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Supporting Information

Euroticins C-E, Three Pairs of Polycyclic Salicylaldehyde Derivative Enantiomers from a Marine-Derived Fungus *Eurotium* sp. SCSIO F452

Weimao Zhong,[†,‡] Yuchan Chen,[‖] Xiaoyi Wei,[§] Junfeng Wang,[†] Qi Zeng,[†,‡] Xinpeng Tian,[†] Weimin Zhang,[‖] Fazuo Wang,*[,†] and Si Zhang*[,†]

[†]CAS Key Laboratory of Tropical Marine Bio-resources and Ecology, Southern Marine Science and Engineering Guangdong Laboratory (Guangzhou), Guangdong Key Laboratory of Marine Materia Medica, RNAM Center for Marine Microbiology, South China Sea Institute of Oceanology, Chinese Academy of Sciences, 164 West Xingang Road, Guangzhou 510301, China

[‖]State Key Laboratory of Applied Microbiology Southern China, Guangdong Provincial Key Laboratory of Microbial Culture Collection and Application, Guangdong Open Laboratory of Applied Microbiology, Guangdong Institute of Microbiology, 100 Central Xianlie Road, Guangzhou 510070, China

[§]Key Laboratory of Plant Resources Conservation and Sustainable Utilization, South China Botanical Garden, Chinese Academy of Sciences, Guangzhou 510650, China

[‡]University of Chinese Academy of Sciences, 19 Yuquan Road, Beijing 100049, China

* Corresponding authors:

Prof. Fazuo Wang

Tel: +86-20-3406-3746

E-mail: wangfazuo@scsio.ac.cn

Prof. Si Zhang

Tel: +86-20-8902-3103

E-mail: zhsimd@scsio.ac.cn

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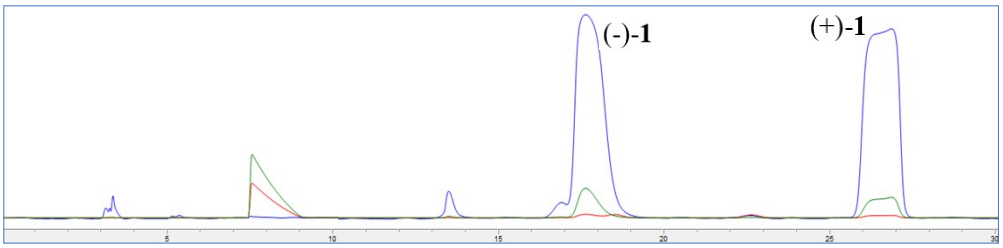


Fig. S1 The chiral HPLC chromatogram of **1.**

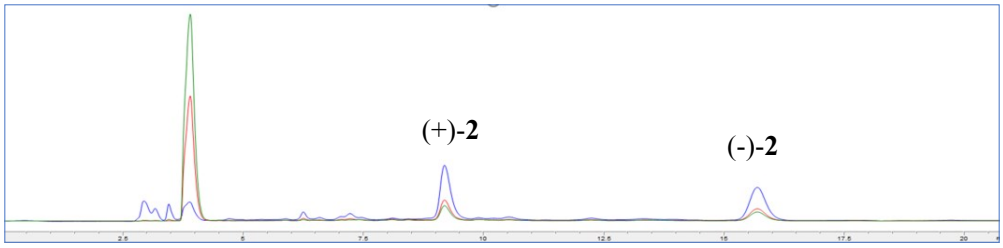


Fig. S2 The chiral HPLC chromatogram of **2.**

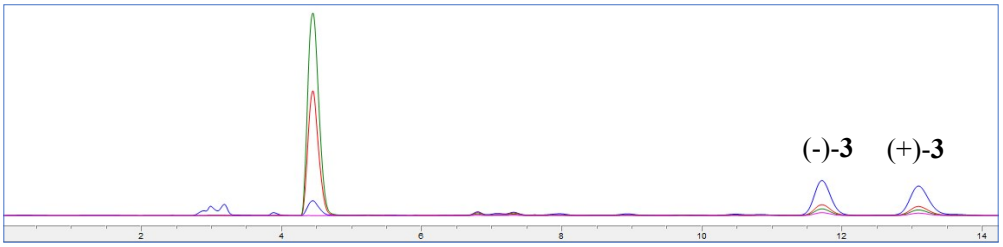


Fig. S3 The chiral HPLC chromatogram of **3.**

Table S1 Cytotoxic activities of compounds (+)-**1**, (-)-**1**, (+)-**3**, and (-)-**3** against tumor cells[a].

Compounds	IC_{50} (μM)			
	SF-268	MCF-7	HepG2	A549
(+)-**1**	11.77 ± 0.14	21.13 ± 0.16	24.89 ± 0.60	27.01 ± 0.24
(-)-**1**	14.76 ± 0.71	18.65 ± 0.45	27.38 ± 0.23	27.04 ± 0.35
(+)-**3**	53.03 ± 5.96	32.13 ± 2.78	94.66 ± 1.58	35.86 ± 1.35
(-)-**3**	59.84 ± 1.48	63.75 ± 2.93	>100	51.17 ± 1.29
Adriamycin	0.57 ± 0.04	0.95 ± 0.06	1.18 ± 0.15	0.70 ± 0.04

[a]The results were mean ± SD (SD = standard deviation). Positive control: Adriamycin.

Table S2 Antioxidative activities of compounds (+)-**1**, (-)-**1**, (+)-**3**, and (-)-**3**[a].

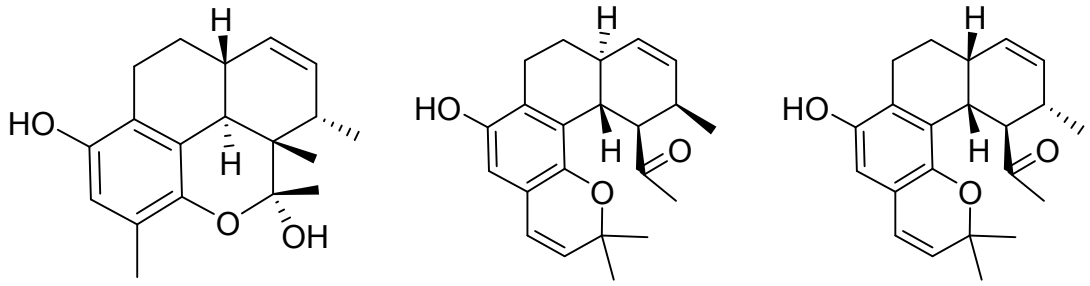
Compounds	EC_{50} (μM)
(+)-**1**	27.00 ± 0.52
(-)-**1**	30.27 ± 1.25
(+)-**3**	>100
(-)-**3**	>100
Ascorbic acid	27.87 ± 0.93

[a]Positive control: Ascorbic acid.

Computational Details

1. Methods

Molecular Merck force field (MMFF) calculations were done using Spartan'14 program (Wavefunction Inc., Irvine, CA, USA). Density functional theory (DFT) and time-dependent density functional theory (TDDFT) calculations were performed with Gaussian09 program package.[1] Truncated structure of (7*S*,8*S*,9*R*,1″*R*,6″*S*)-**1′**, which is corresponding to innate compounds (7*S*,8*S*,9*R*,1″*R*,6″*S*)-**1** to reduce the computational cost, as well as compounds (7*R*,8*R*,3″*S*,6″*R*)-**2**, and (7*R*,8*R*,3″*R*,6″*S*)-**3** (Figure S4) were used in ECD calculations . For conformational analysis, the conformers generated by a MMFF conformational search in an energy window of 10 kcal/mol were subjected to geometry optimization using the DFT method at the B3LYP/def2-SVP level with the PCM for MeOH.[2,3] Frequency calculations were run at the same level to estimate their relative thermal (Δ*E*) and free energies (Δ*G*) at 298.15K. Energies of the low-energy conformers were re-calculated at the M06-2X/def2-TZVP/SMD(MeOH) level.[2,3] The TDDFT calculations were performed using the hybrid PBE1PBE[4] and M06-2X[5] functionals, and the Ahlrichs' basis set TZVP[6]. The ECD spectra were generated by the program SpecDis[7] using a Gaussian band shape from dipole-length dipolar and rotational strengths. The equilibrium population of each conformer at 298.15K was calculated from its Δ*G* using Boltzmann statistics. The calculated spectra of compounds were generated from the low-energy conformers according to the Boltzmann weighting of each conformer in MeOH solution.



(7*S*,8*S*,9*R*,3″*R*,6″*S*)-**1′** (7*R*,8*R*,3″*S*,6″*R*)-**2** (7*R*,8*R*,3″*R*,6″*S*)-**3**

Fig. S4 Structures of compounds applied for theoretical calculations.

2. Results

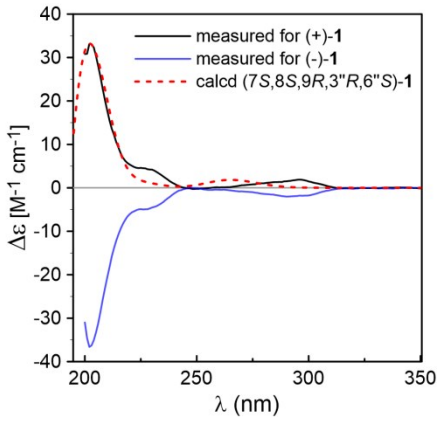


Fig. S5 Comparison between M06-2X/TZVP/PCM calculated and experimental ECD spectra of **1** in MeOH.

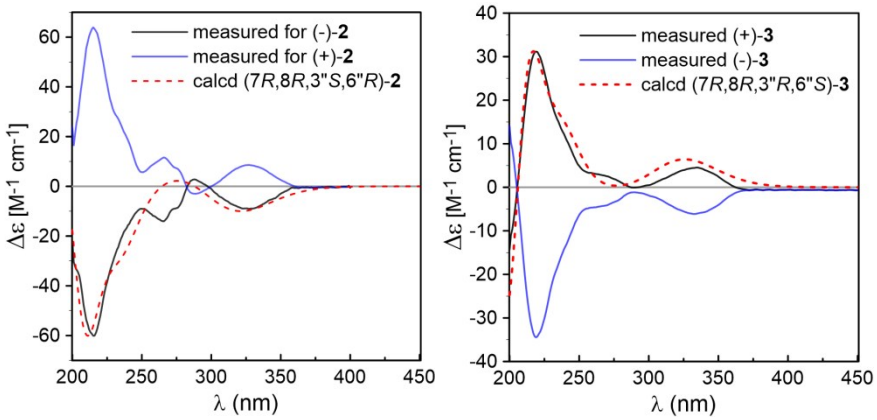


Fig. S6 Comparison between PBE1PBE /TZVP/PCM calculated and experimental ECD spectra of **2** and **3** in MeOH.

Table S3 M06-2X/def2-TZVP/SMD//B3LYP/def2-SVP/PCM calculated relative thermal energies (Δ*E*), relative free energies (Δ*G*), and equilibrium populations (P)[a] of low-energy conformers (7*S*,8*S*,9*R*,1″*R*,6″*S*)-**1′**, (7*R*,8*R*,3″*S*,6″*R*)-**2**, and (7*R*,8*R*,3″*R*,6″*S*)-**3** in MeOH solution.

conformer	Δ*E* (kcal/mol)	Δ*G* (kcal/mol)	P (%)[a]
(7*S*,8*S*,9*R*,1″*R*,6″*S*)-**1′**			
1′a	0.0	0.0	57.0
1′b	0.536	0.449	26.7
1′c	1.059	0.960	11.3
1′d	1.614	1.427	5.1
(7*R*,8*R*,3″*S*,6″*R*)-**2**			
2a	0.0	0.0	76.5
2b	0.773	0.747	21.7
2c[b]	1.303	2.208	1.8

(7*R*,8*R*,3″*R*,6″*S*)-**3**			
3a	0.0	0.0	71.7
3b	0.778	0.745	20.2
3c	0.638	1.404	6.6
3d	1.405	2.106	2.0

[a] From Δ*G* values at 298.15 K.

[b] Conformer not applied to ECD/TDDFT calculations.

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Fig. S7 The ^{1}H NMR (500 MHz) spectrum of euroticin C (**1**) in acetone-d_6.

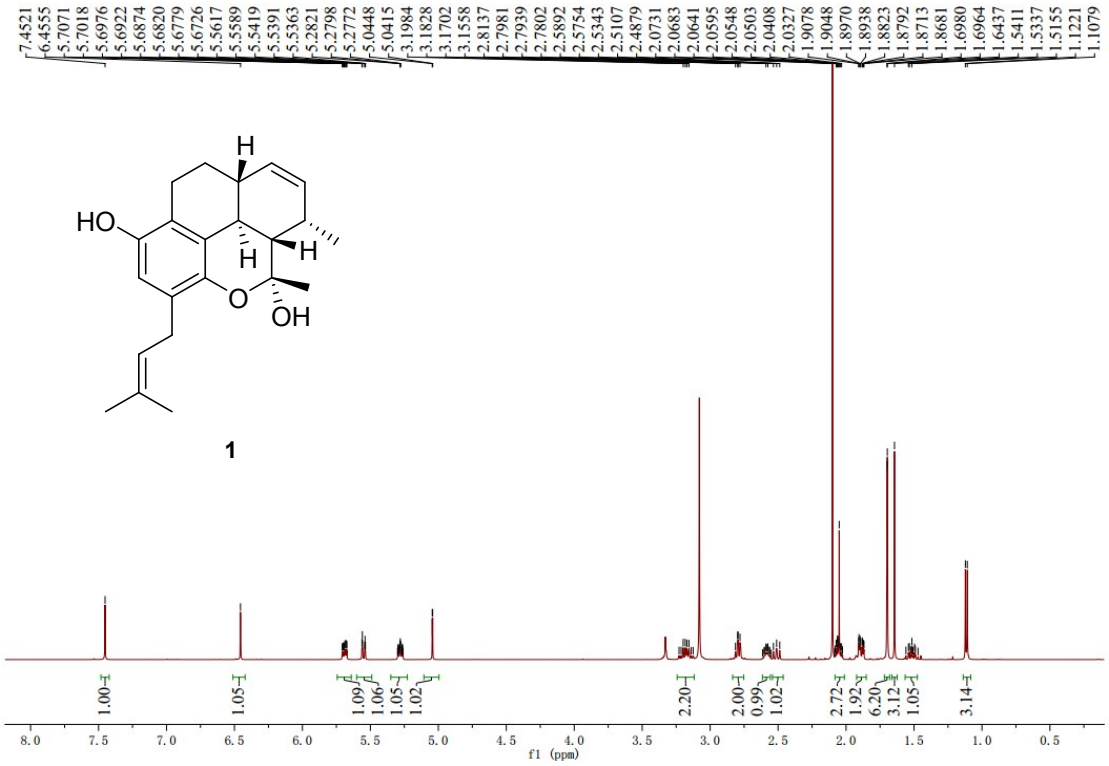

Fig. S8 The ^{13}C NMR (125 MHz) spectrum of euroticin C (**1**) in acetone-d_6.

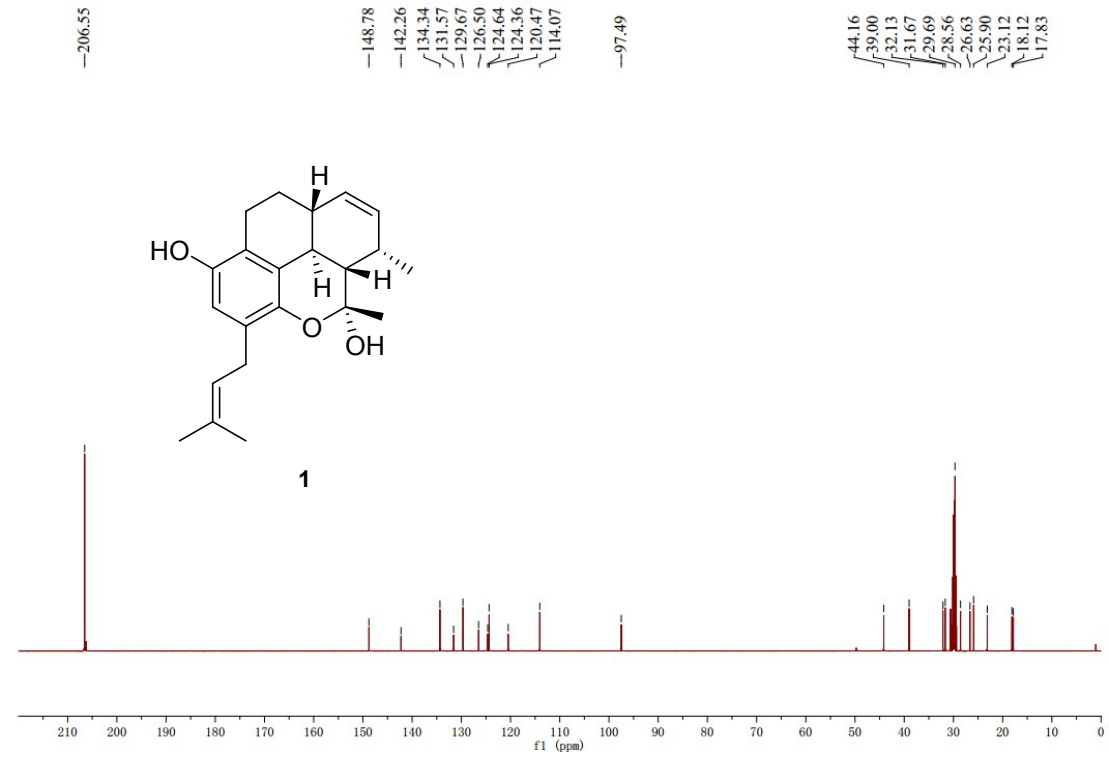

Fig. S9 The HSQC (500 MHz) spectrum of euroticin C (**1**) in acetone-d_6.

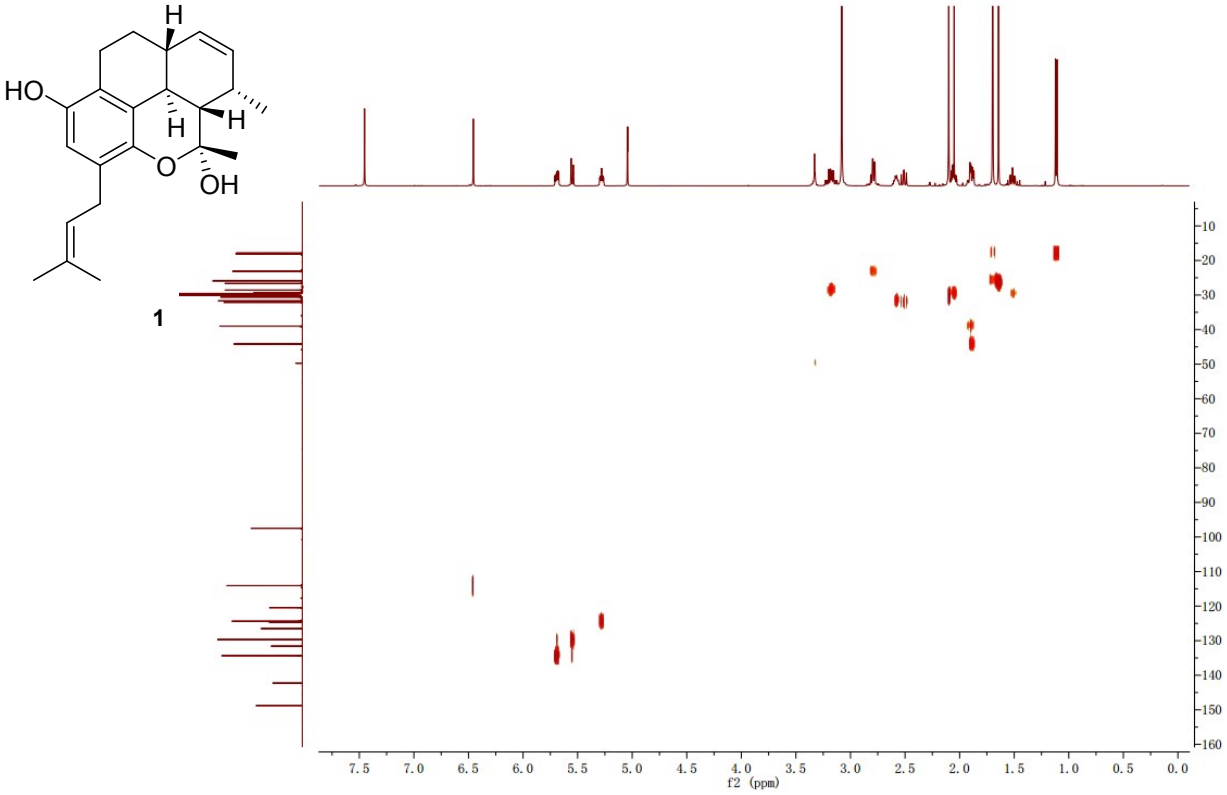

Fig. S10 The HMBC (500 MHz) spectrum of euroticin C (**1**) in acetone-d_6.

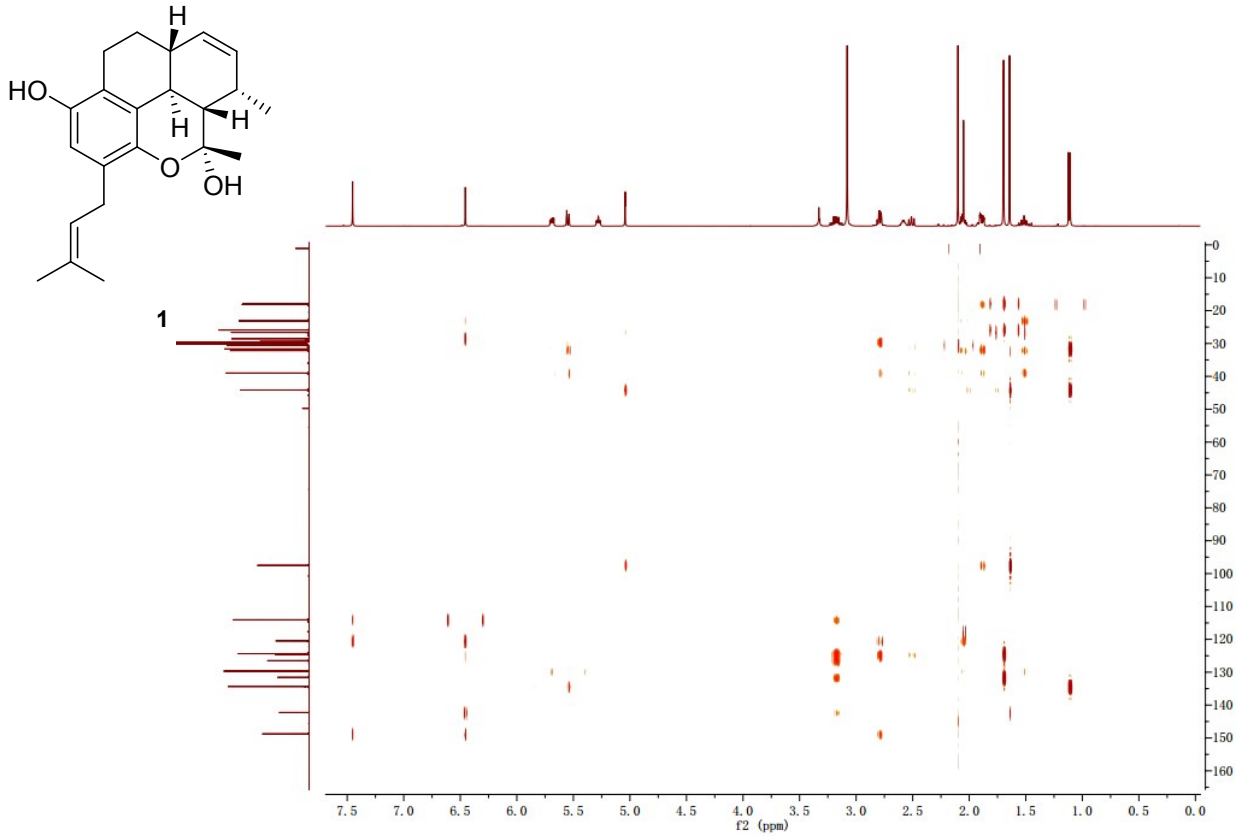

Fig. S11 The ^{1}H-^{1}H COSY (500 MHz) spectrum of euroticin C (**1**) in acetone-d_6.

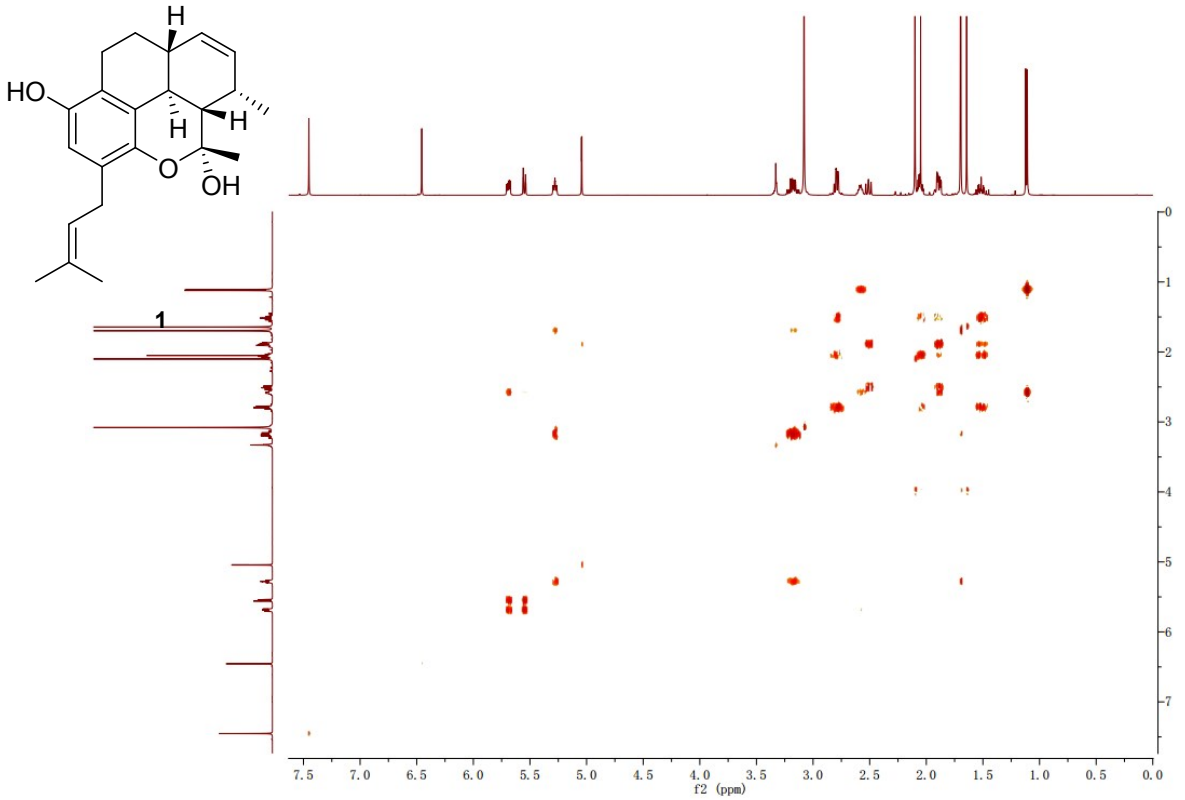

Fig. S12 The NOESY (500 MHz) spectrum of euroticin A (**1**) in acetone-d_6.

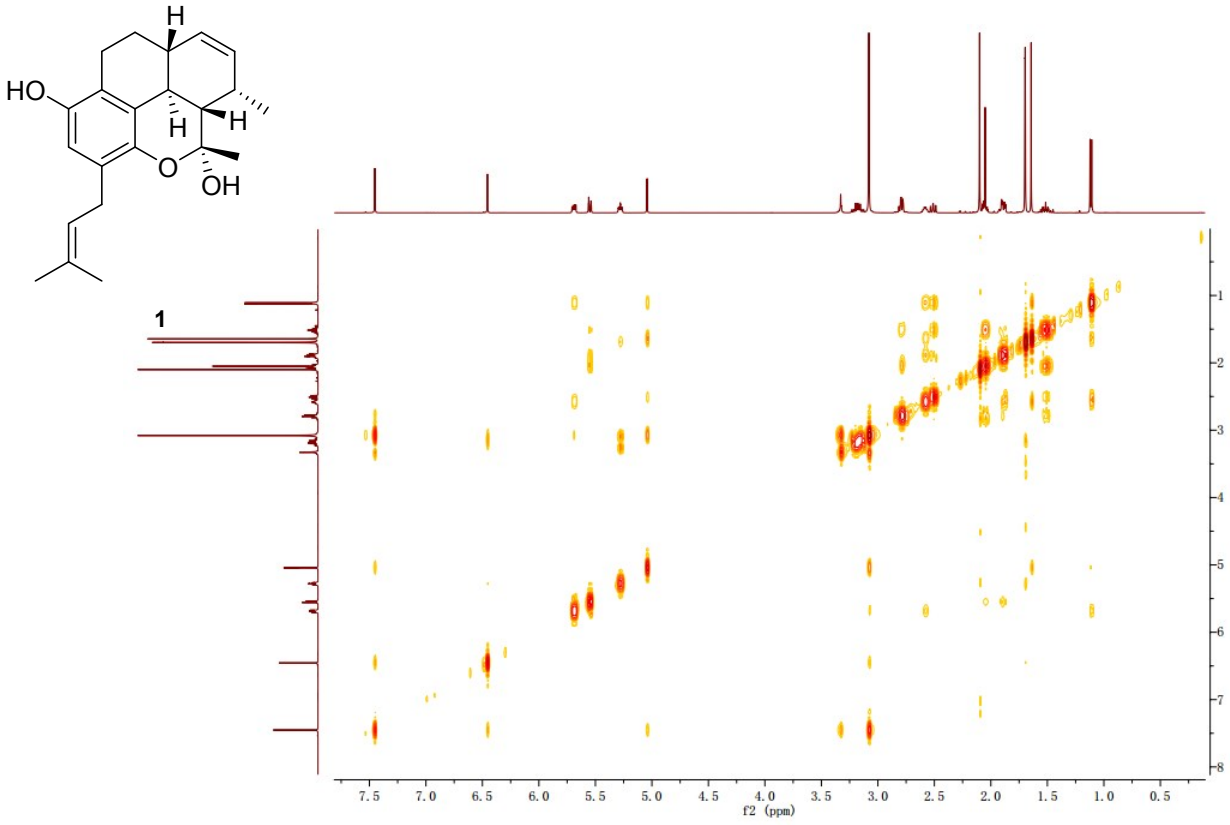

Fig. S13 The HRESIMS spectrum of euroticin C (**1**).

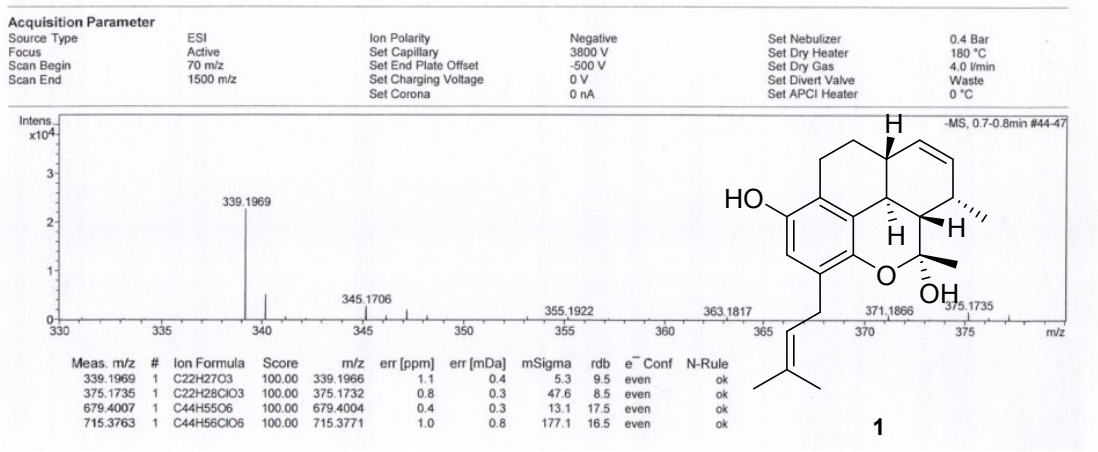

Fig. S14 The UV spectrum of euroticin C (**1**).

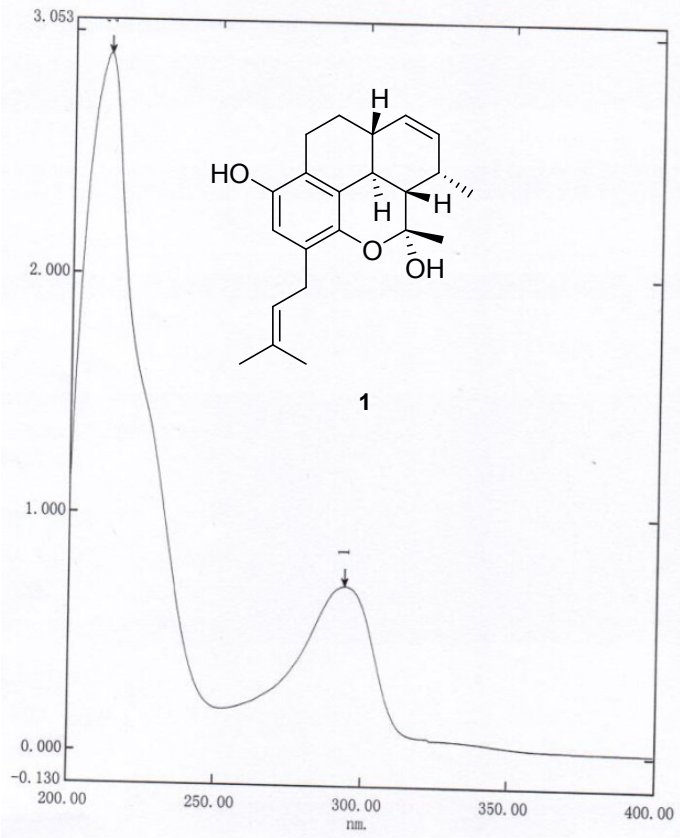

Fig. S15 The ^{1}H NMR (700 MHz) spectrum of euroticin D (**2**) in acetone-d_6.

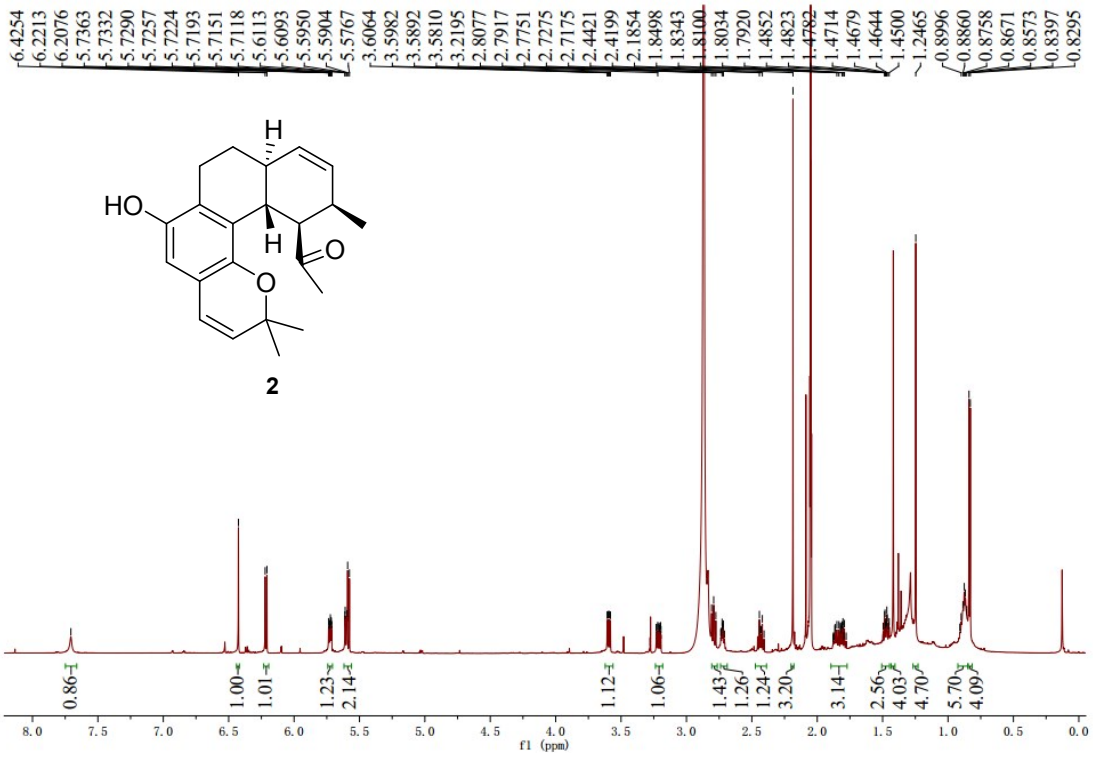

Fig. S16 The ^{13}C NMR (175 MHz) spectrum of euroticin D (**2**) in acetone-d_6.

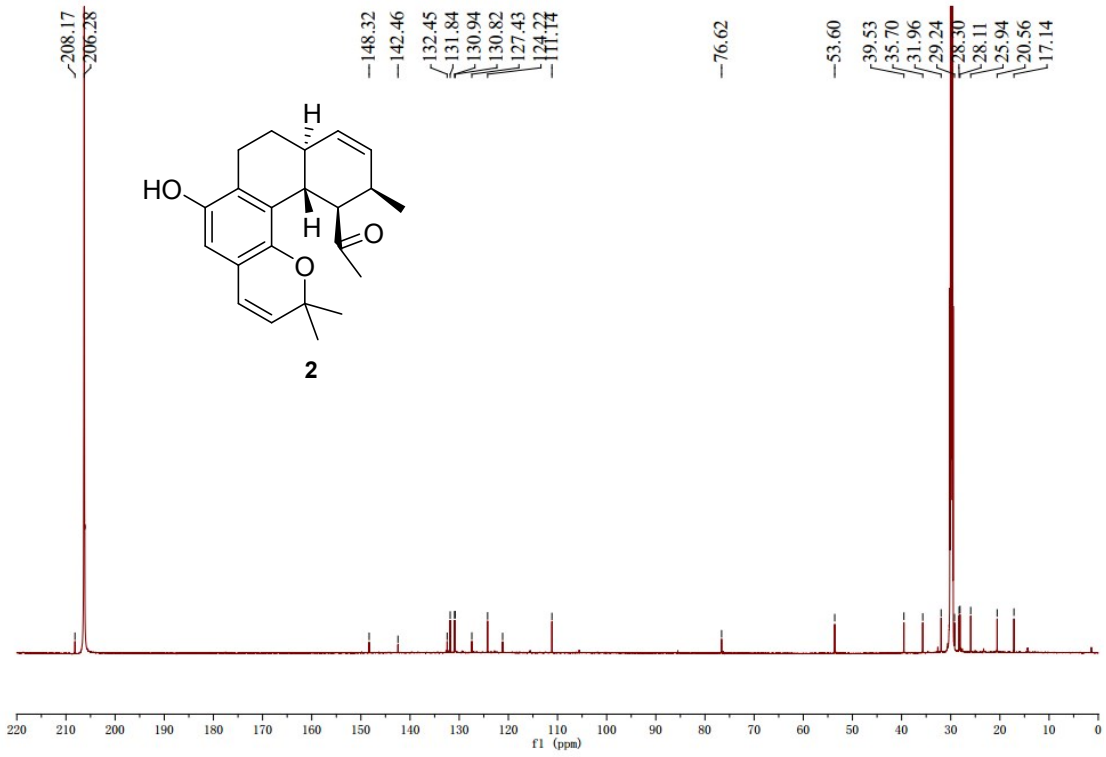

Fig. S17 The HSQC (700 MHz) spectrum of euroticin D (**2**) in acetone-d_6.

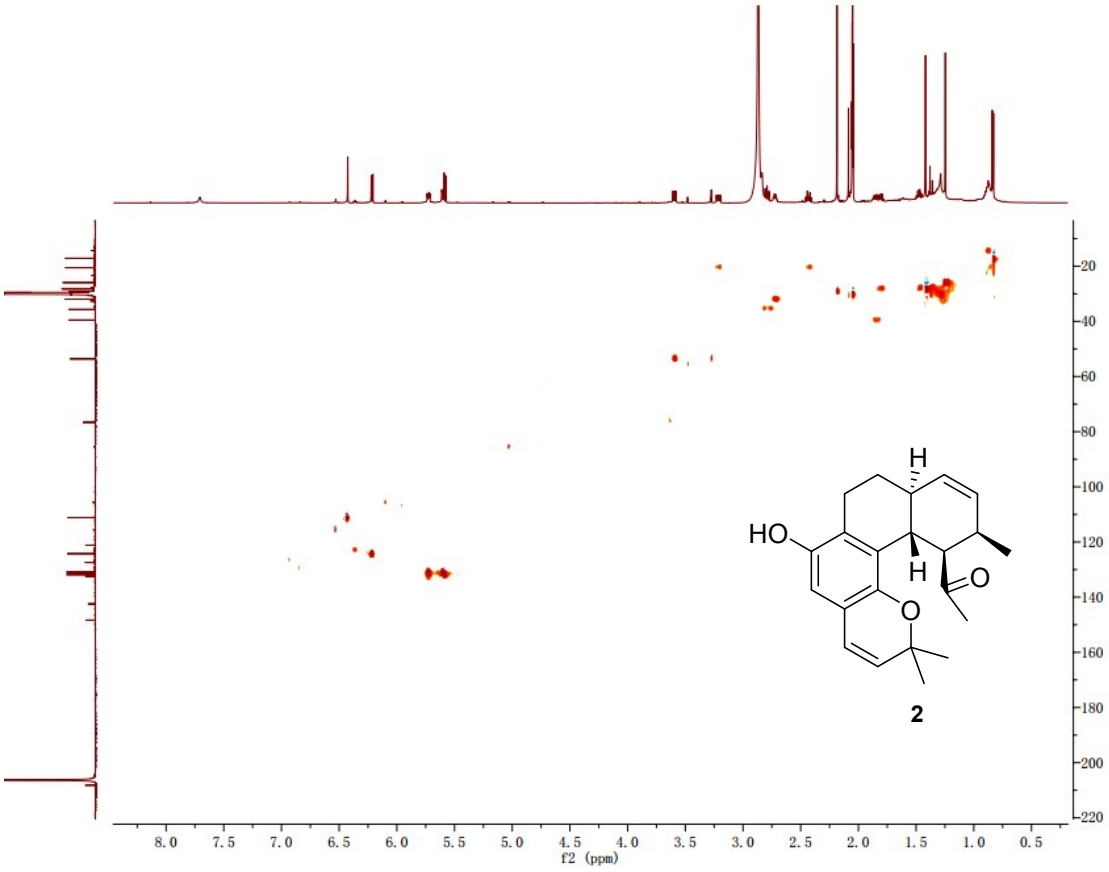

Fig. S18 The HMBC (700 MHz) spectrum of euroticin D (**2**) in acetone-d_6.

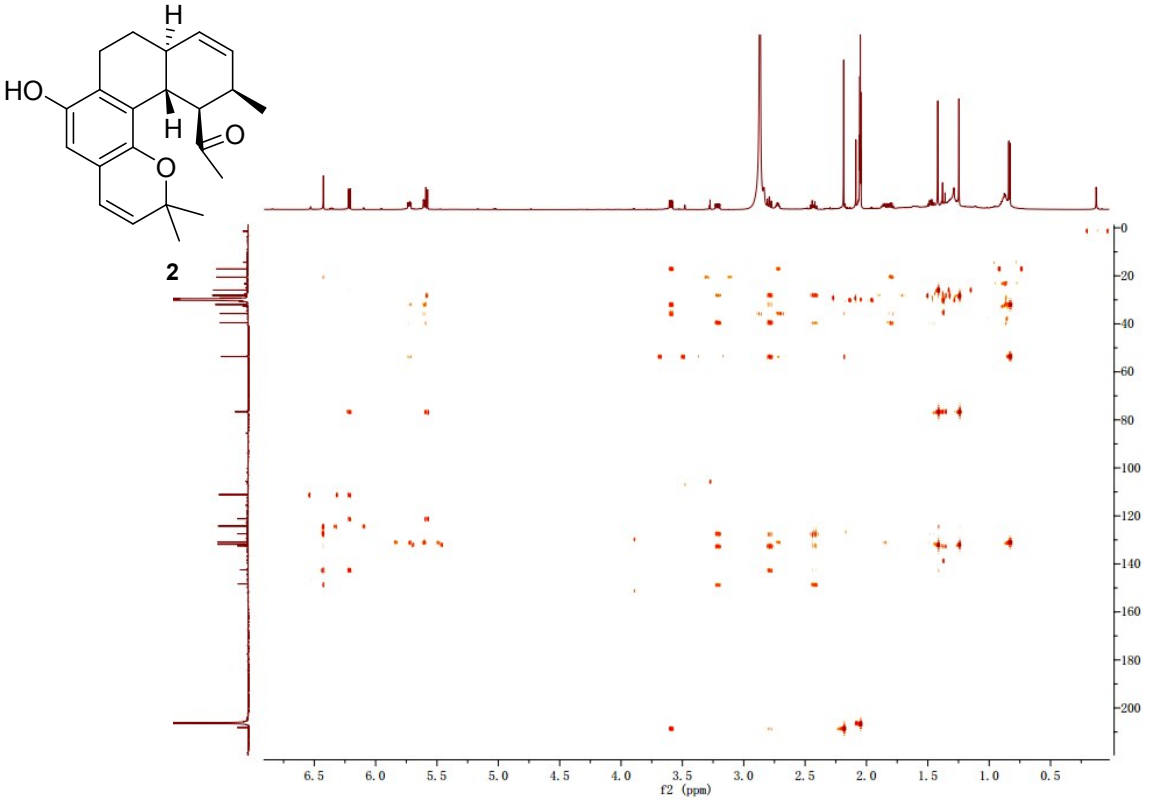

Fig. S19 The ^{1}H-^{1}H COSY (700 MHz) spectrum of euroticin D (**2**) in acetone-d_6.

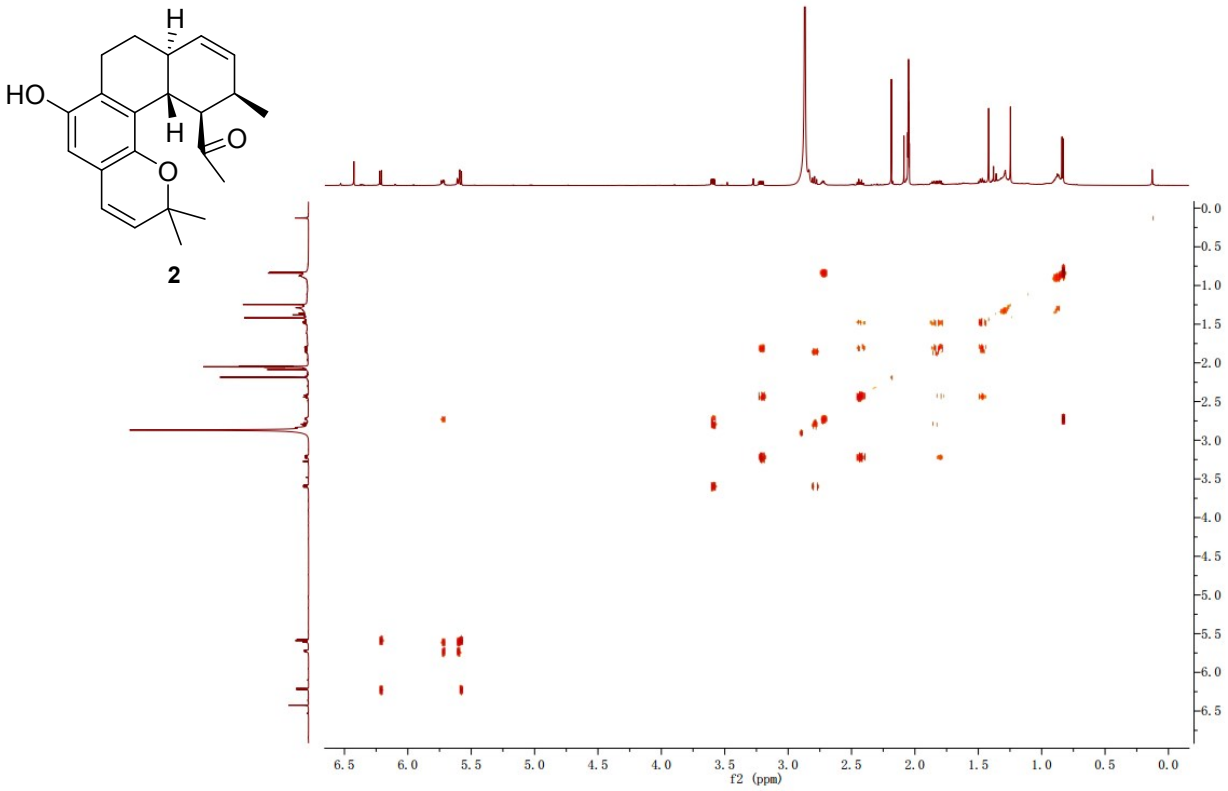

Fig. S20 The NOESY (700 MHz) spectrum of euroticin D (**2**) in acetone-d_6.

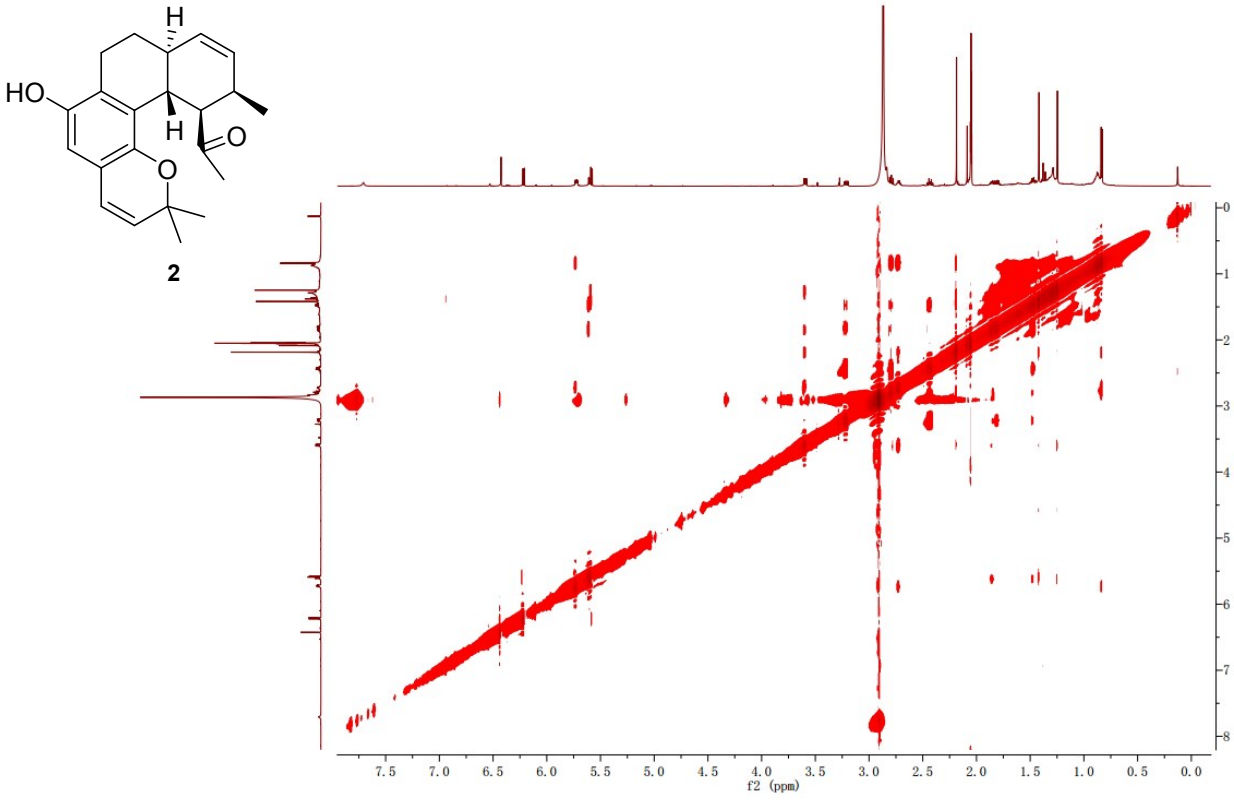

Fig. S21 The HRESIMS spectrum of euroticin D (**2**).

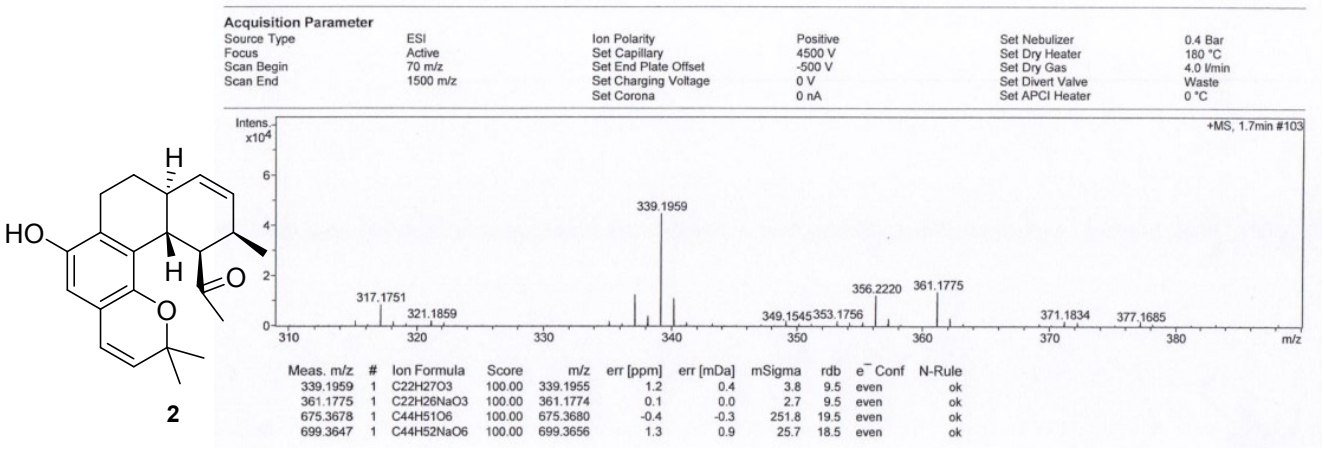

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Fig. S22 The UV spectrum of euroticin D (**2**).

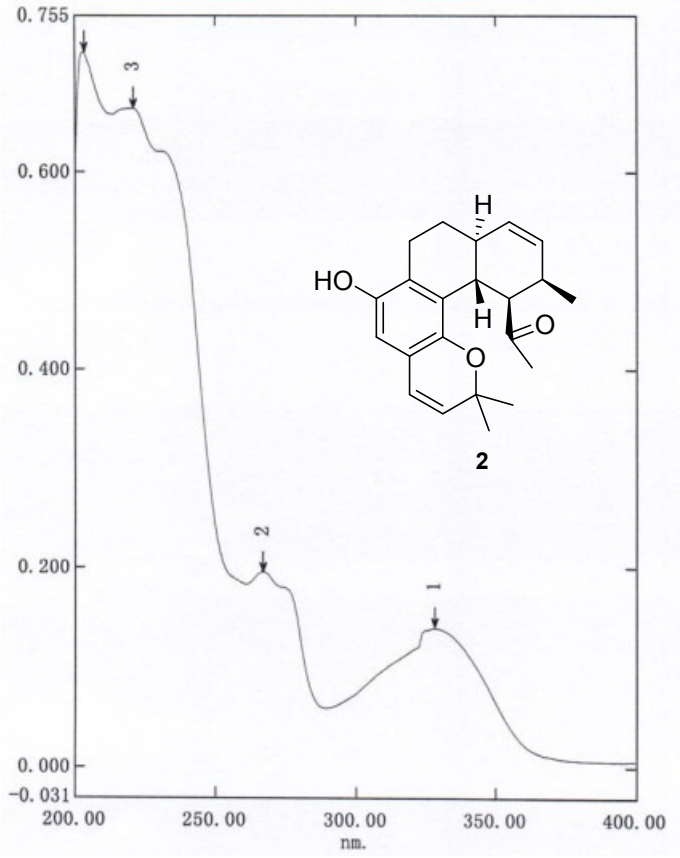

Fig. S23 The ^{1}H NMR (700 MHz) spectrum of euroticin E (**3**) in acetone-d_6.

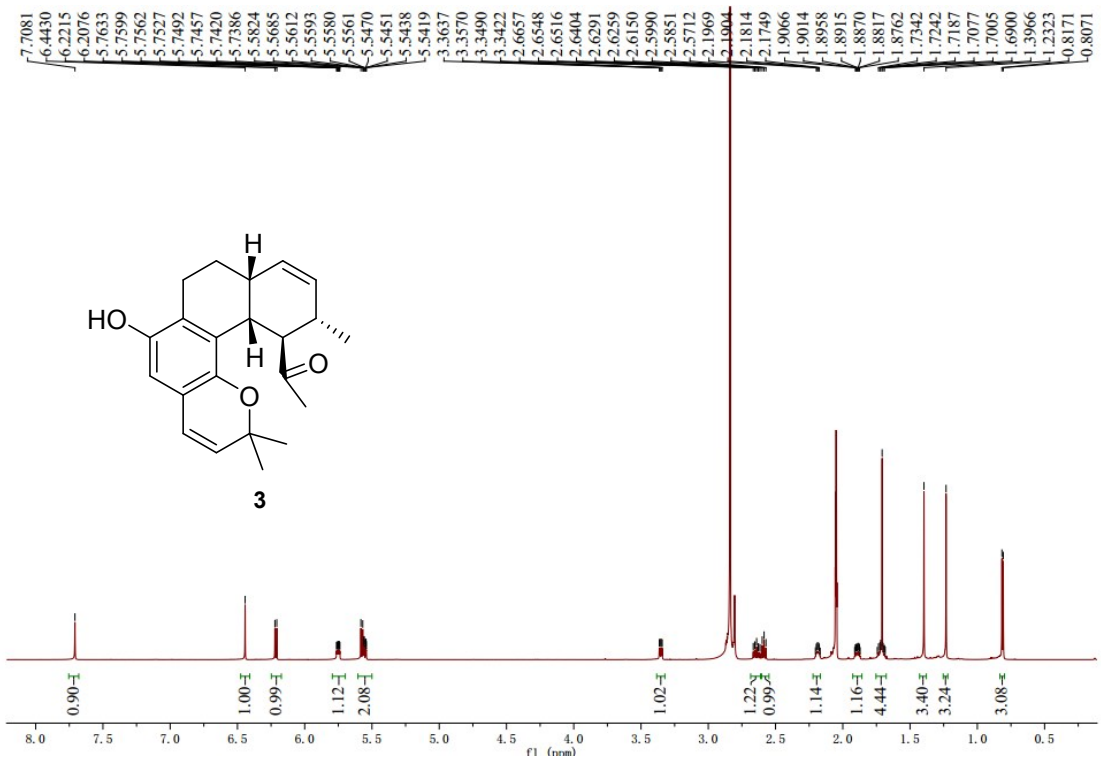

Fig. S24 The ^{13}C NMR (175 MHz) spectrum of euroticin E (**3**) in acetone-d_6.

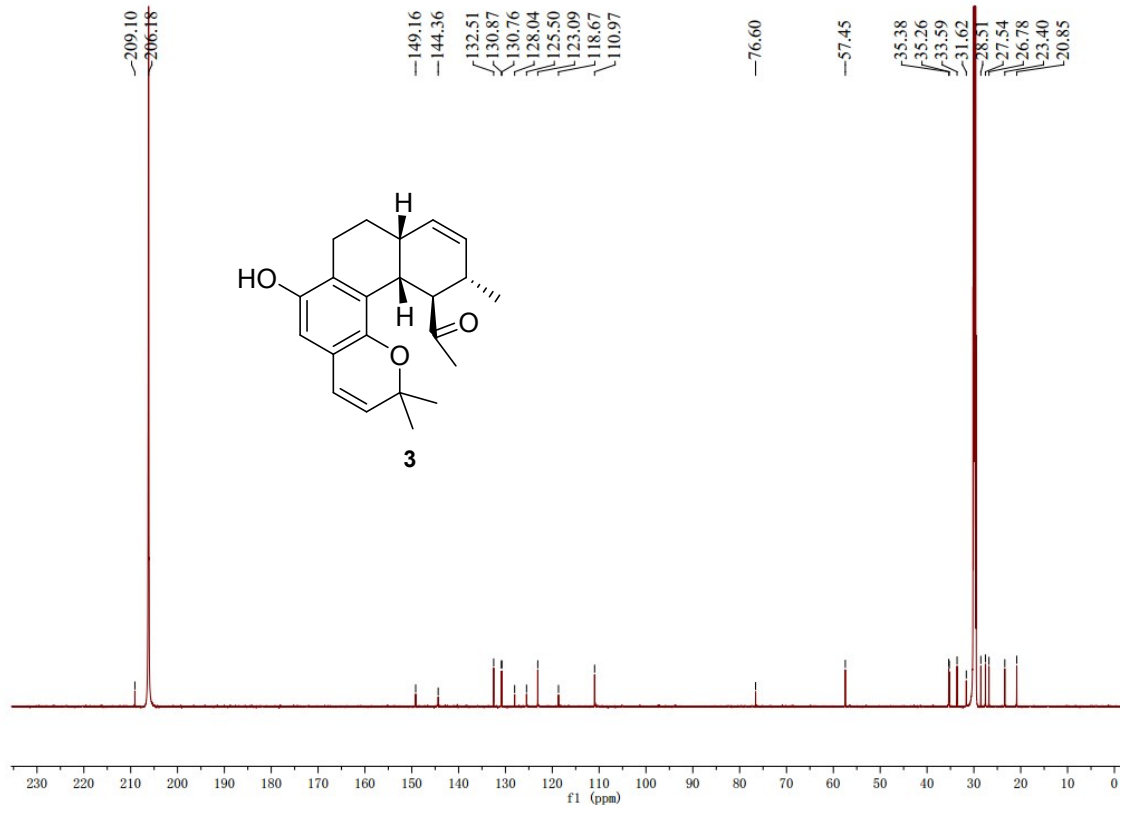

Fig. S25 The HSQC (700 MHz) spectrum of euroticin E (**3**) in acetone-d_6.

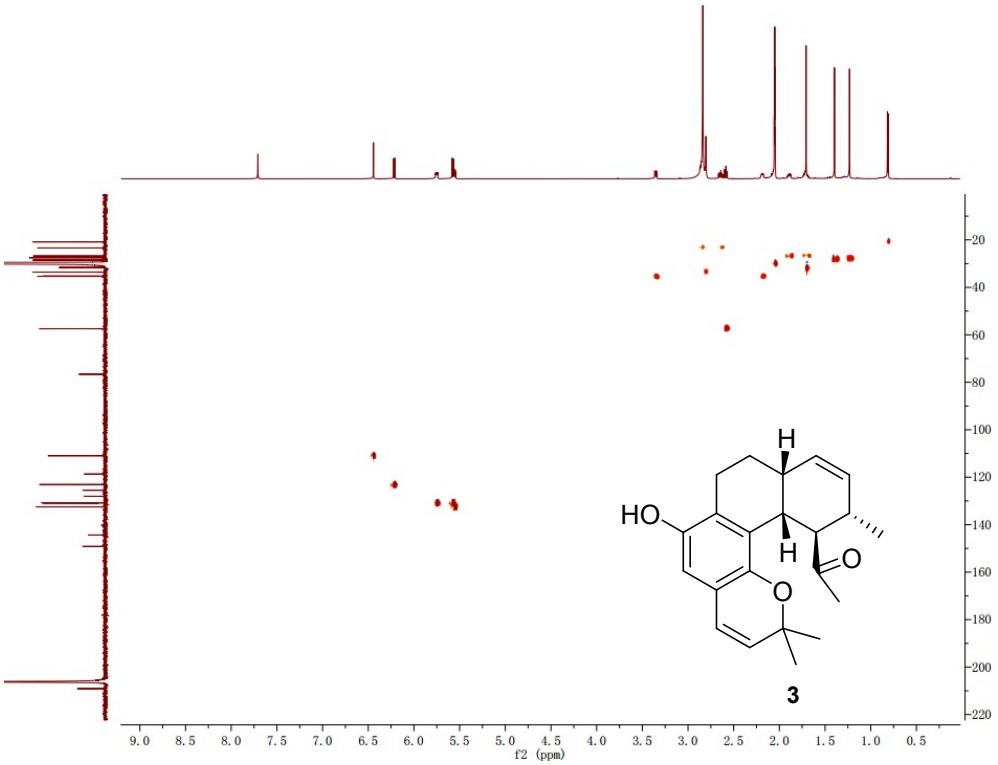

Fig. S26 The HMBC (700 MHz) spectrum of euroticin E (**3**) in acetone-d_6.

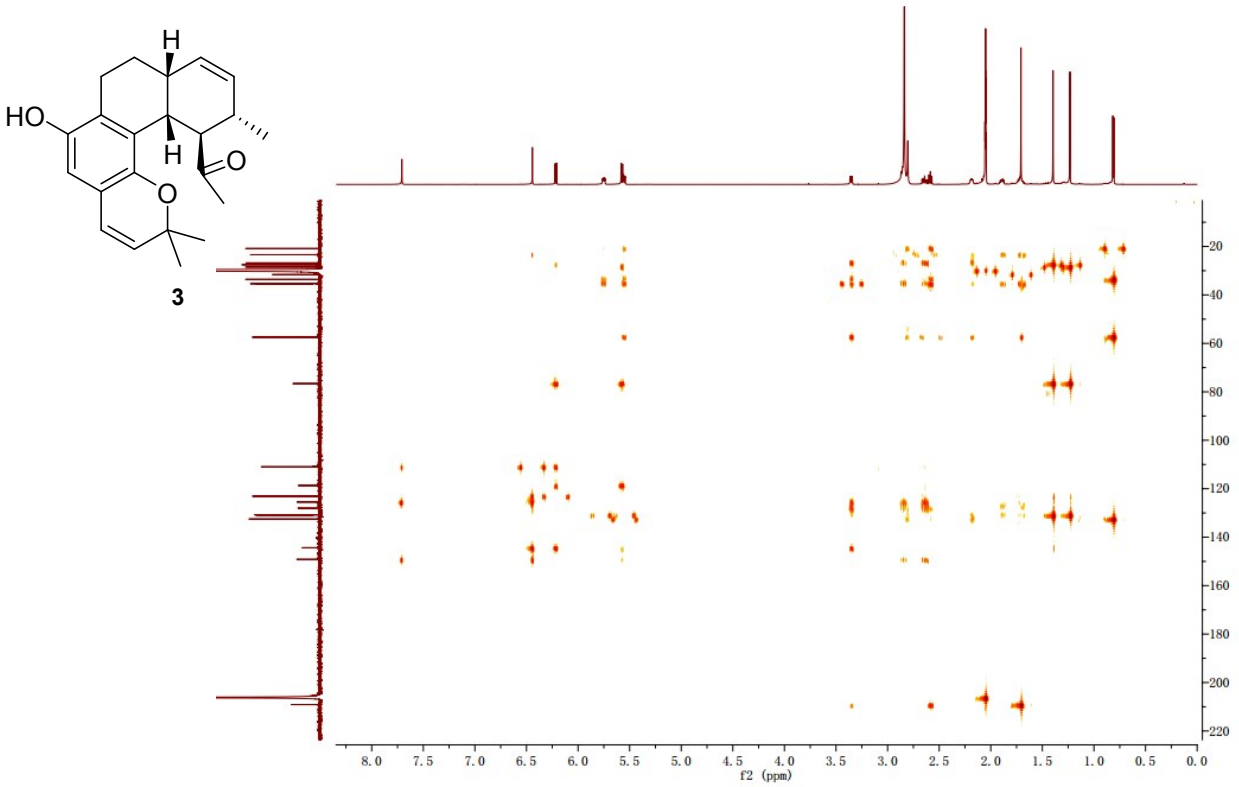

Fig. S27 The ^{1}H-^{1}H COSY (700 MHz) spectrum of euroticin E (**3**) in acetone-d_6.

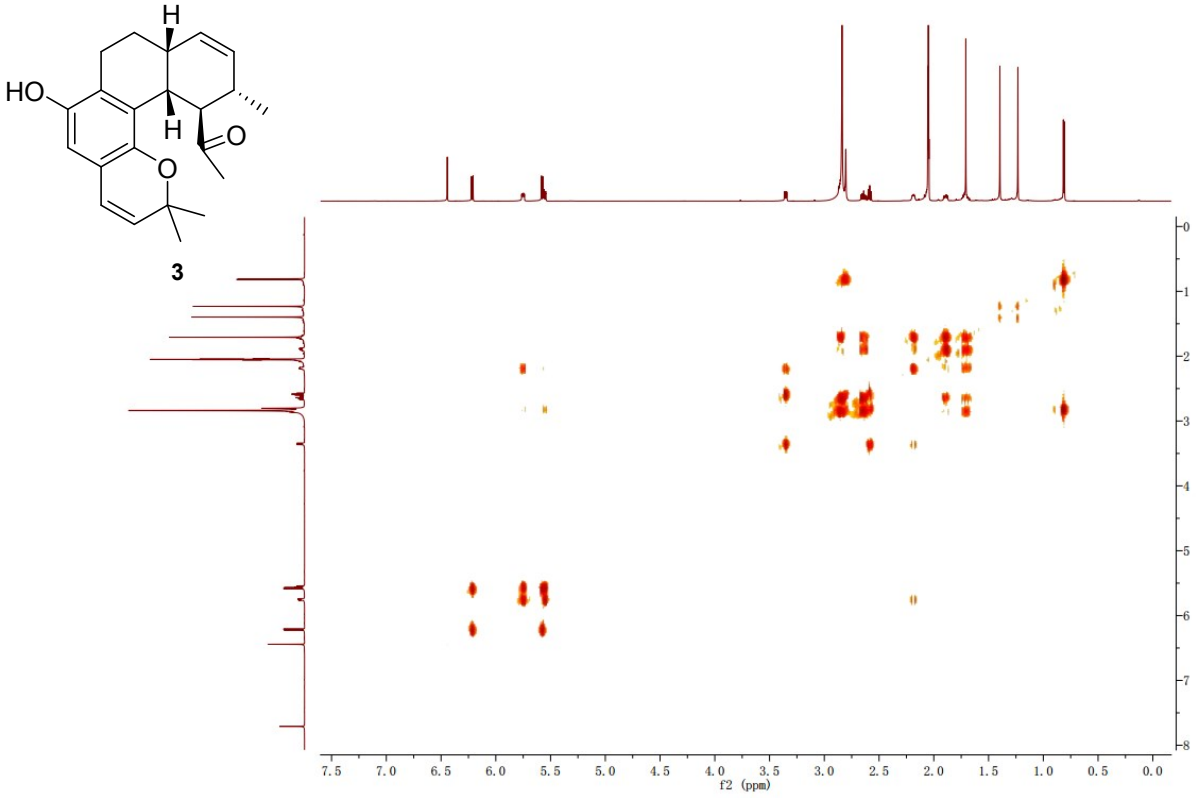

Fig. S28 The NOESY (700 MHz) spectrum of euroticin E (**3**) in acetone-d_6.

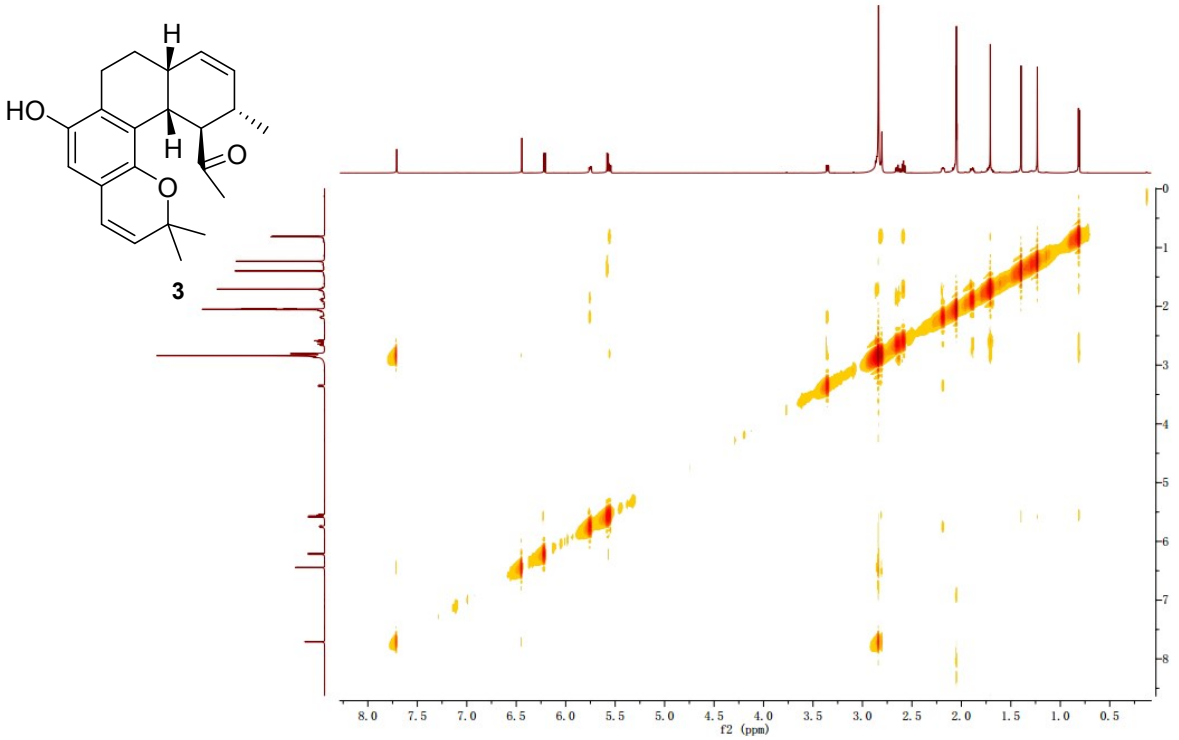

Fig. S29 The HRESIMS spectrum of euroticin E (**3**).

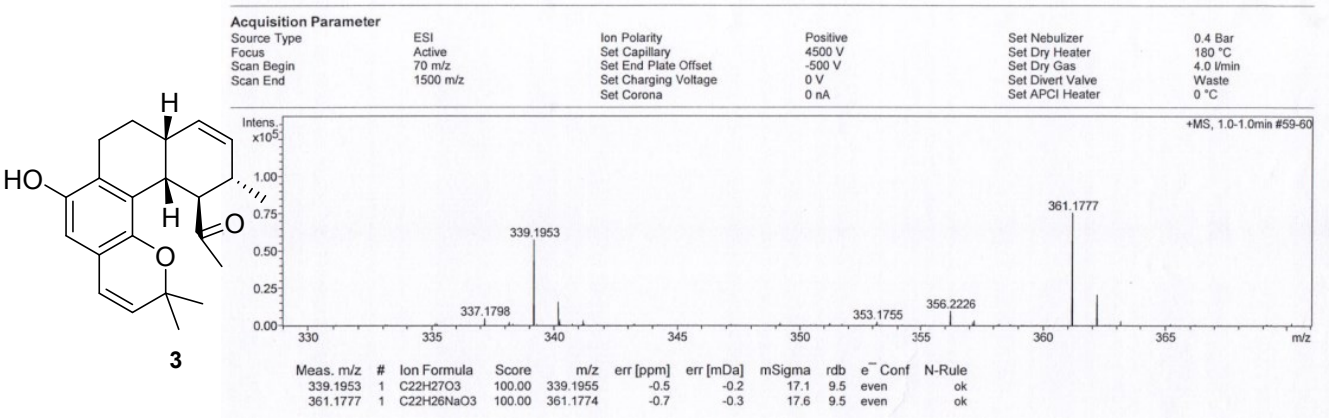

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Fig. S30 The UV spectrum of euroticin E (**3**).