Supporting Information

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(8S, 9R)-Dihydroisoflavipucine, a New Isoflavipucine Derivative from the Endophytic Fungi *Botryosphaeria dothidea*

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AACTTTCAACAACGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAAATGCGAT
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Figure S1: The ITS sequences of *Botryosphaeria dothidea* (D4-2).

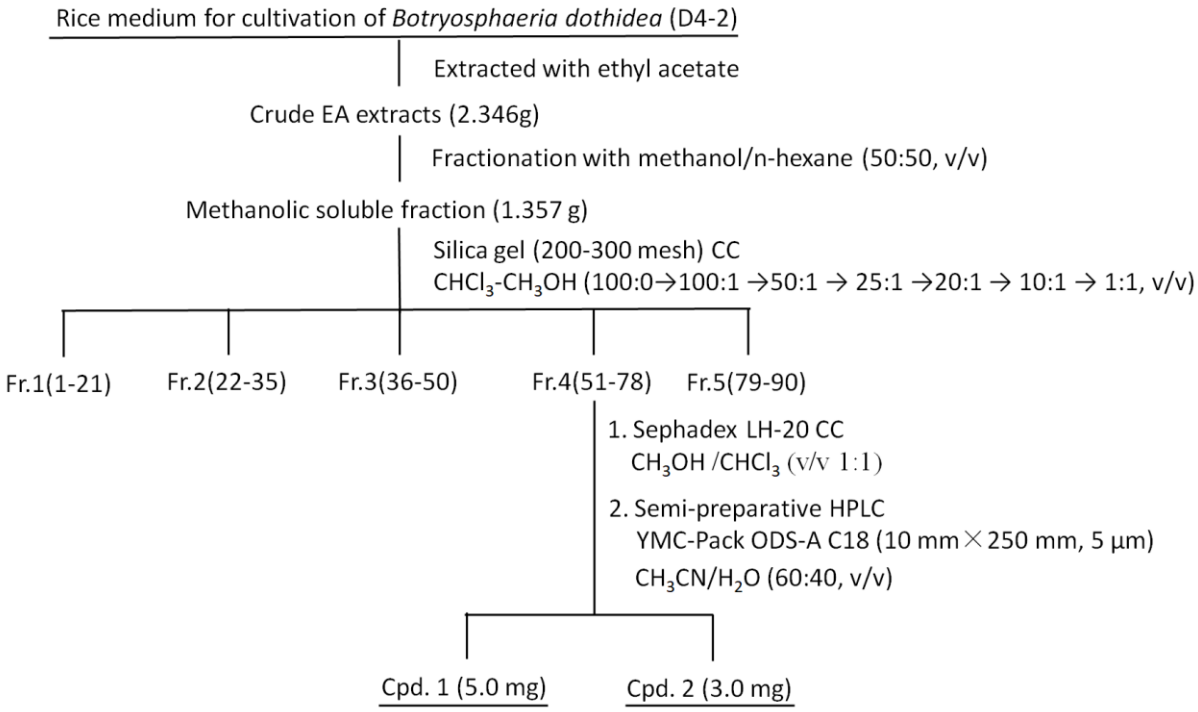


Figure S2 : Extraction, fractionation and purification procedures for compounds **1** and **2**

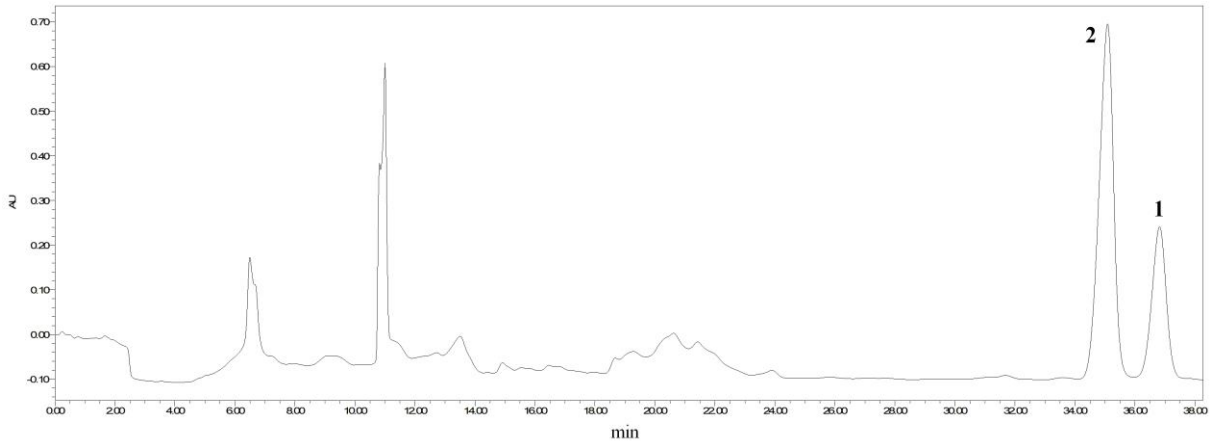


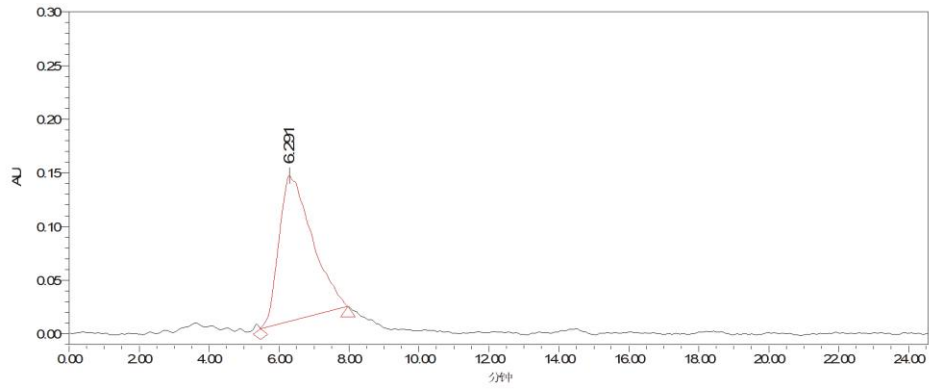
Figure S3 : The semi-preparative HPLC separation of **1** (t_R=35.5 min) and **2** (t_R=34.5 min).

Column: YMC-Pack ODS-A C18 (10 mm ×250 mm, 5 μm)

Mobile phase: Acetonitrile/H_2O (60:40)

Flow rate: 1.5 mL/min

Wavelength: 254 nm

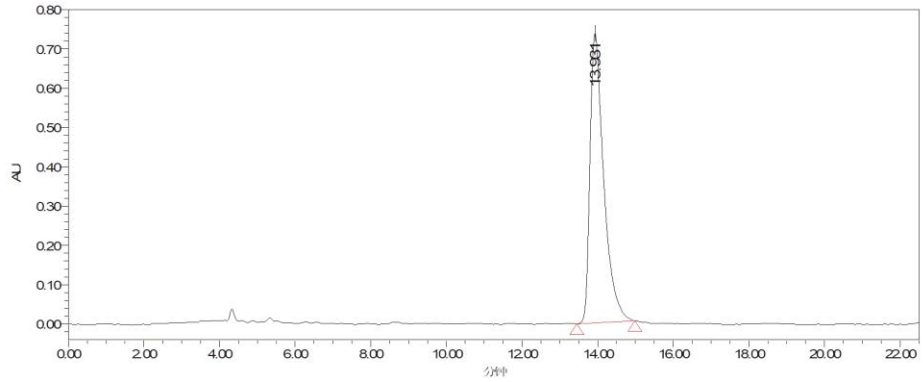


Analysis results

Compound	Retention Time (min)	Height (μV)	Area (μV*S)	Area(%)
1	6.291	136144	8902462	100%

Column: Daicel chiralpak IA-H (4.6 mm ×250mmL, 5 μm)
Mobile phase: n-hexane/ Isopropanol (90:10)
Flow rate: 1.0 mL/min
Wavelength: 210 nm
Injection volume : 5.0μL

Figure S4 : Chiral HPLC chromatogram of compound **1** (t_R=6.291 min).



Analysis results

Compound	Retention Time (min)	Height (μV)	Area (μV*S)	Area(%)
2	13.931	737468	18623660	100%

Column: Daicel chiralpak IA-H (4.6 mm ×250mmL, 5 μm)
Mobile phase: n-hexane/ Isopropanol (90:10)
Flow rate: 1.0 mL/min
Wavelength: 210 nm
Injection volume : 5.0μL

Figure S5 : Chiral HPLC chromatogram of compound **2** (t_R=13.931 min).

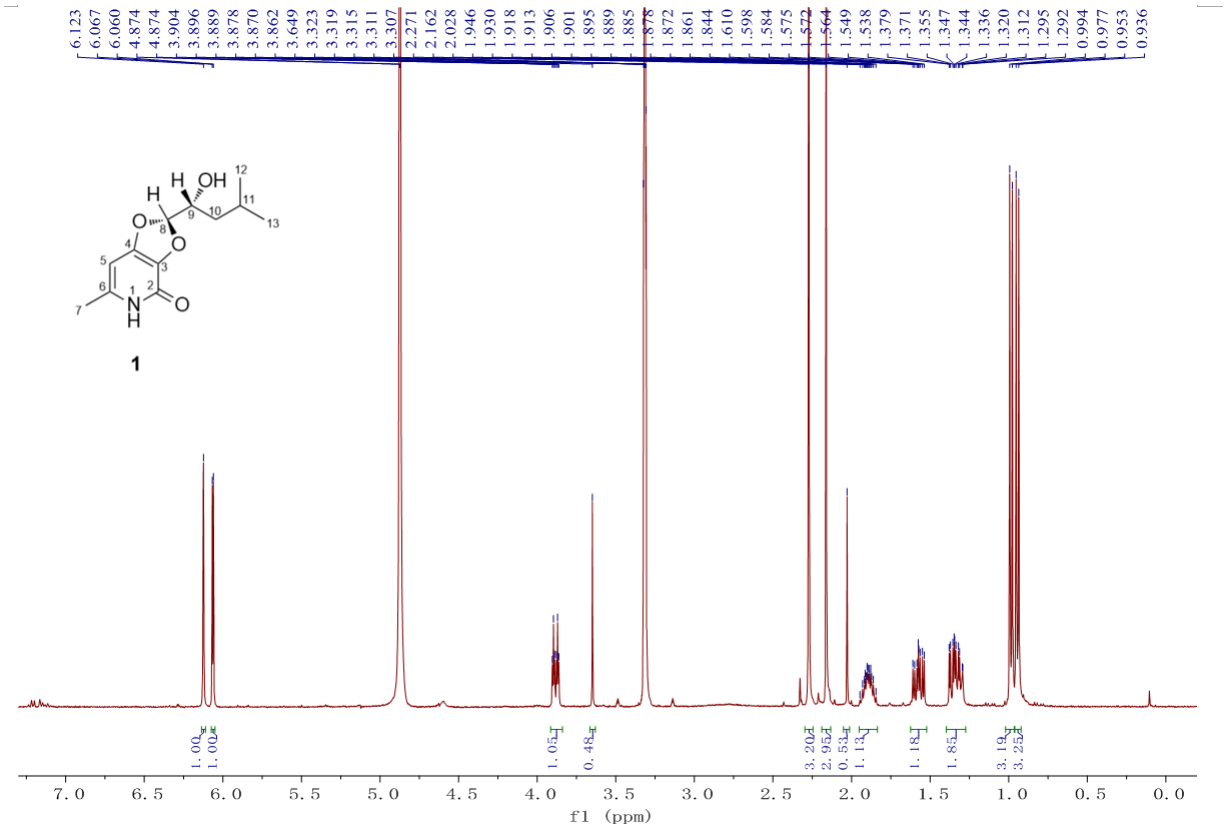


Figure S6 : ^{1}H (400 MHz) NMR Spectroscopic Data of (8S, 9R)-Dihydroisoflavipucine (**1**) in MeOD.

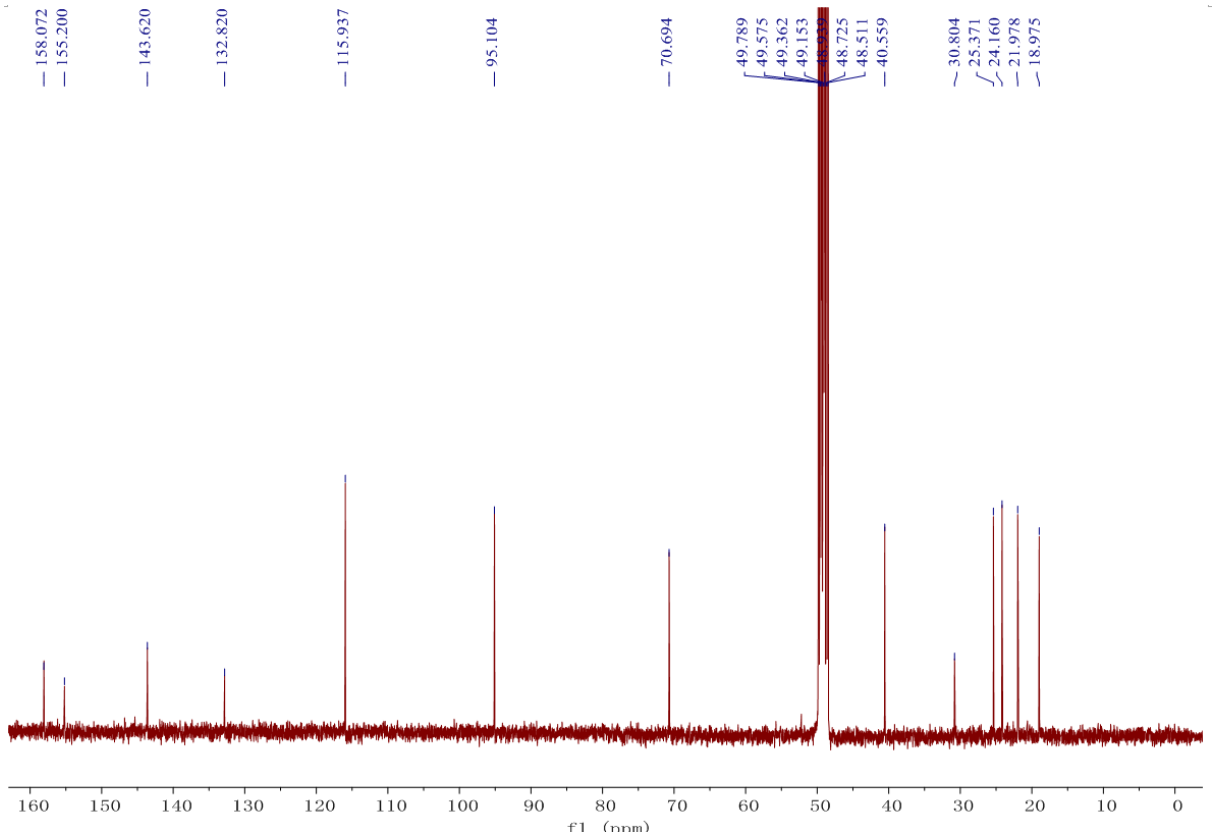


Figure S7 : ^{13}C (100 MHz) NMR Spectroscopic Data of (8S, 9R)-Dihydroisoflavipucine (**1**) in MeOD.

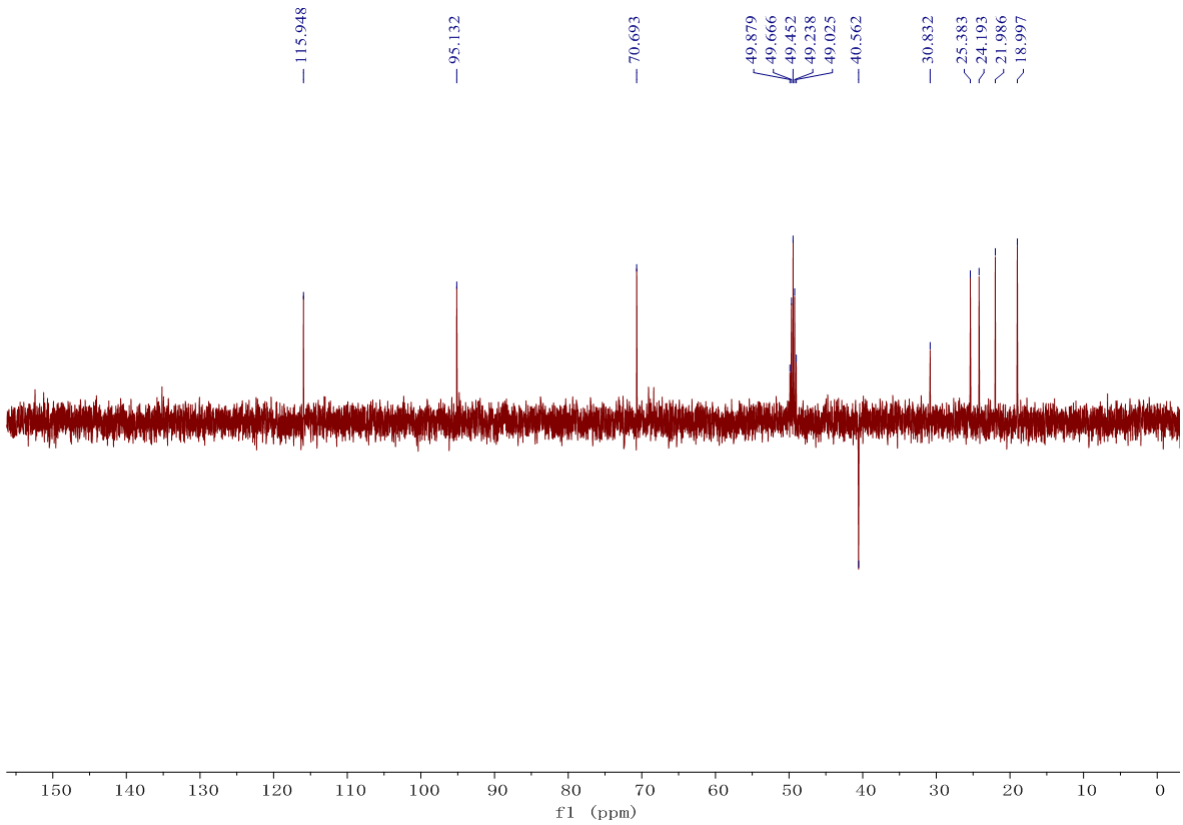


Figure S8 : DEPT135 Spectrum of (8S, 9R)-Dihydroisoflavipucine (**1**) in MeOD.

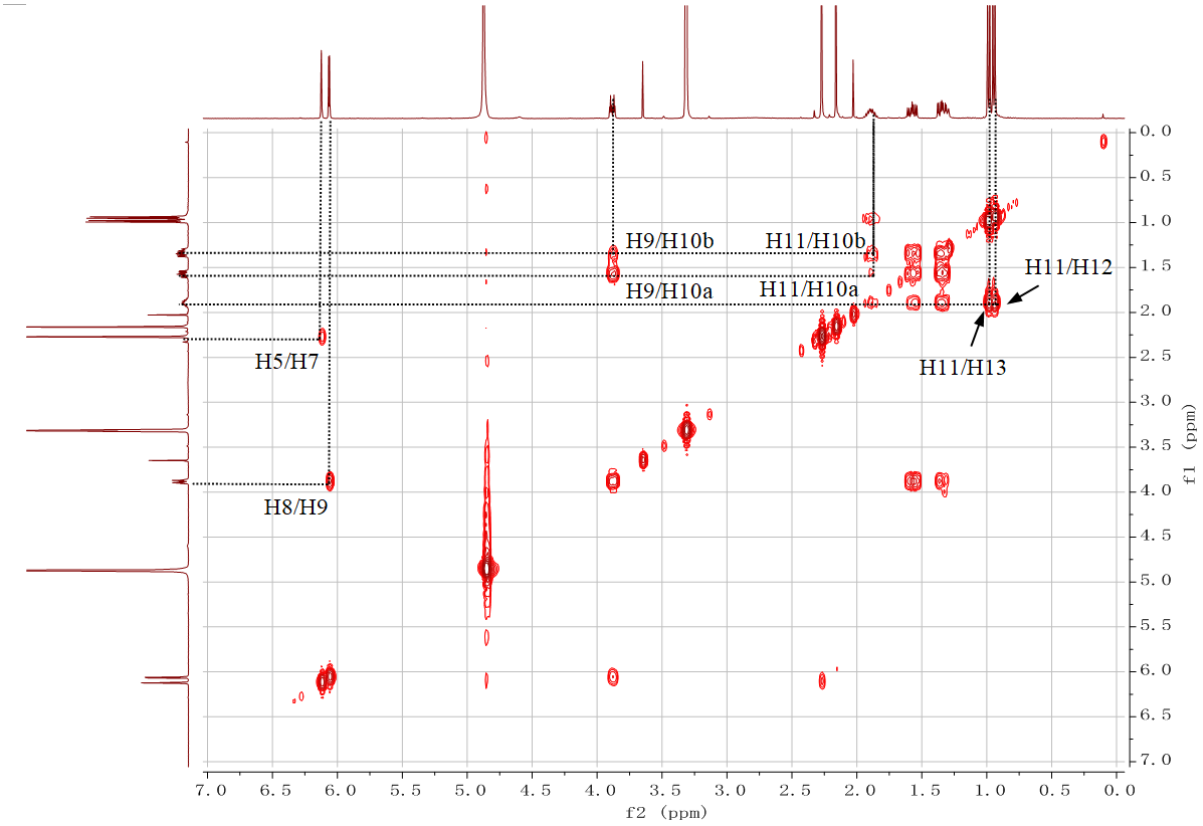


Figure S9 : ^{1}H-^{1}H COSY Spectrum of (8S, 9R)-Dihydroisoflavipucine (**1**) in MeOD.

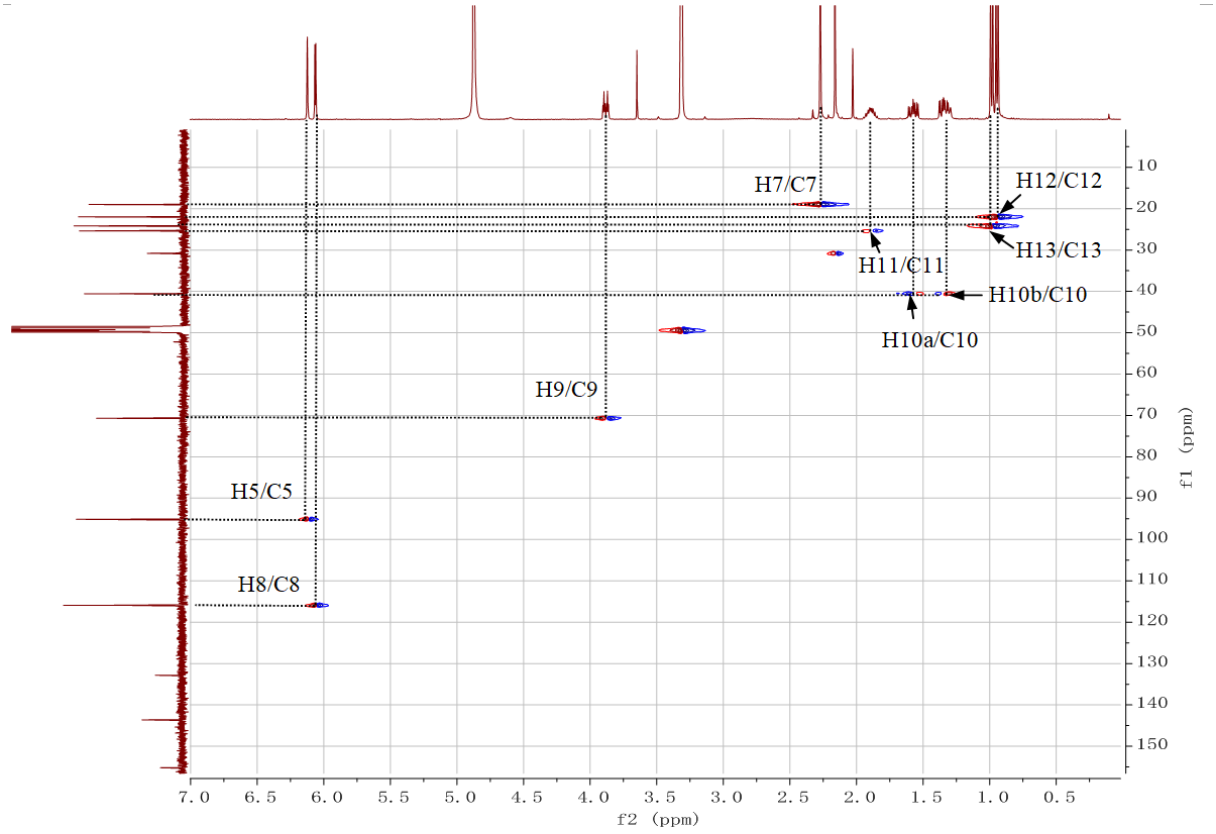


Figure S10 : HSQC Spectrum of (8S, 9R)-Dihydroisoflavipucine (1) in MeOD.

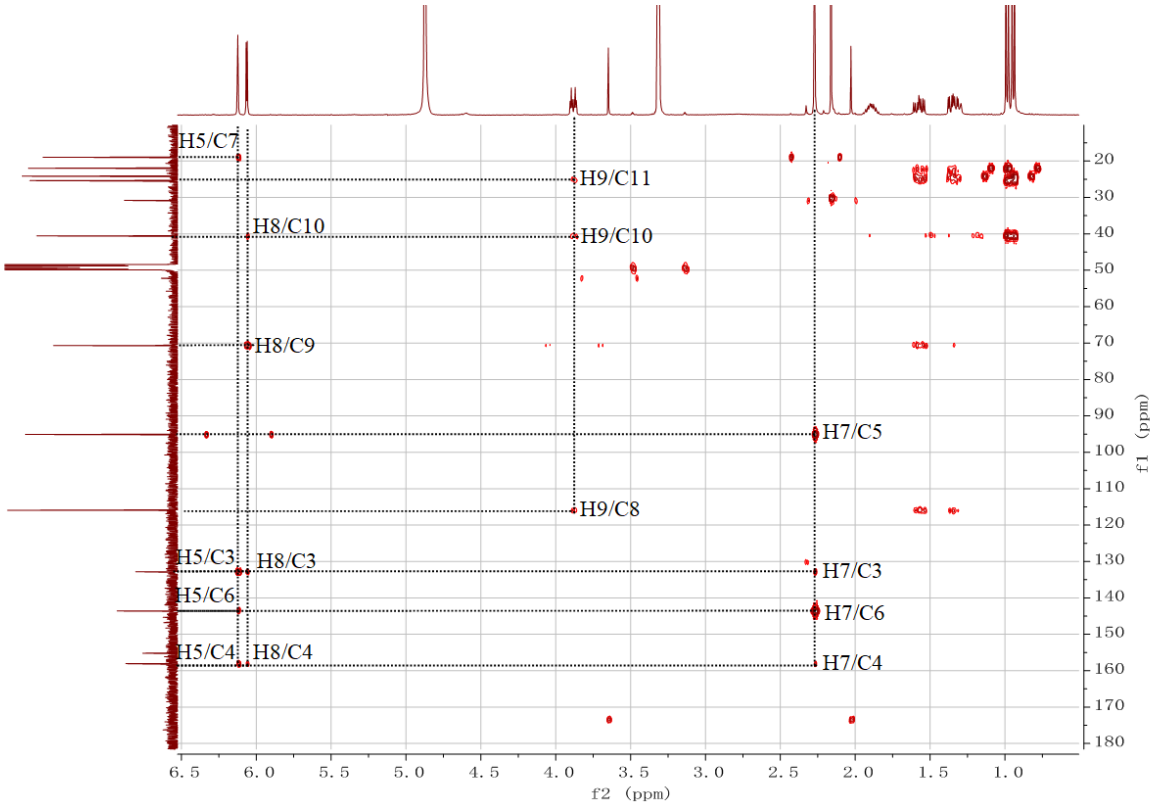


Figure S11 : HMBC Spectrum of (8S, 9R)-Dihydroisoflavipucine (1) in MeOD.

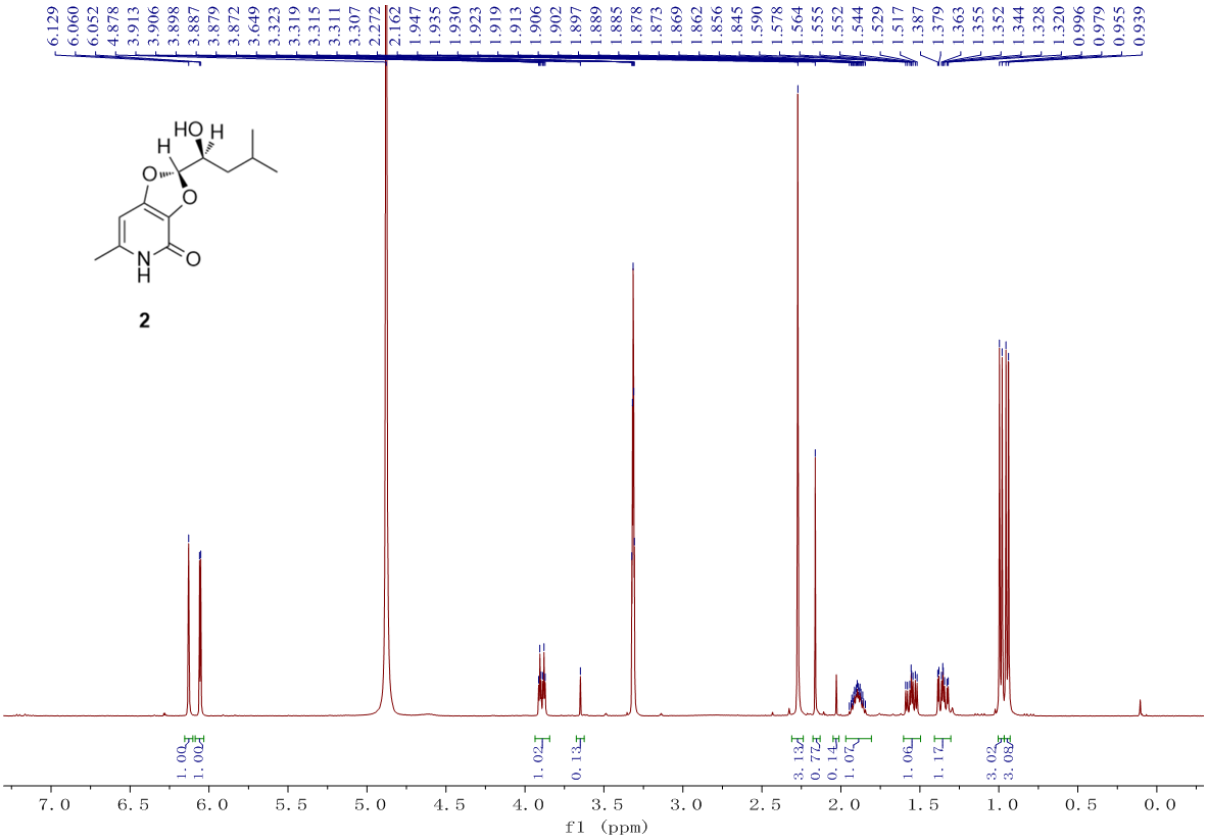


Figure S12 : ^{1}H (400 MHz) NMR Spectroscopic Data of (8S, 9S)-Dihydroisoflavipucine (**2**) in MeOD.

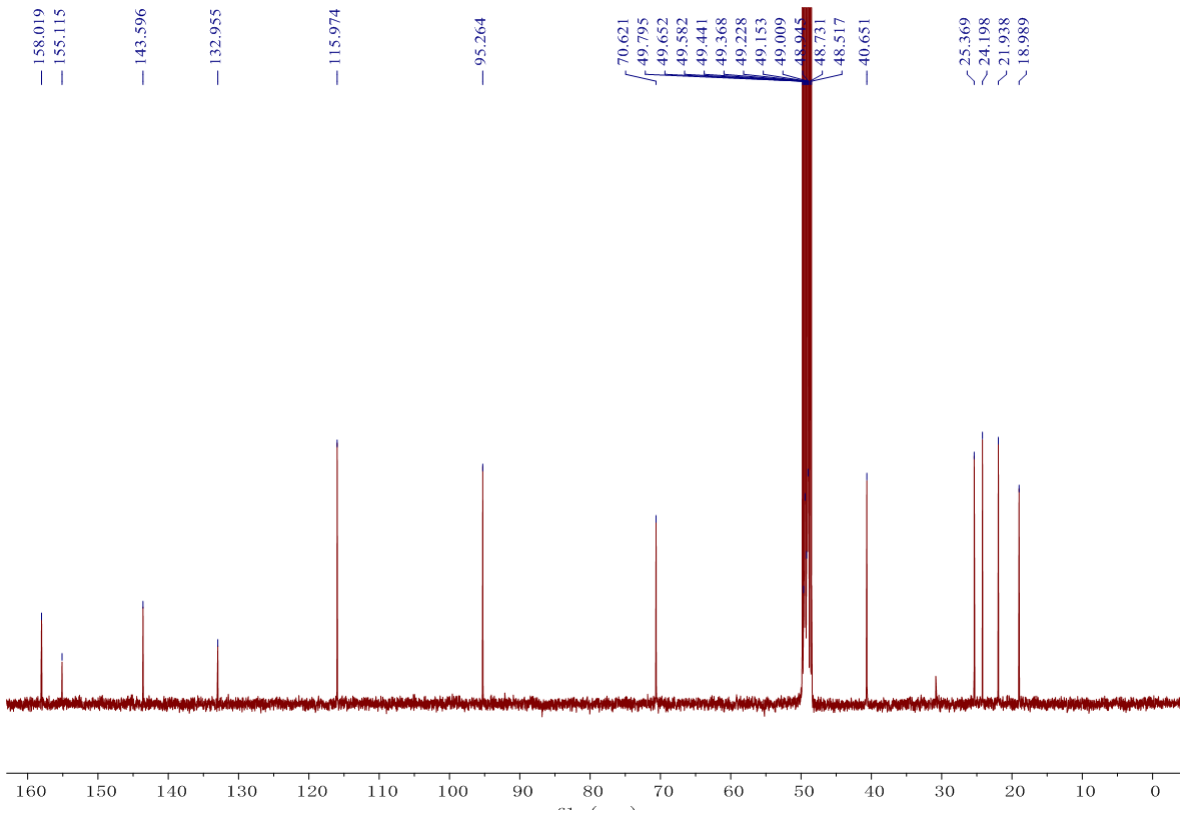


Figure S13 : ^{13}C (100 MHz) NMR Spectroscopic Data of (8S, 9S)-Dihydroisoflavipucine (**2**) in MeOD.

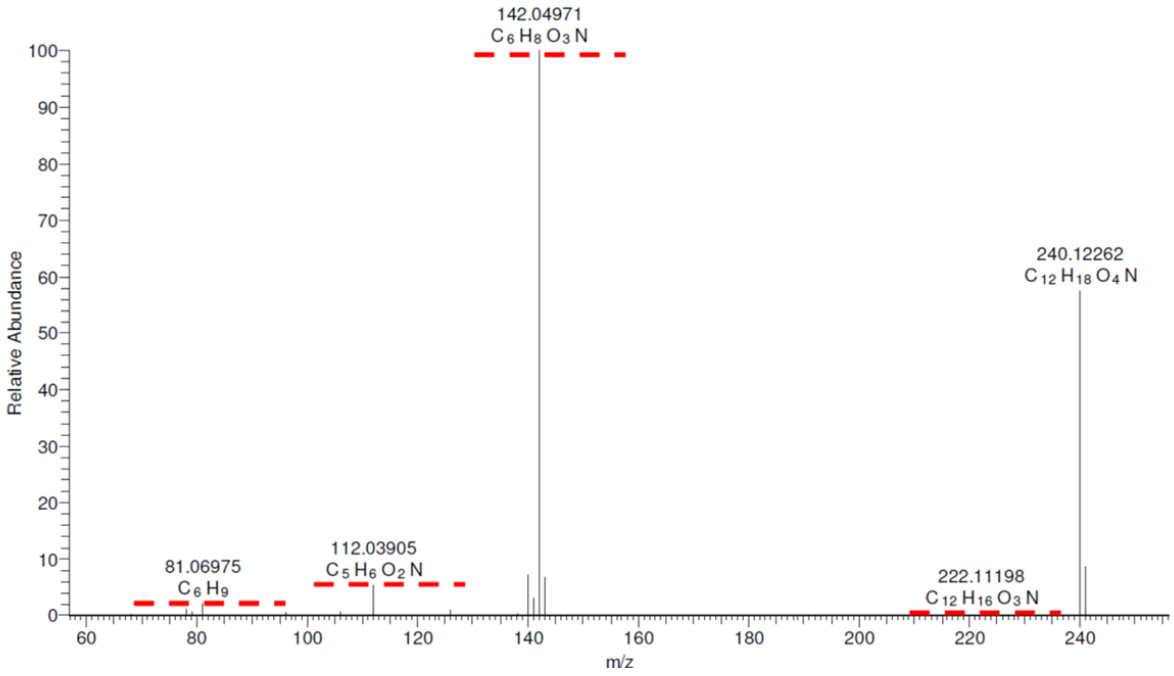


Figure S14 : HRESIMS Spectrum of (8S, 9R)-Dihydroisoflavipucine (**1**).

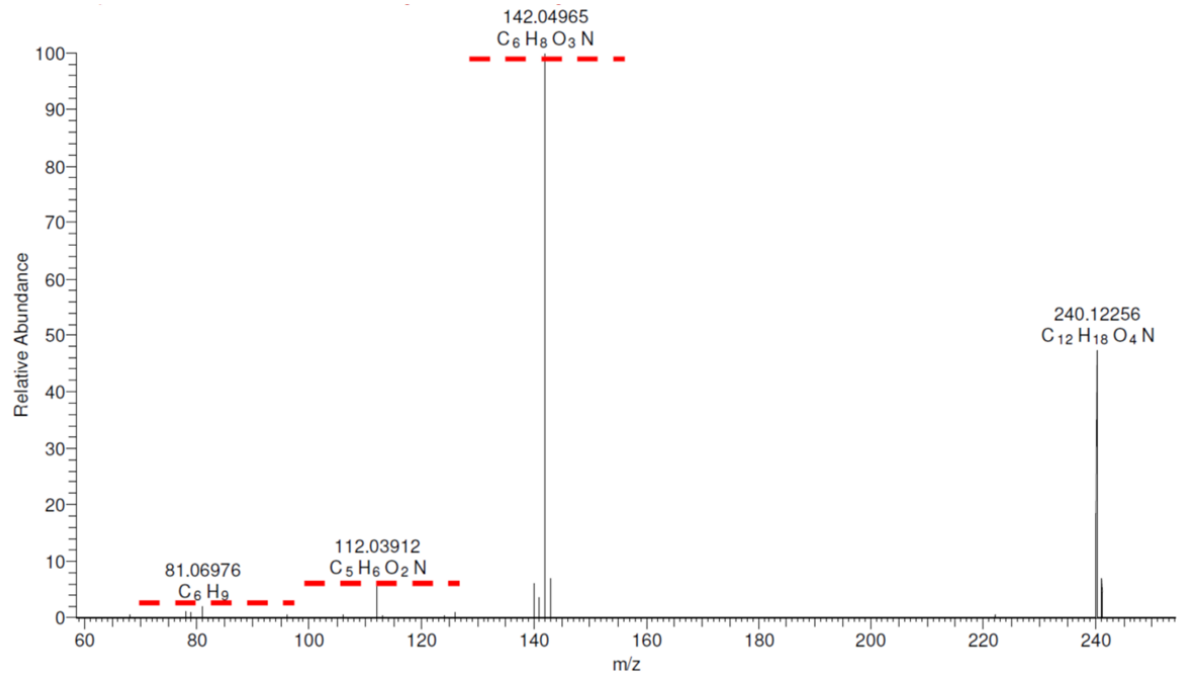


Figure S15 : HRESIMS Spectrum of (8S, 9S)-Dihydroisoflavipucine (**2**).

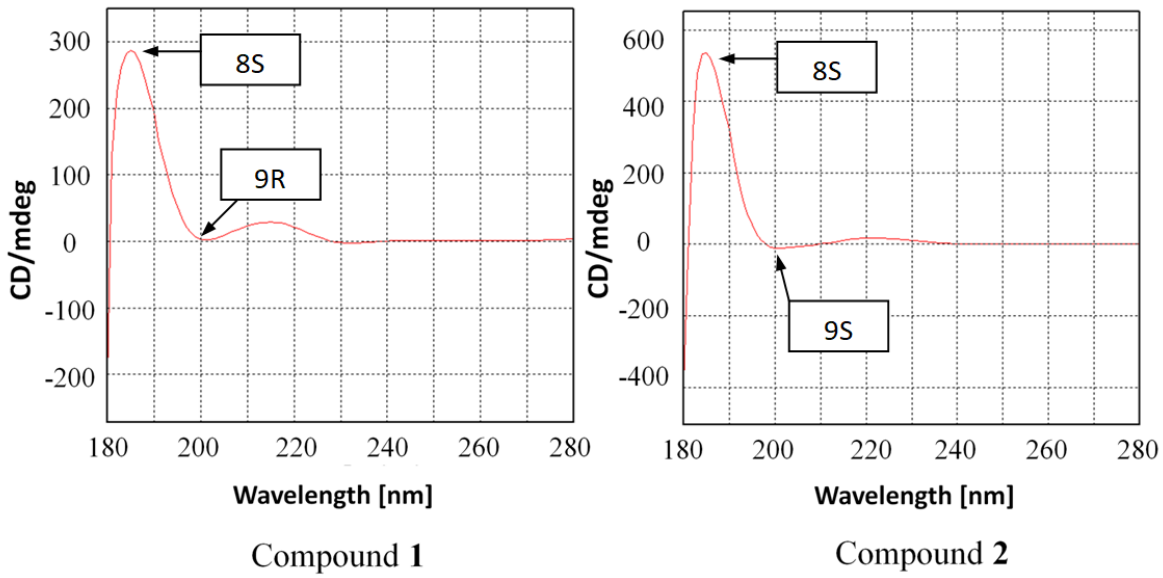


Figure S16 :CD Spectrum of (8S, 9R)-dihydroisoflavipucine (**1**) and (8S, 9S)-dihydroisoflavipucine (**2**) in MeOH.

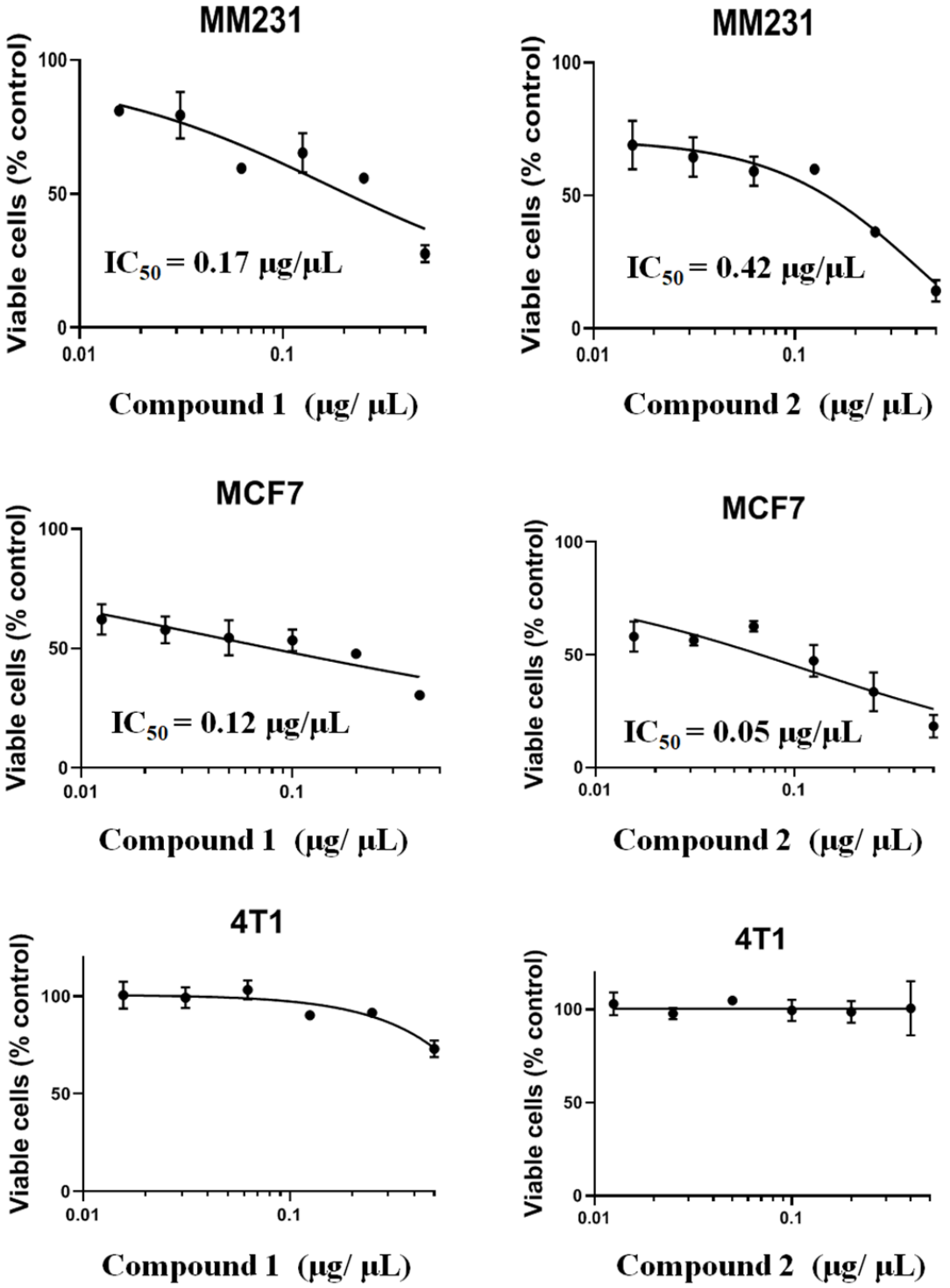
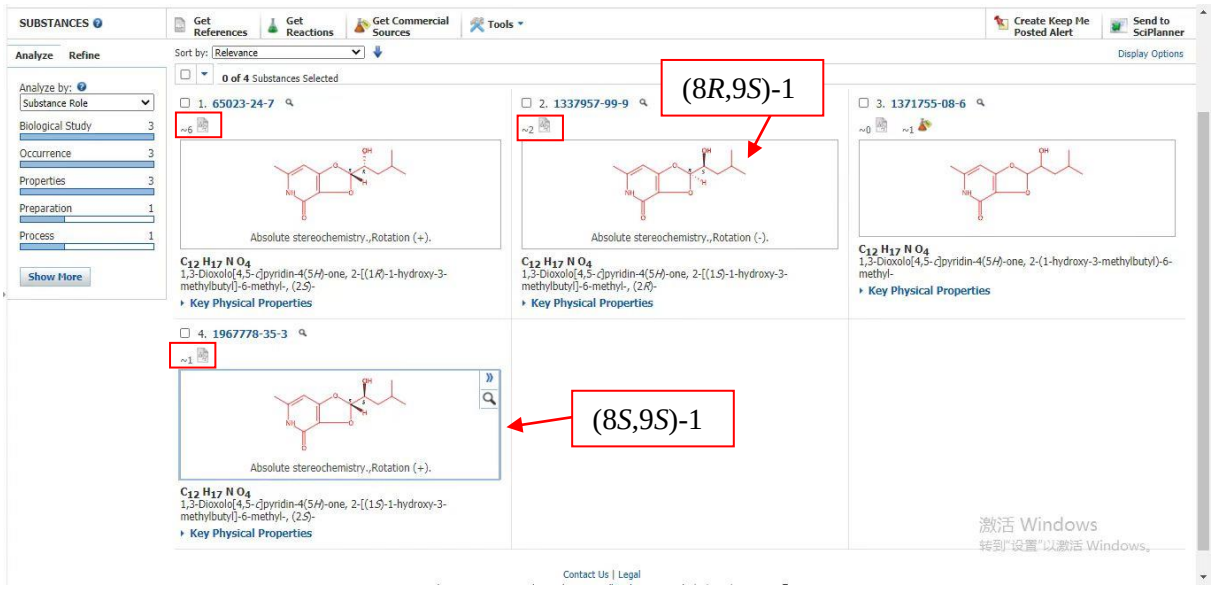


Figure S17 : Antiproliferative effects of (8S, 9R)-dihydroisoflavipucine (**1**) and (8S, 9S)-dihydroisoflavipucine (**2**) on breast cancer cells MDA-MB-231, MCF7 and 4T1.



The literatures mentioned above and their analysis were followed by a list.

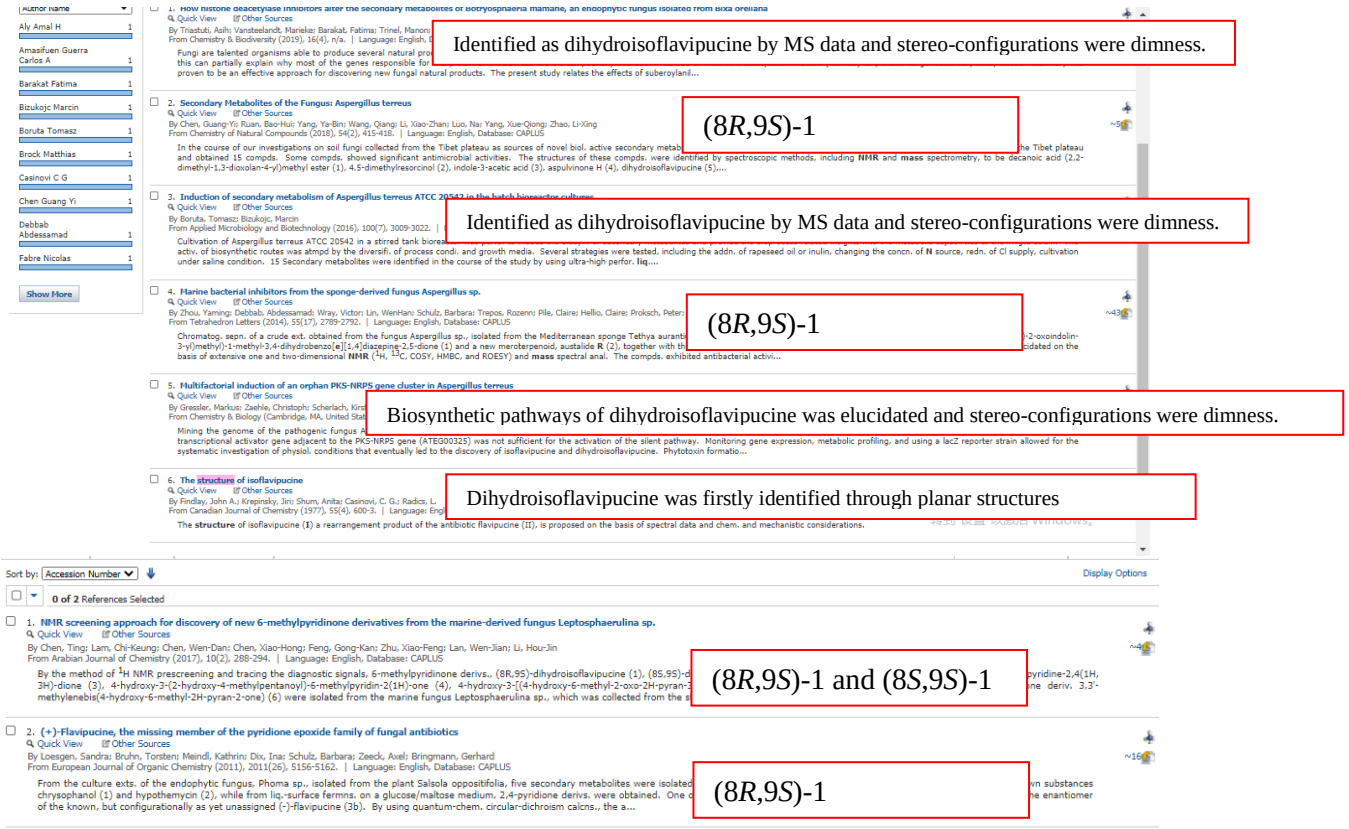


Figure S18: The Scifinder search for the new compound (8*S*, 9*R*)-**1**.