Electronic Supplementary Information

Enantiomeric Neolignans and Sesquineolignans from Jatropha integerrima and Their Absolute Configurations

Jian-Yong Zhu,‡a Bao Cheng,‡b Yin-Jia Zheng,‡c Zhen Dong,a Shu-Ling Lin,a Gui-Hua Tang,a Qiong Gu,a and Sheng Yin*a

‡ These authors have contributed equally to this work.

+a School of Pharmaceutical Sciences, Sun Yat-sen University, Guangzhou, Guangdong 510006, P. R. China
b Institute of Chinese Medical Sciences, Guangdong Pharmaceutical University, Guangzhou, Guangdong 510006, P. R. China
cSchool of Health Management, Guangzhou Medical University, Guangzhou, Guangdong 510182, P. R. China

E-mail: yinsh2@mail.sysu.edu.cn; Fax: +86-20-39943090; Tel: +86-20-39943090.
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YJIZ-9b-20140323
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S4. HSQC spectrum of 1 in CD$_3$OD
S5. HMBC spectrum of 1 in CD$_3$OD
S6. NOESY spectrum of 1 in CD$_3$OD
S7. HRESIMS spectrum of 1

YJIZ-9A-A #364  RT: 2.91  AV: 1  NL: 3.03E6
T: FTMS + p ESI Full ms [300.00-900.00]
S8. IR (KBr disc) spectrum of 1

[Graph showing IR spectrum with wavenumbers and %T values marked]

名称 说明

Administrator 161 样品 161 用户 Administrator 日期 星期二，十月 28 2014
The CD spectra of (±)-1 in MeCN
The Rh$_2$(OCOF$_3$)$_4$ induced CD spectra of (±)-1 in CH$_2$Cl$_2$
S11. $^1$H NMR spectrum of 2 in CD$_3$OD

![NMR Spectrum Image]
S12. $^{13}$C NMR spectrum of 2 in CD$_3$OD

YJ1Z-91500-10-11-12

$^f_1$ (ppm)
S13. HRESIMS spectrum of 2

YJIZ-9A #202  RT: 1.61  AV: 1  NL: 2.38E6
T: FTMS + p ESI Full ms [200.00-1000.00]
S14. IR (KBr disc) spectrum of 2

![IR spectrum graph]

- 2955, 2960, 77 cm⁻¹
- 1735, 45 cm⁻¹
- 1735, 64 cm⁻¹
- 1594, 6 cm⁻¹
- 1376, 28 cm⁻¹
- 1463, 72 cm⁻¹
- 1374, 90 cm⁻¹
- 1125, 21 cm⁻¹
- 1025, 11 cm⁻¹
- 759, 88 cm⁻¹
- 669, 12 cm⁻¹
- 544, 32 cm⁻¹
- 528, 74 cm⁻¹
- 511, 28 cm⁻¹

% T

4000  3500  3000  2500  2000  1500  1000  500

4000  3500  3000  2500  2000  1500  1000  500

7500  8000  8500  9000  9500  10000  10500  11000

名称  说明

Administrator 162 样品 162 用户 Administrator 日期 星期二，十月 28 2014
S15. The CD spectra of (±)-2 in MeCN
The Rh$_2$(OCOCF$_3$)$_4$ induced CD spectrum of (±)-2 in CH$_2$Cl$_2$
S17. $^1$H NMR spectrum of 3 in CDCl$_3$
S18. $^{13}$C NMR spectrum of 3 in CDCl$_3$
S19. $^1$H-$^1$H COSY spectrum of 3 in CDCl$_3$
S20. HSQC spectrum of 3 in CDCl$_3$
S21. HMBC spectrum of 3 in CDCl$_3$
S22. NOESY spectrum of 3 in CDCl₃
S23. HRESIMS spectrum of 3

YJZ-12 #174  RT: 1.39  AV: 1  NL: 2.21E7
T: FTMS + p ESI Full ms [200.00-1000.00]
S24. IR (KBr disc) spectrum of 3
The CD spectra of (±)-3 in MeCN
S26. $^1$H NMR spectrum of 4 in CDCl$_3$
S27. $^{13}$C NMR spectrum of 4 in CDCl$_3$

YJIZ-38-20140509

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S28. $^1$H-$^1$H COSY spectrum of 4 in CDCl$_3$
S29. HSQC spectrum of 4 in CDCl$_3$
S30. HMBC spectrum of 4 in CDCl₃
S31. NOESY spectrum of 4 in CDCl₃
S32. HRESIMS spectrum of 4

yjiz-38 #187  RT: 1.50  AV: 1  NL: 2.48E6
T: FTMS + p ESI Full ms [50.00-1500.00]
S33. IR (KBr disc) spectrum of 4
The CD spectra of (±)-4 in MeCN
S35. $^1$H NMR spectrum of 5 in CDCl$_3$
S36. $^{13}$C NMR spectrum of 5 in CDCl$_3$
S37. HSQC spectrum of 5 in CDCl₃
S38. HMBC spectrum of 5 in CDCl$_3$
HRESIMS spectrum of 5

yjz-22b #189   RT: 1.52  AV: 1  NL: 6.72E5
T: FTMS + p ESI Full ms [50.00-1500.00]
S40. IR (KBr disc) spectrum of 5
S41. The CD spectra of 5a and 5b in MeCN
S42. $^1$H NMR spectrum of 6 in CDCl$_3$
$^{13}$C NMR spectrum of 6 in CDCl$_3$
S44. $^1$H NMR spectrum of 7 in CDCl$_3$
S45. $^{13}$C NMR spectrum of 7 in CDCl$_3$
S46. $^1$H NMR spectrum of 8 in CDCl$_3$
S47. $^{13}$C NMR spectrum of 8 in CDCl$_3$
Key NOE correlations (---) of 1 and 3.
S49. The effects of all compounds on LPS-induced BV-2 microglial cell cytotoxicity. Cells were treated with all compounds at 80 µM for 24 h. MTT assay was performed to detect cell viability. The results are represented as means ± SD based on three independent experiments.