

Integrative Approach Based on HPLC-DAD-MS/MS and NMR for Determination of Ellagic Derivatives from *Bertholletia excelsa* Bark Biomass Residues

Felipe M. A. da Silva, ^{a,b} Anna C. S. Hanna, ^a Abraão A. de Souza, ^{a,c} Francinaldo A. da Silva Filho, ^b Olinda M. F. Canhoto, ^a Alvicler Magalhães, ^a Paulo J. C. Benevides, ^a Mariangela B. M. de Azevedo, ^a Antonio C. Siani, ^{a,d} Adrian M. Pohlit, ^{a,c} Afonso D. L. de Souza ^b and Hector H. F. Koolen ^{*,a,e}

^aCentro de Biotecnologia da Amazônia, 69075-351 Manaus-AM, Brazil

^bDepartamento de Química, Universidade Federal do Amazonas, 69077-000 Manaus-AM, Brazil

^cDepartamento de Tecnologia e Inovação, Instituto Nacional de Pesquisas da Amazônia, 69067-375 Manaus-AM, Brazil

^dInstituto de Tecnologia em Fármacos, Fundação Oswaldo Cruz, 21040-900 Rio de Janeiro-RJ, Brazil

^eGrupo de Pesquisas em Metabolômica e Espectrometria de Massas, Universidade do Estado do Amazonas, 69050-010 Manaus-AM, Brazil

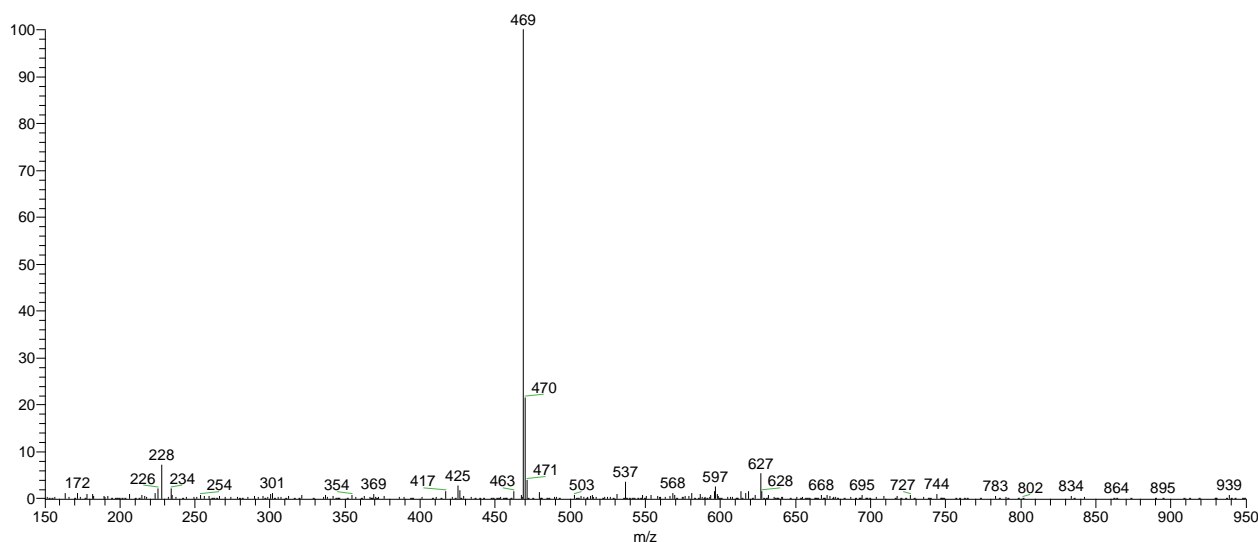


Figure S1. Mass spectrum of the compound **1**.

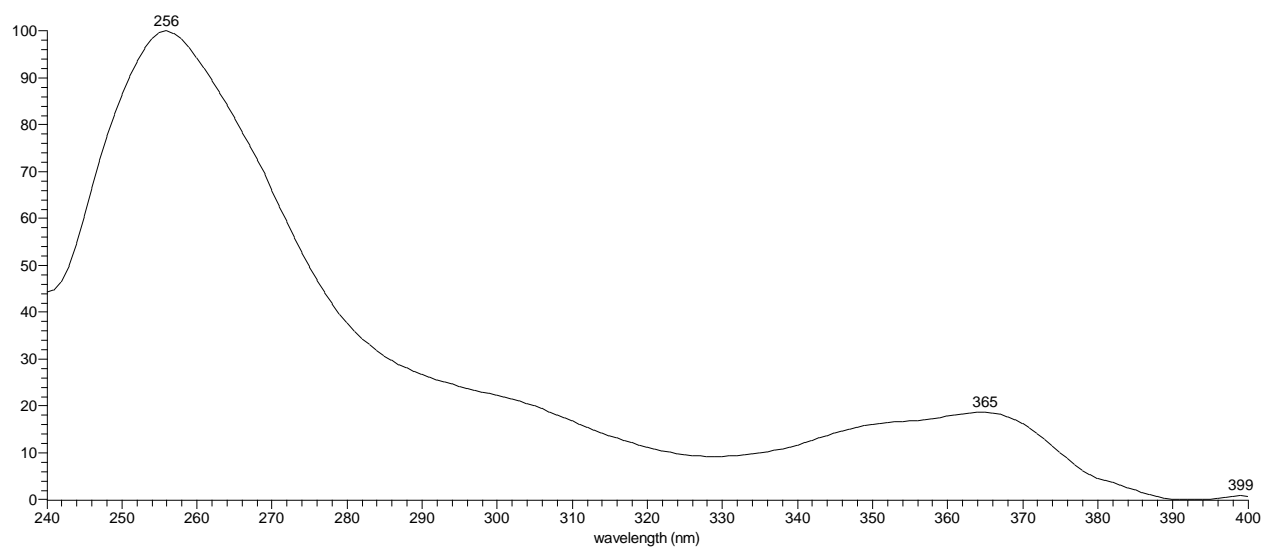


Figure S2. DAD spectra of the compound **1**.

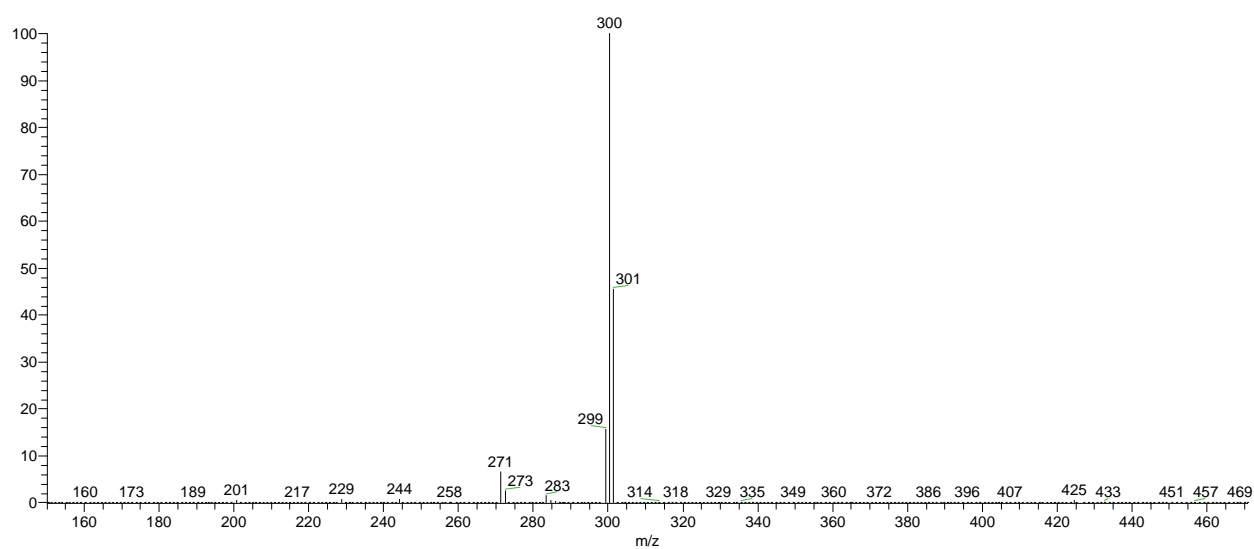


Figure S3. MS^2 spectrum of the ion at m/z 469 (compound **1**).

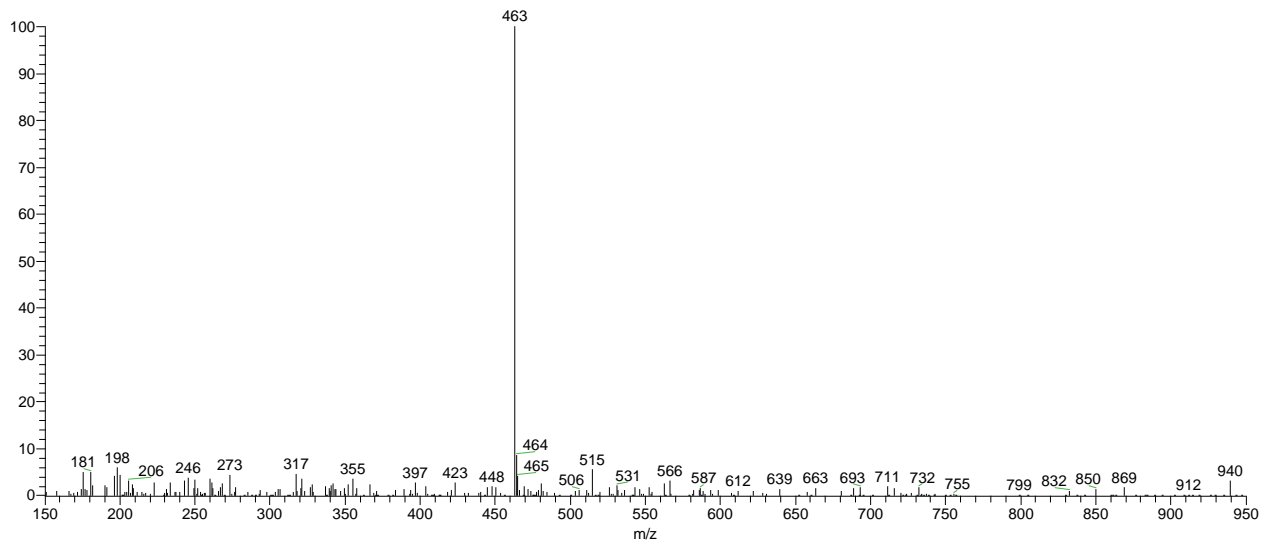


Figure S4. Mass spectrum of the compound **2**.

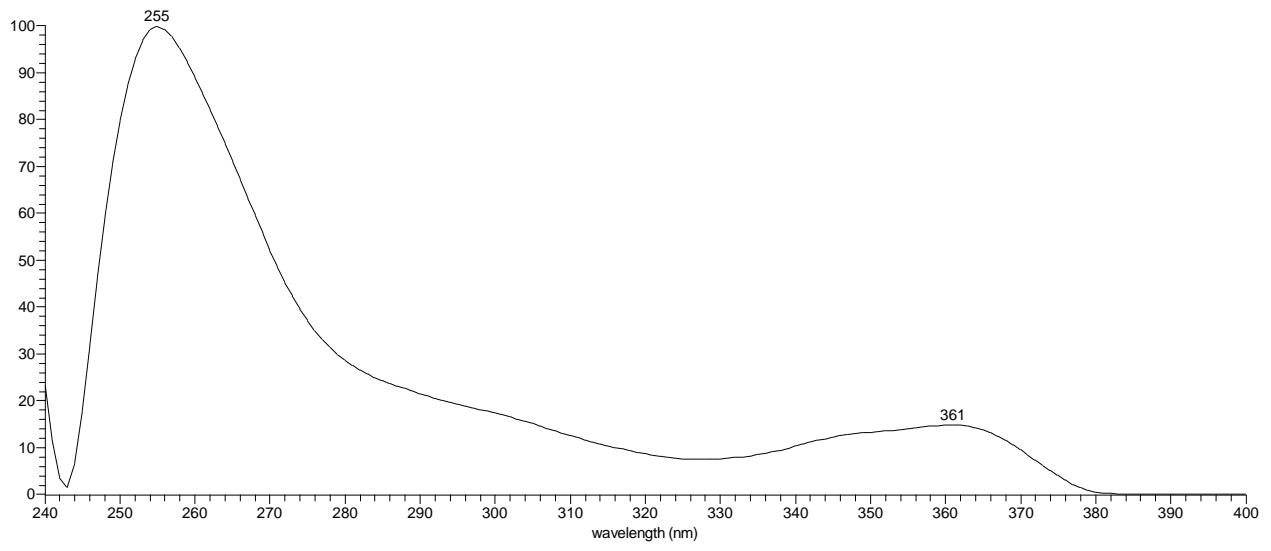


Figure S5. DAD spectra of the compound **2**.

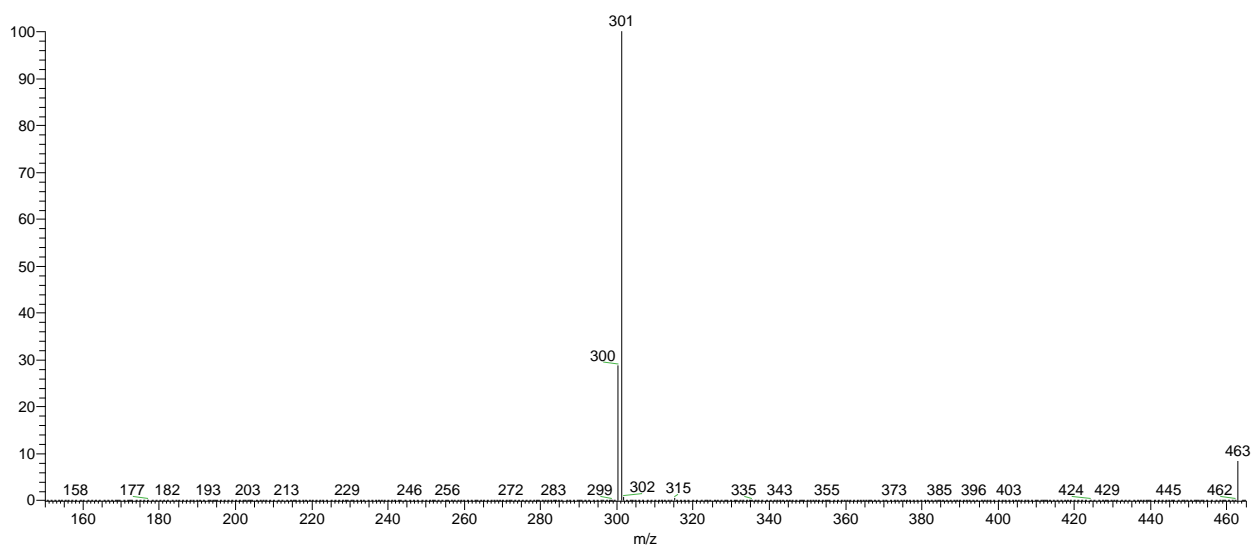


Figure S6. MS² spectrum of the ion at m/z 463 (compound 2).

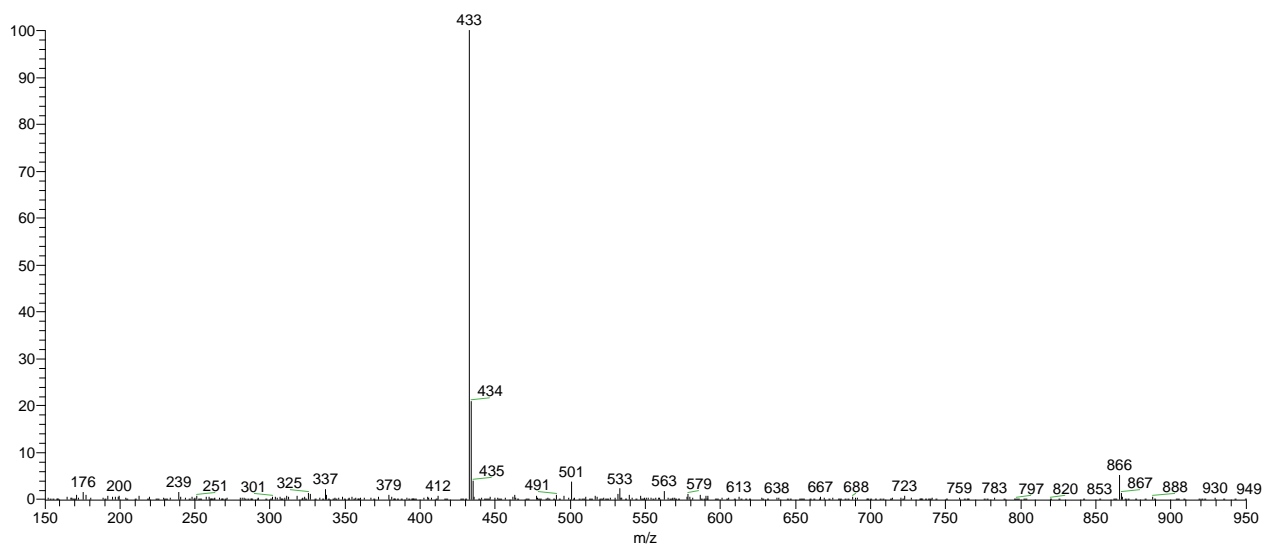


Figure S7. Mass spectrum of the compound 3.

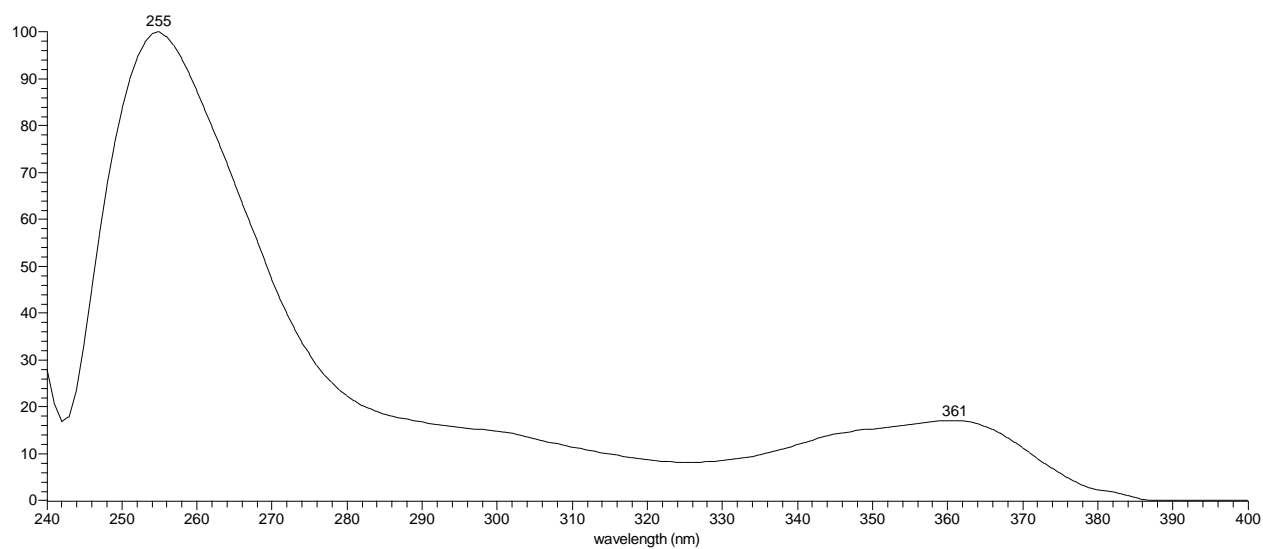


Figure S8. DAD spectra of the compound **3**.

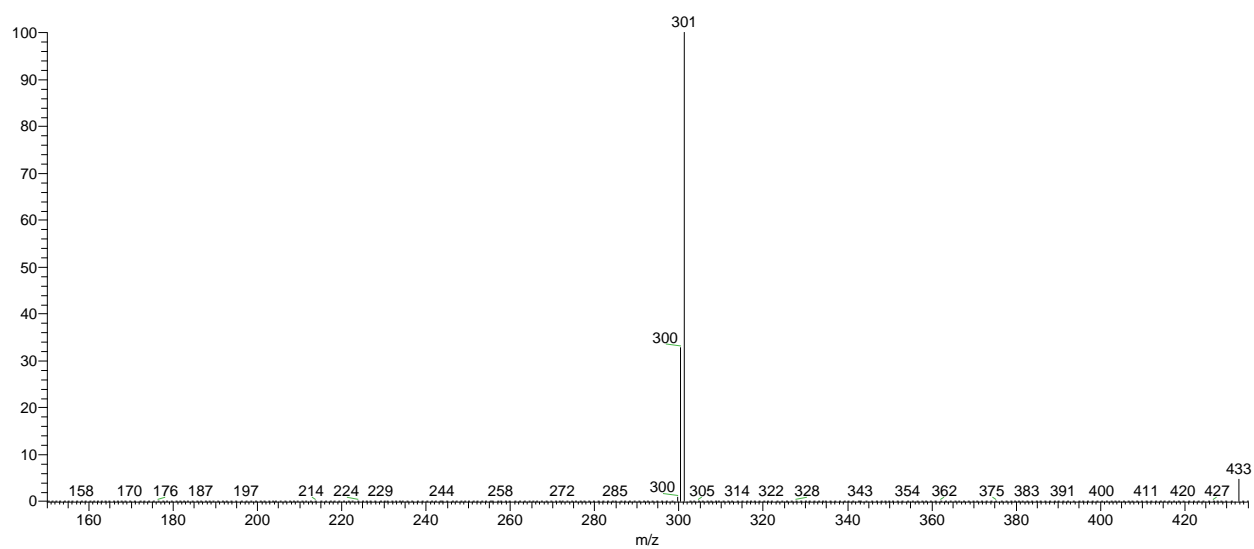


Figure S9. MS^2 spectrum of the ion at m/z 433 (compound **3**).

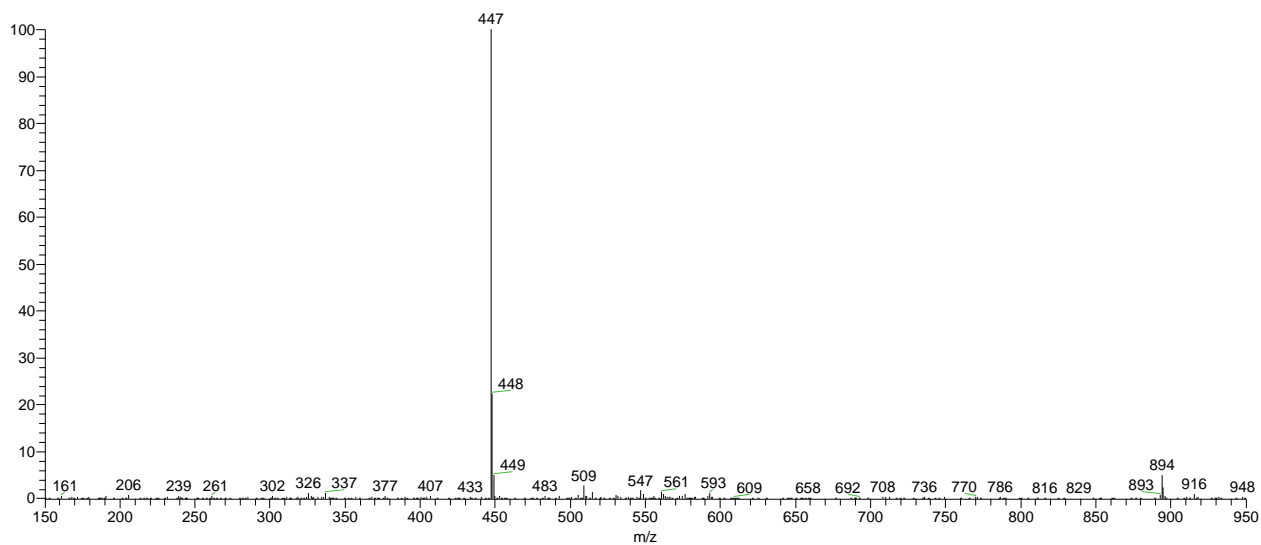


Figure S10. Mass spectrum of the compound **4**.

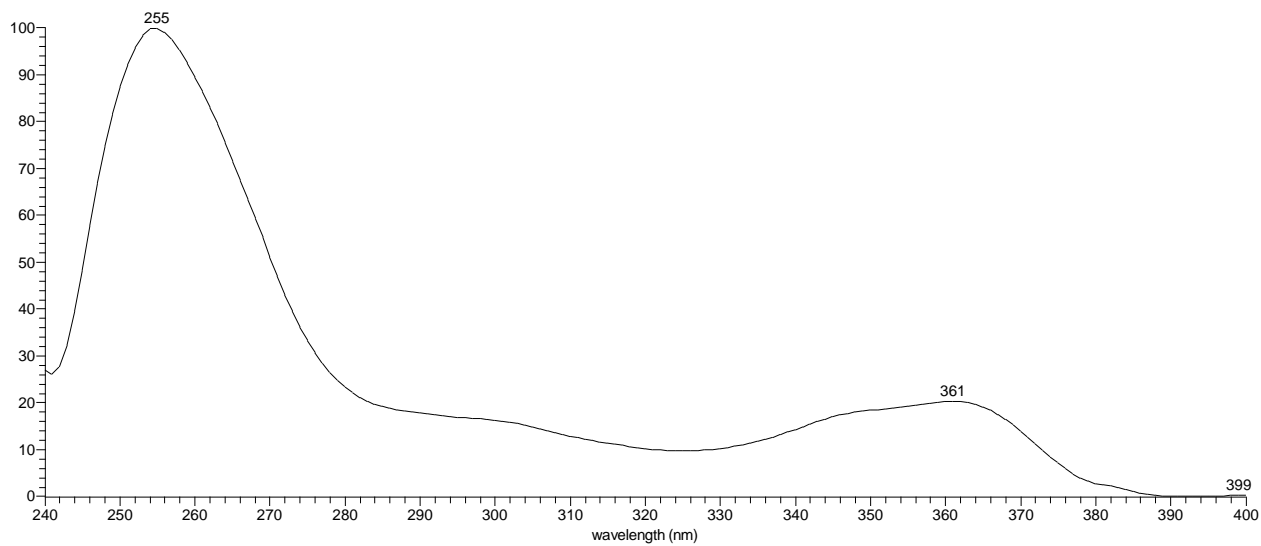


Figure S11. DAD spectra of the compound **4**.

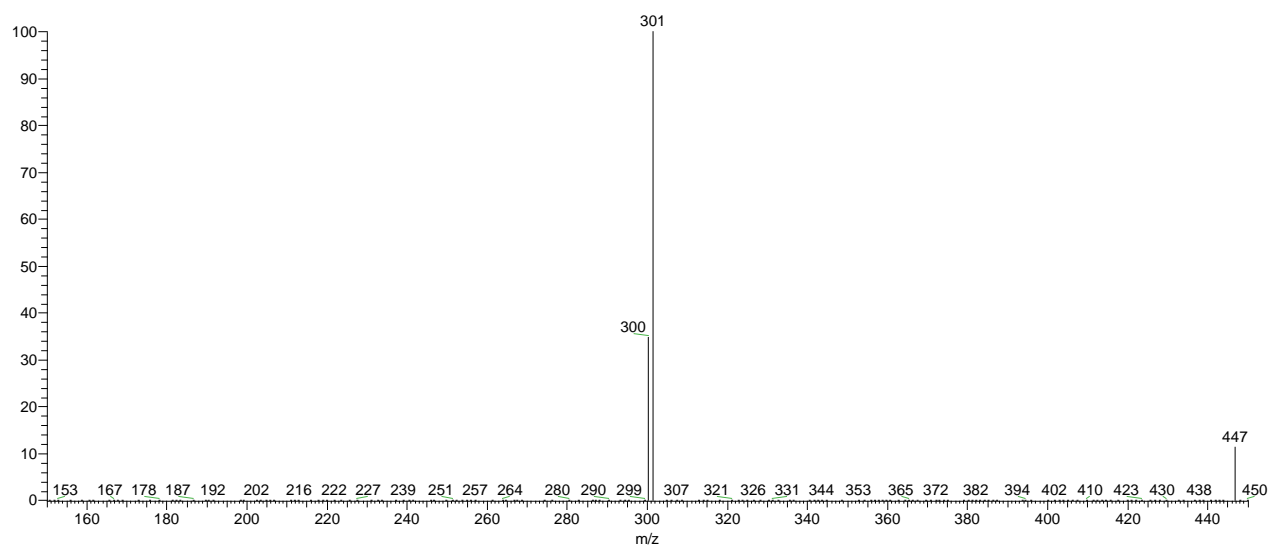


Figure S12. MS² spectrum of the ion at m/z 447 (compound 4).

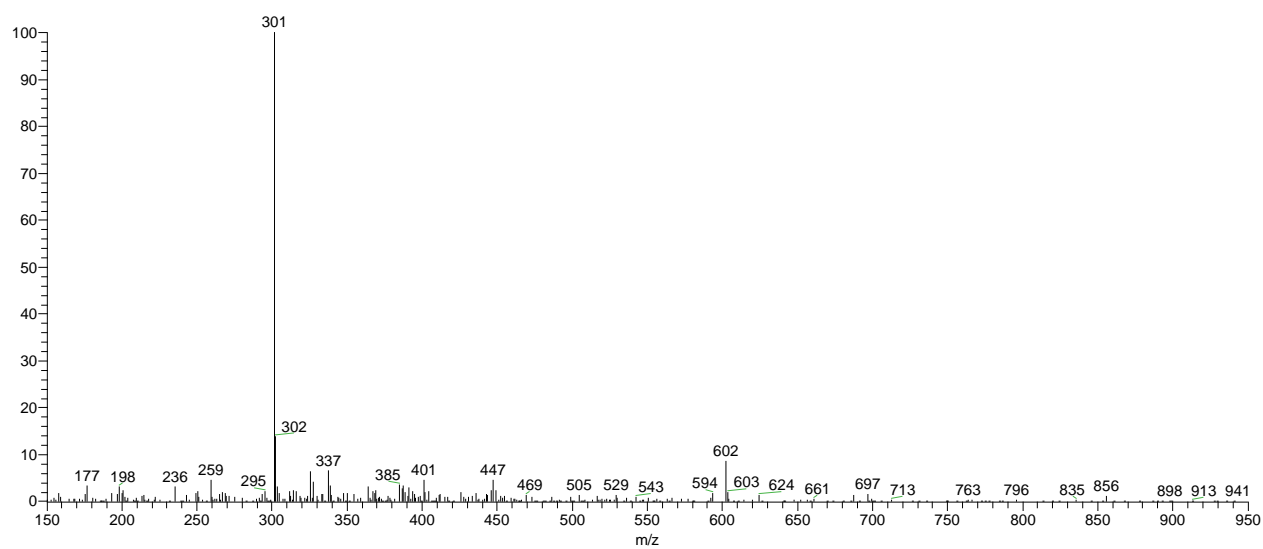


Figure S13. Mass spectrum of the compound 5.

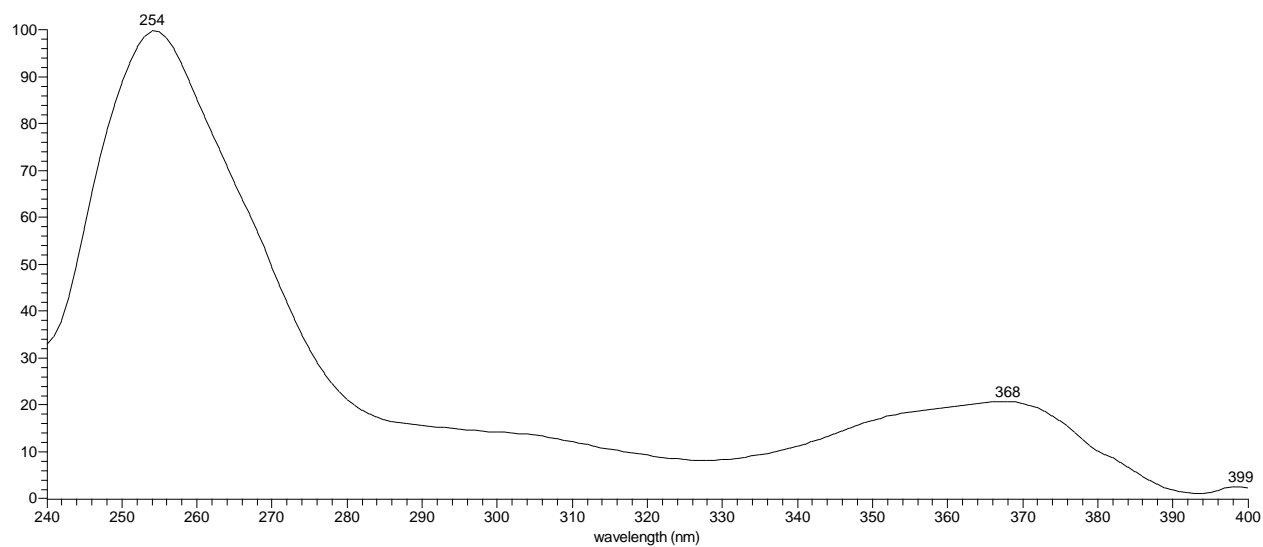


Figure S14. DAD spectra of the compound **5**.

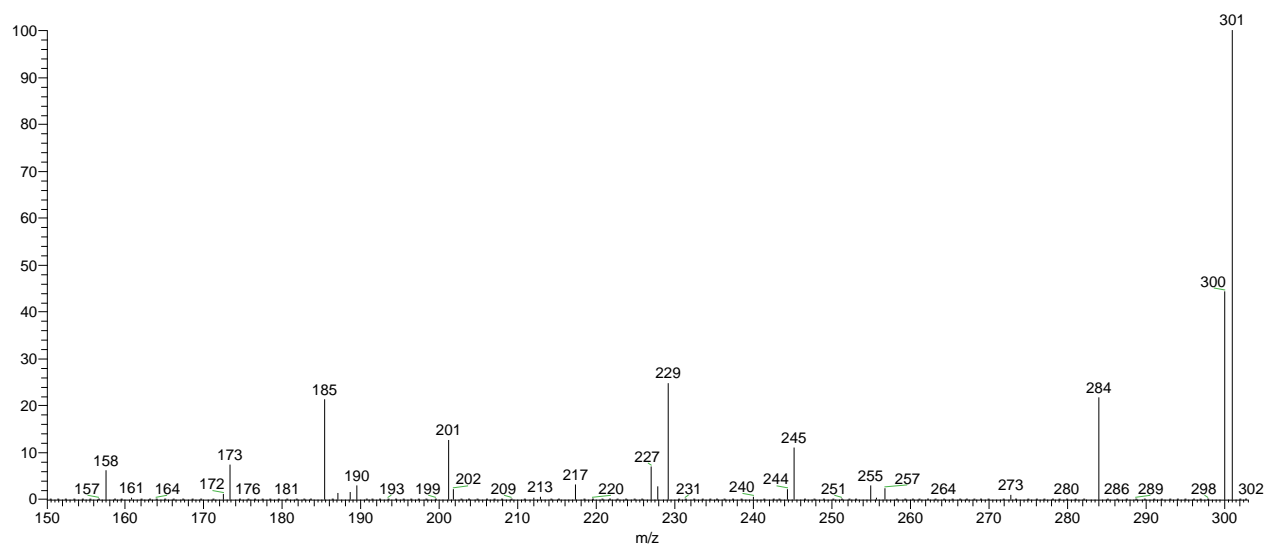


Figure S15. MS^2 spectrum of the ion at m/z 301 (compound **5**).

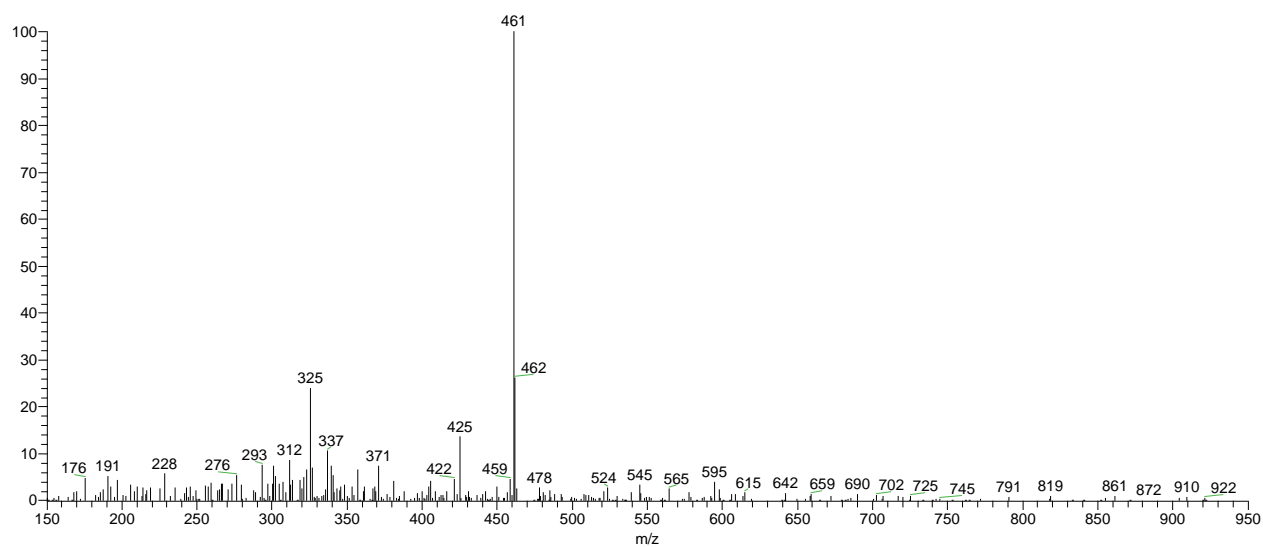


Figure S16. Mass spectrum of the compound **6**.

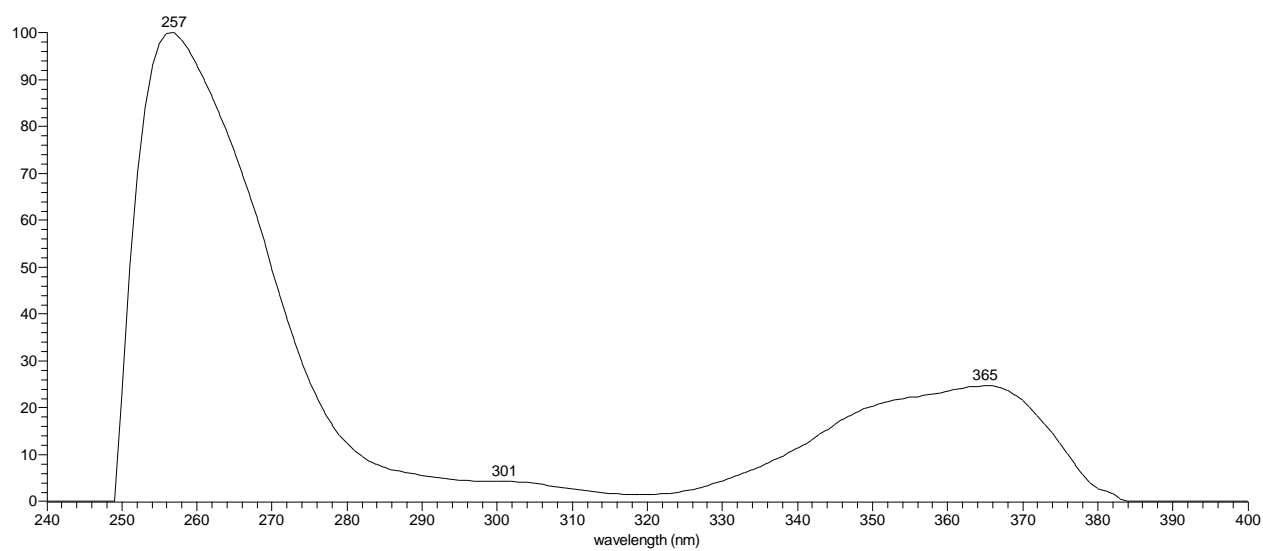


Figure S17. DAD spectra of the compound **6**.

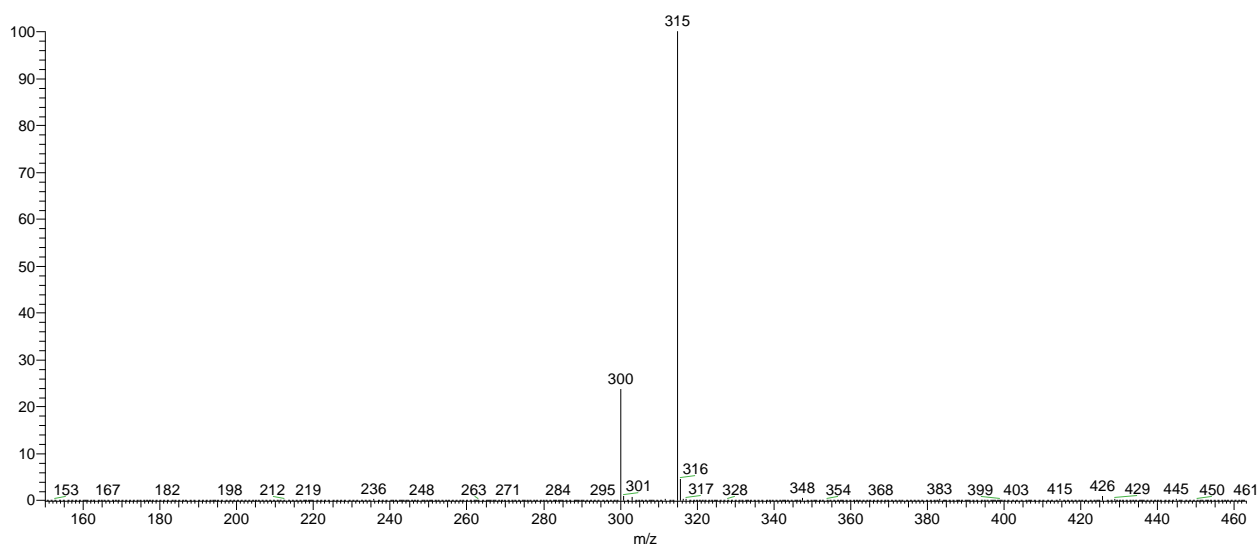


Figure S18. MS² spectrum of the ion at m/z 461 (compound **6**).

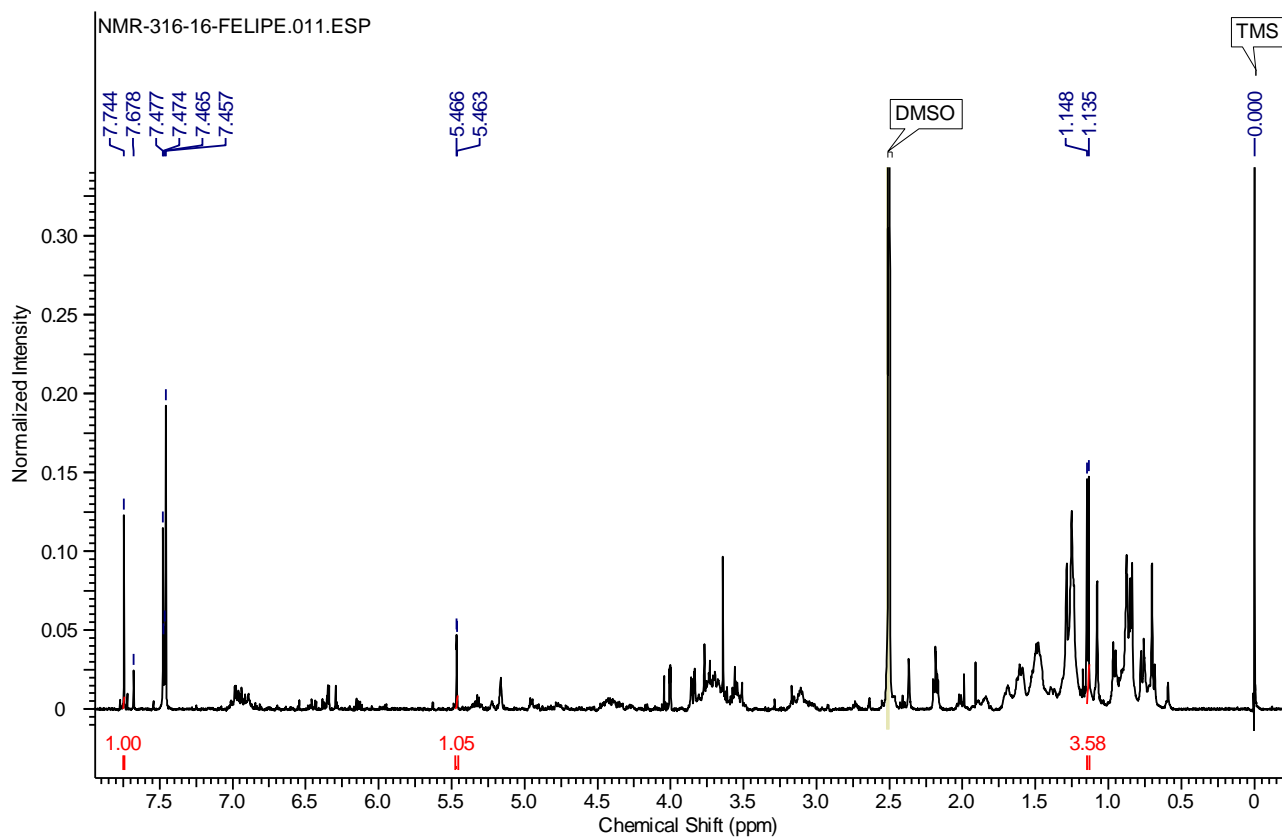


Figure S19. ¹H NMR spectrum (500.13 MHz, DMSO-*d*₆) for the methanol SPE fraction obtained from the SPE fractionation.

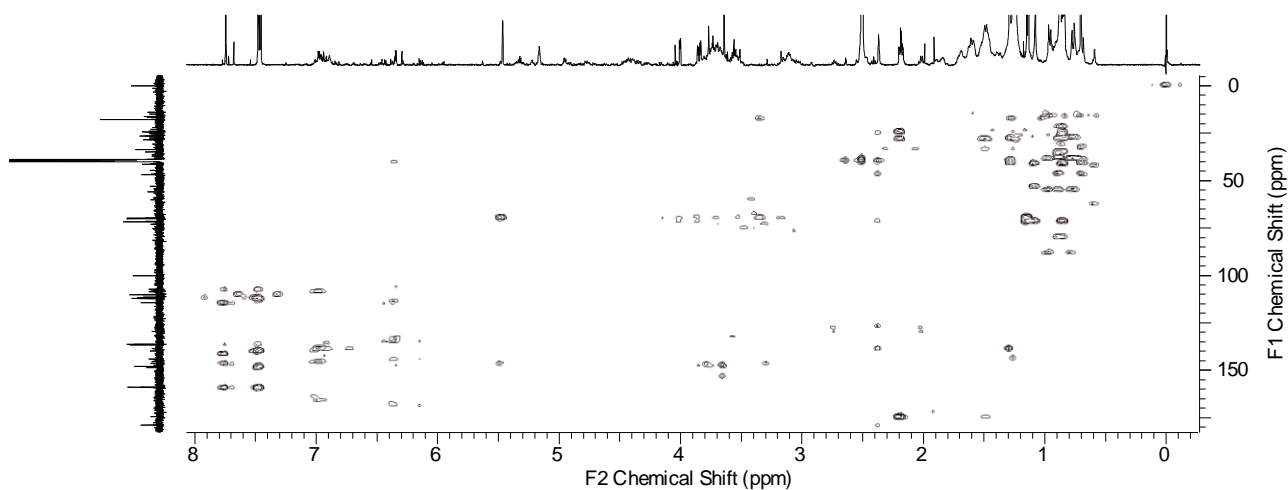


Figure S20. ^1H - ^{13}C correlations observed by HMBC for the methanol SPE fraction obtained from the SPE fractionation.

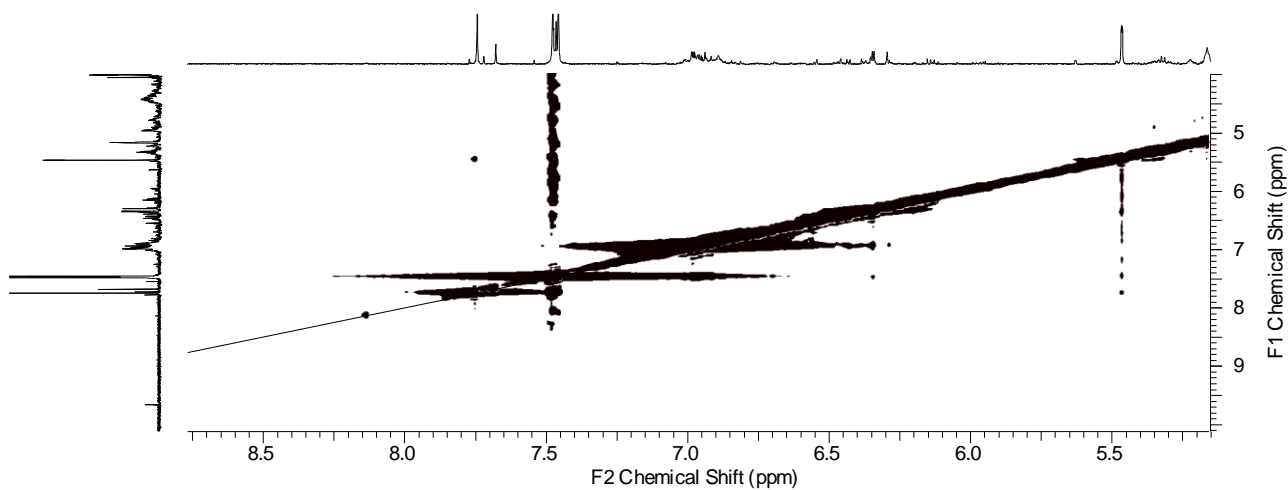


Figure S21. 2D NOESY spectrum (500.13 and 500.13 MHz, $\text{DMSO-}d_6$) for the methanol SPE fraction obtained from the SPE fractionation.

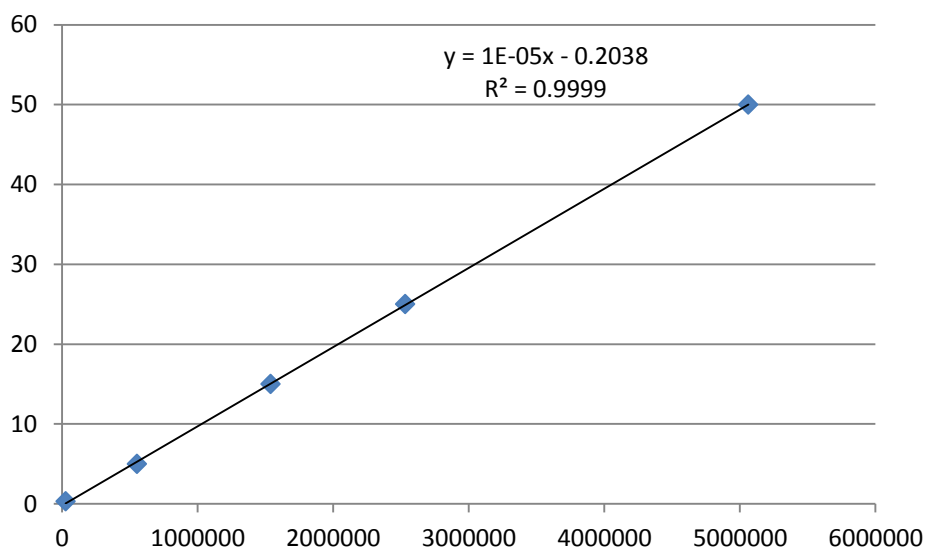


Figure S22. Calibration curve obtained by injecting the ellagic acid standard at 0.3, 5, 15, 25 and 50 $\mu\text{g mL}^{-1}$.

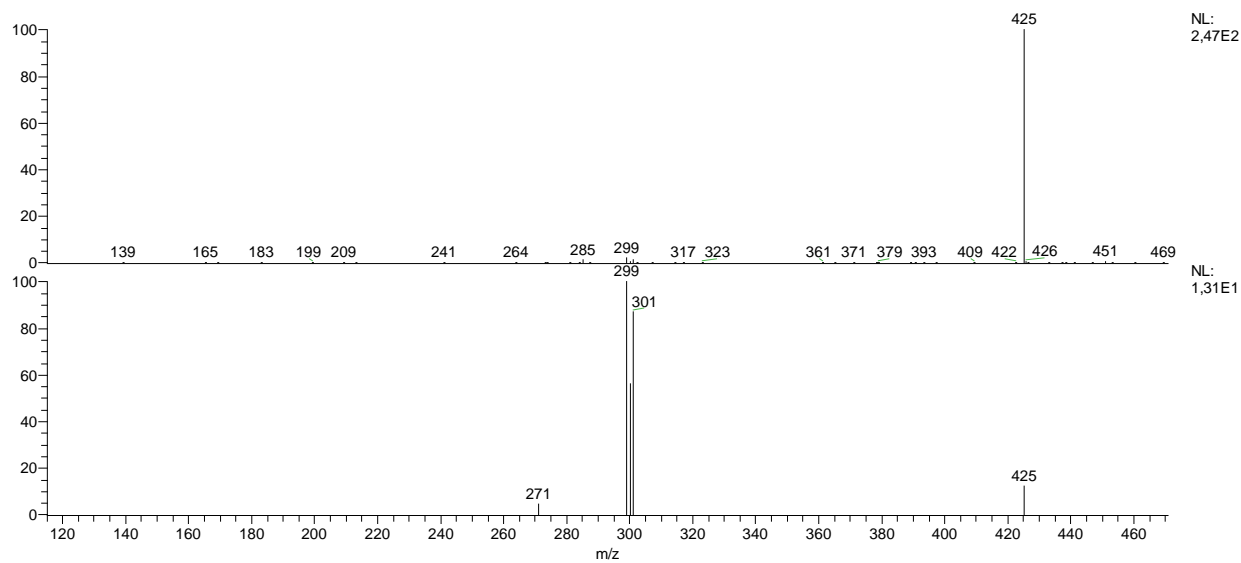


Figure S23. MS³ spectrum of the ion at m/z 469 (compound **1**) through ESI-IT-MS.