Supporting Information

Cytotoxic and Antibacterial Preussomerins from the Mangrove Endophytic Fungus *Lasiodiplodia theobromae*

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Fig. S1 EIMS spectrum of **1**

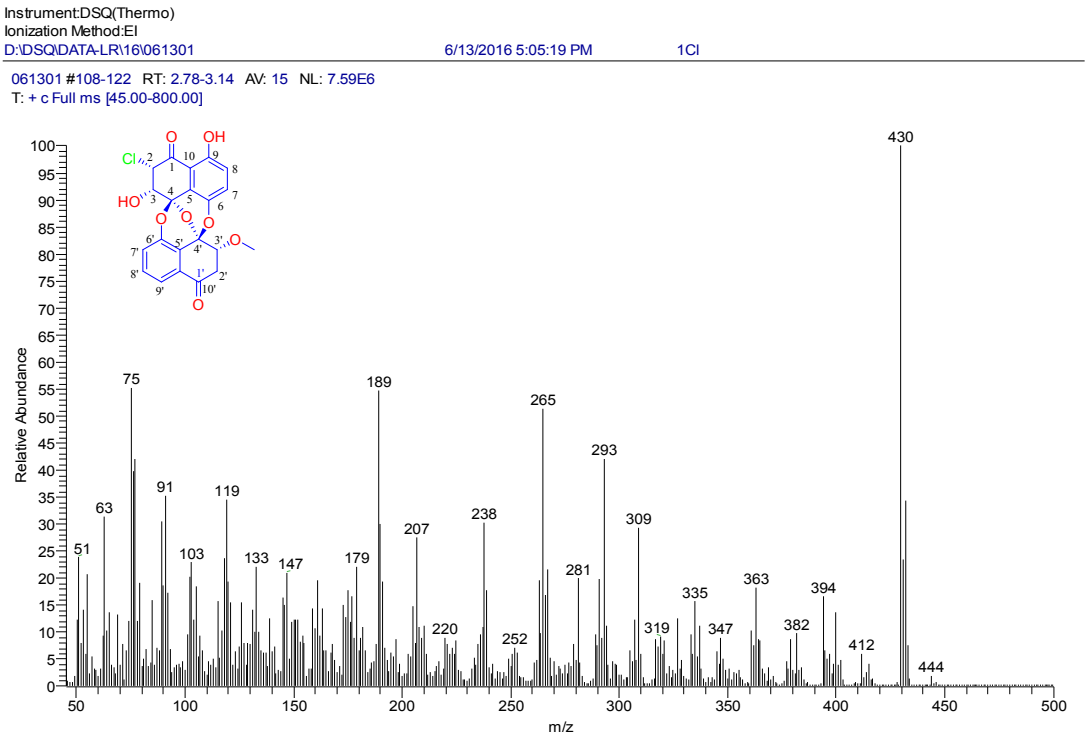


Fig. S2 HREIMS spectrum of **1**

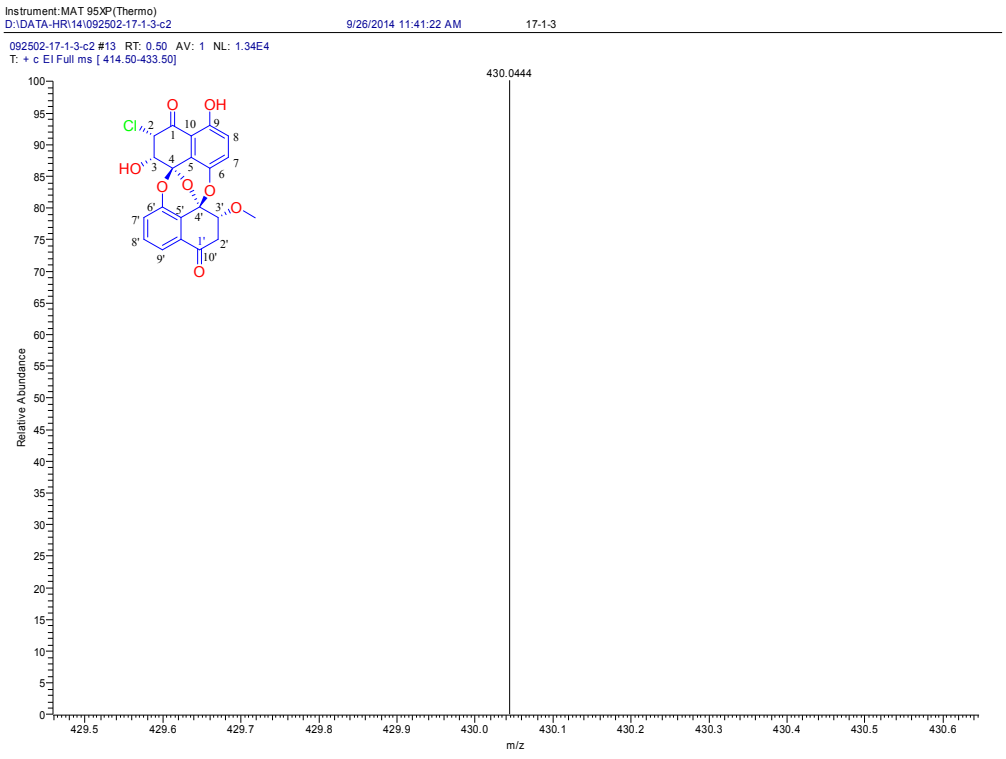


Fig. S3 ^{1}H NMR spectrum of **1** in $CDCl_3$

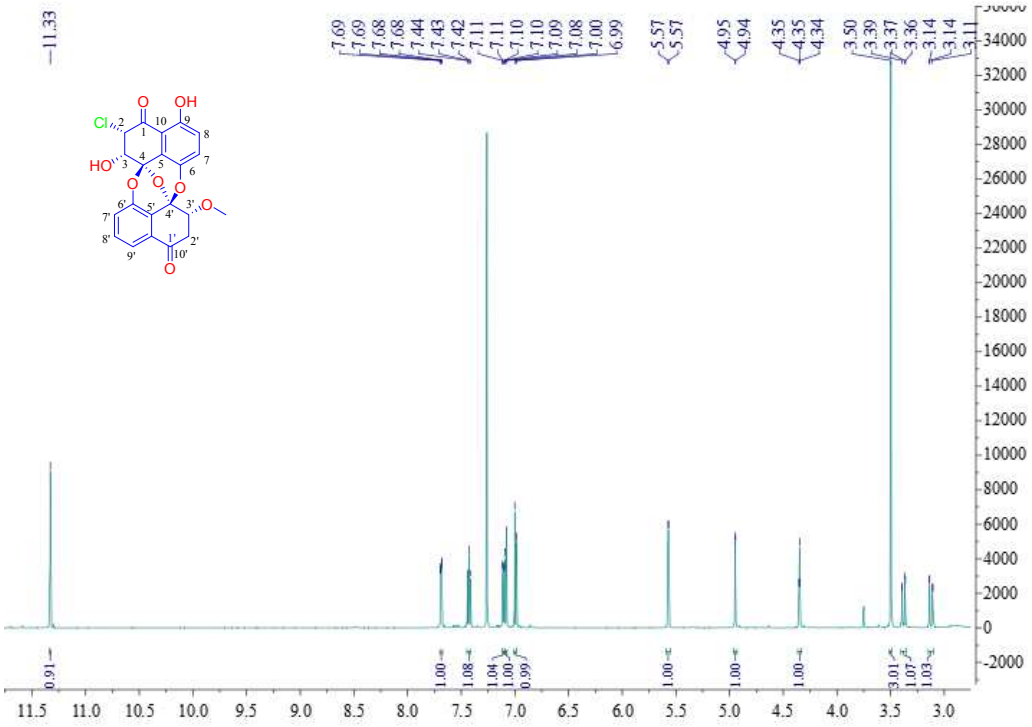


Fig. S4 ^{13}C NMR spectrum of **1** in $CDCl_3$

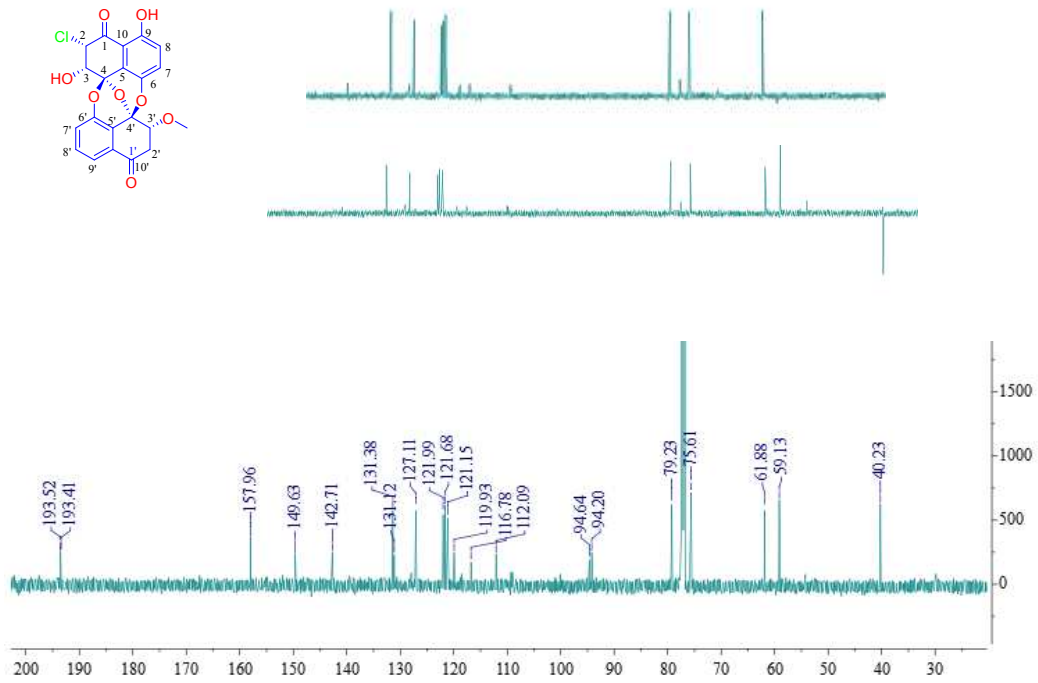


Fig. S5 HSQC spectrum of **1** in $CDCl_3$

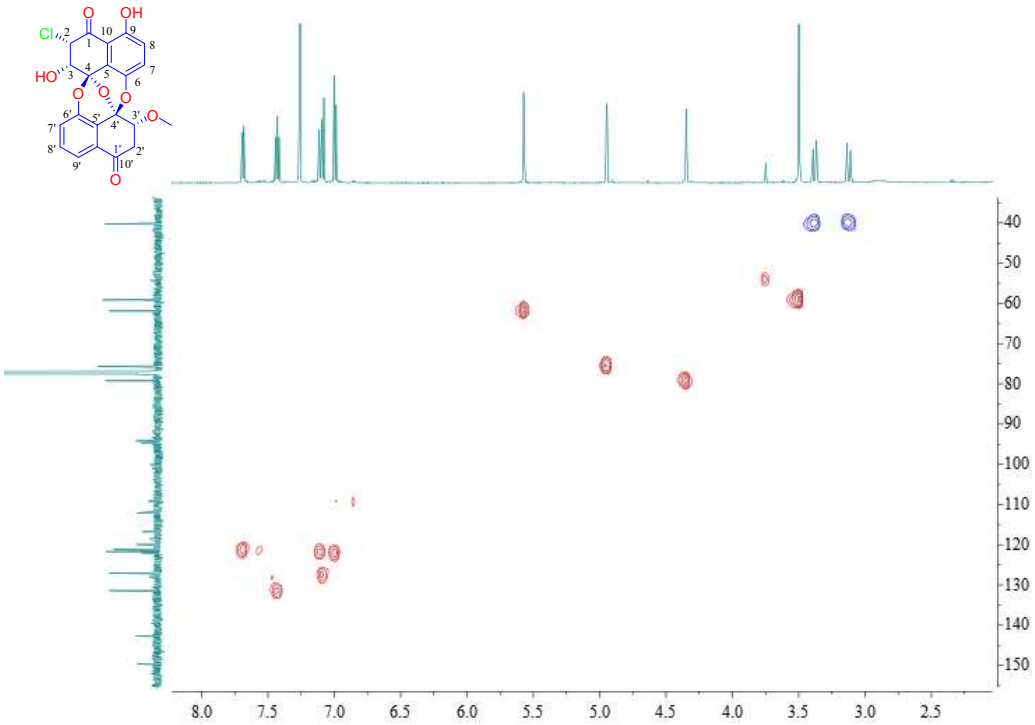


Fig. S6 ^{1}H-^{1}H COSY spectrum of **1** in $CDCl_{35}$

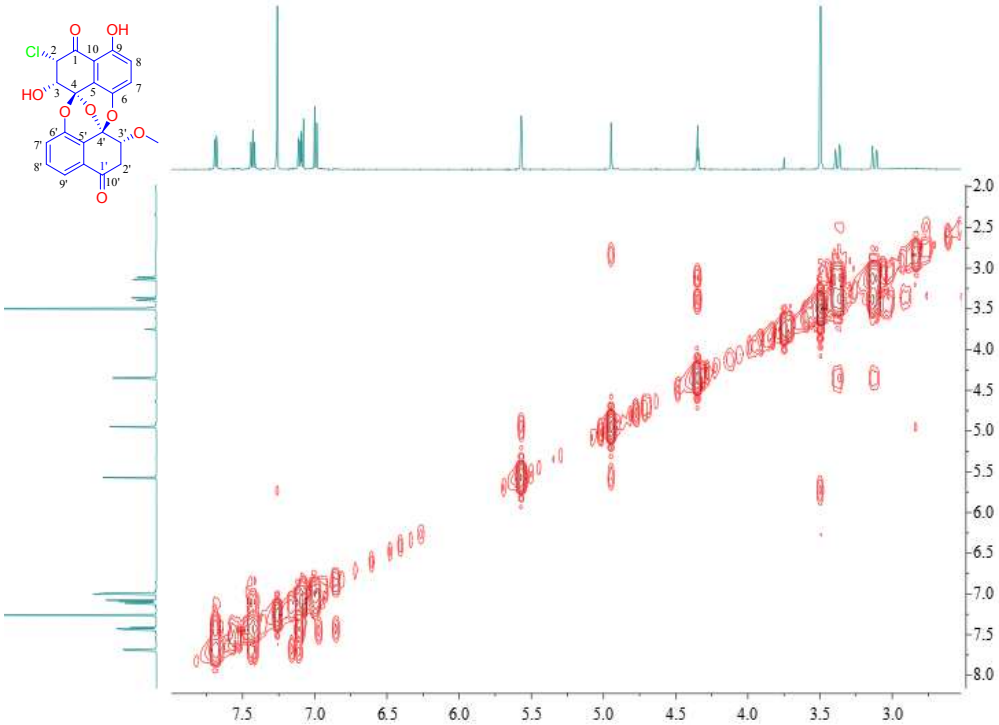


Fig. S7 HMBC spectrum of **1** in $CDCl_3$

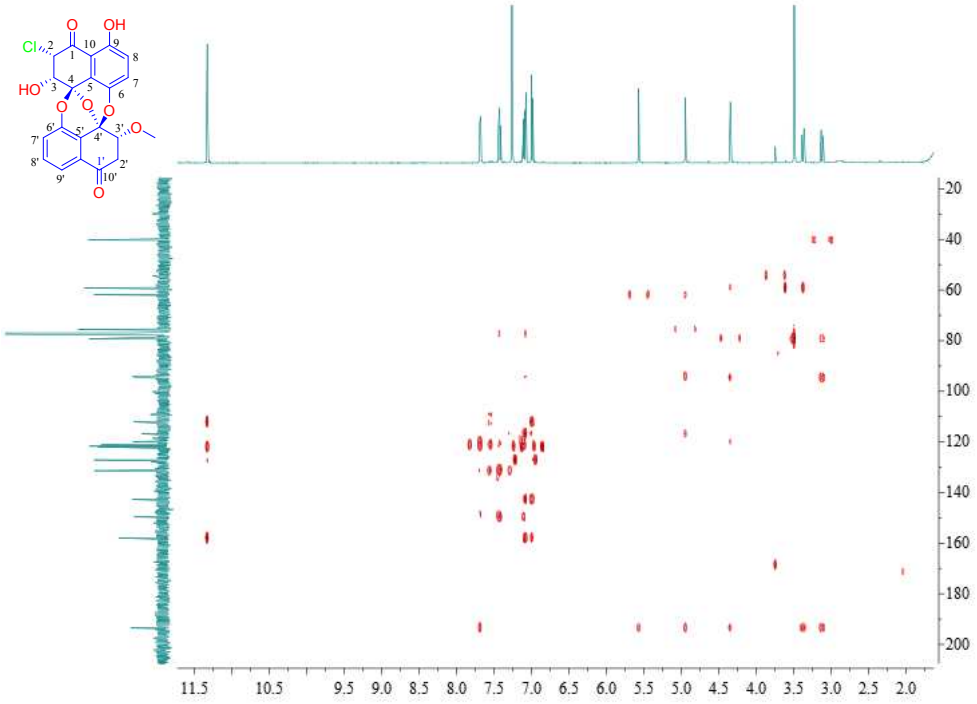


Fig. S8 NOESY spectrum of **1** in $CDCl_3$

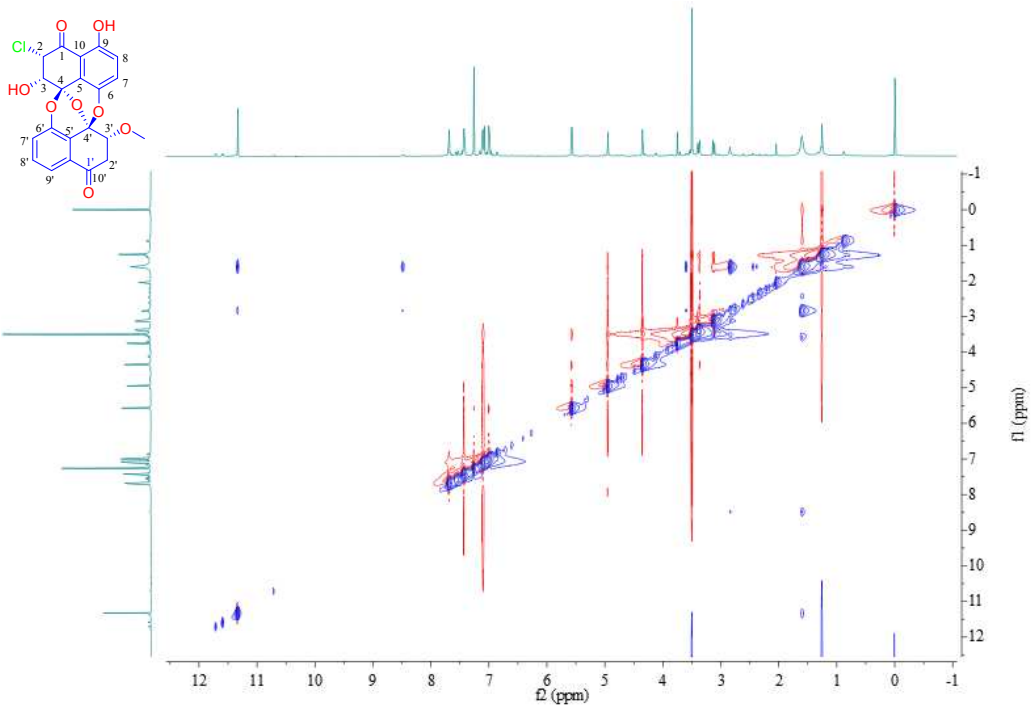


Fig. S9 EIMS spectrum of **2**

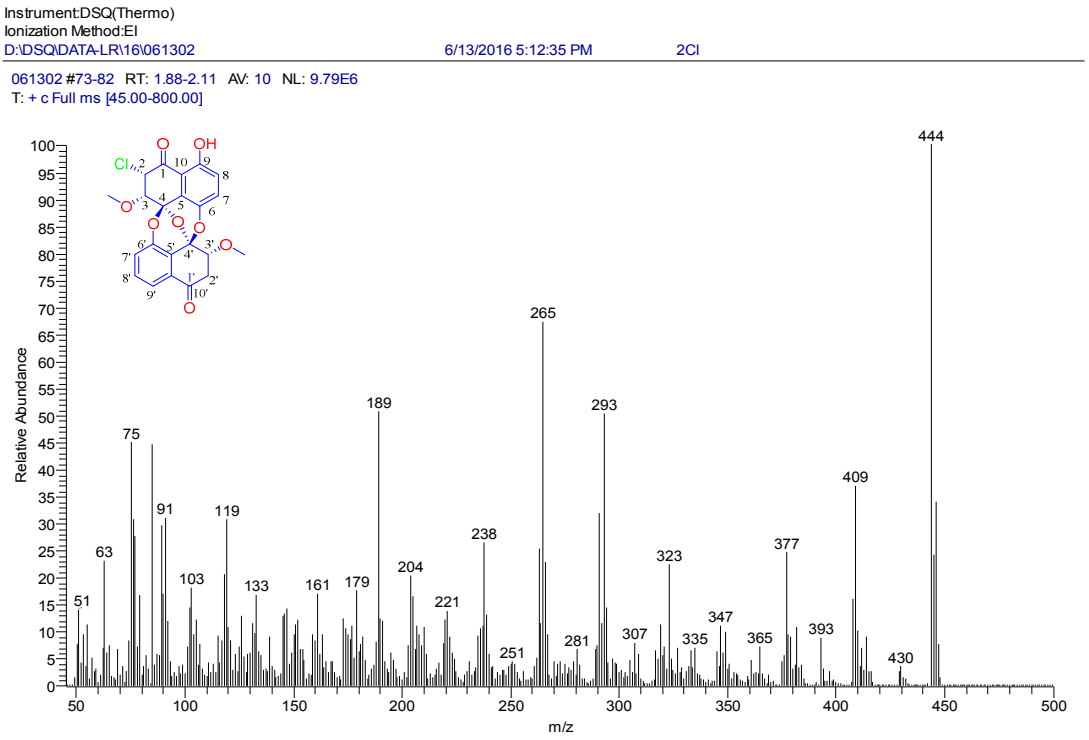


Fig. S10 HREIMS spectrum of **2**

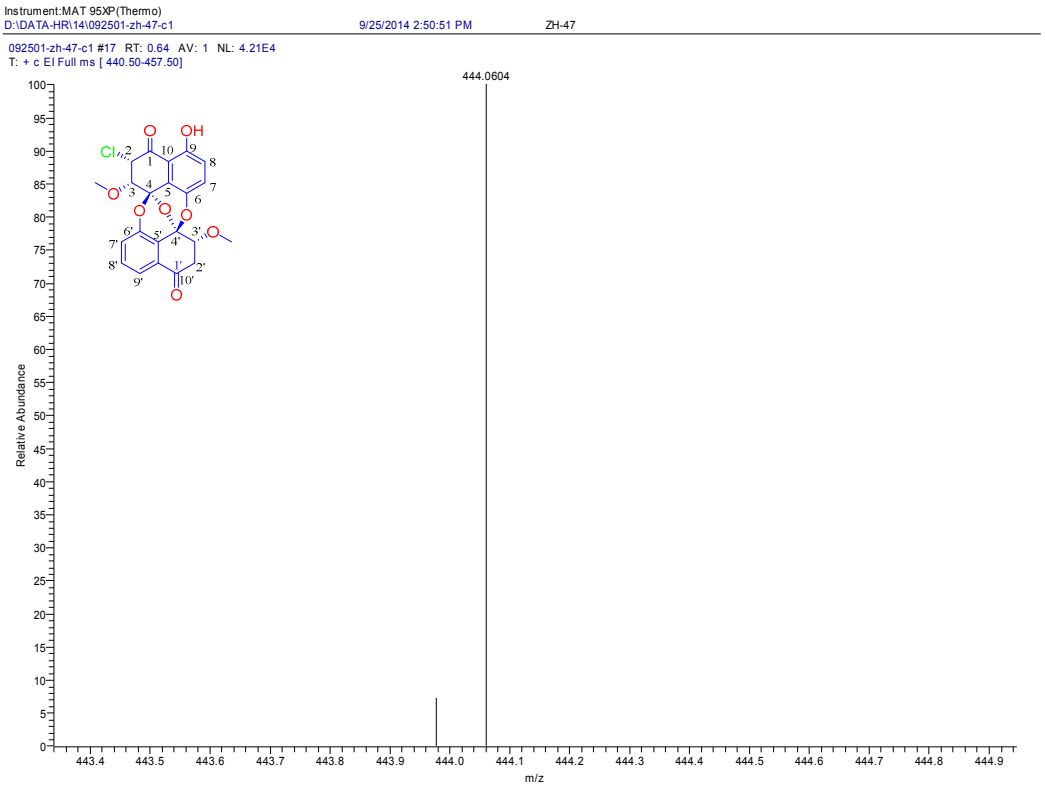


Fig. S11 ^{1}H NMR spectrum of **2** in $CDCl_3$

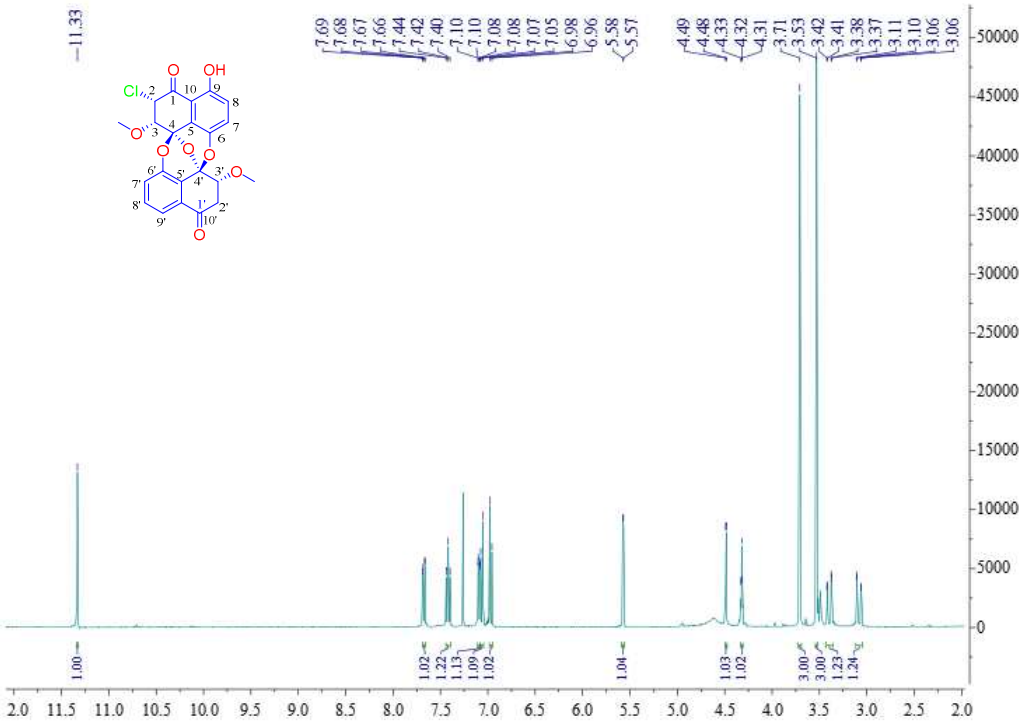


Fig. S12 ^{13}C NMR spectrum of **2** in $CDCl_3$

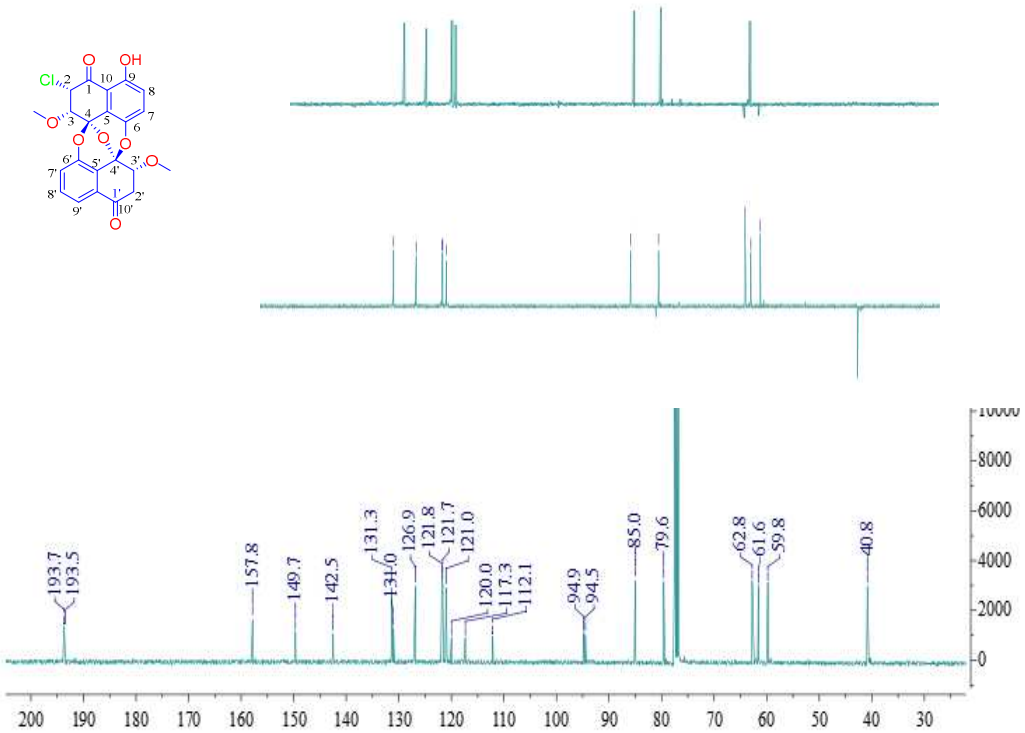


Fig. S13 HSQC spectrum of **2** in $CDCl_3$

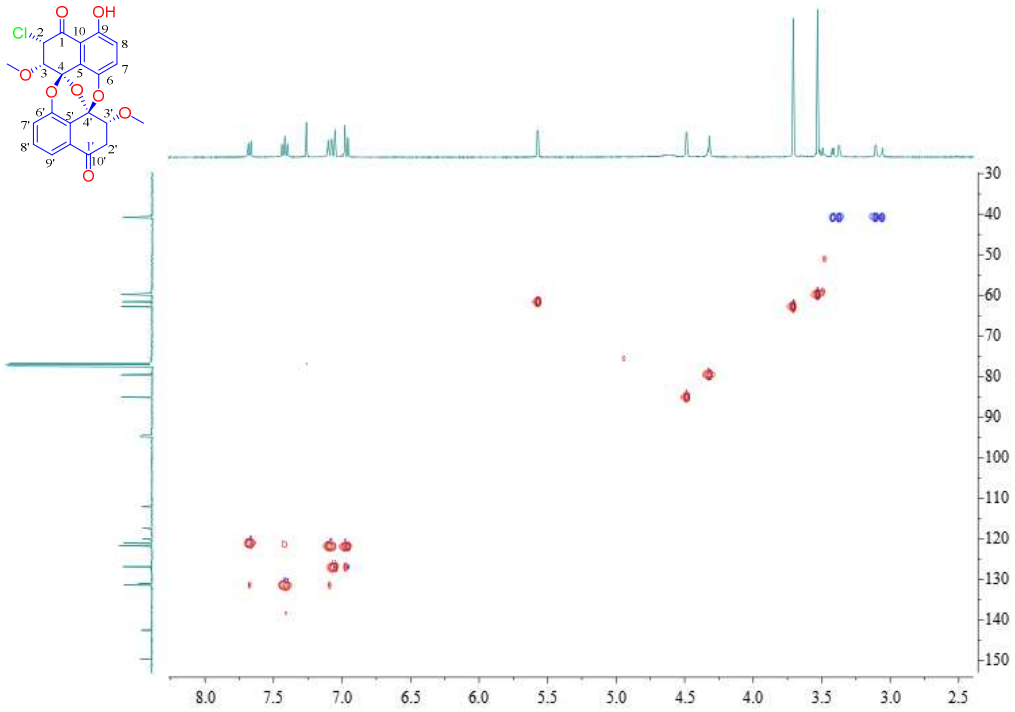


Fig. S14 ^{1}H-^{1}HCOSY spectrum of **2** in $CDCl_3$

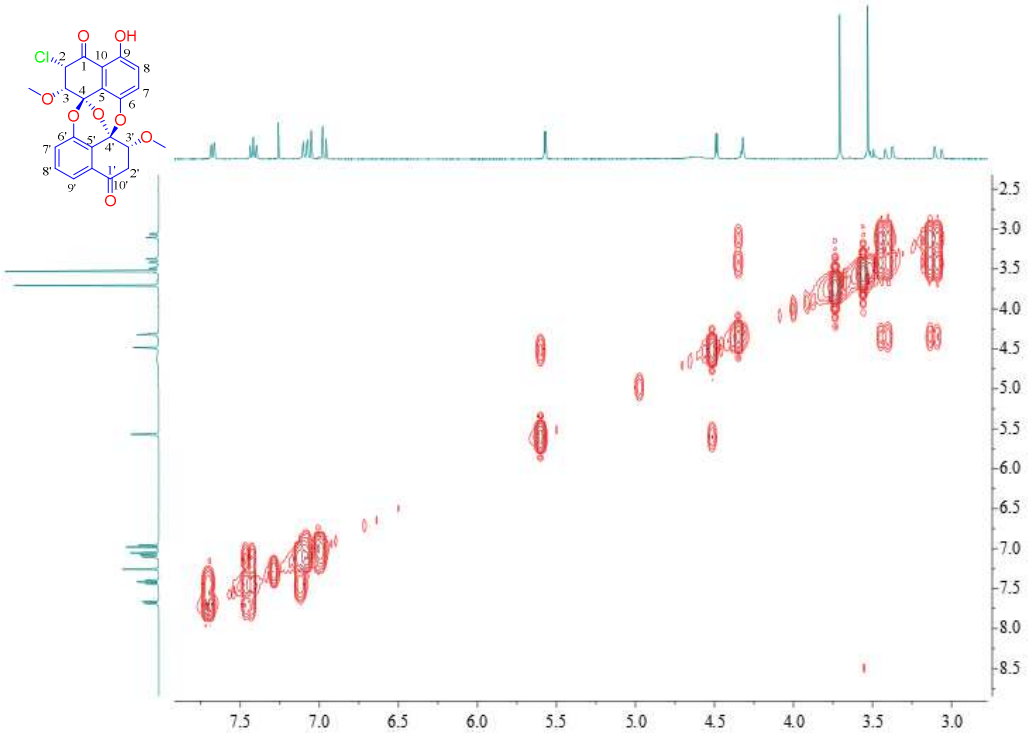


Fig. S15 HMBC spectrum of **2** in $CDCl_3$

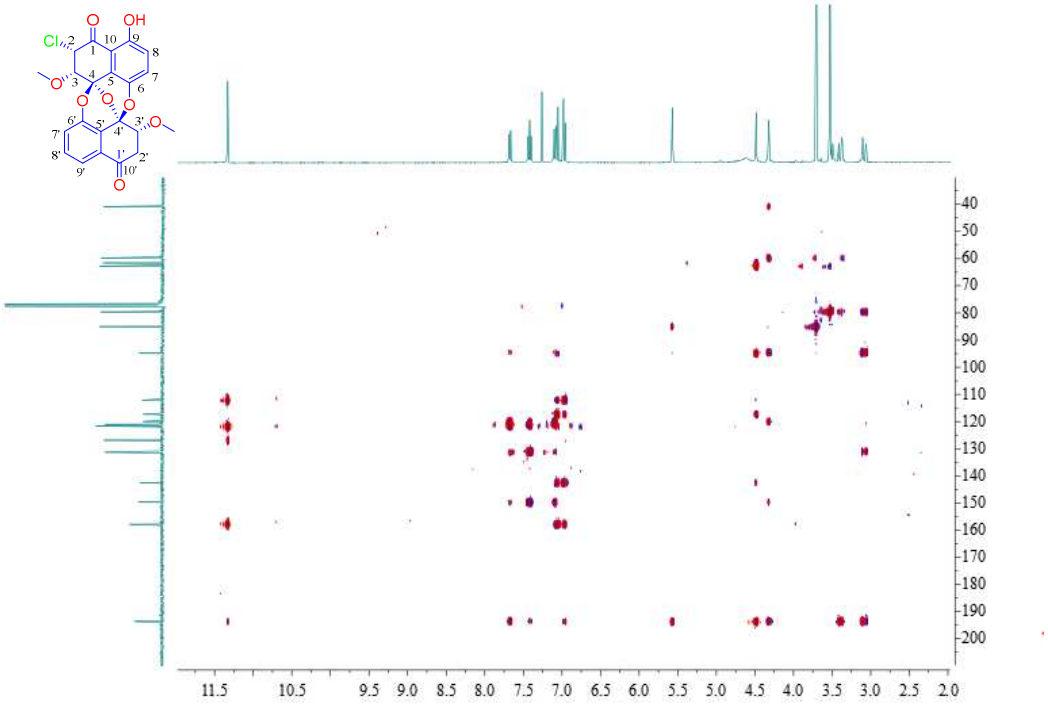


Fig. S16 NOESY spectrum of **2** in $CDCl_3$

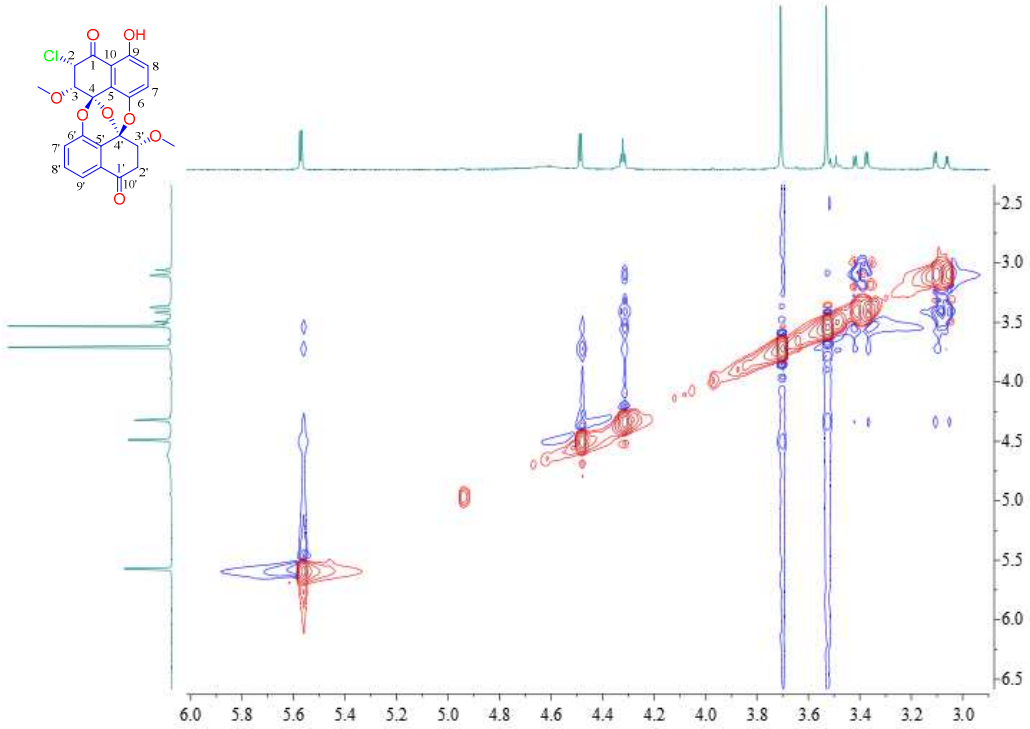


Fig. S17 HRESIMS spectrum of **3**

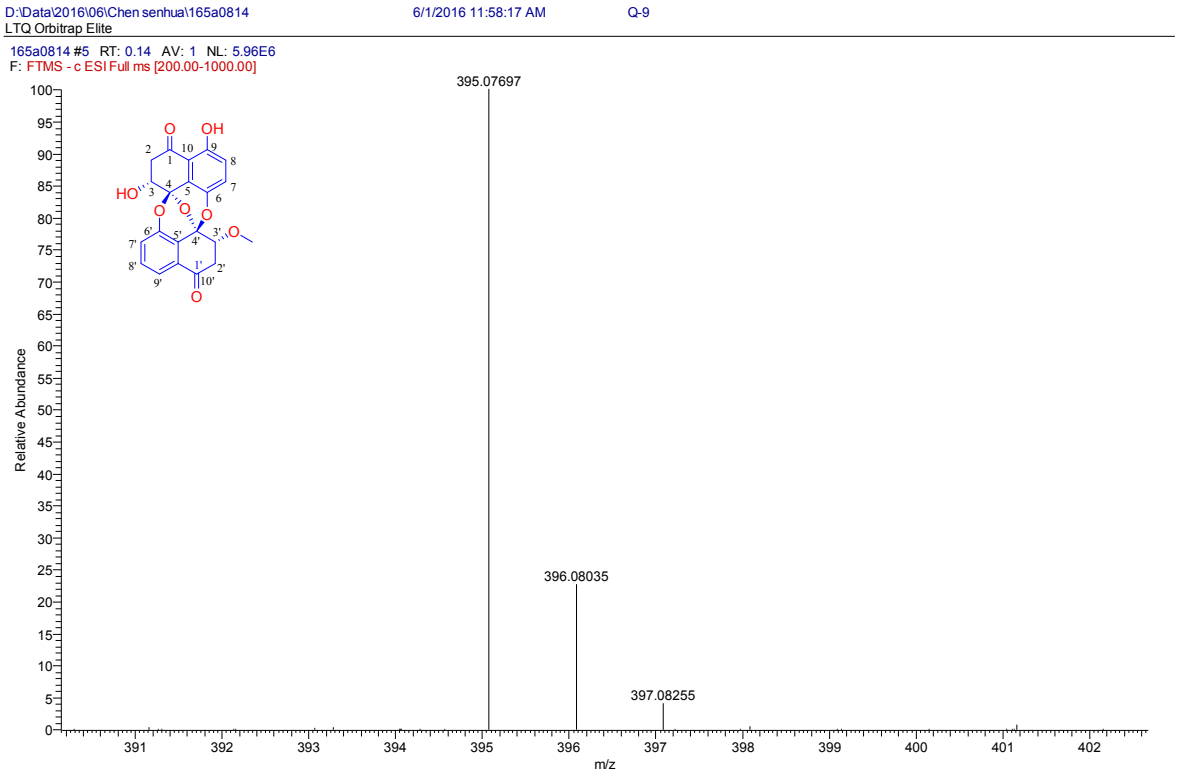


Fig. S18 ^{1}H NMR spectrum of **3** in $CDCl_3$

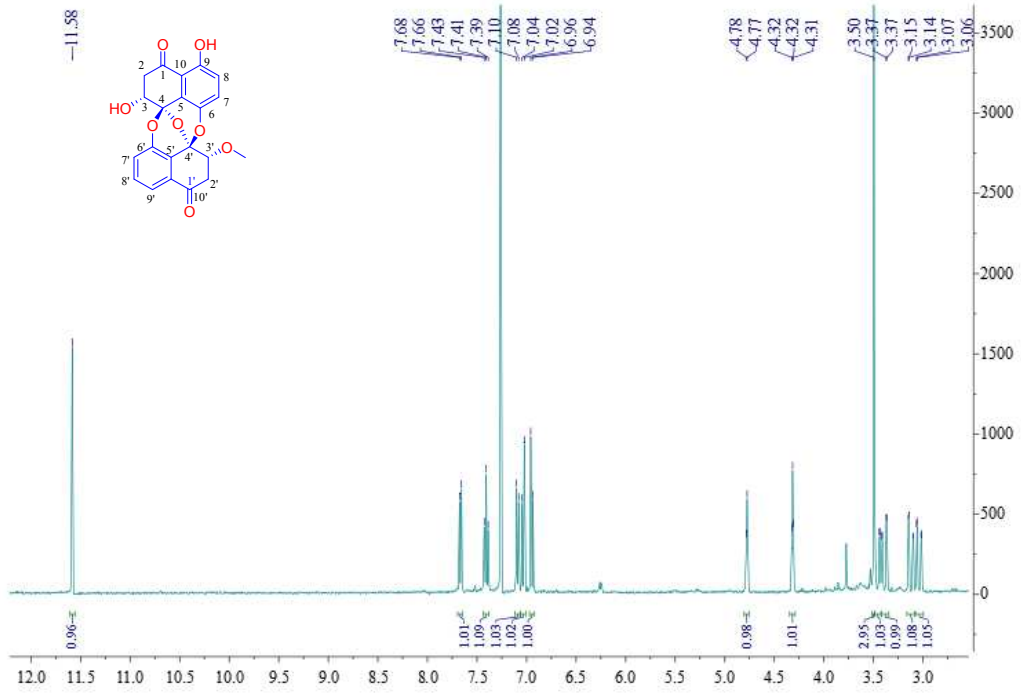


Fig. S19 ^{13}C NMR spectrum of **3** in $CDCl_3$

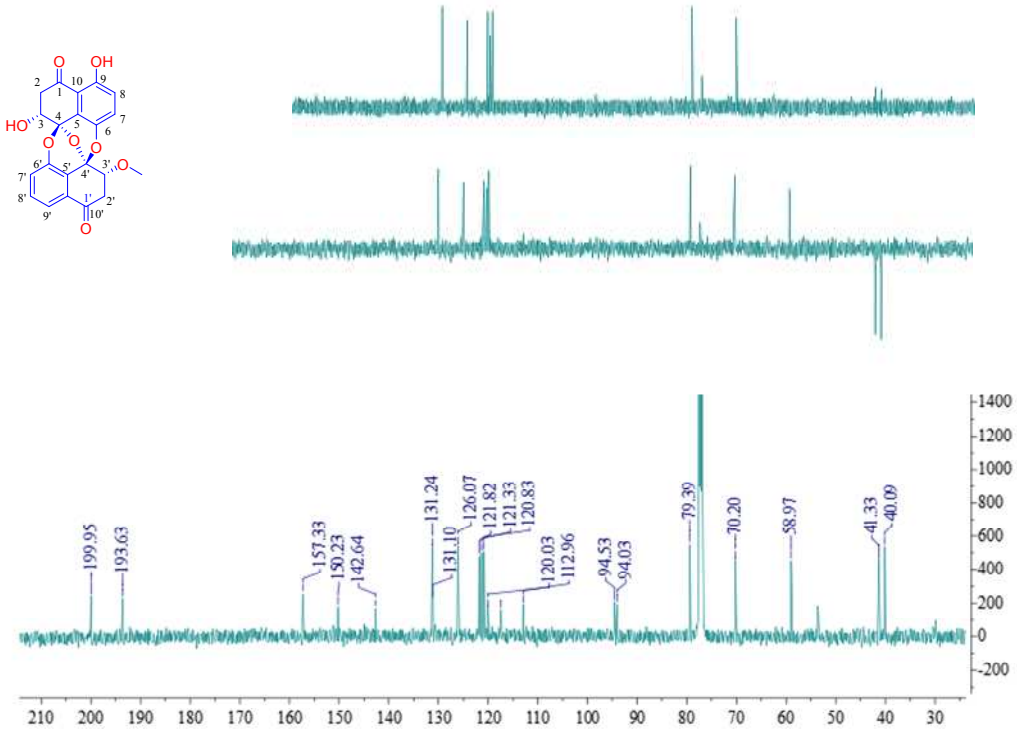


Fig. S20 HSQC spectrum of **3** in $CDCl_3$

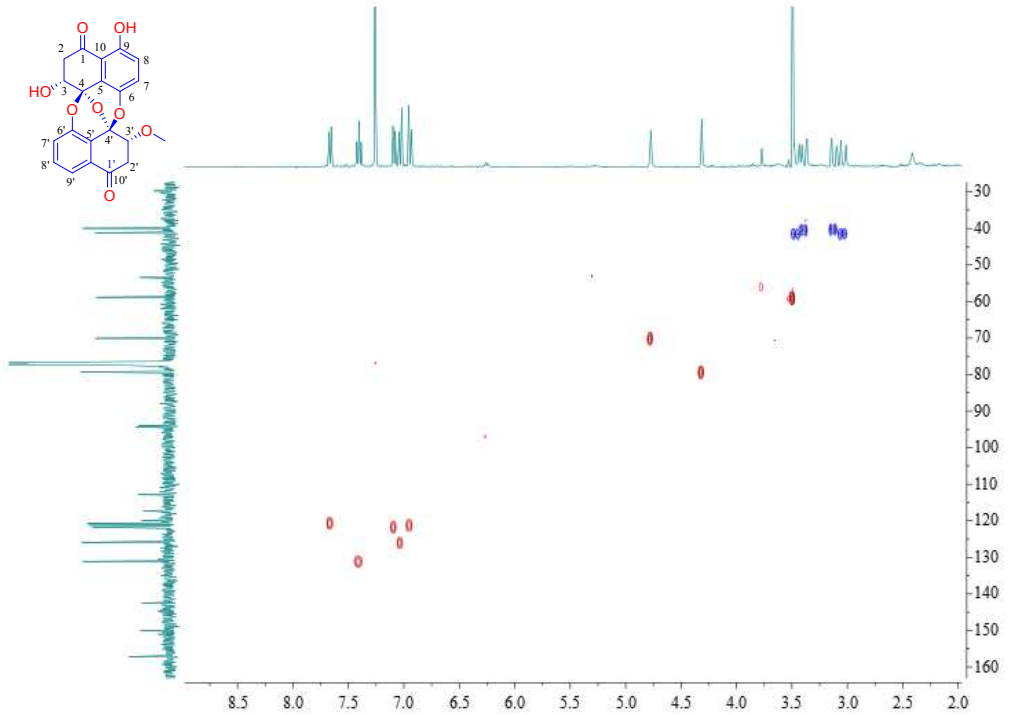


Fig. S21 ^{1}H-^{1}HCOSY spectrum of **3** in $CDCl_3$

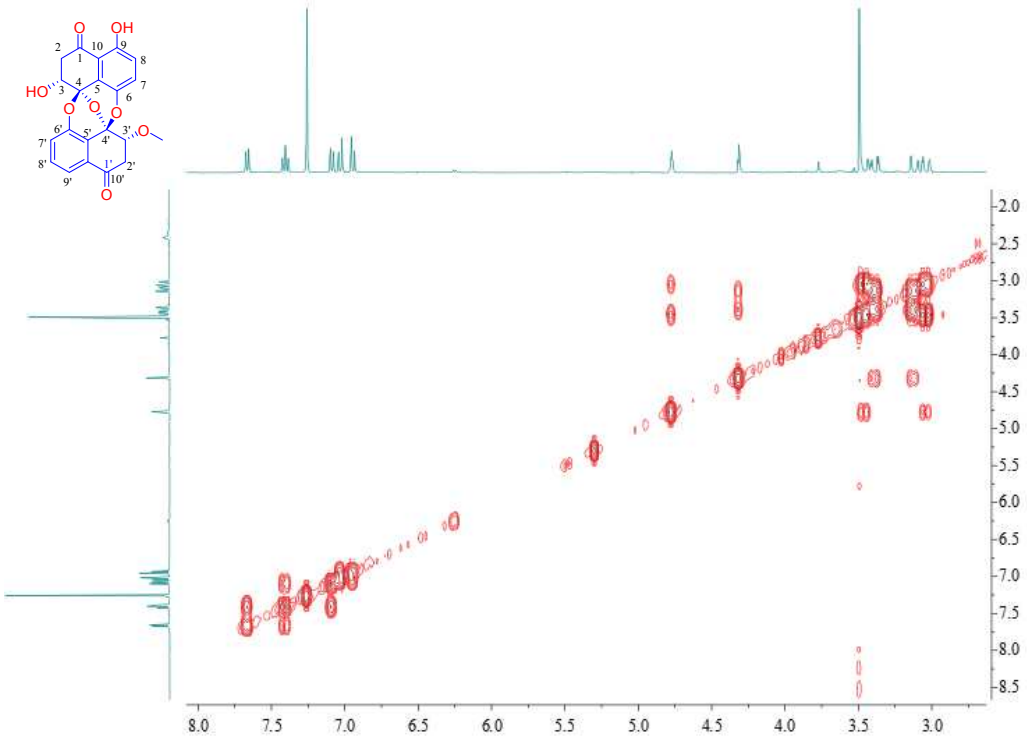
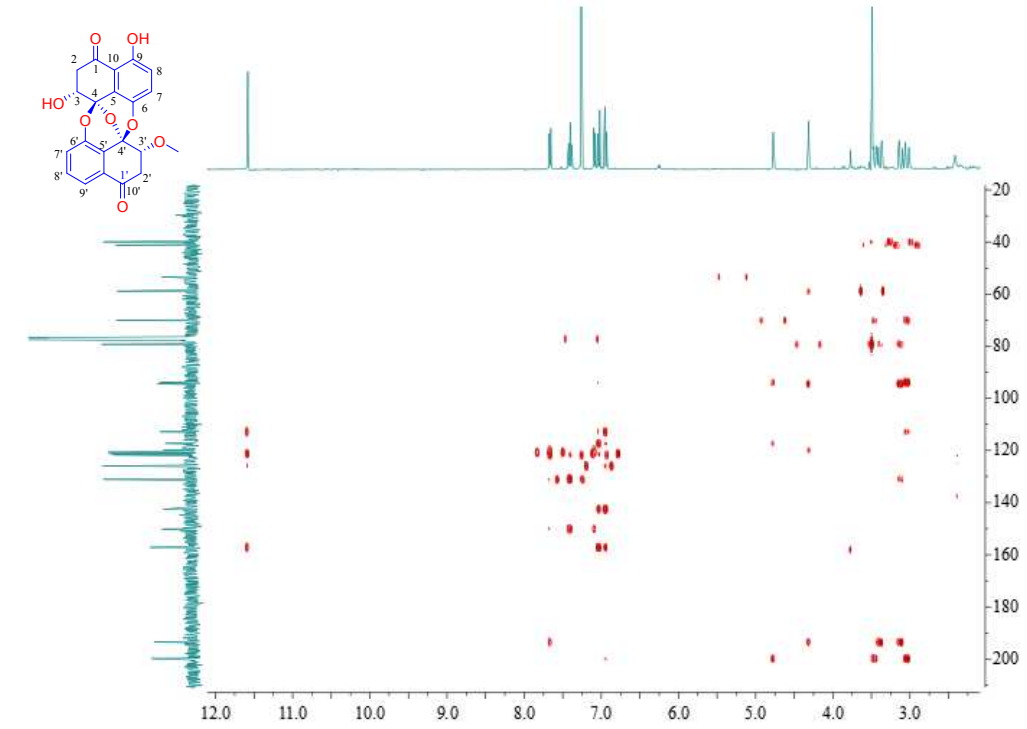


Fig. S22 HMBC spectrum of **3** in $CDCl_3$



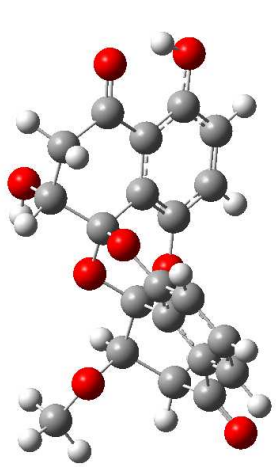
Computational details

Molecular Merck force field (MMFF) and DFT/TD-DFT calculations were carried out with Spartan' 14 software (Wavefunction Inc., Irvine, CA, USA) and Gaussian 09 program, respectively. Conformers within 10 kcal/mol energy window were generated and optimized using DFT calculations at B3LYP/6-31G(d) level. Conformers with Bolzmann distribution over 1% were chosen for ECD calculations in methanol at B3lYP/6-311+g(2d,p) level. The IEF-PCM solvent model for MeOH was used. ECD spectra were generated using the program SpecDis 3.0 (University of Würzburg, Würzburg, Germany) and OriginPro 8.5 (OriginLab, Ltd., Northampton, MA, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.30 ev. All calculations were performed by Tianhe-2 in National Super Computer Center in Guangzhou.

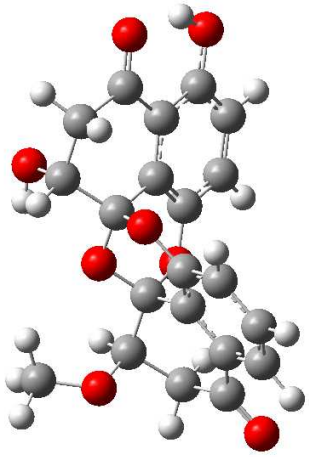
Table S1. Energy Analysis for the Conformers of (3*R*,4*S*,3'*R*,4'*S*)-**3** and (3*S*,4*R*,3'*S*,4'*R*)-**3**.

compound	Conformation	G (Hartree)	G (Kcal/mol)	ΔG (Kcal/mol)	Boltzmann Dist (%)
(3*R*,4*S*,3'*R*,4'*S*) **-3**	**3-1**	−1411.64971334	−885814.2889	0	25.05
(3*R*,4*S*,3'*R*,4'*S*) **-3**	**3-2**	−1411.65074752	−885814.9379	−0.648950949	74.95
(3*S*,4*R*,3'*S*,4'*R*) **-3**	**3e-1**	−1411.64971334	−885814.2889	0	25.05
(3*S*,4*R*,3'*S*,4'*R*) **-3**	**3e-2**	−1411.65074752	−885814.9379	−0.648950949	74.95

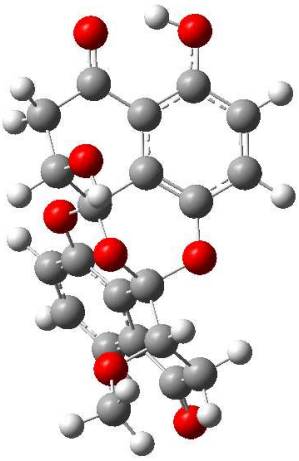
Figure S23. B3LYP/6-31G(d) optimized low-energy conformers of **3** and **3e**.



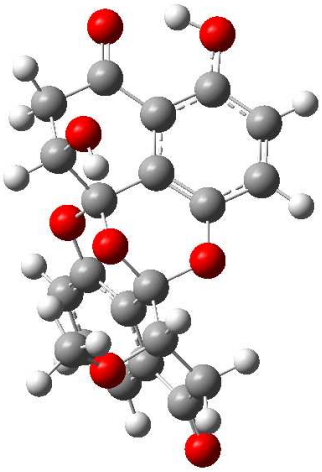
3-1



3-2



3e-1



3e-2

References.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell,

A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision C.01. Gaussian, Inc.: Wallingford CT, 2010.Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Bringmann, G. SpecDis: Quantifying the comparison of calculated and experimental electronic circular dichroism spectra. Chirality 2013, 25, 243–249.