

Supporting Information

Characterization of *Conyza bonariensis* allelochemicals against broomrape weeds

Antonio Cala Peralta^{1,2}, Gabriele Soriano², Jesús G. Zorrilla^{1,2}, Marco Masi^{2,*}, Alessio Cimmino², Mónica Fernández-Aparicio^{3,*}

¹ Department of Chemical Sciences, University of Naples Federico II, Complesso Universitario Monte S. Angelo, Via Cintia 4, 80126 Naples, Italy; antonio.cala@uca.es (A.C.P.); gabriele.soriano@unina.it (G.S.); jesus.garcia@uca.es (J.G.Z.); alessio.cimmino@unina.it (A.C.)

² Allelopathy Group, Department of Organic Chemistry, Facultad de Ciencias, Institute of Biomolecules (INBIO), University of Cadiz, C/Avenida República Saharaui, s/n, 11510 Puerto Real, Spain

³ Department of Plant Breeding, Institute for Sustainable Agriculture (IAS), CSIC, Avenida Menéndez Pidal s/n, 14004 Córdoba, Spain

* Correspondence: marco.masi@unina.it (M.M.); monica.fernandez@ias.csic.es (M.F.-A.)

Supporting Information list

Figure S1. ¹H-NMR spectrum of (4Z)-lachnophyllum methyl ester (**1**) recorded in CDCl₃ at 500 MHz.

Figure S2. ESI MS spectrum of (4Z)-lachnophyllum methyl ester (**1**) recorded in positive modality.

Figure S3. ¹H-NMR spectrum of (4Z)-lachnophyllum lactone (**2**) recorded in CDCl₃ at 500 MHz.

Figure S4. ESI MS spectrum of (4Z)-lachnophyllum lactone (**2**) recorded in positive modality.

Figure S5. ¹H-NMR spectrum of (4Z,8Z)-matricaria lactone (**3**) recorded in CDCl₃ at 500 MHz.

Figure S6. ESI MS spectrum of (4Z,8Z)-matricaria lactone (**3**) recorded in positive modality.

Figure S7. ¹H-NMR spectrum of (4E,8Z)-matricaria lactone (**4**) recorded in CDCl₃ at 500 MHz.

Figure S8. ESI MS spectrum of (4E,8Z)-matricaria lactone (**4**) recorded in positive modality.

Figure S9. ¹H-NMR spectrum of methyl 4-hydroxy-3-methoxybenzoate (**5**) recorded in CDCl₃ at 500 MHz.

Figure S10. ESI MS spectrum of methyl 4-hydroxy-3-methoxybenzoate (**5**) recorded in positive modality.

Figure S11. ¹H-NMR spectrum of methyl 4-hydroxybenzoate (**6**) recorded in CDCl₃ at 500 MHz.

Figure S12. ESI MS spectrum of methyl 4-hydroxybenzoate (**6**) recorded in positive modality.

Figure S13. ¹H-NMR spectrum of hispidulin (**7**) recorded in CDCl₃ at 500 MHz.

Figure S14. ¹³C-NMR spectrum of hispidulin (**7**) recorded in (CD₃)₂CO at 125 MHz.

Figure S15. ESI MS spectrum of hispidulin (**7**) recorded in positive modality.

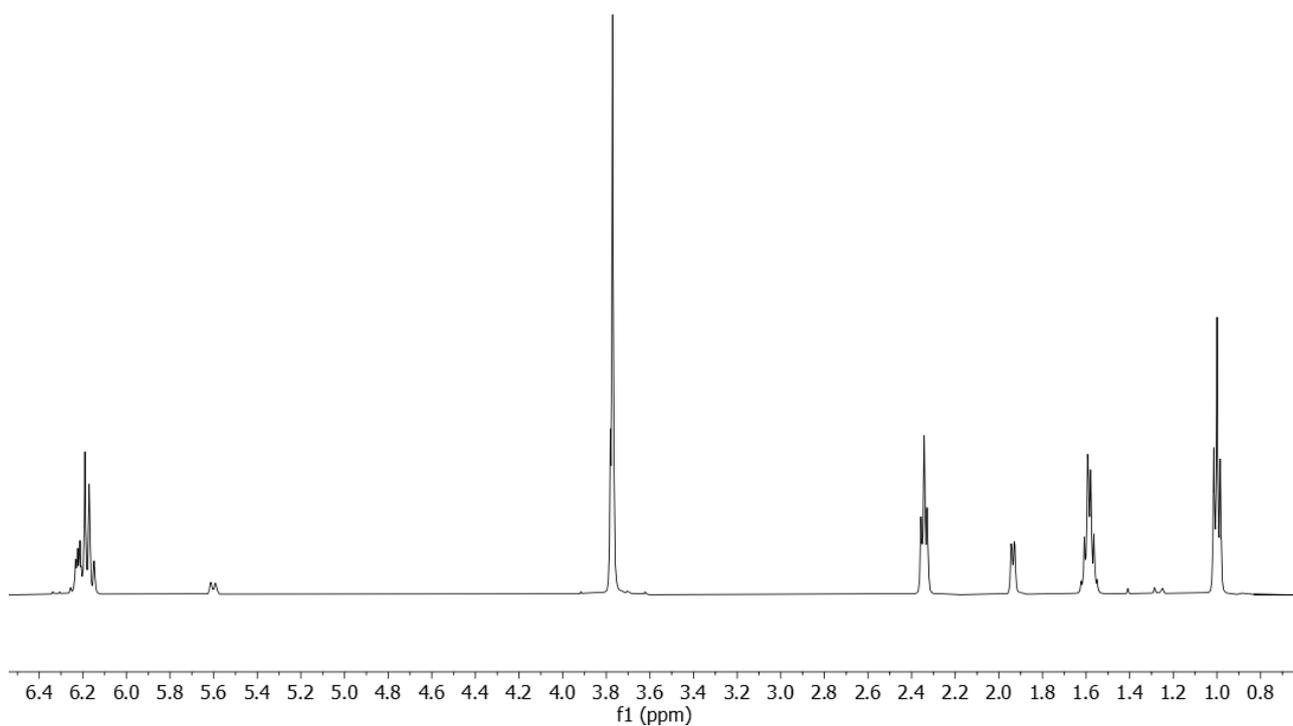


Figure S1. $^1\text{H-NMR}$ spectrum of (4Z)-lachnophyllum methyl ester (**1**) recorded in CDCl_3 at 500 MHz.

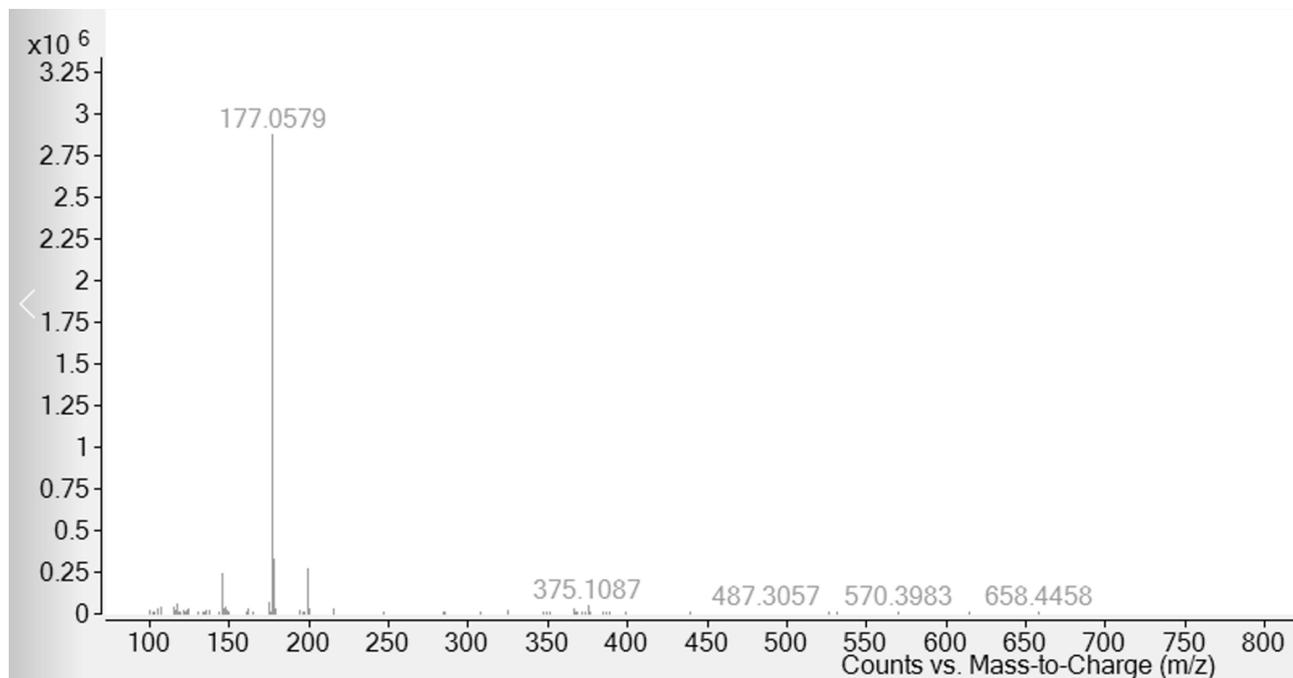


Figure S2. ESI MS spectrum of (4Z)-lachnophyllum methyl ester (**1**) recorded in positive modality.

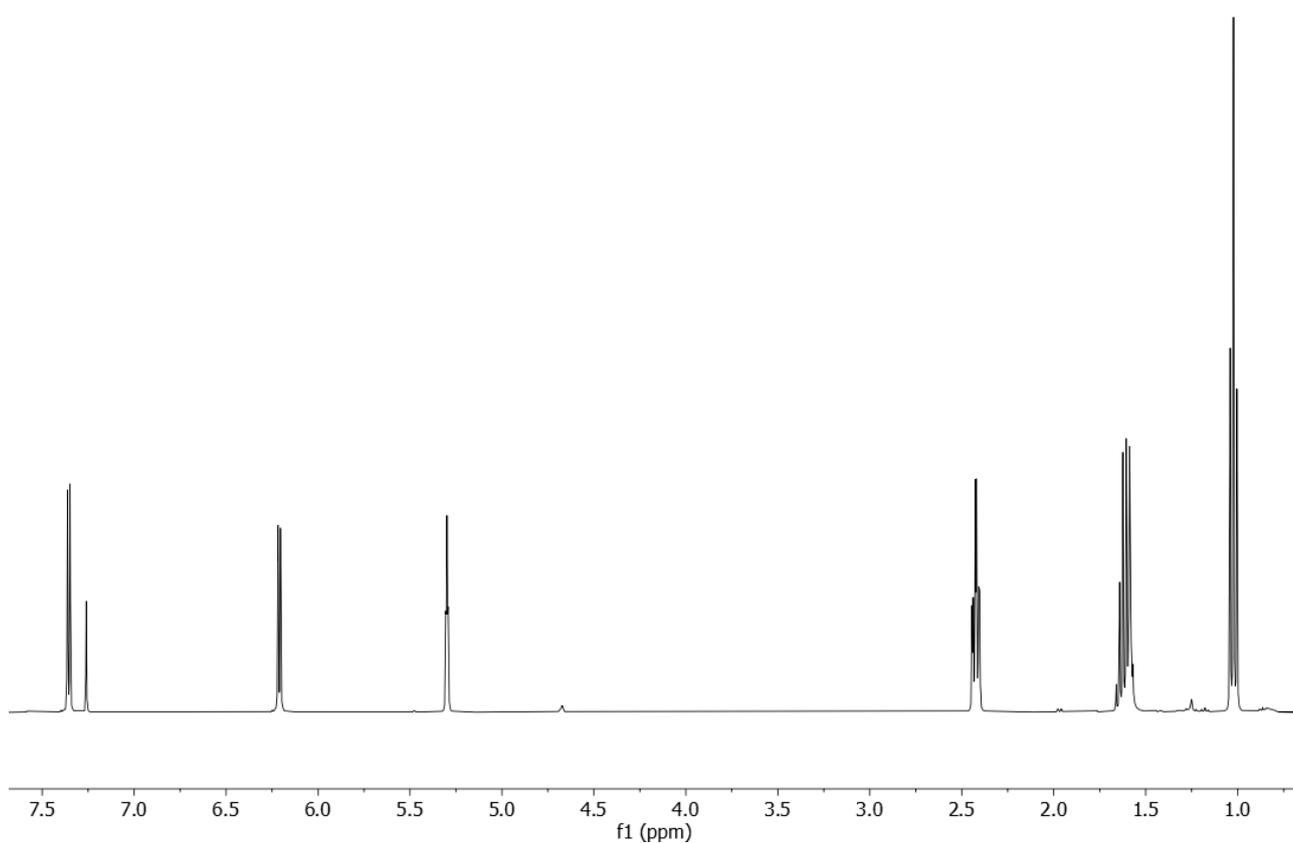


Figure S3. $^1\text{H-NMR}$ spectrum of (4Z)-lachnophyllum lactone (**2**) recorded in CDCl_3 at 500 MHz.

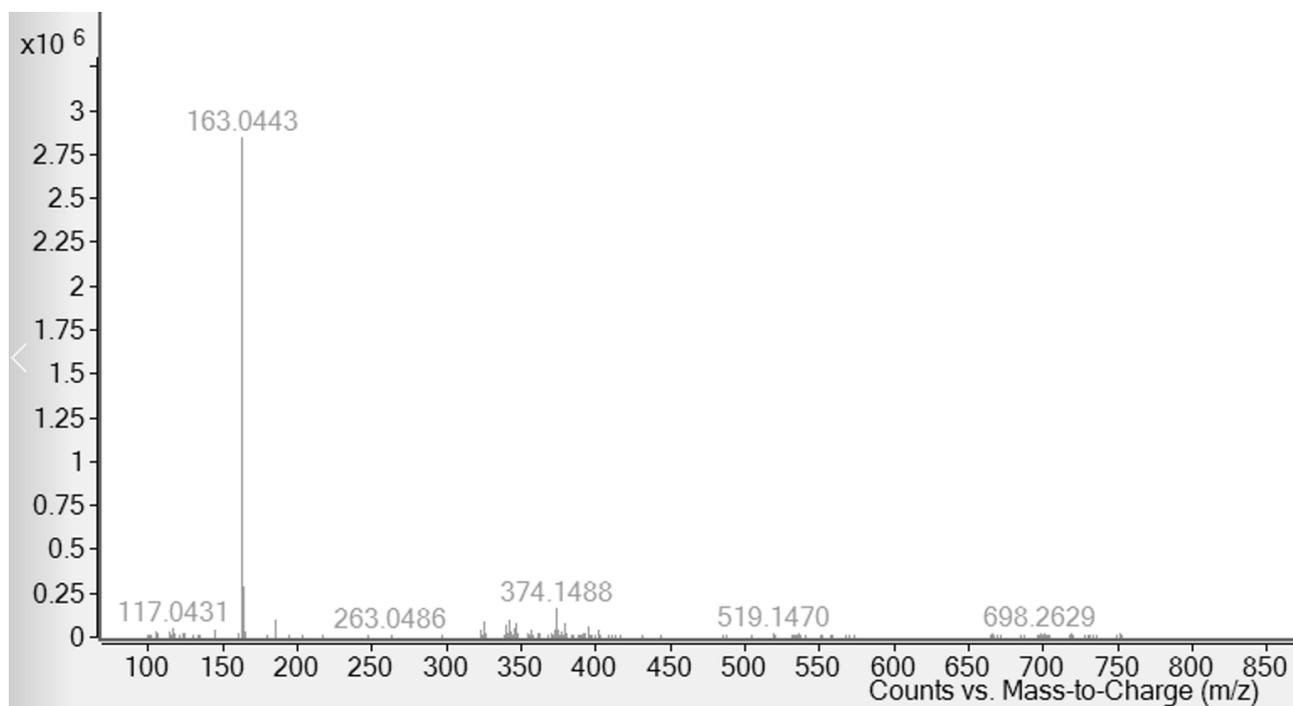


Figure S4. ESI MS spectrum of (4Z)-lachnophyllum lactone (**2**) recorded in positive modality.

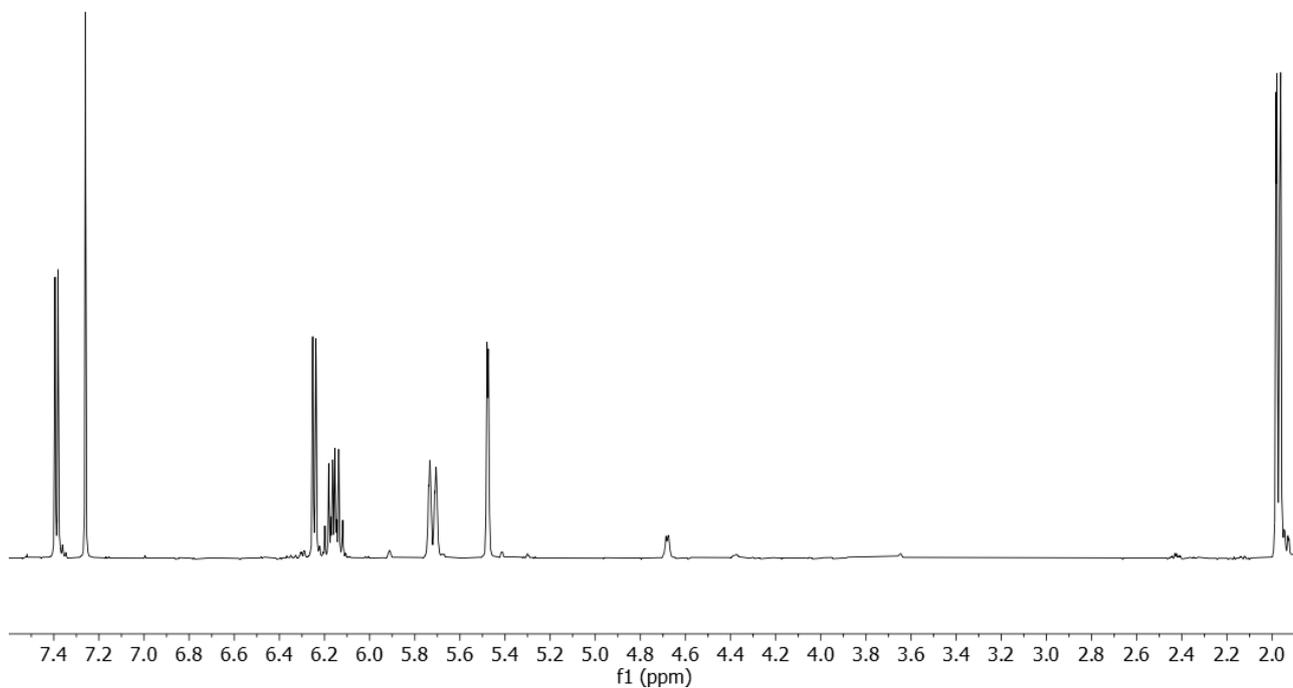


Figure S5. $^1\text{H-NMR}$ spectrum of (4Z,8Z)-matricaria lactone (**3**) recorded in CDCl_3 at 500 MHz.

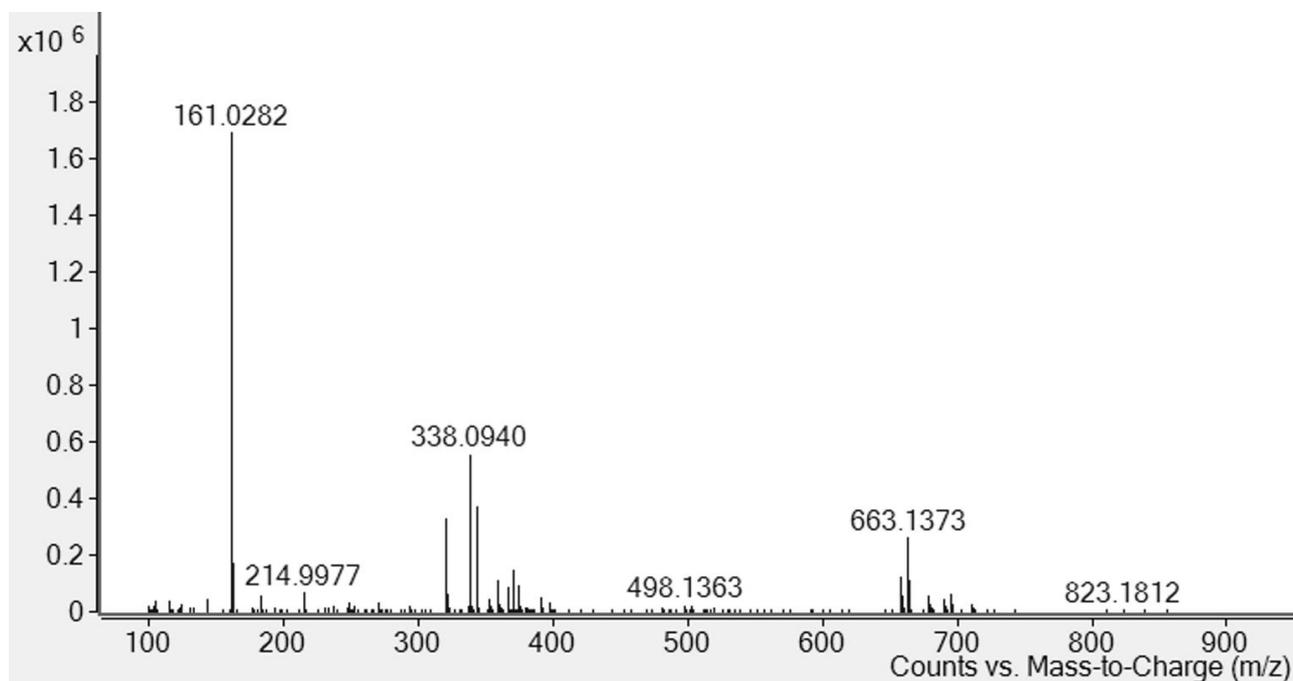


Figure S6. ESI MS spectrum of (4Z,8Z)-matricaria lactone (**3**) recorded in positive modality.

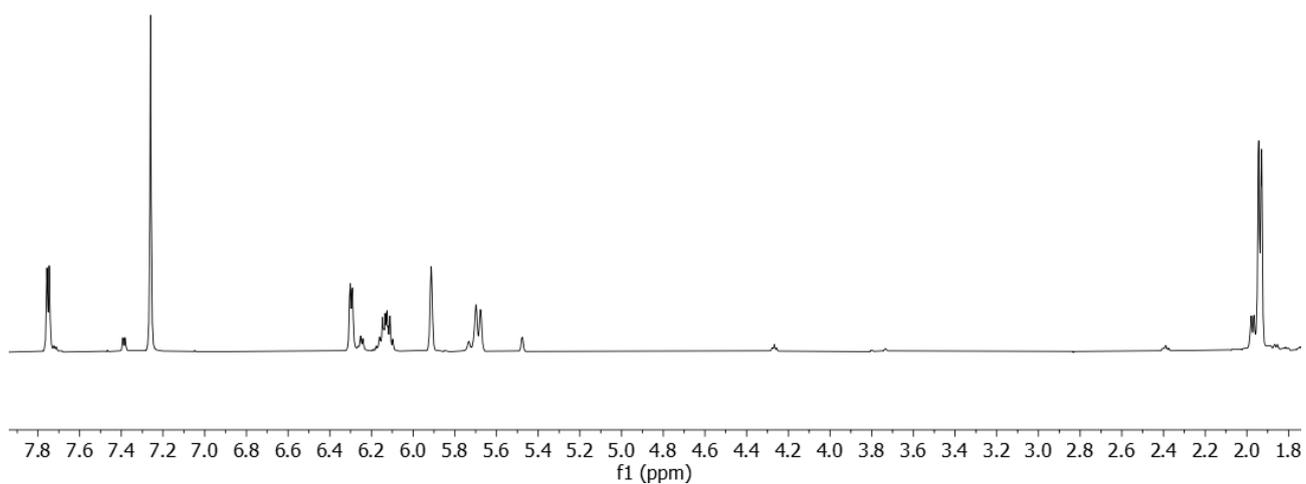


Figure S7. $^1\text{H-NMR}$ spectrum of (4*E*,8*Z*)-matricaria lactone (**4**) recorded in CDCl_3 at 500 MHz.

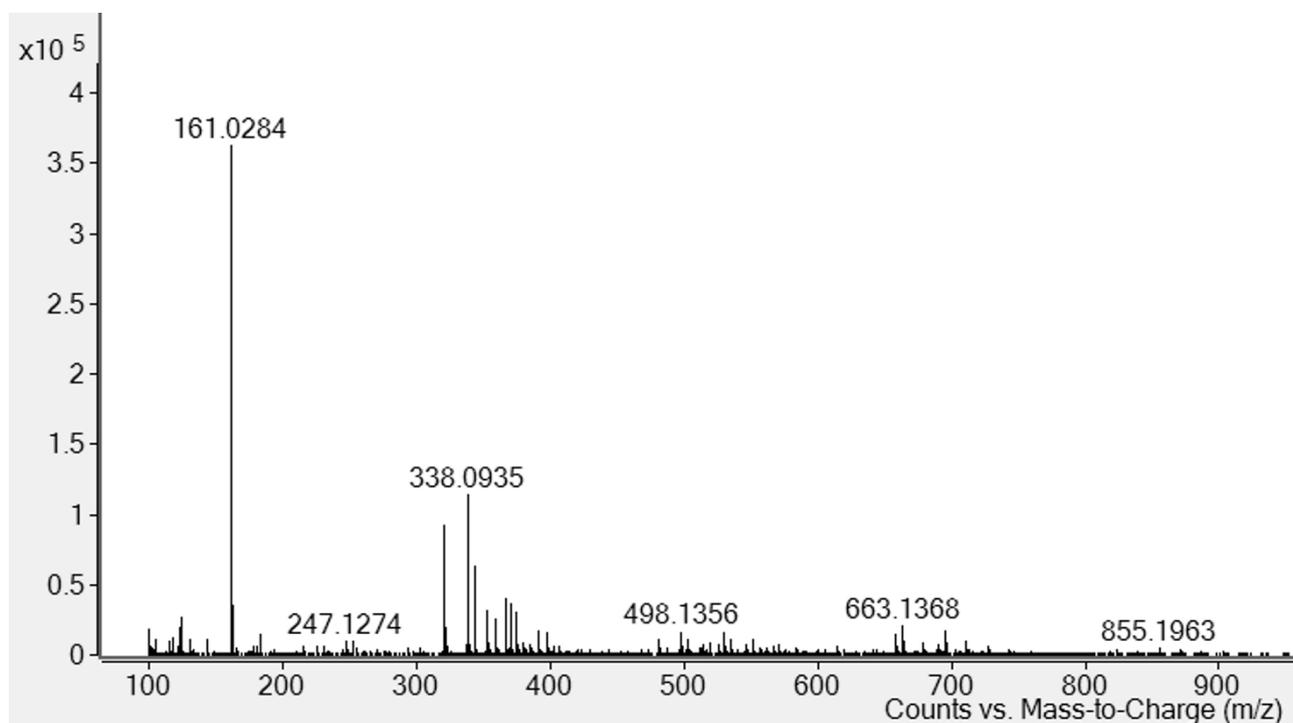


Figure 8. ESI MS spectrum of (4*E*, 8*Z*)-matricaria lactone (**4**) recorded in positive modality.

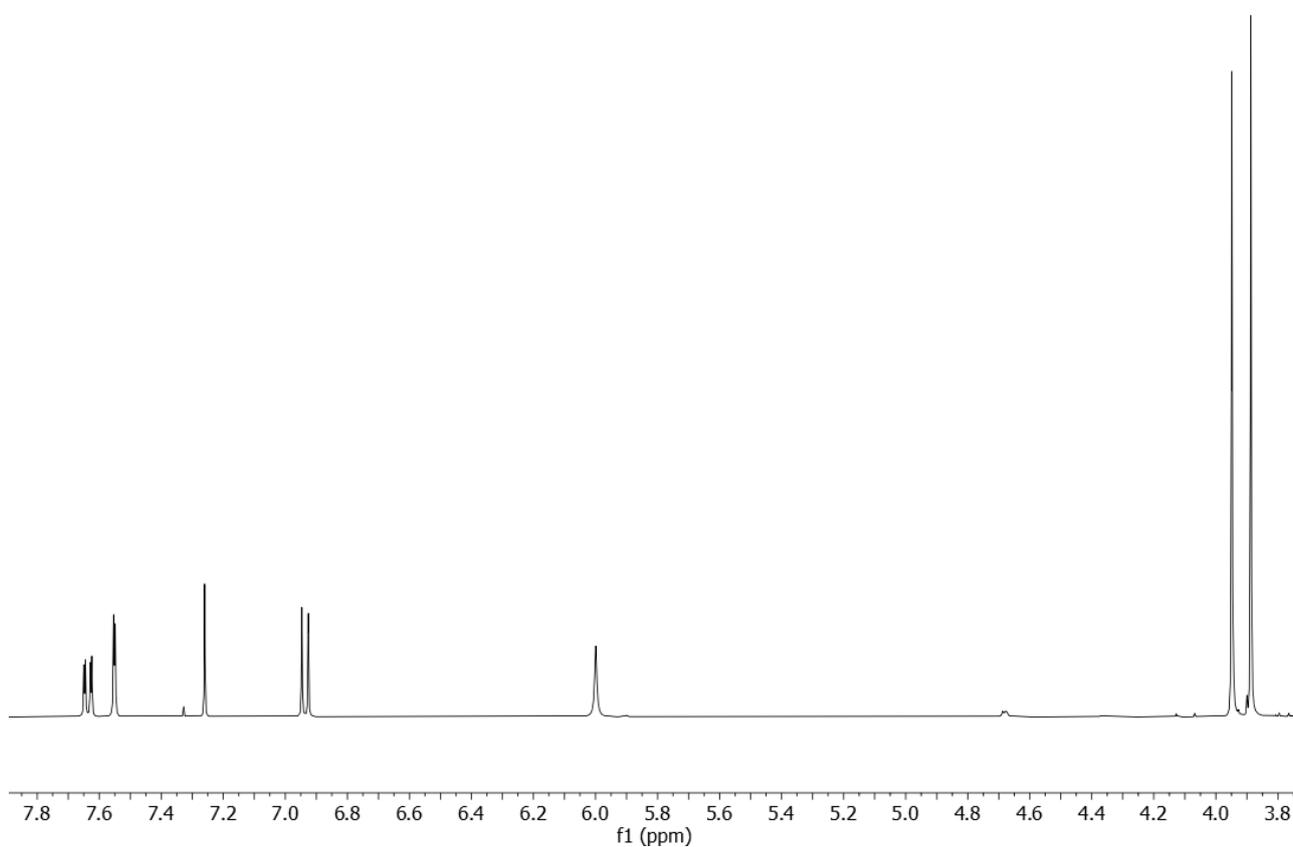


Figure S9. $^1\text{H-NMR}$ spectrum of methyl 4-hydroxy-3-methoxybenzoate (**5**) recorded in CDCl_3 at 500 MHz.

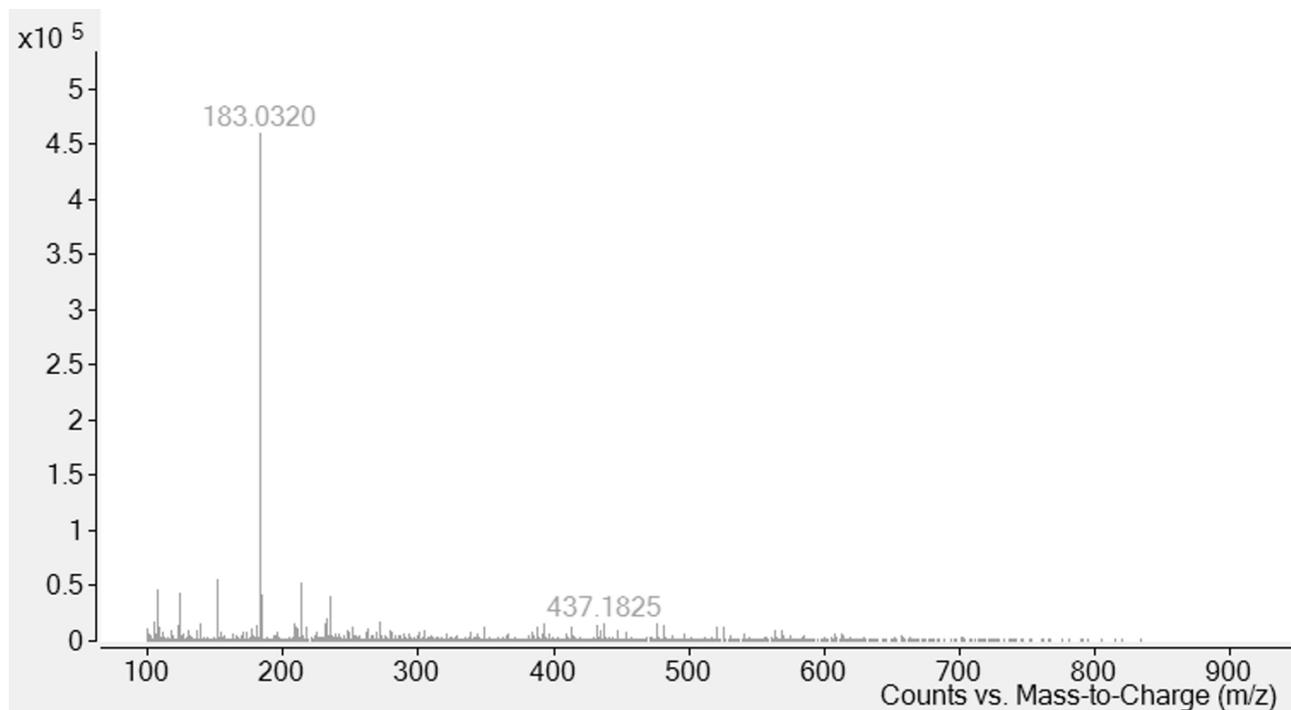


Figure S10. ESI MS spectrum of methyl 4-hydroxy-3-methoxybenzoate (**5**) recorded in positive modality.

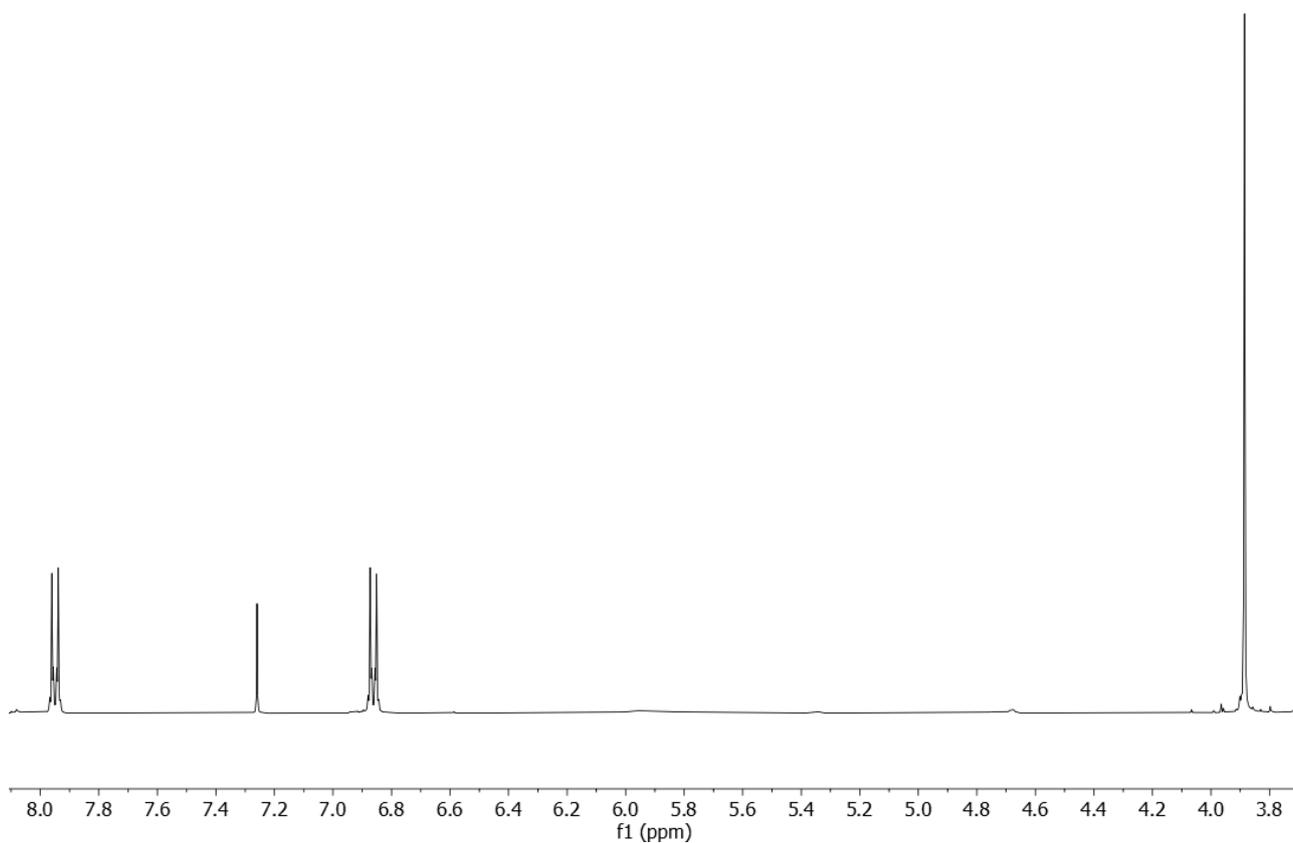


Figure S11. $^1\text{H-NMR}$ spectrum of methyl 4-hydroxybenzoate (**6**) recorded in CDCl_3 at 500 MHz.

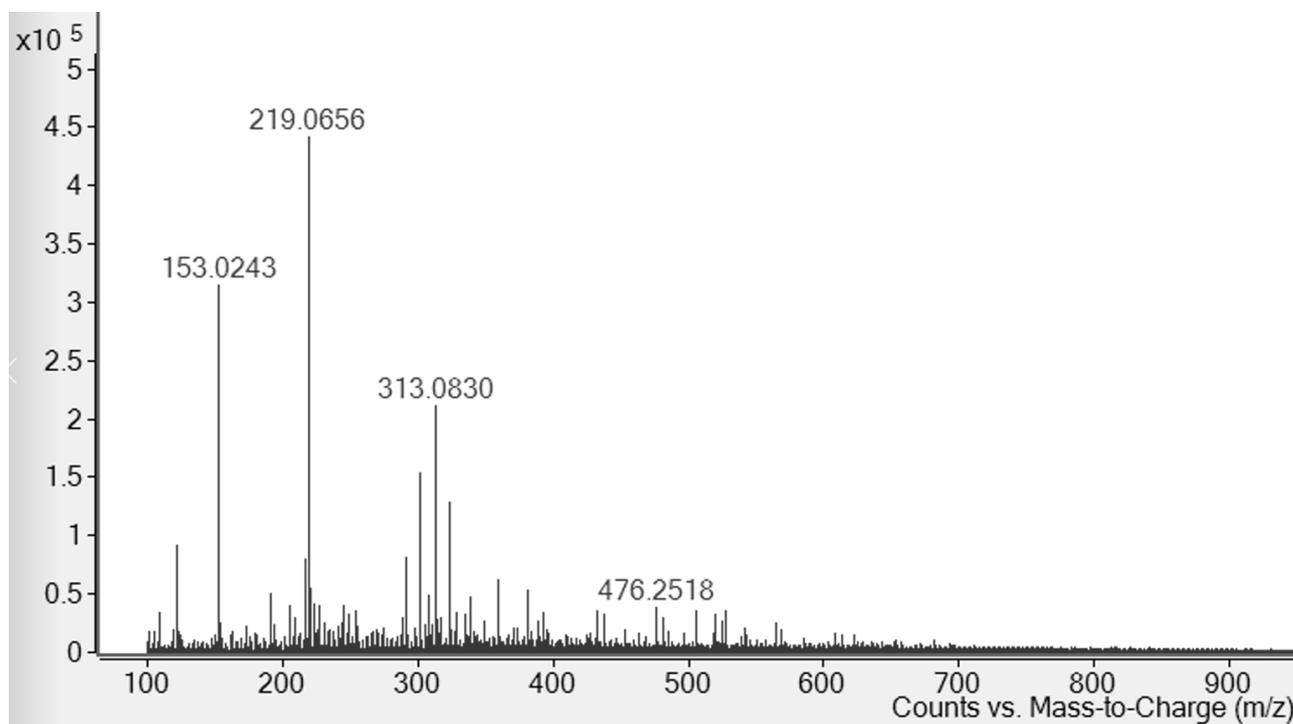


Figure S12. ESI MS spectrum of methyl 4-hydroxybenzoate (**6**) recorded in positive modality.

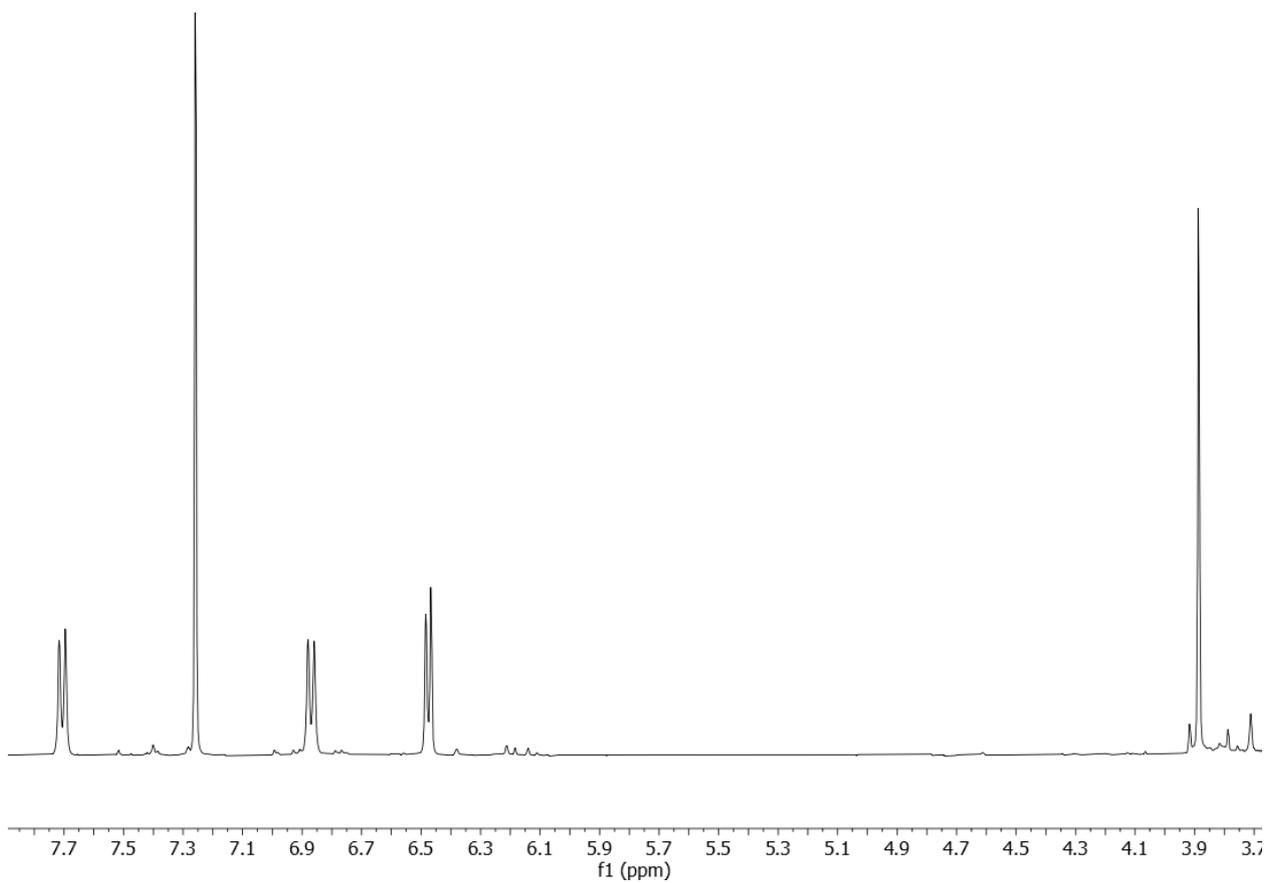


Figure S13. ¹H-NMR spectrum of hispidulin (**7**) recorded in CDCl₃ at 500 MHz.

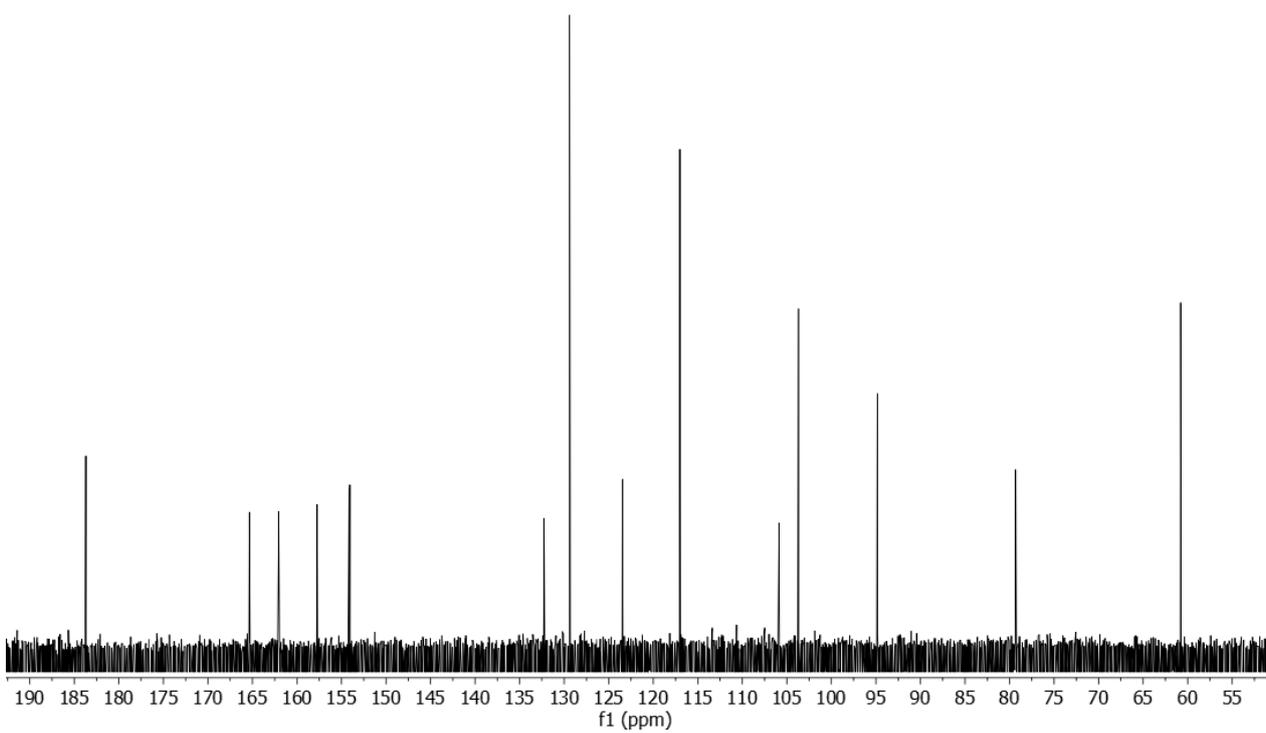


Figure S14. ¹³C-NMR spectrum of hispidulin (**7**) recorded in (CD₃)₂CO at 125 MHz.

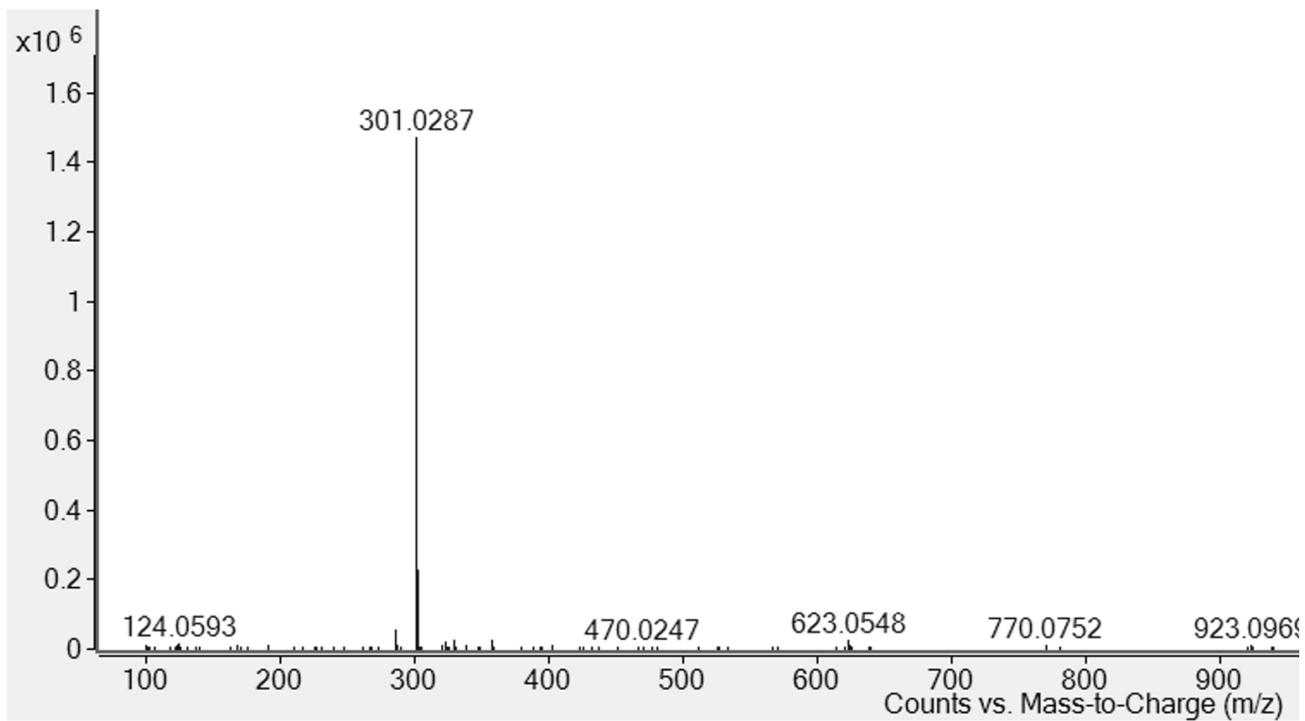


Figure S15. ESI MS spectrum of hispidulin (7) recorded in positive modality.