SUPPORTING INFORMATION

Title: (+)- and (–)-Ascomlactone A, a pair of Novel Dimeric Polyketides from a Mangrove Endophytic Fungus *Ascomycota* sp. SK2YWS-L

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X-ray crystallographic data for (±)-ascomlactone A

Crystal data and structure refinement for **1** are as follows:

Empirical formula	$C_{32}H_{26}O_{11}$	
Formula weight	586.53	
Temperature	293(2) K	
Wavelengh	1.54178 Å	
Crystal system	Monoclinic	
Space group	P_1	
Unit cell dimensions	a= 8.8974(2) Å	α= 102.767(2) °
	b= 11.2339(2) Å	β= 96.993(2) °
	c= 15.5141(3) Å	γ= 90.2390(10) °
Volume	1500.26(5) $Å^3$	
Z	2	
Density (calculated)	1.130 Mg/m^3	
Absorption coefficient	0.832 mm^{-1}	
F(000)	612	
Crystal size	0.35×0.25×0.15 mm^3	
Theta range for data collection	3.9940 to 73.7430°	
Index ranges	−11 <= h <= 11, −14 <= k <= 14, −19 <= l <= 18	
Reflections collected	43057	
Independent reflections	6009 [R(int)= 0.052]	
Completeness to theta = 66.1980°	99.0%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. Transmission	1.0000 to 0.6168	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6009 /1 /396	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1= 0.0623, ωR2= 0.1933	

R indices (all data) R1= 0.0667, ωR2= 0.1977

Data were collected on Agilent Xcalibur Nova single-crystal diffractometer using Cu Kα radiation. The crystal structure was refined by full-matrix least-squares calculation. Crystallographic data for the structure has been deposited in the Cambridge Crystallographic Data Centre (deposition number: CCDC 1570929). Copies of these data can be obtained free of charge via www.ccdc.cam.au.ck/conts/retrieving.html(or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK.; fax: (t44) 1223-336-033; or deposit@ccd.cam.ac.uk)·

Table S1. Energy analysis for the Conformers of **1b**.

compounds	Conformation	G (Hartree)	G (Kcal/mol)	ΔG (Kcal/mol)	Boltzmann Dist (%)
1b	**1b**-a	−2062.50732765	−1294229.329	1.9978	3.13%
	1b-b	−2062.50681352	−1294229.007	2.3204	1.81%
	1b-c	−2062.50630896	−1294228.69	2.6370	1.06%
	1b-d	−2062.50719279	−1294229.245	2.0824	2.71%
	1b-e	−2062.51051138	−1294231.327	0.0000	91.29%

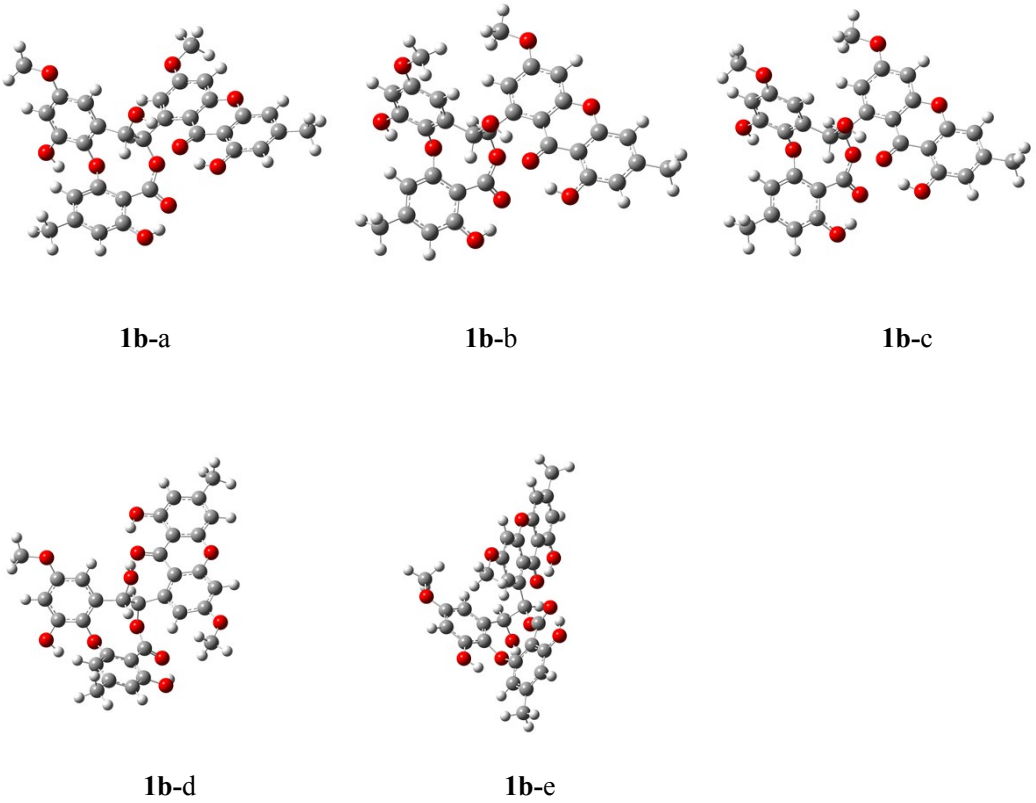


Figure S1. B3LYP/6-31G(d) optimized low-energy conformers of **1b**.

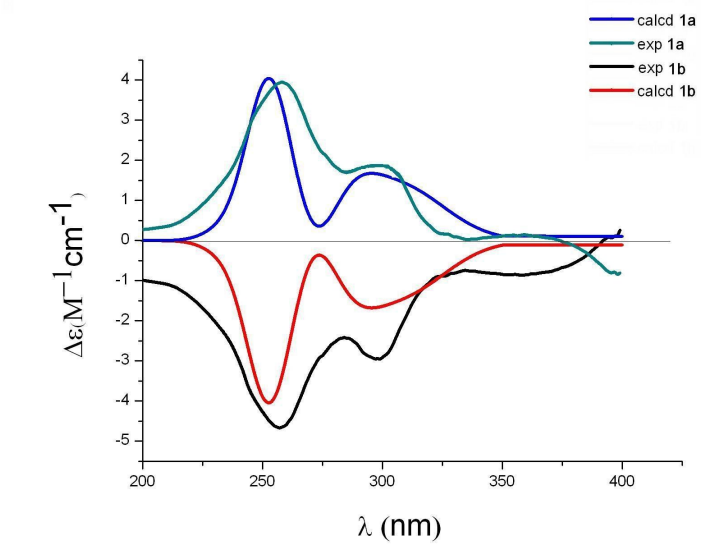


Figure S2. Comparison of the experimental ECD spectra of **1a** and **1b** with the B3lYP/6-311+g(2d,p) calculated spectrum in MeOH. σ = 0.26 eV.

Figure S3. ^{1}H NMR spectrum of (±)-ascomlactone A in DMSO (600 MHz).

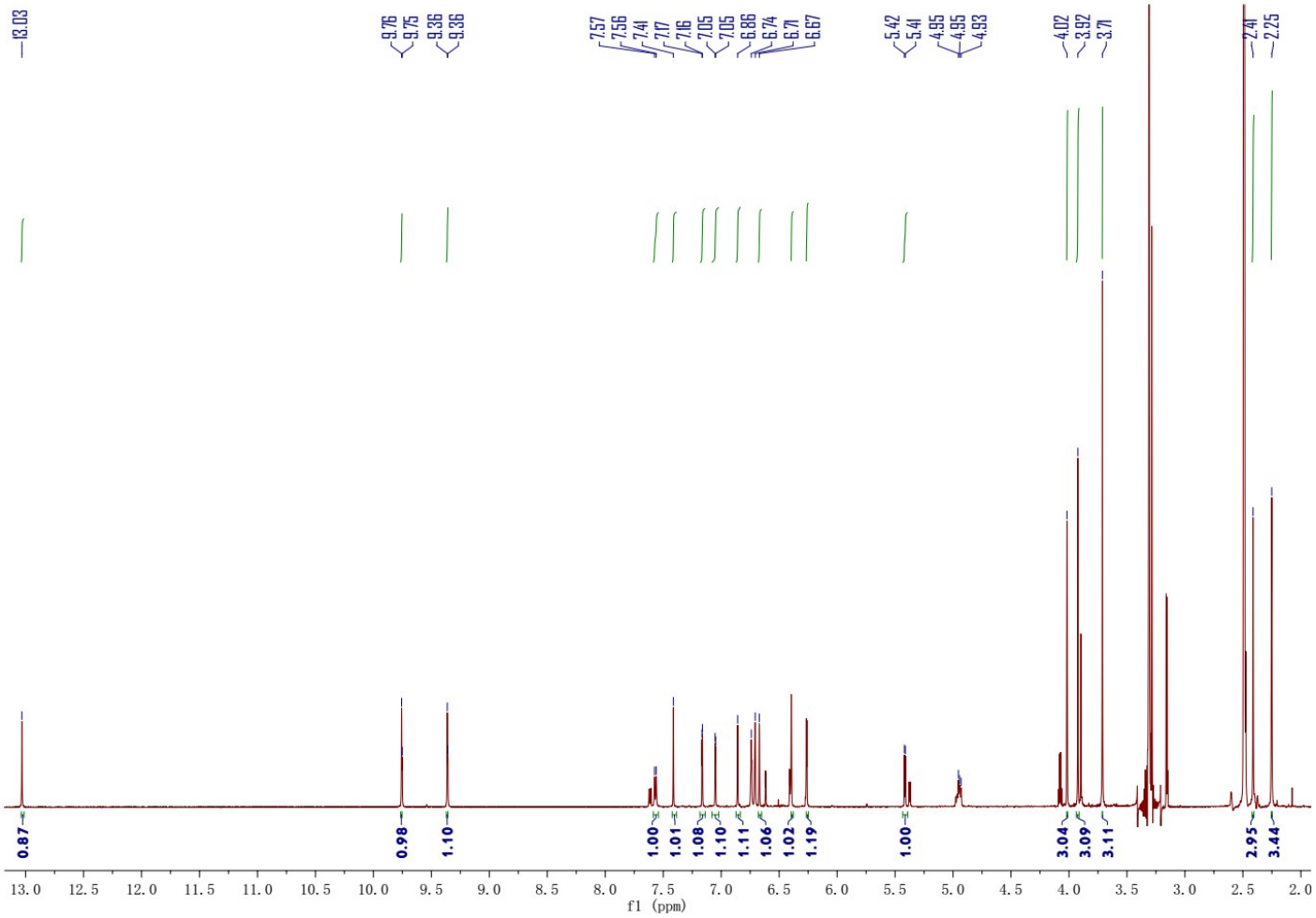


Figure S4. ^{13}C NMR spectrum of (±)-ascomlactone A in DMSO (150 MHz).

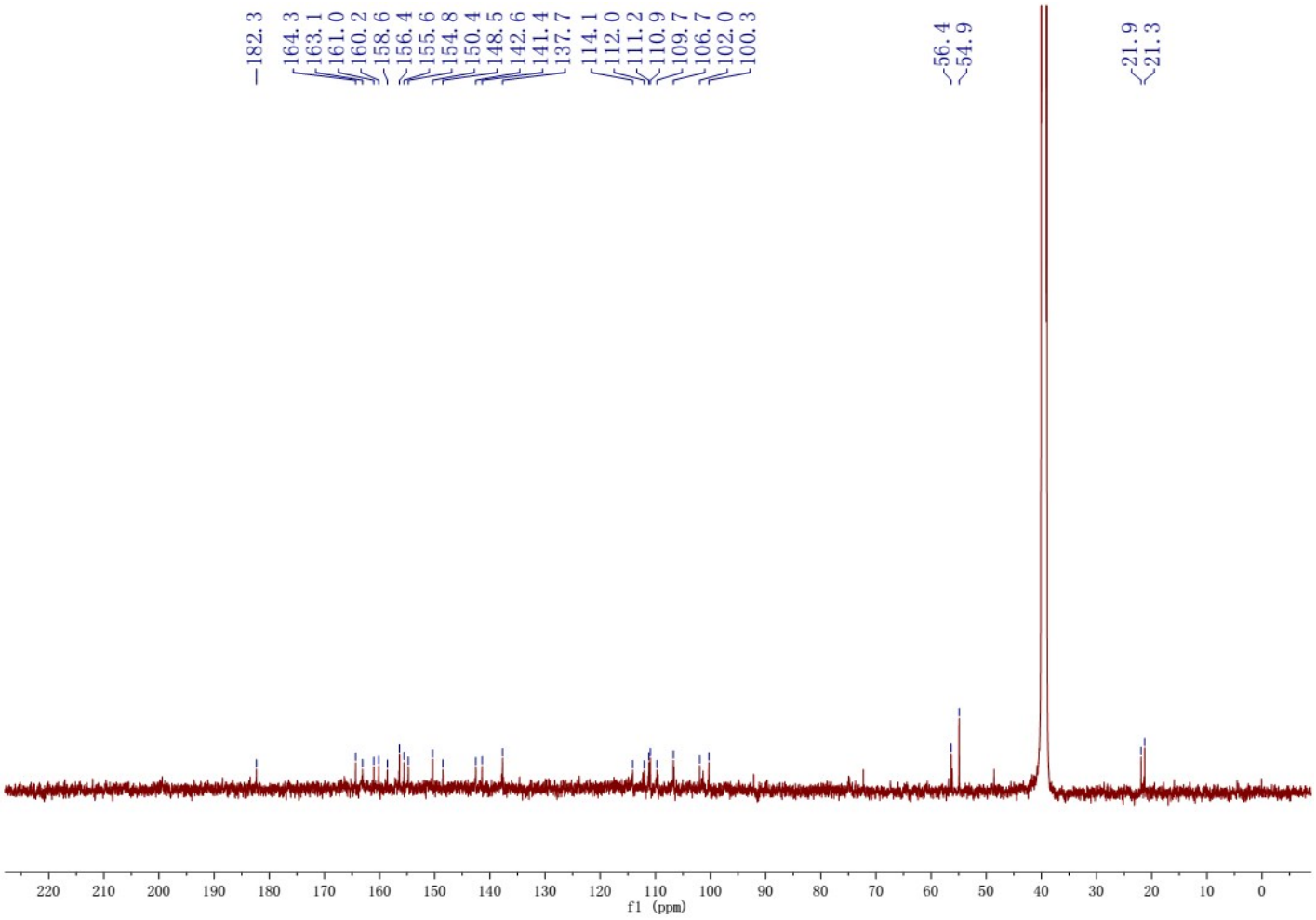


Figure S5. DEPT-90° spectrum of (±)-ascomlactone A in DMSO (150 MHz).

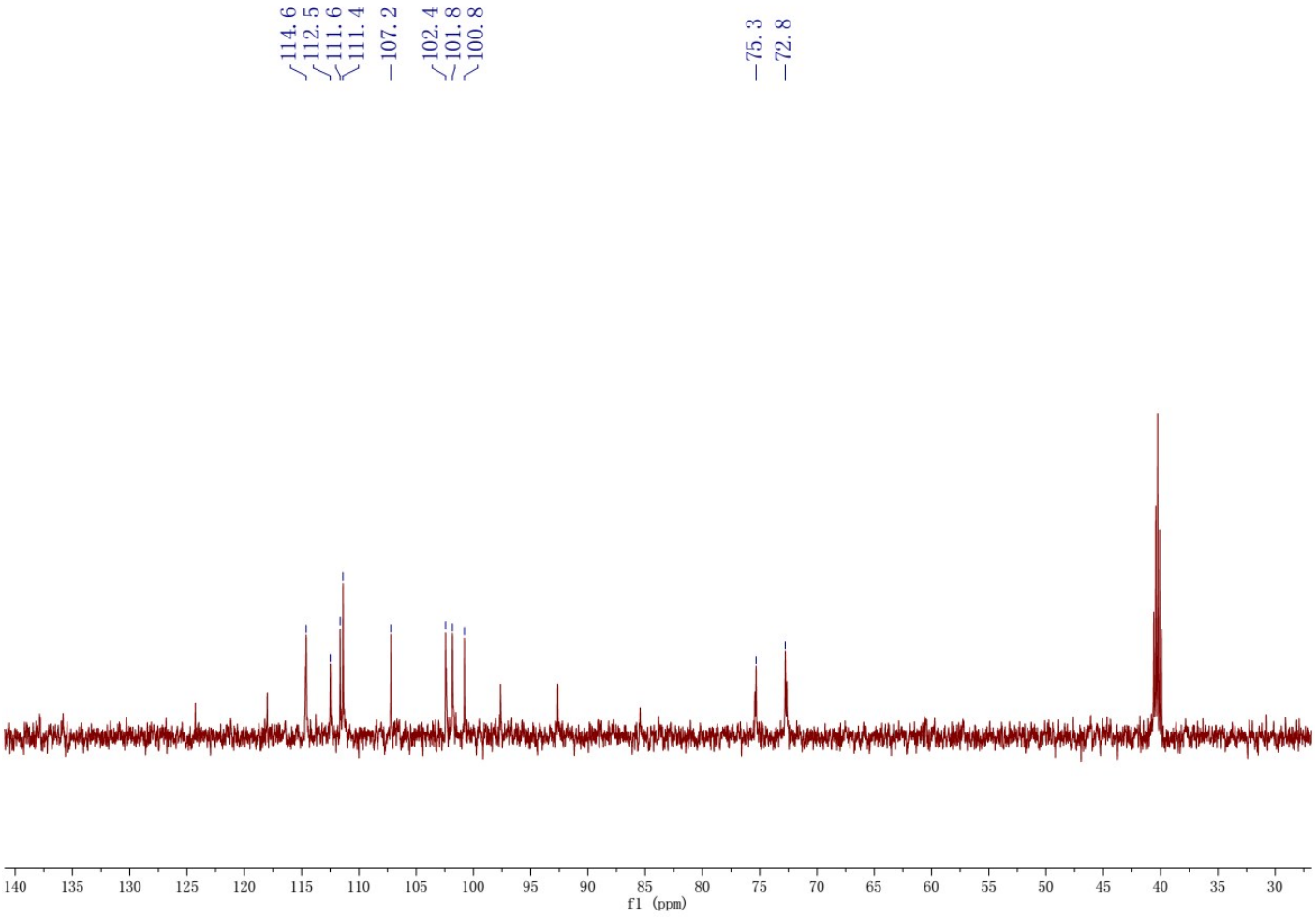


Figure S6. DEPT-135° spectrum of (±)-ascomlactone A in DMSO (150 MHz).

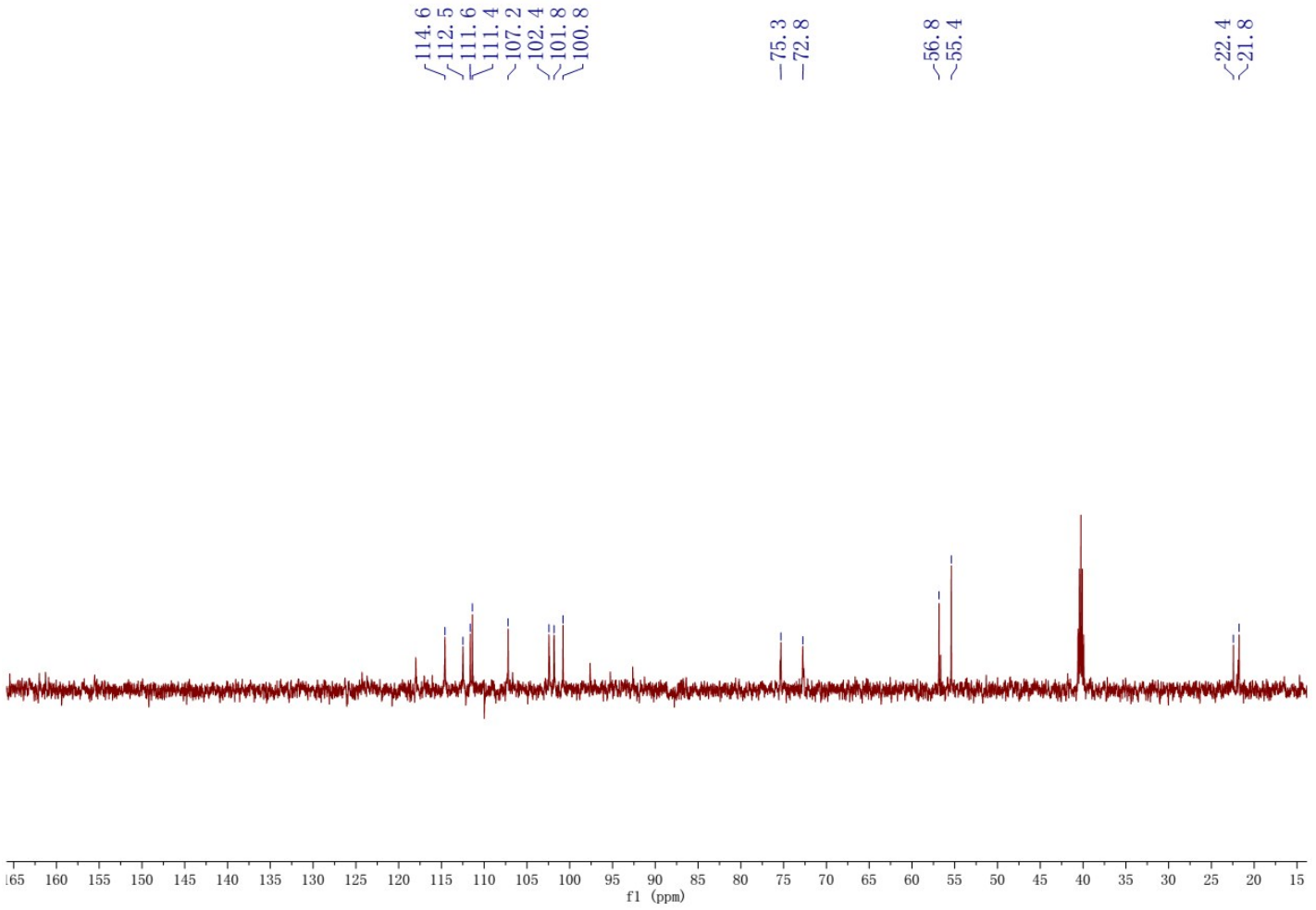


Figure S7. ^{1}H-^{1}H COSY spectrum of (±)-ascomlactone A in DMSO (600 MHz).

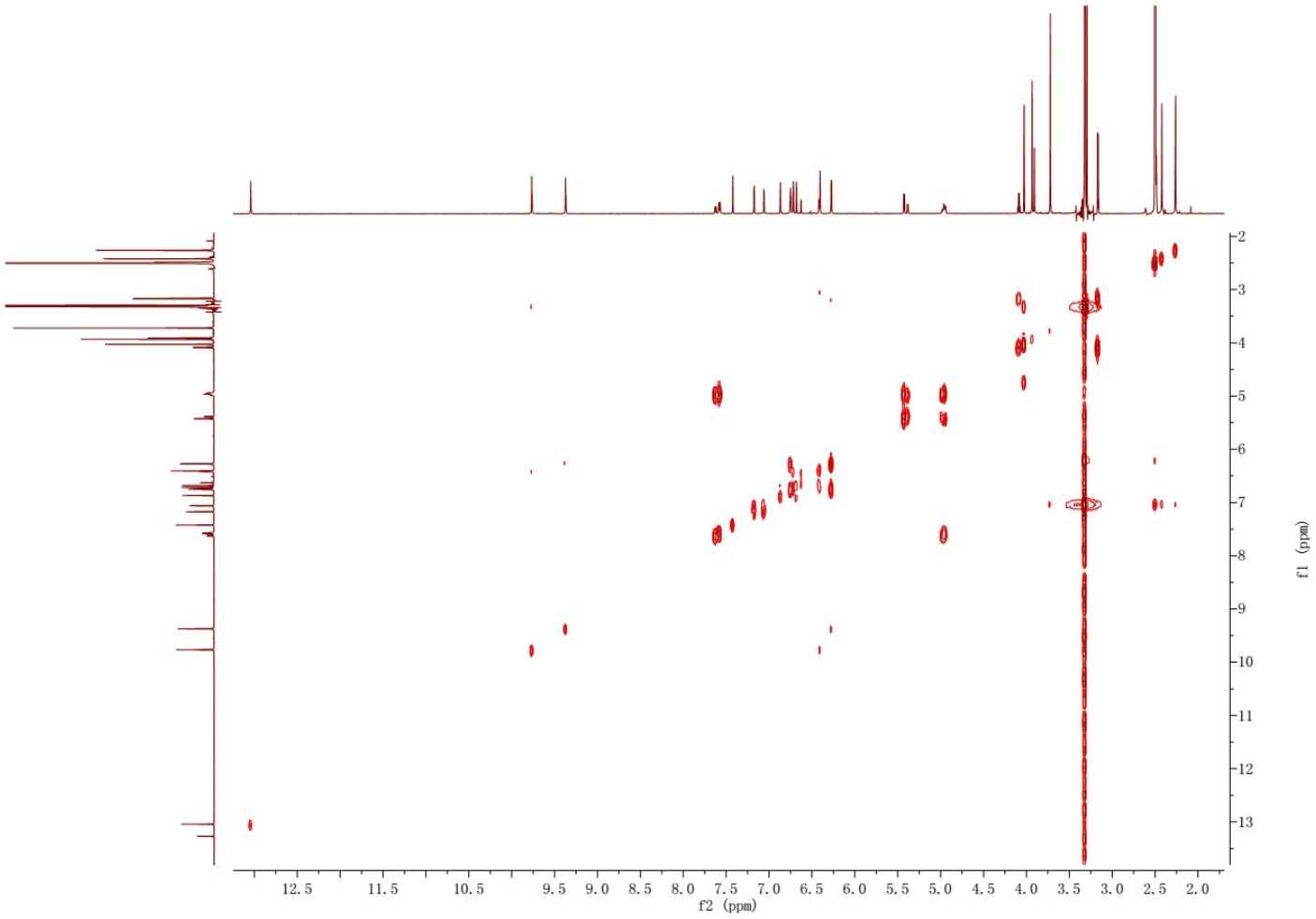


Figure S8. HSQC spectrum of (±)-ascomlactone A in DMSO (600 MHz).

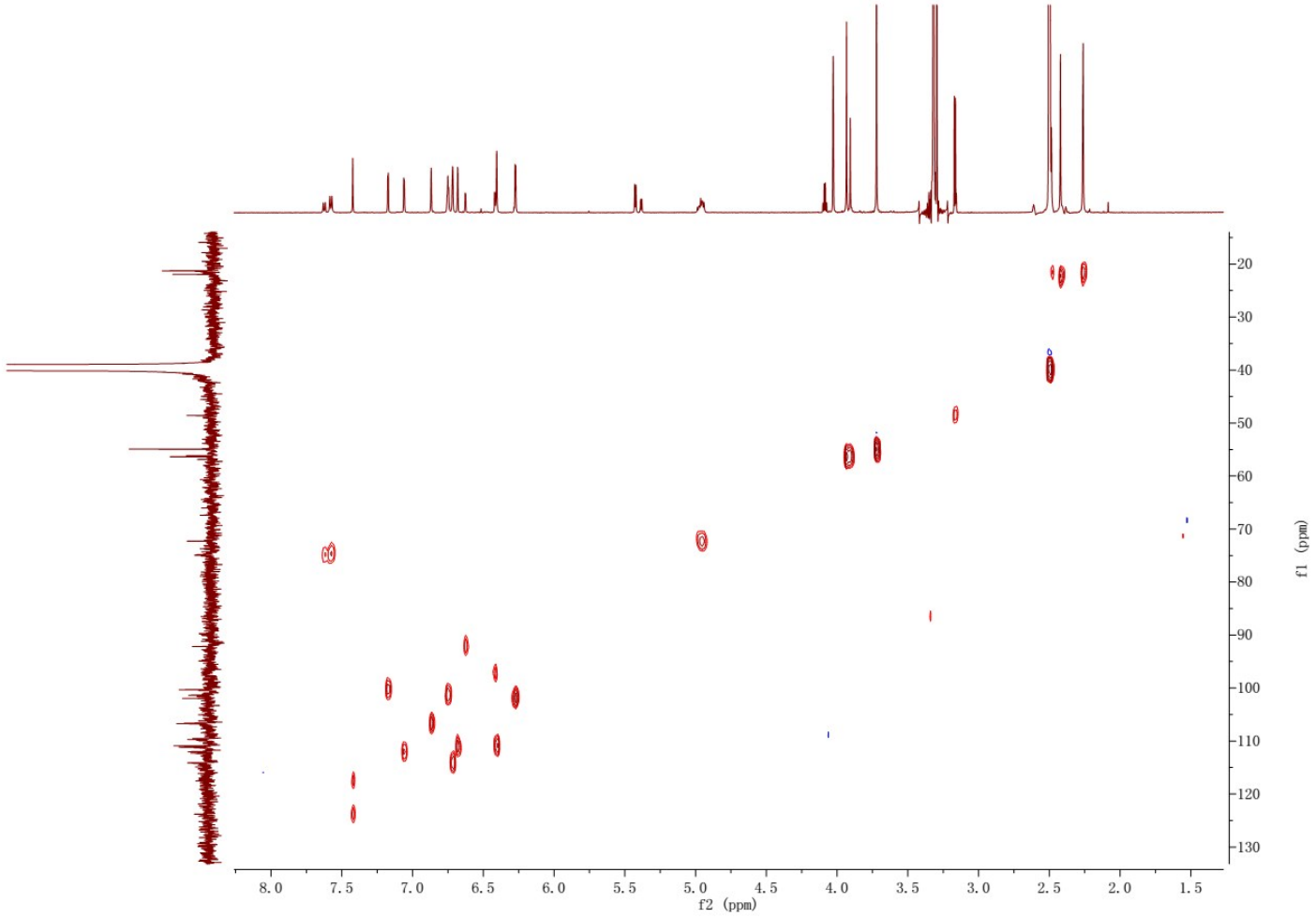


Figure S9. HMBC spectrum of (±)-ascomlactone A in DMSO (600 MHz).

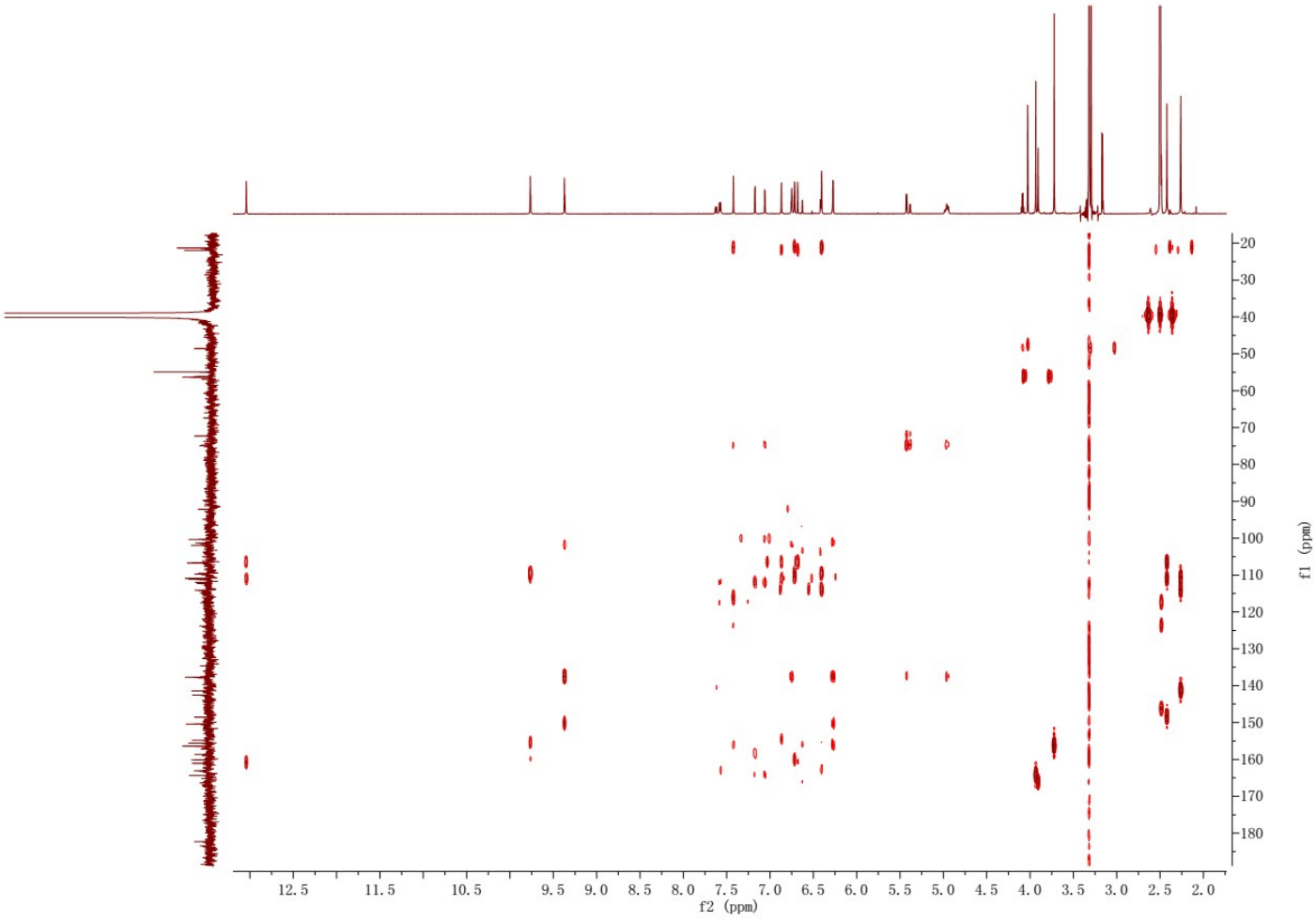
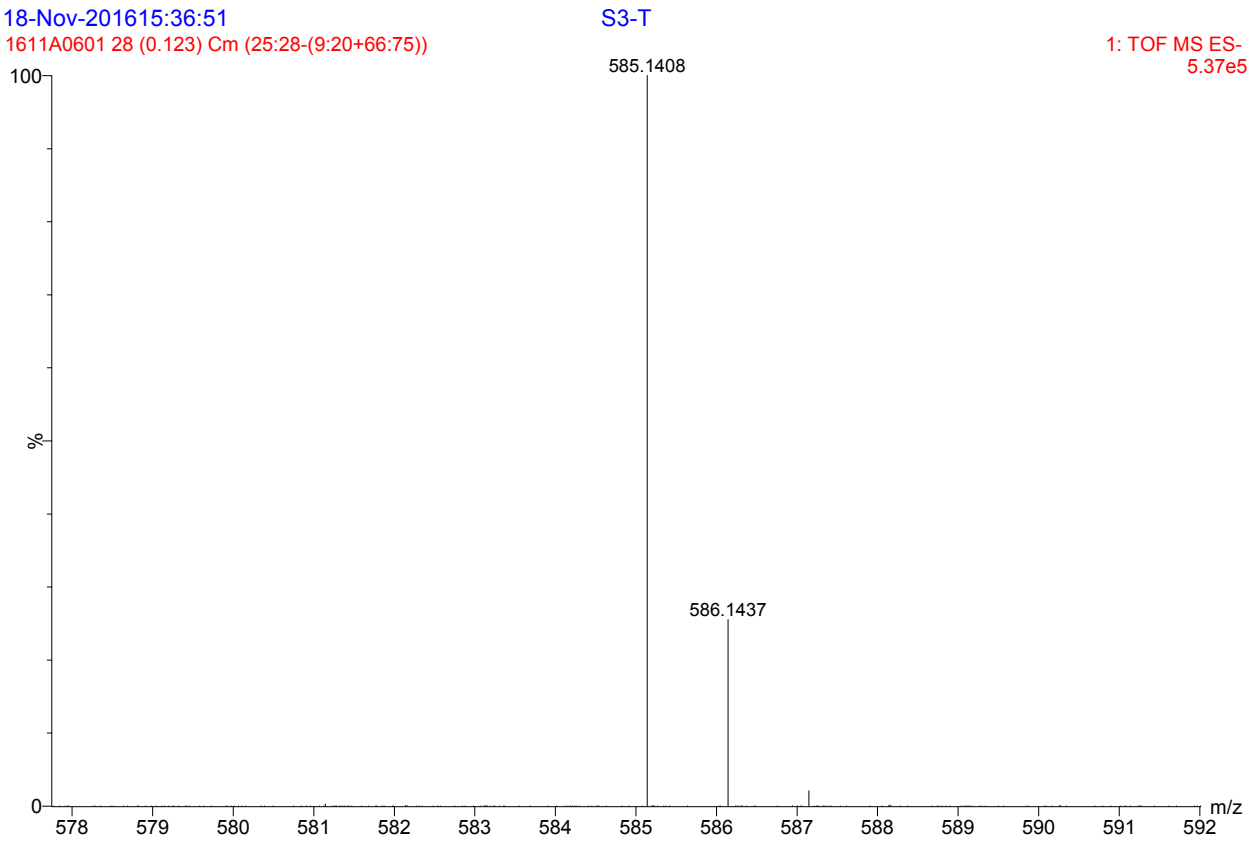


Figure S10. HRESI TOF MS spectrum of (±)-ascomlactone A.



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
585.1408	585.1397	1.1	1.9	20.5	222.1	n/a	n/a	C32 H25 O11

Elemental Composition Report

1. Monoisotopic Mass
2. Elements Used: C: 0-40 H: 0-100 O: 0-20
3. Tolerance = 5.0 PPM

Figure S11. HPCL spectrum of (±)-ascomlactone A: C_{18} column (250 × 10 mm, 5 μm); 85% MeOH/H_20; flow rate; 1.5 mL/min.

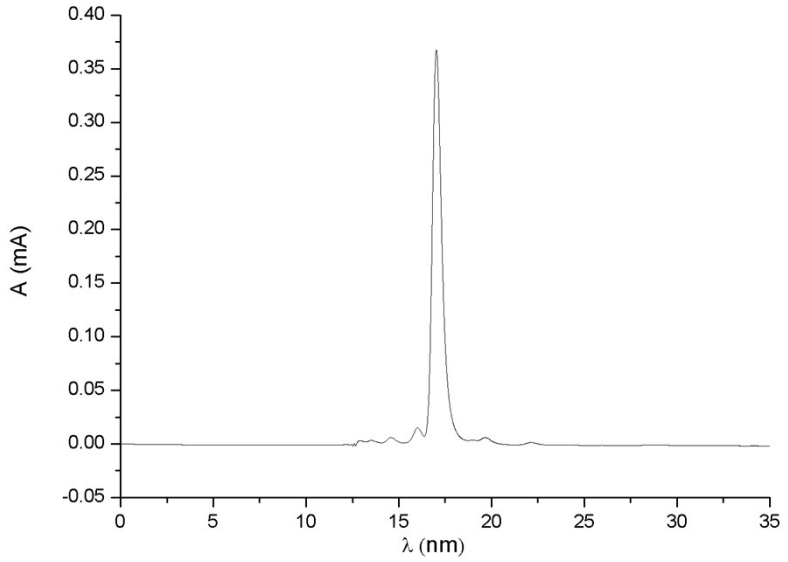


Figure S12. HPLC chiral separation spectrum of (+)-ascomlactone A (**1a**) and (−)-ascomlactone A (**1b**): cellulose-2 (250 × 10 mm, 5 μm); 95% MeOH/H_20; flow rate; 1.0 mL/min. (RT 25.2min with a integration 54.8; RT 28.4 min with a integration 26.1)

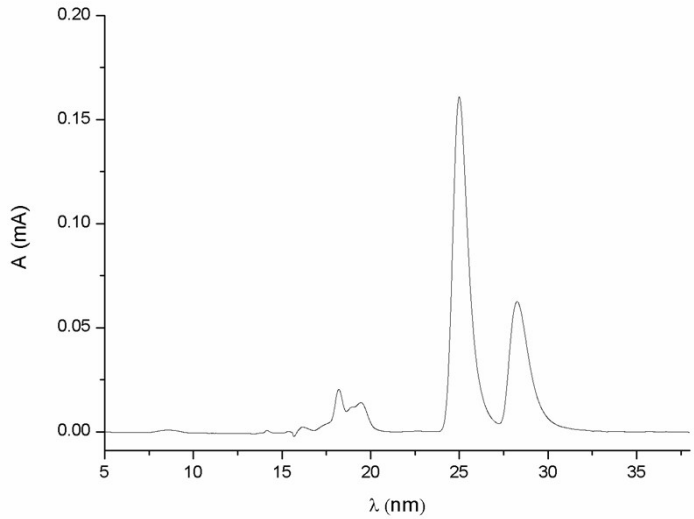


Figure S13. LC-MS of the extract of *Ascomycota* sp. (top), the purified (+)-**1** (middle) and the ESI-MS spectrum of THE peak at RT 4.9 min.