

SUPPLEMENTAL INFORMATION :

Novel *Campylobacter concisus* Lipooligosaccharide is a Determinant of
Inflammatory Potential and Virulence

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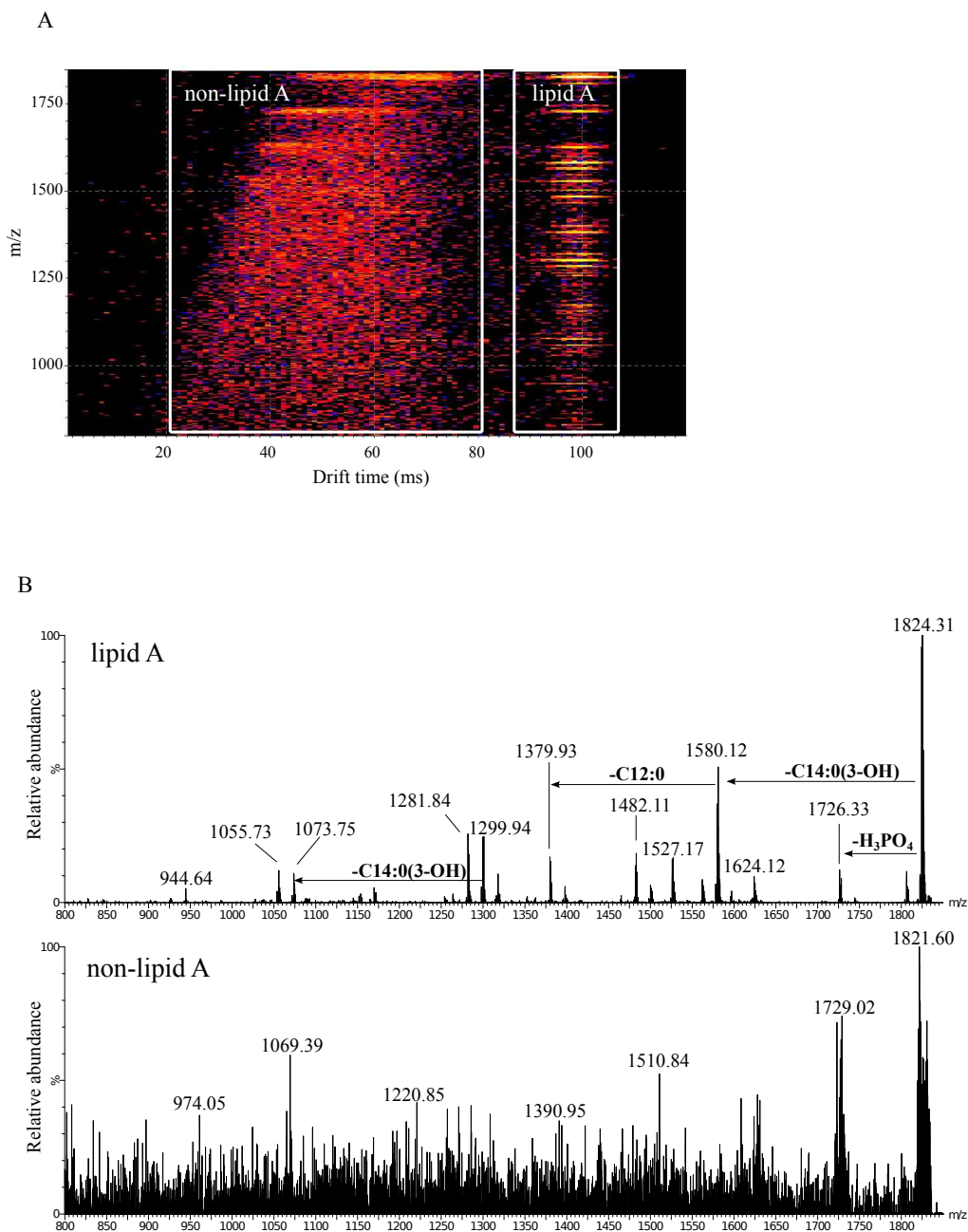
² These authors contributed equally to this work

SUPPLEMENTAL TABLE S1.

Observed and calculated fragment ion peaks of di- and bisphosphorylated lipid A

	<i>O</i> -deacylated		Intact	
	Cal. m/z	Obs. m/z (Δ Da)	Cal. m/z	Obs. m/z (Δ Da)
Full structure	979.49	979.50 (0.01)	1824.24	1824.31 (0.07)
Bis-phosphorylated				
B-ions	466.22	466.22 (0.01)		
Y-ions	512.27	512.26 (0.01)	738.48	738.46 (0.02)
^{0,4} A-ions	526.25	526.26 (-0.01)		
^{0,2} A-ions	586.27	586.24 (0.3)		
Diphosphorylated				
B-ions	546.19	546.19 (0.00)	1164.86	1164.75 (0.09)
Y-ions			658.45	658.49 (-0.04)
^{0,2} A-ions	666.24	666.21 (0.03)		

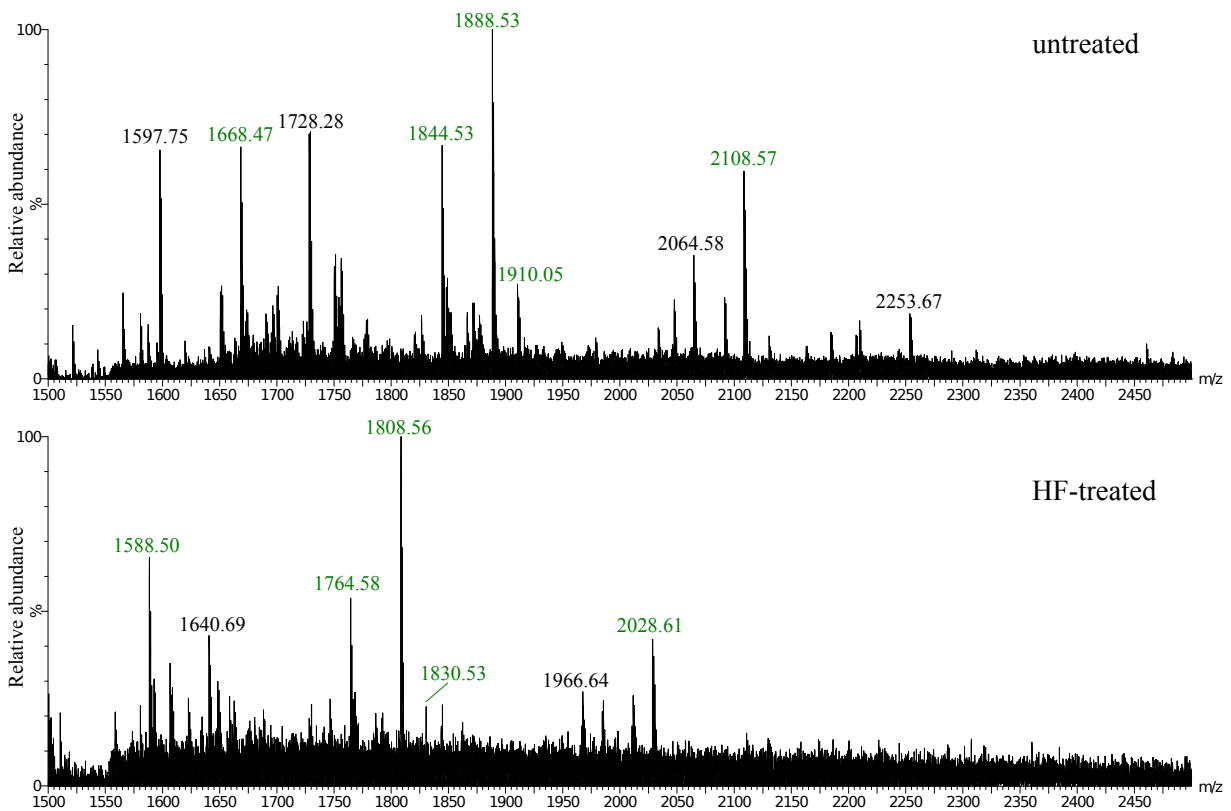
Supplemental Figure S1.



Supplemental Figure S1. Negative-ion IMS-MS/MS analysis of the *C. concisus* 2010-131105 lipid A prompt fragment ions at m/z 1824.31.

Collision-induced dissociation was conducted in the Transfer region of the Triwave device on the Synapt G2 HDMS after the IMS separation. A: Panel shows the two-dimensional plot of the IMS-MS/MS data Under the selection conditions employed to achieve high sensitivity, the interfering non-lipid A prompt fragments at m/z 1821.6-1824.6 were included in the selection window but were readily resolved by IMS due to differences in drift time. B: The lipid A (m/z 1824.31) MS/MS spectrum was selected from the two-dimensional plot as indicated and is shown (top). The spectrum of the non-lipid A prompt fragment ions is also shown (bottom).

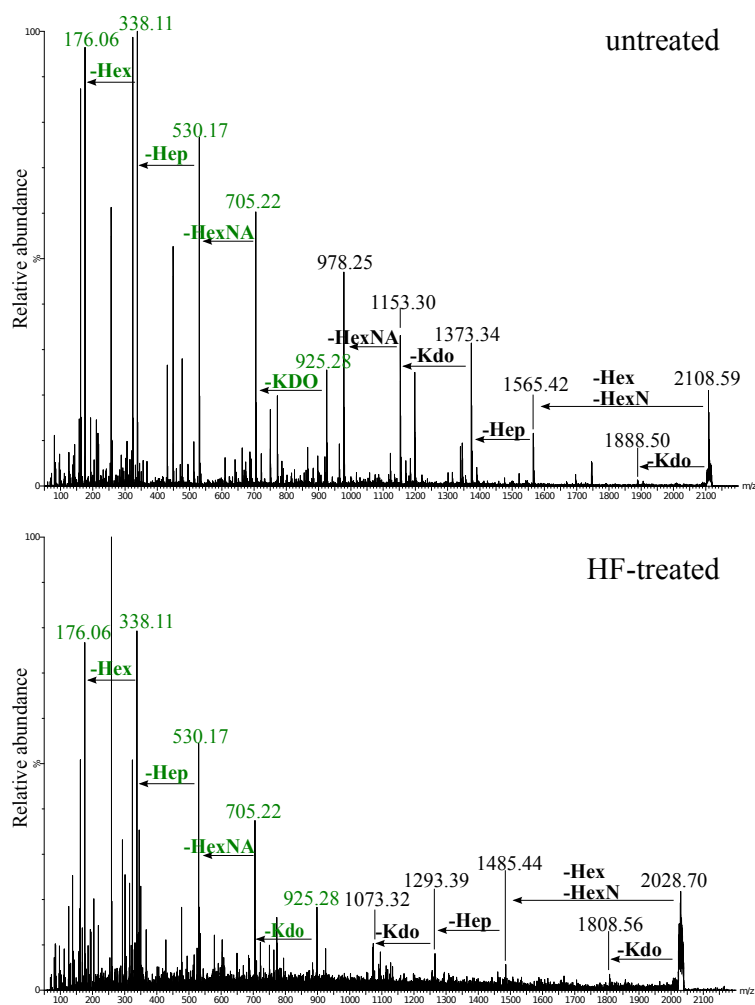
Supplemental Figure S2.



Supplemental Figure S2. Positive-ion MALDI-TOF MS of intact *C. concisus* NCTC 12408 LOS with and without HF treatment.

NCTC 12408 strain LOS was treated with HF to remove phosphoester moieties from the sample. Portions of the positive-ion MALDI-TOF MS spectra of untreated (top) and HF-treated (bottom) LOS are shown. Green-colored labels indicate fragment ion peaks for OS (top) containing a phosphate and (bottom) the corresponding fragment ion peaks that have shifted by m/z 79.97 due to loss of phosphate after HF-treatment.

Supplemental Figure S3.



Supplemental Figure S3. Positive ion MALDI-TOF MS/MS analysis of core OS fragment ions.

LOS of NCTC 12408 was treated with HF to remove phosphoester moieties. Positive-ion MS/MS spectra of untreated OS fragment ions (top $(M+H)^+$ at m/z 2108.59) and HF-treated fragment ions (bottom $(M+H)^+$ at m/z 2028.70) are shown. The mass of losses observed are consistent with the presence of known carbohydrate moieties as indicated. Green-colored labels indicate fragment ions without phosphate that were observed in both spectra.