Electronic Supplementary Information

Two lathyrane diterpenoid stereoisomers containing an unusual *trans-gem*-dimethylcyclopropane from the seeds of *Euphorbia lathyris*

Authors

Linwei Li^{1#}, Jianan Huang^{1#}, Hui Lyu^{1,2}, Fuqin Guan¹, Pirui Li¹, Mei Tian¹, Shu Xu¹, Xingzeng Zhao¹, Fei Liu^{1*}, Christian Paetz², Xu Feng¹, Yu Chen^{1*}

Affiliations

1 Jiangsu Key Laboratory for the Research and Utilization of Plant Resources, The Jiangsu Provincial Platform for Conservation and Utilization of Agricultural Germplasm, Institute of Botany, Jiangsu Province and Chinese Academy of Sciences, Nanjing, China

2 Max-Planck Institute for Chemical Ecology, Jena, Germany

[#]These two authors contributed equally to this work.

* Correspondence: liufeiseu@163.com; Tel.: +86-25-84347041,

yuchen1007@hotmail.com; Tel.: +86-25-84347116.

Contents

No.	Content	Page
1	Figure S1. HPLC chromatogram of 1 (UV 280 nm).	S4
2	Figure S2. UV spectrum of 1.	S4
3	Figure S3. HR-ESI-MS spectrum of 1.	S 5
4	Figure S4. ¹ H-NMR spectrum (500 MHz, CDCl ₃) of compound 1.	S5
5	Figure S5. ¹³ C-NMR spectrum (125 MHz, CDCl ₃) of compound 1.	S6
6	Figure S6. DEPT-135 spectrum (125 MHz, CDCl ₃) of compound 1.	S 6
7	Figure S7. DEPT-90 spectrum (125 MHz, CDCl ₃) of compound 1.	S 7
8	Figure S8. HSQC spectrum (500 MHz, CDCl ₃) of compound 1.	S7
9	Figure S9. HMBC spectrum (500 MHz, CDCl ₃) of compound 1.	S 8
10	Figure S10. ¹ H - ¹ H COSY spectrum (500 MHz, CDCl ₃) of compound 1 .	S8
11	Figure S11. NOESY spectrum (500 MHz, CDCl ₃) of compound 1.	S9
12	Figure S12. HPLC chromatogram of 2 (UV 280 nm).	S10
13	Figure S13. UV spectrum of 2.	S10
14	Figure S14. HR-ESI-MS spectrum of 2.	S11
15	Figure S15. ¹ H-NMR spectrum (500 MHz, CDCl ₃) of compound 2.	S11
16	Figure S16. ¹³ C-NMR spectrum (125 MHz, CDCl ₃) of compound 2.	S12
17	Figure S17. DEPT-135 spectrum (125 MHz, CDCl ₃) of compound 2.	S12
18	Figure S18. DEPT-90 spectrum (125 MHz, CDCl ₃) of compound 2.	S13
19	Figure S19. HSQC spectrum (500 MHz, CDCl ₃) of compound 2.	S13
20	Figure S20. HMBC spectrum (500 MHz, CDCl ₃) of compound 2.	S14

21	Figure S21. ¹ H - ¹ H COSY spectrum (500 MHz, CDCl ₃) of compound 2 .	S14
22	Figure S22. NOESY spectrum (500 MHz, CDCl ₃) of compound 2.	S15
23	Figure S23. Relative stable conformers of a pair of enantiomers for compound 2 with their Boltzmann weighting factor.	S15
24	Figure S24. HPLC chromatogram of 3 (UV 280 nm).	S16
25	Figure S25. UV spectrum of compound 3.	S16
26	Figure S26. HR-ESI-MS spectrum of compound 3.	S17
27	Figure S27. ¹ H-NMR spectrum (300 MHz, CDCl ₃) of compound 3 .	S17
28	Figure S28. ¹³ C-NMR spectrum (75 MHz, CDCl ₃) of compound 3.	S18



Chemical structure of 1



Figure S1. HPLC chromatogram of 1 (UV 280 nm).



Figure S2. UV spectrum of compound 1.



Figure S3. HR-ESI-MS spectrum of 1.



Figure S4. ¹H-NMR spectrum (500 MHz, CDCl₃) of compound 1.



Figure S5. ¹³C-NMR spectrum (125 MHz, CDCl₃) of compound 1.



Figure S6. DEPT-135 spectrum (125 MHz, CDCl₃) of compound 1.



Figure S7. DEPT-90 spectrum (125 MHz, CDCl₃) of compound 1.



Figure S8. HSQC spectrum (500 MHz, CDCl₃) of compound 1.



Figure S9. HMBC spectrum (500 MHz, CDCl₃) of compound 1.



Figure S10. ¹H -¹H COSY spectrum (500 MHz, CDCl₃) of compound 1.



Figure S11. NOESY spectrum (500 MHz, CDCl₃) of compound 1.







Figure S12. HPLC chromatogram of 2 (UV 280 nm).



Figure S13. UV spectrum of compound 2.



Figure S15. ¹H-NMR spectrum (500 MHz, CDCl₃) of compound 2.



Figure S16. ¹³C-NMR spectrum (125 MHz, CDCl₃) of compound 2.



Figure S17. DEPT-135 spectrum (125 MHz, CDCl₃) of compound 2.



Figure S18. DEPT-90 spectrum (125 MHz, CDCl₃) of compound 2.



Figure S19. HSQC spectrum (500 MHz, CDCl₃) of compound 2.



Figure S20. HMBC spectrum (500 MHz, CDCl₃) of compound 2.



Figure S21. ¹H -¹H COSY spectrum (500 MHz, CDCl₃) of compound 2.



Figure S22. NOESY spectrum (500 MHz, CDCl₃) of compound 2.



Figure S23. Relative stable conformers of a pair of enantiomers for compound 2 with their Boltzmann weighting factor.



Chemical structure of **3**



Figure S24. HPLC chromatogram of 3 (UV 280 nm).



Figure S25. UV spectrum of compound 3.



Figure S26. HR-ESI-MS spectrum of compound 3.



Figure S27. ¹H-NMR spectrum (300 MHz, CDCl₃) of compound 3.



Figure S28. ¹³C-NMR spectrum (75 MHz, CDCl₃) of compound 3.