VOLUME 289 (2017) PAGES 2745–2754
DOI 10.1074/jbc.AAC118.004605

## First evidence for a covalent linkage between enterobacterial common antigen and lipopolysaccharide in *Shigella sonnei* phase II $ECA_{LPS}$.

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There was an error in the structure of *Shigella sonnei* phase II $ECA_{LPS}$. The anomeric configuration of residue **J** should be assigned as a β anomer [→4)-β-D-Glc*p*NAc-(1→] based on its chemical shifts (Tables 1 and 2) and $J_{H1,C1}$ (162 Hz). The correction results in an inverted anomeric configuration of the D-GlcNAc residue in the first ECA unit linked to the core oligosaccharide, whereas an α-configuration is characteristic for polymeric chain (Fig. 3). Chemical shifts of the residue **J** were in agreement with predictions carried out by the CASPER program (http://www.casper.organ.su.se/casper/),[1] where professor Göran Widmalm is kindly acknowledged for the error identification (1, 2). This correction does not affect the general results and conclusions of this work.

**Table 1**
**$^{1}H$ and $^{13}C$ NMR chemical shifts of fraction IV containing core OS substituted by ECA trisaccharide ([ECA]-dLOS) isolated from *S. sonnei* phase II LOS**

| | | Chemical shift (ppm) | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Residue | Description | H-1/C-1 | H-2/C-2 | H-3(H3ax,eq)/C-3 | H-4/C-4 | H-5/C-5 | H-6a, H-6b/C-6 | H-7a, H-7b/C-7 (NHAc) | H-8a, H-8b/C-8 [C(O)] |
| A | →5)-α-Kdo*p* | ND[a] | −/96.3 | (1.90, 2.25)/34.1 | 4.11/66.3 | 4.17/73.3 | 3.69/69.7 | 3.80/72.6 | 3.47, 3.93/64.7 |
| B | →3)-L-α-D-Hep*p*4PPEtn-(1→ | 5.20/100.1 | 4.01/71.6 | 4.08/78.5 | 4.61/72.3 | 4.22/72.0 | 4.10/69.3 | 3.72, 3.72/63.8 | |
| C | →3,7)-L-α-D-Hep*p*4P-(1→ | 5.10/103.5 | 4.38/70.6 | 4.12/79.8 | 4.40/69.4 | 3.80/73.2 | 4.23/68.5 | 3.58, 3.75/68.4 | |
| D | L-α-D-Hep*p*-(1→ | 4.98/100.2 | 3.93/70.7 | 3.87/71.4 | 3.84/66.9 | 3.61/71.9 | 4.04/69.5 | 3.65, 3.72/63.7 | |
| E | →3)-α-D-Glc*p*-(1→ | 5.20/102.0 | 3.66/71.0 | 4.07/76.7 | 3.77/71.2 | 3.91/73.1 | 3.79,3.92/60.5 | | |
| F | →2,3)-α-D-Glc*p*-(1→ | 5.80/95.3 | 3.87/73.3 | 4.17/78.7 | 3.56/68.7 | 4.10/71.9 | 3.78,3.95/61.0 | | |
| F′[b] | →2,3)-α-D-Glc*p*-(1→ | 5.81/95.1 | 3.88/73.3 | 4.19/78.8 | 3.57/68.7 | 4.11/72.0 | 3.79,3.96/61.0 | | |
| G | →2)-α-D-Gal*p*-(1→ | 5.61/92.1 | 3.98/73.2 | 4.19/68.9 | 3.98/70.7 | 4.13/72.0 | 3.74,3.74/61.9 | | |
| H | α-D-Gal*p*-(1→ | 5.31/96.6 | 3.85/69.0 | 3.95/70.1 | 3.99/70.1 | 4.13/72.0 | 3.75,3.75/61.9 | | |
| I | →3)-β-D-Glc*p*-(1→ | 4.73/103.1 | 3.39/73.6 | 3.68/85.4 | 3.49/68.9 | 3.44/76.3 | 3.72,3.89/61.4 | | |
| I′[c] | β-D-Glc*p*-(1→ | 4.75/103.1 | 3.33/73.9 | 3.51/76.6 | 3.40/70.4 | 3.45/76.6 | 3.73,3.91/61.4 | | |
| J | →4)-β-D-Glc*p*NAc-(1→ | 4.78/102.3 | 3.75/56.3 | 3.74/72.7 | 3.68/79.5 | 3.54/75.2 | 3.86,3.70/60.9 | (2.03/23.0) | [175.5] |
| K | →4)-β-D-Man*p*NAcA-(1→ | 4.93/99.7 | 4.49/54.2 | 4.07/73.2 | 3.82/74.8 | 3.86/77.2 | −/175.1 | (2.07/22.6) | [176.2] |
| L | α-D-Fuc*p*4NAc-(1→ | 5.35/99.5 | 3.64/69.3 | 4.00/69.1 | 4.20/54.6 | 4.18/66.5 | 1.06/16.2 | (2.07/22.6) | [176.3] |
| PPEtn | | 4.20/63.1 | 3.29/40.7 | | | | | | |

[a] ND, not determined.
[b] Residue F′ is a variant of residue F present in the core OS that is devoid of ECA trisaccharide.
[c] Residue I′ is a terminal residue I present in the core OS that is devoid of ECA trisaccharide.

**Table 2**
**Selected inter-residue NOE and $^{3}J_{H,C}$ connectivities from the anomeric atoms of ([ECA]-dLOS) dodecasaccharide isolated from *S. sonnei* phase II LOS**

Data indicating the covalent linkage between ECA and LOS are shown in boldface type.

| | | | Connectivity to | | |
|---|---|---|---|---|---|
| Residue | Description | Atom $\delta_H/\delta_C$ (ppm) | $\delta_C$ | $\delta_H$ | Inter-residue atom/residue |
| B | →3)-L-α-D-Hep*p*4PPEtn-(1→ | 5.20/100.1 | − | 4.17[a] | H-5 of A |
| C | →3,7)-L-α-D-Hep*p*4P-(1→ | 5.10/103.5 | 78.5 | 4.08[a] | C-3, H-3 of B |
| D | L-α-D-Hep*p*-(1→ | 4.98/100.2 | 68.5 | 3.59/3.74[a] | C-7, H-7a, H-7b of C |
| E | →3)-α-D-Glc*p*-(1→ | 5.20/102.0 | − | 4.12 | H-3 of C |
| F | →2,3)-α-D-Glc*p*-(1→ | 5.80/95.3 | − | 4.07 | H-3 of E |
| F′ | →2,3)-α-D-Glc*p*-(1→[b] | 5.81/95.1 | − | 4.07 | H-3 of E |
| G | →2)-α-D-Gal*p*-(1→ | 5.61/92.1 | − | 3.87[a] | H-2 of F |
| H | α-D-Gal*p*-(1→ | 5.31/96.6 | − | 3.97[a] | H-2 of G |
| I | →3)-β-D-Glc*p*-(1→ | 4.73/103.1 | 78.7 | 4.17 | H-3 of F |
| I′ | β-D-Glc*p*-(1→[c] | 4.75/103.1 | 78.8 | 4.19 | H-3 of F′ |
| **J** | **→4)-β-D-Glc*p*NAc-(1→** | **4.78/102.3** | **85.3** | **3.68** | **H-3 of I** |
| K | →4)-β-D-Man*p*NAcA-(1→ | 4.93/99.7 | 79.4 | 3.69[a] | H-4 of J |
| L | α-D-Fuc*p*4NAc-(1→ | 5.35/99.5 | 74.7 | 3.81 | H-4 of K |

[a] Value represents NOE connectivities only.
[b] Residue F′ is a variant of residue F present in the core OS that is devoid of ECA trisaccharide.
[c] Residue I′ is a terminal residue I present in the core OS that is devoid of ECA trisaccharide.

[1] Please note that the JBC is not responsible for the long-term archiving and maintenance of this site or any other third party-hosted site.

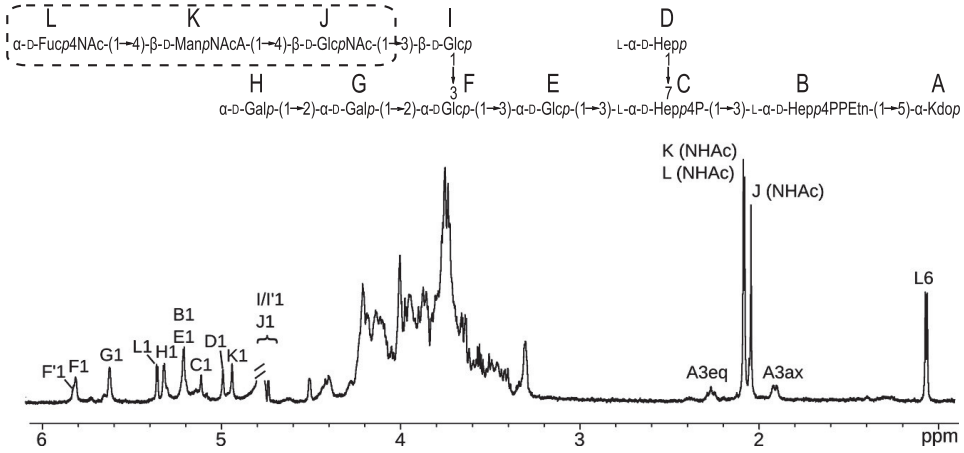


Fig. 3

## References


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