SUPPLEMENTARY MATERIAL

Two new xanthone glycosides from *Swertia punicea* Hemsl. and their anti-inflammatory activity

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Acknowledgement

This work was financially supported by Technology Center, China Tobacco Yunnan Industrial Co., Ltd [grant number JSZX20151008-52].

ABSTRACT

Two new xanthone glycosides (**1**–**2**), together with seven known analogues (**3**–**9**), were isolated from whole herb of *Swertia punicea*. The structures of these metabolites were established on the basis of detailed spectroscopic analysis and comparison with data reported in the literature. In an *in vitro* test, All isolates were evaluated for their anti-inflammatory activity. The results revealed that all of them showed significant anti-inflammatory activity with IC_{50} values ranging from 1.237 to 3.319 mM. Compounds **3**, **4,** and **5** (IC_{50} values in the range 1.237 to 1.987 mM) displayed more potent anti-inflammatory activity than the positive control, indomethacin (IC_{50} value of 2.004 mM).

Keywords：*Swertia punicea*, xanthone glycosides, anti-inflammatory activity

Table S1. ^{1}H and ^{13}C NMR data for compounds **1** and **2** (Data obtained in C_5D_5N)

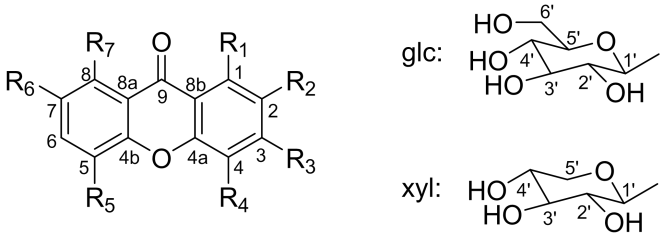
Position	1		2	
No.	δ_C	δ_H (mult, *J*, Hz)	δ_C	δ_H (mult, *J*, Hz)
1	149.9 (s)		149.9 (s)	
2	97.8 (d)	6.95 s	97.4 (d)	6.51 s
3	160.1 (s)		160.0 (s)	
4	140.6 (s)		140.5 (s)	
4a	154.7 (s)		154.8 (s)	
4b	145.8 (s)		145.6 (s)	
5	148.7 (s)		147.6 (s)	
6	115.6 (d)	7.25 overlap	120.6 (d)	7.52 d (7.3)
7	123.8 (d)	7.24 overlap	124.3 (d)	7.26 overlap
8	117.5 (d)	7.99 m	116.2 (d)	7.95 d (7.7)
8a	123.4 (s)		123.3 (s)	
8b	109.9 (s)		109.8 (s)	
9	176.6 (s)		177.2 (s)	
Glc-1'	106.4 (d)	5.68 d (7.8)	106.5 (d)	5.68 d (7.7)
2'	75.8 (d)	4.51 m	75.8 (d)	4.50 m
3'	78.4 (d)	4.12 overlap	78.4 (d)	4.30 overlap
4'	71.5 (d)	4.14 overlap	71.3 (d)	4.27 overlap
5'	78.3 (d)	3.86 overlap	78.2 (d)	4.18 overlap
6'	69.8 (t)	4.86 d (11.0) 4.29 overlap	69.5 (t)	4.29 m 4.13 m
(6-1)-Glc			(6-1)-Xyl	
1"	105.0 (d)	4.94 d (7.7)	105.5 (d)	4.83 d (7.8)
2"	75.1 (d)	3.96 m	74.9 (d)	3.91 m
3"	78.3 (d)	4.31 m	78.0 (d)	4.06 m
4"	71.3 (d)	4.18 overlap	71.2 (d)	4.16 overlap
5"	78.1 (d)	4.16 overlap	67.1 (t)	4.26 overlap
6"	62.6 (t)	4.46 overlap 4.33 overlap		
3-OMe	56.3 (q)	3.84 s	56.5 (q)	3.73 s
4-OMe	61.8 (q)	4.22 s	61.8 (q)	4.22 s
5-OMe	56.5 (q)	3.92 s		

^{1}H NMR Recorded at 500 MHz. ^{13}C NMR Recorded at 125 MHz.

Table S2 The anti-inflammatory activity of compounds **1–9** (IC_{50})

Sample	IC_{50} (mM)	Sample	IC_{50} (mM)
Indomethacin	2.004	5	1.987
1	2.158	6	2.251
2	3.319	7	2.607
3	1.732	8	2.523
4	1.237	9	2.049

Indomethacin was used as positive control.



	R_1	R_2	R_3	R_4	R_5	R_6	R_7
1	O-glc(6-1)-glc	H	OMe	OMe	OMe	H	H
2	O-glc(6-1)-xyl	H	OMe	OMe	OH	H	H
3	O-glc(6-1)-xyl	H	OMe	OMe	H	H	OMe
4	O-glc(6-1)-xyl	H	OMe	OMe	OMe	H	H
5	O-glc(6-1)-glc	OMe	OMe	OMe	H	OMe	H
6	O-glc(6-1)-xyl	OMe	OMe	OMe	OMe	H	H
7	O-glc(6-1)-xyl	OMe	OMe	OMe	H	OMe	H
8	O-glc(6-1)-xyl	OMe	OMe	H	OMe	H	H
9	O-glc(6-1)-glc	OMe	OMe	OMe	OMe	H	H

Figure 1. The structures of compounds **1–9**.

Supplemental file (Figure) Legend

Figure S1. Lift: UV spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in MeOH

Right: UV spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in MeOH

Figure S2. Up: IR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**)

Down: IR spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**)

Figure S3. ^{1}H NMR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

Figure S4. ^{13}C NMR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 125 MHz

Figure S5. ^{13}C NMR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in DMSO at 125 MHz

Figure S6. HSQC spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

Figure S7. HMBC spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

Figure S8. COSY spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

Figure S9. Key HMBC and COSY correlations of compound **1**.

Figure S10. ^{1}H NMR spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in C_5D_5N at 500 MHz

Figure S11. ^{13}C NMR spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in C_5D_5N at 125 MHz

Figure S12. HSQC spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in C_5D_5N at 500 MHz

Figure S13. HMBC spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in C_5D_5N at 500 MHz

Figure S14. COSY spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in C_5D_5N at 500 MHz

Figure S15. Key HMBC and COSY correlations of compound **2**.

Figure S16. ^{1}H NMR spectrum of compound **3** recorded in C_5D_5N at 500 MHz

Figure S17. ^{13}C NMR spectrum of compound **3** recorded in C_5D_5N at 125 MHz

Figure S18. ^{1}H NMR spectrum of compound **4** recorded in C_5D_5N at 500 MHz

Figure S19. ^{13}C NMR spectrum of compound **4** recorded in C_5D_5N at 125 MHz

Figure S20. ^{1}H NMR spectrum of compound **5** recorded in C_5D_5N at 500 MHz

Figure S21. ^{13}C NMR spectrum of compound **5** recorded in C_5D_5N at 125 MHz

Figure S22. ^{1}H NMR spectrum of compound **6** recorded in C_5D_5N at 500 MHz

Figure S23. ^{13}C NMR spectrum of compound **6** recorded in C_5D_5N at 125 MHz

Figure S24. ^{1}H NMR spectrum of compound **7** recorded in C_5D_5N at 500 MHz

Figure S25. ^{13}C NMR spectrum of compound **7** recorded in C_5D_5N at 125 MHz

Figure S26. ^{1}H NMR spectrum of compound **8** recorded in DMSO and C_5D_5N at 500 MHz

Figure S27. ^{13}C NMR spectrum of compound **8** recorded in DMSO and C_5D_5N at 125 MHz

Figure S28. ^{1}H NMR spectrum of compound **9** recorded in C_5D_5N at 500 MHz

Figure S29. ^{13}C NMR spectrum of compound **9** recorded in C_5D_5N at 125 MHz

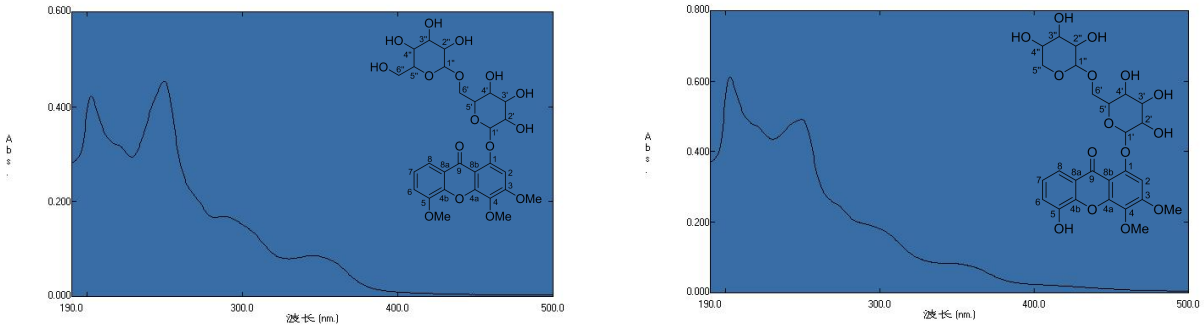


Figure S1. LIFT: UV spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in MeOH

Right: UV spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in MeOH

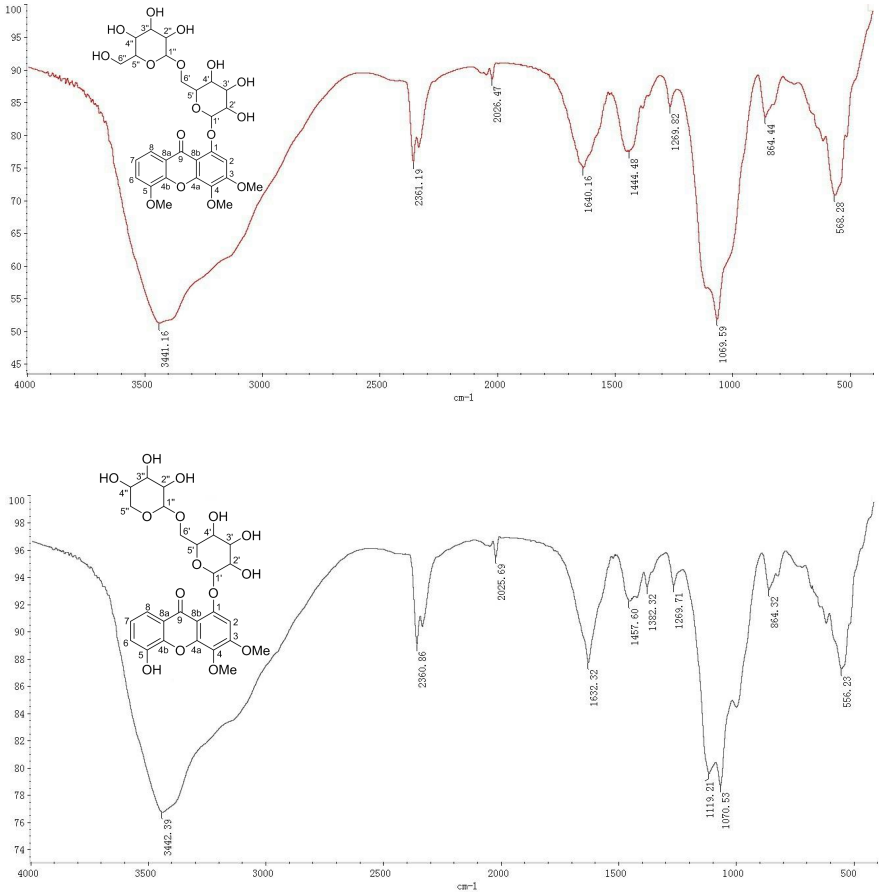


Figure S2. Up: IR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**)

Down: IR spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**)

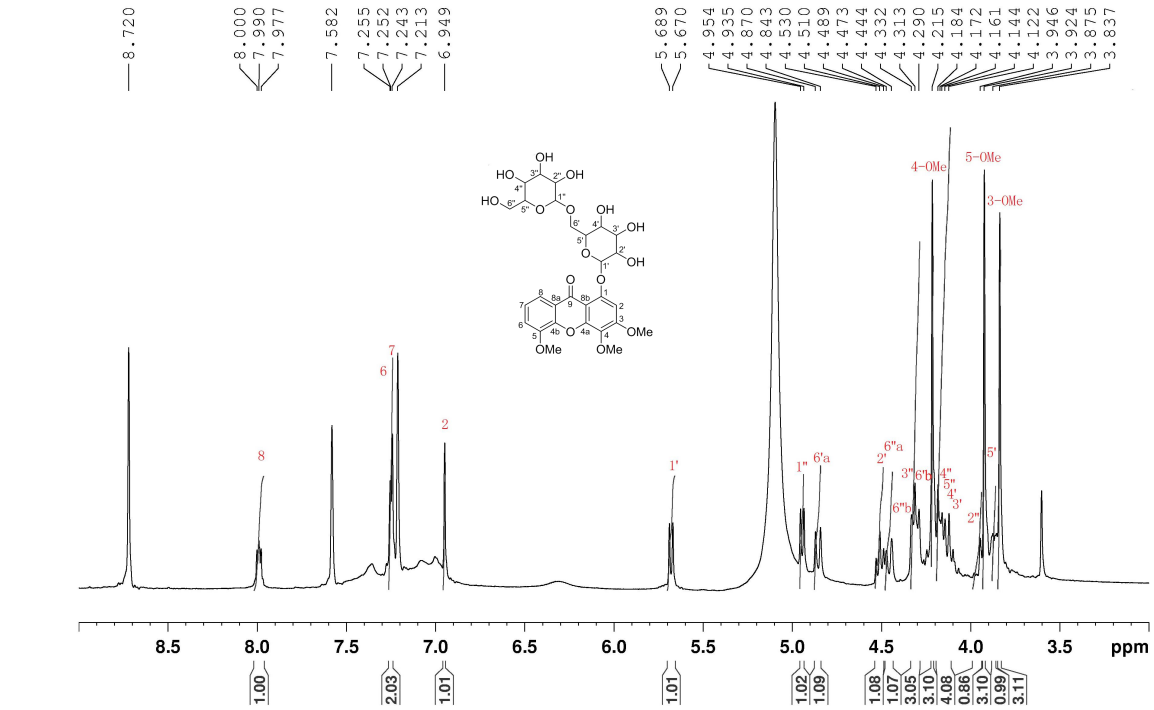


Figure S3. [1]H NMR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

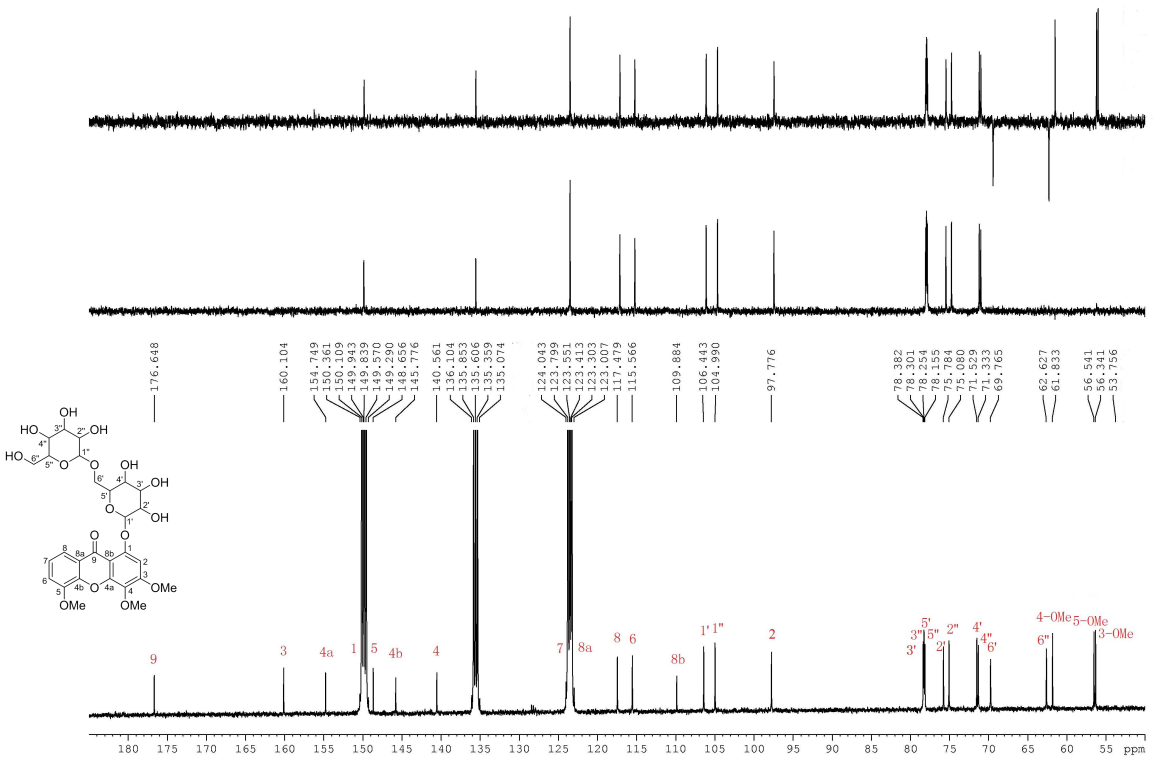


Figure S4. [13]C NMR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 125 MHz

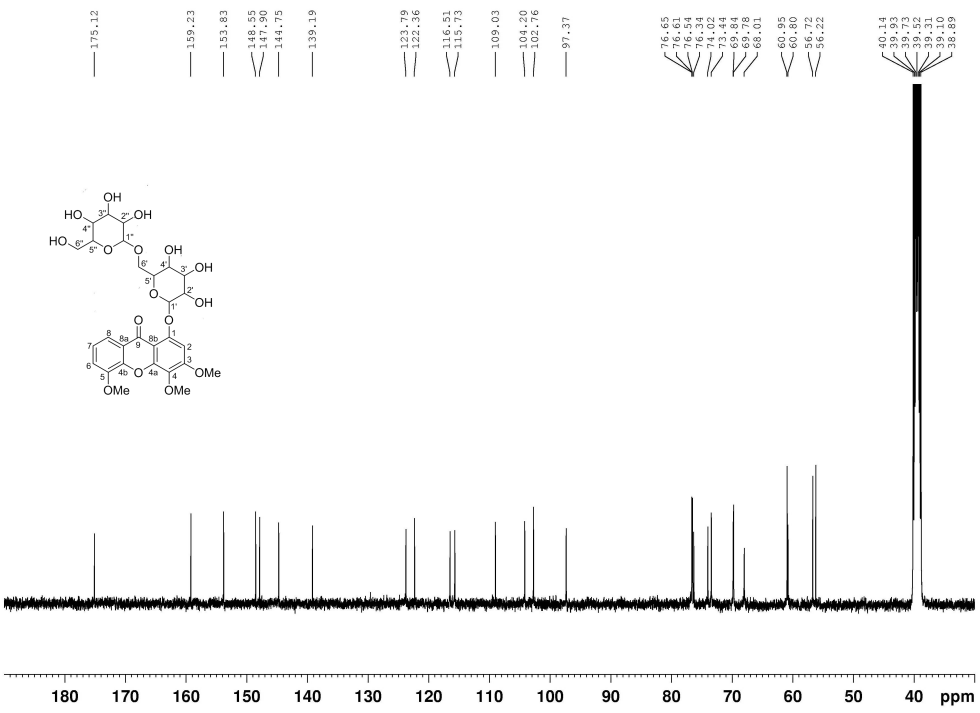


Figure S5. ^{13}C NMR spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in DMSO at 125 MHz

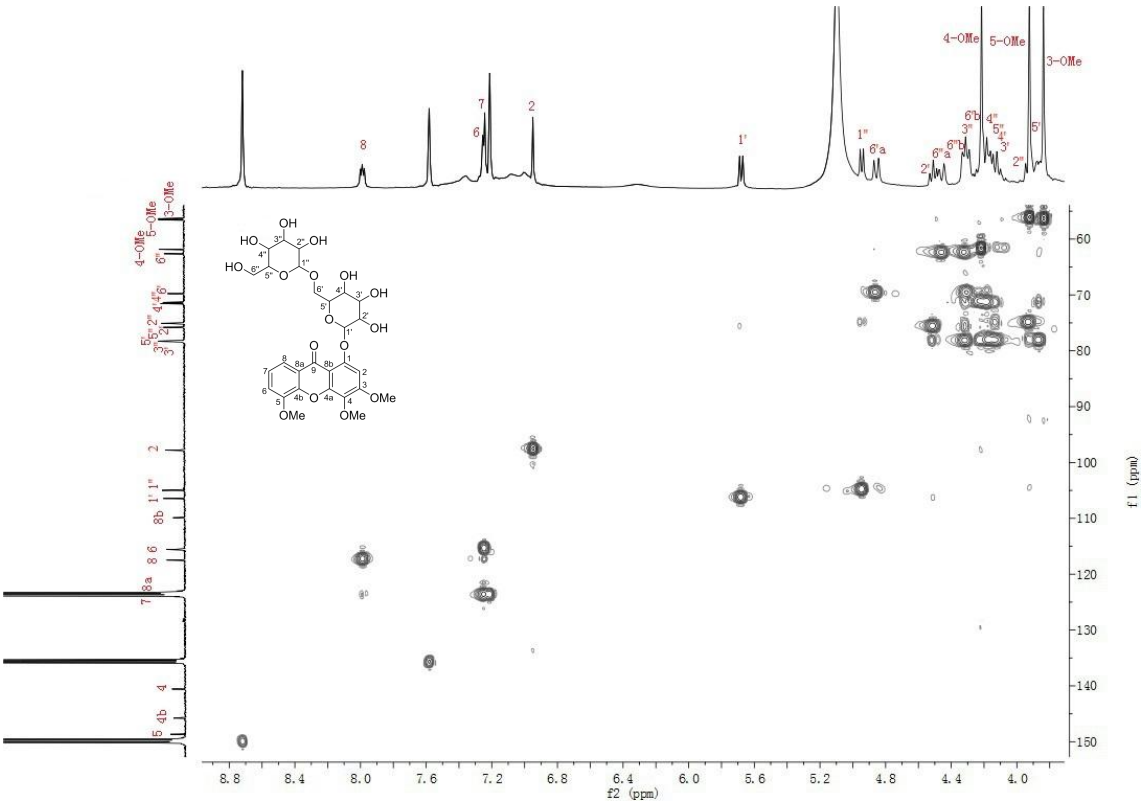


Figure S6. HSQC spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

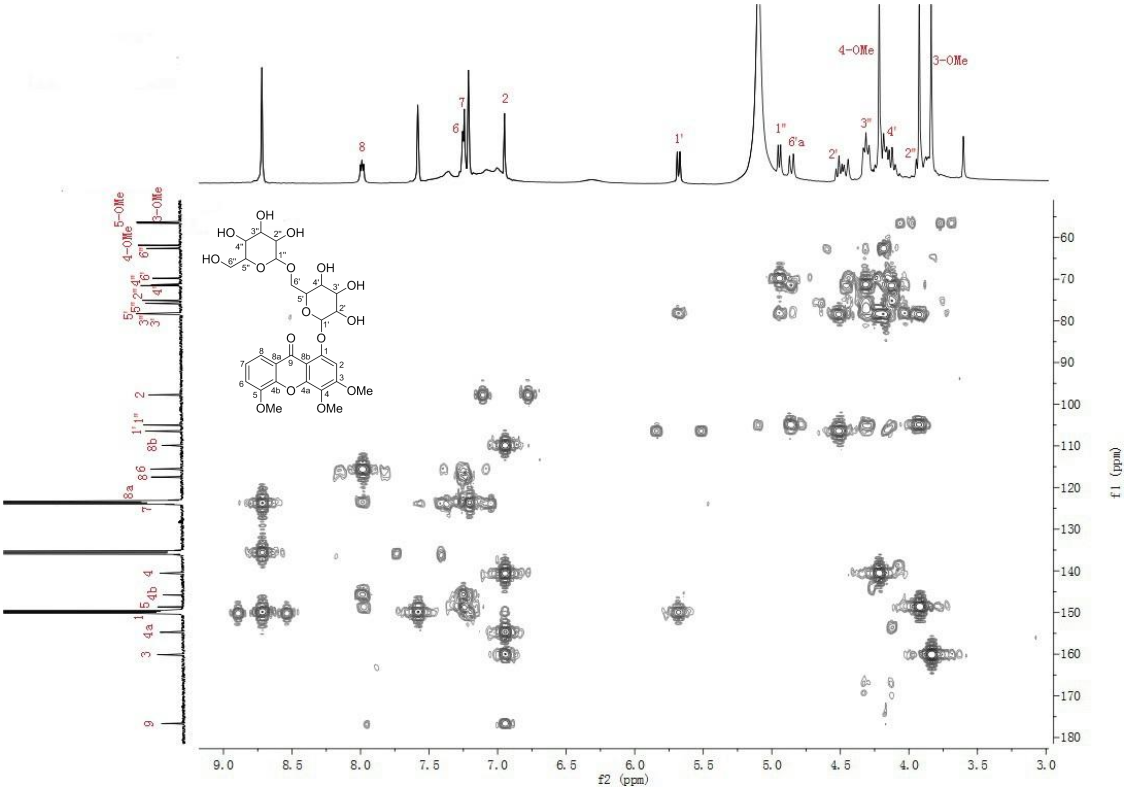


Figure S7. HMBC spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

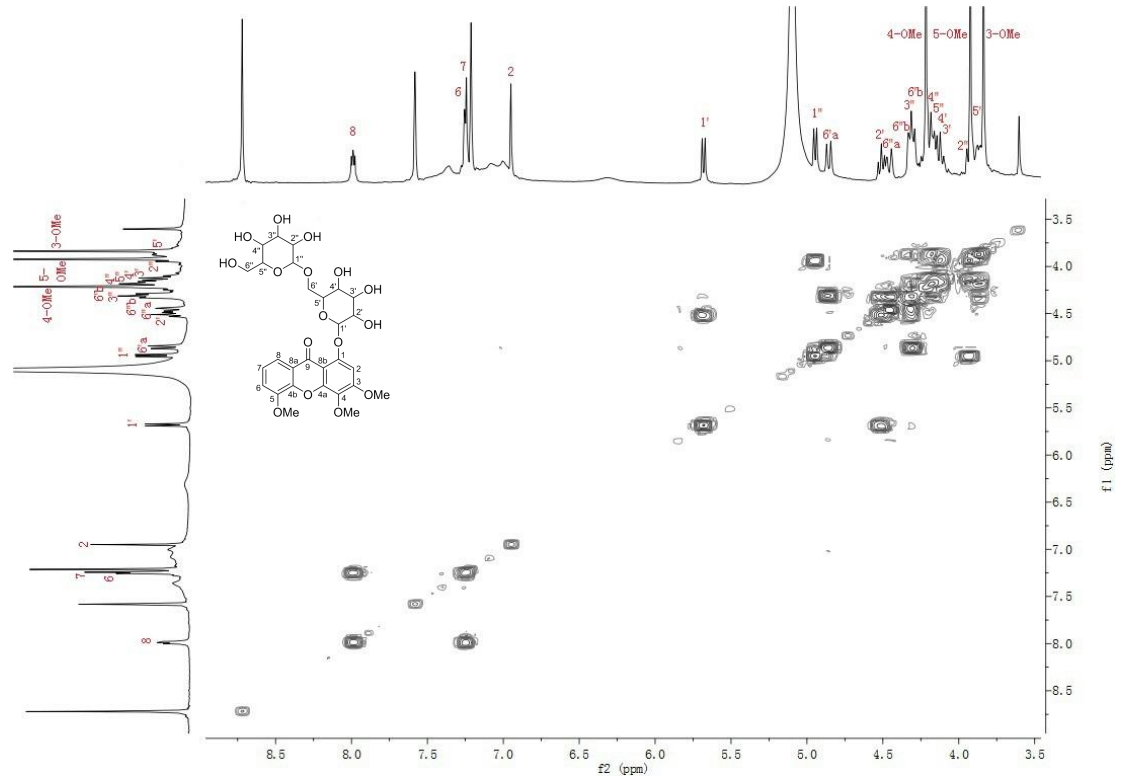


Figure S8. COSY spectrum of 3,4,5-trimethoxy-1-*O*-gentiobiosyloxyxanthone (**1**) recorded in C_5D_5N at 500 MHz

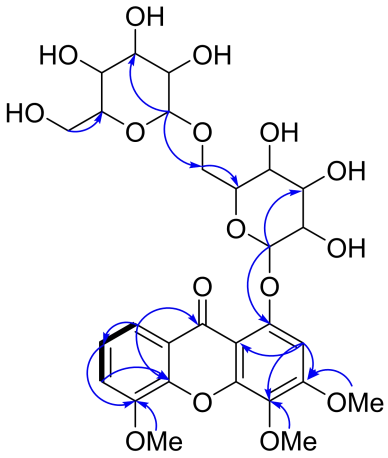


Figure S9. Key HMBC ( ) and COSY ( ) correlations of compound **1**.

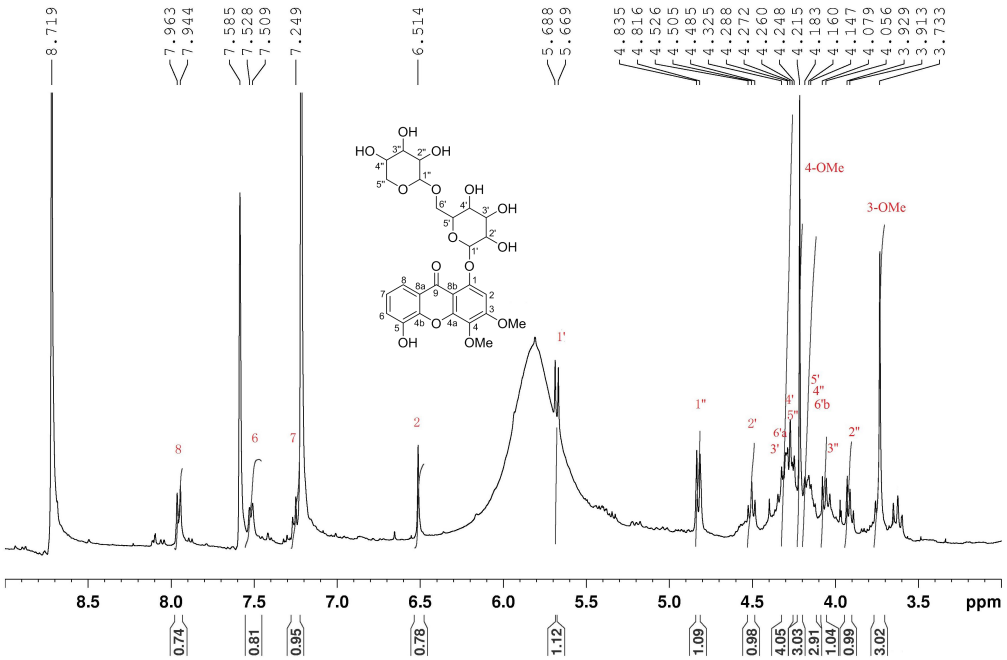


Figure S10. ^{1}H NMR spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in C_5D_5N at 500 MHz

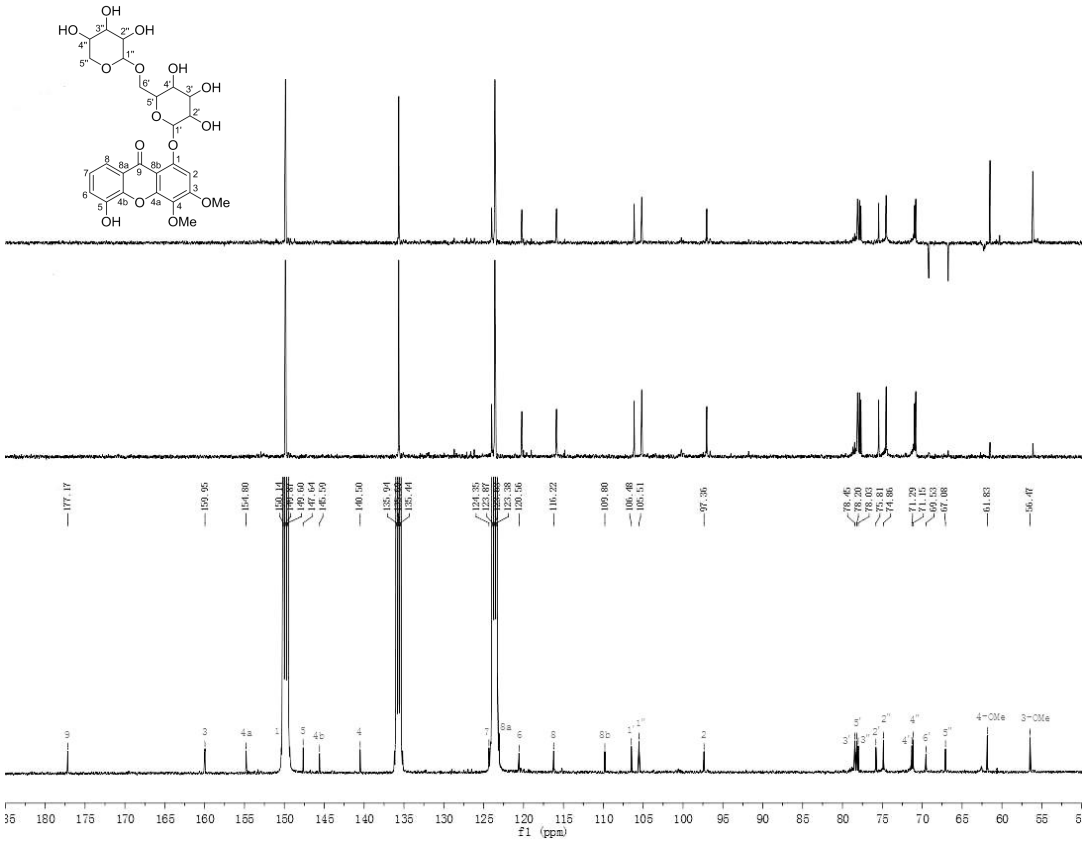


Figure S11. ^{13}C NMR spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone (**2**) recorded in C_5D_5N at 125 MHz

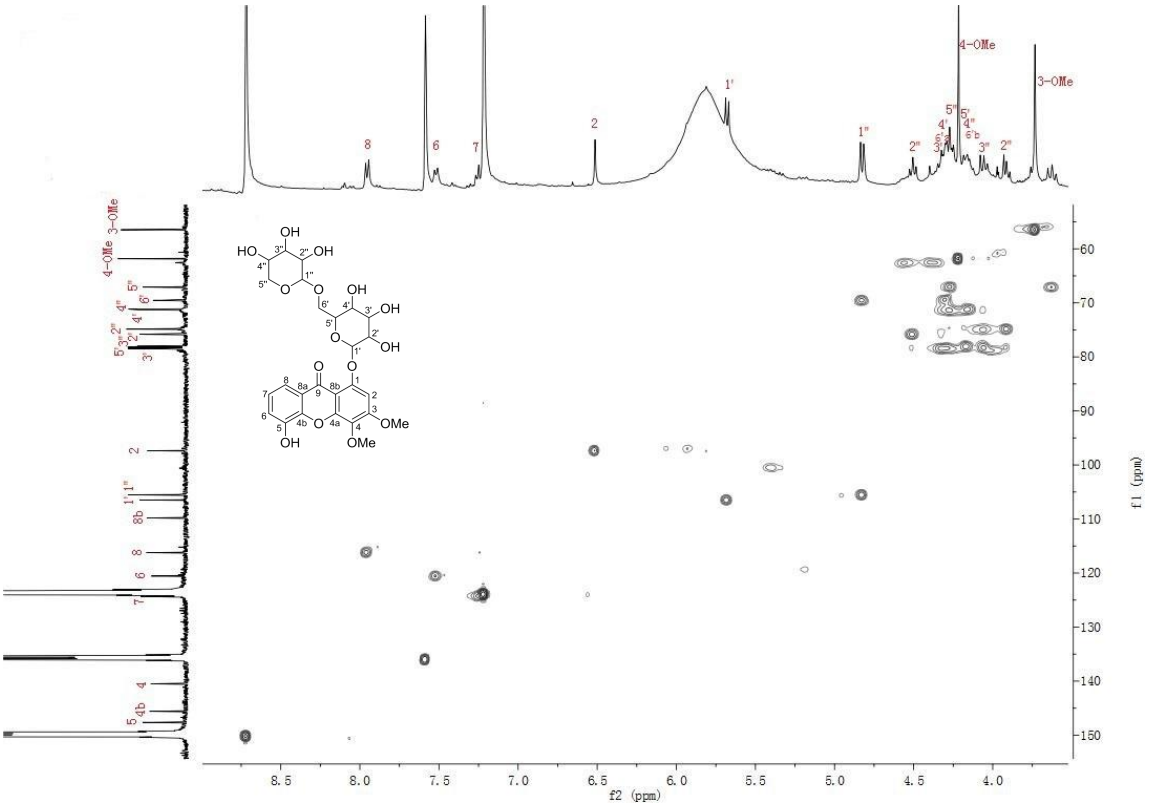


Figure S12. HSQC spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone recorded in C_5D_5N at 500 MHz

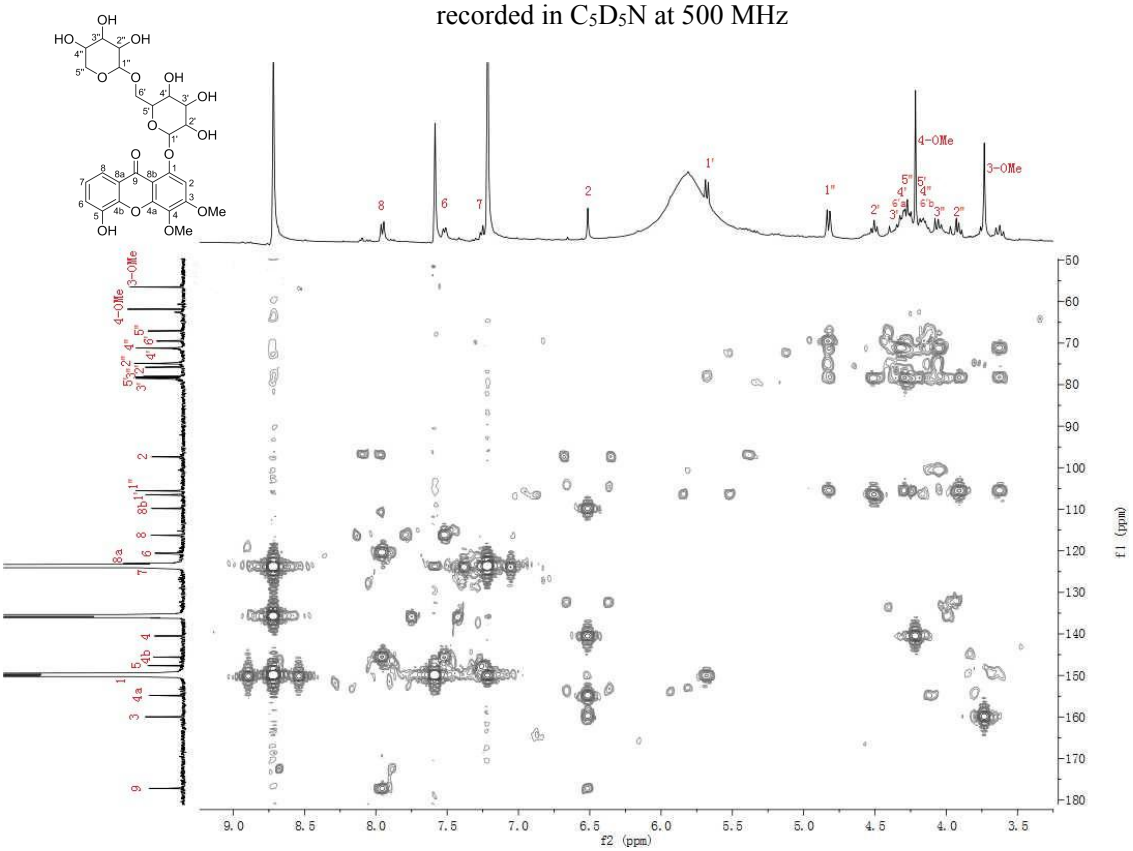


Figure S13. HMBC spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone recorded in C_5D_5N at 500 MHz

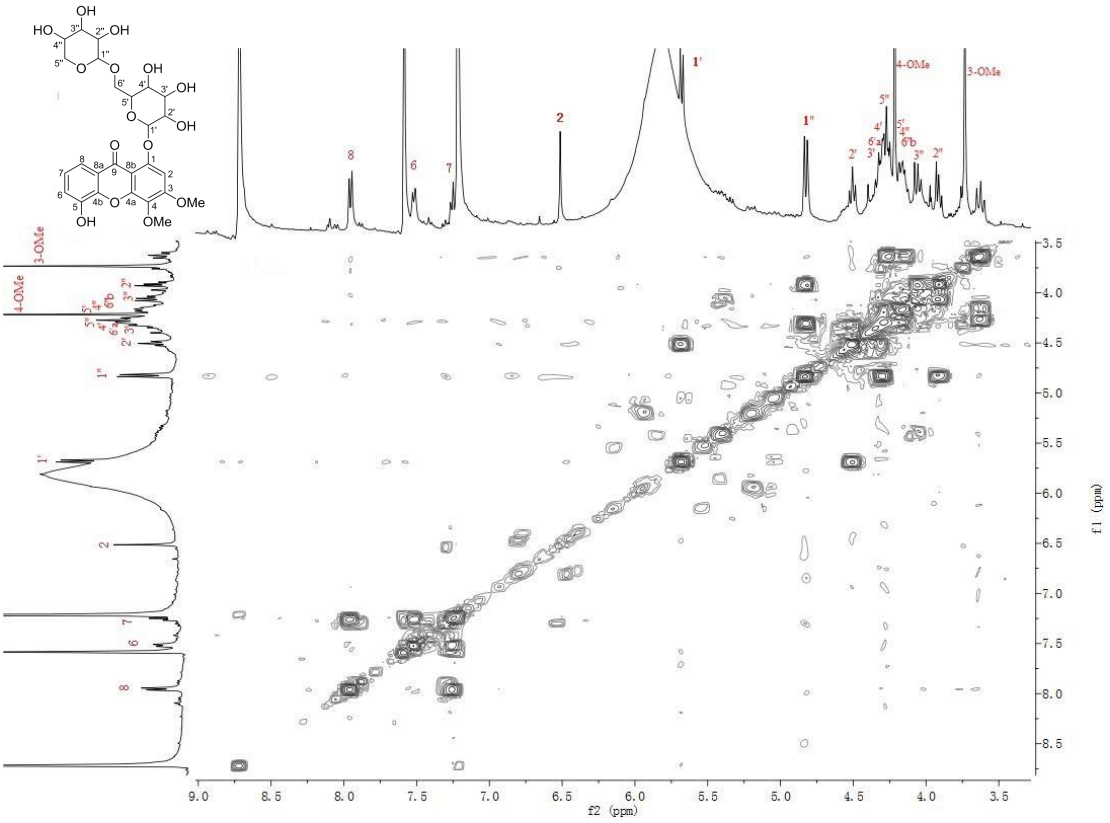


Figure S14. COSY spectrum of 5-hydroxy-3,4-dimethoxy-1-*O*-primeverosyloxyxanthone recorded in C_5D_5N at 500 MHz

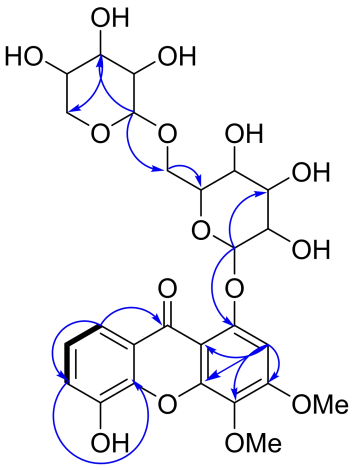


Figure S15. Key HMBC ( ) and COSY ( ) correlations of compound **2**.

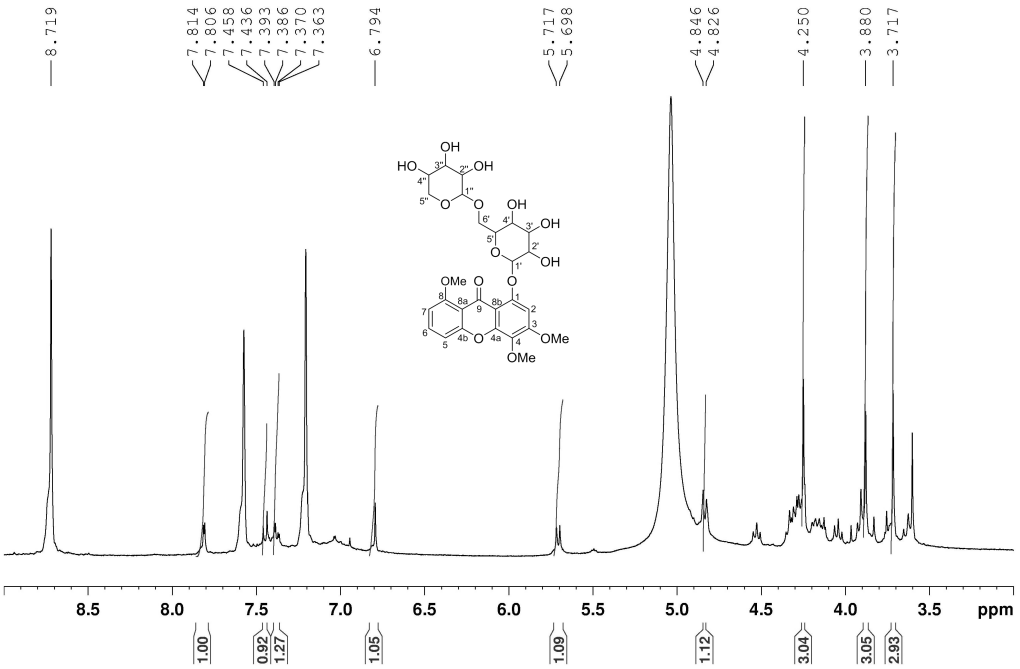


Figure S16. ^{1}H NMR spectrum of compound **3** recorded in C_5D_5N at 500 MHz

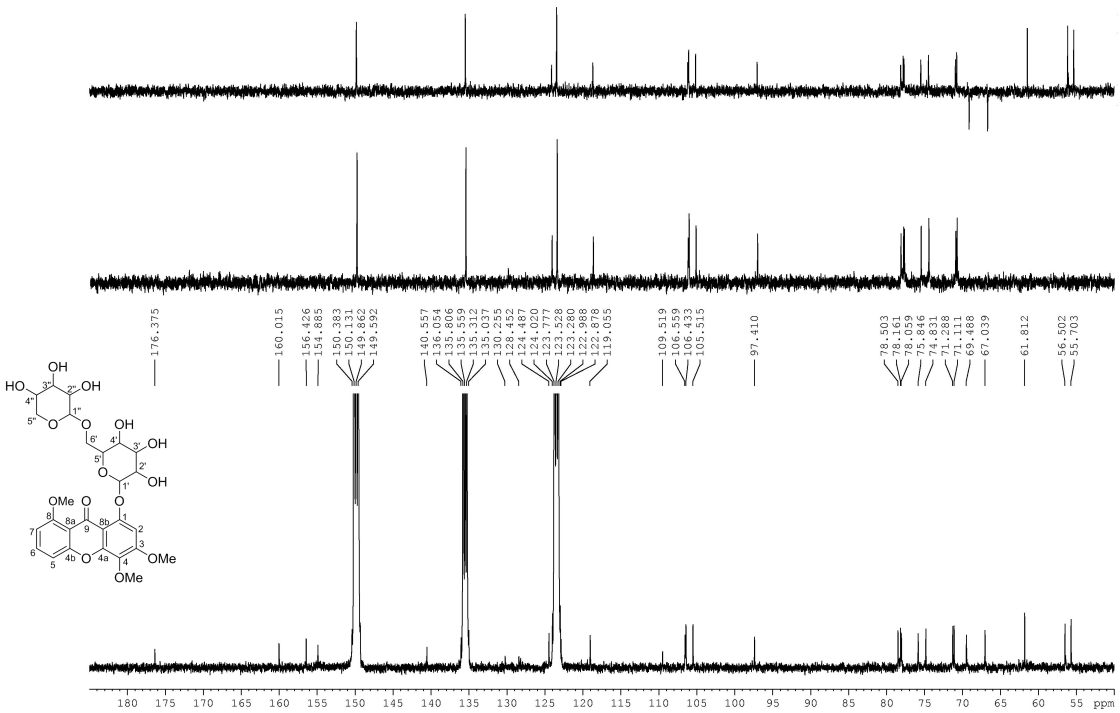


Figure S17. ^{13}C NMR spectrum of compound **3** recorded in C_5D_5N at 125 MHz

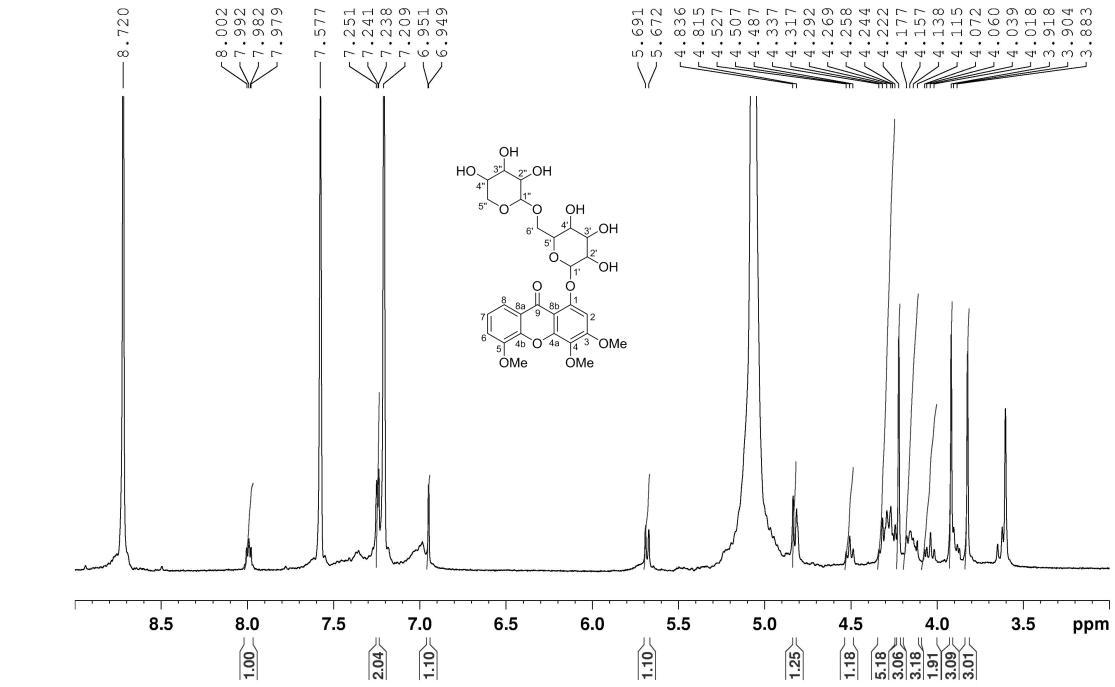


Figure S18. ^{1}H NMR spectrum of compound **4** recorded in C_5D_5N at 500 MHz

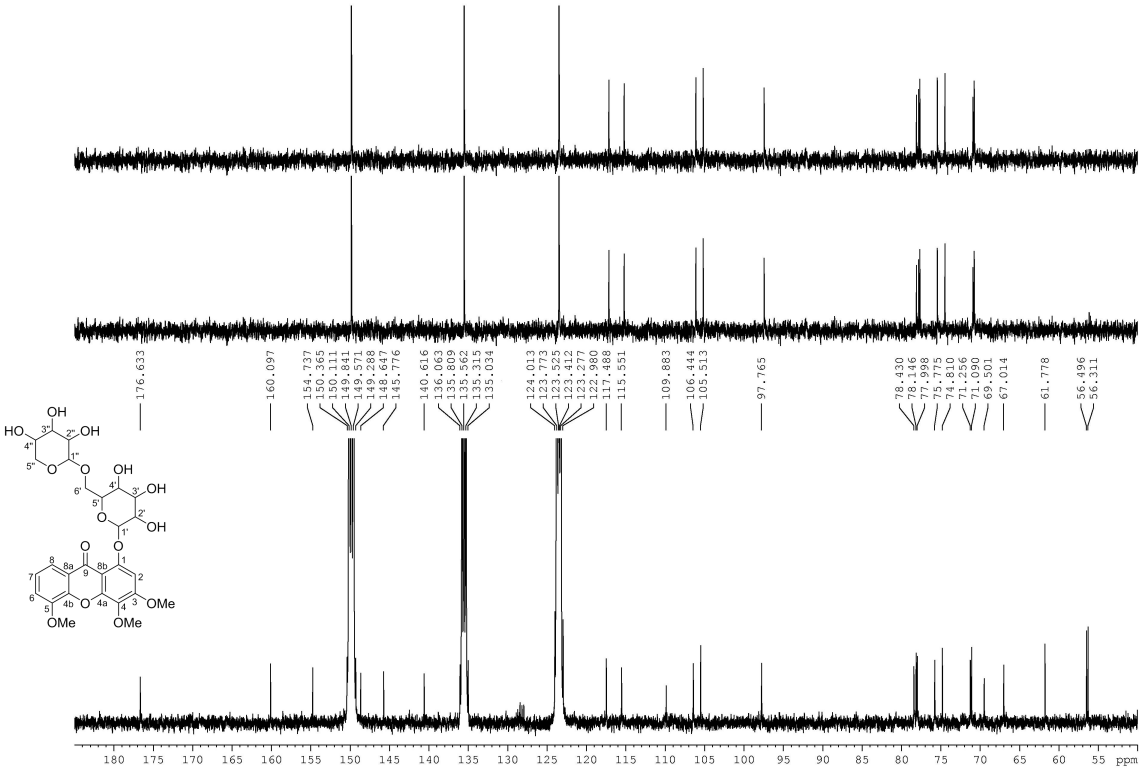


Figure S19. ^{13}C NMR spectrum of compound **4** recorded in C_5D_5N at 125 MHz

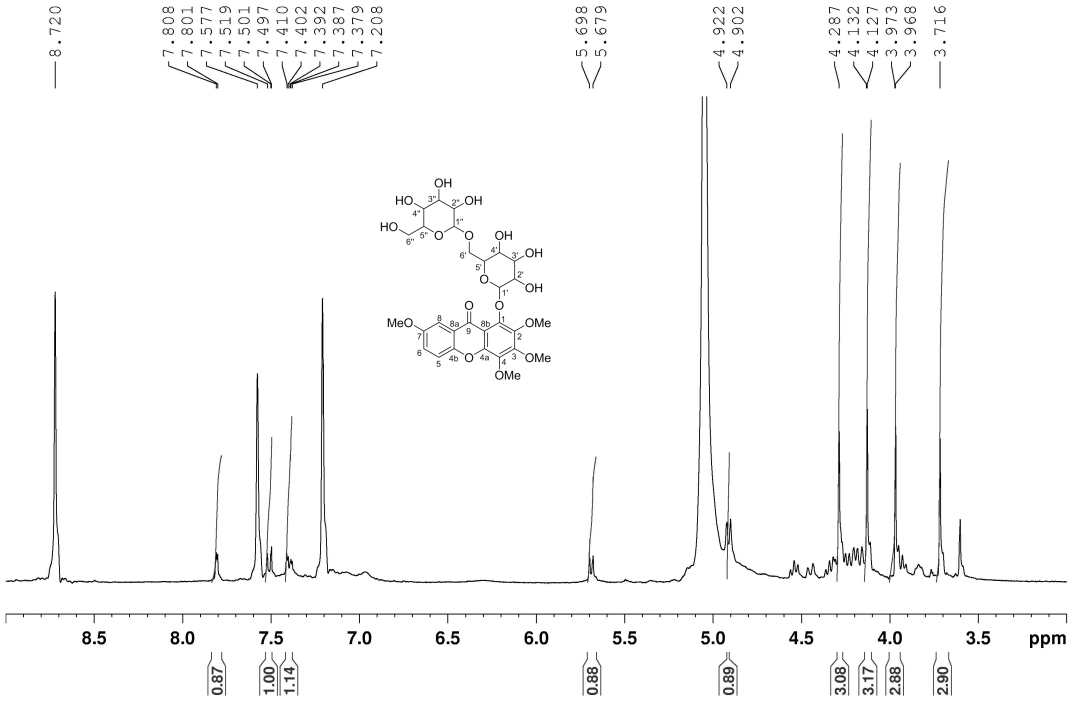


Figure S20. ^{1}H NMR spectrum of compound **5** recorded in C_5D_5N at 500 MHz

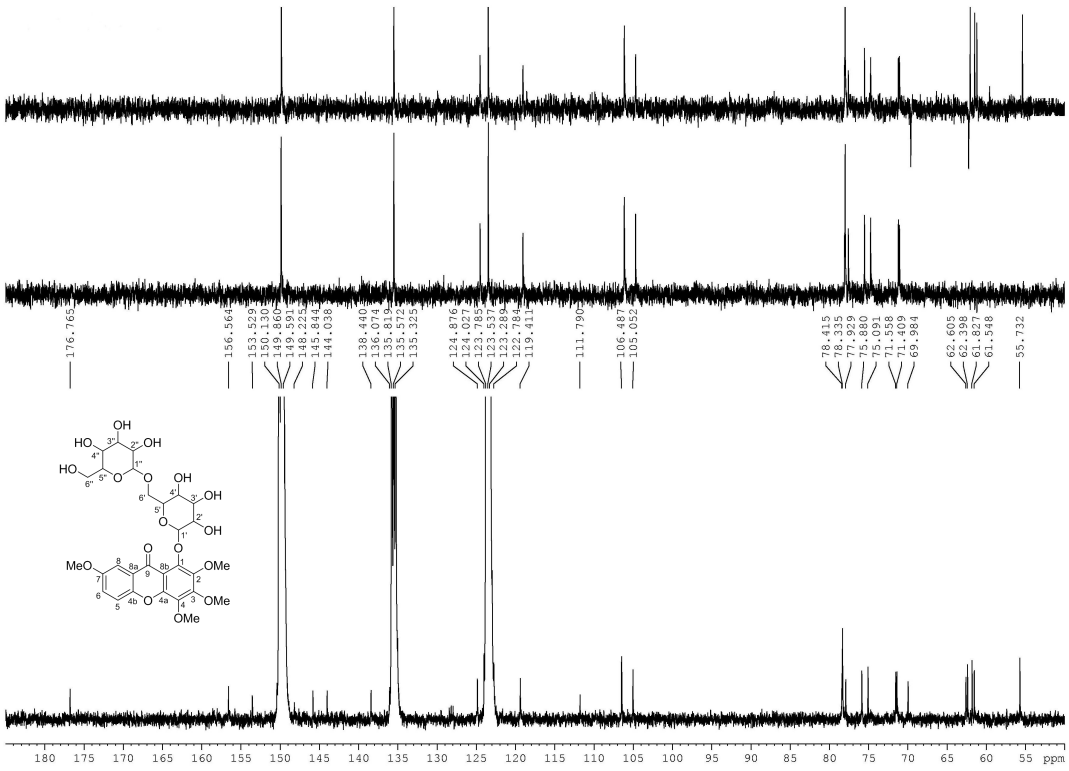


Figure S21. ^{13}C NMR spectrum of compound **5** recorded in C_5D_5N at 125 MHz

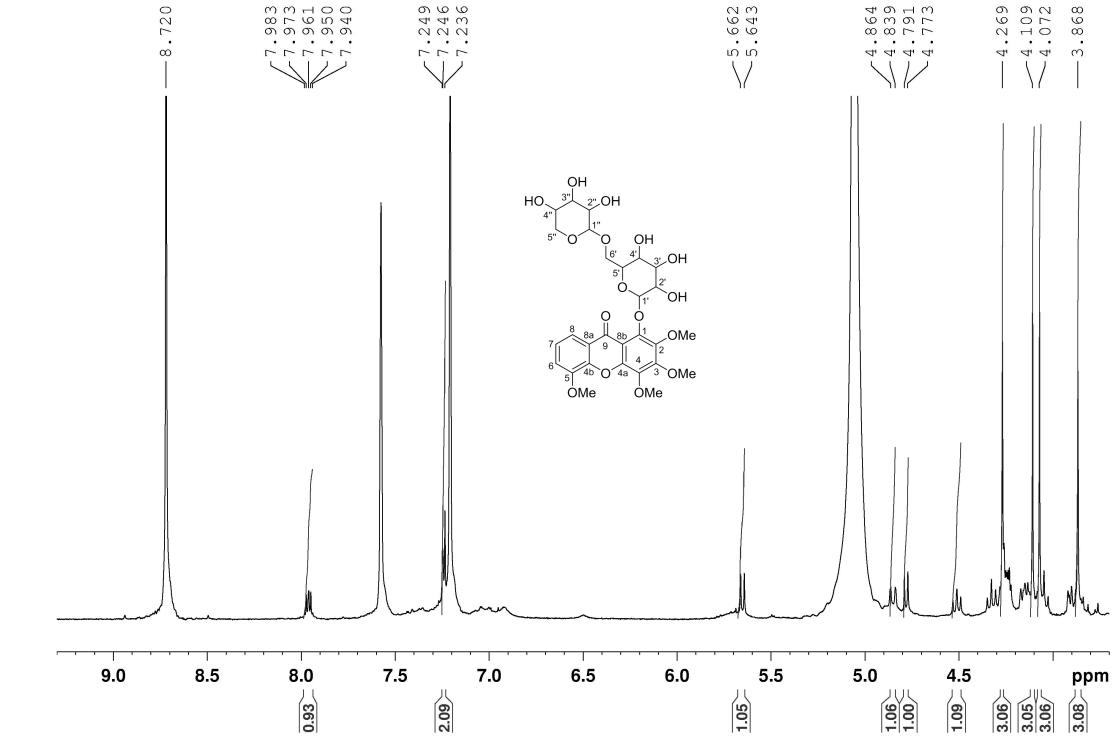


Figure S22. ^{1}H NMR spectrum of compound **6** recorded in C_5D_5N at 500 MHz

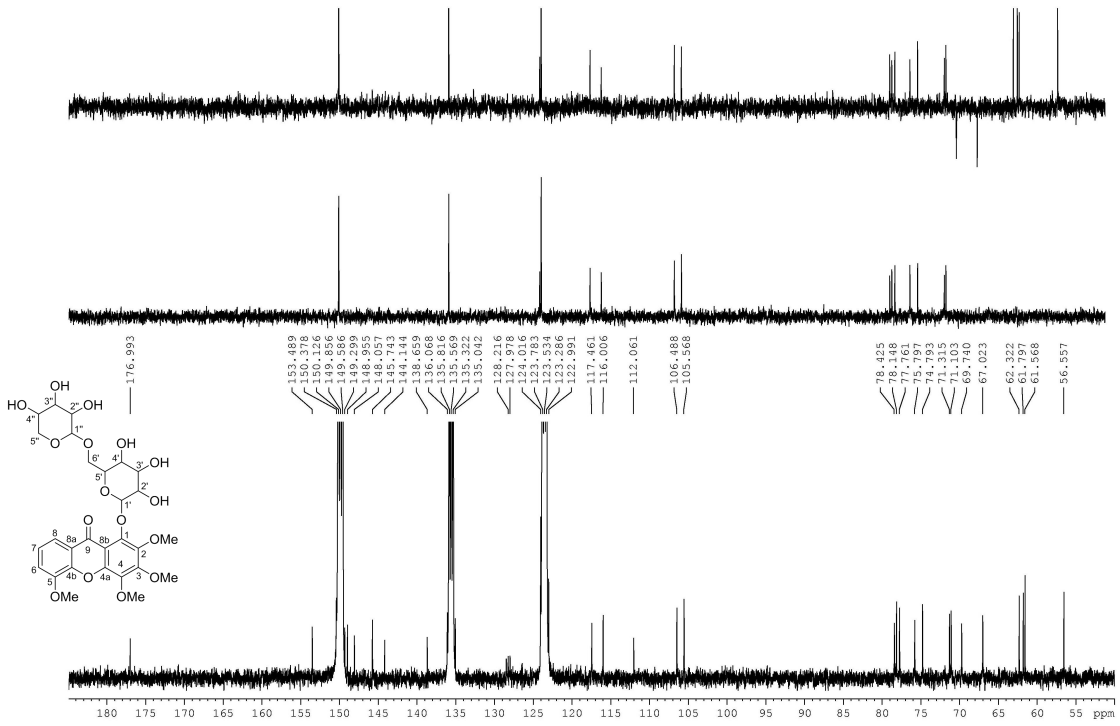


Figure S23. ^{13}C NMR spectrum of compound **6** recorded in C_5D_5N at 125 MHz

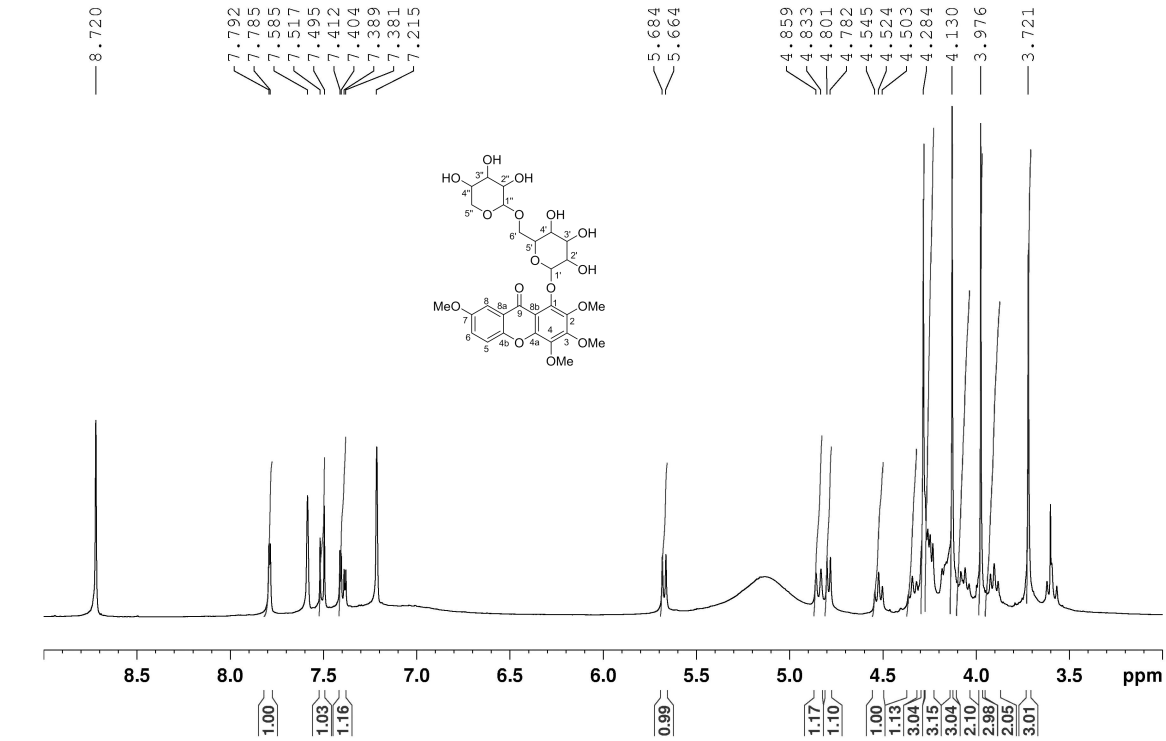


Figure S24. ^{1}H NMR spectrum of compound **7** recorded in C_5D_5N at 500 MHz

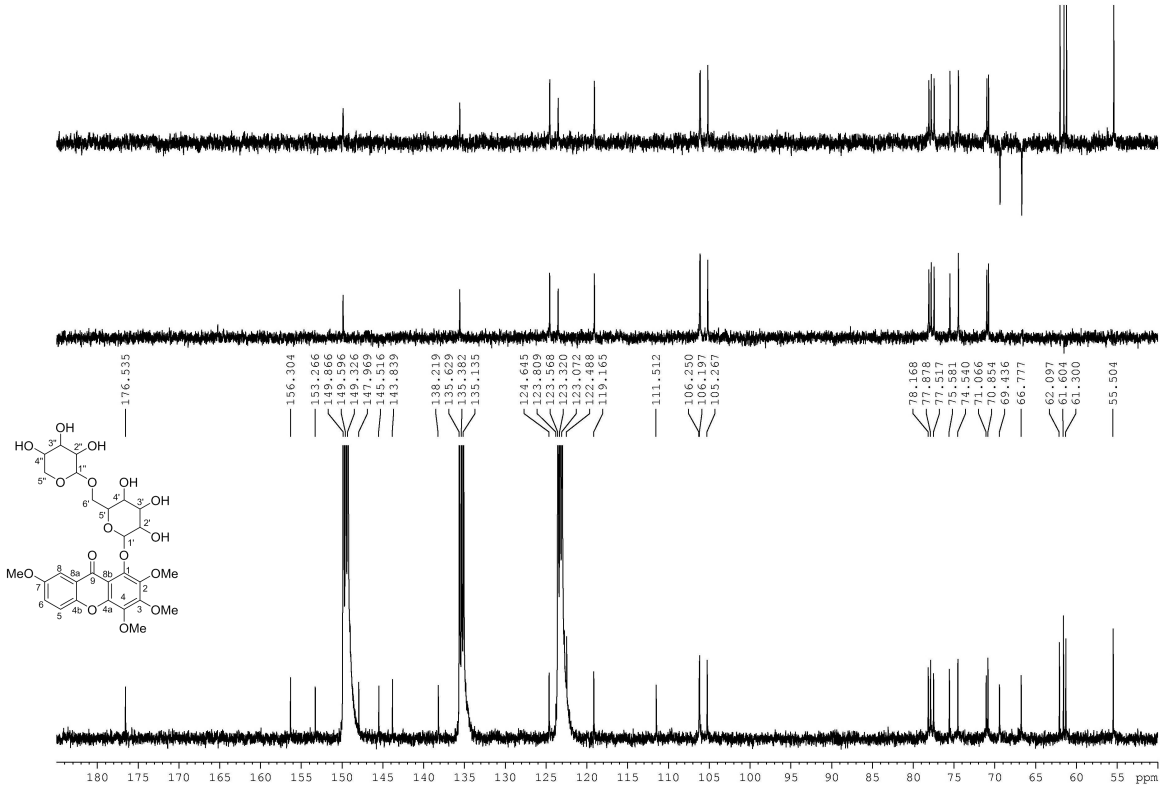


Figure S25. ^{13}C NMR spectrum of compound **7** recorded in C_5D_5N at 125 MHz

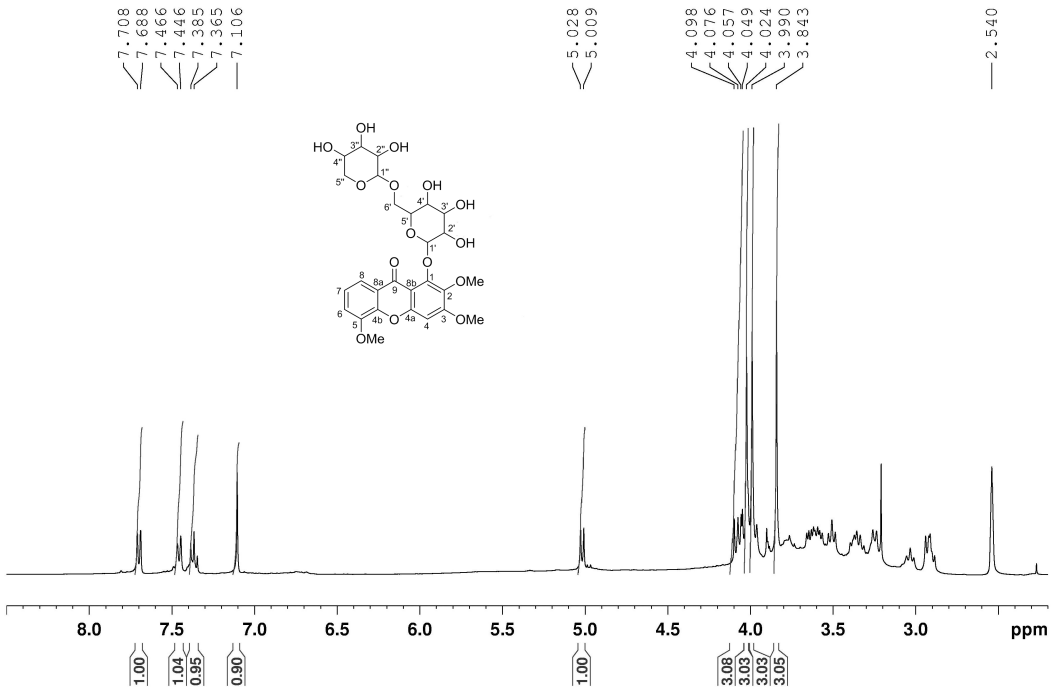


Figure S26. ^{1}H NMR spectrum of compound **8** recorded in DMSO and C_5D_5N at 500 MHz

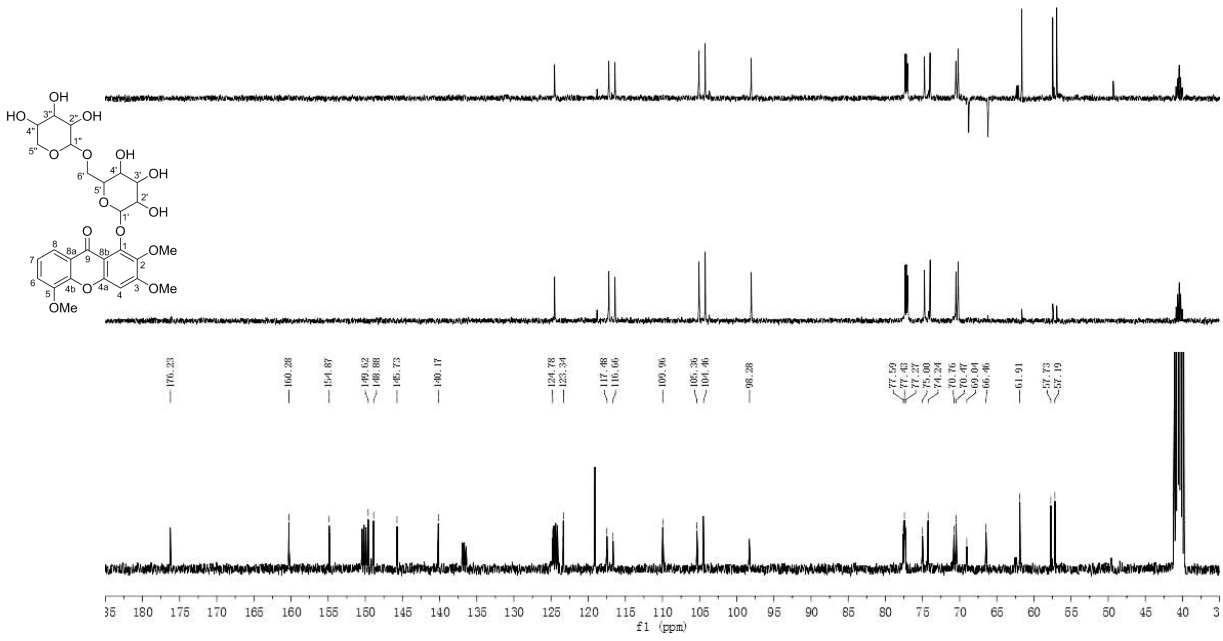


Figure S27. ^{13}C NMR spectrum of compound **8** recorded in DMSO and C_5D_5N at 125 MHz

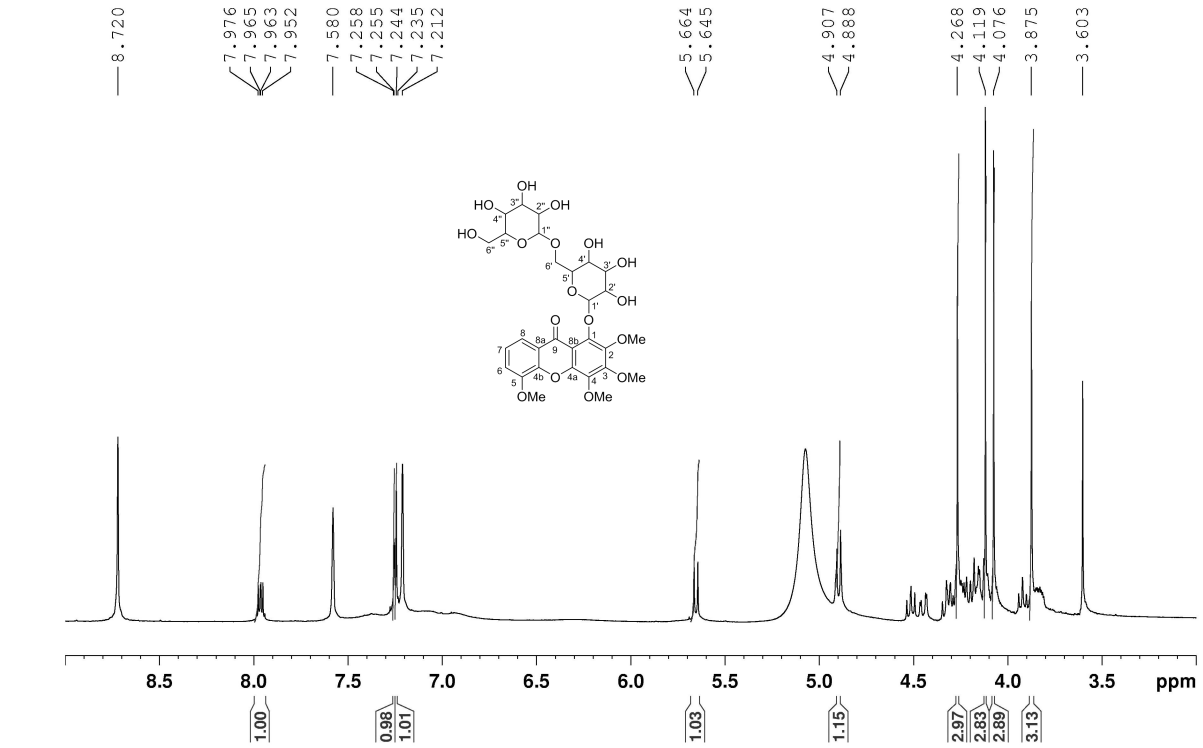


Figure S28. ^{1}H NMR spectrum of compound **9** recorded in C_5D_5N at 500 MHz

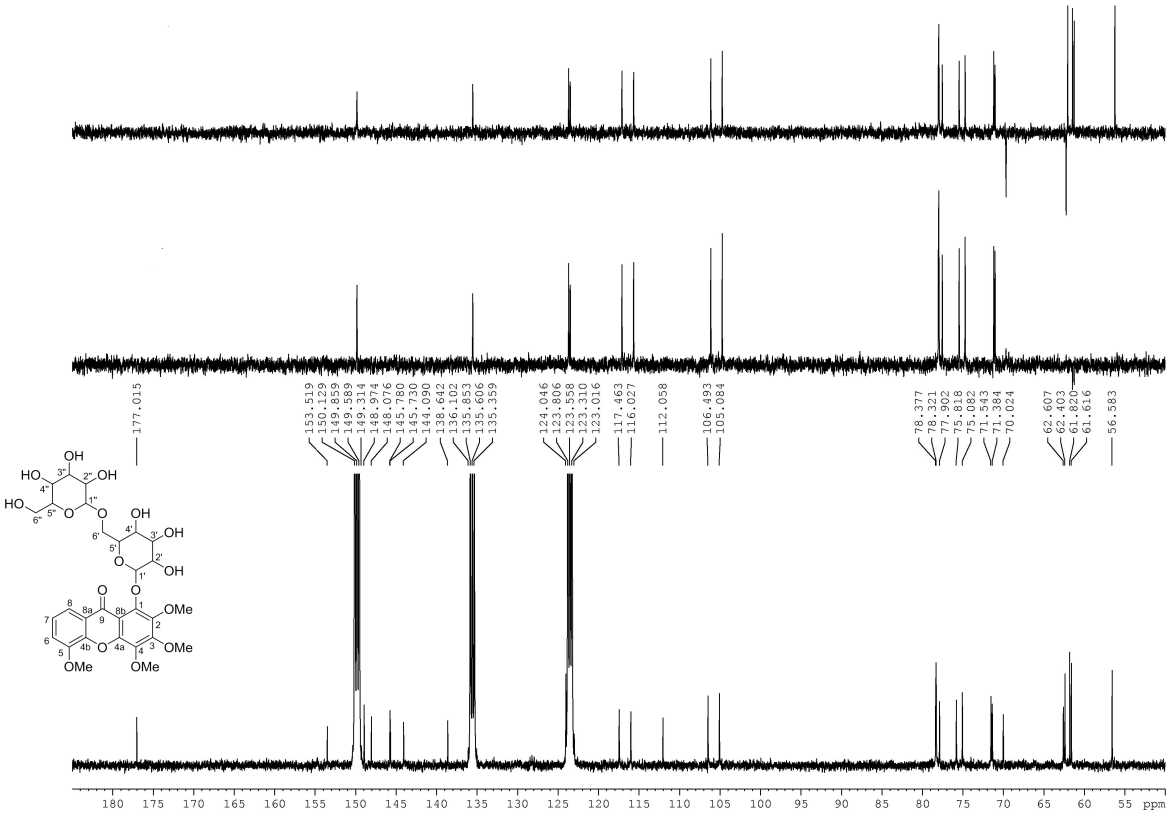


Figure S29. ^{13}C NMR spectrum of compound **9** recorded in C_5D_5N at 125 MHz