

Supplementary Information

Dereplication of Secondary Metabolites from *Isabelcristinia aromatica* (Linderniaceae) by Untargeted Tandem Mass Spectrometry-Based Molecular Networking

Jackson R. G. S. Almeida,*^a Eluiza M. N. Afonso,^a Elaine M. B. Nunes,^b José A. de Siqueira Filho,^b Gibson G. de Oliveira,^c Fausto Carnevale-Neto^d and Norberto P. Lopes^e

^a*Núcleo de Estudos e Pesquisas de Plantas Medicinais (NEPLAME), Universidade Federal do Vale do São Francisco, 56304-205 Petrolina-PE, Brazil*

^b*Centro de Referência para Recuperação de Áreas Degradadas da Caatinga, Universidade Federal do Vale do São Francisco, 56300-000 Petrolina-PE, Brazil*

^c*Centro Universitário FACOL, 56612-285 Vitória de Santo Antão-PE, Brazil*

^d*Northwest Metabolomics Research Center, Department of Anesthesiology and Pain Medicine, University of Washington, 850 Republican Street, Seattle, WA 98109, United States*

^e*Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, 14040-903 Ribeirão Preto-SP, Brazil*

This publication is part of the special issue “Omics Sciences”

*e-mail: jackson.guedes@univasf.edu.br

ORCIDs:

Jackson, R. G. da S. Almeida: <https://orcid.org/0000-0002-0867-1357>

Eluiza M. N. Afonso: <https://orcid.org/0009-0007-8028-2077>

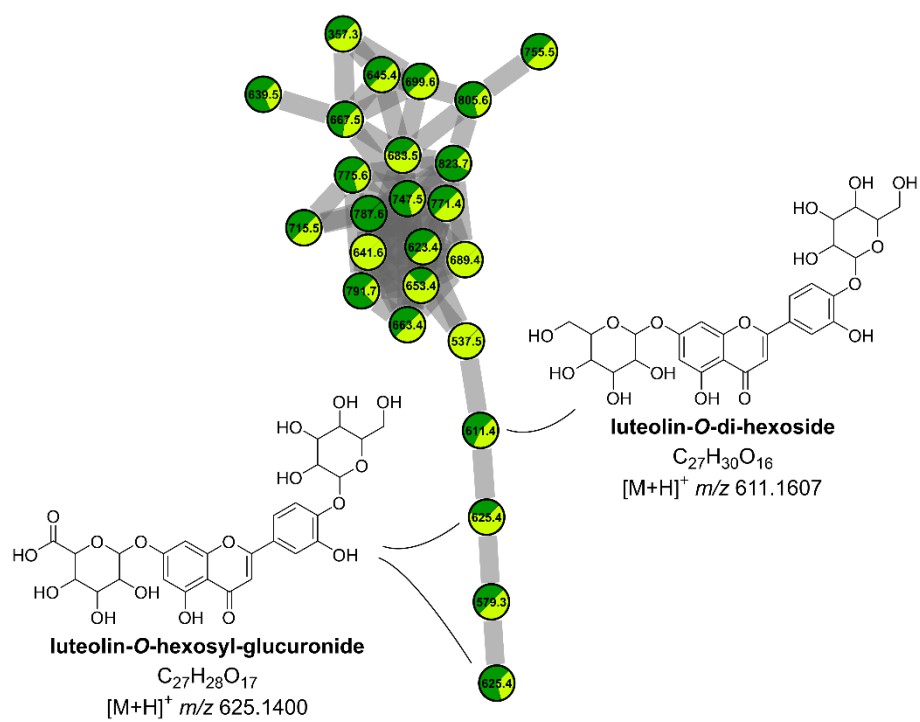
Elaine M. B. Nunes: <https://orcid.org/0000-0001-7064-4328>

José A. de Siqueira Filho: <https://orcid.org/0000-0002-8499-1424>

Gibson G. de Oliveira: <https://orcid.org/0000-0001-7784-9676>

Fausto C. Neto: <https://orcid.org/0000-0002-9364-933X>

Norberto P. Lopes: <https://orcid.org/0000-0002-8159-3658>



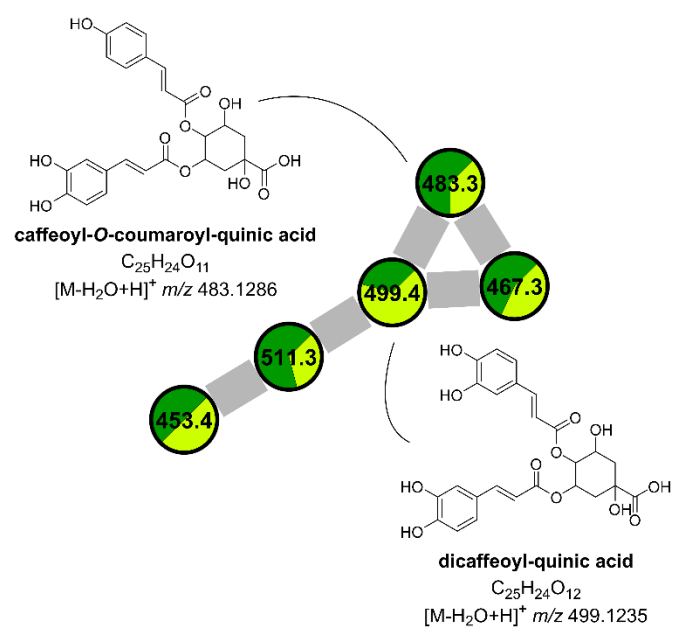


Figure S2. MN applied to LC-(+)-ESI-MS² data showing caffeoylquinic acid derivatives.

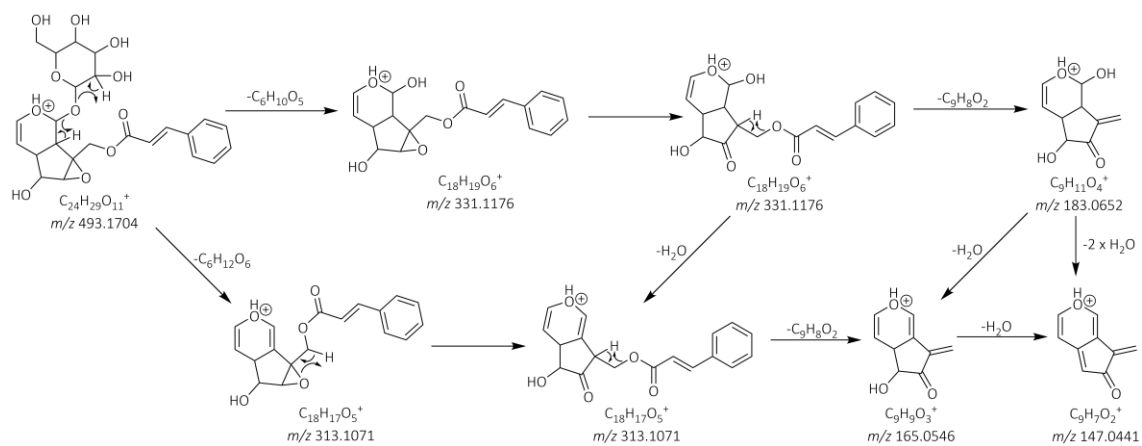


Figure S3. Main fragmentation of protonated globularin ($[M + H]^+$ m/z 493) indicating the neutral loss of hexose moiety followed by alpha-elimination of cynamoyl group and dehydration from the aglycone.

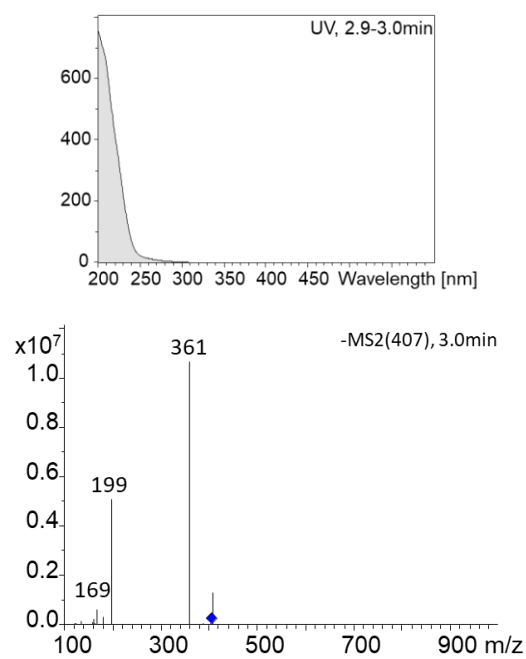


Figure S4. UV and (-)-ESI-MS² spectra of compound **1**.

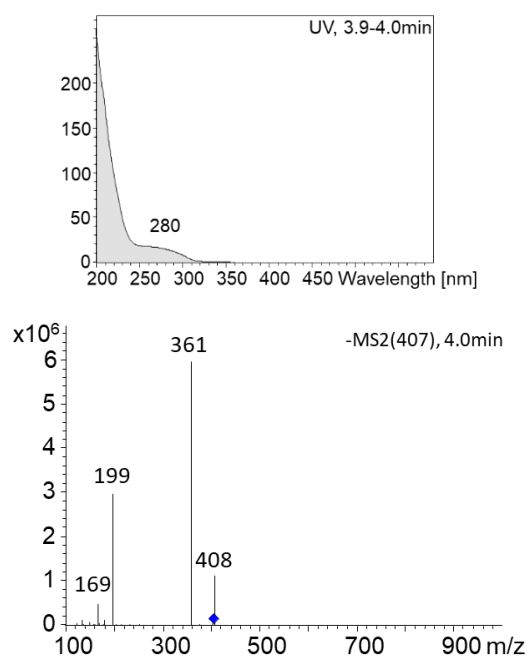


Figure S5. UV and (-)-ESI-MS² spectra of compound 2.

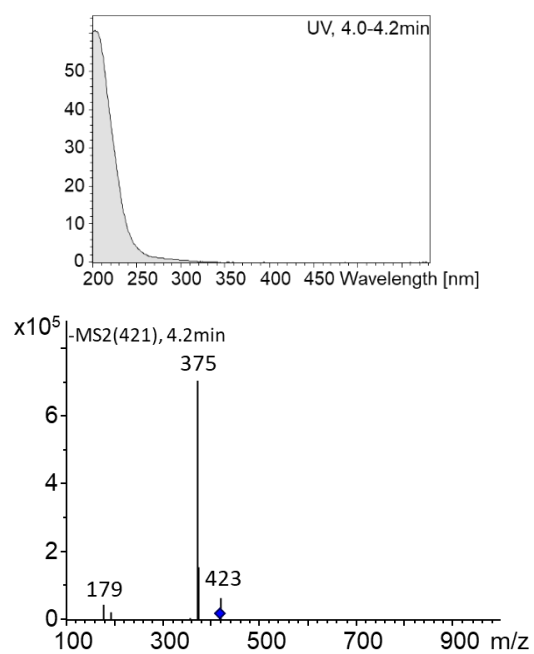


Figure S6. UV and (-)-ESI-MS² spectra of compound **3**.

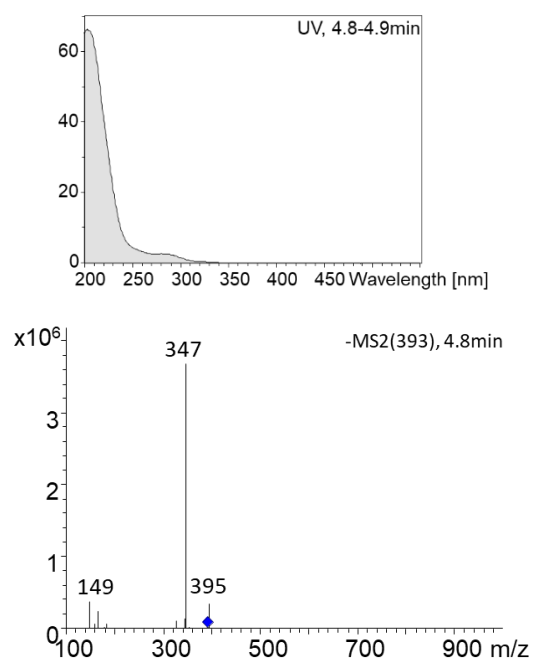


Figure S7. UV and (-)-ESI-MS² spectra of compound 4.

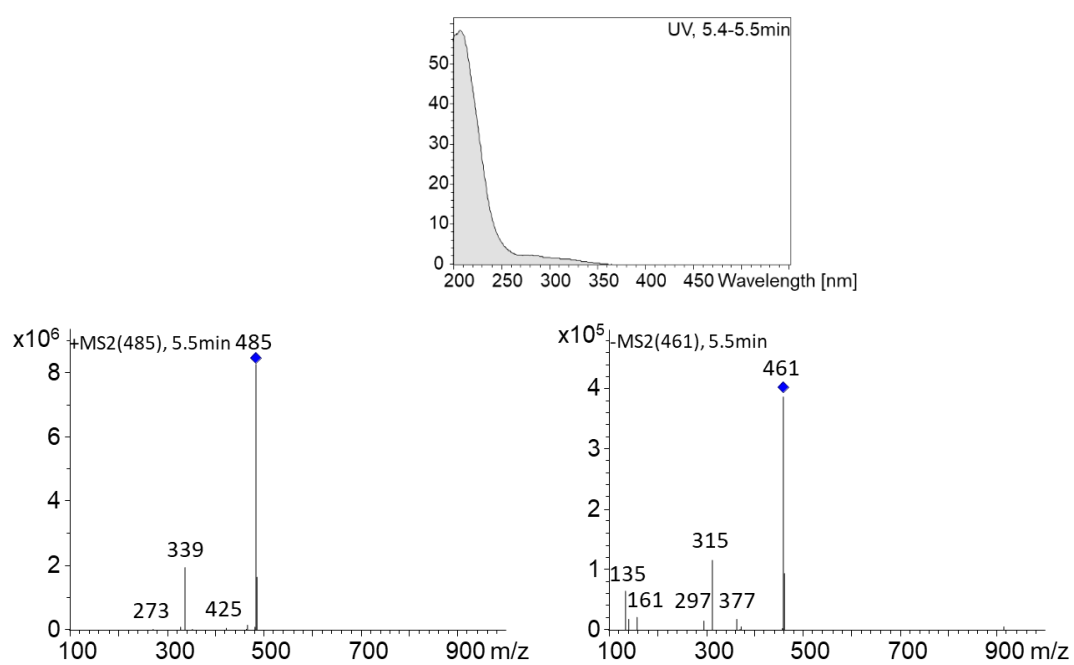


Figure S8. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound 5.

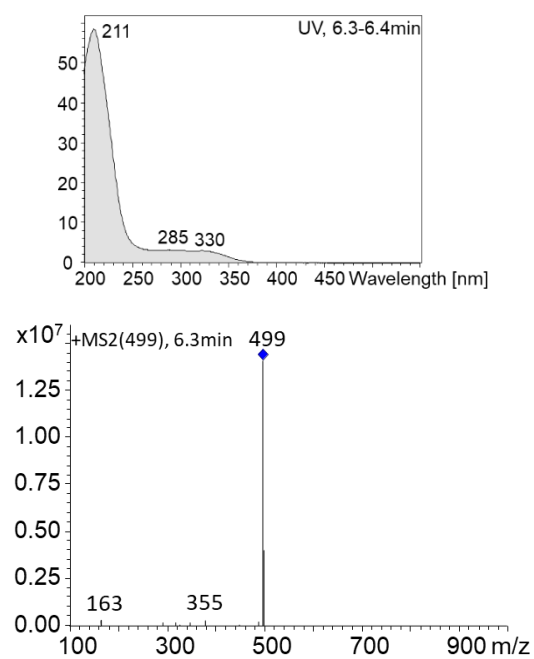


Figure S9. UV and (+)-ESI-MS² spectra of compound **6**.

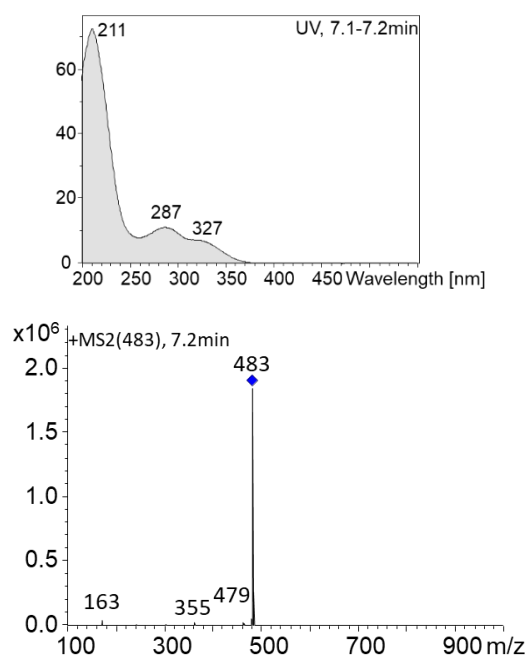


Figure S10. UV and (+)-ESI-MS² spectra of compound 7.

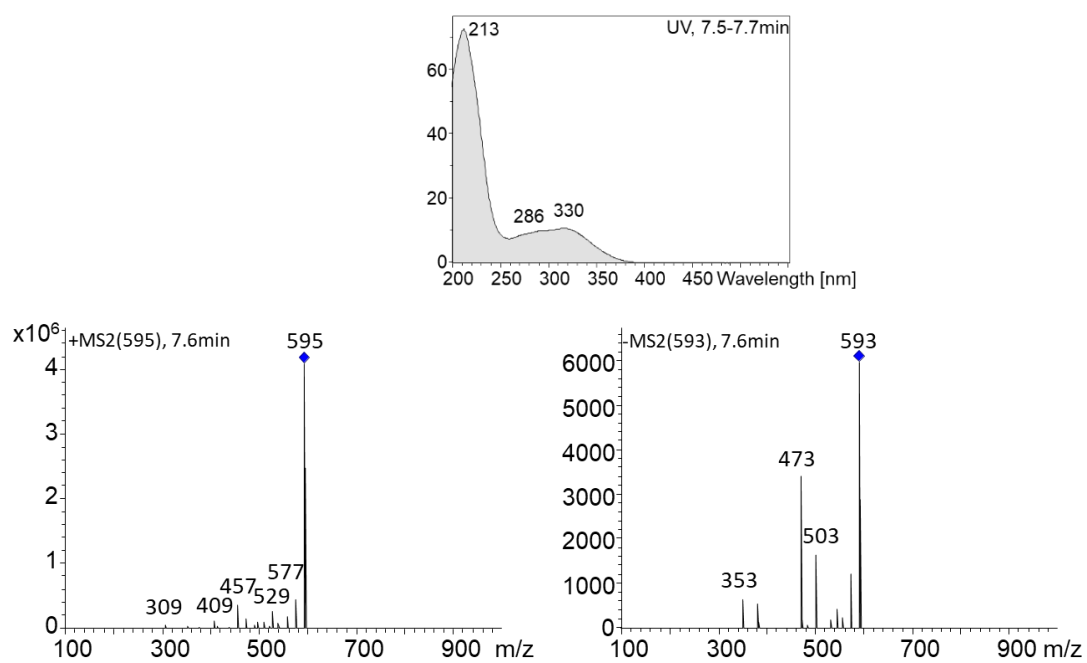


Figure S11. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound 8.

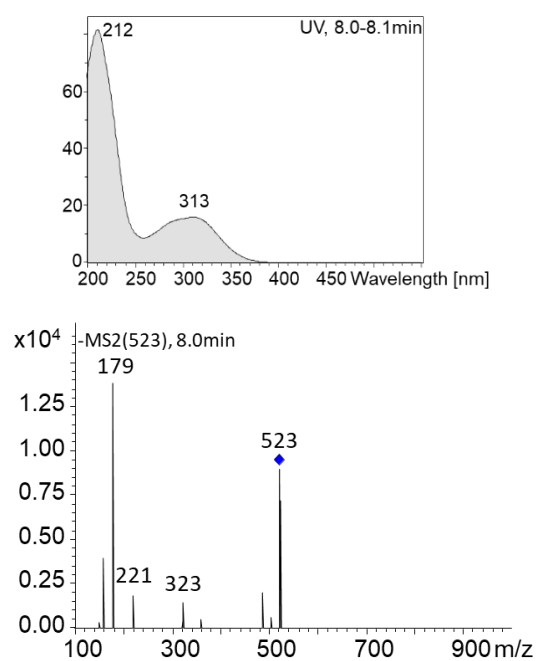


Figure S12. UV and (–)-ESI-MS² spectra of compound **9**.

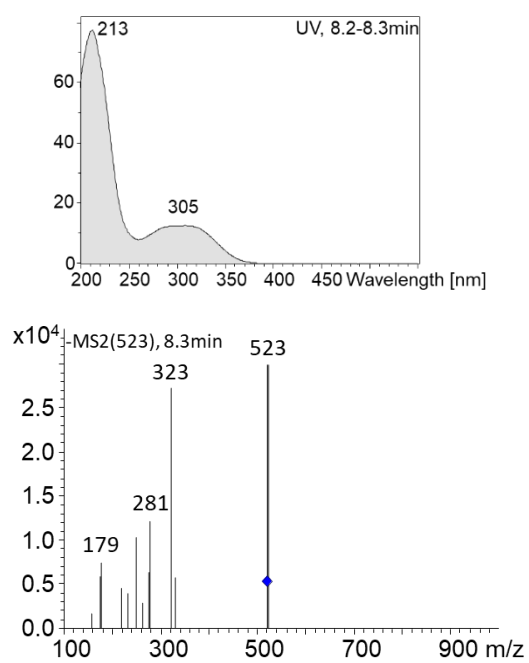


Figure S13. UV and (–)-ESI-MS² spectra of compound **10**.

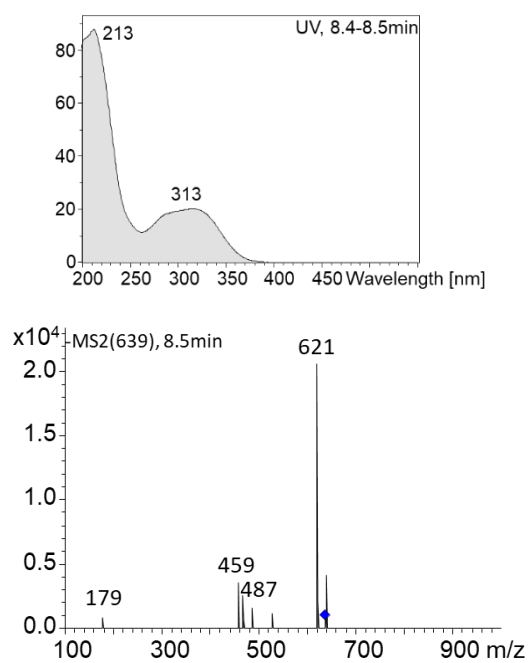


Figure S14. UV and (-)-ESI-MS² spectra of compound **11**.

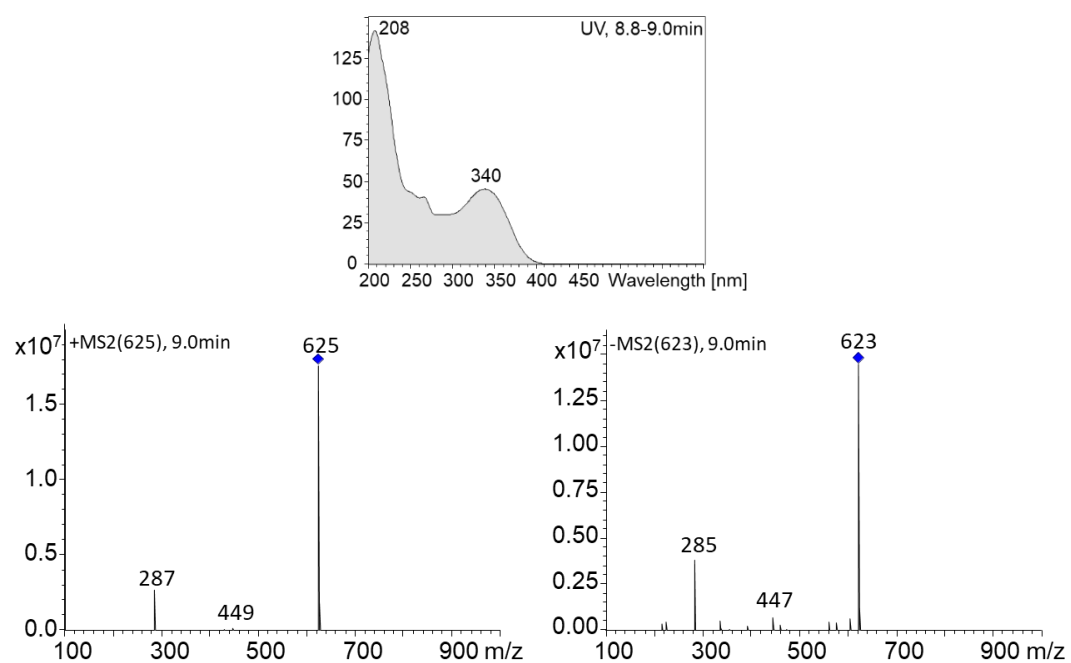


Figure S15. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound **12**.

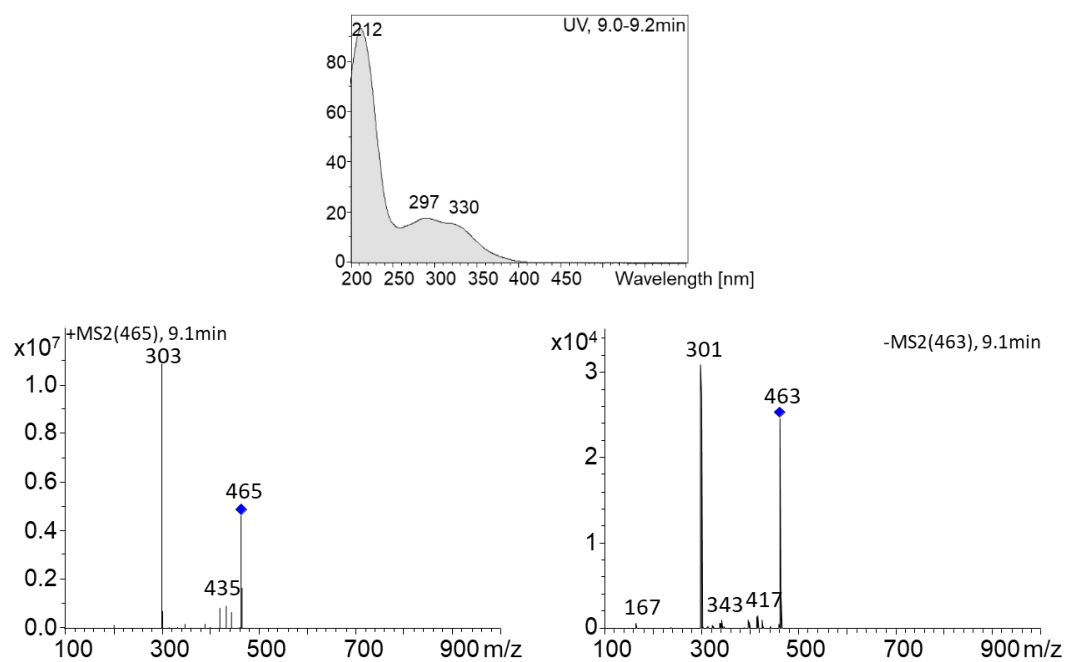


Figure S16. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound **13**.

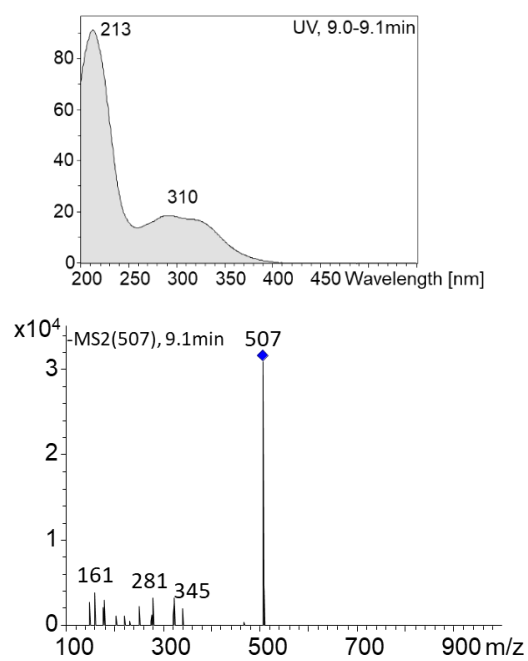


Figure S17. UV and (–)-ESI-MS² spectra of compound **14**.

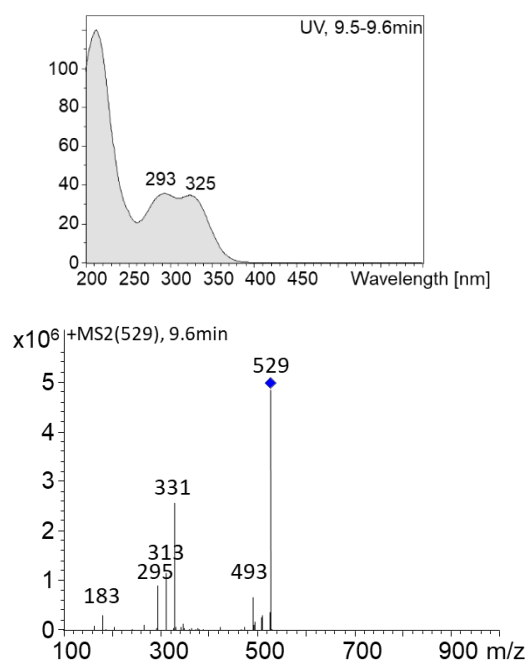


Figure S18. UV and (+)-ESI-MS² spectra of compound **15**.

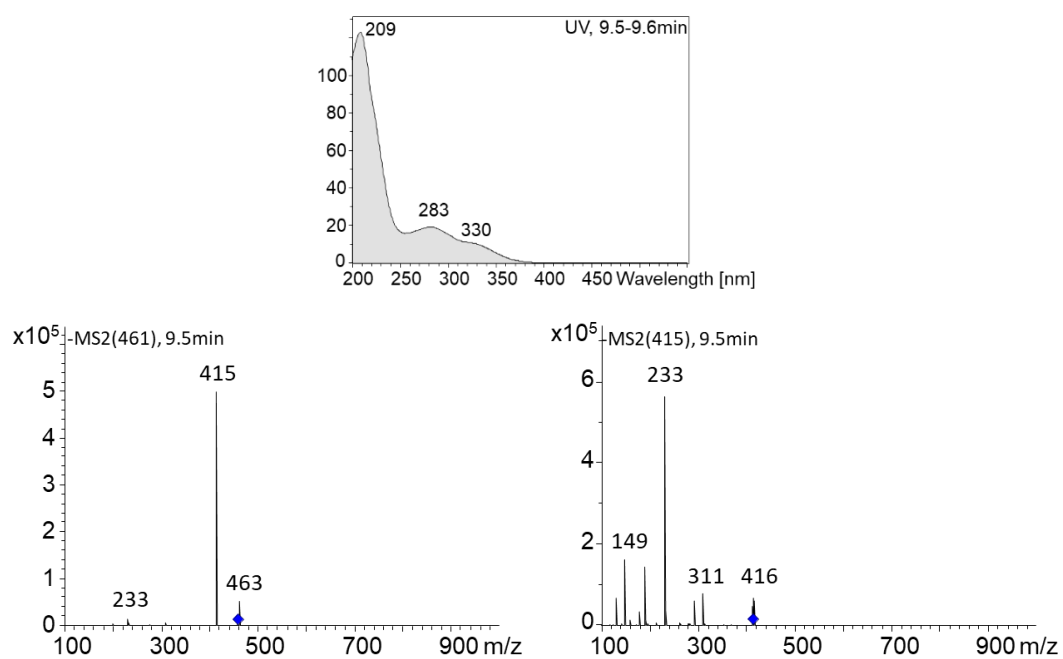


Figure S19. UV and (–)-ESI-MS² spectra of compound **16**.

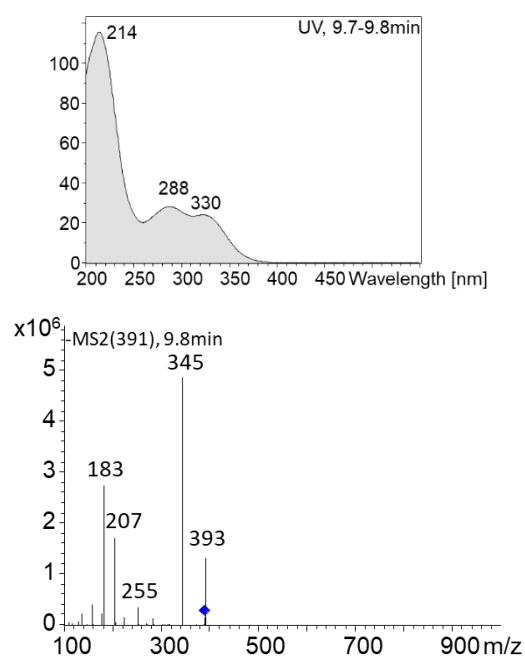


Figure S20. UV and (–)-ESI-MS² spectra of compound **17**.

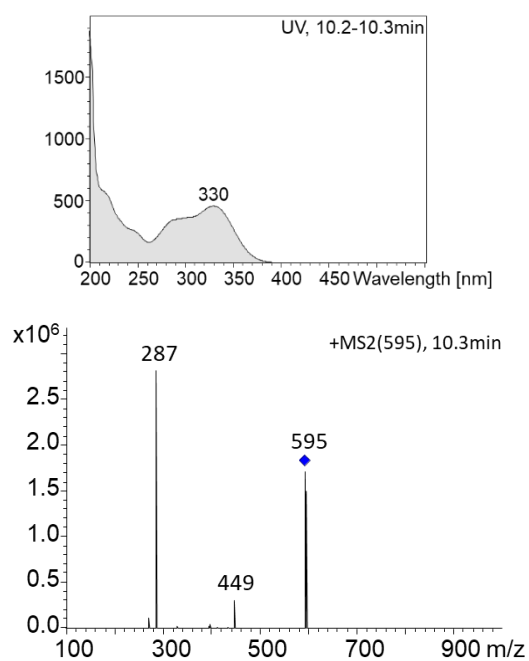


Figure S21. UV and (+)-ESI-MS² spectra of compound **18**.

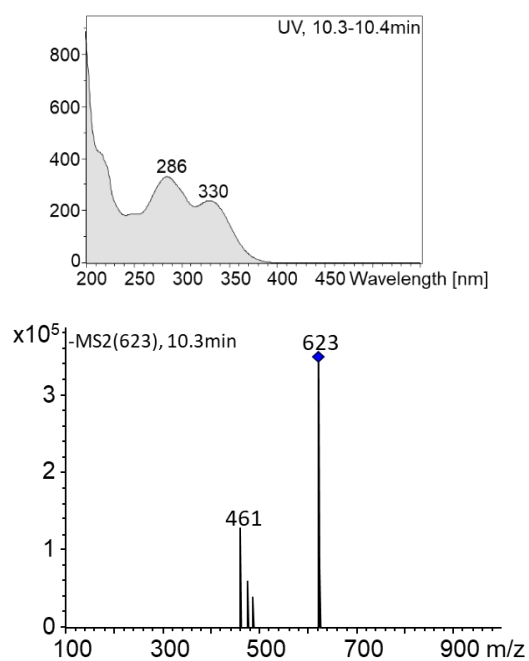


Figure S22. UV and (–)-ESI-MS² spectra of compound **19**.

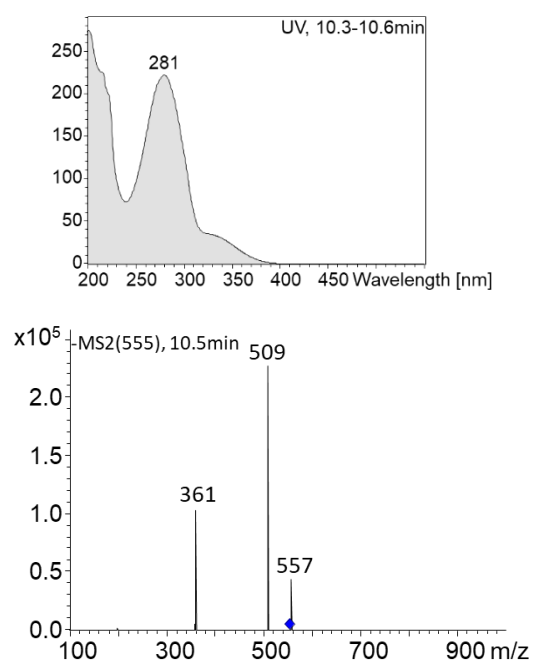


Figure S23. UV and (-)-ESI-MS² spectra of compound **20**.

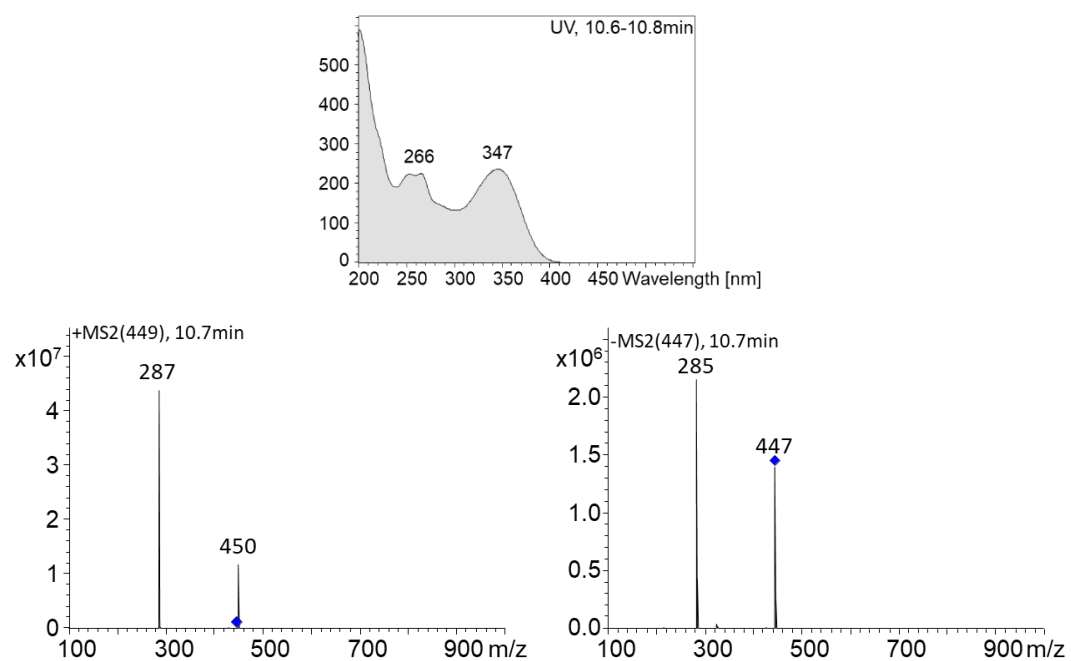


Figure S24. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound 21.

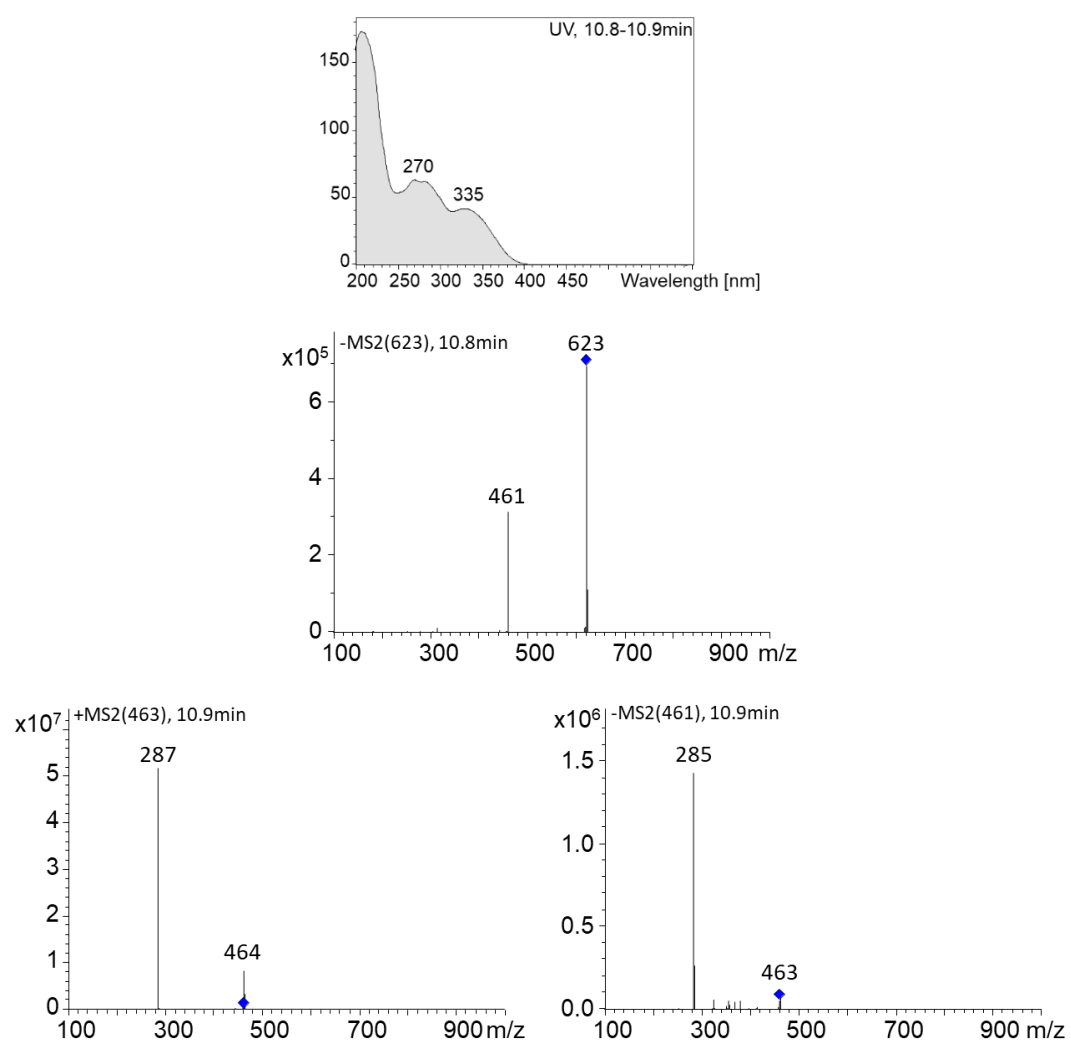


Figure S25. UV, (+)-ESI, and (–)-ESI-MS² spectra of compound **22**.

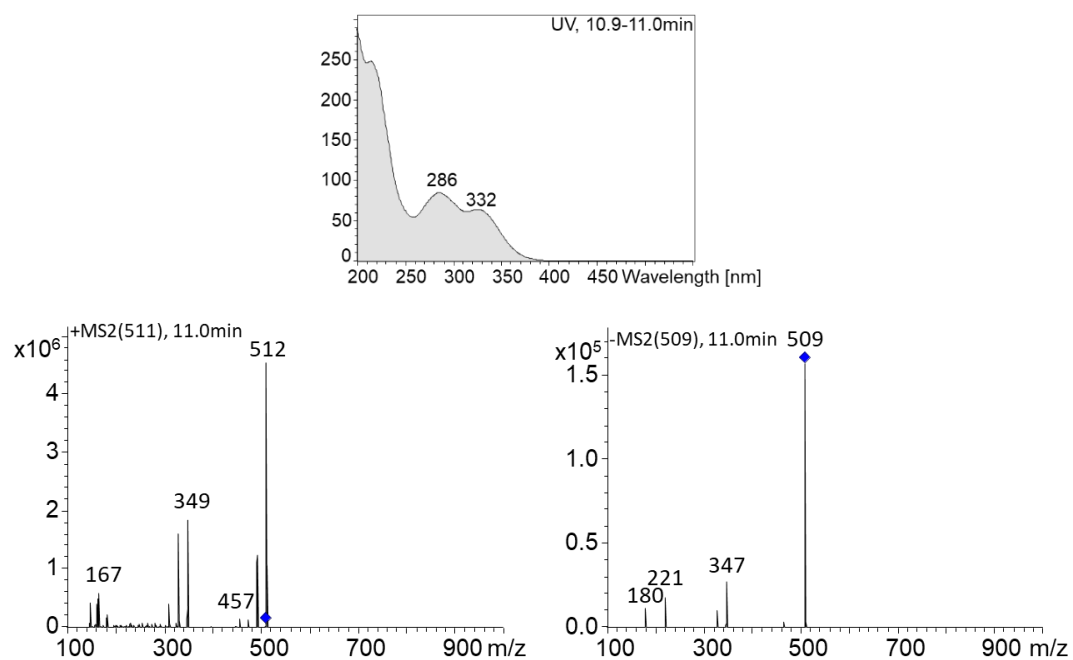


Figure S26. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound 23.

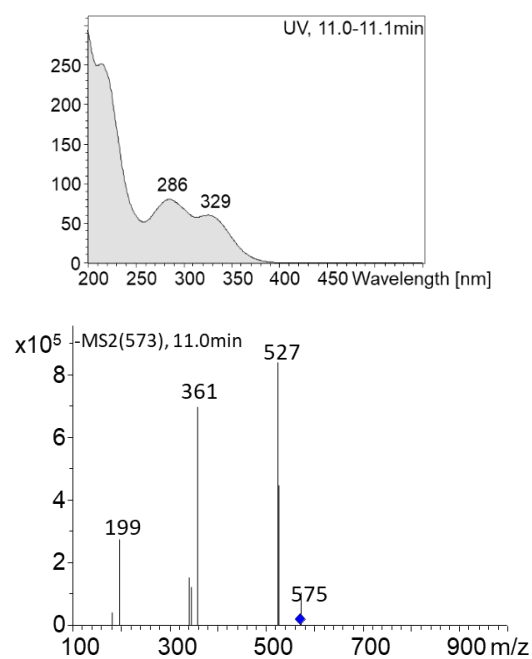


Figure S27. UV and (–)-ESI-MS² spectra of compound **24**.

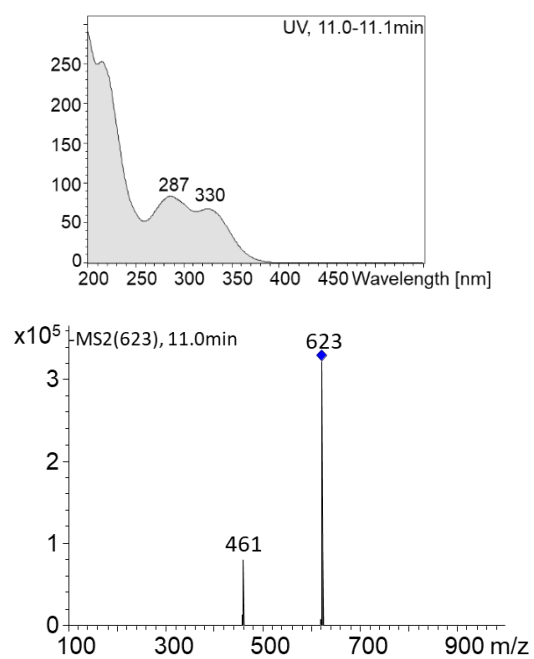


Figure S28. UV and (–)-ESI-MS² spectra of compound 25.

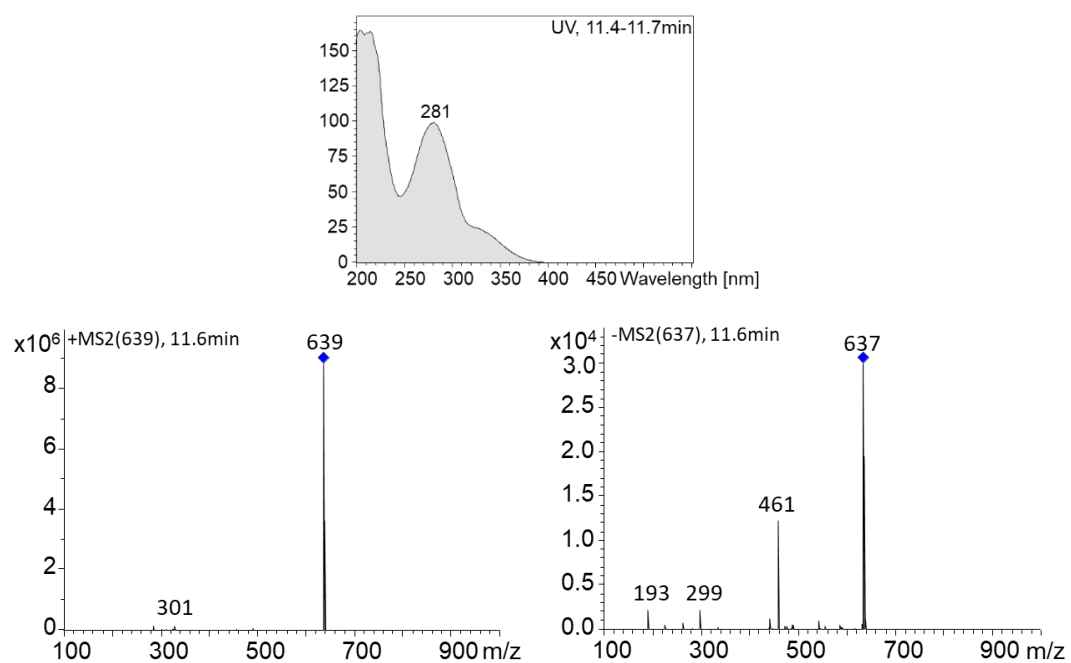


Figure S29. UV, (+)-ESI, and (–)-ESI-MS² spectra of compound 26.

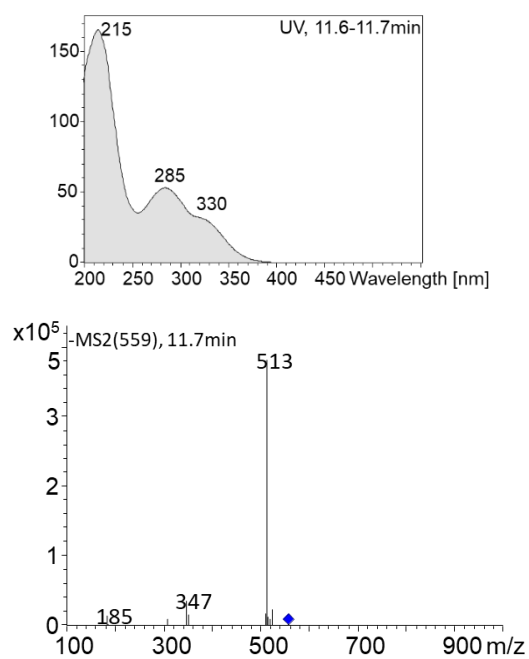


Figure S30. UV and (–)-ESI-MS² spectra of compound 27.

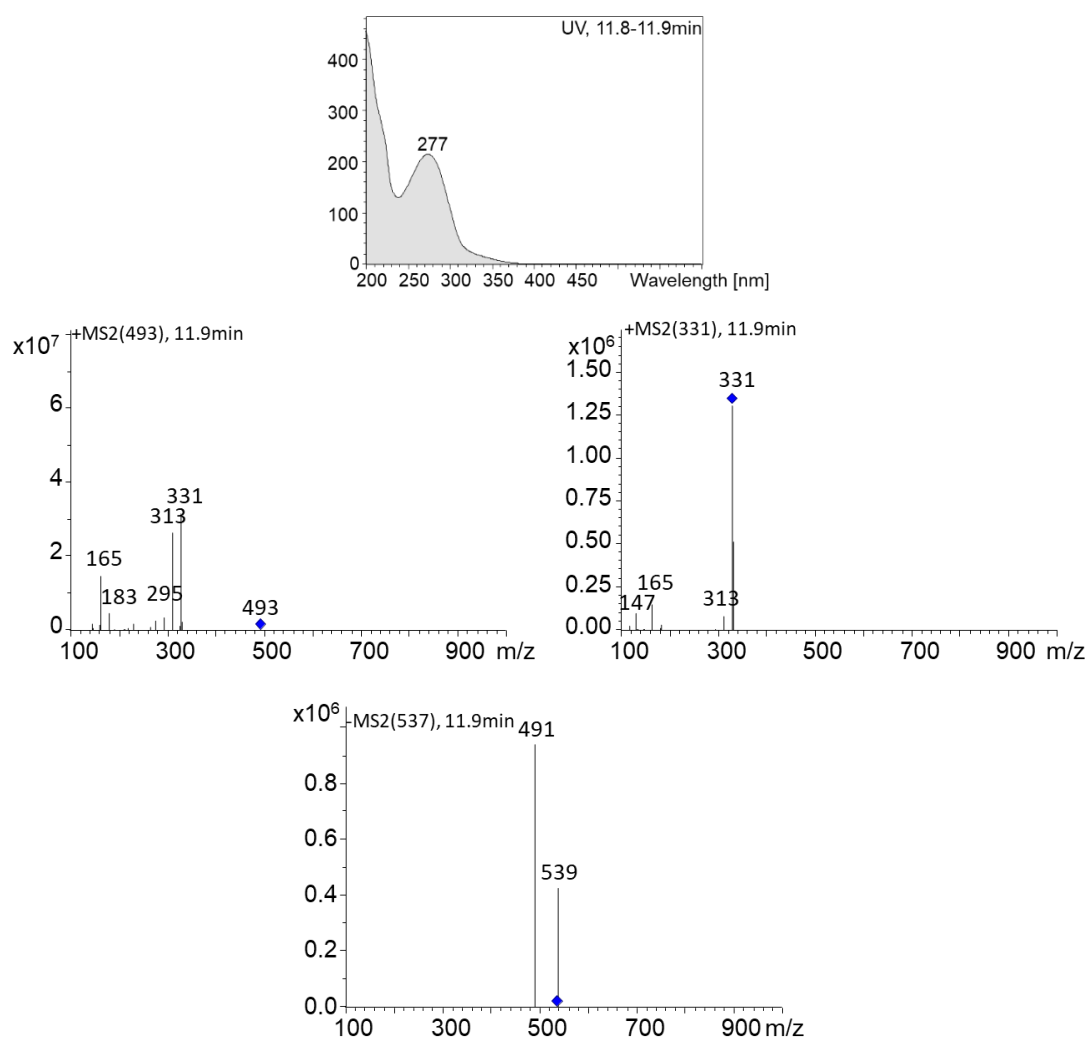


Figure S31. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound **28**.

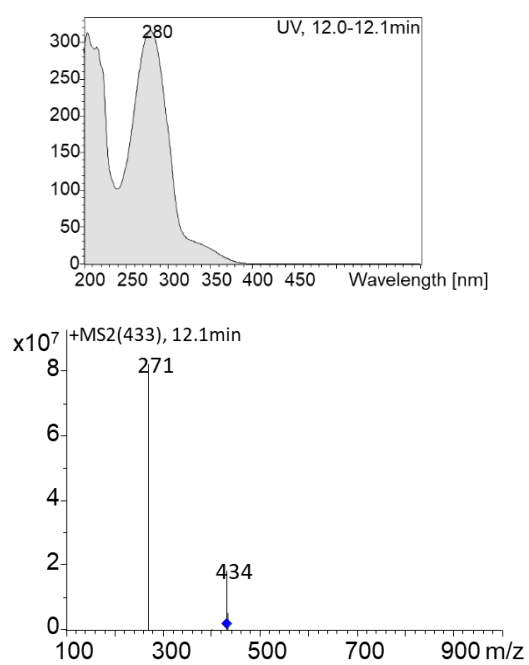


Figure S32. UV and (+)-ESI-MS² spectra of compound **29**.

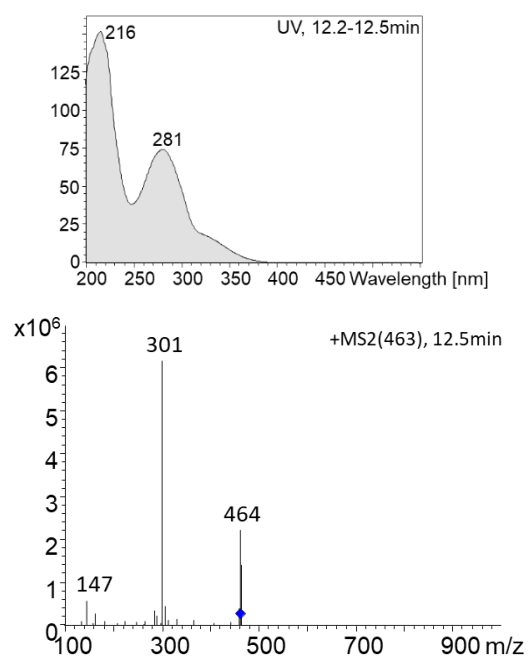


Figure S33. UV and (+)-ESI-MS² spectra of compound **30**.

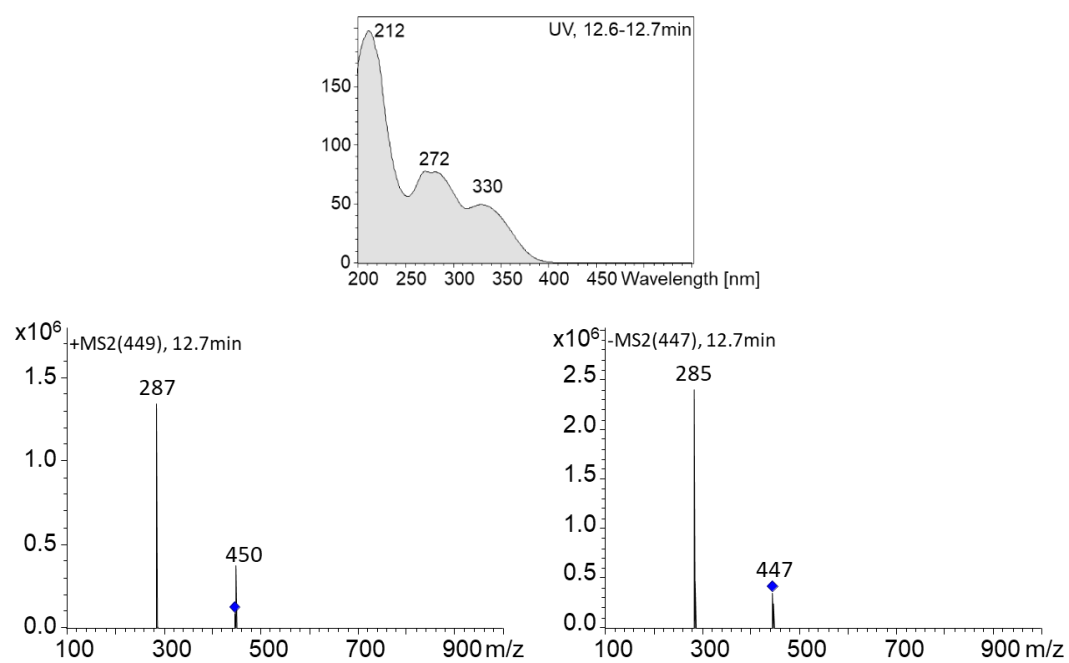


Figure S34. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound **31**.

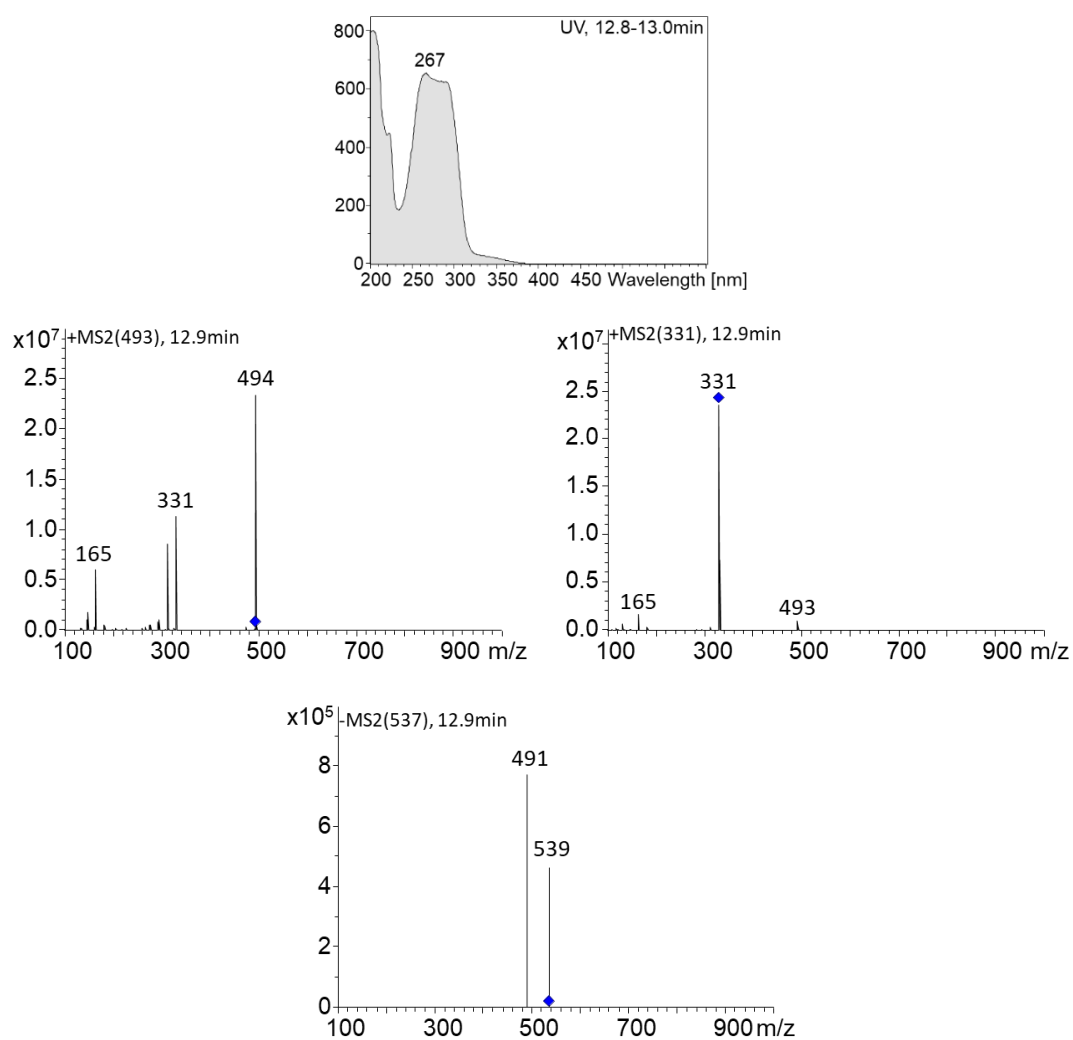


Figure S35. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound **32**.

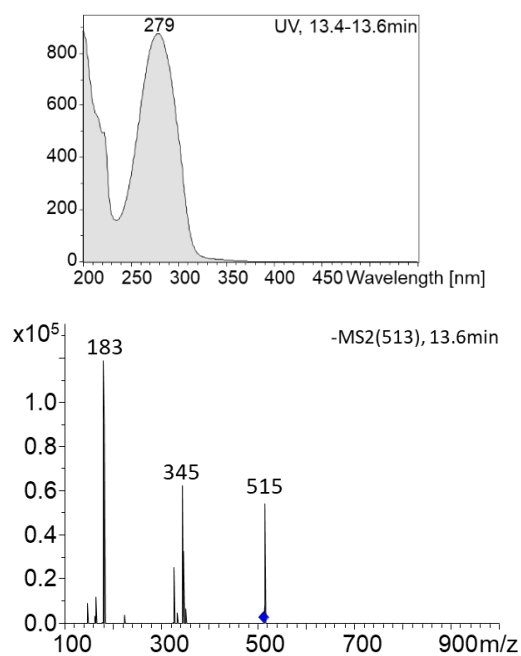


Figure S36. UV and (-)-ESI-MS² spectra of compound **33**.

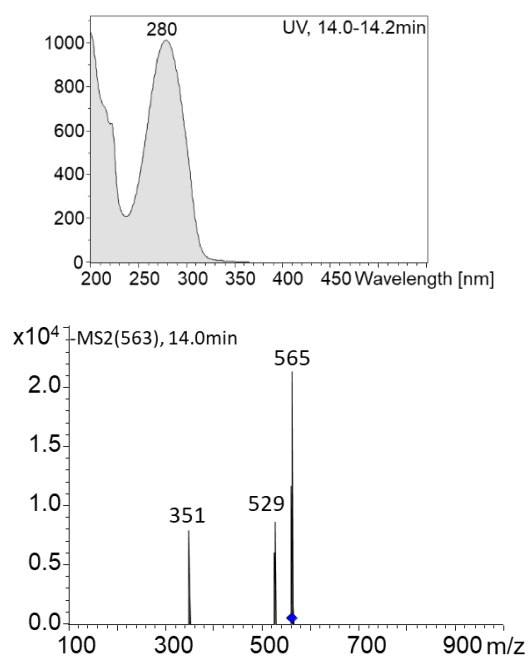


Figure S37. UV and (-)-ESI-MS² spectra of compound **34**.

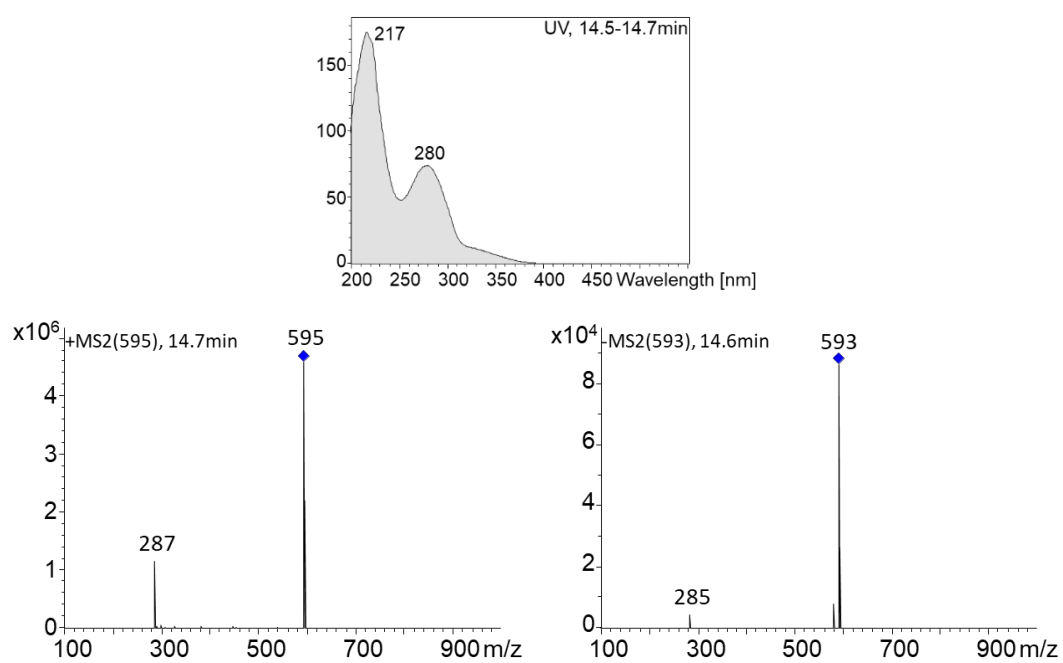


Figure S38. UV, (+)-ESI, and (-)-ESI-MS² spectra of compound **35**.

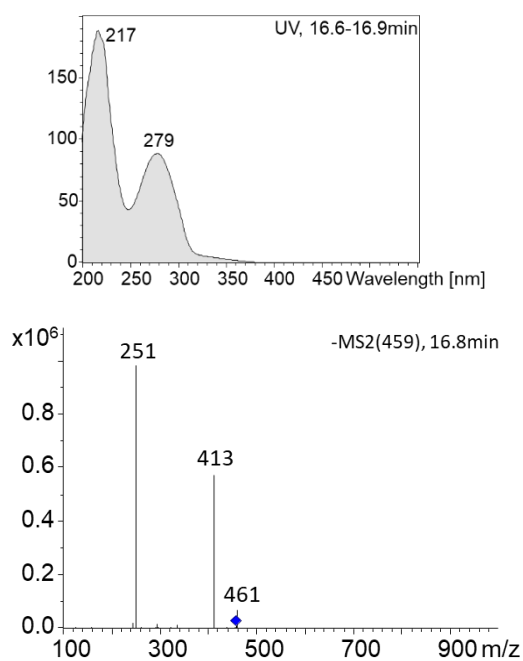


Figure S39. UV and (–)-ESI-MS² spectra of compound **36**.

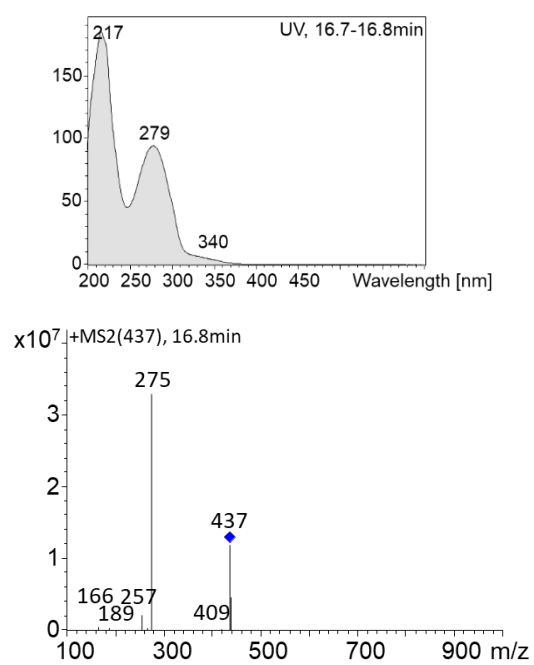


Figure S40. UV and (+)-ESI-MS² spectra of compound 37.

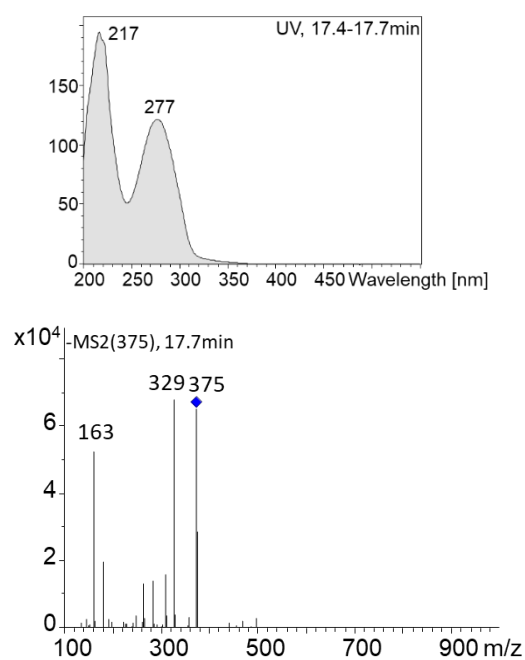


Figure S41. UV and (–)-ESI-MS² spectra of compound **38**.