Supporting Information

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A New Megastigmane Glycoside And Anti-Inflammatory Bibenzyls And From The Stems of *Dendrobium henanense*

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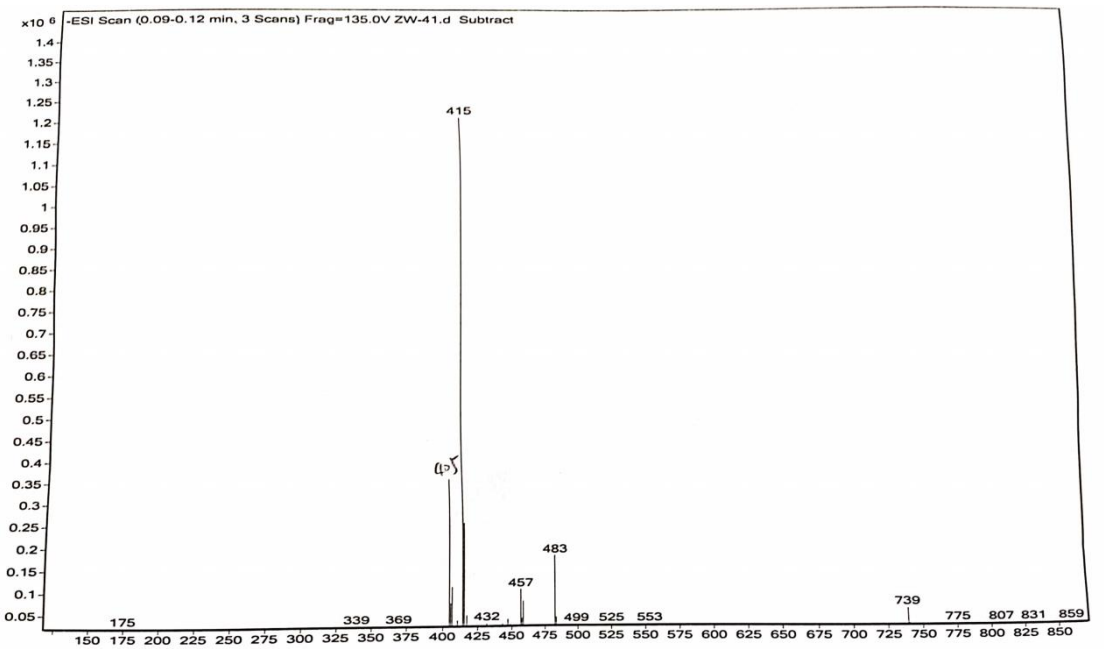
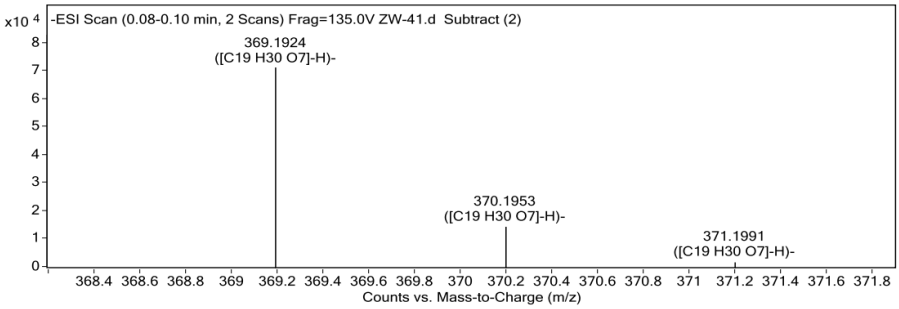


Figure S1: ESI-MS Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
112.9855	1	16070.53		
369.1924	1	71310.68	C19 H30 O7	(M-H)-
405.1689	1	22914.64		
415.1981	1	83379.62		
416.2011	1	18338.2		
432.1879	1	15022.06		
483.1858	1	149955.14		
484.1889	1	34733.03		
739.3917	1	40807.55		
740.3954	1	17841.75		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	300
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C19 H30 O7	370.1992	369.1919	369.1924	-0.50	-1.35	5.0000

Figure S2: HR-ESI-MS Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

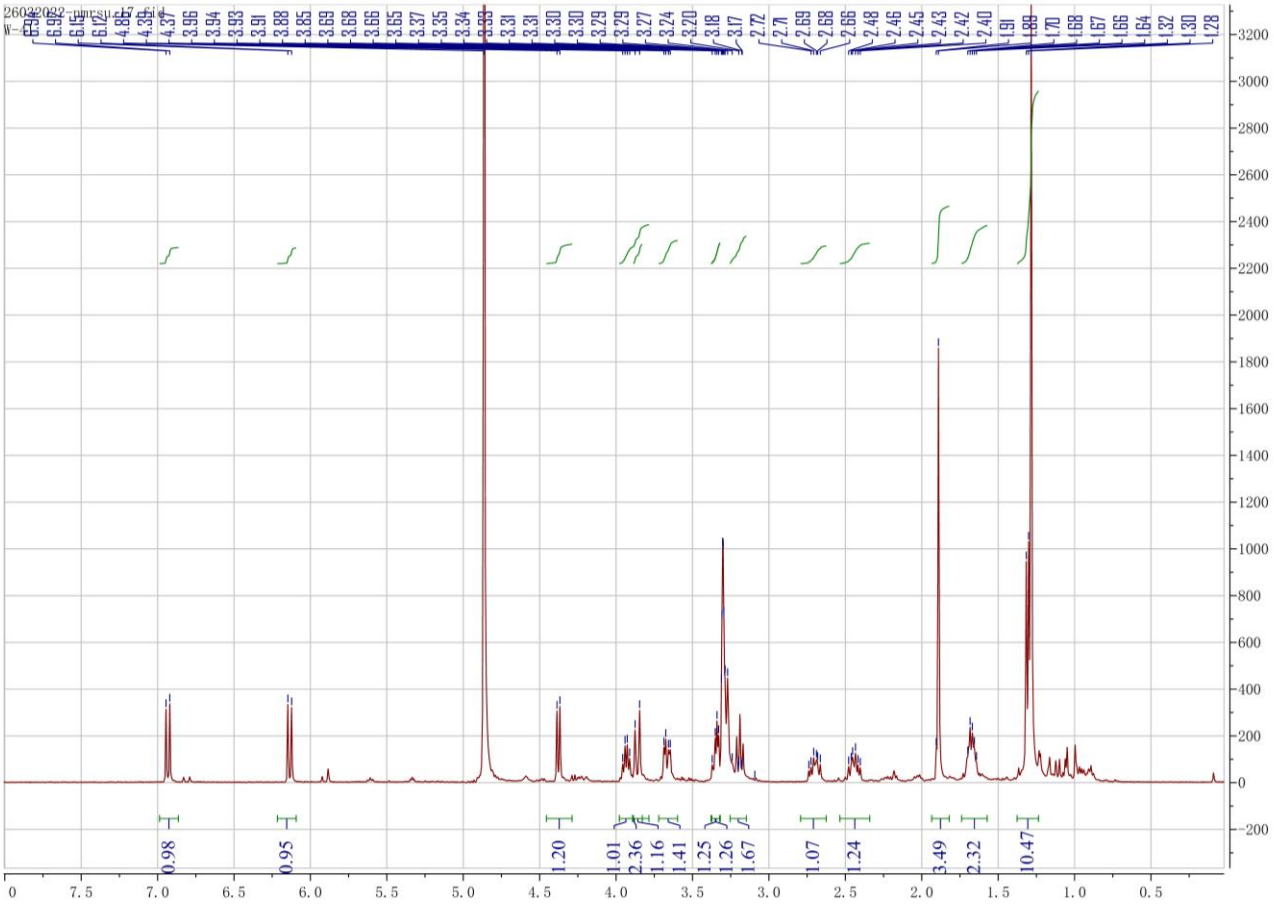


Figure S3: ^{1}H-NMR (400 MHz, CD_3OD) Spectrum of **1** (((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

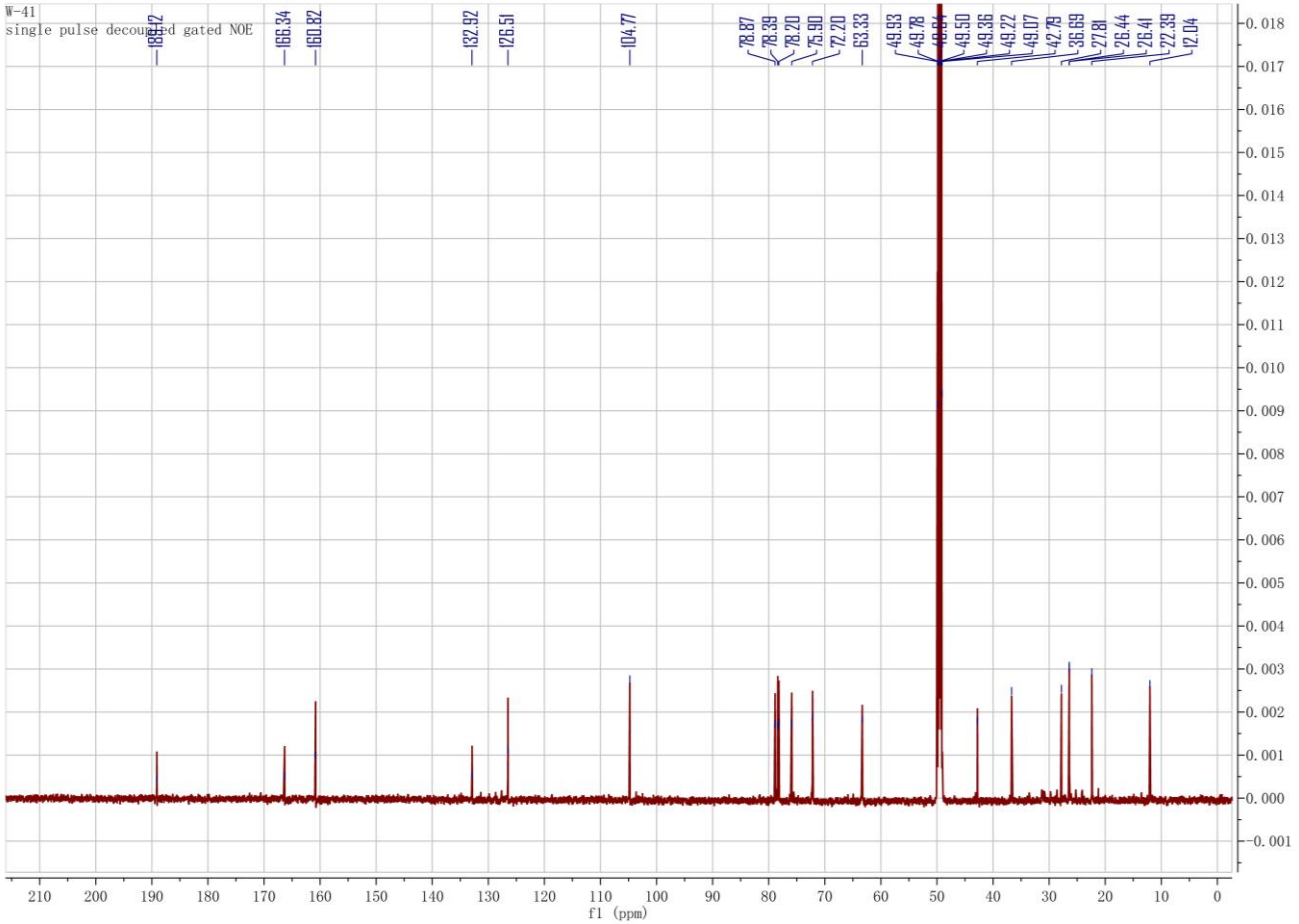


Figure S4: ^{13}C-NMR (150 MHz, CD_3OD) Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

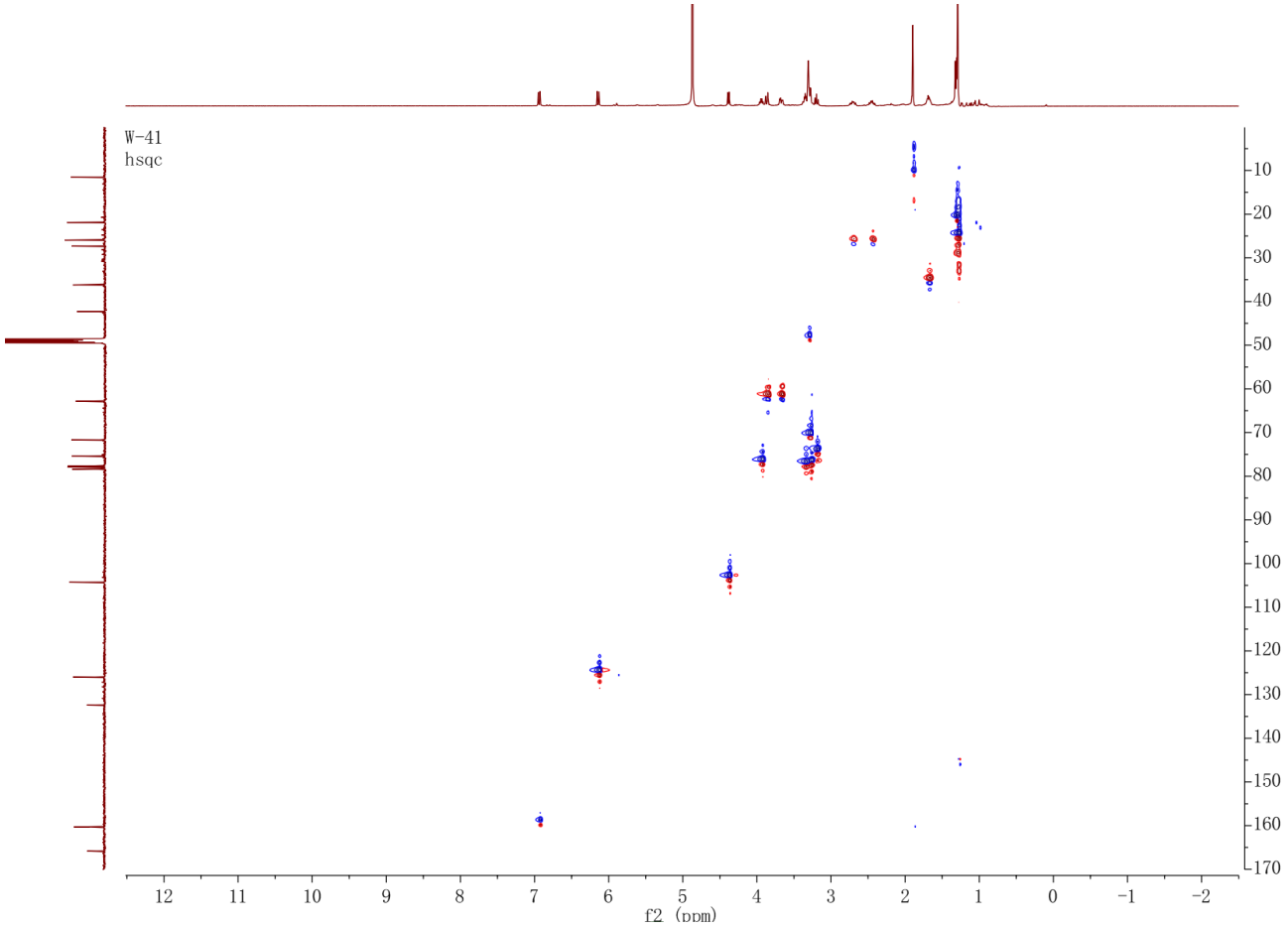


Figure S5: HSQC Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

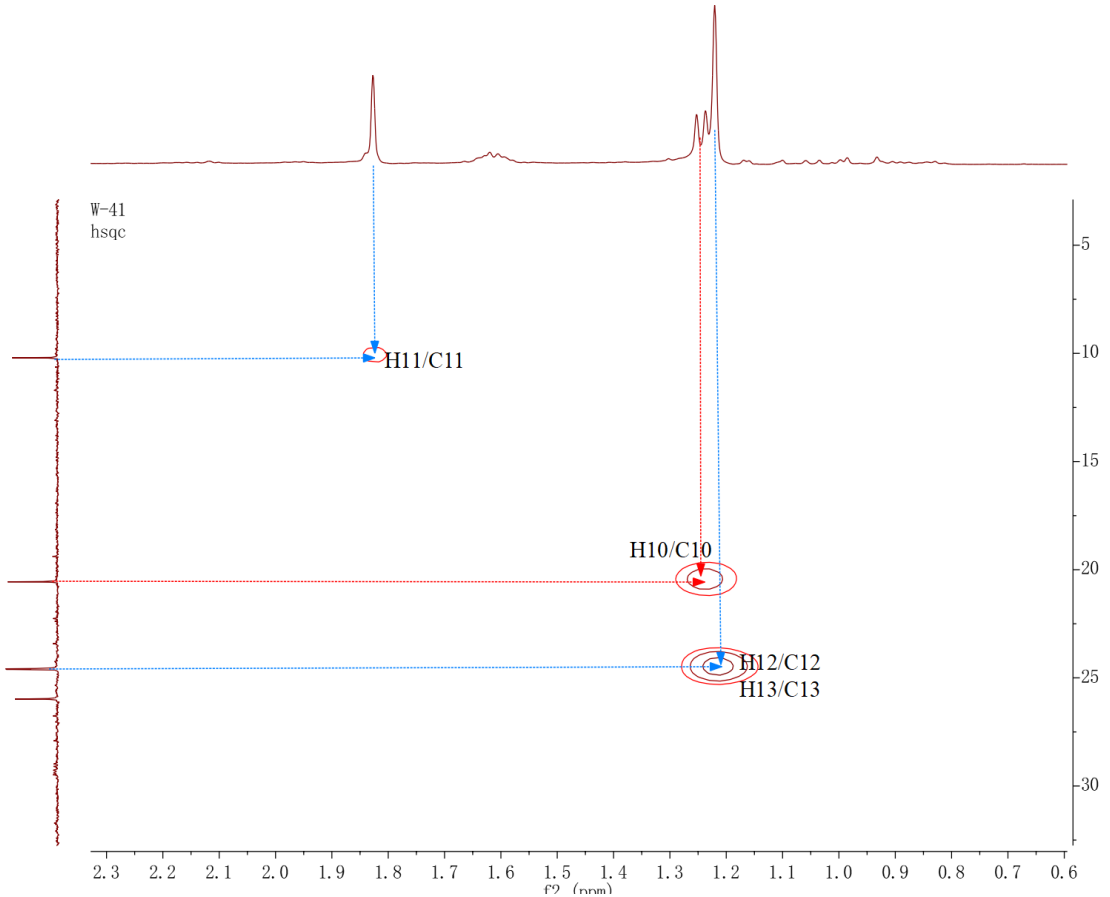


Figure S6: HSQC spectrum of **1** ((9S)-O-β-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 0.6 ppm to δ_H 2.3 ppm)

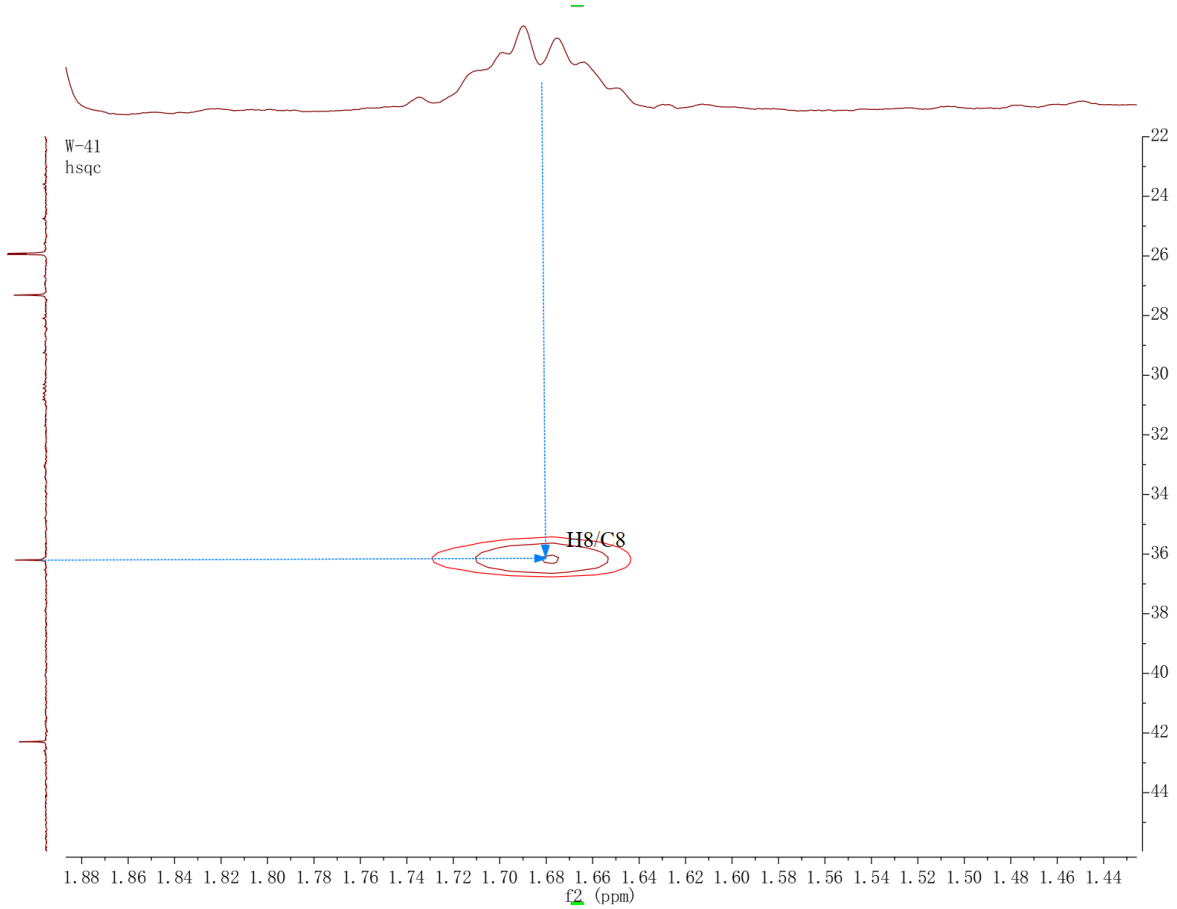


Figure S7: HSQC spectrum of **1** ((9S)-O-β-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 1.44 ppm to δ_H 1.88 ppm)

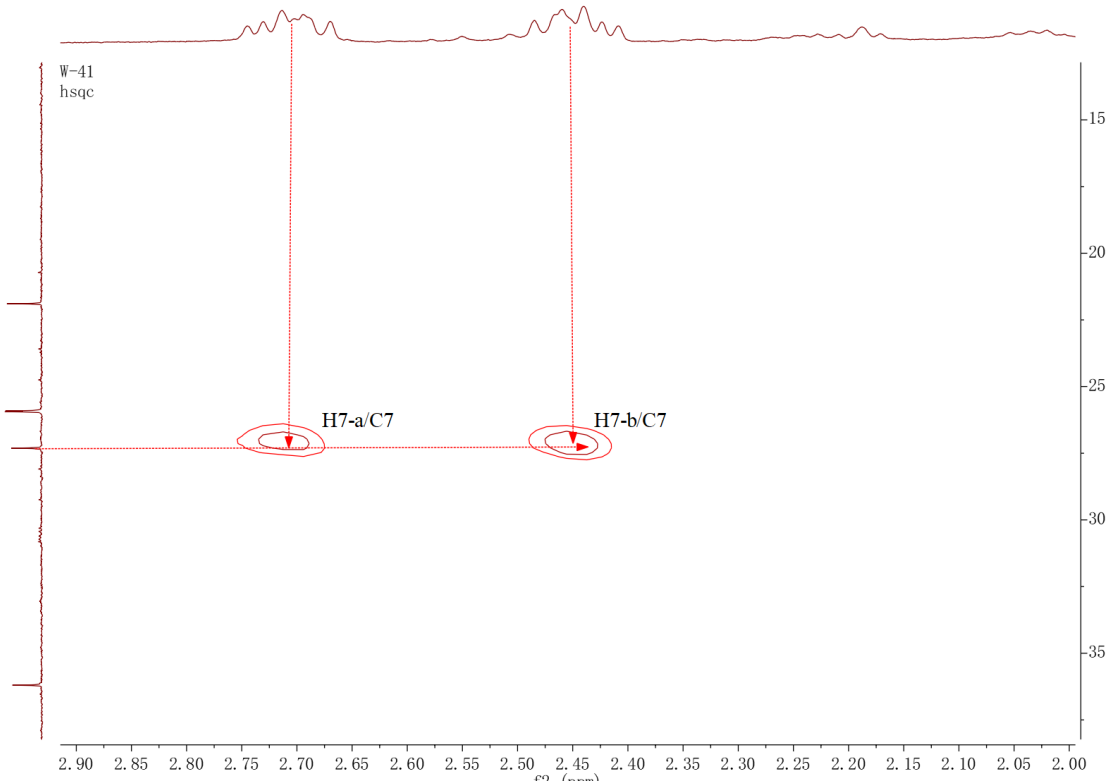


Figure S8: HSQC spectrum of **1** ((9S)-O-β-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 2.0 ppm to δ_H 2.9 ppm)

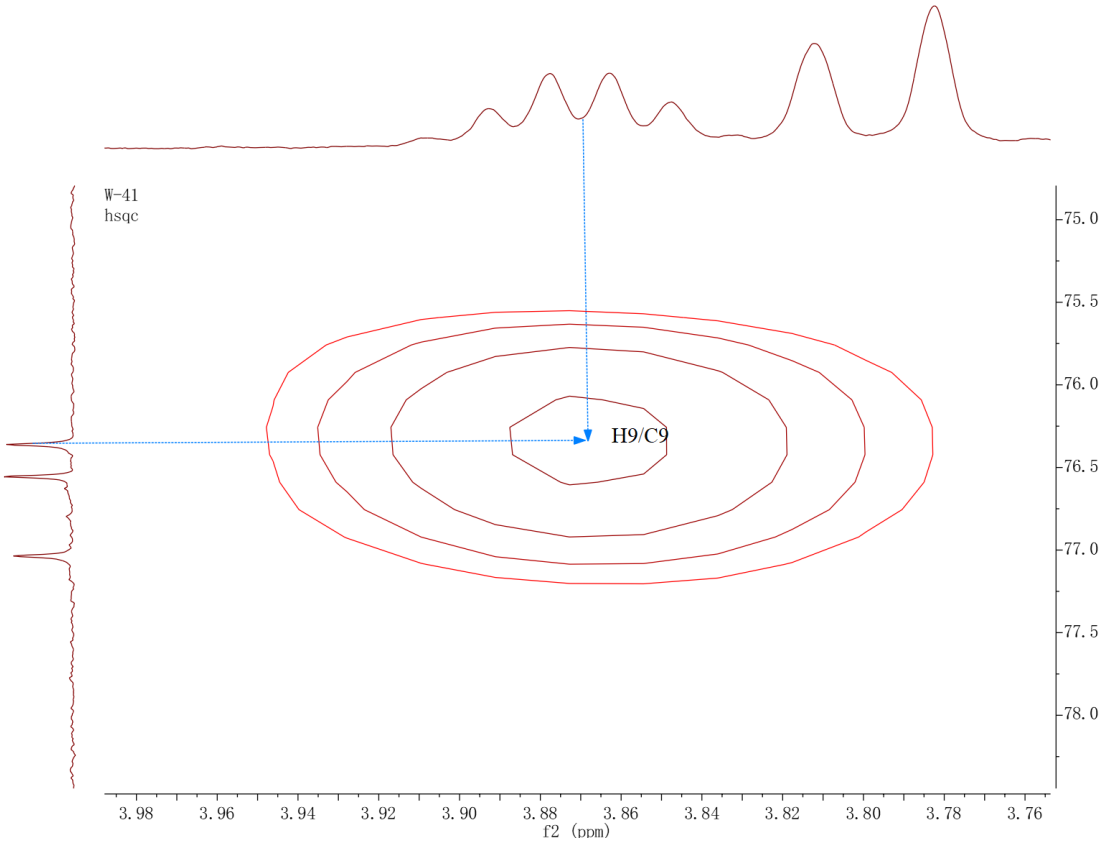


Figure S9: HSQC spectrum of **1** ((9S)-O-β-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 3.76 ppm to δ_H 3.98 ppm)

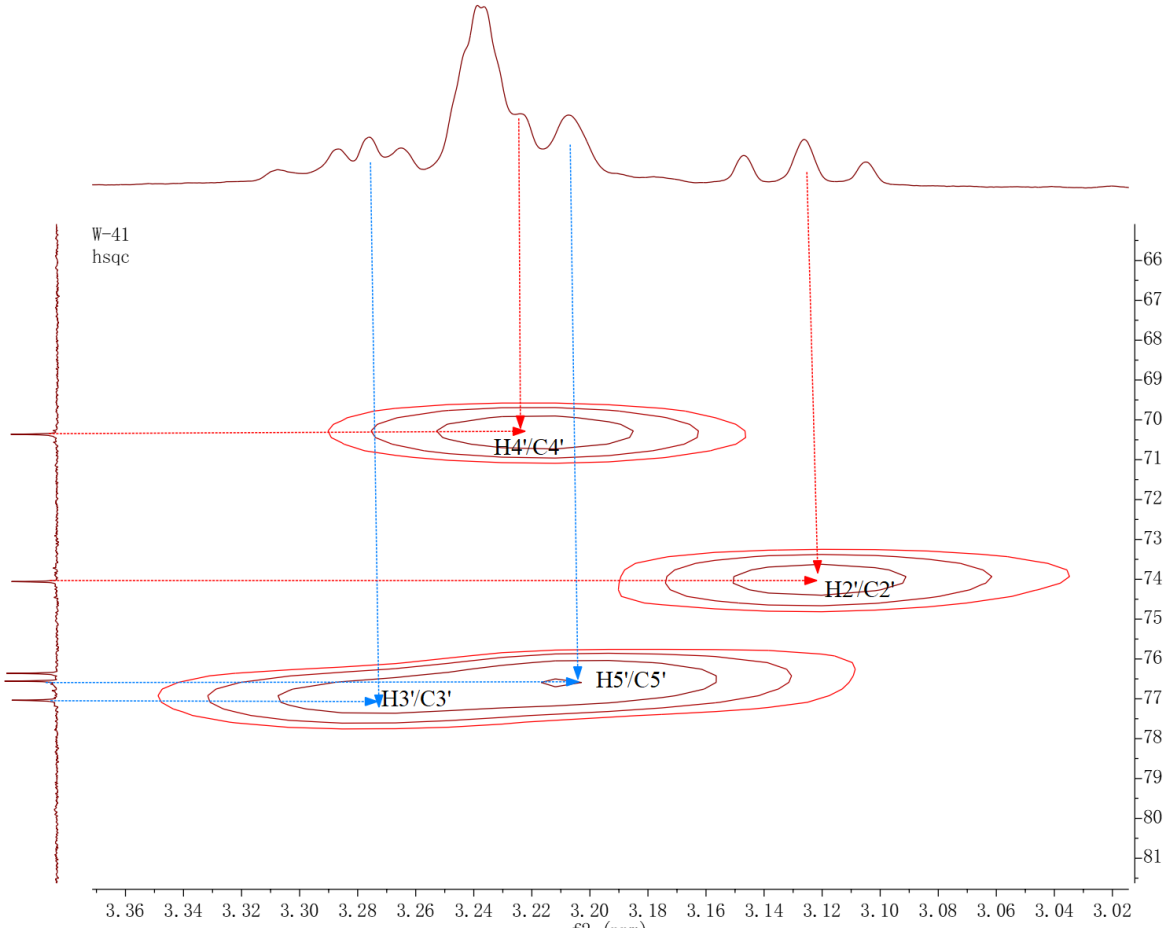


Figure S10: HSQC spectrum of **1** ((9S)-O-β-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 3.02 ppm to δ_H 3.36 ppm)

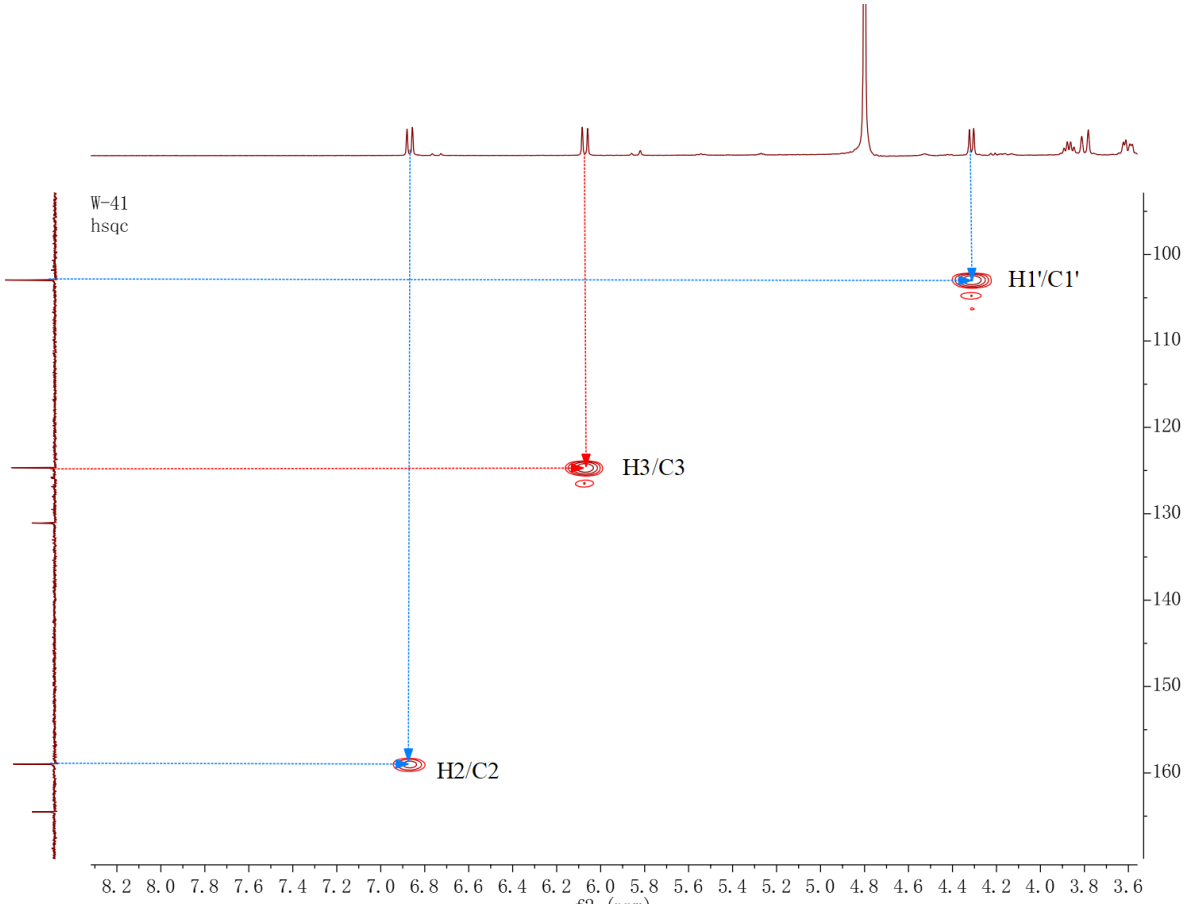


Figure S11: HSQC spectrum of **1** ((9S)-O-β-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 3.6 ppm to δ_H 8.2 ppm)

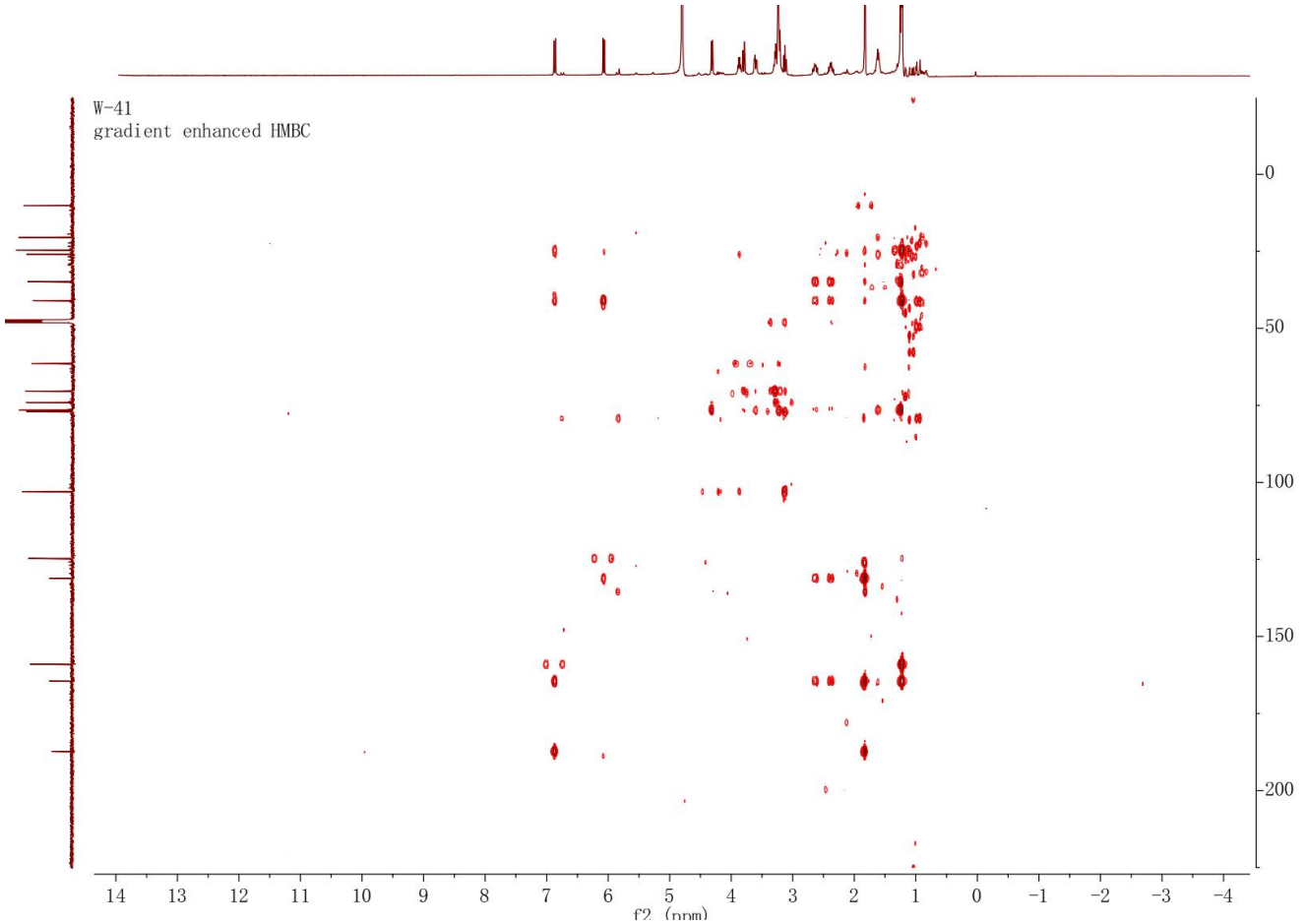


Figure S12: HMBC Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

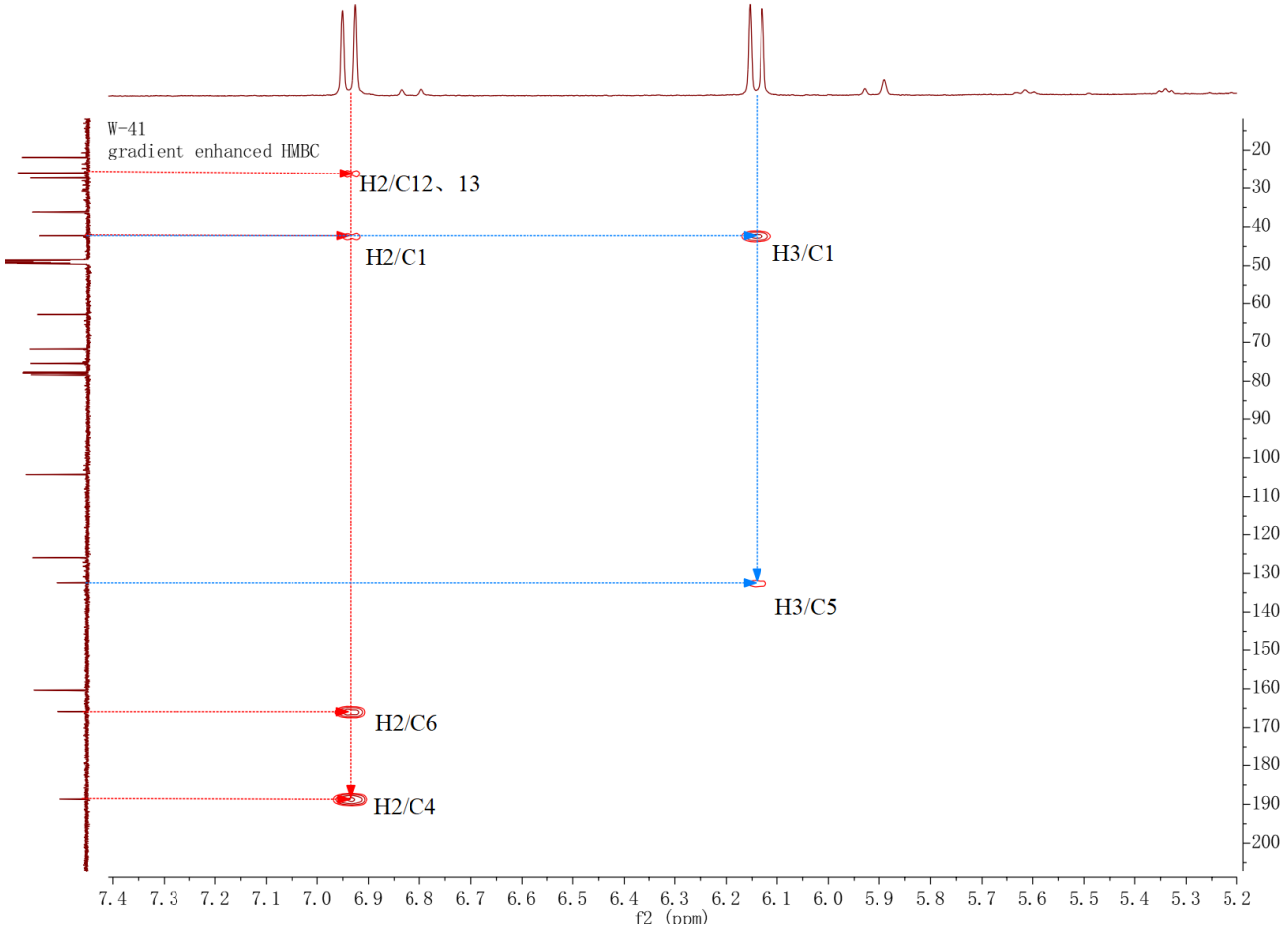


Figure S13: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 5.2 ppm to δ_H7.4 ppm)

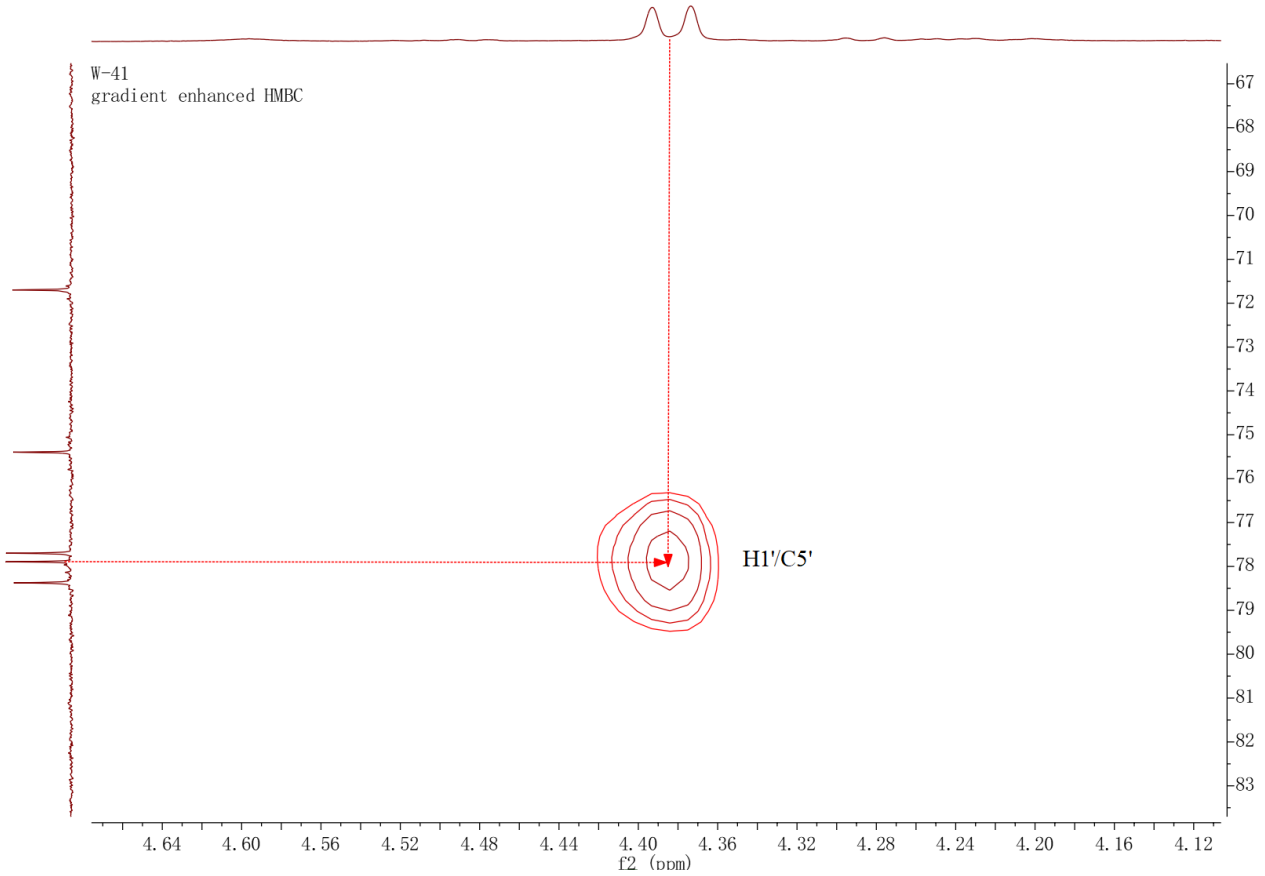


Figure S14: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 4.12 ppm to δ_H 4.64 ppm)

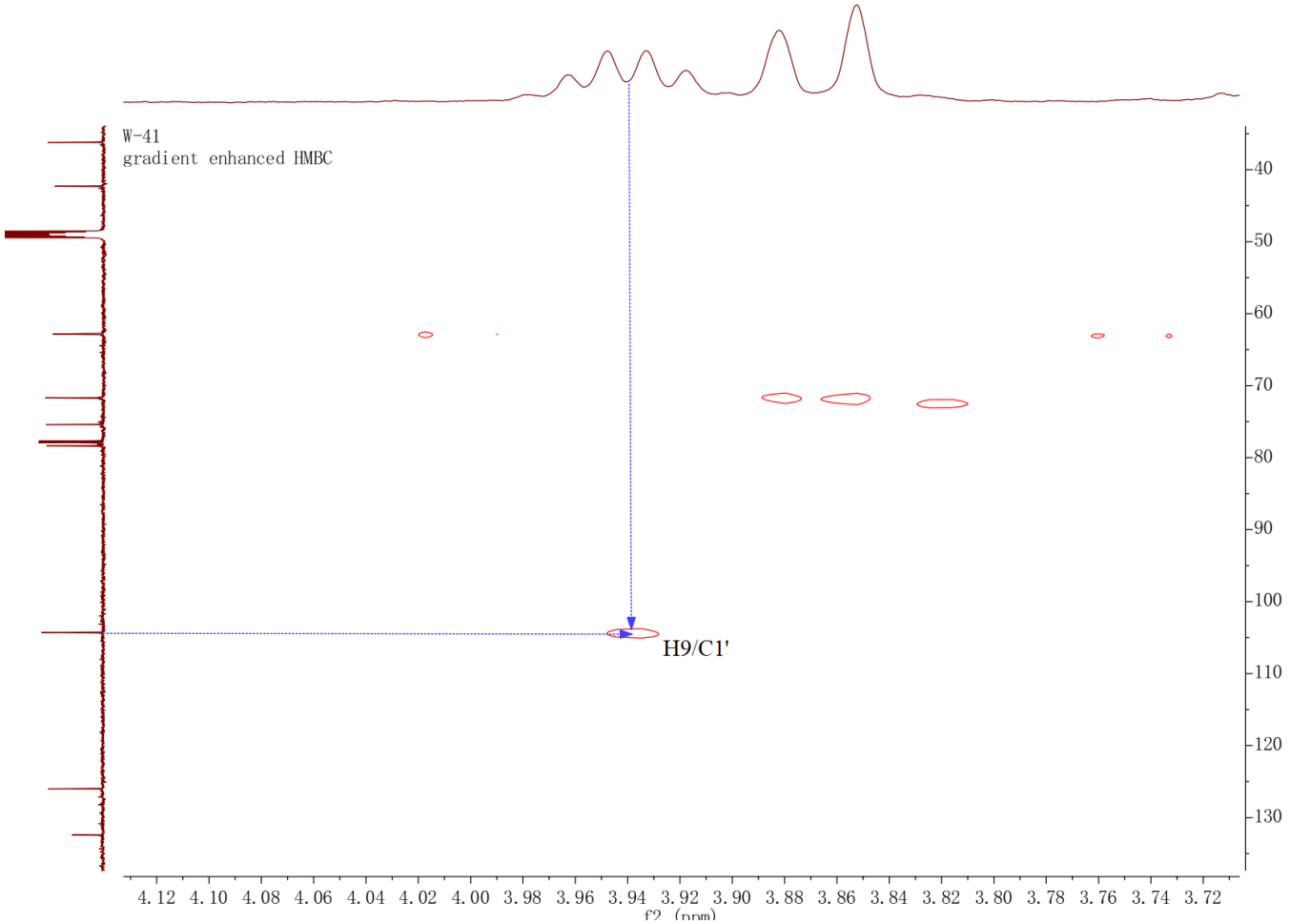


Figure S15: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 3.72 ppm to δ_H 4.12 ppm)

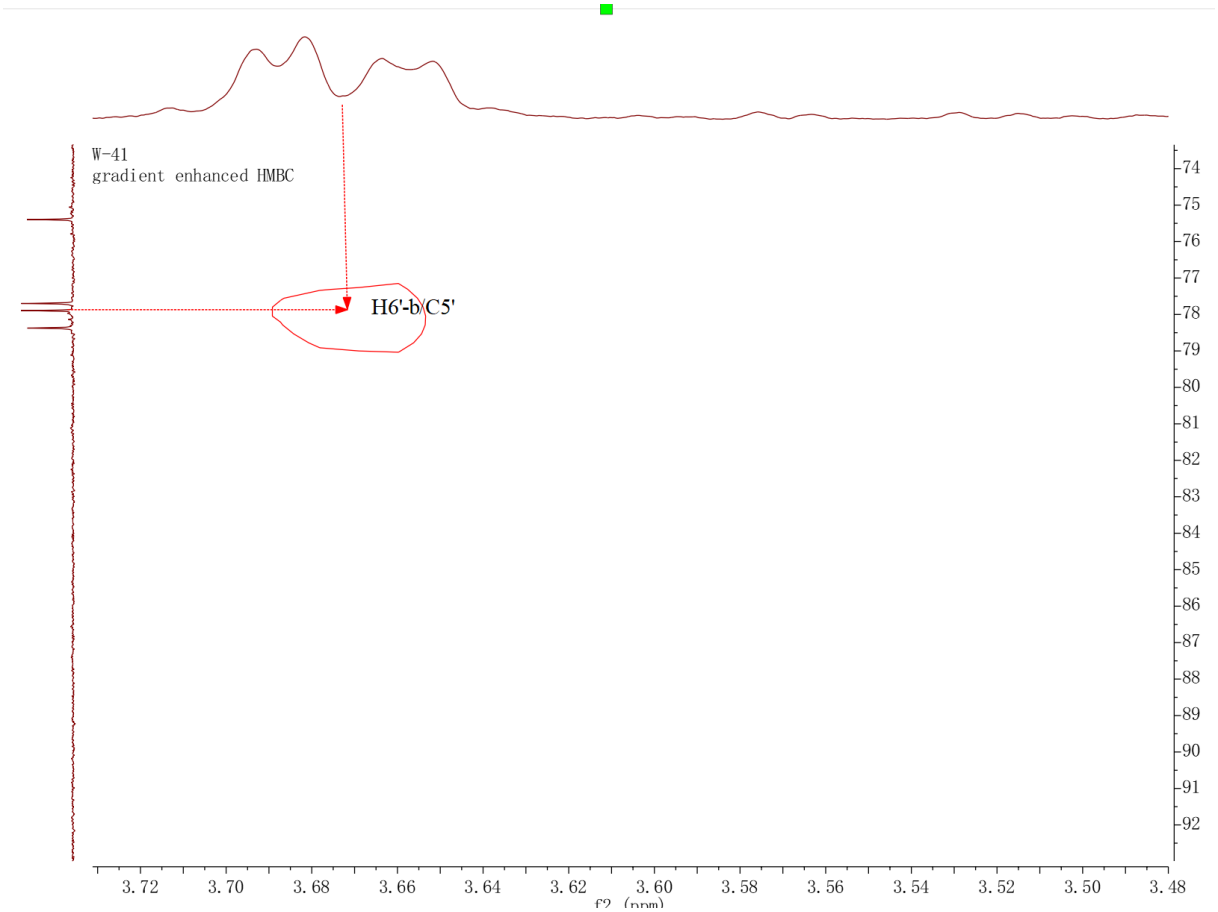


Figure S16: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 3.48 ppm to δ_H 3.72 ppm)

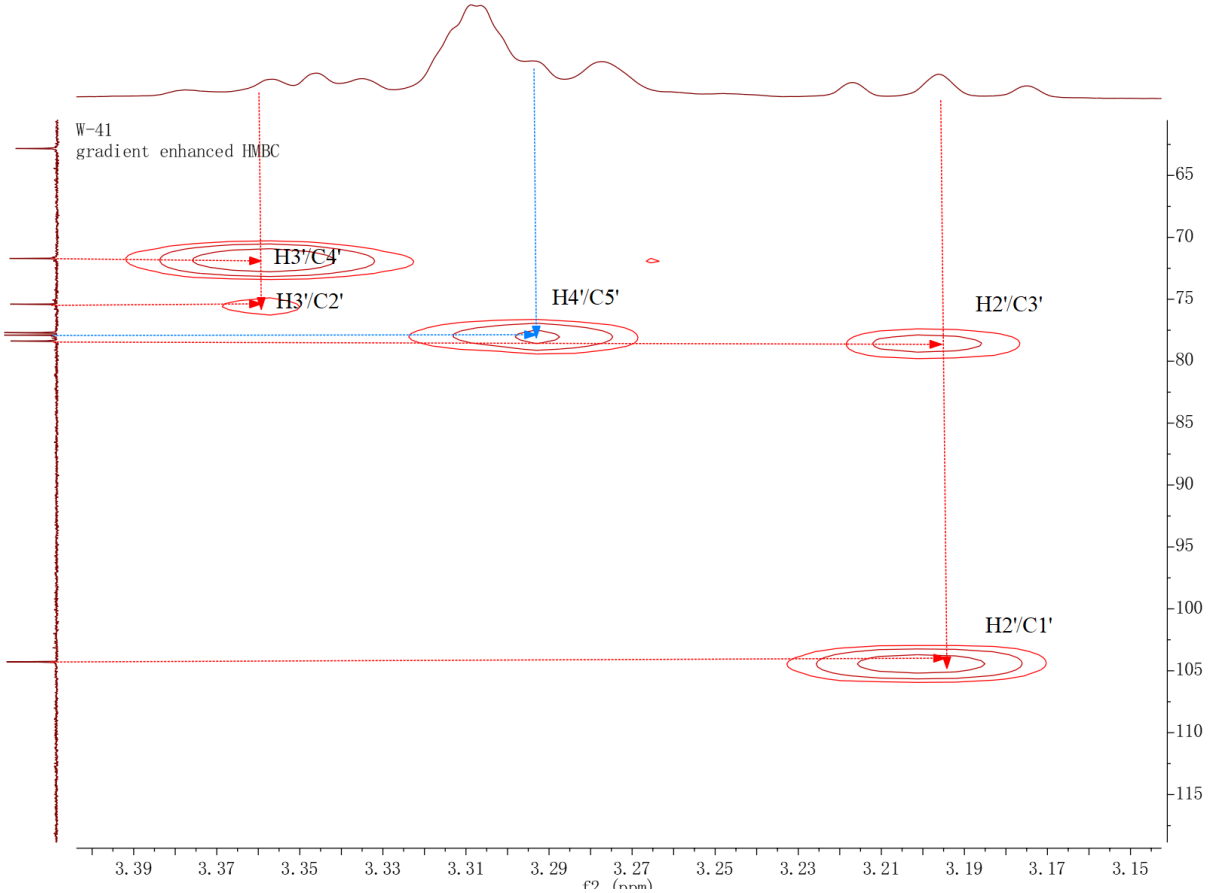


Figure S17: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 3.15 ppm to δ_H 3.39 ppm)

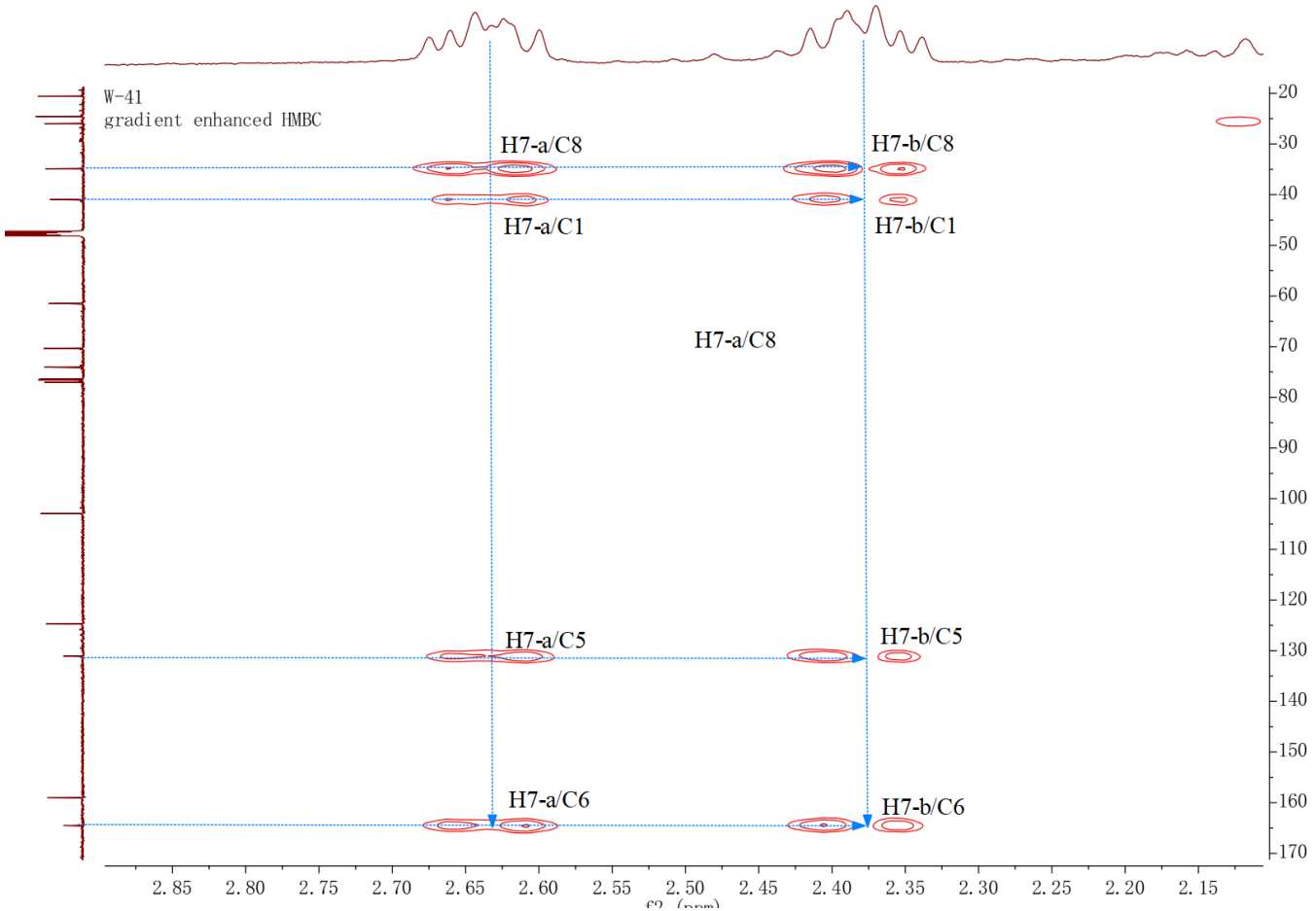


Figure S18: HMBC spectrum of **1** ((9S)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 2.15 ppm to δ_H 2.85 ppm)

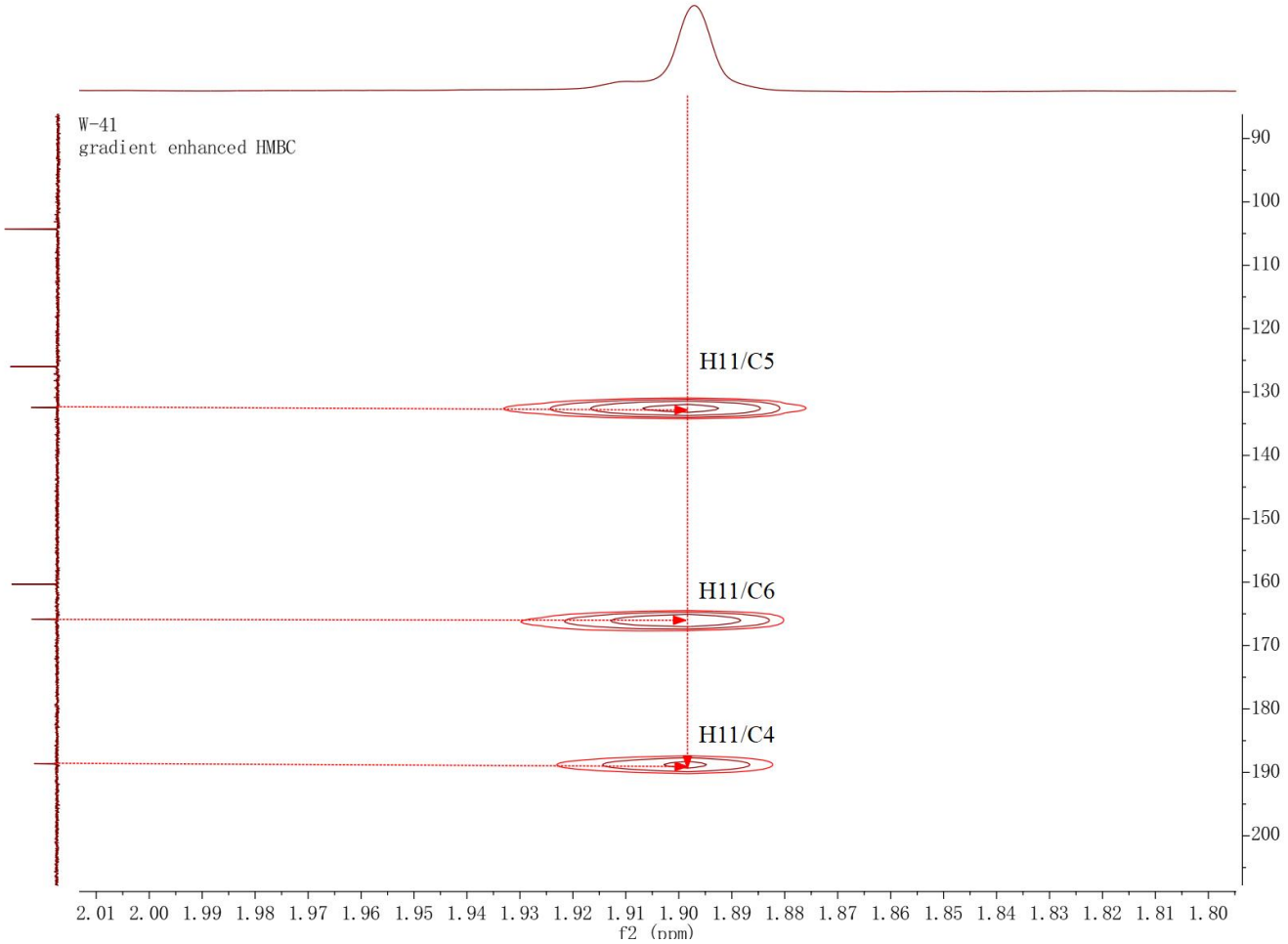


Figure S19: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 1.80 ppm to δ_H 2.01 ppm)

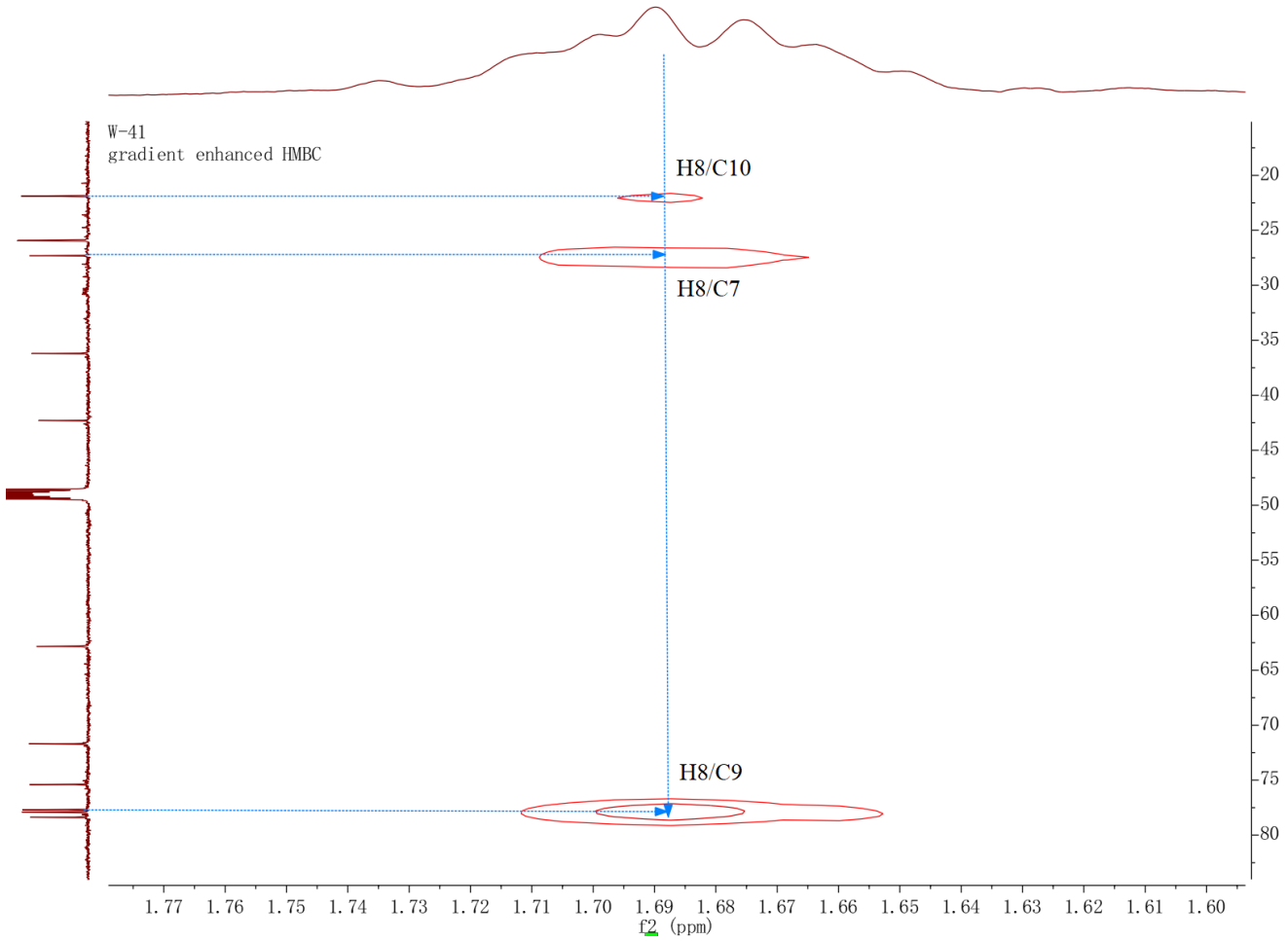


Figure S20: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 1.60 ppm to δ_H 1.77 ppm)

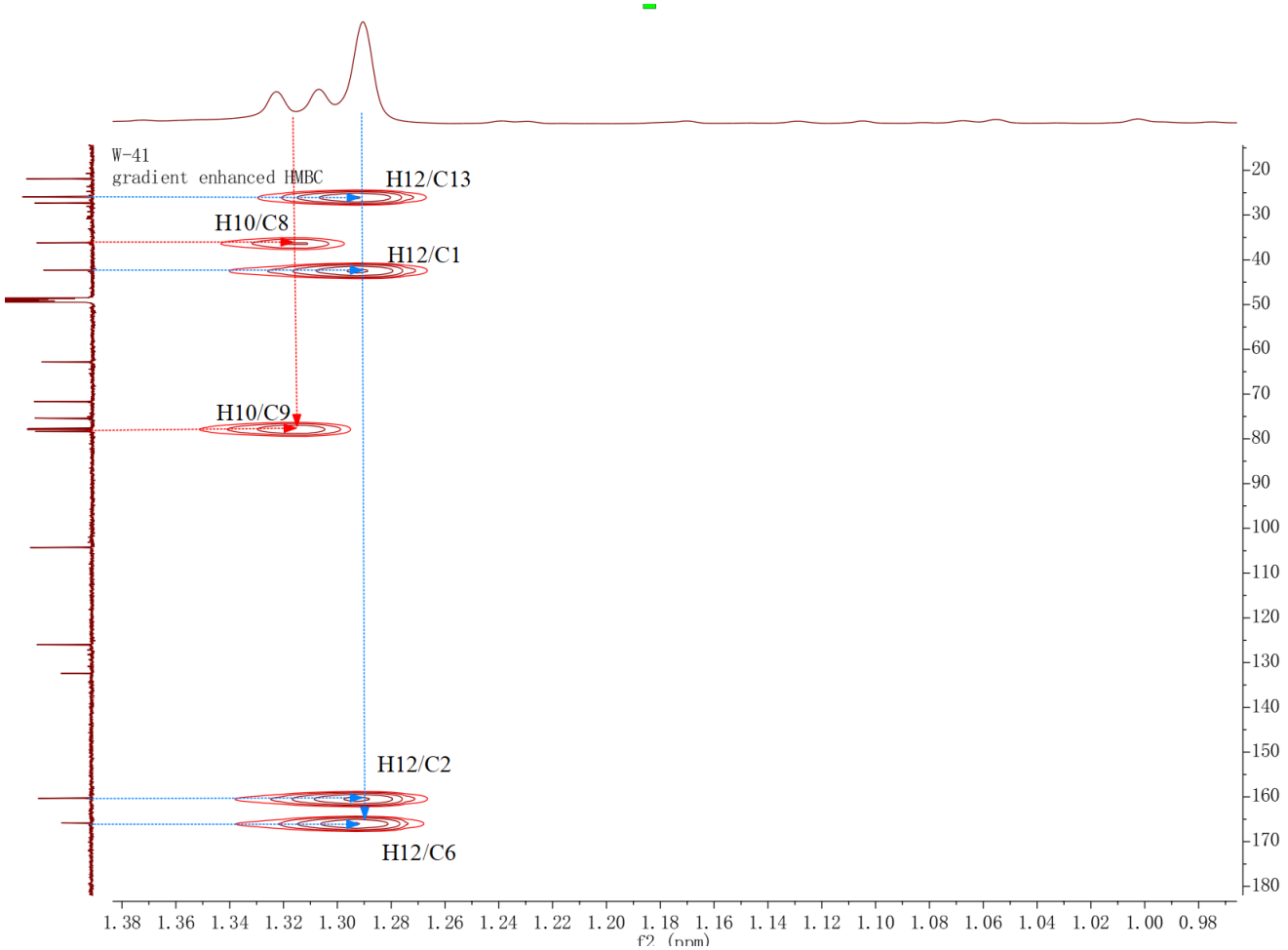


Figure S21: HMBC spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 0.98 ppm to δ_H 1.38 ppm)

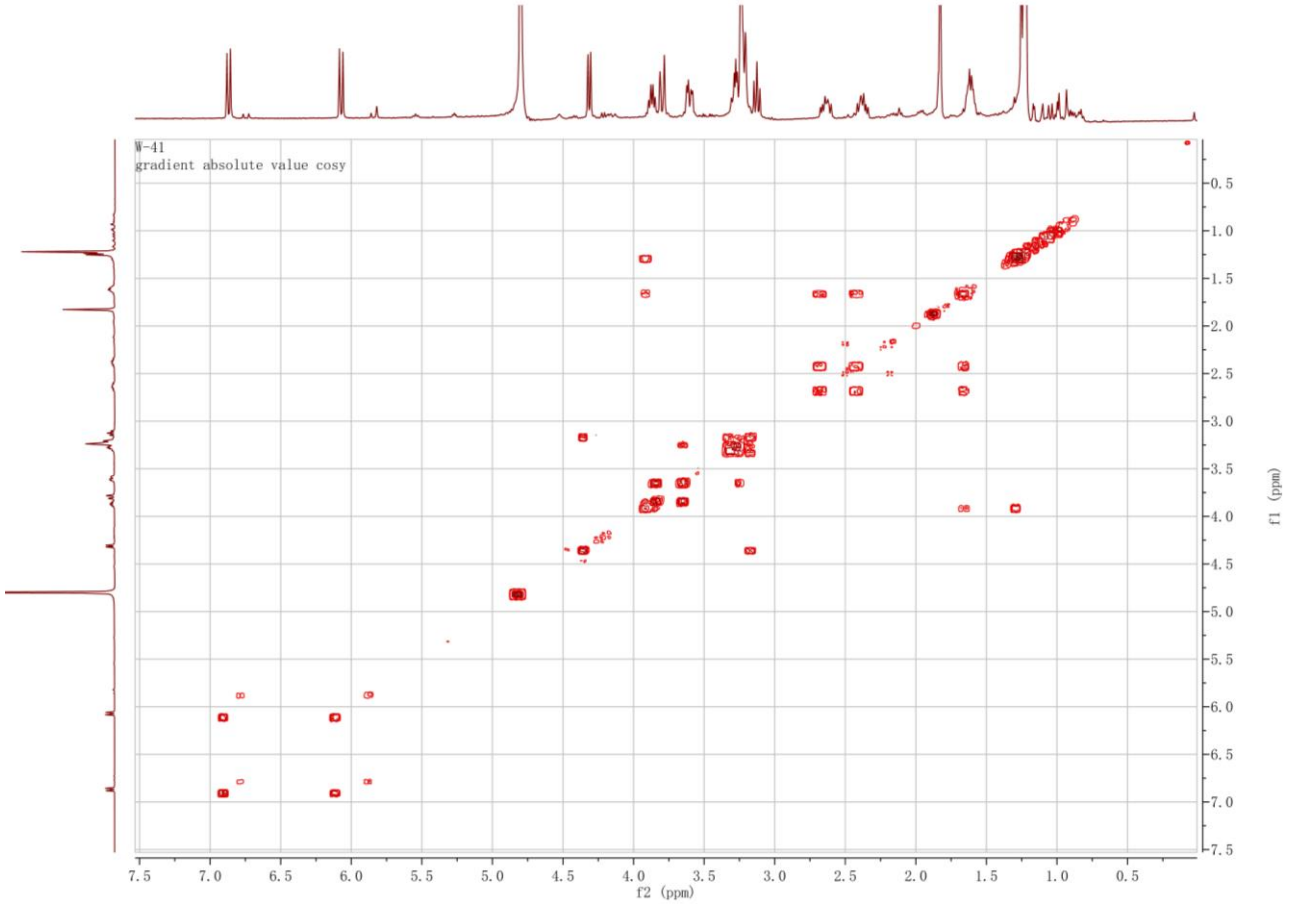


Figure S22: ^{1}H-^{1}H COSY Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

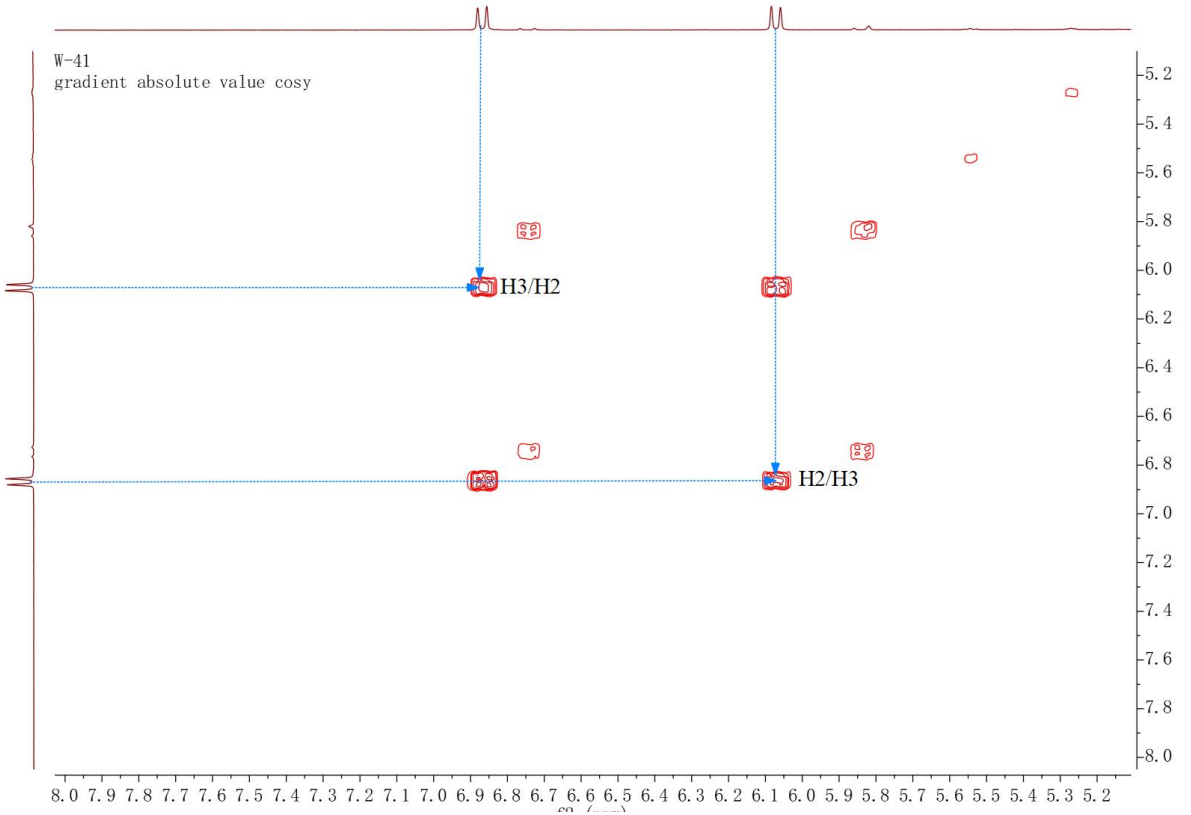


Figure S23: ^{1}H-^{1}H COSY Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 5.2 ppm to δ_H 8.0 ppm)

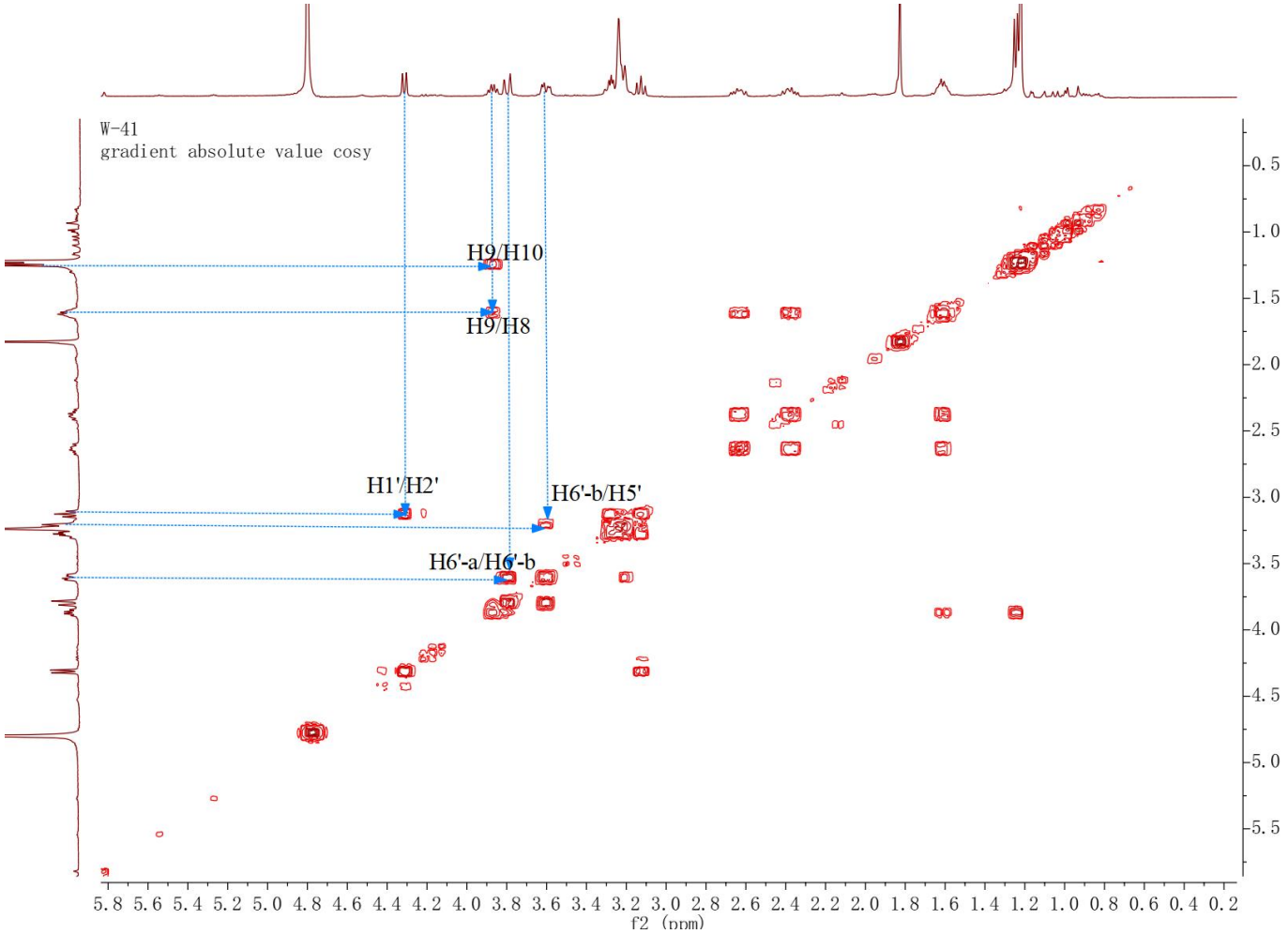


Figure S24: ^{1}H-^{1}H COSY Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 0.2 ppm to δ_H 5.8 ppm)

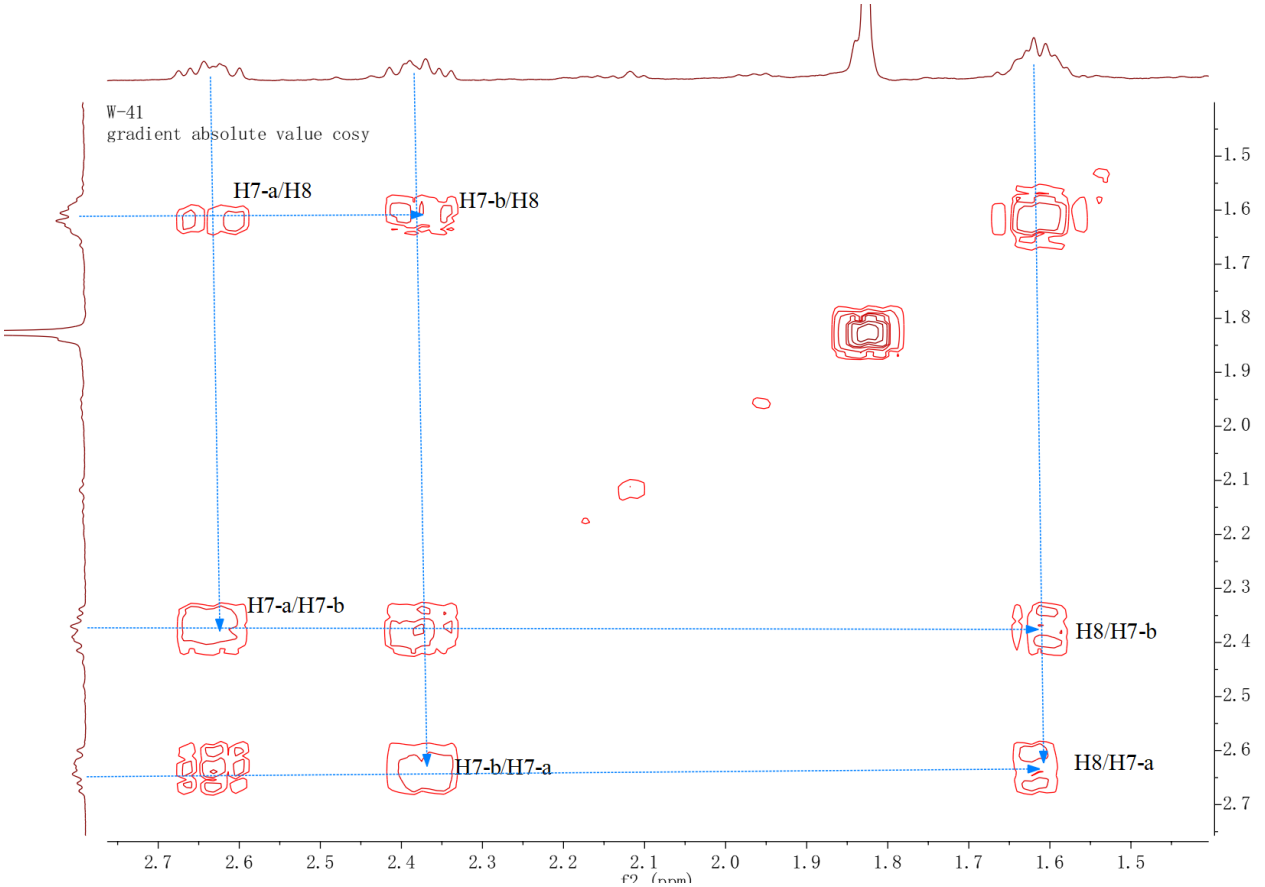


Figure S25: ^{1}H-^{1}H COSY Spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one) (From δ_H 1.5 ppm to δ_H 2.7 ppm)

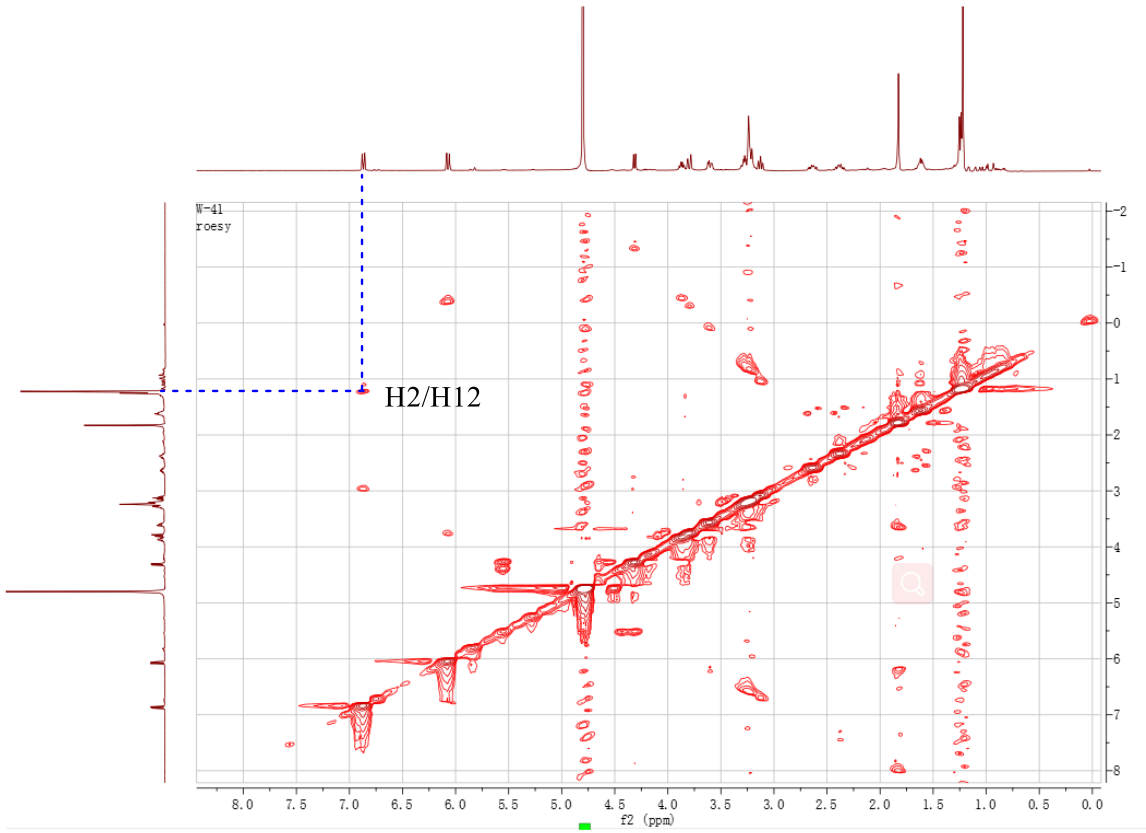
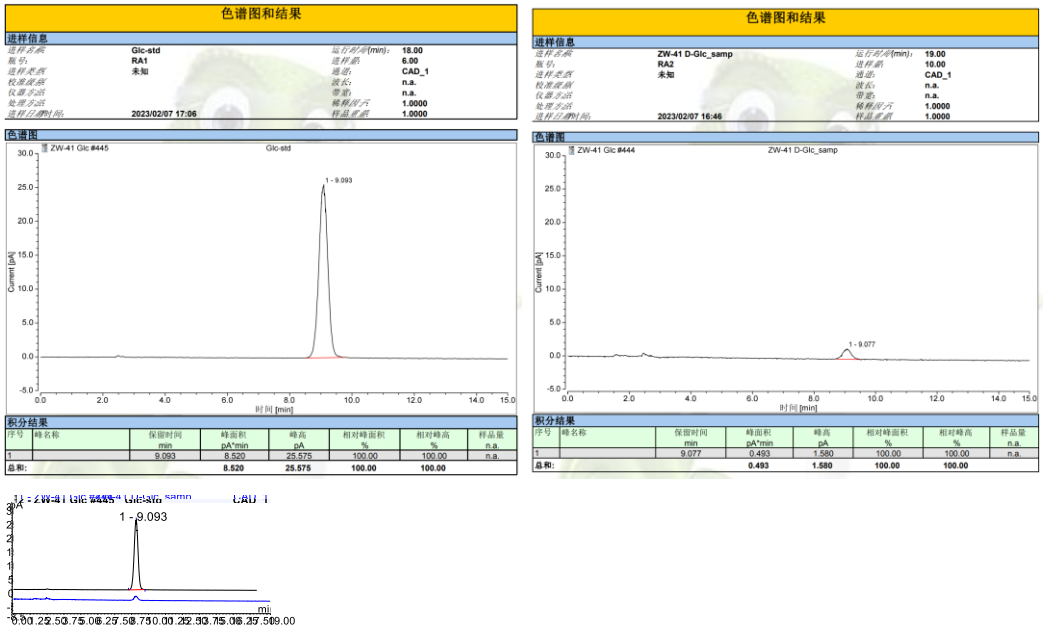


Figure S26: ROESY spectrum of **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)



a hydrolysis experiment to determine the absolute configuration of sugar moiety in 1.

Compound **1** was acid hydrolyzed according to the method described in the literature. Compound **1** (3 mg) was individually refluxed with 5 % HCl in MeOH (5 mL) for 2 hrs. The solution was diluted with H_2O (5 mL) and extracted with EtOAc (10 mL) for 3 times. The aqueous layer was neutralized with $NaHCO_3$ and concentrated in vacumn to give a residue. Purification of the residue was performed by RP-18 column, eluted with 20% MeOH-H_2O, to afford the purified sugar. The optical rotation was determined after dissolving the sugar in MeOH: [α]22.3 D: +40.1 (c 0.09, MeOH). And the sugar molecule were determined to be D-glc using HPLC-CAD, in contrast with the reference D-glc. Chromatographic analyses were performed on a Ulimate 3000 HPLC system equipped with a CAD detector. Chromatographic separation was carried out at 30 °C on a Shodex Asahipak NH_2-P-50 4E column (250 mm × 4.6 mm, 5 µm, USA). The mobile phase was composed of acetonitrile-water (25 : 75, v/v) at 1.0 ml·min^{-1}, every 3 µL sample solution was injected for each run and the CAD spectra were recorded at the frequency was 5 Hz, the filter was 3.6F, the atomizer temperature was 35 °C, the air source was N_2, and the pressure was 4.328×10^5 Pa.

Figure S27: The HPLC of sugar in compound **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

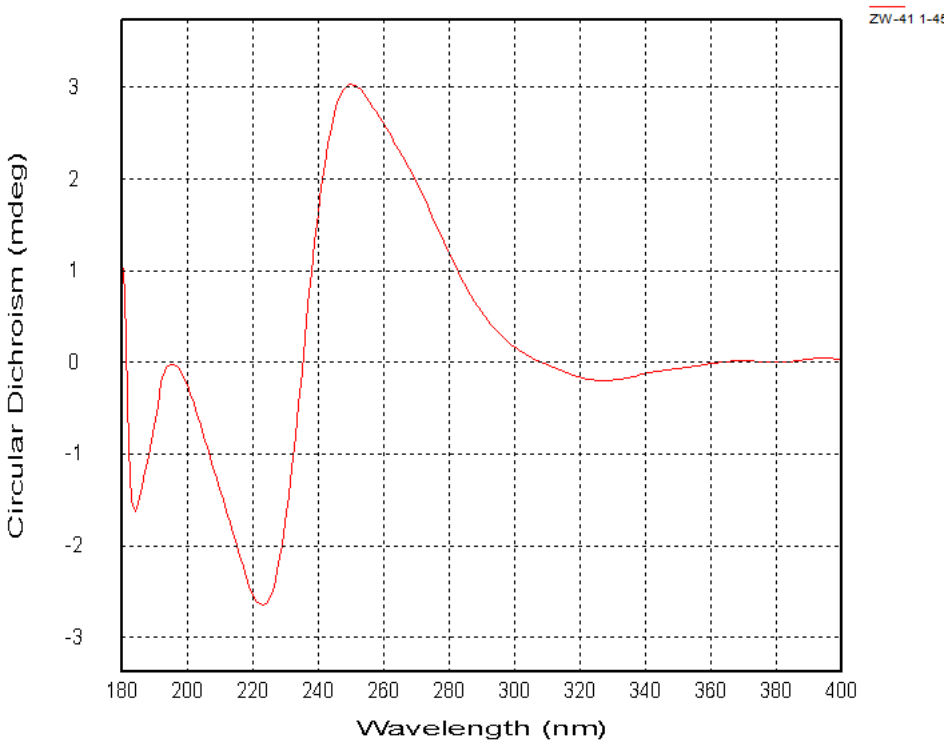


Figure S28: The circular dichroism spectrum of compound **1** ((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

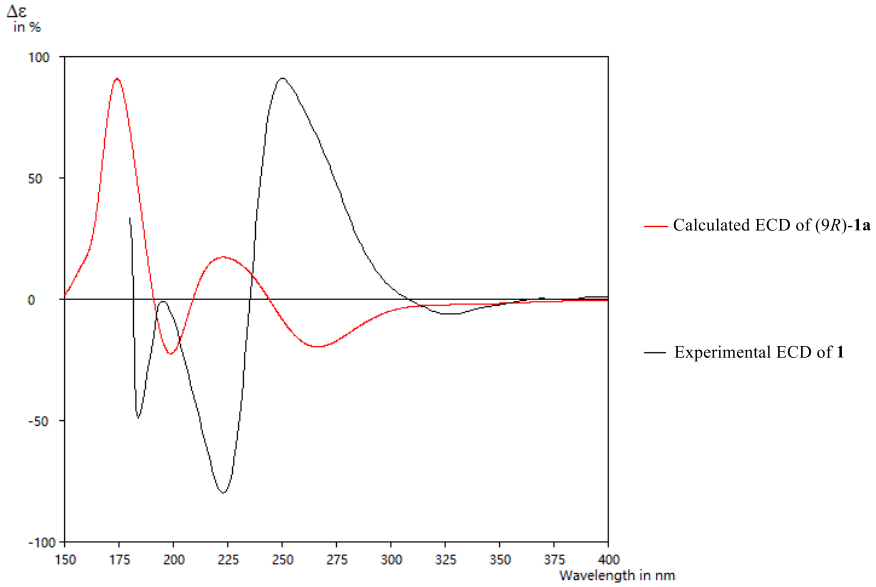


Figure S29: Calculated and experimental ECD spectra of compound **1**((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4-one)

Figure S30: Similarity report of compound **1**((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4- one)

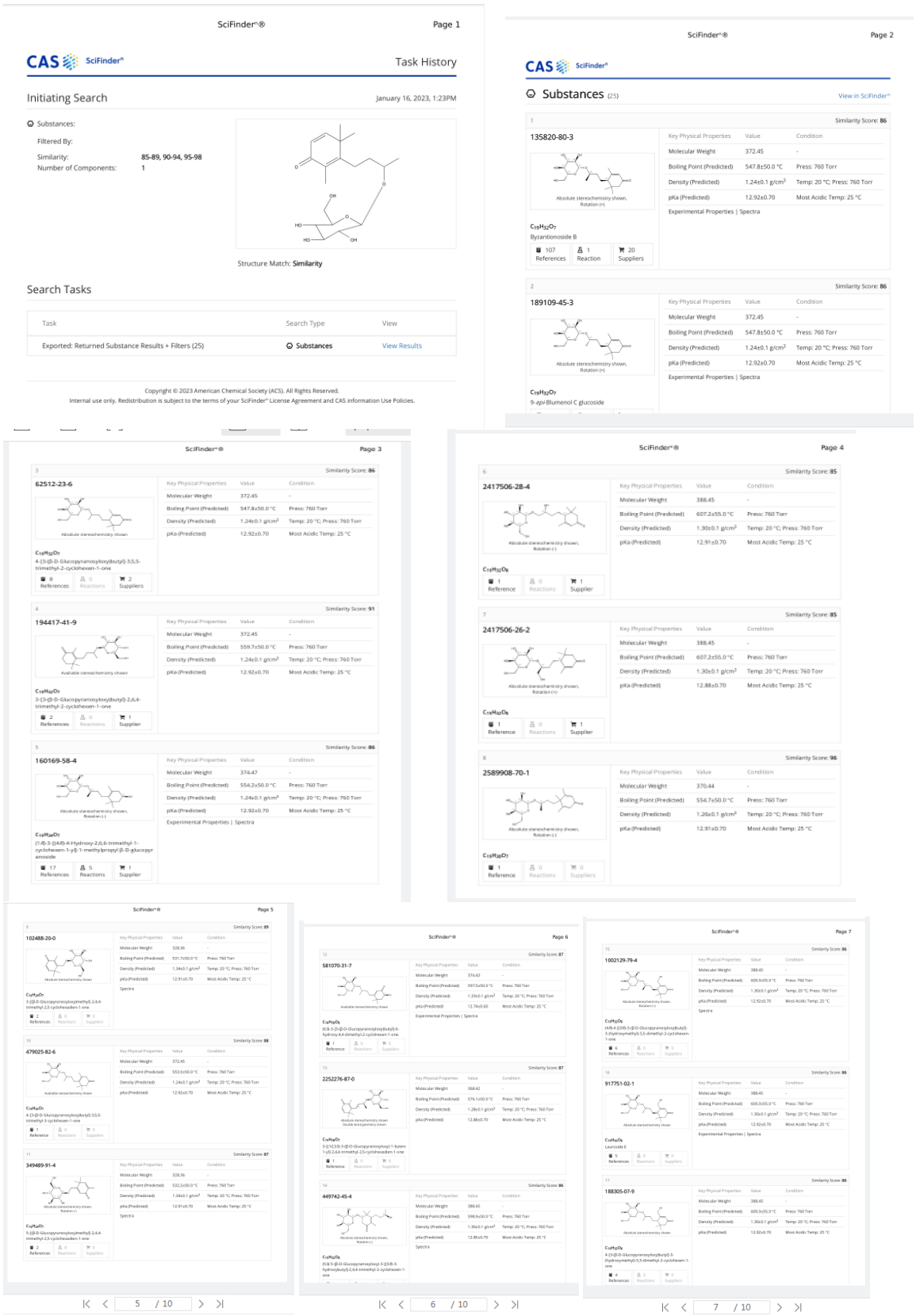


Figure S30: Similarity report of compound **1**((9*S*)-O-*β*-D-glucopyranosyl-2,5-megastigmen-4-one)