

Supplementary File

New chlamydospore derivatives from the endophytic fungus
Pleosporeles sp. Sigrf05 and their cytotoxic and antimicrobial activities

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Table S1. NCBI blastn results for the ITS sequence of Sigrf05 (Accession No. KT369815.1)

Description	Max Score	Total Score	Query cover	E Value	Per. Ident	Accession
<i>Pleosporales</i> sp. LH70	1061	1160	99%	0	99.83	HQ832808.1
<i>Pleosporales</i> sp. YF04U3	1061	1160	99%	0	99.83	JQ809679.1
<i>Pleosporales</i> sp. Sigrf03	1050	1149	98%	0	100	KT369813.1
<i>Pleosporales</i> sp. C1	1029	1112	95%	0	99.82	LC168756.1
<i>Pleosporales</i> sp. p47	1014	1095	93%	0	100	LC169795.1
<i>Pleosporales</i> sp. d75	1005	1076	91%	0	100	LC169832.1
<i>Setophoma</i> sp. HD-2014 isolate DO97	1000	1084	97%	0	98.93	KP050652.1
<i>Pleosporales</i> sp. p103	992	992	85%	0	99.82	LC169822.1
<i>Setophoma</i> <i>yingyisheniae</i> CGMCC 3.19527	939	939	80%	0	100	NR_164602.1
<i>Setophoma</i> sp. FL-2019d isolate LF1420	939	939	80%	0	100	MK511912.1
Uncultured fungus clone LX042399-122-056-B0 7	935	935	91%	0	95.35	GQ999533.1
<i>Setophoma</i> sp. FL-2019d isolate LF556	933	933	80%	0	99.8	MK511942.1
<i>Setophoma</i> sp. FL-2019d isolate LF448	933	933	80%	0	99.8	MK511939.1
<i>Setophoma</i> sp. FL-2019d isolate LF407	933	933	80%	0	99.8	MK511937.1
<i>Setophoma</i> sp. FL-2019d isolate LF341	933	933	80%	0	99.8	MK511929.1
Fungal endophyte isolate 5470	915	915	80%	0	99.02	JQ846051.1

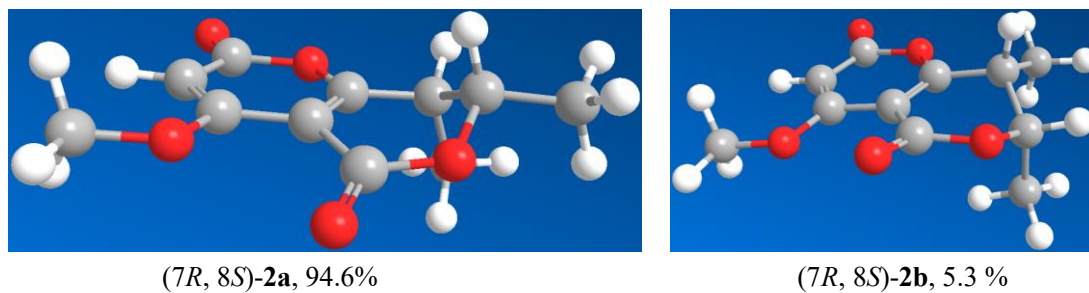


Figure S1. Optimized geometries of the predominant conformers for (7R, 8S)-**2** at the B3LYP/6-31G(d) level in the gas phase.

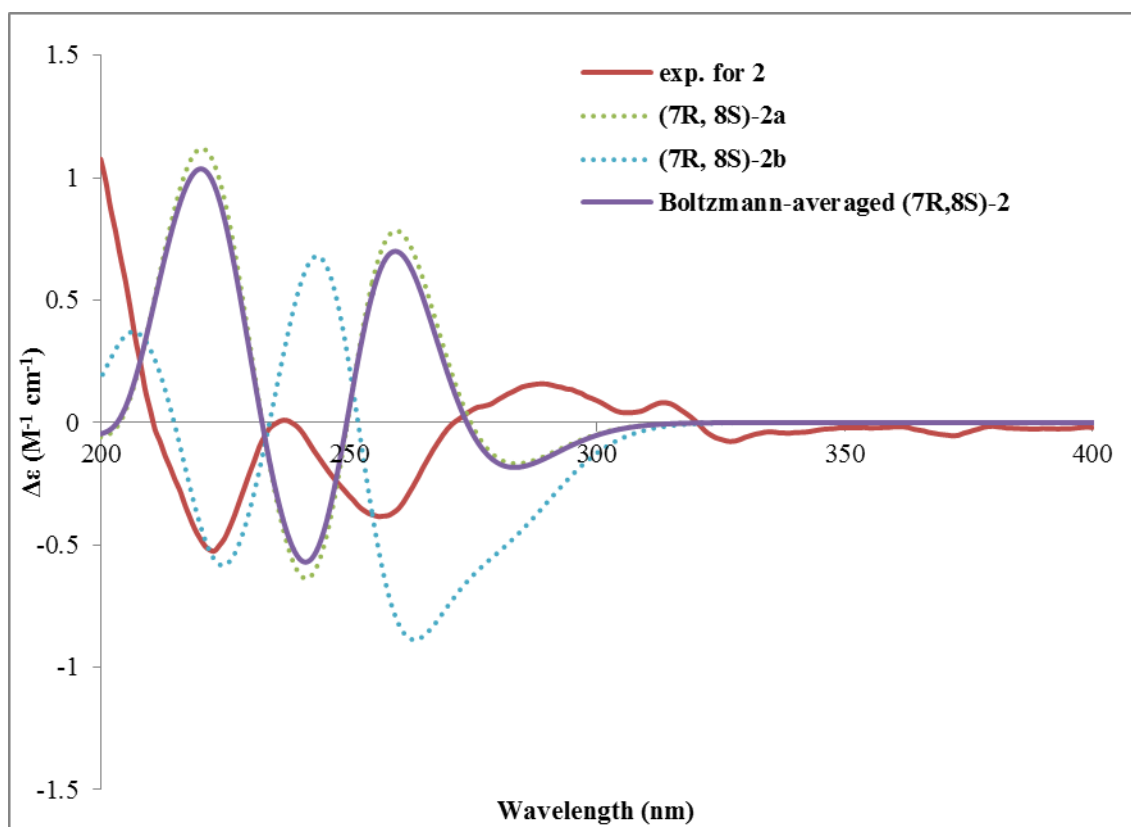
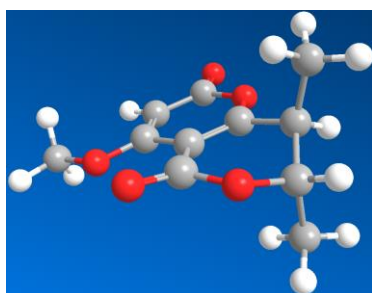
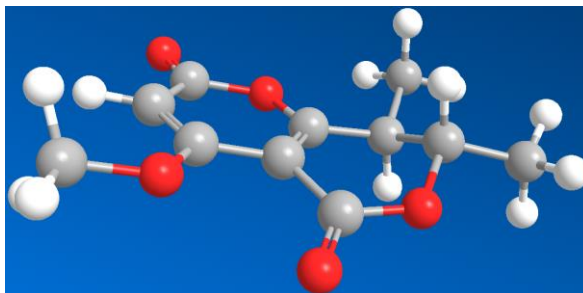


Figure S2. Calculated ECD spectra for (7R,8S)-**2a**, (7R,8S)-**2b**, and the Boltzmann-averaged spectrum.



(7*S*, 8*S*)-**3a**, 24.7%



(7*S*, 8*S*)-**3b**, 75.2%

Figure S3. Optimized geometries of the predominant conformers for (7*S*, 8*S*)-**3** at the B3LYP/6-31G(d) level in the gas phase.

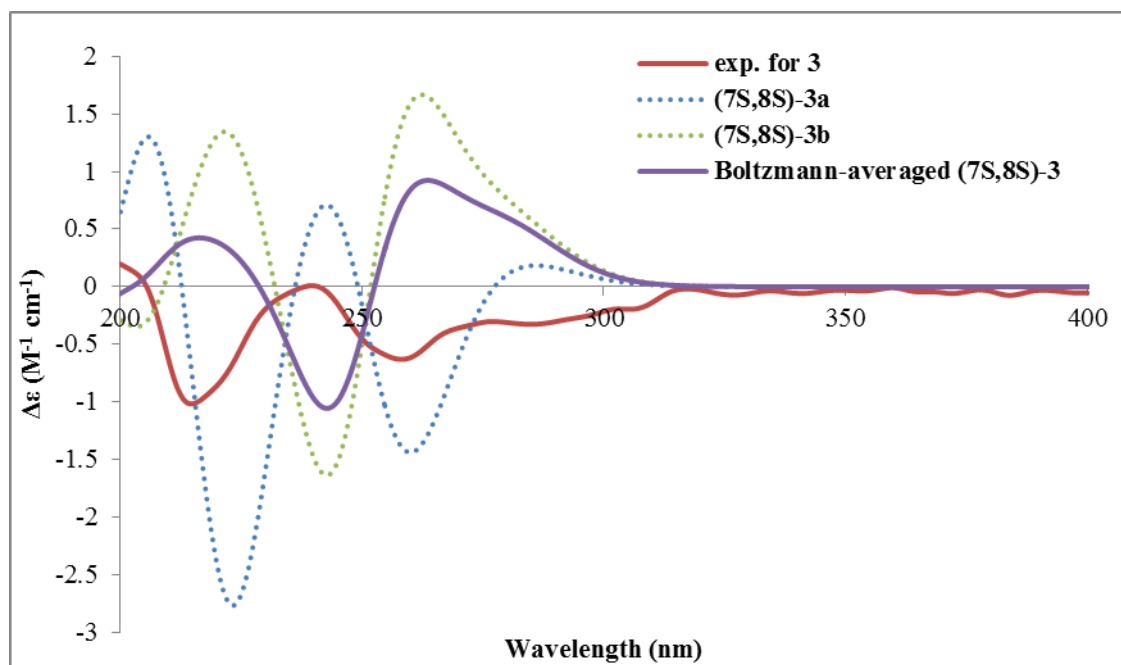


Figure S4. Calculated ECD spectra for (7*S*,8*S*)-**3a**, (7*S*,8*S*)-**3b**, and the Boltzmann-averaged spectrum.

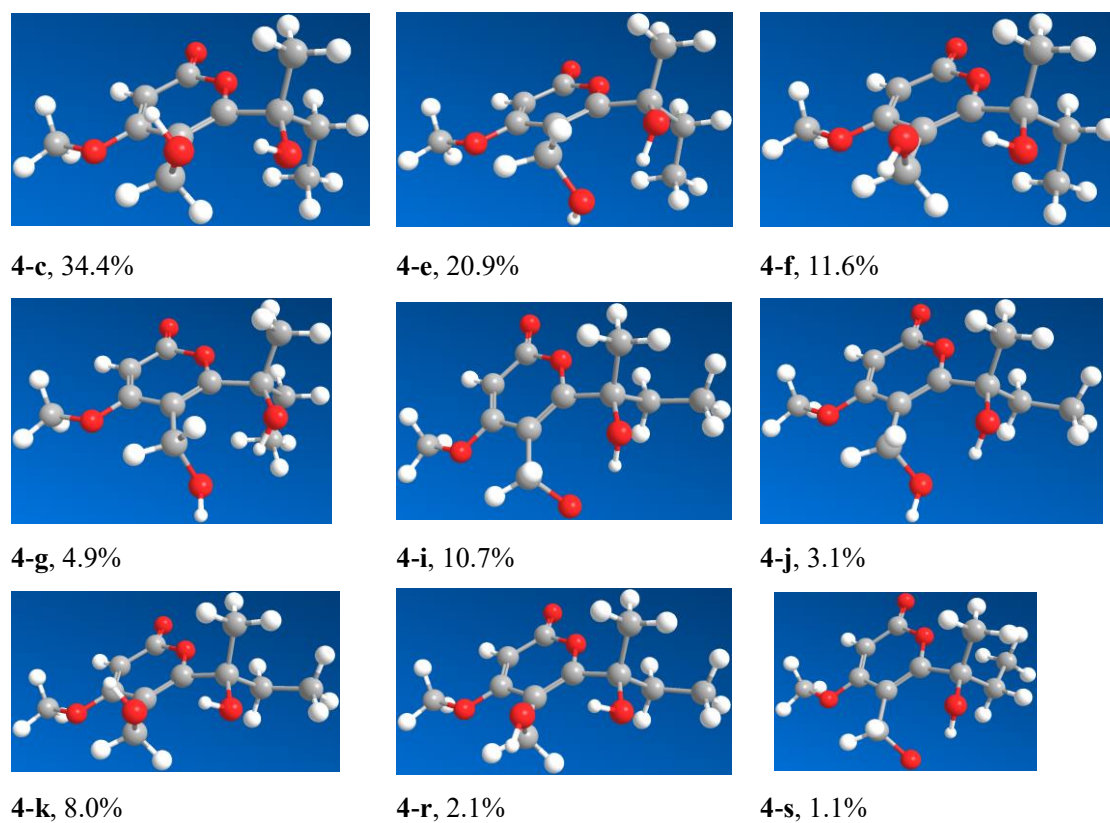


Figure S5. Optimized geometries of the predominant conformers for **4** at the B3LYP/6-31G(d) level in the gas phase.

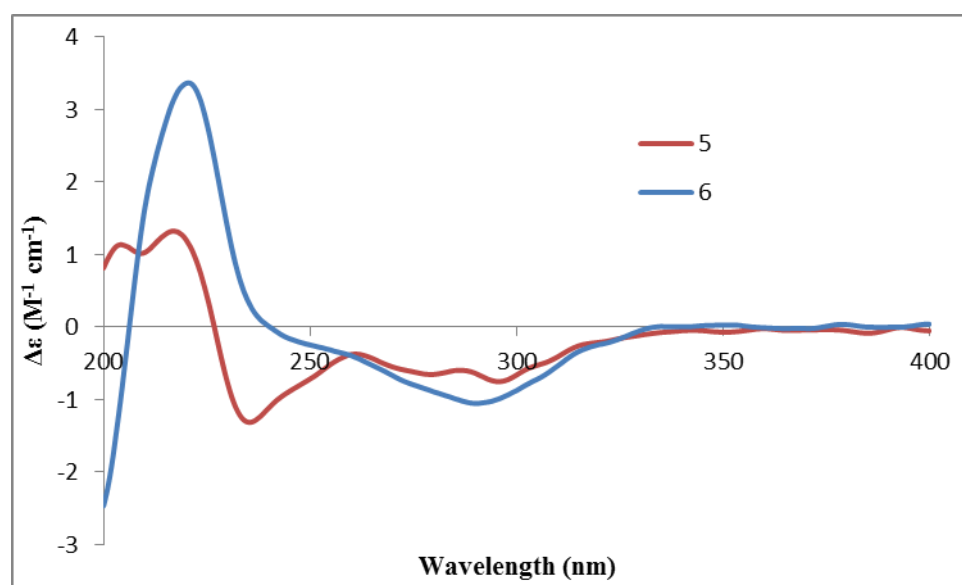
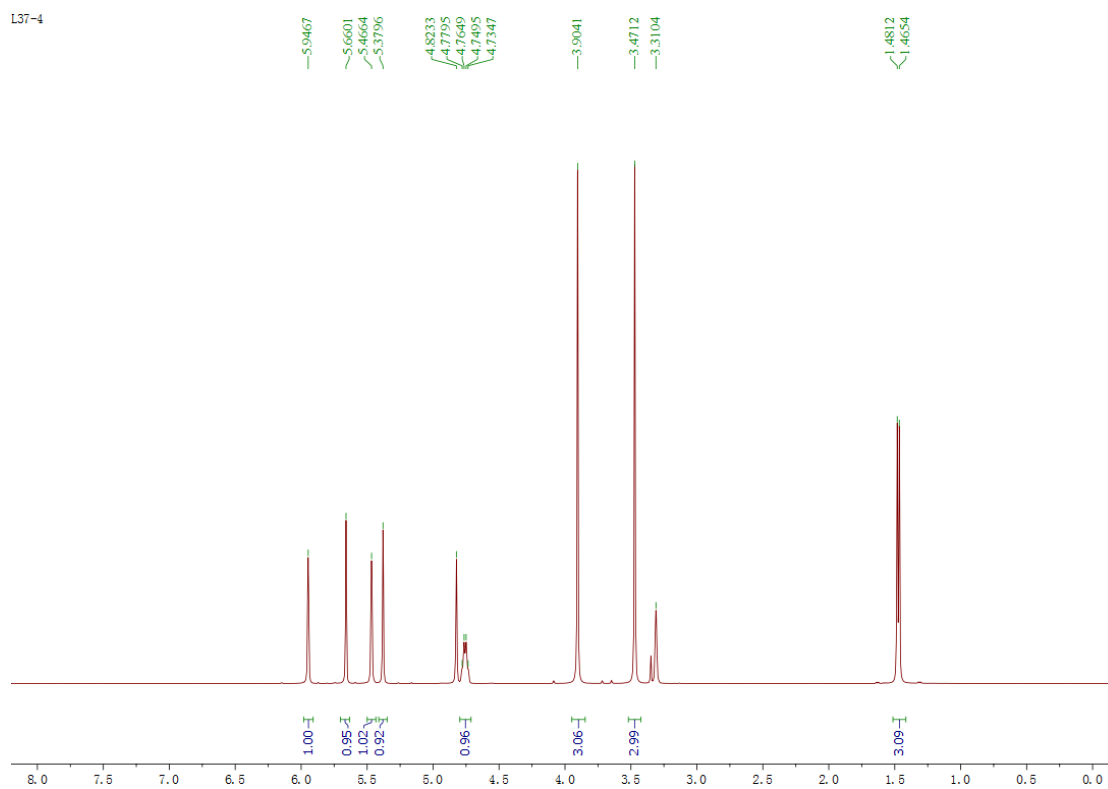
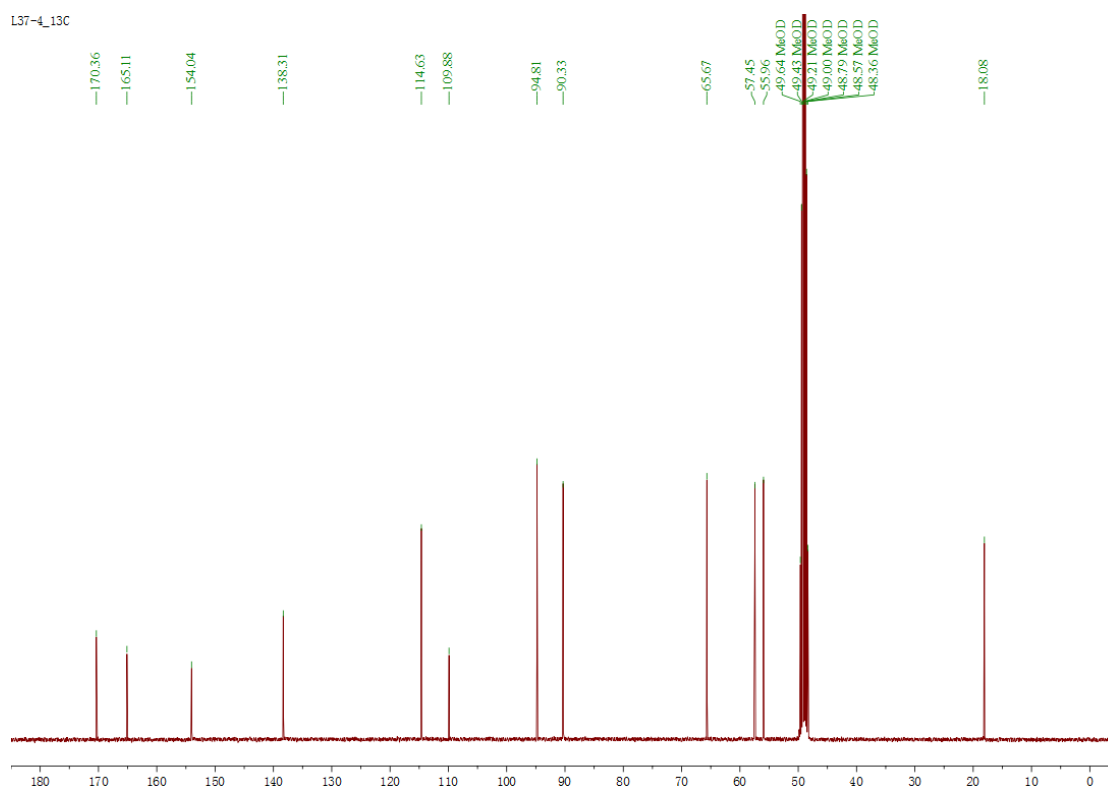


Figure S6. ECD spectra of **5** and **6**.

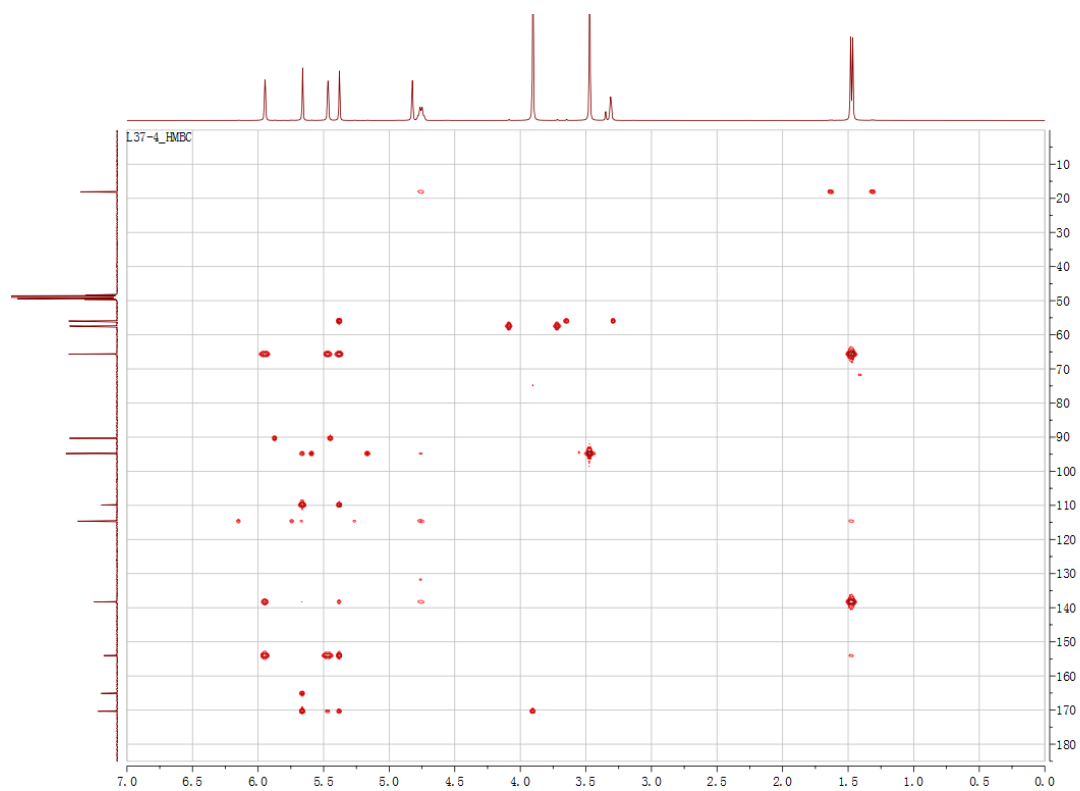
NMR, HRESIMS, and CD spectra of **1**



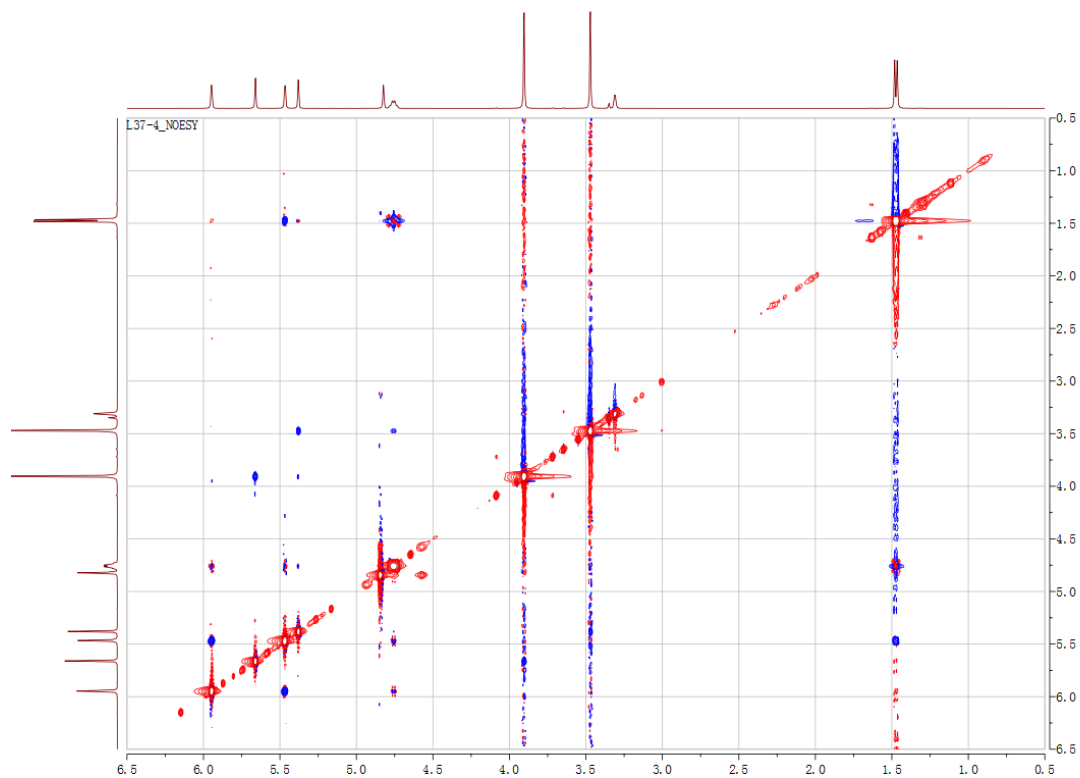
^1H NMR spectrum of **1** (CD_3OD , 400MHz).



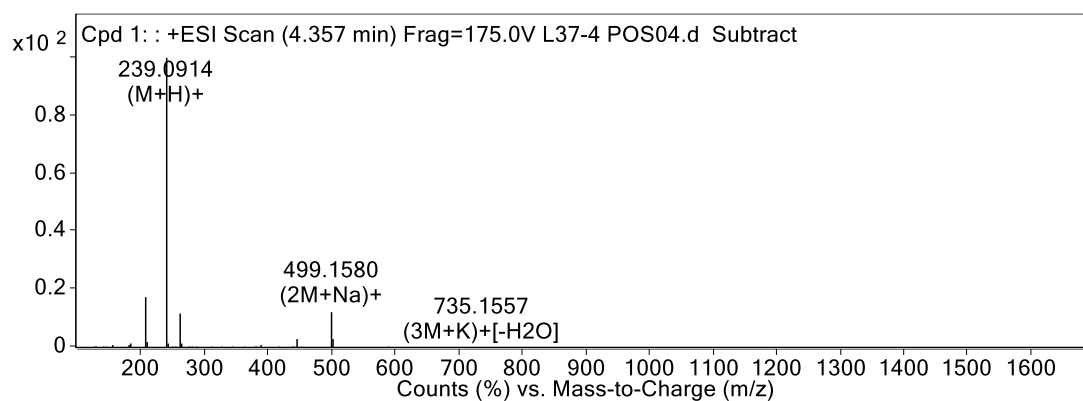
^{13}C NMR spectrum of **1** (CD_3OD , 100MHz).



HMBC spectrum of **1** (CD₃OD).



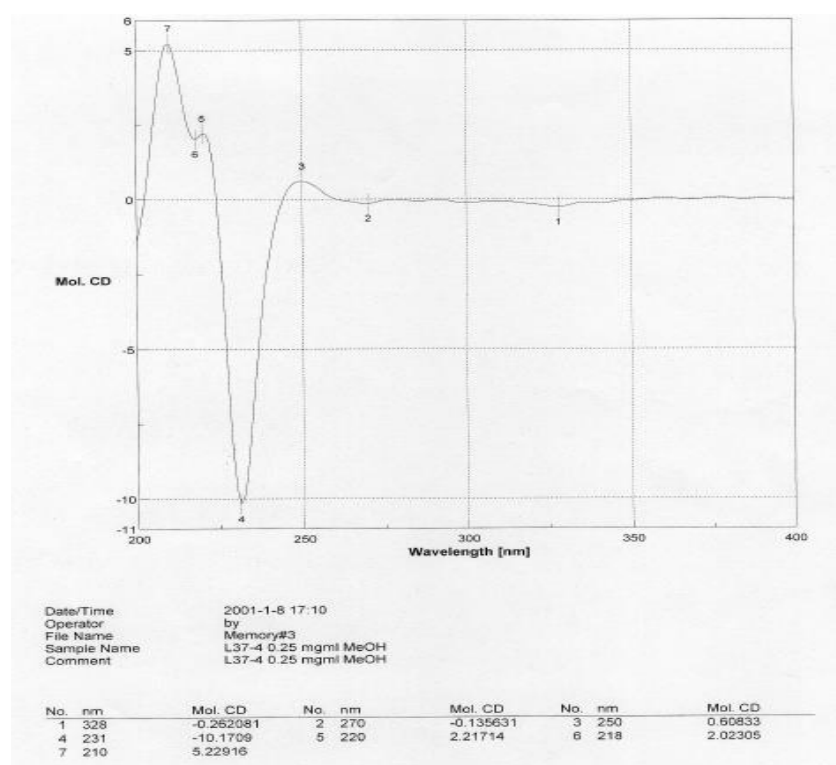
NOESY spectrum of **1** (CD₃OD).



MS Spectrum Peak List

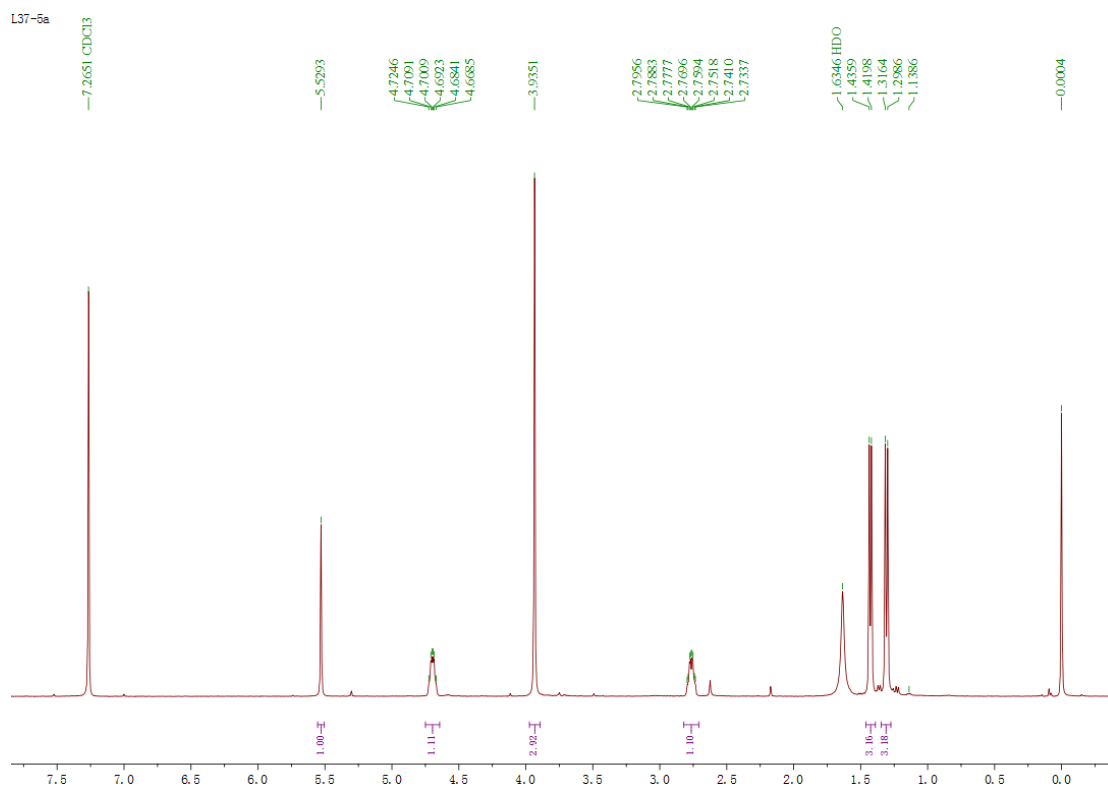
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
239.0914	239.0914	0.04	1	988227.8	C ₁₂ H ₁₅ O ₅	(M+H) ⁺
499.1580	499.1575	1.04	1	124132.2	C ₂₄ H ₂₈ NaO ₁₀	(2M+Na) ⁺

HRESIMS spectrum of **1**.

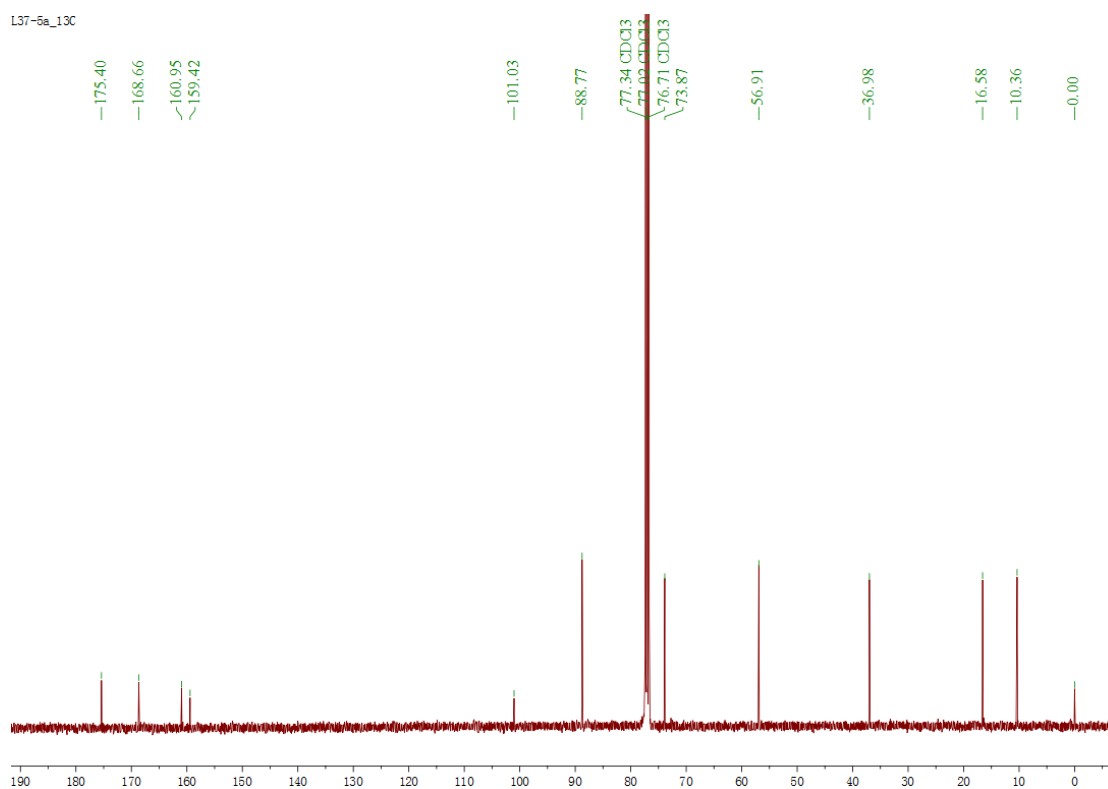


CD spectrum of **1** (CH₃OH).

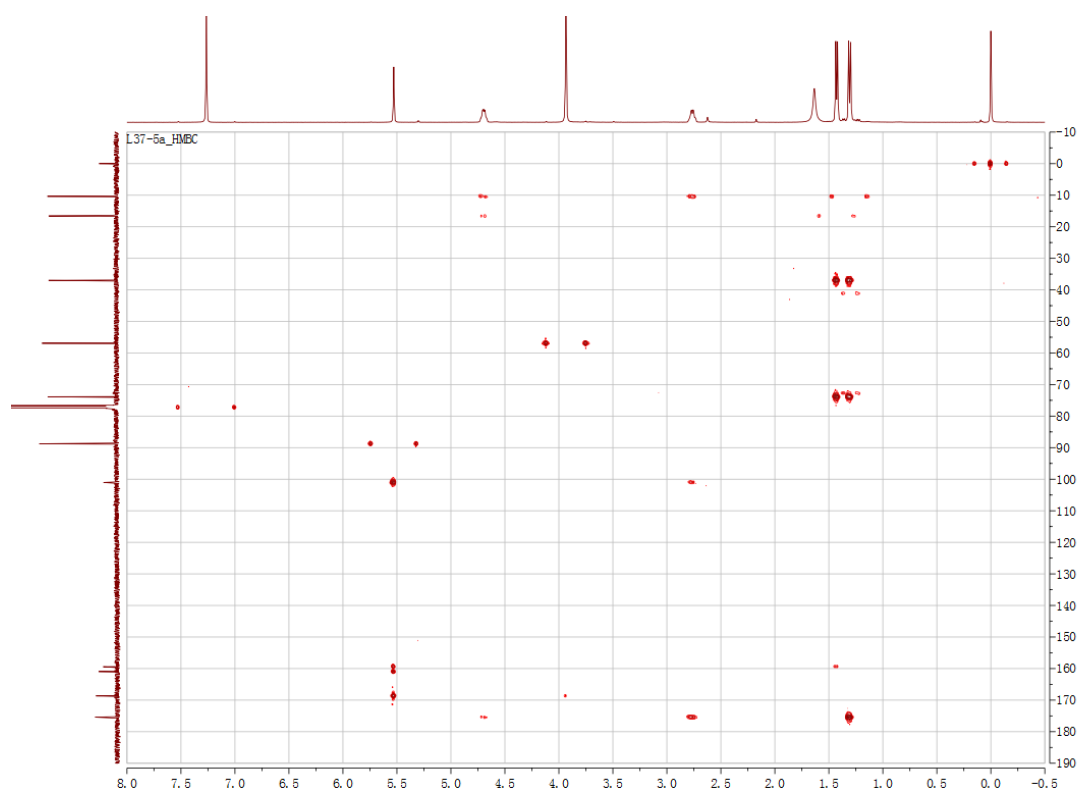
NMR, HRESIMS, and CD spectra of **2**.



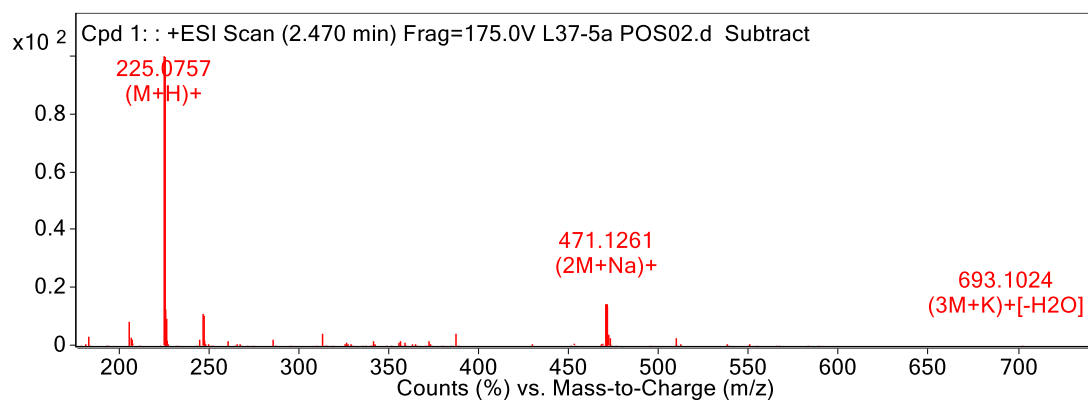
¹H NMR spectrum of **2** (CDCl₃, 400MHz).



¹³C NMR spectrum of **2** (CDCl₃, 100MHz).



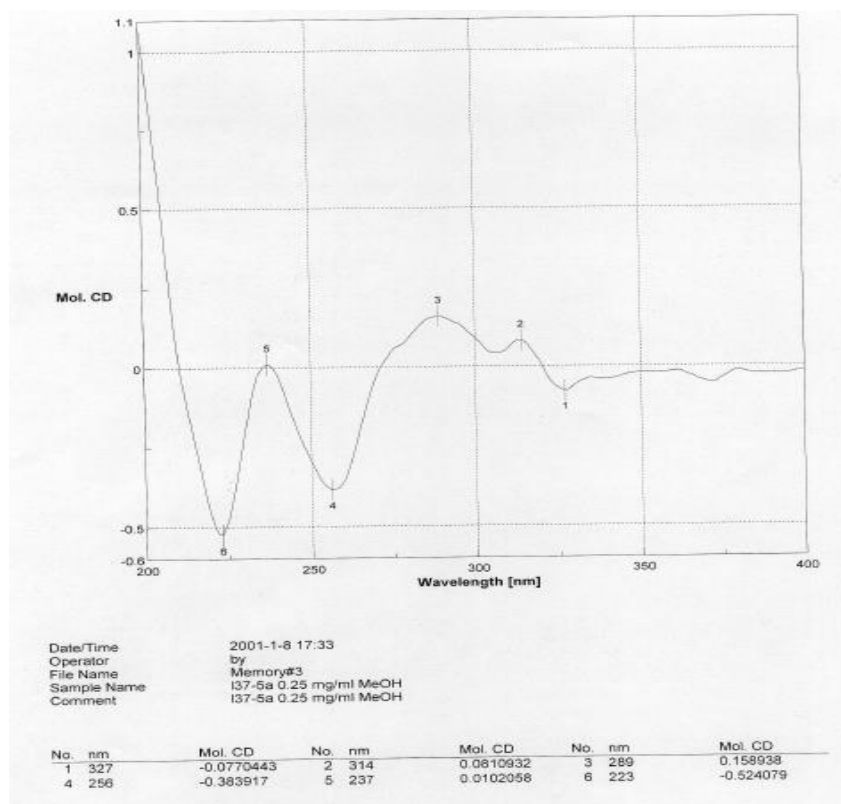
HMBC spectrum of **2** (CDCl₃).



MS Spectrum Peak List

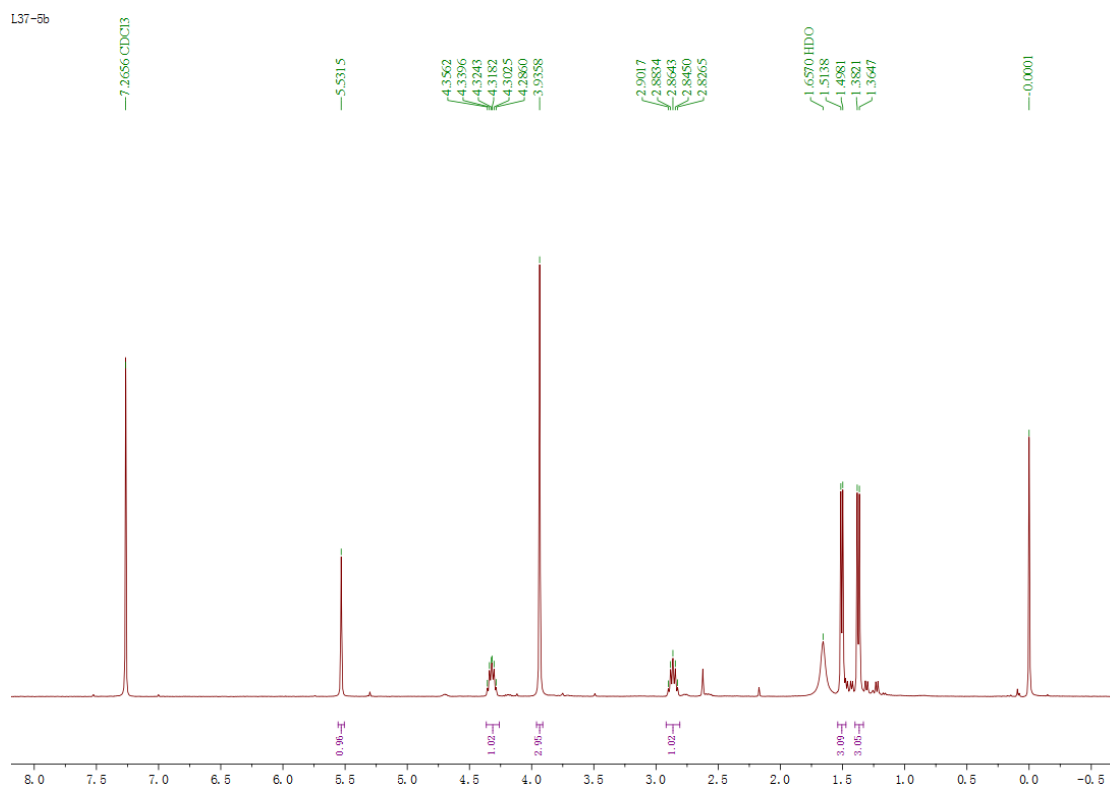
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
225.0757	225.0757	-0.28	1	714381.8	C ₁₁ H ₁₃ O ₅	(M+H) ⁺
247.0578	247.0577	0.4	1	77244.8	C ₁₁ H ₁₂ NaO ₅	(M+Na) ⁺
471.1261	471.1262	-0.19	1	98268.8	C ₂₂ H ₂₄ NaO ₁₀	(2M+Na) ⁺

HRESIMS spectrum of **2**.

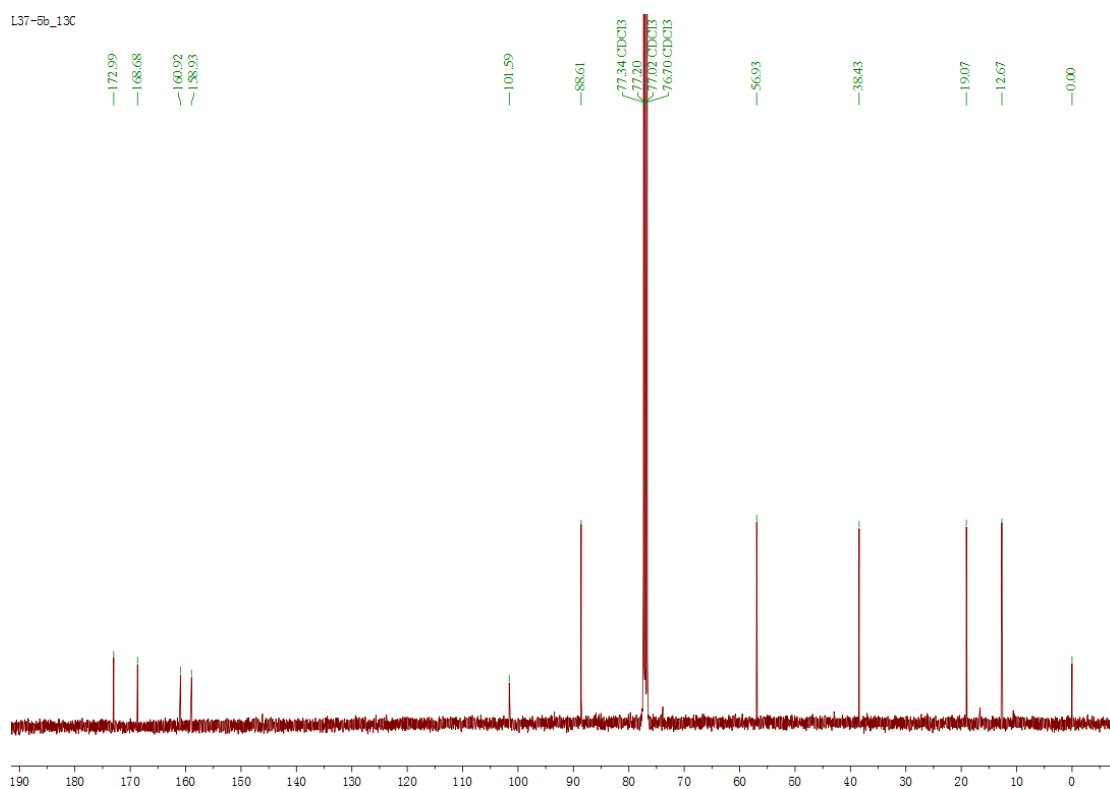


CD spectrum of **2** (CH₃OH).

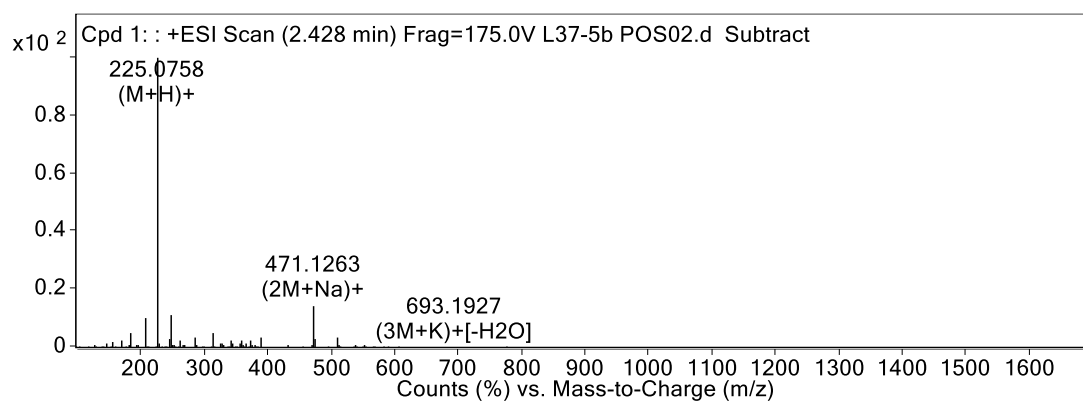
NMR, HRESIMS, and CD spectra of **3**.



¹H NMR spectrum of **3** (CDCl₃, 400MHz).



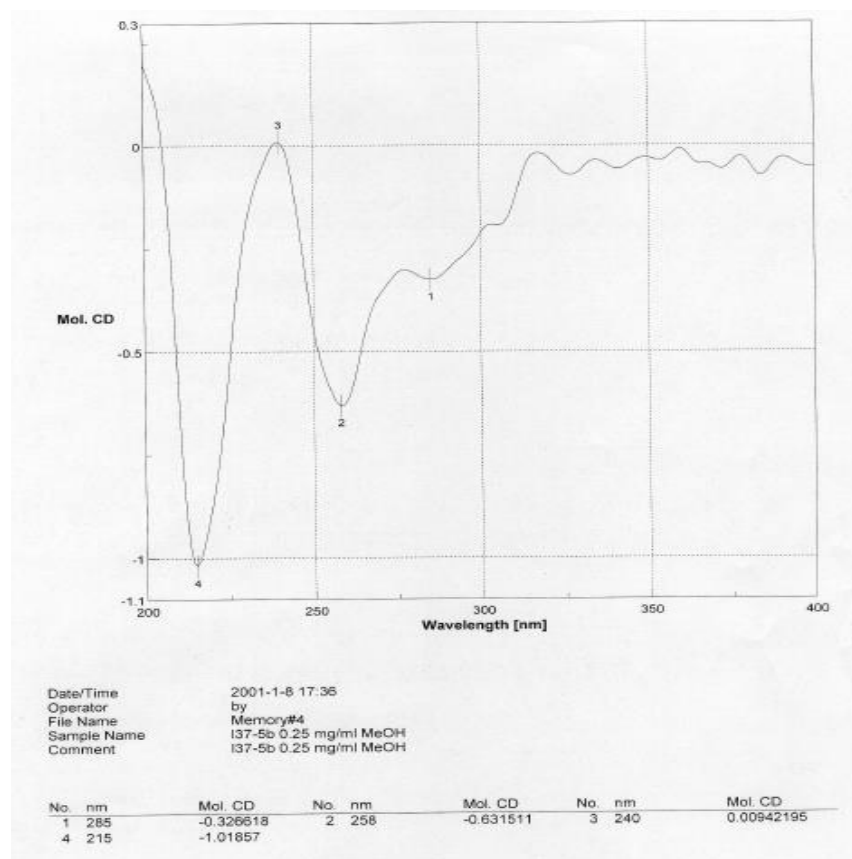
¹³C NMR spectrum of **3** (CDCl₃, 100MHz).



MS Spectrum Peak List

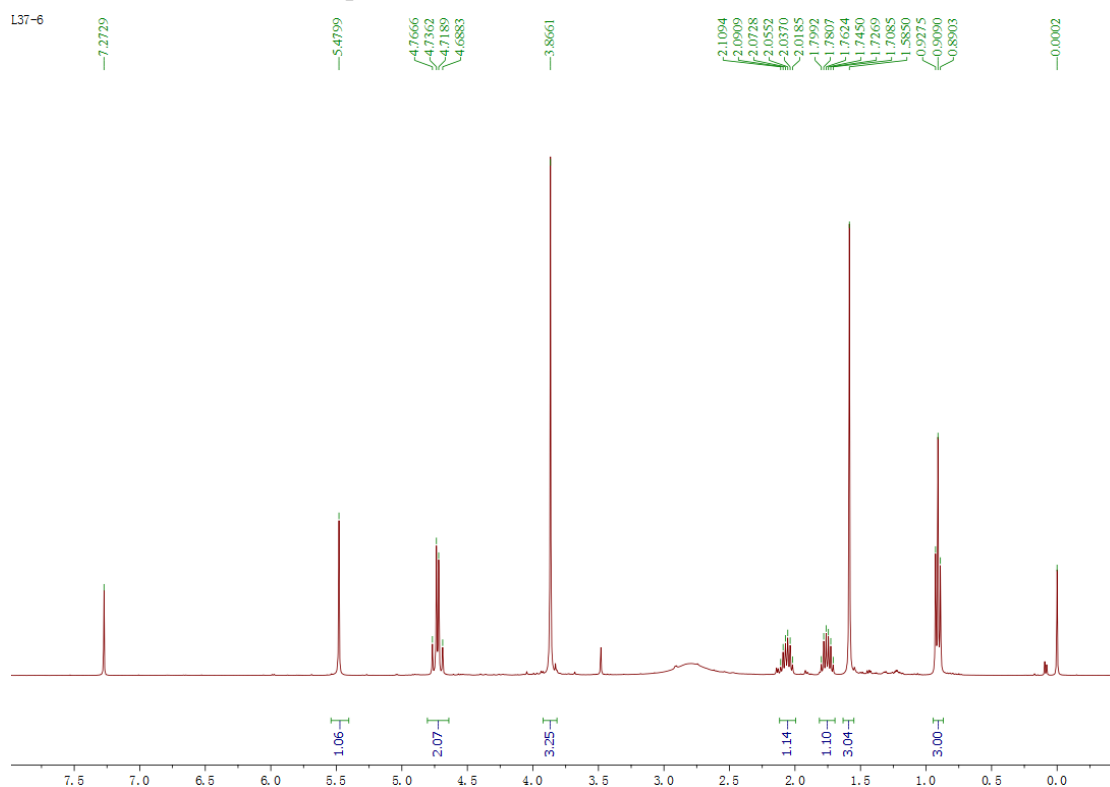
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
225.0758	225.0757	0.28	1	768202.1	C ₁₁ H ₁₃ O ₅	(M+H) ⁺
247.0579	247.0577	0.96	1	86776.8	C ₁₁ H ₁₂ NaO ₅	(M+Na) ⁺
471.1263	471.1262	0.38	1	111611.3	C ₂₂ H ₂₄ NaO ₁₀	(2M+Na) ⁺

HRESIMS spectrum of **3**.

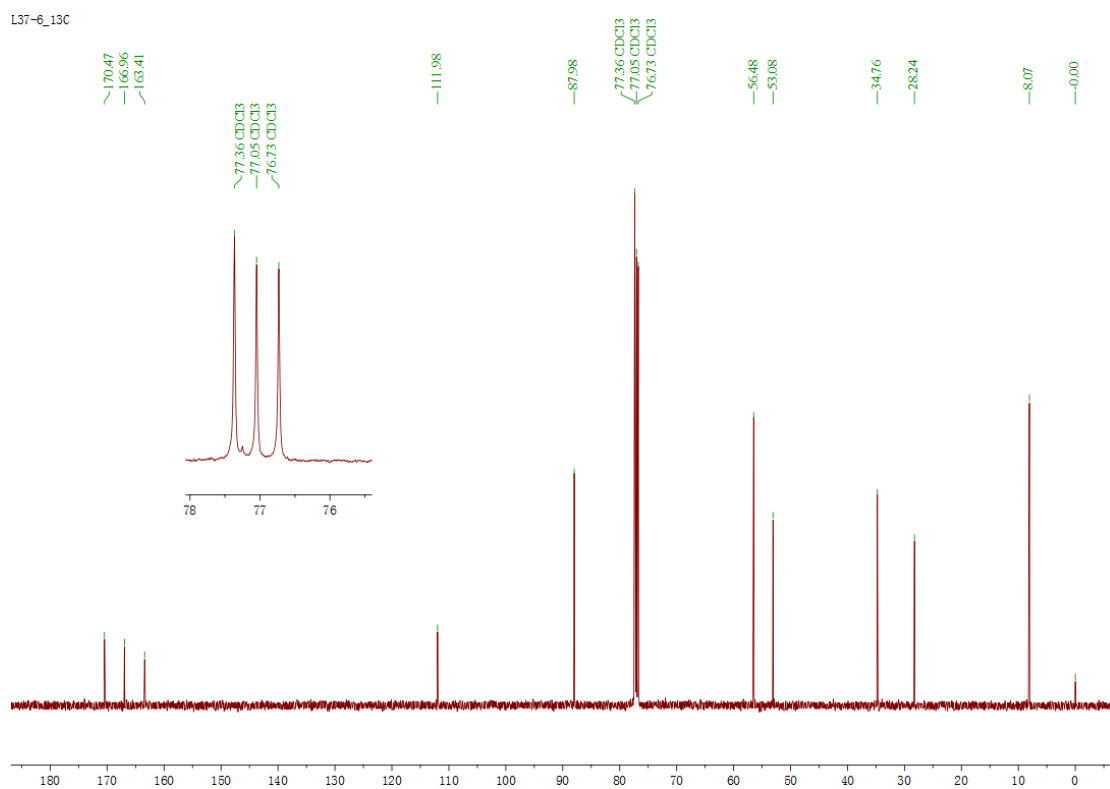


CD spectrum of **3** (CH₃OH).

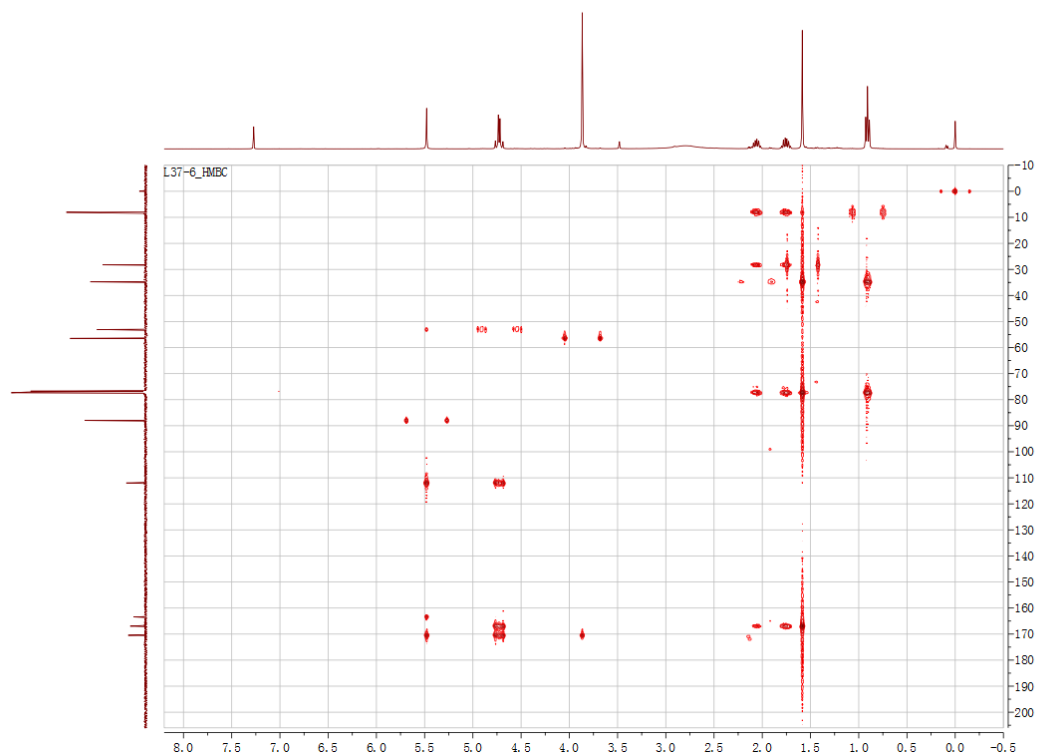
NMR, HRESIMS, and CD spectra of **4**.



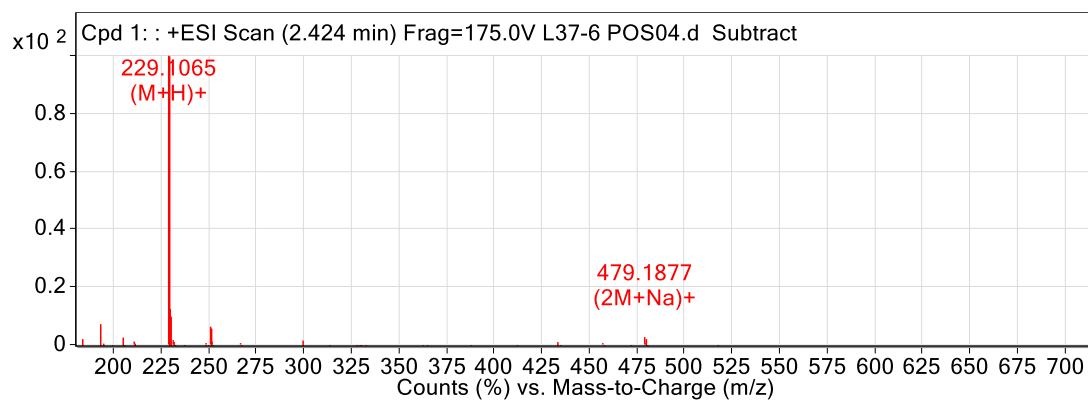
^1H NMR spectrum of **4** (CDCl_3 , 400MHz).



^{13}C NMR spectrum of **4** (CDCl_3 , 100MHz).



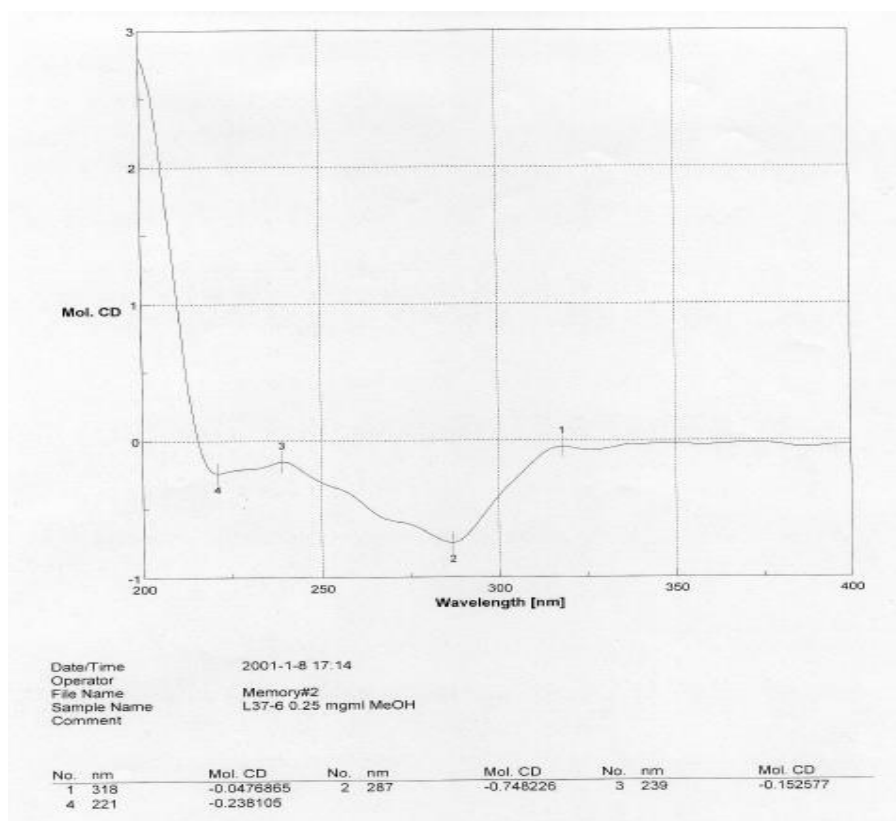
HMBC spectrum of **4** (CDCl₃).



MS Spectrum Peak List

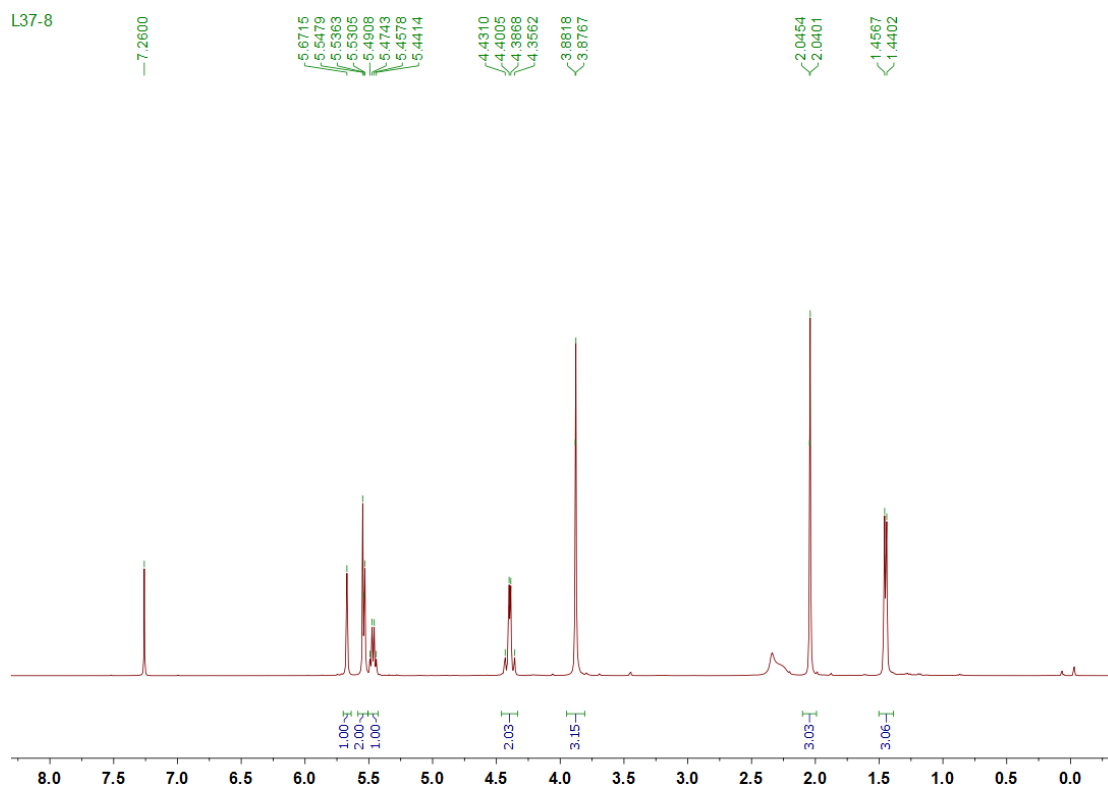
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>z</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
229.1065	229.1071	-2.57	1	651402.5	C ₁₁ H ₁₇ O ₅	(M+H) ⁺
251.0885	251.089	-2	1	41712.8	C ₁₁ H ₁₆ NaO ₅	(M+Na) ⁺
479.1877	479.1888	-2.27	1	15476.9	C ₂₂ H ₃₂ NaO ₁₀	(2M+Na) ⁺

HRESIMS spectrum of **4** (CDCl₃).

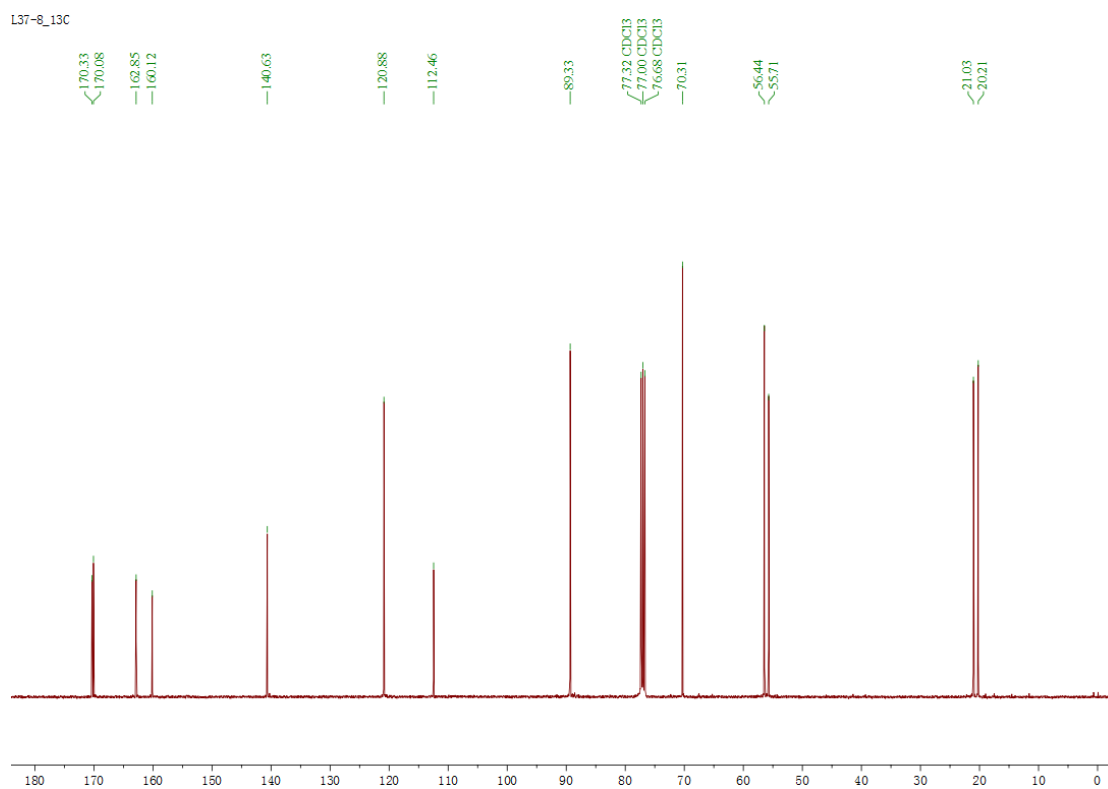


CD spectrum of **4** (CH₃OH).

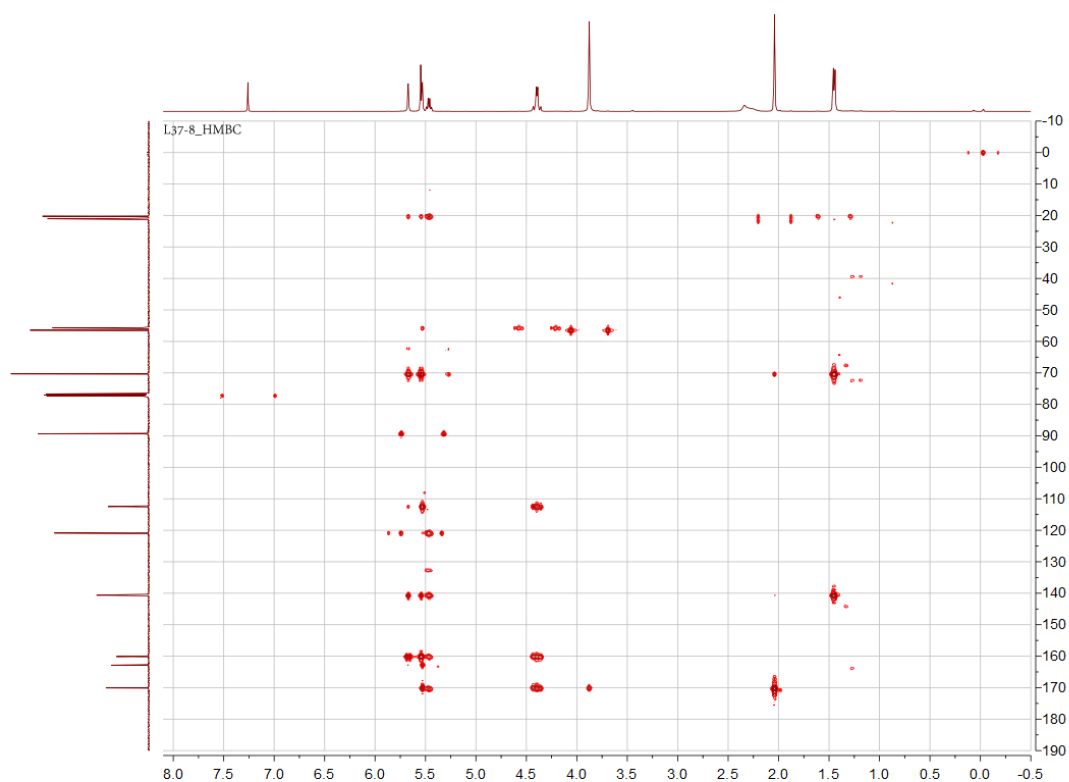
NMR, HRESIMS, and CD spectra of **5**.



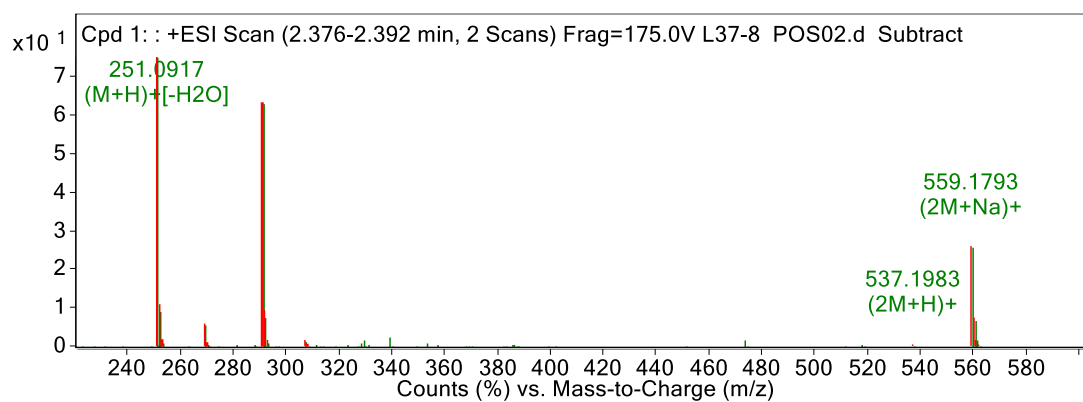
^1H NMR spectrum of **5** (CDCl_3 , 400MHz).



^{13}C NMR spectrum of **5** (CDCl_3 , 100MHz).



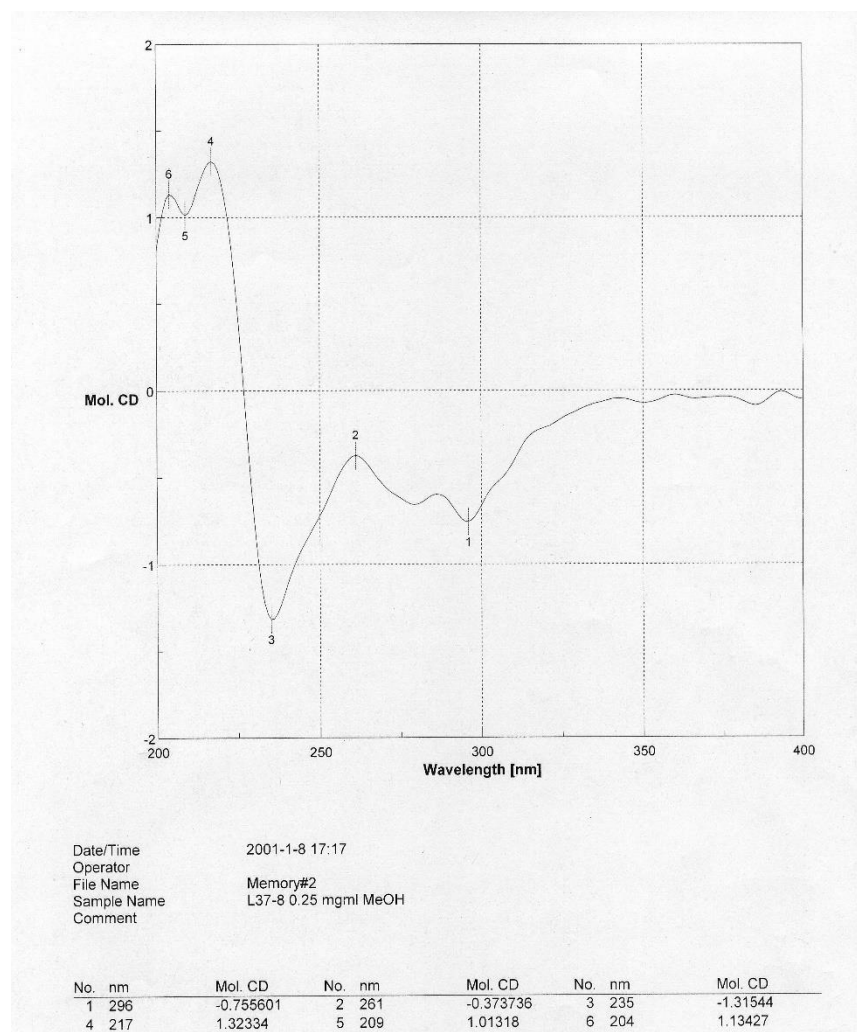
HMBC spectrum of **5** (CDCl₃).



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
251.0917	251.0914	1.16	1	412711.1	C ₁₃ H ₁₅ O ₅	(M+H)+[-H ₂ O]
269.1025	269.102	1.93	1	31363.3	C ₁₃ H ₁₇ O ₆	(M+H)+
291.0842	291.0839	1.01	1	346023.3	C ₁₃ H ₁₆ NaO ₆	(M+Na)+
537.1983	537.1967	3.01	1	2765.8	C ₂₆ H ₃₃ O ₁₂	(2M+H)+
559.1793	559.1786	1.28	1	141551.9	C ₂₆ H ₃₂ NaO ₁₂	(2M+Na)+

HRESIMS spectrum of **5**.



CD spectrum of **5** (MeOH).