

Supporting Information

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Structure, Absolute Configuration and Biological Evaluation of a New Labdane Diterpenoid from *Jatropha podagrica*

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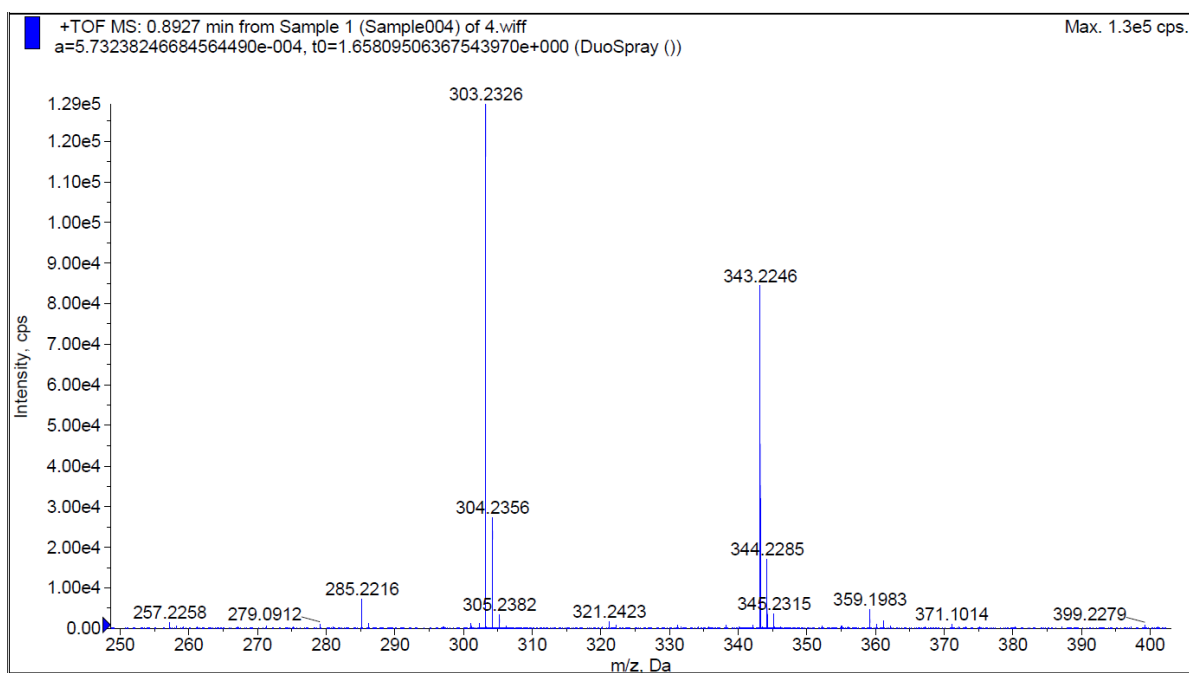


Figure S1: HR-ESI-MS spectrum of **1** (jatrodagricaine A)

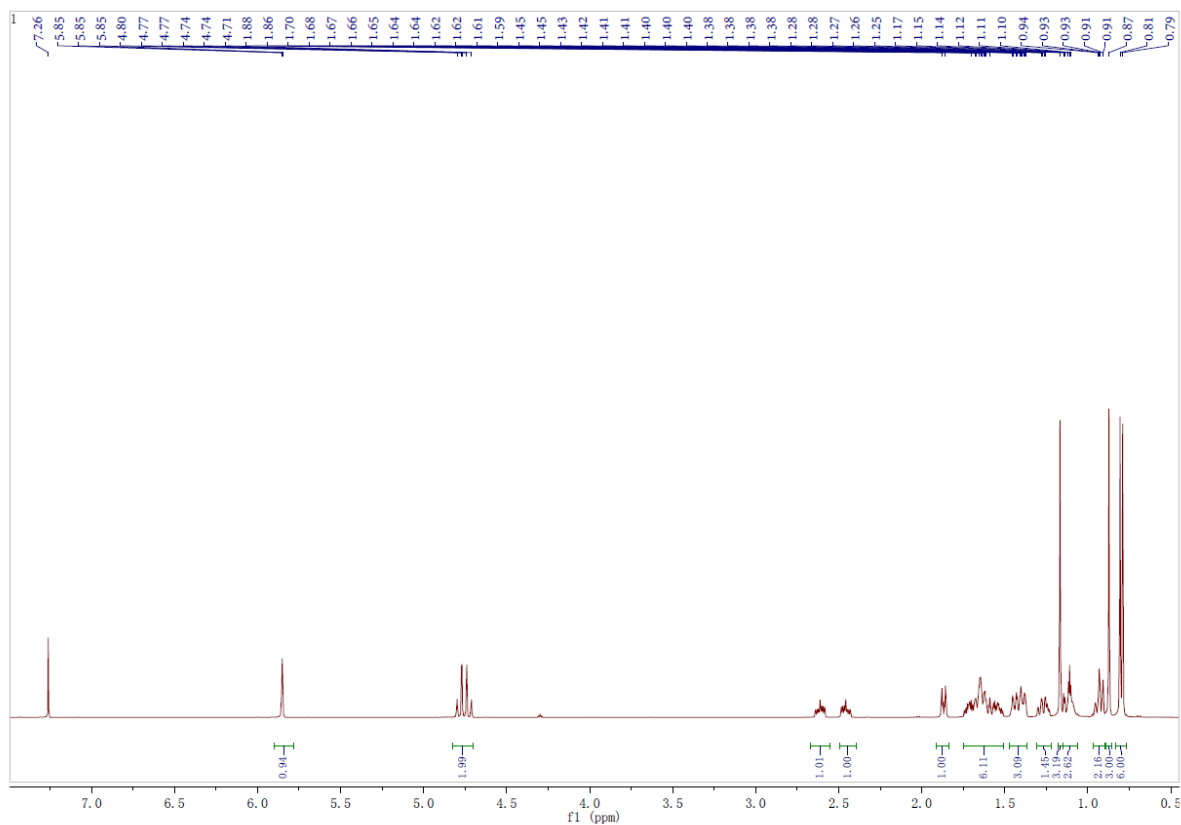


Figure S2: $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum of **1** (jatrodagicaine A)

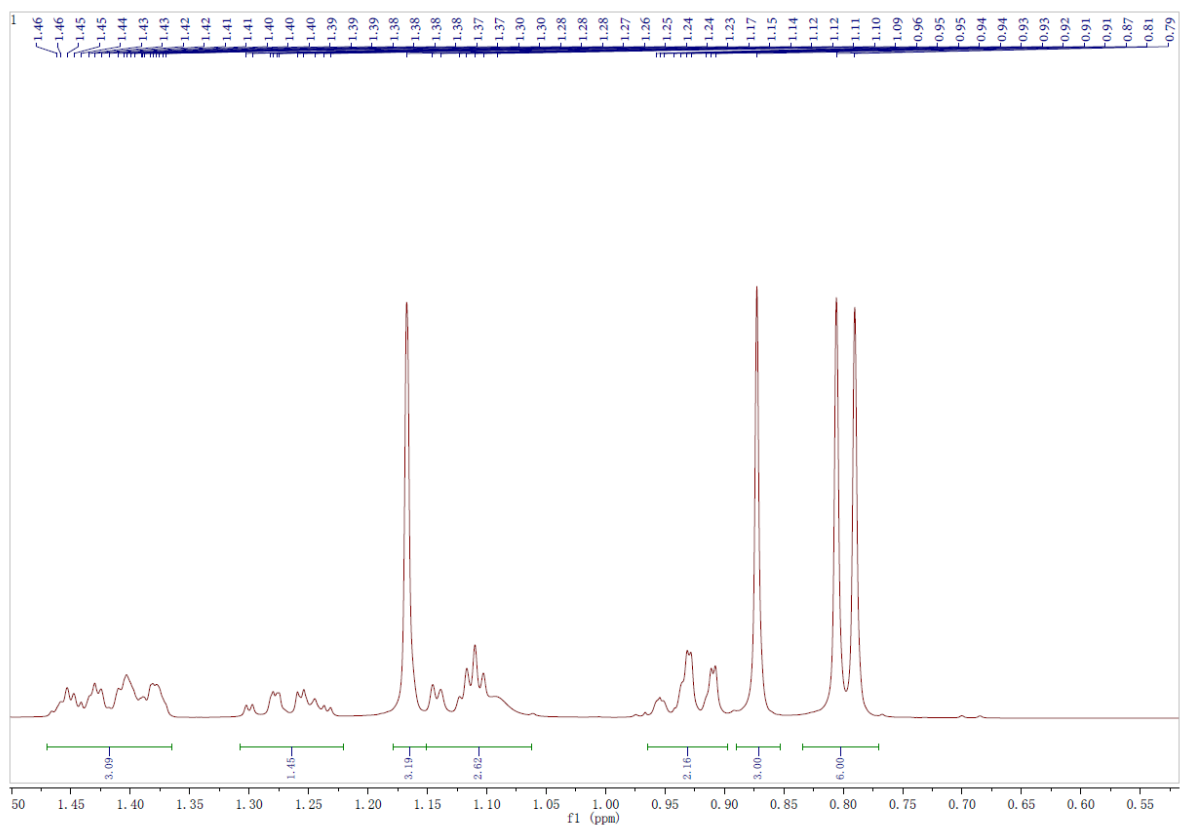


Figure S3: ¹H-NMR (600 MHz, CDCl₃) spectrum of **1** (jatrodagricaine A) (from δ_H 0.5 ppm to δ_H 1.5 ppm)

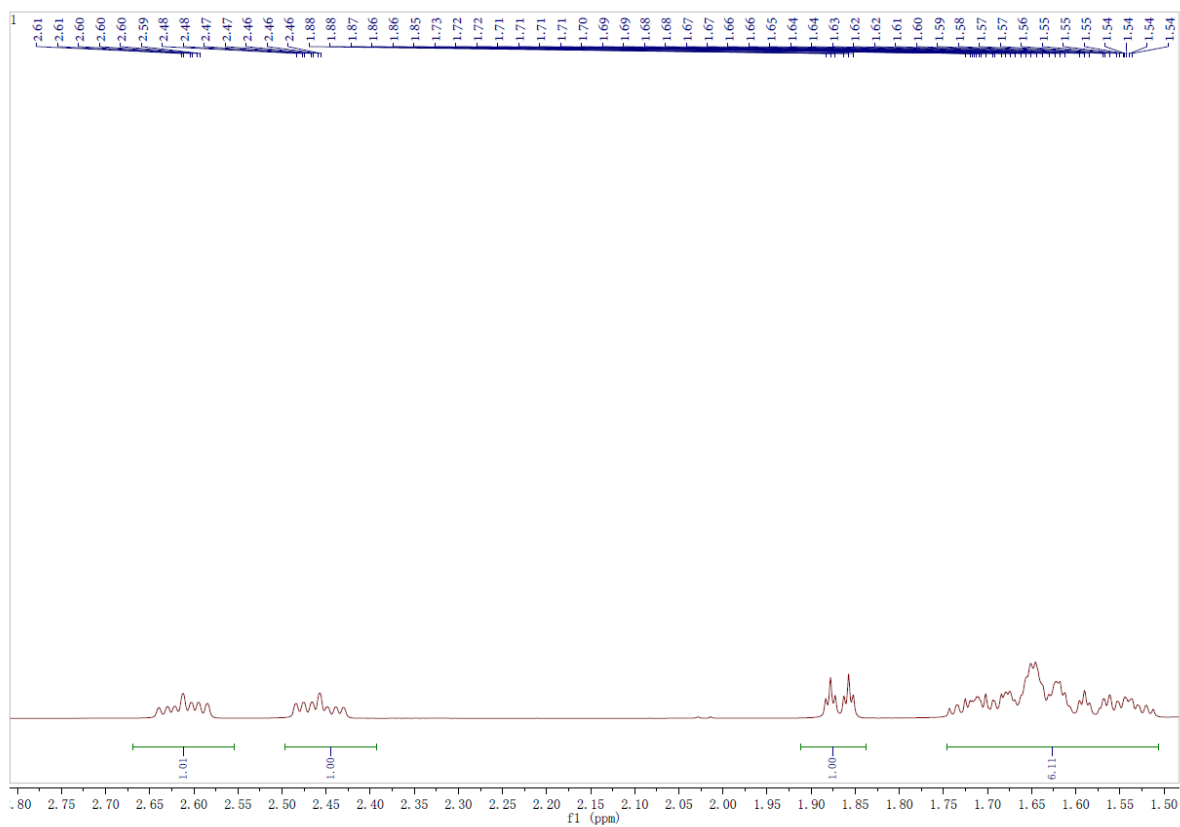


Figure S4: $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum of **1** (jatrodagricaine A) (from δ_{H} 1.5 ppm to δ_{H} 2.8 ppm)



Figure S5: ^{13}C -NMR (150 MHz, CDCl_3) spectrum of **1** (jatrodagricaine A)

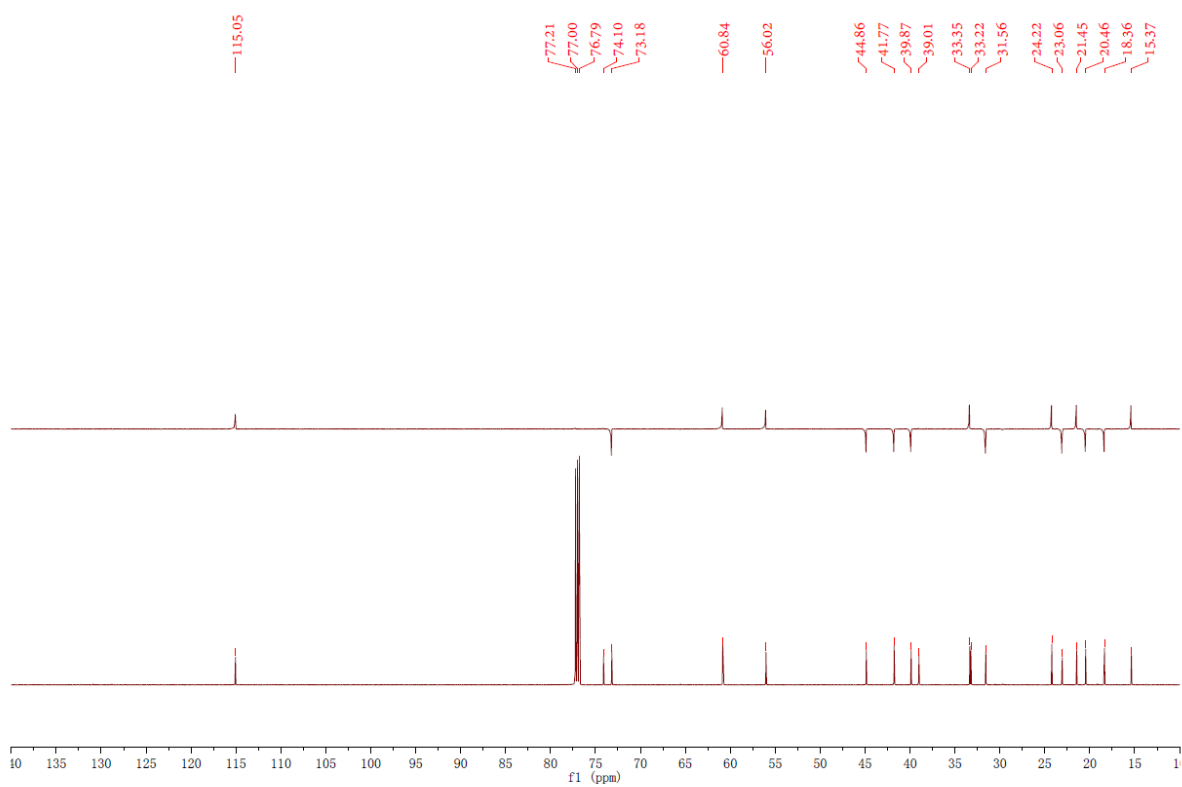


Figure S6: DEPT135 (150 MHz, CDCl₃) spectrum of **1** (jatrodagricaine A)

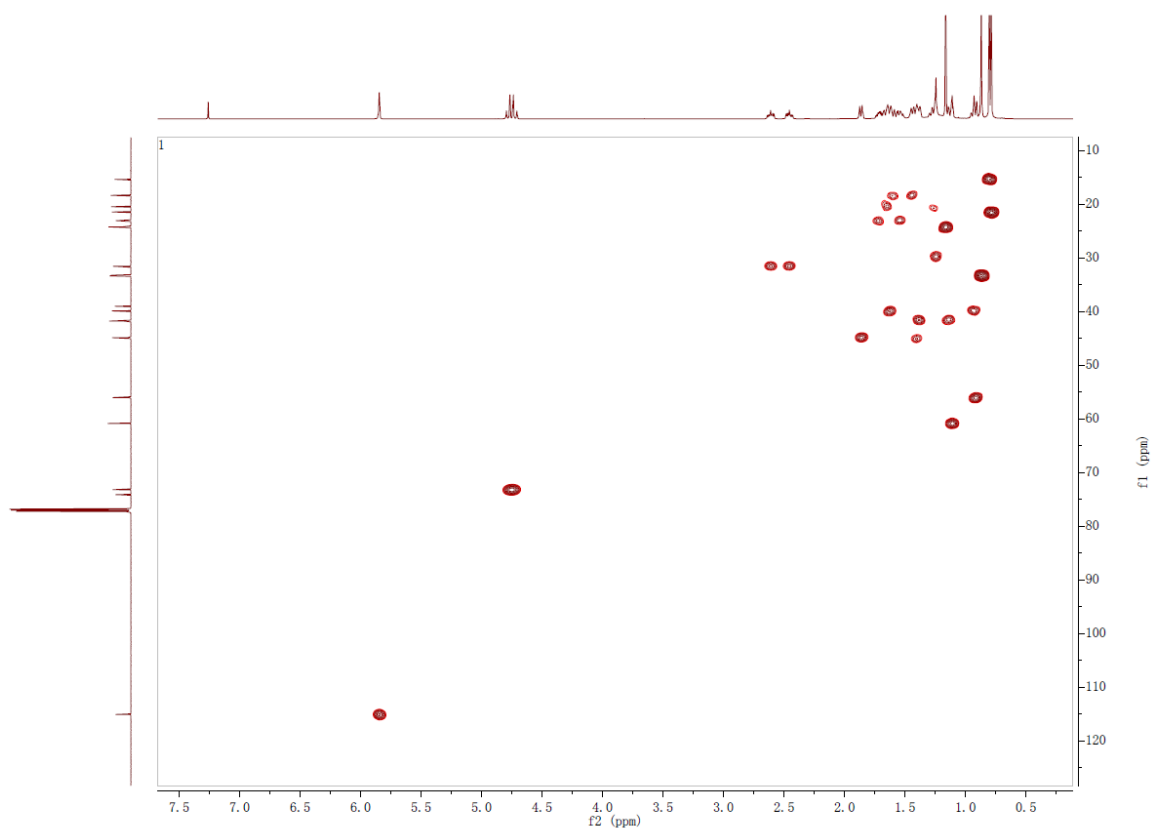


Figure S7: HSQC spectrum of **1** (jatrodagricaine A)

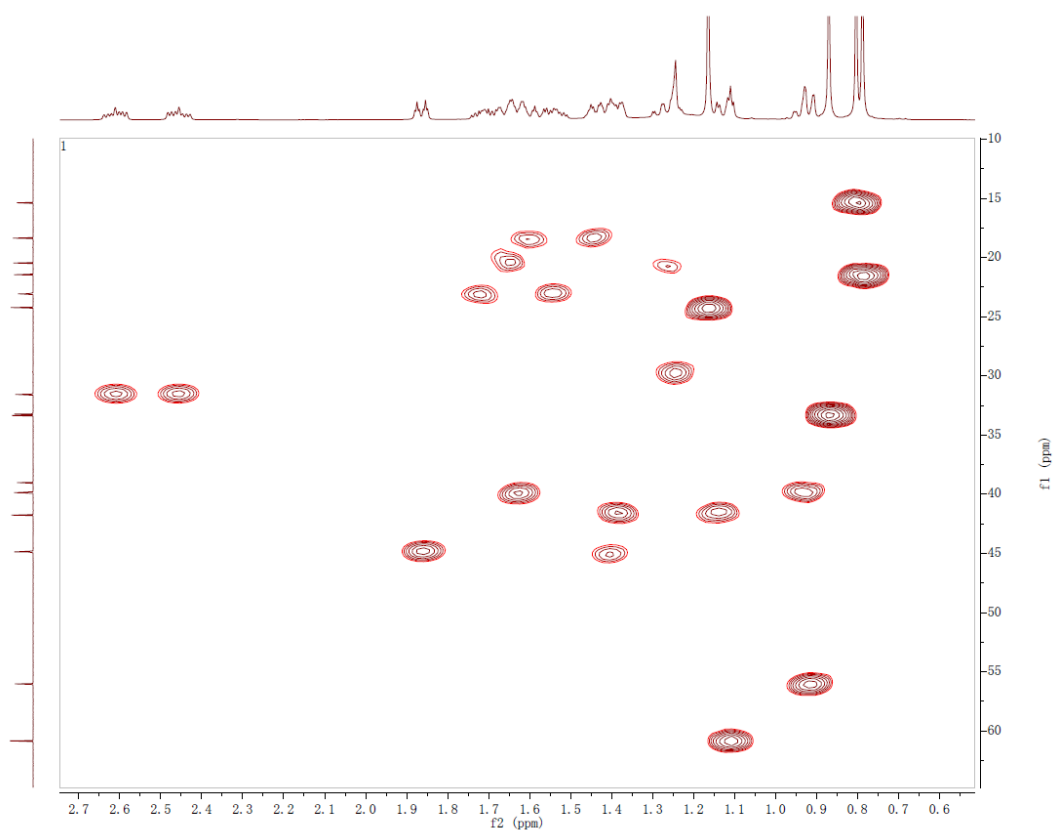


Figure S8: HSQC spectrum of **1** (jatrodagricaine A) (from δ_c 10 ppm to δ_c 65 ppm)

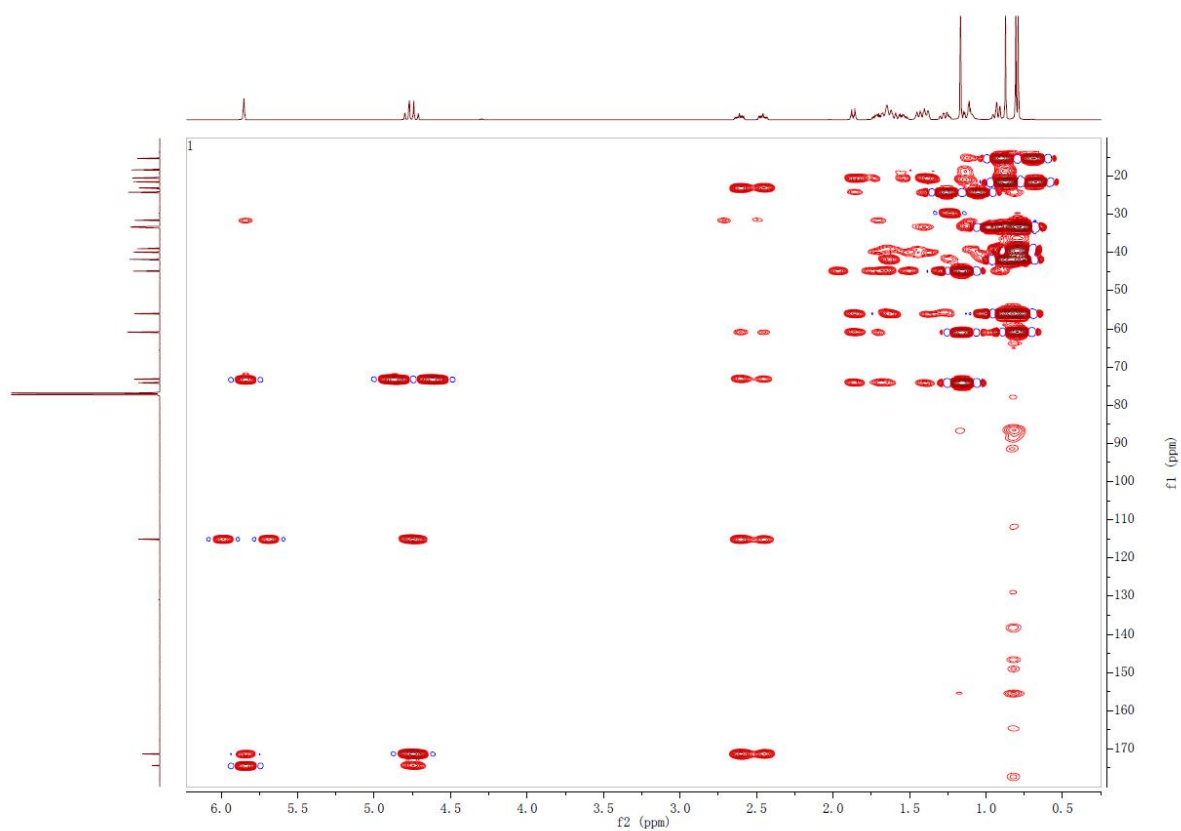


Figure S9: HMBC spectrum of **1** (jatrodagricaine A)

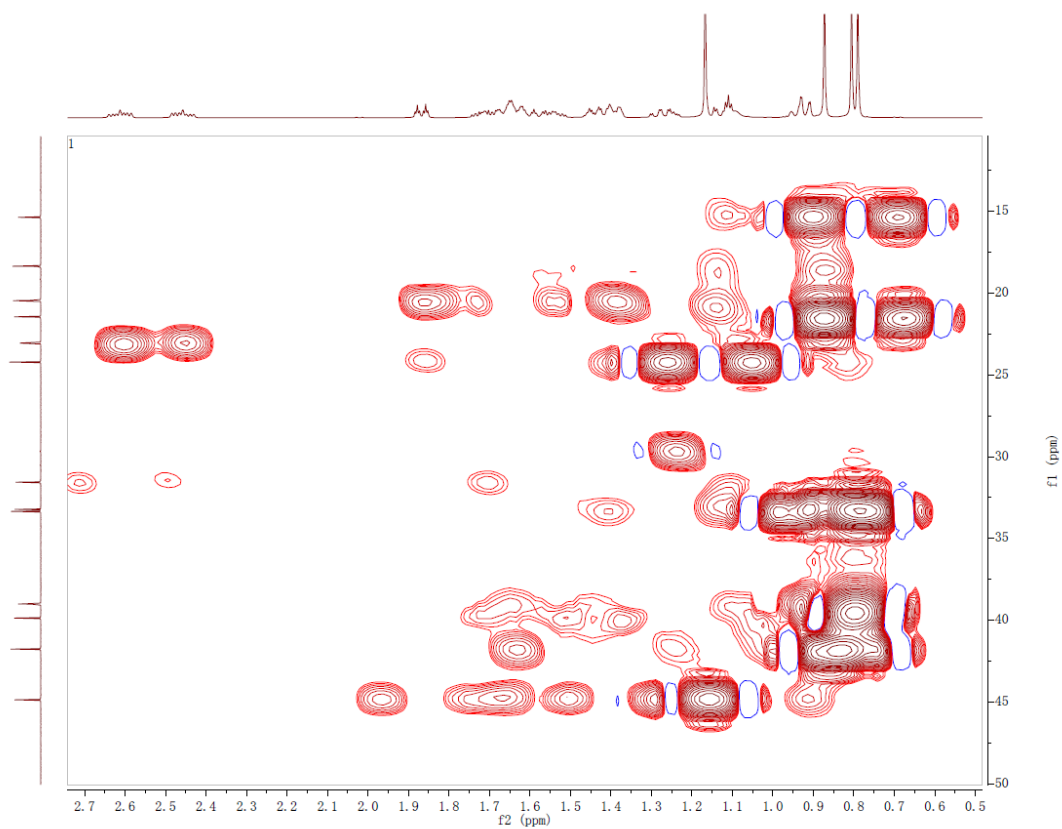


Figure S10: HMBC spectrum of **1** (jatrodagricaine A) (from δ_C 10 ppm to δ_C 50 ppm)

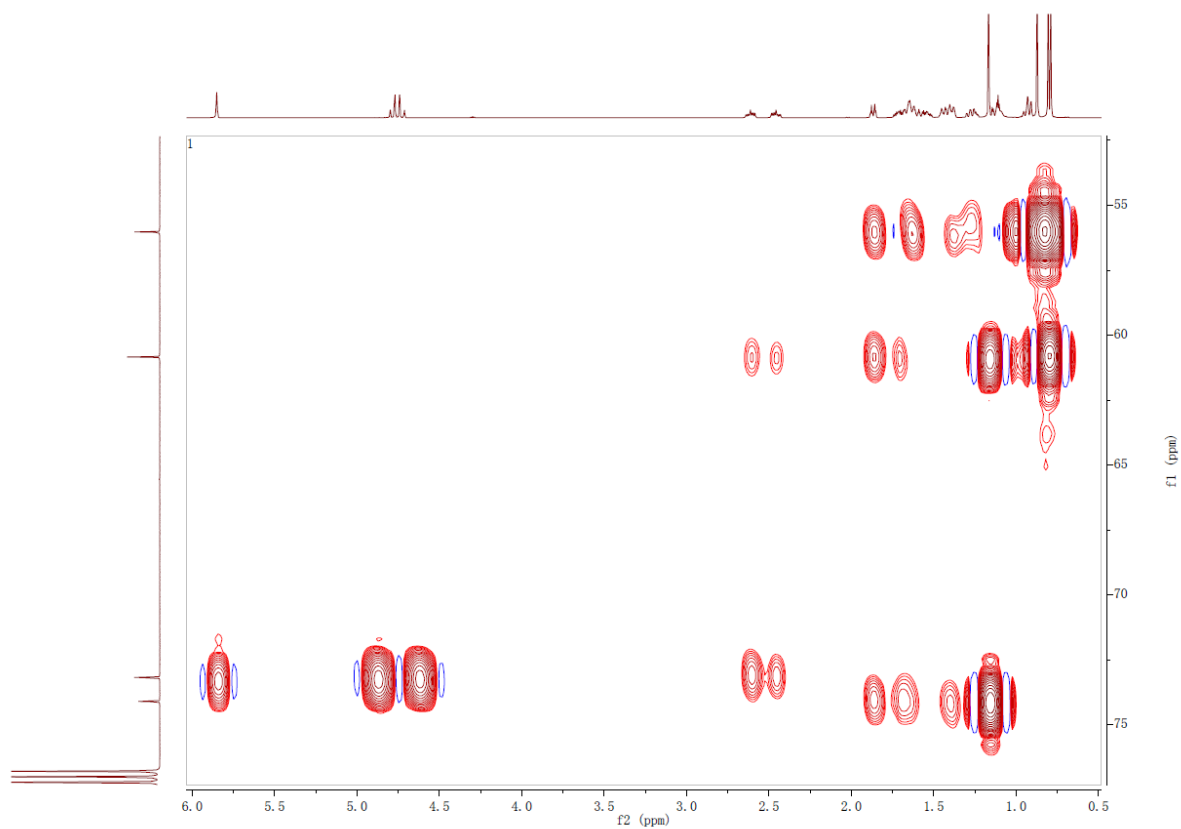


Figure S11: HMBC spectrum of **1** (jatrodagricaine A) (from δ_C 52.5 ppm to δ_C 77.5 ppm)

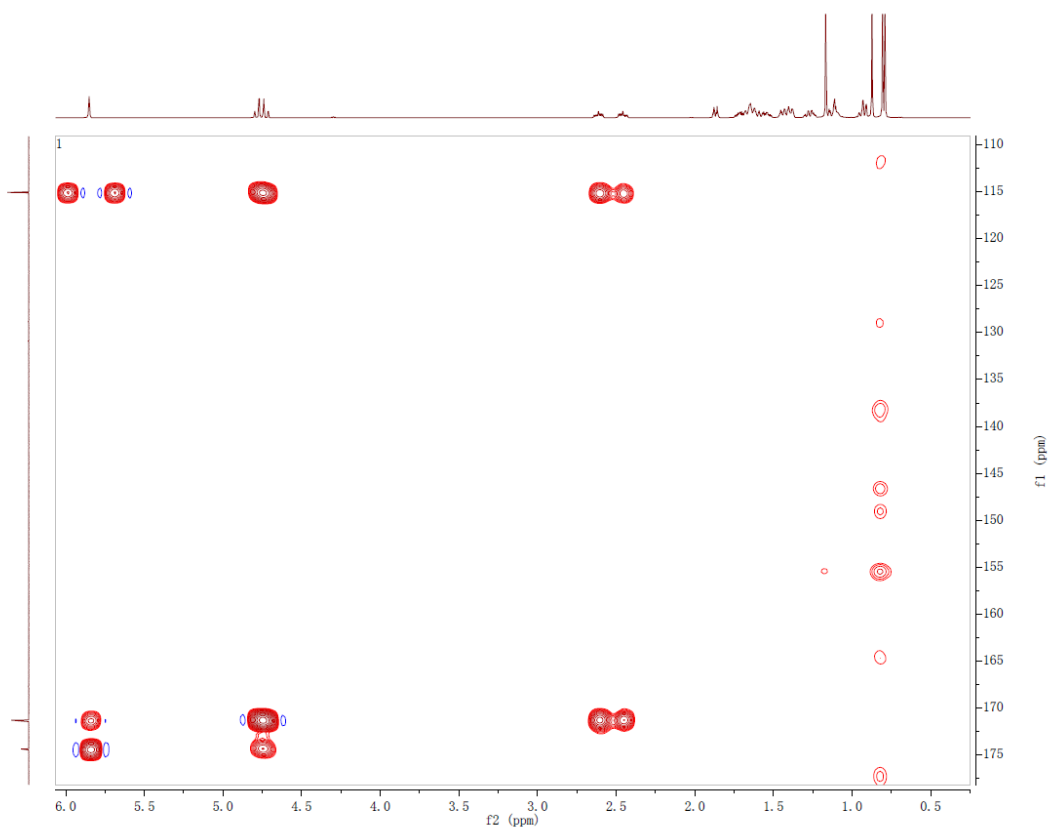


Figure S12: HMBC spectrum of **1** (jatrodagricaine A) (from δ_C 110 ppm to δ_C 178 ppm)

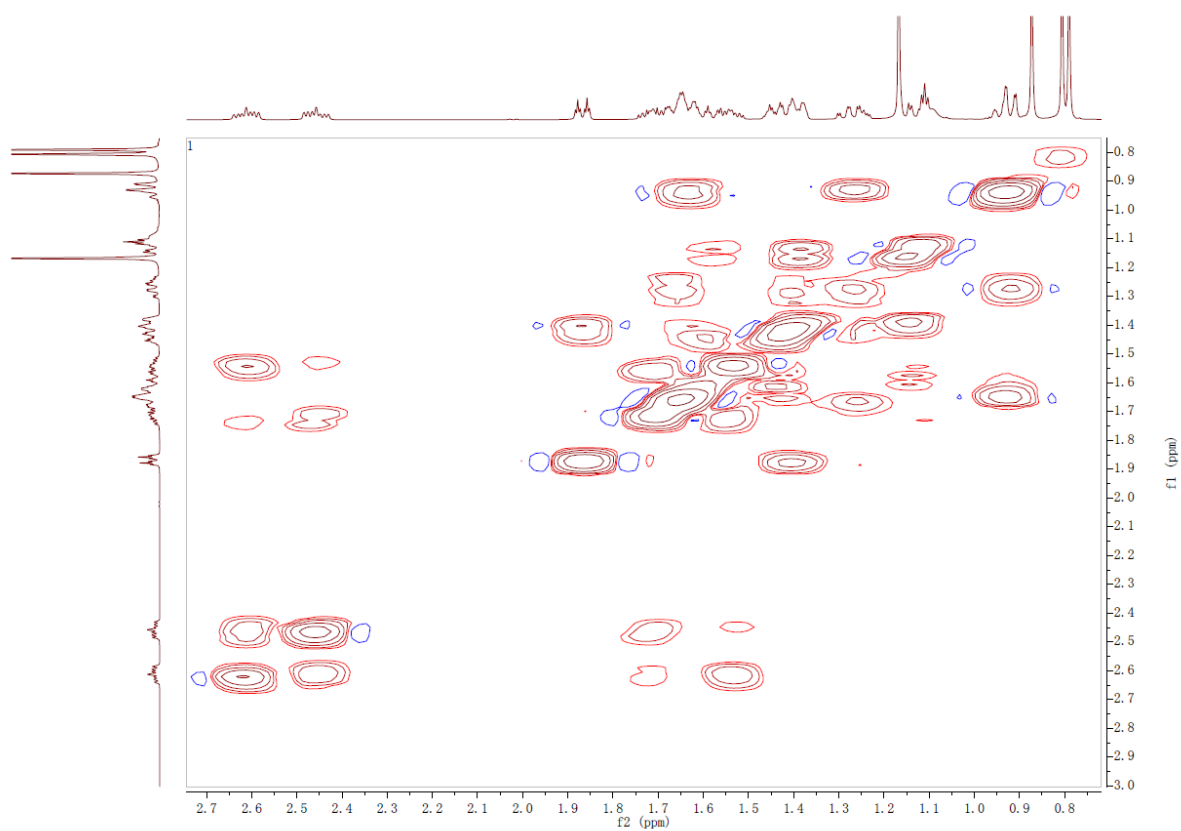


Figure S13: ^1H - ^1H COSY spectrum of **1** (jatrodagricaine A)

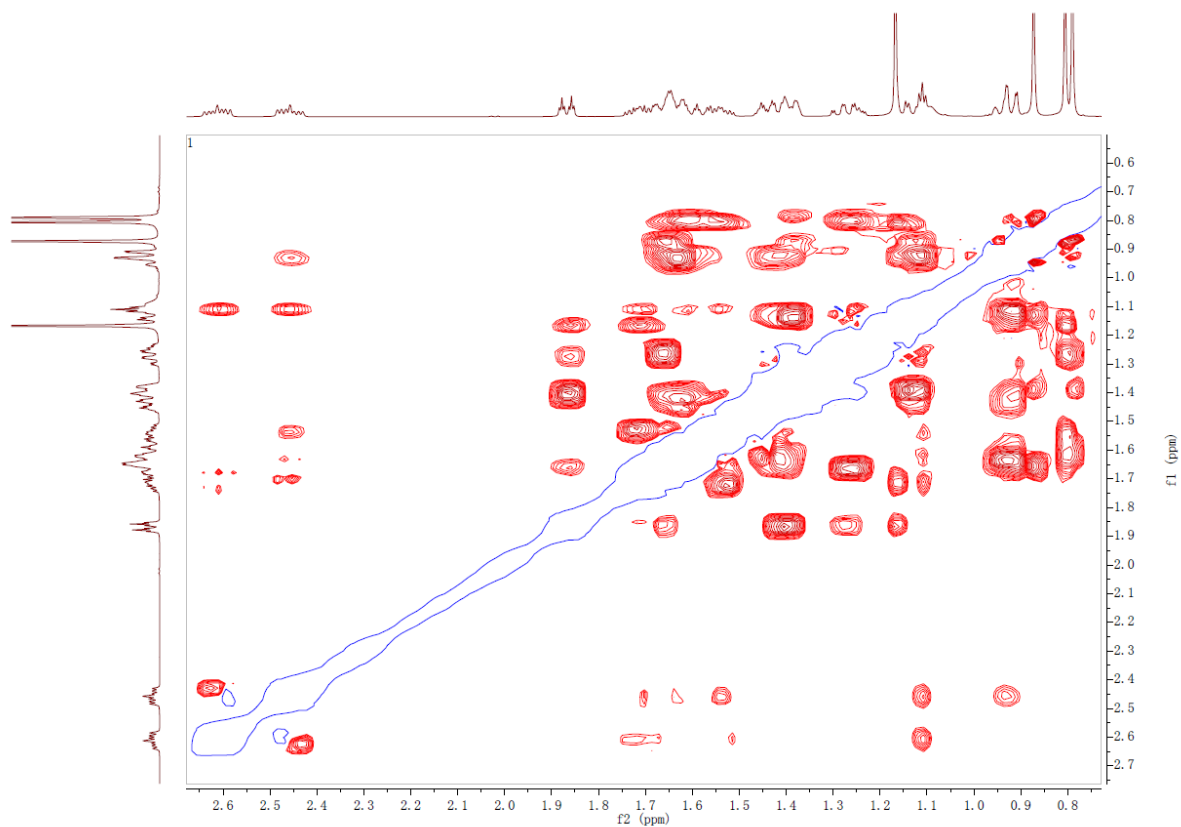


Figure S14: NOESY spectrum of **1** (jatrodagricaine A)

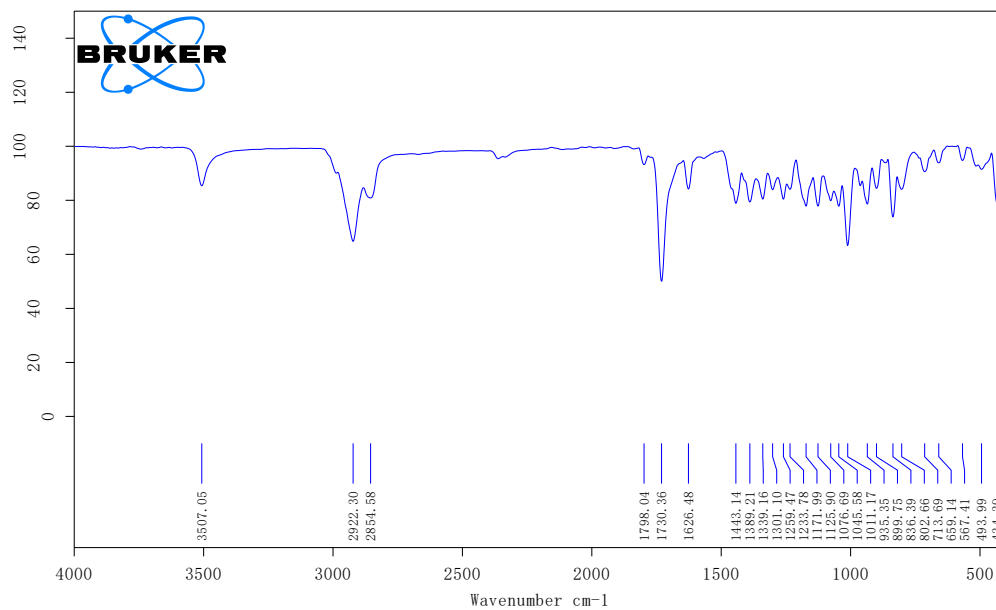


Figure S15: IR spectrum of **1** (jatrodagricaine A)

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320.47

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Figure S16: New compound search report of SciFinder

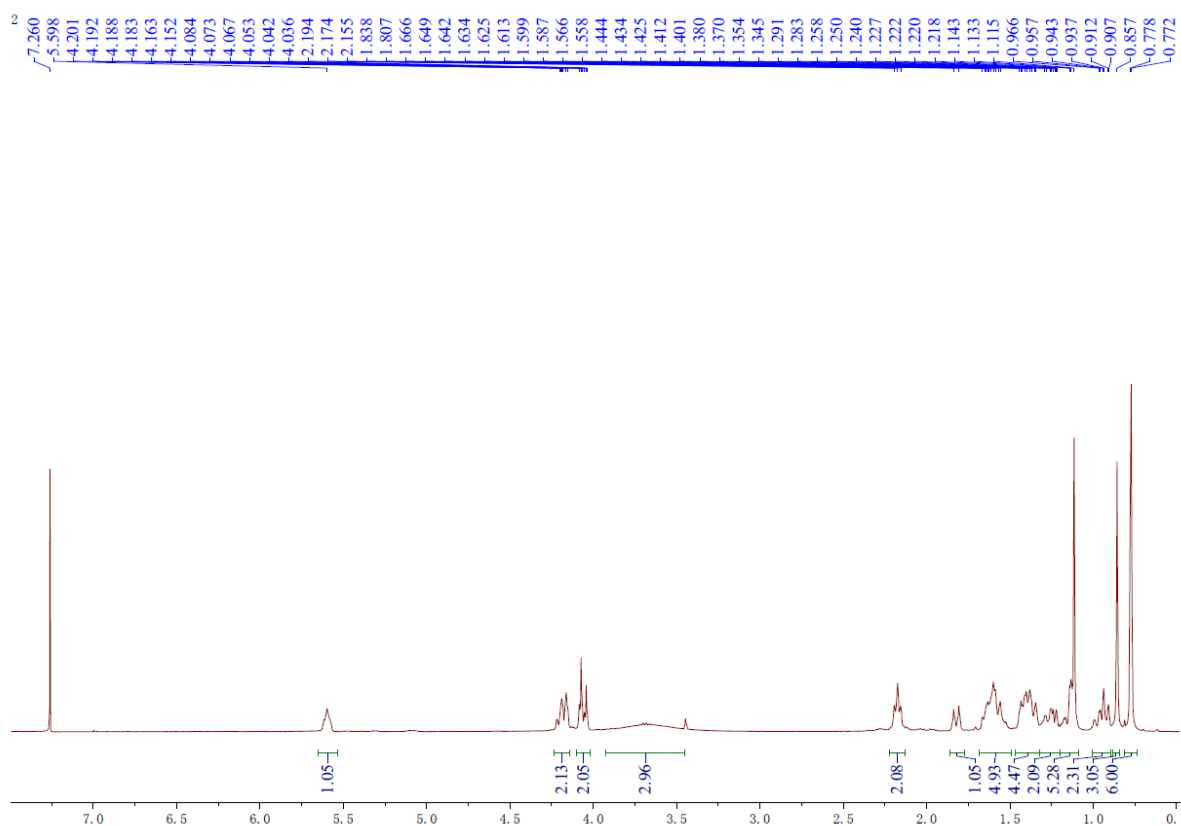


Figure S17: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **2** ($8\alpha,15,16$ -trihydroxy-labd-13E-ene)

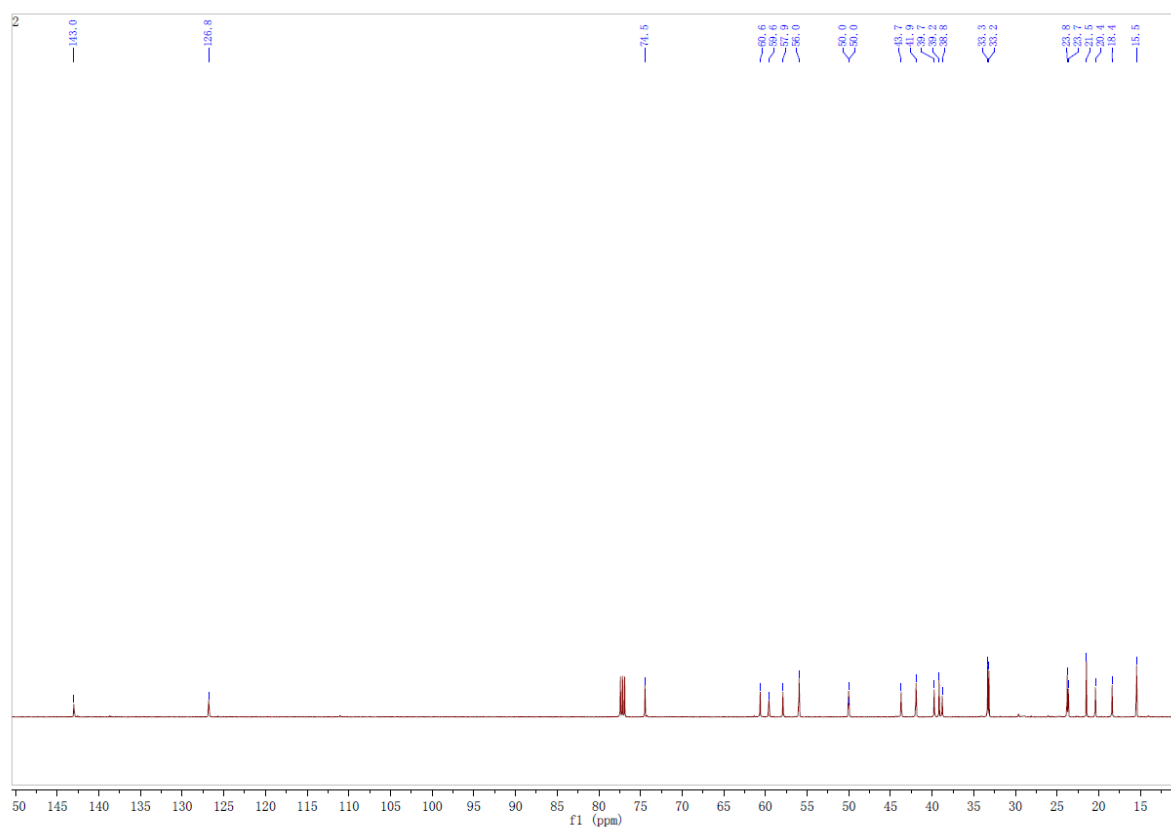


Figure S18: ^{13}C -NMR (125 MHz, CDCl_3) spectrum of **2** ($8\alpha,15,16$ -trihydroxy-labd-13E-ene)

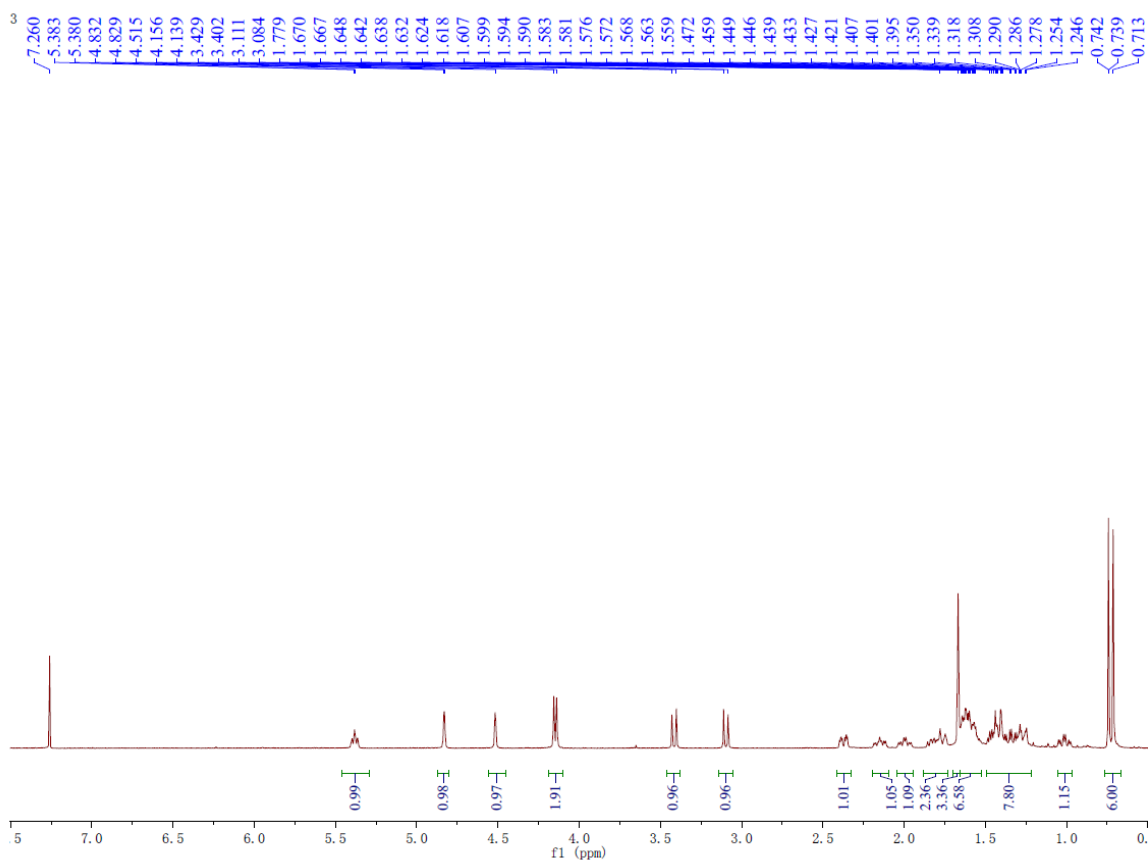


Figure S19: $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum of **3** (kayadiol)

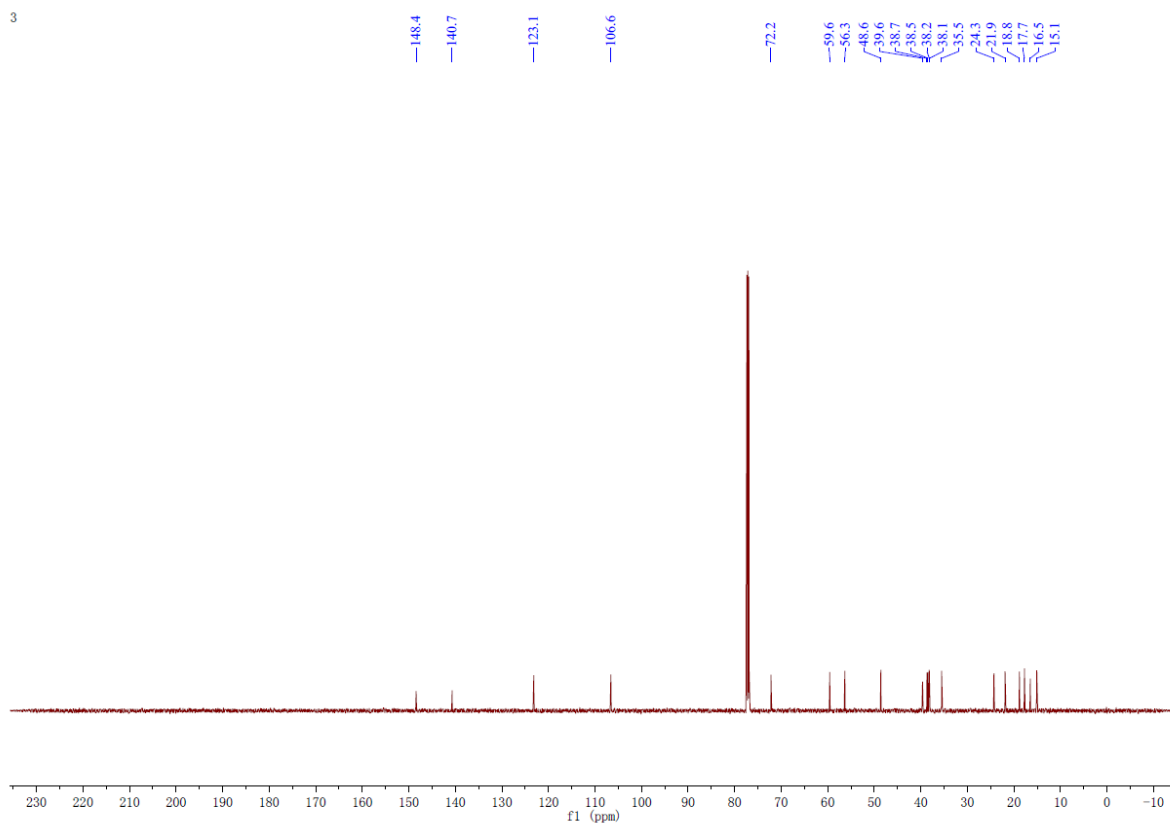


Figure S20: ^{13}C -NMR (150 MHz, CDCl_3) spectrum of **3** (kayadiol)

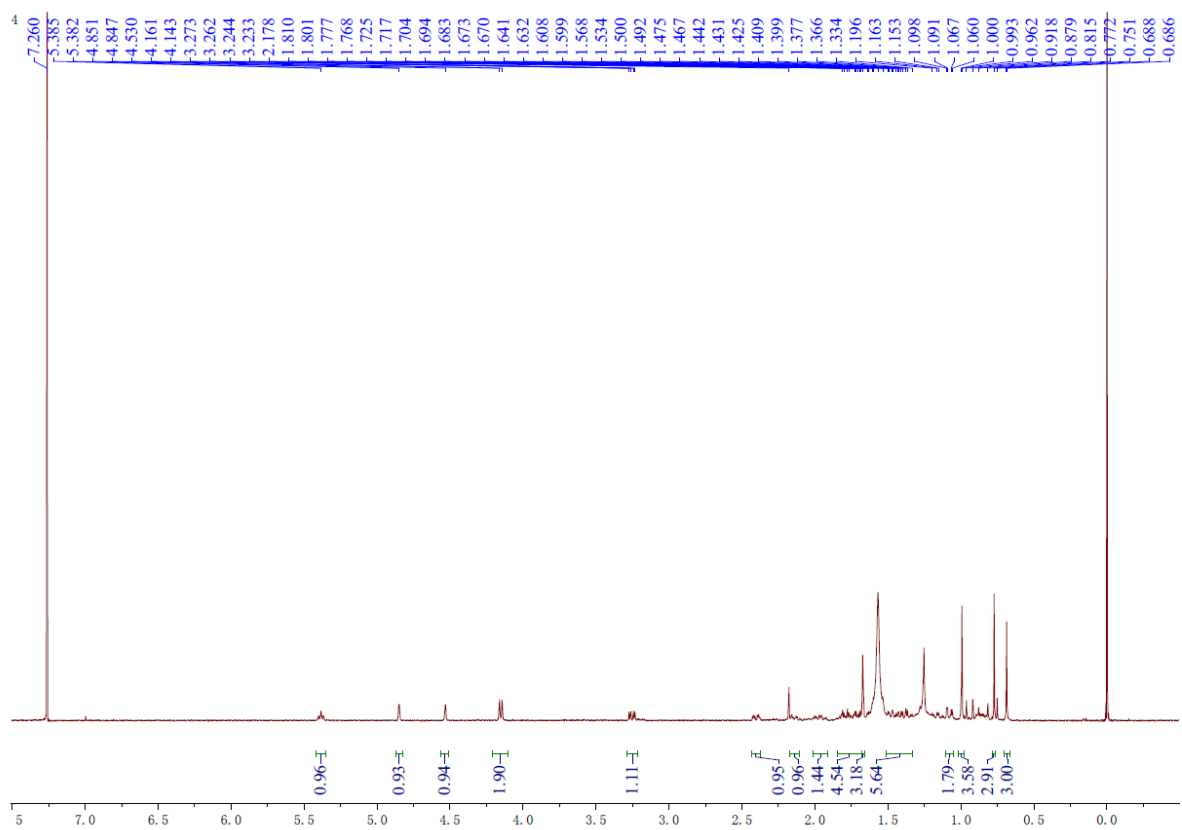


Figure S21: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **4** (labda-8(17),13E-diene-3,15-diol)

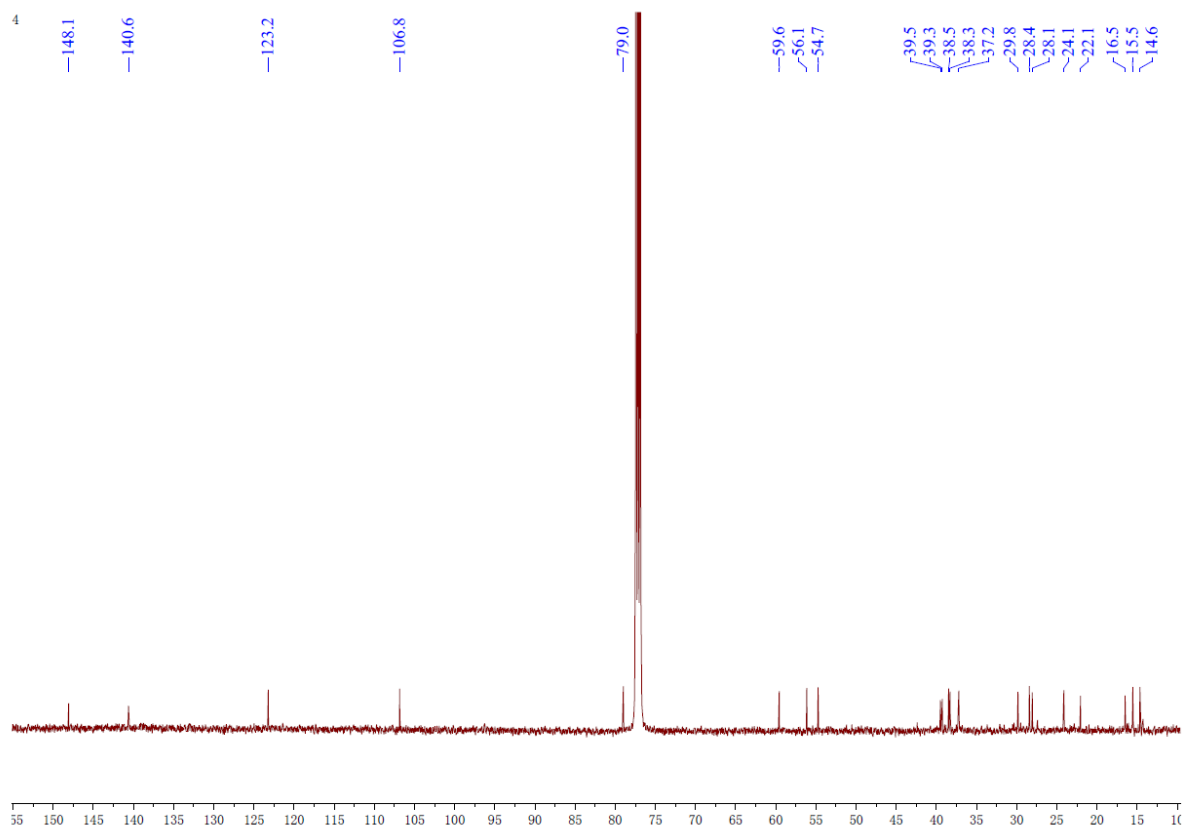


Figure S22: ^{13}C -NMR (125 MHz, CDCl_3) spectrum of **4** (lambda-8(17),13E-diene-3,15-diol)

Table S1. ¹³C NMR data for compounds **1–4** and 9-hydroxylabd-13-en-15,16-olide in CDCl₃.

Position	1 ^{a,c}	2 ^{b,c}	3 ^{a,c}	4 ^{b,c}	9-hydroxylabd-13-en-15,16-olide ^{a,d}
1	39.9 (t)	39.8 (t)	38.1 (t)	37.2 (t)	32.6 (t)
2	18.4 (t)	18.4 (t)	17.7 (t)	28.1 (t)	18.2 (t)
3	41.8 (t)	41.9 (t)	35.5 (t)	79.0 (d)	41.5 (t)
4	33.2 (s)	33.2 (s)	39.6 (s)	39.3 (s)	33.4 (s)
5	56.0 (d)	56.0 (d)	48.6 (d)	54.7 (d)	47.5 (d)
6	20.5 (t)	20.4 (t)	21.9 (t)	24.1 (t)	17.3 (t)
7	44.9 (t)	43.7 (t)	38.7 (t)	38.5 (t)	29.2 (t)
8	74.1 (s)	74.5 (s)	148.4 (s)	148.1 (s)	35.7 (d)
9	60.8 (d)	60.6 (d)	56.3 (d)	56.1 (d)	78.4 (s)
10	39.0 (s)	39.2 (s)	38.5 (s)	39.5 (s)	42.6 (s)
11	23.1 (t)	23.7 (t)	18.8 (t)	22.1 (t)	29.6 (t)
12	31.6 (t)	38.8 (t)	38.2 (t)	38.3 (t)	22.6 (t)
13	171.3 (s)	143.0 (s)	140.7 (s)	140.6 (s)	171.6 (s)
14	115.0 (d)	126.8 (d)	123.1 (d)	123.2 (d)	115.0 (d)
15	174.4 (s)	57.9 (t)	59.6 (t)	59.6 (t)	174.2 (s)
16	73.2 (t)	59.6 (t)	16.5 (q)	16.5 (q)	73.2 (t)
17	24.2 (q)	23.8 (q)	106.6 (t)	106.8 (t)	17.9 (q)
18	33.4 (q)	33.3 (q)	72.2 (t)	28.4 (q)	33.8 (q)
19	21.5 (q)	21.5 (q)	24.3 (q)	15.5 (q)	21.8 (q)
20	15.4 (q)	15.5 (q)	15.1 (q)	14.6 (q)	17.1 (q)

^a Recorded at 150 MHz. ^b Recorded at 125 MHz. ^c Obtained from the paper. ^d Obtained from the literature.