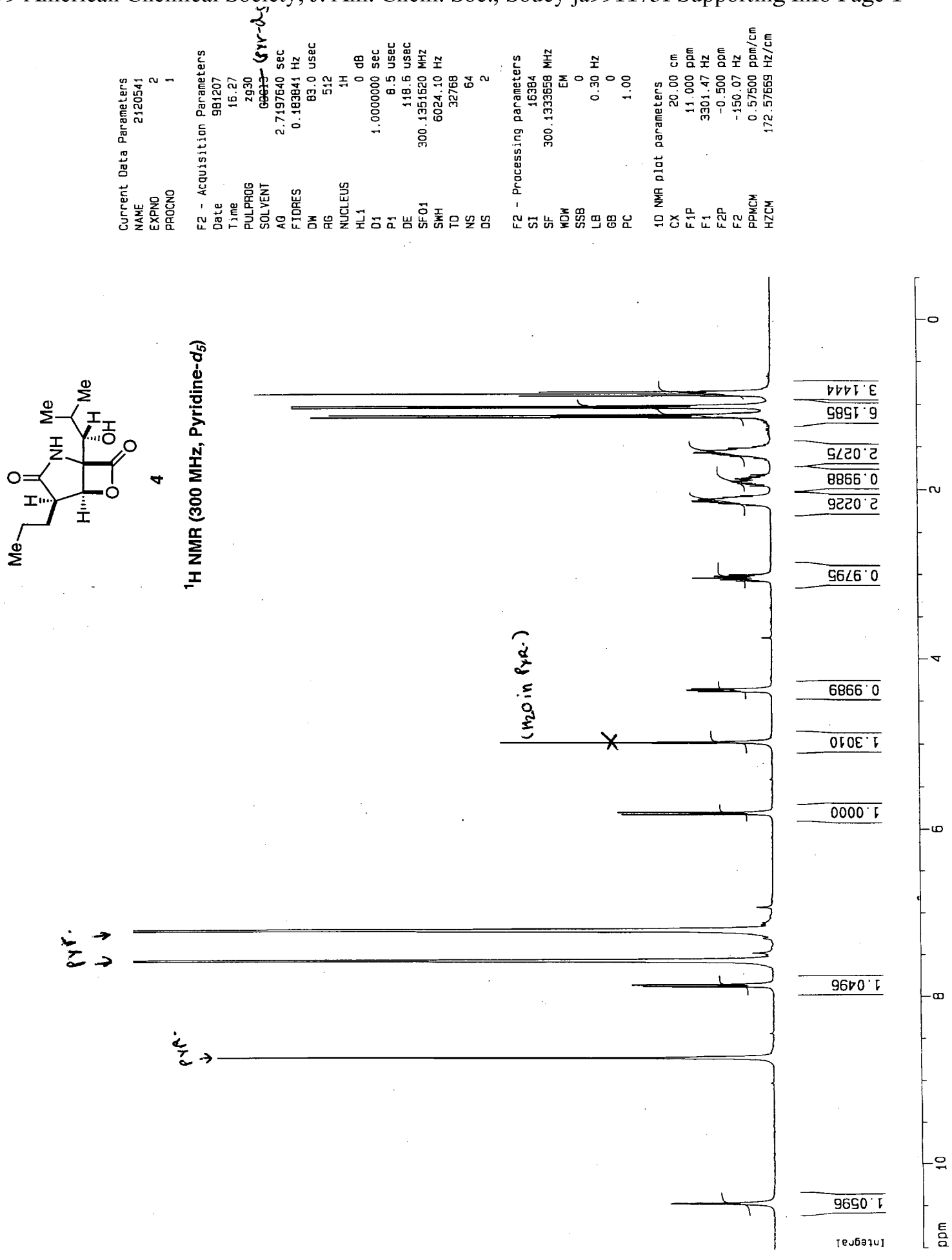

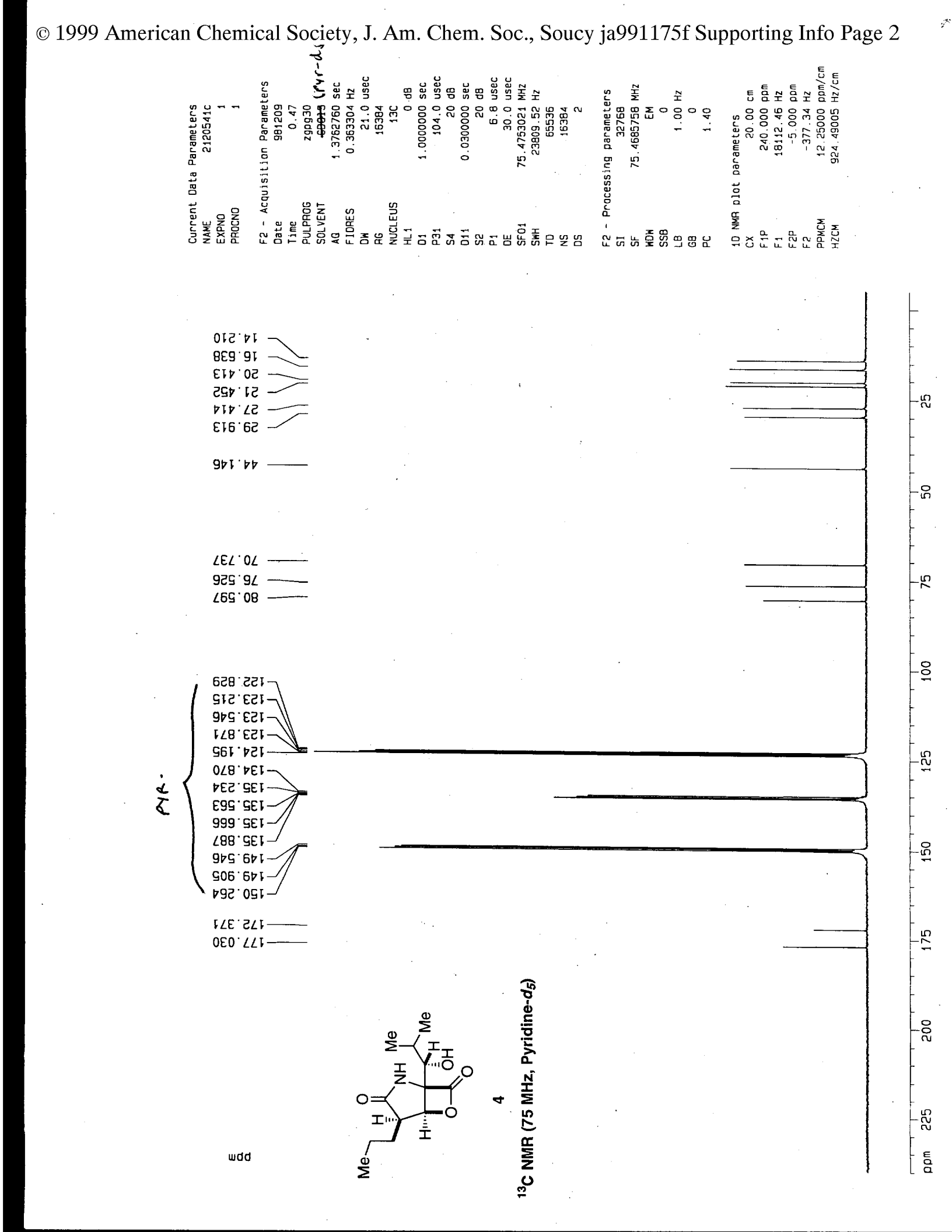

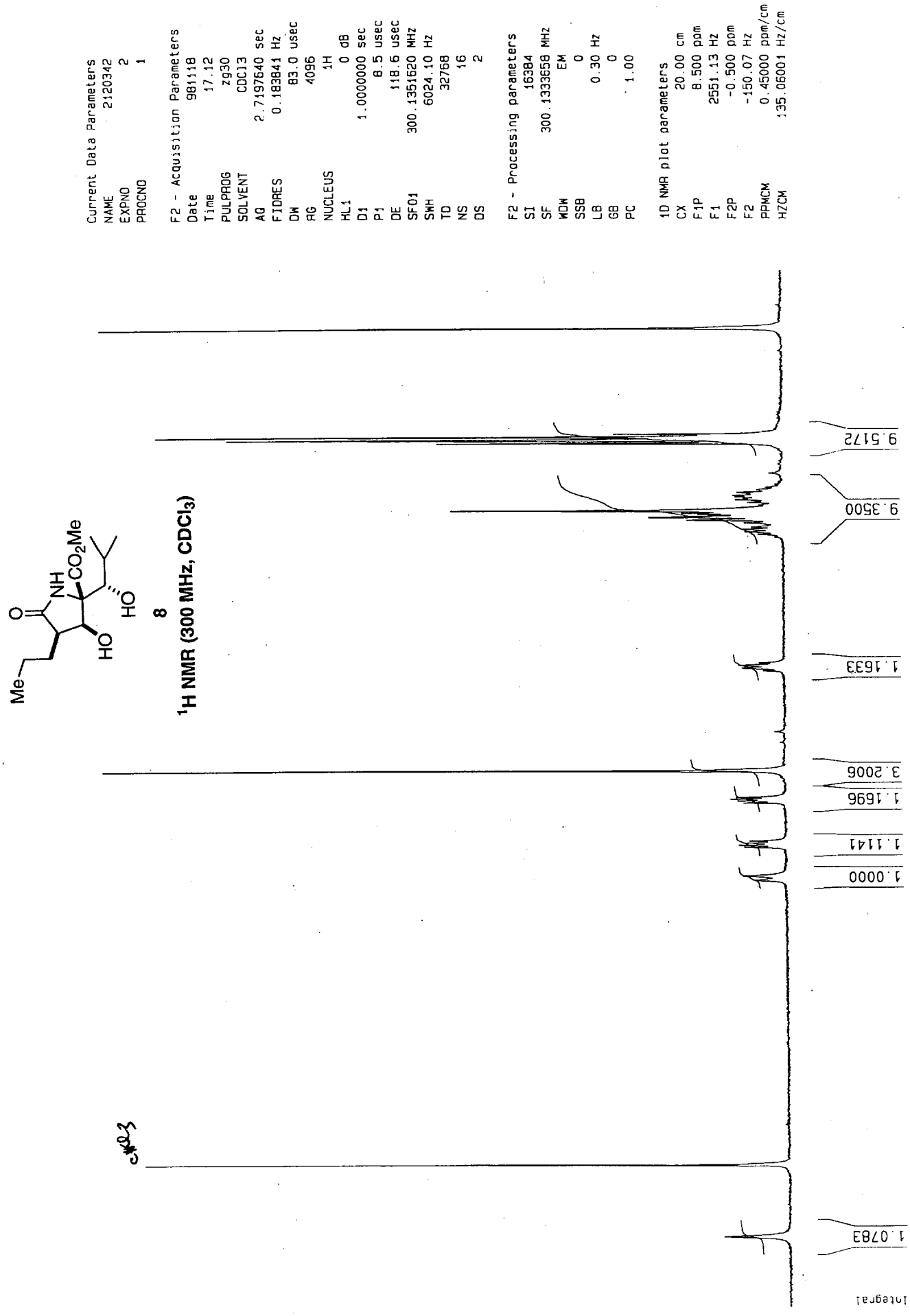

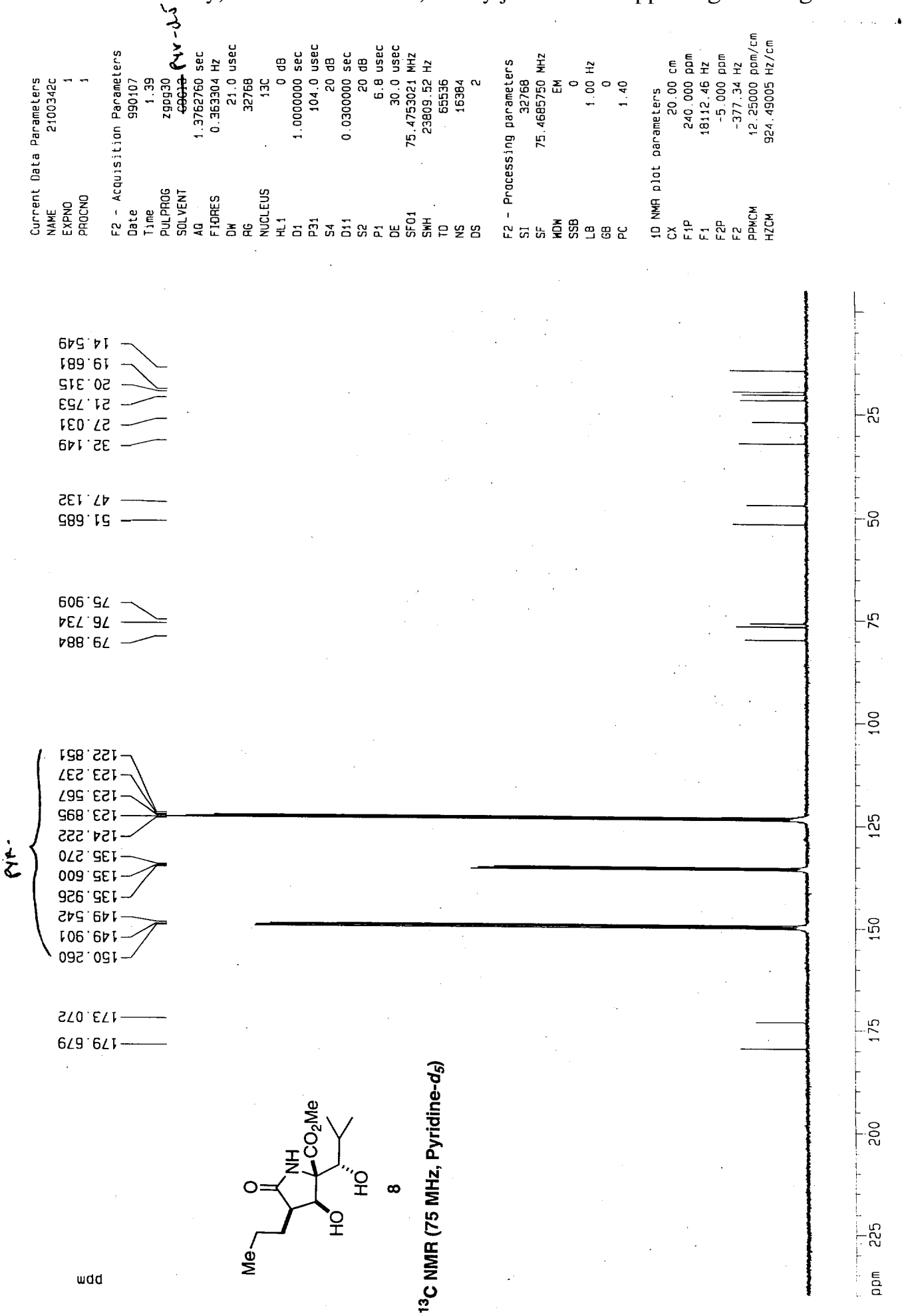

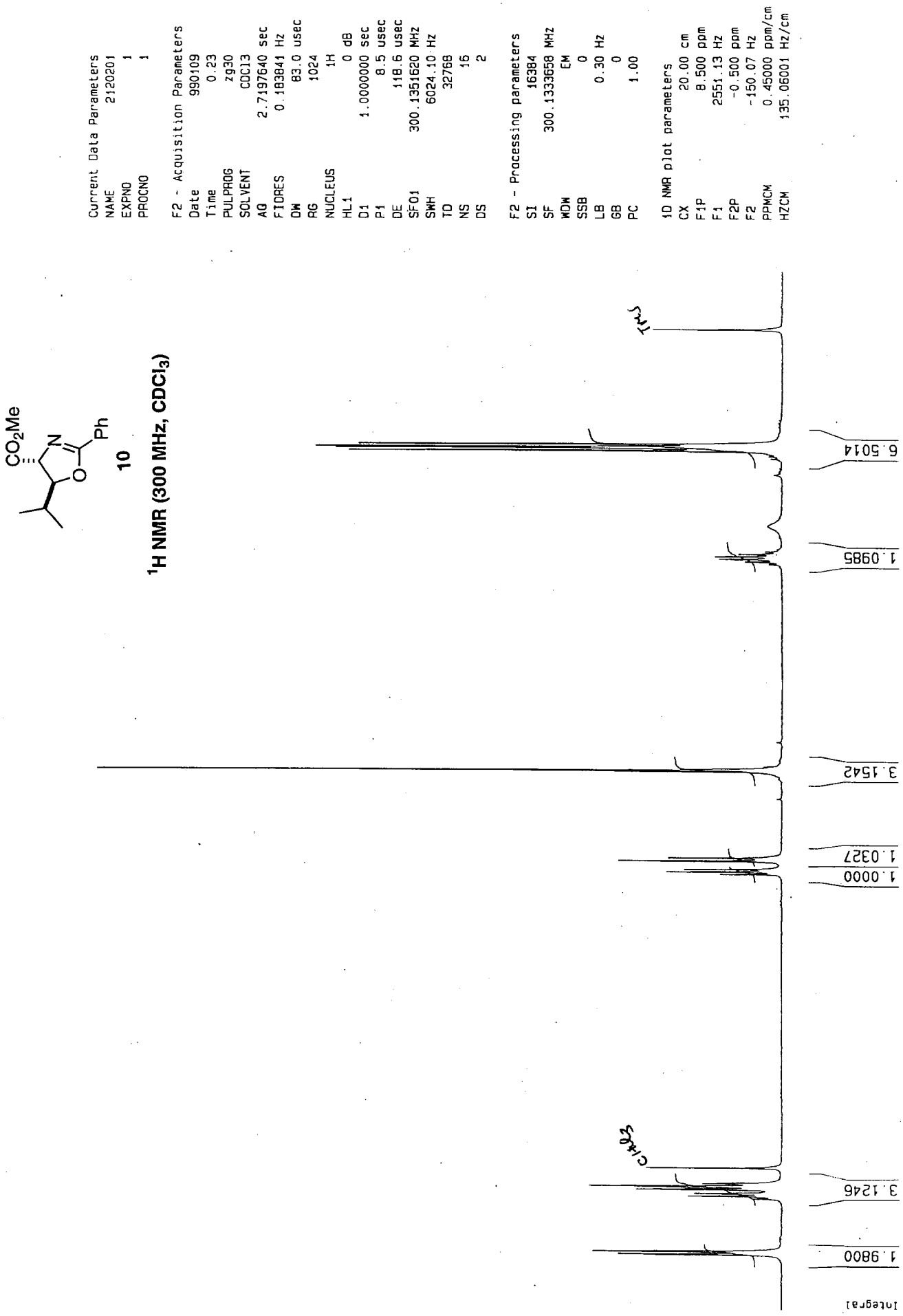

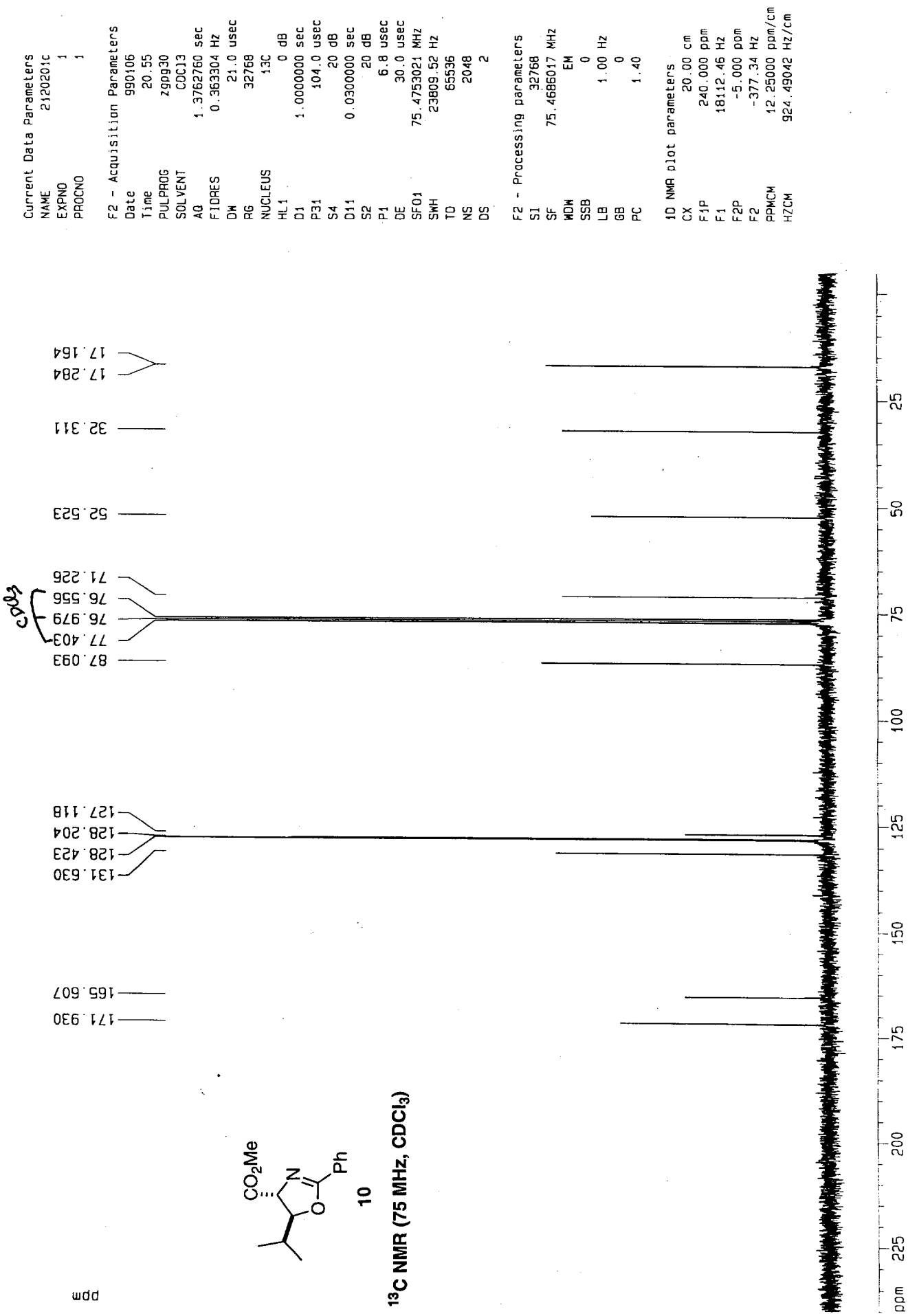

**X-Ray Crystallographic Analysis of 3*S*-Hydroxy-2*R*-(1*S*-hydroxy-2-methyl-propyl)-4*R*-*n*-propyl-5-oxo-pyrrolidine-2-carboxylic acid methyl ester (8):**

Data were collected using a Bruker SMART CCD (charge coupled device) based diffractometer equipped with an LT-2 low-temperature apparatus operating at 213 K. A suitable crystal was chosen and mounted on a glass fiber using grease. Data were measured using omega scans of 0.3 ° per frame for 45 seconds, such that a hemisphere was collected. A total of 1271 frames were collected with a maximum resolution of 0.75 Å. The first 50 frames were recollected at the end of data collection to monitor for decay. Cell parameters were retrieved using SMART[1] software and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software[2] which corrects for Lp and decay. Absorption corrections were applied using SADABS[6] supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97[3] program and refined by least squares method on $F^2$, SHELXL-97,[4] incorporated in SHELXTL-PC V 5.10.[5]

The structure was solved in the space group $P2_12_12_1$ (# 19) by analysis of systematic absences. All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. The crystal used for the diffraction study showed no decomposition during data collection. All drawing are done at 50% ellipsiods.

**References**


1. SMART V 5.050 (NT) *Software for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (1998).
2. SAINT V 5.01 (NT) *Software for the CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (1998).
3. Sheldrick, G. M. SHELXS-90, *Program for the Solution of Crystal Structure*, University of Göttingen, Germany, 1990.
4. Sheldrick, G. M. SHELXL-97, *Program for the Refinement of Crystal Structure*, University of Göttingen, Germany, 1997.
5. SHELXTL 5.10 (PC-Version), *Program library for Structure Solution and Molecular Graphics*; Bruker Analytical X-ray Systems, Madison, WI (1998).
6. SADABS. *Program for absorption corrections using Siemens CCD based on the method of Robert Blessing*; Blessing, R.H. Acta Cryst. A51 (1995) 33-38.

Table 1. Crystal data and structure refinement for psc1.

| | | |
|---|---|---|
| Identification code | psc1 | |
| Empirical formula | C13 H23 N O5 | |
| Formula weight | 273.32 | |
| Temperature | 213(2) K | |
| Wavelength | 0.71073 ≈ | |
| Crystal system | Orthorhombic | |
| Space group | P2(1)2(1)2(1) | |
| Unit cell dimensions | a = 10.536(2) ≈ | α= 90∞. |
| | b = 20.451(4) ≈ | β= 90∞. |
| | c = 27.557(6) ≈ | γ = 90∞. |
| Volume | 5938(2) ≈$^3$ | |
| Z | 16 | |
| Density (calculated) | 1.223 Mg/m$^3$ | |
| Absorption coefficient | 0.093 mm$^{-1}$ | |
| F(000) | 2368 | |
| Crystal size | 0.05 x 0.10 x 0.25 mm$^3$ | |
| Theta range for data collection | 1.48 to 22.50∞. | |
| Index ranges | -10<=h<=11, -22<=k<=18, -29<=l<=29 | |
| Reflections collected | 25661 | |
| Independent reflections | 7779 [R(int) = 0.0727] | |
| Completeness to theta = 22.50∞ | 100.0 % | |
| Absorption correction | None | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 7779 / 456 / 685 | |
| Goodness-of-fit on F$^2$ | 1.026 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0736, wR2 = 0.1714 | |
| R indices (all data) | R1 = 0.1156, wR2 = 0.1957 | |
| Absolute structure parameter | 1(2) | |
| Largest diff. peak and hole | 0.566 and -0.817 e.≈$^3$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for psc1. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| O(1A) | 13689(5) | 10040(2) | 10864(2) | 44(1) |
| O(2A) | 12523(4) | 8614(2) | 9856(2) | 43(1) |
| O(3A) | 11024(4) | 8510(2) | 11254(2) | 45(1) |
| O(4A) | 9658(4) | 8655(2) | 9913(2) | 43(1) |
| O(5A) | 10400(4) | 9663(2) | 9760(2) | 43(1) |
| N(1A) | 11744(5) | 9666(3) | 10622(2) | 43(1) |
| C(1A) | 11097(7) | 9071(3) | 10474(3) | 43(1) |
| C(2A) | 12248(7) | 8611(4) | 10361(3) | 43(1) |
| C(3A) | 13323(7) | 8874(3) | 10678(3) | 44(1) |
| C(4A) | 12974(7) | 9592(4) | 10727(3) | 43(1) |
| C(5A) | 10224(7) | 8782(4) | 10889(3) | 45(1) |
| C(6A) | 9274(7) | 9262(4) | 11112(3) | 47(1) |
| C(7A) | 8441(7) | 8892(4) | 11477(3) | 48(1) |
| C(8A) | 8439(7) | 9609(4) | 10760(3) | 49(1) |
| C(9A) | 10348(7) | 9173(4) | 10012(3) | 43(1) |
| C(10A) | 8983(7) | 8670(4) | 9453(2) | 44(1) |
| C(11A) | 14675(7) | 8772(3) | 10506(3) | 46(1) |
| C(12A) | 15032(7) | 8043(4) | 10492(3) | 49(1) |
| C(13A) | 16424(7) | 7934(4) | 10371(3) | 51(1) |
| O(1B) | 11415(4) | 9312(2) | 12051(2) | 41(1) |
| O(2B) | 14302(4) | 8860(2) | 13019(2) | 40(1) |
| O(3B) | 15285(4) | 9654(2) | 11624(2) | 41(1) |
| O(4B) | 15899(4) | 9997(2) | 13081(2) | 40(1) |
| O(5B) | 13982(4) | 10478(2) | 13127(2) | 40(1) |
| N(1B) | 13180(5) | 9878(3) | 12292(2) | 39(1) |
| C(1B) | 14492(6) | 9777(3) | 12444(2) | 40(1) |
| C(2B) | 14516(7) | 9017(3) | 12523(2) | 40(1) |
| C(3B) | 13465(7) | 8759(3) | 12193(3) | 42(1) |
| C(4B) | 12564(7) | 9333(4) | 12165(3) | 41(1) |
| C(5B) | 15494(7) | 9999(3) | 12056(2) | 41(1) |
| C(6B) | 15645(7) | 10744(4) | 11997(3) | 43(1) |

| | | | | |
|---|---|---|---|---|
| C(7B) | 14455(7) | 11112(3) | 11853(3) | 44(1) |
| C(8B) | 16698(7) | 10872(4) | 11631(3) | 44(1) |
| C(9B) | 14733(6) | 10121(4) | 12919(2) | 39(1) |
| C(10B) | 16150(7) | 10240(3) | 13562(2) | 41(1) |
| C(11B) | 12816(7) | 8110(3) | 12340(3) | 47(1) |
| C(12B) | 13699(8) | 7525(4) | 12343(3) | 51(1) |
| C(13B) | 14254(8) | 7355(4) | 11877(3) | 54(1) |
| O(1C) | 11861(4) | 9168(2) | 13355(2) | 41(1) |
| O(2C) | 9176(4) | 9932(2) | 12393(2) | 42(1) |
| O(3C) | 9245(4) | 10622(2) | 13838(2) | 44(1) |
| O(4C) | 9446(4) | 11387(2) | 12475(2) | 43(1) |
| O(5C) | 11363(4) | 10969(2) | 12326(2) | 43(1) |
| N(1C) | 11288(5) | 10211(3) | 13156(2) | 41(1) |
| C(1C) | 10184(7) | 10603(4) | 13031(3) | 42(1) |
| C(2C) | 9200(7) | 10056(3) | 12897(3) | 42(1) |
| C(3C) | 9643(7) | 9458(3) | 13195(3) | 42(1) |
| C(4C) | 11059(7) | 9581(4) | 13245(3) | 41(1) |
| C(5C) | 9742(7) | 11032(4) | 13460(3) | 44(1) |
| C(6C) | 10750(7) | 11495(4) | 13676(3) | 48(1) |
| C(7C) | 10133(7) | 11912(4) | 14075(3) | 49(1) |
| C(8C) | 11416(7) | 11934(4) | 13315(3) | 50(1) |
| C(9C) | 10418(7) | 10994(3) | 12574(3) | 42(1) |
| C(10C) | 9541(7) | 11766(4) | 12030(3) | 44(1) |
| C(11C) | 9304(6) | 8780(4) | 13002(3) | 45(1) |
| C(12C) | 7881(7) | 8649(4) | 13015(3) | 48(1) |
| C(13C) | 7480(7) | 7990(4) | 12845(3) | 49(1) |
| O(1D) | 11234(5) | 10249(2) | 14502(2) | 46(1) |
| O(2D) | 10729(5) | 8722(2) | 15516(2) | 49(1) |
| O(3D) | 11528(5) | 8214(2) | 14081(2) | 49(1) |
| O(4D) | 13038(5) | 7897(2) | 15405(2) | 52(1) |
| O(5D) | 13723(5) | 8927(2) | 15506(2) | 49(1) |
| N(1D) | 12427(6) | 9354(3) | 14696(2) | 47(1) |
| C(1D) | 12284(7) | 8668(4) | 14849(3) | 48(1) |
| C(2D) | 10851(7) | 8648(4) | 15009(3) | 49(1) |
| C(3D) | 10233(7) | 9206(4) | 14719(3) | 49(1) |
| C(4D) | 11314(7) | 9670(4) | 14626(3) | 47(1) |

| | | | | |
|---|---|---|---|---|
| C(5D) | 12537(7) | 8172(4) | 14425(3) | 50(1) |
| C(6D) | 13804(8) | 8247(4) | 14162(3) | 53(1) |
| C(7D) | 13966(8) | 7682(4) | 13809(3) | 54(1) |
| C(8D) | 14928(7) | 8309(4) | 14458(3) | 55(1) |
| C(9D) | 13109(8) | 8535(4) | 15287(3) | 49(1) |
| C(10D) | 13655(8) | 7709(4) | 15848(3) | 53(1) |
| C(11D) | 9050(7) | 9553(4) | 14913(3) | 52(1) |
| C(12D) | 7798(8) | 9180(4) | 14846(3) | 56(1) |
| C(13D) | 7620(8) | 8668(4) | 15197(3) | 58(1) |

Table 3. Bond lengths [≈] and angles [∞] for psc1.

| | |
|---|---|
| O(1A)-C(4A) | 1.244(8) |
| O(2A)-C(2A) | 1.422(8) |
| O(3A)-C(5A) | 1.424(8) |
| O(4A)-C(9A) | 1.315(8) |
| O(4A)-C(10A) | 1.452(8) |
| O(5A)-C(9A) | 1.221(8) |
| N(1A)-C(4A) | 1.337(9) |
| N(1A)-C(1A) | 1.454(9) |
| C(1A)-C(9A) | 1.512(10) |
| C(1A)-C(2A) | 1.566(10) |
| C(1A)-C(5A) | 1.583(10) |
| C(2A)-C(3A) | 1.529(10) |
| C(3A)-C(11A) | 1.516(10) |
| C(3A)-C(4A) | 1.519(10) |
| C(5A)-C(6A) | 1.531(10) |
| C(6A)-C(8A) | 1.489(10) |
| C(6A)-C(7A) | 1.534(10) |
| C(11A)-C(12A) | 1.538(10) |
| C(12A)-C(13A) | 1.520(10) |
| O(1B)-C(4B) | 1.252(8) |
| O(2B)-C(2B) | 1.421(8) |
| O(3B)-C(5B) | 1.400(8) |
| O(4B)-C(9B) | 1.331(8) |
| O(4B)-C(10B) | 1.438(8) |
| O(5B)-C(9B) | 1.220(8) |
| N(1B)-C(4B) | 1.336(9) |
| N(1B)-C(1B) | 1.459(9) |
| C(1B)-C(9B) | 1.507(10) |
| C(1B)-C(5B) | 1.569(10) |
| C(1B)-C(2B) | 1.571(10) |
| C(2B)-C(3B) | 1.527(10) |
| C(3B)-C(4B) | 1.511(10) |
| C(3B)-C(11B) | 1.548(10) |
| C(5B)-C(6B) | 1.540(10) |

| | |
|---|---|
| C(6B)-C(7B) | 1.516(10) |
| C(6B)-C(8B) | 1.523(10) |
| C(11B)-C(12B) | 1.516(10) |
| C(12B)-C(13B) | 1.453(10) |
| O(1C)-C(4C) | 1.234(8) |
| O(2C)-C(2C) | 1.413(8) |
| O(3C)-C(5C) | 1.436(8) |
| O(4C)-C(9C) | 1.330(8) |
| O(4C)-C(10C) | 1.453(8) |
| O(5C)-C(9C) | 1.209(8) |
| N(1C)-C(4C) | 1.335(9) |
| N(1C)-C(1C) | 1.453(9) |
| C(1C)-C(9C) | 1.511(10) |
| C(1C)-C(5C) | 1.543(10) |
| C(1C)-C(2C) | 1.570(10) |
| C(2C)-C(3C) | 1.546(9) |
| C(3C)-C(4C) | 1.519(10) |
| C(3C)-C(11C) | 1.528(10) |
| C(5C)-C(6C) | 1.543(10) |
| C(6C)-C(8C) | 1.512(10) |
| C(6C)-C(7C) | 1.536(10) |
| C(11C)-C(12C) | 1.523(9) |
| C(12C)-C(13C) | 1.488(10) |
| O(1D)-C(4D) | 1.235(8) |
| O(2D)-C(2D) | 1.411(9) |
| O(3D)-C(5D) | 1.429(9) |
| O(4D)-C(9D) | 1.346(9) |
| O(4D)-C(10D) | 1.436(8) |
| O(5D)-C(9D) | 1.195(8) |
| N(1D)-C(4D) | 1.353(9) |
| N(1D)-C(1D) | 1.473(9) |
| C(1D)-C(9D) | 1.512(11) |
| C(1D)-C(5D) | 1.569(10) |
| C(1D)-C(2D) | 1.574(11) |
| C(2D)-C(3D) | 1.537(10) |
| C(3D)-C(4D) | 1.505(10) |

| | |
|---|---|
| C(3D)-C(11D) | 1.531(10) |
| C(5D)-C(6D) | 1.528(11) |
| C(6D)-C(8D) | 1.443(11) |
| C(6D)-C(7D) | 1.521(10) |
| C(11D)-C(12D) | 1.535(11) |
| C(12D)-C(13D) | 1.439(10) |

| | |
|---|---|
| C(9A)-O(4A)-C(10A) | 115.8(5) |
| C(4A)-N(1A)-C(1A) | 114.9(6) |
| N(1A)-C(1A)-C(9A) | 111.4(6) |
| N(1A)-C(1A)-C(2A) | 101.3(6) |
| C(9A)-C(1A)-C(2A) | 108.7(6) |
| N(1A)-C(1A)-C(5A) | 112.5(6) |
| C(9A)-C(1A)-C(5A) | 110.9(6) |
| C(2A)-C(1A)-C(5A) | 111.6(6) |
| O(2A)-C(2A)-C(3A) | 114.0(6) |
| O(2A)-C(2A)-C(1A) | 110.4(6) |
| C(3A)-C(2A)-C(1A) | 104.4(5) |
| C(11A)-C(3A)-C(4A) | 112.9(6) |
| C(11A)-C(3A)-C(2A) | 117.9(6) |
| C(4A)-C(3A)-C(2A) | 102.2(6) |
| O(1A)-C(4A)-N(1A) | 124.7(7) |
| O(1A)-C(4A)-C(3A) | 126.3(7) |
| N(1A)-C(4A)-C(3A) | 109.0(6) |
| O(3A)-C(5A)-C(6A) | 110.8(6) |
| O(3A)-C(5A)-C(1A) | 108.2(6) |
| C(6A)-C(5A)-C(1A) | 115.5(6) |
| C(8A)-C(6A)-C(5A) | 115.5(6) |
| C(8A)-C(6A)-C(7A) | 108.8(6) |
| C(5A)-C(6A)-C(7A) | 108.7(6) |
| O(5A)-C(9A)-O(4A) | 124.6(6) |
| O(5A)-C(9A)-C(1A) | 124.7(7) |
| O(4A)-C(9A)-C(1A) | 110.6(6) |
| C(3A)-C(11A)-C(12A) | 111.8(6) |
| C(13A)-C(12A)-C(11A) | 112.5(7) |
| C(9B)-O(4B)-C(10B) | 114.4(5) |

| | |
|---|---|
| C(4B)-N(1B)-C(1B) | 114.6(6) |
| N(1B)-C(1B)-C(9B) | 110.1(5) |
| N(1B)-C(1B)-C(5B) | 113.6(5) |
| C(9B)-C(1B)-C(5B) | 110.1(6) |
| N(1B)-C(1B)-C(2B) | 101.3(6) |
| C(9B)-C(1B)-C(2B) | 109.8(6) |
| C(5B)-C(1B)-C(2B) | 111.7(5) |
| O(2B)-C(2B)-C(3B) | 112.4(6) |
| O(2B)-C(2B)-C(1B) | 110.7(5) |
| C(3B)-C(2B)-C(1B) | 104.3(5) |
| C(4B)-C(3B)-C(2B) | 102.6(5) |
| C(4B)-C(3B)-C(11B) | 113.7(6) |
| C(2B)-C(3B)-C(11B) | 117.4(6) |
| O(1B)-C(4B)-N(1B) | 124.4(7) |
| O(1B)-C(4B)-C(3B) | 126.4(7) |
| N(1B)-C(4B)-C(3B) | 109.3(6) |
| O(3B)-C(5B)-C(6B) | 115.1(6) |
| O(3B)-C(5B)-C(1B) | 109.1(5) |
| C(6B)-C(5B)-C(1B) | 115.3(6) |
| C(7B)-C(6B)-C(8B) | 110.1(6) |
| C(7B)-C(6B)-C(5B) | 115.7(6) |
| C(8B)-C(6B)-C(5B) | 108.4(6) |
| O(5B)-C(9B)-O(4B) | 123.6(6) |
| O(5B)-C(9B)-C(1B) | 125.3(6) |
| O(4B)-C(9B)-C(1B) | 111.1(6) |
| C(12B)-C(11B)-C(3B) | 114.1(6) |
| C(13B)-C(12B)-C(11B) | 115.5(7) |
| C(9C)-O(4C)-C(10C) | 116.3(5) |
| C(4C)-N(1C)-C(1C) | 115.6(6) |
| N(1C)-C(1C)-C(9C) | 110.9(6) |
| N(1C)-C(1C)-C(5C) | 112.0(6) |
| C(9C)-C(1C)-C(5C) | 112.7(6) |
| N(1C)-C(1C)-C(2C) | 101.0(5) |
| C(9C)-C(1C)-C(2C) | 106.8(6) |
| C(5C)-C(1C)-C(2C) | 112.7(6) |
| O(2C)-C(2C)-C(3C) | 112.8(6) |

| | |
|---|---|
| O(2C)-C(2C)-C(1C) | 111.8(6) |
| C(3C)-C(2C)-C(1C) | 103.9(5) |
| C(4C)-C(3C)-C(11C) | 114.3(6) |
| C(4C)-C(3C)-C(2C) | 102.3(6) |
| C(11C)-C(3C)-C(2C) | 117.5(6) |
| O(1C)-C(4C)-N(1C) | 125.7(7) |
| O(1C)-C(4C)-C(3C) | 125.6(6) |
| N(1C)-C(4C)-C(3C) | 108.7(6) |
| O(3C)-C(5C)-C(1C) | 109.5(6) |
| O(3C)-C(5C)-C(6C) | 109.2(6) |
| C(1C)-C(5C)-C(6C) | 115.8(6) |
| C(8C)-C(6C)-C(7C) | 109.8(6) |
| C(8C)-C(6C)-C(5C) | 115.5(6) |
| C(7C)-C(6C)-C(5C) | 109.0(6) |
| O(5C)-C(9C)-O(4C) | 122.9(6) |
| O(5C)-C(9C)-C(1C) | 125.7(6) |
| O(4C)-C(9C)-C(1C) | 111.4(6) |
| C(12C)-C(11C)-C(3C) | 112.4(6) |
| C(13C)-C(12C)-C(11C) | 115.5(6) |
| C(9D)-O(4D)-C(10D) | 116.0(6) |
| C(4D)-N(1D)-C(1D) | 114.0(6) |
| N(1D)-C(1D)-C(9D) | 110.0(6) |
| N(1D)-C(1D)-C(5D) | 112.6(6) |
| C(9D)-C(1D)-C(5D) | 112.3(6) |
| N(1D)-C(1D)-C(2D) | 101.7(6) |
| C(9D)-C(1D)-C(2D) | 108.9(6) |
| C(5D)-C(1D)-C(2D) | 110.8(6) |
| O(2D)-C(2D)-C(3D) | 113.4(6) |
| O(2D)-C(2D)-C(1D) | 111.3(6) |
| C(3D)-C(2D)-C(1D) | 104.0(6) |
| C(4D)-C(3D)-C(11D) | 112.5(6) |
| C(4D)-C(3D)-C(2D) | 103.6(6) |
| C(11D)-C(3D)-C(2D) | 120.5(6) |
| O(1D)-C(4D)-N(1D) | 123.8(7) |
| O(1D)-C(4D)-C(3D) | 126.9(7) |
| N(1D)-C(4D)-C(3D) | 109.3(6) |

| | |
|---|---|
| O(3D)-C(5D)-C(6D) | 109.2(6) |
| O(3D)-C(5D)-C(1D) | 109.2(6) |
| C(6D)-C(5D)-C(1D) | 115.9(7) |
| C(8D)-C(6D)-C(7D) | 109.6(7) |
| C(8D)-C(6D)-C(5D) | 117.2(7) |
| C(7D)-C(6D)-C(5D) | 109.0(7) |
| O(5D)-C(9D)-O(4D) | 124.0(7) |
| O(5D)-C(9D)-C(1D) | 126.4(7) |
| O(4D)-C(9D)-C(1D) | 109.6(7) |
| C(3D)-C(11D)-C(12D) | 115.3(6) |
| C(13D)-C(12D)-C(11D) | 113.1(7) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x $10^3$) for psc1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| O(1A) | 52(2) | 37(1) | 42(1) | -1(1) | -11(1) | 1(1) |
| O(2A) | 53(1) | 36(1) | 39(1) | -1(1) | -6(1) | 1(1) |
| O(3A) | 54(2) | 41(1) | 40(1) | 0(1) | -8(1) | 5(1) |
| O(4A) | 54(1) | 38(1) | 38(1) | 2(1) | -10(1) | -1(1) |
| O(5A) | 52(2) | 37(1) | 39(1) | 3(1) | -8(1) | 0(1) |
| N(1A) | 52(1) | 36(1) | 39(1) | -1(1) | -9(1) | 2(1) |
| C(1A) | 52(1) | 37(1) | 39(1) | 0(1) | -8(1) | 2(1) |
| C(2A) | 53(1) | 36(1) | 39(1) | -1(1) | -7(1) | 2(1) |
| C(3A) | 53(1) | 37(1) | 41(1) | -1(1) | -8(1) | 3(1) |
| C(4A) | 52(1) | 36(1) | 41(1) | -1(1) | -9(1) | 2(1) |
| C(5A) | 54(1) | 40(1) | 40(1) | 0(1) | -7(1) | 4(1) |
| C(6A) | 55(2) | 43(1) | 43(1) | -1(1) | -5(1) | 5(1) |
| C(7A) | 55(2) | 44(2) | 45(2) | -1(2) | -5(2) | 5(2) |
| C(8A) | 56(2) | 46(2) | 45(2) | -1(2) | -4(2) | 5(2) |
| C(9A) | 53(1) | 37(1) | 38(1) | 1(1) | -9(1) | 1(1) |
| C(10A) | 55(2) | 39(2) | 38(2) | 1(2) | -11(2) | -1(2) |
| C(11A) | 55(2) | 39(1) | 44(1) | -2(1) | -8(1) | 4(1) |
| C(12A) | 58(2) | 42(2) | 47(2) | -3(2) | -8(2) | 5(2) |
| C(13A) | 59(2) | 44(2) | 49(2) | -4(2) | -8(2) | 6(2) |
| O(1B) | 37(1) | 42(1) | 45(1) | -6(1) | -6(1) | 4(1) |
| O(2B) | 38(1) | 41(1) | 41(1) | -2(1) | -3(1) | 5(1) |
| O(3B) | 40(1) | 43(1) | 39(1) | -5(1) | -1(1) | 7(1) |
| O(4B) | 35(1) | 46(1) | 39(1) | -9(1) | -4(1) | 4(1) |
| O(5B) | 34(1) | 44(1) | 41(1) | -9(1) | -1(1) | 4(1) |
| N(1B) | 36(1) | 40(1) | 41(1) | -5(1) | -4(1) | 5(1) |
| C(1B) | 37(1) | 42(1) | 40(1) | -5(1) | -3(1) | 5(1) |
| C(2B) | 38(1) | 41(1) | 42(1) | -4(1) | -3(1) | 5(1) |
| C(3B) | 40(1) | 42(1) | 45(1) | -5(1) | -4(1) | 5(1) |
| C(4B) | 37(1) | 41(1) | 43(1) | -5(1) | -5(1) | 4(1) |
| C(5B) | 39(1) | 43(1) | 41(1) | -5(1) | -1(1) | 5(1) |
| C(6B) | 42(1) | 44(1) | 43(1) | -3(1) | 2(1) | 4(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(7B) | 43(2) | 45(2) | 45(2) | -3(2) | 2(2) | 3(2) |
| C(8B) | 43(2) | 45(2) | 45(2) | -3(2) | 2(2) | 3(2) |
| C(9B) | 35(1) | 43(1) | 40(1) | -7(1) | -2(1) | 4(1) |
| C(10B) | 36(2) | 48(2) | 39(2) | -9(2) | -4(2) | 4(2) |
| C(11B) | 46(1) | 45(1) | 49(1) | -4(1) | -4(1) | 5(1) |
| C(12B) | 51(2) | 49(2) | 54(2) | -4(2) | -2(2) | 6(2) |
| C(13B) | 54(2) | 51(2) | 57(2) | -3(2) | -2(2) | 7(2) |
| O(1C) | 36(1) | 40(1) | 47(2) | 5(1) | -1(1) | 5(1) |
| O(2C) | 38(1) | 41(1) | 46(1) | 3(1) | -2(1) | 3(1) |
| O(3C) | 40(1) | 45(2) | 47(2) | 3(1) | 1(1) | 1(1) |
| O(4C) | 37(1) | 43(1) | 49(1) | 9(1) | -1(1) | 4(1) |
| O(5C) | 37(1) | 42(1) | 48(2) | 5(1) | 1(1) | 4(1) |
| N(1C) | 36(1) | 41(1) | 47(1) | 4(1) | -1(1) | 3(1) |
| C(1C) | 37(1) | 42(1) | 47(1) | 4(1) | -1(1) | 3(1) |
| C(2C) | 37(1) | 41(1) | 47(1) | 4(1) | -2(1) | 3(1) |
| C(3C) | 37(1) | 41(1) | 49(1) | 5(1) | -2(1) | 3(1) |
| C(4C) | 36(1) | 40(1) | 47(1) | 5(1) | -2(1) | 4(1) |
| C(5C) | 41(1) | 44(1) | 48(1) | 3(1) | 1(1) | 2(1) |
| C(6C) | 46(1) | 47(2) | 51(2) | 1(1) | 0(1) | 1(1) |
| C(7C) | 48(2) | 47(2) | 52(2) | 0(2) | 0(2) | 2(2) |
| C(8C) | 48(2) | 48(2) | 53(2) | 0(2) | 1(2) | 0(2) |
| C(9C) | 37(1) | 42(1) | 48(1) | 6(1) | -1(1) | 4(1) |
| C(10C) | 39(2) | 44(2) | 50(2) | 10(2) | -1(2) | 4(2) |
| C(11C) | 40(1) | 43(1) | 53(1) | 4(1) | -3(1) | 2(1) |
| C(12C) | 42(2) | 44(2) | 56(2) | 4(2) | -4(2) | 0(2) |
| C(13C) | 43(2) | 46(2) | 58(2) | 4(2) | -5(2) | 0(2) |
| O(1D) | 56(2) | 36(1) | 46(2) | 2(1) | -1(1) | -1(1) |
| O(2D) | 62(2) | 40(1) | 45(1) | 1(1) | 2(1) | -3(1) |
| O(3D) | 62(2) | 40(1) | 45(2) | 0(1) | -1(1) | 1(1) |
| O(4D) | 71(2) | 38(1) | 46(2) | 2(1) | -6(1) | 3(1) |
| O(5D) | 66(2) | 37(1) | 45(2) | 0(1) | -6(1) | 2(1) |
| N(1D) | 59(1) | 36(1) | 45(1) | 1(1) | -1(1) | -1(1) |
| C(1D) | 62(1) | 38(1) | 45(1) | 1(1) | -2(1) | 0(1) |
| C(2D) | 61(1) | 39(1) | 46(1) | 1(1) | 0(1) | -2(1) |
| C(3D) | 60(1) | 40(1) | 47(1) | 0(1) | 0(1) | -2(1) |
| C(4D) | 58(1) | 37(1) | 46(1) | 1(1) | -1(1) | -1(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(5D) | 63(1) | 40(1) | 47(1) | 0(1) | -1(1) | 0(1) |
| C(6D) | 65(2) | 44(1) | 50(2) | -2(1) | 0(1) | 1(1) |
| C(7D) | 66(2) | 44(2) | 51(2) | -2(2) | 1(2) | 1(2) |
| C(8D) | 67(2) | 46(2) | 52(2) | -2(2) | 0(2) | 1(2) |
| C(9D) | 66(1) | 37(1) | 45(1) | 1(1) | -5(1) | 1(1) |
| C(10D) | 73(2) | 39(2) | 48(2) | 3(2) | -7(2) | 3(2) |
| C(11D) | 62(2) | 44(1) | 52(2) | 0(1) | 0(1) | -3(1) |
| C(12D) | 64(2) | 47(2) | 56(2) | -1(2) | -1(2) | -4(2) |
| C(13D) | 66(2) | 49(2) | 58(2) | 0(2) | -3(2) | -4(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($\approx^2$x $10^3$) for psc1.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2AA) | 12888 | 8961 | 9784 | 64 |
| H(3AA) | 11091 | 8771 | 11482 | 67 |
| H(1AA) | 11360 | 10042 | 10641 | 51 |
| H(2AB) | 12038 | 8159 | 10464 | 51 |
| H(3AB) | 13243 | 8671 | 11003 | 52 |
| H(5AA) | 9730 | 8418 | 10746 | 54 |
| H(6AA) | 9761 | 9597 | 11294 | 56 |
| H(7AA) | 7854 | 9195 | 11629 | 72 |
| H(7AB) | 8973 | 8694 | 11723 | 72 |
| H(7AC) | 7967 | 8554 | 11309 | 72 |
| H(8AA) | 7895 | 9912 | 10933 | 73 |
| H(8AB) | 7920 | 9292 | 10589 | 73 |
| H(8AC) | 8957 | 9847 | 10529 | 73 |
| H(10A) | 8505 | 8268 | 9414 | 66 |
| H(10B) | 9588 | 8713 | 9190 | 66 |
| H(10C) | 8406 | 9039 | 9450 | 66 |
| H(11A) | 15258 | 9003 | 10723 | 55 |
| H(11B) | 14770 | 8958 | 10180 | 55 |
| H(12A) | 14848 | 7847 | 10809 | 59 |
| H(12B) | 14506 | 7821 | 10250 | 59 |
| H(13A) | 16602 | 7469 | 10366 | 76 |
| H(13B) | 16949 | 8144 | 10615 | 76 |
| H(13C) | 16608 | 8121 | 10055 | 76 |
| H(2BA) | 13565 | 8961 | 13094 | 60 |
| H(3BA) | 14776 | 9859 | 11452 | 61 |
| H(1BA) | 12827 | 10263 | 12284 | 47 |
| H(2BB) | 15345 | 8838 | 12418 | 48 |
| H(3BB) | 13834 | 8697 | 11866 | 51 |
| H(5BA) | 16322 | 9842 | 12179 | 49 |
| H(6BA) | 15931 | 10920 | 12313 | 52 |

| | | | | |
|---|---|---|---|---|
| H(7BA) | 14652 | 11573 | 11817 | 66 |
| H(7BB) | 13814 | 11058 | 12102 | 66 |
| H(7BC) | 14138 | 10942 | 11548 | 66 |
| H(8BA) | 16800 | 11340 | 11587 | 67 |
| H(8BB) | 16478 | 10672 | 11323 | 67 |
| H(8BC) | 17487 | 10686 | 11749 | 67 |
| H(10D) | 17013 | 10132 | 13653 | 61 |
| H(10E) | 15563 | 10041 | 13789 | 61 |
| H(10F) | 16041 | 10711 | 13566 | 61 |
| H(11C) | 12449 | 8161 | 12664 | 56 |
| H(11D) | 12118 | 8022 | 12114 | 56 |
| H(12C) | 14389 | 7612 | 12573 | 61 |
| H(12D) | 13228 | 7145 | 12465 | 61 |
| H(13D) | 14808 | 6979 | 11916 | 81 |
| H(13E) | 14740 | 7722 | 11755 | 81 |
| H(13F) | 13583 | 7249 | 11649 | 81 |
| H(2CA) | 9845 | 9748 | 12311 | 62 |
| H(3CA) | 9827 | 10518 | 14026 | 66 |
| H(1CA) | 12048 | 10377 | 13171 | 49 |
| H(2CB) | 8344 | 10190 | 13006 | 50 |
| H(3CB) | 9265 | 9498 | 13523 | 51 |
| H(5CA) | 9033 | 11307 | 13341 | 53 |
| H(6CA) | 11407 | 11220 | 13832 | 57 |
| H(7CA) | 10766 | 12198 | 14218 | 73 |
| H(7CB) | 9786 | 11628 | 14324 | 73 |
| H(7CC) | 9457 | 12174 | 13936 | 73 |
| H(8CA) | 12055 | 12191 | 13481 | 75 |
| H(8CB) | 10802 | 12224 | 13165 | 75 |
| H(8CC) | 11817 | 11668 | 13067 | 75 |
| H(10G) | 8783 | 12030 | 11991 | 66 |
| H(10H) | 9625 | 11472 | 11756 | 66 |
| H(10I) | 10279 | 12048 | 12047 | 66 |
| H(11E) | 9606 | 8740 | 12667 | 54 |
| H(11F) | 9740 | 8448 | 13197 | 54 |
| H(12E) | 7583 | 8708 | 13349 | 57 |
| H(12F) | 7456 | 8978 | 12814 | 57 |

| | | | | |
|---|---|---|---|---|
| H(13G) | 6564 | 7953 | 12867 | 74 |
| H(13H) | 7873 | 7658 | 13046 | 74 |
| H(13I) | 7741 | 7930 | 12510 | 74 |
| H(2DA) | 10917 | 9102 | 15594 | 73 |
| H(3DA) | 11695 | 8500 | 13877 | 74 |
| H(1DA) | 13162 | 9539 | 14653 | 56 |
| H(2DB) | 10472 | 8226 | 14910 | 58 |
| H(3DB) | 9996 | 9020 | 14400 | 59 |
| H(5DA) | 12515 | 7727 | 14566 | 60 |
| H(6DA) | 13745 | 8650 | 13965 | 63 |
| H(7DA) | 14765 | 7729 | 13637 | 80 |
| H(7DB) | 13272 | 7683 | 13578 | 80 |
| H(7DC) | 13965 | 7272 | 13986 | 80 |
| H(8DA) | 14827 | 8673 | 14680 | 82 |
| H(8DB) | 15658 | 8385 | 14251 | 82 |
| H(8DC) | 15054 | 7909 | 14641 | 82 |
| H(10J) | 13525 | 7245 | 15904 | 80 |
| H(10K) | 13300 | 7956 | 16116 | 80 |
| H(10L) | 14557 | 7798 | 15823 | 80 |
| H(11G) | 8976 | 9978 | 14751 | 63 |
| H(11H) | 9170 | 9637 | 15260 | 63 |
| H(12G) | 7090 | 9490 | 14870 | 67 |
| H(12H) | 7780 | 8990 | 14520 | 67 |
| H(13J) | 6834 | 8439 | 15129 | 87 |
| H(13K) | 7580 | 8856 | 15520 | 87 |
| H(13L) | 8325 | 8364 | 15180 | 87 |