

SUPPORTING INFORMATION

Ring Opening of Nonactivated 2-(1-Aminoalkyl) Aziridines: Unusual Regio- and Stereoselective C-2 and C-3 Cleavage

*José M. Concellón** and *Estela Riego*

Departamento de Química Orgánica e Inorgánica, Facultad de Química, Universidad de Oviedo,

Julián Clavería 8, 33071 Oviedo, Spain

Email: jmcg@sauron.quimica.uniovi.es

List of Contents

General Experimental	S1
Spectroscopic Data of Compounds 7	S2
¹³ C NMR Spectra of Compounds 3 , 4 , and 7a	S3-S8

GENERAL EXPERIMENTAL

¹H NMR spectra were recorded at 300 MHz. ¹³C NMR spectra were recorded at 75 MHz. Chemical shifts are reported in ppm relative to TMS in CDCl₃. Only the molecular ions and/or base peaks in MS are given. Optical rotations were measured in CHCl₃. Analytical TLC was conducted in precoated silica gel 60 F-254 on aluminum sheets; compounds were visualized with UV light or iodine. Flash chromatography was carried out on Merck silica gel 60 (230-400 mesh). BF₃·OEt₂ was distilled before using. Amino aziridines **1** were prepared according to literature procedure.¹ Acetonitrile was distilled from CaH₂ and stored over activated 4Å molecular sieves.

SPECTROSCOPIC DATA OF COMPOUNDS **7**

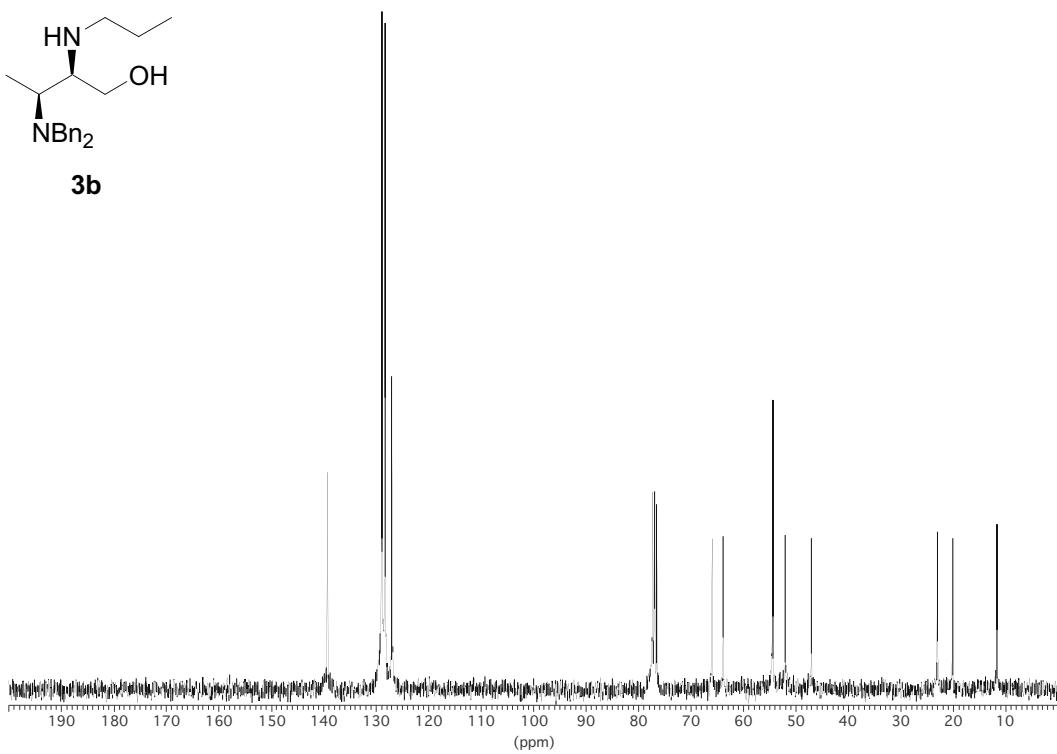
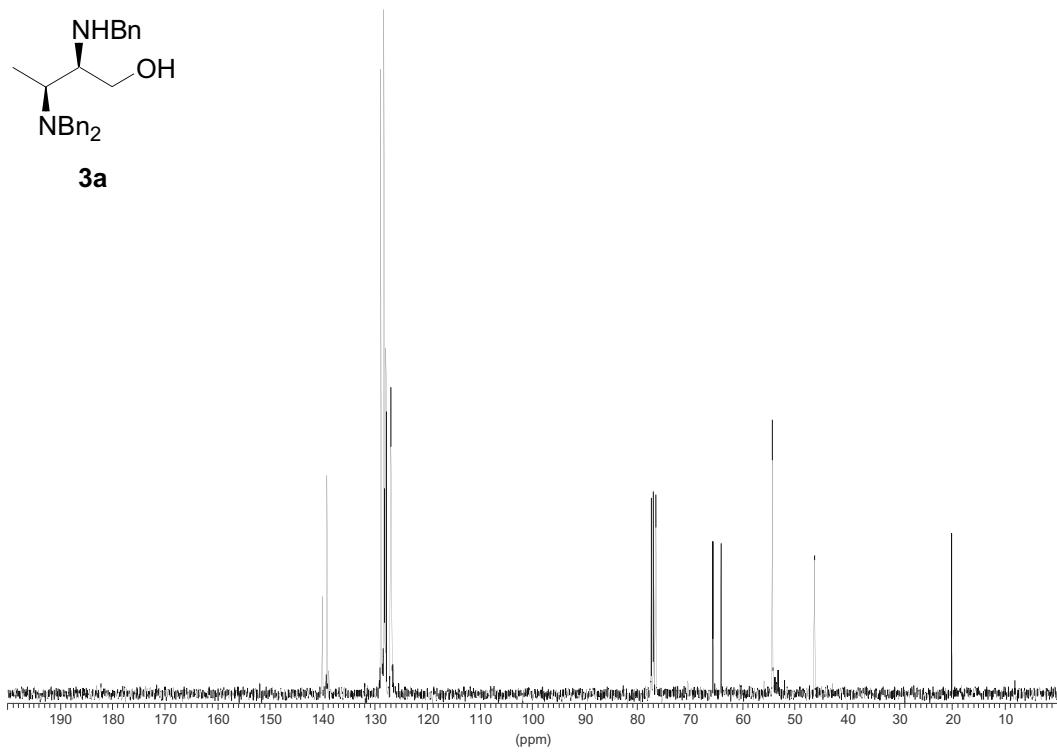
(1) Concellón, J. M.; Bernad, P. L.; Riego, E.; García-Granda, S.; Forcén-Acebal, A. *J. Org. Chem.* **2001**, *66*, 2764.

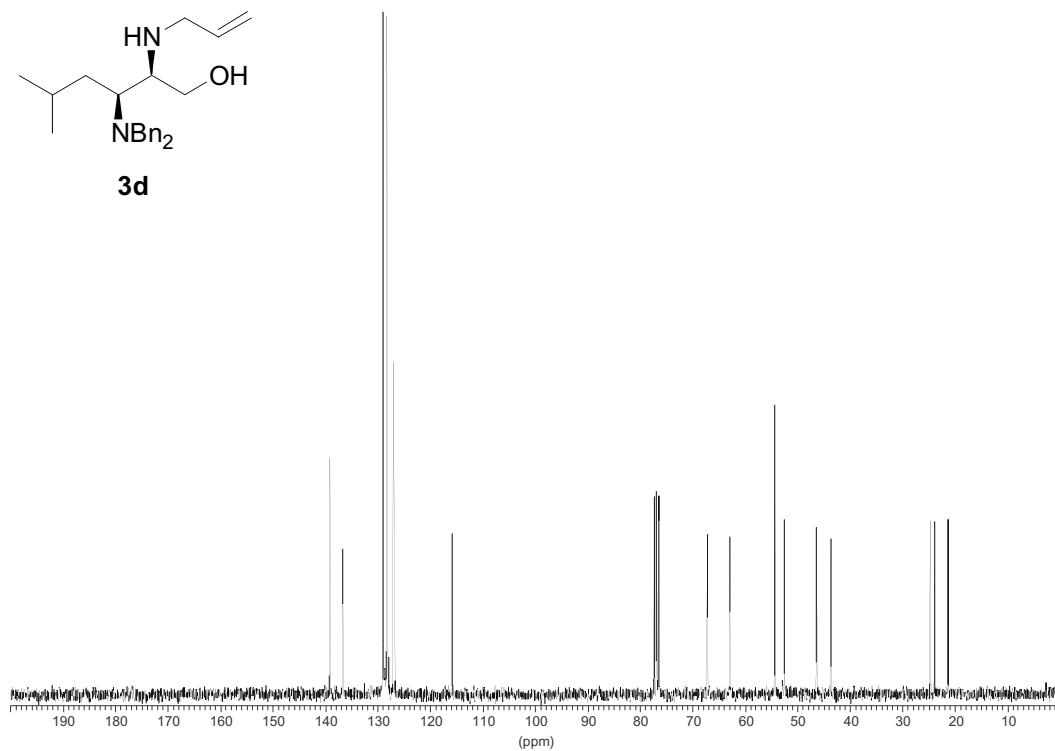
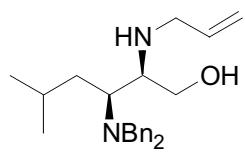
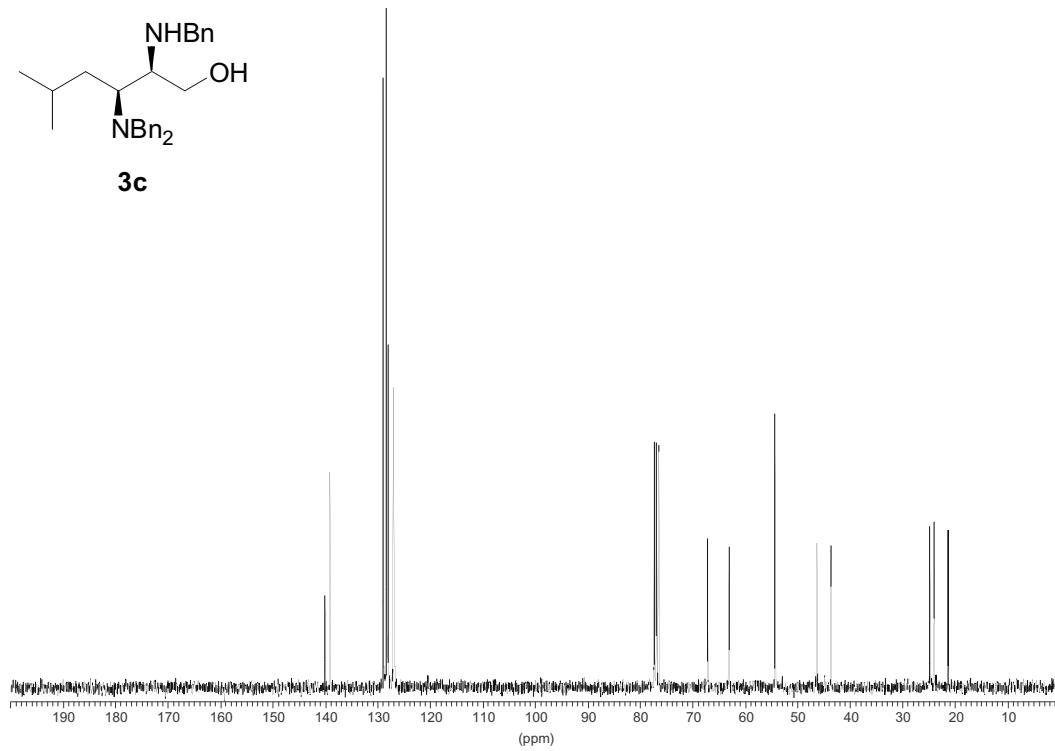
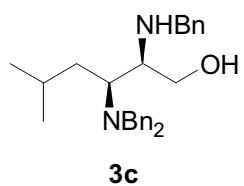
(2*R*,3*S*)-1-Benzylamino-3-(dibenzylamino)butan-2-ol (7a): ^1H NMR (300 MHz, CDCl_3): $\delta =$ 7.48-7.28 (m, 15 H), 3.94-3.63 (m, 3 H), 3.60 (AB syst., $J = 13.5$, 2 x 2 H), 3.01-2.97 (m, 1 H), 2.85-2.51 (m, 2 H), 1.25 (d, $J = 6.5$ Hz, 3 H); ^{13}C NMR (75 MHz, CDCl_3): $\delta =$ 139.7 (3 C), 128.4 (4 CH), 128.1 (2 CH), 128.0 (2 CH), 127.8 (4 CH), 126.5 (3 CH), 70.9 (CH), 55.3 (CH), 53.8 (2 CH₂), 53.3 (CH₂), 51.9 (CH₂), 8.1 (CH₃).

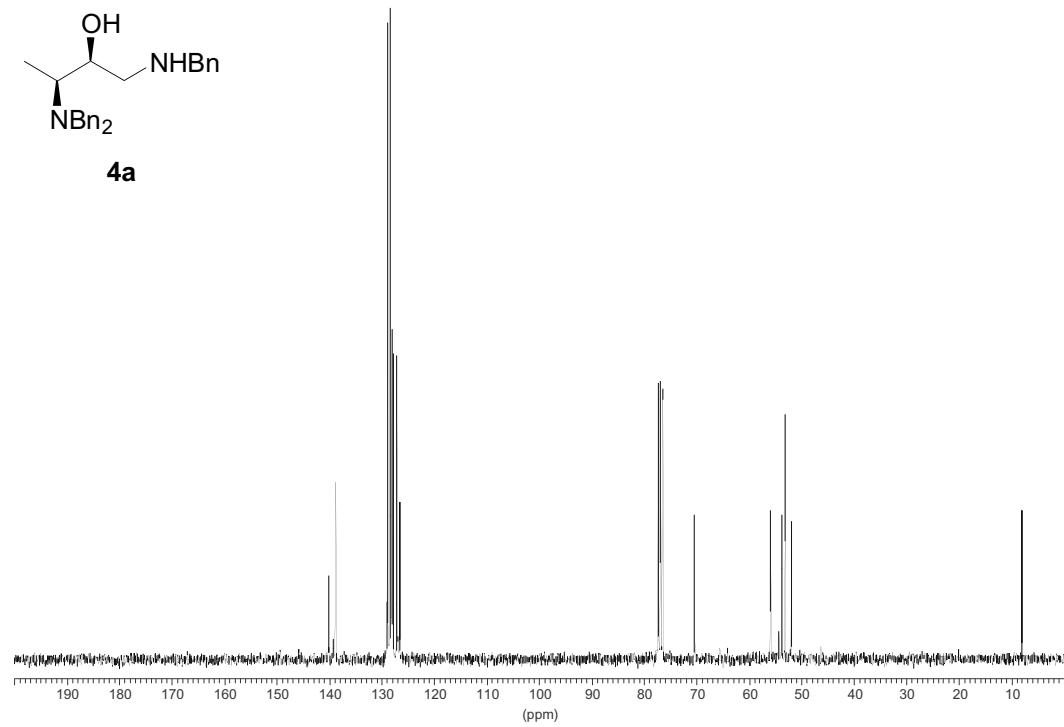
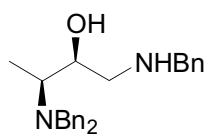
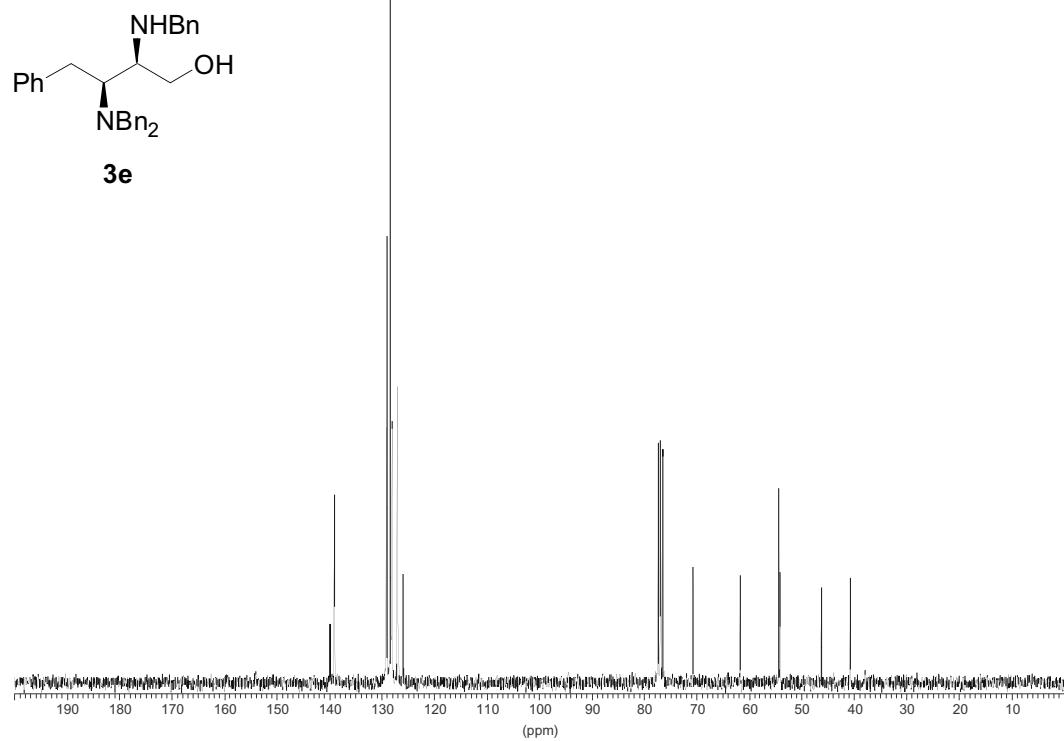
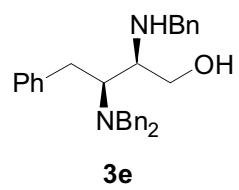
(2*R*,3*S*)-1-Benzylamino-3-dibenzylamino-4-phenylbutan-2-ol (7e)²

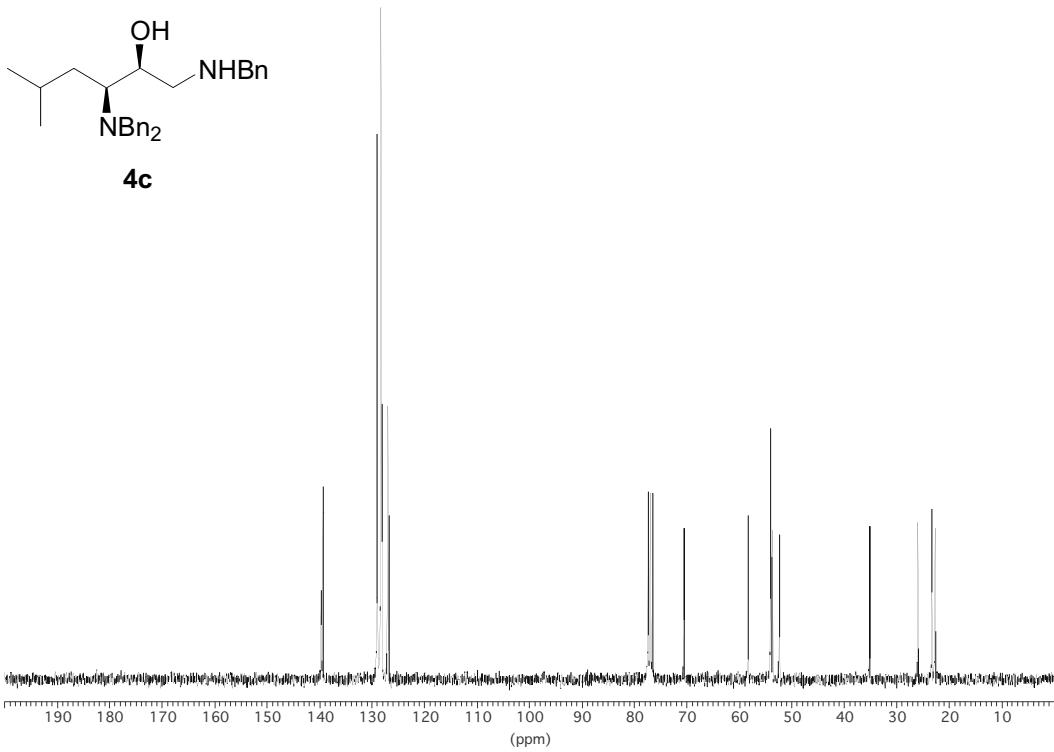
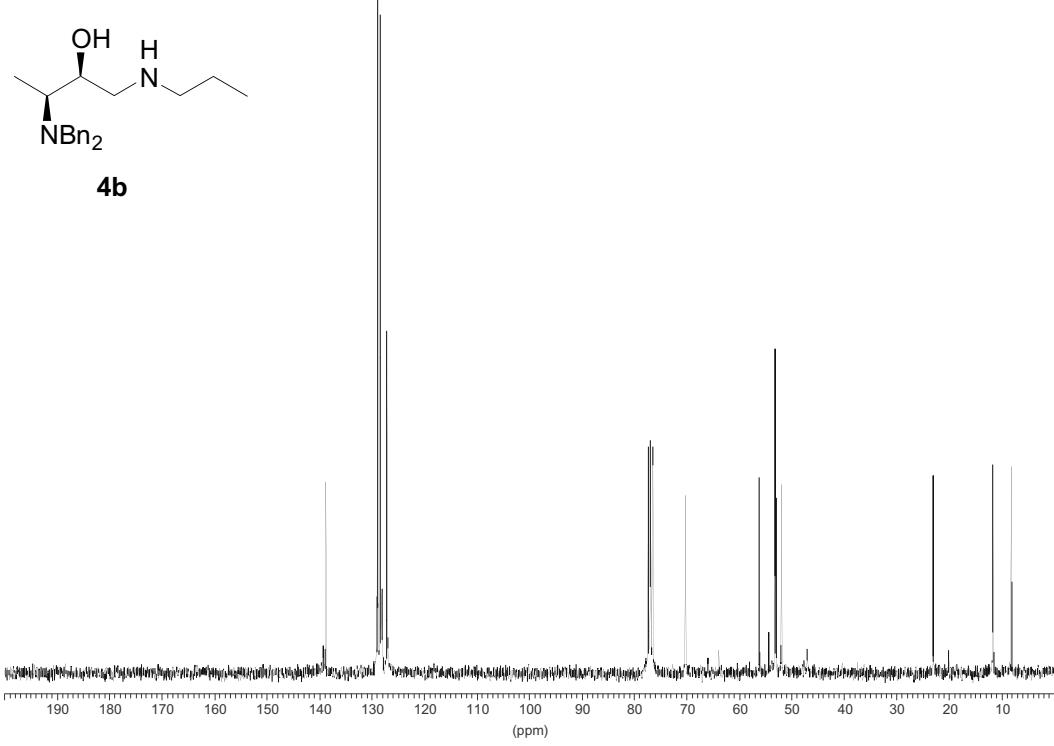
(2) Concellón, J. M.; Cuervo, H.; Fernández-Fano, R. *Tetrahedron* **2001**, *57*, 8983.

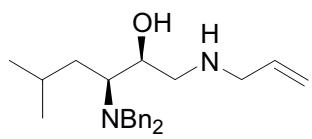
¹³C NMR SPECTRA



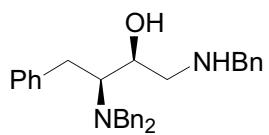
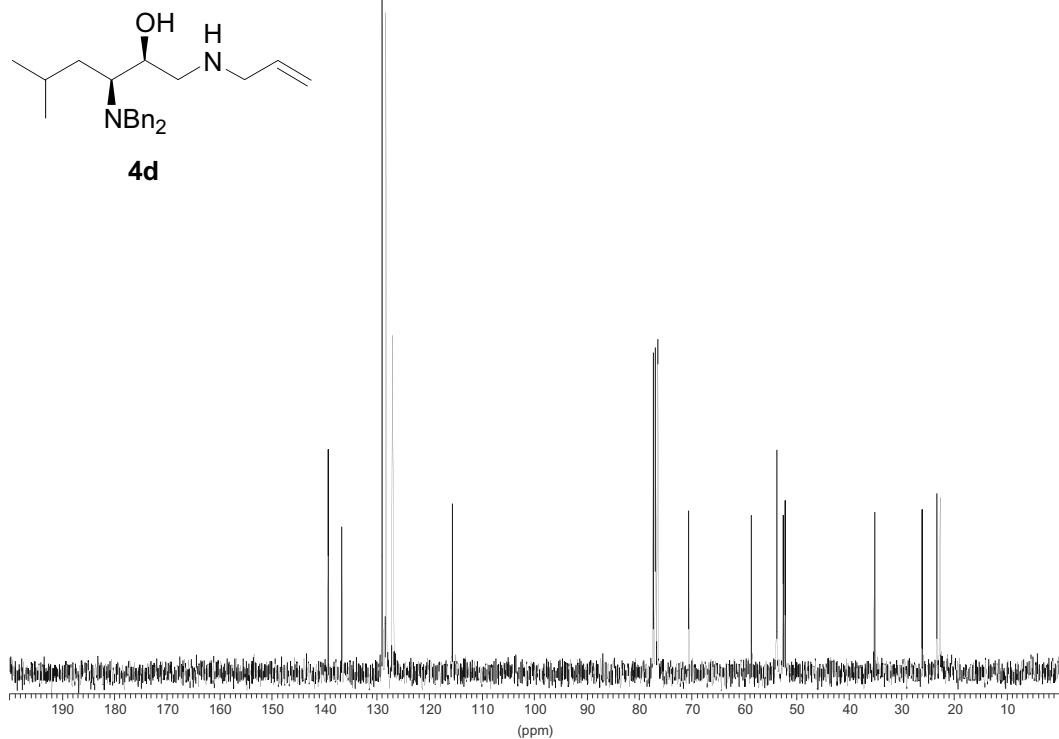




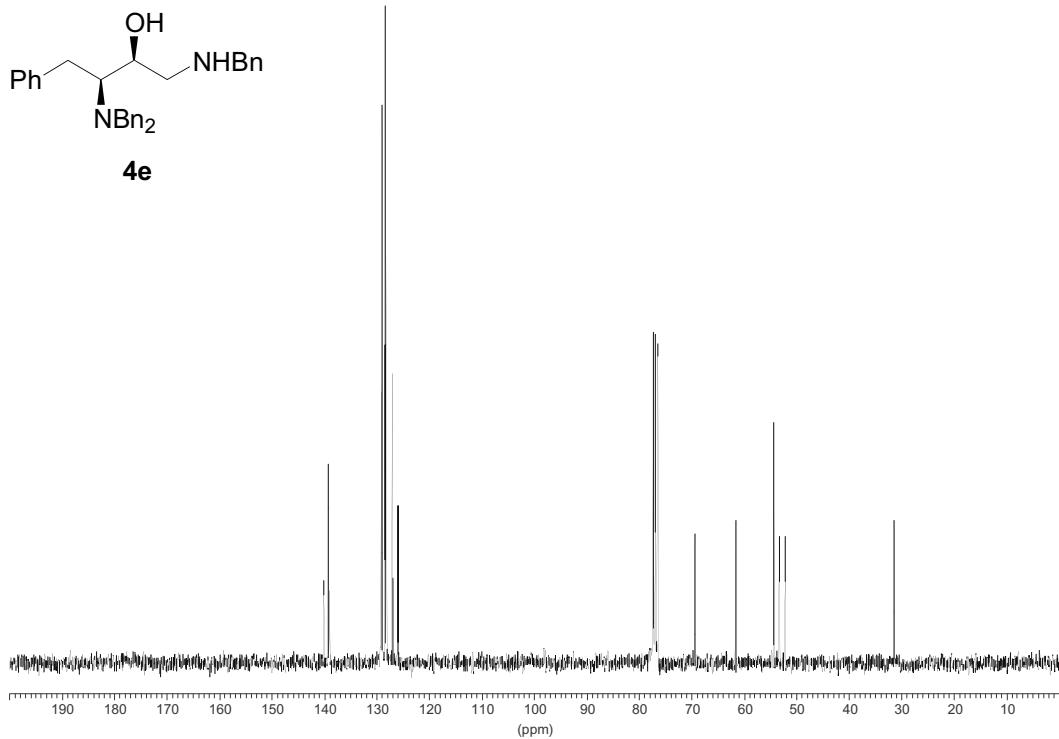


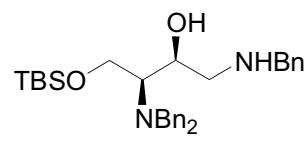


4d

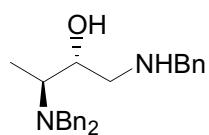
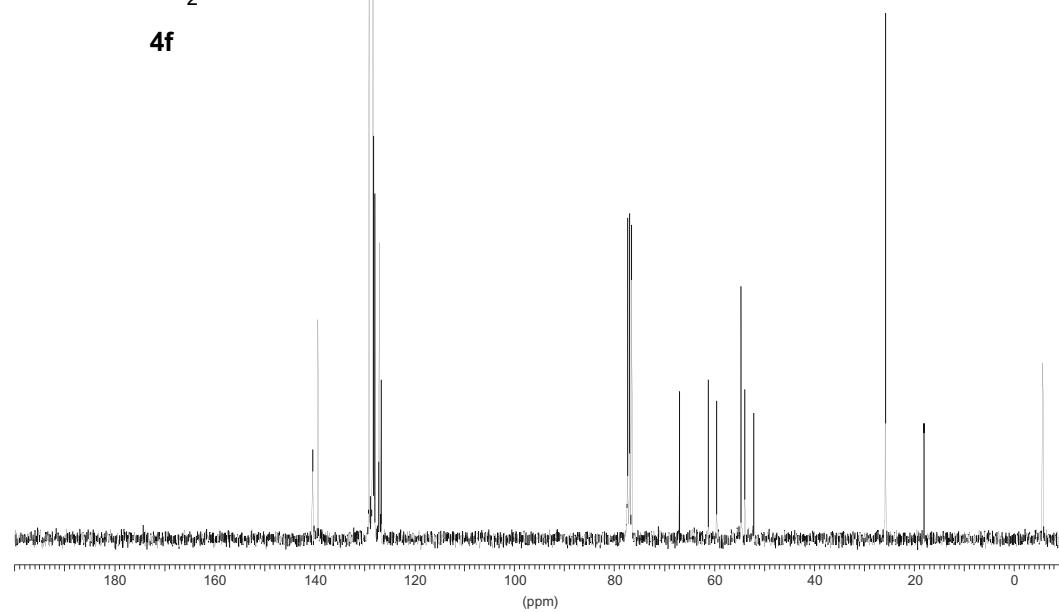


4e





4f



7a

