SUPPLEMENTARY MATERIAL

A new phenylpropanoid glucoside and a chain compound from the roots of *Allium tuberosum*

Yun-Shan Fang ^{a, b, 1}, Shi-Xi Liu ^{b, 1}, Ying-Cong Ma ^b, Jian-Wei Dong ^b,
Le Cai ^{b,*}, Zhong-Tao Ding ^b

^a*School of Chemical Science and Technology, Kunming University, Kunming 650214, China*

^b*School of Chemical Science and Technology, Yunnan University, Kunming 650091, China*

caile@ynu.edu.cn

Abstract: A new phenylpropanoid glucoside tuberosinine D (**1**) and a chain compound (Z)-11*R*,12*S*,13*S*-trihydroxy-9-octadecenoate (**2**) were isolated from the roots of *Allium tuberosum*. The absolute configuration of **1** was established by comparing of experimental and calculated electronic circular dichroism (ECD). The absolute configuration of **2** was determined by using the modified Mosher's method for the first time.

Keywords: *Allium tuberosum*; tuberosinine D; (Z)-11*R*,12*S*,13*S*-trihydroxy-9-octadecenoate; absolute configuration; the modified Mosher's method.

Figure S1: The key ^1H - ^1H COSY (—), HMBC (—) and ROESY (---) correlations of **1**.

Figure S2 NOE correlations (---) and *threo* configuration of **1**.

Figure S3: Calculated and experimental ECD spectra of **1**.

Figure S4 The key ^1H - ^1H COSY (—) and HMBC (↷) correlations of **2**.

Figure S5 The EIMS analysis of **2**.

Figure S6 NOE correlations (↷) and configuration analysis of **2**: (A) 11,12-*erythro* configuration; (B) 12,13-*erythro* configuration

Figure S7 $\Delta\delta_{S-R}$ of ^1H NMR for *S*- and *R*-MTPA esters of **2**.

Figure S8. ^1H NMR (500 MHz, CD_3OD) spectrum of compound **1**.

Figure S9. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **1**.

Figure S10. ^1H - ^1H COSY spectrum of compound **1**.

Figure S11. HSQC spectrum of compound **1**.

Figure S12. HMBC spectrum of compound **1**.

Figure S13. ROESY spectrum of compound **1**.

Figure S14. HRESIMS (+) spectrum of compound **1**

Figure S15. ¹H NMR (600 MHz, CD₃OD) spectrum of compound **2**.

Figure S16. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **2**.

Figure S17. ^1H - ^1H COSY spectrum of compound **2**.

Figure S18. HSQC spectrum of compound **2**.

Figure S19. HMBC spectrum of compound **2**.

Figure S20. ROESY spectrum of compound **2**.

User Spectra

Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
185.1018	2	22105.54		
205.6151	2	14176.7		
353.2298	1	138782.56	C18 H34 O5	(M+Na)+
354.233	1	28688.52	C18 H34 O5	(M+Na)+
369.2003	1	45937.58		
683.4698	1	29491.58		
684.4728	1	11138.21		
699.4353	1	16455.28		

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C18 H34 O5	330.2406	353.2298	353.2298	0.1	0.3	2.0000

Figure S21. HRESIMS (+) spectrum of compound **2**.

Figure S22. EIMS (+) spectrum of compound **2**.

Figure S23. ^1H NMR (400 MHz, CD_3OD) spectrum of compound **11,13-di-(R)-MTPA-2**.

Figure S24. ^1H - ^1H COSY spectrum of compound 11,13-di-(*R*)-MTPA-2.

Figure S25. ESIMS (+) spectrum of compound 11,13-di-(*R*)-MTPA-2.

Figure S28. ESIMS (+) spectrum of compound 11-(*S*)-MTPA-2.