

Supporting Information

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A New Megastigmane Glycoside and Other Constituents from *Amomum muricarpum* Elmer

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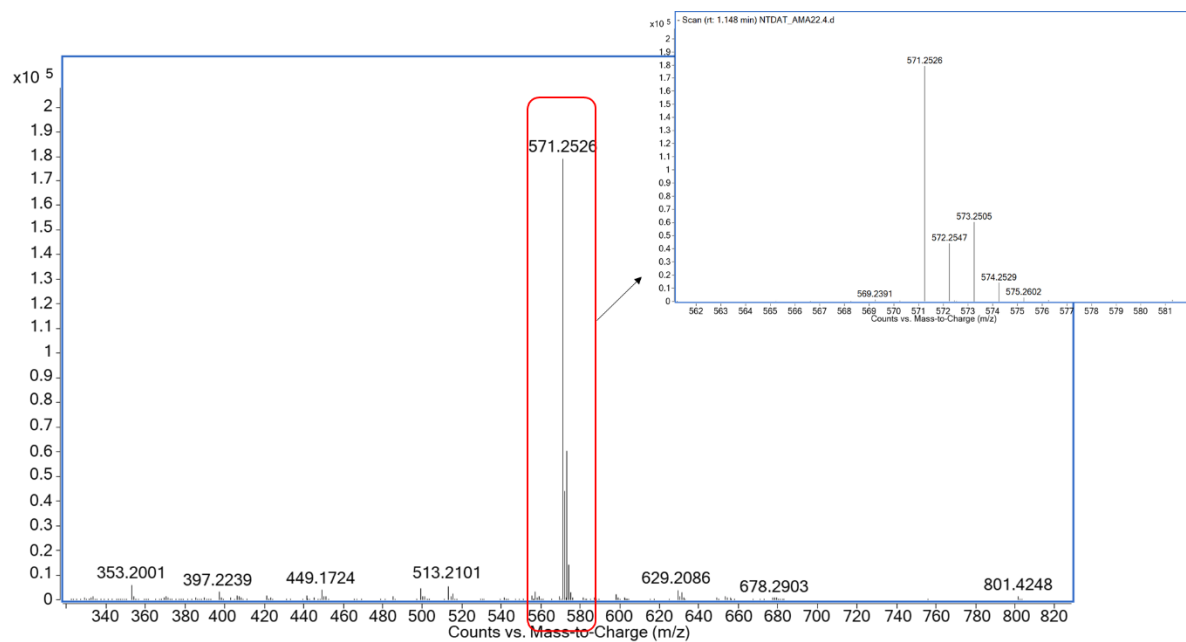


Figure S1: HRESIMS spectrum of compound (1)

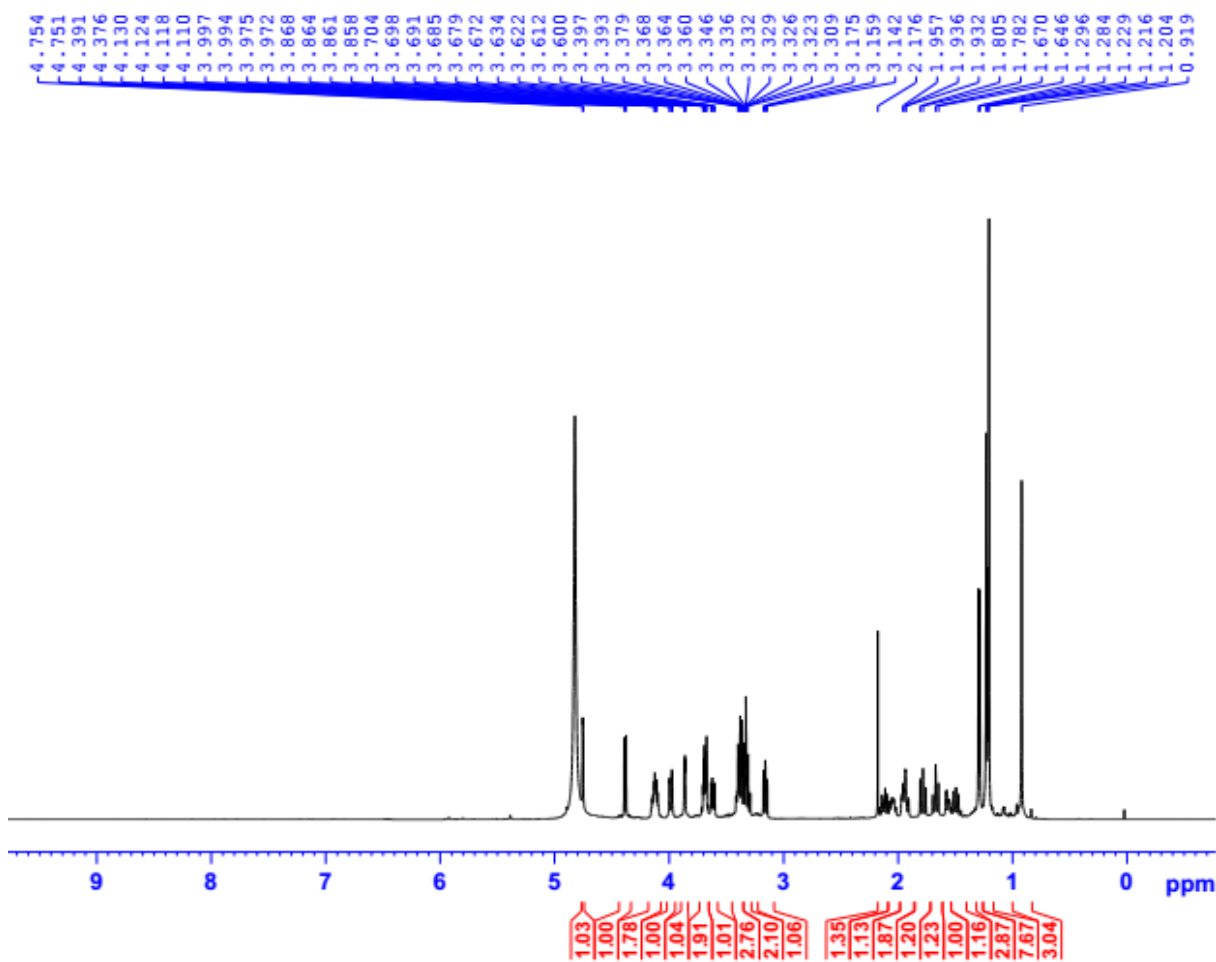


Figure S2: ¹H NMR spectrum of compound (1). Measured in CD₃OD, 500 MHz

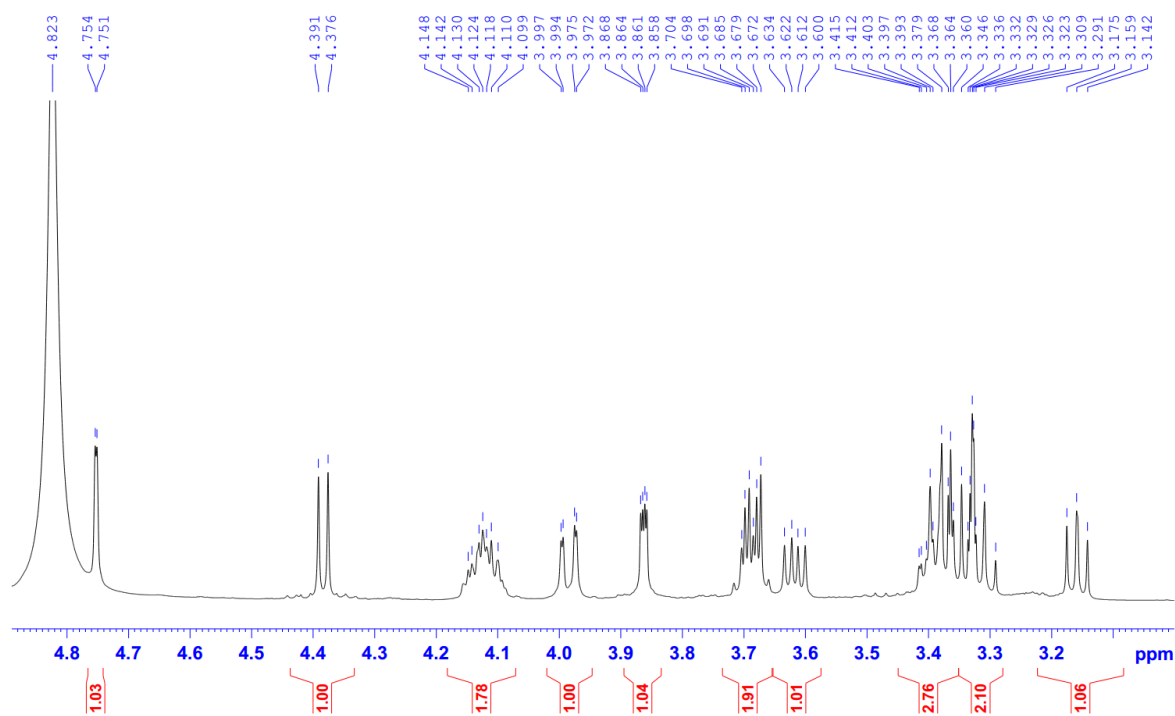


Figure S3: ^1H NMR spectrum (3.0-5.0 ppm) of compound **(1)**. Measured in CD_3OD , 500 MHz

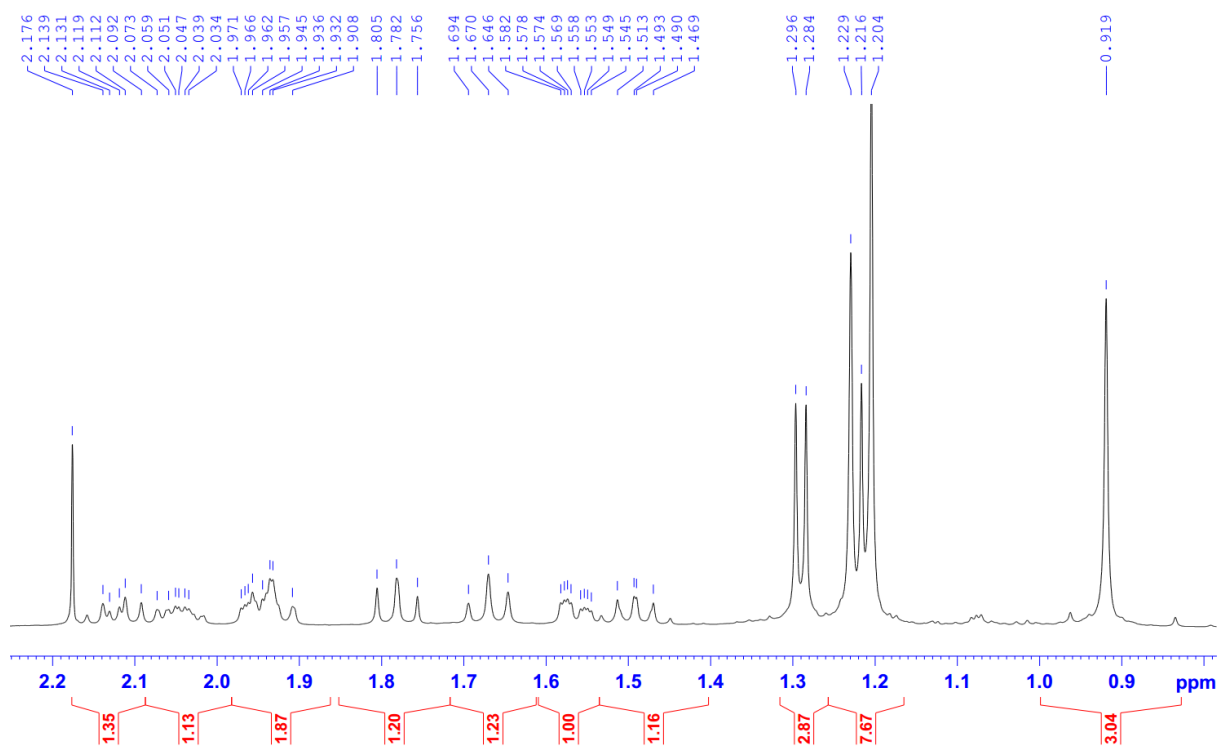


Figure S14: ^1H NMR spectrum (0.8-2.2 ppm) of compound **(1)**. Measured in CD_3OD , 500 MHz

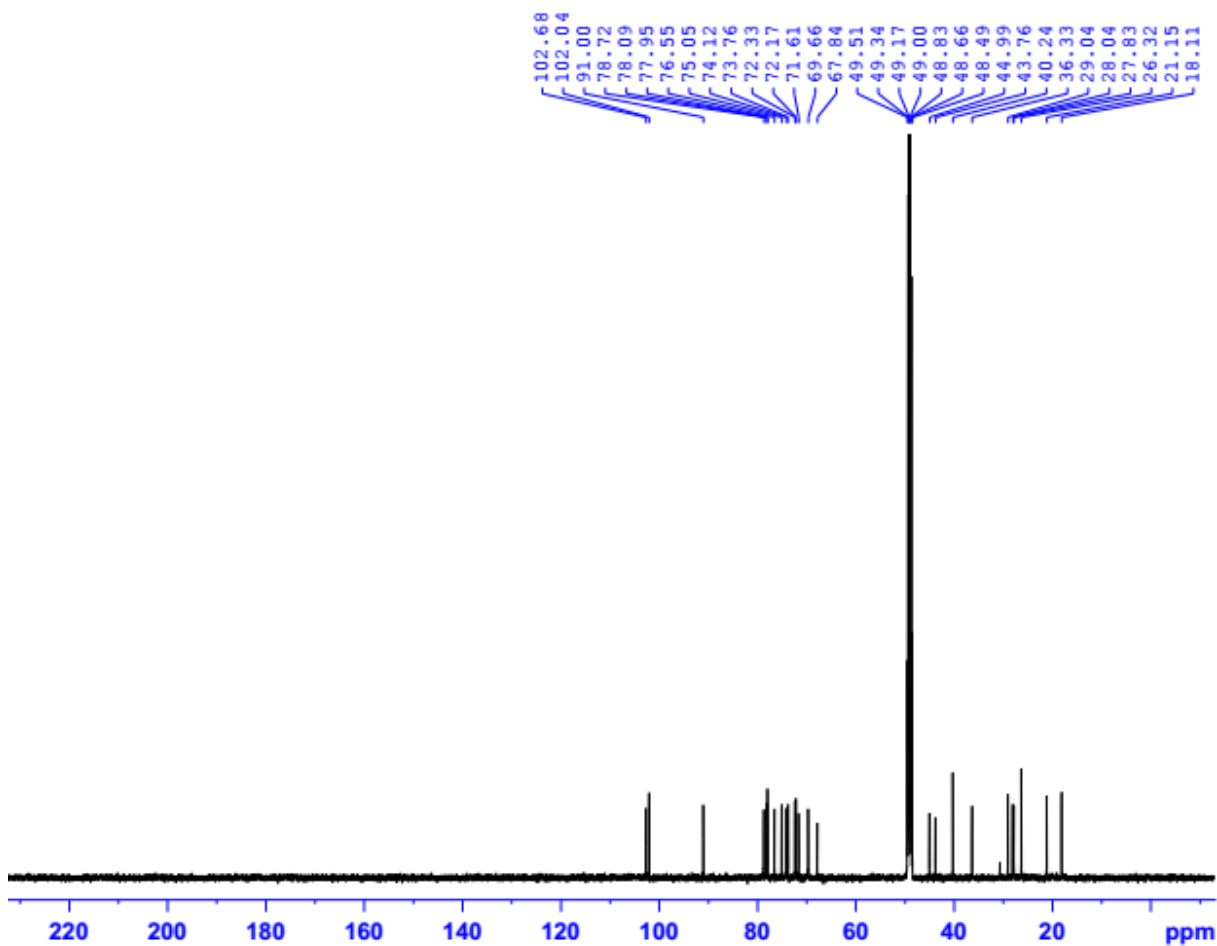


Figure S5: ^{13}C NMR spectrum of compound (1). Measured in CD_3OD , 125 MHz

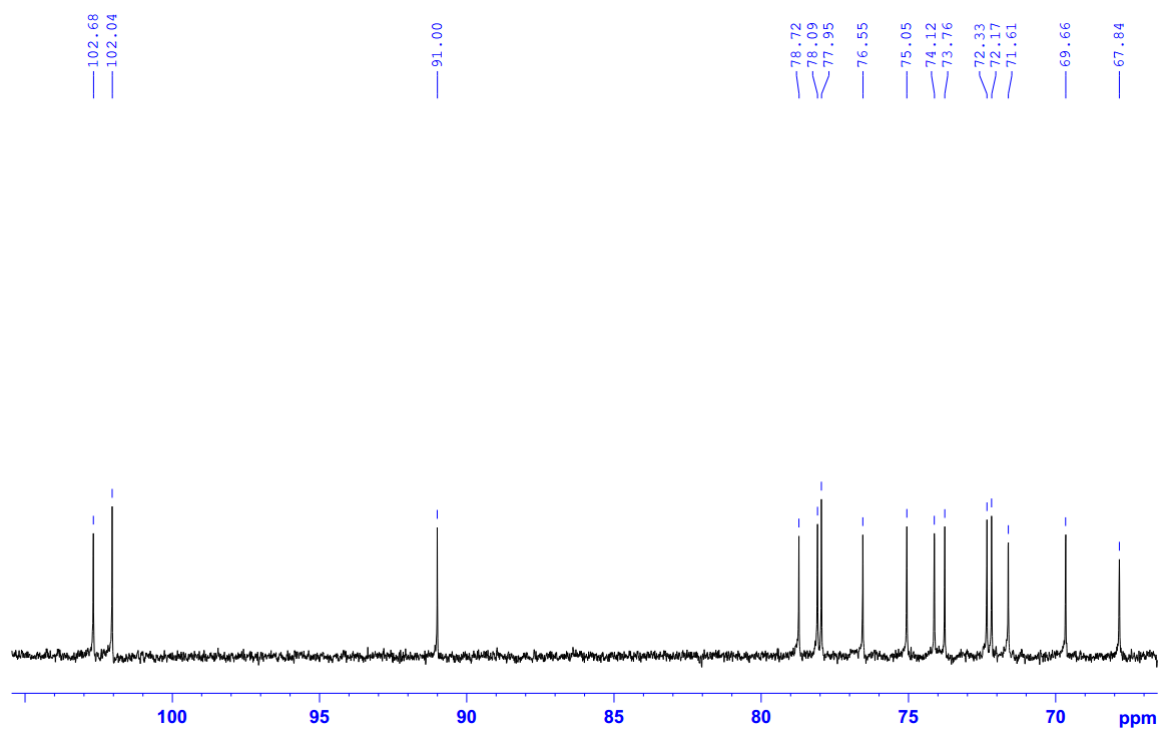


Figure S6: ^{13}C NMR spectrum (67-115 ppm) of compound (1). Measured in CD_3OD , 125 MHz

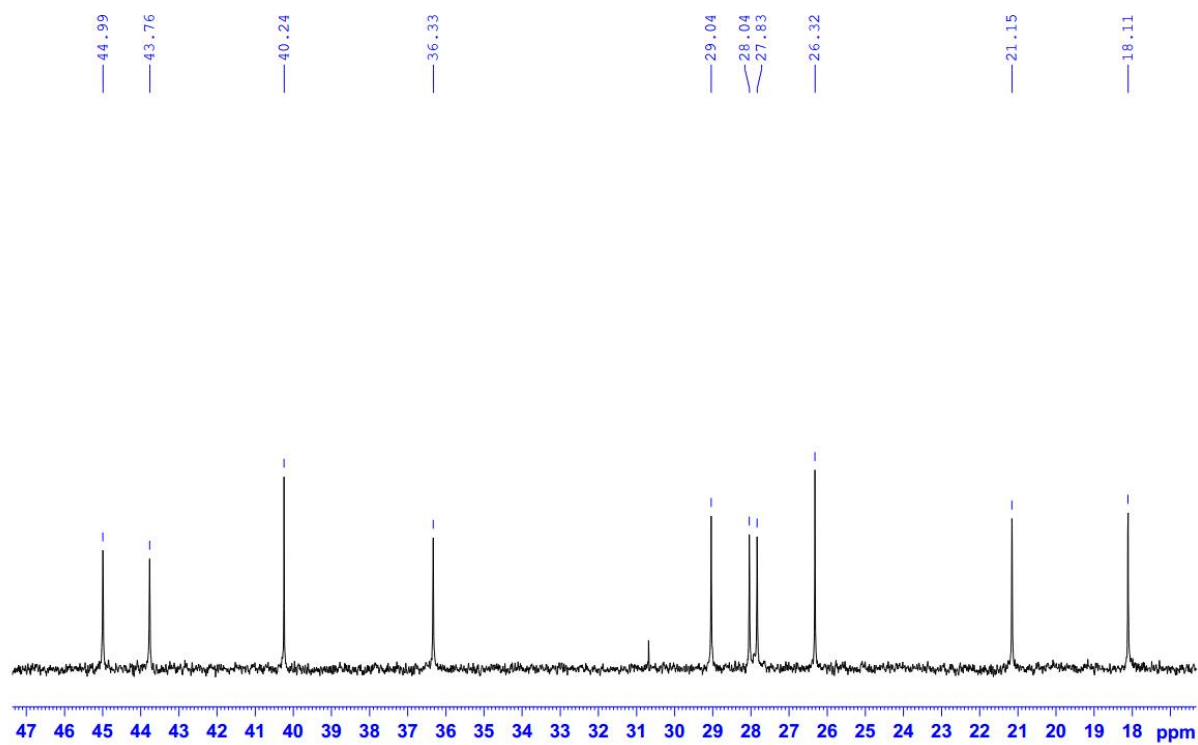


Figure S7: ^{13}C NMR spectrum (17-47 ppm) of compound (1). Measured in CD_3OD , 125 MHz

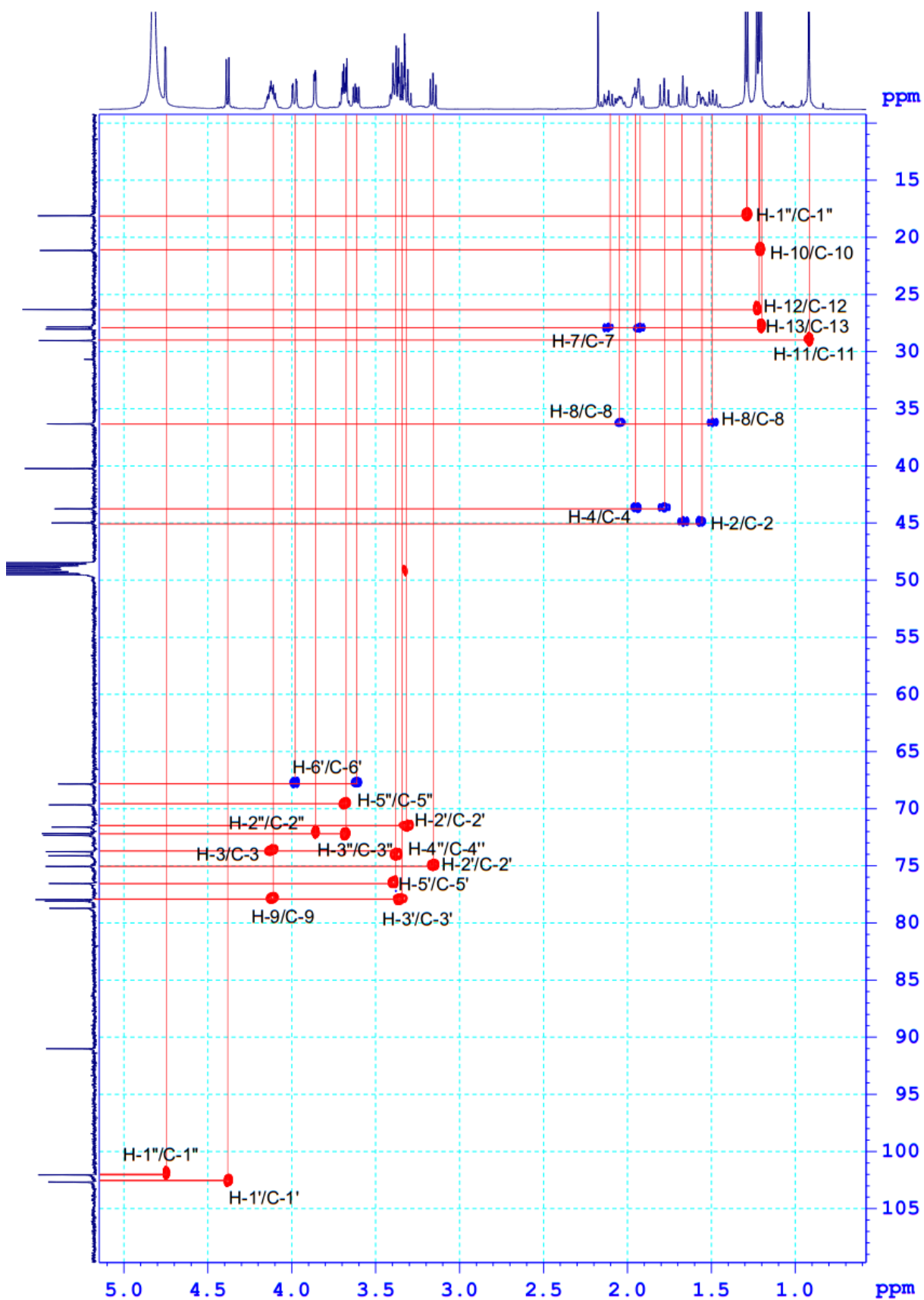


Figure S8: HSQC NMR spectrum of compound (1). Measured in CD₃OD

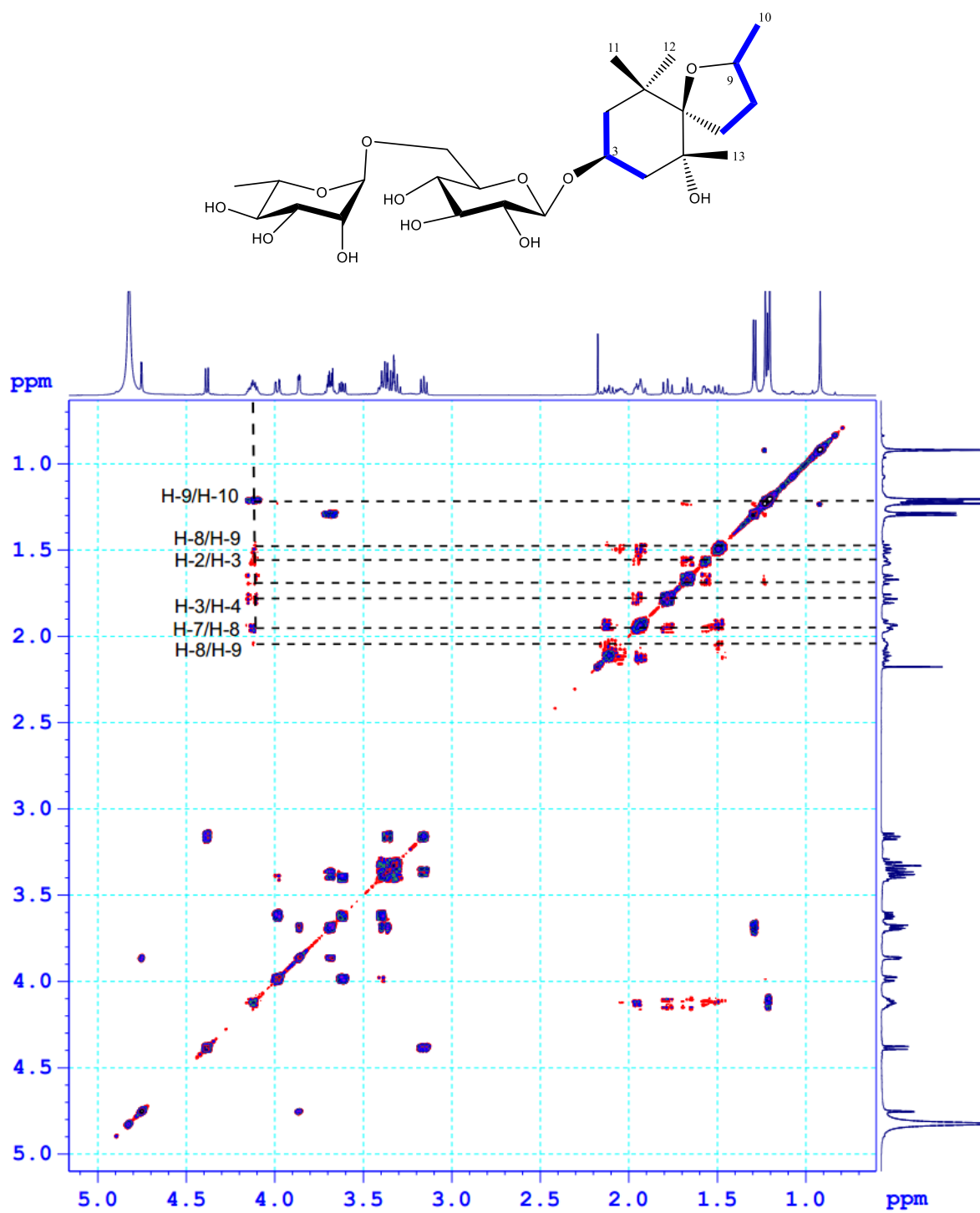


Figure S9: COSY NMR spectrum of compound (1). Measured in CD₃OD.
— COSY correlation

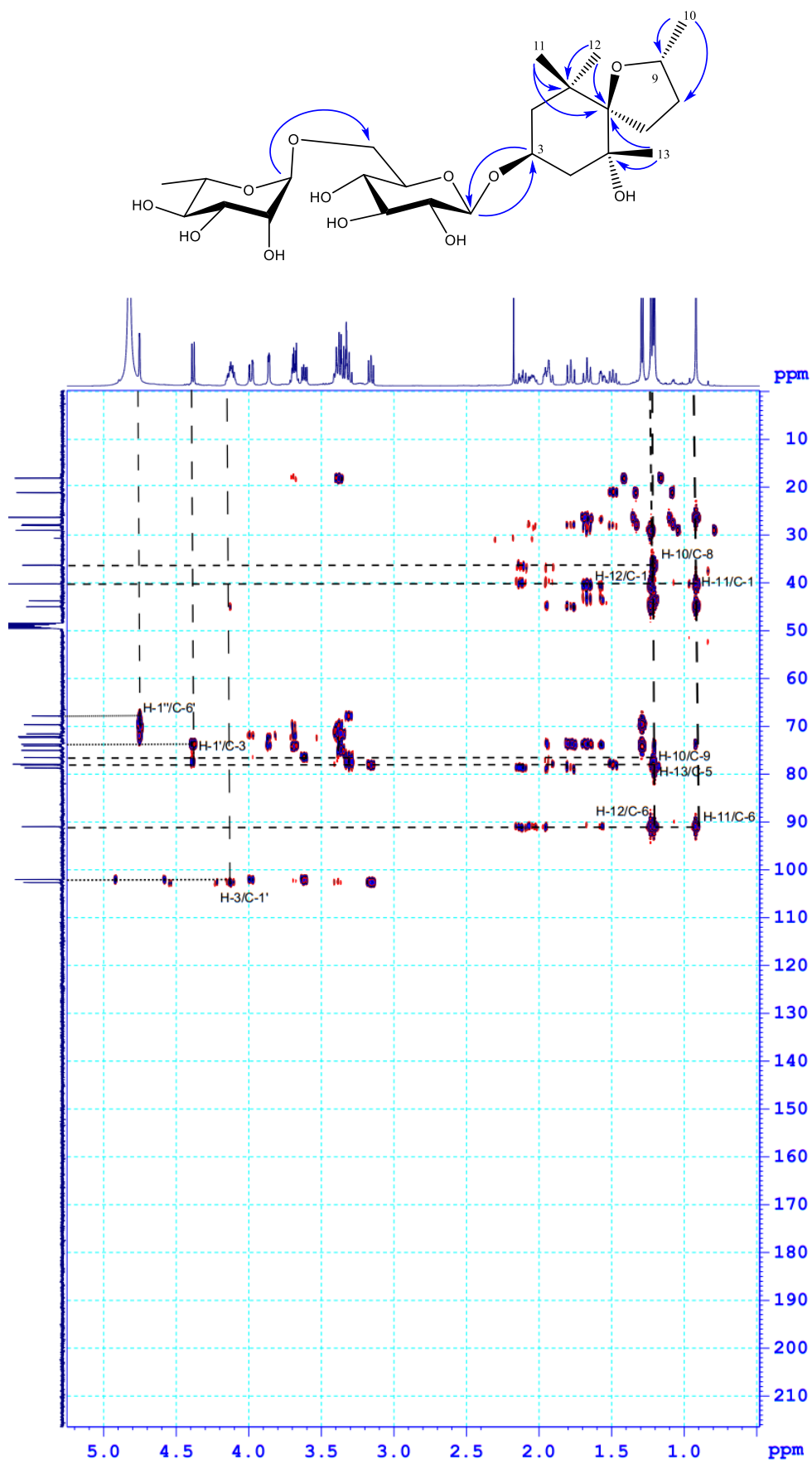


Figure S10: HMBC NMR spectrum of compound (1). Measured in CD₃OD
Key HMBC → correlations

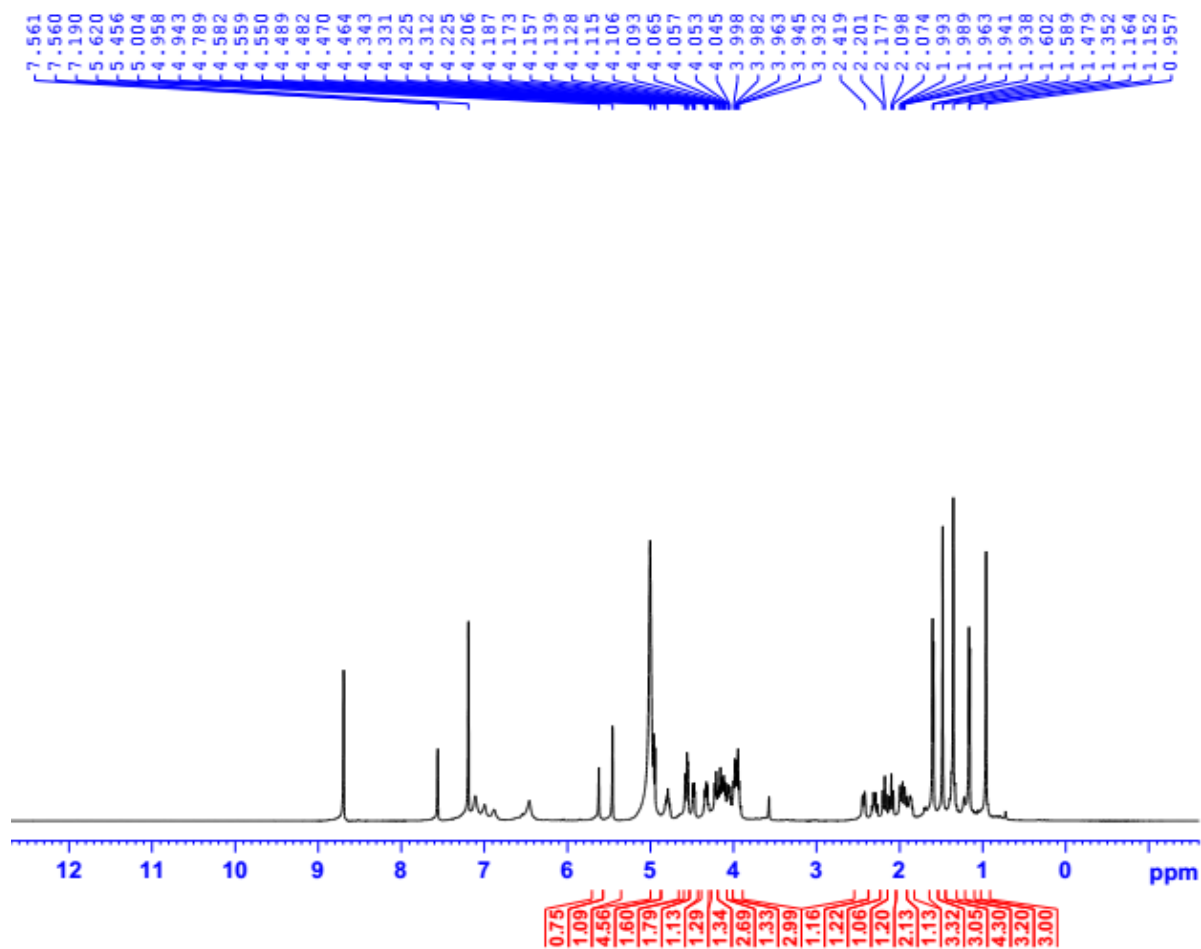


Figure S11: ^1H NMR spectrum of compound (**1**). Measured in Pyridine- d_5 , 500 MHz

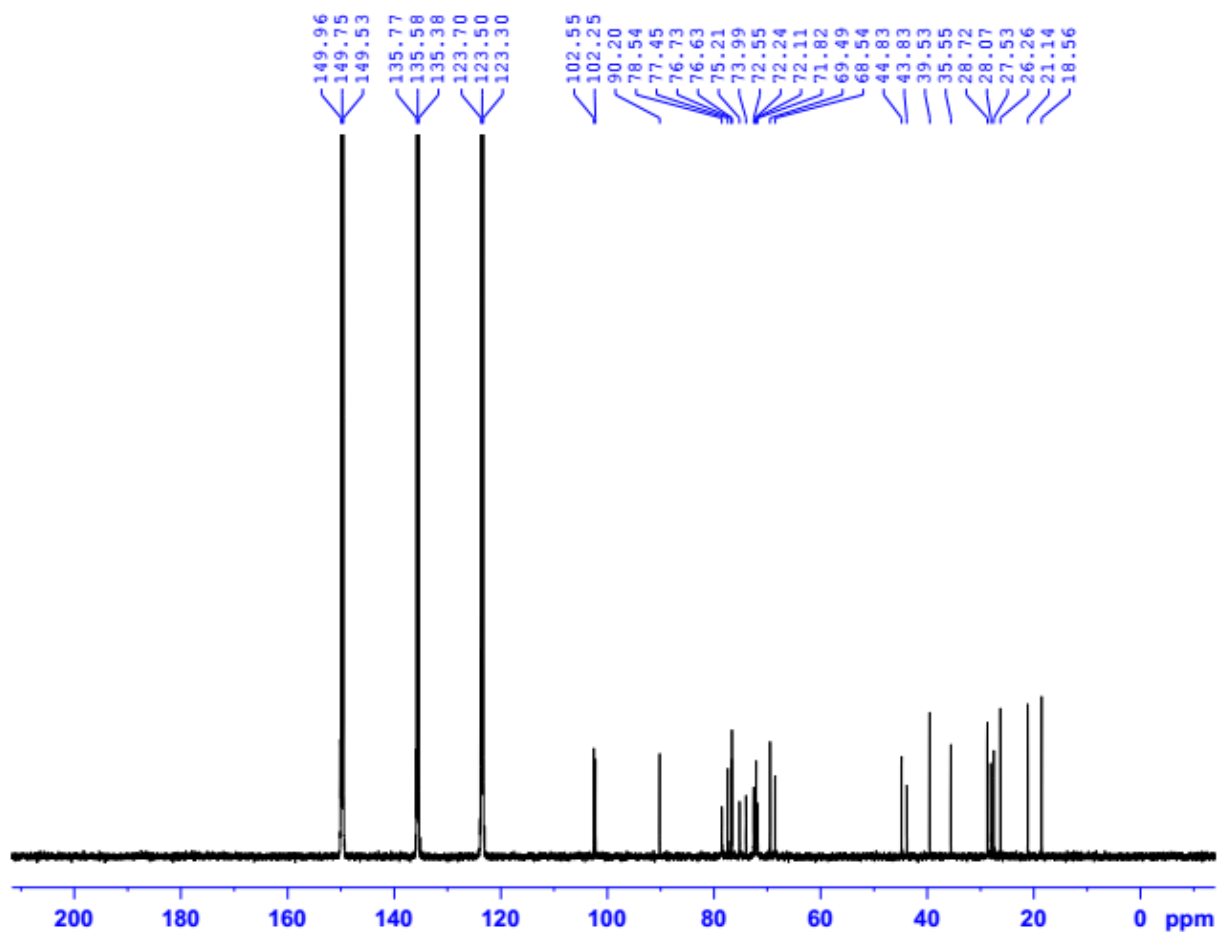


Figure S12: ^{13}C NMR spectrum of compound (1). Measured in Pyridine- d_5 , 125 MHz

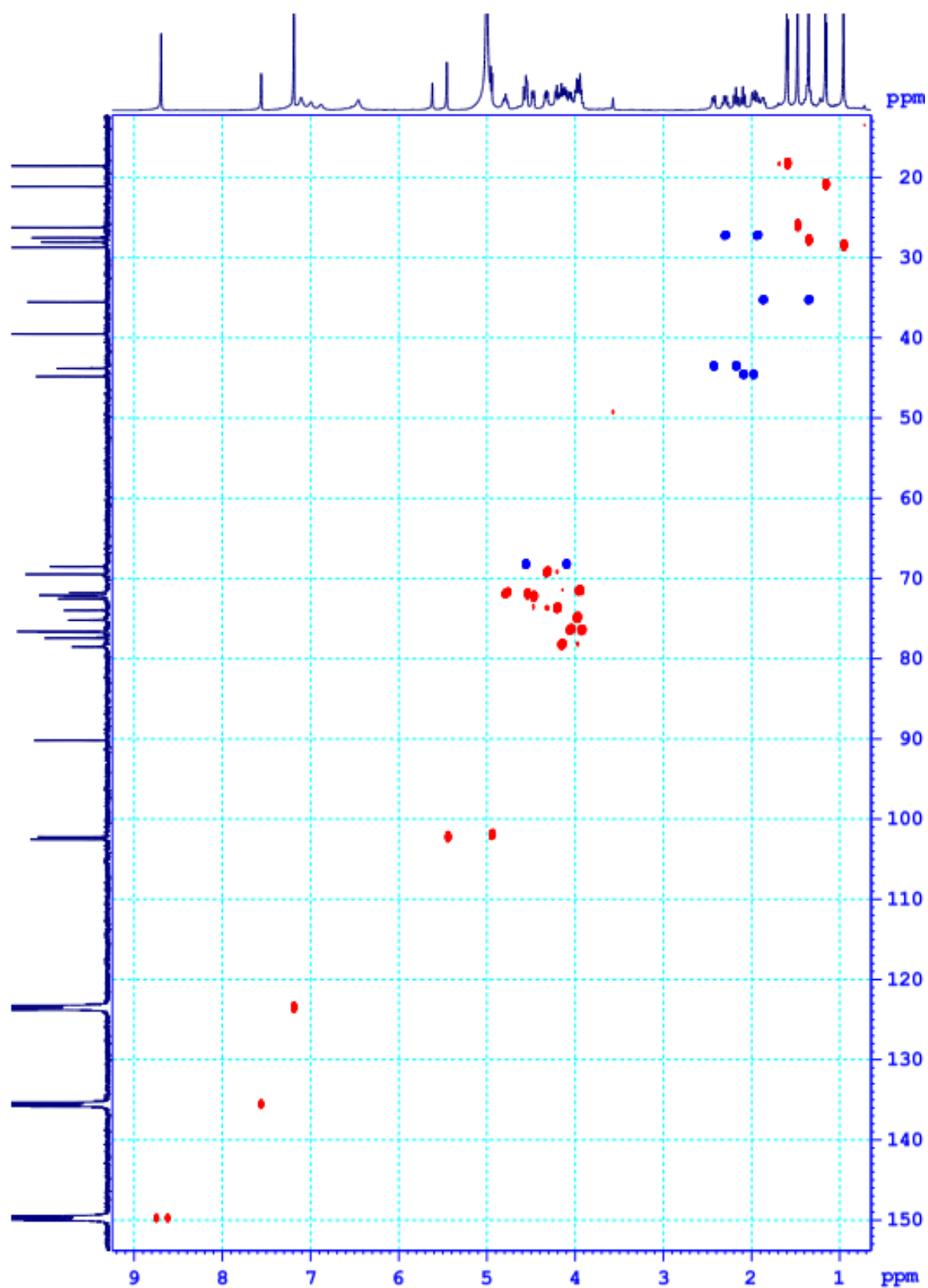


Figure S13: HSQC NMR spectrum of compound (1). Measured in Pyridine- d_5

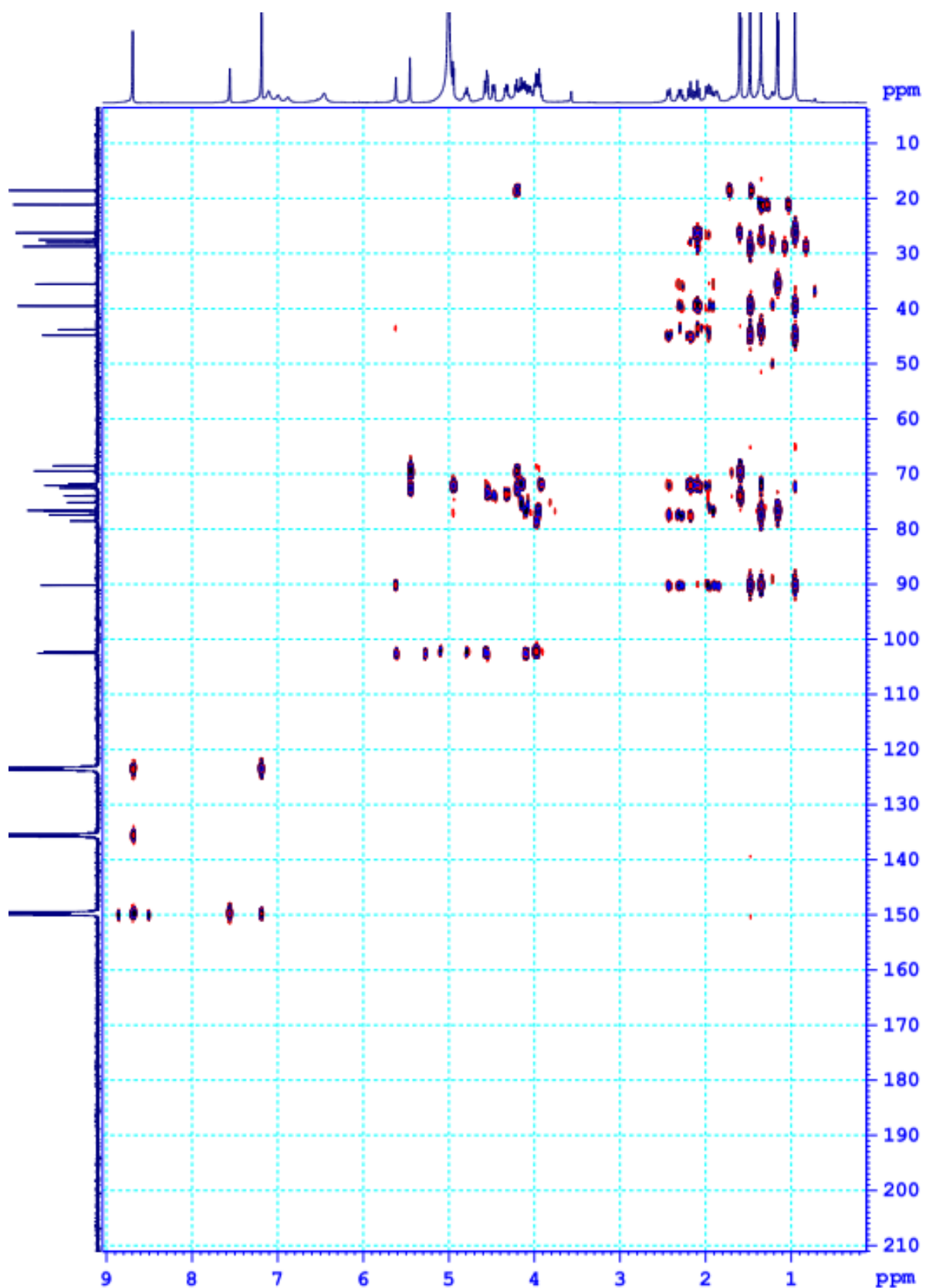


Figure S14: HMBC NMR spectrum of compound (1). Measured in Pyridine-*d*₅

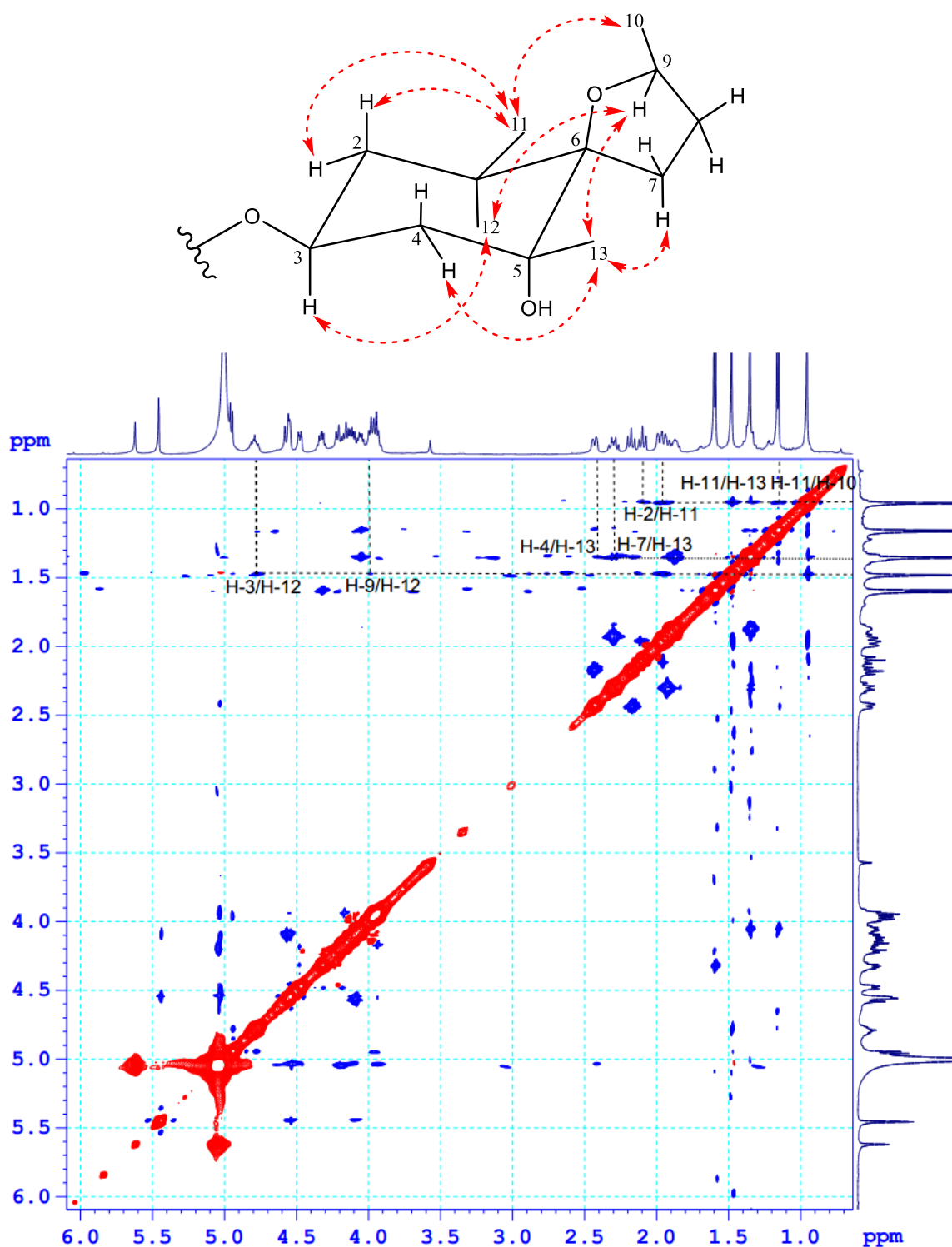


Figure S15: NOESY NMR spectrum of compound (1). Measured in Pyridine-*d*₅

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Substances

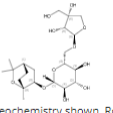
References Reactions Suppliers

Filtering: Similarity: 85-89 Number of Components: 1

24 Results Sort: Relevance View: Full

1 90

1082606-94-7



Absolute stereochemistry shown, Rotation (-)

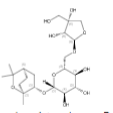
C₂₁H₃₆O₁₁
 (1R,4S,6R)-1,3,3-Trimethyl-2-oxabicyclo [2.2.2]oct-6-yl 6-O-D-apio-β-D-furanosyl-β-D-glucopyranoside

3 References 0 Reactions 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	464.50	-
Boiling Point (Predicted)	674.6±55.0 °C	Press: 760 Torr
Density (Predicted)	1.45±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.77±0.60	Most Acidic Temp: 25 °C

2 90

217975-07-0

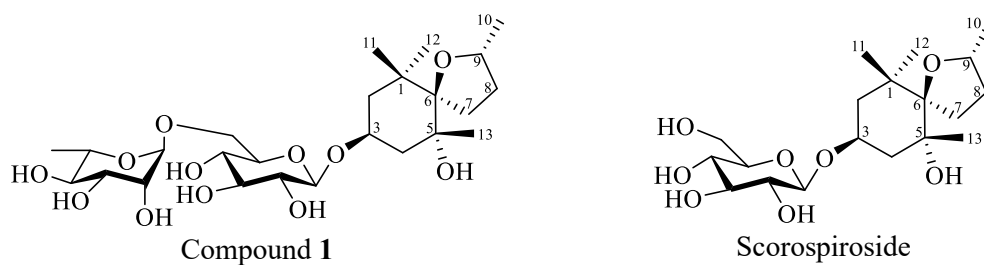


Absolute stereochemistry shown, Rotation (+)

Key Physical Properties	Value	Condition
Molecular Weight	464.50	-
Boiling Point (Predicted)	674.6±55.0 °C	Press: 760 Torr
Density (Predicted)	1.45±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.77±0.60	Most Acidic Temp: 25 °C

Figure S16: The Scifinder search for the new compound (1)

Table S1: Structure and NMR data of compound **1** and the most similar compound, scorospiroside



No.	δ_C #,a	δ_H #,c	δ_C #,b	δ_H #,d
1	39.5		39.5	
2	44.8	2.09 (1H, t, $J = 12.0$ Hz) 1.97 (1H, dd, $J = 12.0, 4.0$ Hz)	44.8	2.13 (1H, t, $J = 12.0$ Hz) 1.96 (1H, dd, $J = 12.0, 4.0$ Hz)
3	72.1	4.80 (1H, m)	72.4	4.79 (1H, tt, $J = 12.0, 4.0$ Hz)
4	43.8	2.43 (1H, brd, $J = 11.0$ Hz) 2.17 (1H, dd, $J = 13.0, 12.0$ Hz)	44.0	2.50 (1H, brd, $J = 13.0$ Hz) 2.23 (1H, dd, $J = 13.0$ Hz)
5	77.4		77.4	
6	90.2		90.2	
7	27.5	2.30 (1H, m) 1.93 (1H, m)	27.5	2.34 (1H, m) 1.88-2.00 (1H, m)
8	35.5	1.87 (1H, m) 1.34 (1H, m)	35.6	1.88-2.00 (1H, m) 1.42 (1H, m)
9	76.6	4.04 (1H, m)	76.7	4.10 (1H, m)
10	21.1	1.16 (3H, d, $J = 6.5$ Hz)	21.2	1.21 (3H, d, $J = 6.0$ Hz)
11	28.7	0.95 (3H, s)	28.7	0.96 (3H, s)
12	26.2	1.47 (3H, s)	26.2	1.43 (3H, s)
13	28.0	1.35 (3H, s)	28.1	1.37 (3H, s)
1'	102.6	4.96 (1H, d, $J = 7.5$ Hz)	102.6	5.01 (1H, d, $J = 8.0$ Hz)
2'	75.2	3.99 (1H, m)	75.3	4.00 (1H, dd, $J = 8.0, 9.0$ Hz)
3'	76.6	4.12 (1H, m)	78.6	4.19 (1H, t, $J = 9.0$ Hz)
4'	71.8	4.82 (1H, m)	71.7	4.25 (1H, t, $J = 9.0$ Hz)
5'	73.9	4.20 (1H, m)	78.1	3.81 (1H, m)
6'	68.5	4.09 (1H, m) 4.56 (1H, m)	62.8	4.34 (1H, dd, $J = 12.0, 5.0$ Hz) 4.45 (1H, dd, $J = 12.0, 5.0$ Hz)
1''	102.3	5.46 (1H, brs)		
2''	72.6	4.22 (1H, m)		
3''	72.2	4.47 (1H, m)		
4''	69.5	4.33 (1H, m)		
5''	69.5	4.30 (1H, m)		
6''	18.6	1.60 (3H, d, $J = 6.5$ Hz)		

Measure in pyridine- d_5 , ^a 125 MHz; ^b 100 MHz; ^c 500 MHz; ^d 400 MHz;

F. Abe and T. Yamauchi (1993). Megastigmanes and flavonoids from the leaves of *Scorodocarpus borneensis*, *Phytochemistry* **33** (6), 1499-1501.