Supporting Information

Eurotiumins A-E, Five New Alkaloids from the Marine-Derived

Fungus Eurotium sp. SCSIO F452

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Computational Details



Figure S1. Structures applied for theoretical calculations of 1, and 2.

Table S1. Relative thermal energies (ΔE), relative free energies (ΔG), and equilibrium populations (P) of low-energy conformers of structures **1** and **2** in MeOH.

conformer	ΔE (kcal/mol) ^{<i>a</i>}	ΔG (kcal/mol) ^{<i>a</i>}	$P(\%)^b$
Compound 1			
1a	0.0	0.0	69.7
1b	1.22	1.29	8.0
1c	1.33	1.31	7.6
1d	1.50	1.33	7.3
1e	1.62	1.56	5.0
1f ^{<i>c</i>}	1.82	1.99	2.4
Compound 2			
2a	0.0	0.0	38.3
2b	0.35	0.31	22.8
2c	0.63	0.51	16.3
2d	0.58	0.70	11.7
2e	0.66	0.85	9.2
2f ^c	1.87	1.82	1.8

^{*a*} At the M06-2X/def2-TZVP/ IEFPCM level of theory.

^{*b*} From ΔG values at 298.15 K.

^c Conformer not applied to ECD/TDDFT calculations.













1d







Figure S2. Conformations of low-energy conformers of 1, and 2.



Figure S3. The ¹H NMR spectrum of eurotiumin A (1) in CD₃COCD₃.



Figure S4. The ¹³C NMR spectrum of eurotiumin A (1) in CD₃COCD₃.

Figure S5. The HSQC spectrum of eurotiumin A (1) in CD₃COCD₃.





Figure S6. The HMBC spectrum of eurotiumin A (1) in CD₃COCD₃.





(mqq) fi



Figure S8. The NOESY spectrum of eurotiumin A (1) in CD₃COCD₃.

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Figure S10. The IR spectrum of eurotiumin A (1).





Figure S11. The UV spectrum of eurotiumin A (1).



Figure S12. The ¹H NMR spectrum of eurotiumin B (2) in CD₃COCD₃.



Figure S13. The ¹³C NMR spectrum of eurotiumin B (2) in CD₃COCD₃.







Figure S15. The HMBC spectrum of eurotiumin B (2) in CD₃COCD₃.



Figure S16. The ¹H–¹H COSY spectrum of eurotiumin B (2) in CD₃COCD₃.





(uidd) Li



Figure S18. The HRESIMS spectrum of eurotiumin B (2).



Figure S19. The IR spectrum of eurotiumin B (2).

Figure S20. The UV spectrum of eurotiumin B (2).



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Figure S21. The ¹H NMR spectrum of eurotiumin C (3) in DMSO-d₆.



Figure S22. The ¹³C NMR spectrum of eurotiumin C (3) in DMSO-d₆.

Figure S23. The HSQC spectrum of eurotiumin C (3) in DMSO-d₆.





Figure S24. The HMBC spectrum of eurotiumin C (3) in DMSO-d6.



Figure S25. The ¹H–¹H COSY spectrum of eurotiumin C (3) in DMSO-*d*₆.



Figure S26. The NOESY spectrum of eurotiumin C (3) in DMSO-d6.



Figure S27. The HRESIMS spectrum of eurotiumin C (3).

Figure S28. The IR spectrum of eurotiumin C (3).







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Figure S30. The ¹H NMR spectrum of eurotiumin D (4) in CD₃COCD₃.





Figure S31. The ¹³C NMR spectrum of eurotiumin D (4) in CD₃COCD₃.



Figure S32. The HSQC spectrum of eurotiumin D (4) in CD₃COCD₃.



Figure S33. The HMBC spectrum of eurotiumin D (4) in CD₃COCD₃.



Figure S34. The ¹H–¹H COSY spectrum of eurotiumin D (4) in CD₃COCD₃.





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Figure S36. The HRESIMS spectrum of eurotiumin D (4).



Figure S37. The IR spectrum of eurotiumin D (4).





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Figure S40. The ¹³C NMR spectrum of eurotiumin E (14) in CD₃COCD₃.







Figure S42. The HMBC spectrum of eurotiumin E (14) in CD₃COCD₃.



Figure S43. The ¹H–¹H COSY spectrum of eurotiumin E (14) in CD₃COCD₃.



Figure S44. The HRESIMS spectrum of eurotiumin E (14).

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2018-03-15 17:57:40 数据集: F452-46-1 - RawData 3.962 [测定属性] 波长范围 (nm.): 200.00 到 400.00 因长犯固(min.) 扫描速度: 采样间隔: 自动采样间隔: 扫描模式: 中速 0.2 启用 单个 [仪器属性] 3.000 【仪器属性】 仪器类型: 测定方式: 狭缝宽: 积分时间: 光源转换波长: 检测器单元: C/P 結舟. UV-2600 系列 吸收值 2.0 0.1 秒. 0.1 D. 323.0 nm 直接 标准 S/R 转换: 阶梯校正: OFF 2.000 Abs. [附件属性] 附件: 无 [数据处理参数] 阈值: 点: 内插: 平均: 0.0100000 5 。 停用 停用 1.000 [样品准备属性] 重量: 体积: 稀释: 光程长: 附加信息: 0.000 -0.179 200.00 250.00 300.00 350.00 400.00 nm. No. P/V 波长(nm) 吸收值 描述 ٢ 280.40 2.346 226.20 3.541 ۲ 207.60 3.773 1 О. N 14 页1/1

光谱峰值检测报告

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MS and NMR data of compounds 5-13

Compound 5: yellow solid, positive HRESIMS *m*/*z* 482.2775 [M + Na]⁺ (calcd for C₂₉H₃₇N₃NaO₂, 482.2778). ¹³C NMR (acetone-*d*₆, 175 MHz) , δ_C : 144.4 (C-2), 104.8 (C-3), 127.6 (C-3a), 110.9 (C-4), 133.4 (C-5), 125.4 (C-6), 126.4 (C-7), 134.6 (C-7a), 116.8 (C-8), 125.1 (C-9), 160.3 (C-10), 52.3 (C-12), 166.7 (C-13), 40.1 (C-15), 146.1 (C-16), 112.4 (C-17), 27.9 (C-18/19), 20.8 (C-20), 35.1 (C-21), 123.0 (C-22), 131.9 (C-23), 25.9 (C-24), 17.9 (C-25), 32.6 (C-26), 123.4 (C-27), 133.2 (C-28), 25.9 (C-29), 17.9 (C-30).

Compound **6**: yellow solid, positive ESIMS *m*/*z* 414.4 [M + Na]⁺. ¹³C NMR (acetone-*d*₆, 175 MHz), δ_C: 144.3 (C-2), 105.0 (C-3), 125.4 (C-3a), 117.7 (C-4), 121.2 (C-5), 123.2 (C-6), 126.8 (C-7), 134.9 (C-7a), 110.7 (C-8), 127.4 (C-9), 160.2 (C-10), 52.2 (C-12), 166.9 (C-13), 40.1 (C-15), 146.1 (C-16), 112.4 (C-17), 27.9 (C-18/19), 20.7 (C-20), 28.9 (C-21), 123.2 (C-22), 133.4 (C-23), 25.9 (C-24), 17.9 (C-25).

Compound 7: yellow solid, positive HRESIMS *m/z* 392.2344 [M + H]⁺ (calcd for C₂₄H₃₀N₃O₂, 392.2333). ¹³C NMR (acetone-*d*₆, 125 MHz), δ_C: 145.2 (C-2), 103.8 (C-3), 127.2 (C-3a), 118.6 (C-4), 134.0 (C-5), 123.1 (C-6), 112.3 (C-7), 134.7 (C-7a), 111.8 (C-8), 125.5 (C-9), 160.8 (C-10), 52.2 (C-12), 167.1 (C-13), 40.0 (C-15), 145.9 (C-16), 112.2 (C-17), 27.9 (C-18/19), 20.8 (C-20), 35.0 (C-21), 125.5 (C-22), 131.9 (C-23), 25.8 (C-24), 17.8 (C-25).

Compound 8: red solid, positive HRESIMS *m*/*z* 460.2967 [M + H]⁺ (calcd for C₂₉H₃₈N₃O₂, 460.2959). ¹³C NMR (acetone-*d*₆, 175 MHz), δ_C: 142.7 (C-2), 103.0 (C-3), 127.6 (C-3a), 131.8 (C-4), 131.7 (C-5), 124.3 (C-6), 110.0 (C-7), 135.5 (C-7a), 113.4 (C-8), 130.2 (C-9), 159.3 (C-10), 52.2 (C-12), 166.8 (C-13), 39.8 (C-15), 146.4 (C-16), 111.7 (C-17), 27.5 (C-18/19), 21.2 (C-20), 28.7 (C-21), 127.6 (C-22), 131.0 (C-23), 25.8 (C-24), 18.2 (C-25), 31.9 (C-26), 127.6 (C-27), 131.1 (C-28), 25.9 (C-29), 17.9 (C-30).

Compound **9**: yellow solid, negative ESIMS *m*/*z* 338.2 [M - H]⁻. ¹³C NMR (dimethyl sulfoxide-*d*₆, 175 MHz), *δ*_C: 144.2 (C-2), 103.8 (C-3), 126.2 (C-3a), 111.5 (C-4), 119.5 (C-5), 120.7 (C-6), 119.3 (C-7), 135.1 (C-7a), 111.3 (C-8), 125.1 (C-9), 165.8 (C-10), 79.1 (C-12), 161.4 (C-13), 39.1 (C-15), 145.2 (C-16), 111.7 (C-17), 27.8 (C-18), 27.5 (C-19), 24.7 (C-20).

Compound **10**: yellow oil, positive HRESIMS *m*/*z* 322.1560 [M + H]⁺ (calcd for C₁₉H₂₀N₃O₂, 322.1550). ¹³C NMR (acetone-*d*₆, 125 MHz), δ_C: 145.3 (C-2), 104.2 (C-3), 127.1 (C-3a), 119.7 (C-4), 120.9 (C-5), 122.3 (C-6), 112.5 (C-7), 136.3 (C-7a), 112.2 (C-8), 126.3 (C-9), 157.8 (C-10), 136.1 (C-12), 156.6 (C-13), 40.1 (C-15), 145.9 (C-16), 112.4 (C-17), 27.9 (C-18/19), 100.1 (C-20). Compound **11**: yellow oil, positive HRESIMS *m*/*z* 392.1972 [M + H]⁺ (calcd for C₂₃H₂₆N₃O₃,

392.1969). ¹³C NMR (acetone-*d*₆, 125 MHz), *δ*C: 146.9 (C-2), 104.3 (C-3), 127.3 (C-3a), 119.2 (C-4), 134.8 (C-5), 123.5 (C-6), 112.5 (C-7), 135.0 (C-7a), 117.3 (C-8), 124.6 (C-9), 157.5 (C-10), 152.6 (C-12), 160.6 (C-13), 40.2 (C-15), 145.7 (C-16), 112.7 (C-17), 28.1 (C-18/19), 35.2 (C-21), 125.4 (C-22), 131.9 (C-23), 25.8 (C-24), 17.9 (C-25).

Compound **12**: yellow oil, positive HRESIMS *m*/*z* 462.3121 [M + H]⁺ (calcd for C₂₉H₄₀N₃O₂, 462.3115). ¹³C NMR (acetone-*d*₆, 125 MHz), δ_C: 141.5 (C-2), 104.2 (C-3), 129.1 (C-3a), 115.2 (C-4), 134.0 (C-5), 123.0 (C-6), 123.5 (C-7), 132.4 (C-7a), 29.7 (C-8), 54.7 (C-9), 168.8 (C-10), 50.9 (C-12), 168.0 (C-13), 39.1 (C-15), 145.9 (C-16), 112.5 (C-17), 28.1 (C-18), 28.0 (C-19), 20.0 (C-20), 34.7 (C-21), 124.6 (C-22), 131.7 (C-23), 25.8 (C-24), 18.0 (C-25), 31.5 (C-26), 123.0 (C-27), 133.0 (C-28), 25.9 (C-29), 18.0 (C-30).

Compound **13**: white solid, positive ESIMS *m*/*z* 245 [M + H]⁺. ¹³C NMR (acetone-*d*₆, 125 MHz) , δ_C: 166.9 (C-1), 45.9 (C-3), 22.8 (C-4), 29.3 (C-5), 60.0 (C-6), 170.9 (C-7), 57.6 (C-9), 38.1 (C-10), 137.4 (C-1'), 131.0 (C-2'/6'), 131.0 (C-3'/5'), 128.0 (C-4').