

# Insights into in the metabolome of the cyanobacterium *Leibleinia gracilis* from the lagoon of Tahiti and first inspection of its variability

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P2 Figure S1. Analytical HPLC chromatograms of the F2 fraction of *L. gracilis* on C18 reverse phase (UV at 210 nm and ELSD)

Figure S2. UHPLC-HRMS chromatogram and MS/MS fragmentation of the isolated major (9*E*)-11-oxopalmitoleic acid

P3 Figure S3. <sup>1</sup>H NMR of (9*E*)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (600 MHz)

Figure S4. <sup>13</sup>C NMR spectrum of (9*E*)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (150 MHz)

P4 Figure S5. COSY spectrum of (9*E*)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (600 MHz)

Figure S6. HSQC NMR of (9*E*)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (600 MHz)

P5 Figure S7. HMBC NMR of (9*E*)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (600 MHz)

P6 Figure S8. UHPLC-HRMS chromatogram showing the MS/MS fragmentation spectrum of the main annotated compound Erucamide (*m/z* 338.3449)

Figure S9. MS/MS fragmentation of the Erucamide: confirmation matching with Metlin database

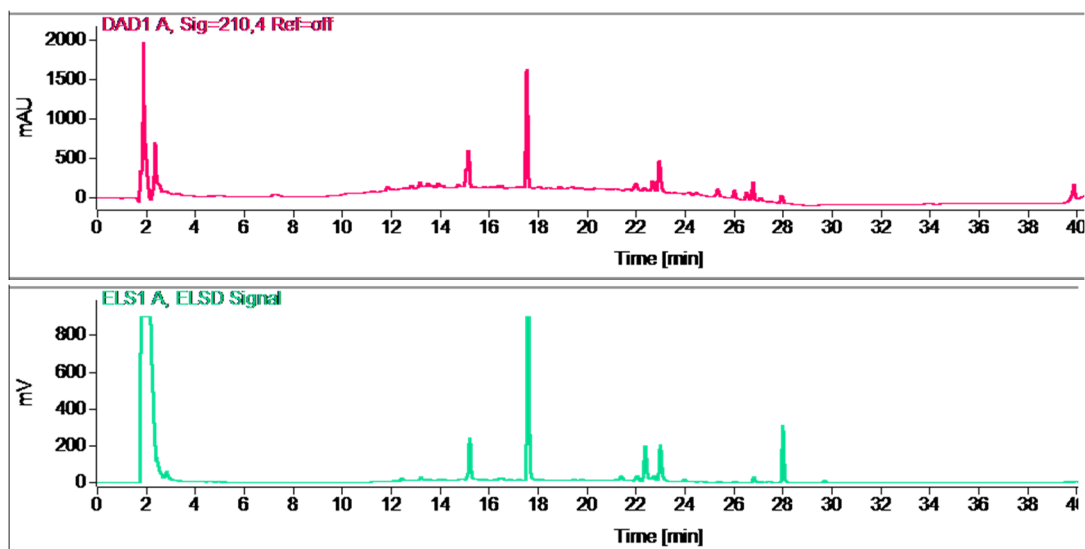


Figure S1. Analytical HPLC chromatograms of the F2 fraction of *L. gracilis* on C18 reverse phase (UV at 210 nm and ELSD)

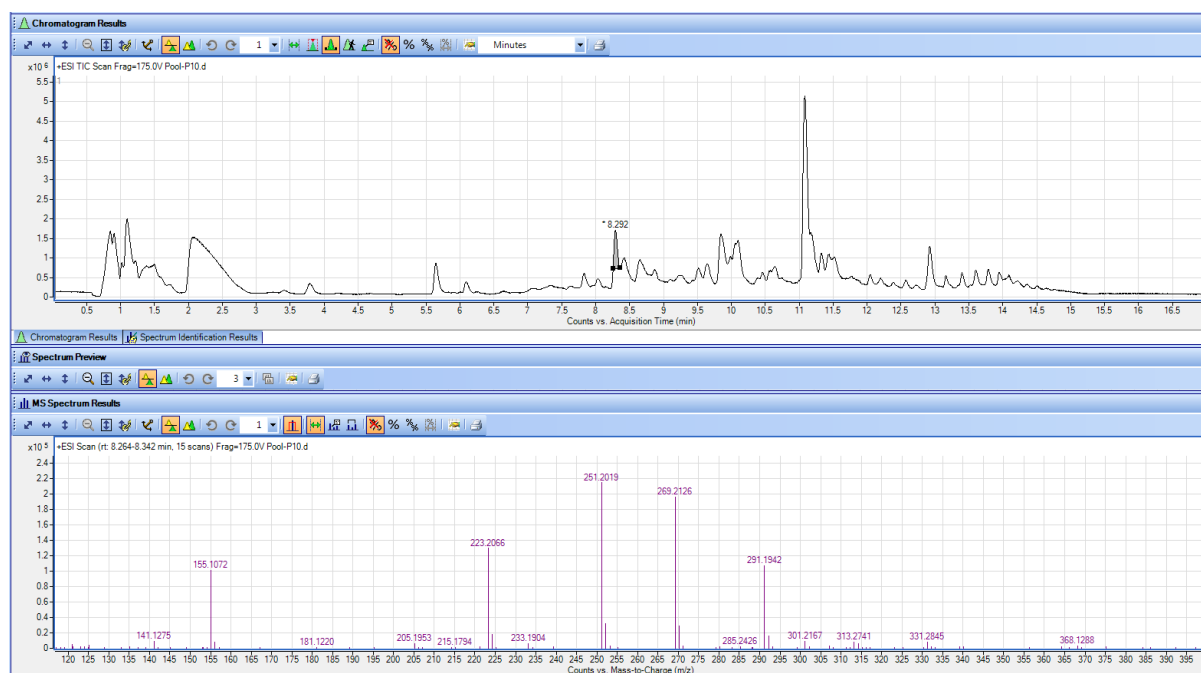


Figure S2. UHPLC-HRMS chromatogram and MS/MS fragmentation of the isolated major (9E)-11-oxopalmitoleic acid

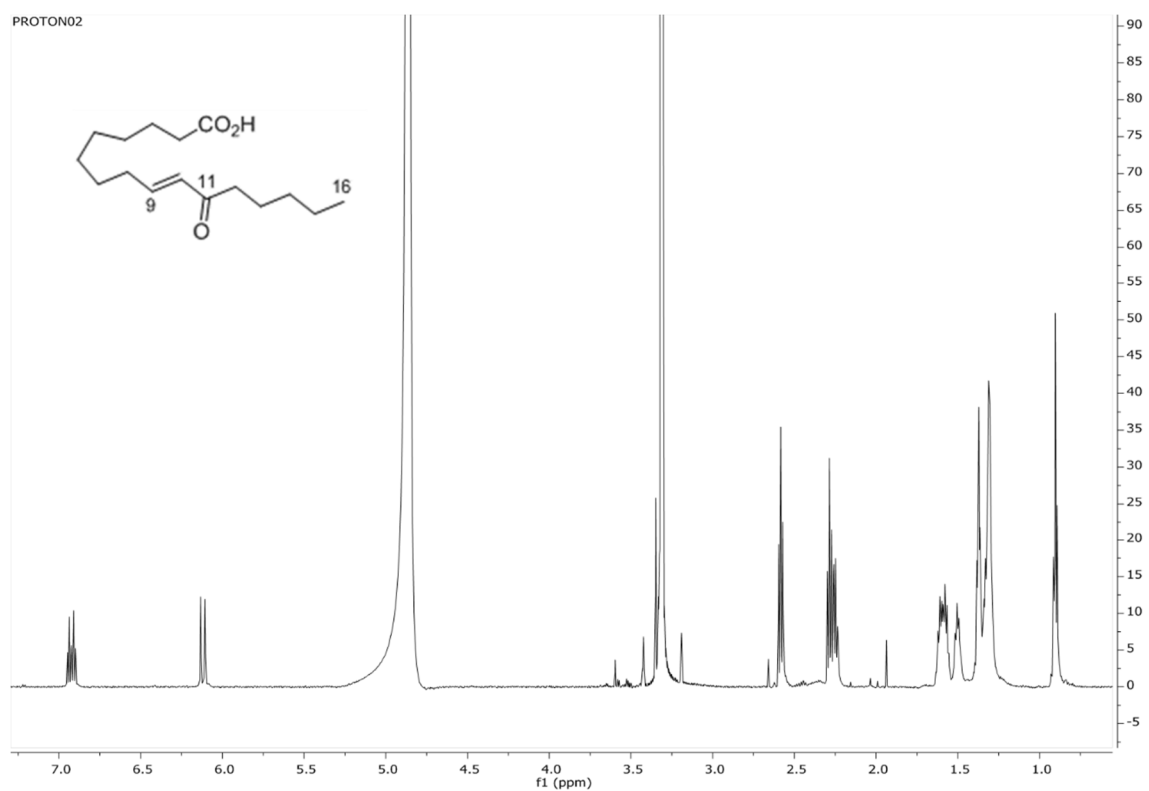


Figure S3.  $^1\text{H}$  NMR of (*9E*)-11-oxopalmitoleic acid in  $\text{CD}_3\text{OD}$  (600 MHz)

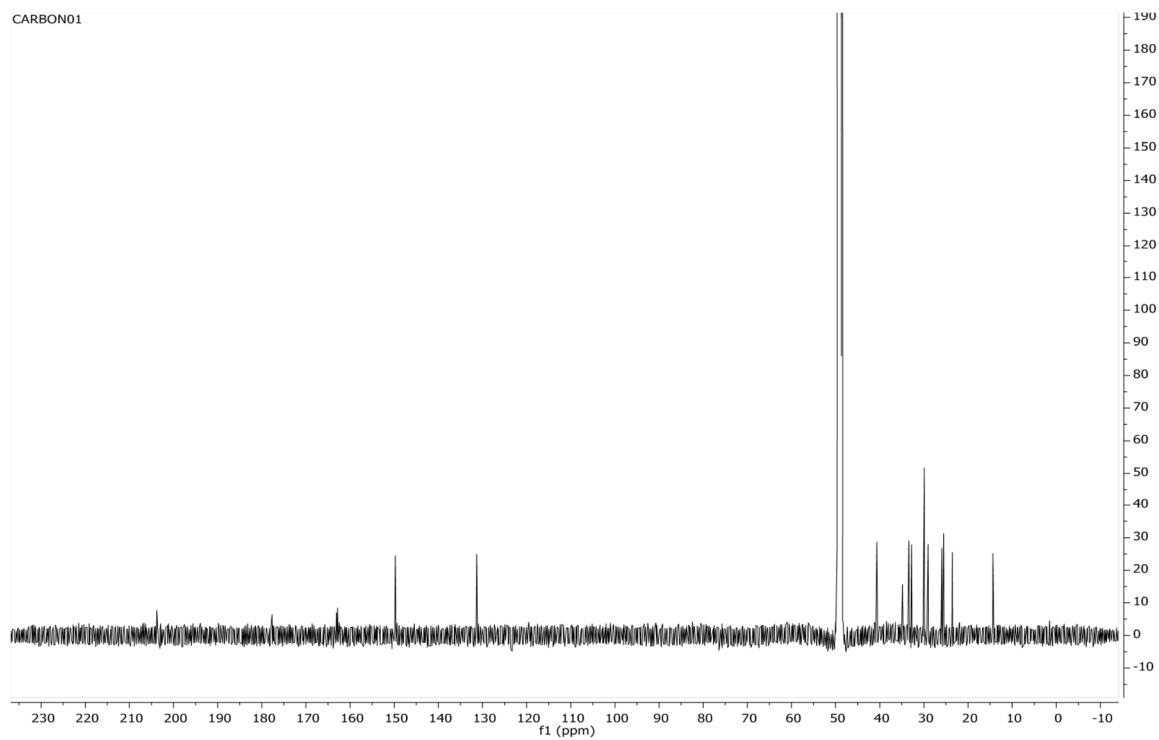


Figure S4.  $^{13}\text{C}$  NMR spectrum of (*9E*)-11-oxopalmitoleic acid in  $\text{CD}_3\text{OD}$  (150 MHz)

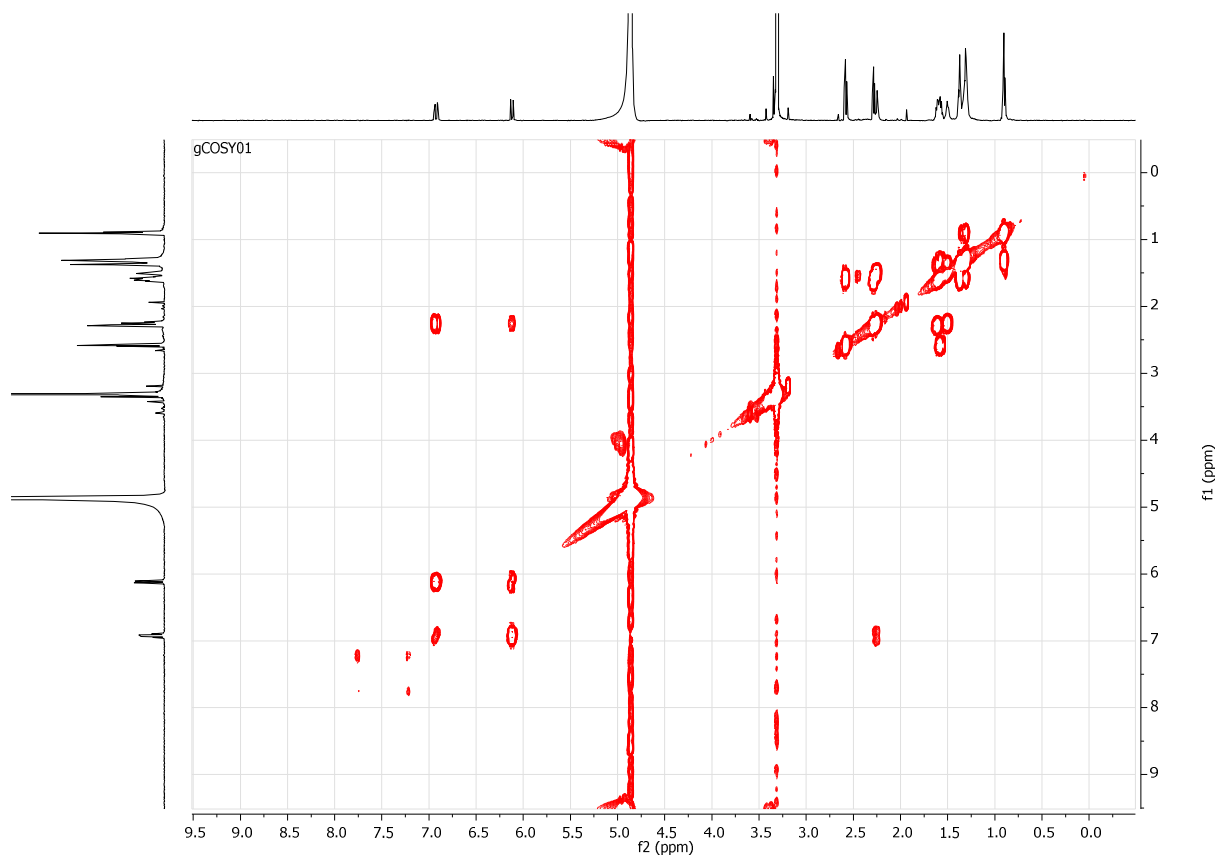


Figure S5. COSY spectrum of (9E)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (600 MHz)

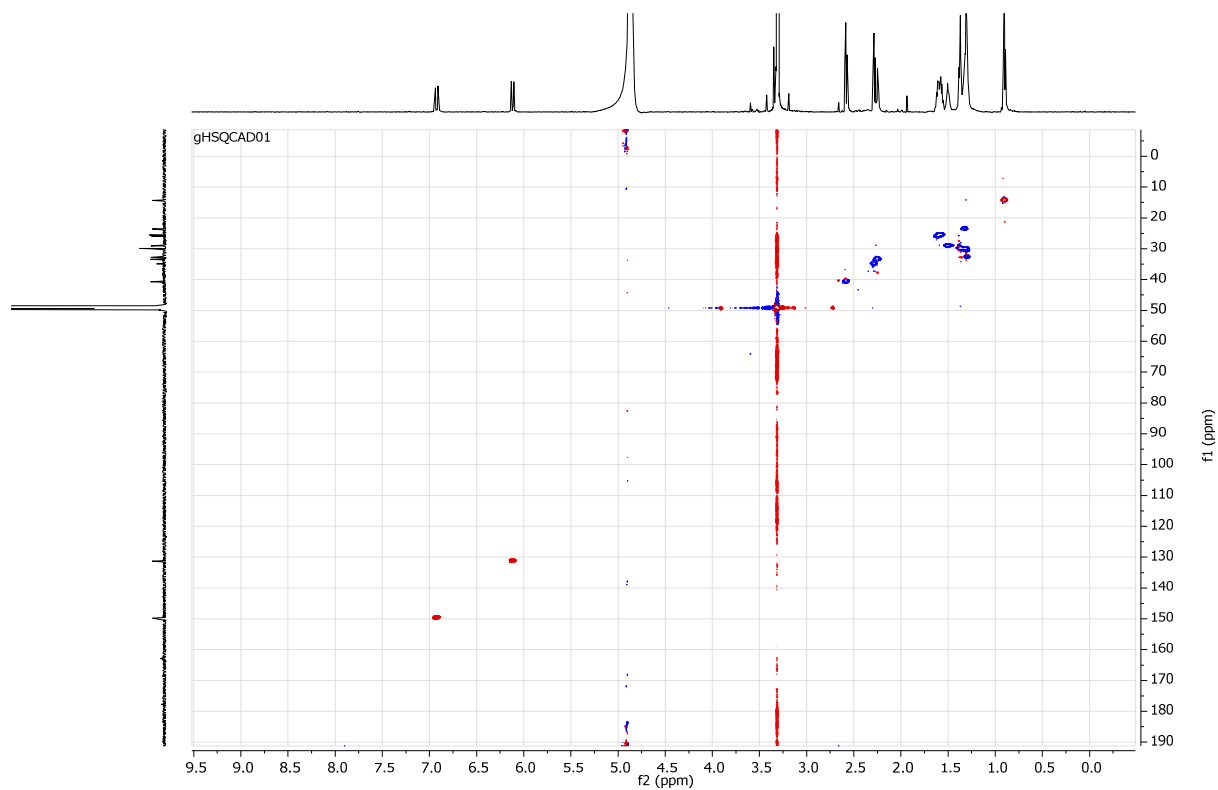


Figure S6. HSQC NMR of (9E)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (600 MHz)

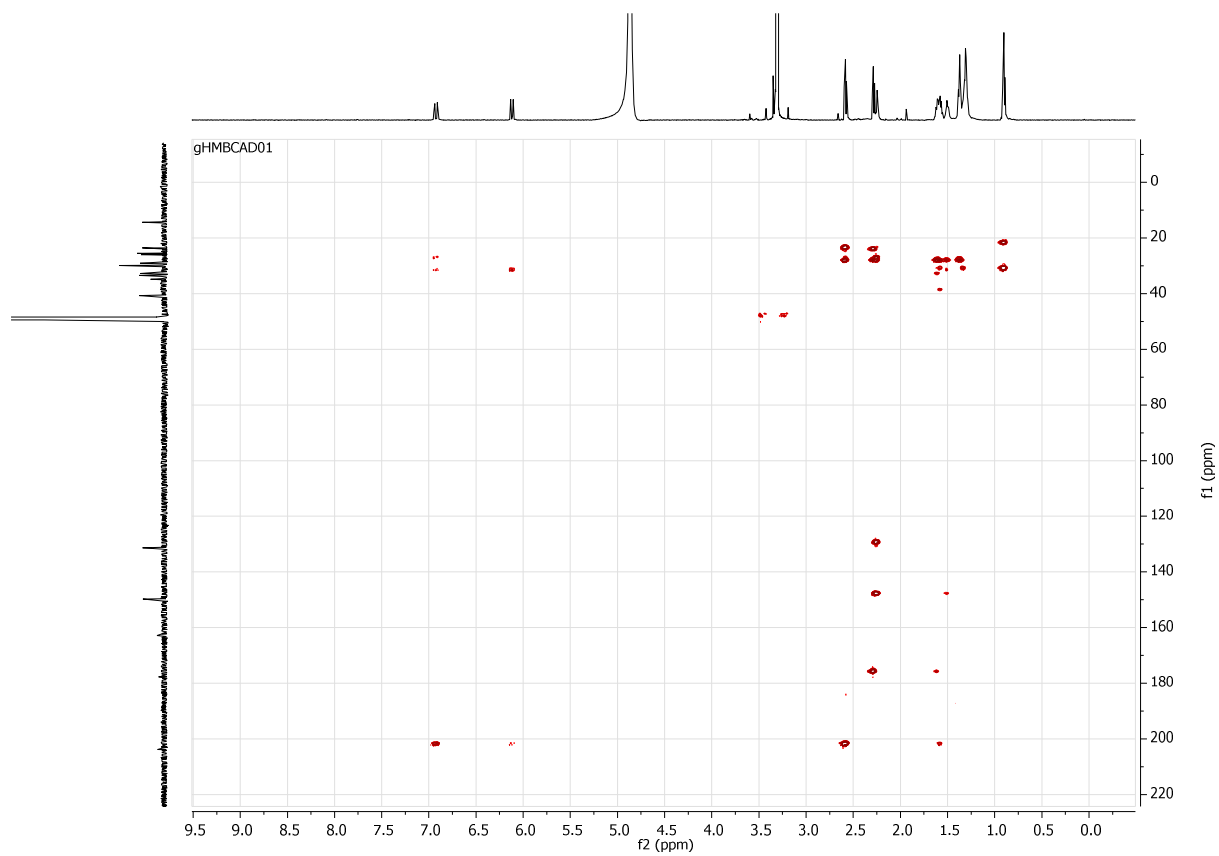


Figure S7. HMBC NMR of (9E)-11-oxopalmitoleic acid in CD<sub>3</sub>OD (600 MHz)

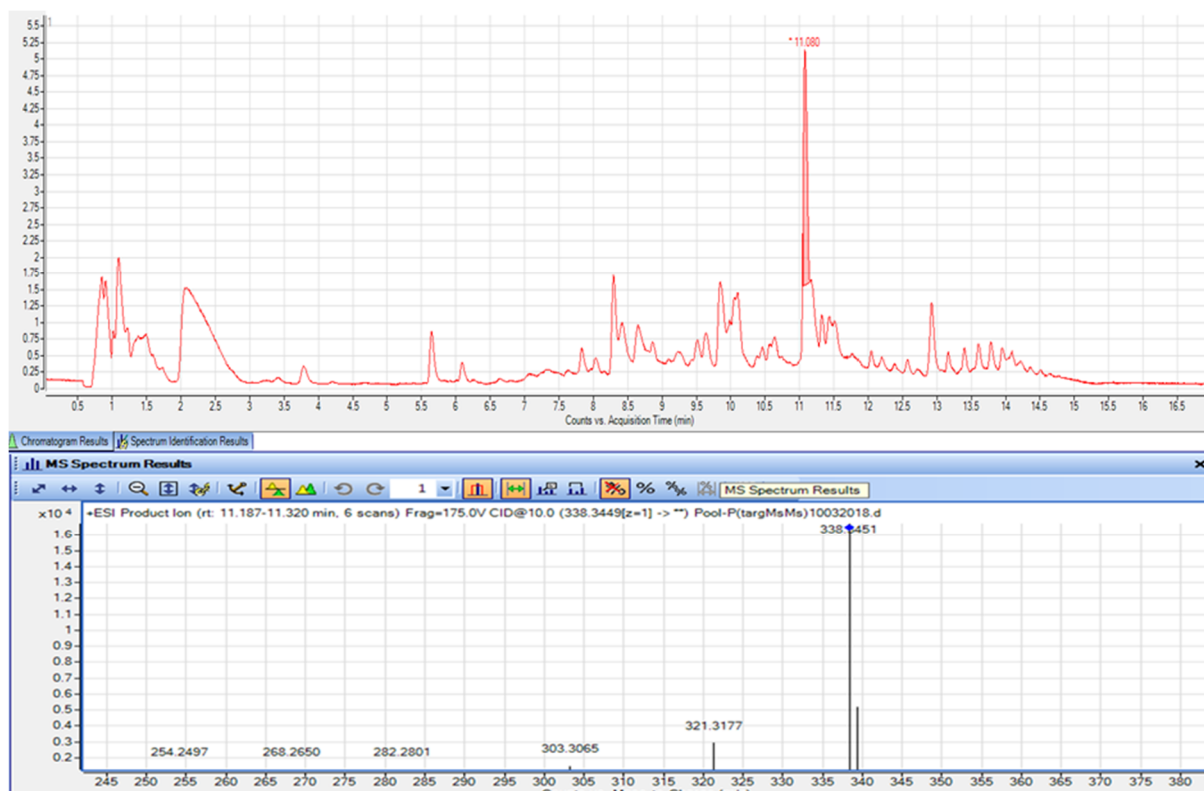


Figure S8. UHPLC-HRMS chromatogram showing the MS/MS fragmentation spectrum of the main annotated compound Erucamide ( $m/z$  338.3449)

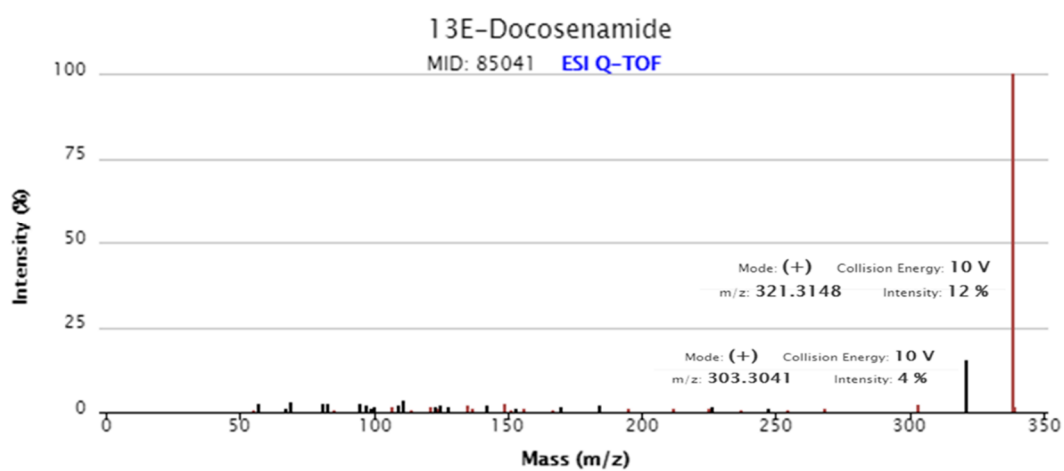


Figure S9. MS/MS fragmentation of the Erucamide: confirmation matching with Metlin database