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SUPPORTING INFORMATION

Synthesis of the tetrasaccharide repeating unit of the *O*-antigen of *Escherichia coli* O69 strain and its conformational analysis

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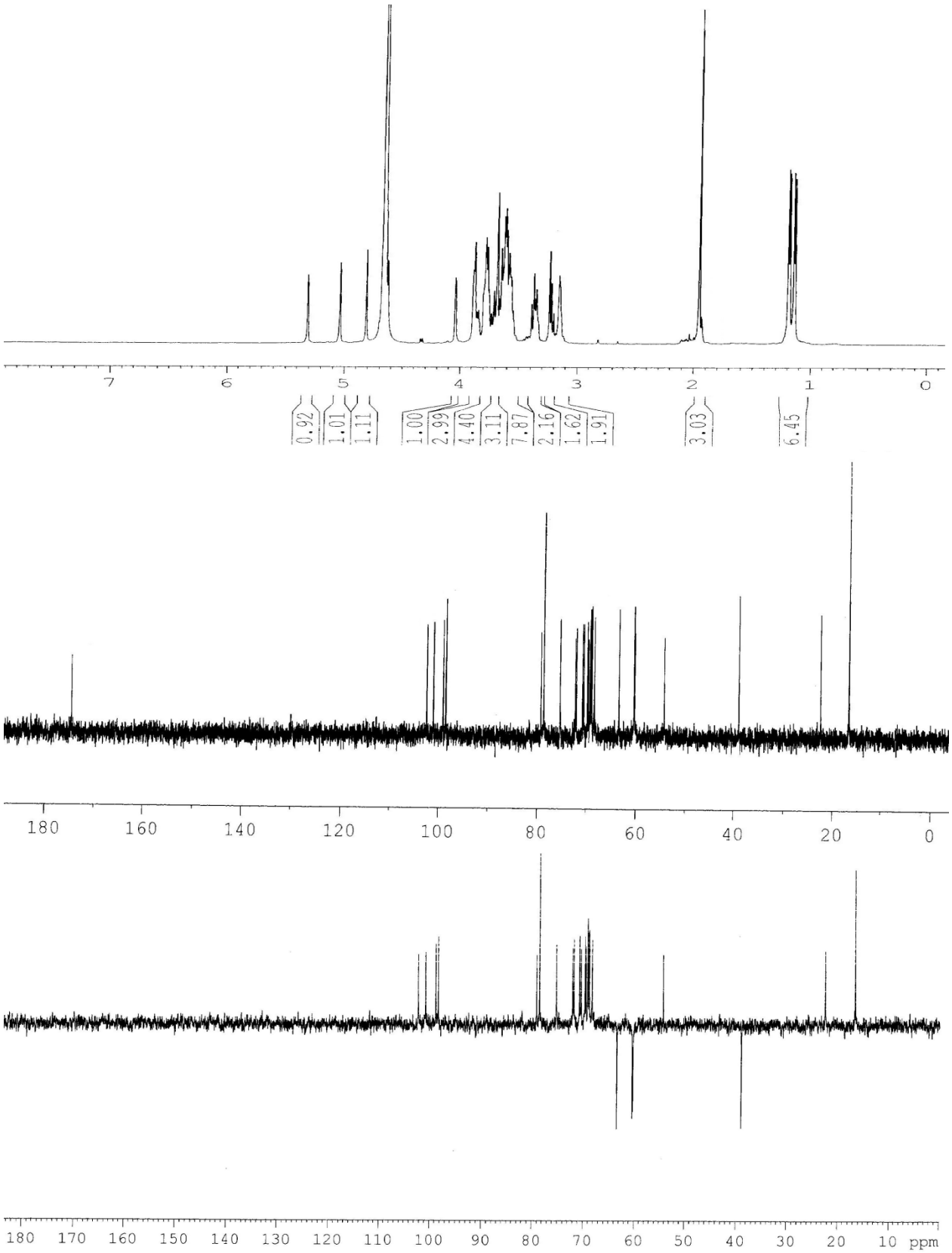
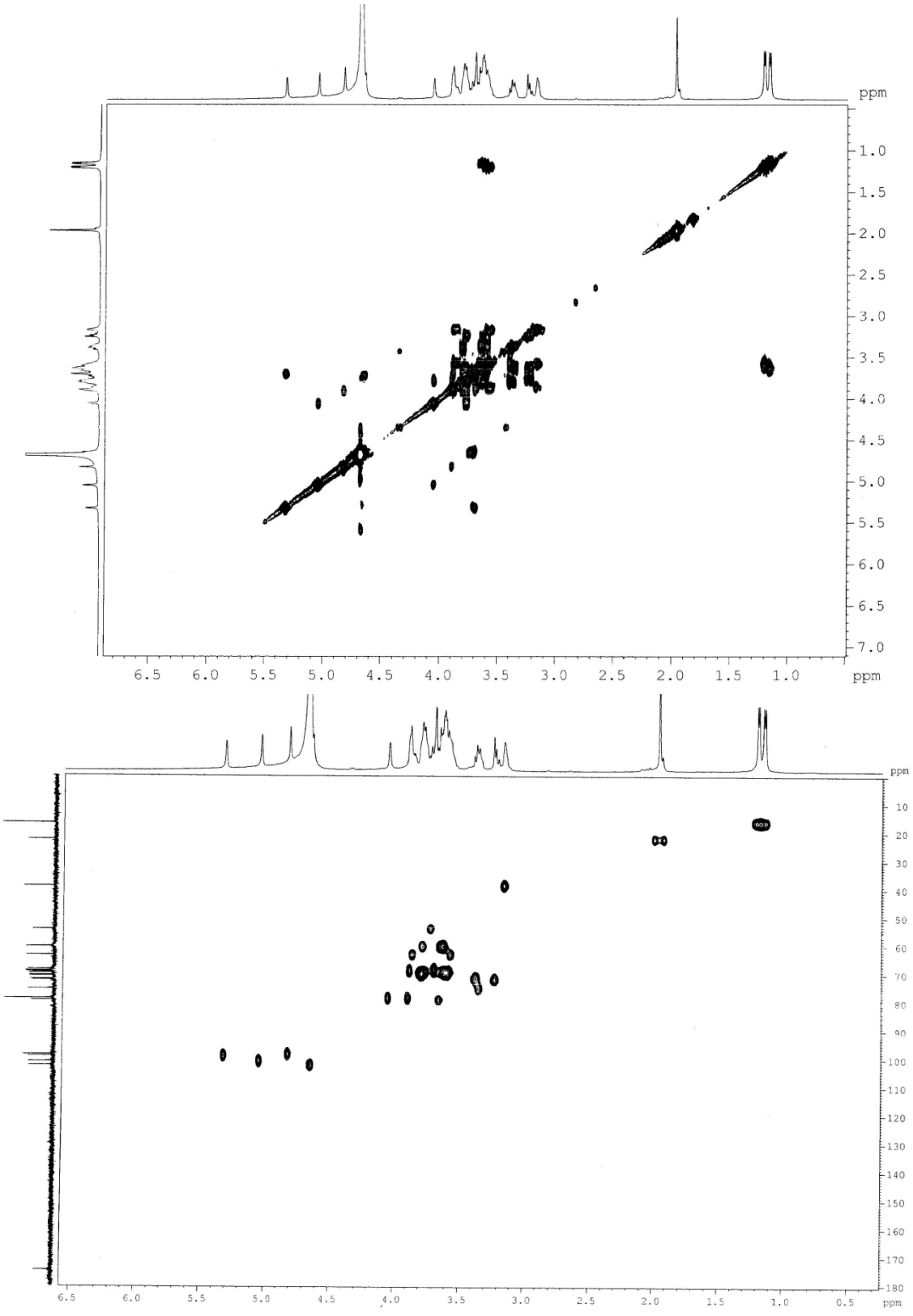
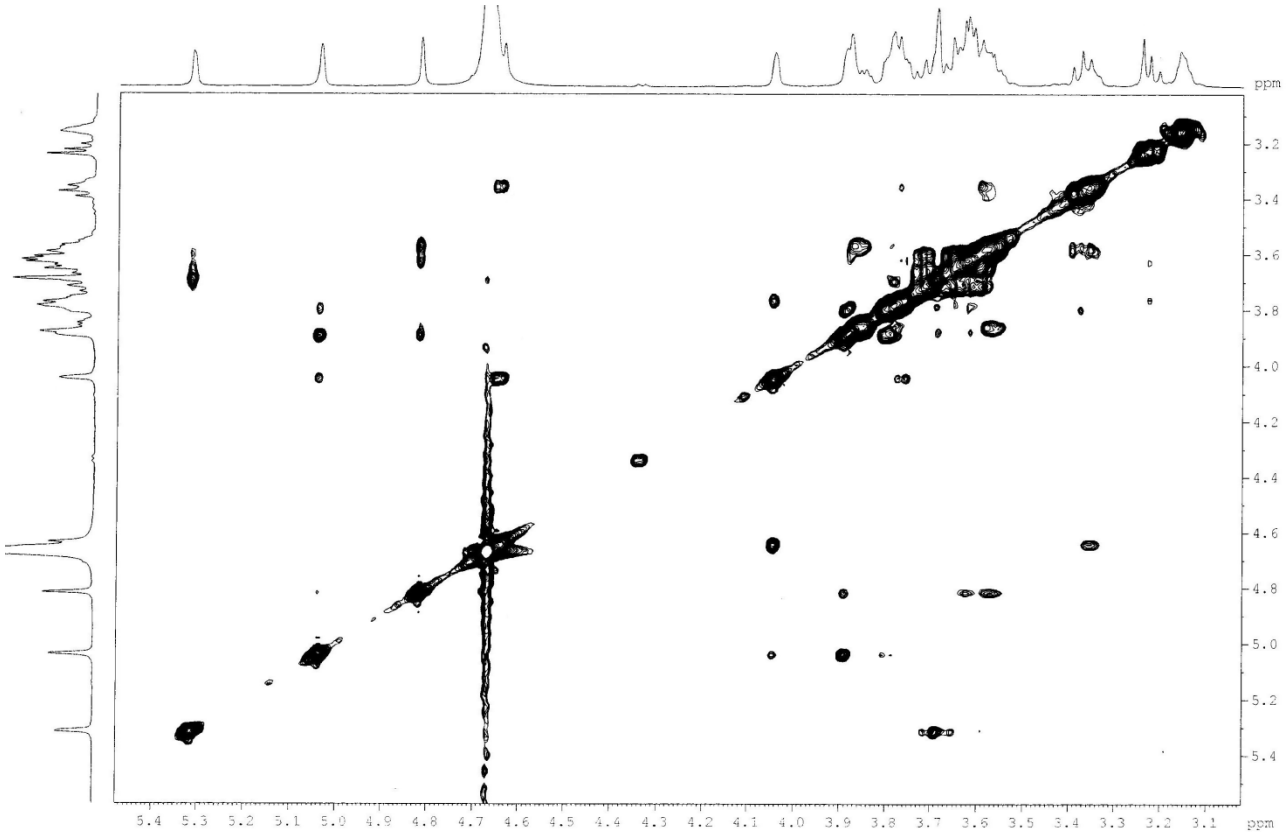
Index



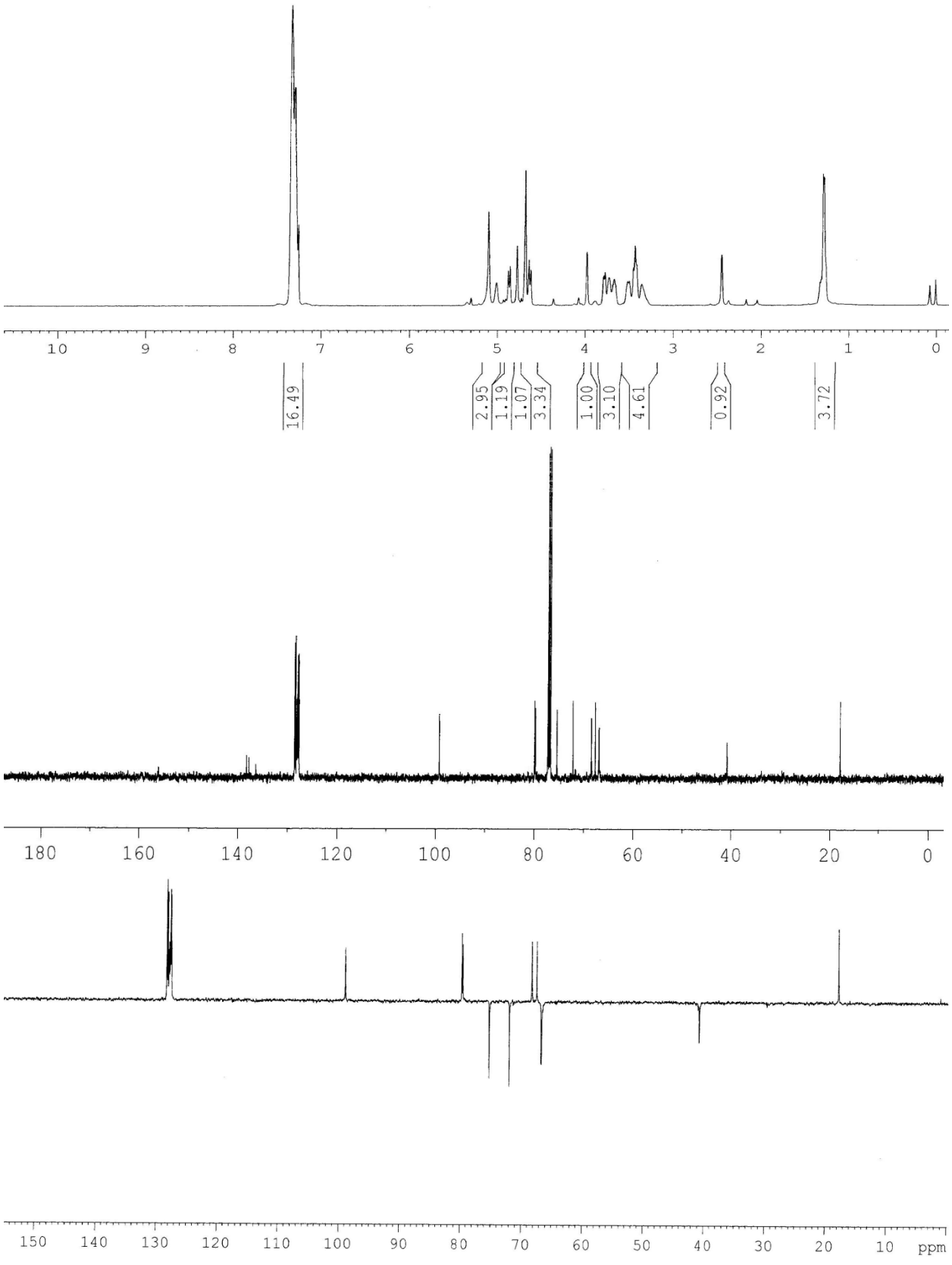
^{1}H, ^{13}C and DEPT 135 NMR spectra of 2-aminoethyl (α-D-galactopyranosyl)-(1→3)-(2-acetamido-2-deoxy-β-D-glucopyranosyl)-(1→2)-(α-L-rhamnopyranosyl)-(1→2)-α-L-rhamnopyranoside **(1)** (D_2O)**.**



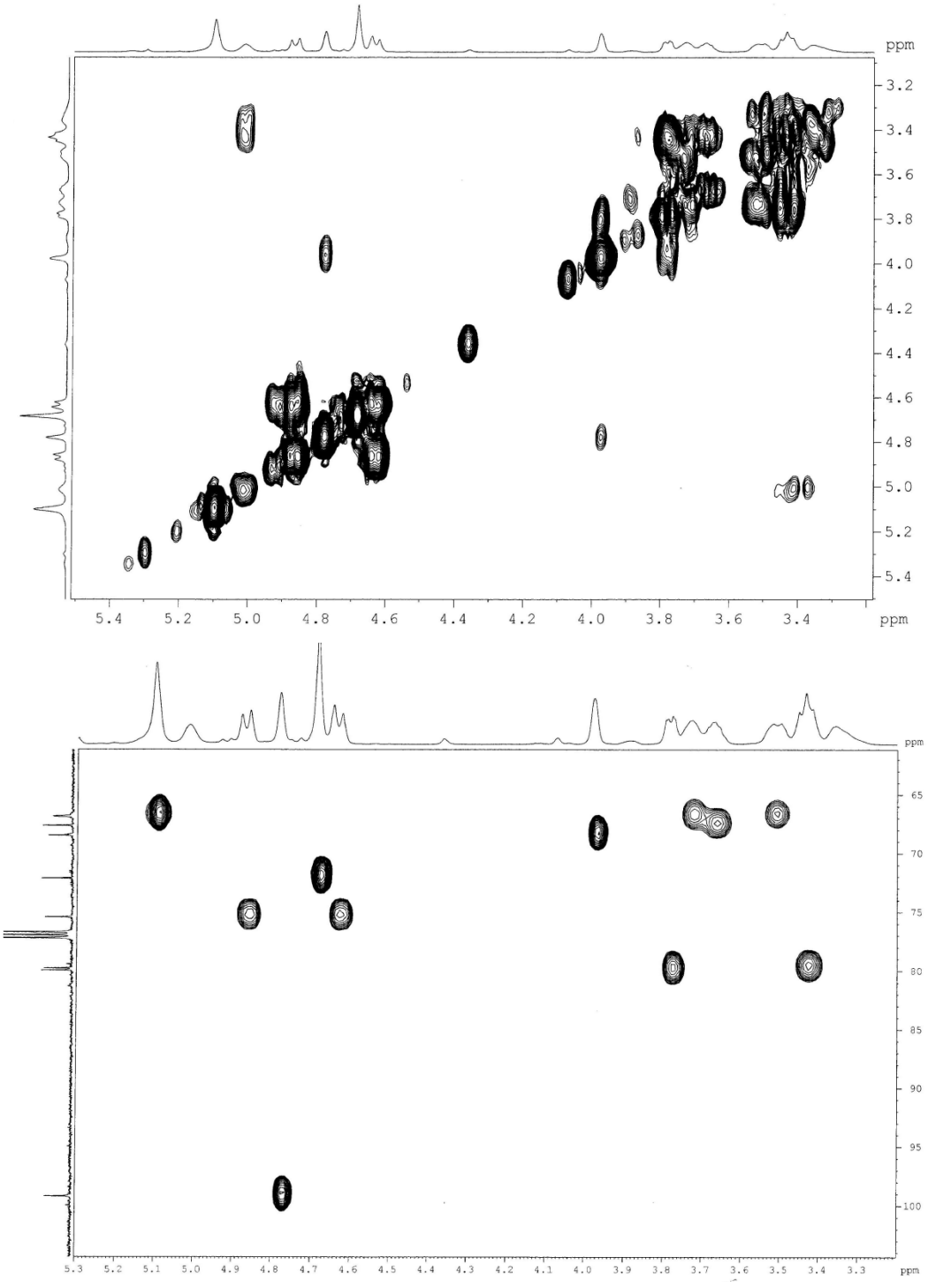
2D COSY and HSQC NMR spectra (selected regions) of 2-aminoethyl (α-D-galactopyranosyl)-(1→3)-(2-acetamido-2-deoxy-β-D-glucopyranosyl)-(1→2)-(α-L-rhamnopyranosyl)-(1→2)-α-L-rhamnopyranoside **(1)** (D_2O)**.**



2D ^{1}H-^{1}H ROESY (300 ms spin lock) spectrum of 2-aminoethyl (α-D-galactopyranosyl)-(1→3)-(2-acetamido-2-deoxy-β-D-glucopyranosyl)-(1→2)-(α-L-rhamnopyranosyl)-(1→2)-α-L-rhamnopyranoside (**1**) showing the inter-glycosidic ROEs.



^{1}H, ^{13}C and DEPT 135 NMR spectra of 2-(carbobenzyloxy)aminoethyl 3,4-di-*O*-benzyl-α-L-rhamnopyranoside **(3)** ($CDCl_3$).



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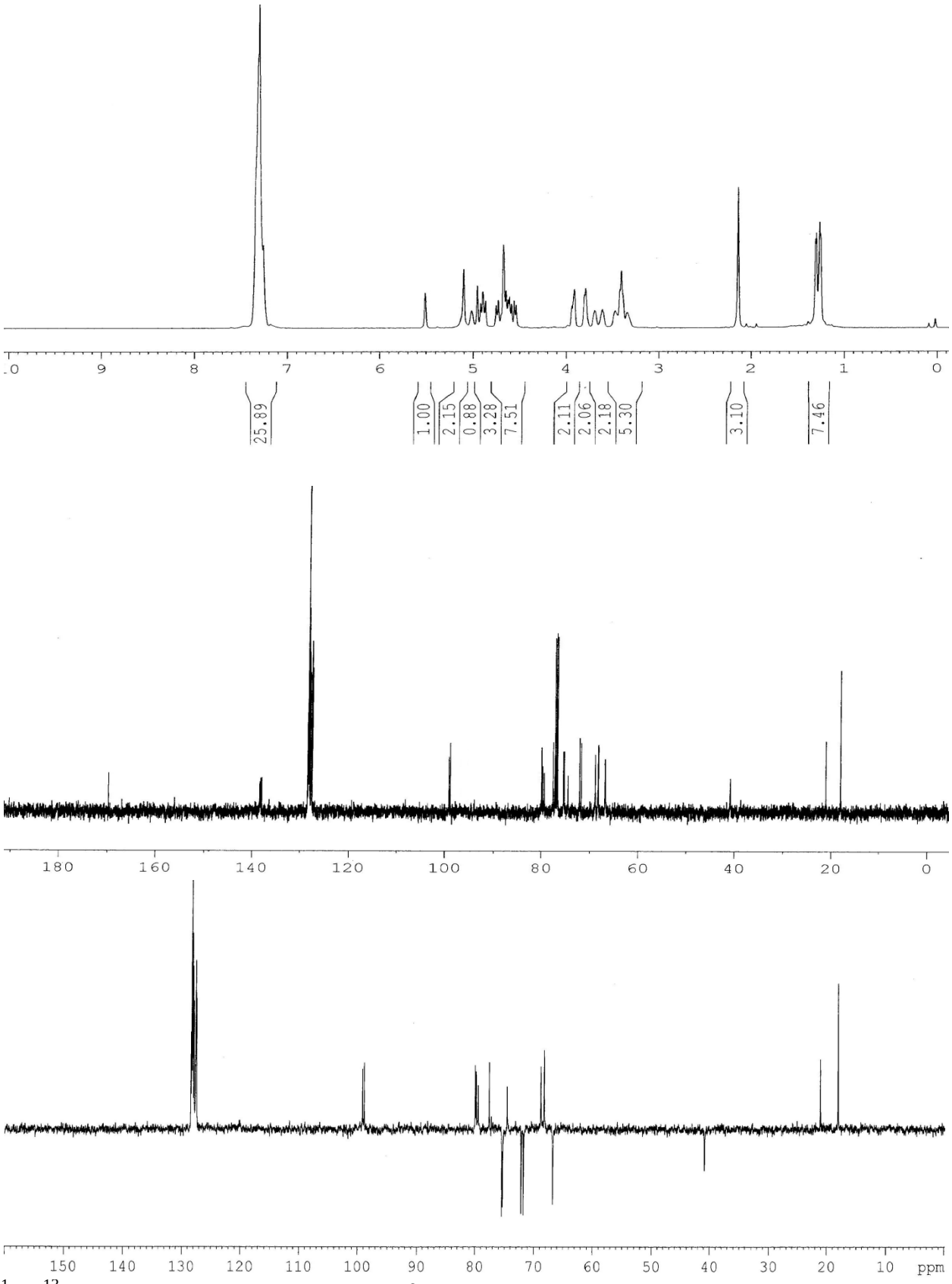
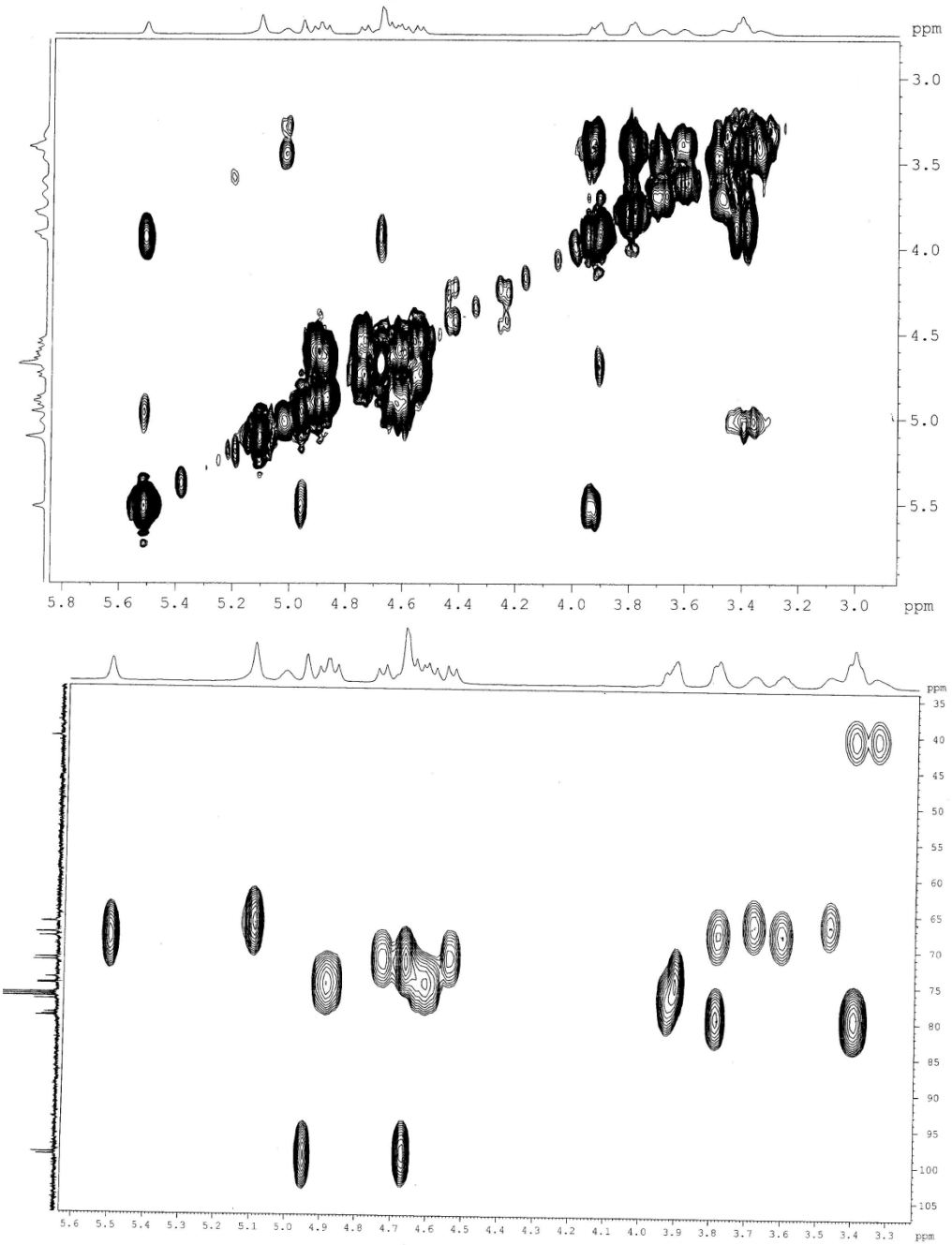


^{1}H, ^{13}C and DEPT 135 NMR spectra of 2-(carbobenzyloxy)aminoethyl (2-*O*-acetyl-3,4-di-*O*-benzyl-α-L-rhamnopyranosyl)-(1→2)-3,4-di-*O*-benzyl-α-L-rhamnopyranoside **(6)** ($CDCl_3$)**.**



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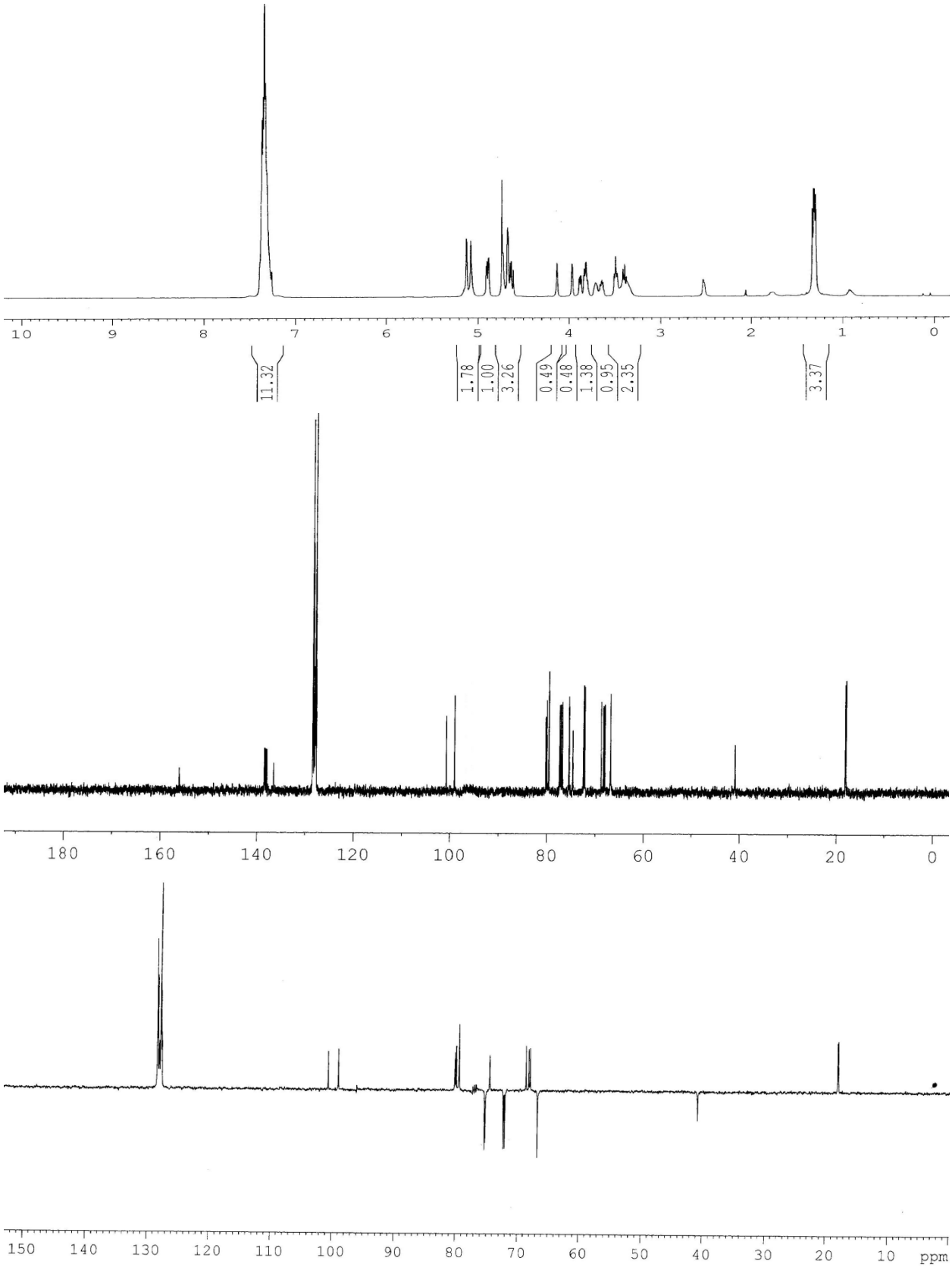

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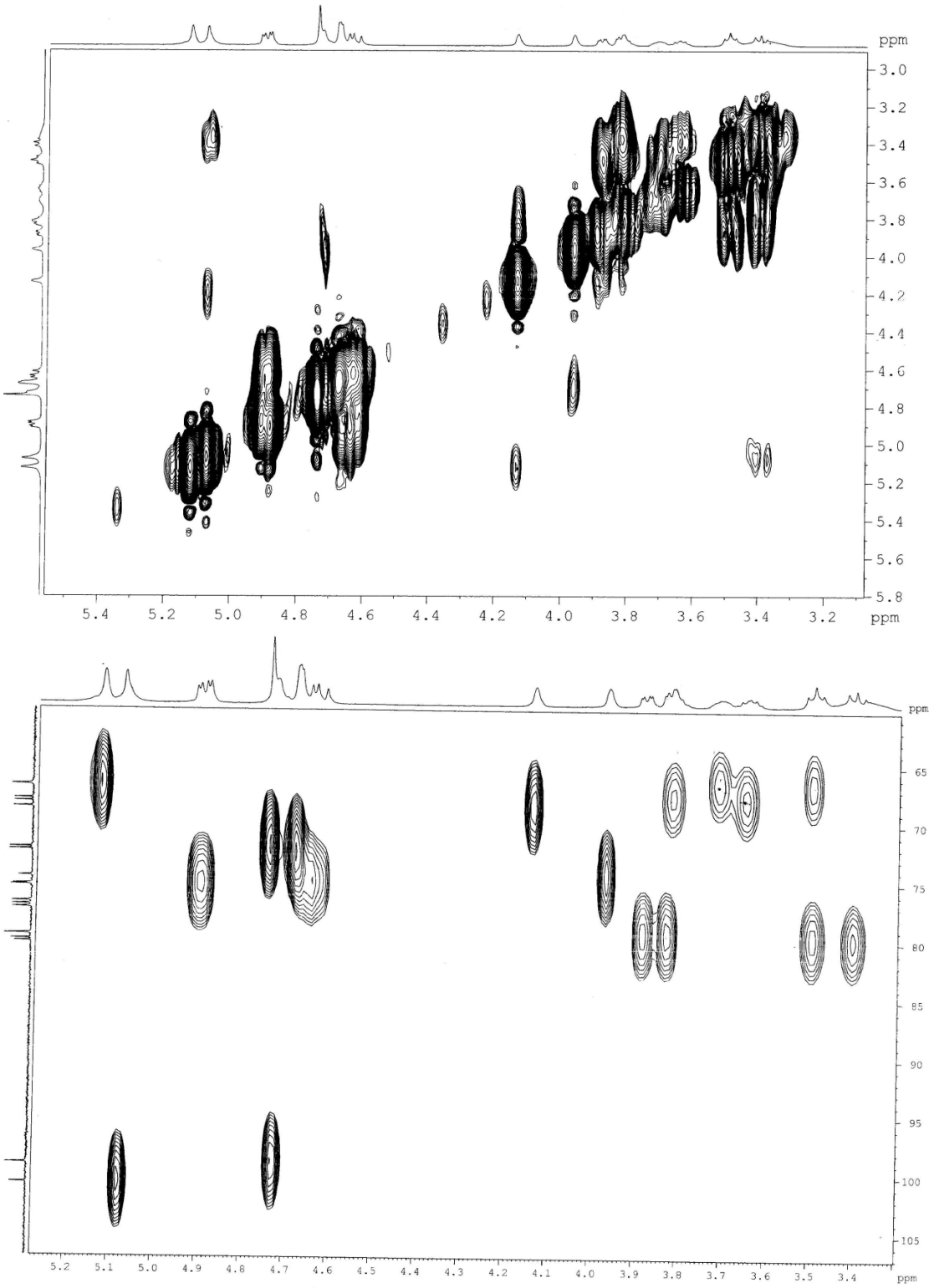

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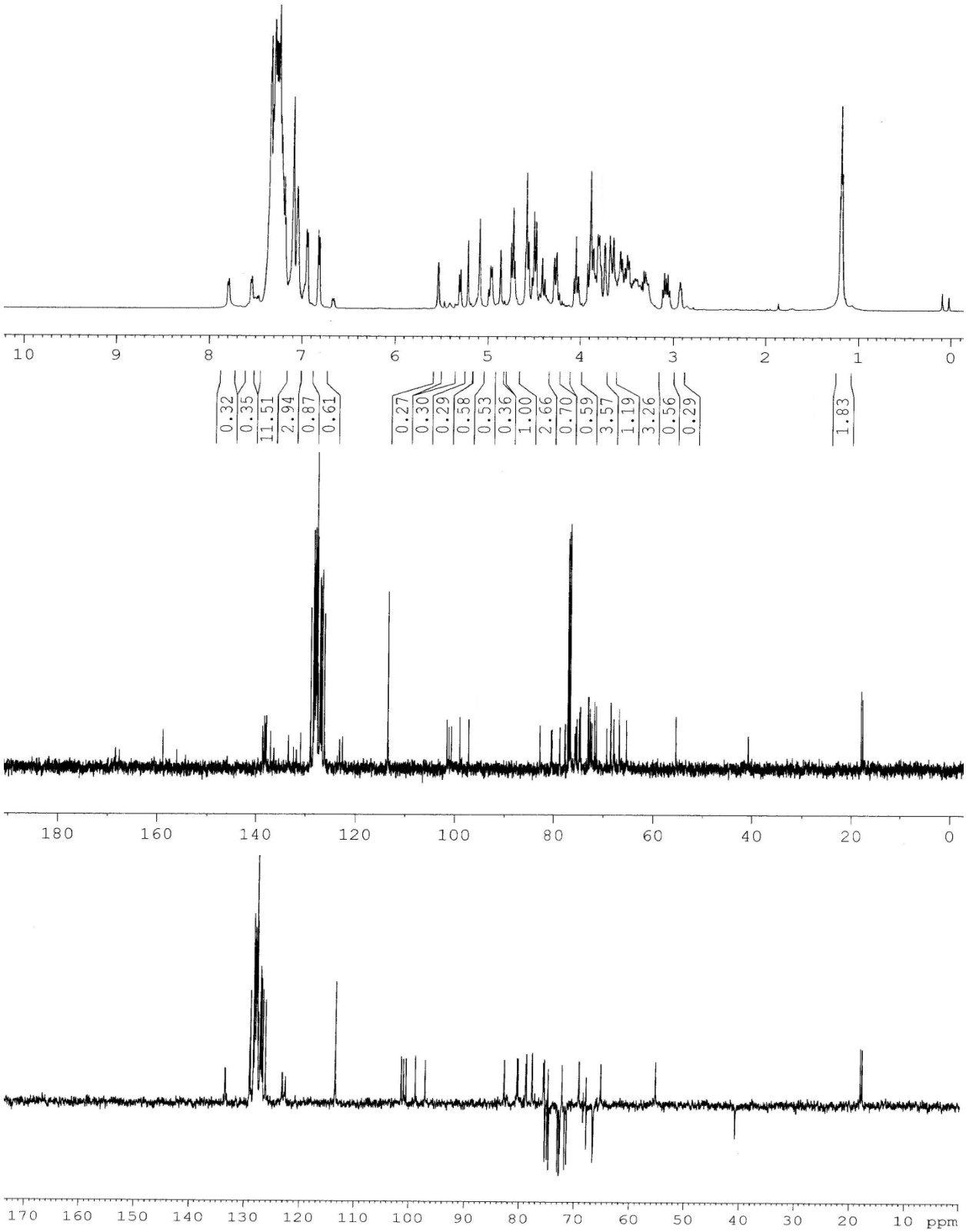

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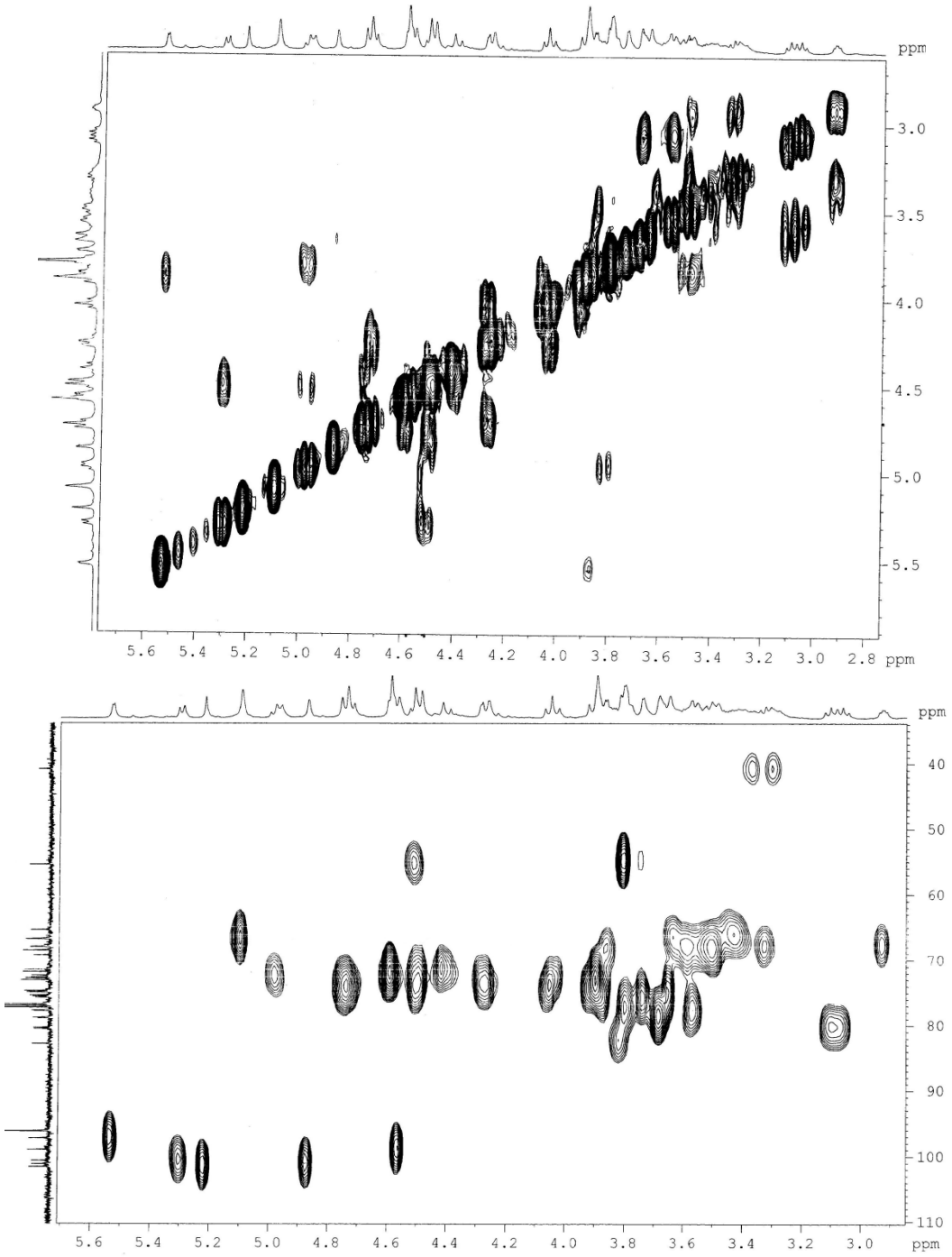

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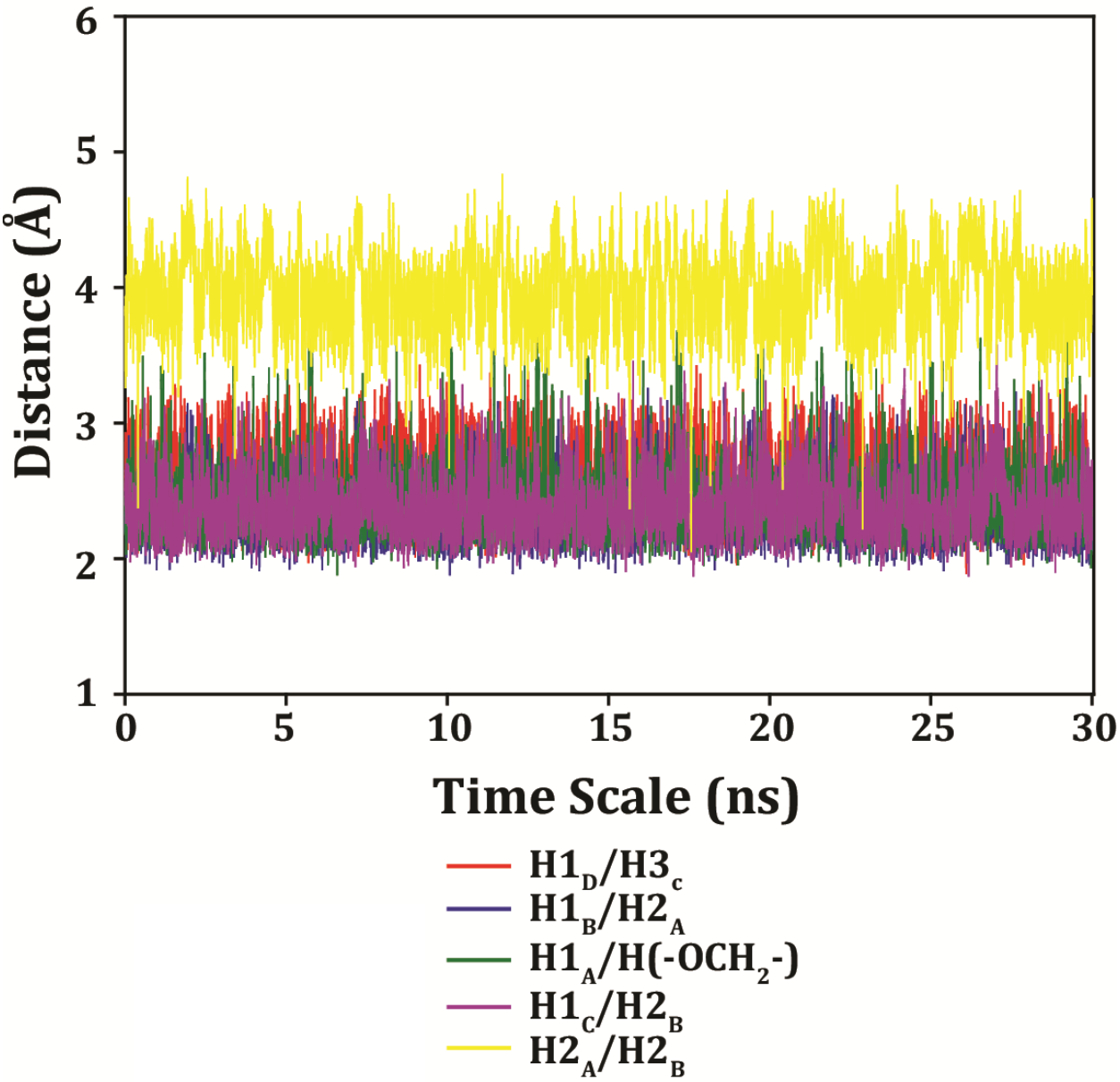

Figure 1: Inter-proton distances of each inter-glycosidic linkage.

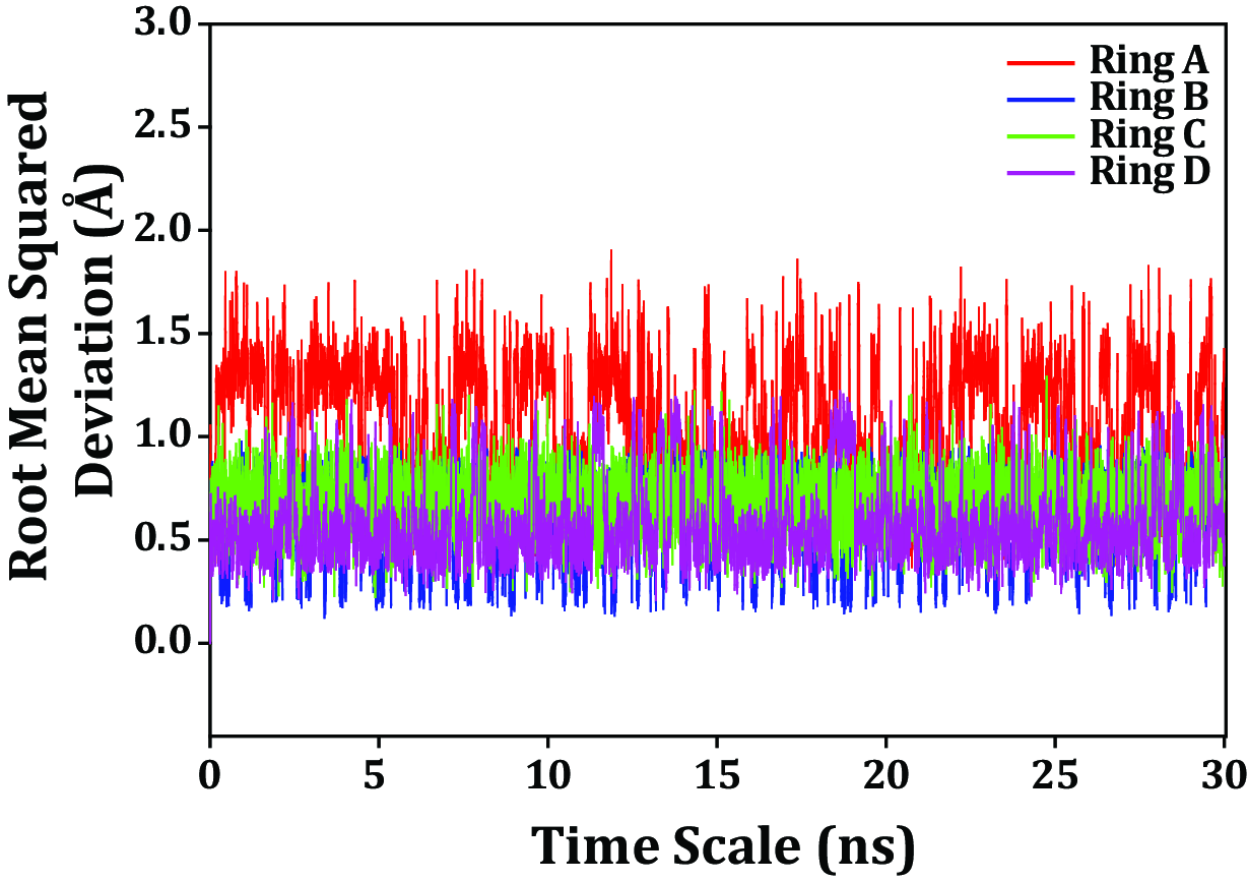

Figure 2: Root-mean-squared-deviation (RMSD) plot with respect to the individual carbohydrate rings.

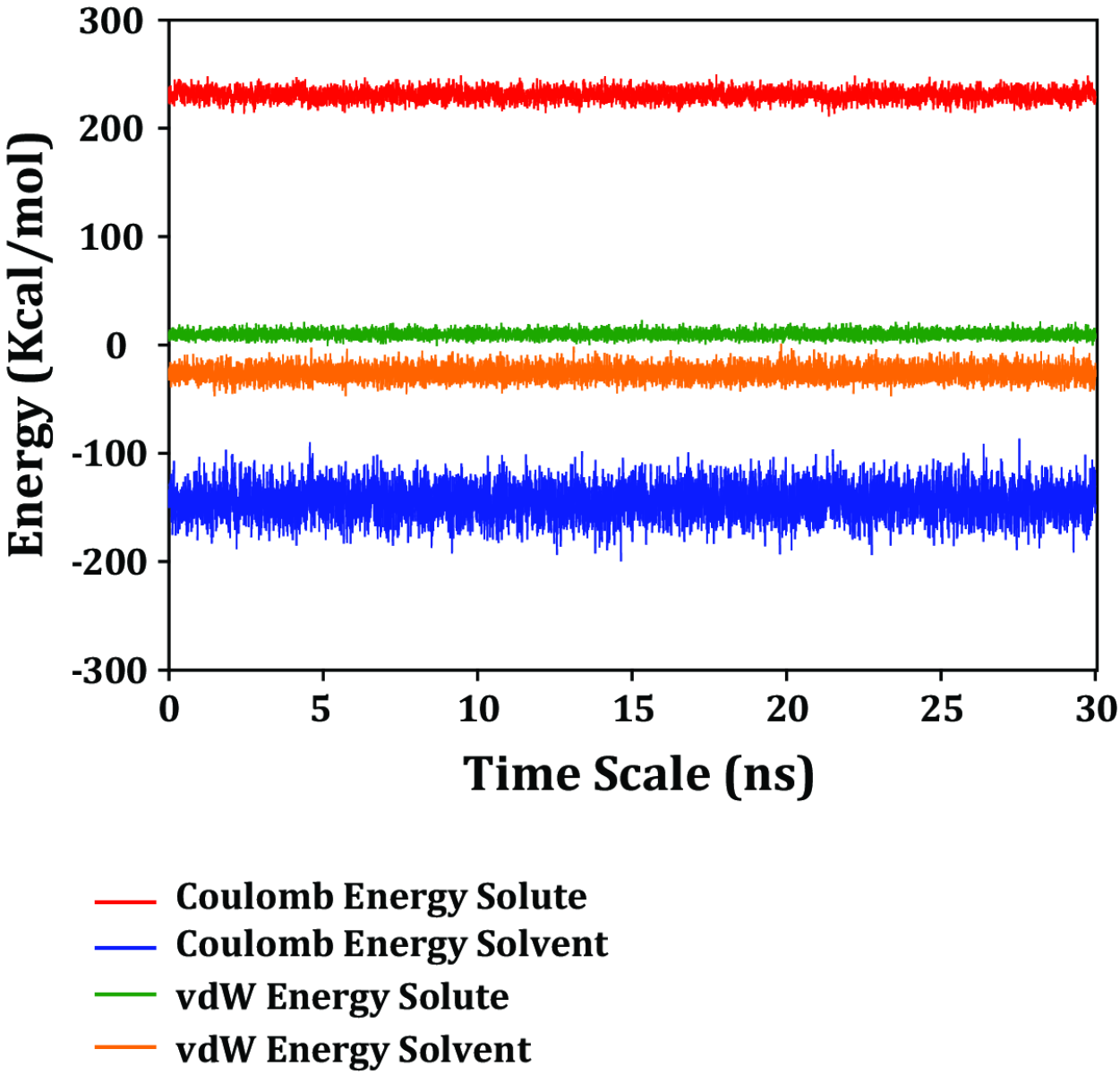

Figure 3: Coulombic and van der Waals (vdW) contribution.