

SUPPLEMENTARY MATERIAL

A new iridoid from the roots of *Valeriana jatamansi* Jones with α -glucosidase activity

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ABSTRACT

One new iridoid namely rupesin F (**1**) together with four known ones (**2** - **5**) were isolated from the roots of *Valeriana jatamansi* Jones. The structures were established using spectroscopic methods (1D and 2D NMR including HSQC, HMBC, COSY and NOESY) and by comparison with previously published literature data. The isolated compounds **1** and **3** exhibited strong α -glucosidase inhibition activity with IC_{50} values of 10.13 ± 0.11 and 9.13 ± 0.03 $\mu\text{g/mL}$, respectively. This study enriched the chemical diversity of metabolites and provides a direction for the development of antidiabetic agents.

KEYWORDS: *Valeriana jatamansi*; iridoids; rupesin F; α -glucosidase

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Table S1. ^1H NMR and ^{13}C NMR data for compounds 1 and 2 in CD_3OD (δ in ppm; J in Hz).

Position	1^{a} δ_{H} (J in Hz)	δ_{C}
1	6.33 d (3.3)	91.5
2	-	-
3	5.08 s	95.1
4	-	150.4
5	3.17 t (6.1)	38.0
6	2.14 m, 1.93 m	43.4
7	3.84 dd (3.1, 7.2)	79.5
8	-	83.6
9	2.41 t (3.6)	43.0
10	1.42 s	19.1
11	4.94 s, 4.87 s	108.0
1'	-	173.8
2'	2.31 dd (6.4, 14.7), 2.20 m	42.3
3'	1.88 m	33.2
4'	0.97 d (6.7)	19.5
5'	1.43 m, 1.28 m	30.1
6'	0.94 t (7.4)	11.9

^aRecorded at 600 MHz for ^1H NMR and 150 MHz for ^{13}C NMR.

Assignments are based on COSY, HSQC, HMBC and NOESY experiments.

Table S2. The IC₅₀ value of the extract, fractions and isolated compounds from *V. jatamansi* for the *in-vitro* inhibition of α -glucosidase

Compound	IC₅₀ ($\mu\text{g/mL}$)
Parent extract (ethanolic extract)	17.45 \pm 0.30
Water fraction	12.16 \pm 0.10
<i>n</i> -Butanol fraction	13.00 \pm 0.11
Rupesin F (1)	10.13 \pm 0.11
Rupesin E (2)	13.31 \pm 0.04
valerianoside A (3)	9.13 \pm 0.03
8,9-didehydro-7-hydro-xydolichodial (4)	11.9 \pm 0.03
Acarbose	3.74 \pm 0.12

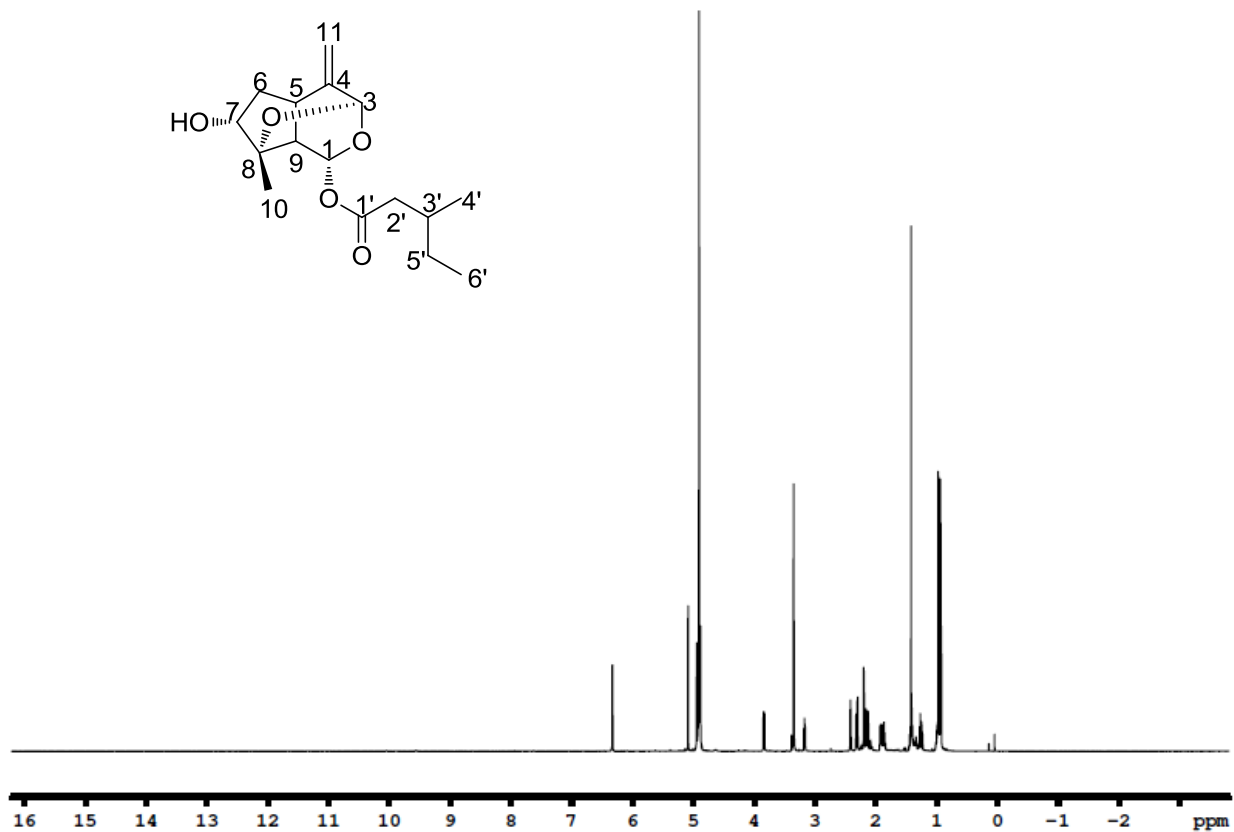


Figure S1. ¹H NMR spectrum of Rupesin F in CD₃OD

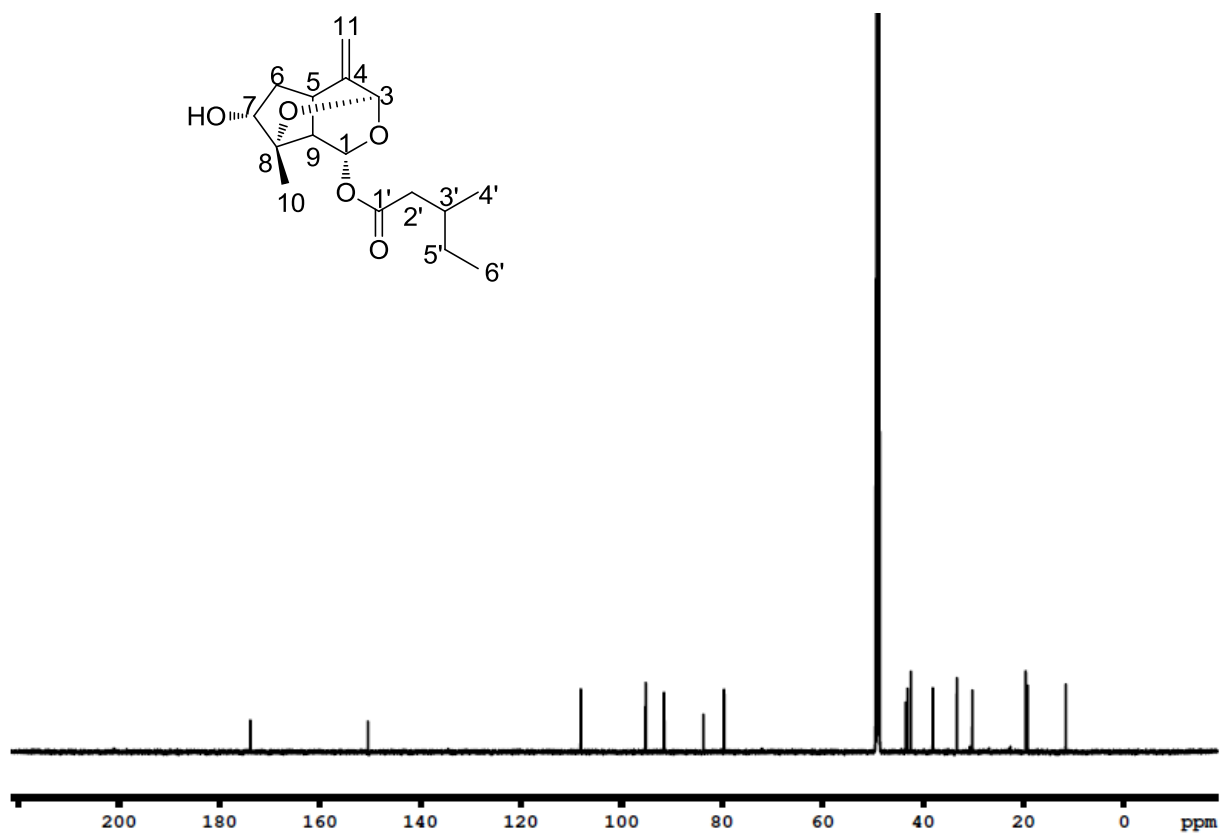


Figure S2. ^{13}C NMR spectrum of Rupesin F in CD_3OD

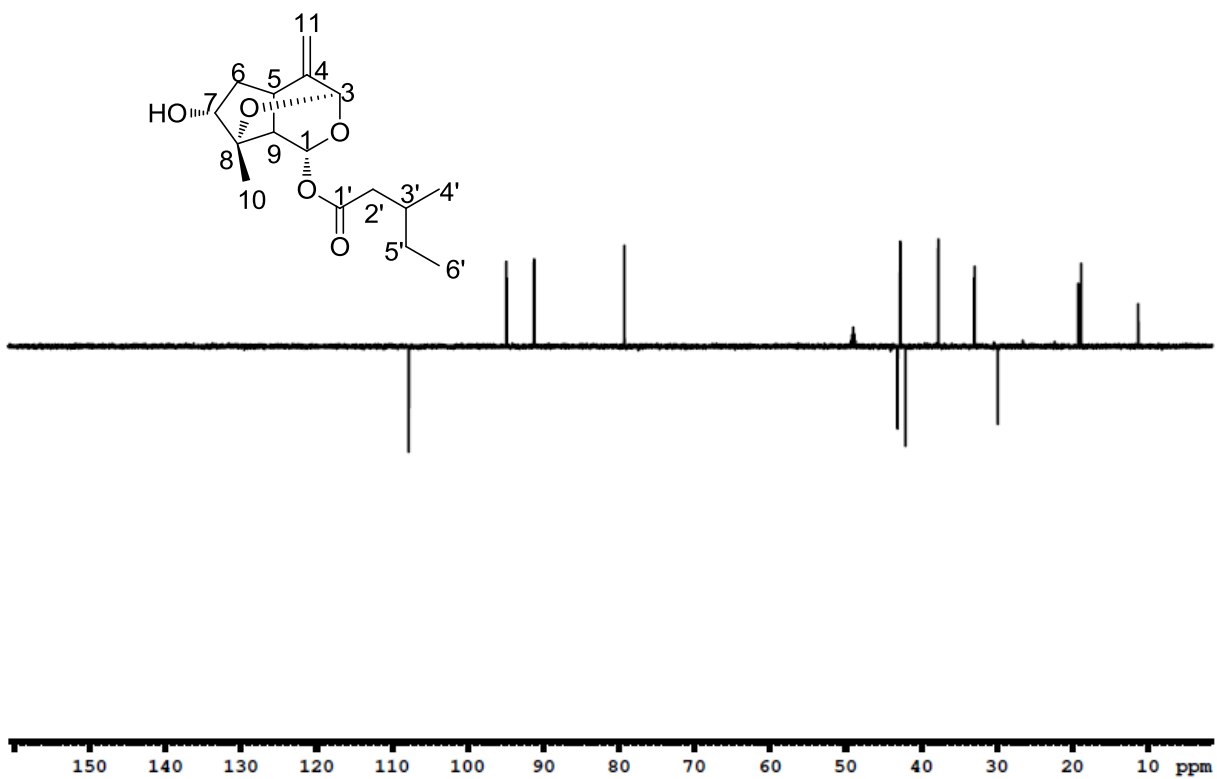


Figure S3. DEPT 135 spectrum of Rupesin F in CD₃OD

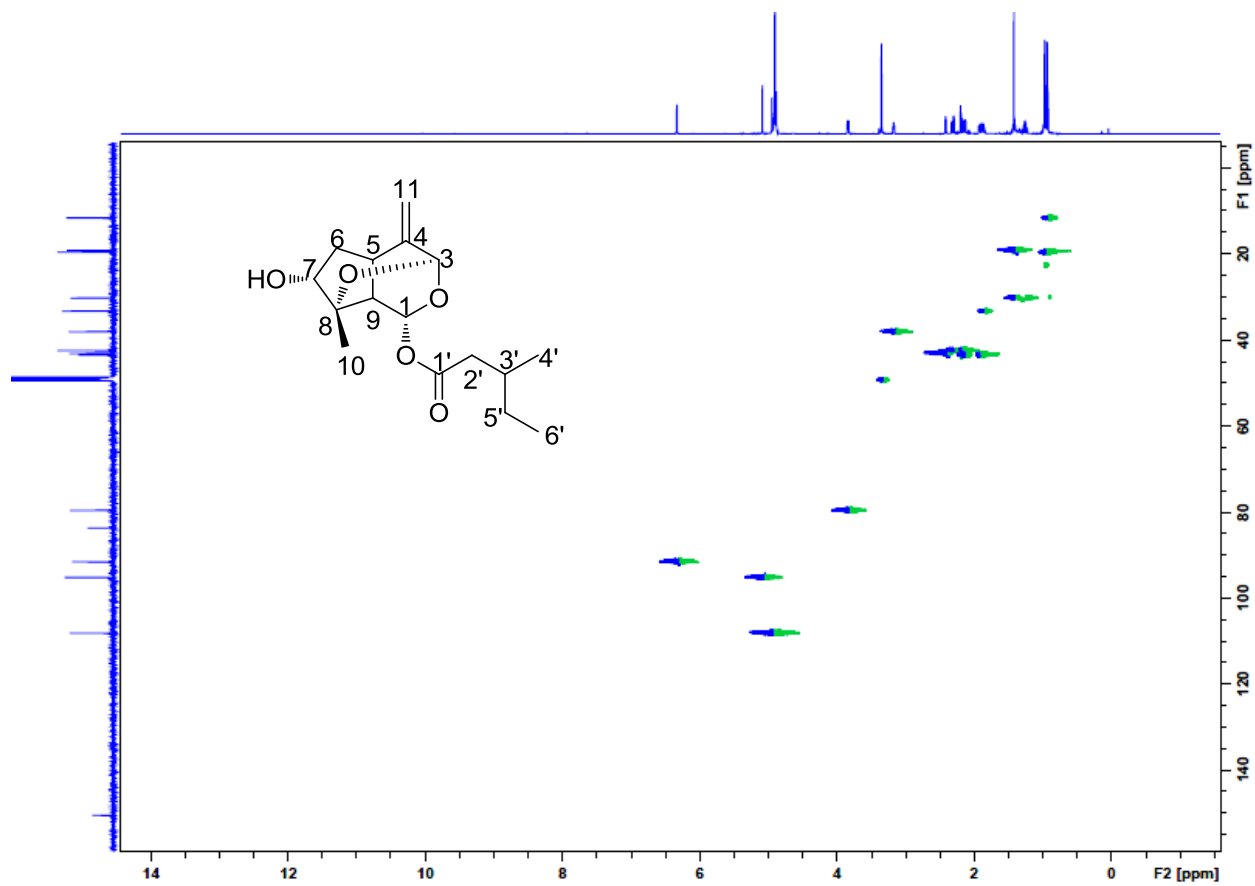


Figure S4. HSQC spectrum of Rupesin F in CD₃OD

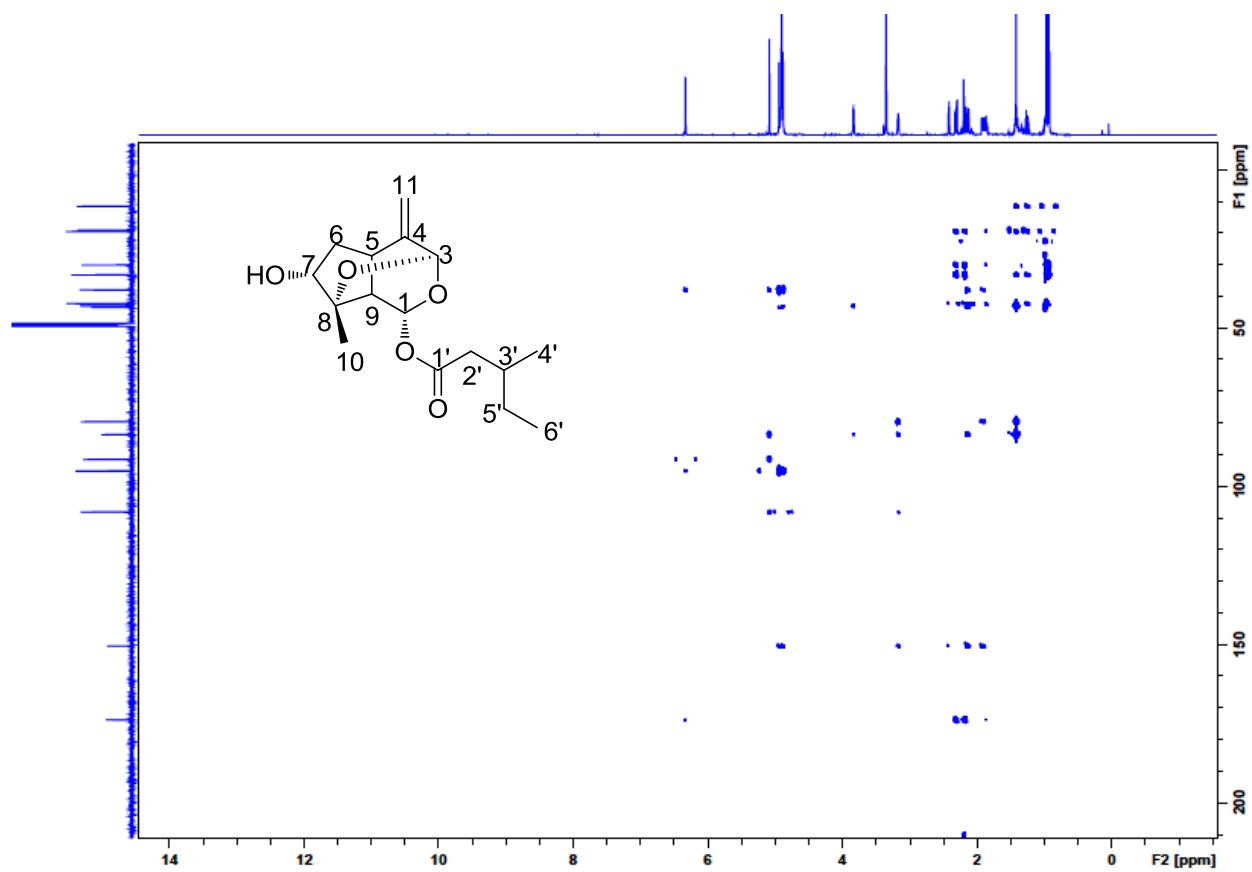


Figure S5. HMBC spectrum of Rupesin F in CD₃OD

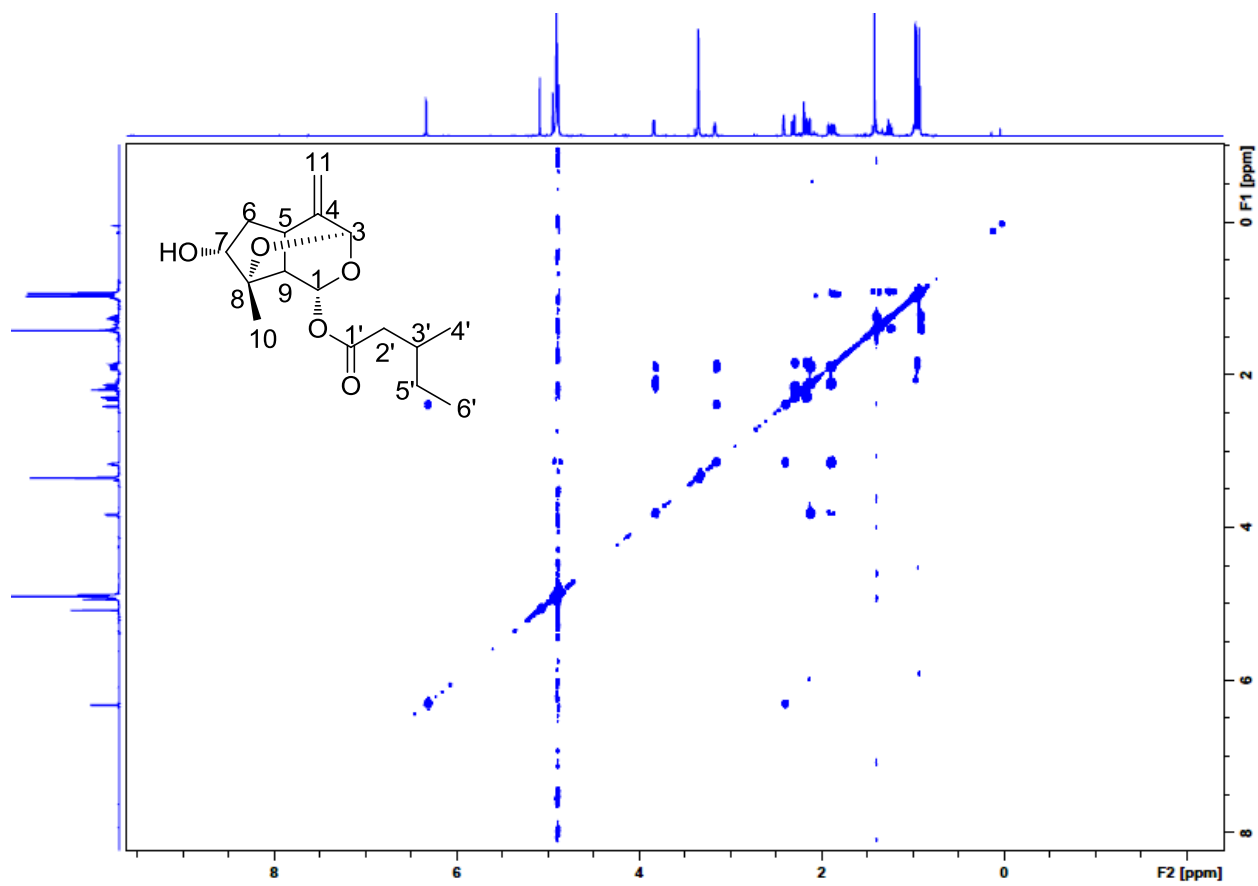


Figure S6. COSY spectrum of Rupesin F in CD₃OD

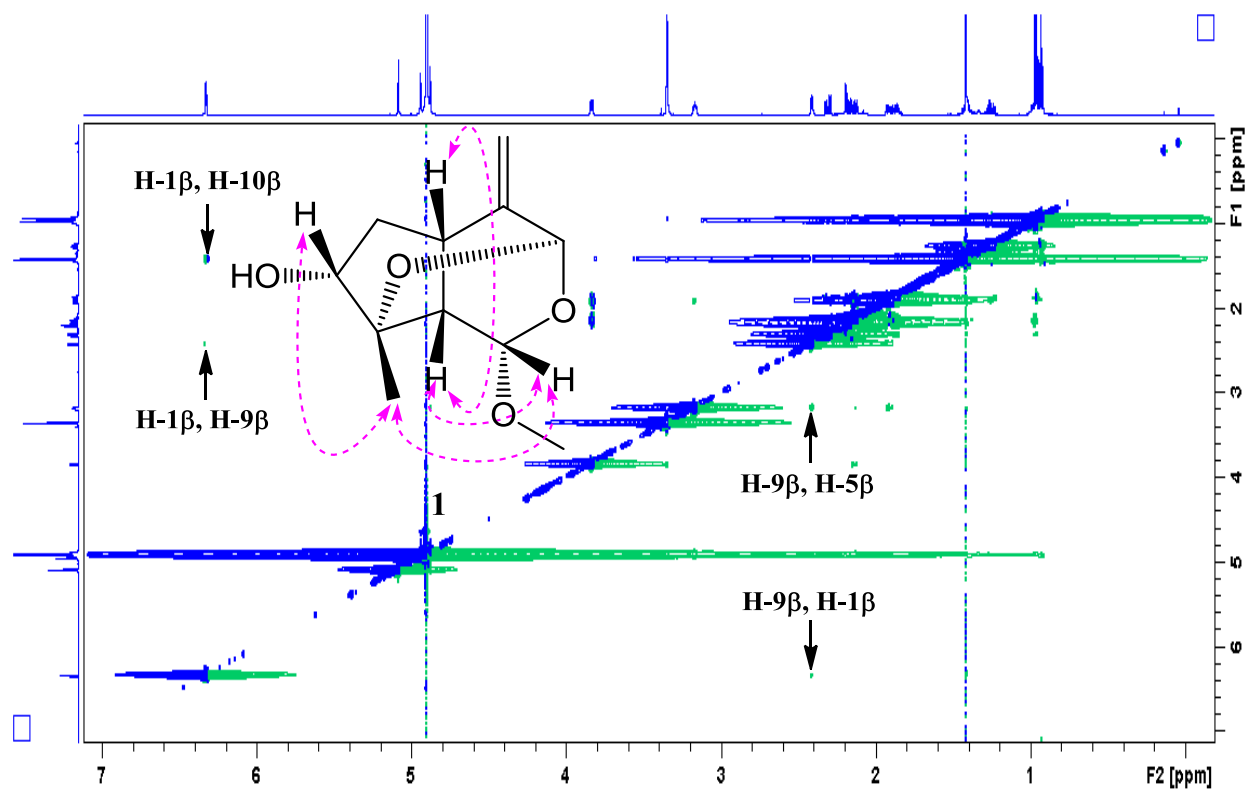


Figure S7. NOESY spectrum of Rupesin F in CD₃OD

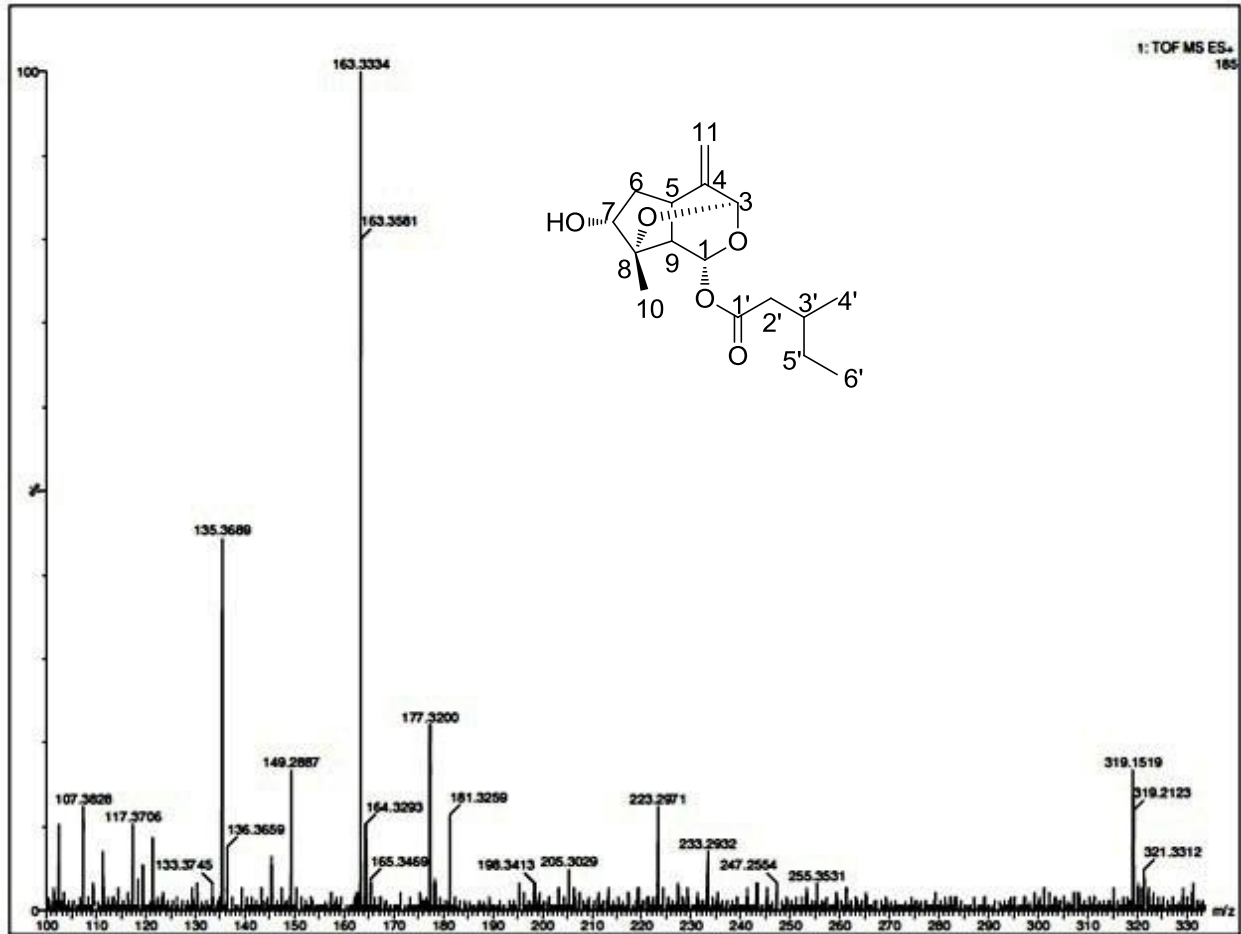
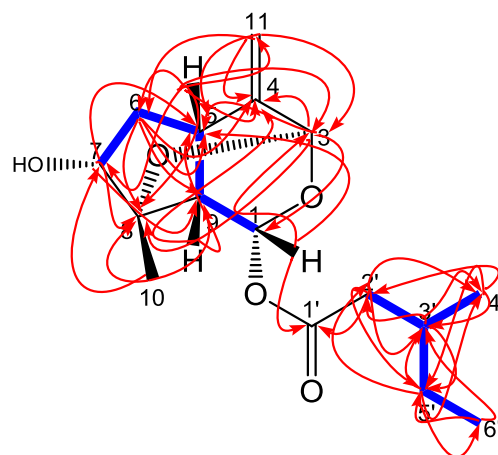


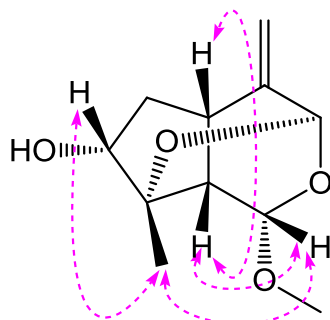
Figure S8. HRESIMS mass spectra of Rupesin F

HMBC 
COSY 



1

NOE 



1

Figure S9. Key HMBC, COSY and NOESY correlations of Rupesin F

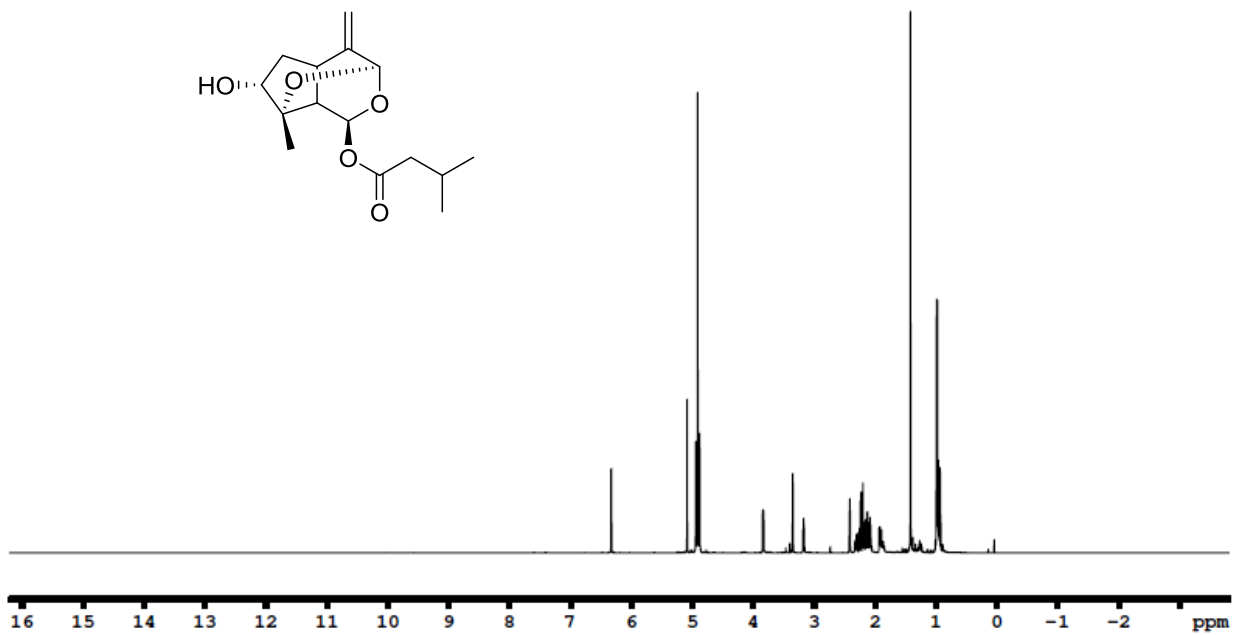


Figure S10. ¹H NMR spectrum of Rupesin E in CD₃OD

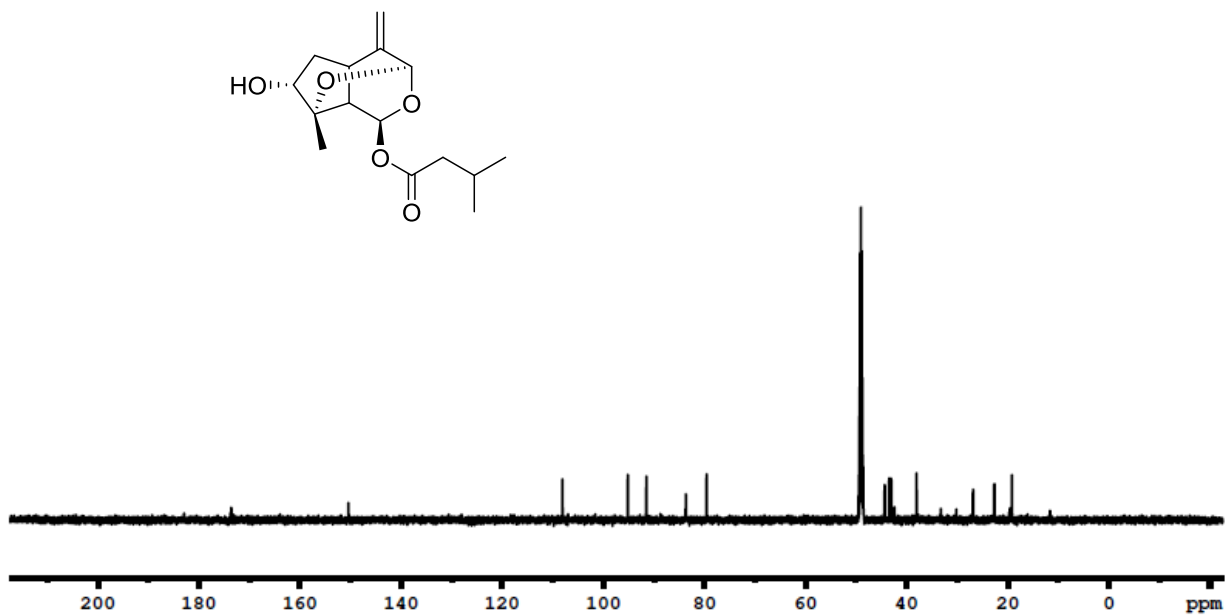


Figure S11. ¹³C NMR spectrum of Rupesin E in CD₃OD

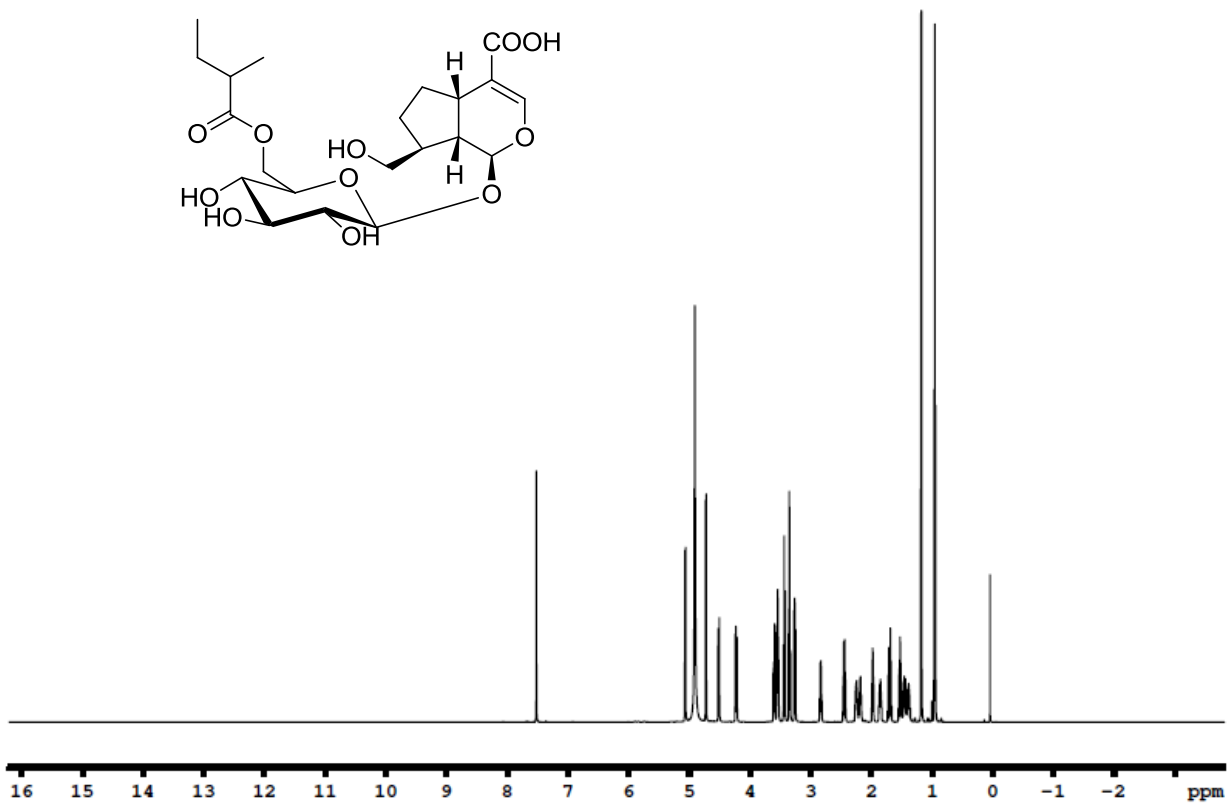


Figure S12. ¹H spectrum of Valerianoside A in CD₃OD

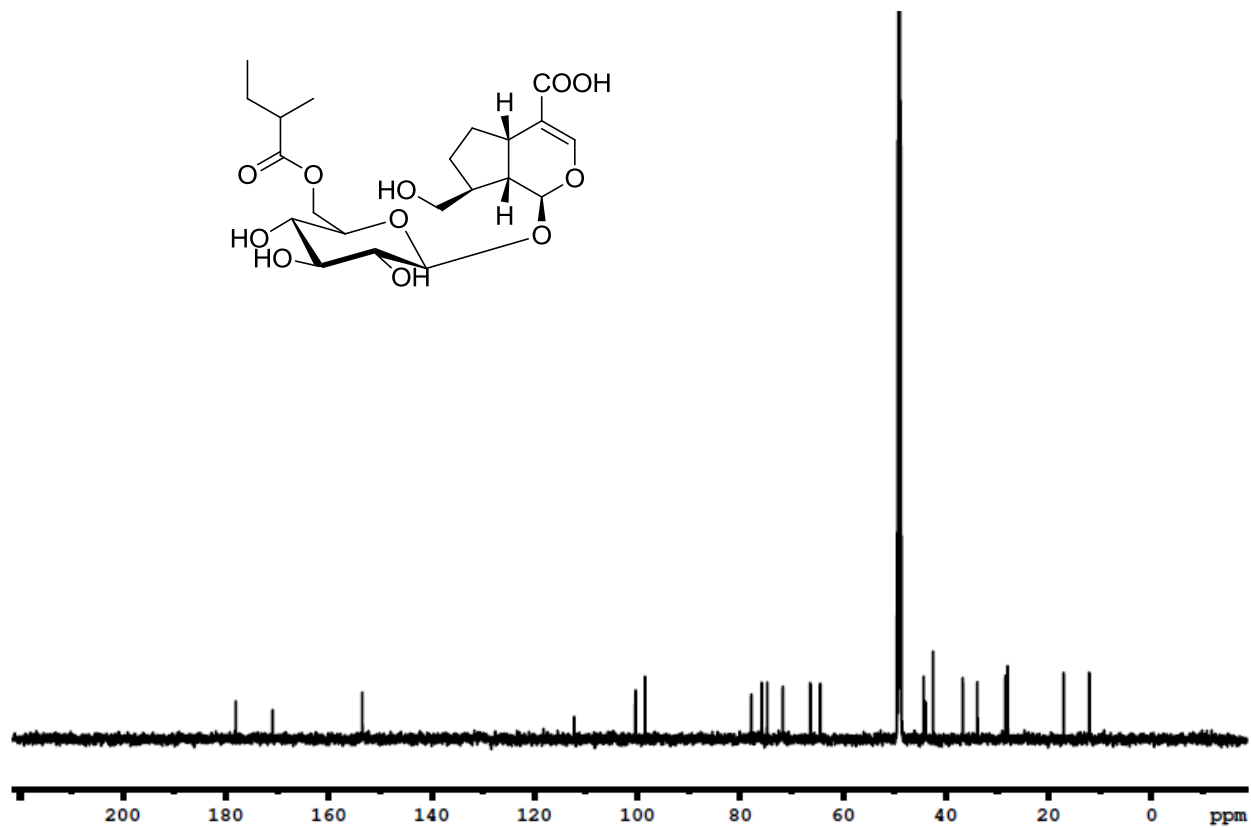


Figure S13. ¹³C NMR spectrum of Valerianoside A in CD₃OD

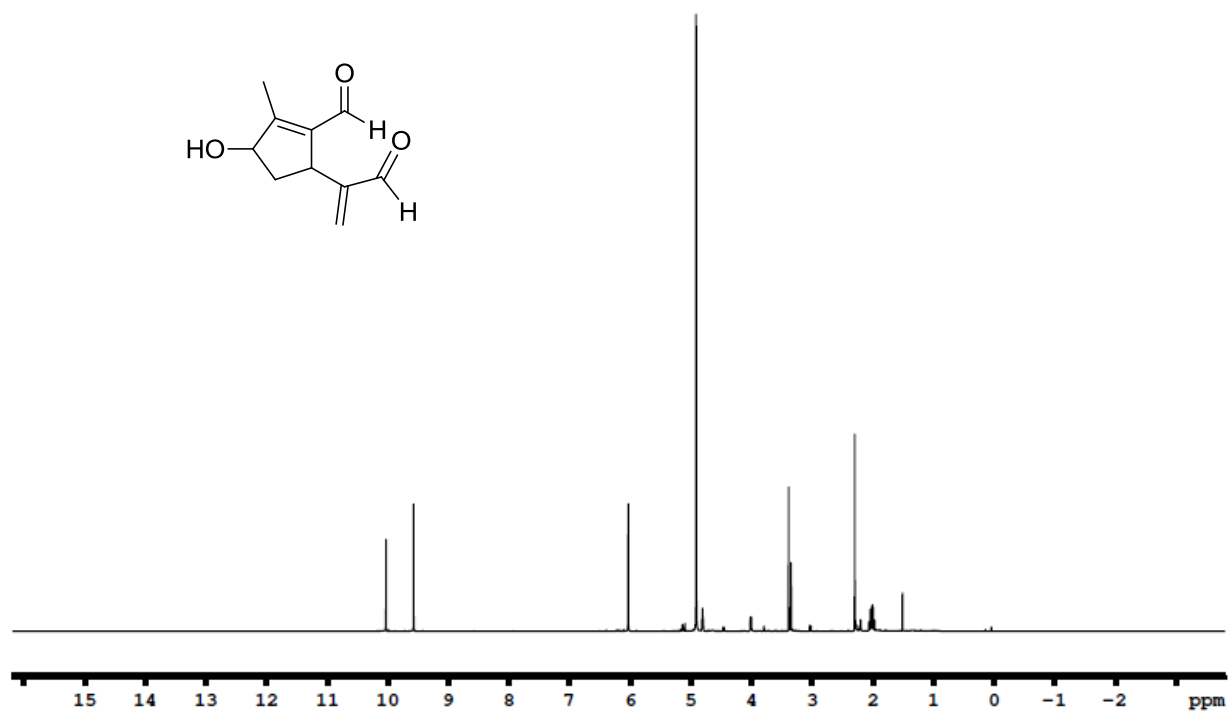


Figure S14. ^1H NMR spectrum of 8,9-didehydro-7-hydro-xydolichodial in CD_3OD

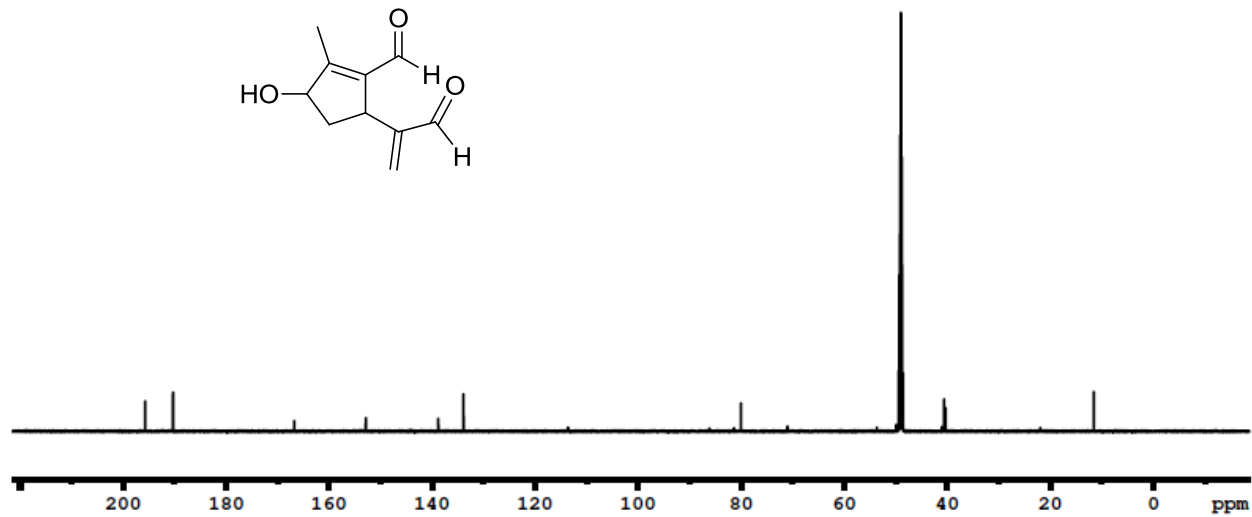


Figure S15. ^{13}C NMR spectrum of 8,9-didehydro-7-hydro-xydolichodial in CD_3OD

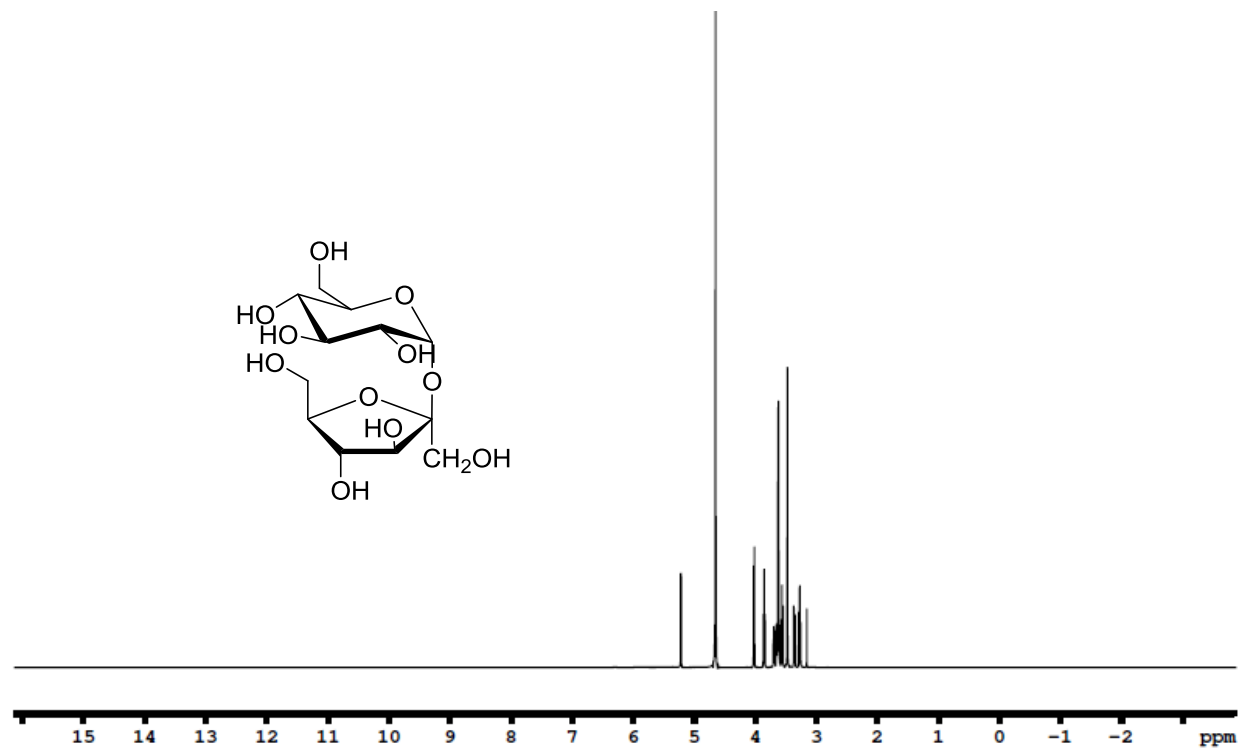


Figure S16. ^1H NMR spectrum of sucrose in D_2O

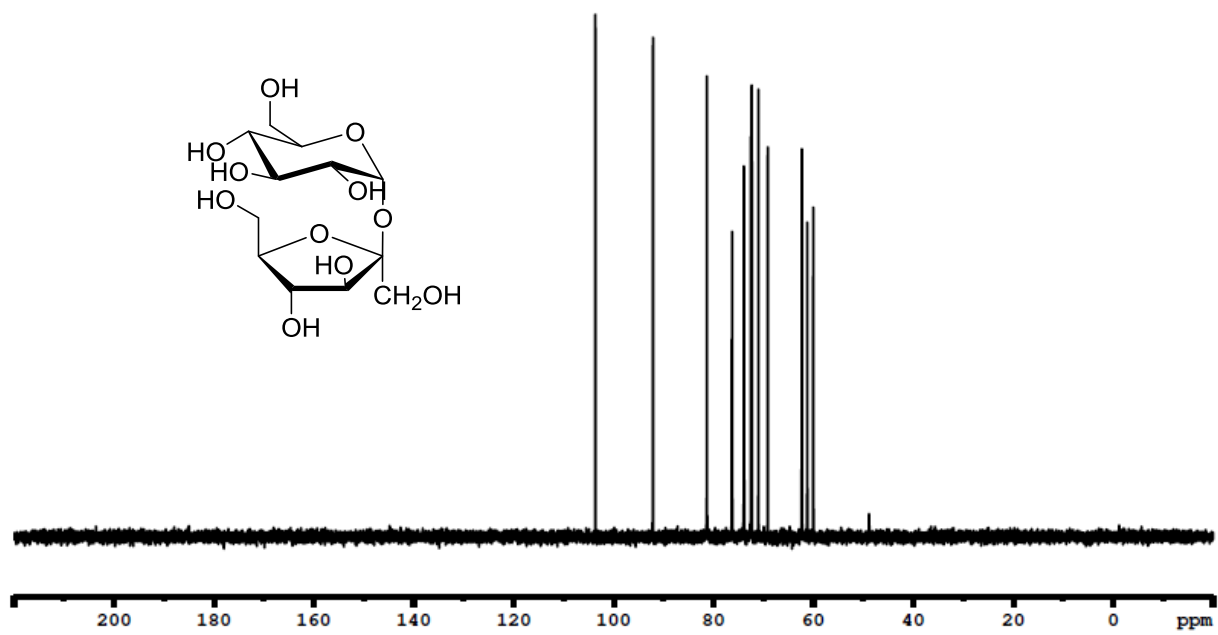


Figure S17. ^{13}C NMR spectrum of sucrose in D_2O