

# Sophorolipid suppresses LPS-induced inflammation in RAW264.7 cells through NF- $\kappa$ B signaling pathway

Rui-Qi Xu<sup>1,†</sup>, Ling Ma<sup>2,†</sup>, Timson Chen<sup>2</sup>, Jing Wang<sup>1,\*</sup>

<sup>1</sup> Key Laboratory of Synthetic and Biological Colloids, Ministry of Education, School of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, China

<sup>2</sup> Adolph Innovation Laboratory, Guangzhou Degu Personal Care Products Co., Ltd., Guangzhou 510000, China

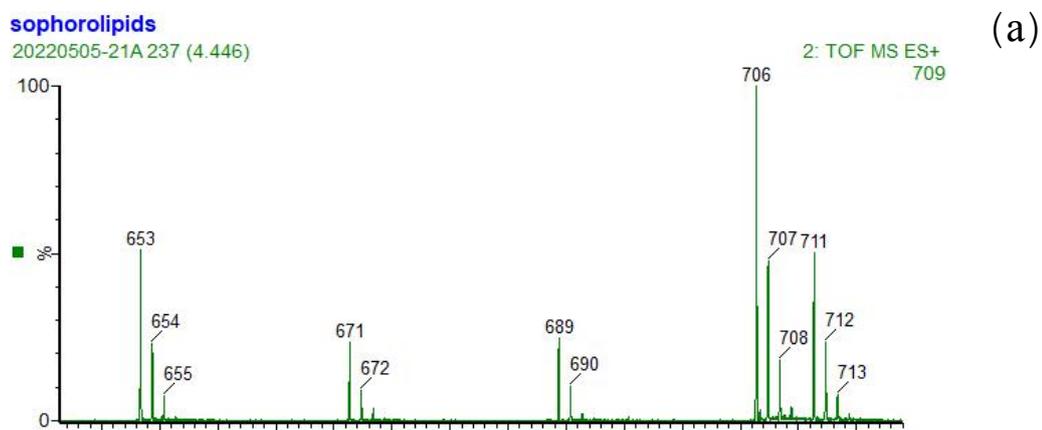
\* Correspondence: jingwang@jiangnan.edu.cn

<sup>†</sup>These authors contributed equally to this work.

Liquid chromatography - mass spectrometry:

Acidic components (R.T- 0.5-4.0) are eluted first while the lactonic (R.T- 3.0-10.0) are eluted later due to their higher hydrophobicity.

The following figures depict the liquid chromatography and mass spectra of SL we got: to identify the presence of different modifications. Figure S1(a) reveals the mass spectrum of SL with molecular formula C<sub>34</sub>H<sub>56</sub>O<sub>14</sub>. The spectrum shows presences of amine adduct at m/z 706 and sodium adduct at m/z 711 respectively.



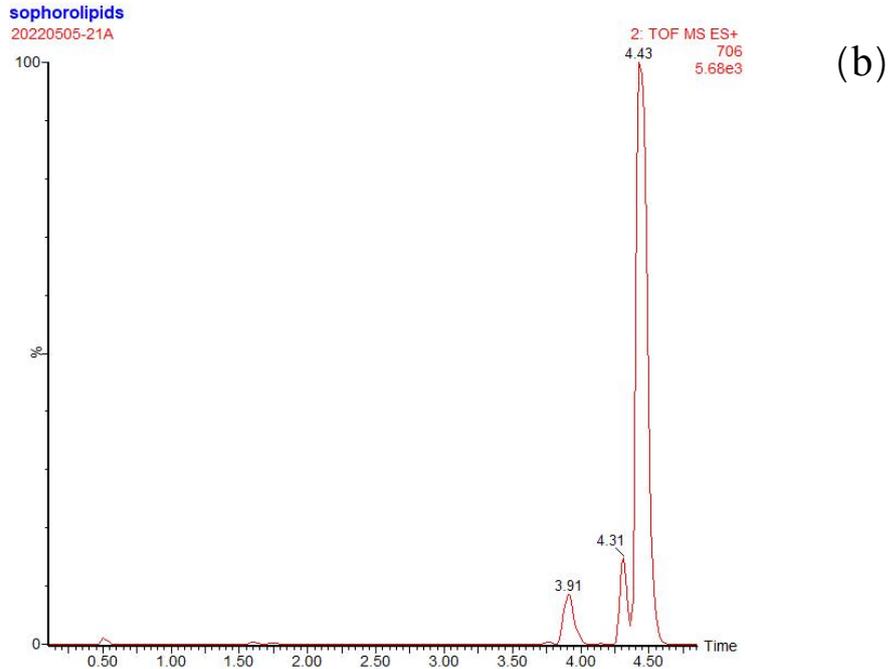
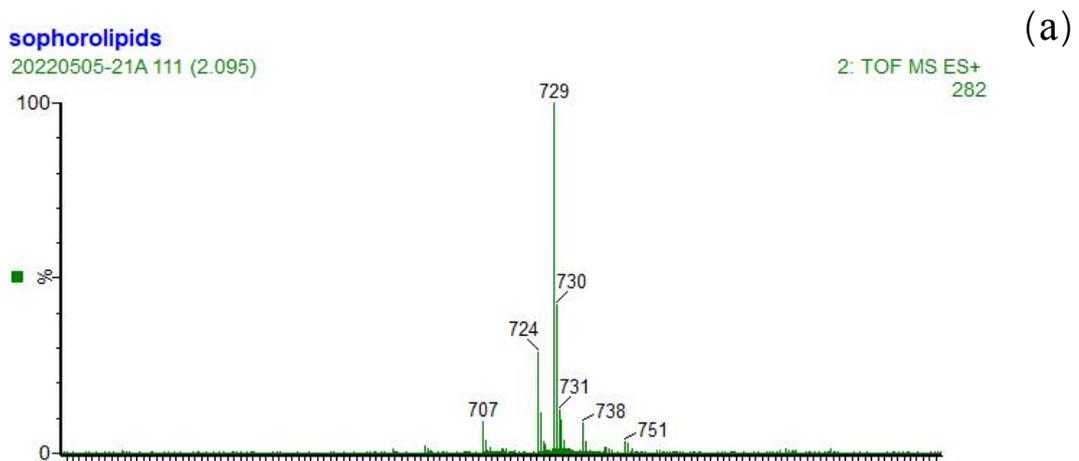
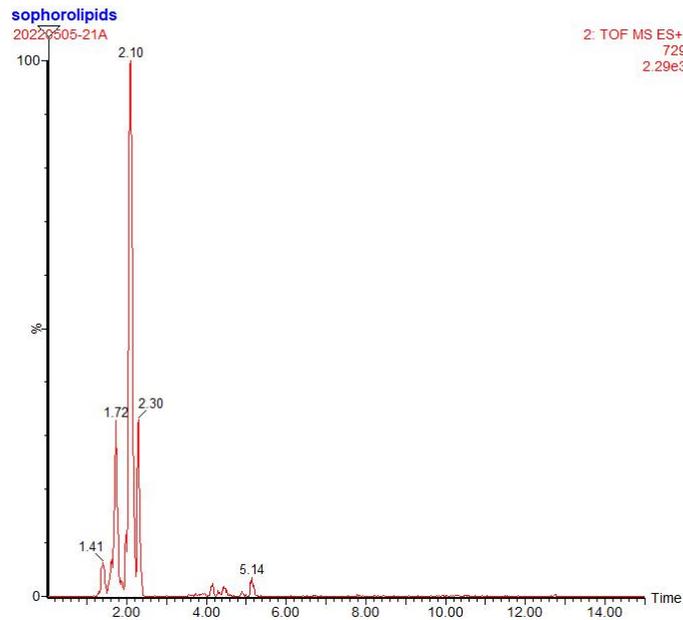


Figure S1 (a): Mass spectrum of di-acetylated lactonic form S1 (b): Liquid chromatography of di-acetylated lactonic form

Figure S2(a) reveals the mass spectrum of SL with molecular formula  $C_{34}H_{58}O_{15}$  and  $C_{34}H_{60}O_{15}$ . The spectrum shows presences of sodium adduct at  $m/z$  729, 731 and amine adduct at  $m/z$  724 respectively. The mass spectrum also shows presence of protonated molecular ion peak at  $m/z$  707.

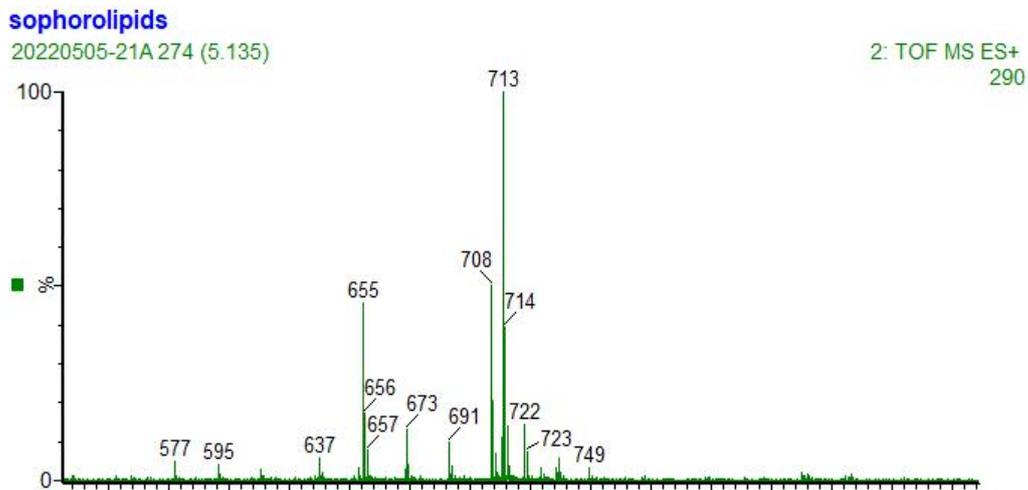




(b)

Figure S2 (a): Mass spectrum of di-acetylated acidic form S2 (b): Liquid chromatography of di-acetylated acidic form

Figure S3(a) reveals the mass spectrum of SL with molecular formula  $C_{34}H_{58}O_{14}$ . The spectrum shows presences of amine adduct at  $m/z$  708 and sodium adduct at  $m/z$  713 respectively.



(a)

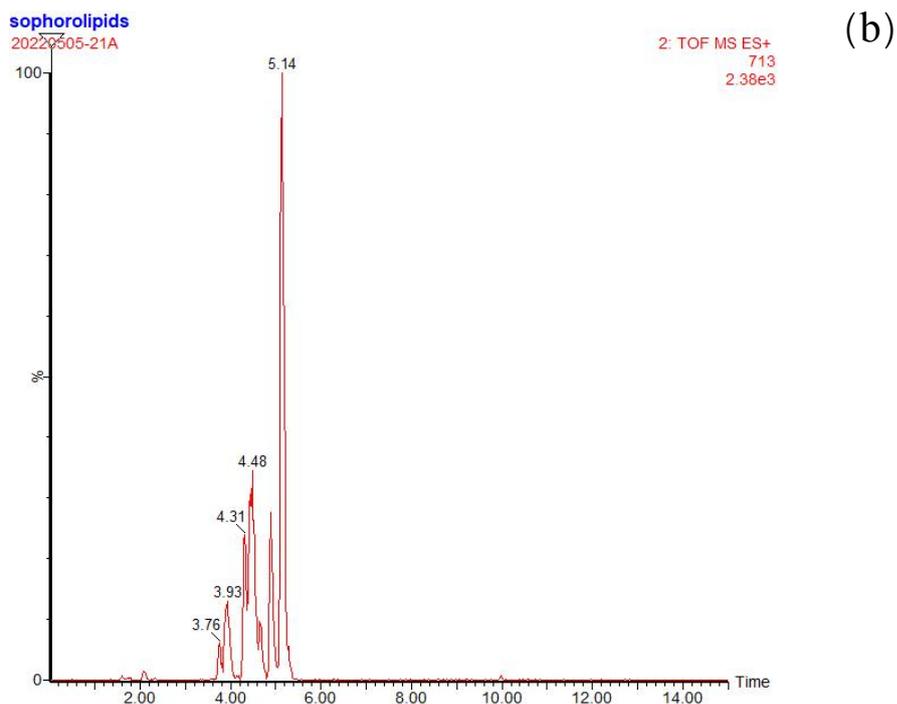
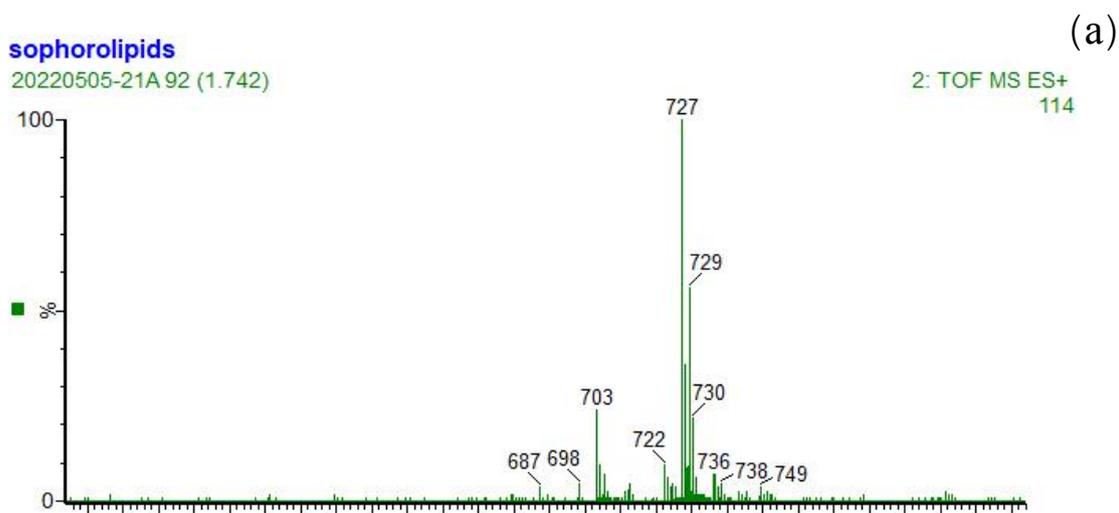


Figure S3 (a): Mass spectrum of di-acetylated lactonic form S3 (b): Liquid chromatography of di-acetylated lactonic form

Figure S4(a) reveals the mass spectrum of SL with molecular formula  $C_{34}H_{56}O_{15}$ . The spectrum shows presences of sodium adduct at  $m/z$  727 and amine adduct at  $m/z$  722 respectively. The mass spectrum also shows presence of deprotonated molecular ion peak at  $m/z$  703.



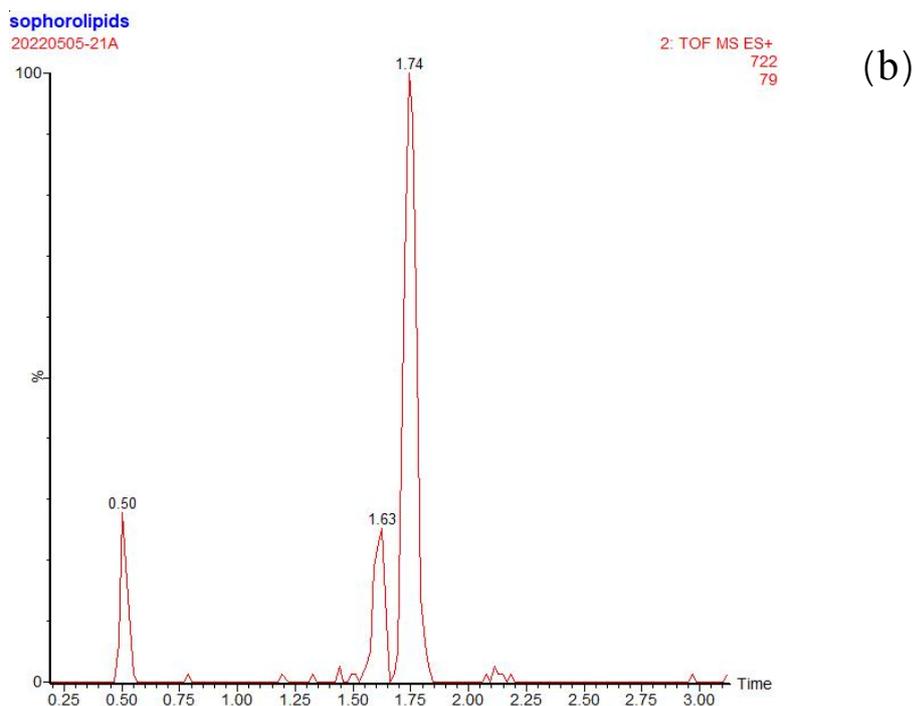
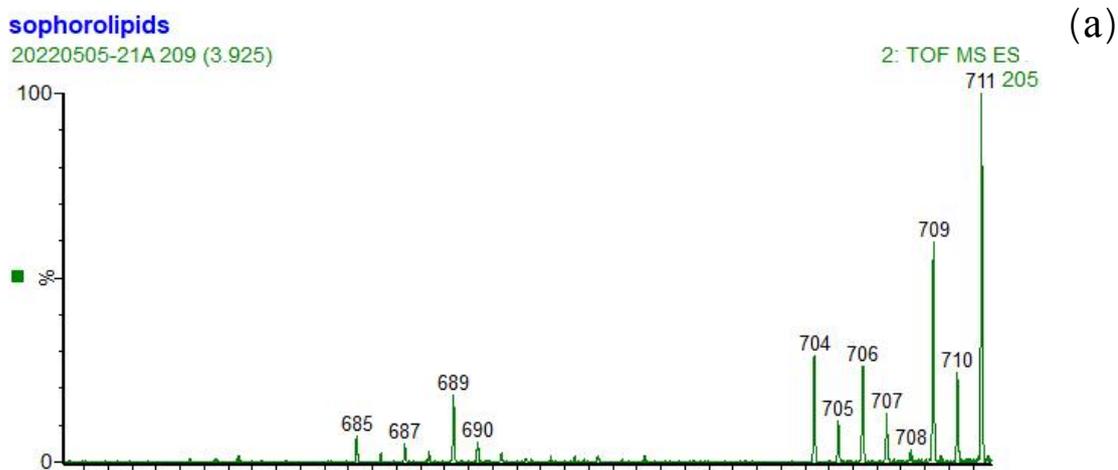


Figure S4 (a): Mass spectrum of di-acetylated acidic form S4 (b): Liquid chromatography of di-acetylated acidic form

Figure S5(a) reveals the mass spectrum of SL with molecular formula  $C_{34}H_{54}O_{14}$ . The spectrum shows presences of amine adduct at  $m/z$  708 and sodium adduct at  $m/z$  713 respectively.



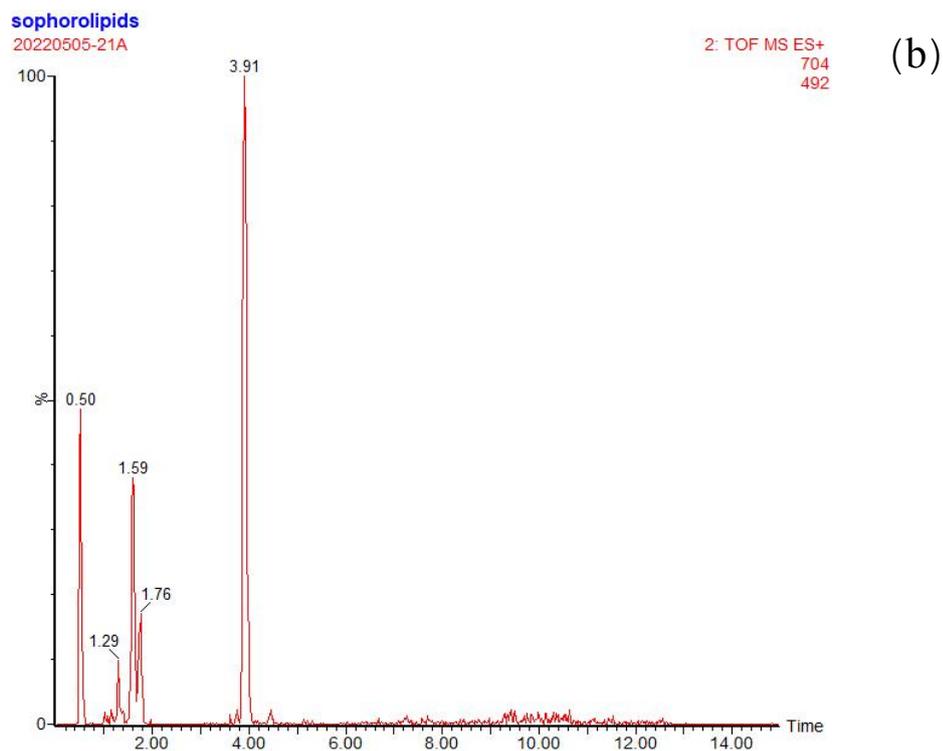
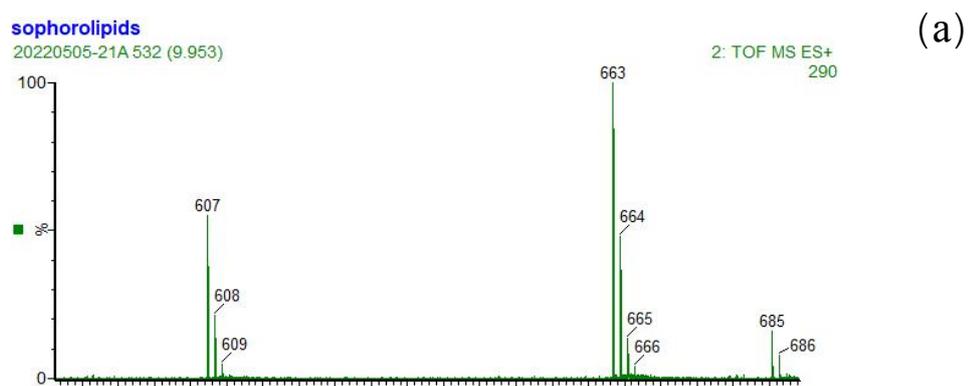
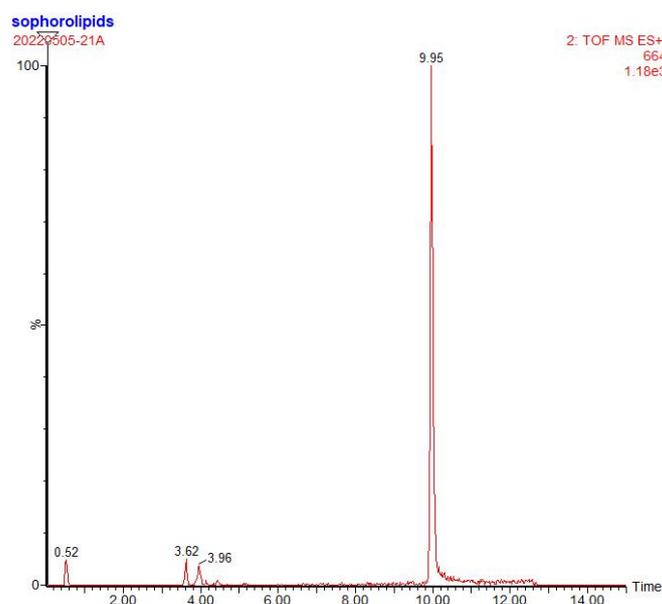
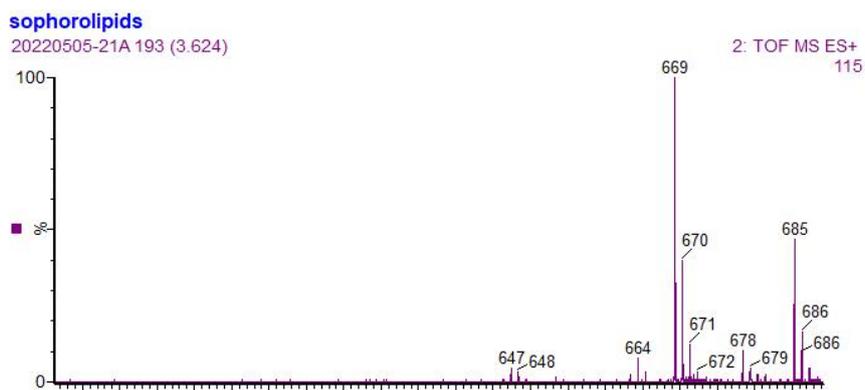


Figure S5 (a): Mass spectrum of di-acetylated lactonic form S5 (b): Liquid chromatography of di-acetylated lactonic form

Figure S6(a) reveals the mass spectrum of SL with molecular formula  $C_{34}H_{54}O_{13}$ . The spectrum shows presences of amine adduct at  $m/z$  664 and sodium adduct at  $m/z$  669 respectively.

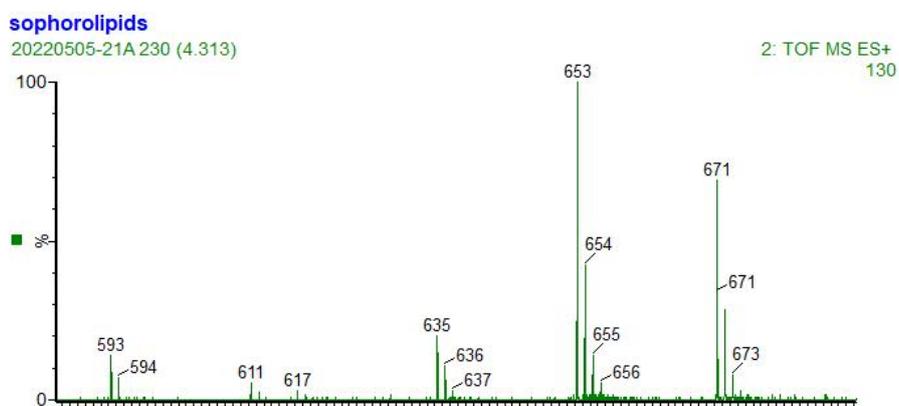




(b)

Figure S6 (a): Mass spectrum of mona-acetylated lactonic form S6 (b): Liquid chromatography of mona-acetylated lactonic form

Figure S7(a) reveals the mass spectrum of SL with molecular formula  $C_{34}H_{56}O_{13}$ . The spectrum shows presences of sodium adduct at m/z 671.



(a)

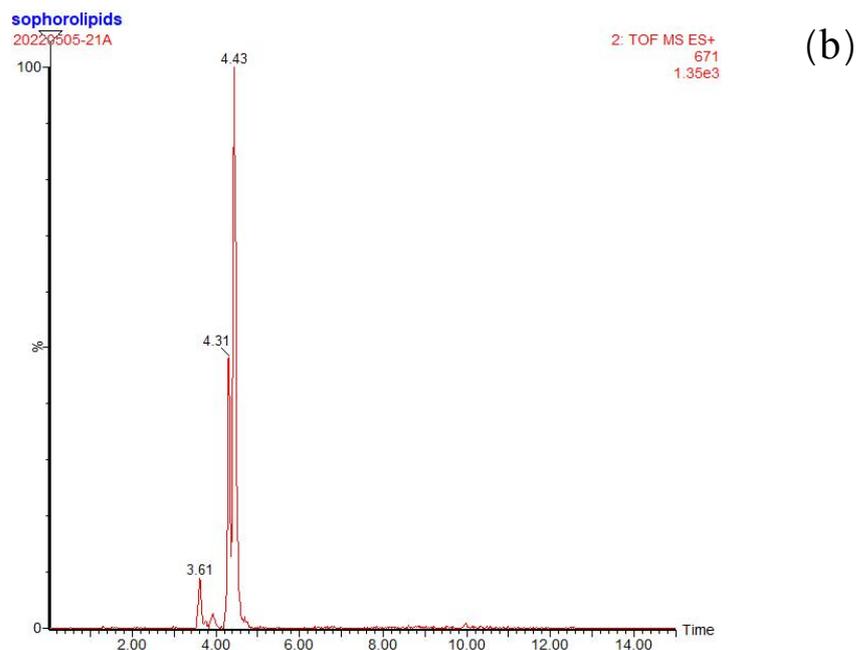
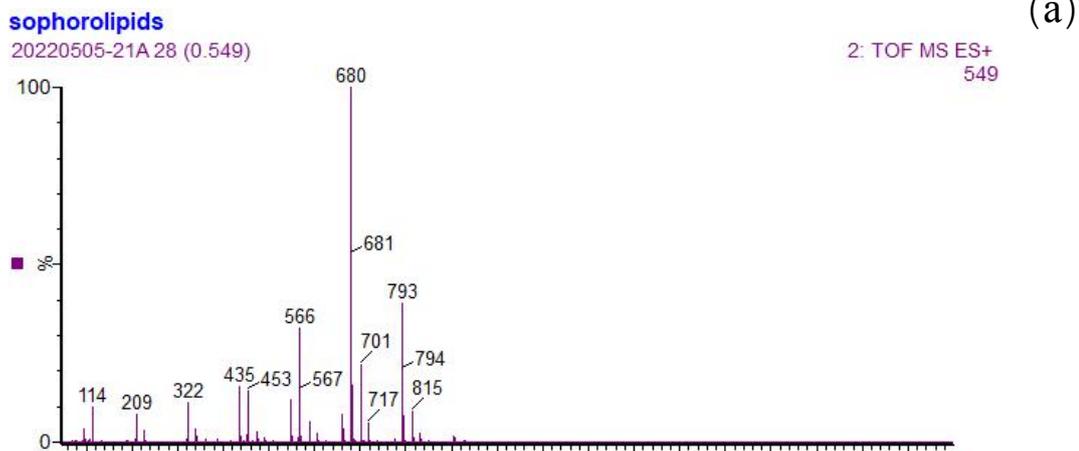


Figure S7 (a): Mass spectrum of mona-acetylated lactonic form S7 (b): Liquid chromatography of mona-acetylated lactonic form

Figure S8(a) reveals the mass spectrum of SL with molecular formula  $C_{32}H_{54}O_{14}$ . The spectrum shows presences of amine adduct at  $m/z$  680.



sophorolipids  
20220505-21A

2: TOF MS ES+  
680  
3.62e3

(b)

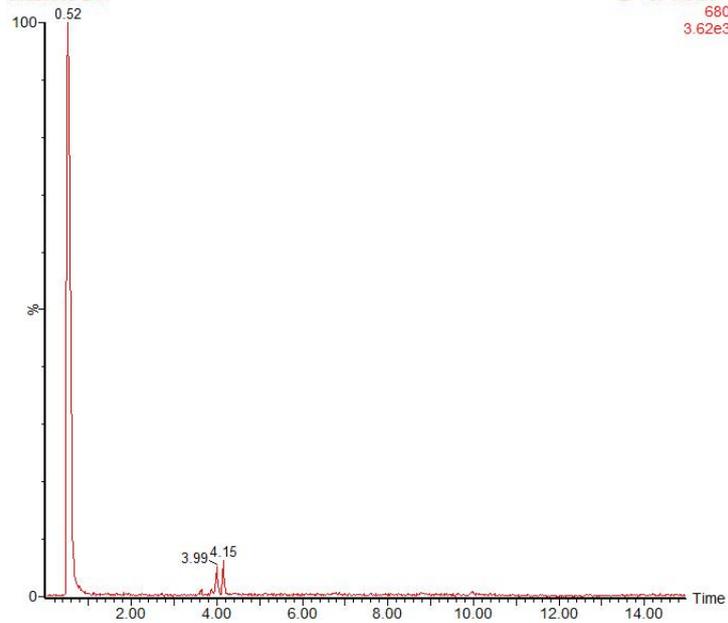


Figure S8 (a): Mass spectrum of mona-acetylated acidic form S8 (b): Liquid chromatography of mona-acetylated acidic form