

Supplementary materials

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

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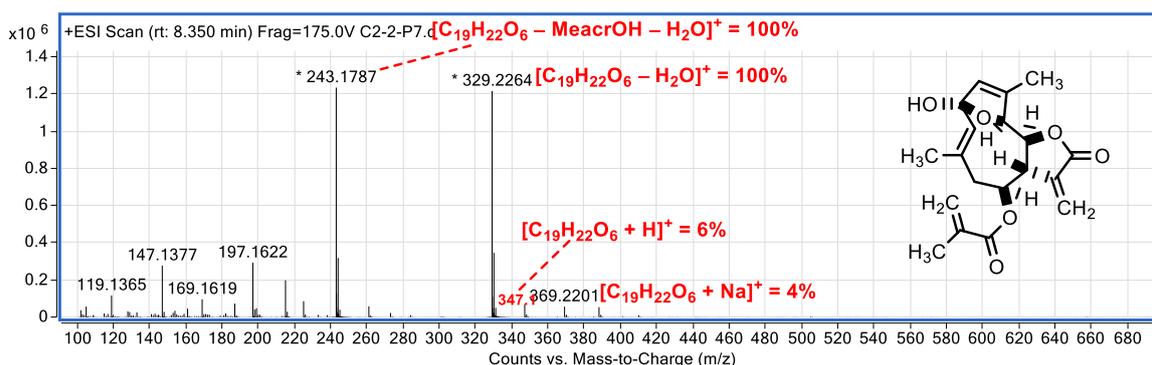


Figure S1. ESI-TOF-MS of compound 1.

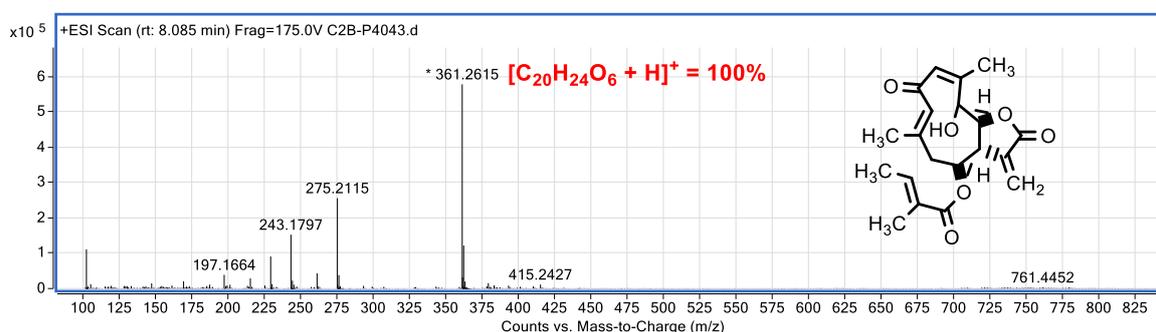


Figure S2. ESI-TOF-MS of compound 7.

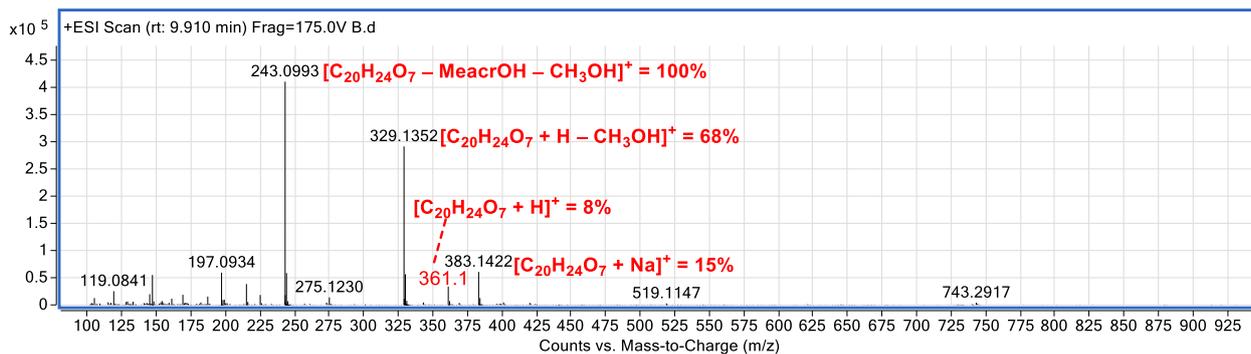


Figure S3. ESI-TOF-MS of compound 2.

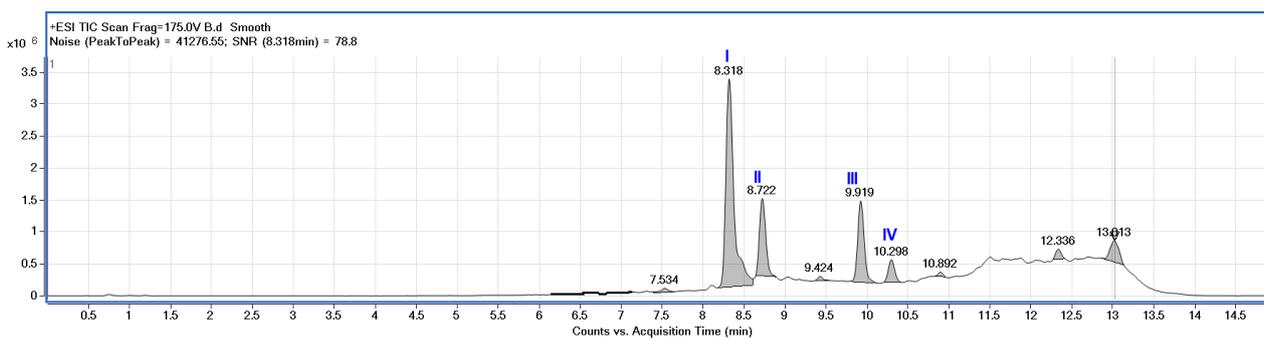
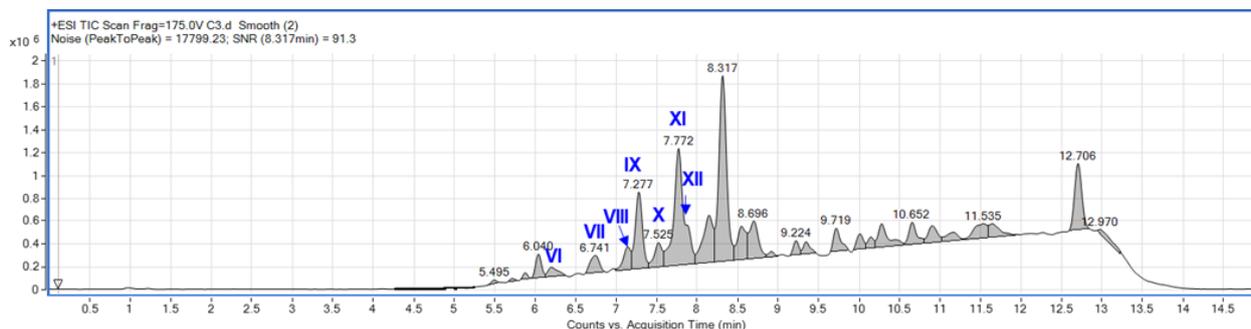


Figure S4. LC chromatogram of main fraction B.



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

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

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

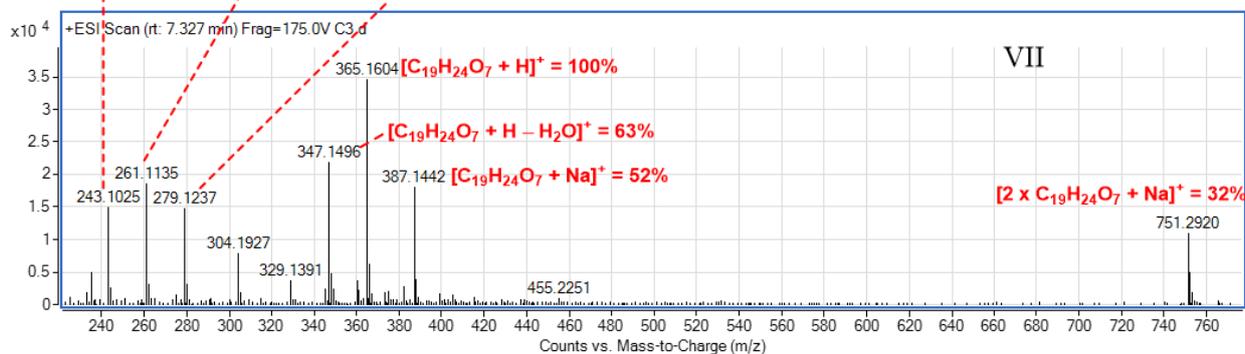


Figure S5. LC profile of subfraction C3 and ESI-TOF-MS of compound 4.

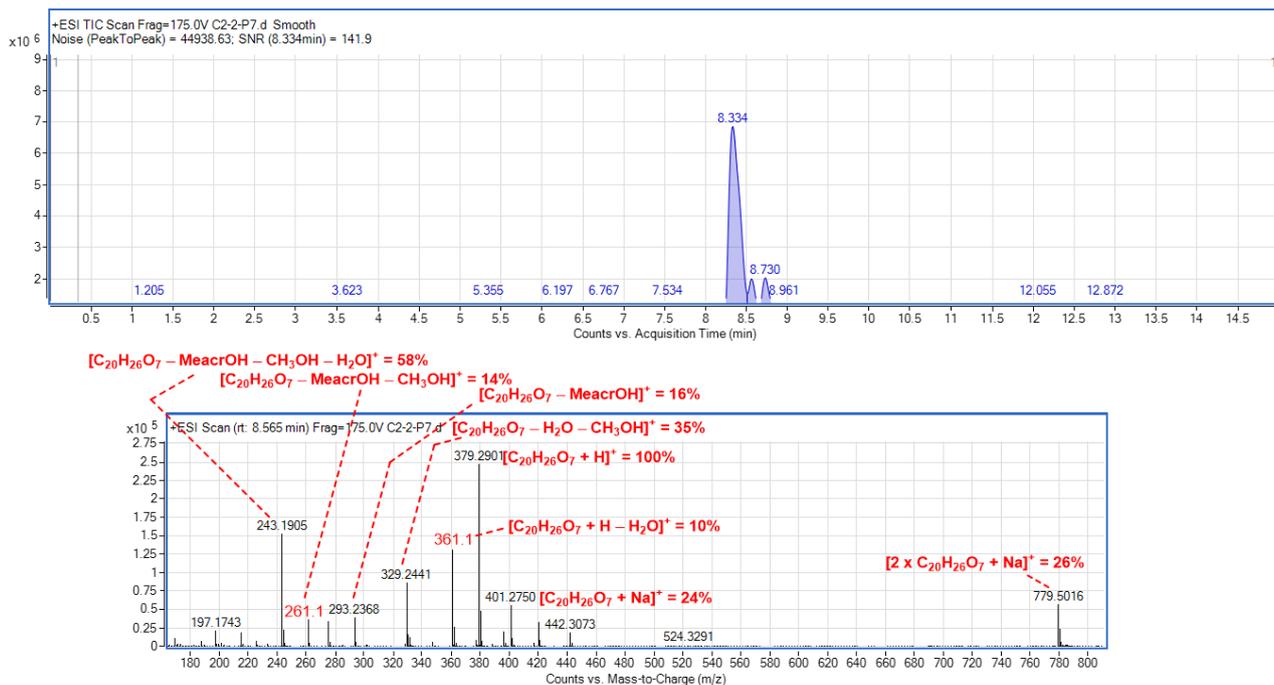


Figure S6. LC chromatogram of sub-fraction P1C-C2-2P7.

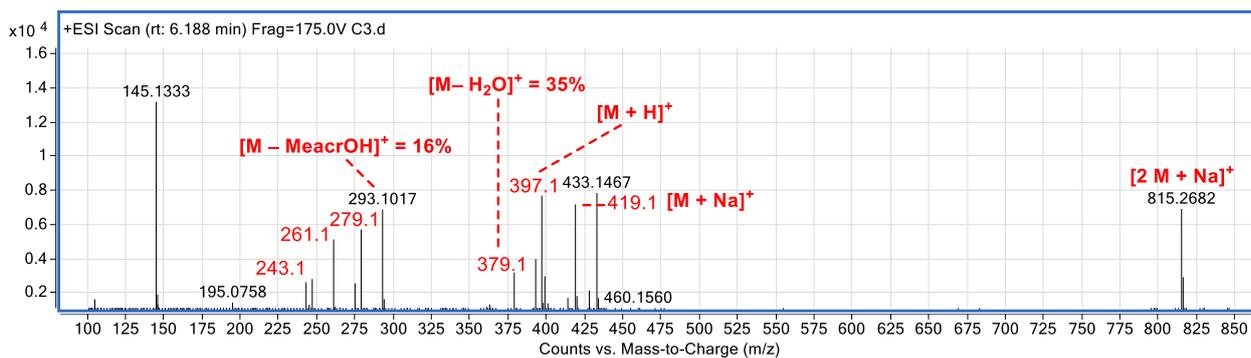


Figure S7. ESI-TOF-MS of peak VI.

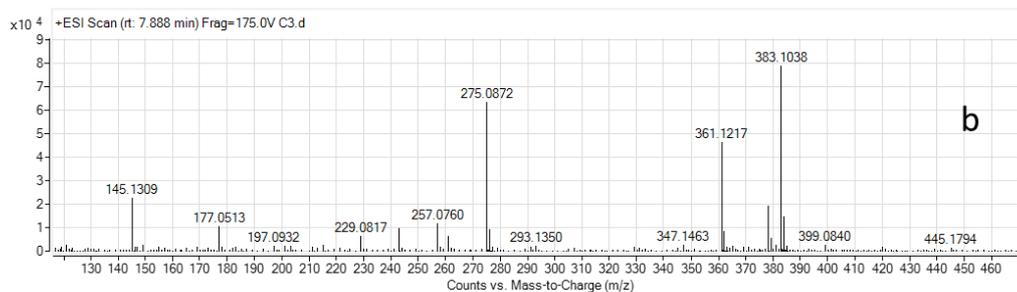
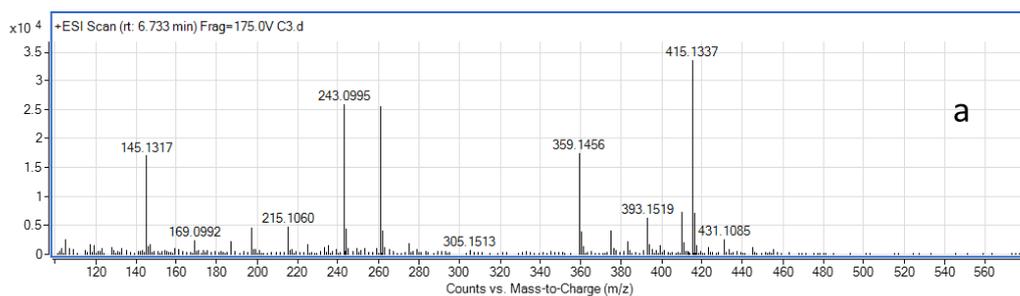


Figure S8. LC chromatogram of (a) peak VII and (b) peak XII.

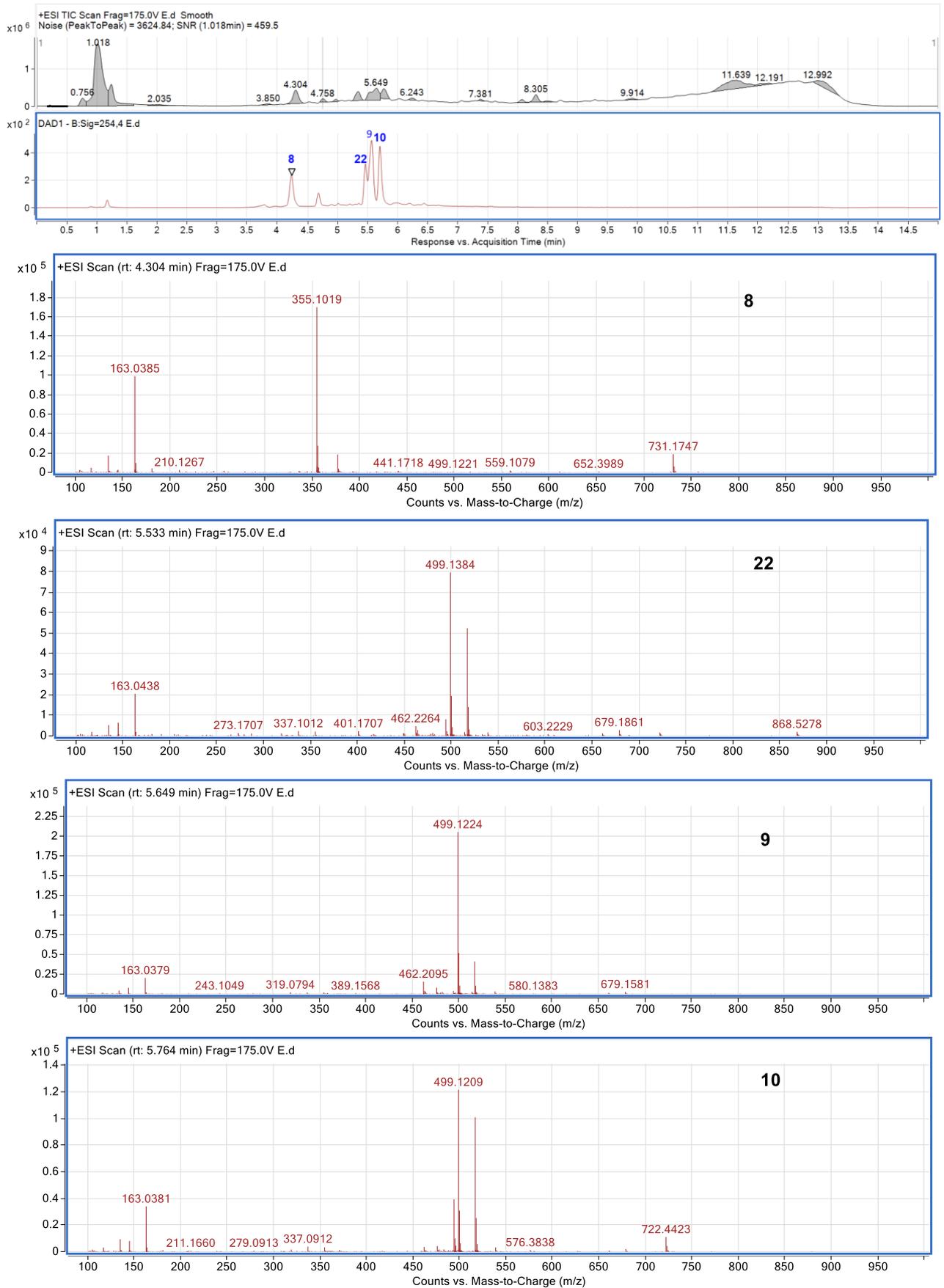


Figure S9. LC chromatogram of quinic acid derivations 8-10 and 22.

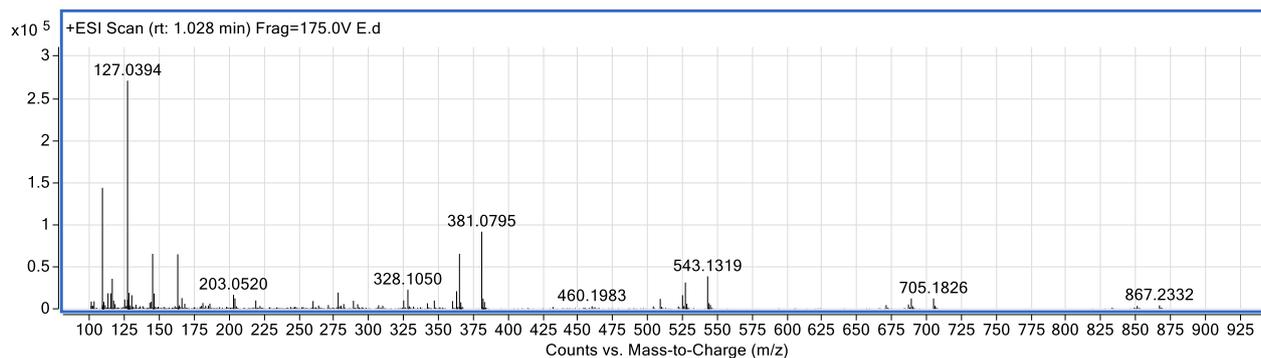


Figure S10. LC chromatogram of crude extract P1E and MS profiles of sugars.

Reveleris[®]
X2

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



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

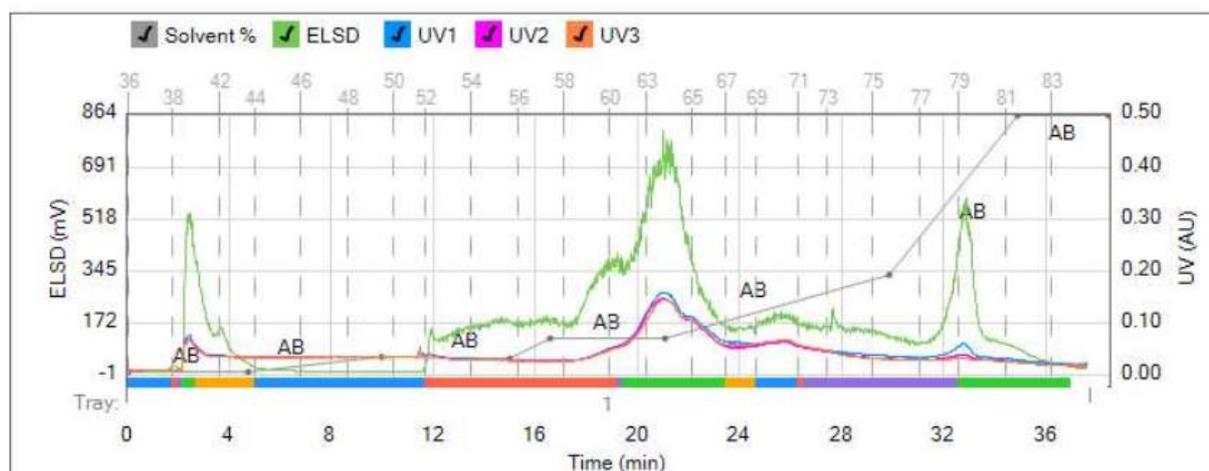


Figure S11. MPLC chromatogram of fraction P1B.

Reveleris[®]
X2

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



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

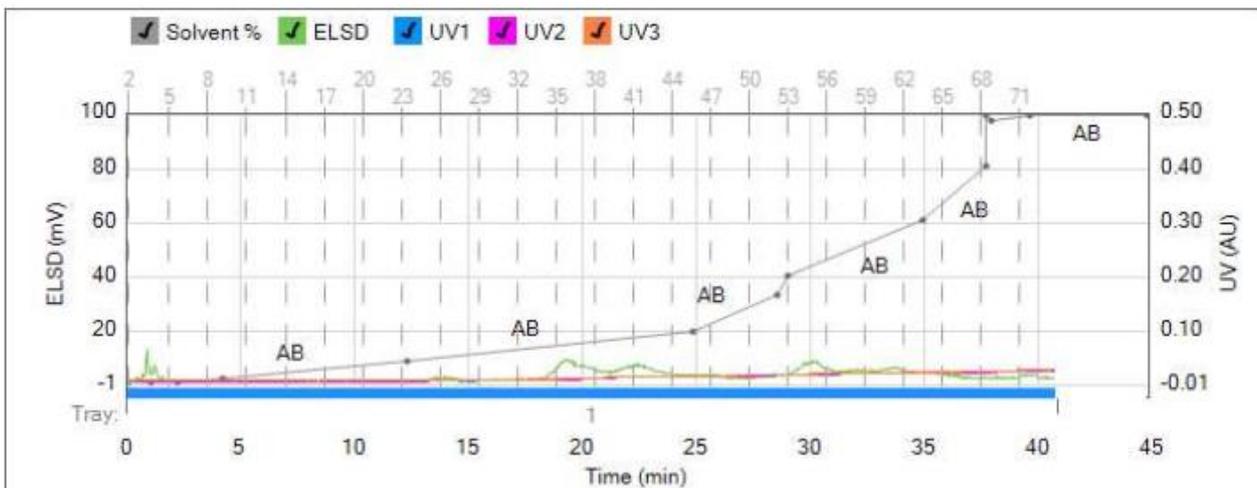


Figure S12. MPLC chromatogram of fraction P1C2.

Reveleris[®]
X2

Method Name:
Run Name: 2020-03-13_08-03-10-p1-c2-2
Run Date: 2020-03-13 08:14



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

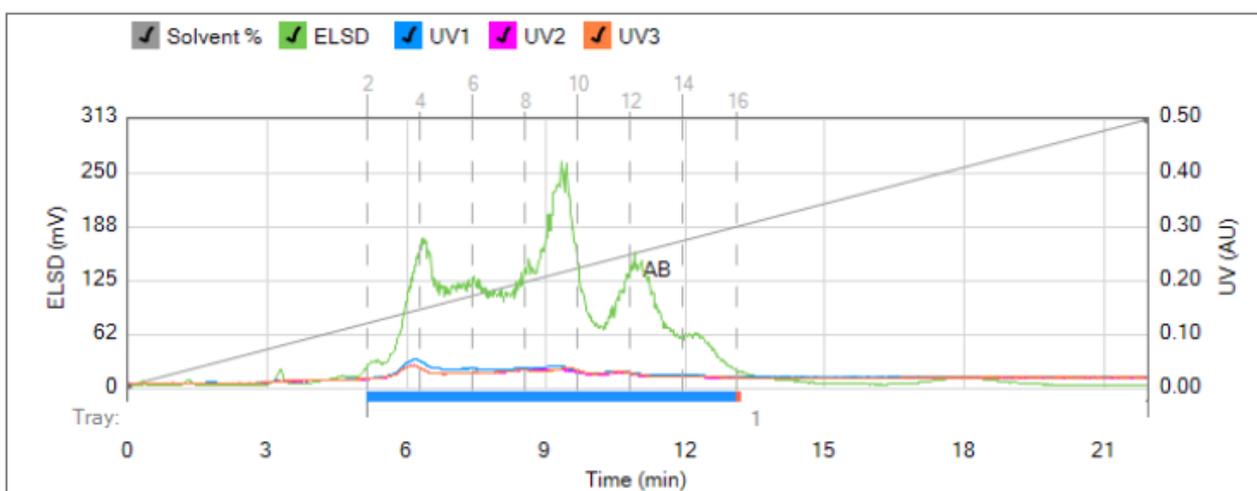


Figure S13. MPLC chromatogram of sub-fraction P1C2-2.

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

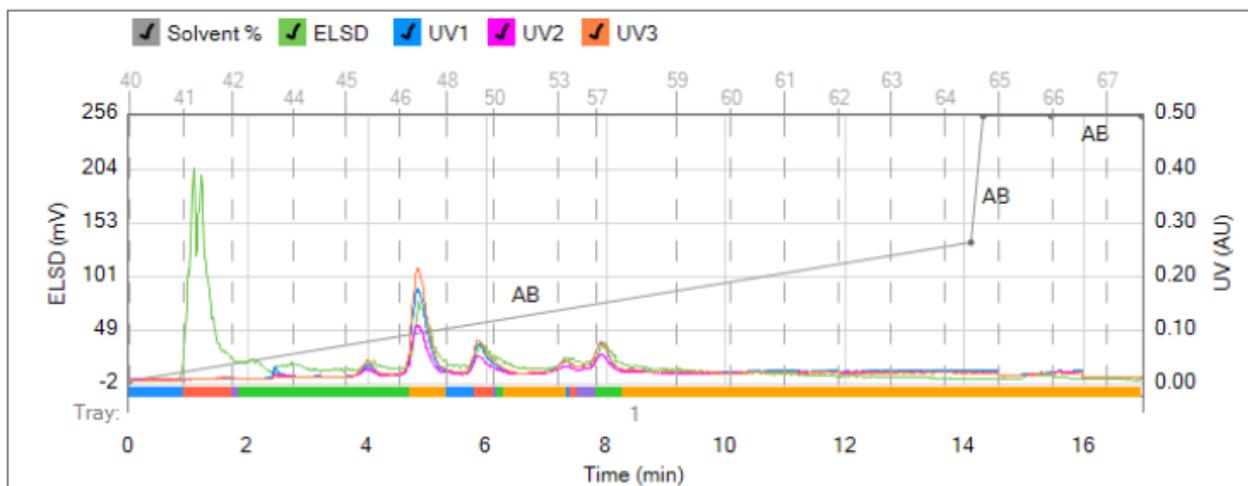


Figure 14. MPLC chromatogram of sub-fraction P1E3.