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

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

\textsuperscript{a}School of Chemical Science and Technology, Kunming University, Kunming 650214, China
\textsuperscript{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)-11R,12S,13S-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)-11R,12S,13S-trihydroxy-9-octadecenoate; absolute configuration; the modified Mosher’s method.
Figure S1: The key $^1$H-$^1$H 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 $^1$H-$^1$H 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 $^1$H NMR for S- and R-MTPA esters of 2.
Figure S8. $^1$H NMR (500 MHz, CD$_3$OD) spectrum of compound 1.

Figure S9. $^{13}$C NMR (125 MHz, CD$_3$OD) spectrum of compound 1.
Figure S10. $^1$H-$^1$H 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, CD$_3$OD) spectrum of compound 2.
Figure S16. $^{13}$C NMR (150 MHz, CD$_3$OD) spectrum of compound 2.

Figure S17. $^1$H-$^1$H 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.

Figure S21. HRESIMS (+) spectrum of compound 2.
Figure S22. EIMS (+) spectrum of compound 2.

Figure S23. $^1$H NMR (400 MHz, CD$_3$OD) spectrum of compound 11,13-di-(R)-MTPA-2.
Figure S24. $^1$H-$^1$H COSY spectrum of compound 11,13-di-(R)-MTPA-2.

Figure S25. ESIMS (+) spectrum of compound 11,13-di-(R)-MTPA-2.
Figure S26. $^1$H NMR (400 MHz, CD$_3$OD) spectrum of compound 11-(S)-MTPA-2

Figure S27. $^1$H-$^1$H COSY spectrum of compound 11-(S)-MTPA-2.
Figure S28. ESIMS (+) spectrum of compound 11-(S)-MTPA-2.