

Supporting Information

Synthesis of a tetrasaccharide and its glycoconjugate corresponding to the capsular polysaccharide of *Neisseria meningitidis* serogroup X and its immunochemical studies

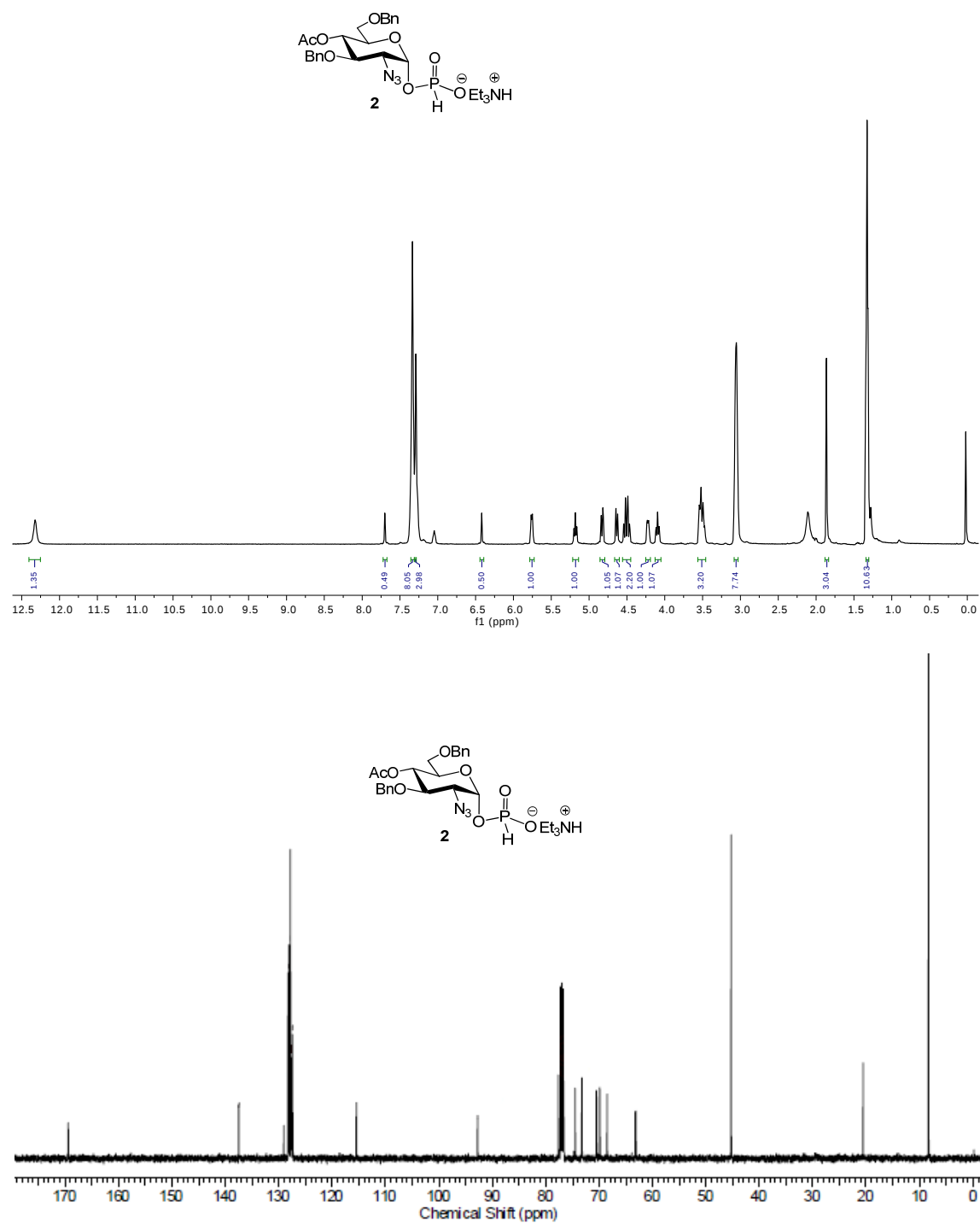
Kishore R. Harale,¹ Nilesh B. Dumare,¹ Deepti Singh,¹ Anup Kumar Misra,² Manoj Kumar Chhikara^{1*}

¹MSD Wellcome Trust Hilleman Laboratories Pvt. Ltd.,
2nd Floor, Nanotechnology Building, Jamia Hamdard, Hamdard Nagar, New Delhi 110062,
India; E-mail: manoj.kumar@hillemanlabs.org

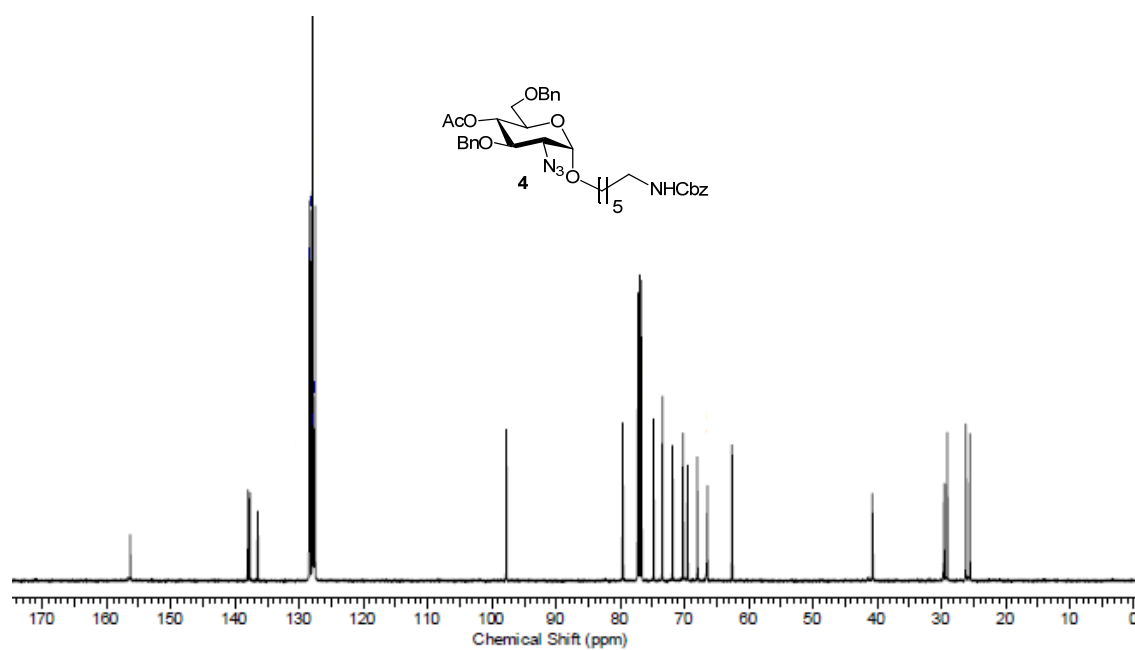
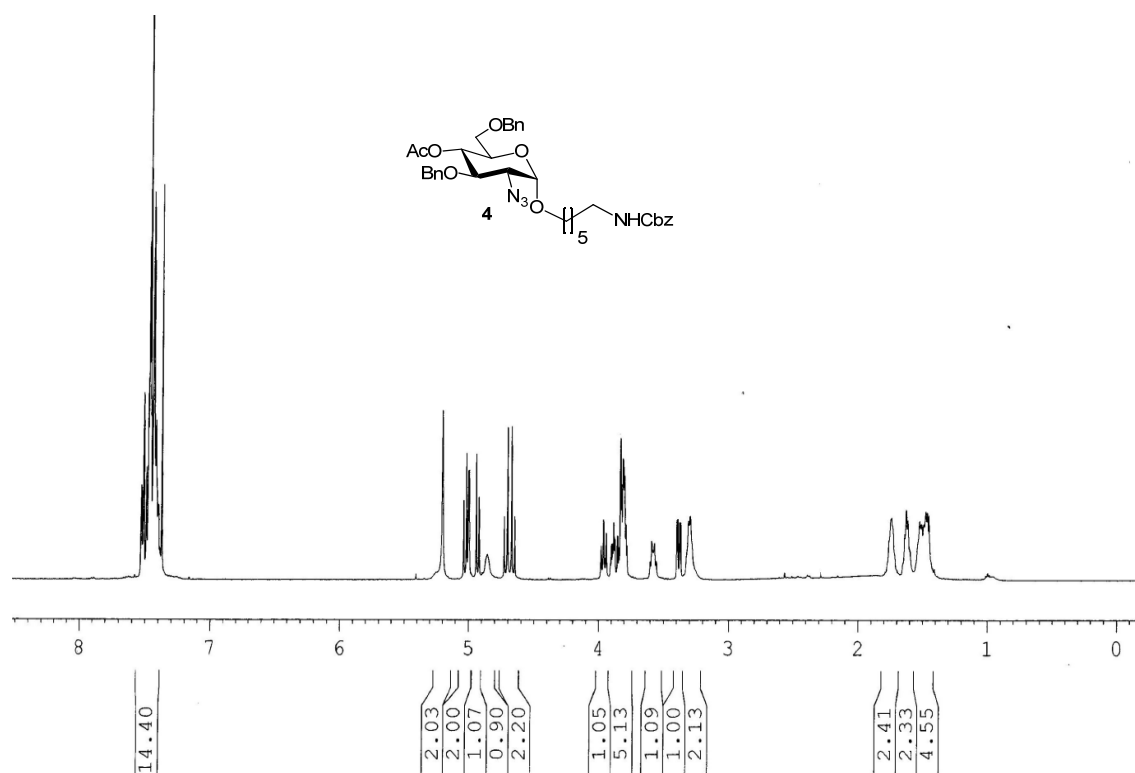
²Bose Institute, Division of Molecular Medicine, P-1/12, C.I.T. Scheme VII M, Kolkata
700054, India

Index

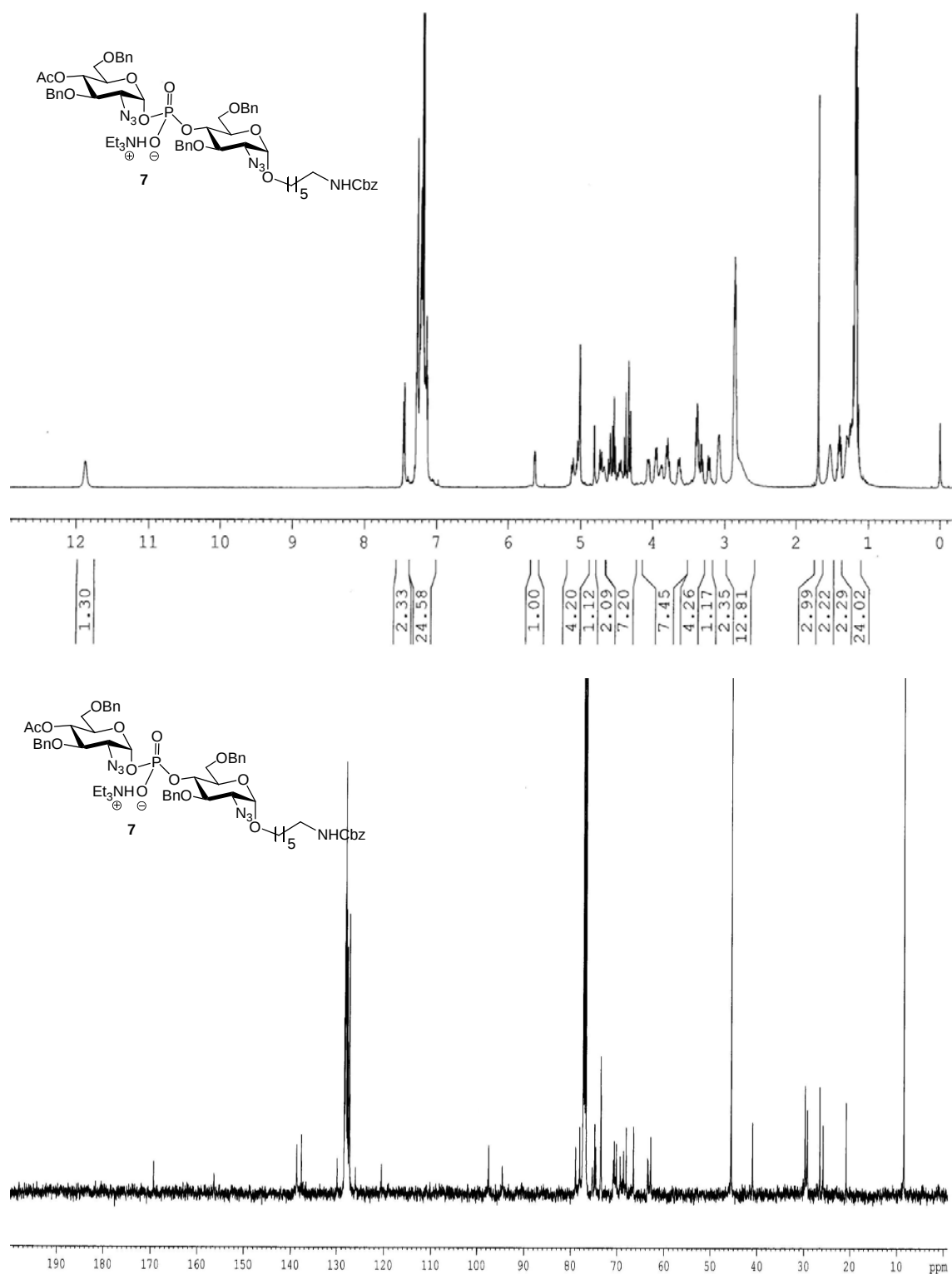
Subject	Page No.
1D and 2D NMR spectra of compounds 2 , 4 , 7-11 and 1	2-19



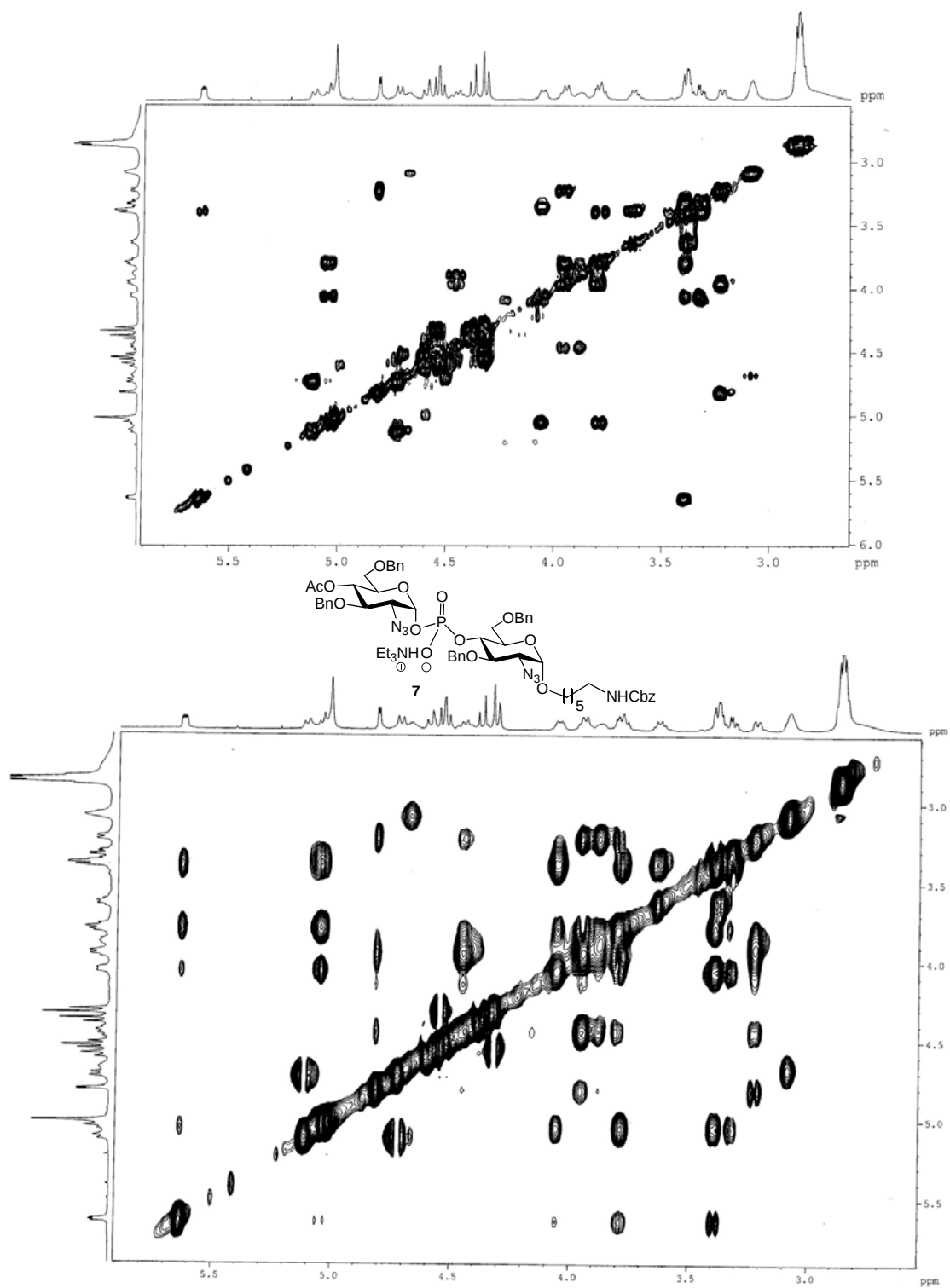
¹H and ¹³C NMR spectra of 4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl hydrogen phosphonate triethylammonium salt (**2**) (CDCl₃).



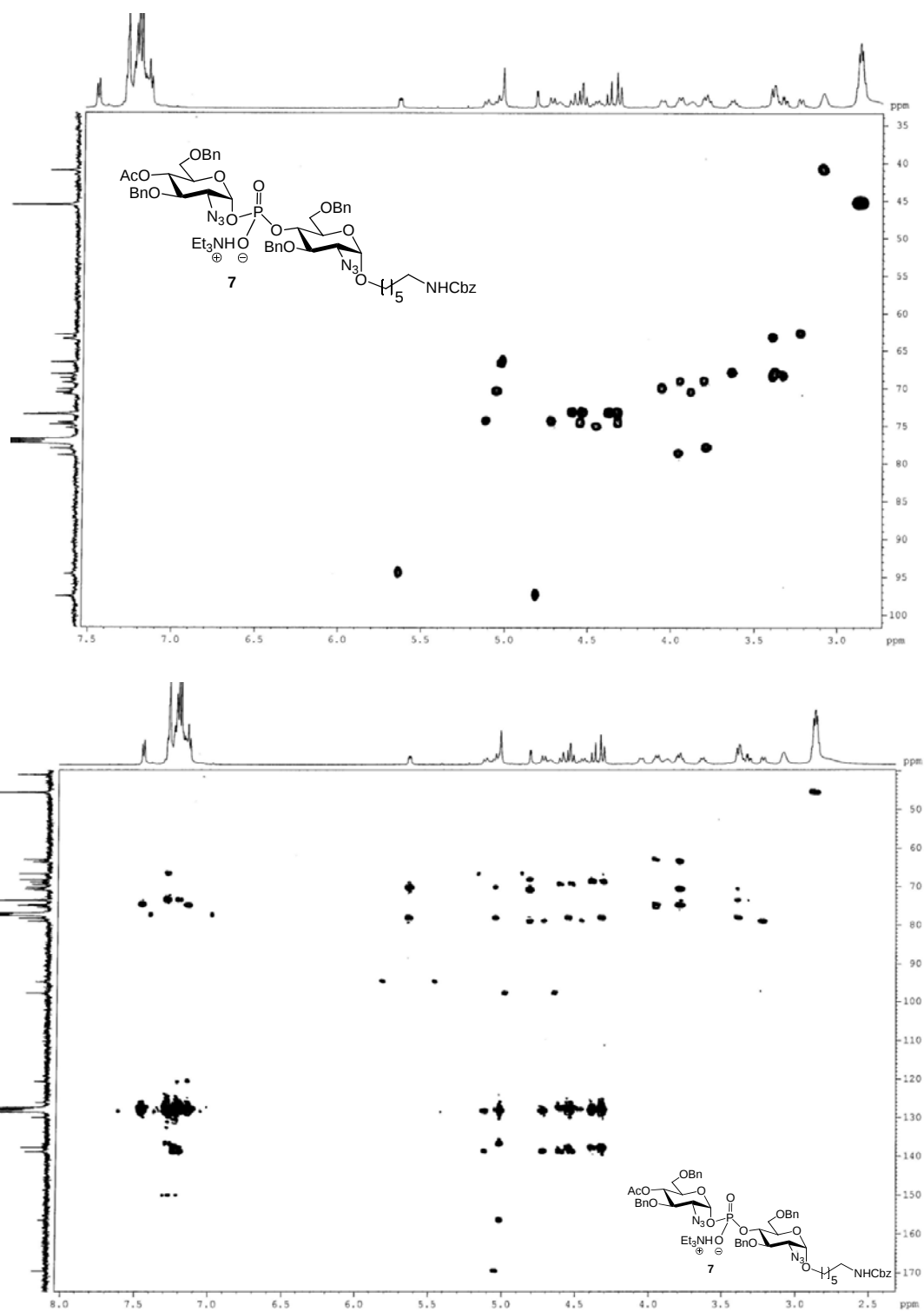
^1H and ^{13}C NMR spectra of 6-(*N*-benzyloxycarbonyl)aminohexyl 2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside (**4**) (CDCl₃).



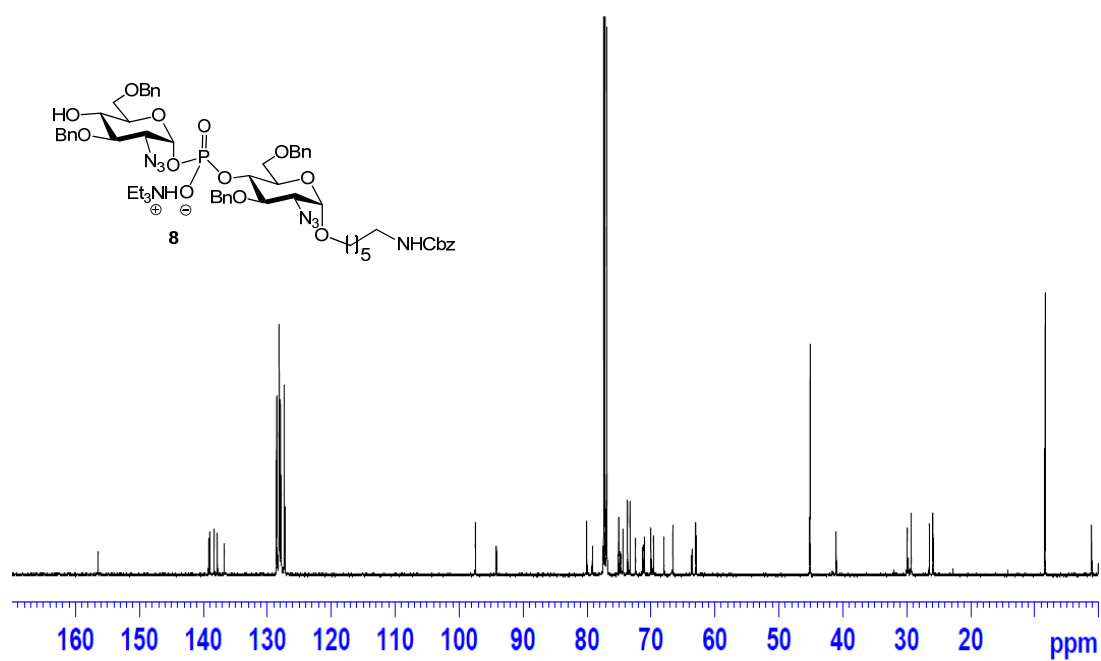
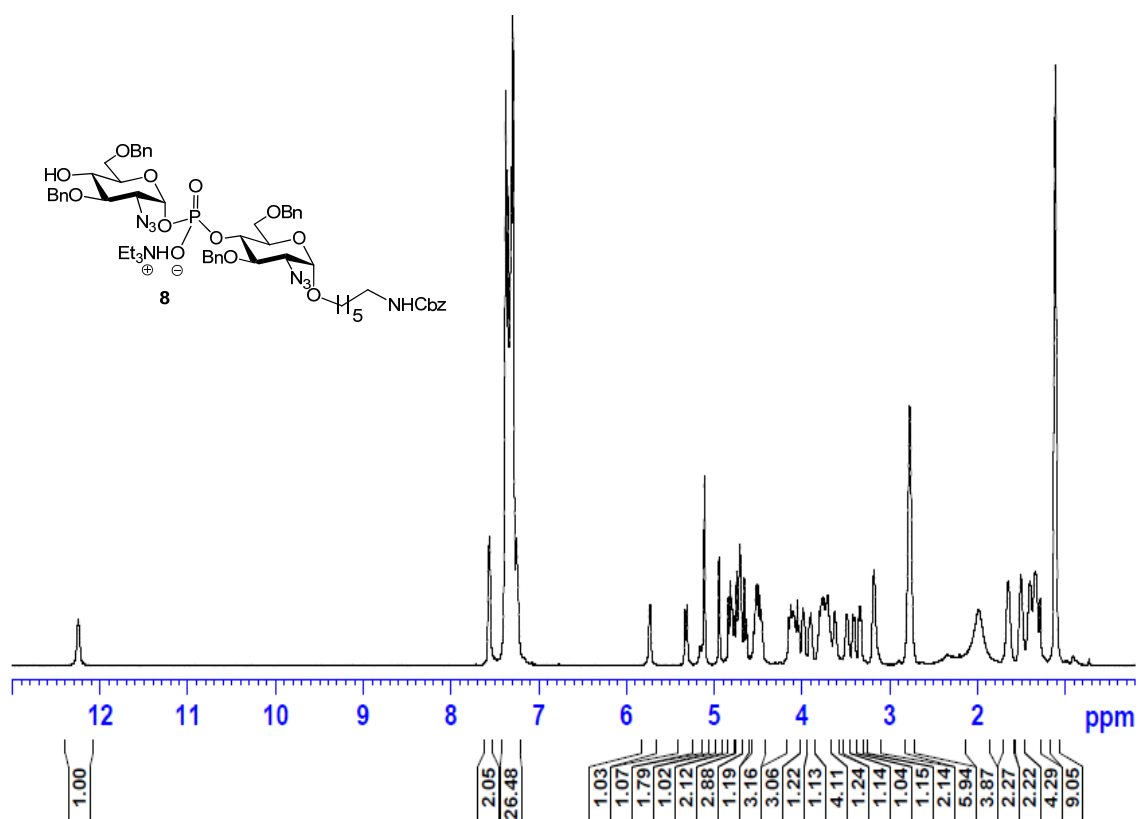
¹H and ¹³C NMR spectra of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, triethylammonium salt (**7**) (CDCl₃).



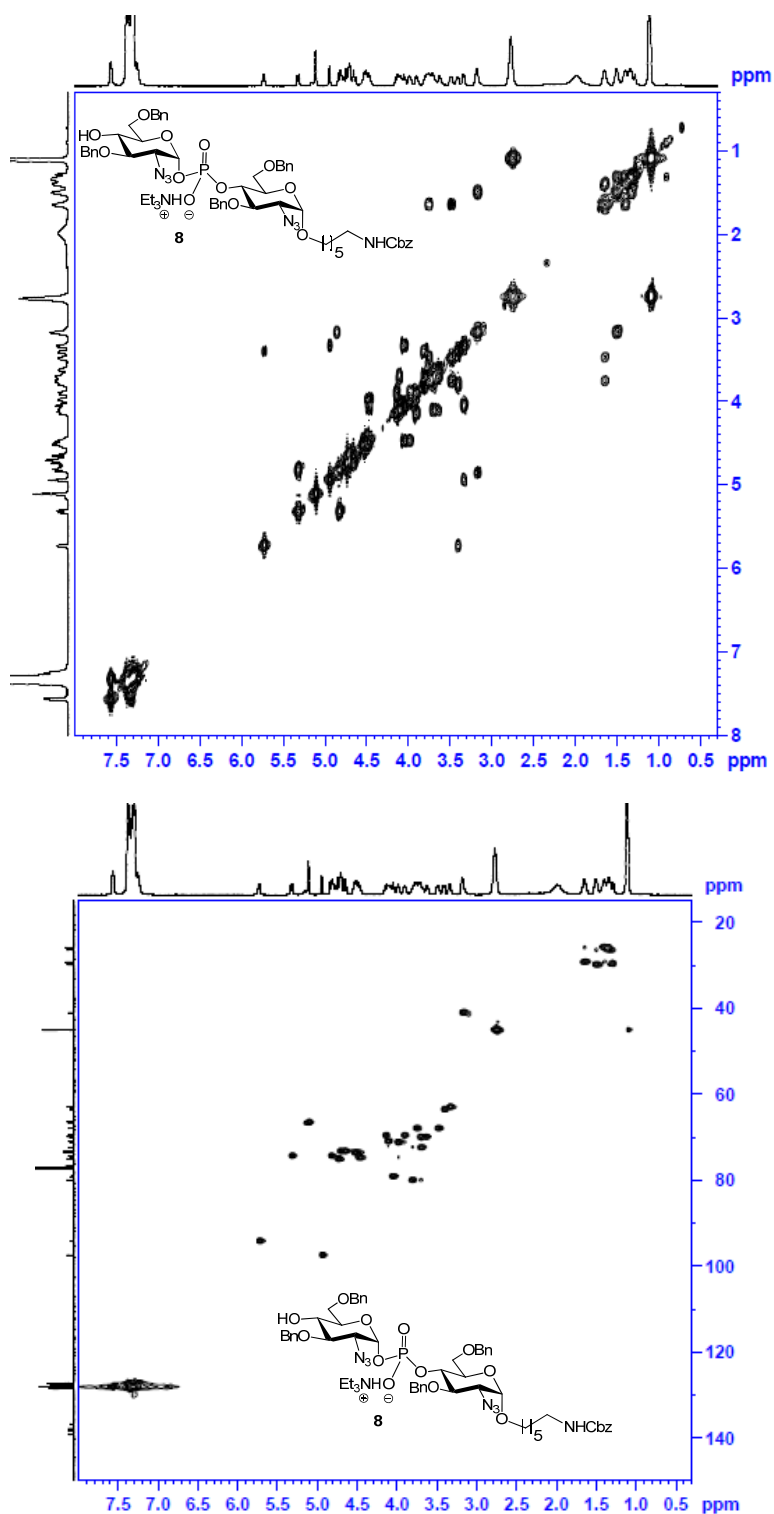
2D COSY and 2D TOCSY NMR spectra (selected regions) of 6-(*N*-benzyloxycarbonyl) aminoheptyl *O*-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, triethylammonium salt (**7**) (CDCl_3).



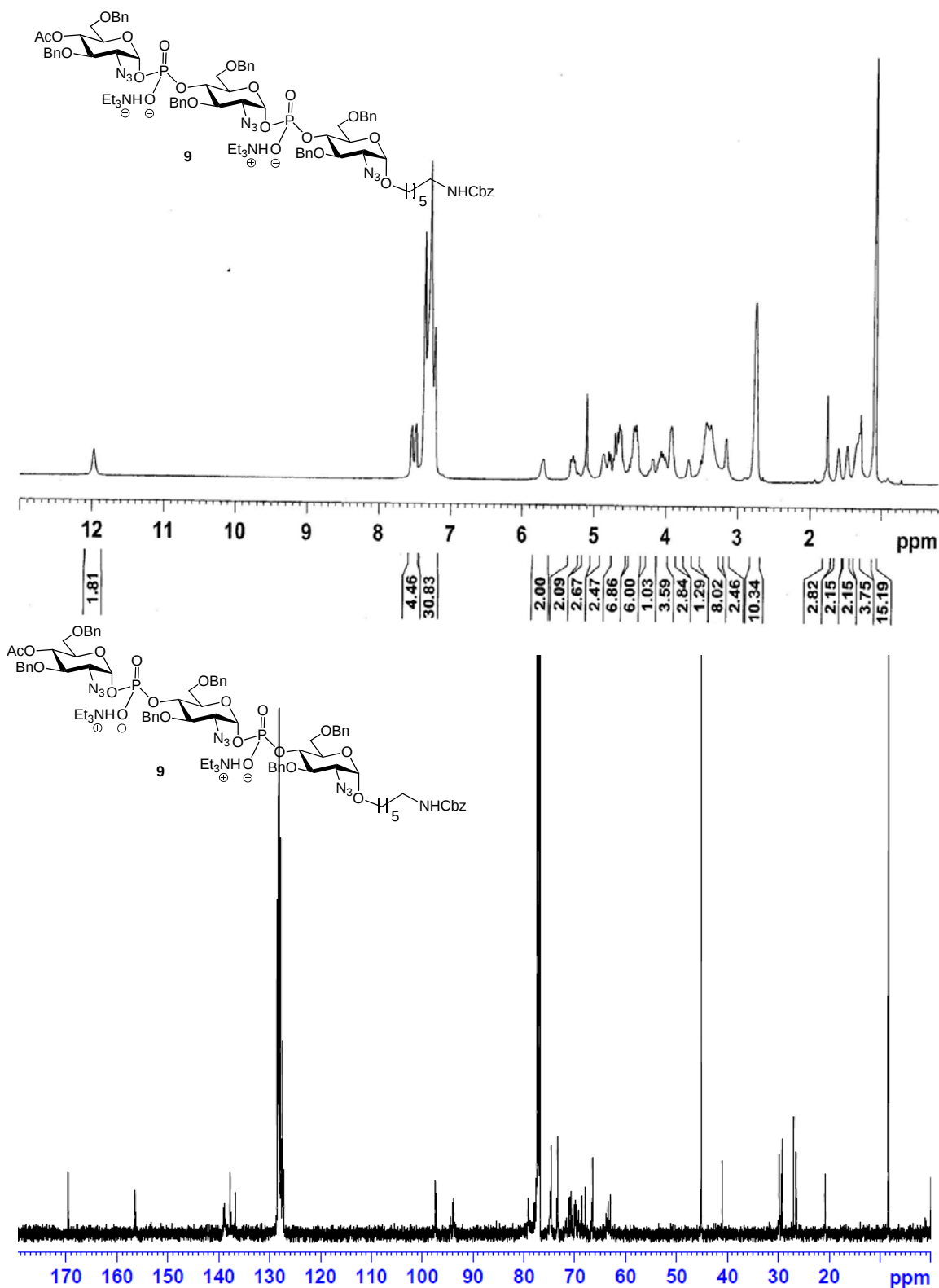
2D HSQC and 2D HMBC NMR spectra (selected regions) of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, triethylammonium salt (**7**) (CDCl_3).



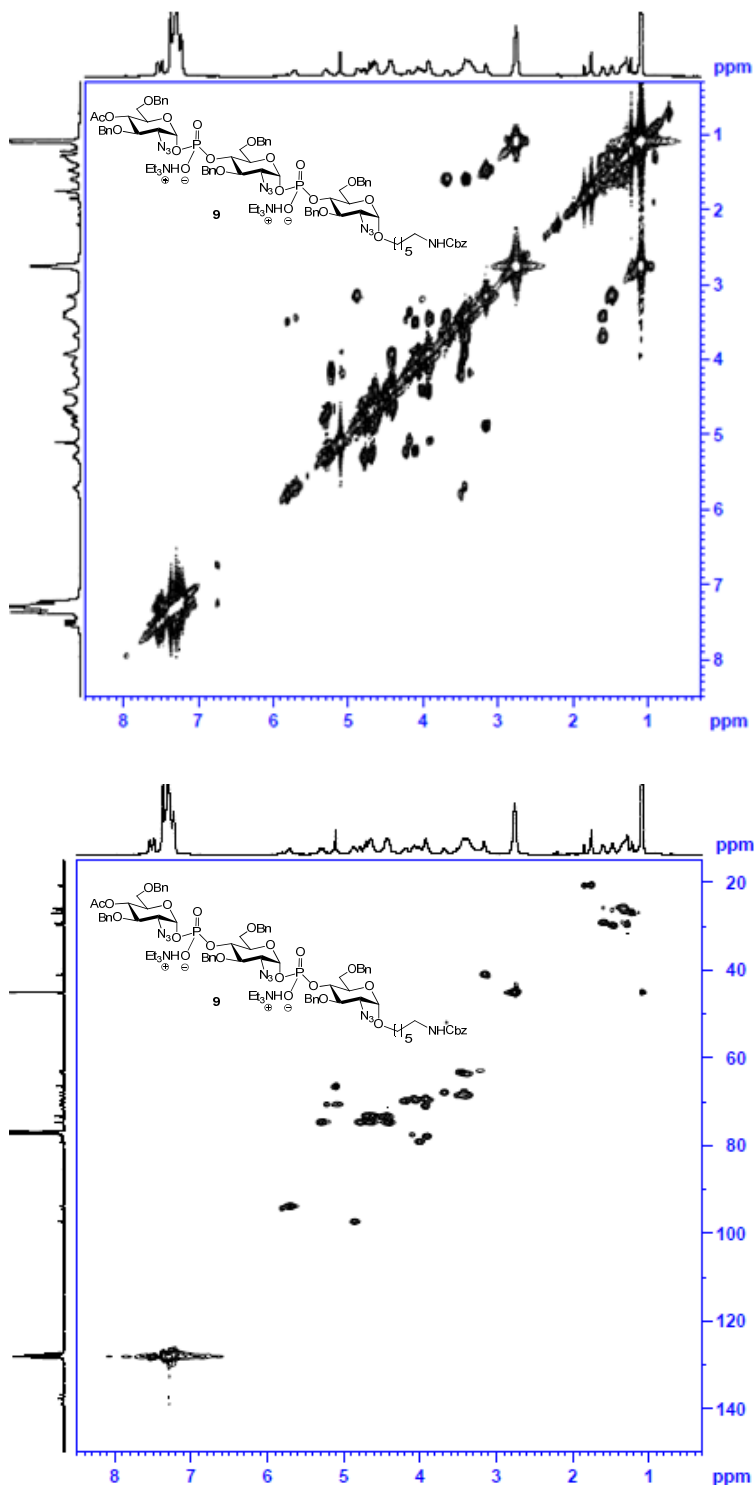
^1H and ^{13}C NMR spectra of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, triethylammonium salt (**8**) (CDCl_3).



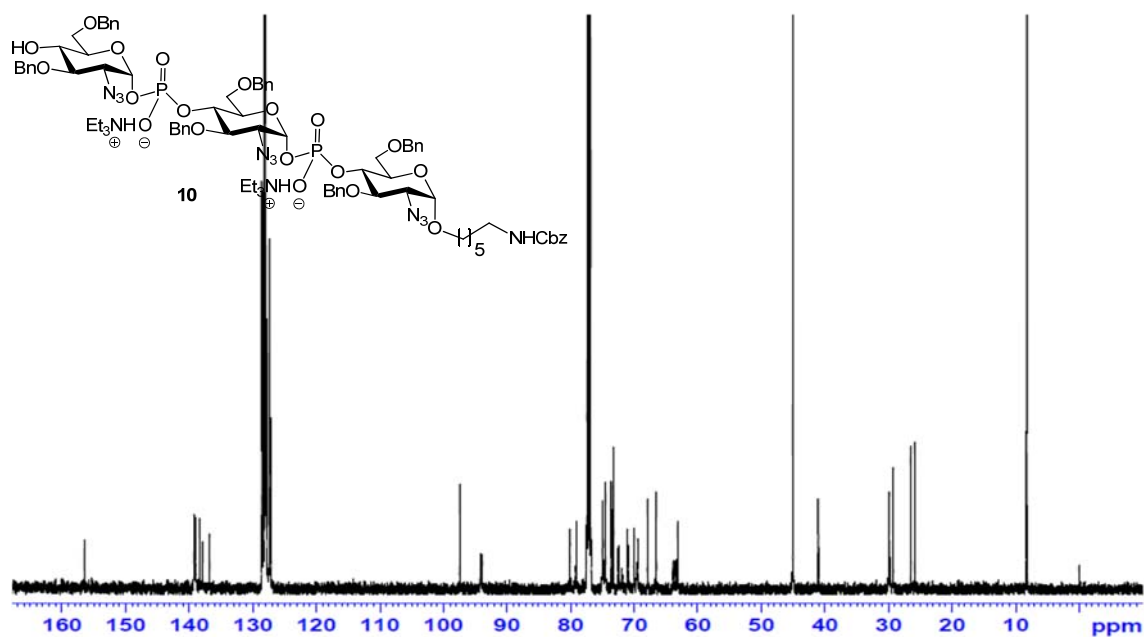
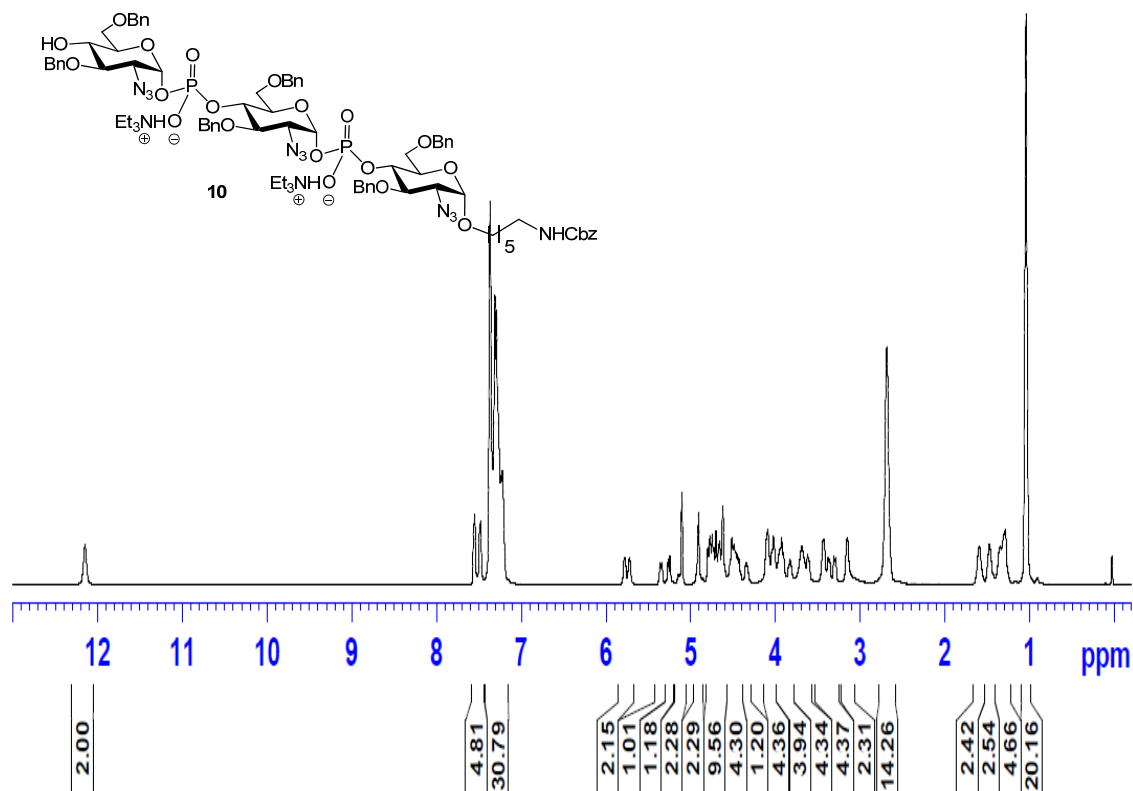
2D COSY and 2D HSQC NMR spectra (selected regions) of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, triethylammonium salt (**8**) (CDCl_3).



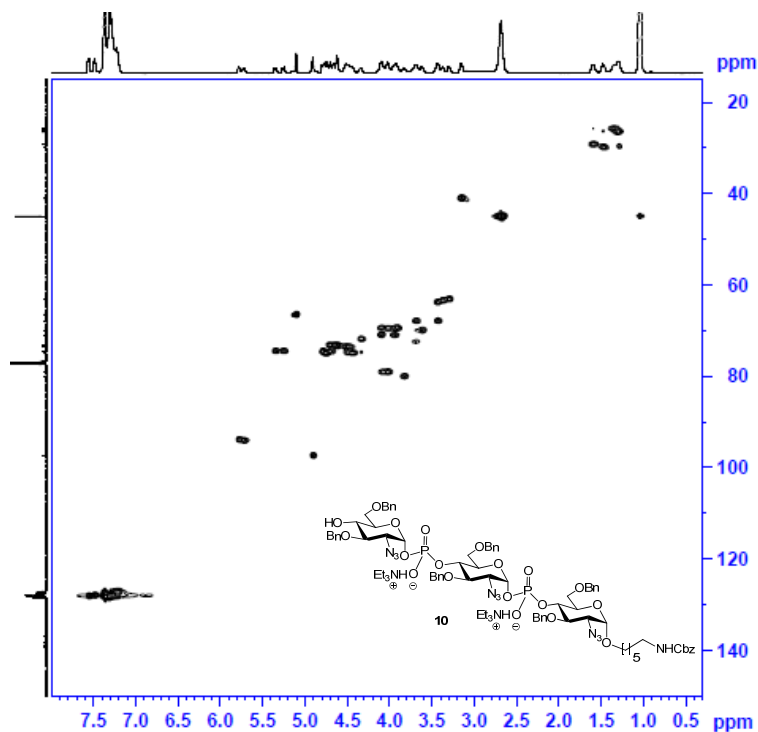
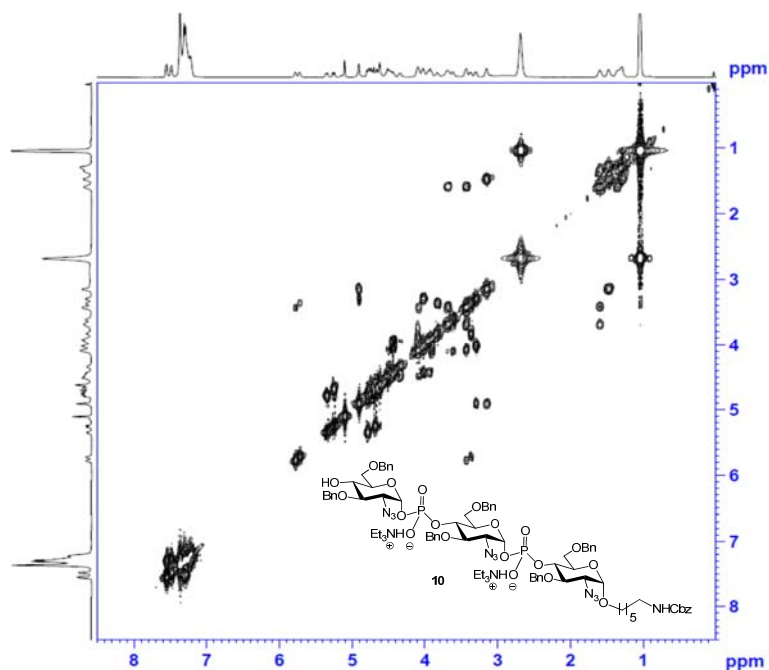
¹H and ¹³C NMR spectra of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, bis-triethylammonium salt (**9**) (CDCl₃).



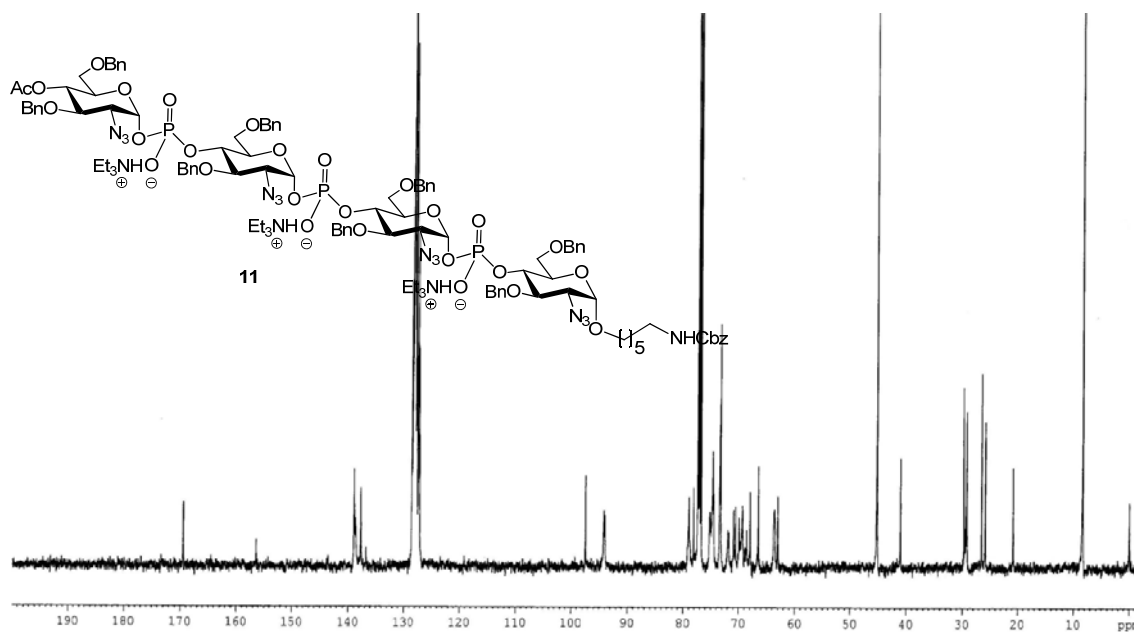
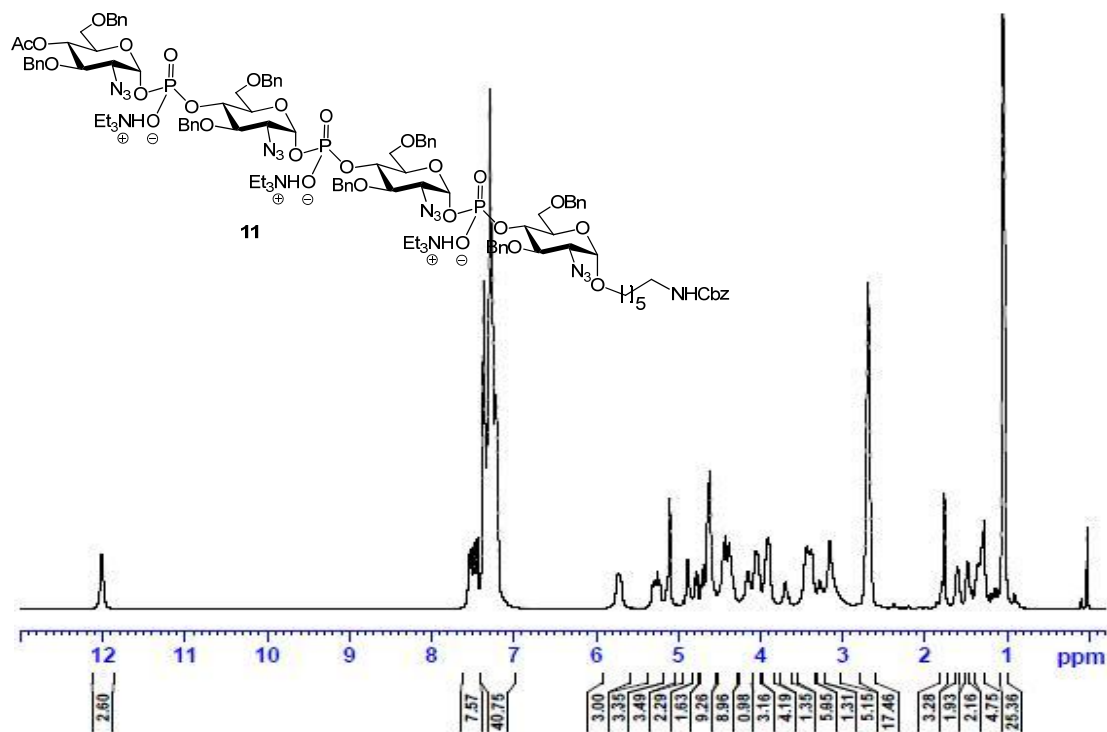
2D COSY and 2D HSQC NMR spectra (selected regions) of 6-(*N*-benzyloxycarbonyl)aminoethyl O-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, bis-triethylammonium salt (**9**) (CDCl₃).



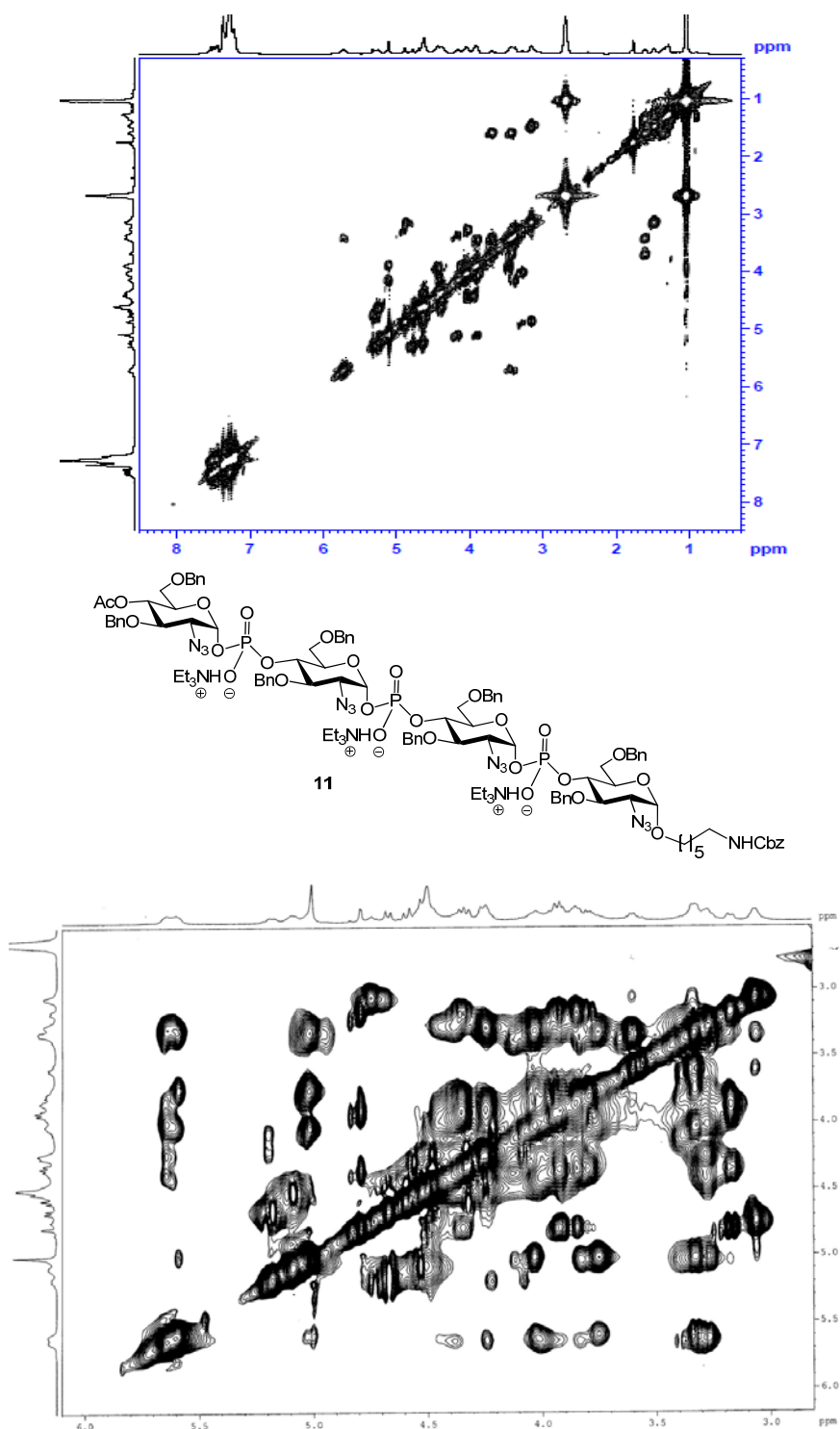
¹H and ¹³C NMR spectra of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, bis-triethylammonium salt (**10**) (CDCl₃).



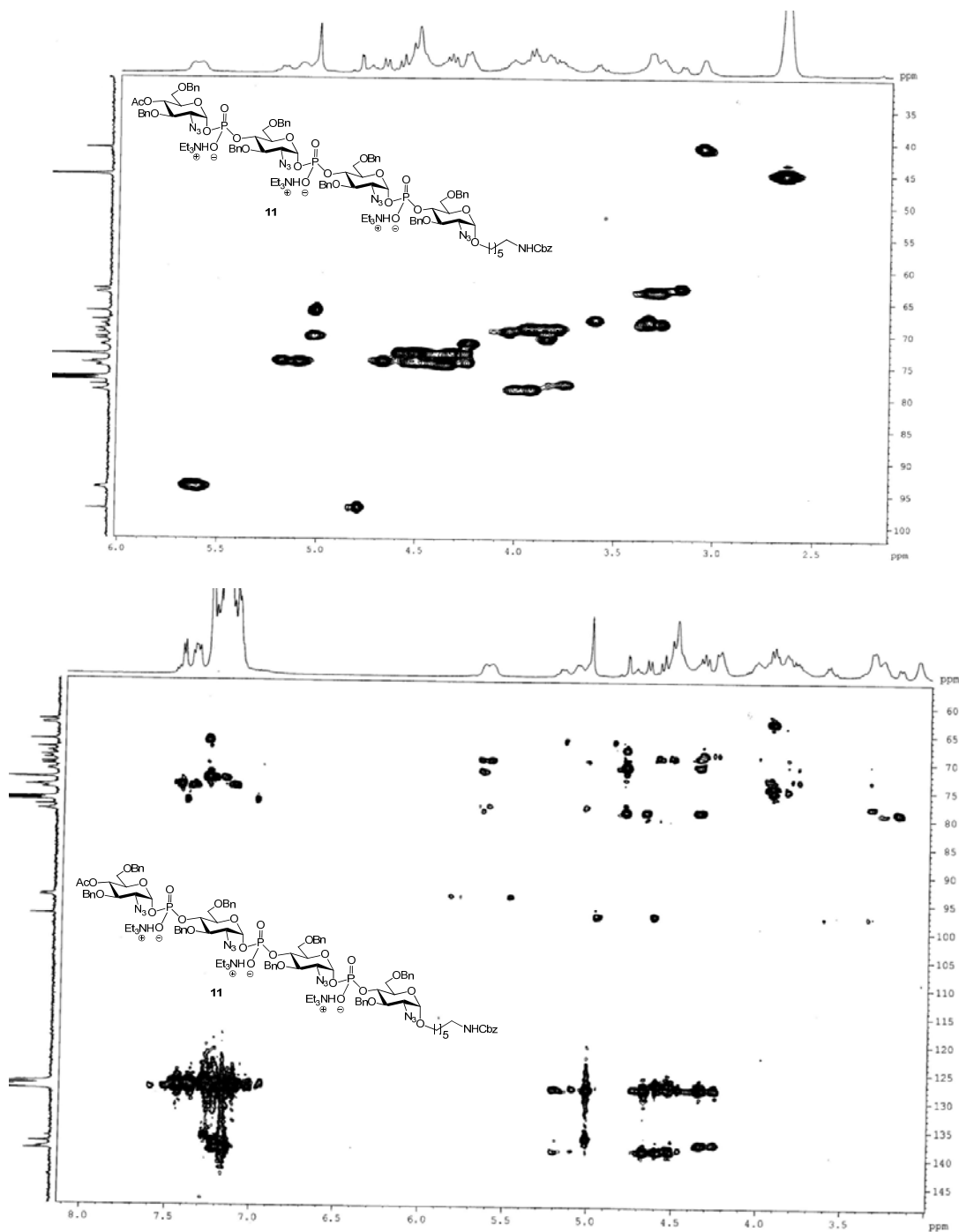
2D COSY and 2D HSQC NMR spectra (selected regions) of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, bis-triethylammonium salt (**10**) (CDCl₃).



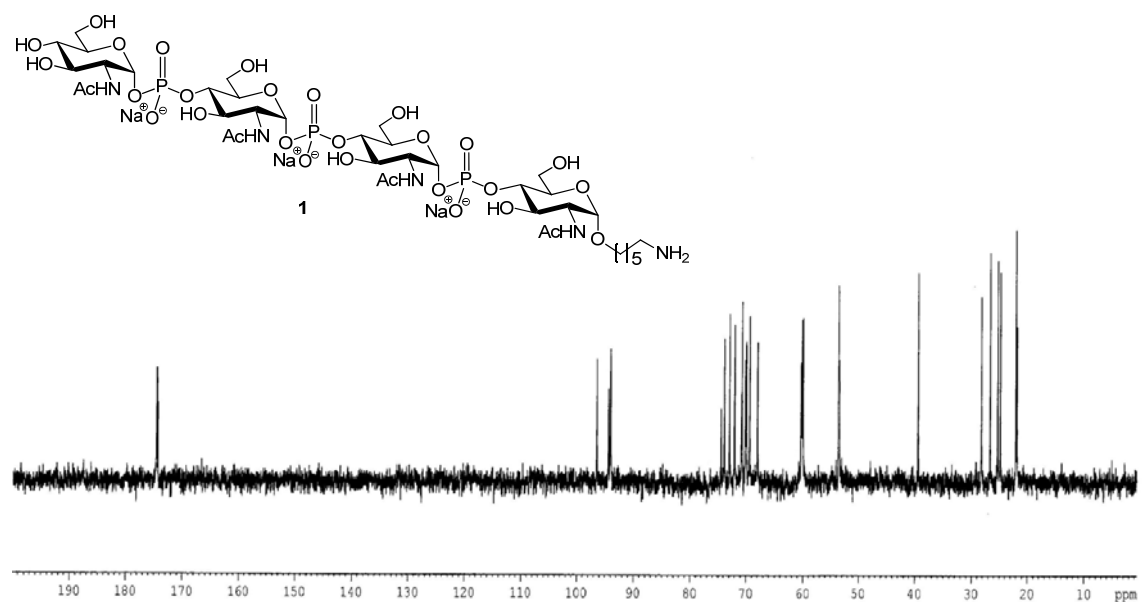
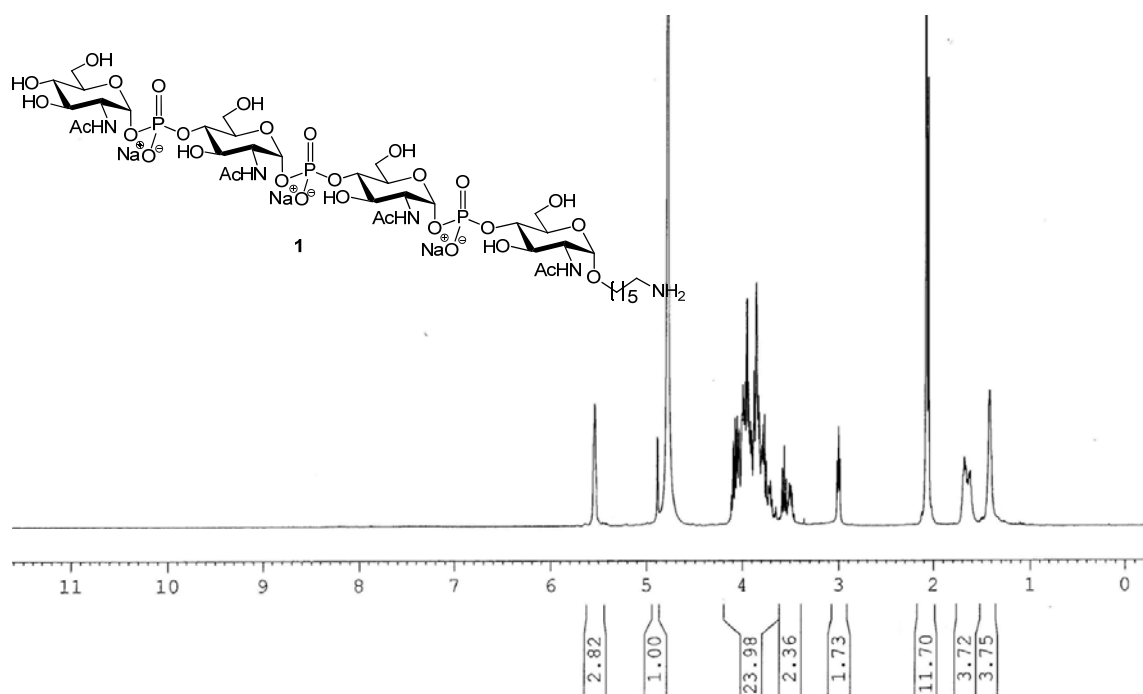
^1H and ^{13}C NMR spectra of 6-(*N*-benzyloxycarbonyl)aminohexyl *O*-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, tris-triethylammonium salt (**11**) (CDCl_3).



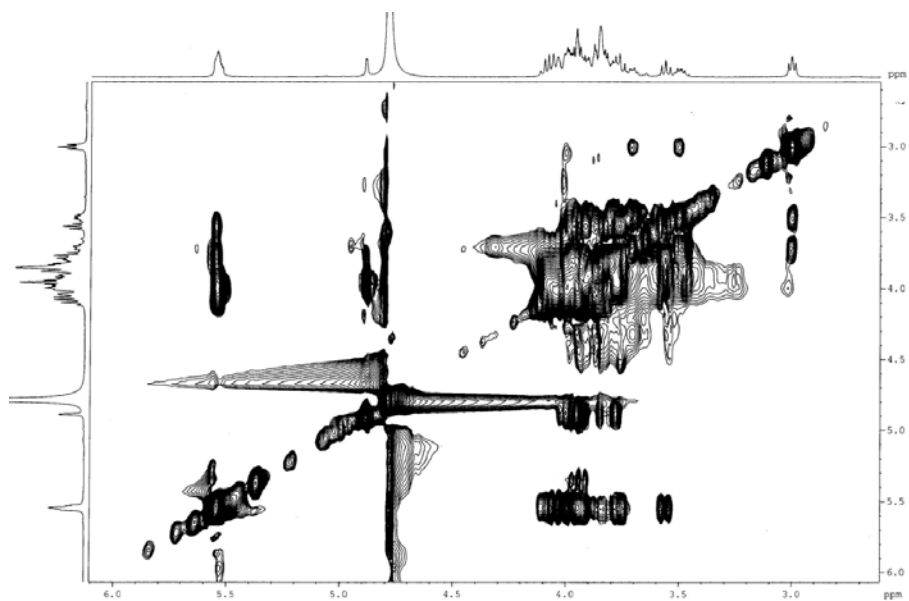
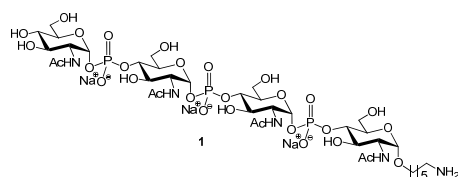
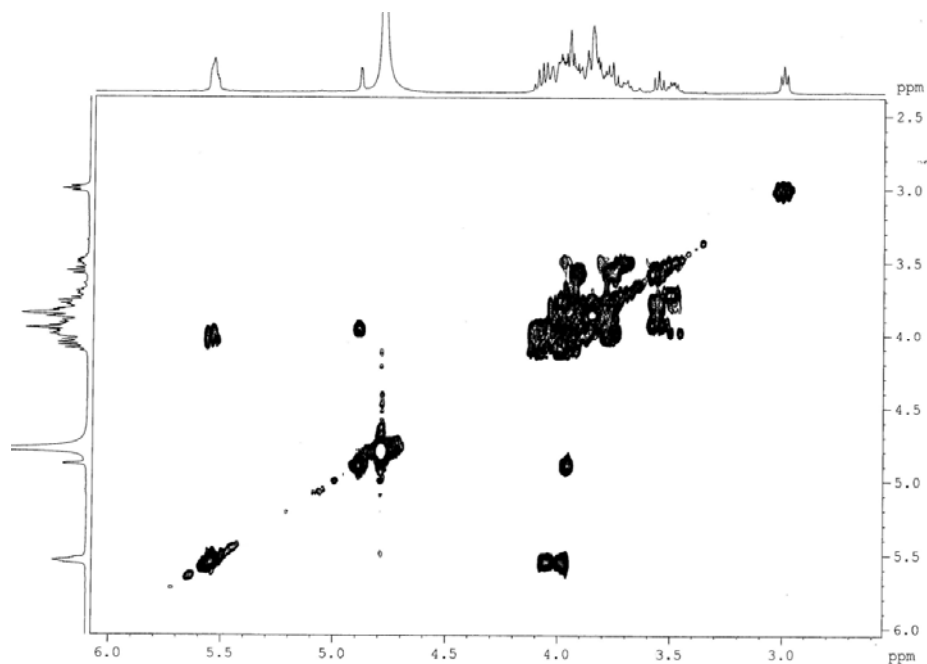
2D COSY and 2D TOCSY NMR spectra (selected regions) of 6-(*N*-benzyloxycarbonyl)aminohexyl O-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1→4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1→4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1→4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, tris-triethylammonium salt (**11**) (CDCl₃).



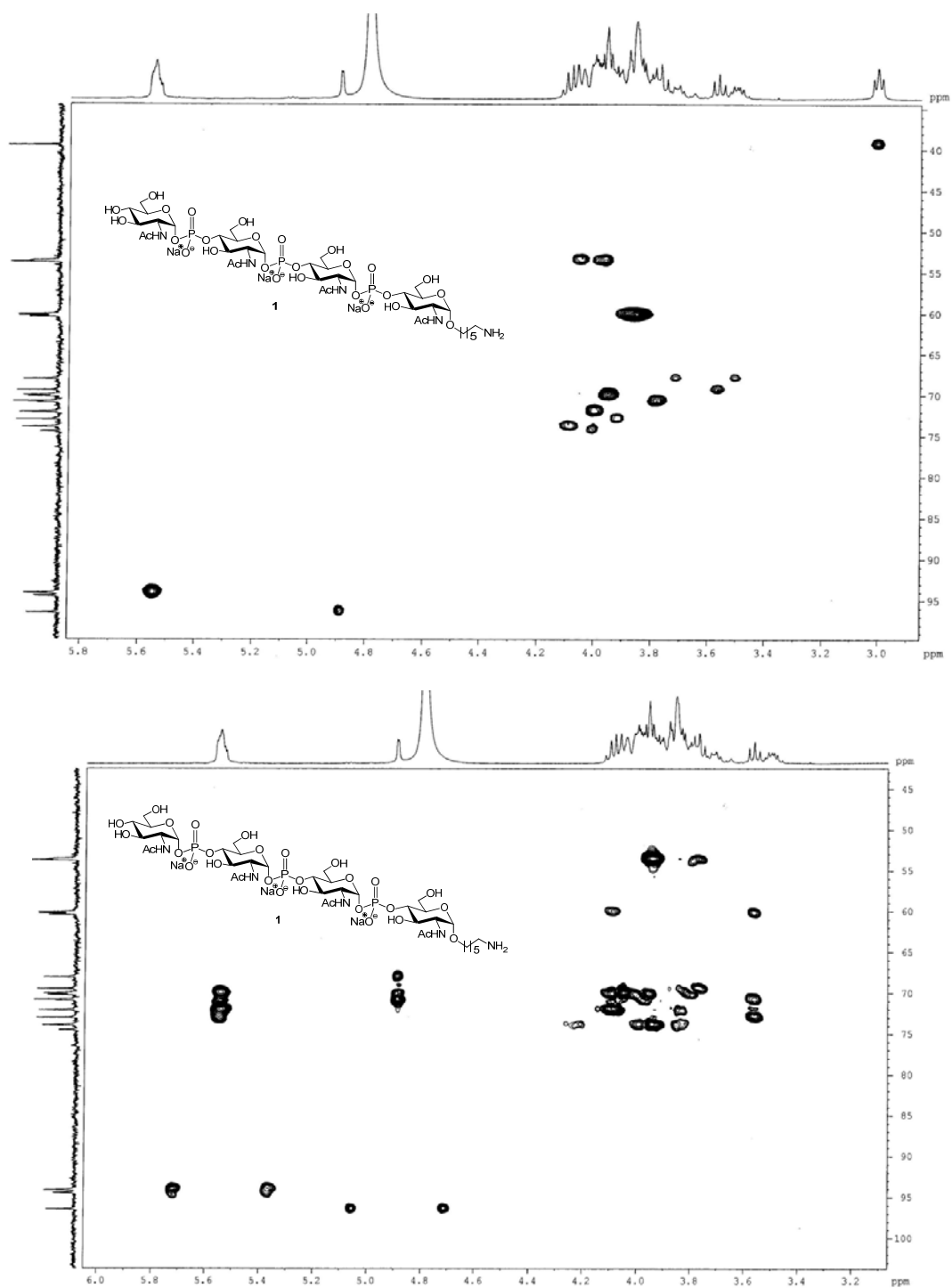
2D HSQC and 2D HMBC NMR spectra (selected regions) of 6-(*N*-benzyloxycarbonyl)aminoethyl *O*-(4-*O*-acetyl-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-azido-3,6-di-*O*-benzyl-2-deoxy- α -D-glucopyranoside, tris-triethylammonium salt (**11**) (CDCl₃).



^1H and ^{13}C NMR spectra of 6-aminoethyl O-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-acetamido-2-deoxy- α -D-glucopyranoside), trisodium salt (**1**) (D₂O).



2D COSY and TOCSY NMR spectra (selected regions) of 6-aminoethyl O-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-acetamido-2-deoxy- α -D-glucopyranoside, trisodium salt (**1**) (D₂O).



2D HSQC and HMBC NMR spectra (selected regions) of 6-aminoethyl O-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-(2-acetamido-2-deoxy- α -D-glucopyranosyl phosphate)-(1 $\rightarrow$ 4)-2-acetamido-2-deoxy- α -D-glucopyranoside, trisodium salt (**1**) (D_2O).