

Triterpenes and Phenolic Compounds from *Euphorbia deightonii* with Antiviral Activity against Herpes Simplex Virus Type 2

SUPPLEMENTARY MATERIAL

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TABLE OF CONTENT

Figure S1. ^1H NMR spectrum of compound 1 (500 MHz, in CDCl_3)	2
Figure S2. ^{13}C JMOD NMR spectrum of compound 1 (125 MHz, in CDCl_3)	2
Figure S3. HSQC spectrum of compound 1 (in CDCl_3)	3
Figure S4. ^1H - ^1H COSY spectrum of compound 1 (in CDCl_3)	3
Figure S5. HMBC spectrum of compound 1 (in CDCl_3)	4
Figure S6. NOESY spectrum of compound 1 (in CDCl_3)	4
Figure S7. ^1H NMR spectrum of compound 3 (500 MHz, in CDCl_3)	4
Figure S8. ^{13}C JMOD NMR spectrum of compound 3 (125 MHz, in CDCl_3)	4
Figure S9. ^1H NMR spectrum of compound 4 (500 MHz, in CDCl_3)	5
Figure S10. ^{13}C JMOD NMR spectrum of compound 4 (125 MHz, in CDCl_3)	5
Figure S11. HSQC spectrum of compound 4 (in CDCl_3)	6
Figure S12. ^1H - ^1H COSY spectrum of compound 4 (in CDCl_3)	6
Figure S13. HMBC spectrum of compound 4 (in CDCl_3)	7
Figure S14. NOESY spectrum of compound 4 (in CDCl_3)	7
Figure S15. HRMS spectrum of compound 1	8
Figure S16. HRMS spectrum of compound 4	8
Figure S17. Chiral chromatographic separation of compound 4	9
Figure S18. HPLC chromatogram of compound 1	9

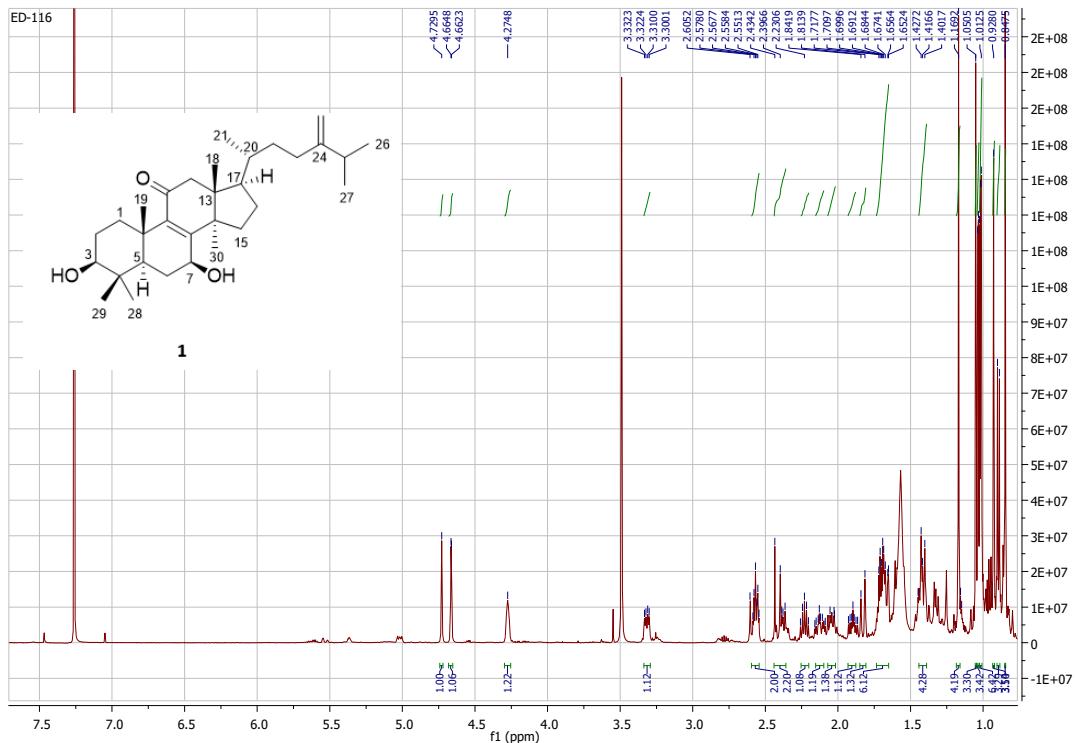


Figure S1. ^1H NMR spectrum of compound **1** (500 MHz, in CDCl_3)

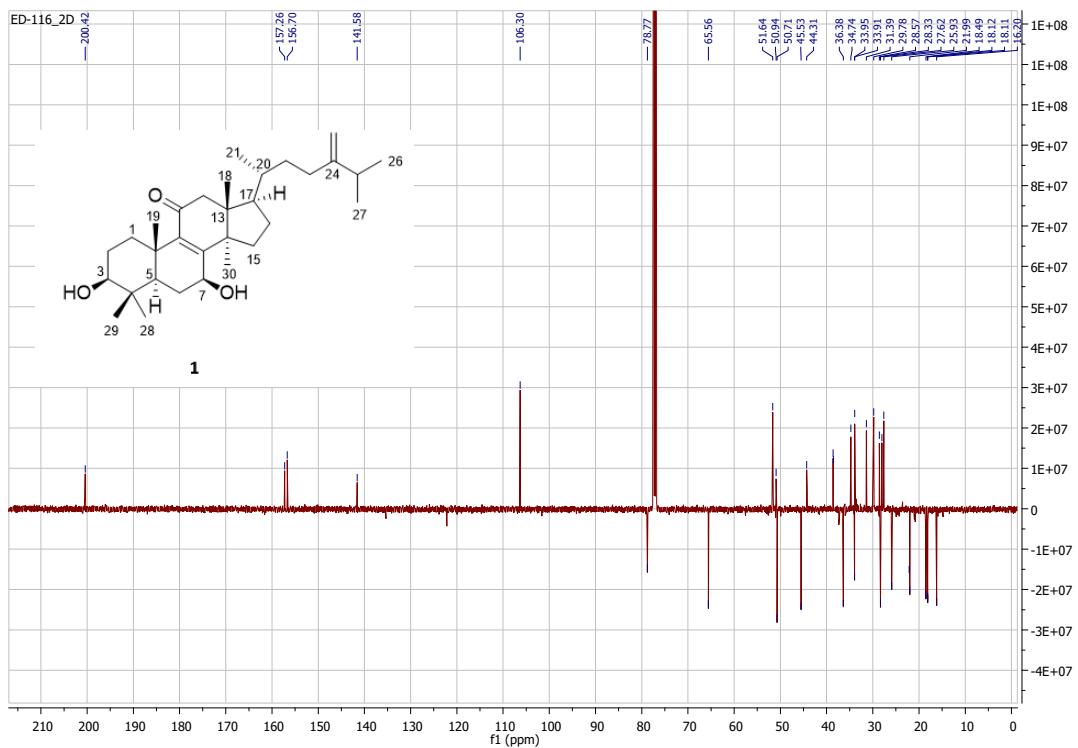


Figure S2. ^{13}C JMOD NMR spectrum of compound **1** (125 MHz, in CDCl_3)

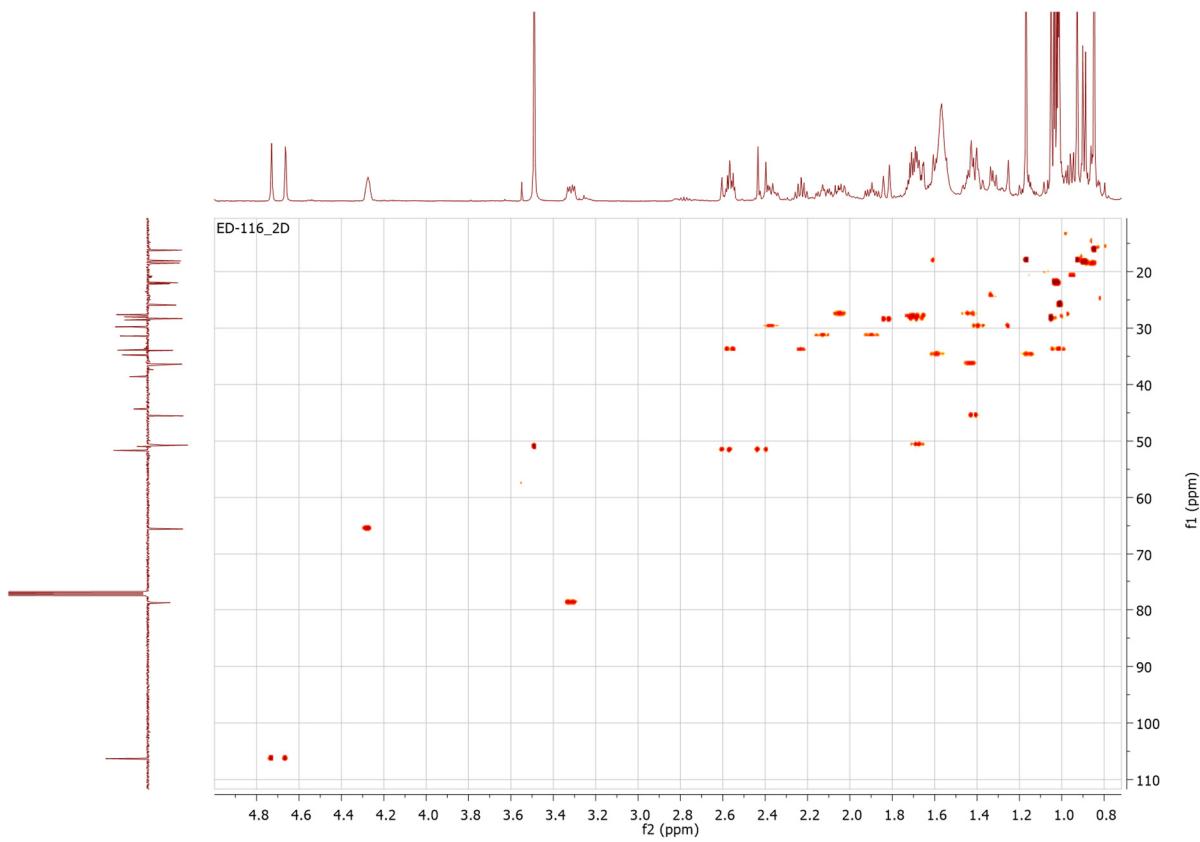


Figure S3. HSQC spectrum of compound **1** (in CDCl_3)

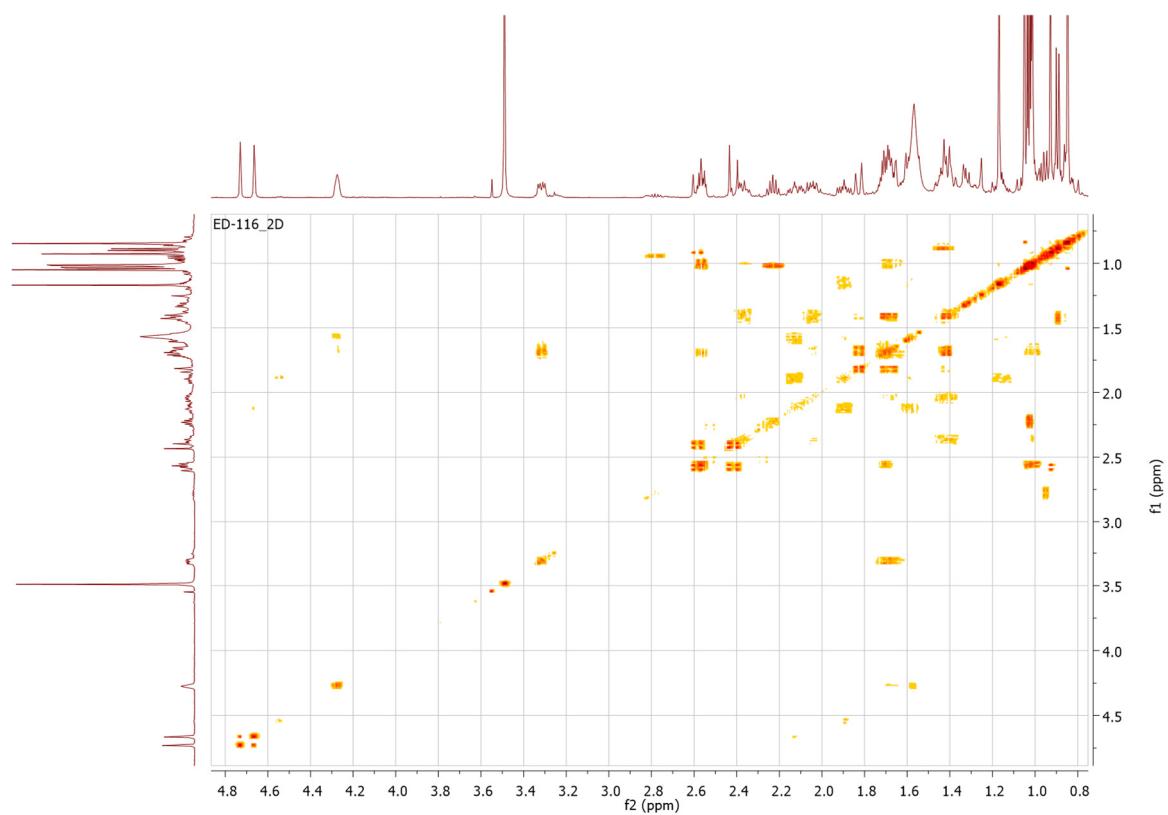


Figure S4. ^1H - ^1H COSY spectrum of compound **1** (in CDCl_3)

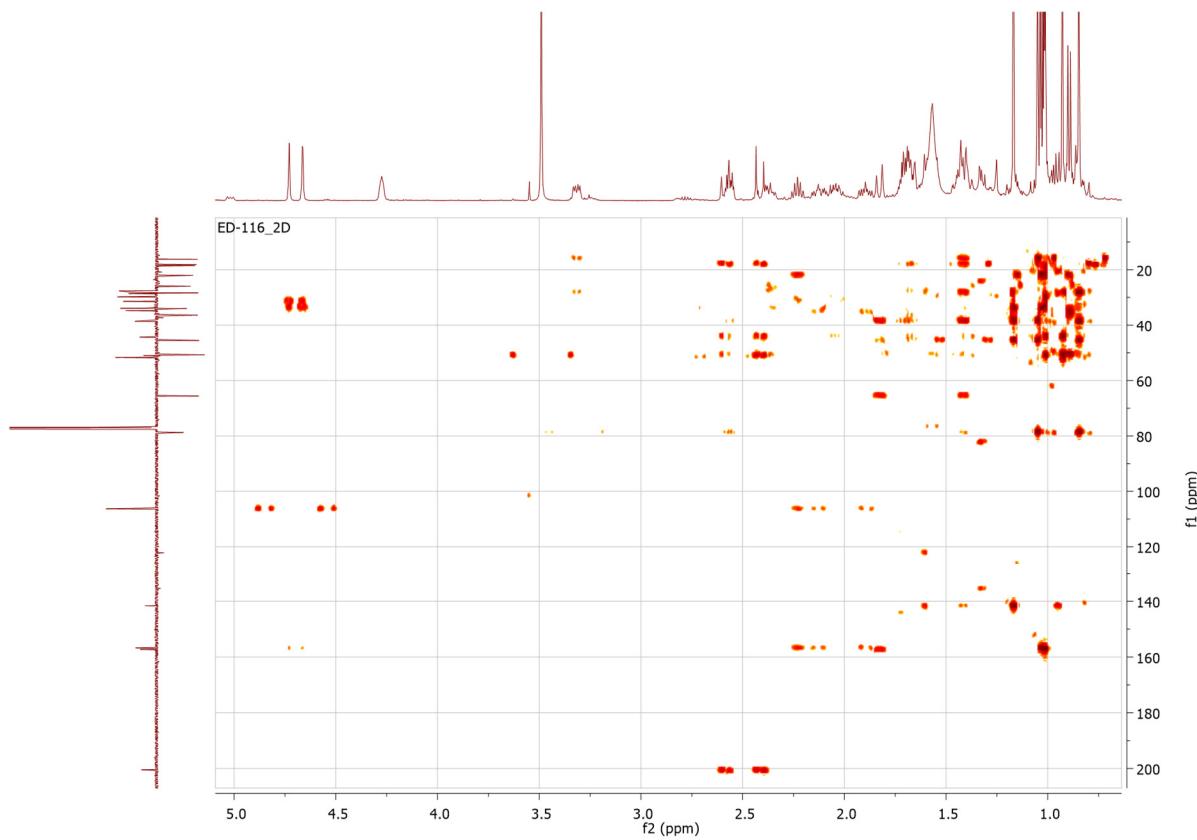


Figure S5. HMBC spectrum of compound **1** (in CDCl_3)

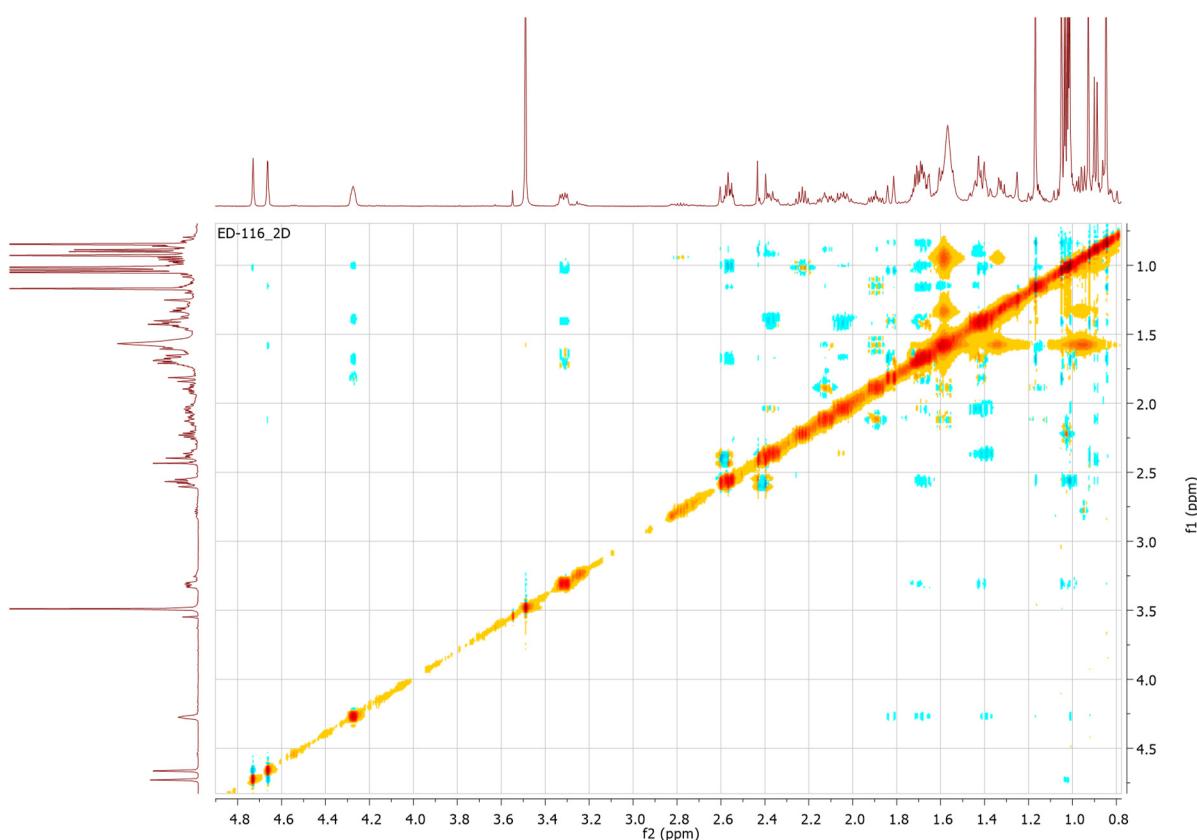


Figure S6. NOESY spectrum of compound **1** (in CDCl_3)

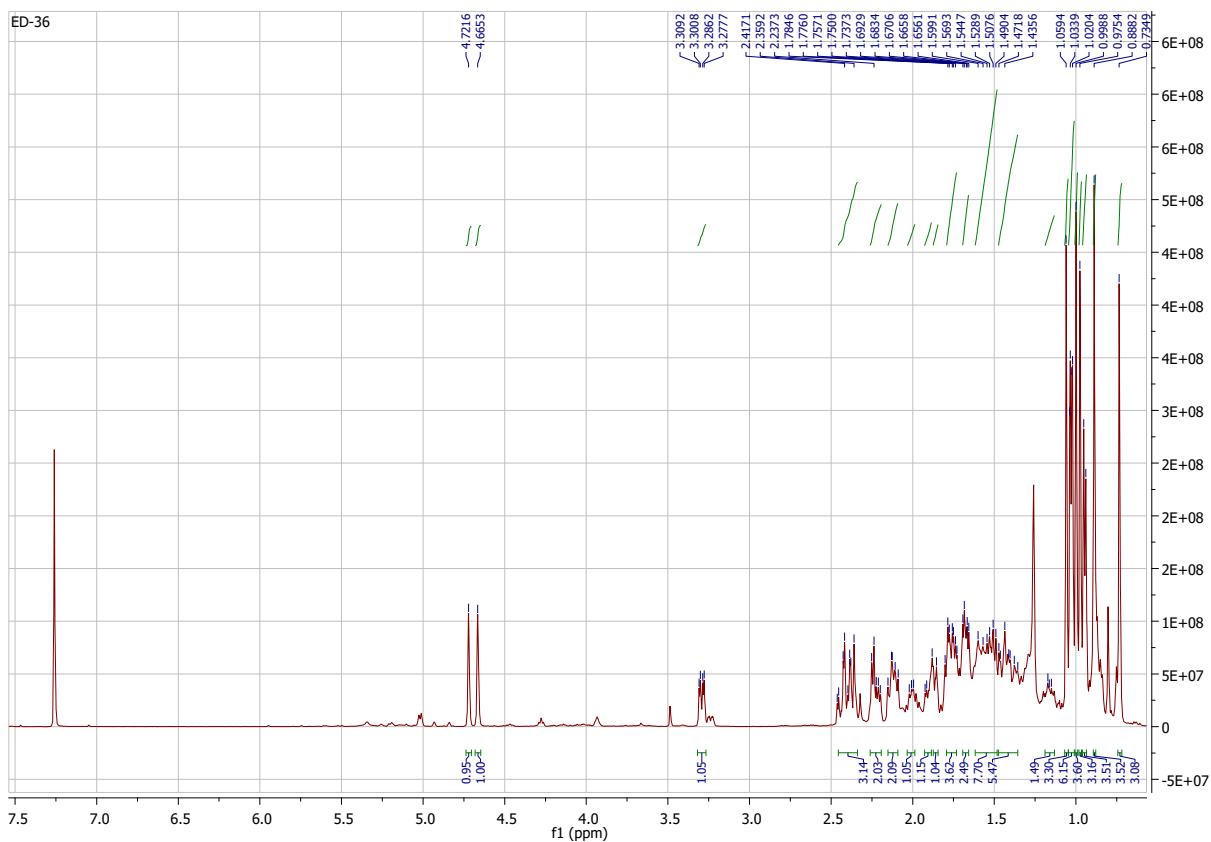


Figure S7. ^1H NMR spectrum of compound **3** (500 MHz, in CDCl_3)

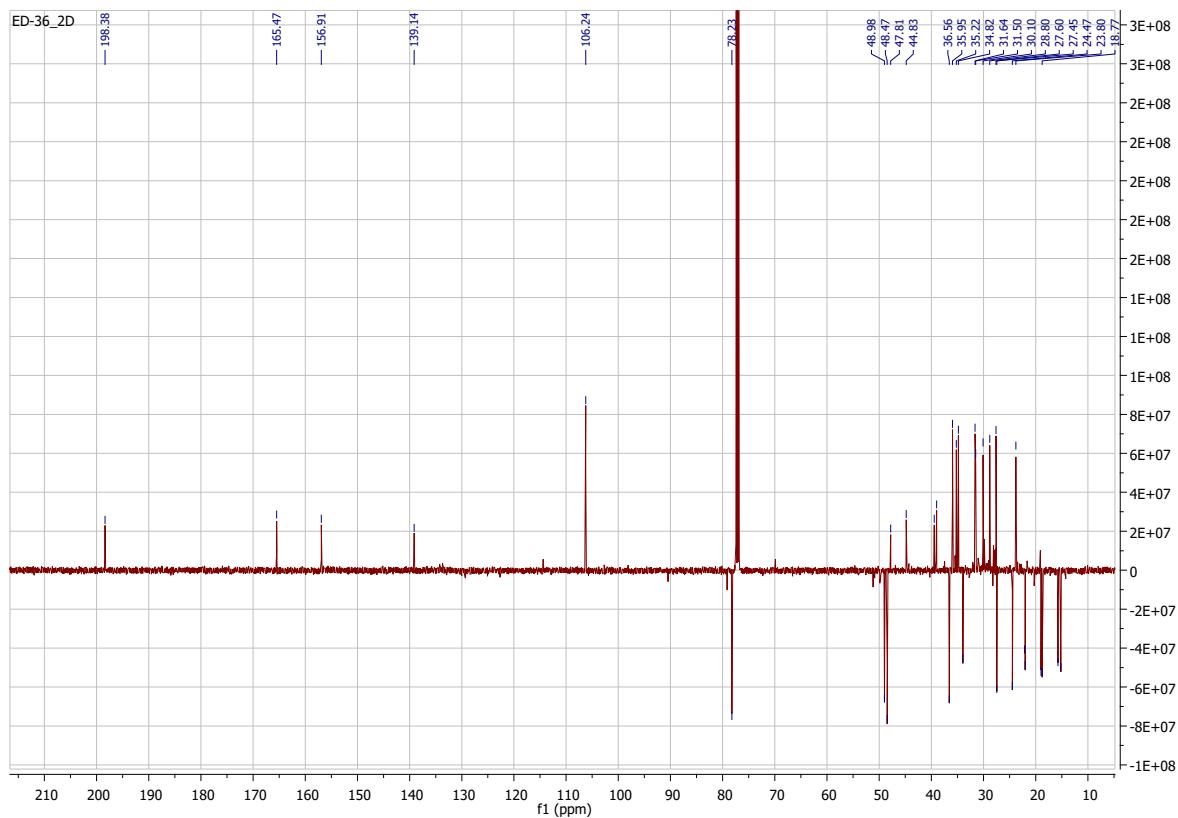


Figure S8. ^{13}C JMOD spectrum of compound **3** (500 MHz, in CDCl_3)

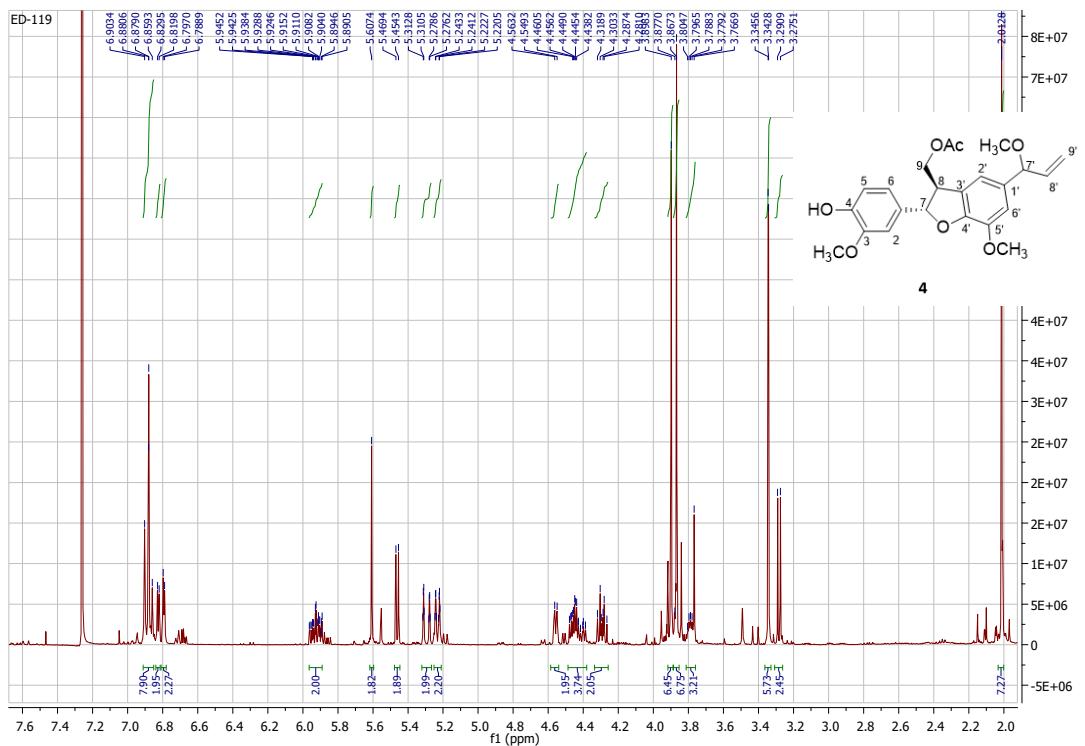


Figure S9. ^1H NMR spectrum of compound **4** (500 MHz, in CDCl_3)

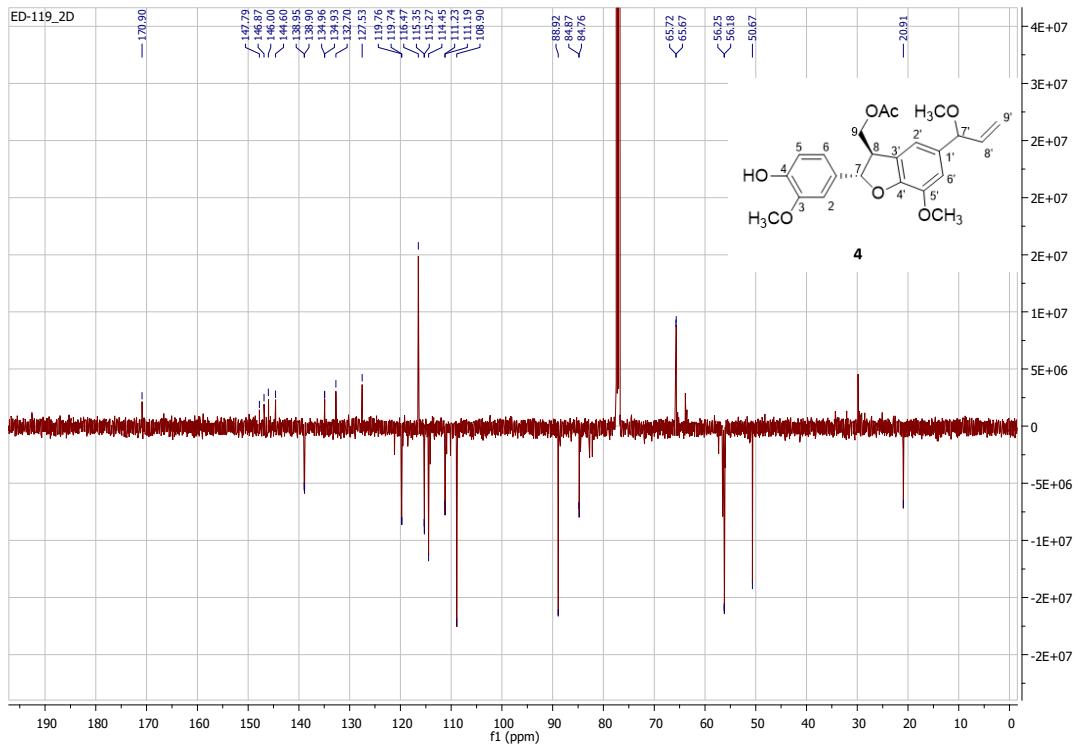


Figure S10. ^{13}C JMOD NMR spectrum of compound 4 (125 MHz, in CDCl_3)

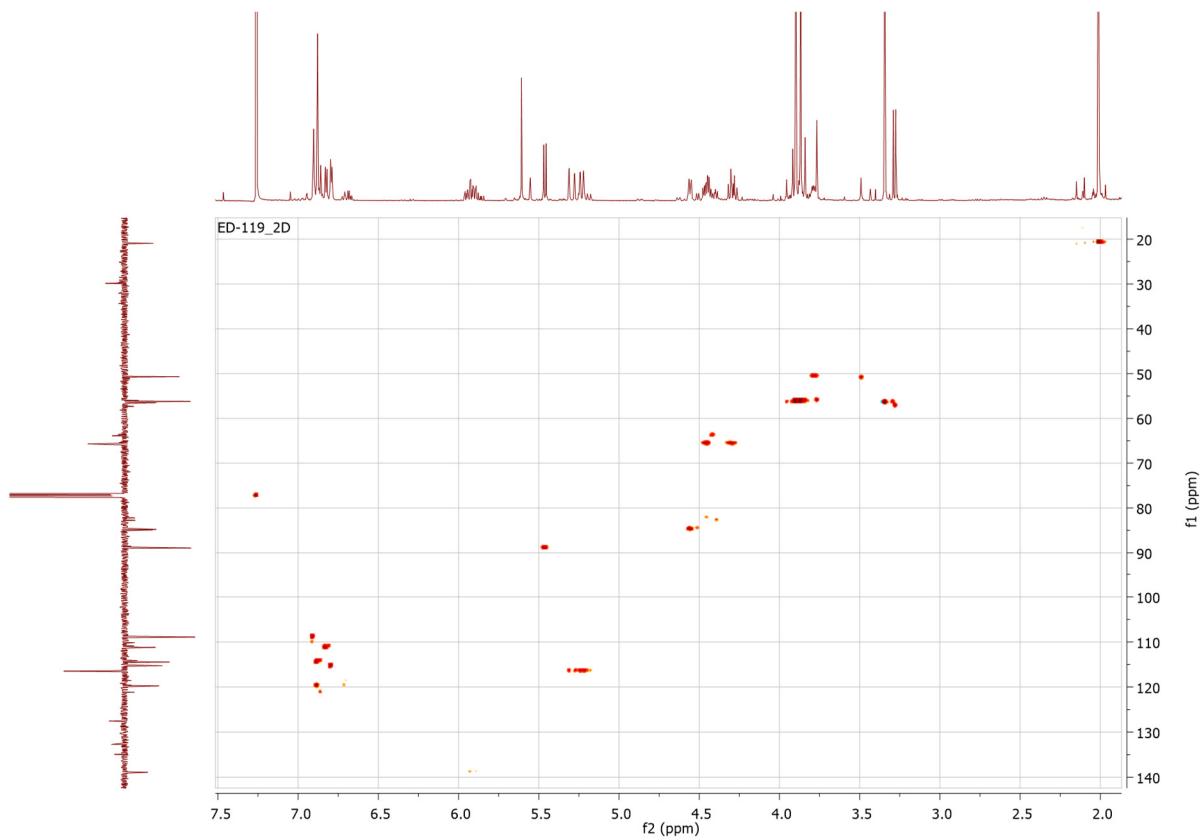


Figure S11. HSQC spectrum of compound 4 (in CDCl_3)

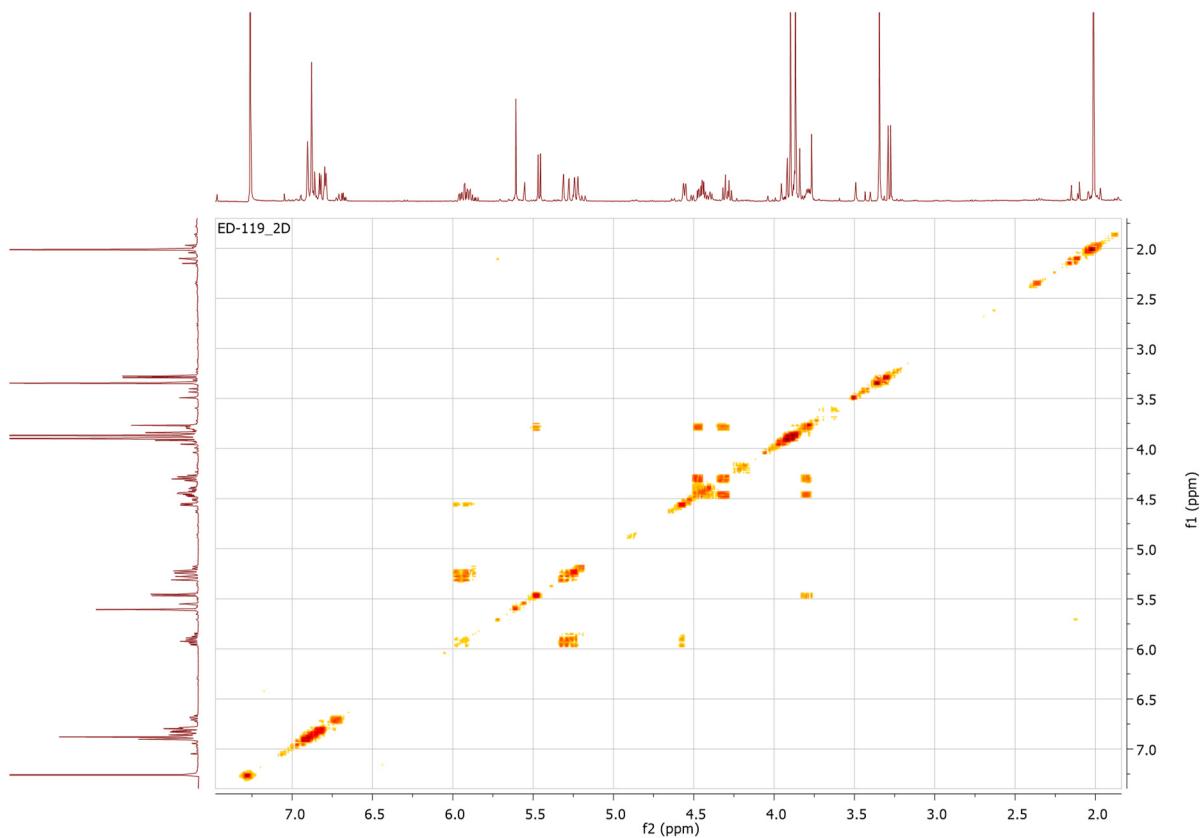


Figure S12. ^1H - ^1H COSY spectrum of compound 4 (in CDCl_3)

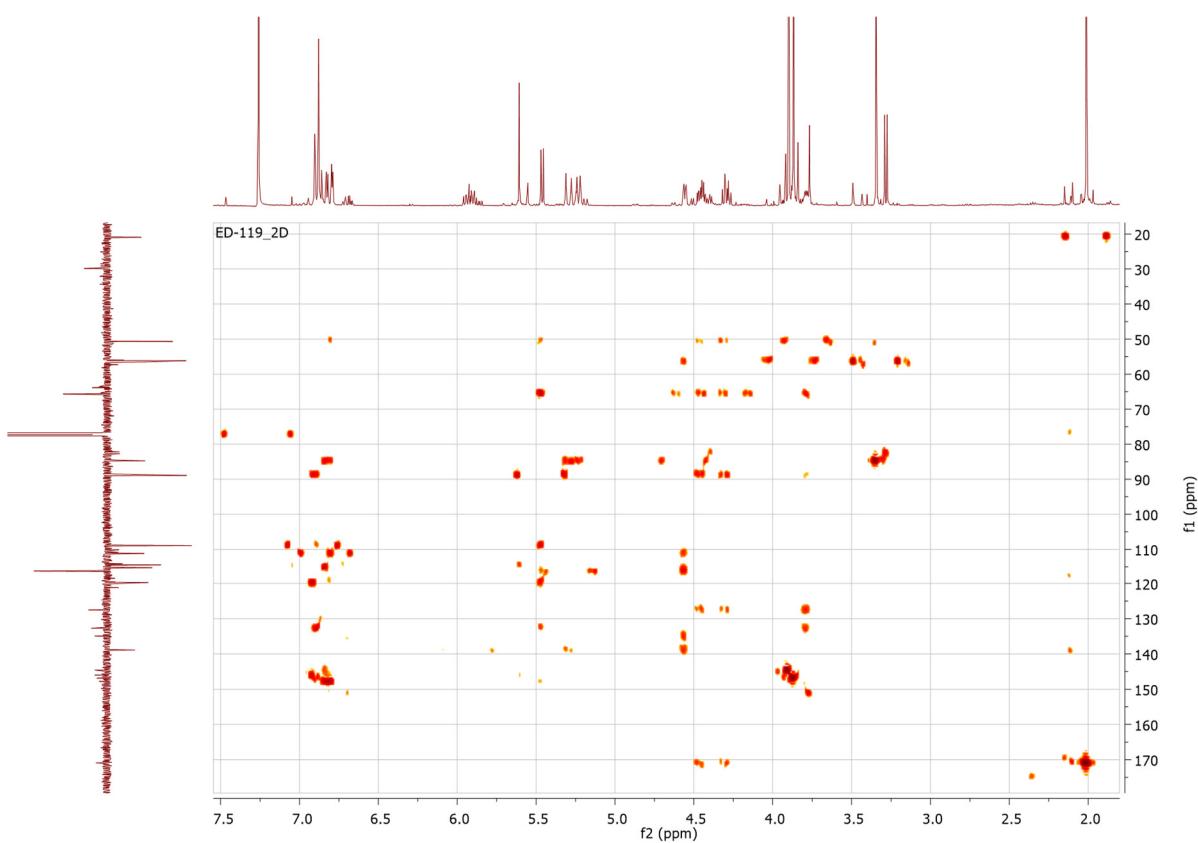


Figure S13. HMBC spectrum of compound 4 (in CDCl_3)

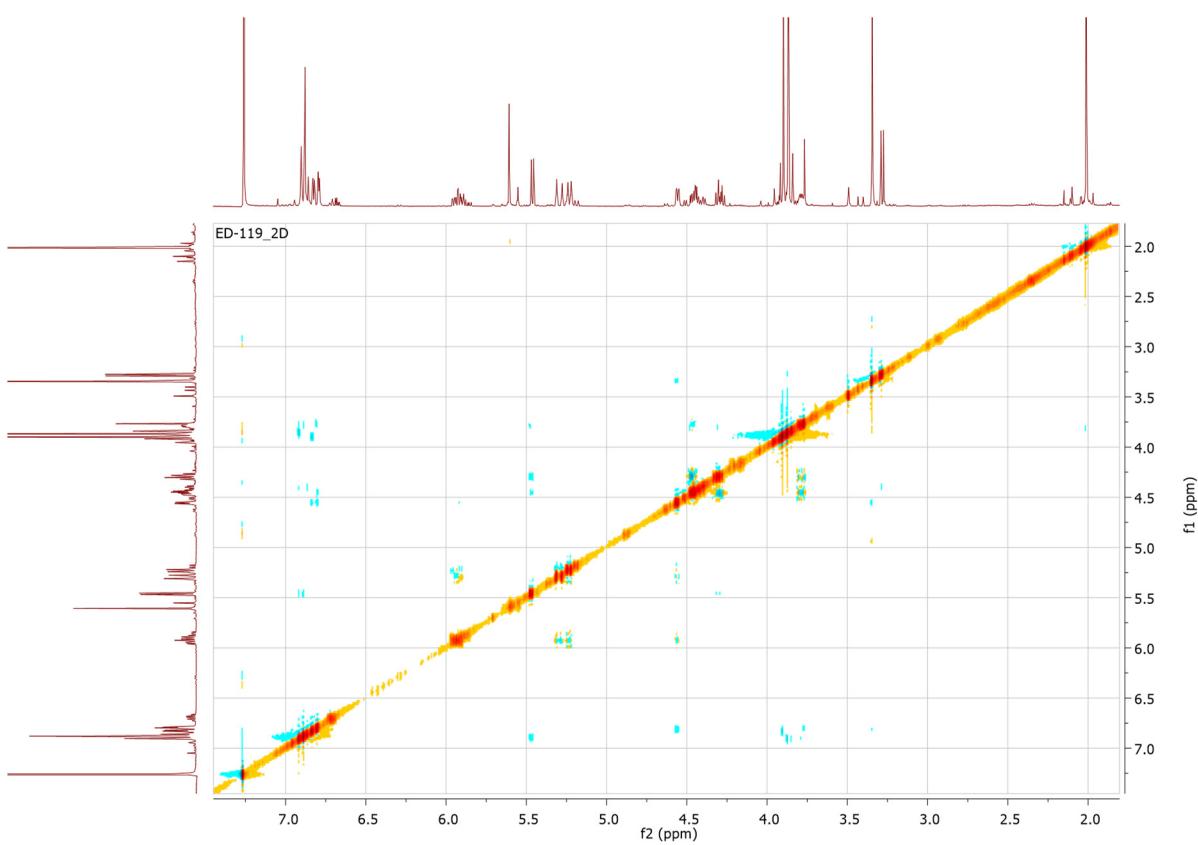
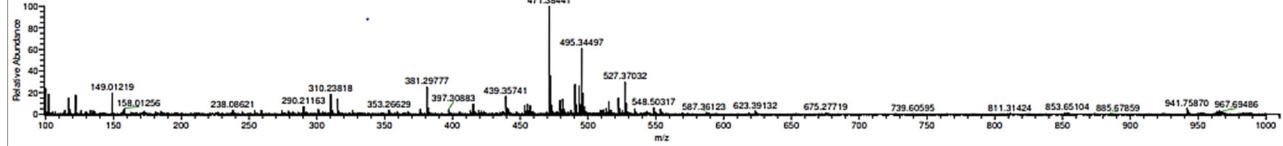


Figure S14. NOESY spectrum of compound 4 (in CDCl_3)

1-5, 11-14

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T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

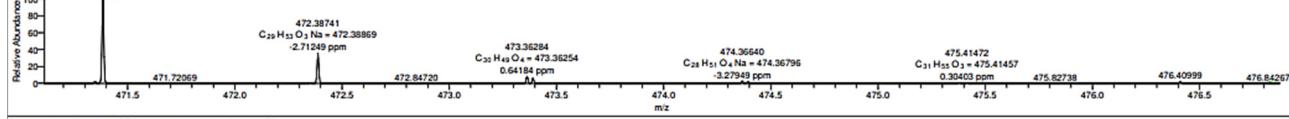


D-20200917 #2550 2568 RT: 13.09-13.18 AV: 19 NL: 1.01E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

C₂₁H₃₁O₃ = 471.38327

2.40955 ppm



D-20200917 #2550 2568 RT: 13.09-13.18 AV: 19 NL: 2.61E7

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

C₂₄H₄₅O₄ = 493.34409

1.89059 ppm

C₂₄H₄₅O₄ = 493.34492

1.89059 ppm

C₂₁H₃₃O₃Na = 493.36532

0.29848 ppm

C₂₄H₄₅O₄ = 493.40617

4.37579 ppm

C₂₄H₄₅O₄ = 493.44474

C31H50O3 +H: C31H51O3 p(ess, s/p40) Chrg 1R: 70...

471.3827

2.40955 ppm

472.38668

473.38864

474.39284

475.39576

476.40999

476.84267

Figure S15. HRMS spectrum of compound 1.

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1-5, 11-14

09/17/20 11:57:43

1:1 FA

D-20200917 #2776 2801 RT: 14.25-14.38 AV: 26 NL: 2.89E8

T: FTMS + p ESI Full lock ms [100.0000-1000.0000]

C₂₅H₄₂O₇ = 415.17572

1.42279 ppm

C₂₄H₄₁O₇Na = 415.17513

415.17572

C₂₁H₃₉O₇Na = 416.18055

-3.74575 ppm

C₂₁H₃₉O₇ = 416.17909

416.17909

C₂₁H₃₉O₇ = 416.18250

-2.34732 ppm

416.27950

417.18162

417.18162

C₂₁H₃₉O₇Na = 417.18250

417.18250

418.18617

418.23289

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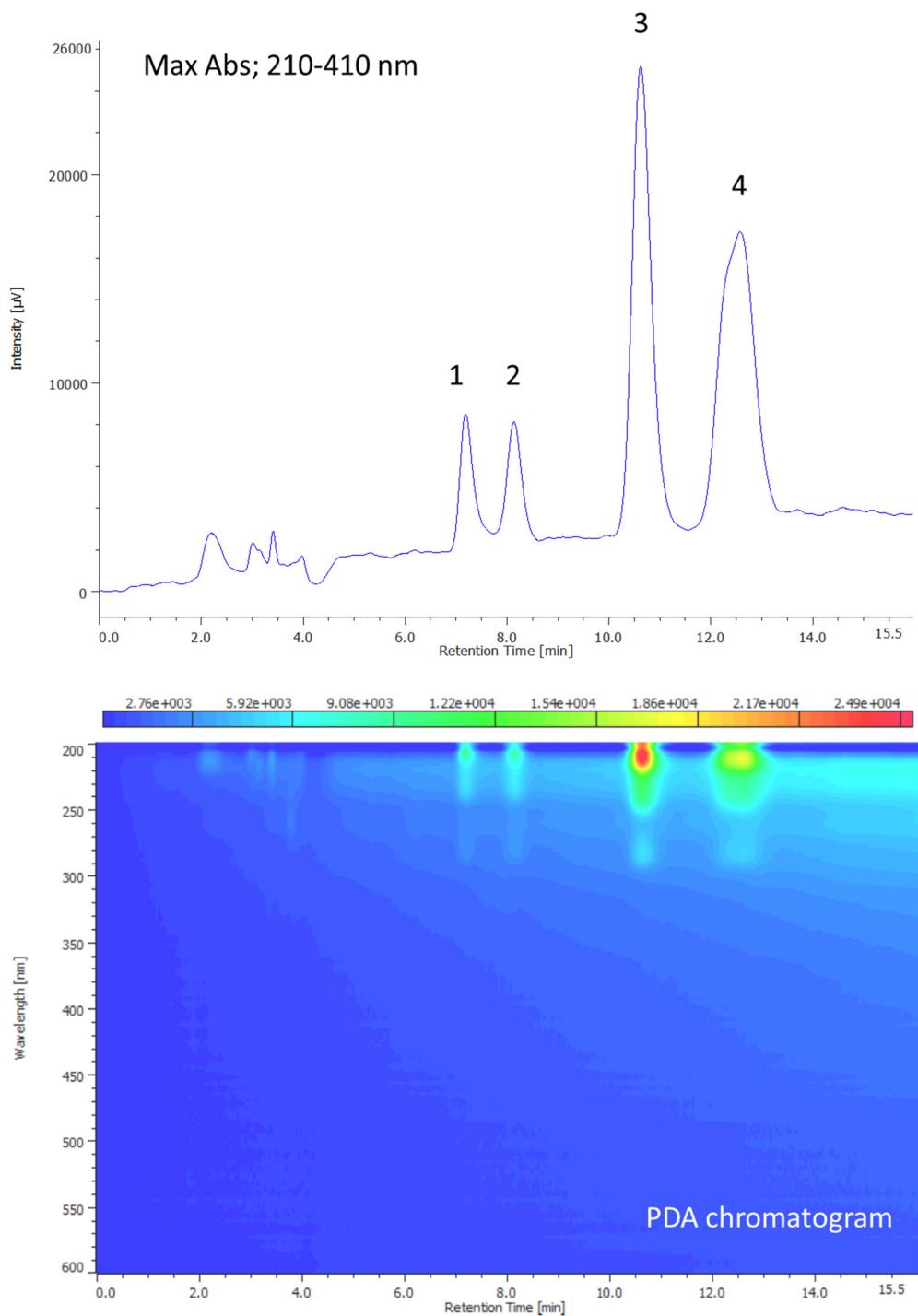


Figure S17. Chiral chromatographic separation of compound **4**. Conditions: chromatographic instrument: Jasco HPLC/SFC instrument (Jasco International Co. Ltd., Hachioji, Tokyo, Japan) equipped with an MD-4015 PDA detector; stationary phase: Phenomenex Lux® 5 µm i-Amylose-1, 250 x 4.6 mm LC column (Phenomenex Inc., Torrance, CA, USA); mobile phase: 1 mL/min flow rate, isocratic elution, cyclohexane (+0.1% TFA) : tetrahydrofuran (+0.1% TFA) – 87 : 13.

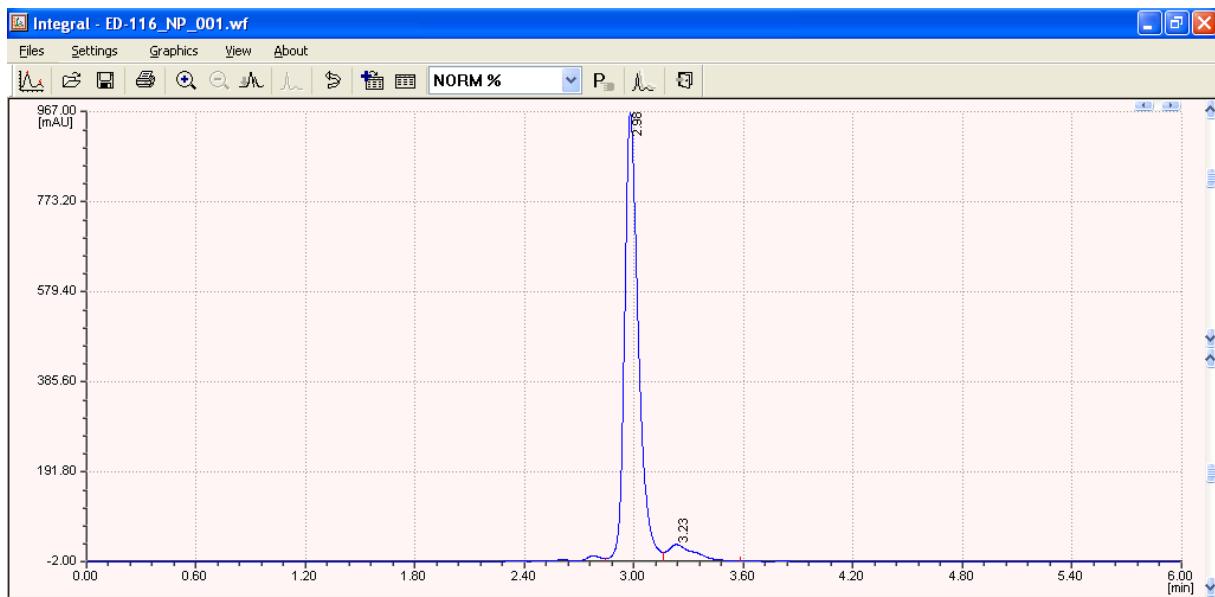


Figure S18. HPLC chromatogram of compound **1**. Conditions: WUFENG HPLC instrument; column: LiChrospher Si 60 (5 μ m, 250-4 mm); mobile phase: *n*-Hexane-EtOAc (3:7); flow rate: 1.0 ml/min; RT 2.98 min