

Supporting Information

Flavonoids from the fruits of *Phyllanthus acidus* (L.) Skeels with anti- α -glucosidase activity

Abstract: Eleven flavonoids including one new flavonol glycoside, quercetin-3-*O*-(2- α -L-rhamnopyranosyl)- β -D-glucuronopyranosyl methyl ester (1), were isolated for the first time from the fruits of *Phyllanthus acidus* (L.) Skeels (Phyllanthaceae). Their structures were determined by extensive spectroscopic data. The known flavonoids, quercetin-3-*O*- β -D-glucuronide methyl ester (3), quercetin-3-*O*-(2"- α -L-rhamnopyranosyl-6"-*O*- α -L-rhamnopyranosyl)- β -D-glucopyranoside (5), myricetin (9), and 6-methoxy-naringenin (11) were isolated for the first time from the genus *Phyllanthus*. Flavonoids 4, 6 and 9 (IC_{50} = 6.01, 6.32, and 7.84 μ M, respectively) showed stronger α -glucosidase inhibitory activities than the positive control, acarbose (IC_{50} = 306.45 μ M). The fruits of *P. acidus* might be further developed as an anti-diabetic food supplement.

Keywords:

Phyllanthaceae; *Phyllanthus acidus* (L.) Skeels; flavonoids; anti- α -glucosidase activity

Contents of Supporting Information

No.	Contents	Pages
1.	Figure S1. Key HMBC (H → C) correlations of compound 1	3
2.	Figure S2. ¹ H NMR spectrum of compound 1	4
3.	Figure S3. ¹³ C NMR spectrum of compound 1	4
4.	Figure S4. HSQC spectrum of compound 1	5
5.	Figure S5. HMBC spectrum of compound 1	5
6.	Figure S6. ¹ H- ¹ H COSY spectrum of compound 1	6
7.	Figure S7. ROESY spectrum of compound 1	6
8.	Figure S8. Negative ESIMS spectrum of compound 1	7
9.	Figure S9. HRESIMS spectrum of compound 1	8
10.	Figure S10. CD and UV spectra of compound 1	9
11.	Table S1. α -Glucosidase inhibitory activities of compounds 2-11	10

Figure S2. Key HMBC (H → C) correlations of compound 1

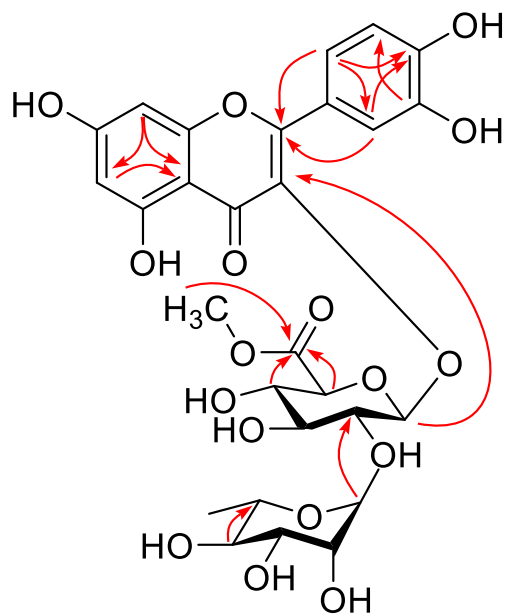


Figure S3. ^1H NMR spectrum of compound 1

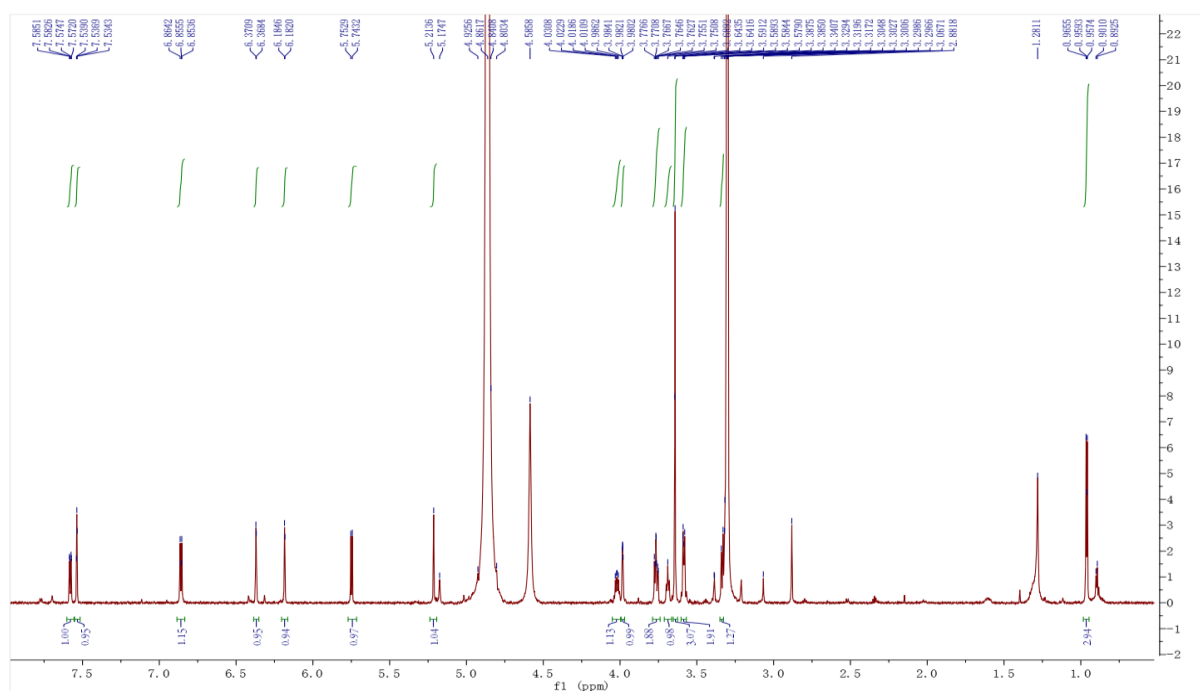


Figure S4. ^{13}C NMR spectrum of compound 1

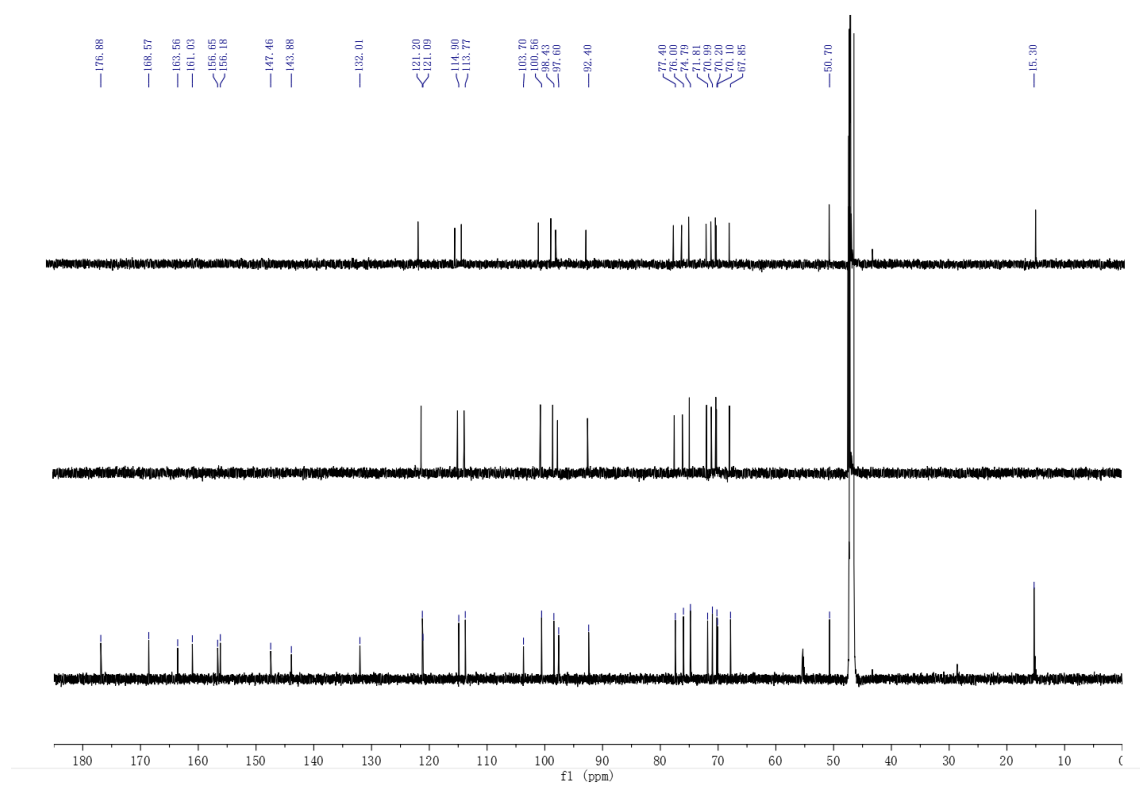


Figure S5. HSQC spectrum of compound 1

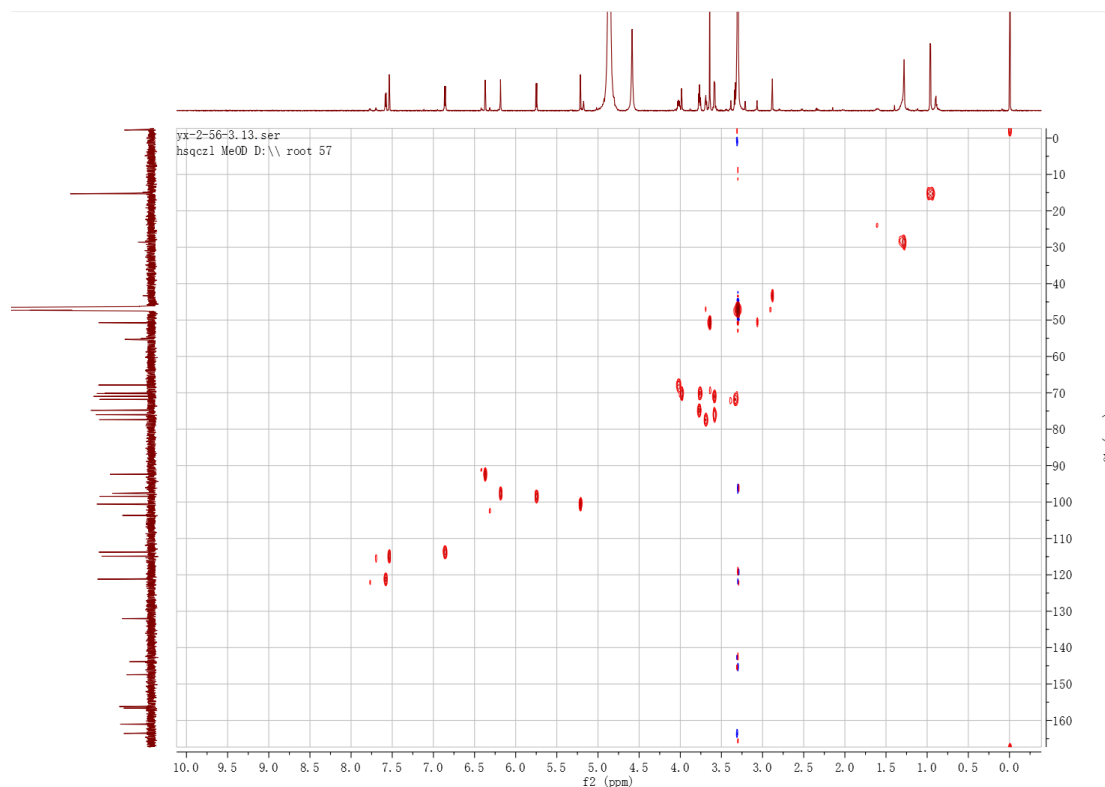


Figure S6. HMBC spectrum of compound 1

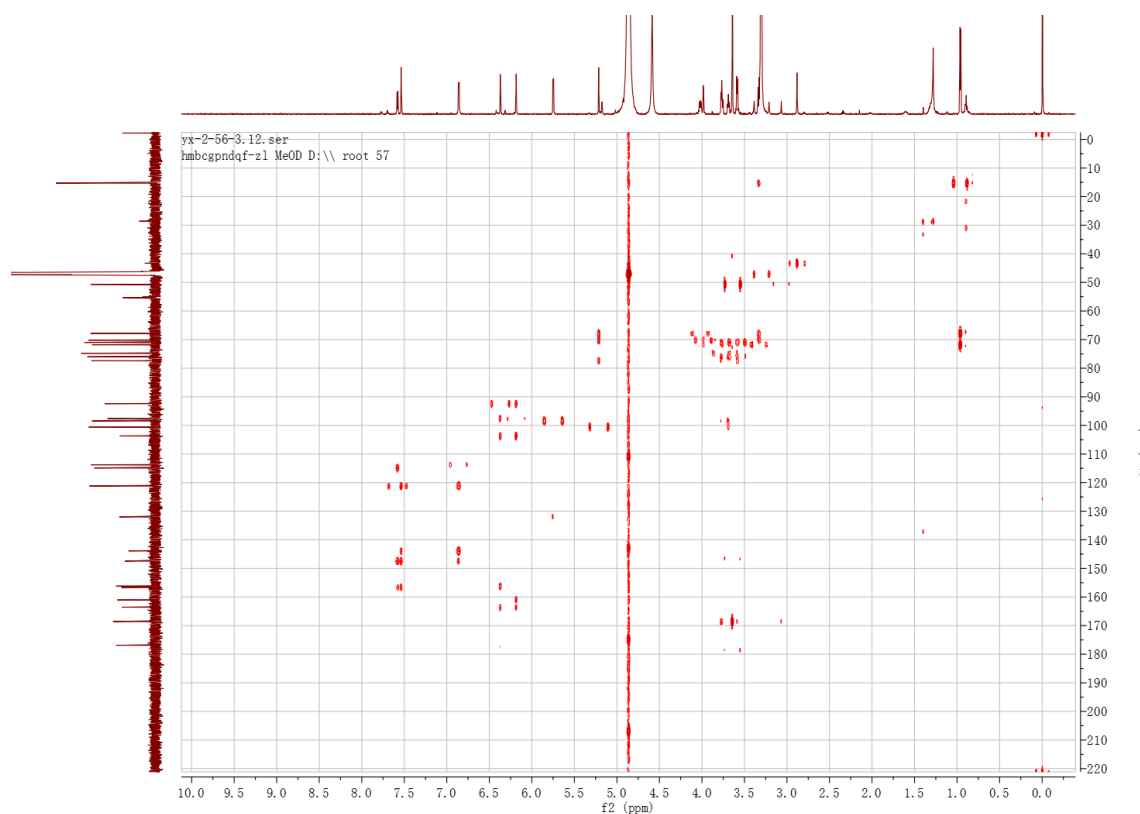


Figure S7. ^1H - ^1H COSY spectrum of compound 1

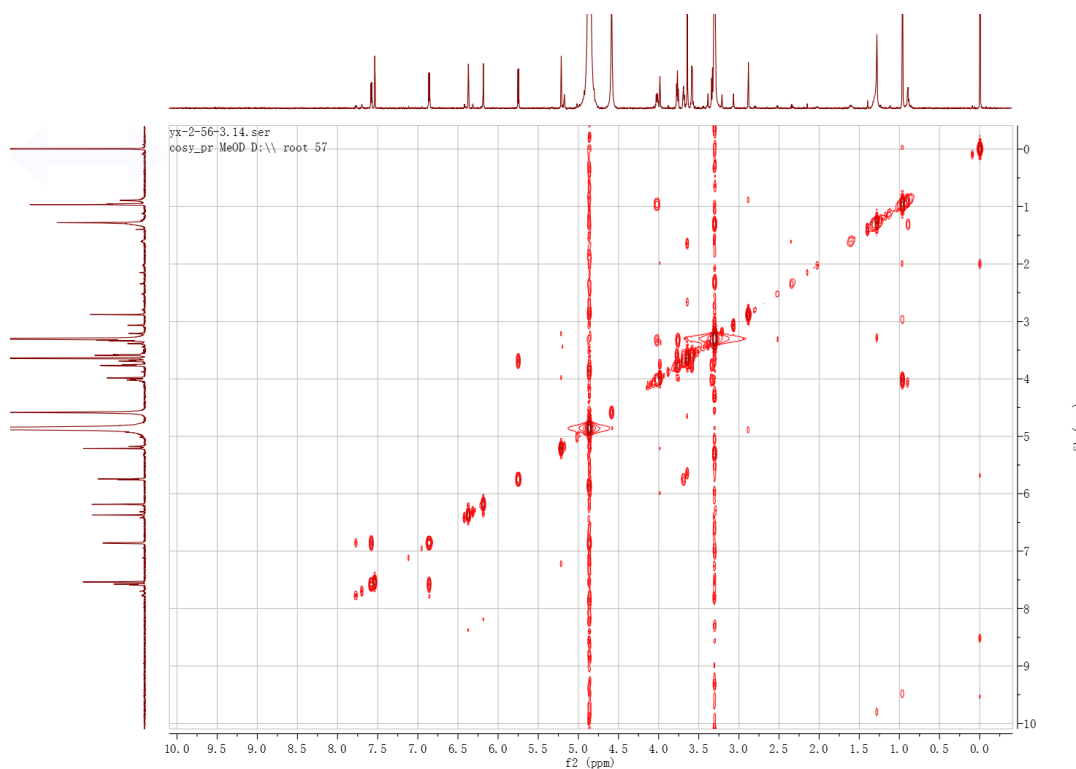


Figure S8. ROESY spectrum of compound 1

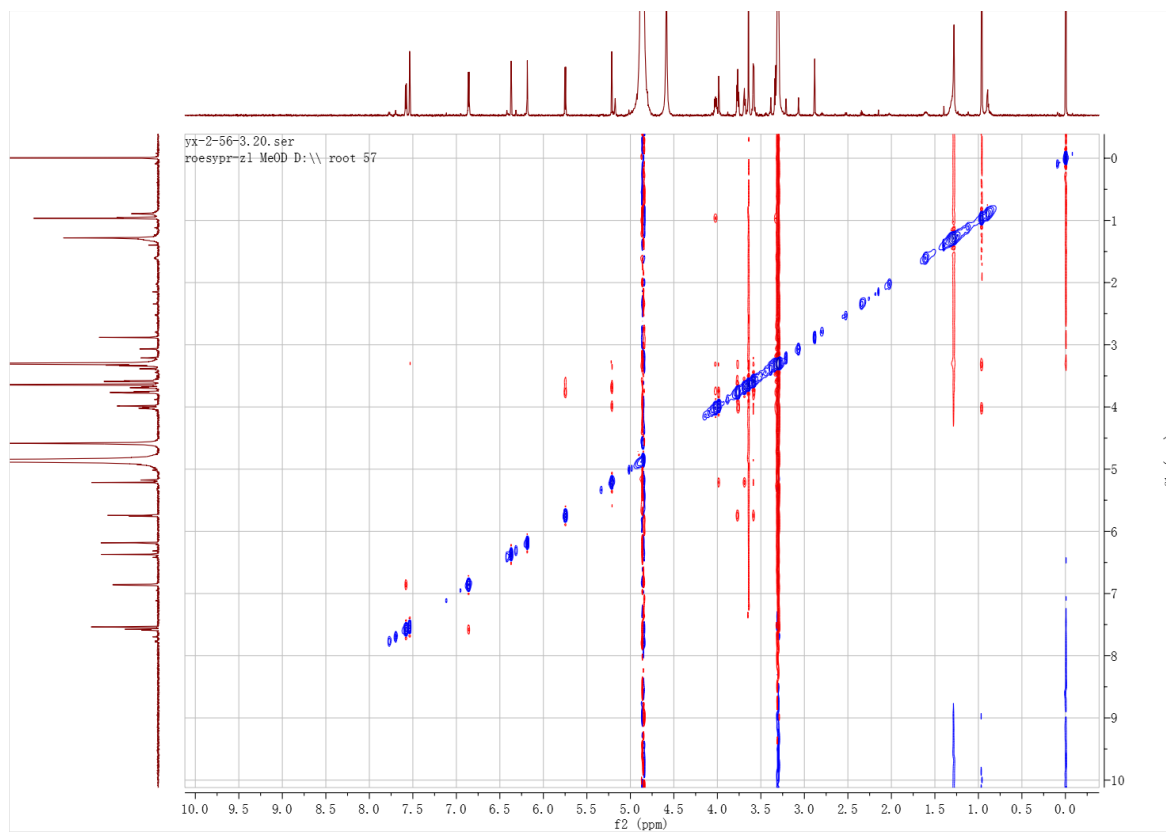


Figure S9. Negative ESIMS spectrum of compound 1

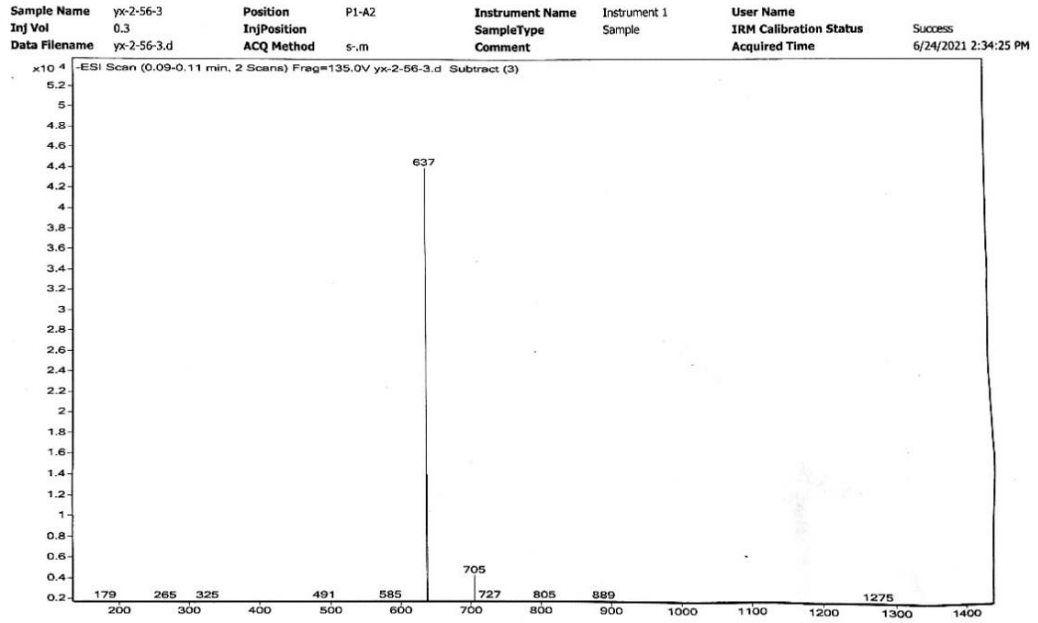
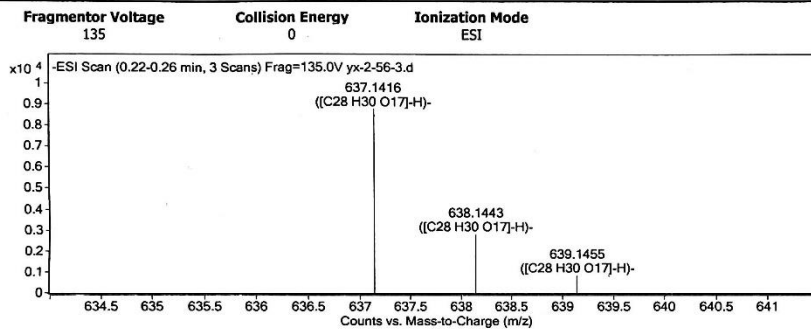


Figure S10. HRESIMS spectrum of compound 1

Qualitative Analysis Report

Data Filename yx-2-56-3.d **Sample Name** yx-2-56-3
Sample Type Sample **Position** P1-A2
Instrument Name Instrument 1 **User Name**
Acq Method S-.m **Acquired Time** 6/24/2021 2:34:25 PM
IRM Calibration Status XXXXXXXXXX **DA Method** Default.m
Comment
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
68.9957		4786.2		
96.9602		4687.82		
112.9856	1	7382.49		
119.0358		3140.37		
637.1416	1	8807.66	C28 H30 O17	(M-H)-
638.1443	1	2817.79	C28 H30 O17	(M-H)-
955.9712	1	2802.36		
966.0006	1	23623.78		
967.0035	1	4847.16		
982.9904	1	9655.19		
1033.9882	1	20229.27		
1034.9912	1	4227.83		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz _{obs}	Diff. (mDa)	Diff. (ppm)	DBE
C28 H30 O17	638.1483	637.1410	637.1416	-0.60	-0.94	14.0000

--- End Of Report ---

Figure S11. CD and UV spectra of compound 1

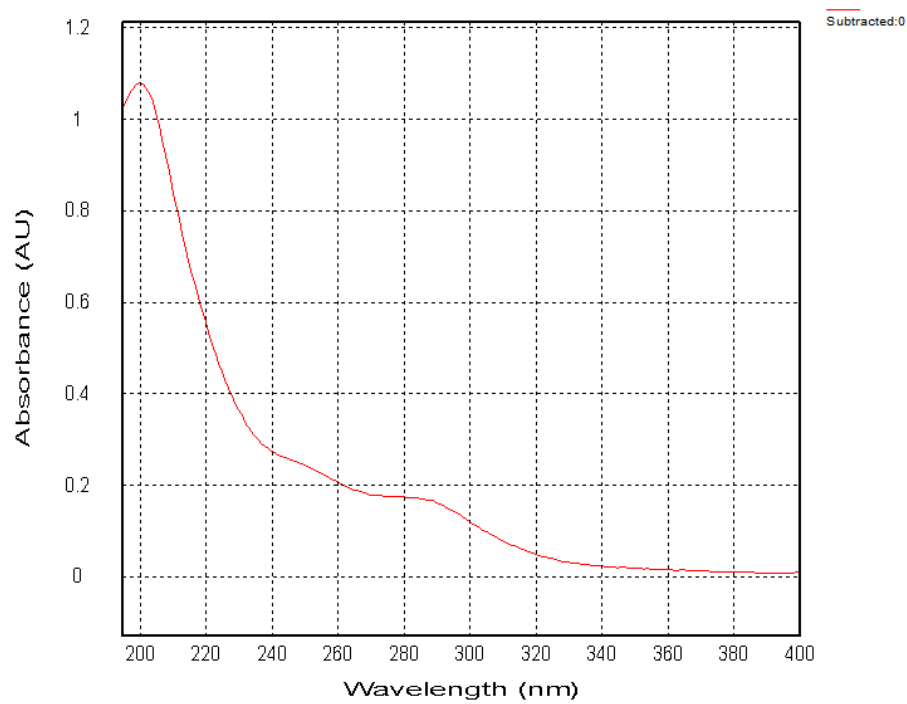
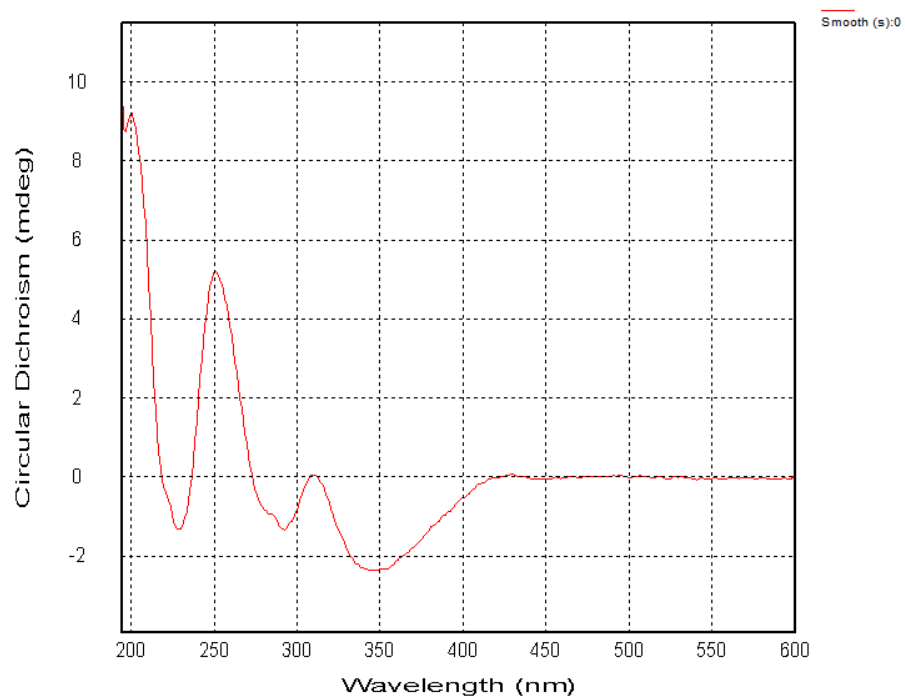


Table S1. α -Glucosidase inhibitory activities of compounds **2-11**

Compd.	Concentration (μM)	IC_{50} (μM)	Inhibition rate (%)
Acarbose	400	306.45 \pm 7.01	55.03 \pm 0.49
2	50		0.51 \pm 1.17
3	50		14.16 \pm 2.52
4		6.01 \pm 0.14	
5	50		-5.45 \pm 1.89
6		6.32 \pm 0.31	
7	50		-3.41 \pm 3.18
8	50		24.46 \pm 2.17
9		7.84 \pm 0.33	
10	50		20.89 \pm 2.35
11	50		9.37 \pm 2.59