

Supplementary Information

Metabolomic Insights on Plant Growth-Promoting Yeast as Bioinput: Biochemical Interactions with Tomato Seedlings

Miria A. Souza,^{a,b} Jorge C. Rodrigues Neto,^a Eder A. Barbosa,^a Catharine A. Bomfim,^a Thais D. Mendes,^a João R. M. de Almeida,^a Silvia B. Gonçalves,^a Félix G. de Siqueira^a and Patrícia V. Abdelnur^{*,a,b}

^a*Empresa Brasileira de Pesquisa Agropecuária, Embrapa Agroenergy, W3 Norte, PqEB, 70770-901 Brasília-DF, Brazil*

^b*Instituto de Química, Universidade Federal de Goiás, Campus Samambaia, 74690-900 Goiânia-GO, Brazil*

*e-mail: patricia.abdelnur@embrapa.br

Miria de Almeida Souza: <https://orcid.org/0000-0003-0243-5182>

Jorge Candido Rodrigues Neto: <https://orcid.org/0000-0002-6173-1451>

Eder Alves Barbosa: <https://orcid.org/0000-0002-7613-4414>

Catharine Abreu Bomfim: <https://orcid.org/0000-0001-7313-1157>

Thais Demarchi Mendes: <https://orcid.org/0000-0002-8505-7924>

João Ricardo Moreira de Almeida: <https://orcid.org/0000-0002-2902-5805>

Silvia Belem Goncalves: <https://orcid.org/0000-0002-6036-4725>

Félix Gonçalves de Siqueira: <https://orcid.org/0000-0001-5239-4994>

Patrícia Verardi Abdelnur: <https://orcid.org/0000-0001-5936-6523>

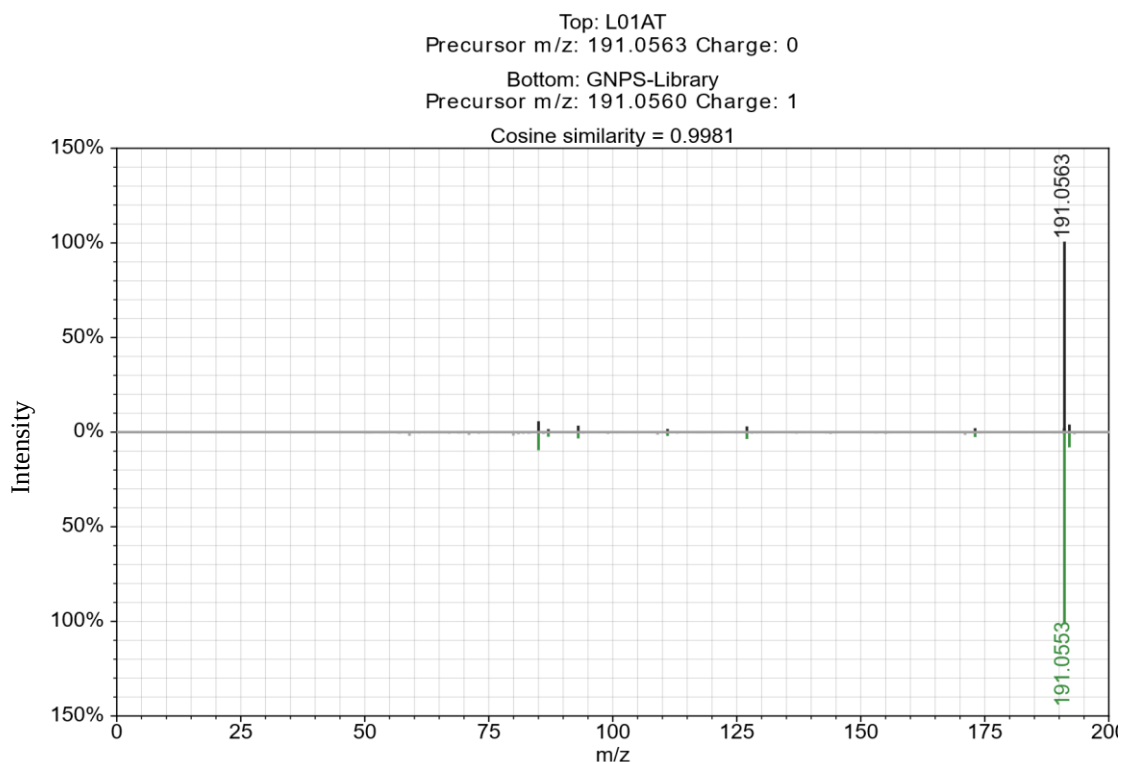


Figure S1. Mass spectrum of the compound (1S,3R,4S,5R)-1,3,4,5-tetrahydrocyclohexane-1-carboxylic acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

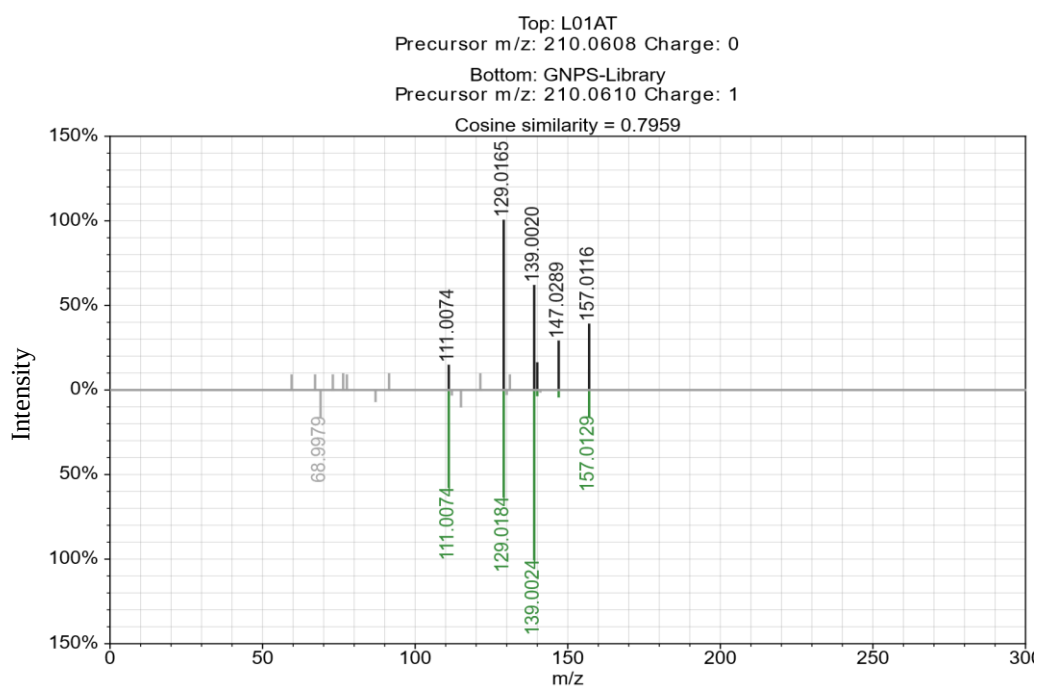


Figure S2. Mass spectrum of the compound citric acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

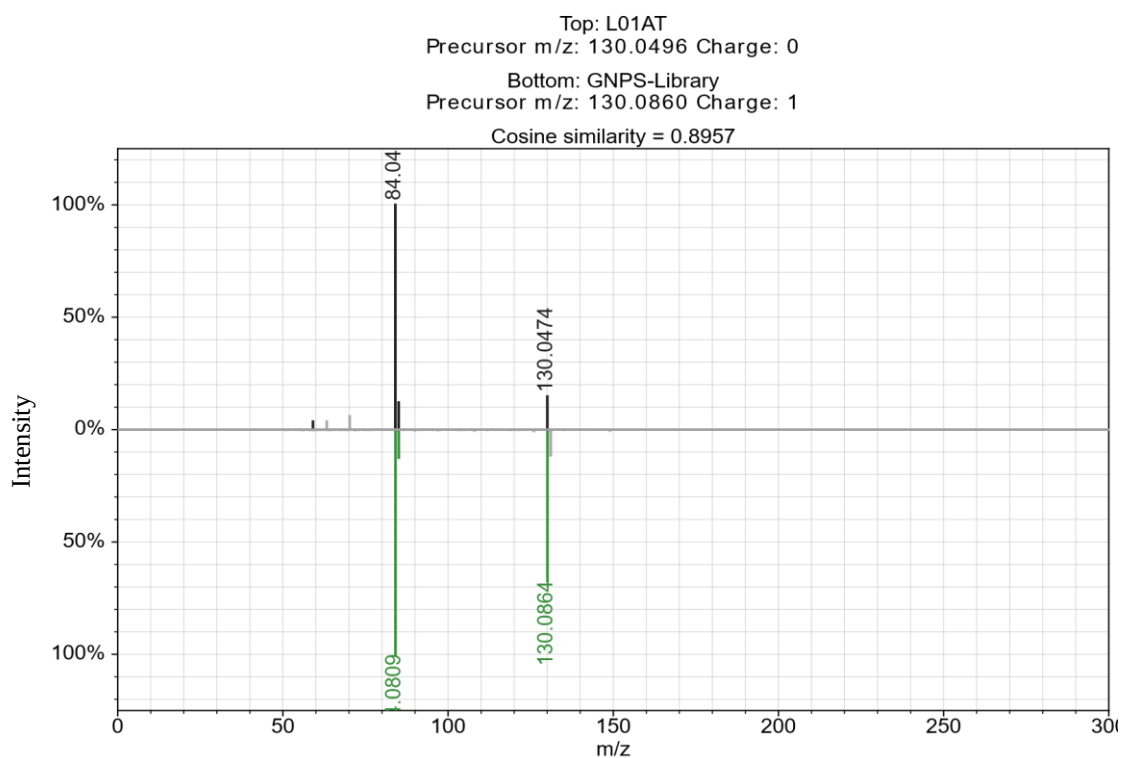


Figure S3. Mass spectrum of the compound pipecolic acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

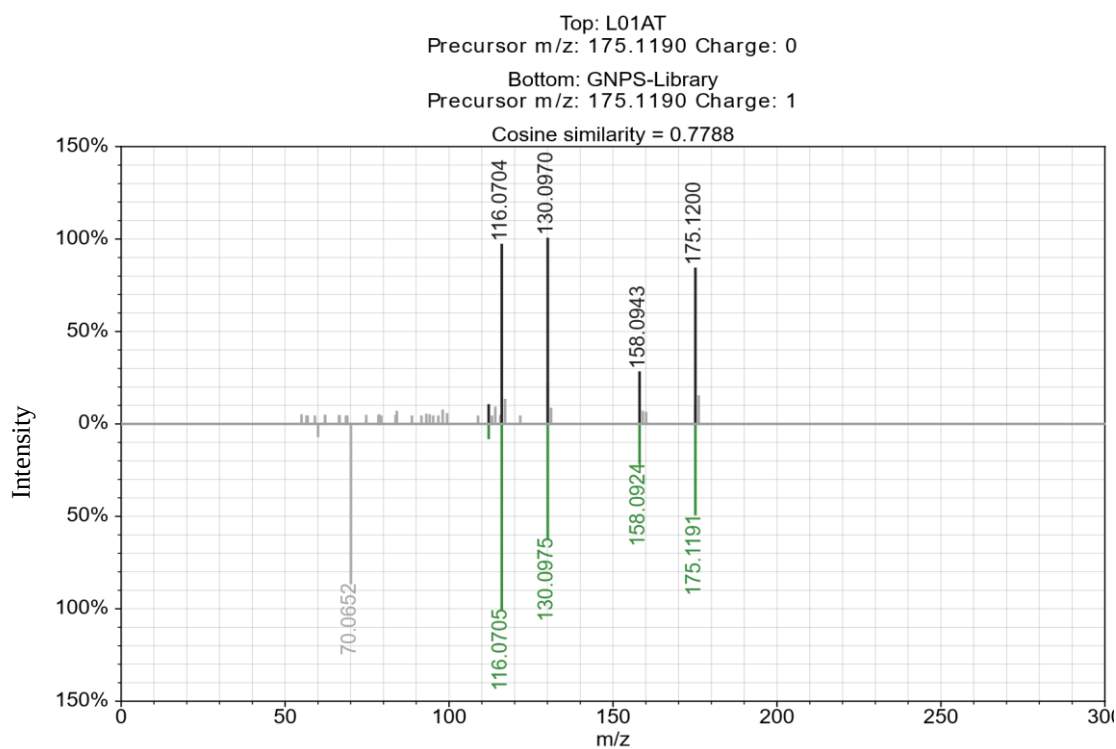


Figure S4. Mass spectrum of the compound arginine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

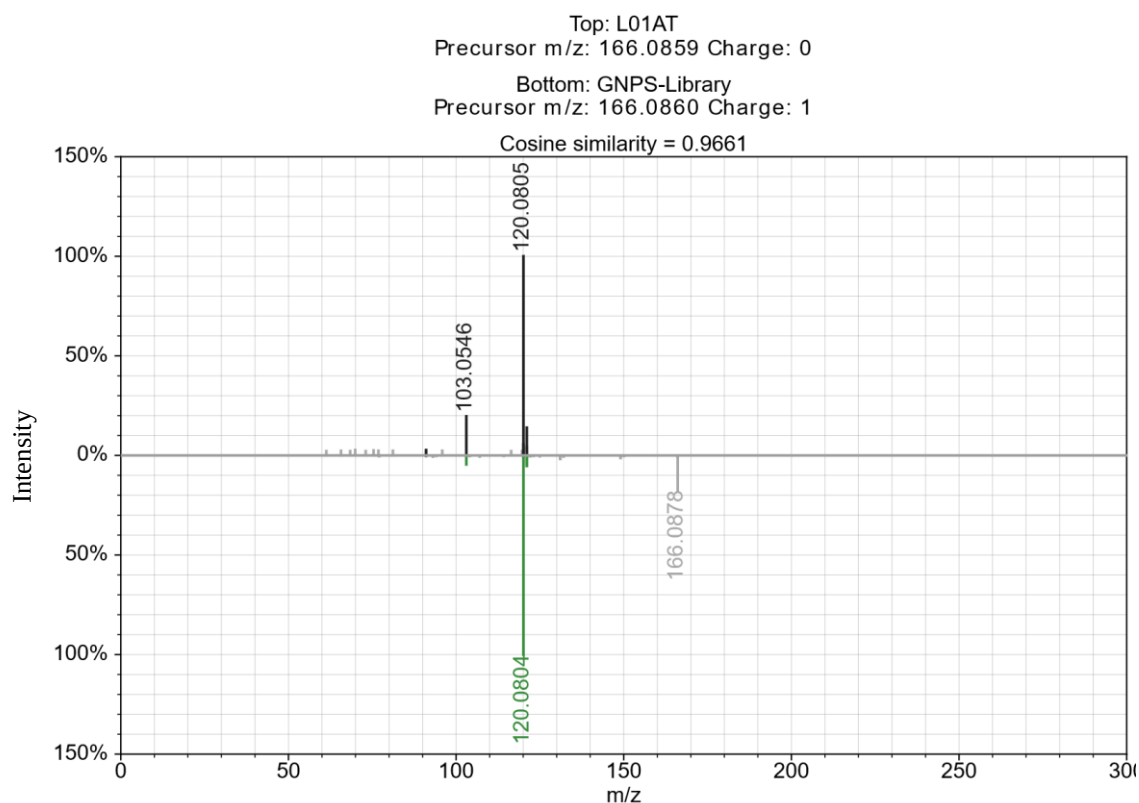


Figure S5. Mass spectrum of the compound phenylalanine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

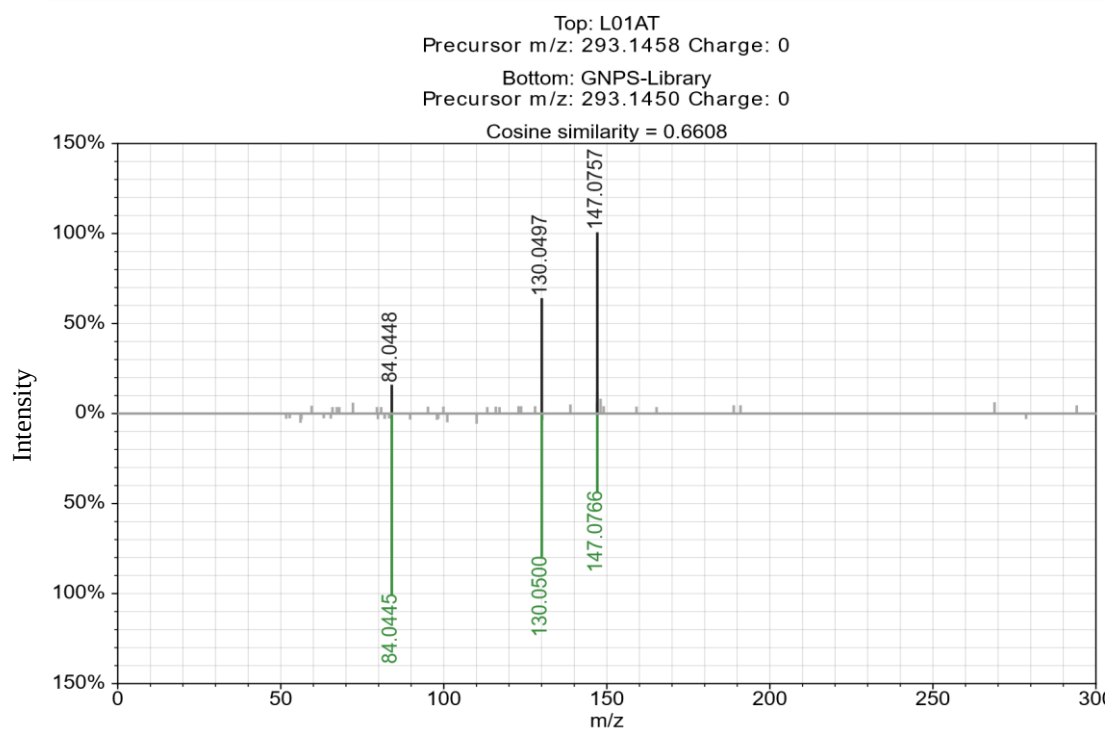


Figure S6. Mass spectrum of the compound glutamine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

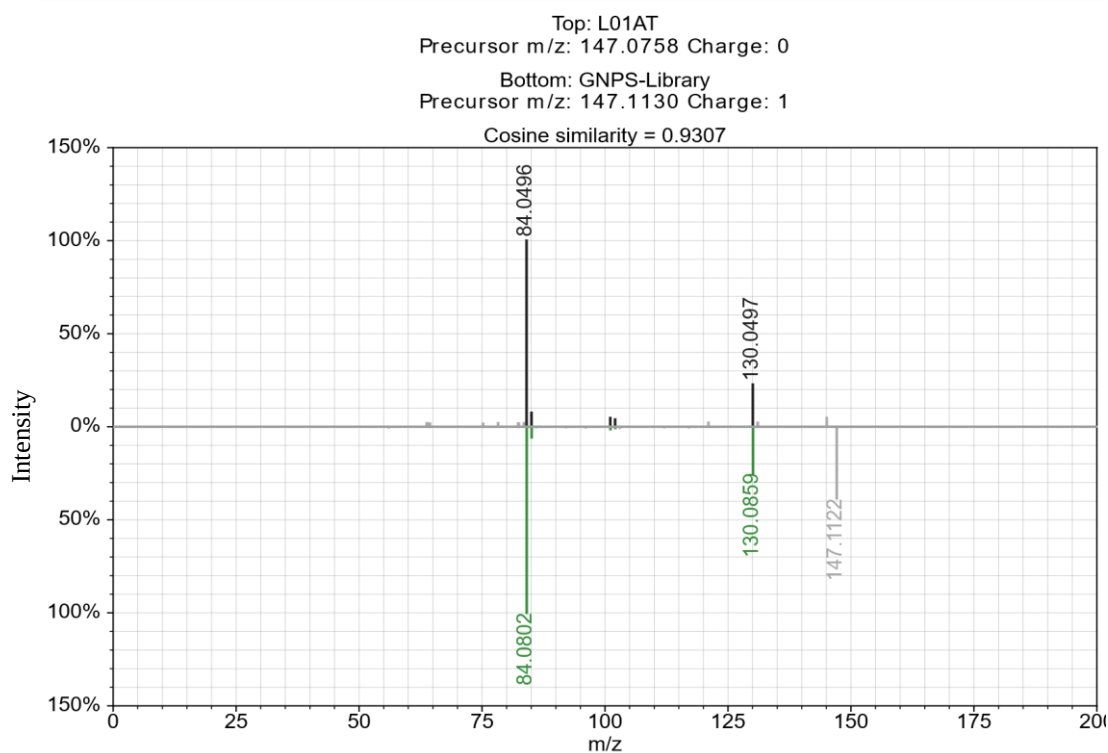


Figure S7. Mass spectrum of the compound lysine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

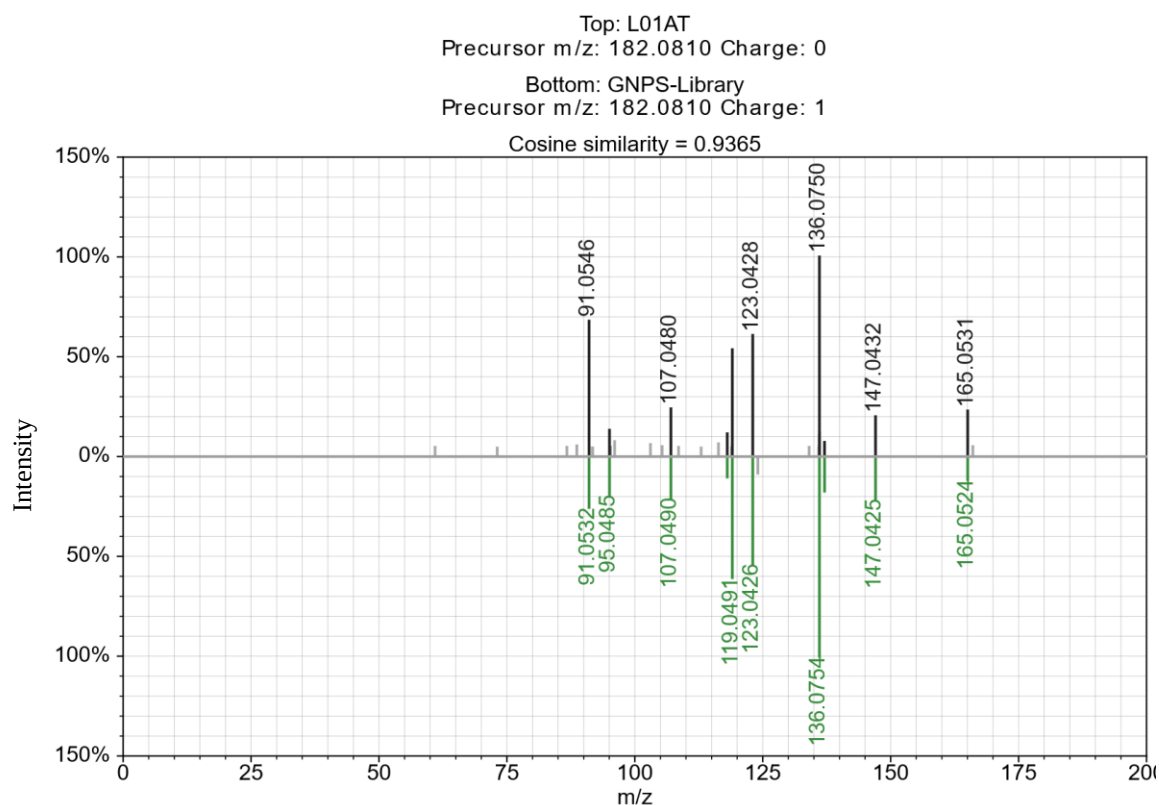


Figure S8. Mass spectrum of the compound tyrosine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

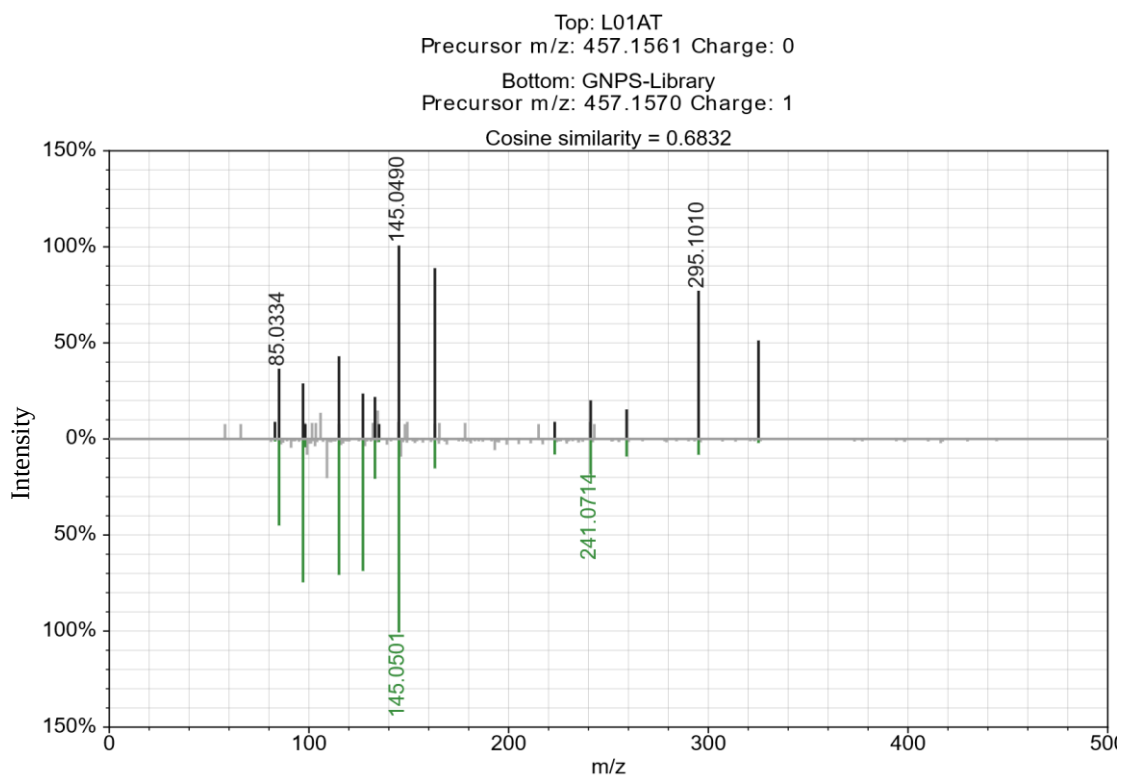


Figure S9. Mass spectrum of the compound trehalose. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

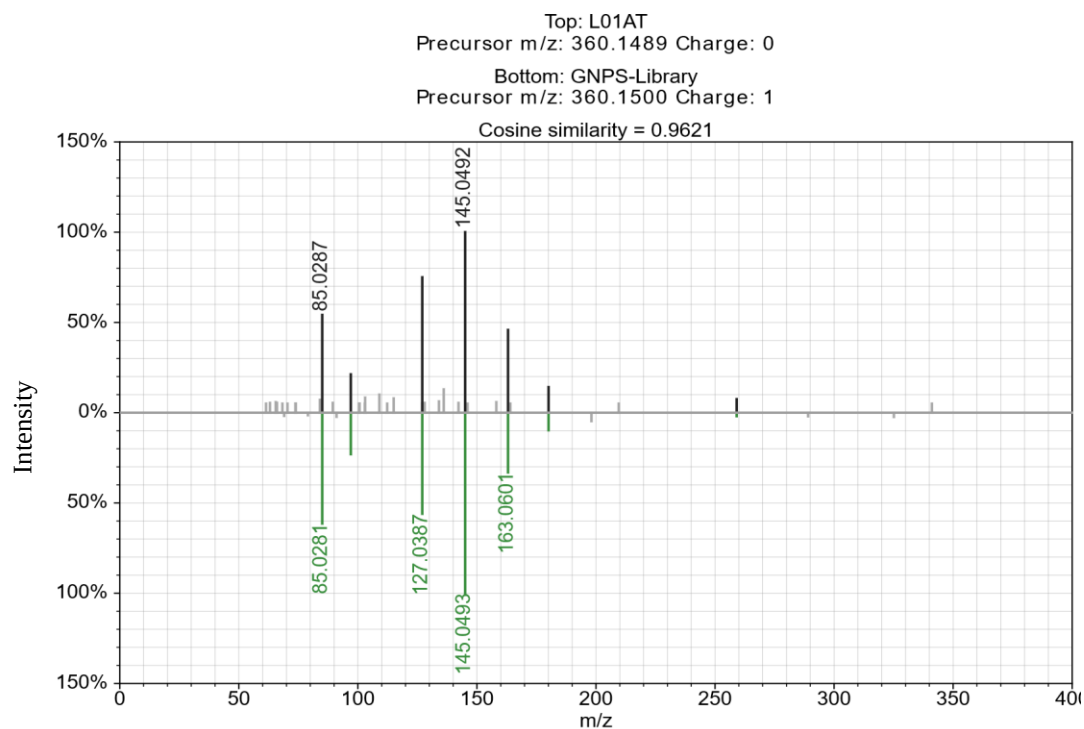


Figure S10. Mass spectrum of the compound sucrose. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

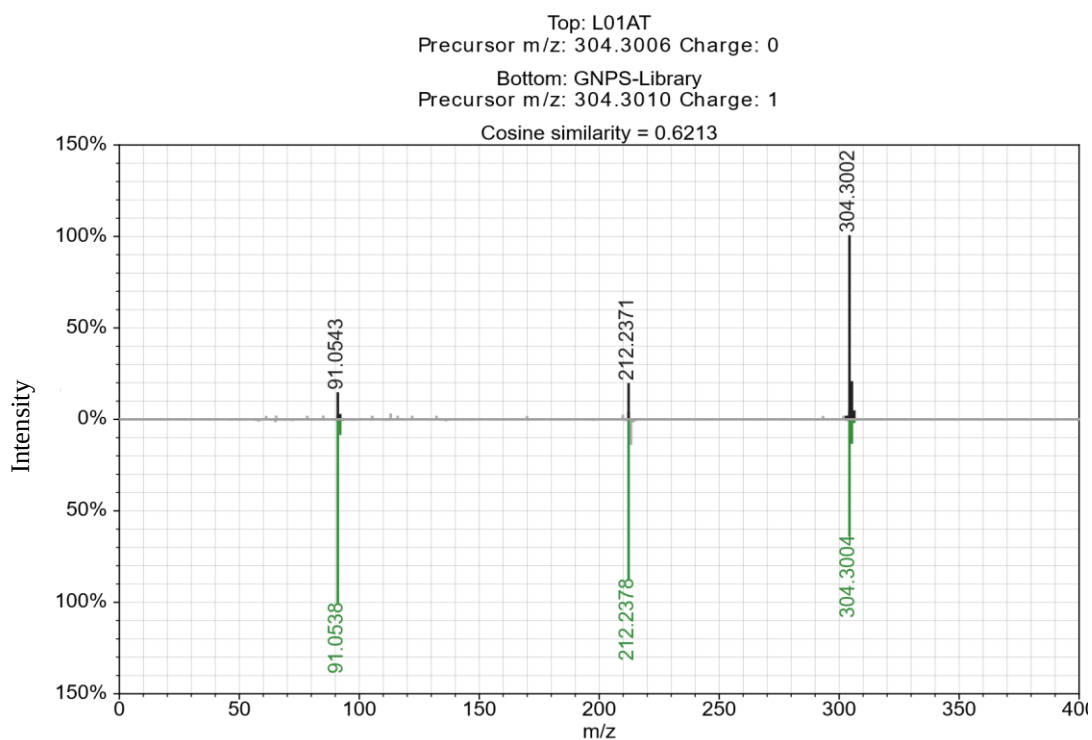


Figure S11. Mass spectrum of the compound 5,6-epoxy-8Z,11Z,14Z-eicosatrienoic acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

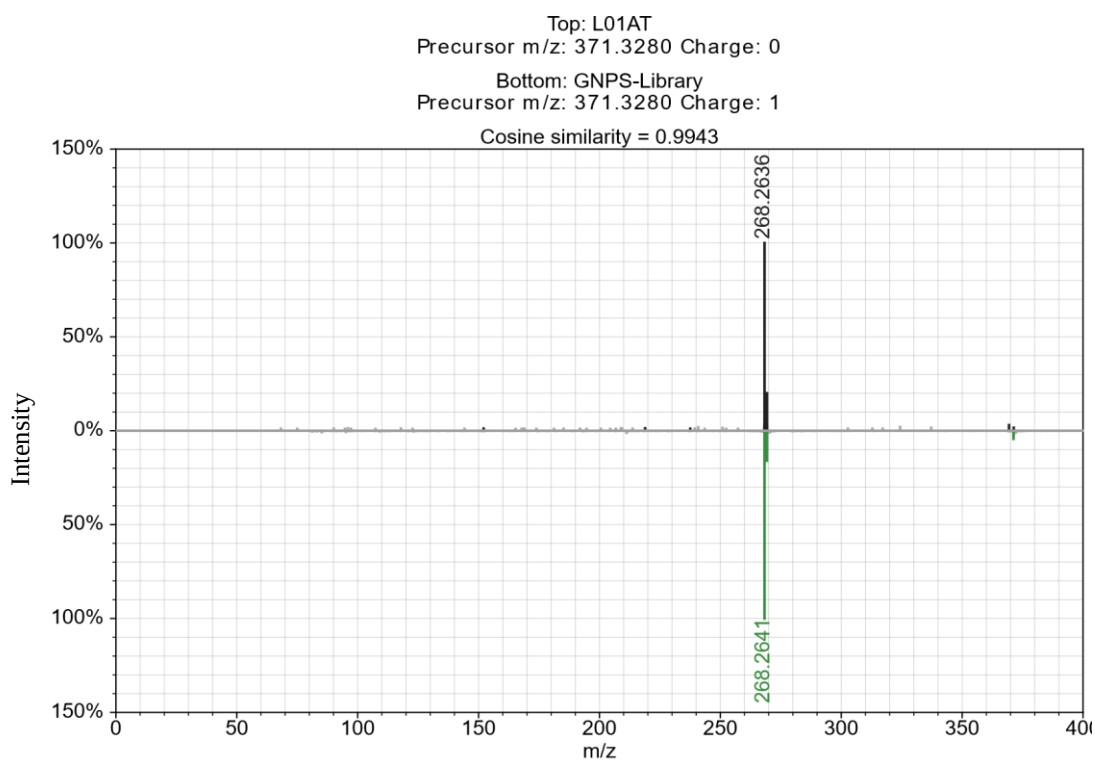


Figure S12. Mass spectrum of the compound heptadecasing-4-ene. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

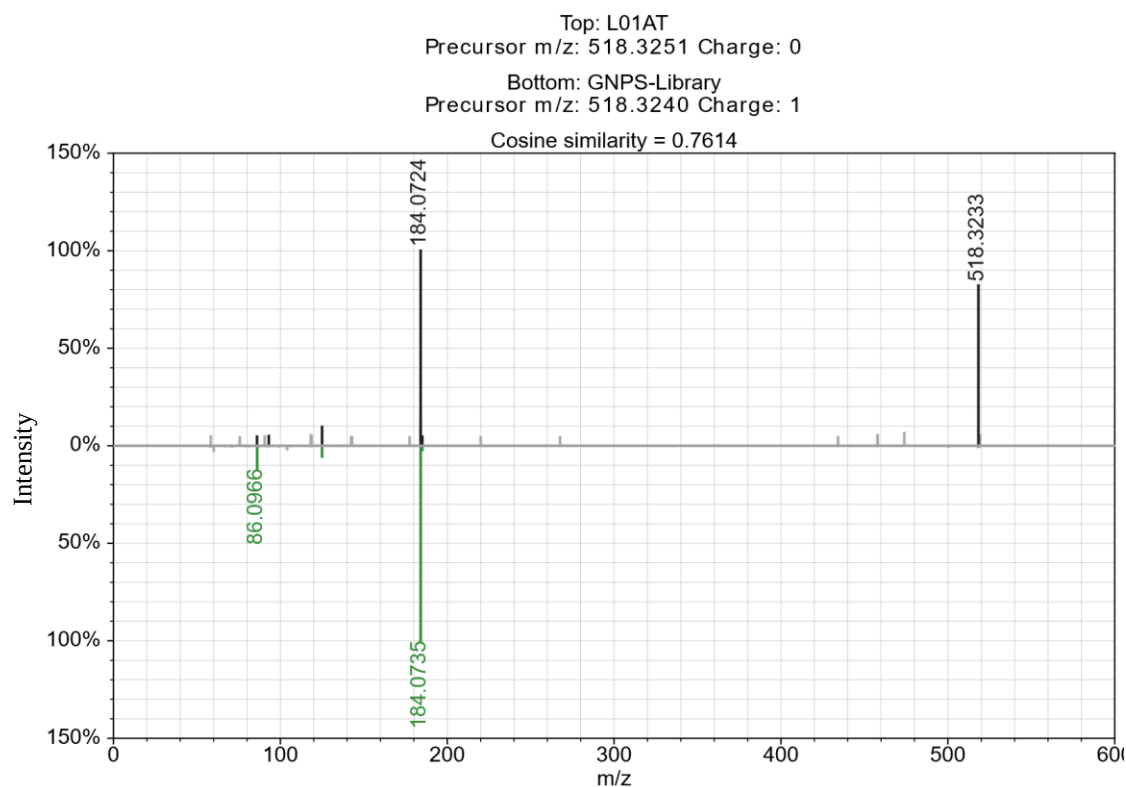


Figure S13. Mass spectrum of the compound lyso-PC(16:0) . The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

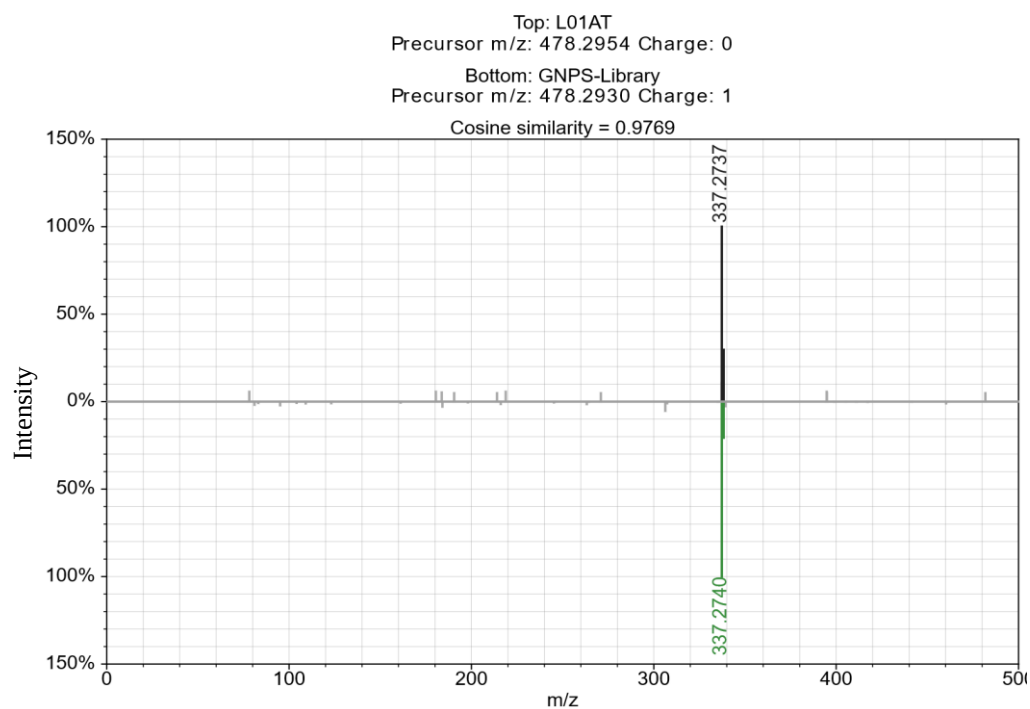


Figure S14. Mass spectrum of the compound 1-stearoyl-2-hydroxy-*sn*-glycero-3-phosphoethanolamine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

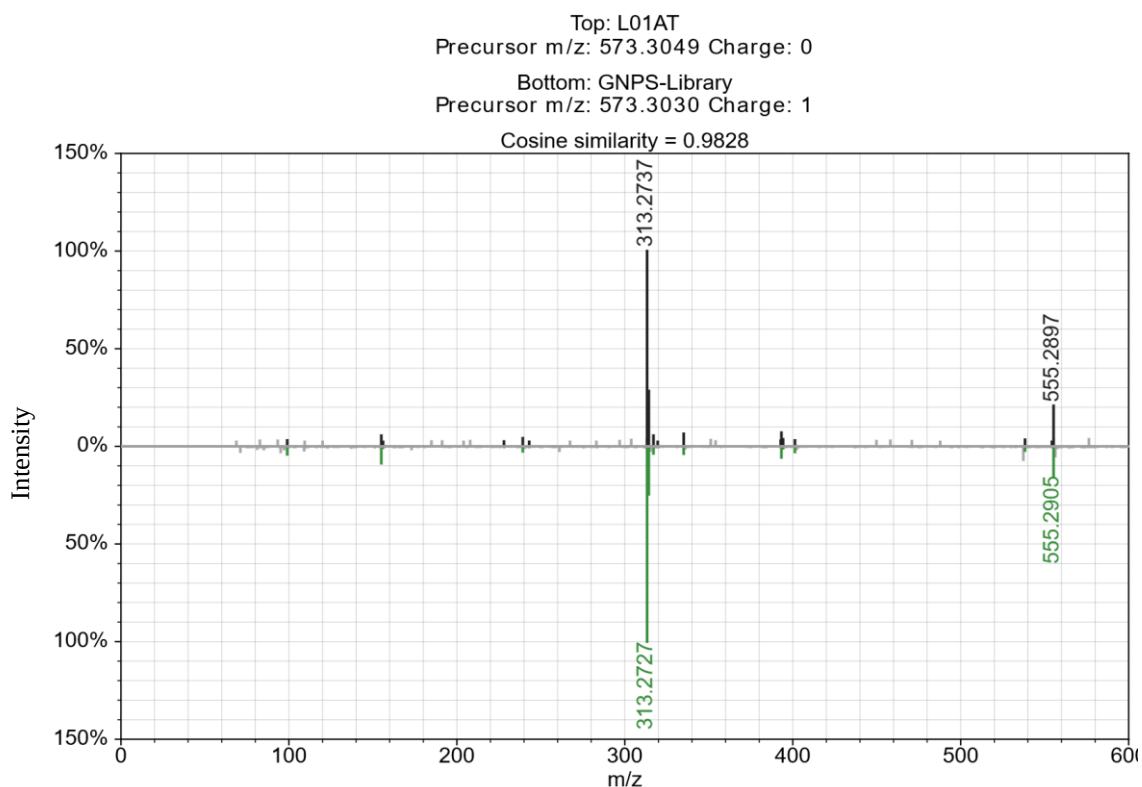


Figure S15. Mass spectrum of the compound 1-palmitoyl-2-hydroxy-*sn*-glycero-3-phosphoethanolamine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

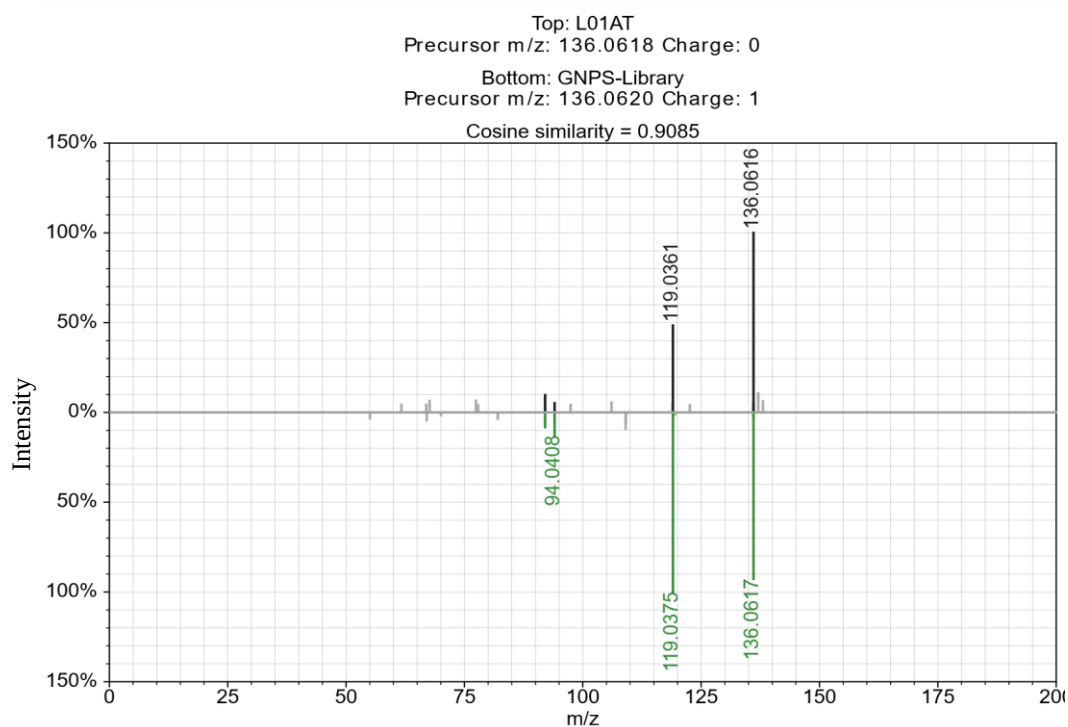


Figure S16. Mass spectrum of the compound adenine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

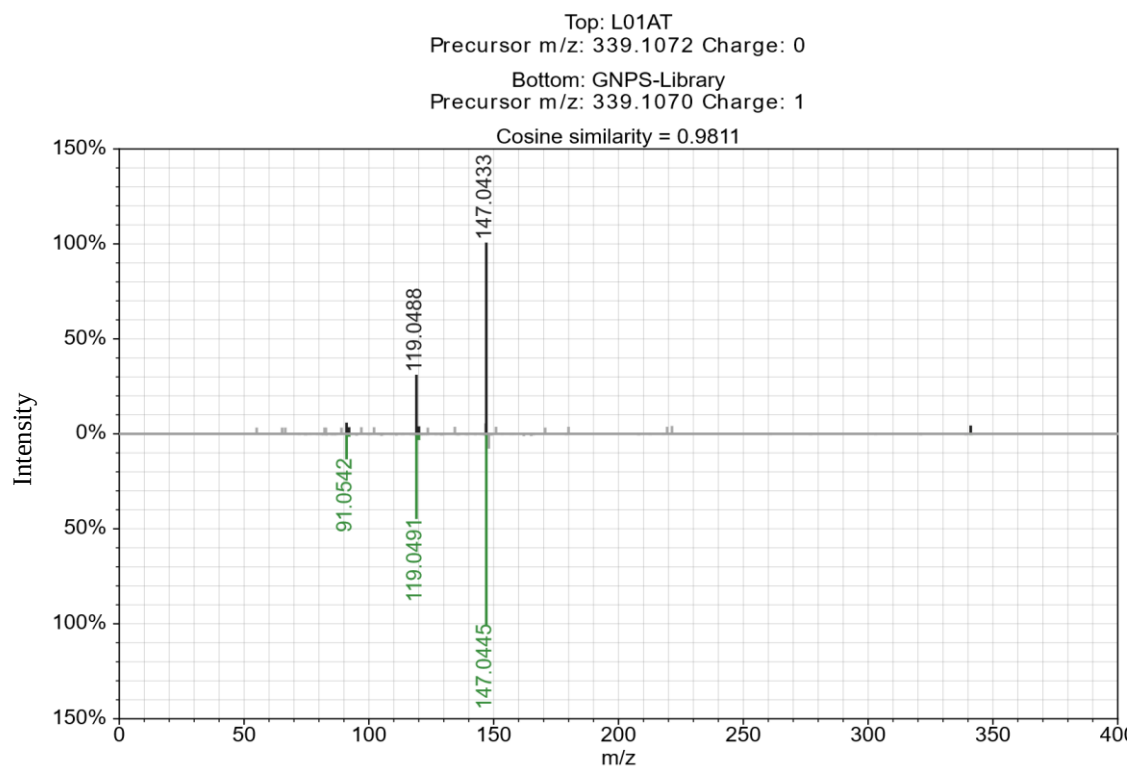


Figure S17. Mass spectrum of the compound 3-*p*-coumaroylquinic acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

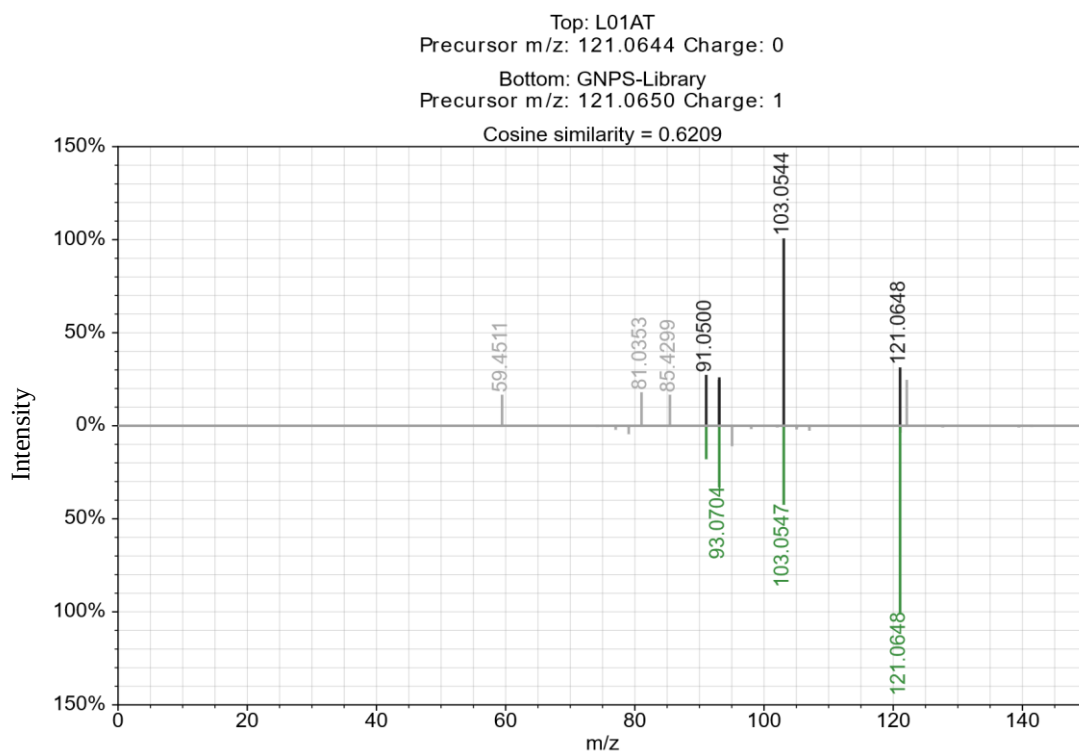


Figure S18. Mass spectrum of the compound tyramine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

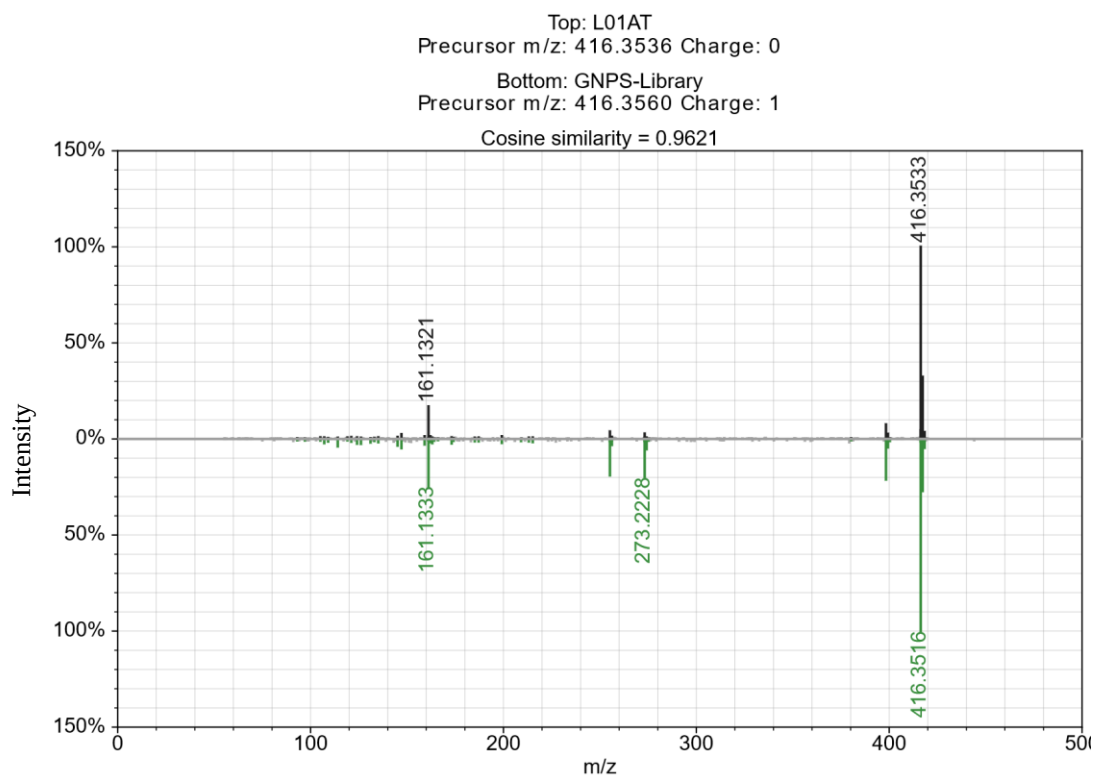


Figure S19. Mass spectrum of the compound solasodine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

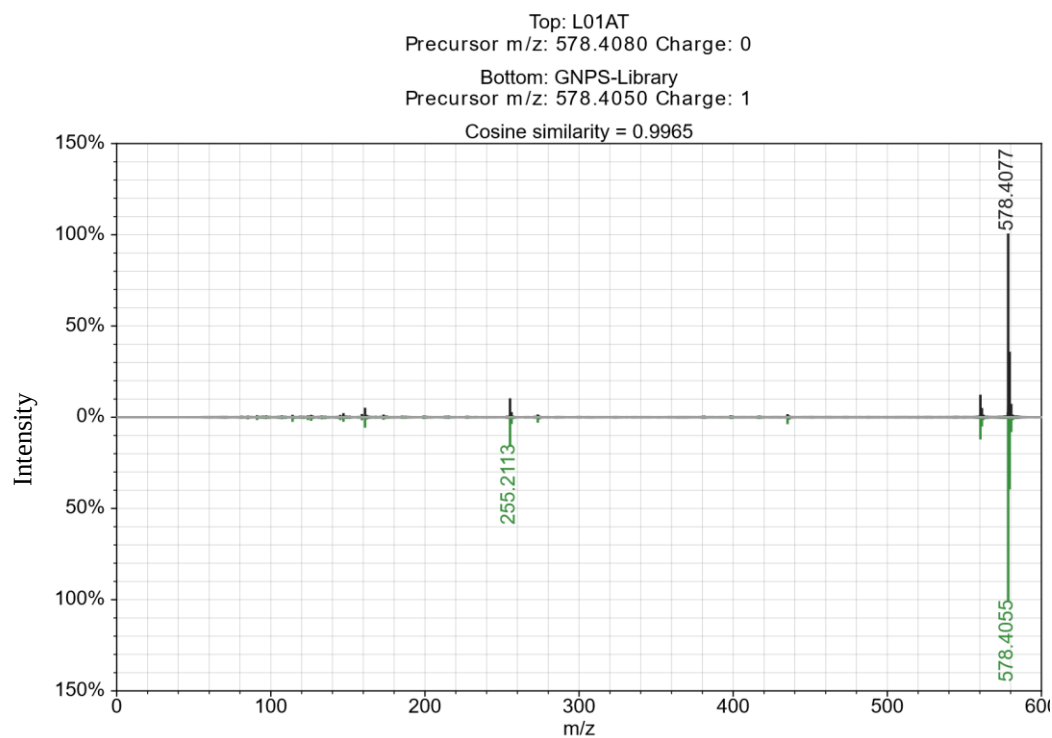


Figure S20. Mass spectrum of the compound tomatidine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

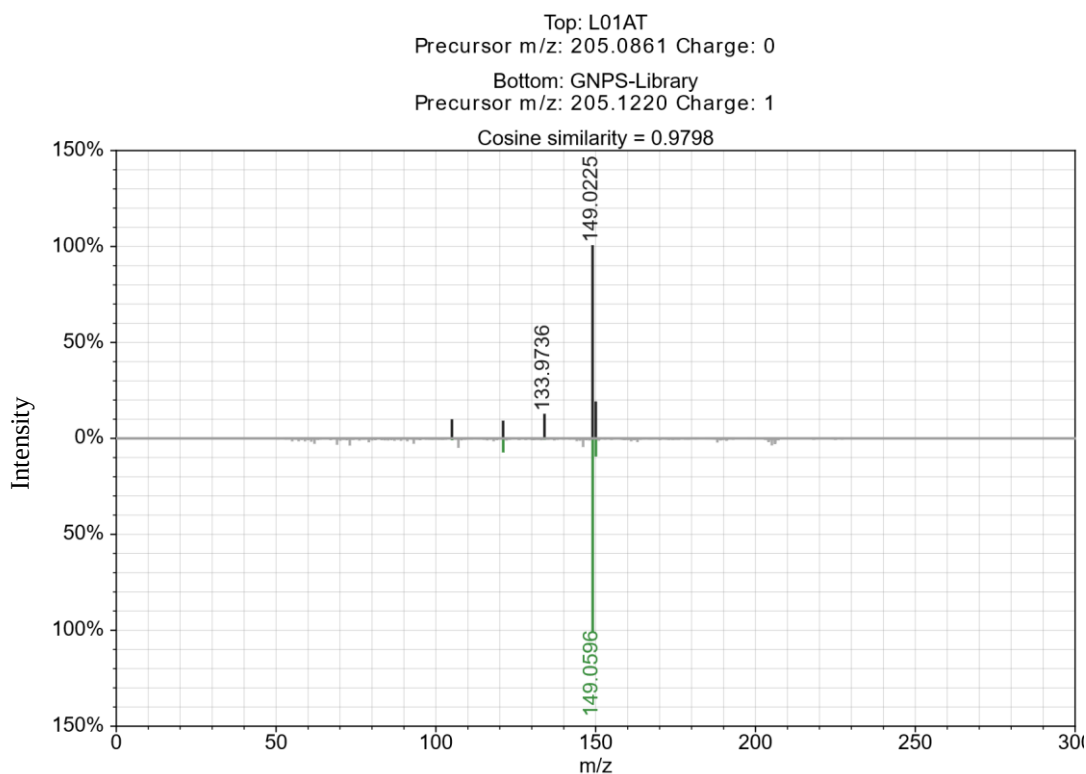


Figure S21. Mass spectrum of the compound 1-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]ethenone. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

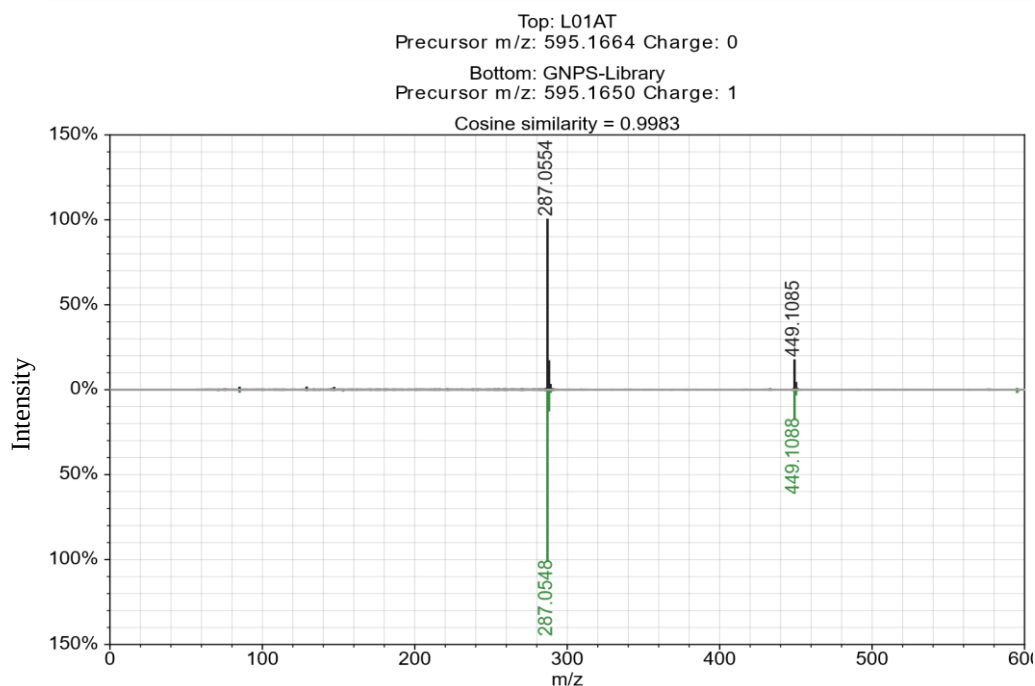


Figure S22. Mass spectrum of the compound 2-(3,4-dihydroxyphenyl)-5-hydroxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxychromen-4-one. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

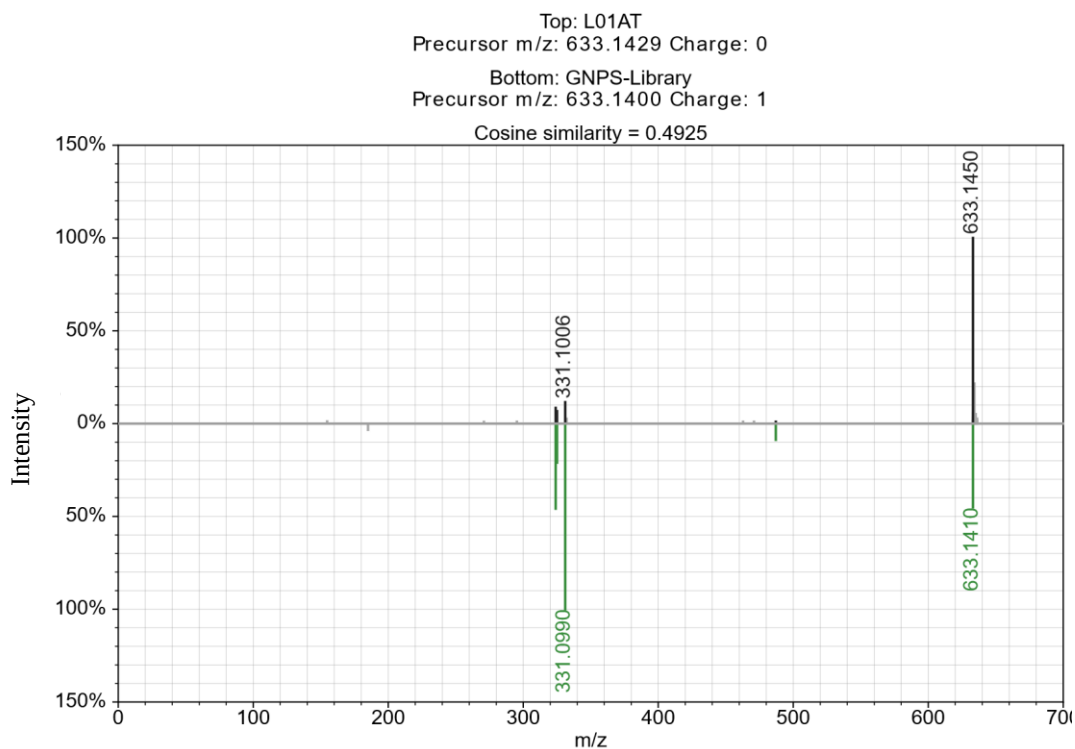


Figure S23. Mass spectrum of the compound 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-(((2*S*,3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(((3*R*,4*R*,5*R*,6*S*)-3,4,5-trihydroxy-6-methyltetrahydro-2*H*-pyran-2-yl)oxy)methyl)tetrahydro-2*H*-pyran-2-yl)oxy)-4*H*-chromen-4-one. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

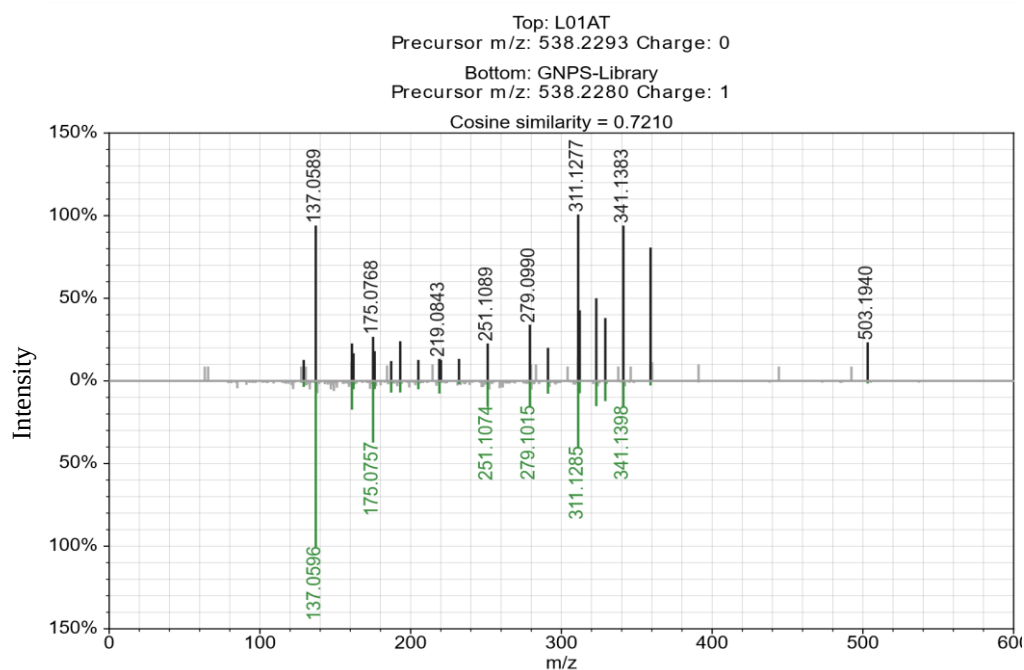


Figure S24. Mass spectrum of the compound 2-(hydroxymethyl)-6-[4-[(2*S*,3*S*)-3-(hydroxymethyl)-5-[(*E*)-3-hydroxyprop-1-enyl]-7-methoxy-2,3-dihydro-1-benzofuran-2-yl]-2-methoxyphenoxy]oxane-3,4,5-triol. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

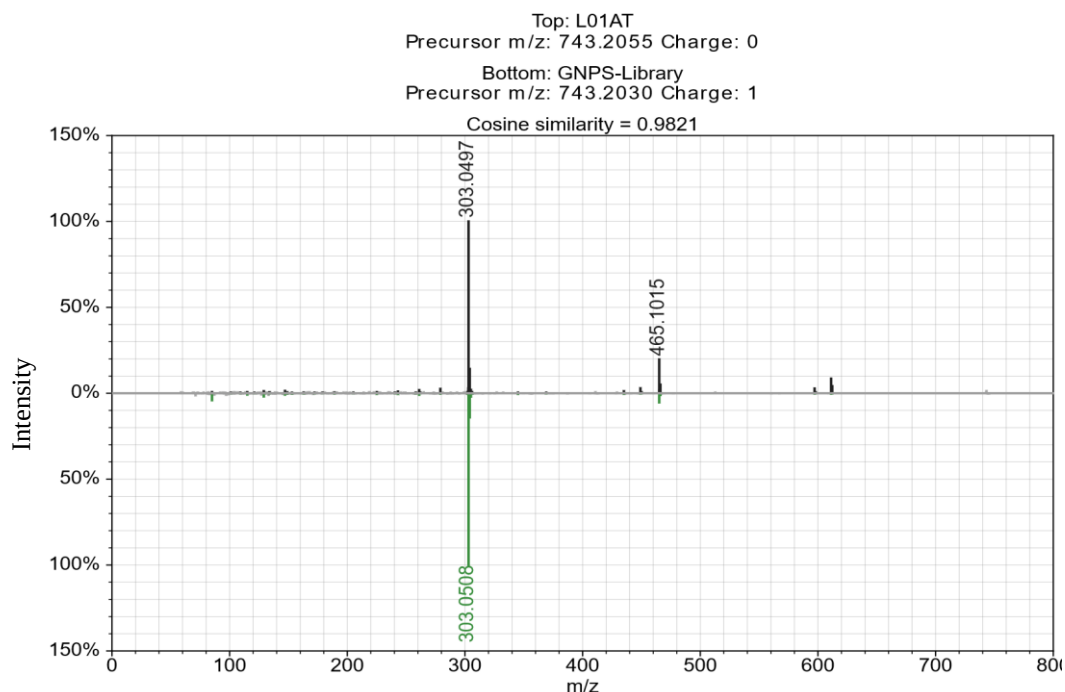


Figure S25. Mass spectrum of the compound 3-[(2*S*,3*R*,4*S*,5*S*,6*R*)-6-[[[(2*R*,3*R*,4*R*,5*R*,6*S*)-3-[(2*S*,3*R*,4*R*)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-4,5-dihydroxy-6-methyloxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxychromen-4-one. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

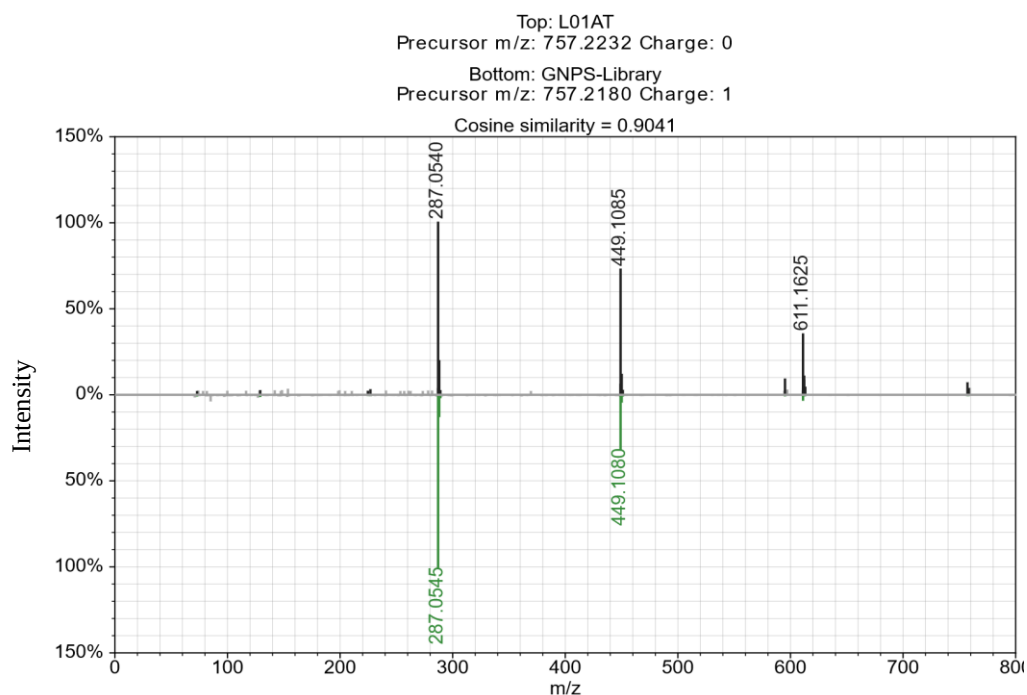


Figure S26. Mass spectrum of the compound 3-[4,5-dihydroxy-6-(hydroxymethyl)-3-[(2*S*,3*R*,4*R*,5*R*,6*S*)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

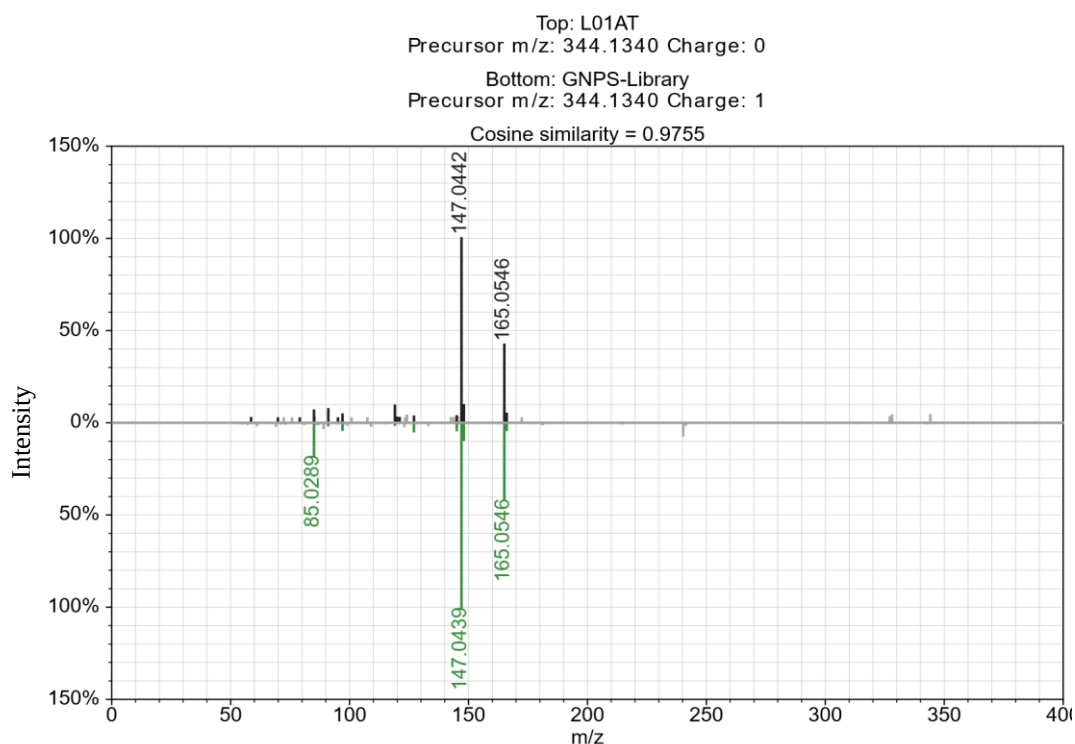


Figure S27. Mass spectrum of the compound (*E*)-3-[4-[(2*S*,3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]prop-2-enoic acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

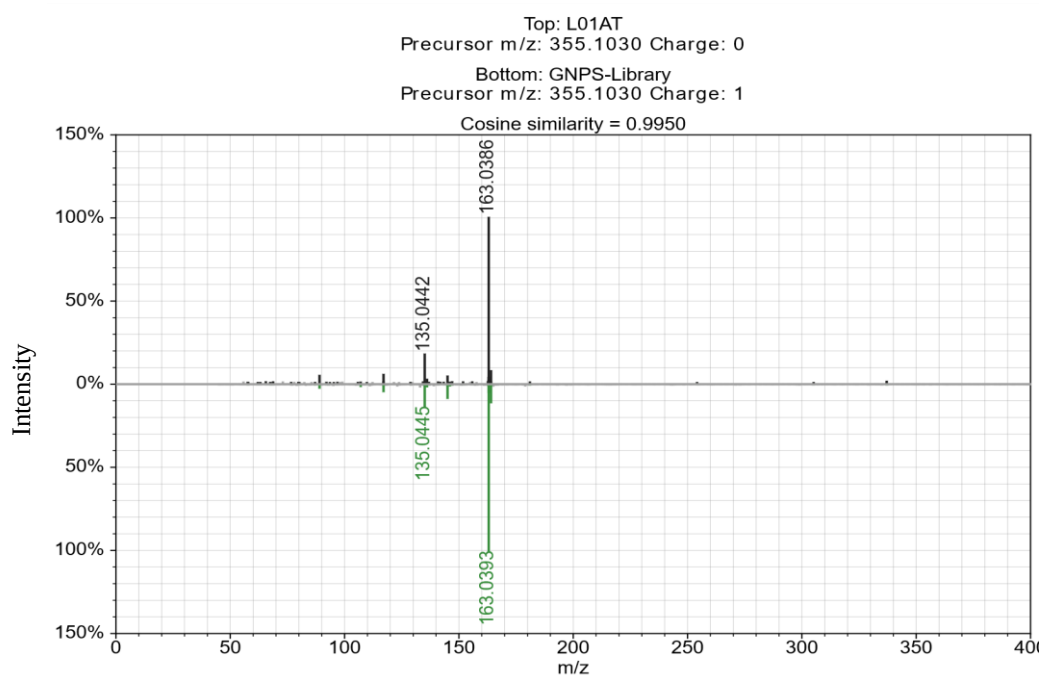


Figure S28. Mass spectrum of the compound cryptochlorogenic acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

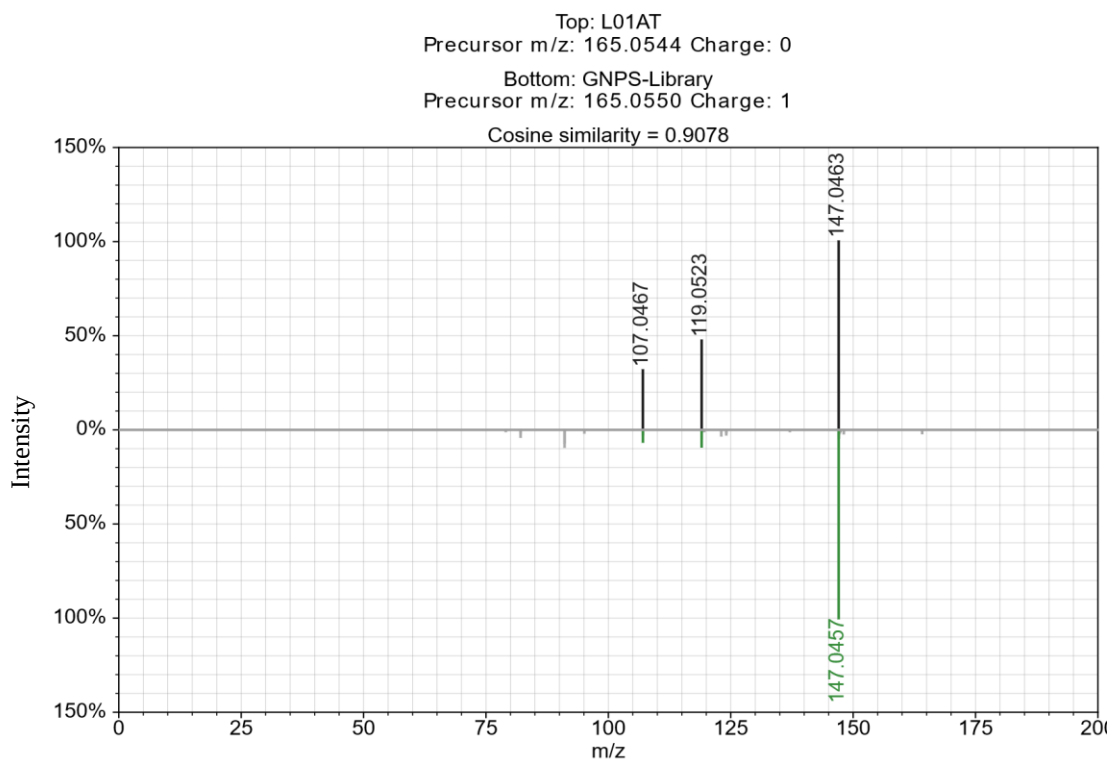


Figure S29. Mass spectrum of the compound *p*-coumaric acid. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

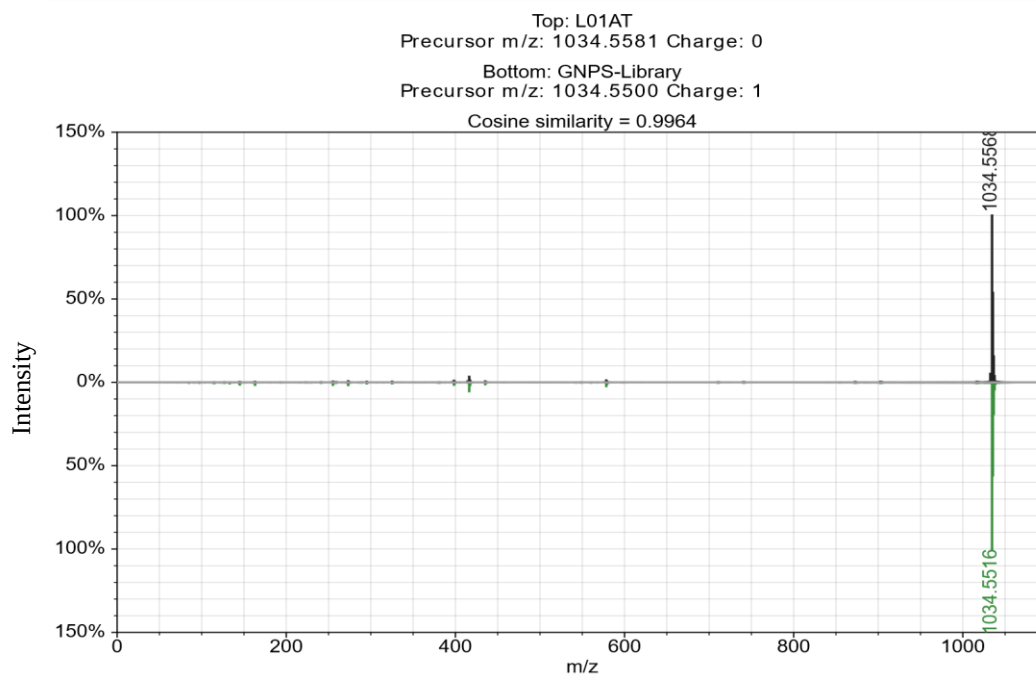


Figure S30. Mass spectrum of the compound furostane base + *O*-Hex, *O*-Hex-Hex-Hex. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

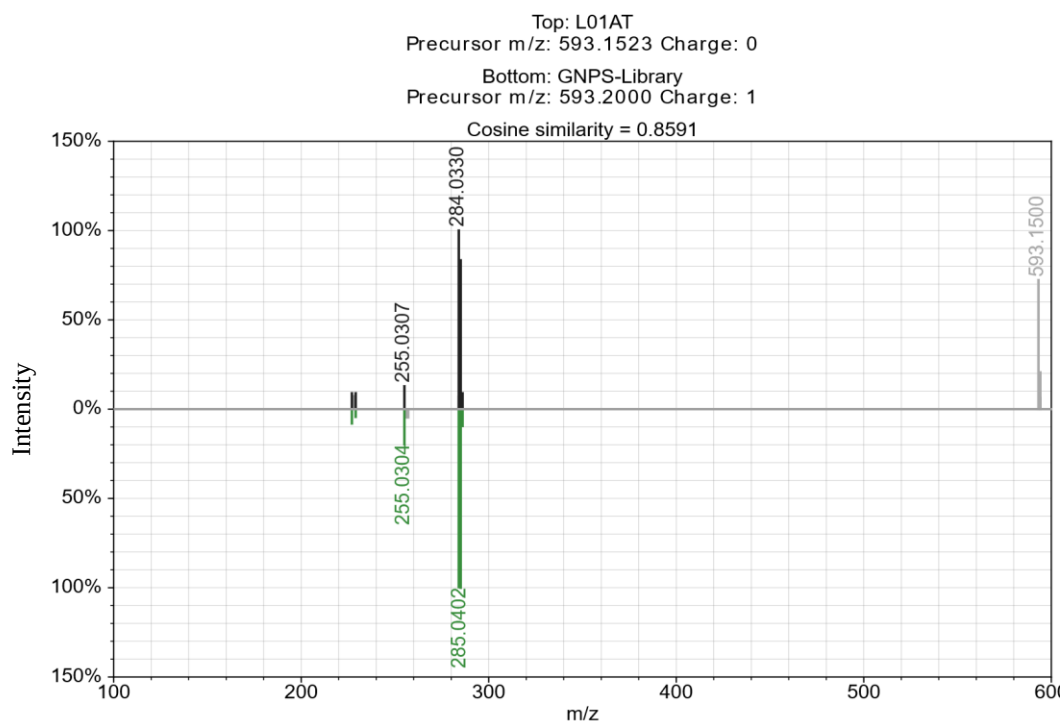


Figure S31. Mass spectrum of the compound kaempferol-3-*O*-rutinoside. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

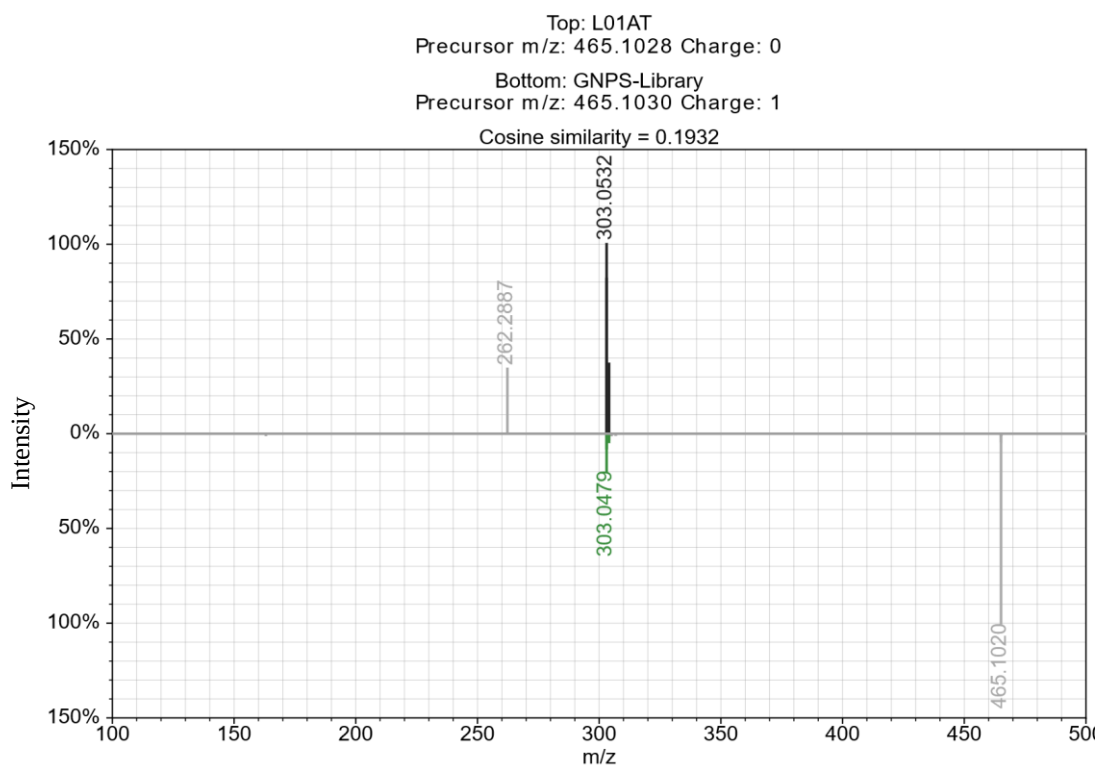


Figure S32. Mass spectrum of the compound quercetin-4'-*O*-glucoside. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

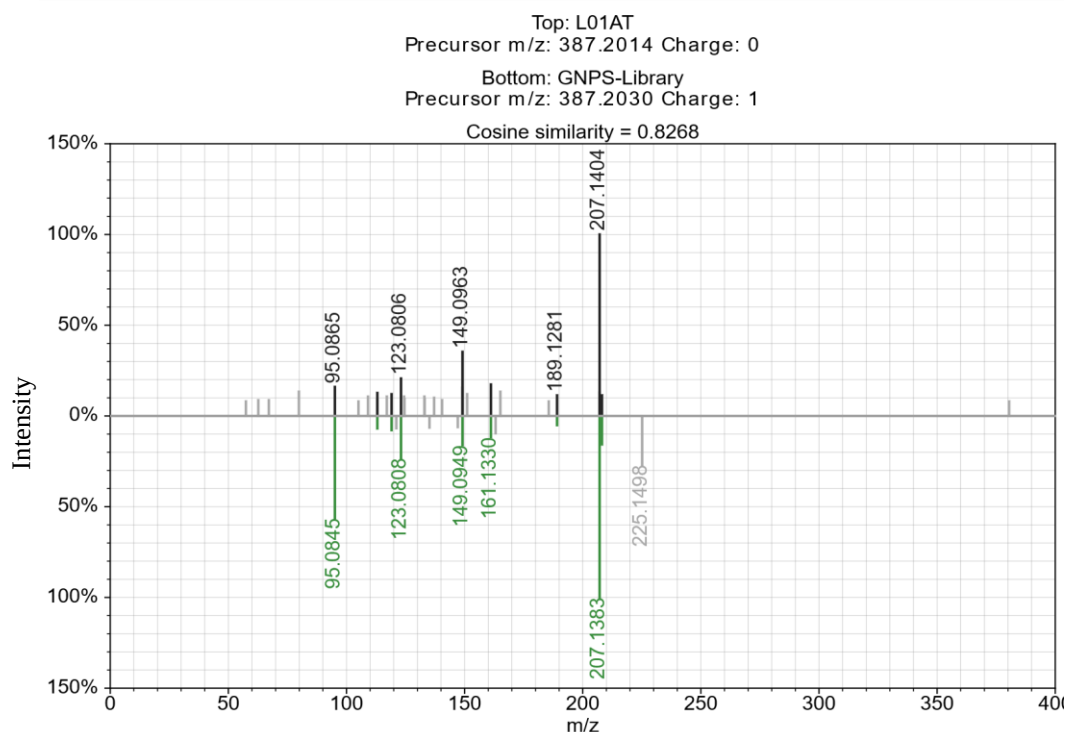


Figure S33. Mass spectrum of the compound roseoside. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

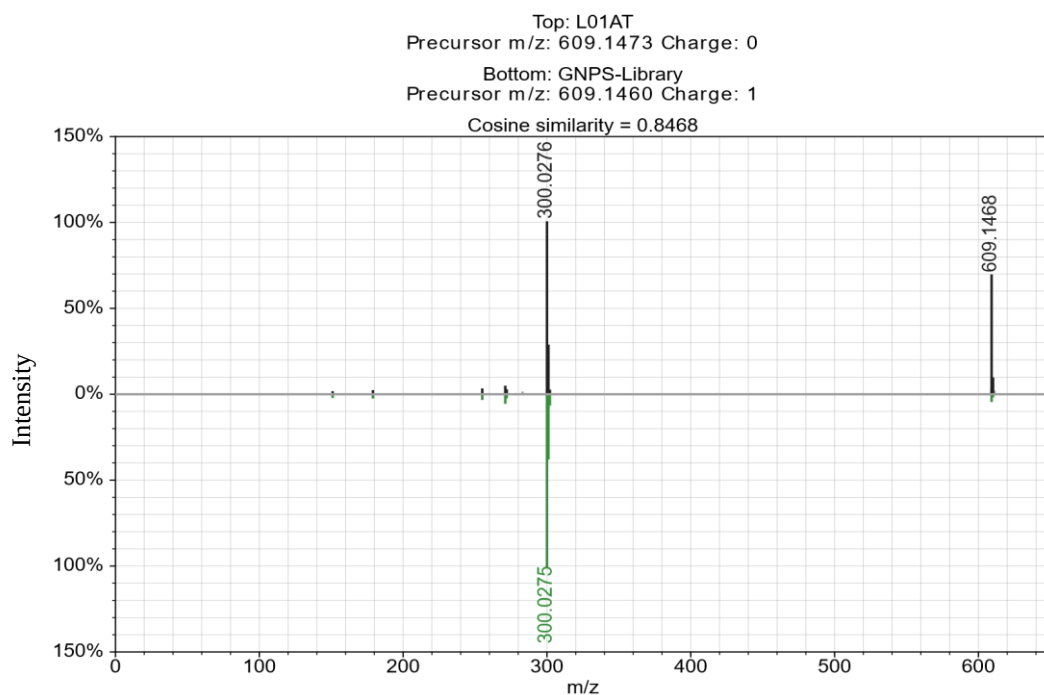


Figure S34. Mass spectrum of the compound routine. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

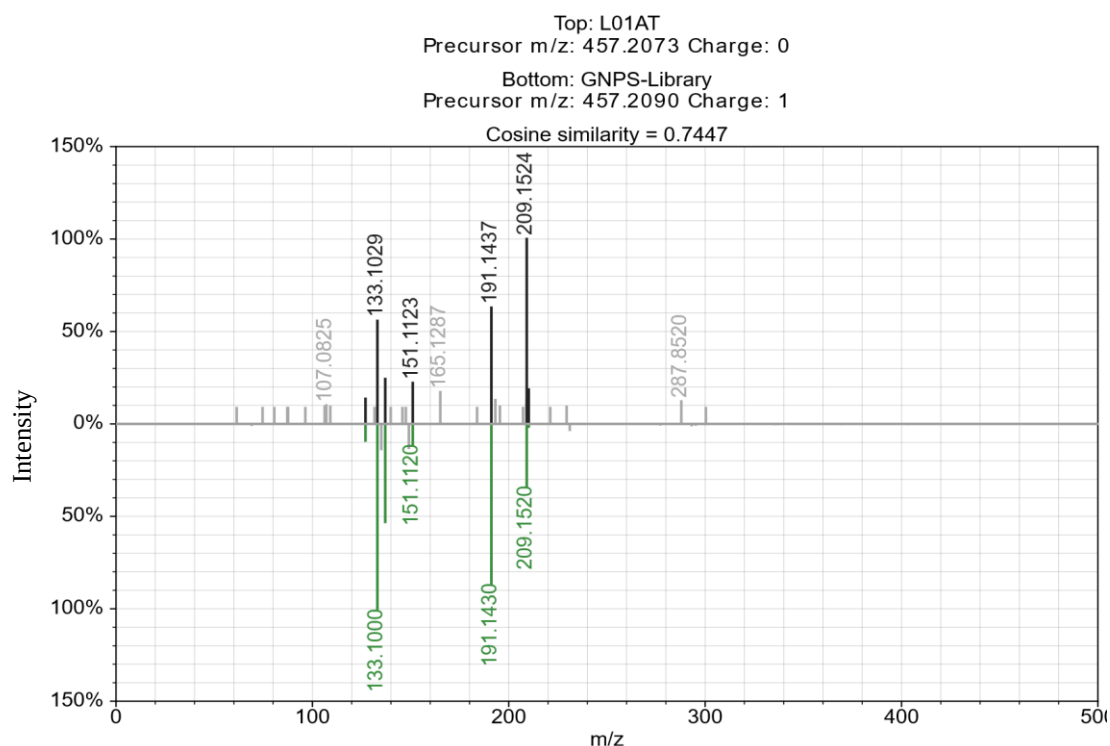


Figure S35. Mass spectrum of the compound 4-[(*E*)-3-[(2*R*,3*R*,4*S*,5*S*,6*R*)-3-[(2*S*,3*R*,4*R*)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

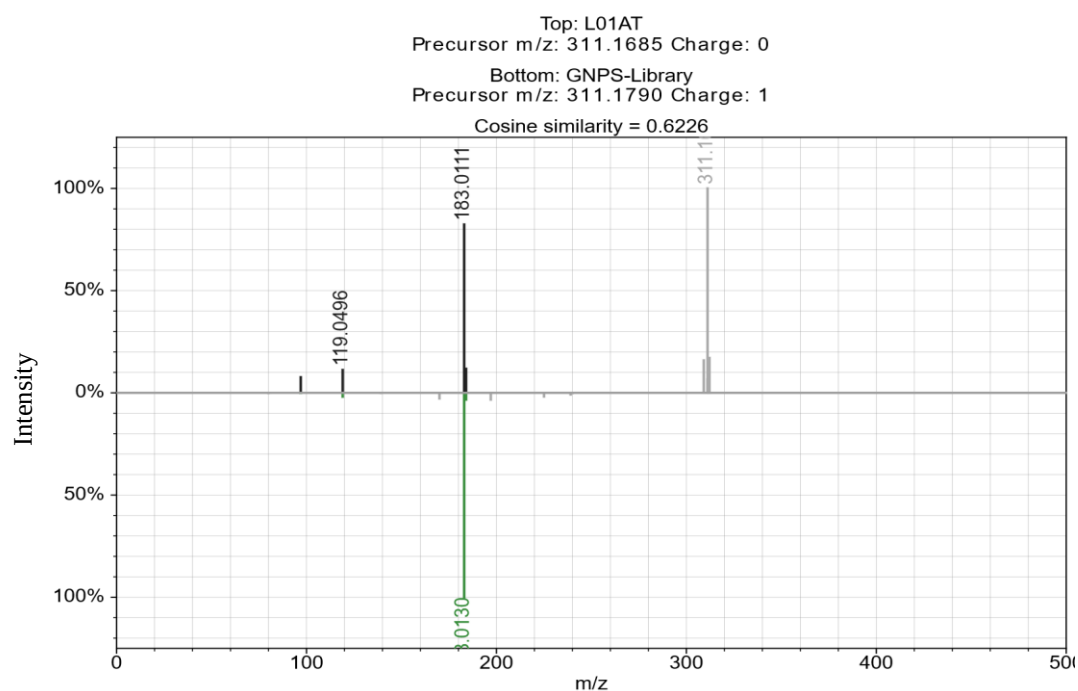


Figure S36. Mass spectrum of the compound canrenone. The upper panel corresponds to the experimental spectrum of sample L01AT, while the lower panel corresponds to the reference spectrum from the Global Natural Product Social Molecular Networking (GNPS) library. The comparison was performed by LC-MS/MS analysis.

