

## Supplementary Materials

# Mining Xanthine Oxidase Inhibitors from an Edible Seaweed *Pterocladia capillacea* by Using in vitro Bioassays, Affinity Ultrafiltration LC-MS/MS, Metabolomics Tools, and In Silico Prediction

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## Figure legends

**Figure S1.** The MS/MS spectrum of compound **1** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S2.** The MS/MS spectrum of compound **2** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S3.** The MS/MS spectrum of the  $[M+NH_4]^+$  ion of compound **3** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S4.** The MS/MS spectrum of the  $[M+H]^+$  ion of compound **3** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S5.** The MS/MS spectrum of compound **4** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S6.** The MS/MS spectrum of compound **5** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S7.** The MS/MS spectrum of compound **6** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S8.** The MS/MS spectrum of compound **7** captured by the affinity ultrafiltration from fractions F4-2(P) and F4-3(P).

**Figure S9.** The MS/MS spectrum of compound **8** captured by the affinity ultrafiltration from fractions F4-2(P) and F4-3(P).

**Figure S10.** The MS/MS spectrum of compound **9** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S11.** The MS/MS spectrum of compound **10** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S12.** The MS/MS spectrum of compound **11** captured by the affinity ultrafiltration from fraction F4-2(P).

**Figure S13.** The MS/MS spectrum of compound **12** captured by the affinity ultrafiltration from fraction F4-3(P).

**Figure S14.** The MS/MS spectrum of compound **13** captured by the affinity ultrafiltration from fraction F4-3(P).

**Figure S15.** The MS/MS spectrum of compound **14** captured by the affinity ultrafiltration from fraction F4-3(P).

**Figure S16.** The MS/MS spectrum of compound **15** captured by the affinity ultrafiltration from fraction F4-3(P).

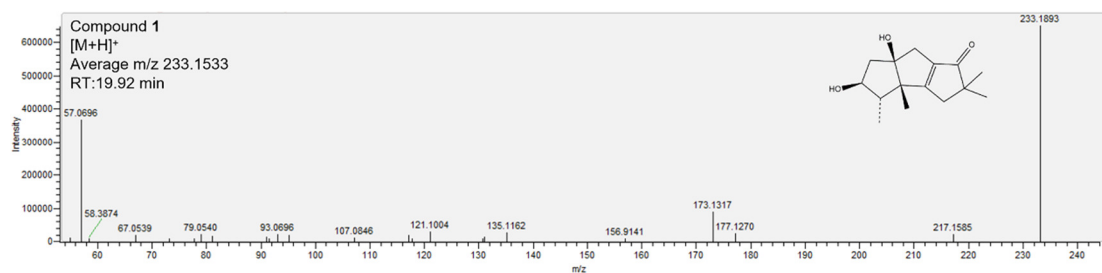
**Figure S17.** The MS/MS spectrum of compound **16** captured by the affinity ultrafiltration from fraction F4-3(P).

**Figure S18.** The MS/MS spectrum of compound **17** captured by the affinity ultrafiltration from fraction F4-3(P).

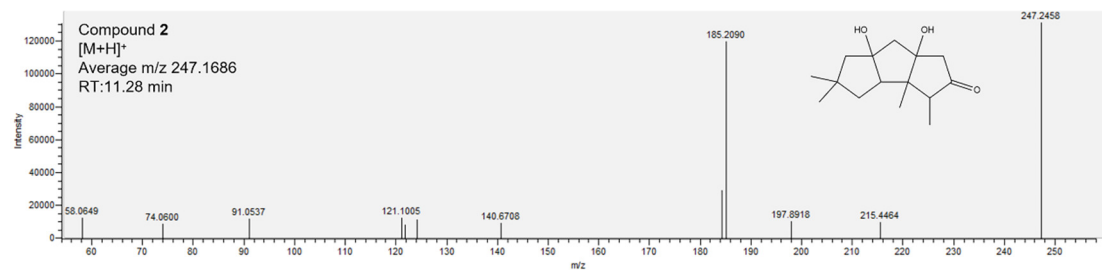
**Figure S19.** The MS/MS spectrum of compound **18** captured by the affinity ultrafiltration from fraction F4-3(P).

**Figure S20.** The MS/MS spectrum of compound **19** captured by the affinity ultrafiltration from fraction F4-3(P).

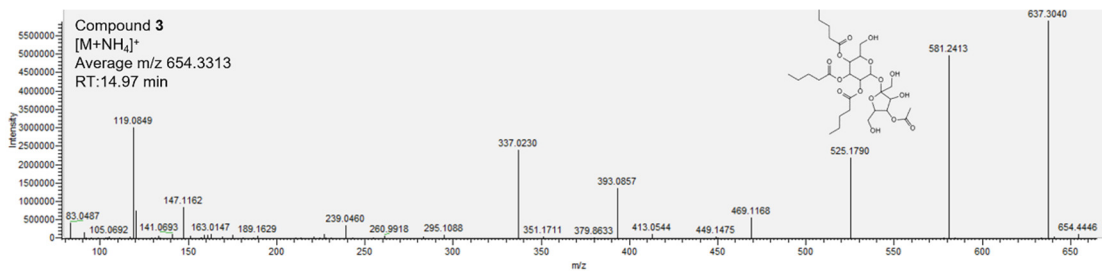
**Figure S21.** The MS/MS spectrum of compound **20** captured by the affinity ultrafiltration from fraction F4-3(P).



**Figure S1**



**Figure S2**



**Figure S3**

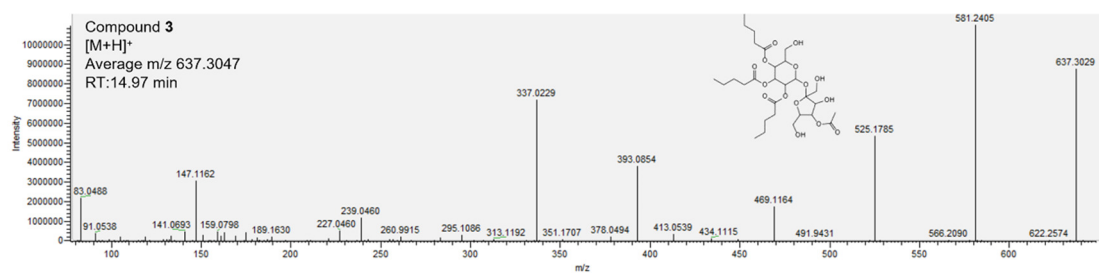


Figure S4

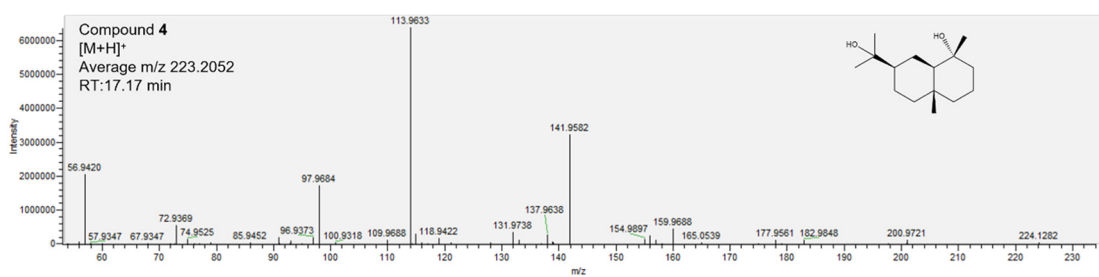


Figure S5

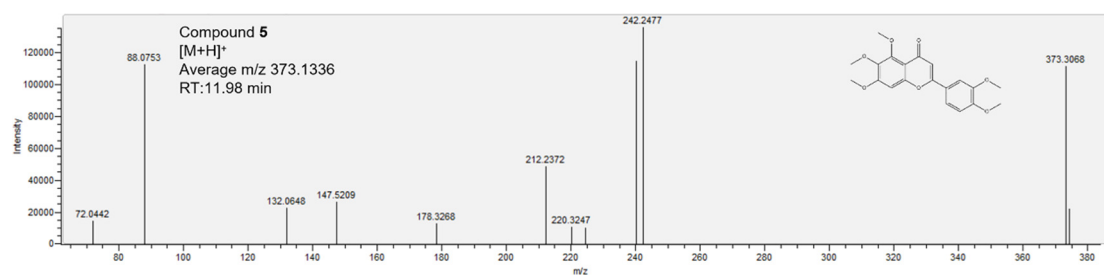


Figure S6

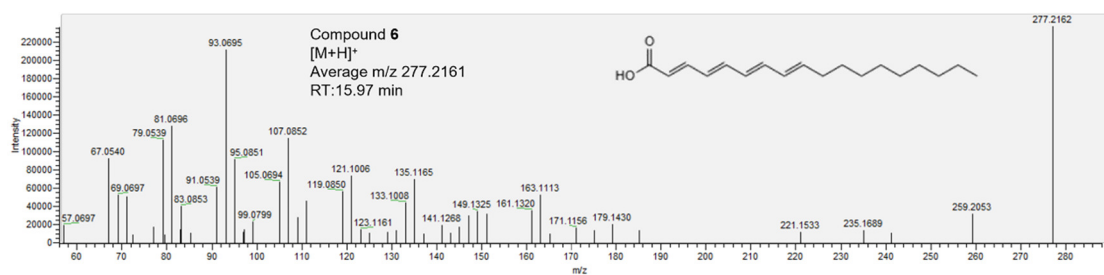


Figure S7

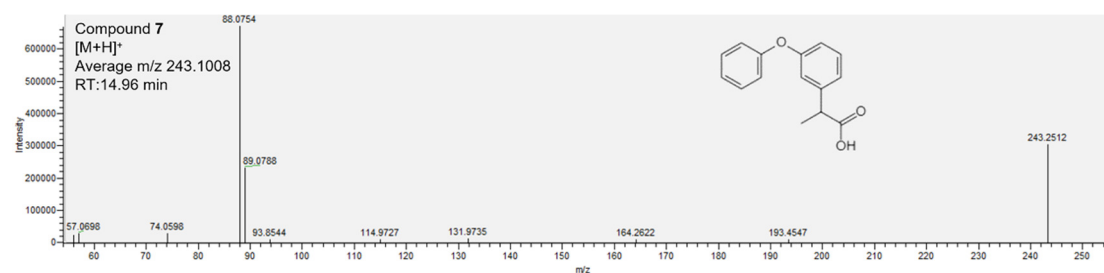


Figure S8

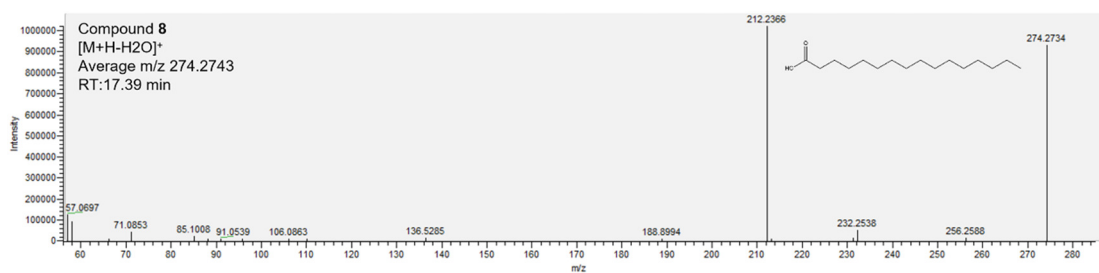


Figure S9

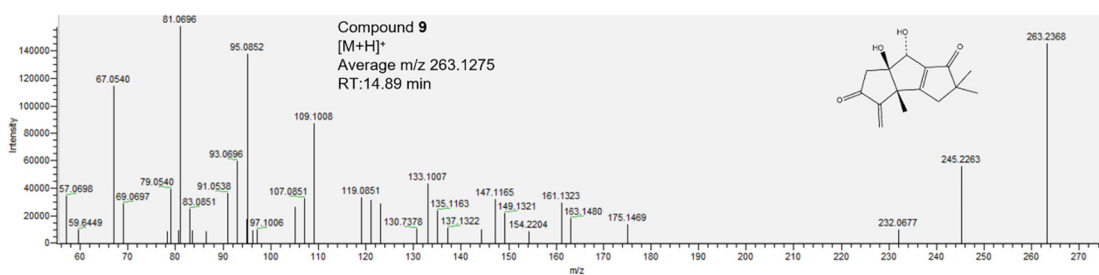


Figure S10

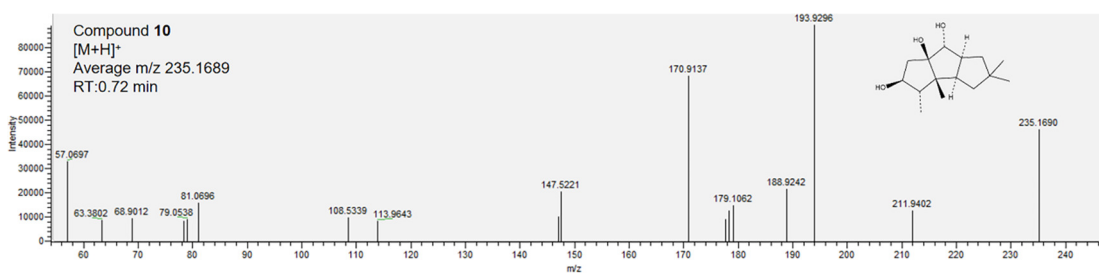


Figure S11

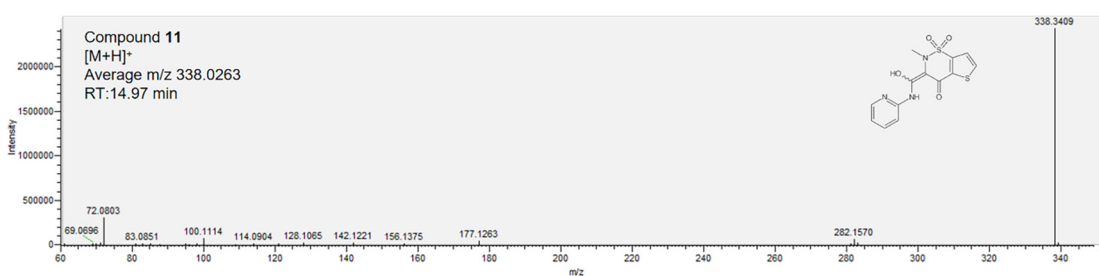


Figure S12

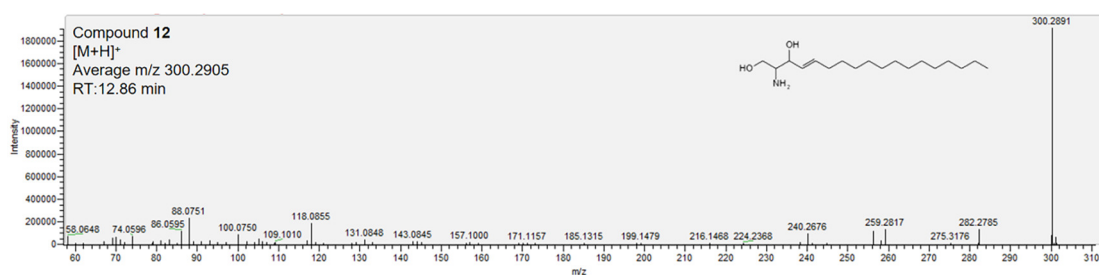


Figure S13

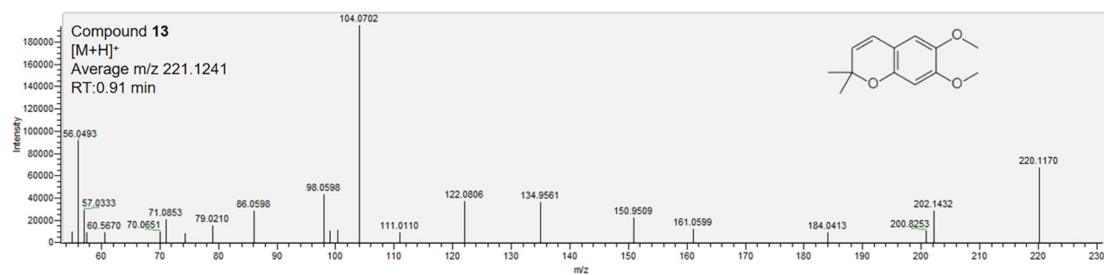


Figure S14

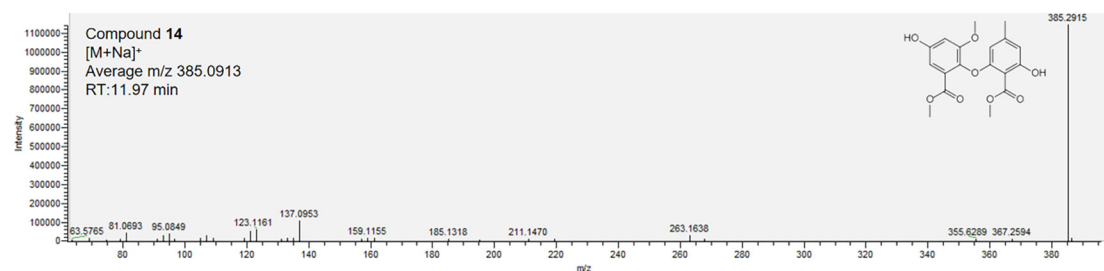


Figure S15

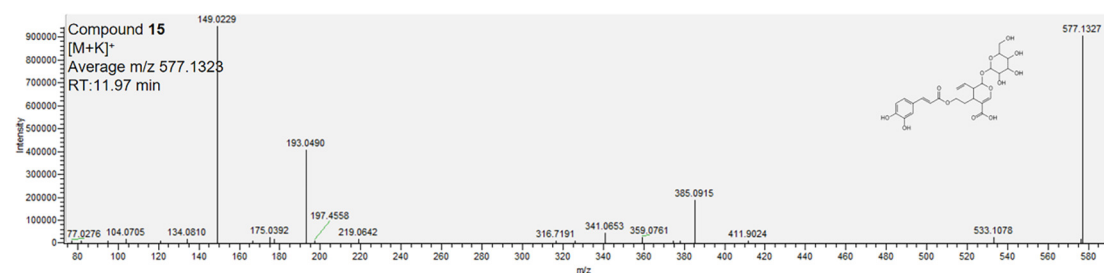


Figure S16

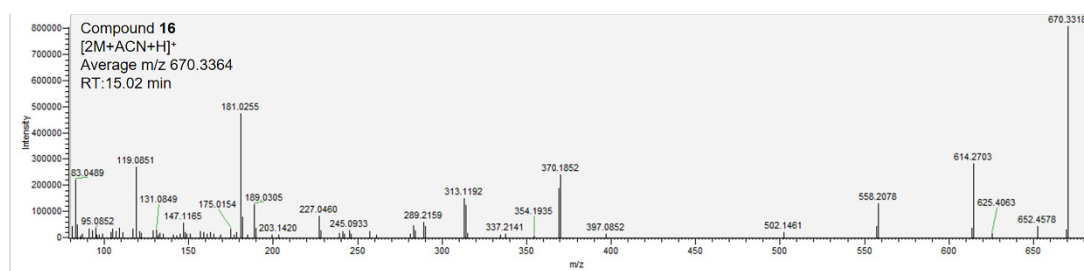
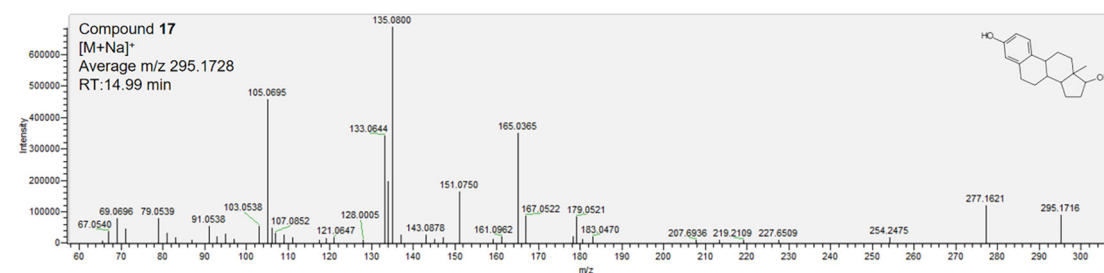
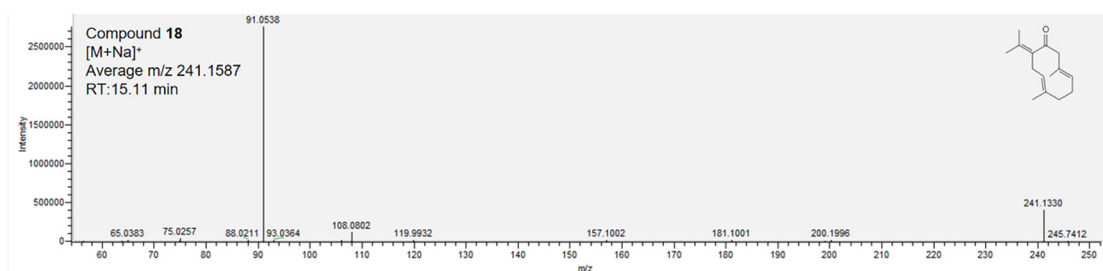


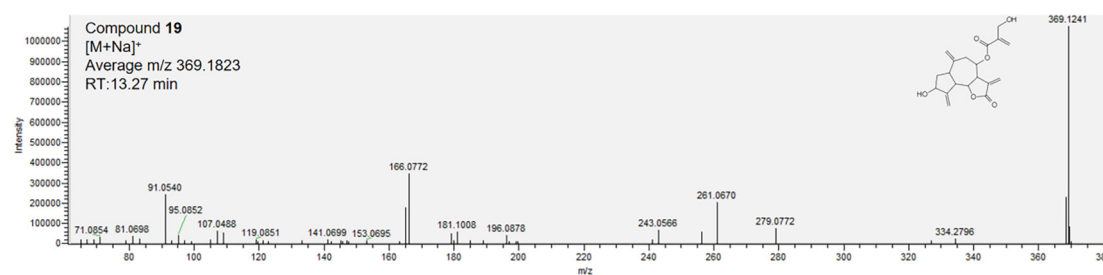
Figure S17



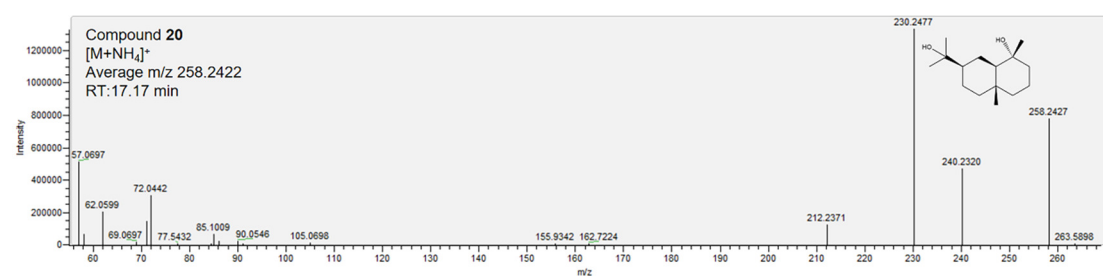
**Figure S18**



**Figure S19**



**Figure S20**



**Figure S21**