

Supplementary materials

# LC-TOF-ESI-MS Patterns of Hirsutinolide-like Sesquiterpenoids from *Elephantopus mollis* Kunth Alongside Chemophenetic significance of its chemical constituents

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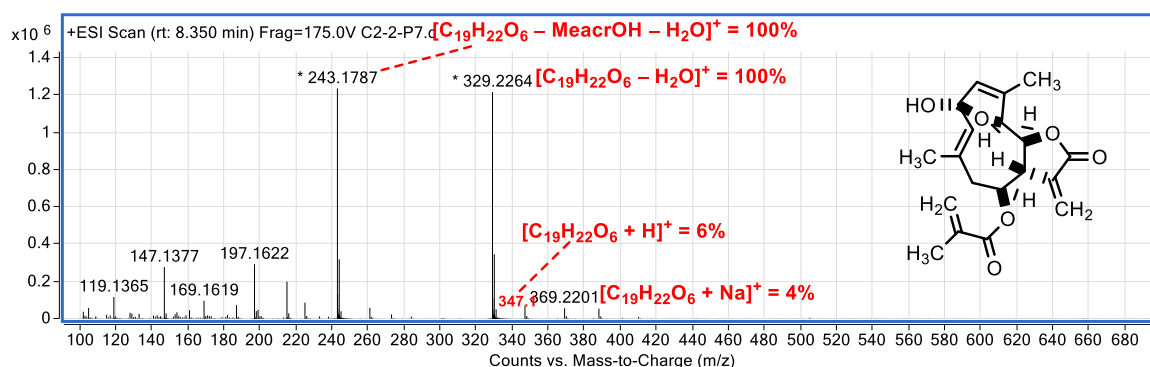


Figure S1. ESI-TOF-MS of compound 1.

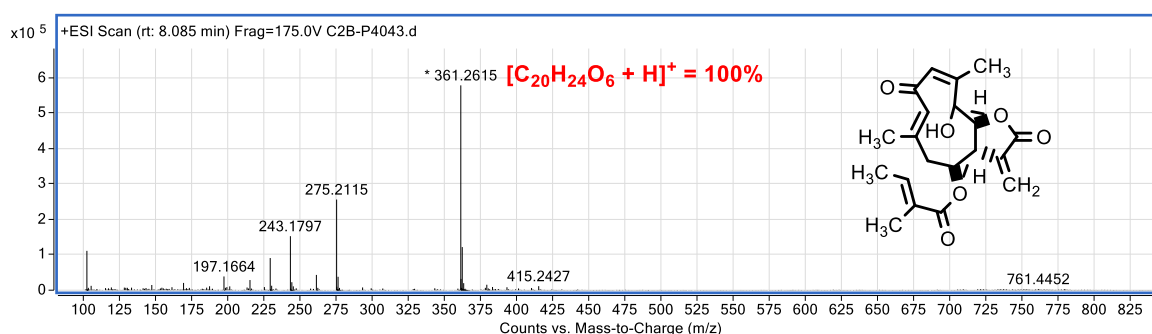


Figure S2. ESI-TOF-MS of compound 7.

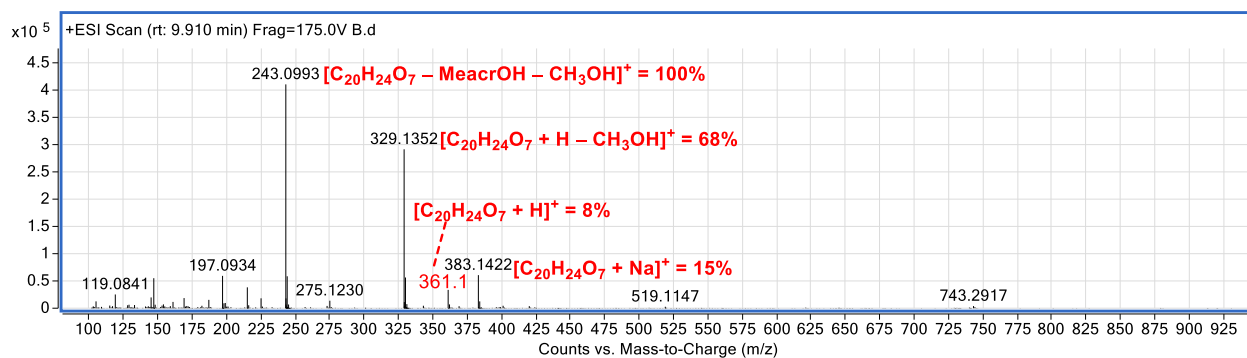


Figure S3. ESI-TOF-MS of compound 2.

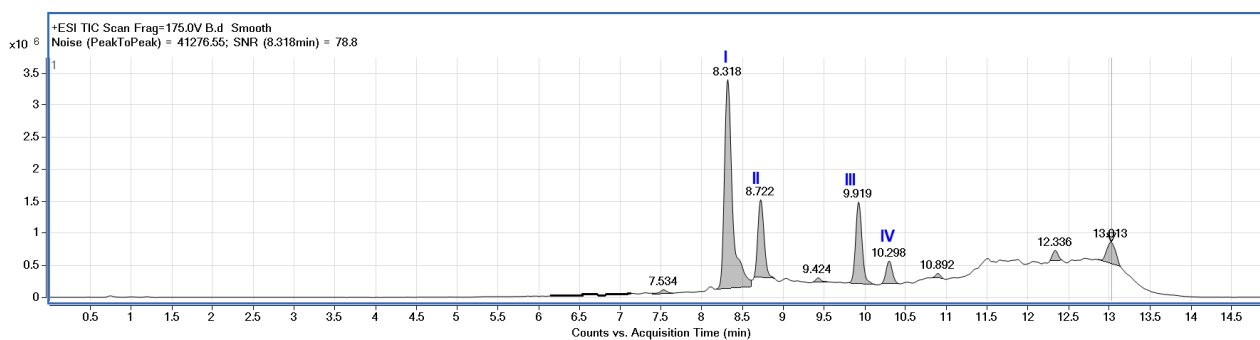
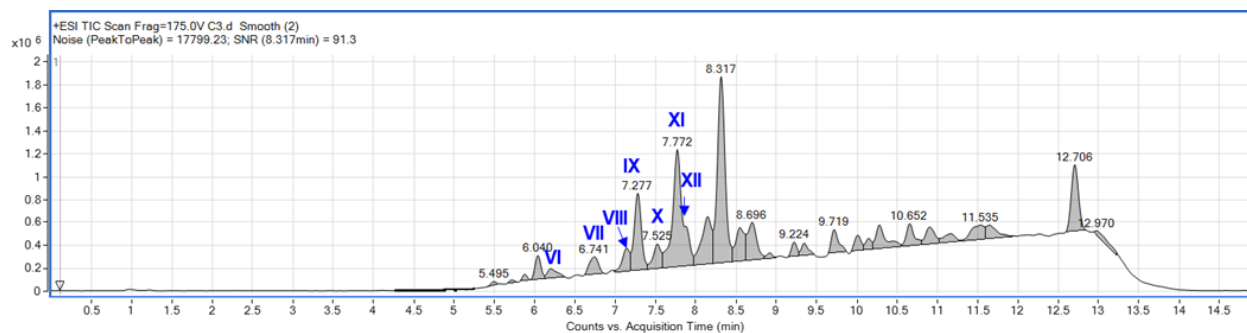


Figure S4. LC chromatogram of main fraction B.



$[C_{19}H_{24}O_7 - MeacrOH - 2H_2O]^+ = 43\%$

$[C_{19}H_{24}O_7 - MeacrOH - H_2O]^+ = 53\%$

$[C_{19}H_{24}O_7 - MeacrOH]^+ = 42\%$

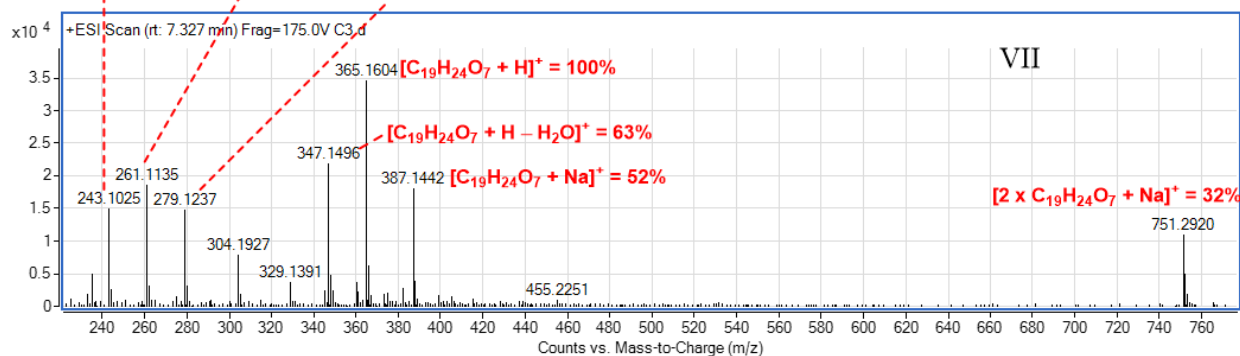


Figure S5. LC profile of subfraction C3 and ESI-TOF-MS of compound 4.

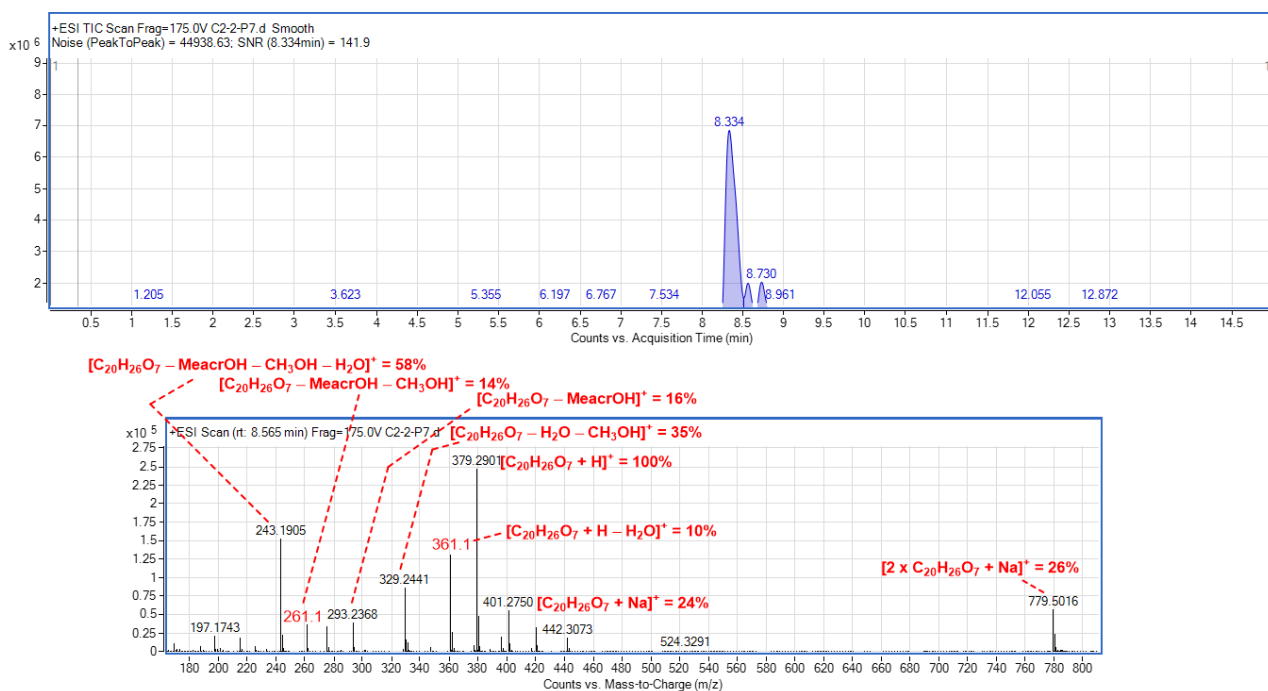


Figure S6. LC chromatogram of sub-fraction P1C-C2-2P7.

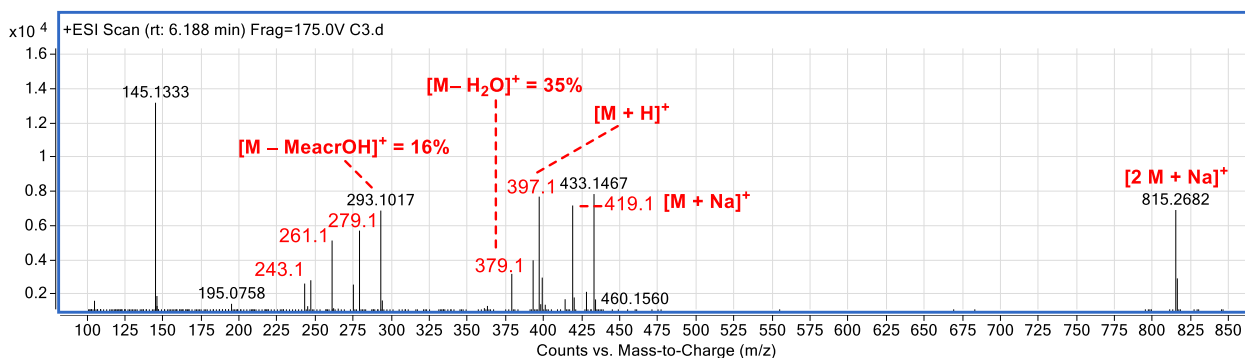


Figure S7. ESI-TOF-MS of peak VI.

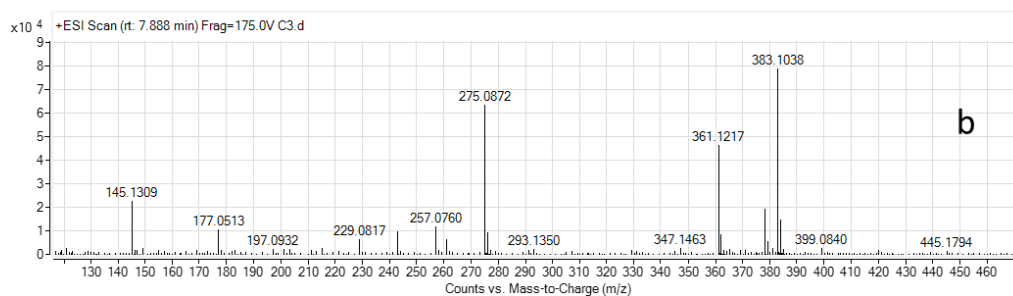
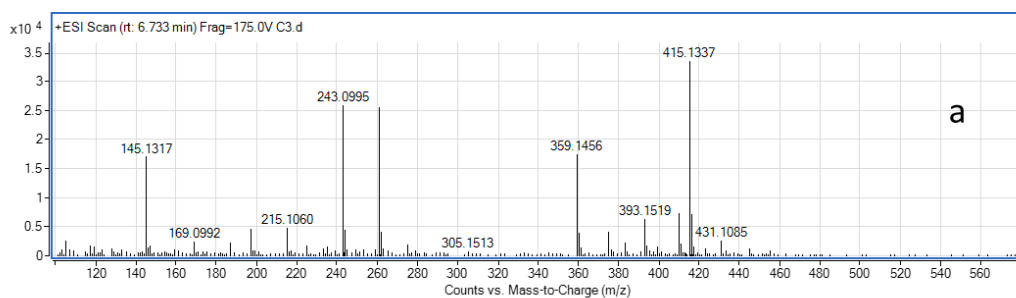


Figure S8. LC chromatogram of (a) peak VII and (b) peak XII.

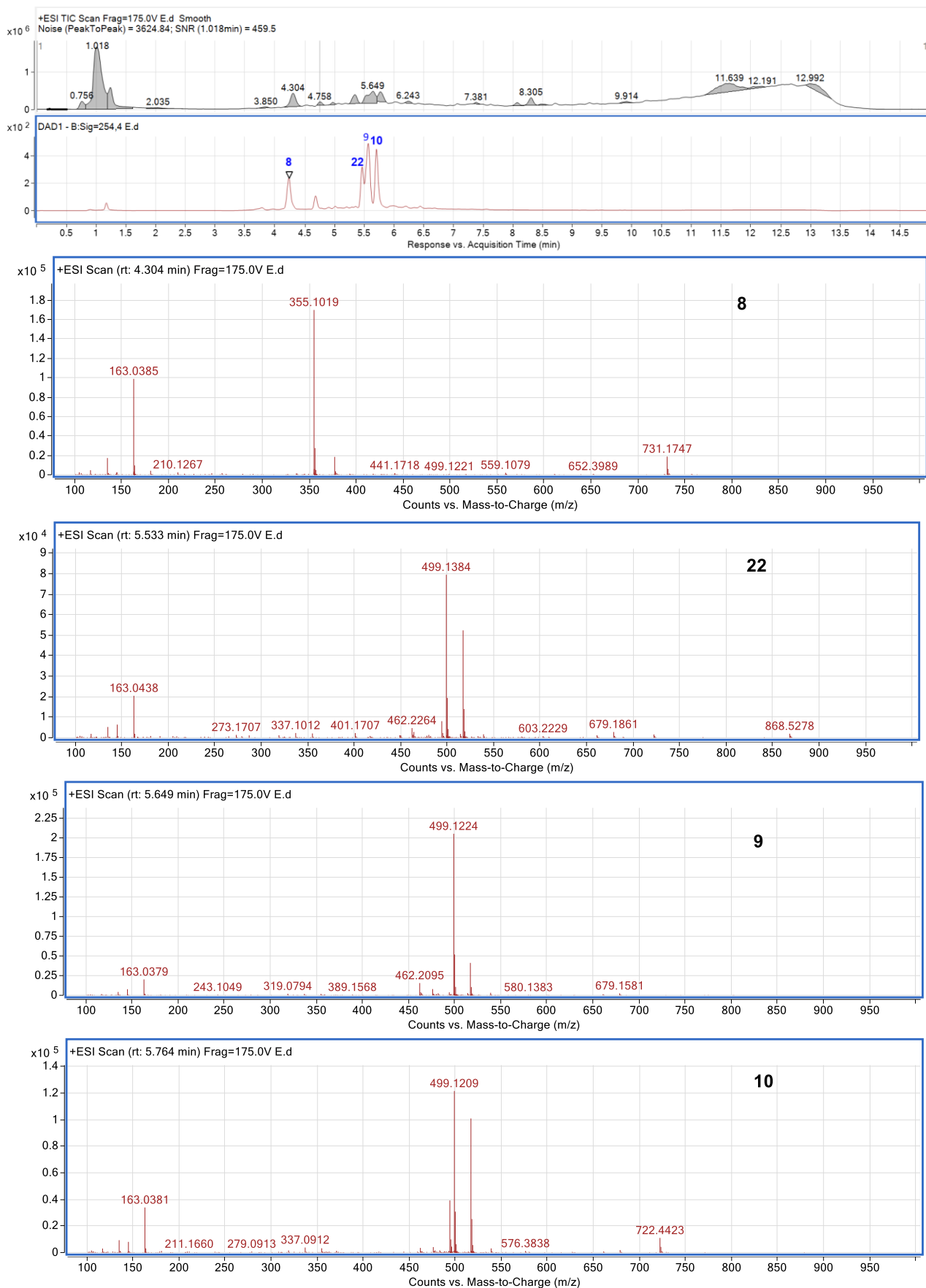


Figure S9. LC chromatogram of quinic acid derivations 8-10 and 22.

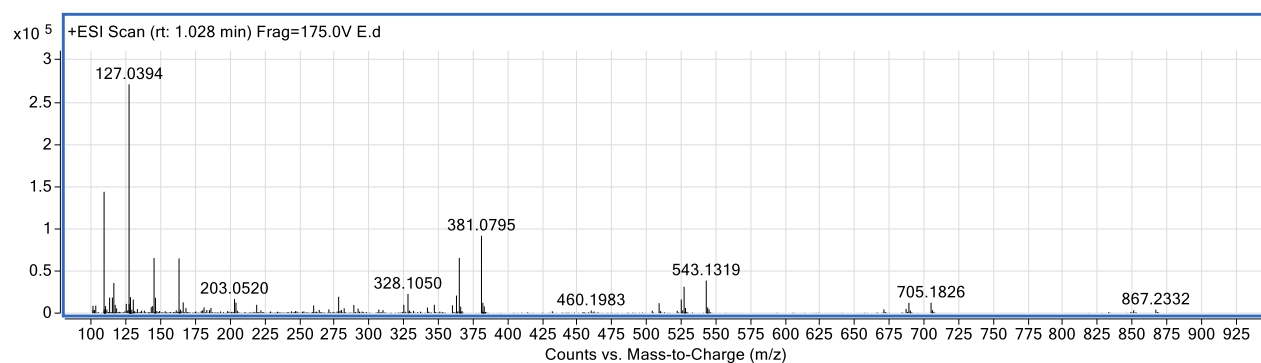


Figure S10. LC chromatogram of crude extract P1E and MS profiles of sugars.

**Reveleris<sup>®</sup>**  
**X2**

Method Name:  
Run Name: 2020-07-04\_12-54-51-b  
Run Date: 2020-07-04 13:09

**BUCHI**

Column: FP Si 24g(weld cap)  
Flow Rate: 20 mL/min  
Equilibration: 6.6 min  
Run Length: 38.6 min  
Mode: Flash Liquid

Solvent A: Petroleum Ether  
Solvent B: Ethyl acetate  
Solvent C: Empty  
Solvent D: Empty  
Slope Detection: Off

UV Threshold: 0.05 AU  
UV Sensitivity: Low  
UV1 Wavelength: 254 nm  
UV2 Wavelength: 265 nm  
UV3 Wavelength: 280 nm

ELSD Threshold: 20 mV  
ELSD Sensitivity: Low  
Collection: Collect Peaks  
Per-Vial Volume: 18 mL  
Non-Peak Volume: 18 mL

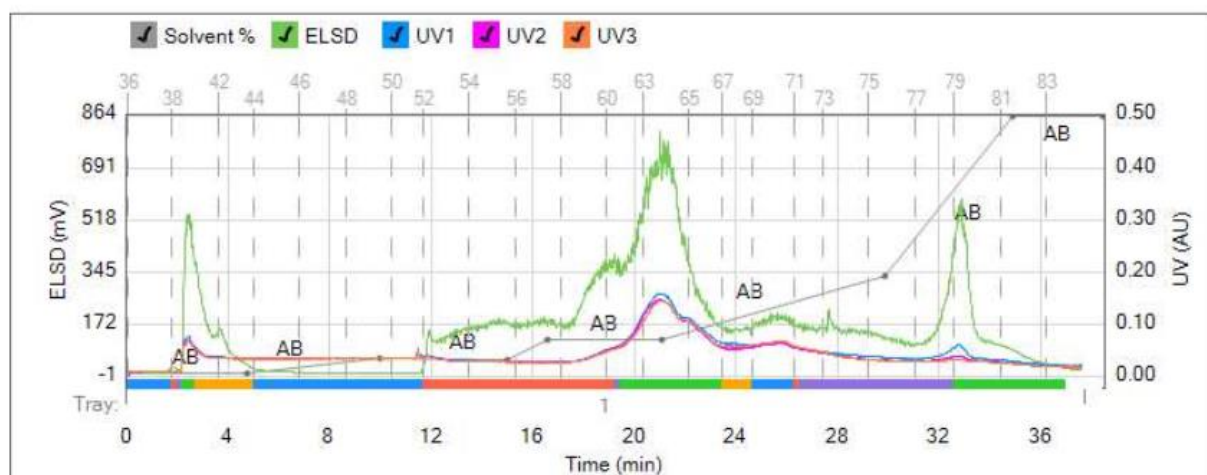


Figure S11. MPLC chromatogram of fraction P1B.

**Reveleris<sup>®</sup>**  
X2

Method Name:  
Run Name: 2020-05-23\_14-43-26-c2-bleue  
Run Date: 2020-05-23 14:57

BUCHI

Column: FP Si 24g(weld cap)  
Flow Rate: 32 mL/min  
Equilibration: 6.6 min  
Run Length: 45.0 min  
Mode: Flash Liquid

Solvent A: Dichloromethane  
Solvent B: Ethyl acetate  
Solvent C: Empty  
Solvent D: Empty  
Slope Detection: Off

UV Threshold: 0.05 AU  
UV Sensitivity: Low  
UV1 Wavelength: 254 nm  
UV2 Wavelength: 265 nm  
UV3 Wavelength: 280 nm

ELSD Threshold: 20 mV  
ELSD Sensitivity: Low  
Collection: Collect All  
Per-Vial Volume: 18 mL  
Non-Peak Volume: 18 mL

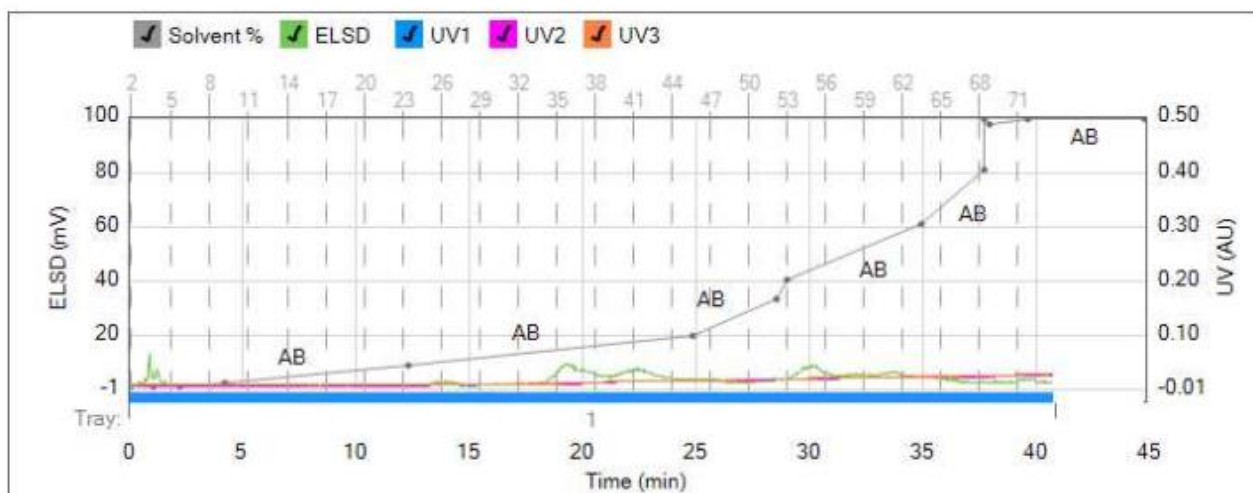


Figure S12. MPLC chromatogram of fraction P1C2.

**Reveleris<sup>®</sup>**  
X2

Method Name:  
Run Name: 2020-03-13\_08-03-10-pl-c2-2  
Run Date: 2020-03-13 08:14

BUCHI

Column: FP Si 24g(weld cap)  
Flow Rate: 32 mL/min  
Equilibration: 4.0 min  
Run Length: 22.0 min  
Mode: Flash Liquid

Solvent A: Petroleum Ether  
Solvent B: Ethyl acetate  
Solvent C: Empty  
Solvent D: Empty  
Slope Detection: Off

UV Threshold: 0.05 AU  
UV Sensitivity: Low  
UV1 Wavelength: 254 nm  
UV2 Wavelength: 265 nm  
UV3 Wavelength: 280 nm

ELSD Threshold: 20 mV  
ELSD Sensitivity: Low  
Collection: Collect Peaks  
Per-Vial Volume: 18 mL  
Non-Peak Volume: 18 mL

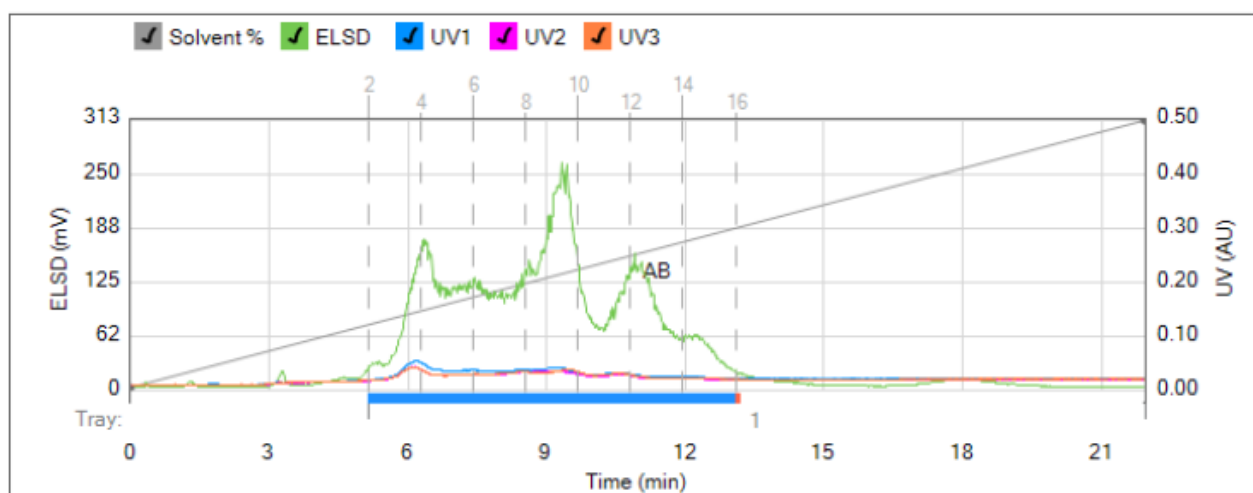


Figure S13. MPLC chromatogram of sub-fraction P1C2-2.

Column: bypass  
Flow Rate: 20 mL/min  
Equilibration: 5.0 min  
Run Length: 17.0 min  
Mode: Flash Liquid

Solvent A: Water  
Solvent B: Acetonitrile  
Solvent C: Empty  
Solvent D: Empty  
Slope Detection: Off

UV Threshold: 0.05 AU  
UV Sensitivity: Low  
UV1 Wavelength: 254 nm  
UV2 Wavelength: 265 nm  
UV3 Wavelength: 280 nm

ELSD Threshold: 20 mV  
ELSD Sensitivity: Low  
Collection: Collect All  
Per-Vial Volume: 18 mL  
Non-Peak Volume: 18 mL

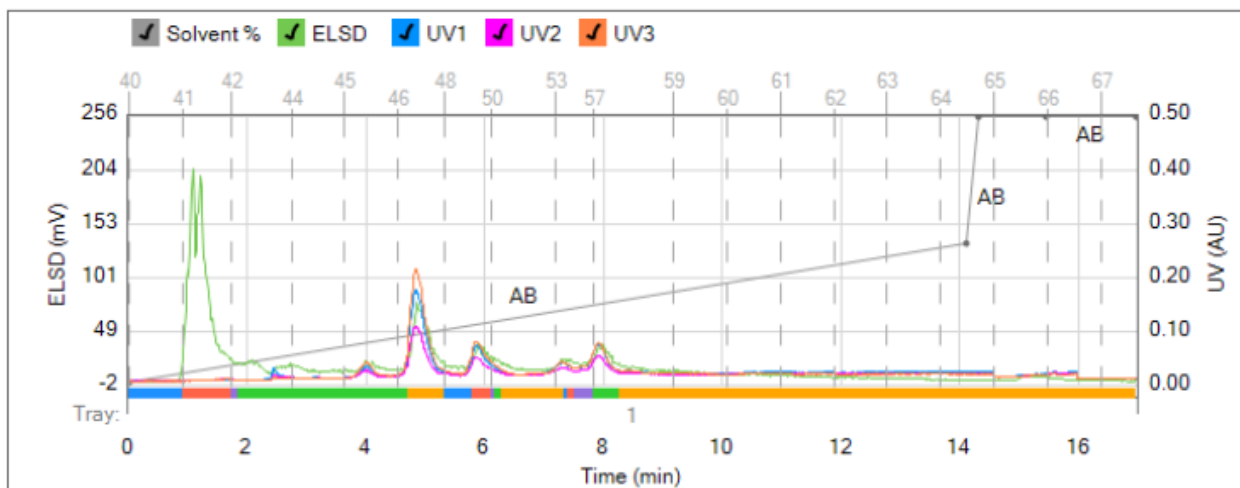


Figure 14. MPLC chromatogram of sub-fraction P1E3.