

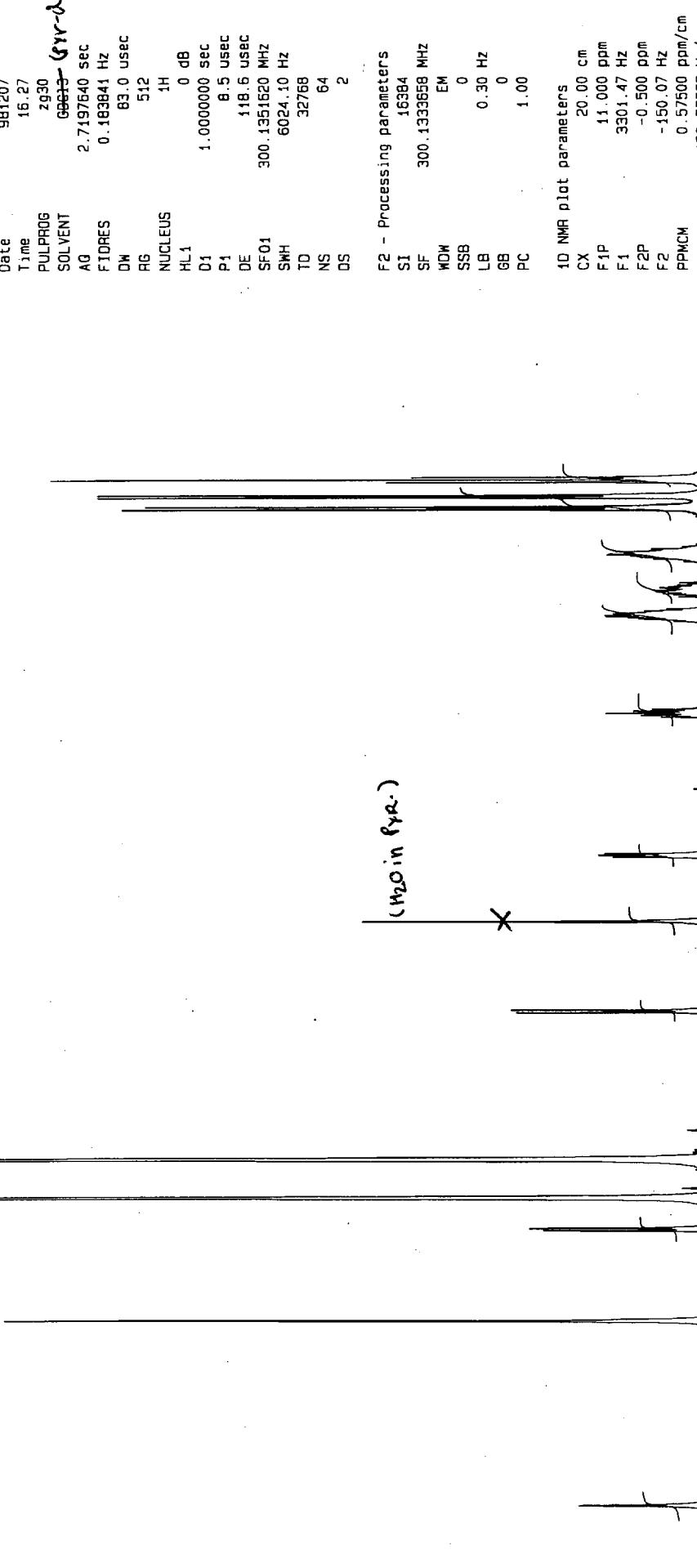
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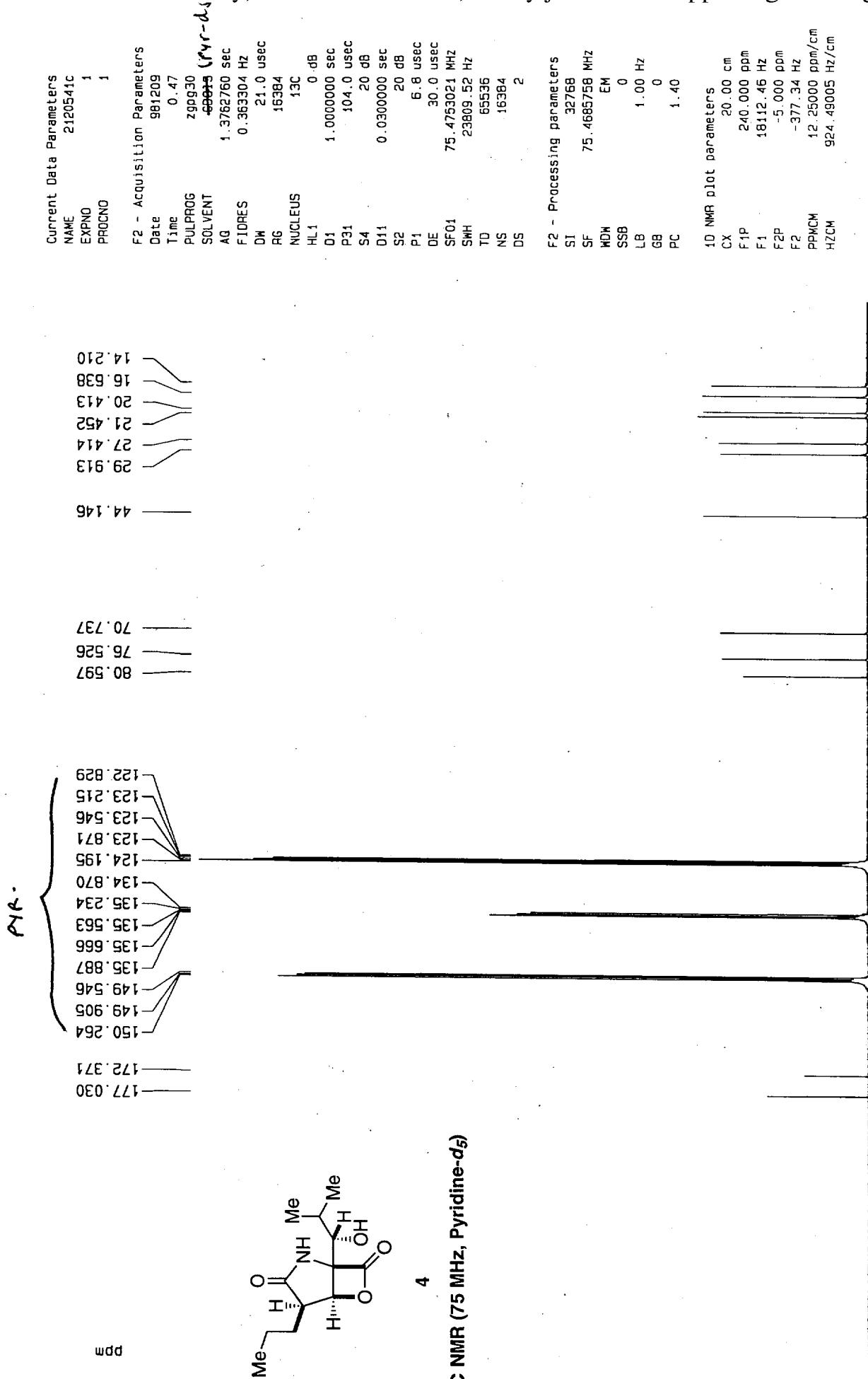
¹H NMR (300 MHz, Pyridine-d₅)

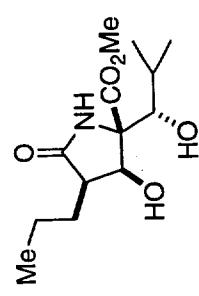
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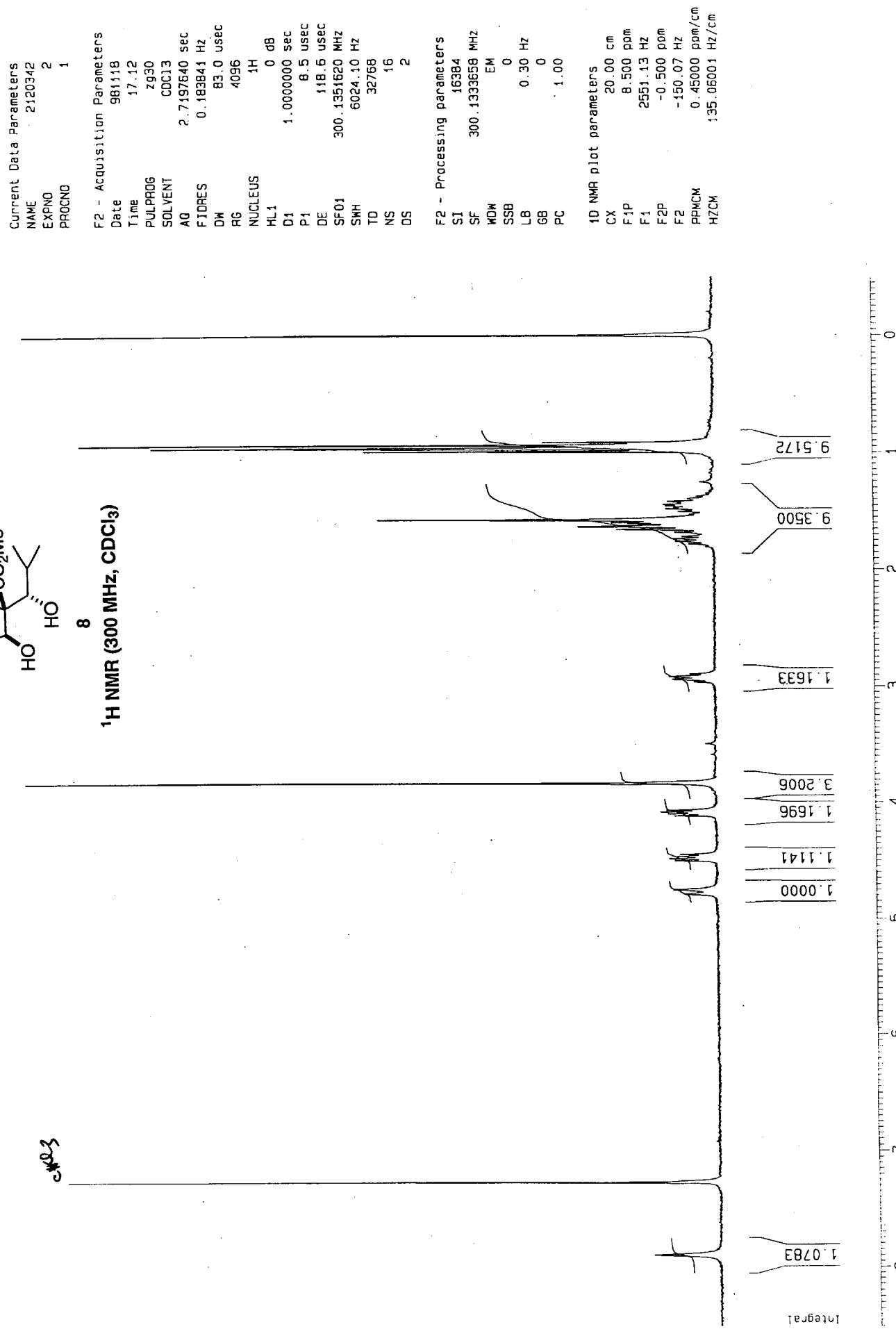
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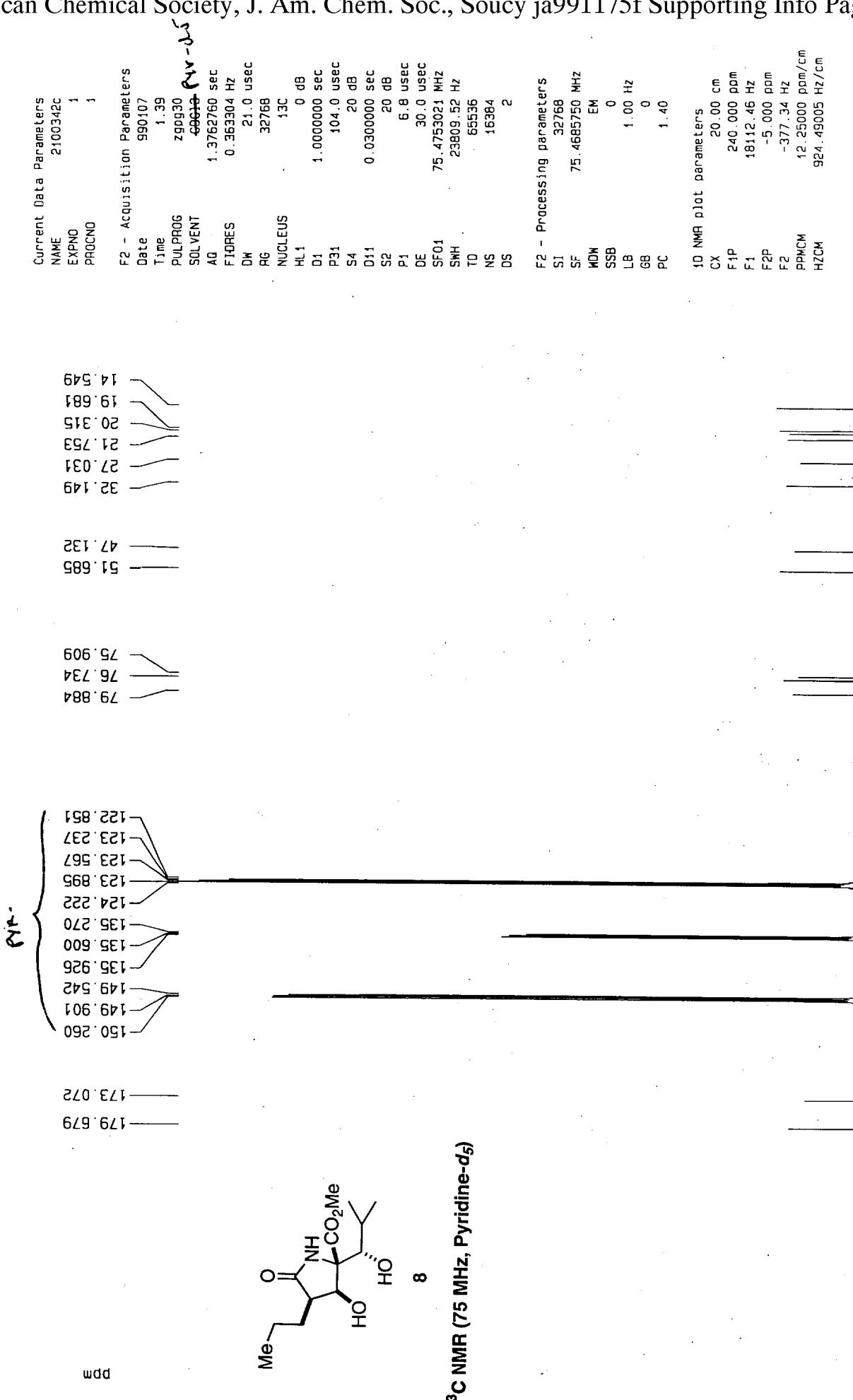


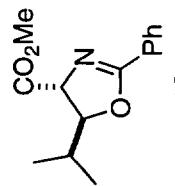




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¹H NMR (300 MHz, CDCl₃)





**¹H NMR (300 MHz, CDCl₃)**

Current Data Parameters
NAME 2120201
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PROCNO 1

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Date 990109
Time 0.23
PULPROG 2930
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DW 83.0 usec
RG 1024
NUCLEUS 1H
HL1 0 dB
D1 1.0000000 sec
P1 8.5 usec
DE 118.6 usec
SF01 300.1351620 MHz
SWH 6024.10 Hz
TD 32768
NS 16
DS 2

F2 - Processing parameters
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SF 300.1333658 MHz
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LB 0.30 Hz
GB 0
PC 1.00

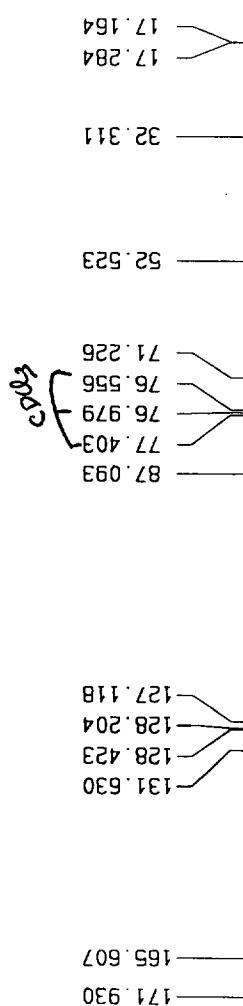


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 PROCN 1

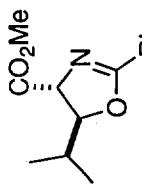
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 RG 32768
 NUCLEUS ¹³C
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 D1 1.0000000 sec
 P31 104.0 usec
 S4 20 dB
 D11 0.0300000 sec
 S2 20 dB
 P1 6.8 usec
 DE 30.0 usec
 SF01 75.4753021 MHz
 SWH 23809.52 Hz
 TD 65536
 NS 2048
 DS 2

F2 - Processing parameters
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 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 240.000 ppm
 F1 18112.46 Hz
 F2P -5.000 ppm
 F2 -377.34 Hz
 PPMCM 12.25000 ppm/cm
 HZCM 924.49042 Hz/cm



ppm



¹³C NMR (75 MHz, CDCl₃)
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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 SMART¹ software and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software² which corrects for Lp and decay. Absorption corrections were applied using SADABS⁶ supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97³ program and refined by least squares method on F², SHELXL-97,⁴ incorporated in SHELXTL-PC V 5.10.⁵

The structure was solved in the space group P2₁2₁2₁ (# 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% ellipsoids.

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 \approx	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.536(2) \approx b = 20.451(4) \approx c = 27.557(6) \approx	$\alpha = 90^\circ$. $\beta = 90^\circ$. $\gamma = 90^\circ$.
Volume	5938(2) \approx^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 \leq h \leq 11, -22 \leq k \leq 18, -29 \leq l \leq 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. \approx^3	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) 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 [\AA] and angles [$^\circ$] 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 ($\approx^2 \times 10^3$) for psc1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	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 ($\times 10^4$) and isotropic displacement parameters ($\approx^2 \times 10^{-3}$)
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
