REVISED

Supporting Information

Crystal data for 7: $C_{24}H_{31}NO_3S$, f.w. 413.56, Monoclinic, space group C2, a = 22.762(3) Å, b = 10.848(1) Å, c = 9.947(1) Å, β = 96.90(1)°, V = 2437.96(40) Å^3, Z = 4, D_c = 1.127 g/cm^3, μ = 1.351 mm^{-1}, F(000) = 888.

Data collection: X-ray diffraction data were collected from a colourless prismatic crystal of **7** (size 0.15 x 0.2 x 0.1), with graphite monochromated Cu-$K\alpha$ radiation (λ = 1.5418 Å) on a Siemens P4 diffractometer (θ-2θ scan technique). 2667 reflections were collected ($3.91<\theta<67.46$; +h,+k,+l and –h,-k,-l), 2495 unique; 3 standard reflections, measured every 100 reflections, showed no significant decay. Data were corrected for Lorentz and polarization effects and an empirical absorption correction was applied.

Structure analysis and refinement: the structure was solved by direct methods using SIR92 (Altomare, A.; Cascarano, G.; Guagliardi, A. *J. Appl. Cryst.* **1993**, *26*, 343) and refined by full-matrix least squares on F2 using SHELXL97 (Sheldrick, G. *SHELXL97, Program for crystal structure refinement*; University of Göttingen, Germany, **1997**). Non hydrogen atoms were refined anisotropically. The N-bonded hydrogen was located by difference-Fourier technique and refined, while all the others have been included at calculated positions and refined with group temperature factors. Final values of the residual R1 for reflections with $I>2\sigma$ and for all reflections were respectively 0.041 and 0.045. The highest peak and hole in the final difference-Fourier map were 0.195 and -0.189 eÅ^3. The refined value of Flack's parameter (Flack, H. D. *Acta Cryst.* **1983**, *A 39*, 876-880) was 0.03(2).

A view of **7** is shown in Figure S1 and selected molecular dimensions are reported in Table S1. Bond lengths and angles fall in the expected range (Allen, F. M.; Kennard, O; Watson, D. G.; Brammer, L.; Orpen, A. G.; Taylor, R. J. *J. Chem. Soc., Perkin Trans. 2* **1987**, S1-S19).
The hydrogen atom found by Fourier-difference map indicates a planar geometry on N, as commonly found in amides. Consistent with the sp2 hybridization on C2, the conformation around C2—C3 bond is skew. An intermolecular hydrogen bond is found between the amidic hydrogen and the S-bonded oxygen, which probably play a significant role in the crystal packing (O---H 1.968(1) Å; O---H—N 163.0(2)°).

Table S1

Bond lengths (Å)		Bond angles (°)	
S(1)-O(1)	1.498(3)	C(1)-C(2)-C(3)	125.1(5)
S(1)-C(41)	1.794(4)	O(1)-S(1)-C(41)	106.90(16)
S(1)-C(4)	1.837(3)	O(1)-S(1)-C(4)	107.85(15)
C(1)-C(2)	1.292(6)	C(41)-S(1)-C(4)	98.11(15)
C(2)-C(3)	1.494(6)	C(9)-N(1)-C(5)	122.4(3)
N(1)-C(9)	1.339(4)	C(9)-O(2)-C(10)	115.2(3)
N(1)-C(5)	1.451(4)	**Torsion angles (°)**	
O(2)-C(10)	1.446(4)	C(1)-C(2)-C(3)-C(4)	119.2(4)
O(2)-C(9)	1.355(4)	C(2)-C(3)-C(4)-C(5)	-39.6(4)
		C(2)-C(3)-C(4)-S(1)	85.4(3)

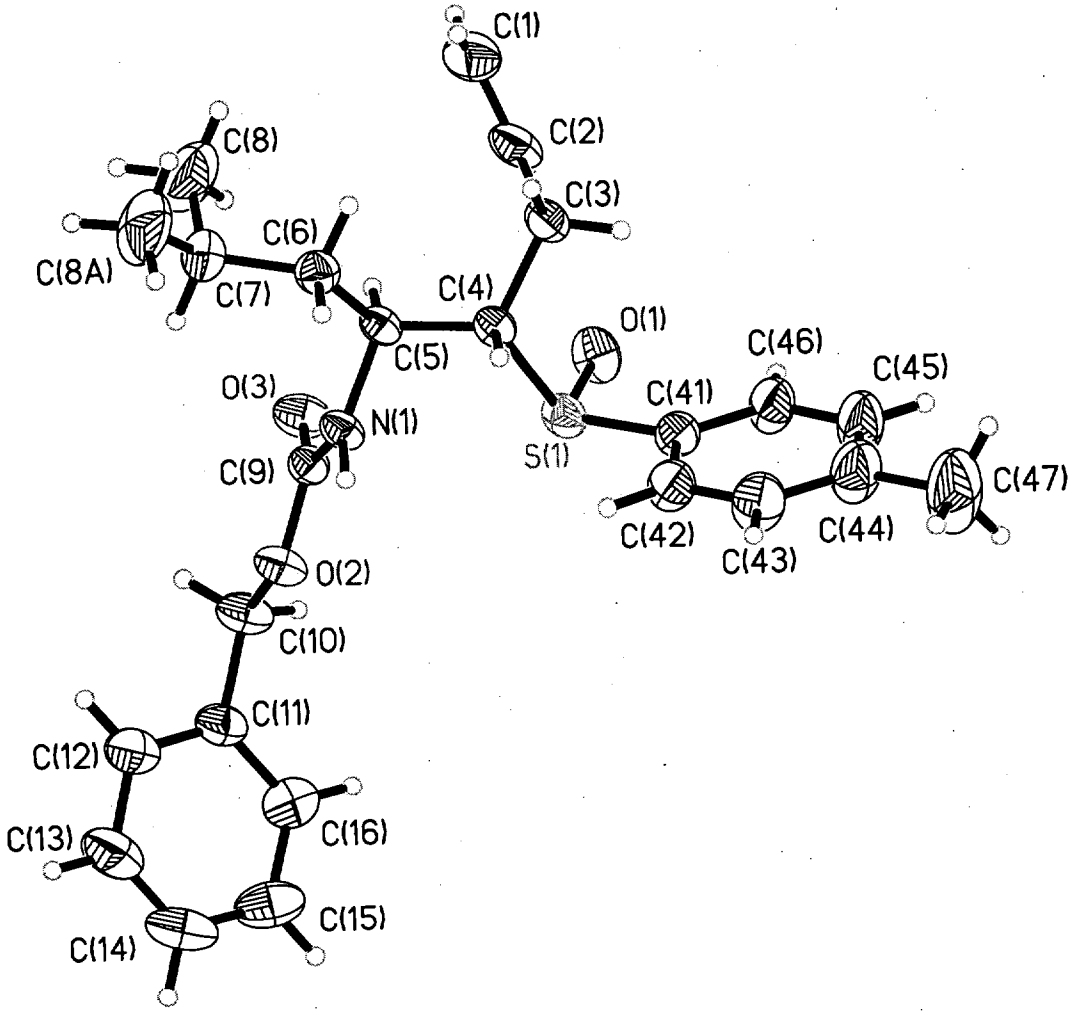
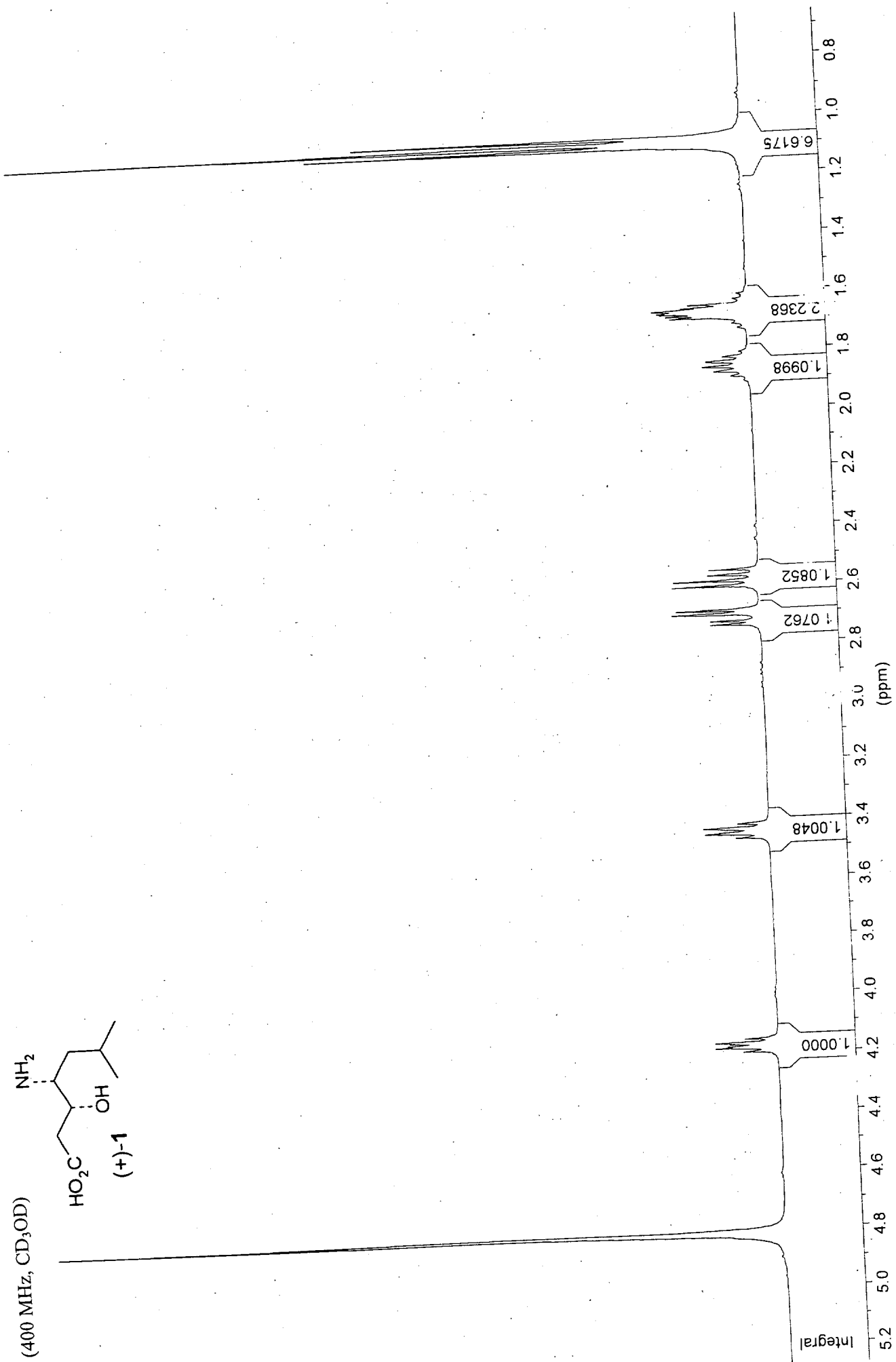
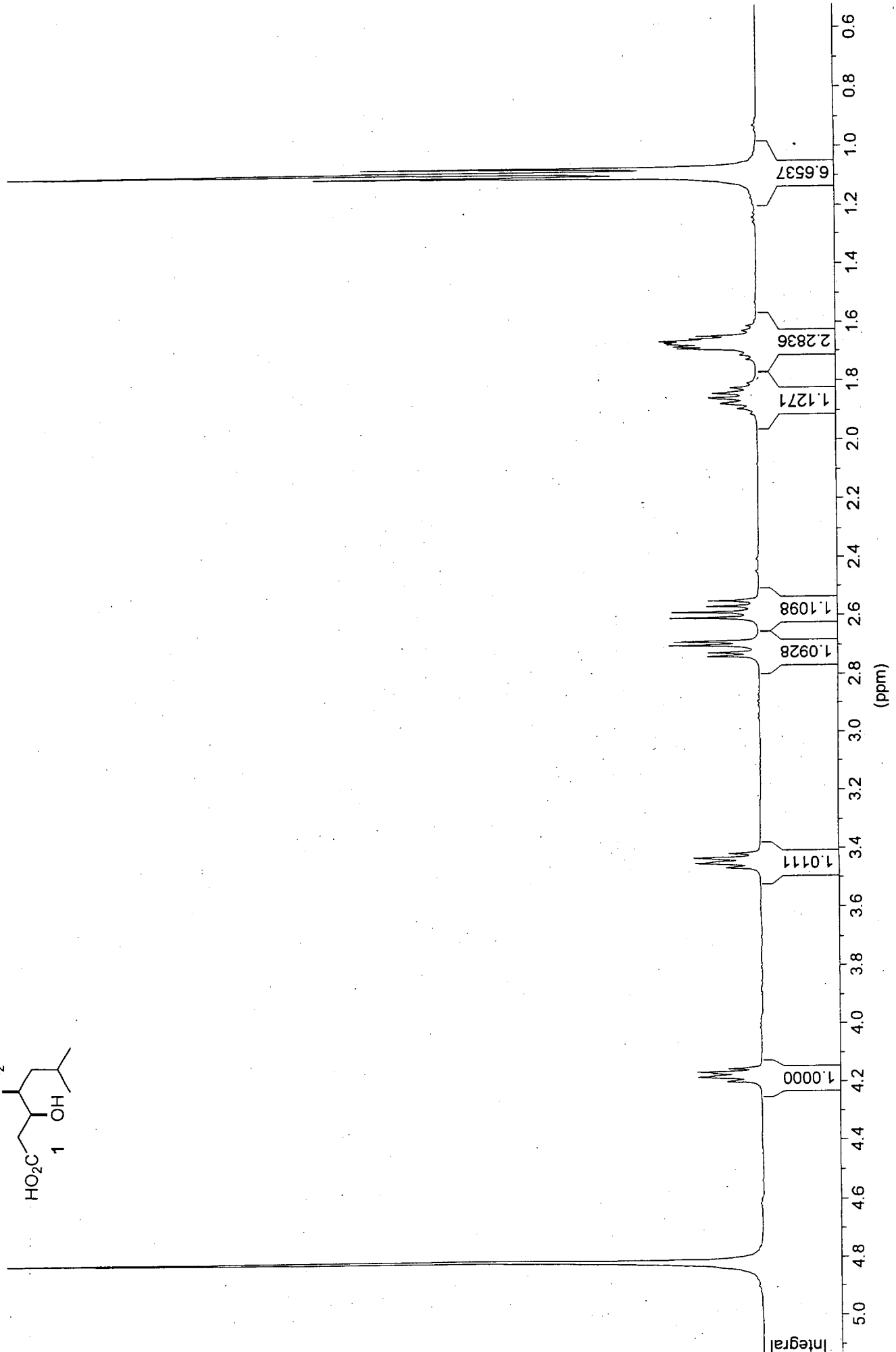


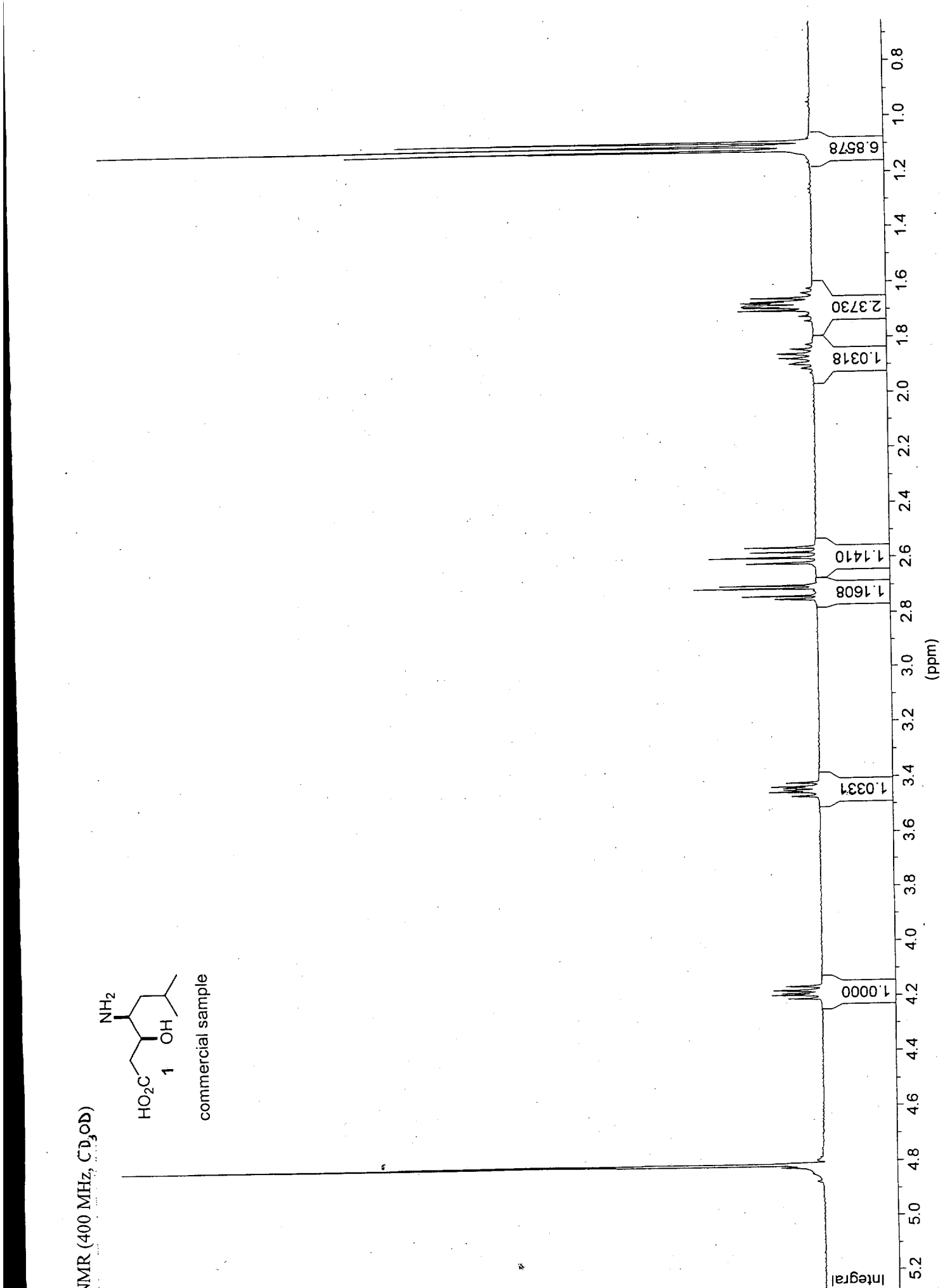
Figure S1. ORTEP view of **7** showing the absolute configuration and the atomic labelling scheme. 30% Thermal ellipsoid for non-hydrogen atoms are shown.

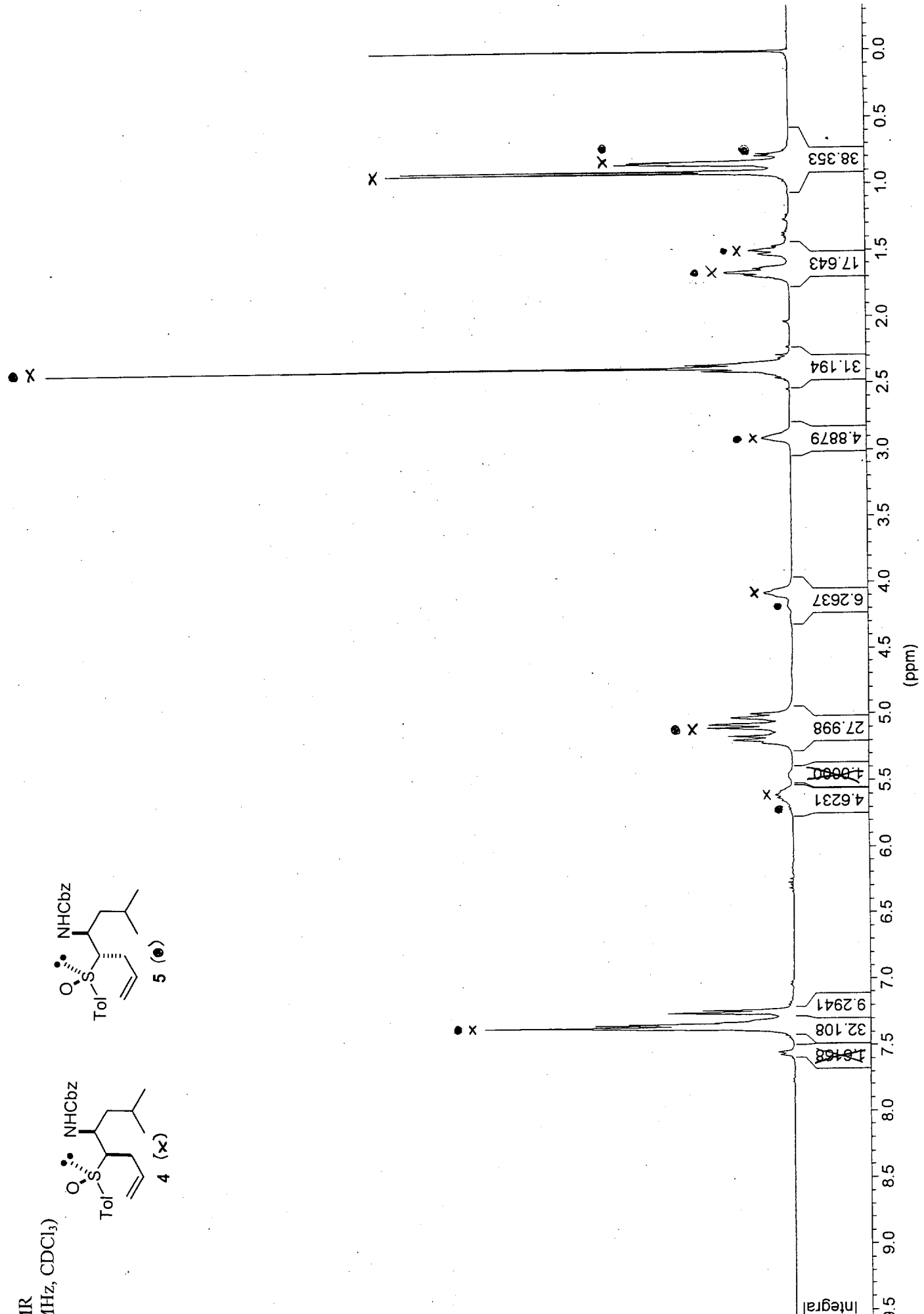


R (400 MHz, CD_3OD)

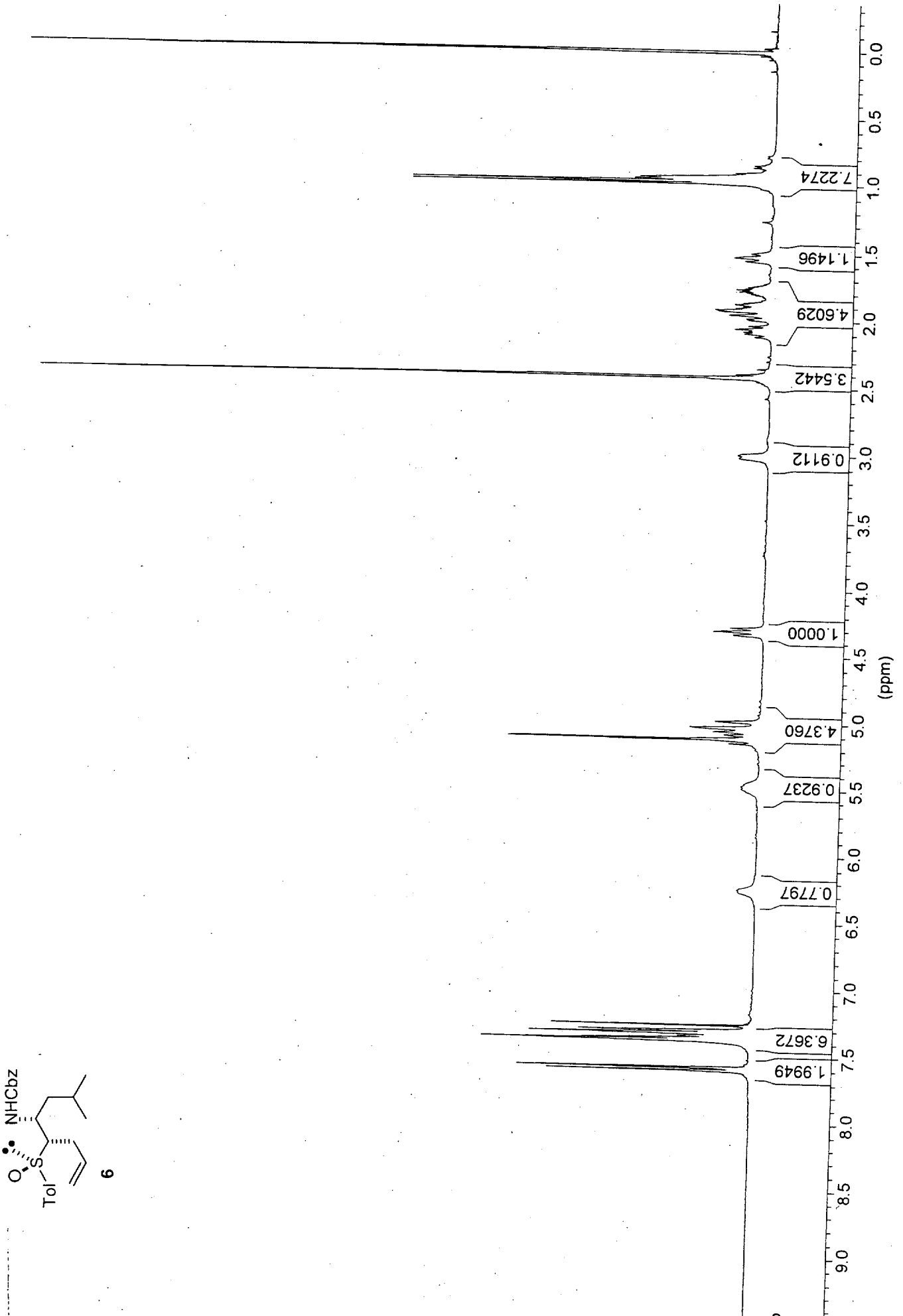


MR (400 MHz, CD_3OD)


NMR (400 MHz, CD3OD)
commercial sample
NH2
OH
HO2C
1
Integral
6.8578
2.3730
1.0318
1.1410
1.1608
1.0331
1.0000
(ppm)

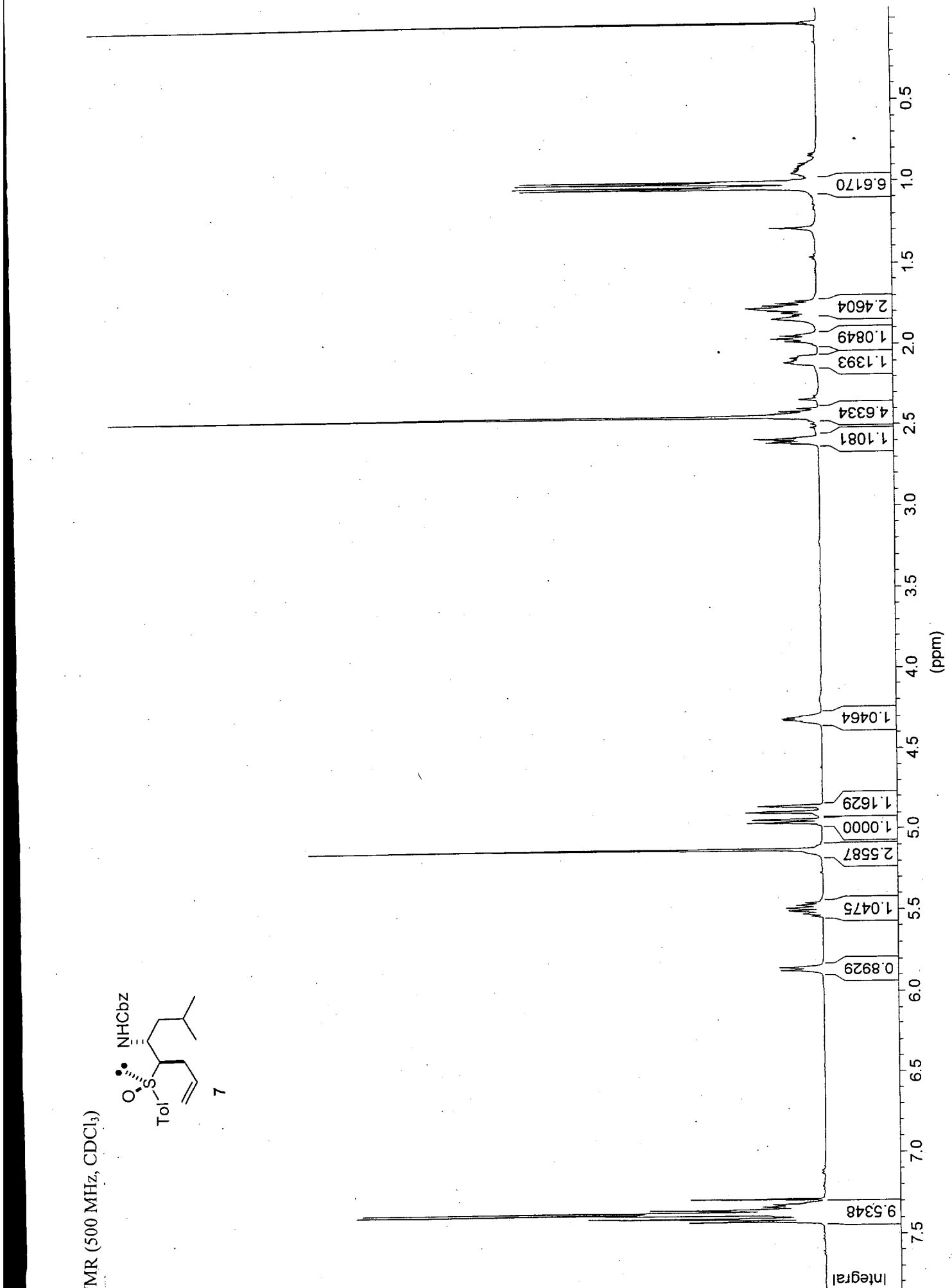

38.353
17.643
31.194
4.8879
6.2637
27.998
4.6231
9.2941
32.108
(ppm)
NHCbz
Tol
5 (●)
NHCbz
Tol
4 (x)

IR
MHz, $CDCl_3$)

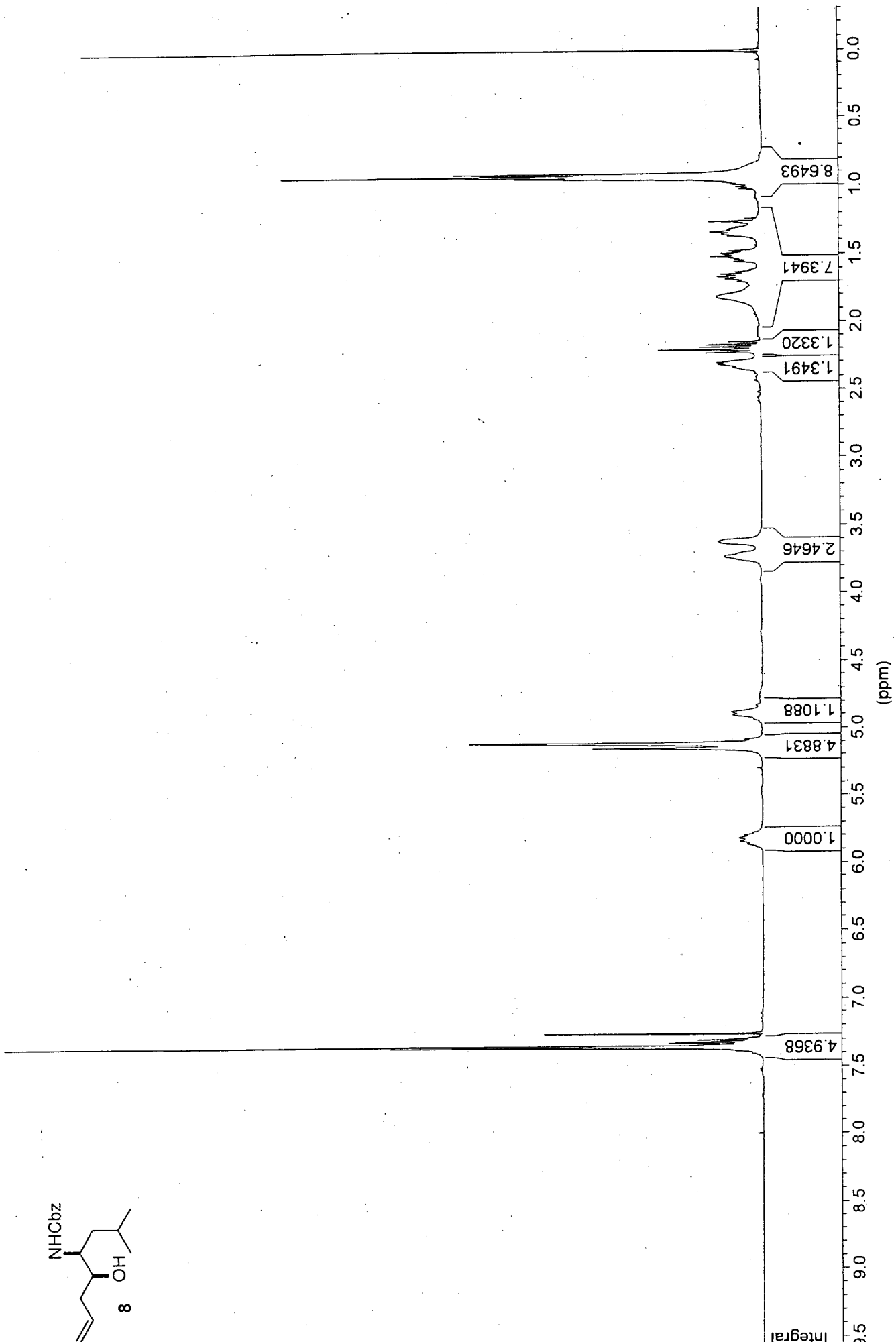


6

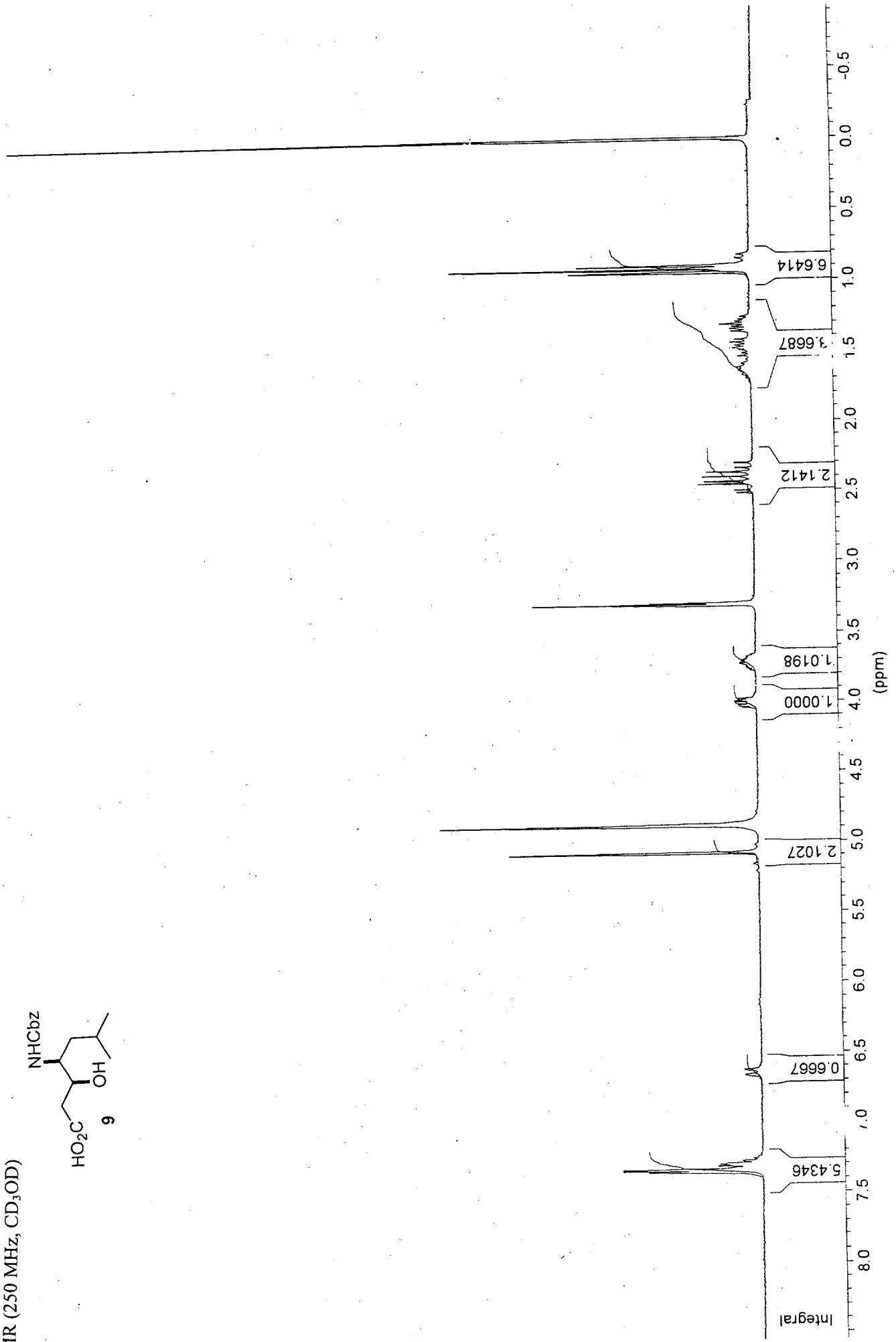
MR (400 MHz, $CDCl_3$)



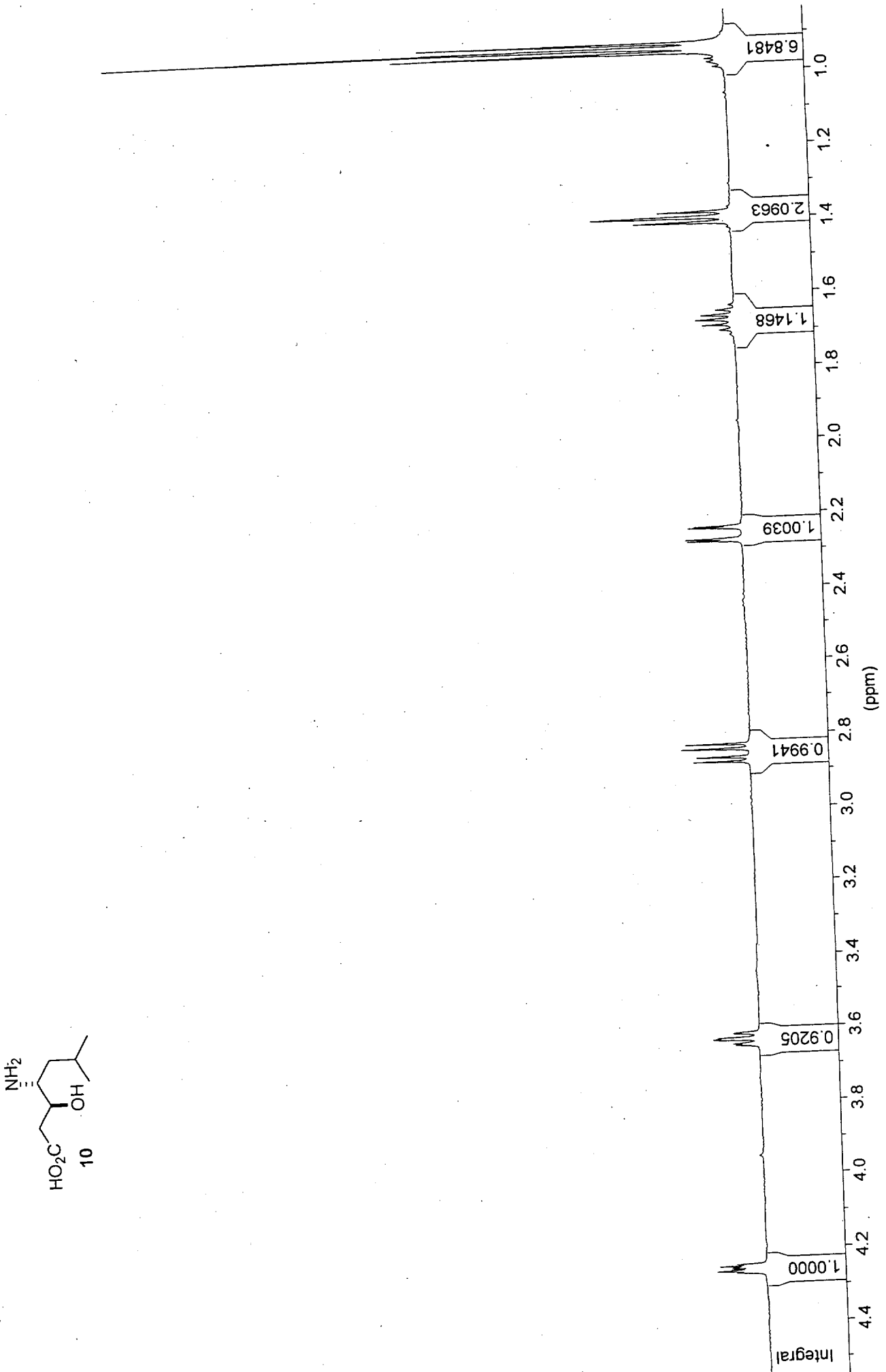
MR (500 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



IR (250 MHz, CD_3OD)



^{1}H NMR (500 MHz, CD_3OD)

10