SUPPORTING INFORMATION

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

Manas Jana,a Rajiv Kumar Kar,b Anirban Bhunia b and Anup Kumar Misraa*

aBose Institute, Division of Molecular Medicine, P-1/12, C.I.T. Scheme VII-M, Kolkata-700054, India; FAX: 91-33-2355 3886; E-mail: akmisra69@gmail.com

bBose Institute, Department of Biophysics, P-1/12, C.I.T. Scheme VII-M, Kolkata-700054, India

* Corresponding author

Index

<table>
<thead>
<tr>
<th>Subject</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D and 2D NMR spectra of compounds 1 and 3, 6, 7, 9</td>
<td>2-12</td>
</tr>
<tr>
<td>Inter-proton distances of each inter-glycosidic linkage</td>
<td>13</td>
</tr>
<tr>
<td>Root-mean-squared-deviation (RMSD) plot with respect to the individual carbohydrate rings</td>
<td>14</td>
</tr>
<tr>
<td>Coulombic and van der Waals (vdW) contribution</td>
<td>15</td>
</tr>
</tbody>
</table>
$^1$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 (I) (D$_2$O).
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) (D₂O).
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-diol-β-D-glucopyranoside (3) (CDCl₃).
2D COSY and HSQC NMR spectra (selected regions) of 2-(carbobenzyloxy)aminoethyl 3,4-di-O-benzyl-α-L-rhamnopyranoside (3) (CDCl₃).
$^1$H, $^{13}$C and DEPT 135 NMR spectra of 2-(carbobenzyloxy)aminoethyl (2-0-acetyl-3,4-di-0-benzyl-α-L-rhamnopyranosyl)-(1→2)-3,4-di-0-benzyl-α-L-rhamnopyranoside (6) (CDCl$_3$).
2D COSY and HSQC NMR spectra (selected regions) 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) (CDCl₃).
$^1$H, $^{13}$C and DEPT 135 NMR spectra of 2-(carbobenzyloxy)aminoethyl (3,4-di-O-benzyl-$\alpha$-L-rhamnopyranosyl)-(1→2)-3,4-di-O-benzyl-$\alpha$-L-rhamnopyranoside (7) (CDCl$_3$).
2D COSY and HSQC NMR spectra (selected regions) of 2-(carbobenzyloxy)aminoethyl (3,4-di-O-benzyl-α-L-rhamnopyranosyl)-(1→2)-3,4-di-O-benzyl-α-L-rhamnopyranoside (7) (CDCl₃).
$^1$H, $^{13}$C and DEPT 135 NMR spectra of 2-(carbobenzyloxy)aminoethyl (2,3,4,6-tetra-$O$-benzyl-$\alpha$-D-galactopyranosyl)-(1→3)-(4,6-$O$-benzylidene-2-deoxy-2-$N$-phthalimido-$\beta$-D-glucopyranosyl)-(1→2)-(3,4-$O$-benzyl-$\alpha$-L-rhamnopyranosyl)-(1→2)-3,4-$O$-benzyl-$\alpha$-L-rhamnopyranoside (9) (CDCl$_3$).
2D COSY and HSQC NMR spectra (selected regions) of 2-(carbobenzyloxy)aminoethyl (2,3,4,6-tetra-O-benzyl-α-D-galactopyranosyl)-(1→3)-(4,6-O-benzylidene-2-deoxy-2-N-phthalimido-β-D-glucopyranosyl)-(1→2)-(3,4-di-O-benzyl-α-L-rhamnopyranosyl)-(1→2)-3,4-di-O-benzyl-α-L-rhamnopyranoside (9) (CDCl₃).
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.