

SUPPORTING INFORMATION

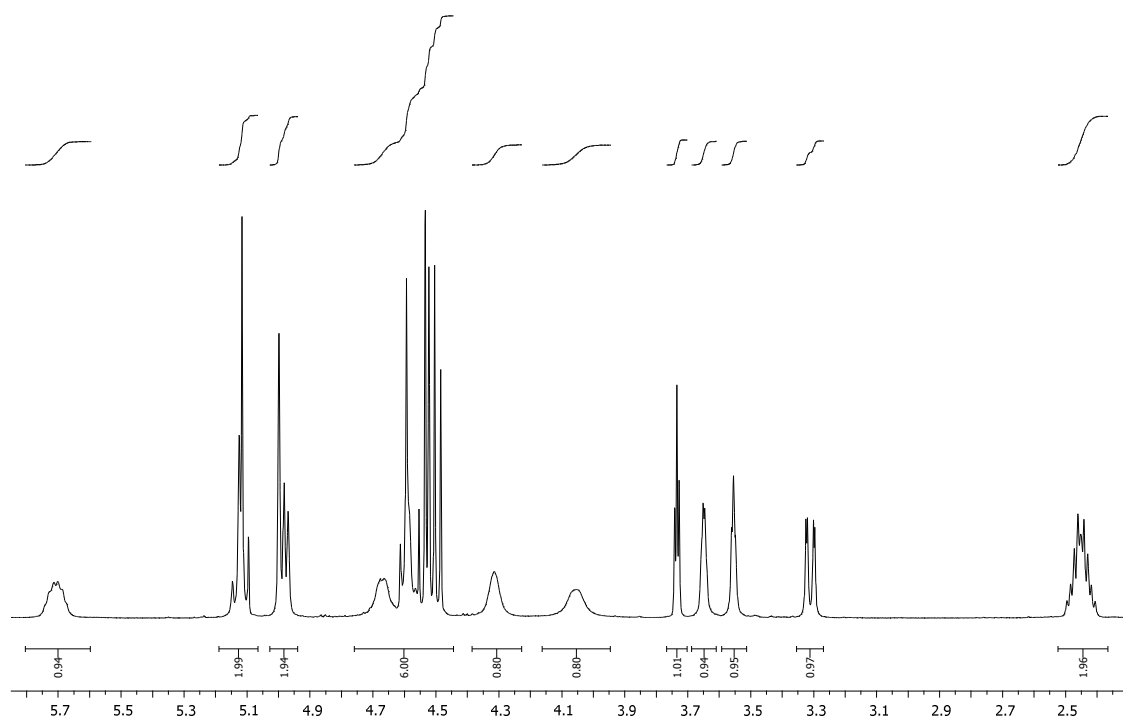
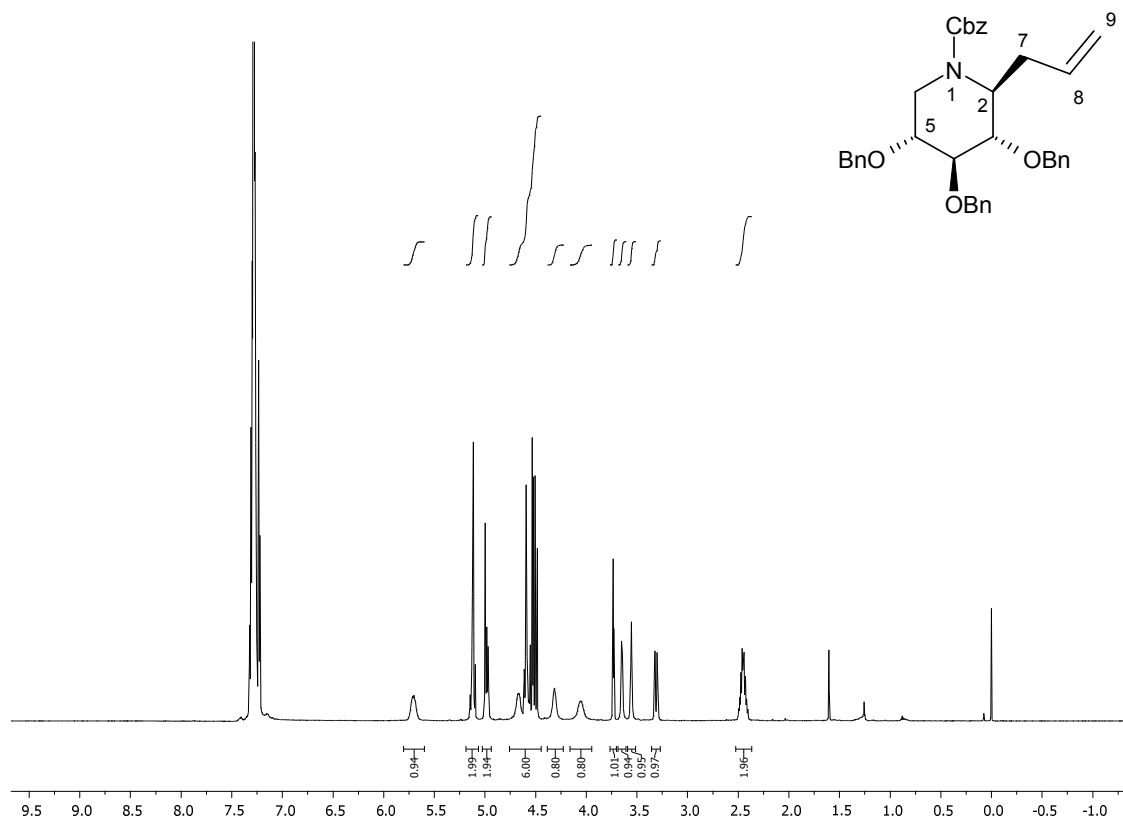
Carboxybenzyl Group as an *O*-Nucleophile in the C-H Allylic Oxidation: Total Synthesis of (–)-Castanospermine

Michał Malik,* Grzegorz Witkowski, Sławomir Jarosz*

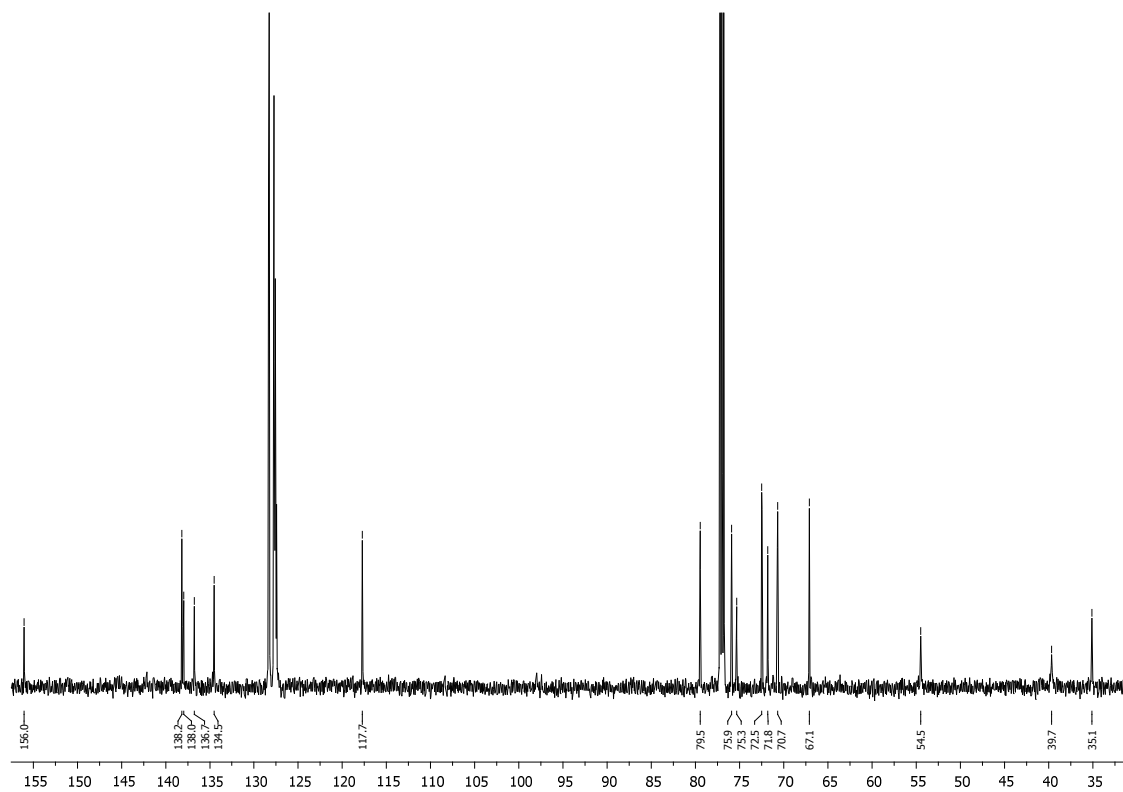
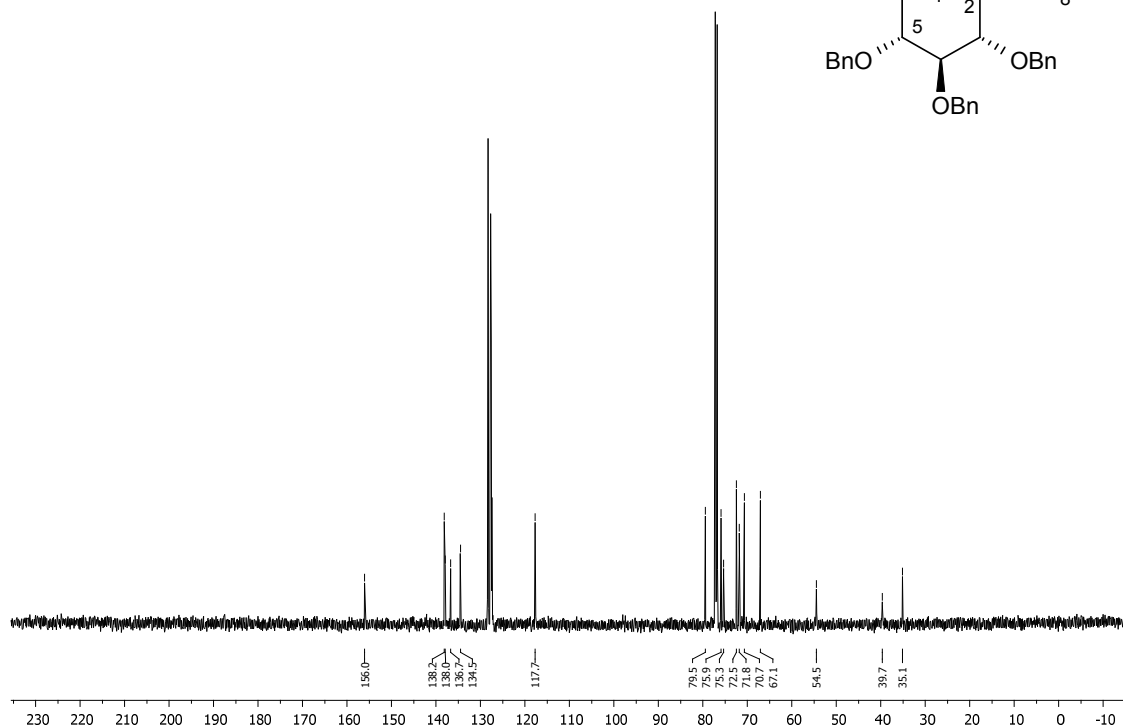
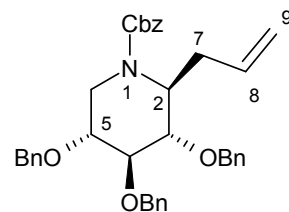
Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw

1) ^1H and ^{13}C NMR spectra of all compounds.....	2
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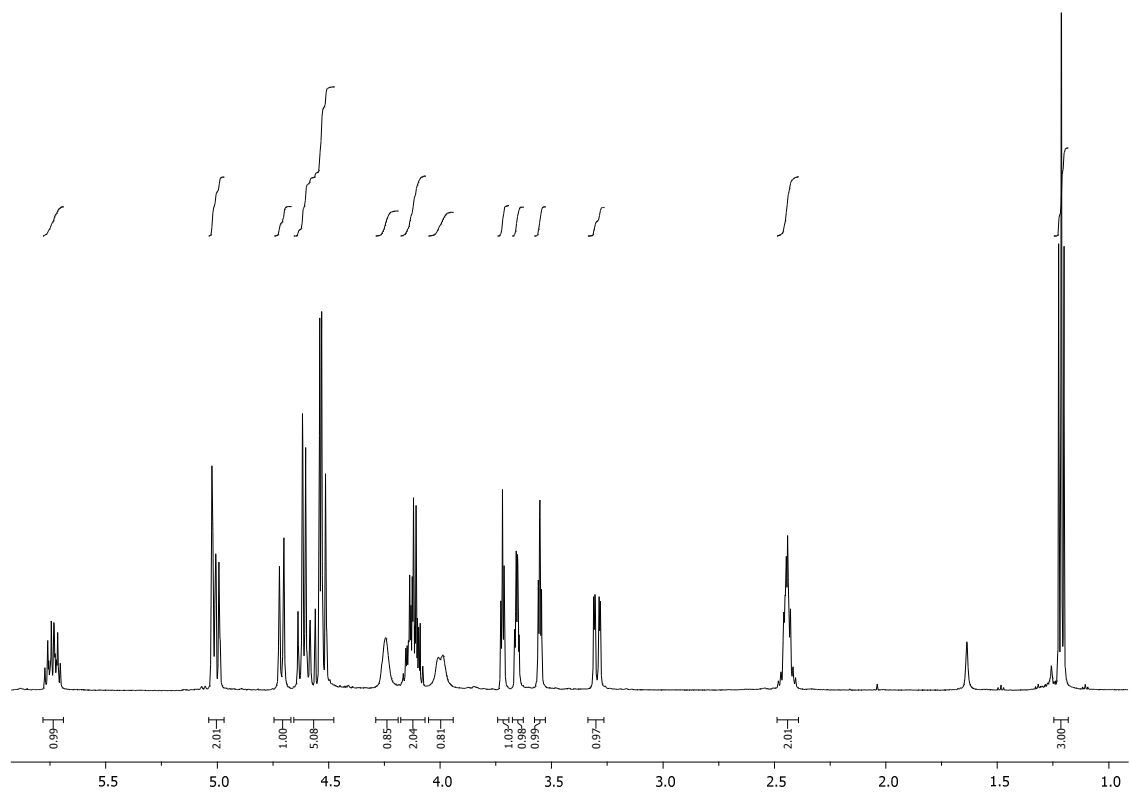
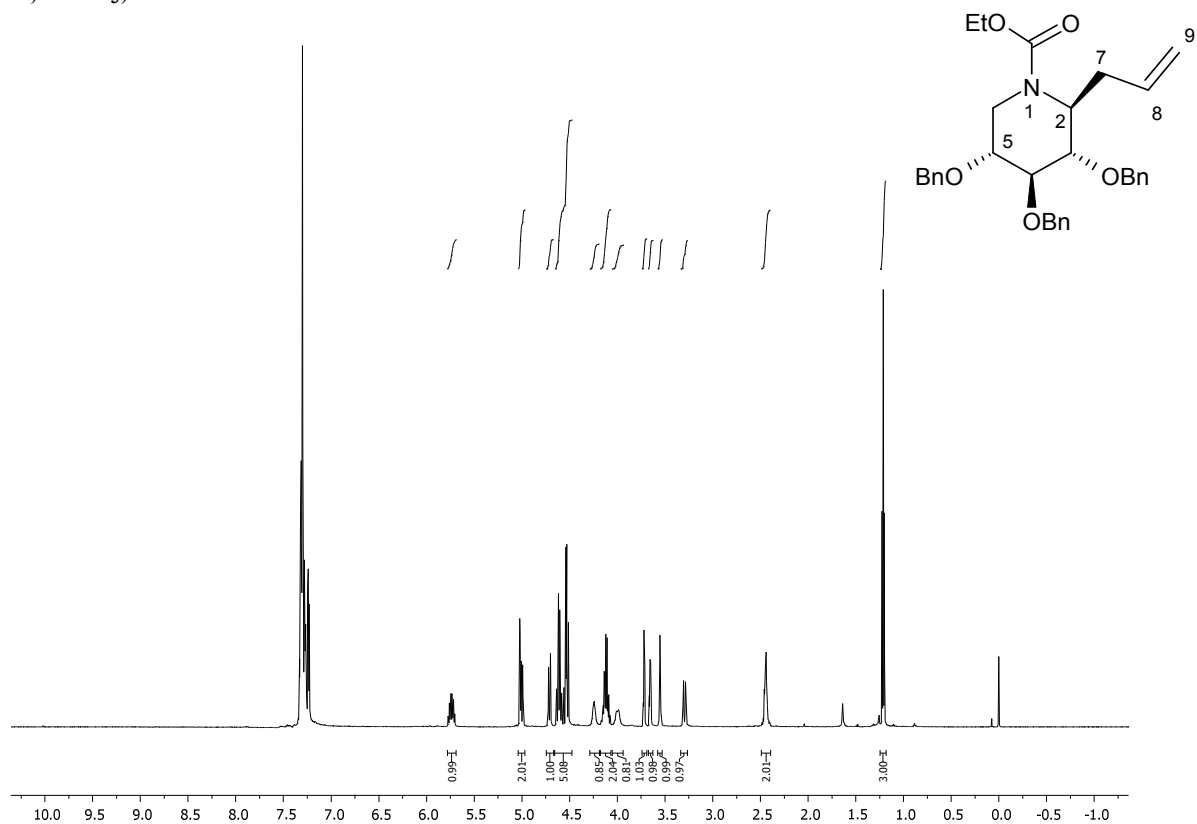
3a, CDCl₃, 600 MHz



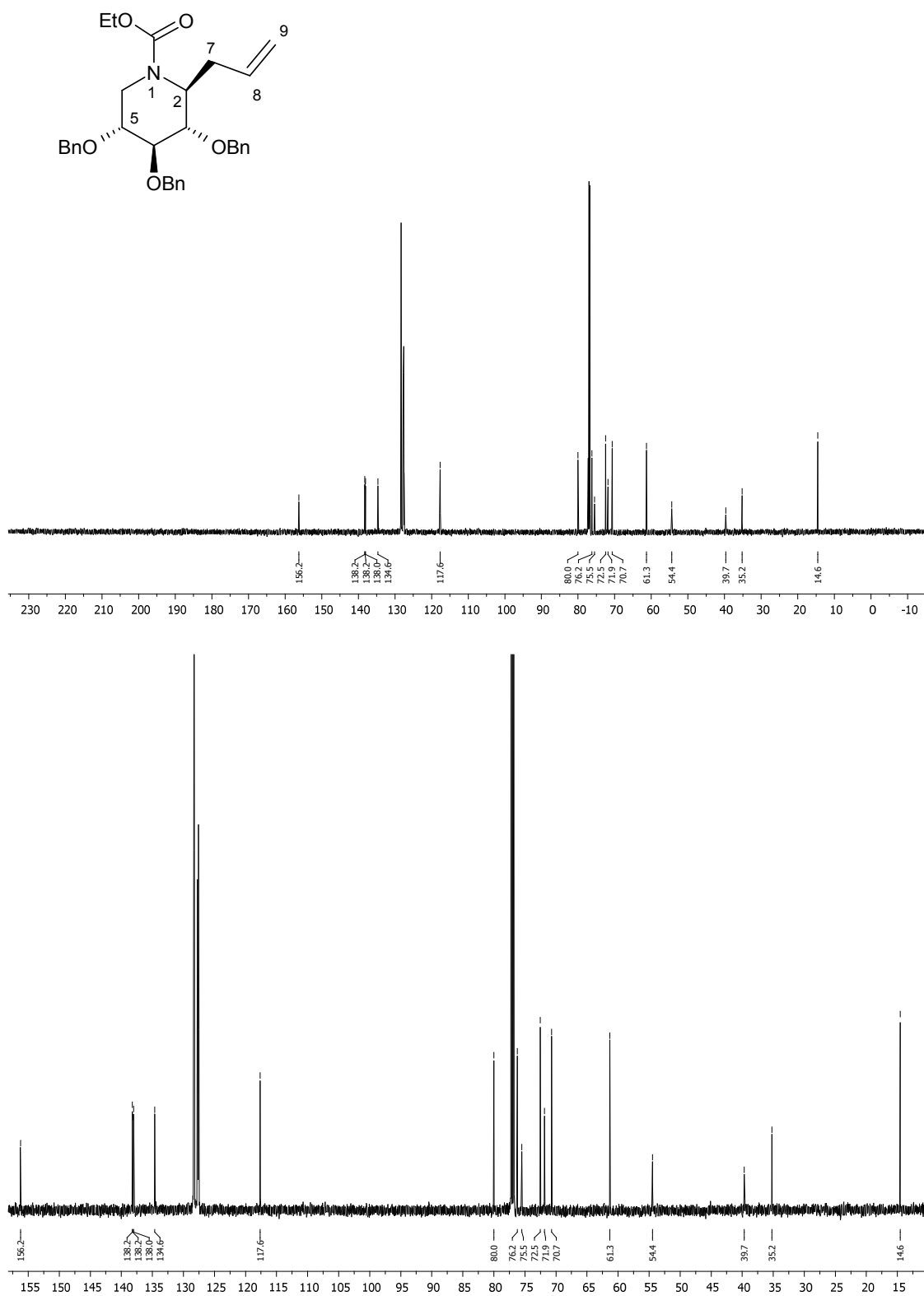
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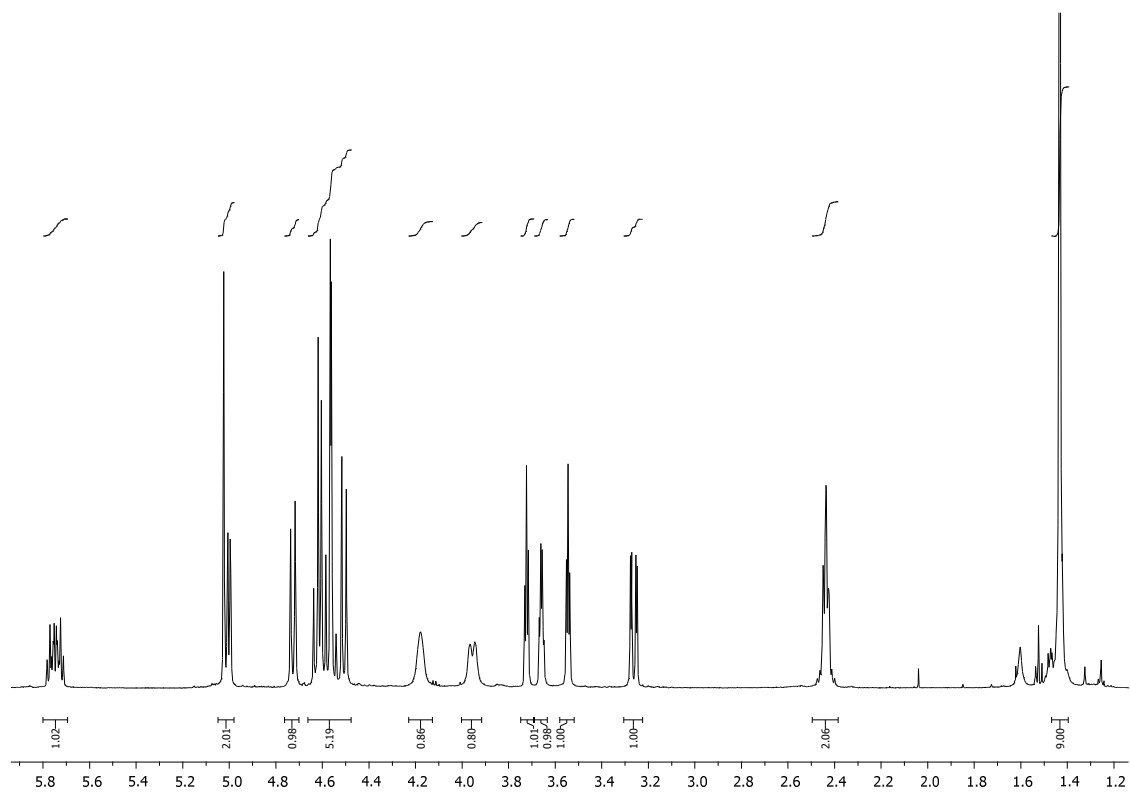
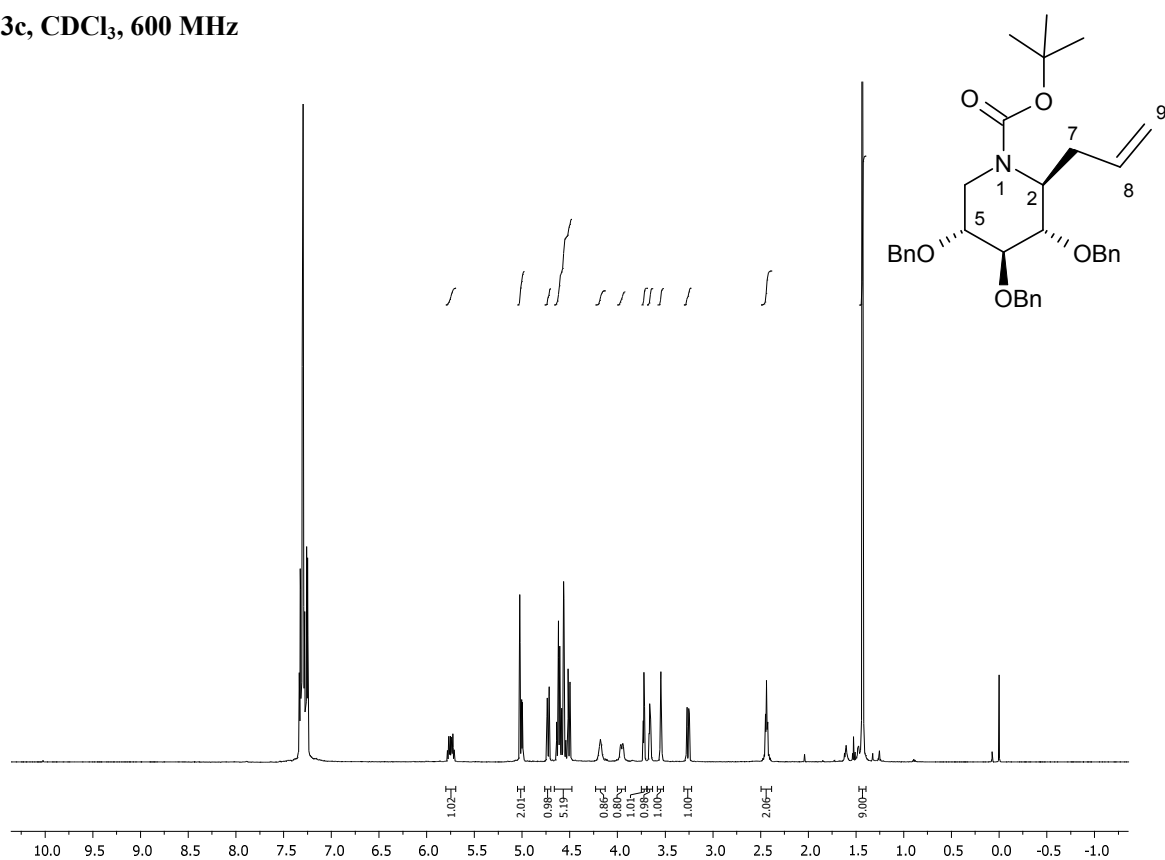
3b, CDCl₃, 600 MHz



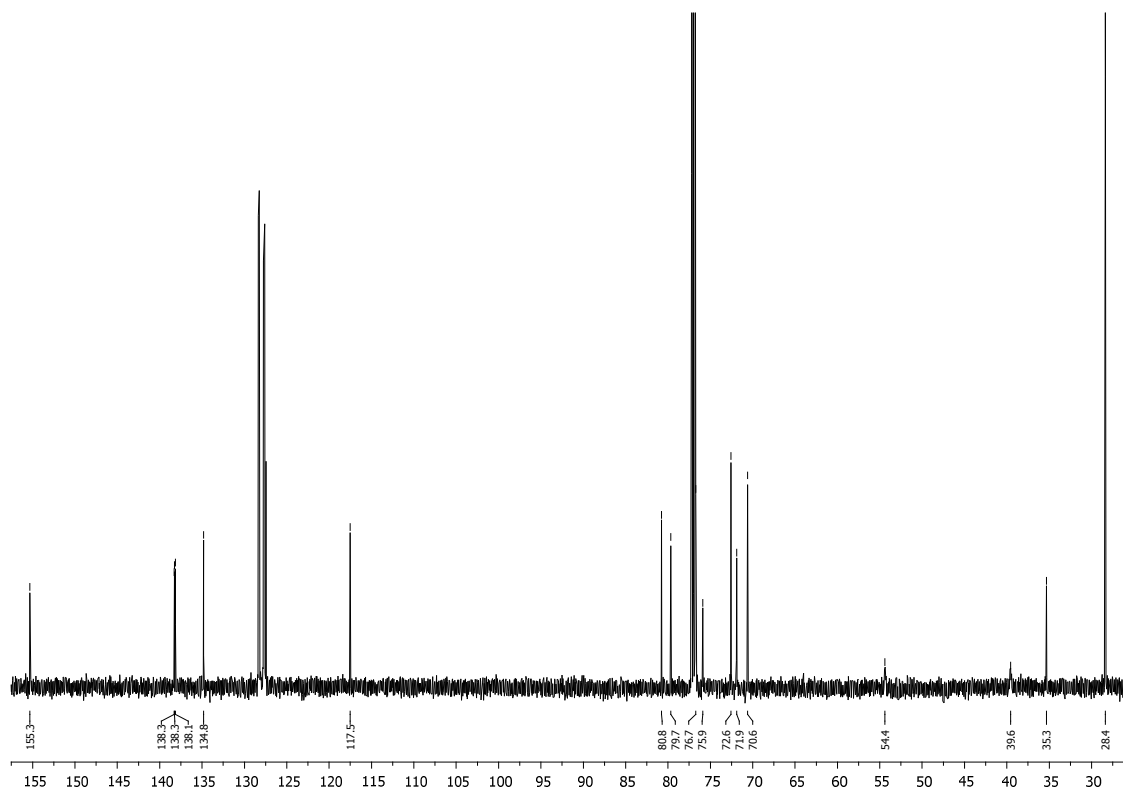
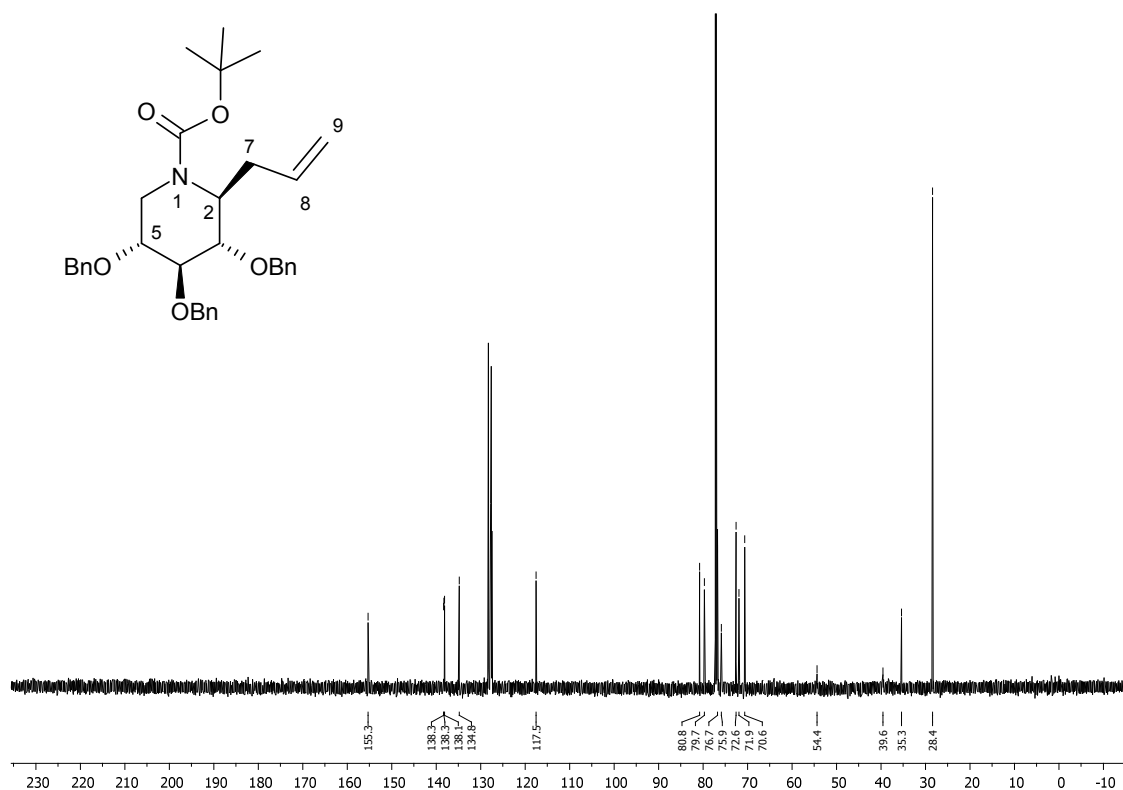
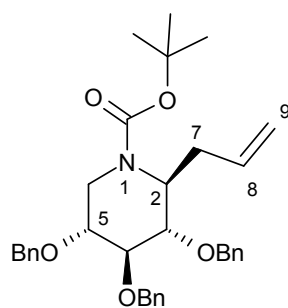
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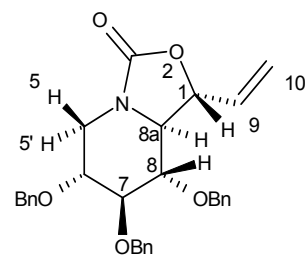
3c, CDCl₃, 600 MHz



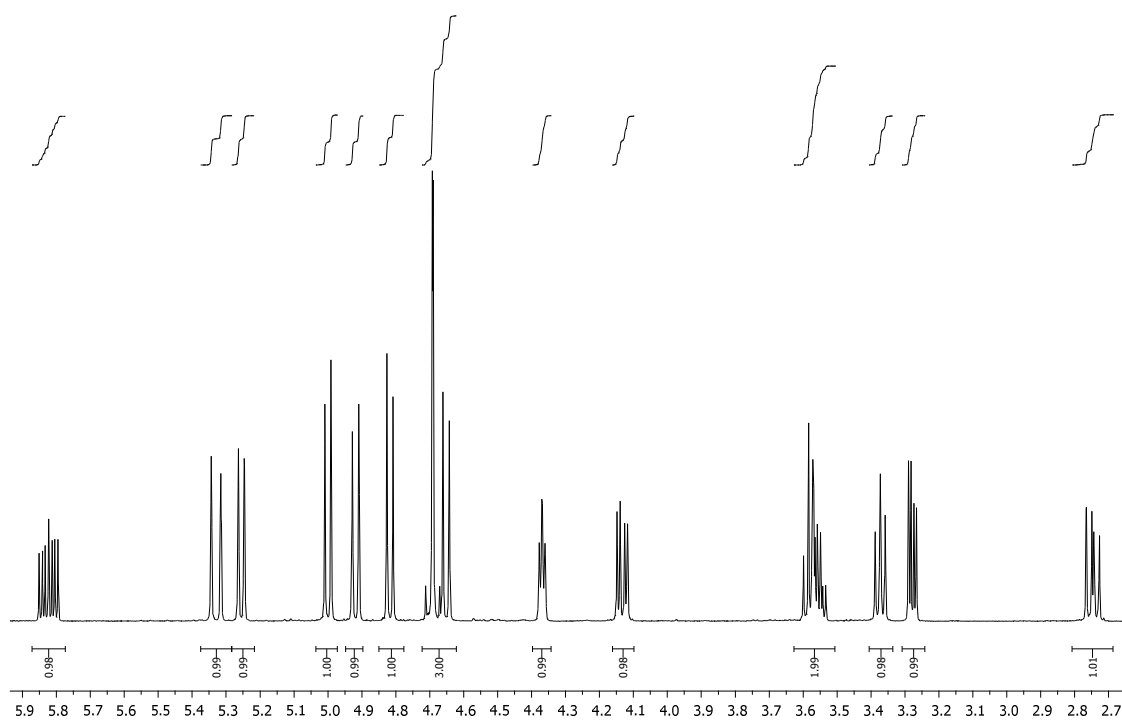
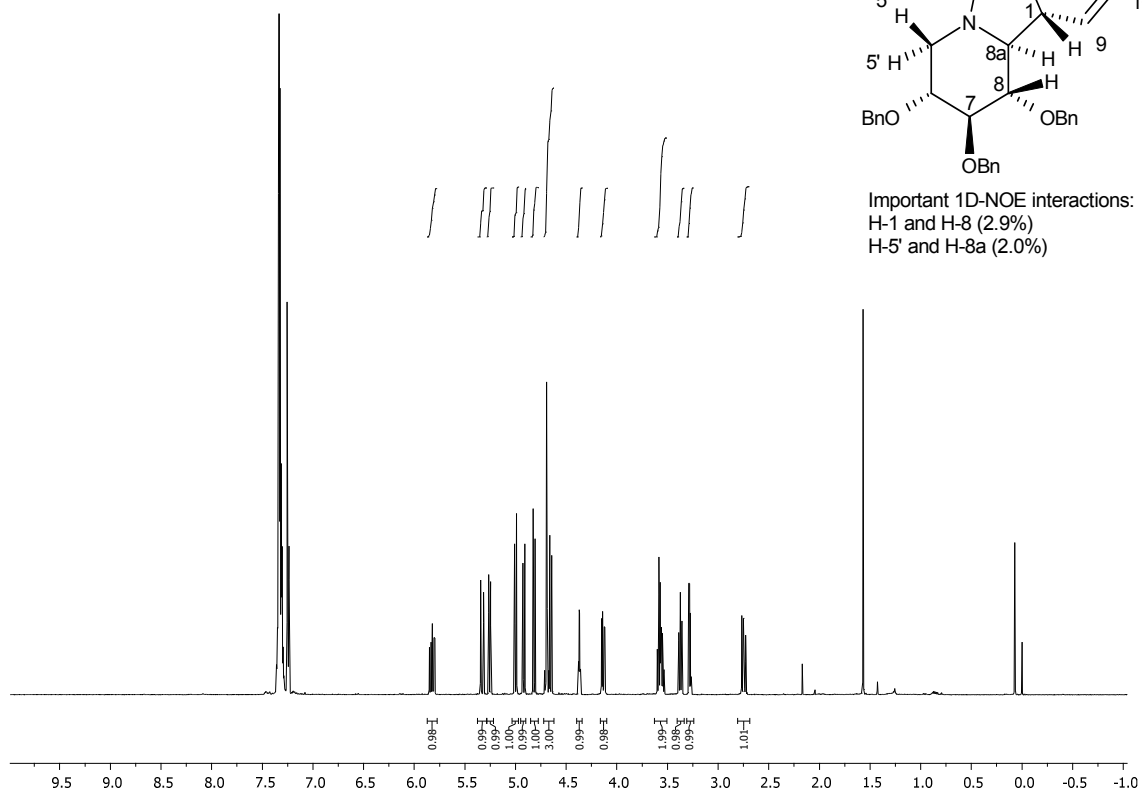
3c, CDCl₃, 150 MHz



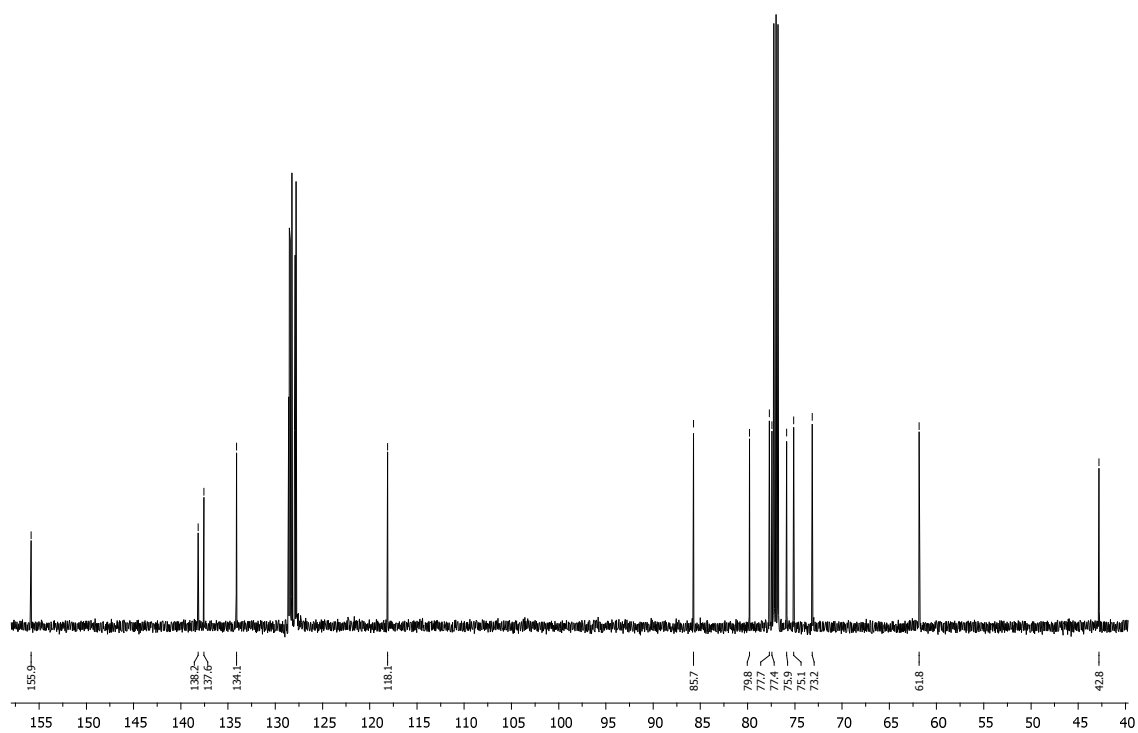
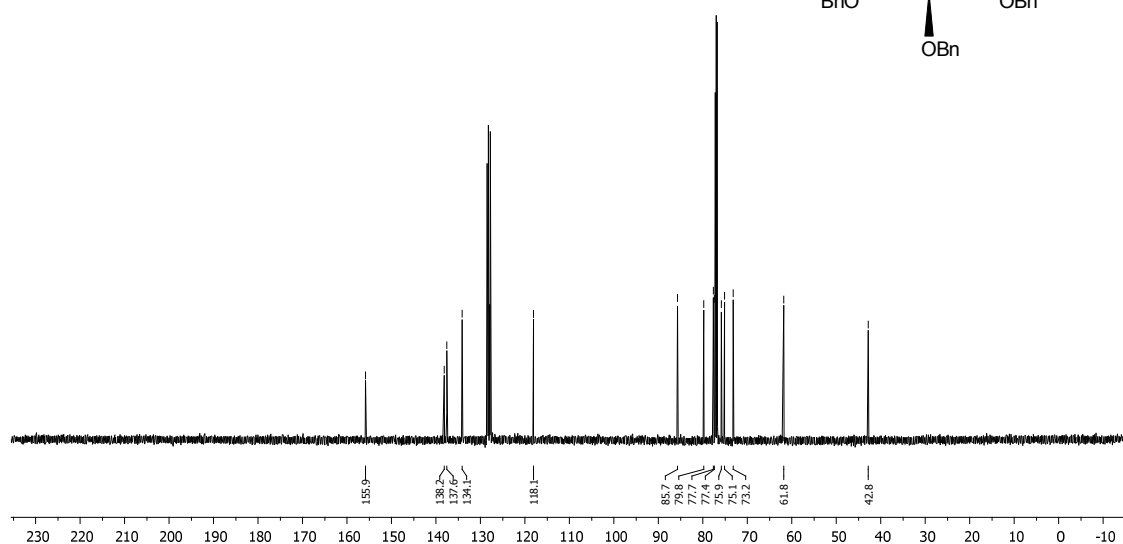
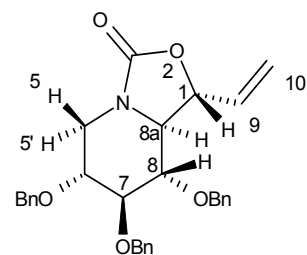
4, CDCl₃, 600 MHz



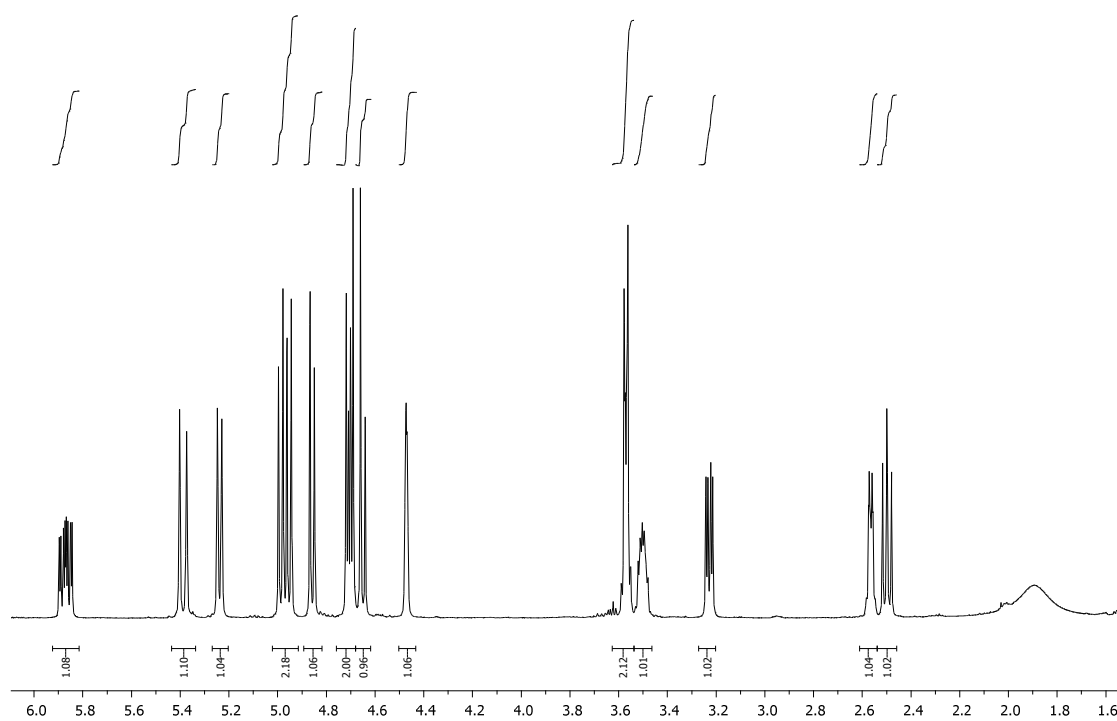
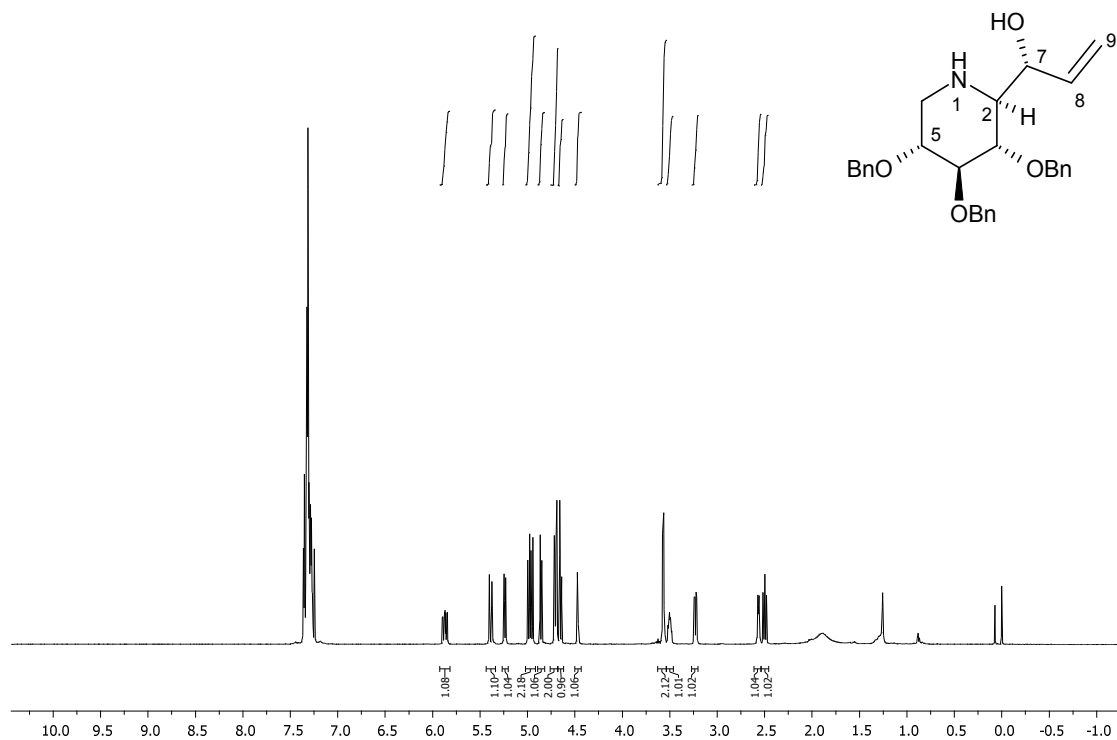
Important 1D-NOE interactions:
H-1 and H-8 (2.9%)
H-5' and H-8a (2.0%)



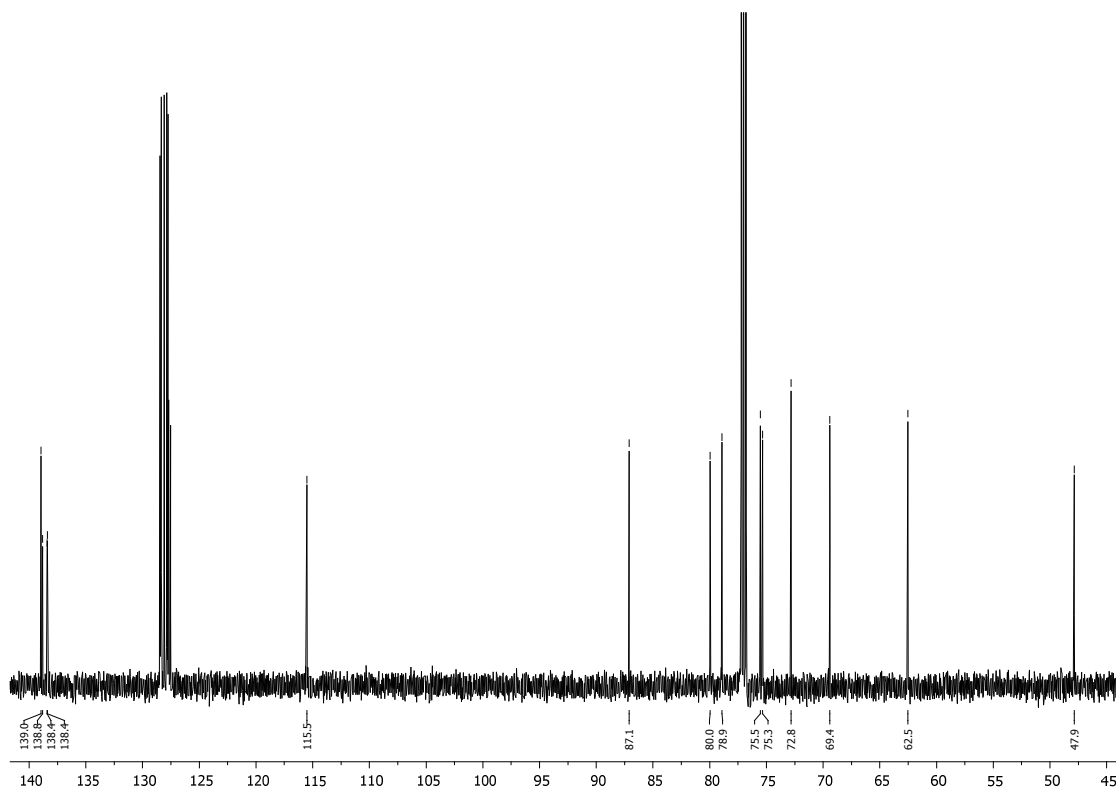
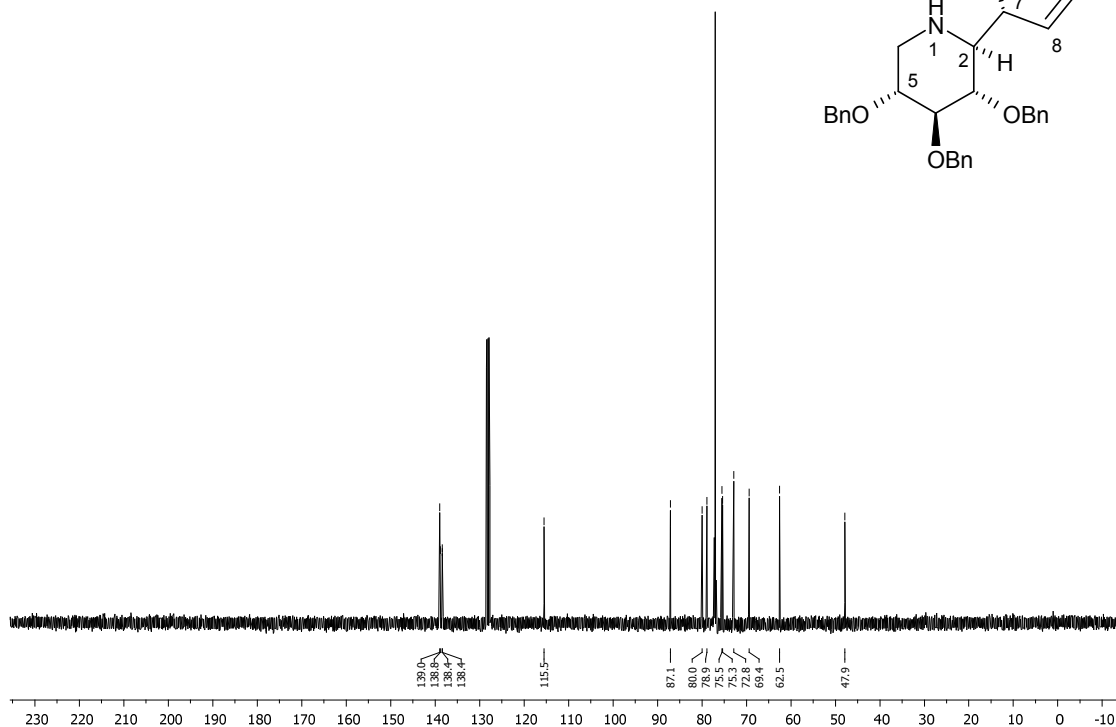
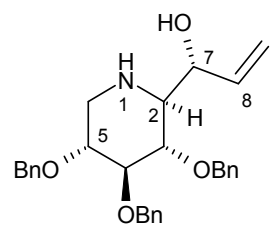
4, CDCl₃, 150 MHz



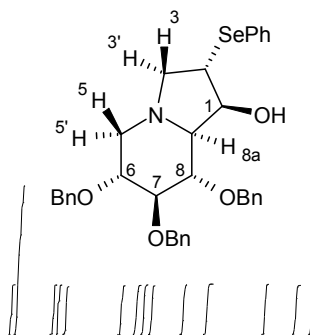
5, CDCl₃, 600 MHz



5, CDCl₃, 150 MHz



6a, C₆D₆, 600 MHz



Important 1D-NOE interactions:

H-1 and H-8a (2.4%)

H-2 and H-3 (1.7%)

H-3 and H-5 (1.1%)

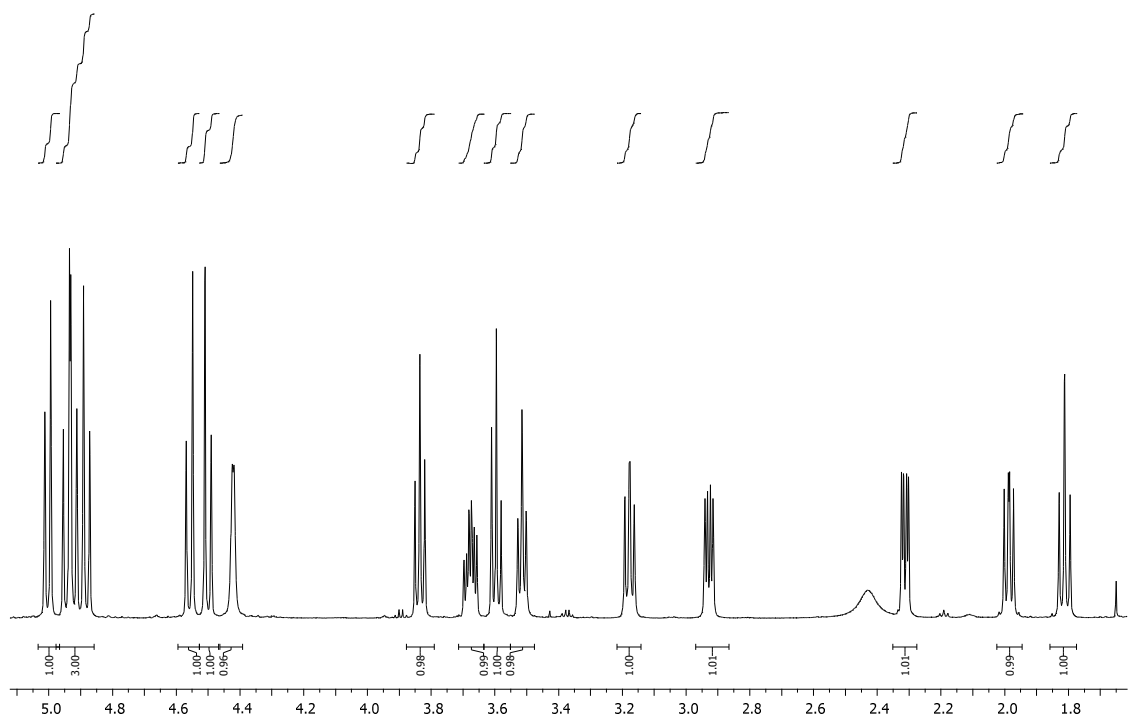
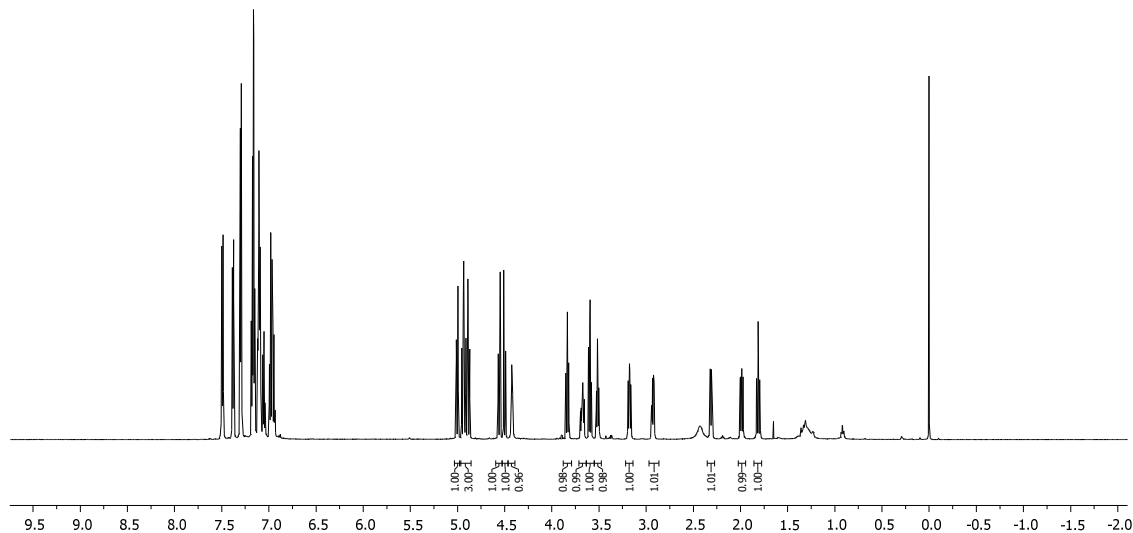
H-5' and H-8a (1.7%)

H-3' and H-8a (1.4%)

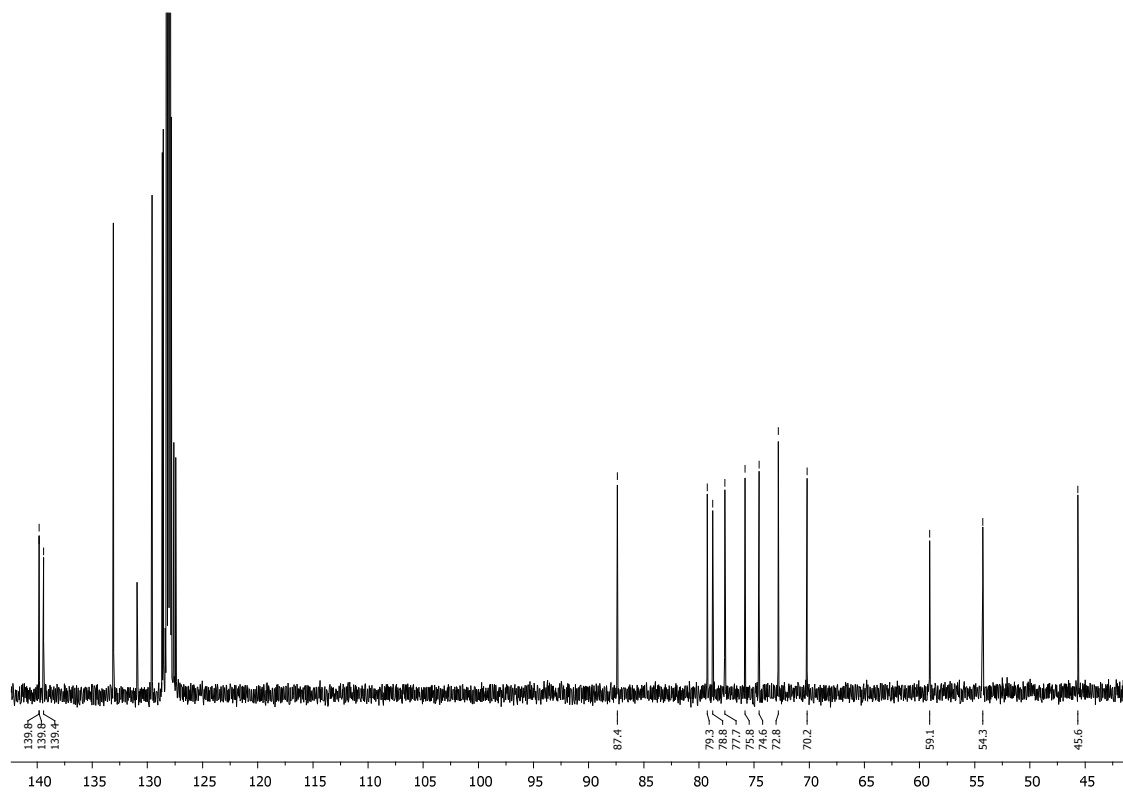
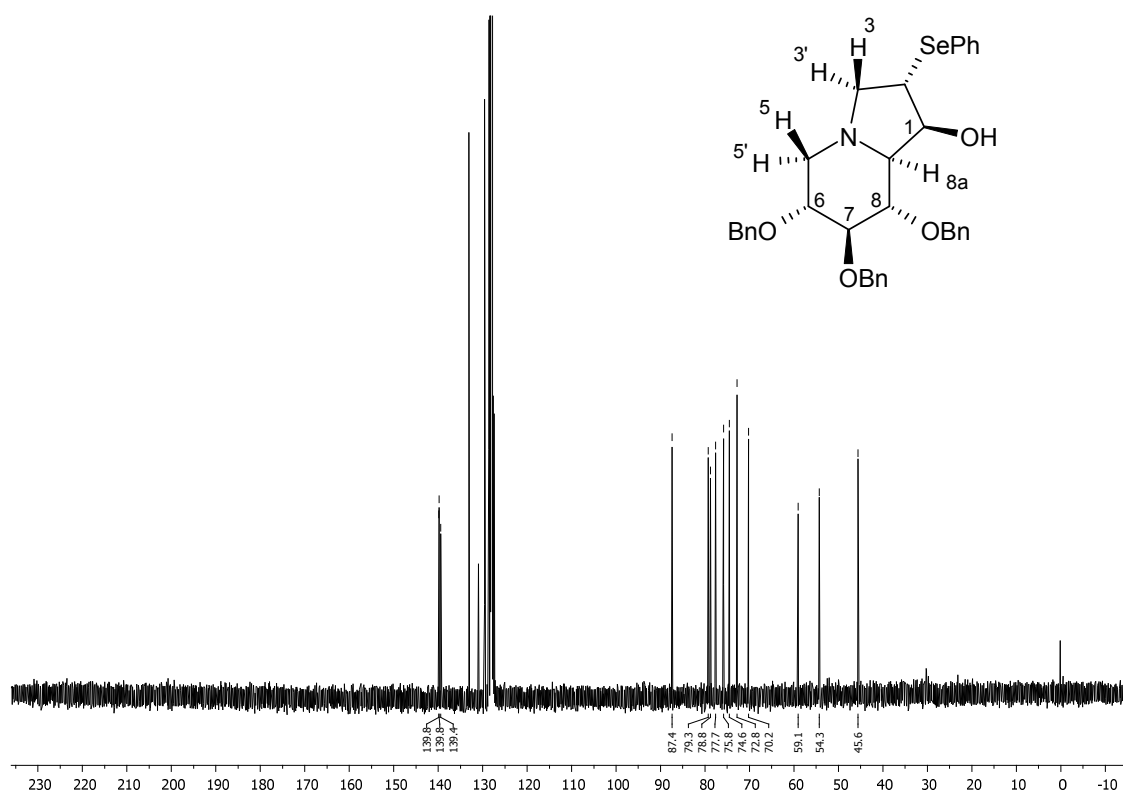
H-3' and H-5' (1.4%)

Important HMBC correlations:

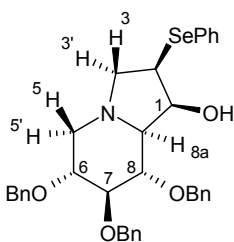
C-3 and H-5; C-3 and H-5'; C-5 and H-3'



6a, C₆D₆, 150 MHz



6b, C₆D₆, 600 MHz

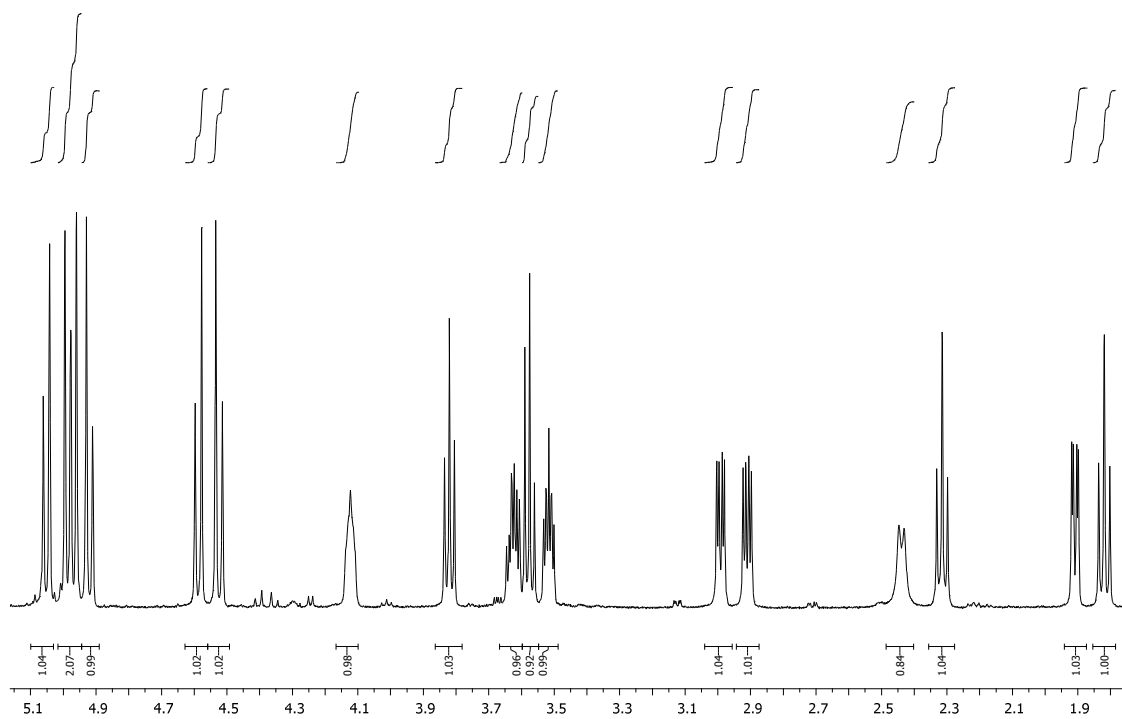
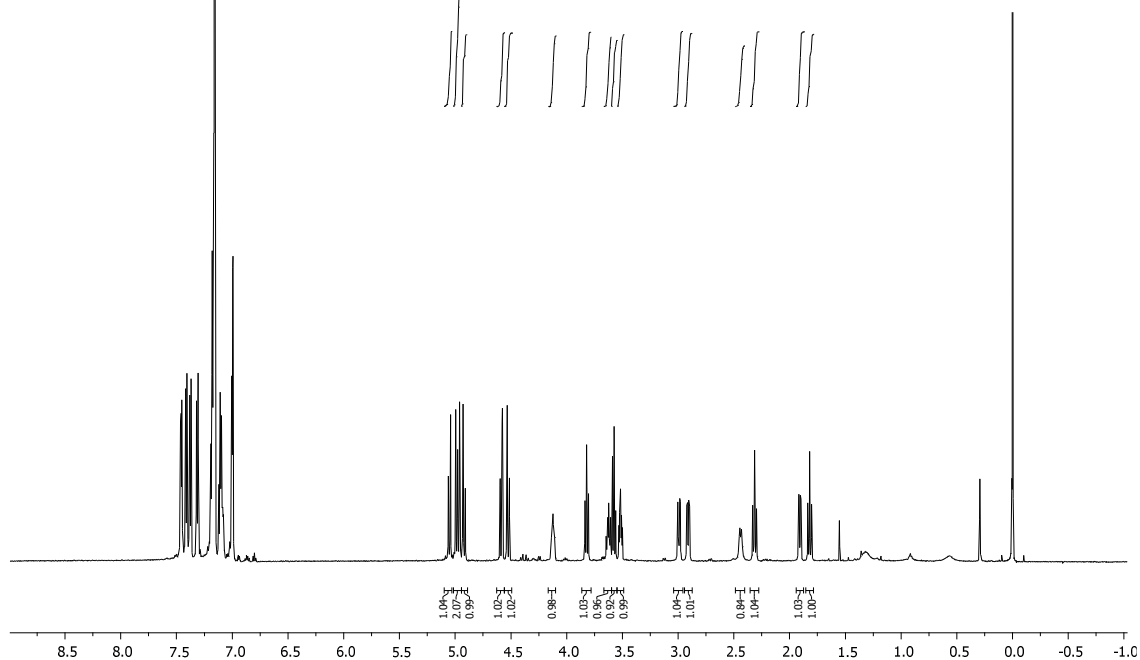


Important 1D-NOE interactions:

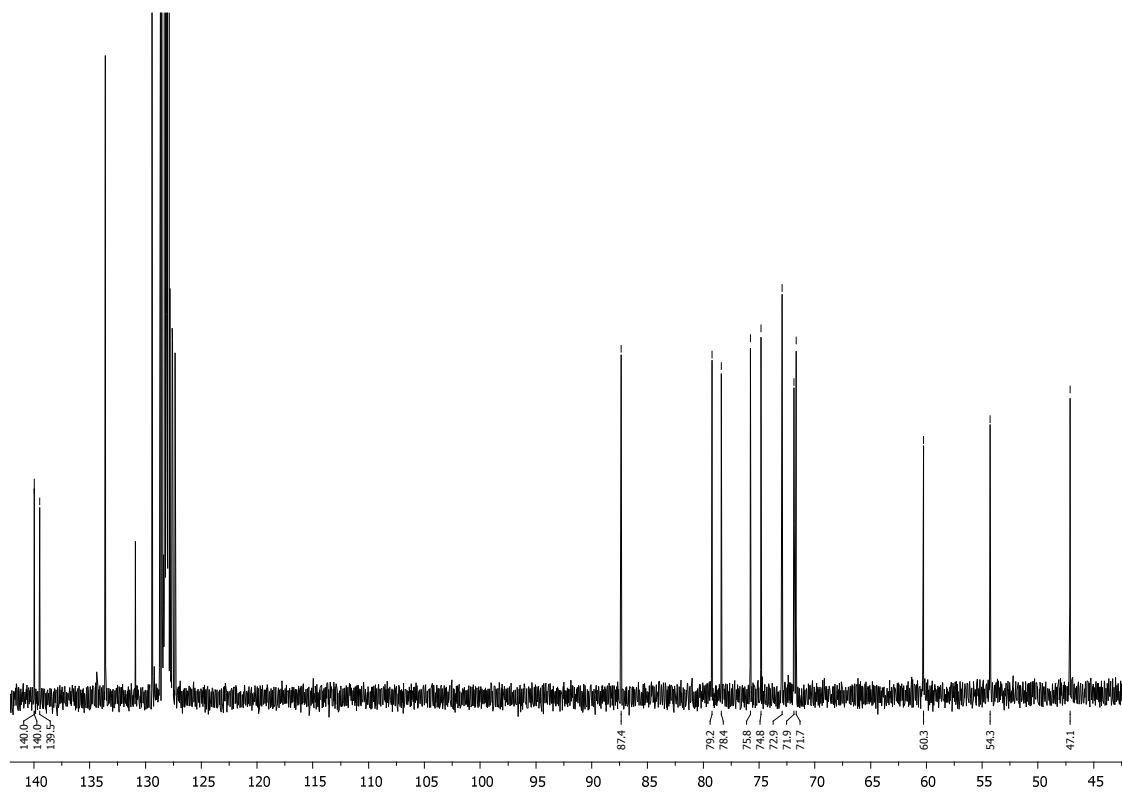
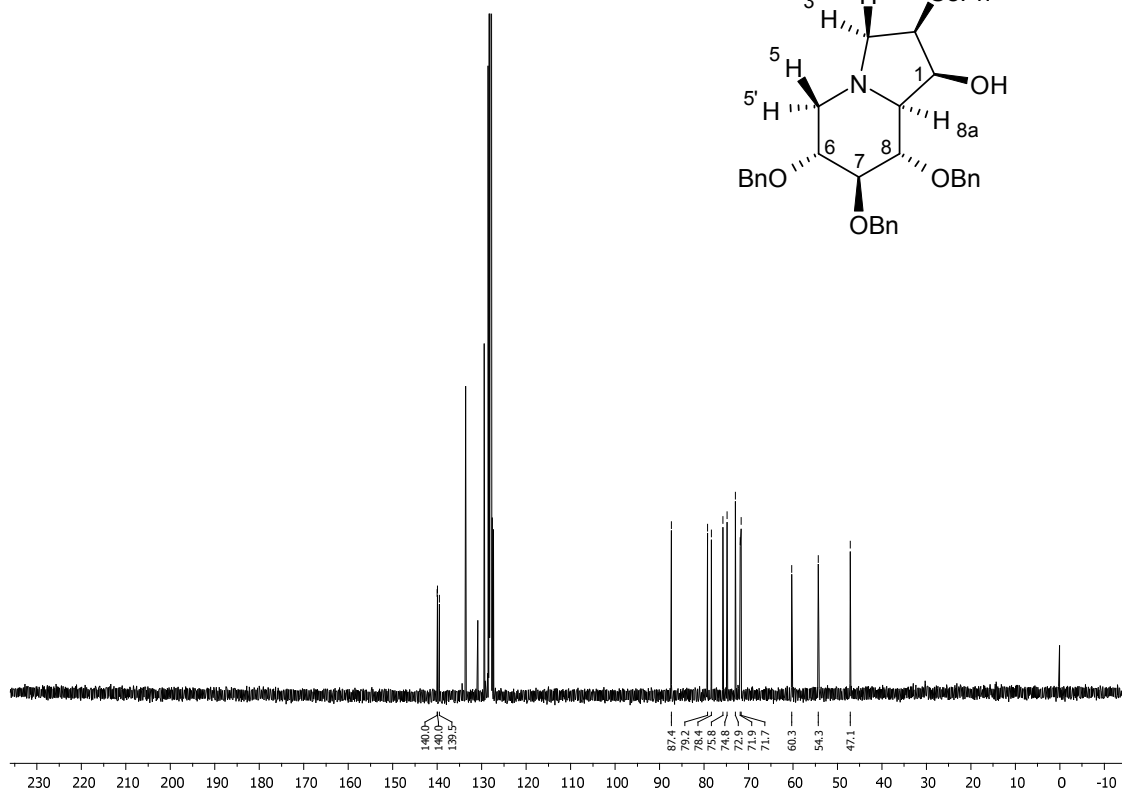
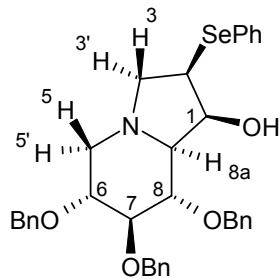
- H-1 and H-8a (2.8%)
- H-2 and H-8a (1.2%)
- H-1 and H-2 (3.3%)
- H-5 and H-3 (1.1%)
- OH and H-3 (0.4%)
- OH and H-8 (1.5%)

Important HMBC correlations:

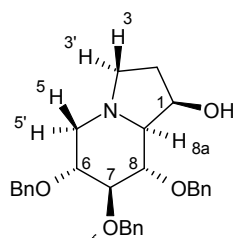
- C-5 and H-3'; C-3 and H-5; C-3 and H-5'



6b, C₆D₆, 150 MHz

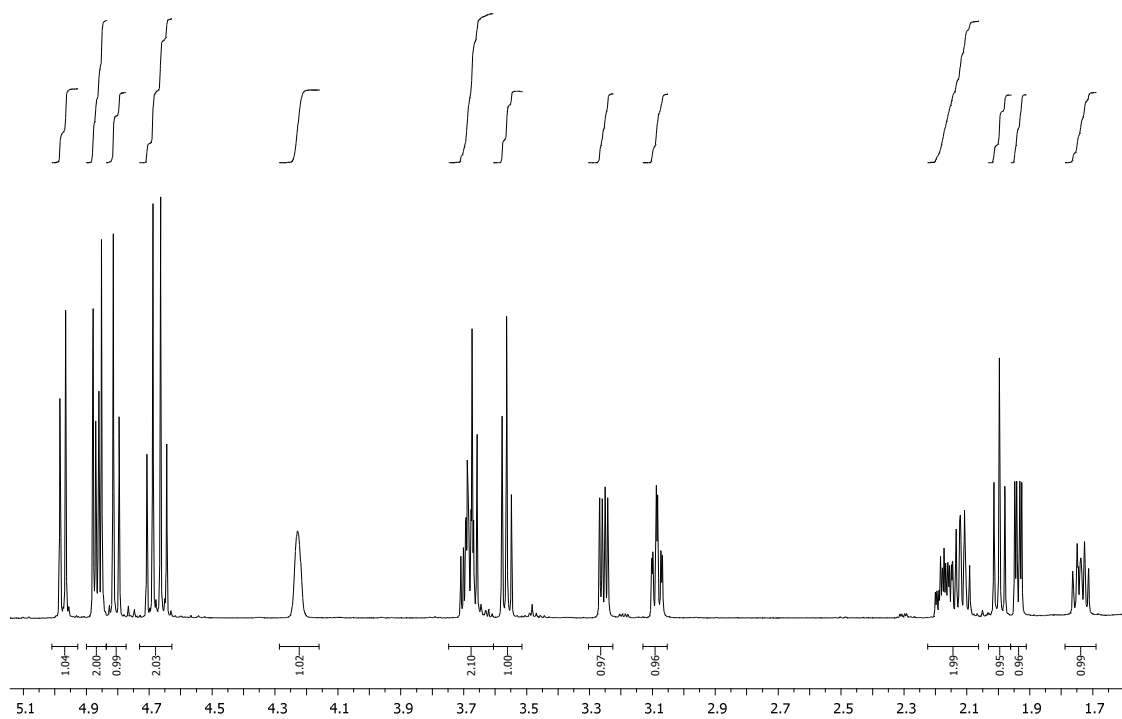
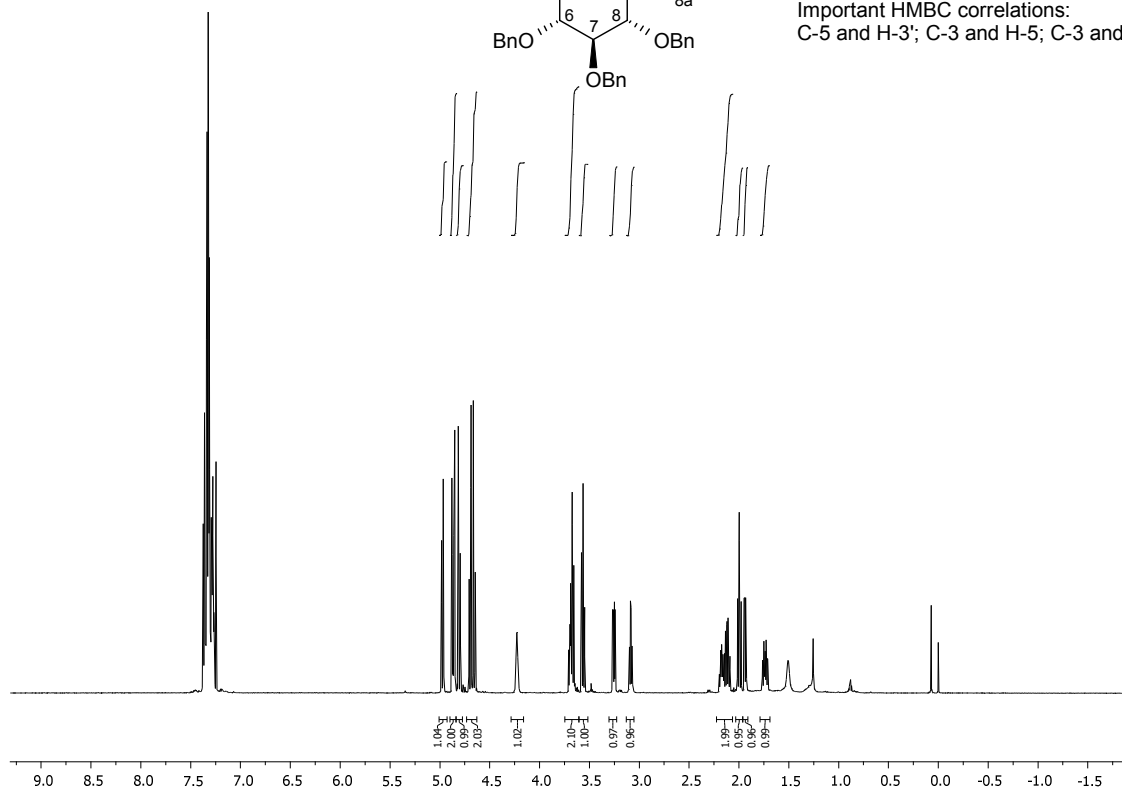


7, CDCl₃, 600 MHz

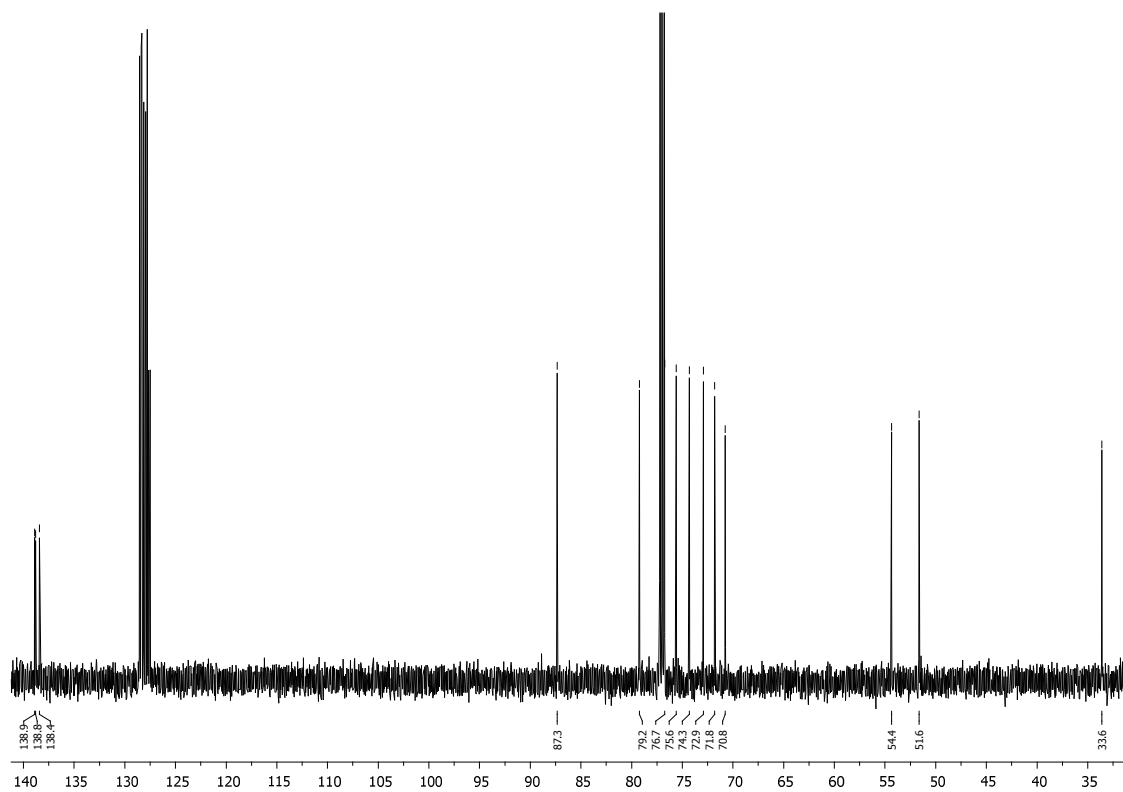
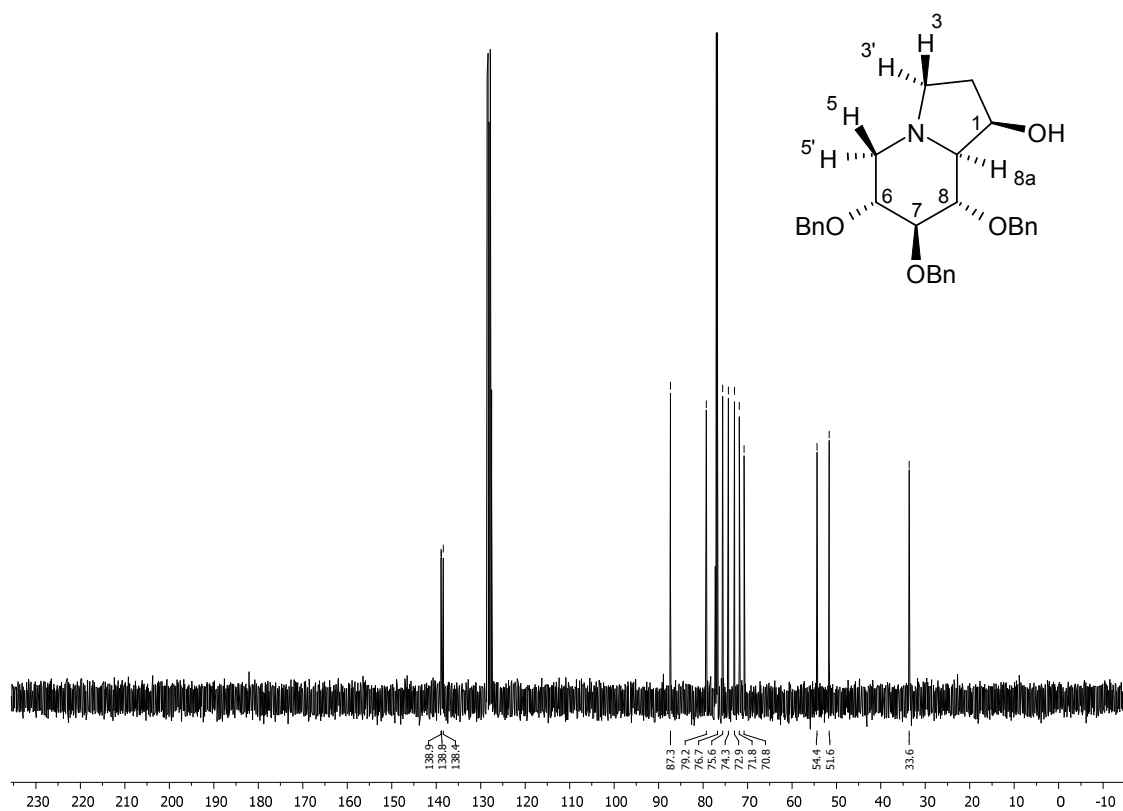


Important 2D-NOESY interactions:
H-3' and H-5'; H-3 and H-5; H-3' and H-8a;
H-1 and H-8a

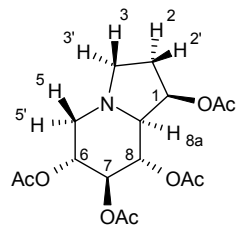
Important HMBC correlations:
C-5 and H-3'; C-3 and H-5; C-3 and H-5'



7, CDCl₃, 150 MHz

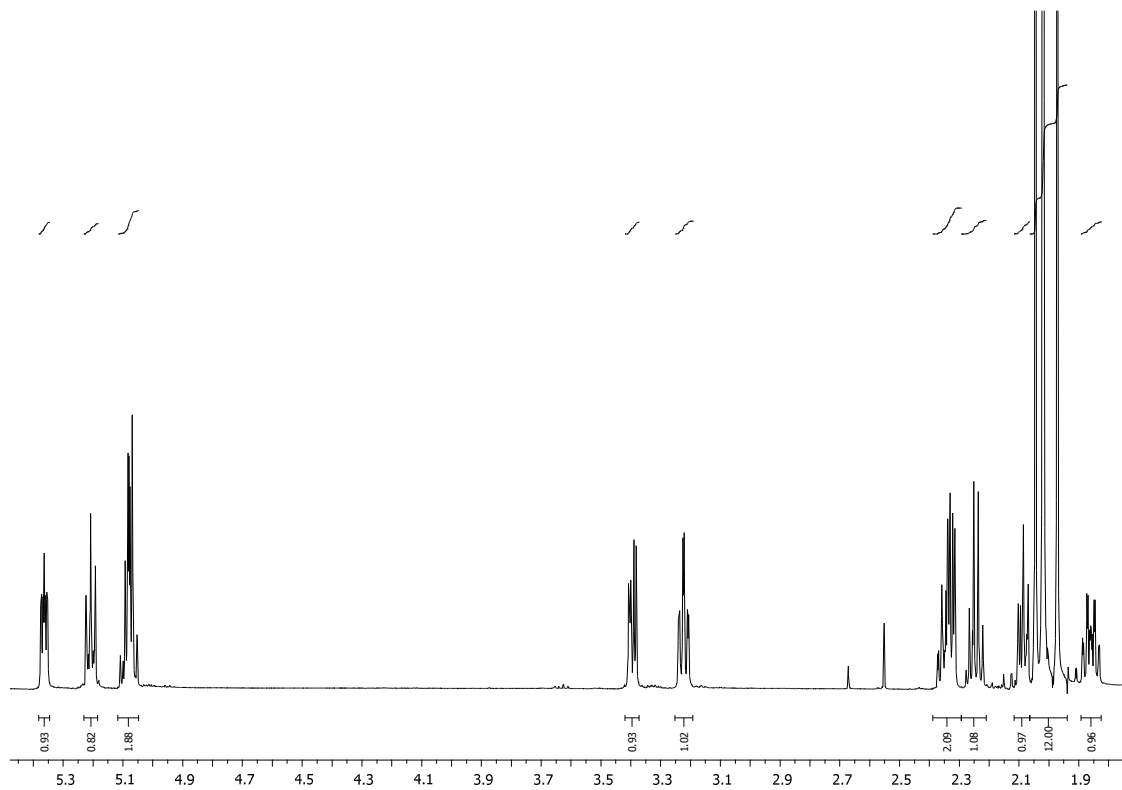
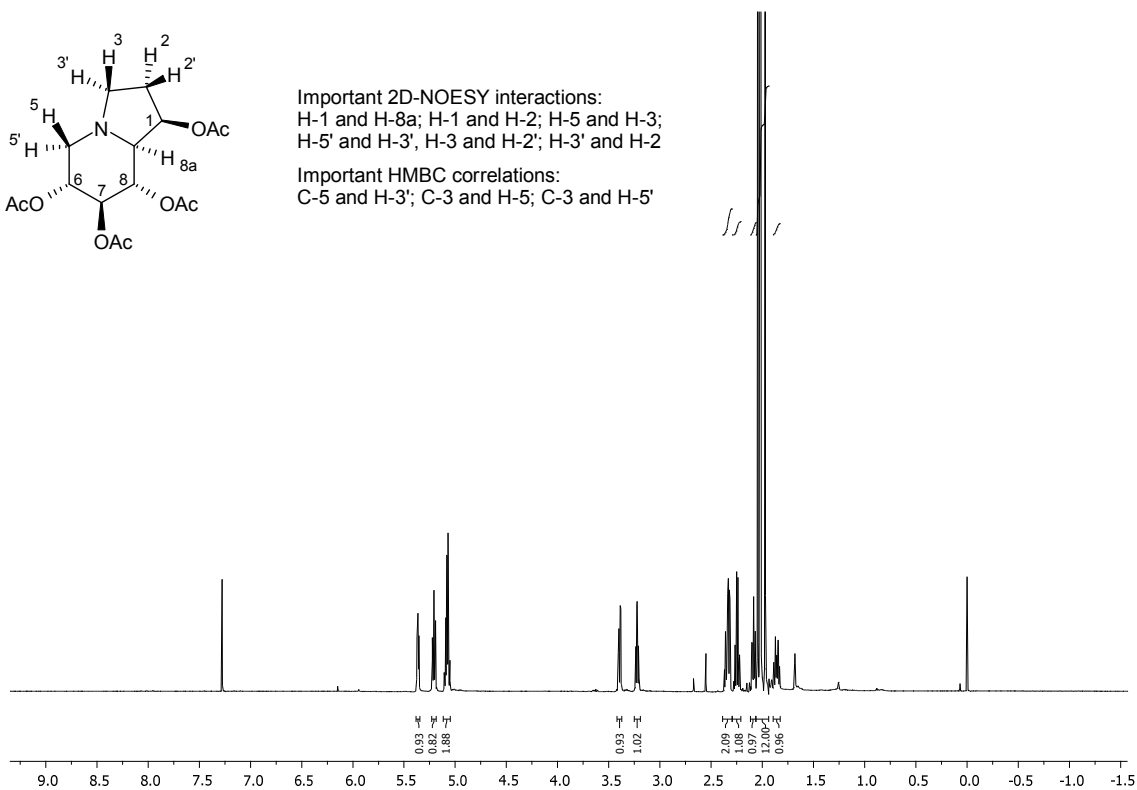


8, CDCl₃, 600 MHz

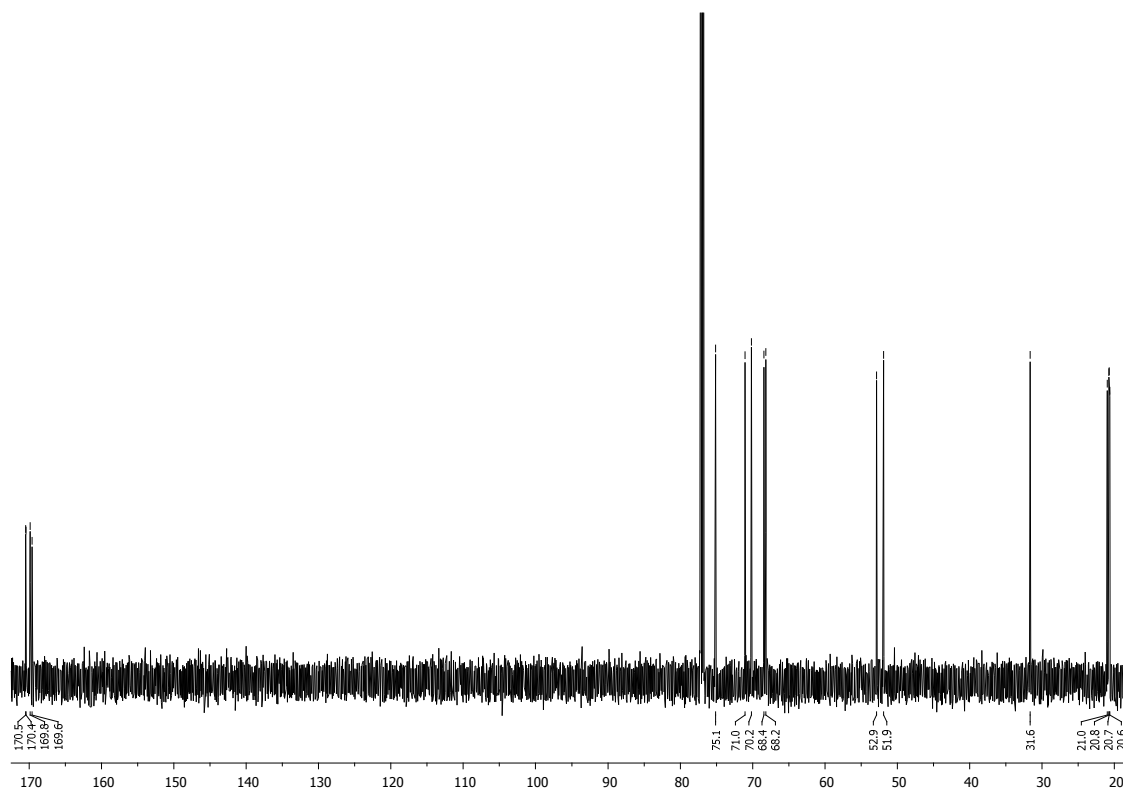
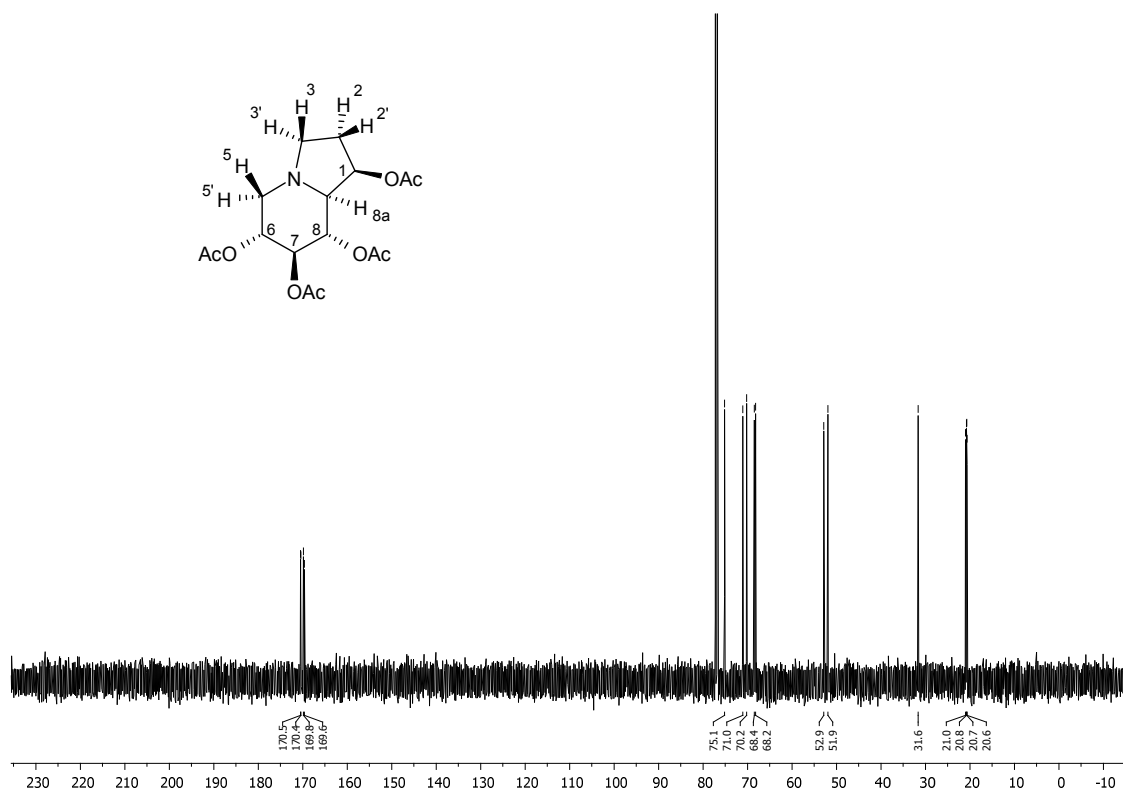


Important 2D-NOESY interactions:
H-1 and H-8a; H-1 and H-2; H-5 and H-3;
H-5' and H-3', H-3 and H-2'; H-3' and H-2

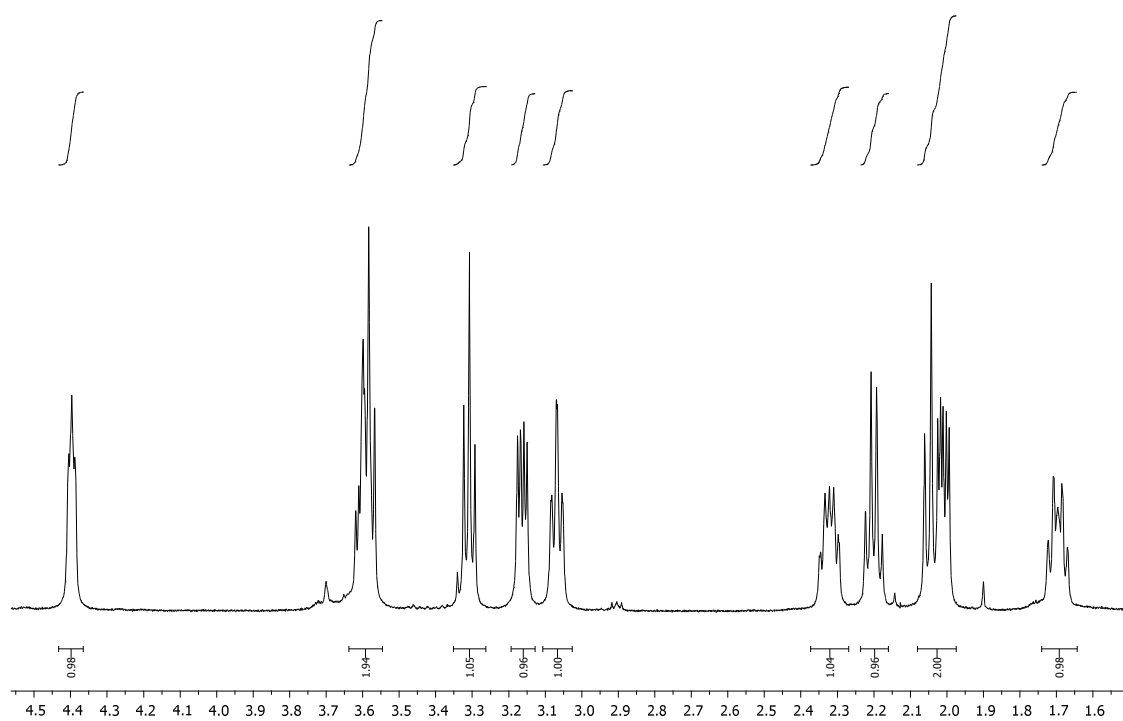
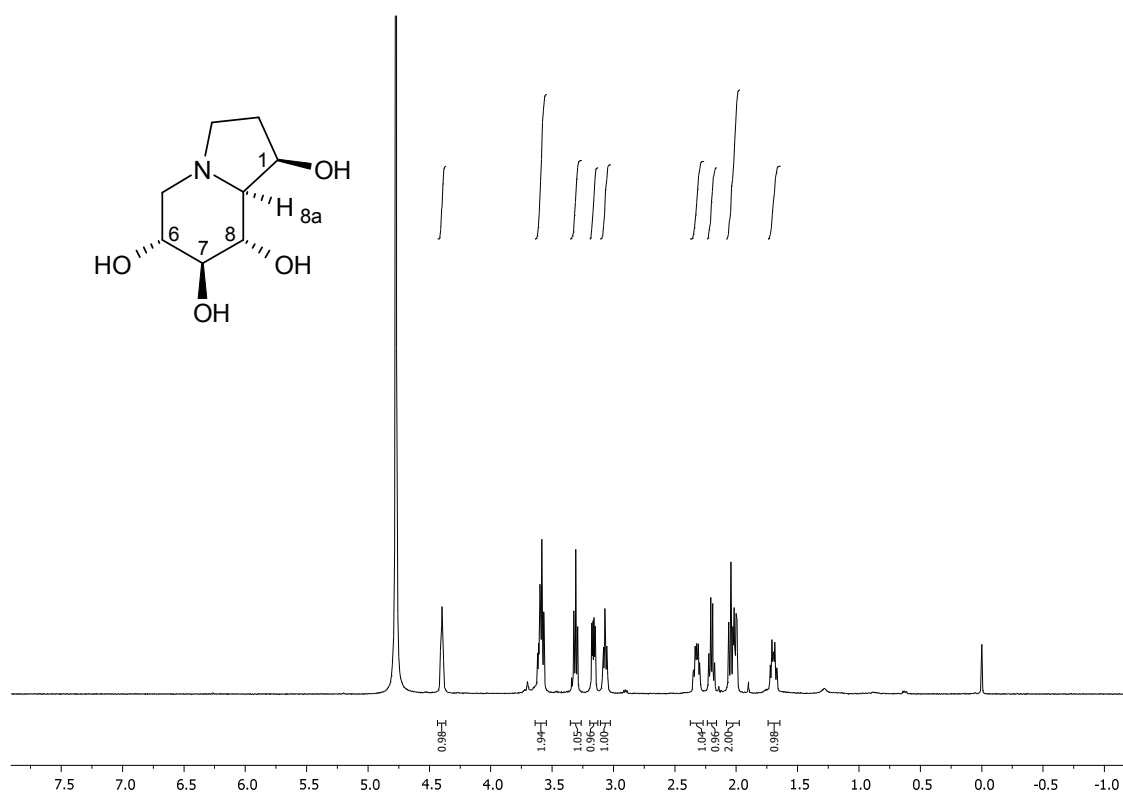
Important HMBC correlations:
C-5 and H-3'; C-3 and H-5; C-3 and H-5'



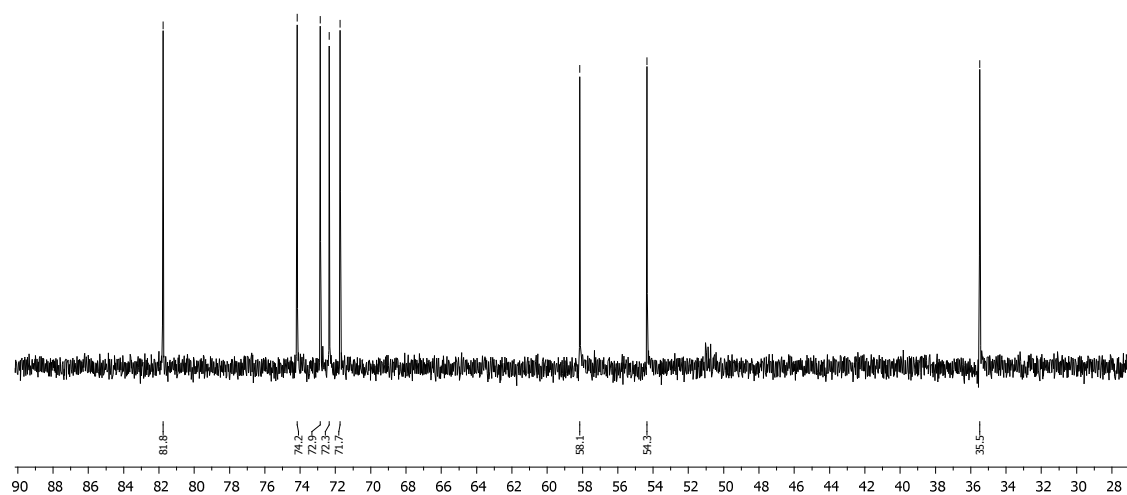
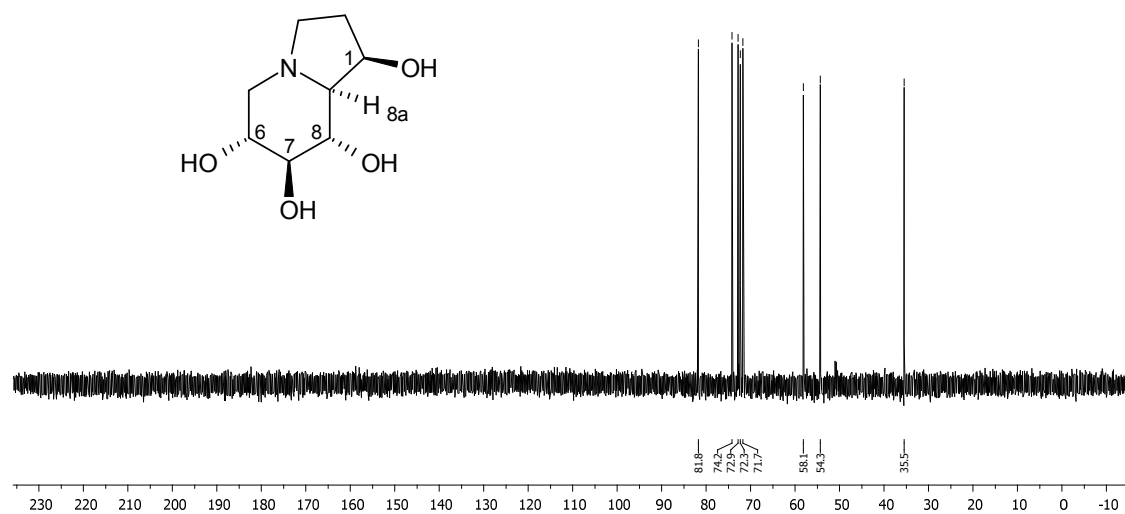
8, CDCl₃, 150 MHz



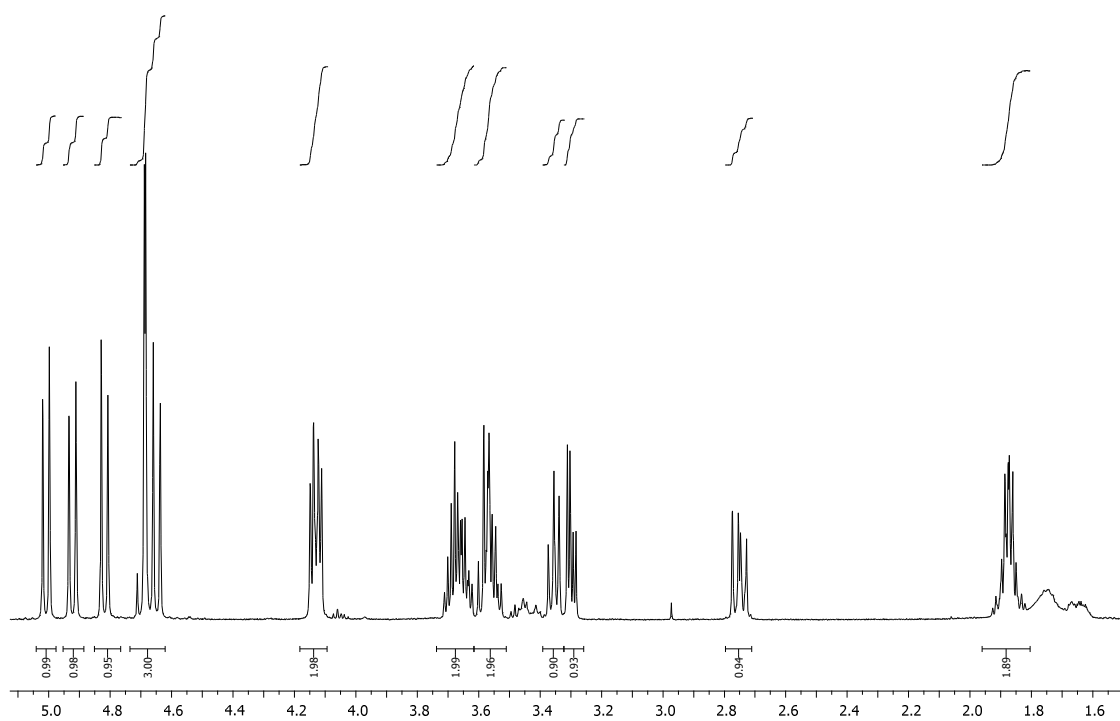
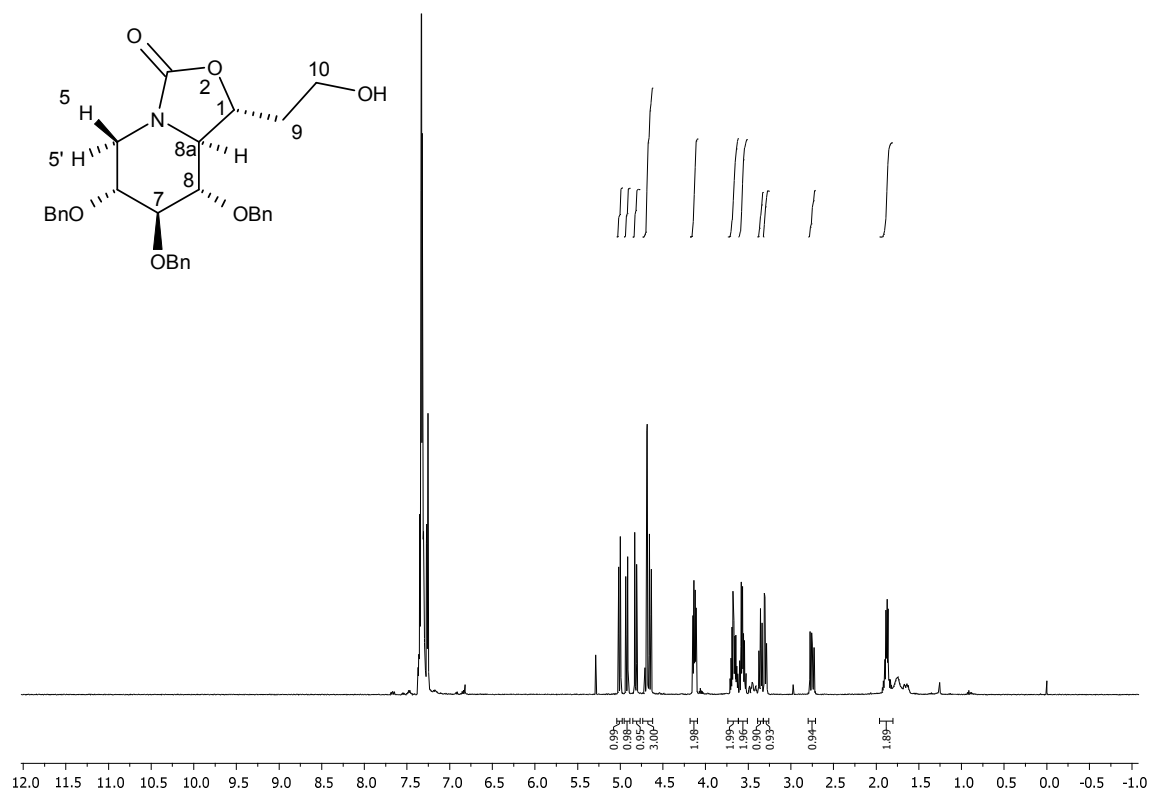
9, D₂O, 600 MHz



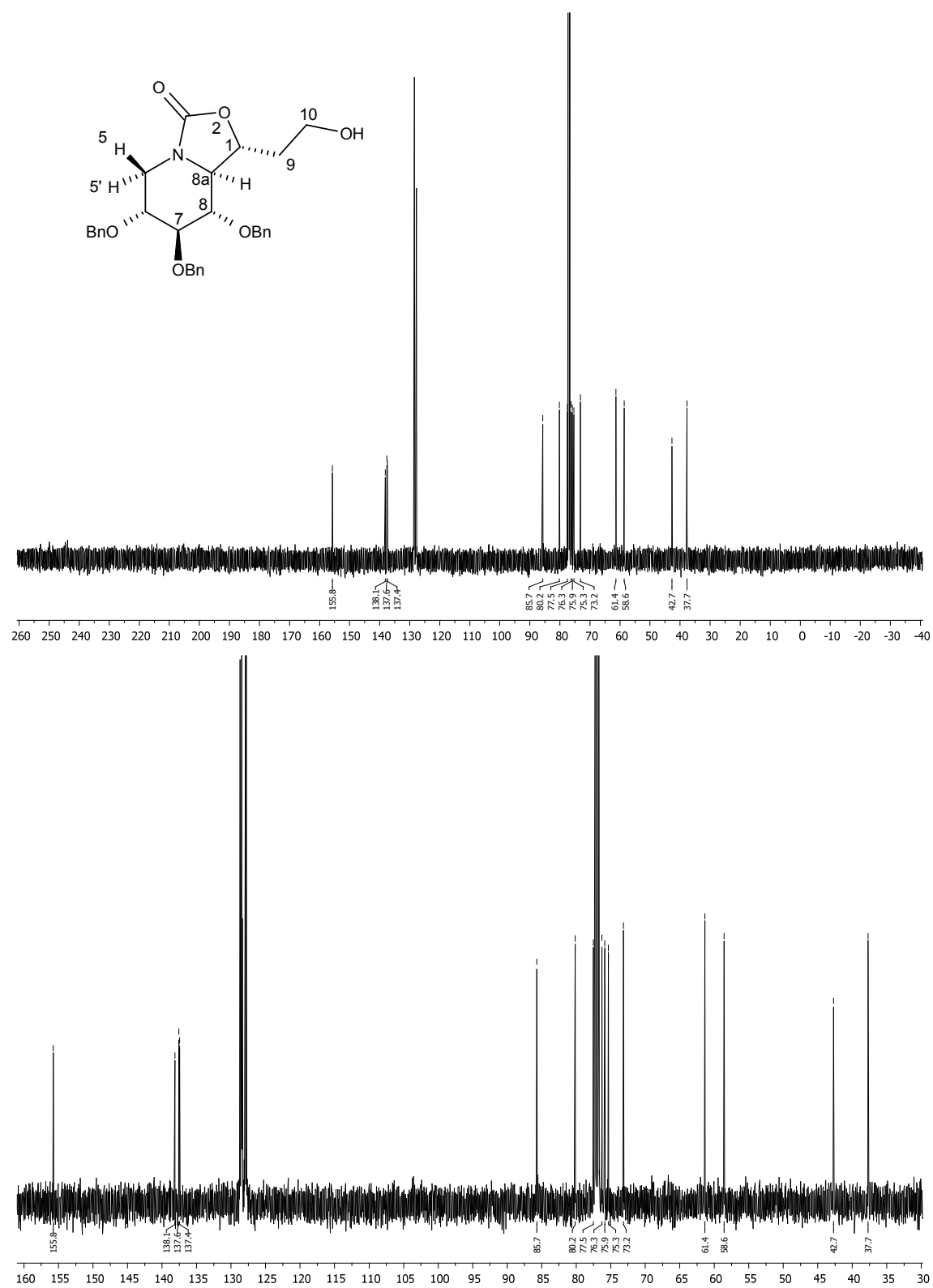
9, D₂O, 150 MHz



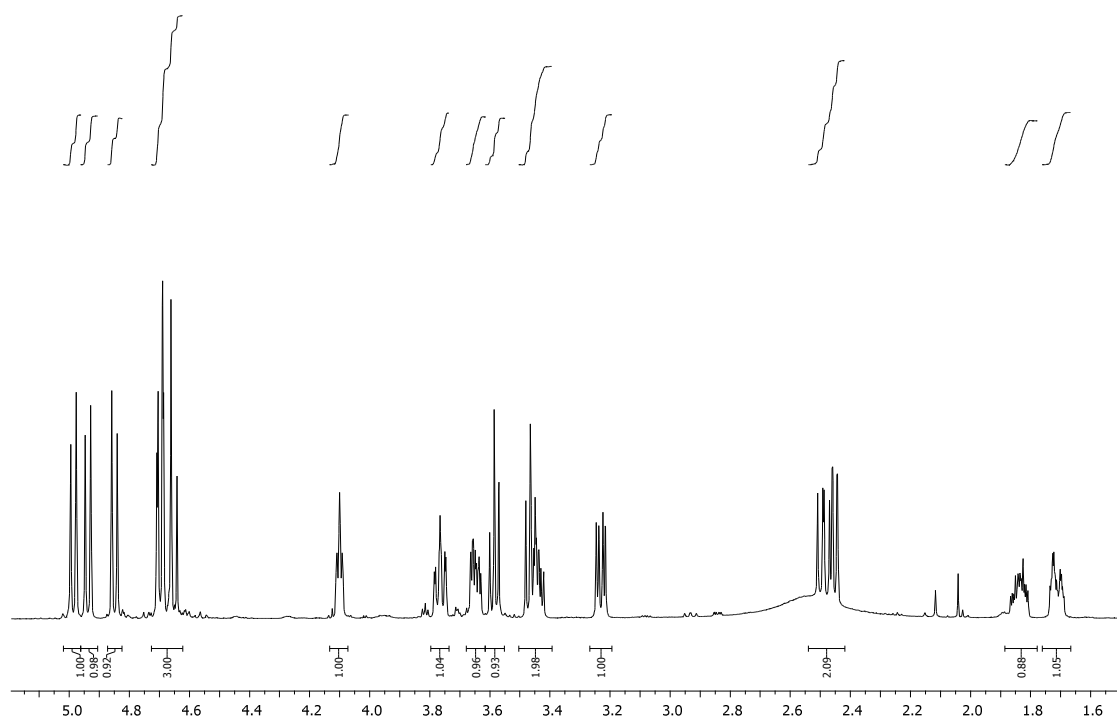
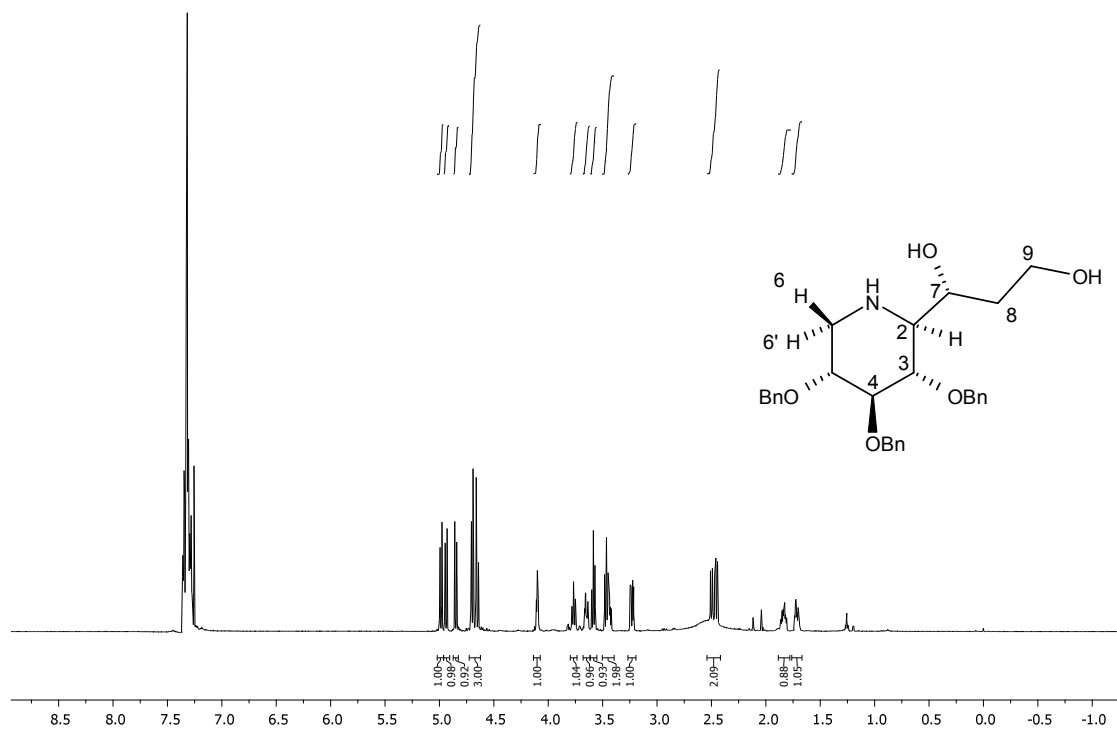
10, CDCl₃, 500 MHz



10, CDCl₃, 125 MHz



11, CDCl₃, 600 MHz



11, CDCl₃, 150 MHz

