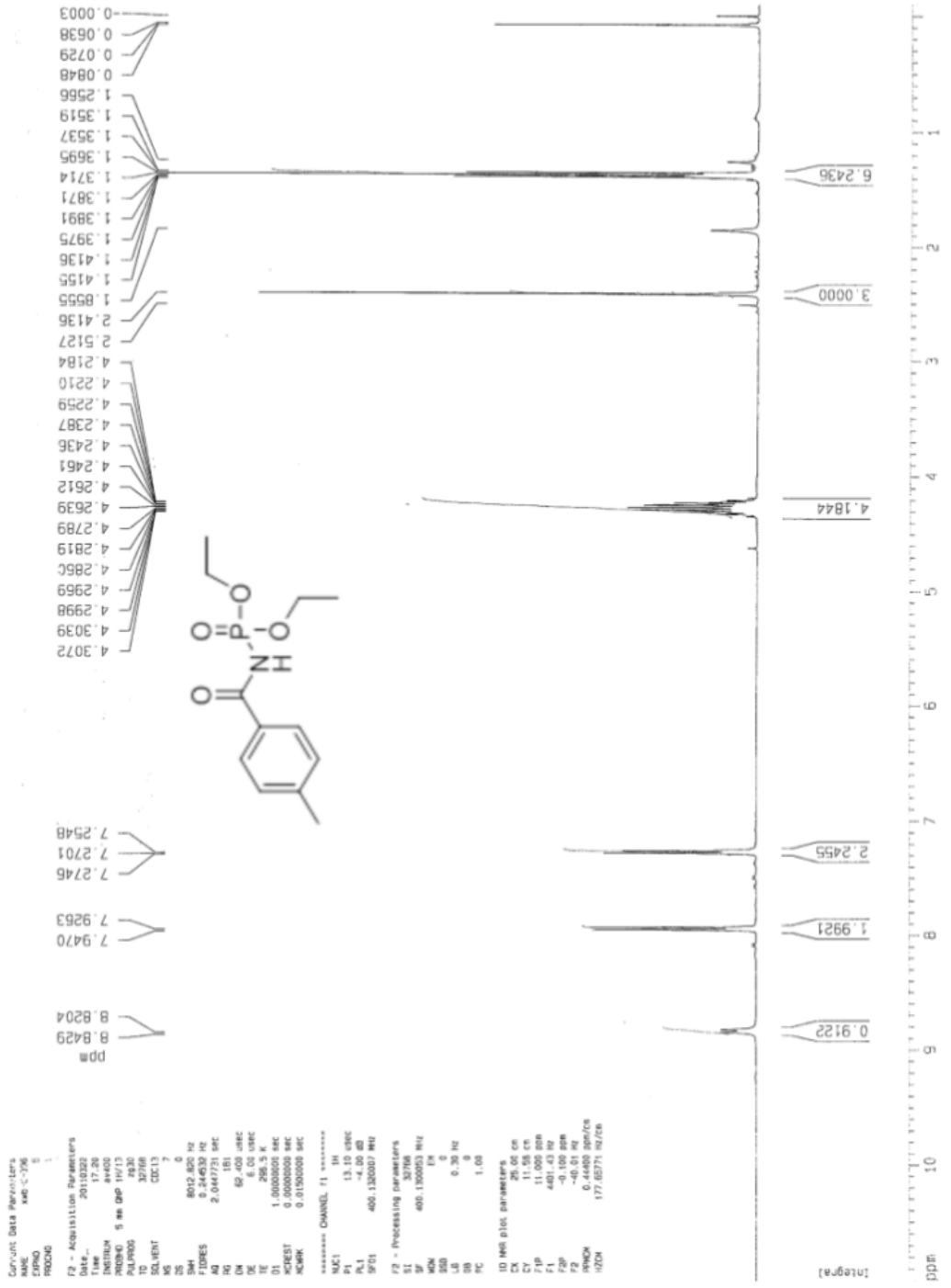

xwb-2o
HSQC
ppm
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
10
20
30
40
50
60
70
80
90
100
110
120
130

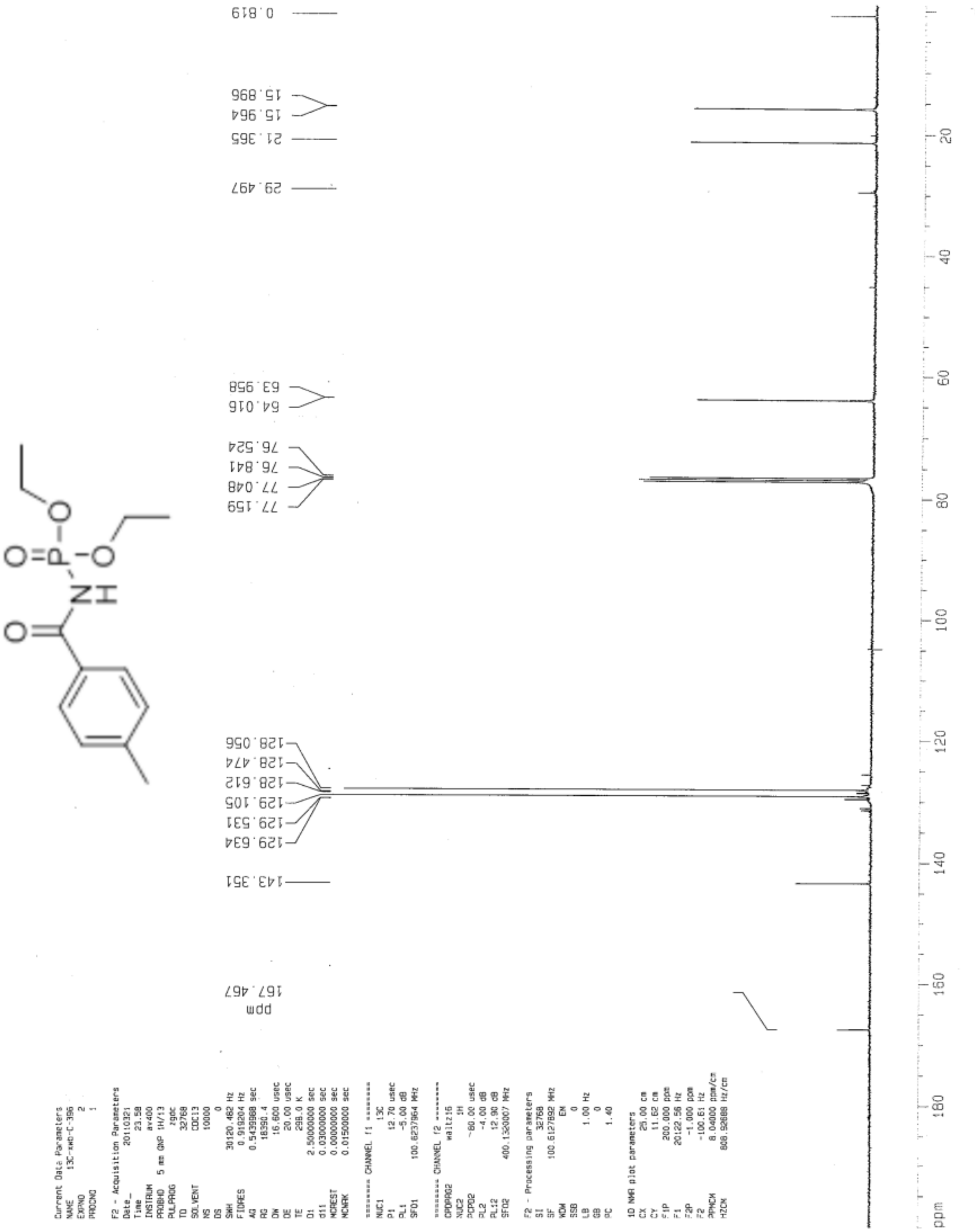
Dimethyl (4-methylbenzoyl)phosphoramidate 2p

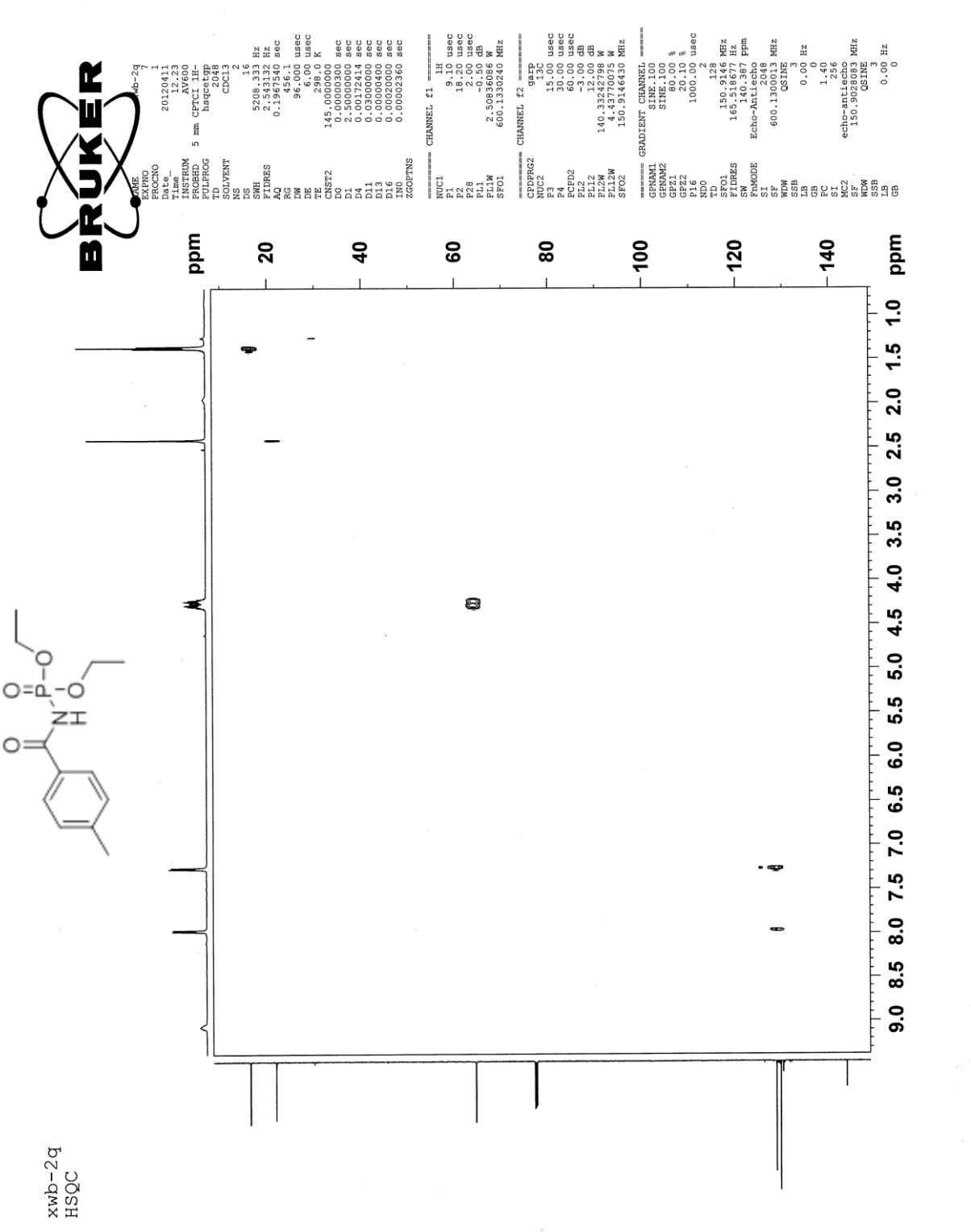

21.696
54.609
54.550
76.839
77.157
77.475
128.080
128.455
128.652
128.826
128.993
129.156
129.239
129.464
129.561
129.666
143.836
167.945
167.965
ppm
20
40
60
80
100
120
140
160
180
ppm


xwb-2p
HSQC
ppm
ppm

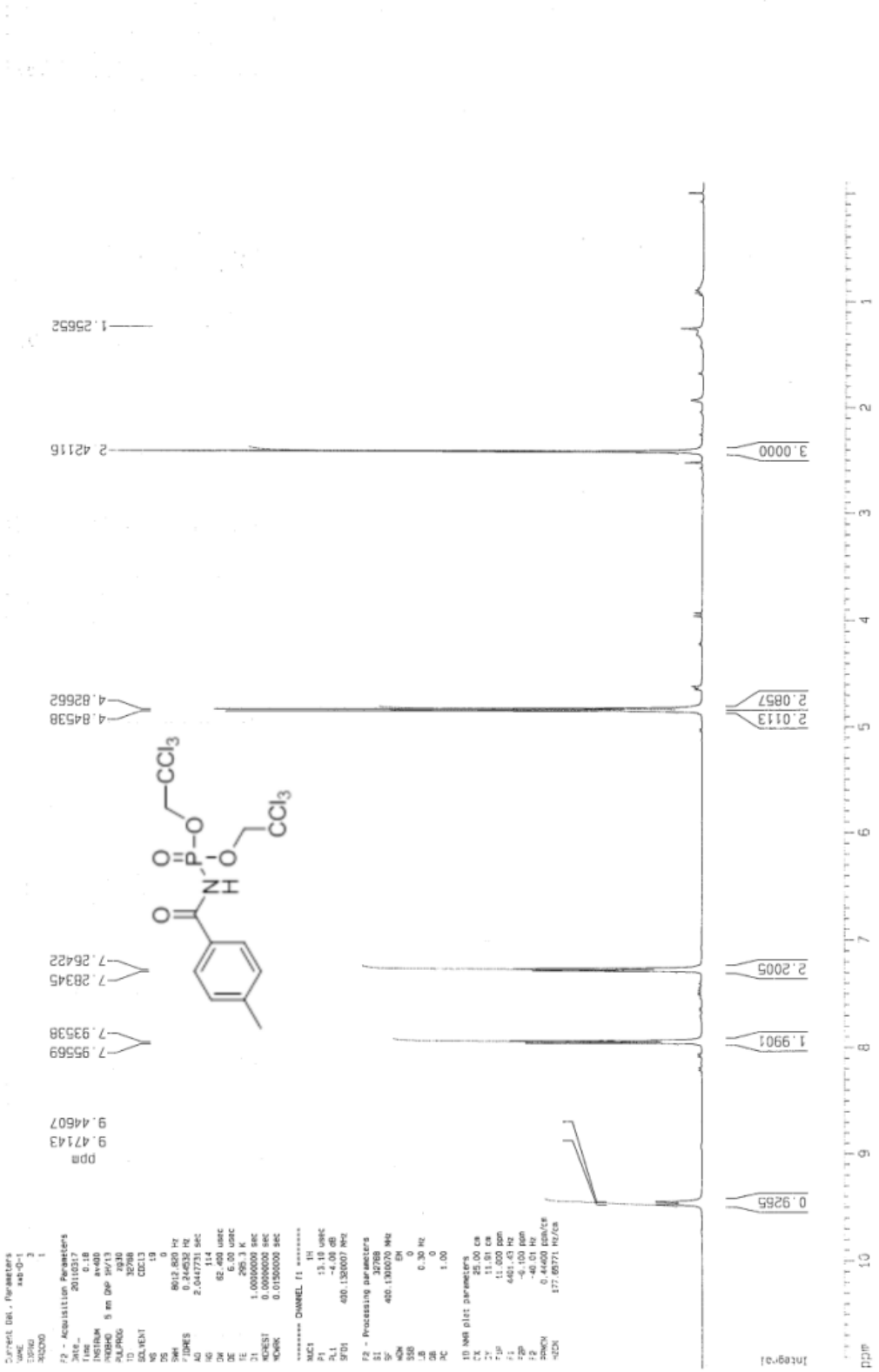
Diethyl (4-methylbenzoyl)phosphoramidate 2q

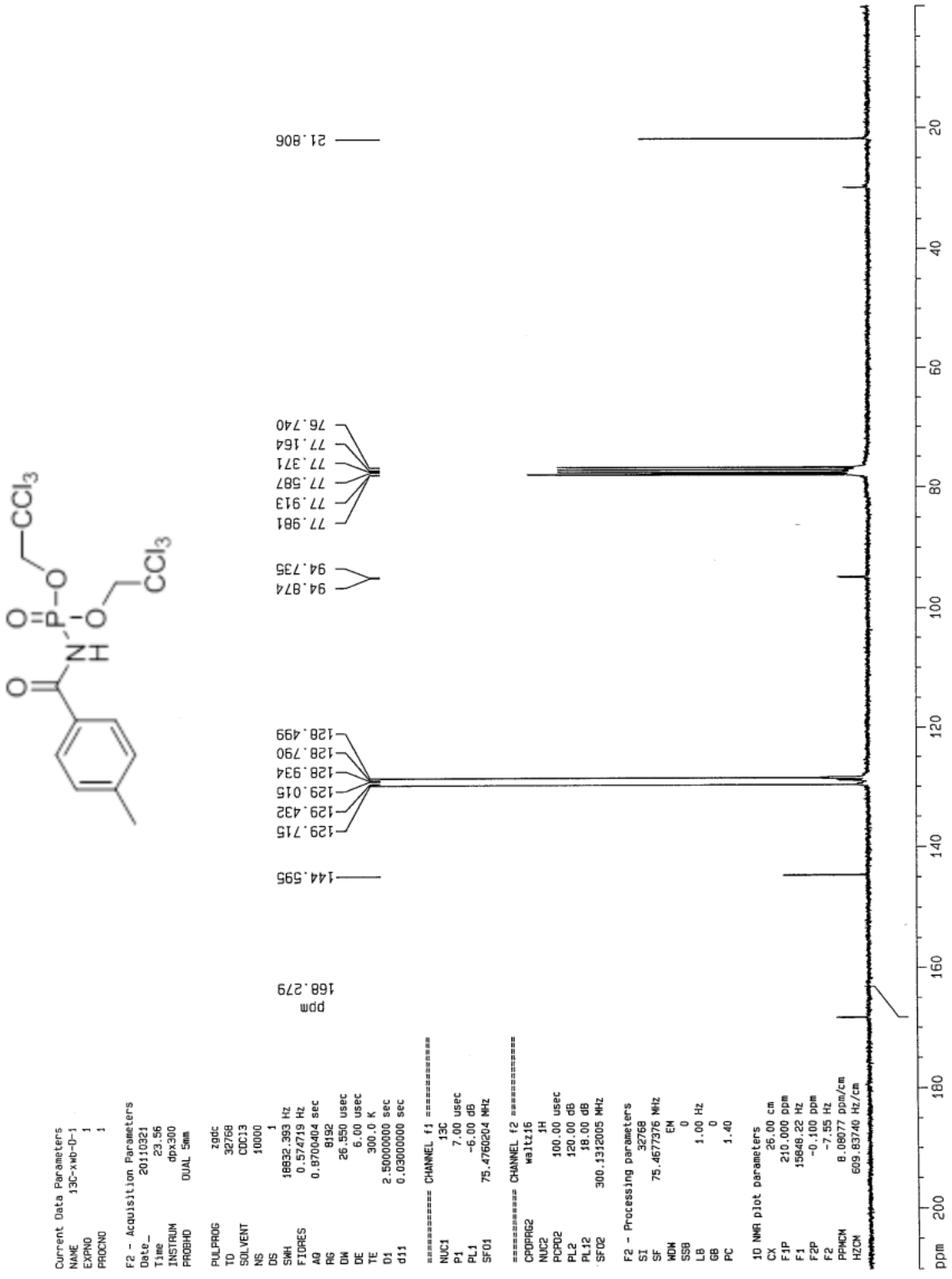



0.819
15.896
15.964
21.365
29.497
63.958
64.016
76.524
76.841
77.048
77.159
128.056
128.474
128.612
129.105
129.531
129.634
143.351
167.467
ppm

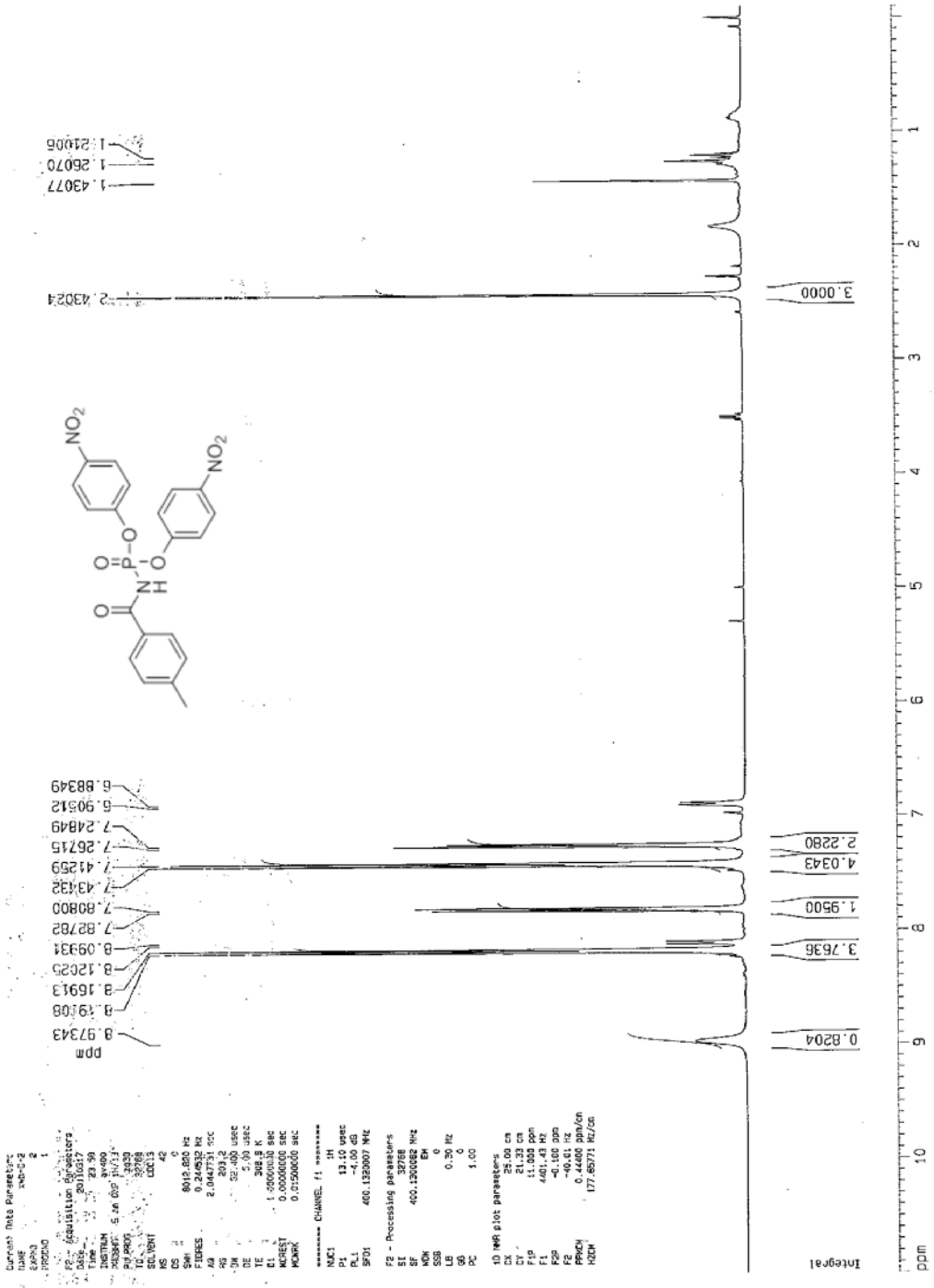

xwb-2q
HSQC
ppm

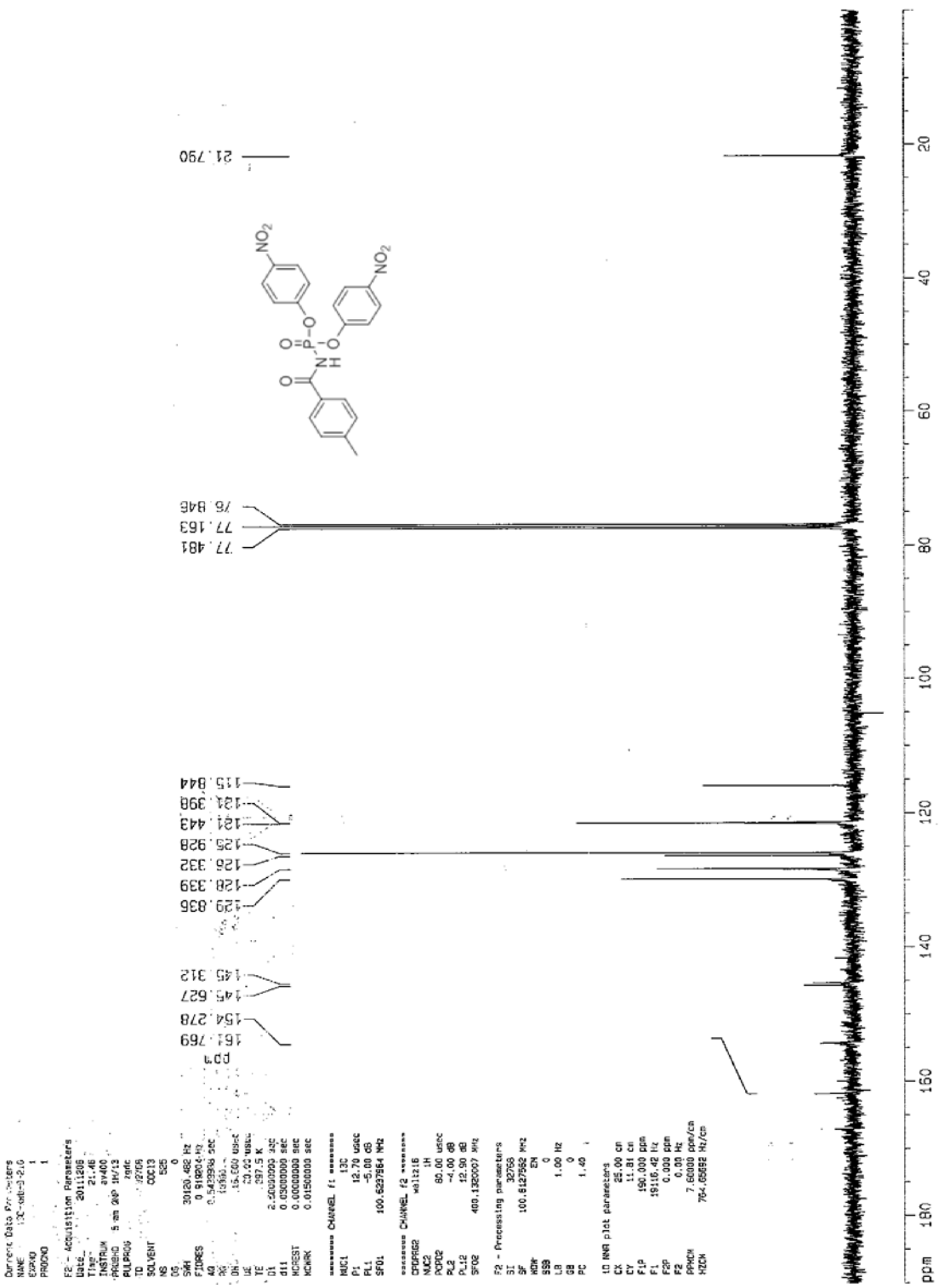
Bis(2,2,2-trichloroethyl) (4-methylbenzoyl)phosphoramidate 2r



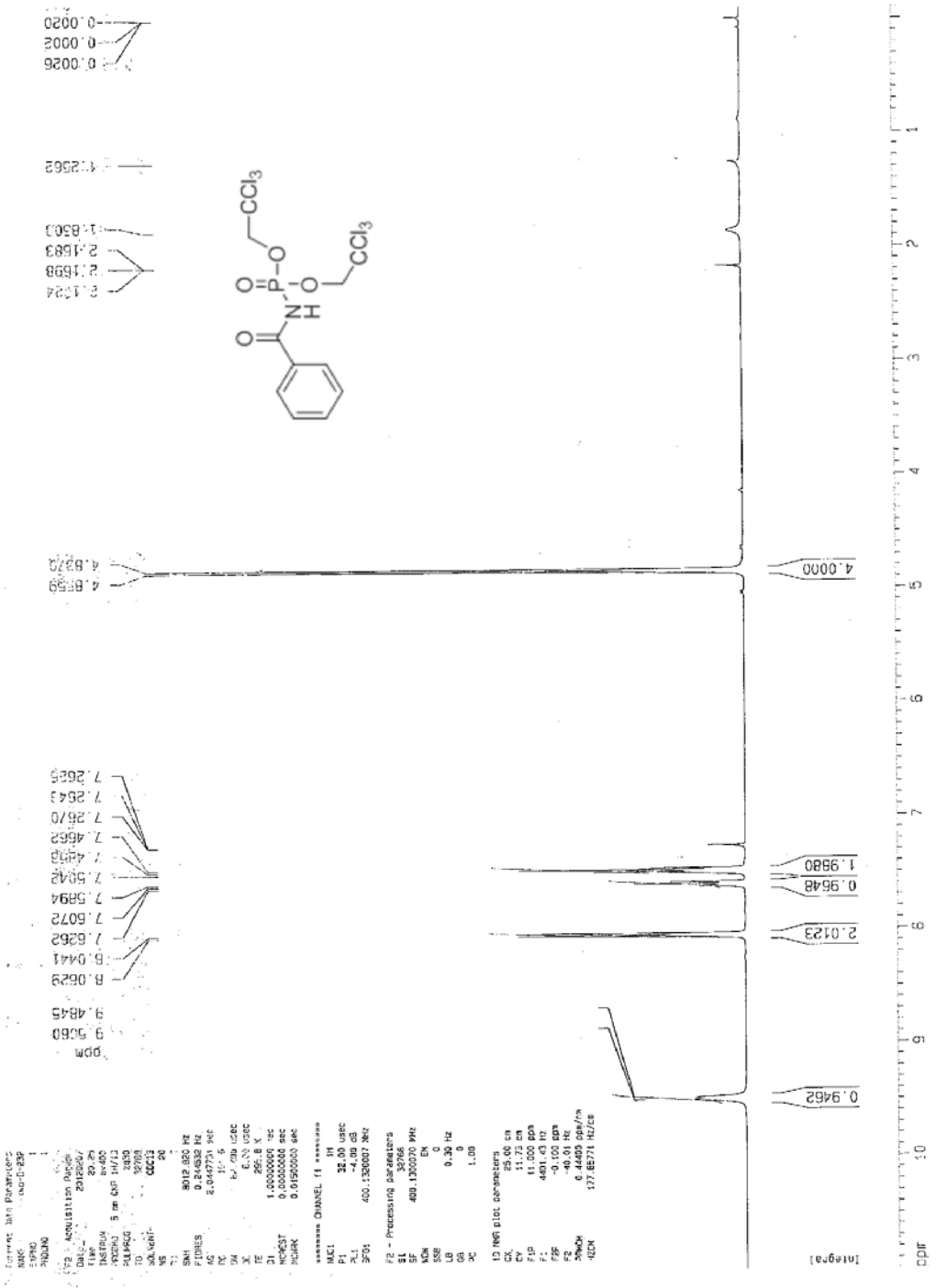

21.806
76.740
77.164
77.371
77.587
77.913
77.981
94.735
94.874
128.499
128.790
128.934
129.015
129.432
129.715
144.595
168.279
ppm
ppm

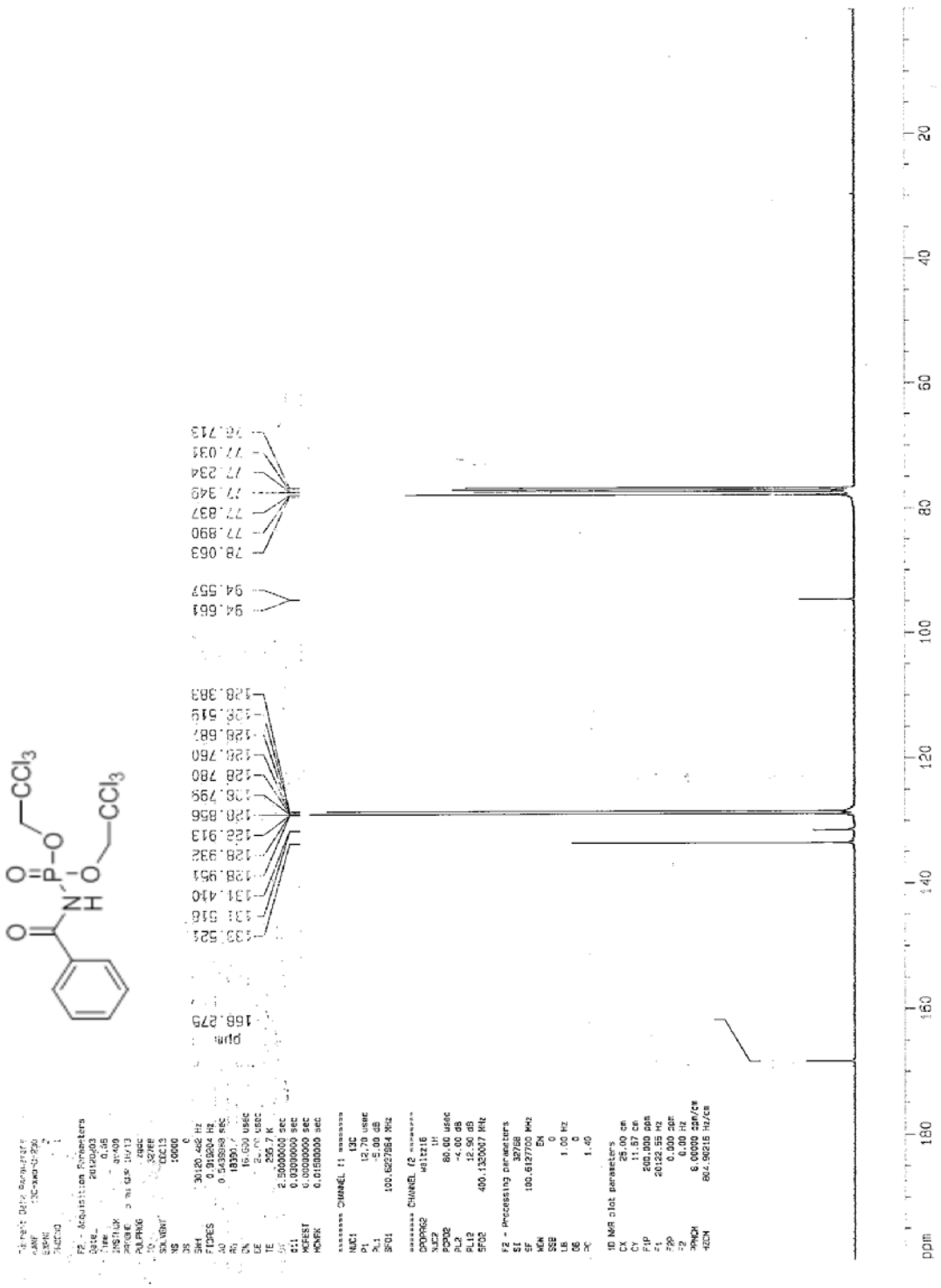
Bis(4-nitrophenyl) (4-methylbenzoyl)phosphoramidate 2s




21.790
77.481
77.163
76.846
115.844
121.398
121.443
125.928
126.332
128.339
129.836
145.312
145.627
154.278
161.769
ppm
20
40
60
80
100
120
140
160
180
ppm

Bis(2,2,2-trichloroethyl) benzoylphosphoramidate 2t




CCl3
CCl3
O
P
O
O
N
H
O
ppm
166.279
133.525
133.516
131.410
128.932
128.913
128.856
128.799
128.780
128.687
128.519
128.383
94.664
94.557
78.063
77.890
77.837
77.349
77.234
77.031
76.713
20
40
60
80
100
120
140
160
180
ppm