

Unveiling the functional components and anti-Alzheimer's activity of *Koelreuteria elegans* (Seem.) A.C. Sm. using UHPLC-MS/MS and molecular networking

Mohamed S. Demerdash^{1a}, Reem T. Attia^{2a}, Moshera M. El-Sherei¹, Wafaa M. Aziz¹, Sherif Ashraf Fahmy^{3*}, Marwa Y. Issa^{1*}

¹Department of Pharmacognosy, Faculty of Pharmacy, Cairo University, Cairo 11562, Egypt

²Department of Pharmacology, Toxicology, and Biochemistry, Faculty of Pharmacy, Future University in Egypt, Cairo11865, Egypt

³Department of Chemistry, School of Life and Medical Sciences, University of Hertfordshire Hosted by Global Academic Foundation, R5 New Garden City, New Administrative Capital, AL109AB, Cairo11835, Egypt

^a **Both authors contributed equally to this work.**

***Corresponding authors: Sherif Ashraf Fahmy, Email: sheriffahmy@aucegypt.edu.**

Marwa Y. Issa, Email: marwa.issa@pharma.cu.edu.eg

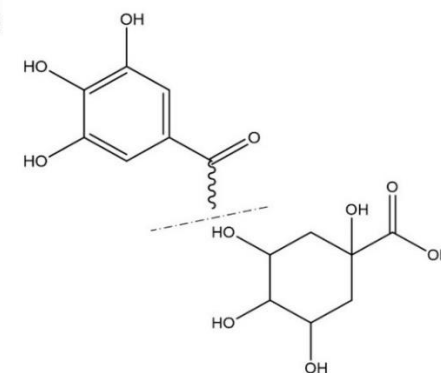
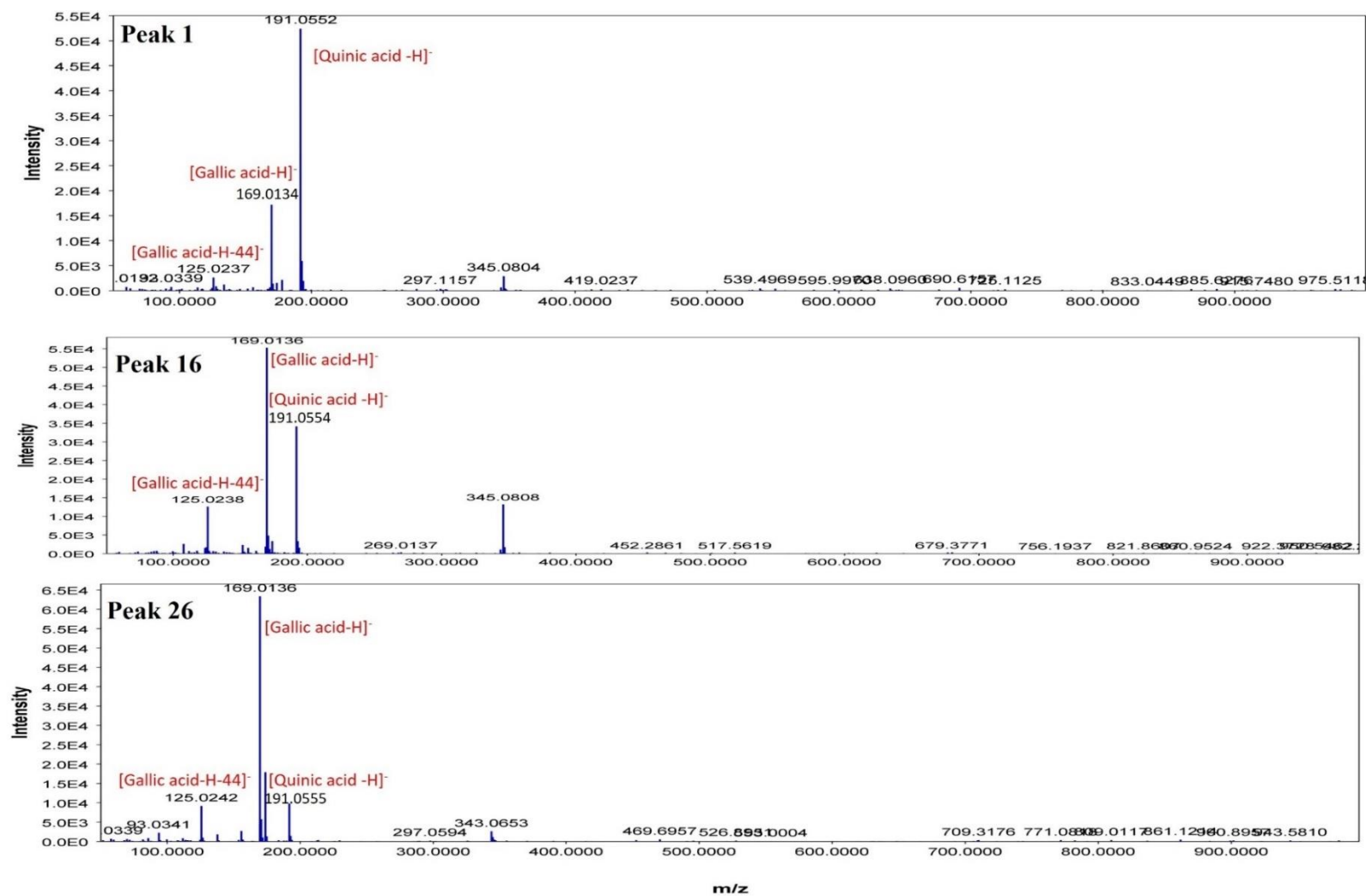


Fig. S1. MS/MS spectra of theogallin isomers (1, 16, 26)

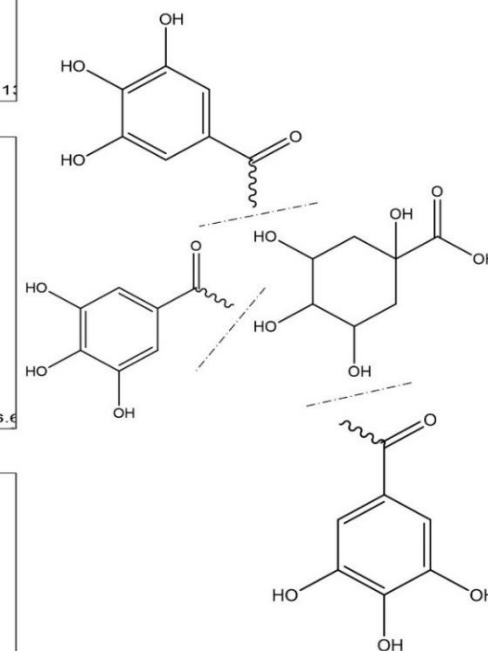
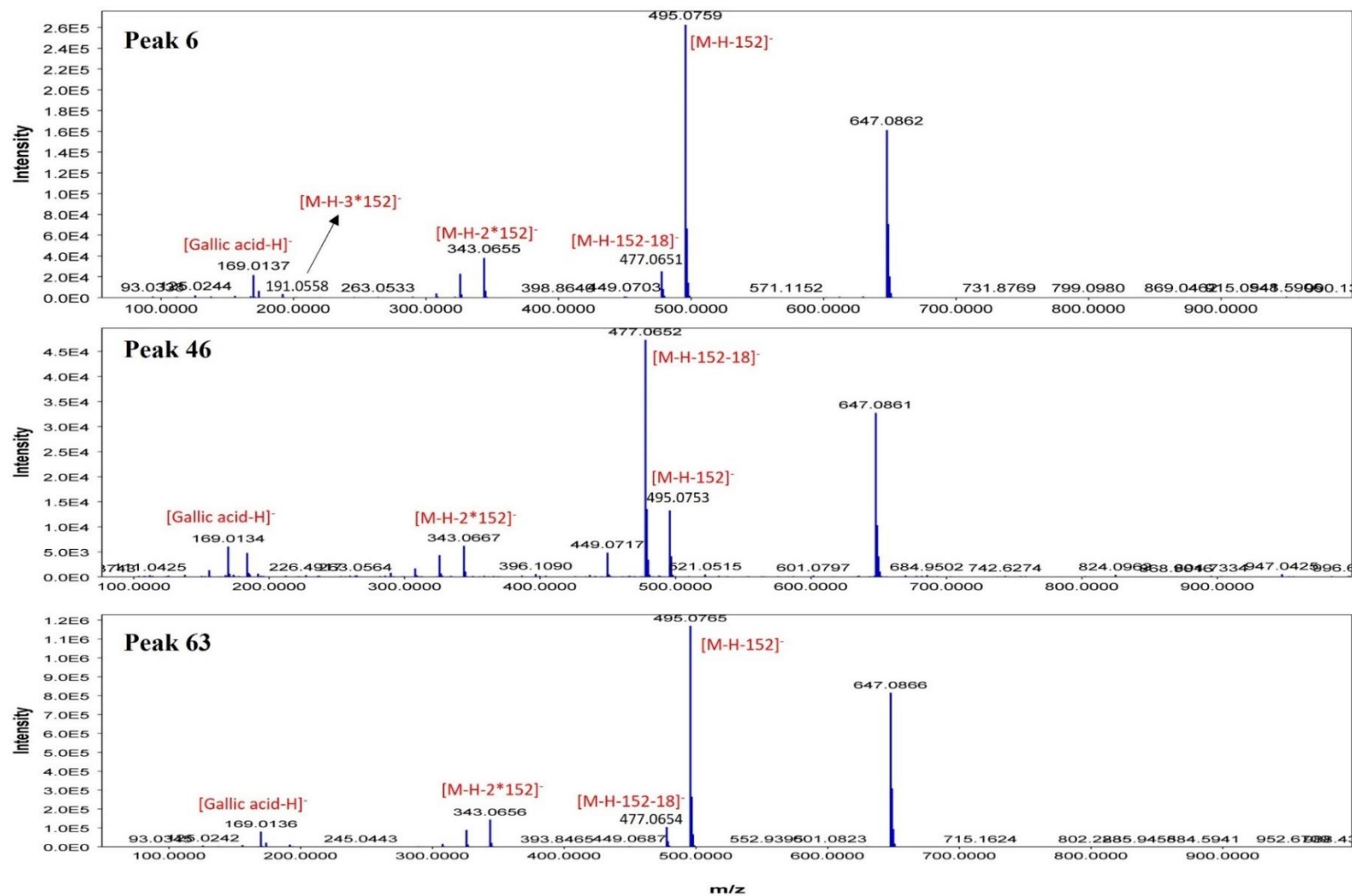


Fig. S2. MS/MS spectra of tri-O-galloylquinic isomers (6, 46, 63)

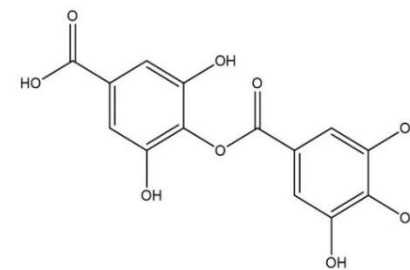
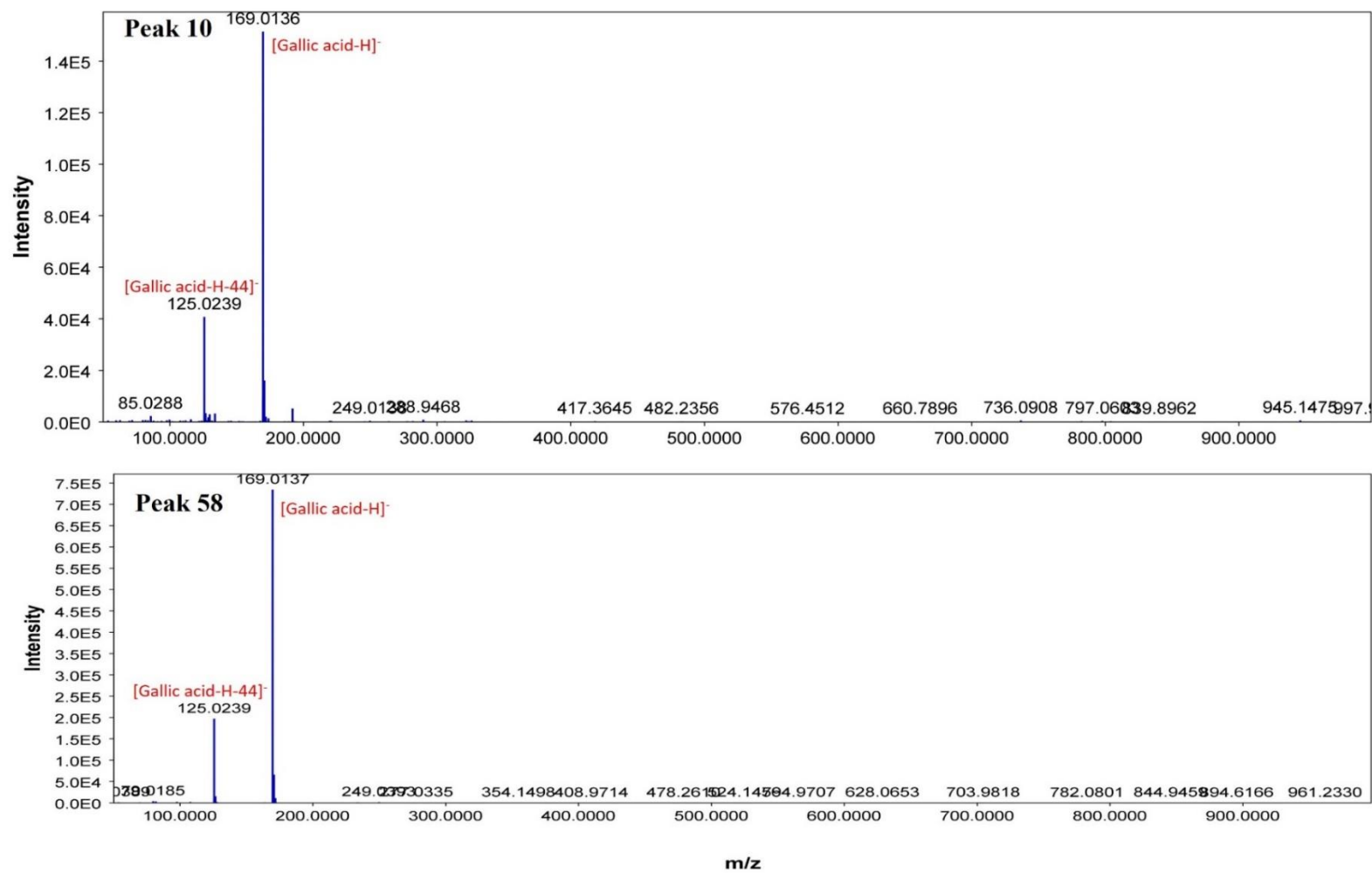


Fig. S3. MS/MS spectra of digallic acid isomers (**10**, **58**)

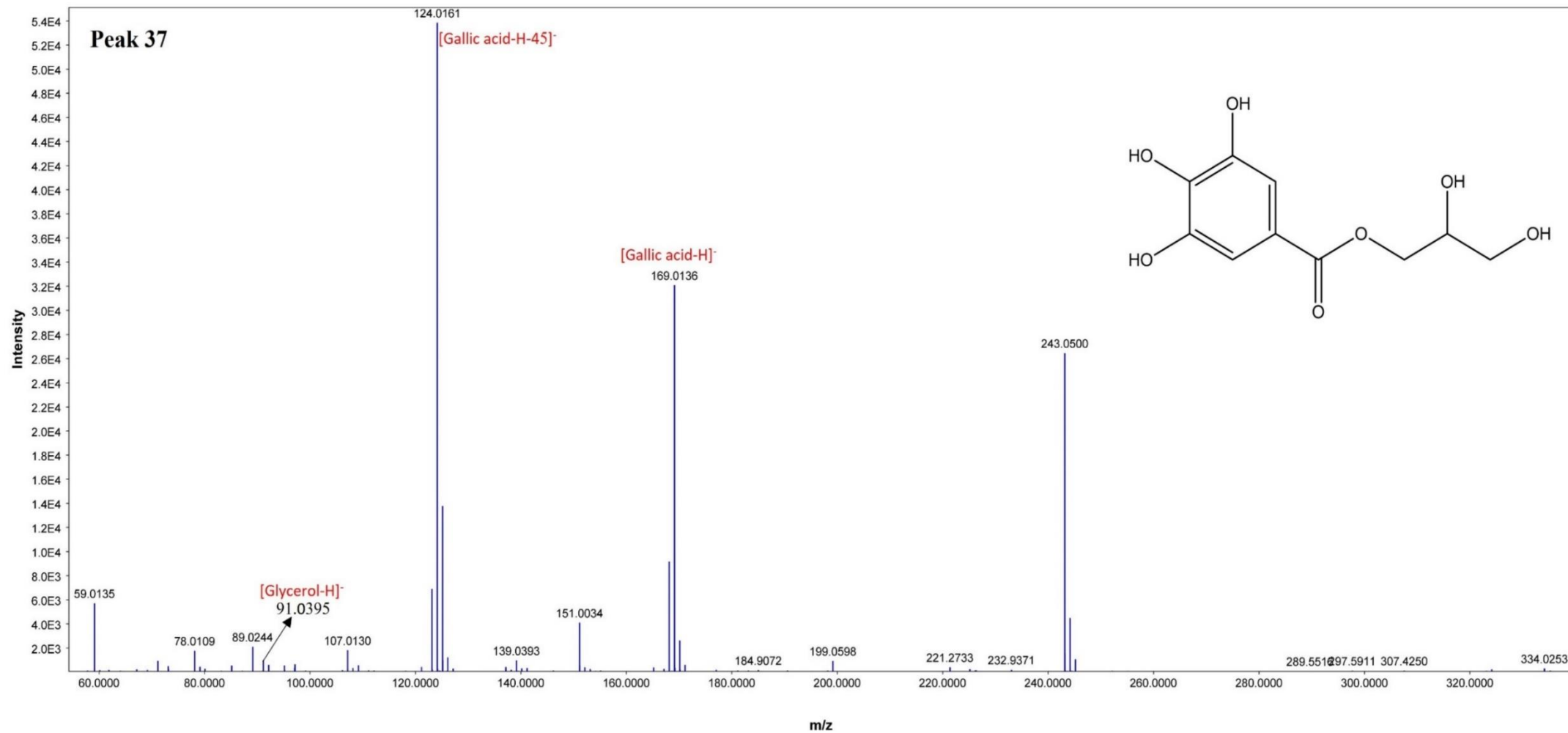


Fig. S4. MS/MS spectrum of galloylglycerol (37)

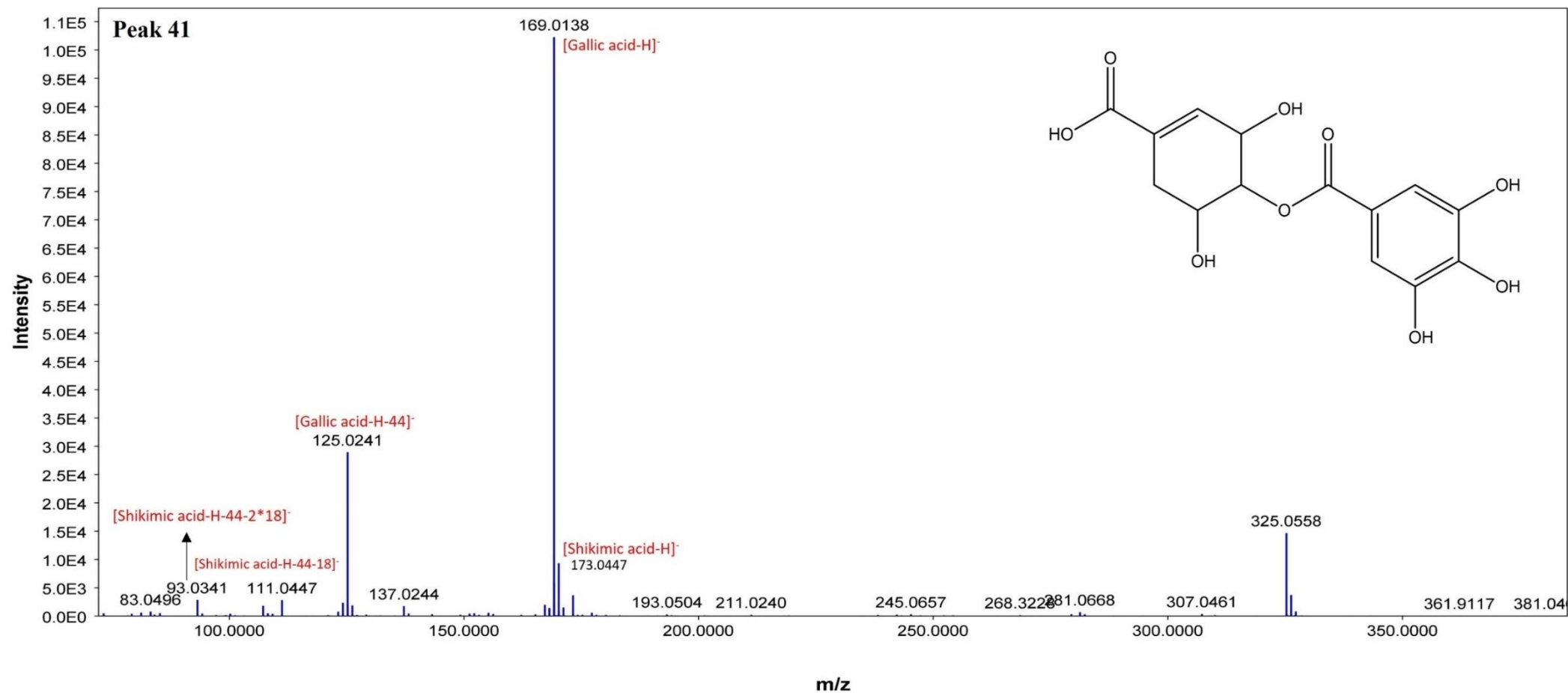


Fig. S5. MS/MS spectrum of galloylshikimic acid (**41**)

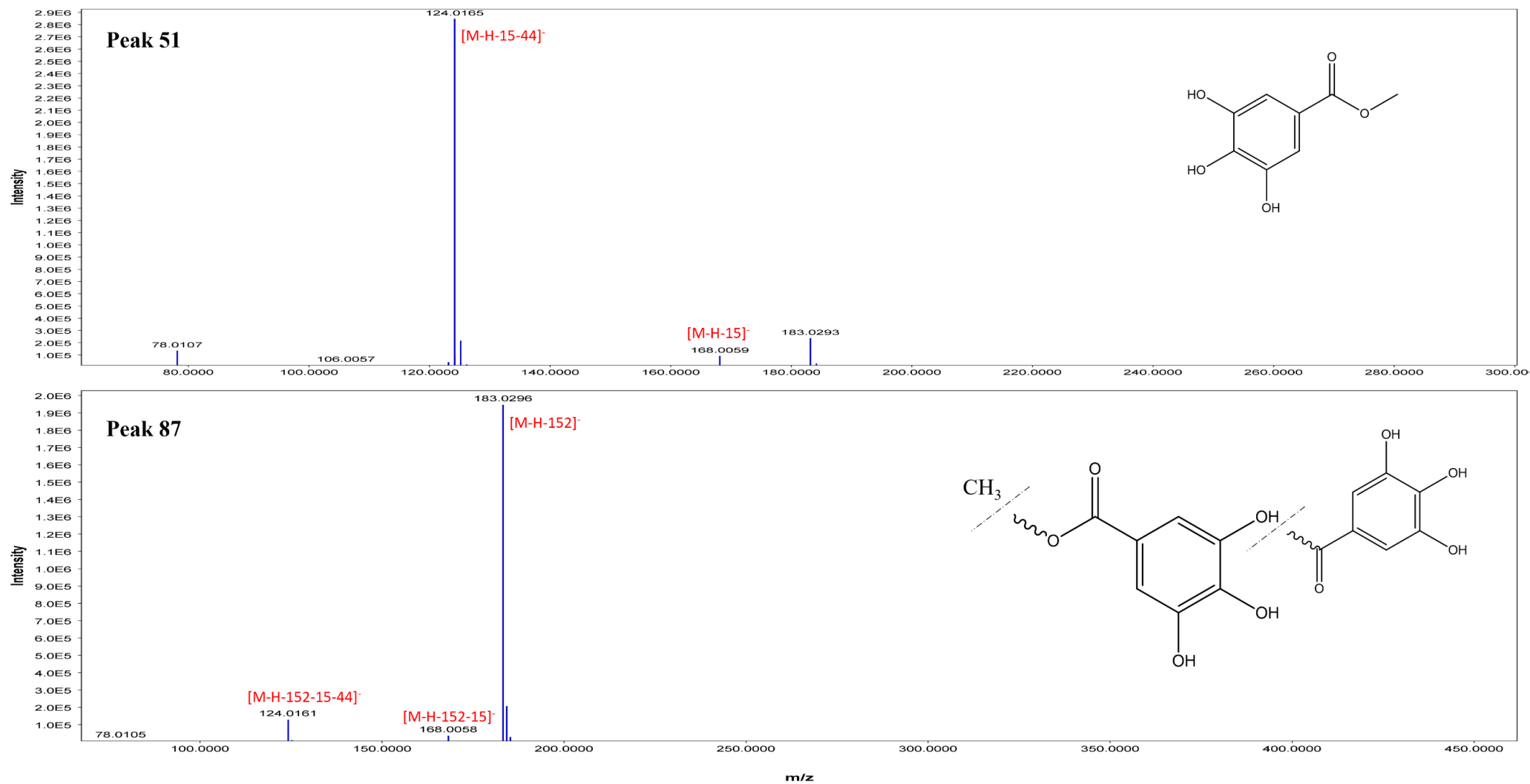


Fig. S6. MS/MS spectra of methyl gallate (**51**) and methyl digallate (**87**)

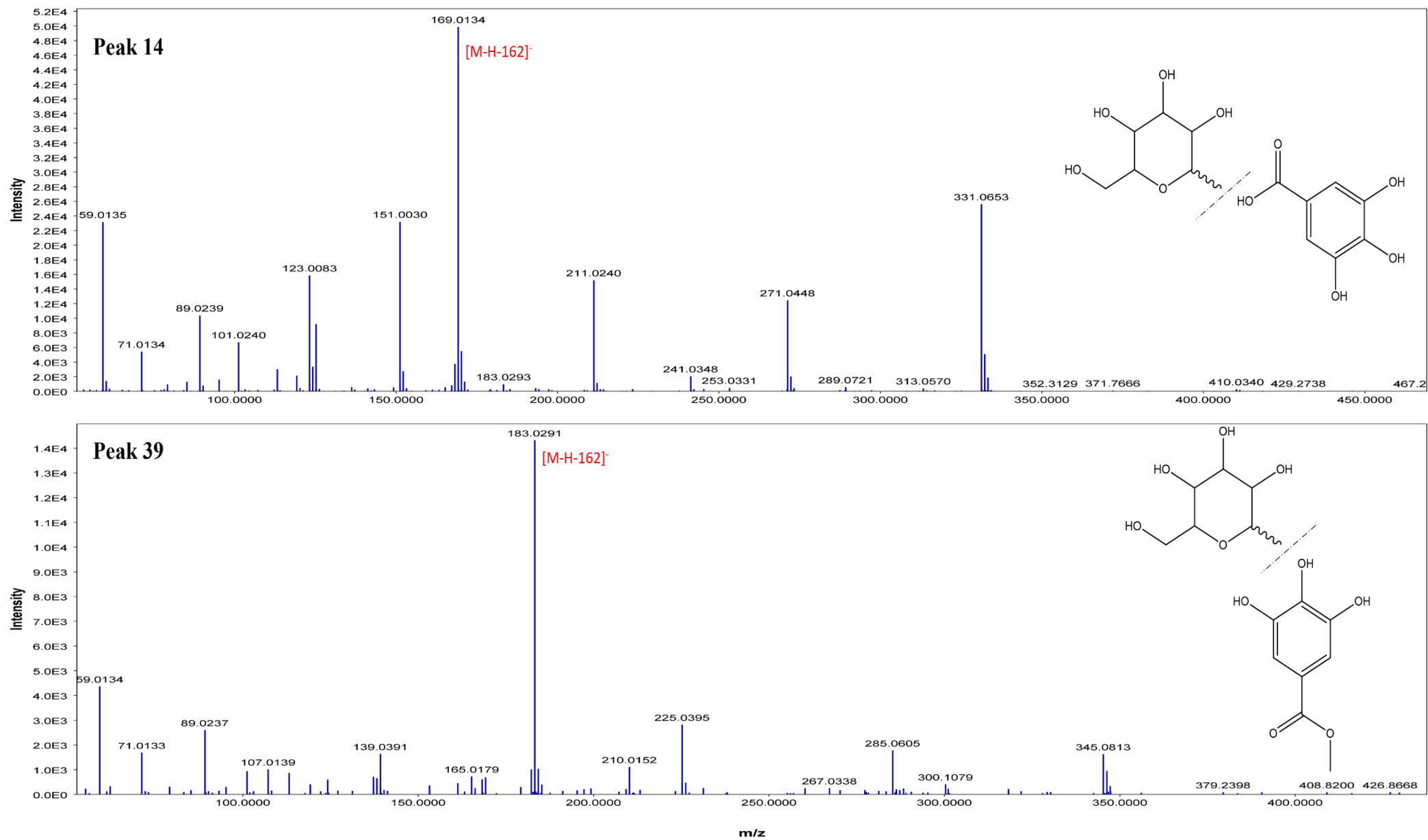


Fig. S7. MS/MS spectra of galloyl hexoside (**14**) and methyl gallate hexoside (**39**)

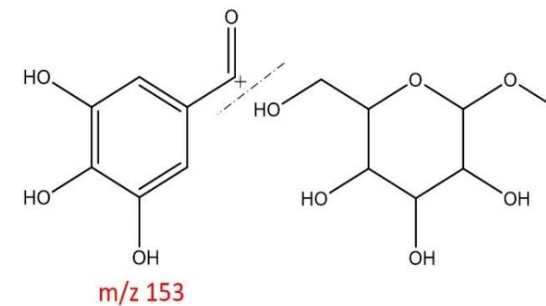
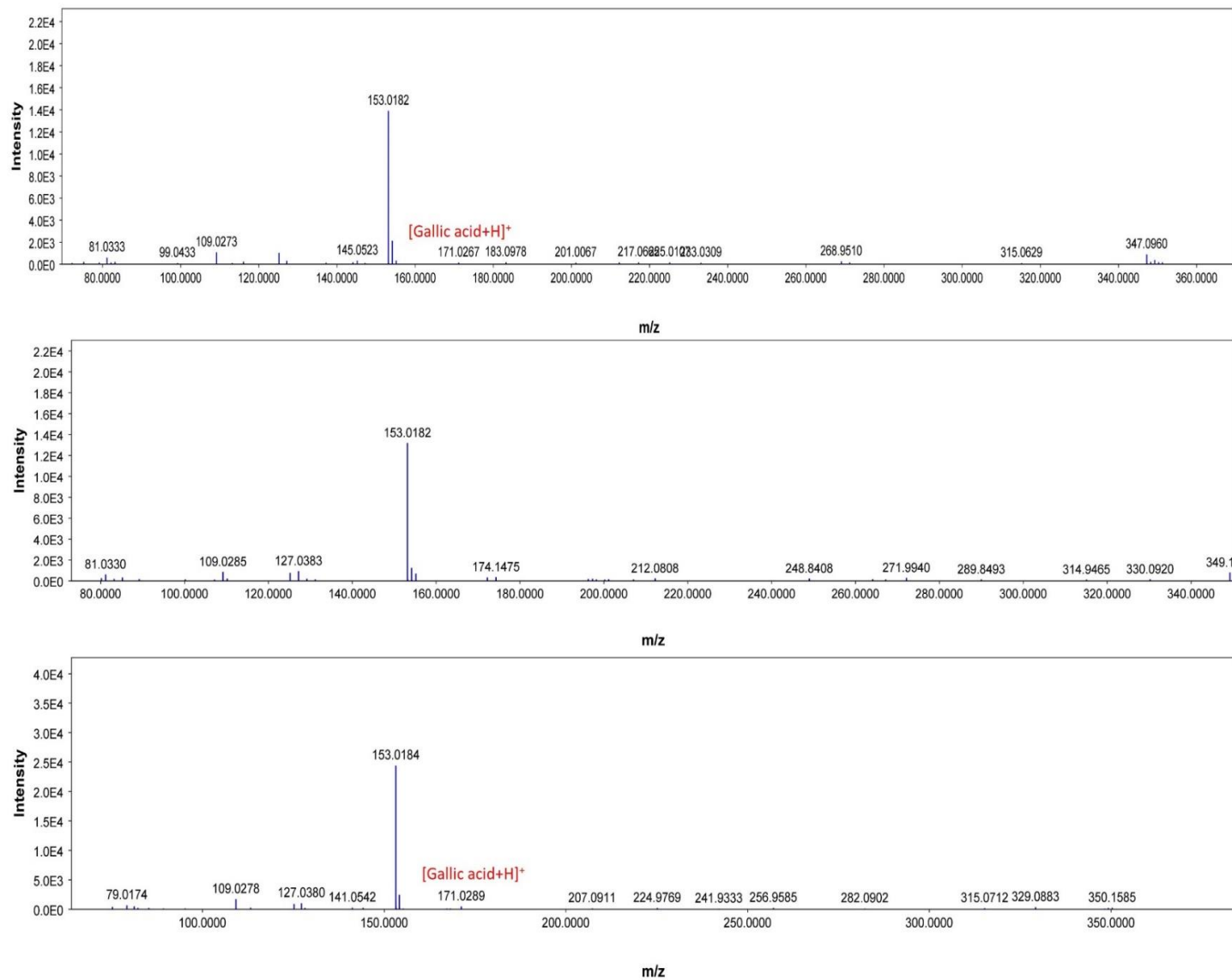


Fig. S8. MS/MS spectra of methyl-O-galloyl hexoside isomers (8, 23, 31)

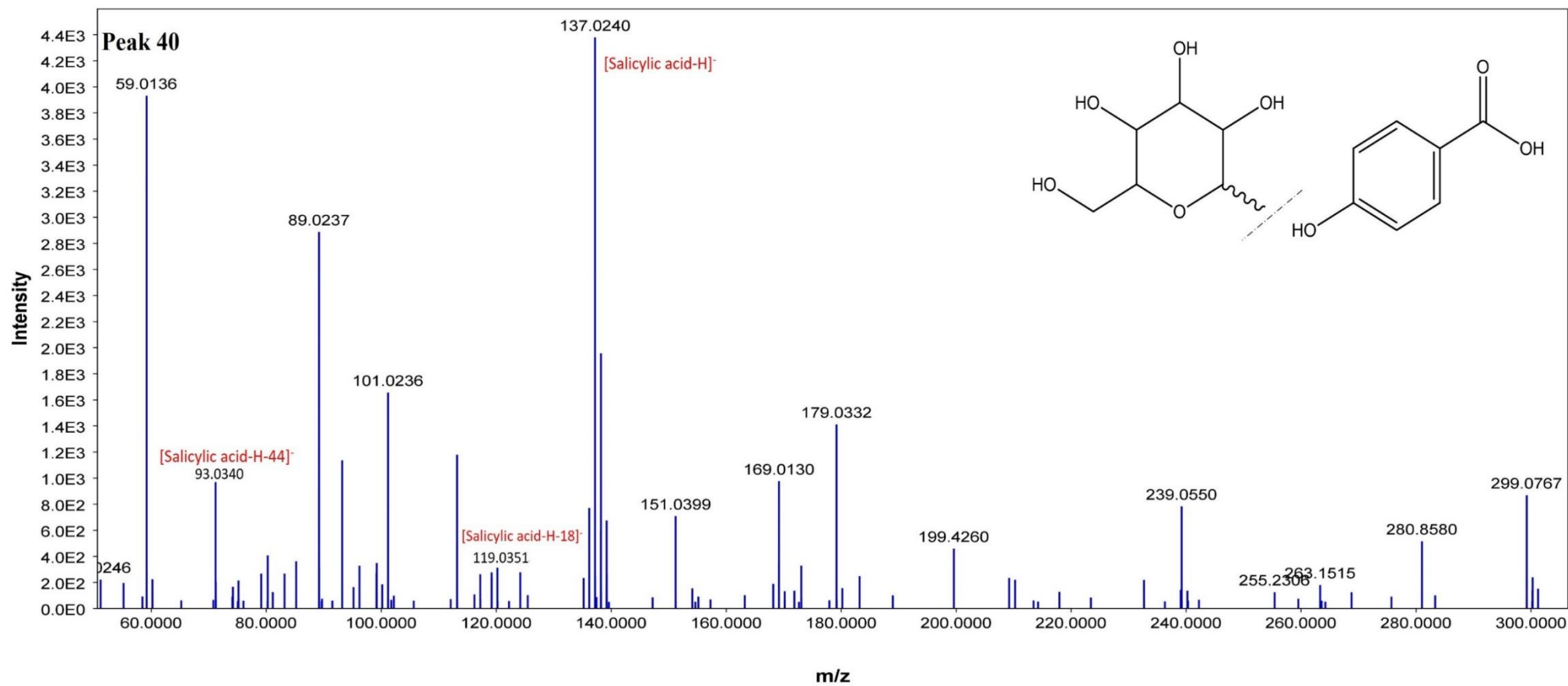


Fig. S9. MS/MS spectrum of salicylic acid hexoside (**40**)

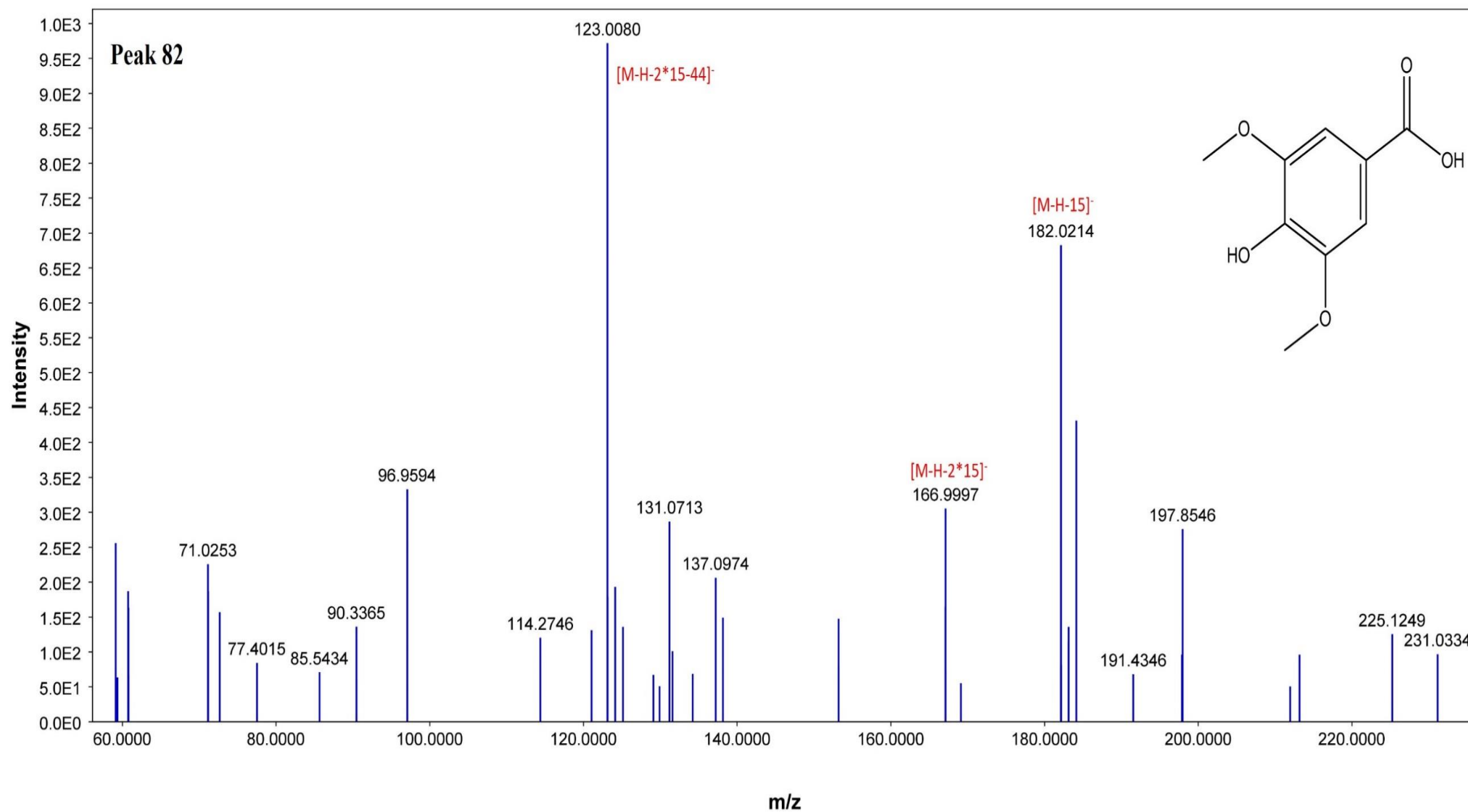


Fig. S10. MS/MS spectrum of syringic acid (**82**)

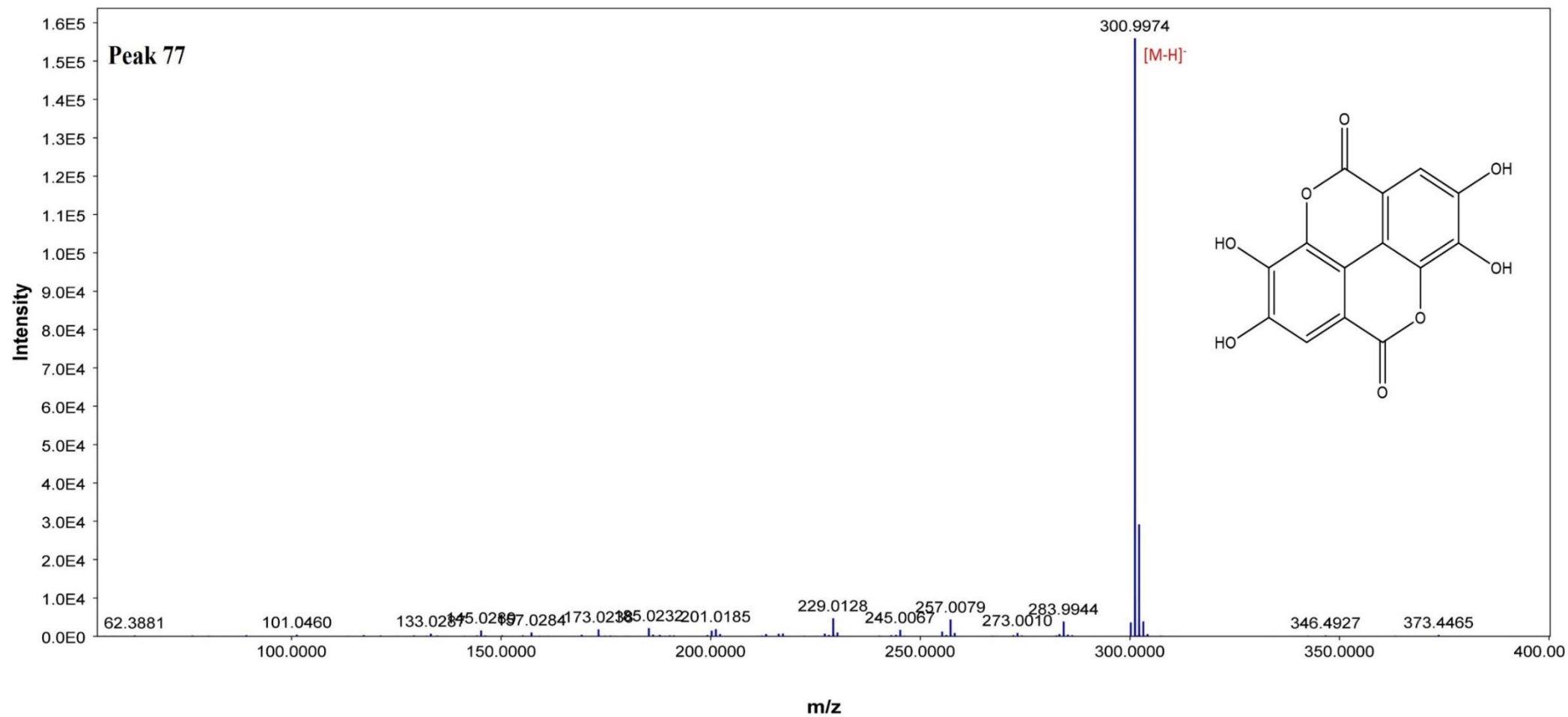


Fig. S11. MS/MS spectrum of ellagic acid (77)

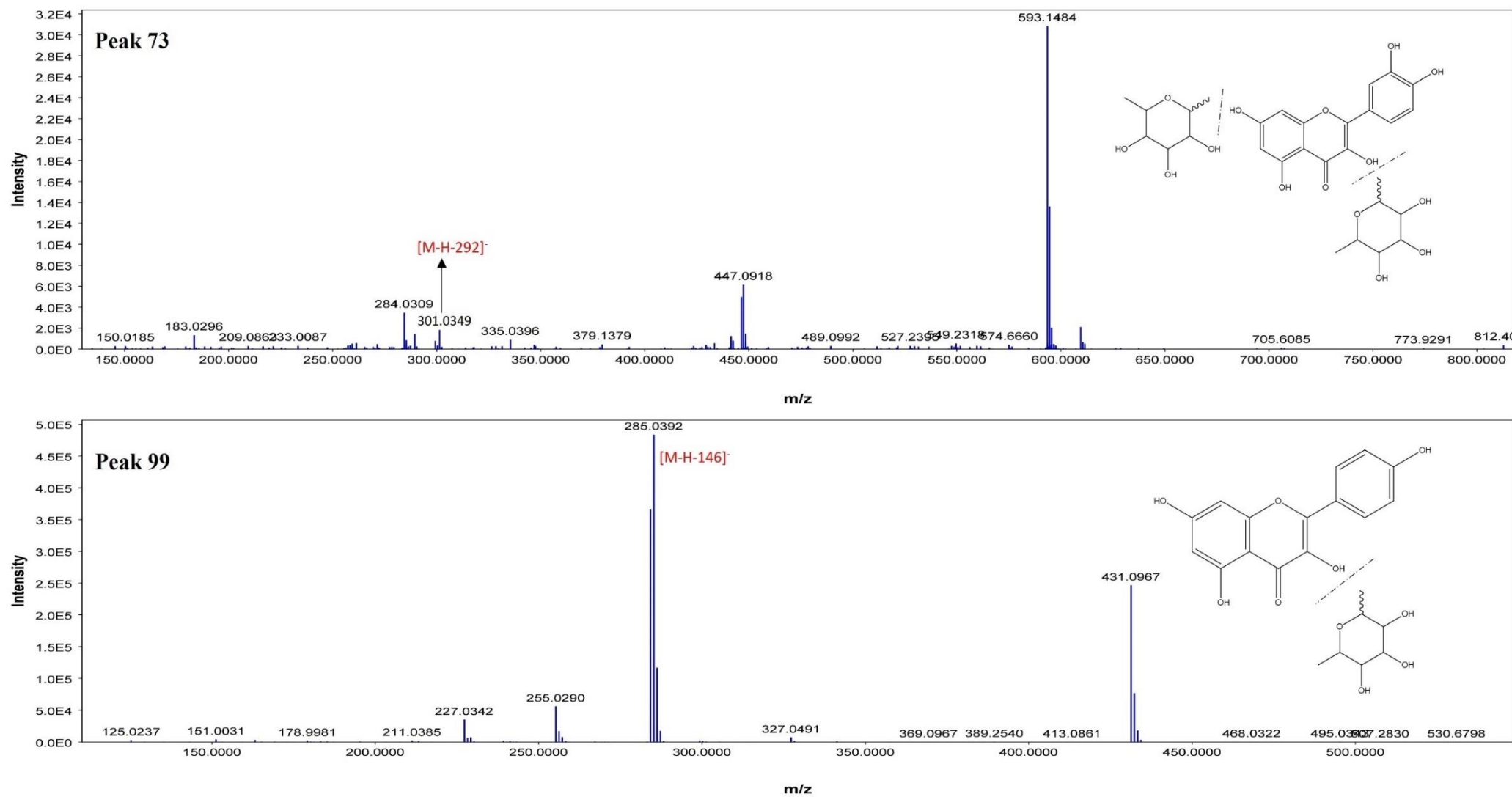


Fig. S12. MS/MS spectra of quercetin di-deoxyhexoside (**73**) and kaempferol deoxyhexoside (**99**)

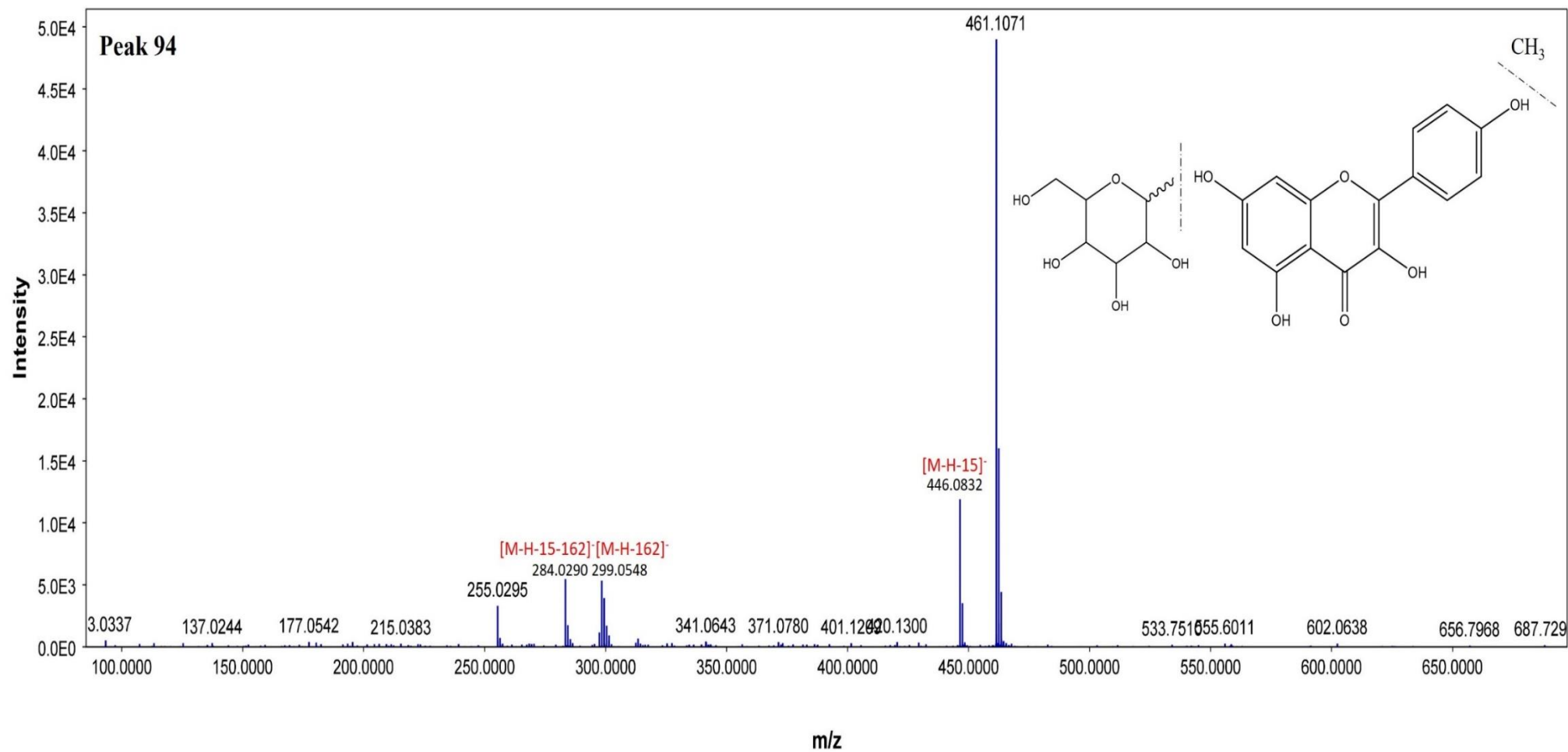


Fig. S13. MS/MS spectrum of kaempferide hexoside (**94**)

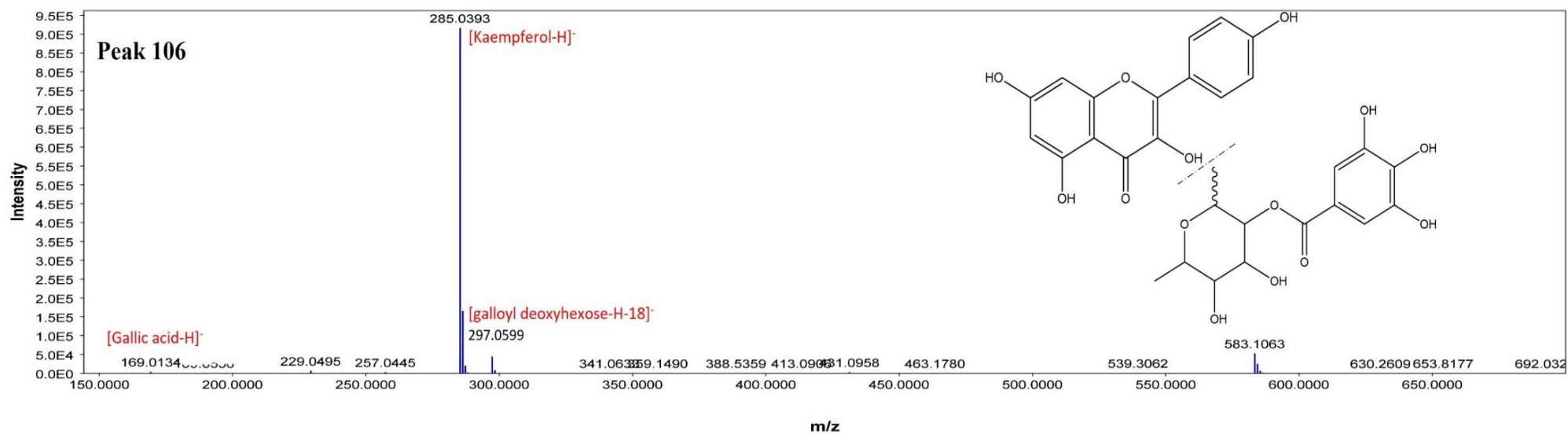
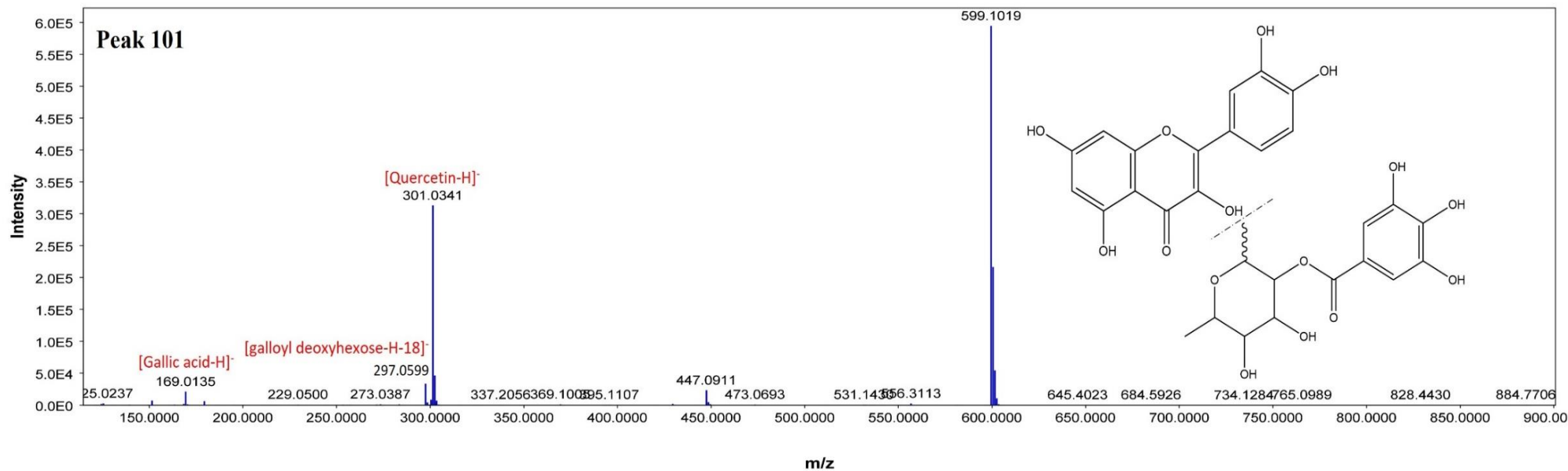


Fig. S14. MS/MS spectra of quercetin galloyl deoxyhexoside (**101**) and kaempferol galloyl deoxyhexoside (**106**)

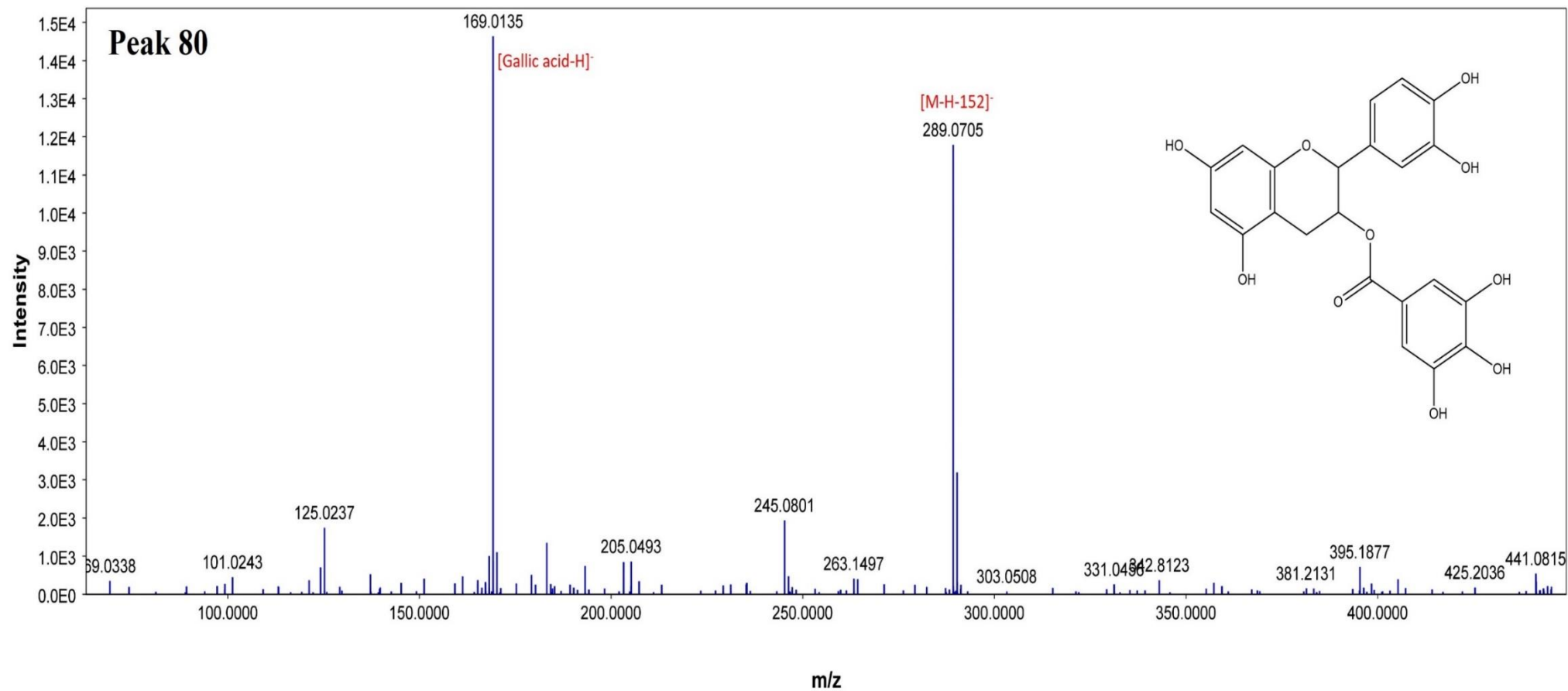


Fig. S15. MS/MS spectrum of catechin gallate (**80**)

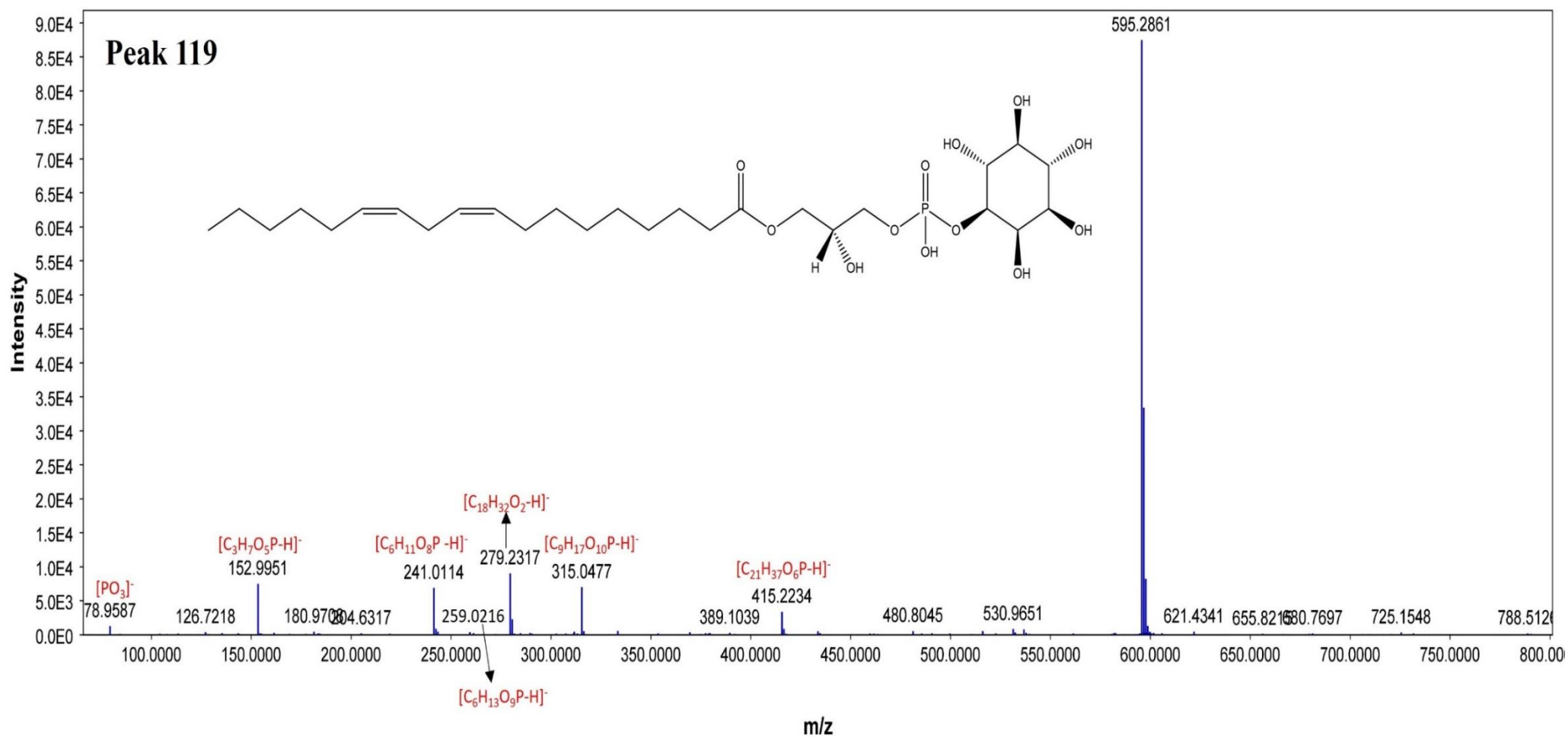


Fig. S16. MS/MS spectrum of phosphoinositol (18:2/0:0) (**119**)

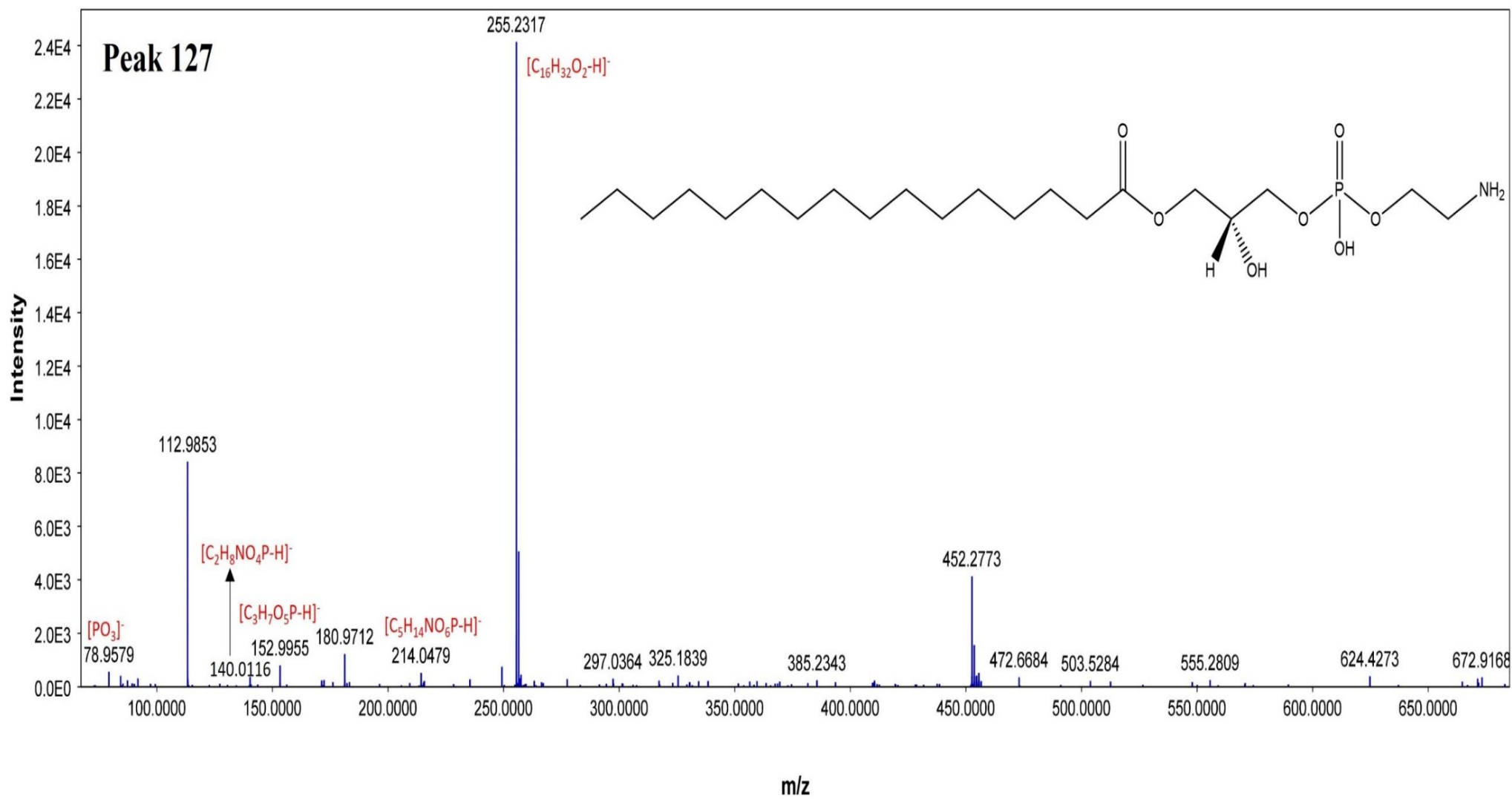


Fig. S17. MS/MS spectrum of phosphoethanolamine (16:0/0:0) (**127**)

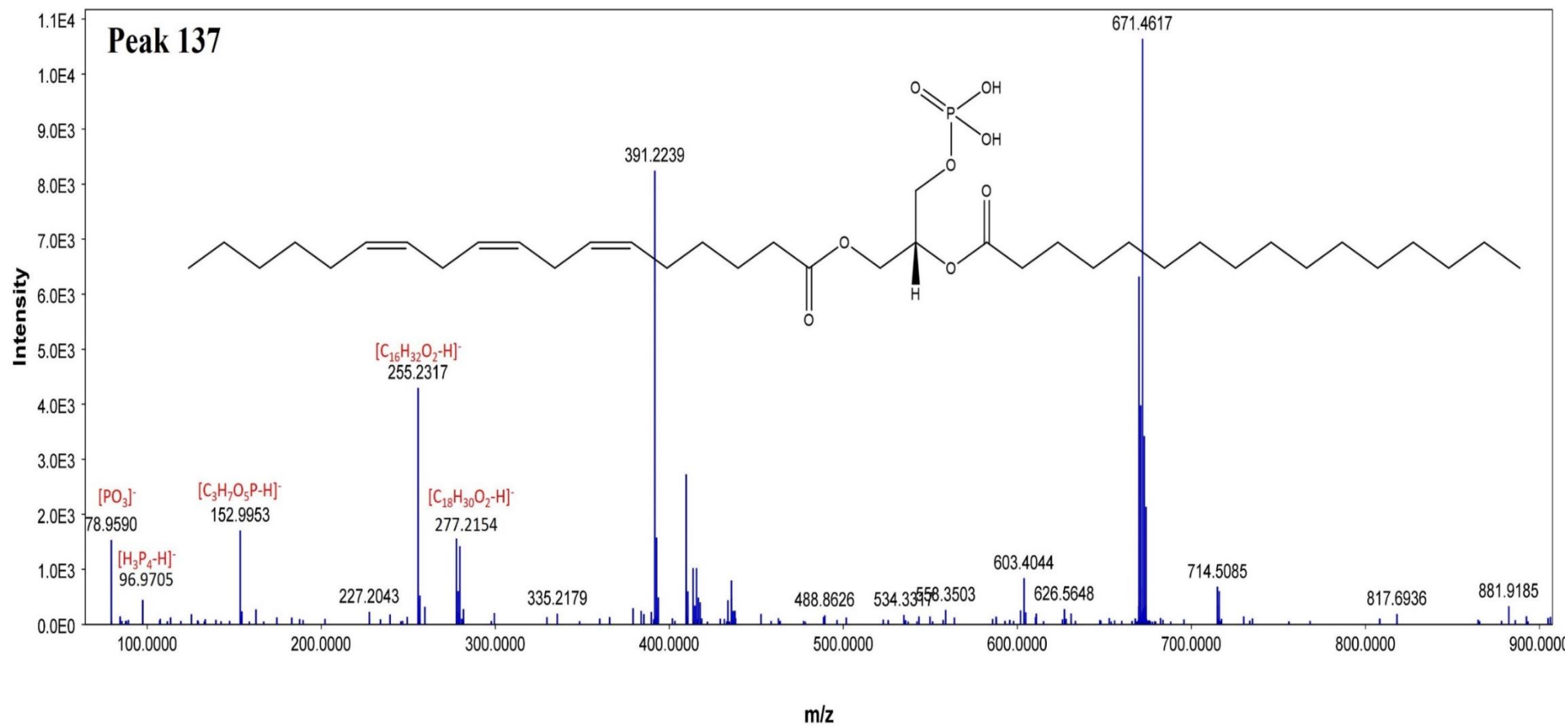


Fig. S18. MS/MS spectrum of phosphatidic acid (18:3/16:0) (**137**)

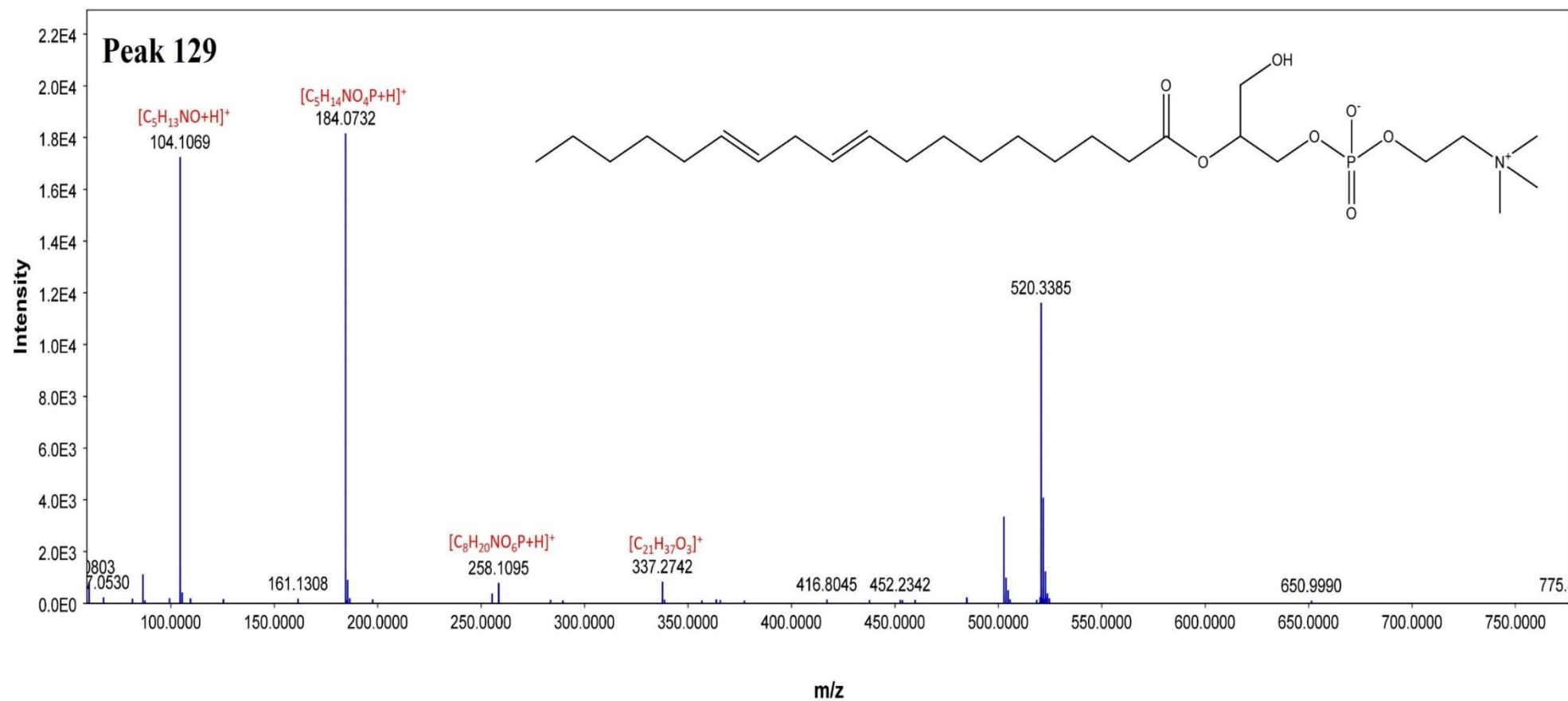


Fig. S19. MS/MS spectrum of phosphocholine (18:2) (**129**)

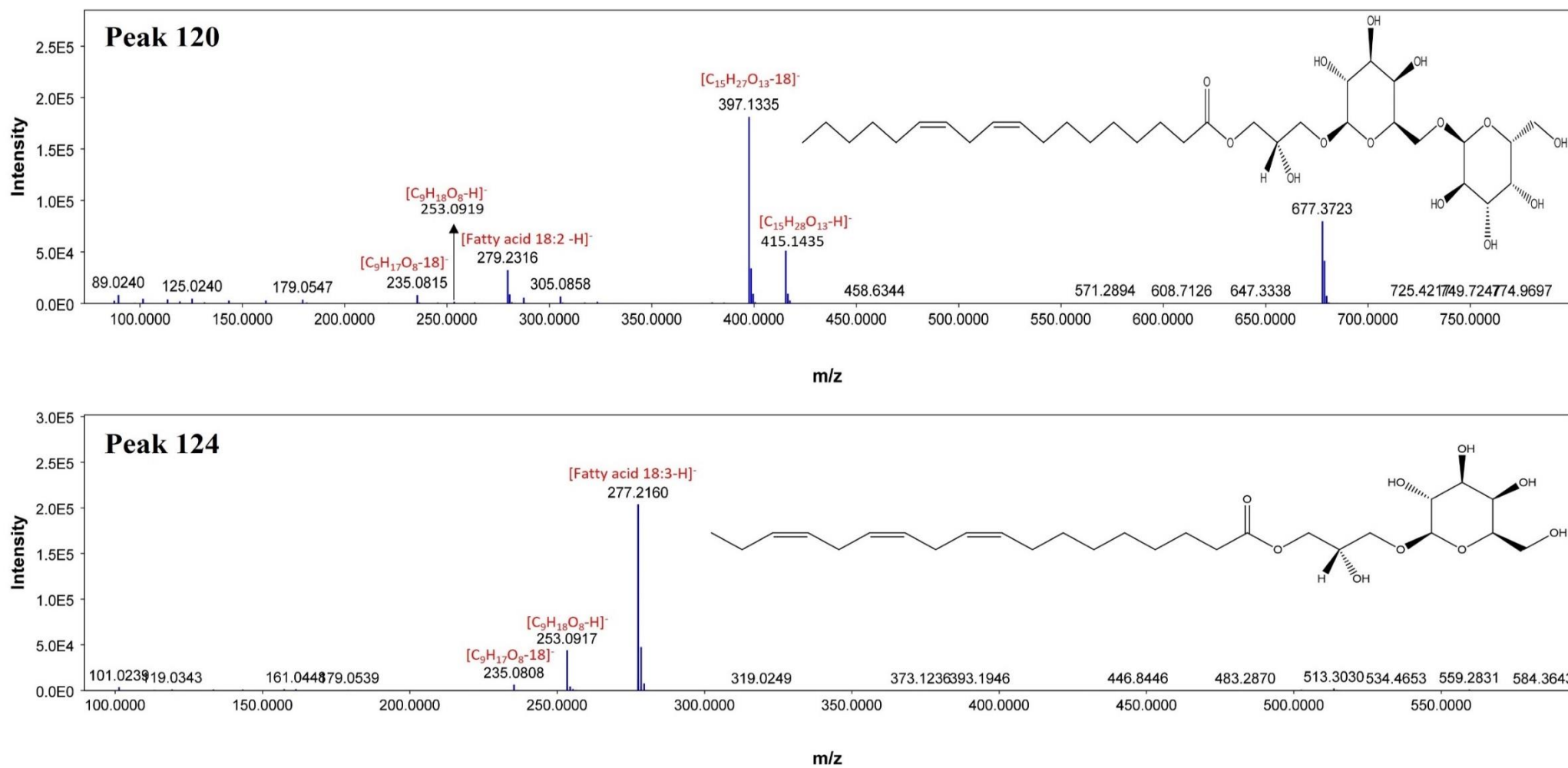


Fig. S20. MS/MS spectra of Digalactosylmonoacylglycerol (DGMG 18:2) (**120**), Monogalactosylmonoacylglycerol (MGMG 18:3) (**124**)

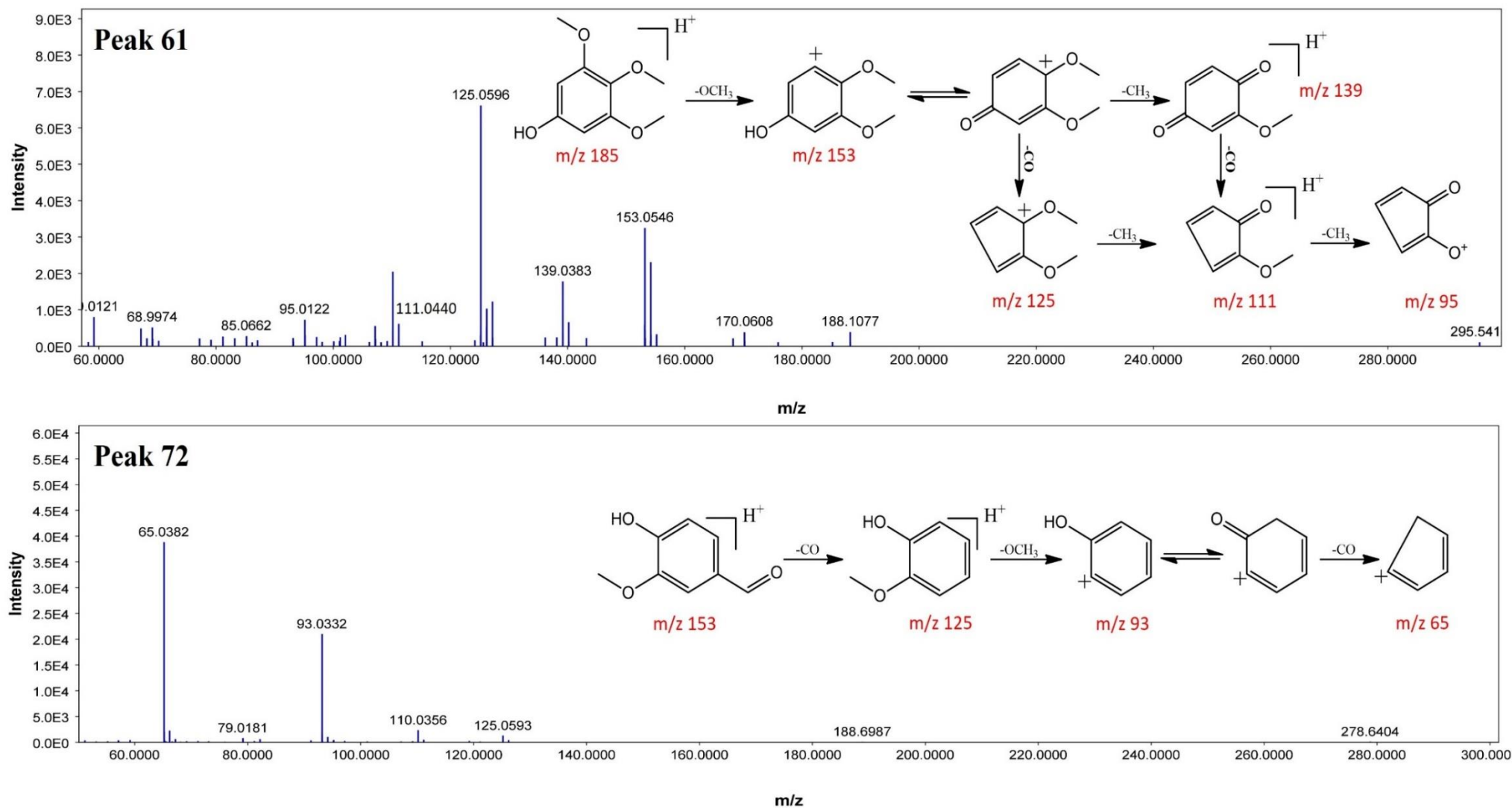


Fig. S21. MS/MS spectra of trimethoxyphenol (**61**), vaniline (**72**)