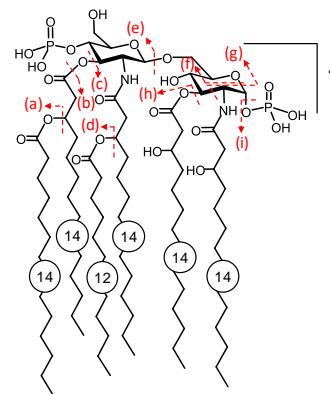
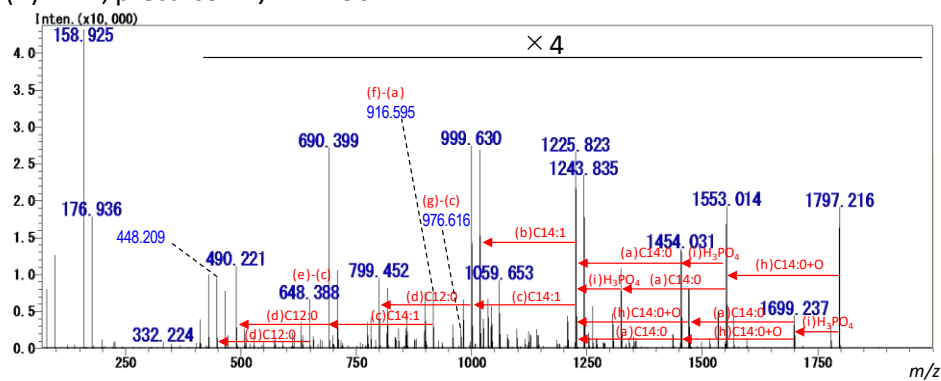
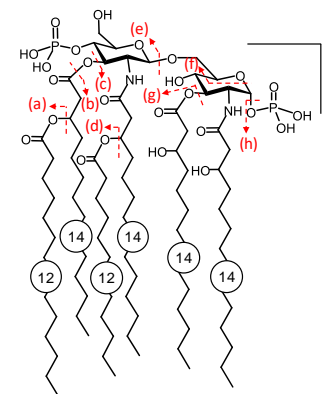
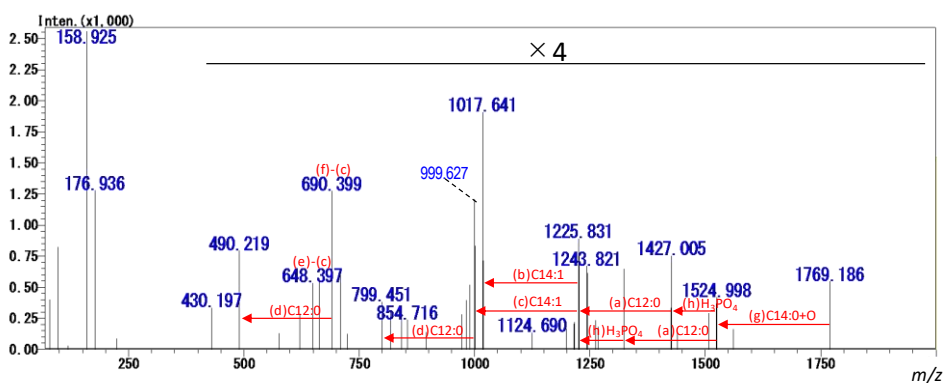


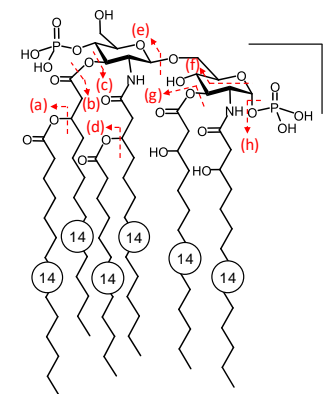
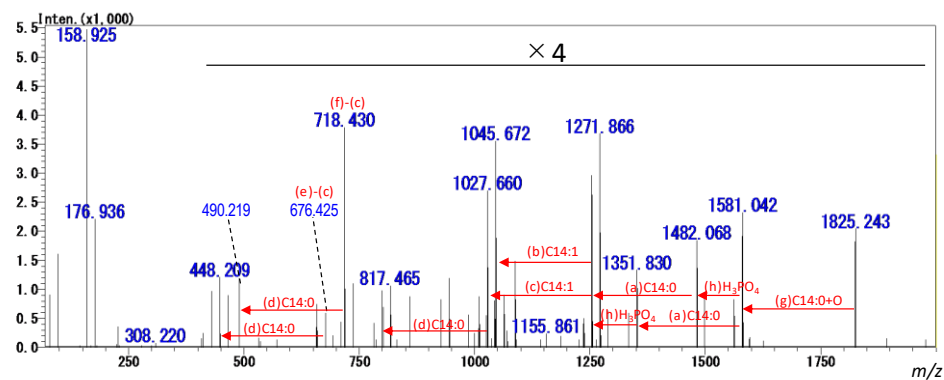
(A) ID: 1, precursor  $m/z = 1796.2$



(B) ID: 2, precursor  $m/z = 1768.2$



(C) ID: 3, precursor  $m/z = 1824.2$



(D) ID: 4, precursor  $m/z = 1359.8$

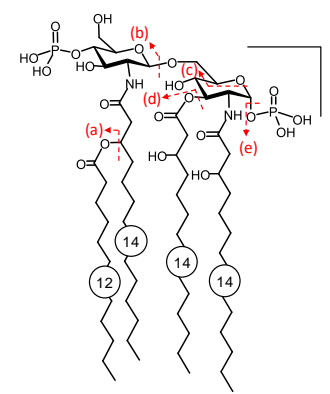
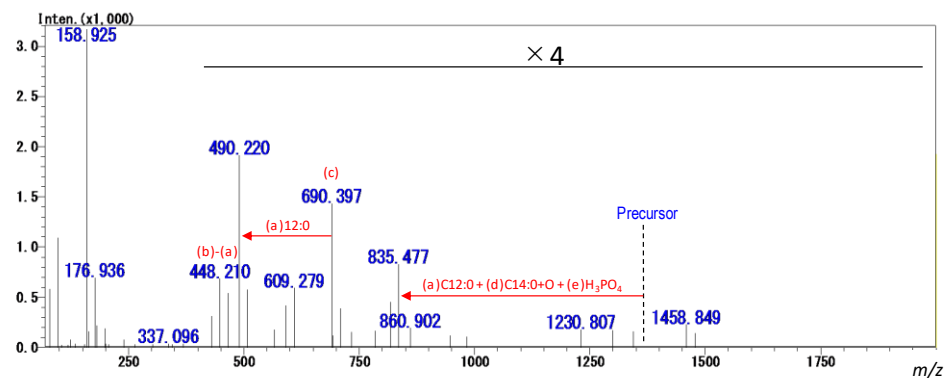
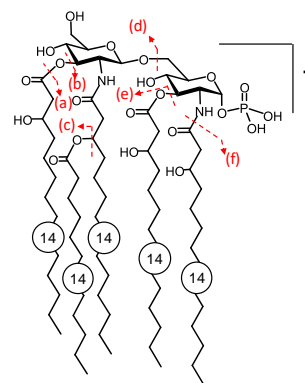
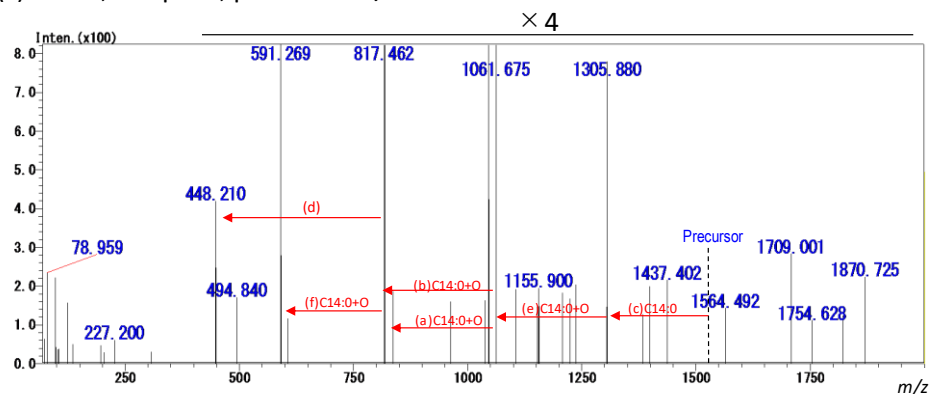


Figure S1. MS/MS spectra of diverse molecular species present in *E. coli* lipid A.

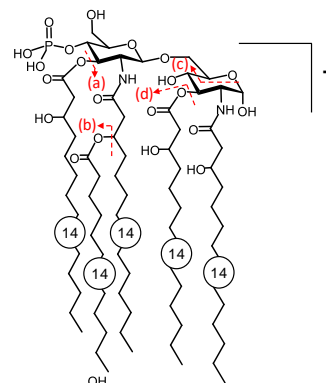
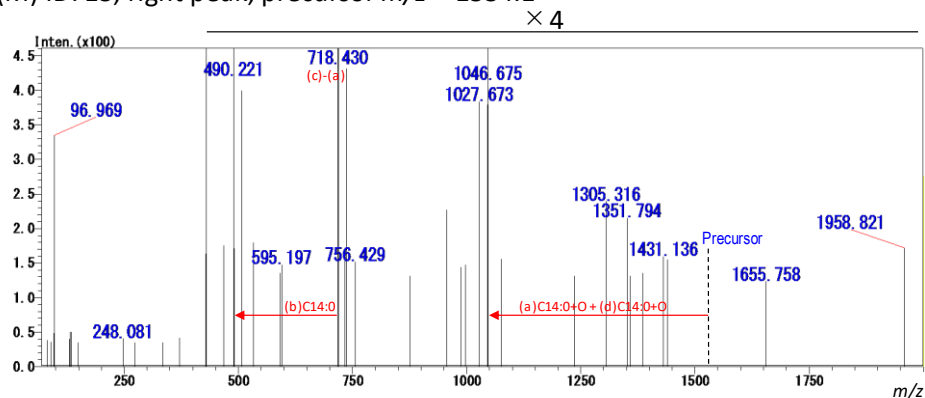




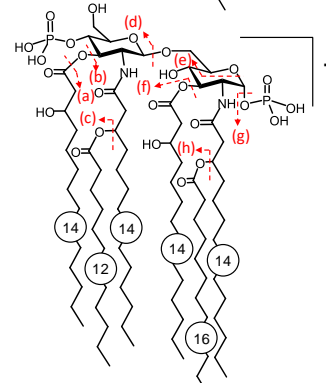
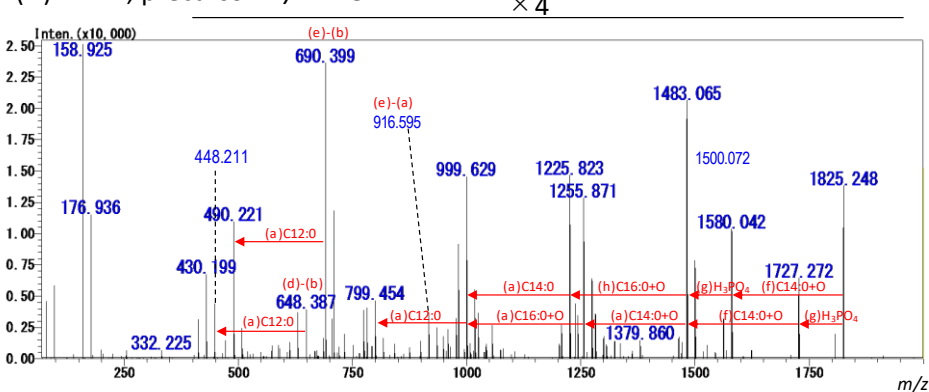
(L) ID: 13, left peak, precursor  $m/z = 1534.1$



(M) ID: 13, right peak, precursor  $m/z = 1534.1$



(N) ID: 14, precursor  $m/z = 1824.2$



(O) ID: 15, precursor  $m/z = 1852.3$

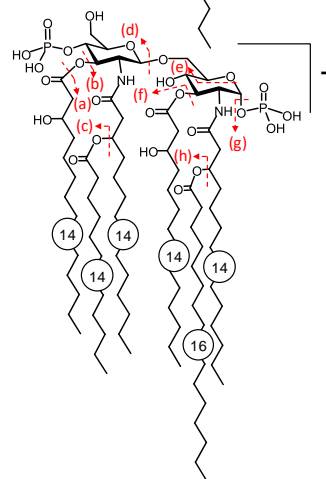
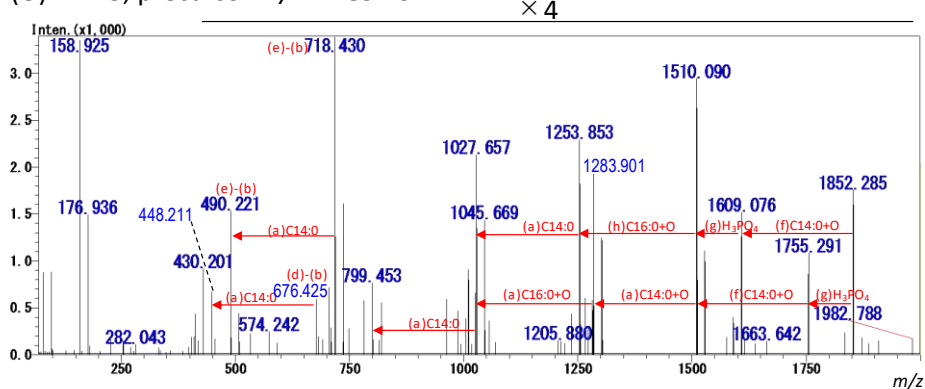
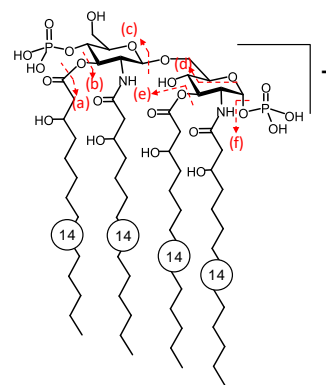
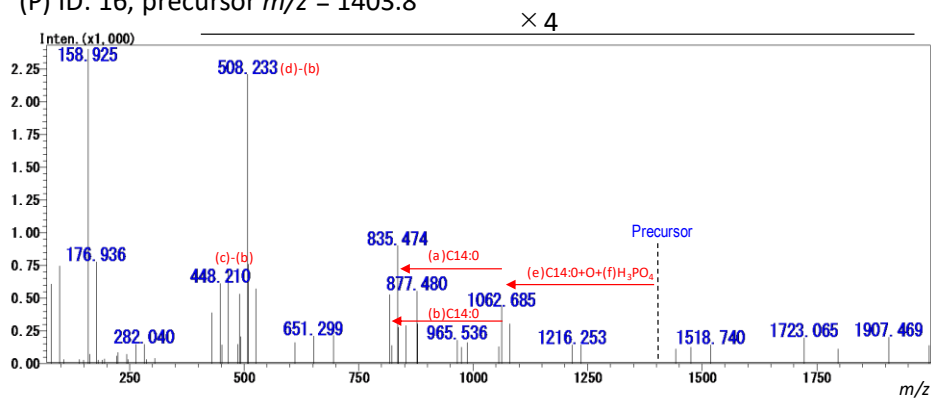
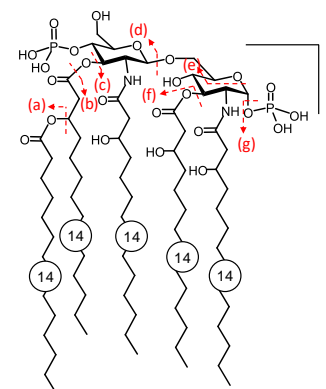
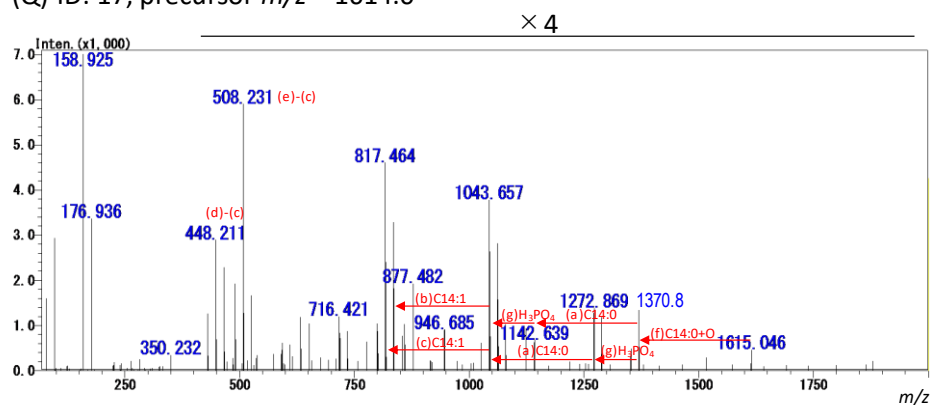


Figure S1. (Continued) MS/MS spectra of diverse molecular species present in *E. coli* lipid A.

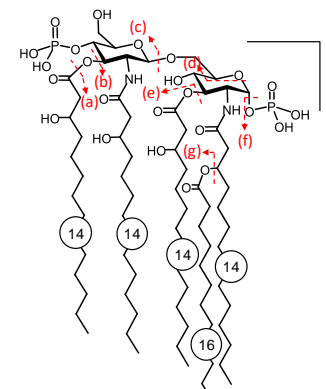
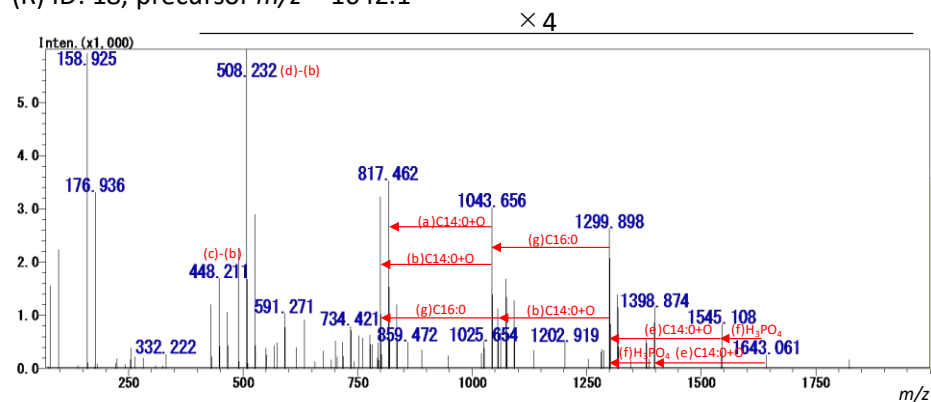
(P) ID: 16, precursor  $m/z = 1403.8$



(Q) ID: 17, precursor  $m/z = 1614.0$



(R) ID: 18, precursor  $m/z = 1642.1$



(S) ID: 19, precursor  $m/z = 1852.3$

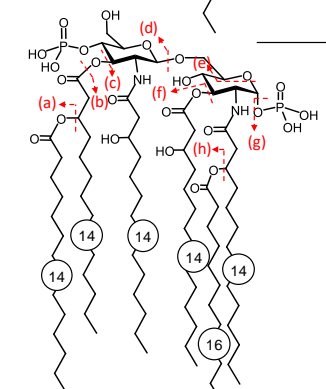
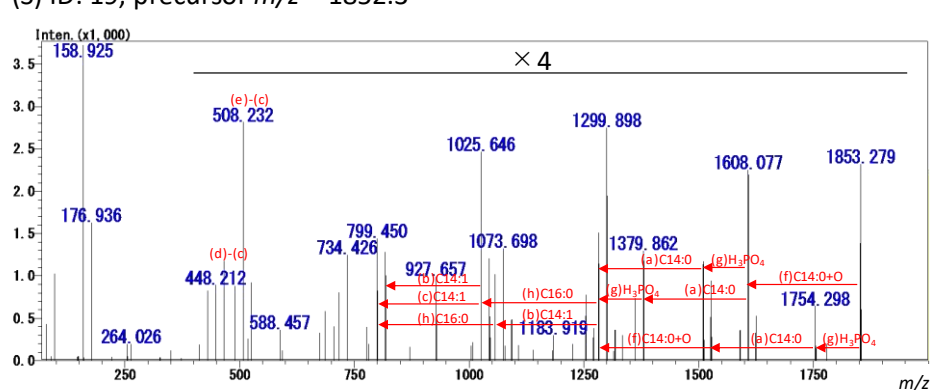


Figure S1. (Continued) MS/MS spectra of diverse molecular species present in *E. coli* lipid A.

(T) ID: 20, precursor  $m/z = 1850.3$

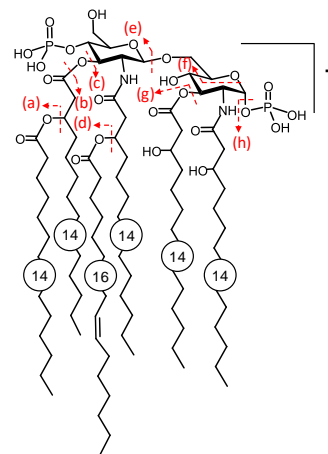
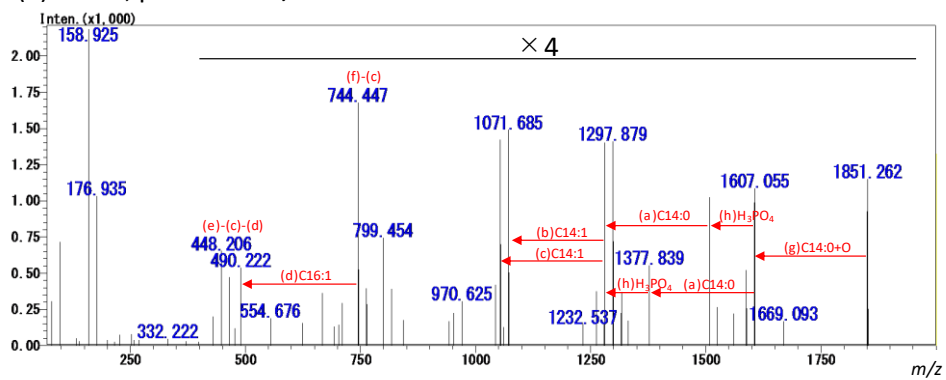
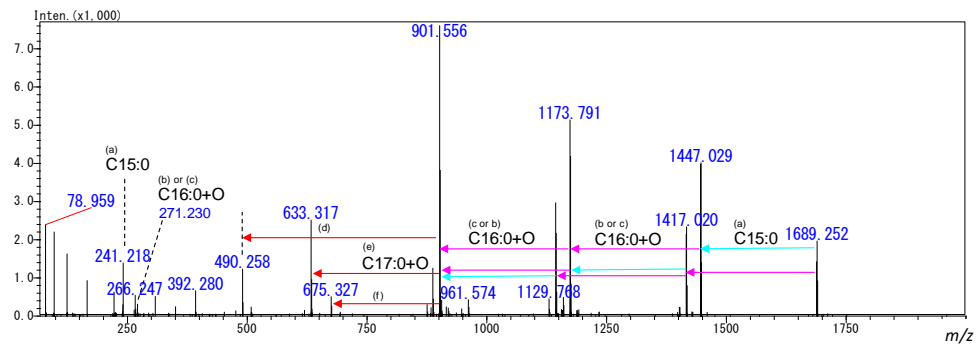
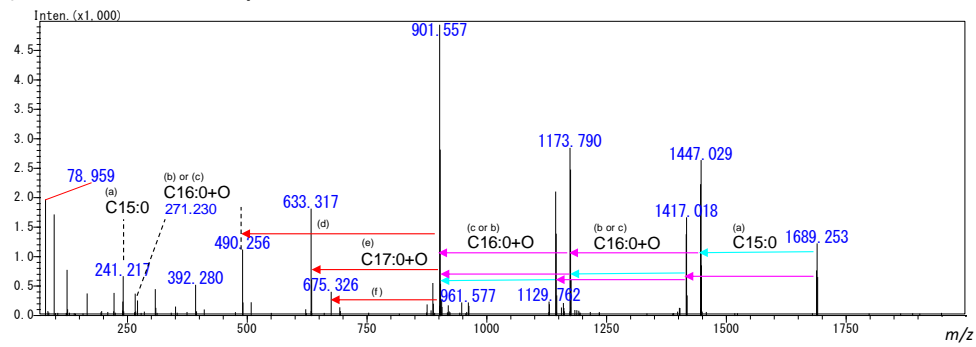


Figure S1. (Continued) MS/MS spectra of diverse molecular species present in *E. coli* lipid A.

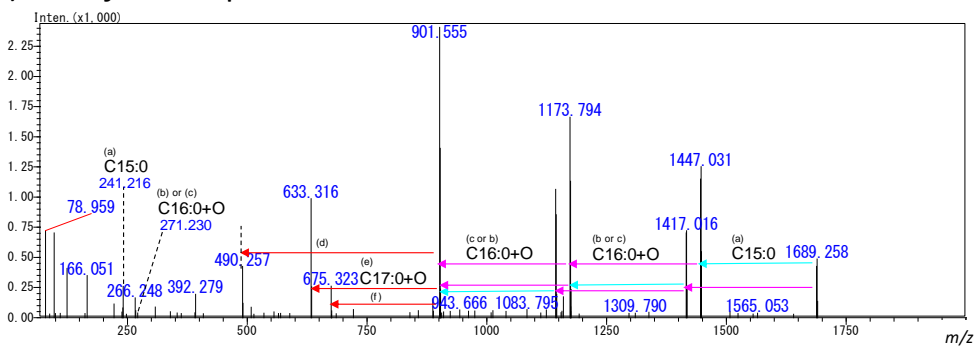
(A) *B. thetaiotaomicron* lipid A 81:0



(B) *B. intestinalis* lipid A 81:0



(C) *B. uniformis* lipid A 81:0



(D) *P. johnsonii* lipid A 81:0

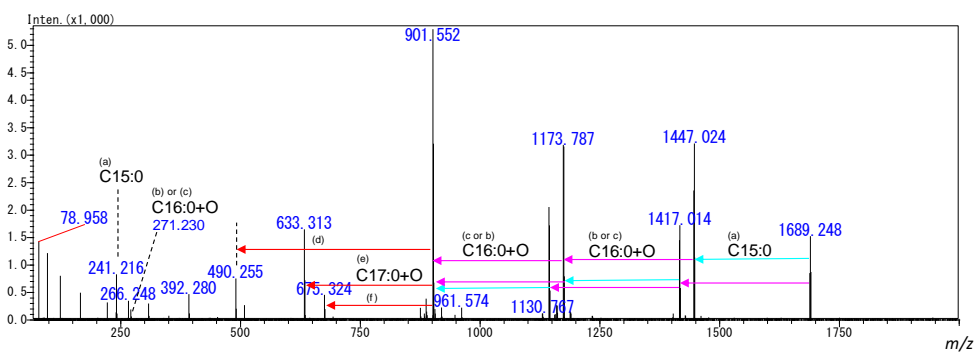
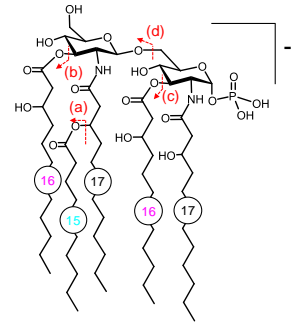
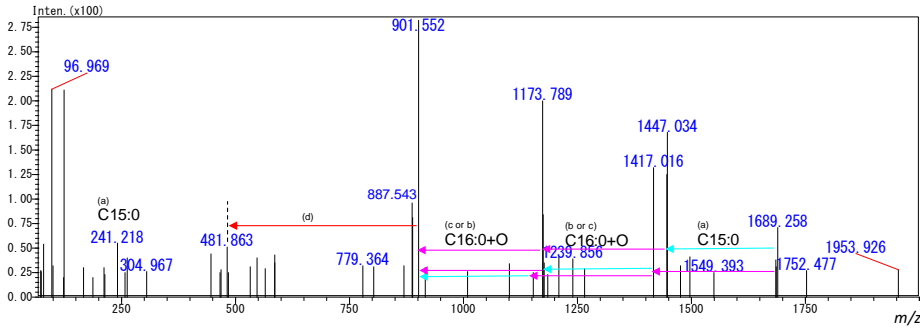
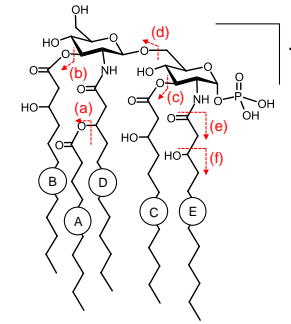
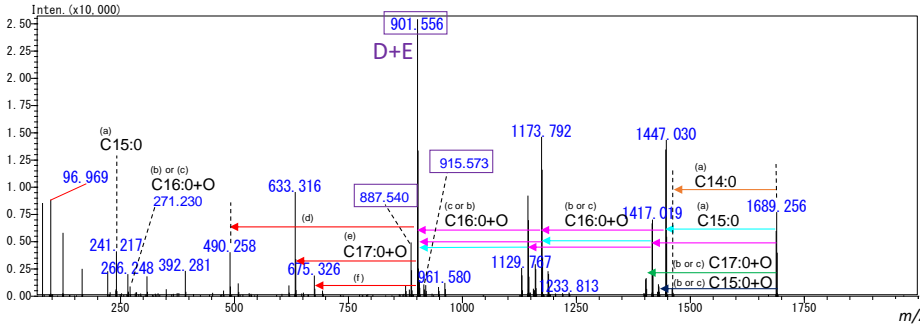


Figure S2. MS/MS spectra of lipid A 81:0 from Bacteroidetes strains.

(E) *P. xylaniphila* lipid A 81:0



(F) *B. vulgatus* lipid A 81:0



A = 14 or 15

D, E = 16 or 17 (D+E = 33, 34 or 35)

B, C = 15, 16 or 17 (B+C = 81-A-D-E)

(G) *O. laneus* lipid A 81:0

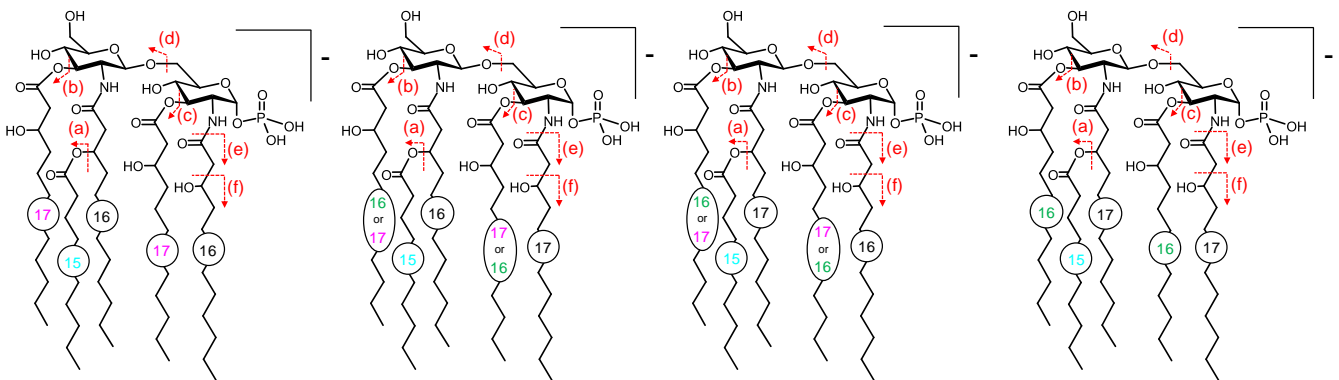
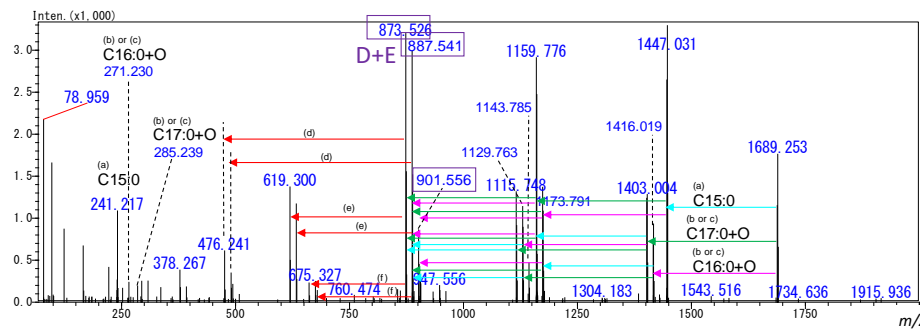
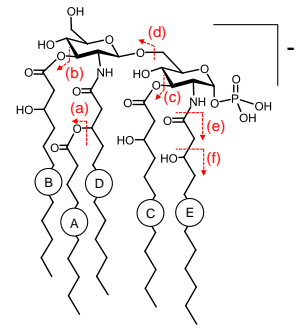
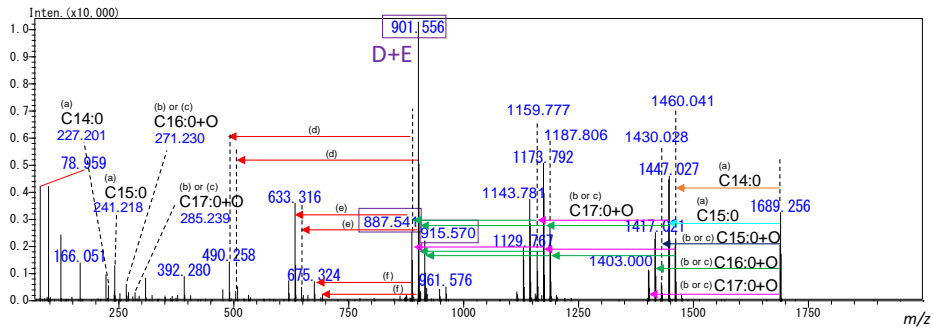


Figure S2. (Continued) MS/MS spectra of lipid A 81:0 from Bacteroidetes strains.



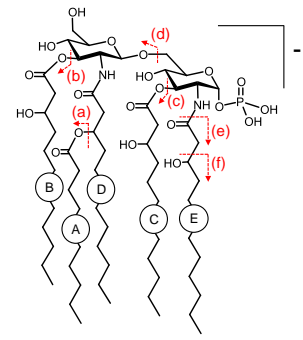
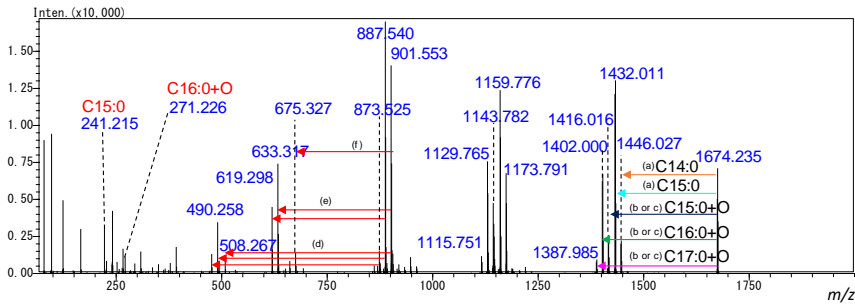
(H) *P. copri* lipid A 81:0



A = 14 or 15  
 D, E = 16 or 17 (D+E = 33, 34 or 35)  
 B, C = 15, 16 or 17 (B+C = 81-A-D-E)

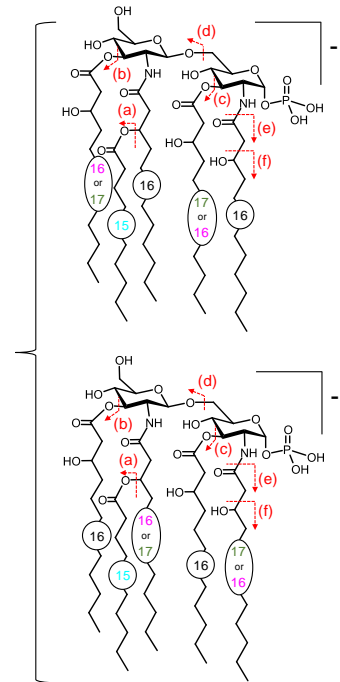
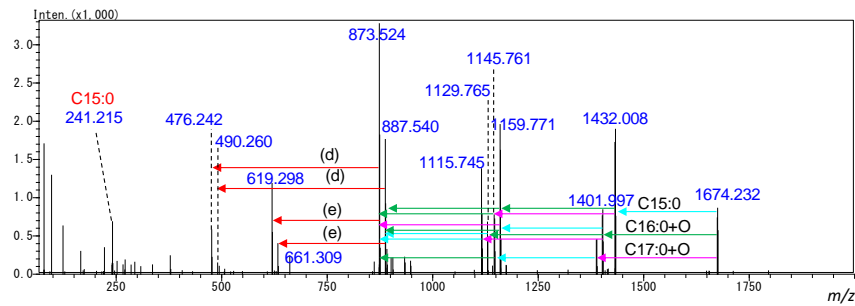
Figure S2. (Continued) MS/MS spectra of lipid A 81:0 from Bacteroidetes strains.

(A) Major *B. vulgatus* lipid A 80:0, precursor  $m/z = 1674.2$

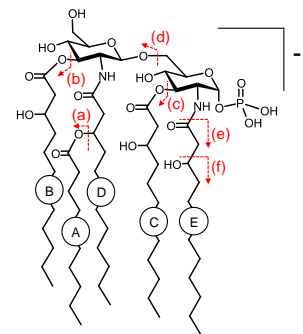
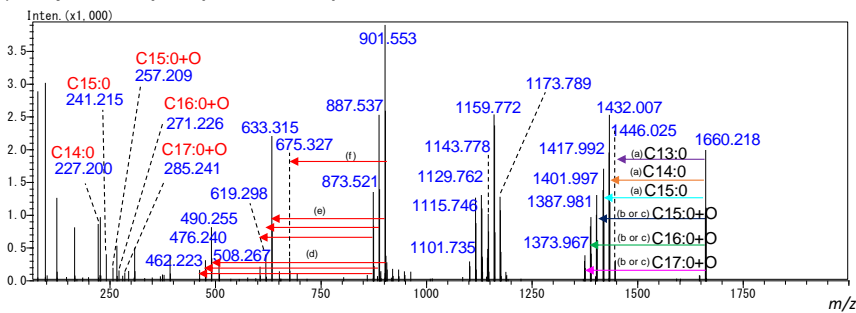


A = 14 or 15  
 D, E = 16 or 17 (D+E = 33, 34 or 35)  
 B, C = 15, 16 or 17 (B+C = 81-A-D-E)

(B) Major *O. laneus* lipid A 80:0, precursor  $m/z = 1674.2$



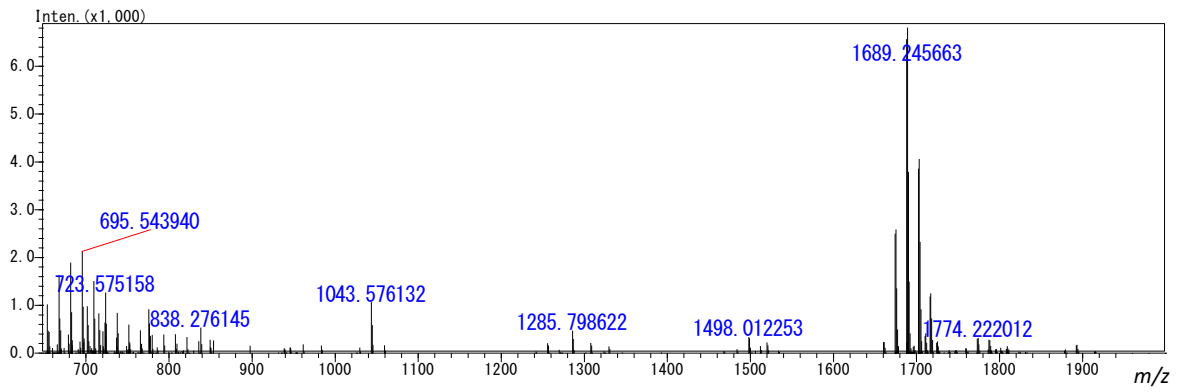
(C) Major *P. copri* lipid A 79:0, precursor  $m/z = 1660.2$



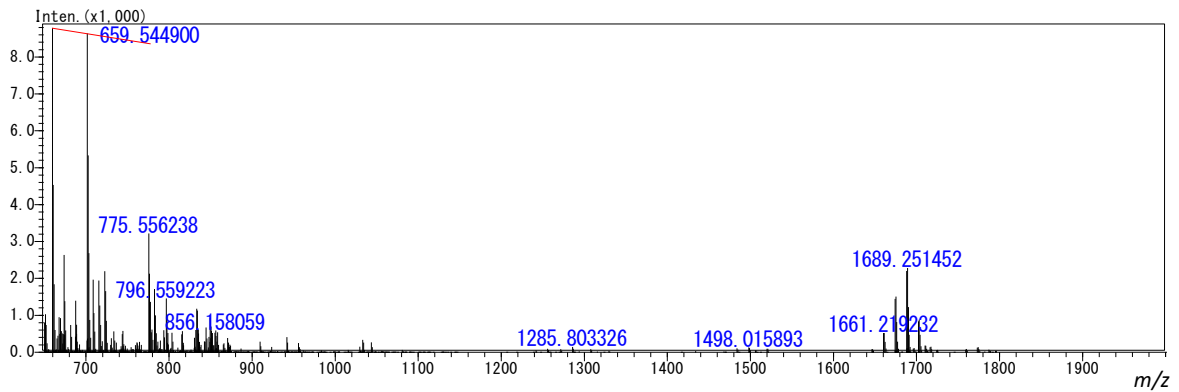
A = 13, 14 or 15  
 D, E = 16 or 17 (D+E = 32, 33, or 34)  
 B, C = 15, 16 or 17 (B+C = 81-A-D-E)

Figure S3. MS/MS spectra of dominant lipid A species in each Bacteroidetes strain.

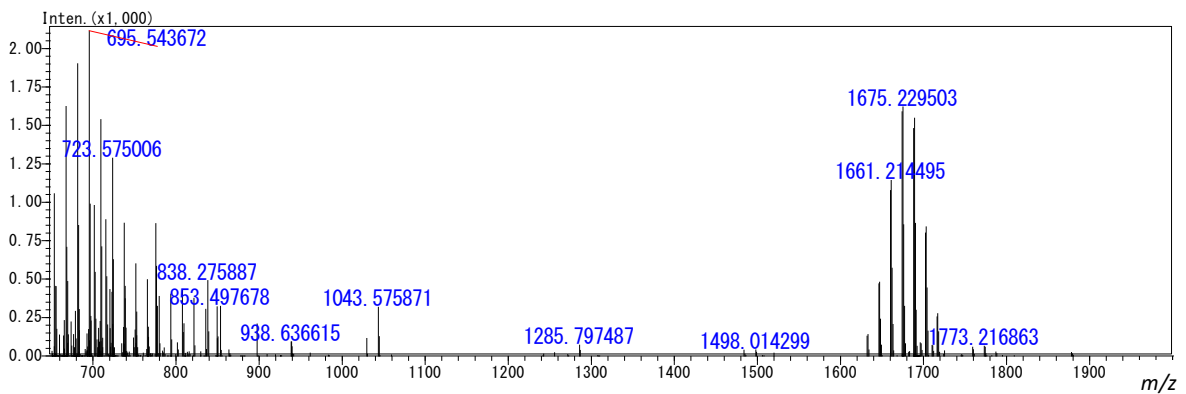
(A) *B. fragilis*



(B) *B. thetaiotaomicron*



(C) *B. vulgatus*



(D) *B. intestinalis*

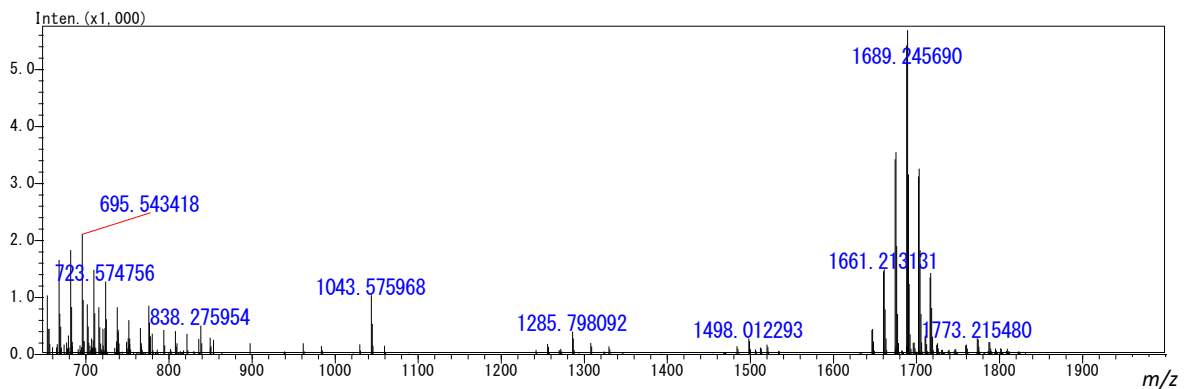
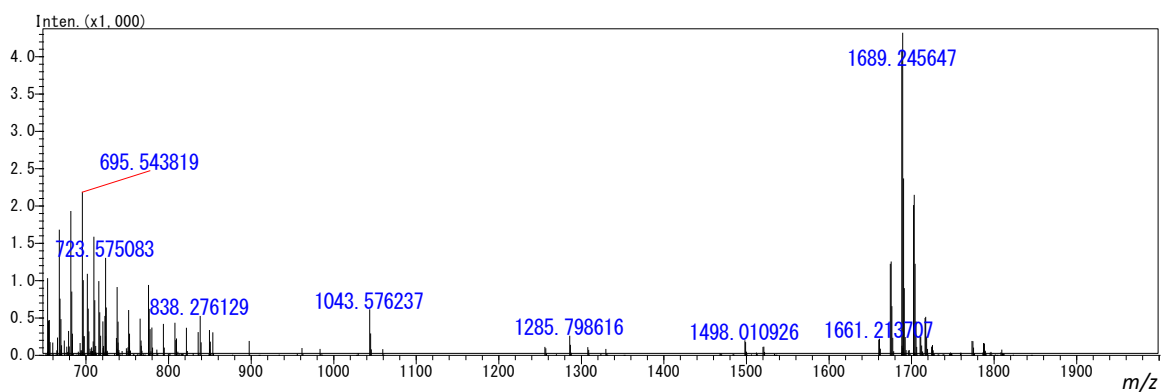


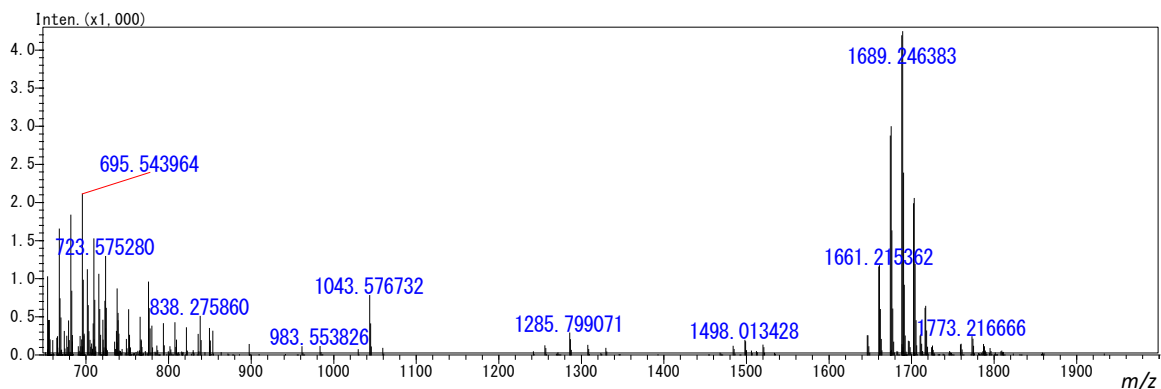
Figure S4. MS1 spectra of lipid A extracts in each Bacteroidetes strain.

Average MS1 spectra of RT=10–12 min were presented.

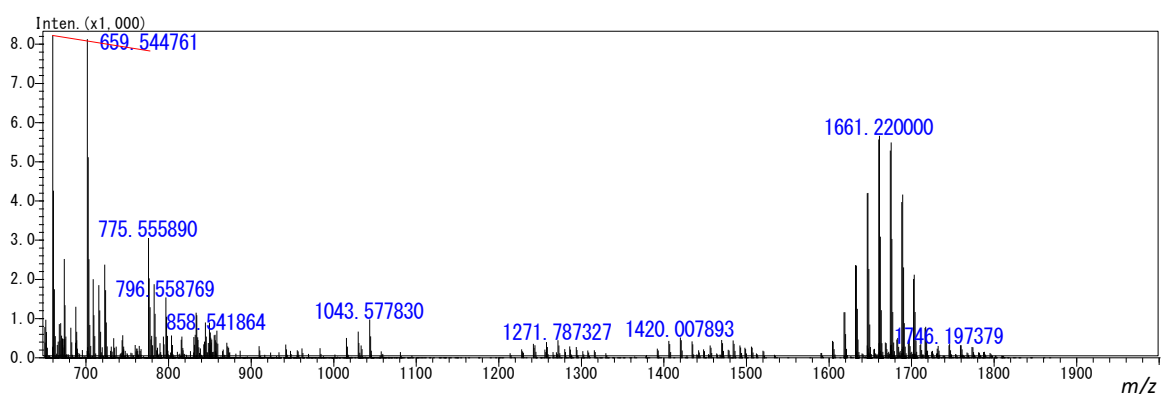
(E) *B. uniformis*



(F) *P. johnsonii*



(G) *P. copri*



(H) *P. xylaniphila*

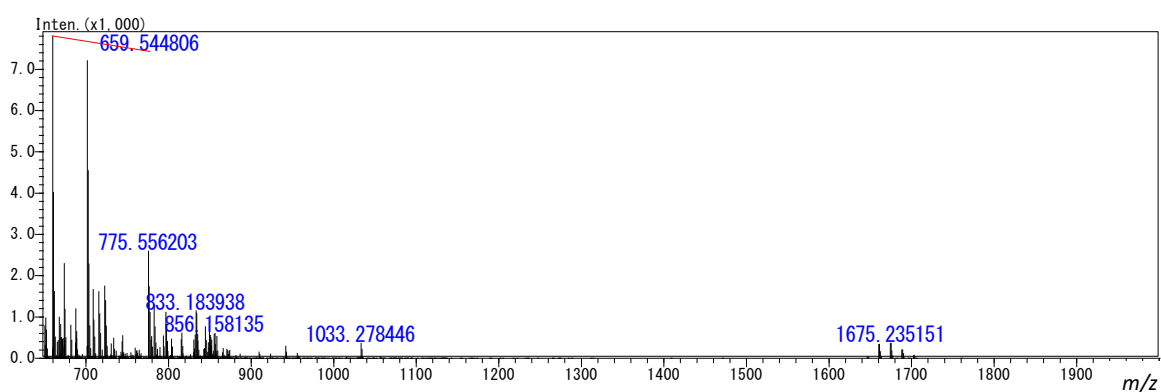
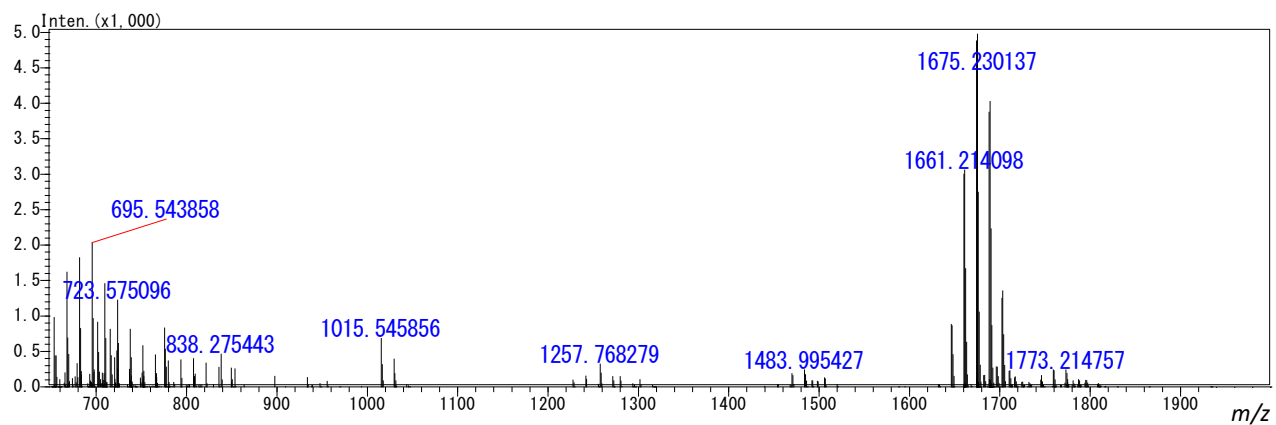


Figure S4. (Continued) MS1 spectra of lipid A extracts in each Bacteroidetes strain.

Average MS1 spectra of RT=10–12 min were presented.

(I) *O. laneus*



**Figure S4.** (Continued) MS1 spectra of lipid A extracts in each Bacteroidetes strain. Average MS1 spectra of RT=10–12 min were presented.