

Supporting Information

Vitepyrroloids A-D, 2-Cyanopyrrole-containing Labdane Diterpenoid Alkaloids from the Leaves of *Vitex trifolia*

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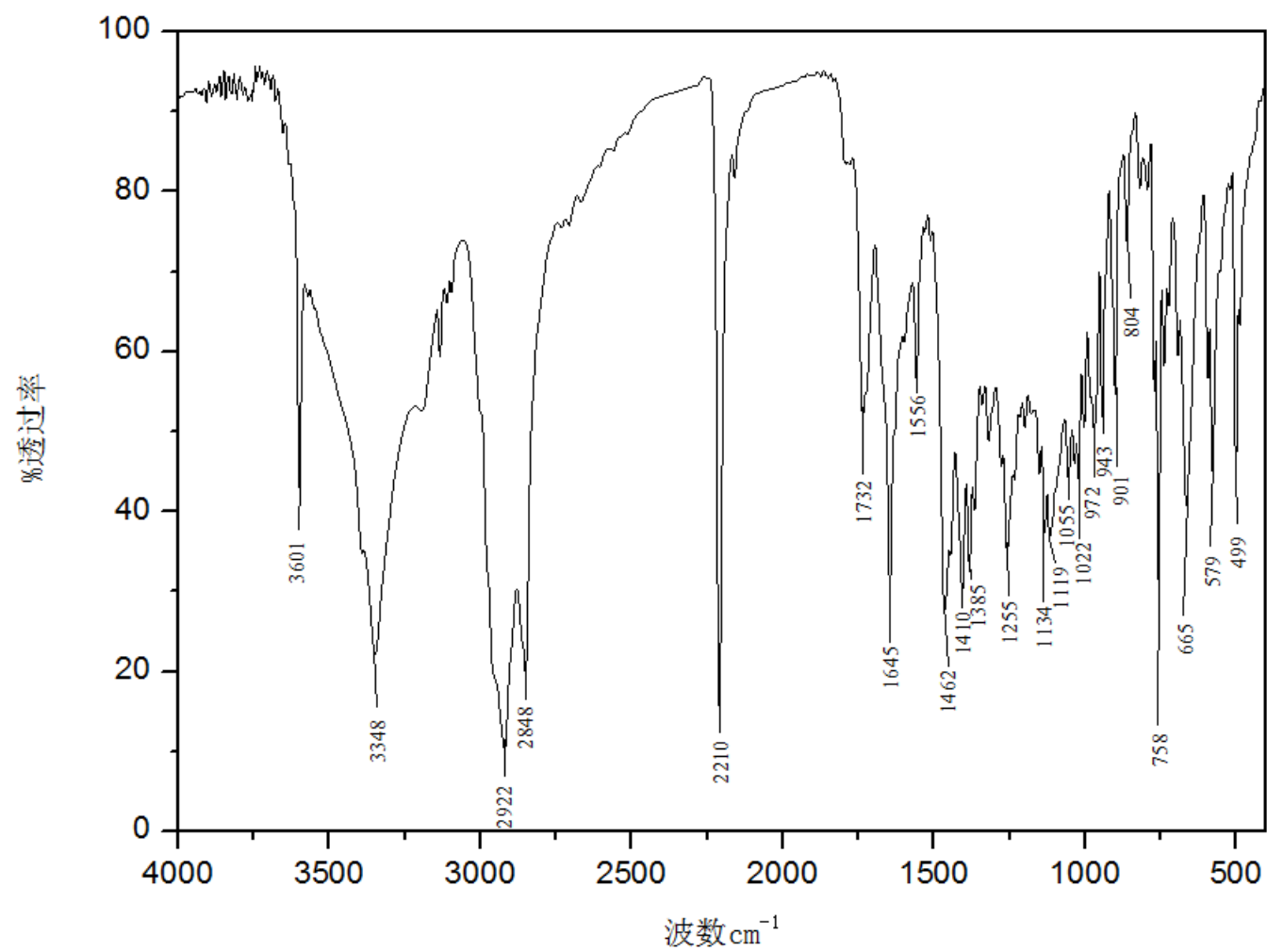


Figure S1. The IR Spectra of Compound **1**

Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQDATA-LR\16\090209

9/

mjy-zh

090209 #56 RT: 1.45 AV: 1 NL: 2.24E7
T: + c Full ms [45.00-800.00]

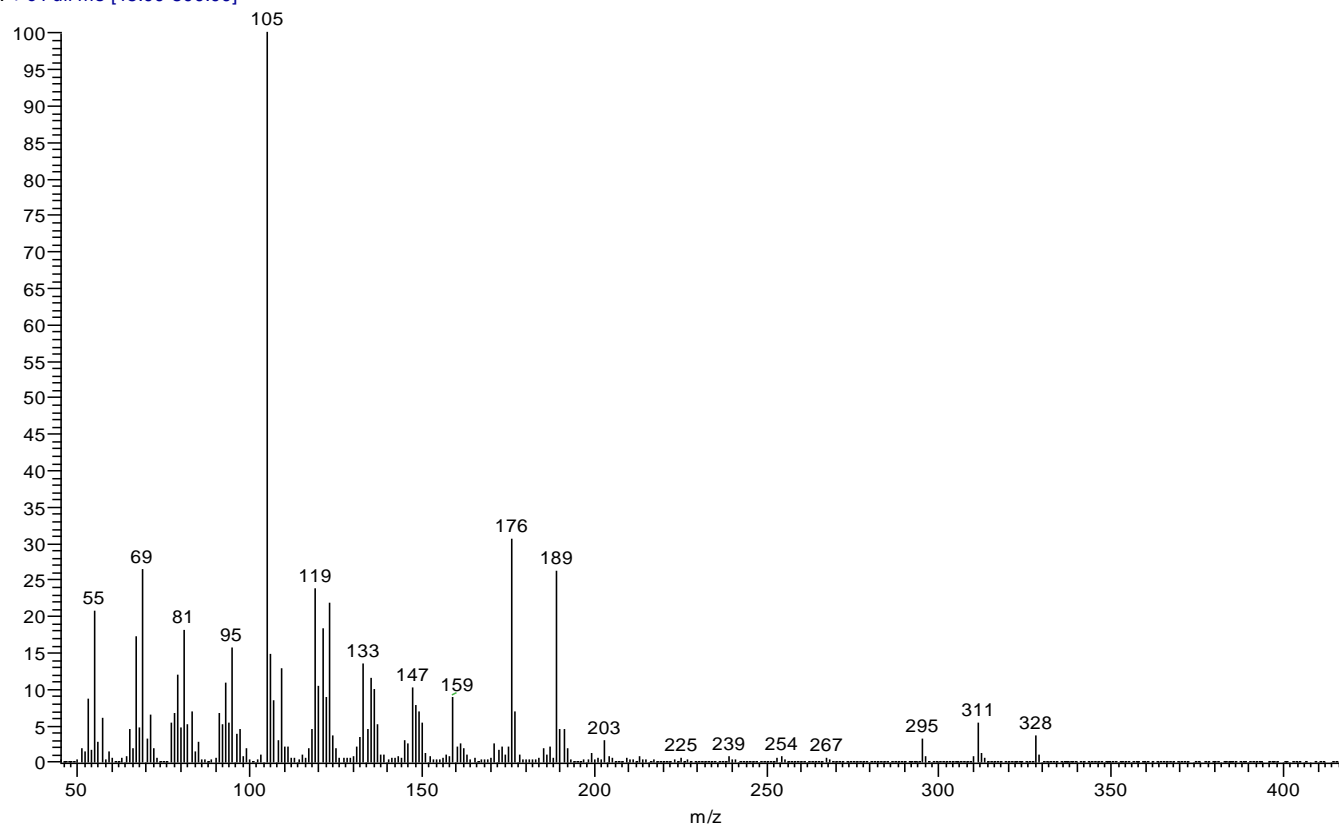


Figure S2. The EIMS Spectroscopic Data of Compound 1

SPECTRUM-MS
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Full ms [316.500 - 333.500] - Range: 328.200 - 328.300
Scan No. 9 of 16
Scan #: 9
RT: 0.33
Data points: 1

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
328.2507	100.0	328.2509	-0.6	-0.2	7.0	C ₂₁ H ₃₂ O ₁ N ₂

Instrument: MAT 95XP(Thermo)
D:\DATA-HR\16\090902-mjy-zh-c1
090902-mjy-zh-c1 #9 RT: 0.33 AV: 1 NL: 1.07E5
T: + c EI Full ms [316.50-333.50]

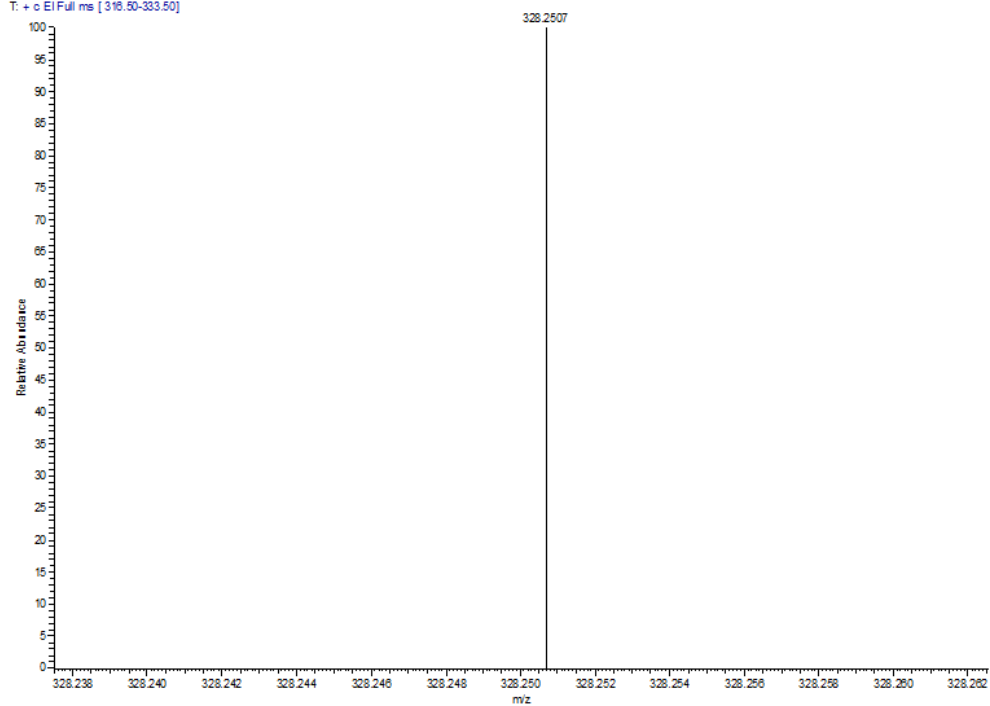


Figure S3. The HREIMS Spectroscopic Data of Compound 1

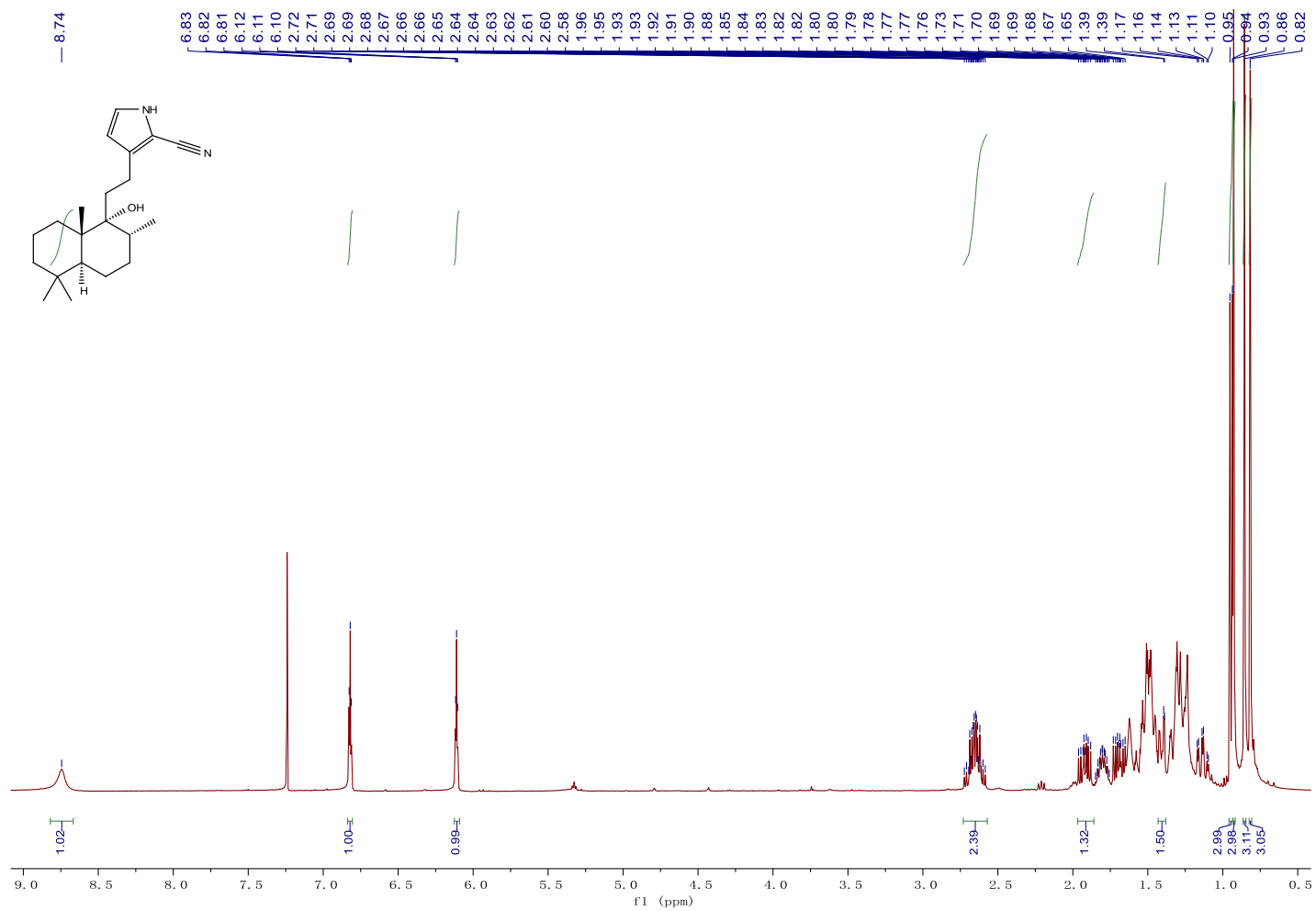


Figure S4. The ¹H NMR Spectrum of Compound 1 in CDCl₃

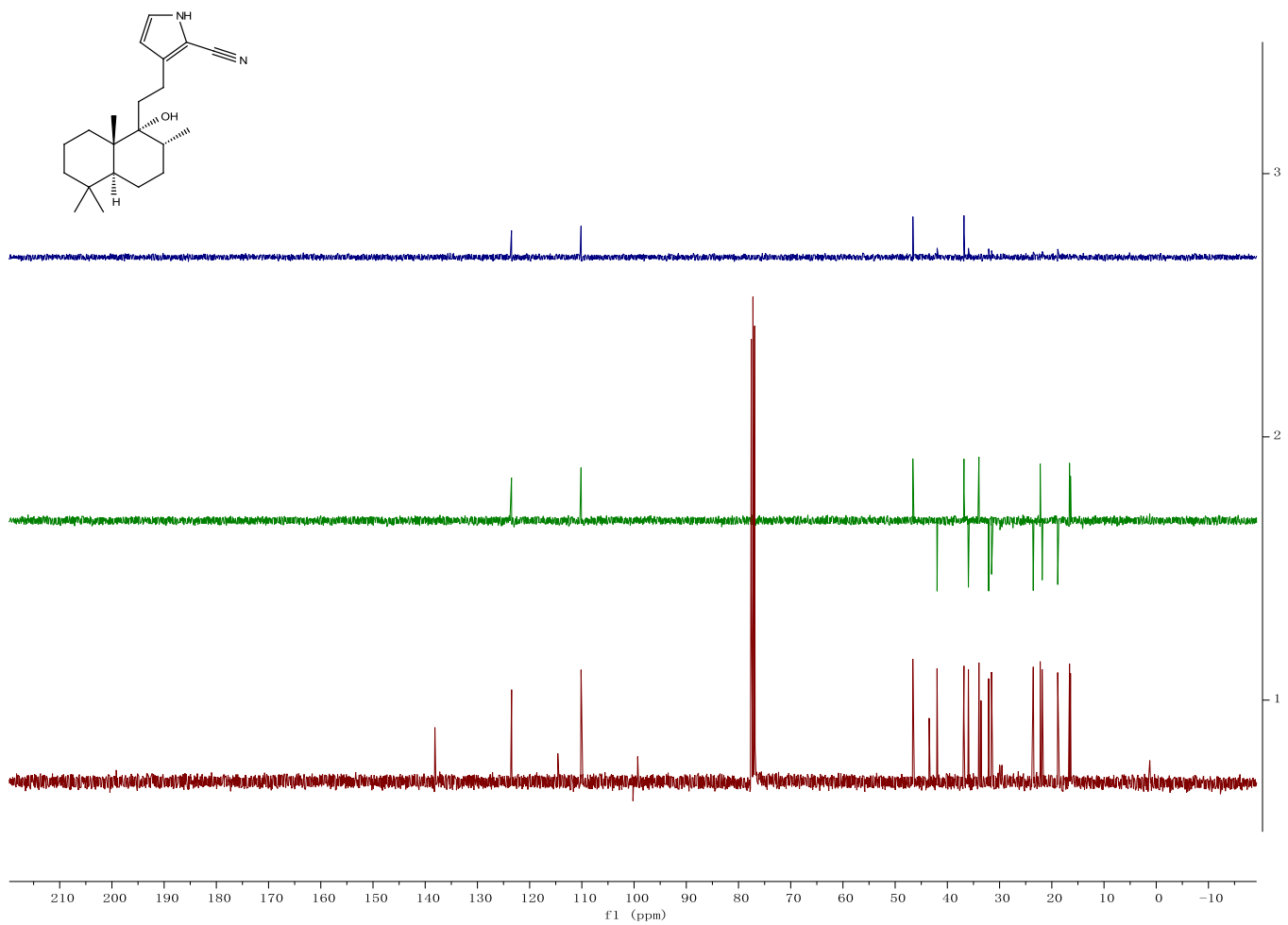


Figure S5. The ^{13}C NMR Spectrum of Compound 1 in CDCl_3

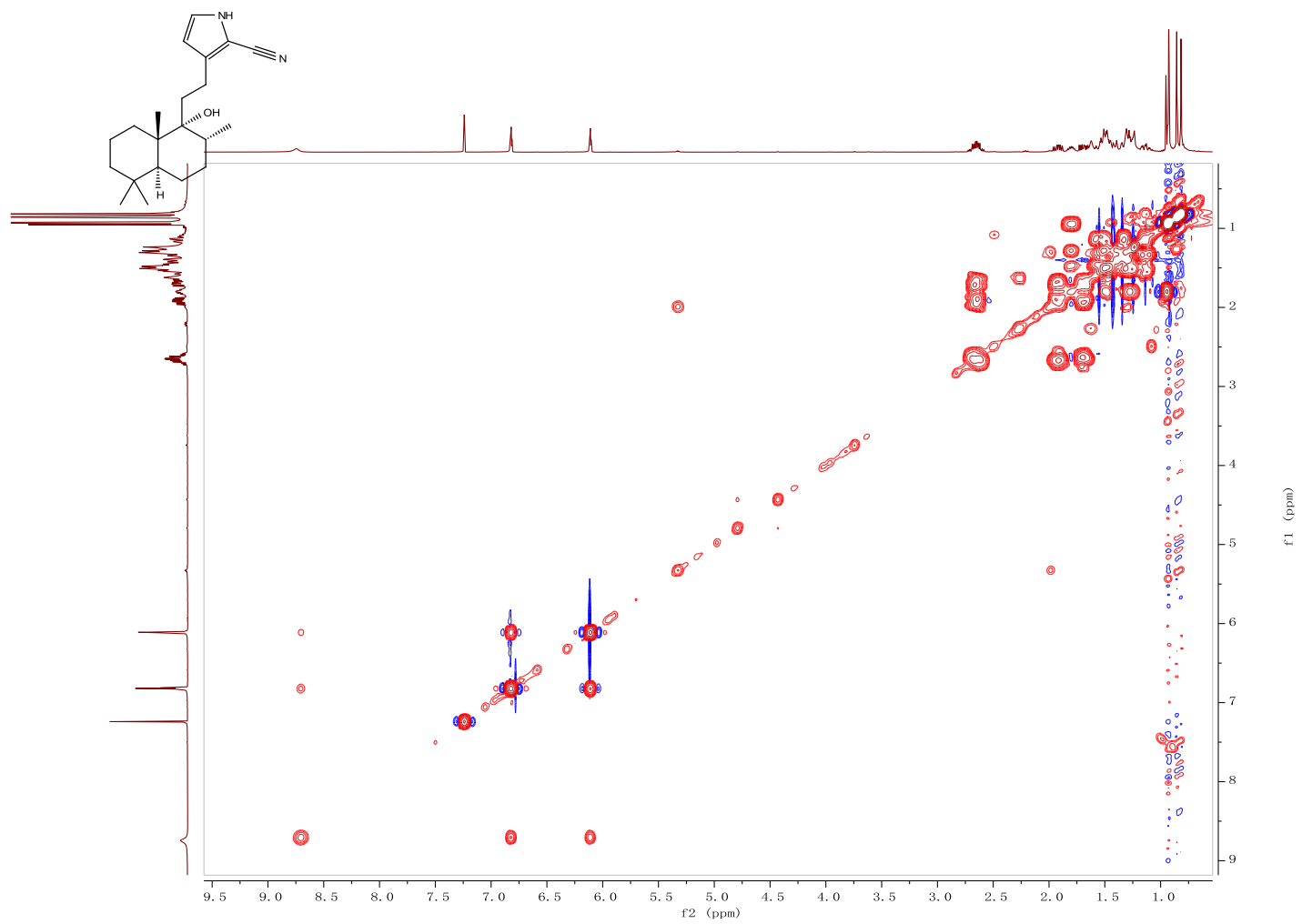


Figure S6. The ^1H - ^1H COSY Spectrum of Compound **1** in CDCl_3

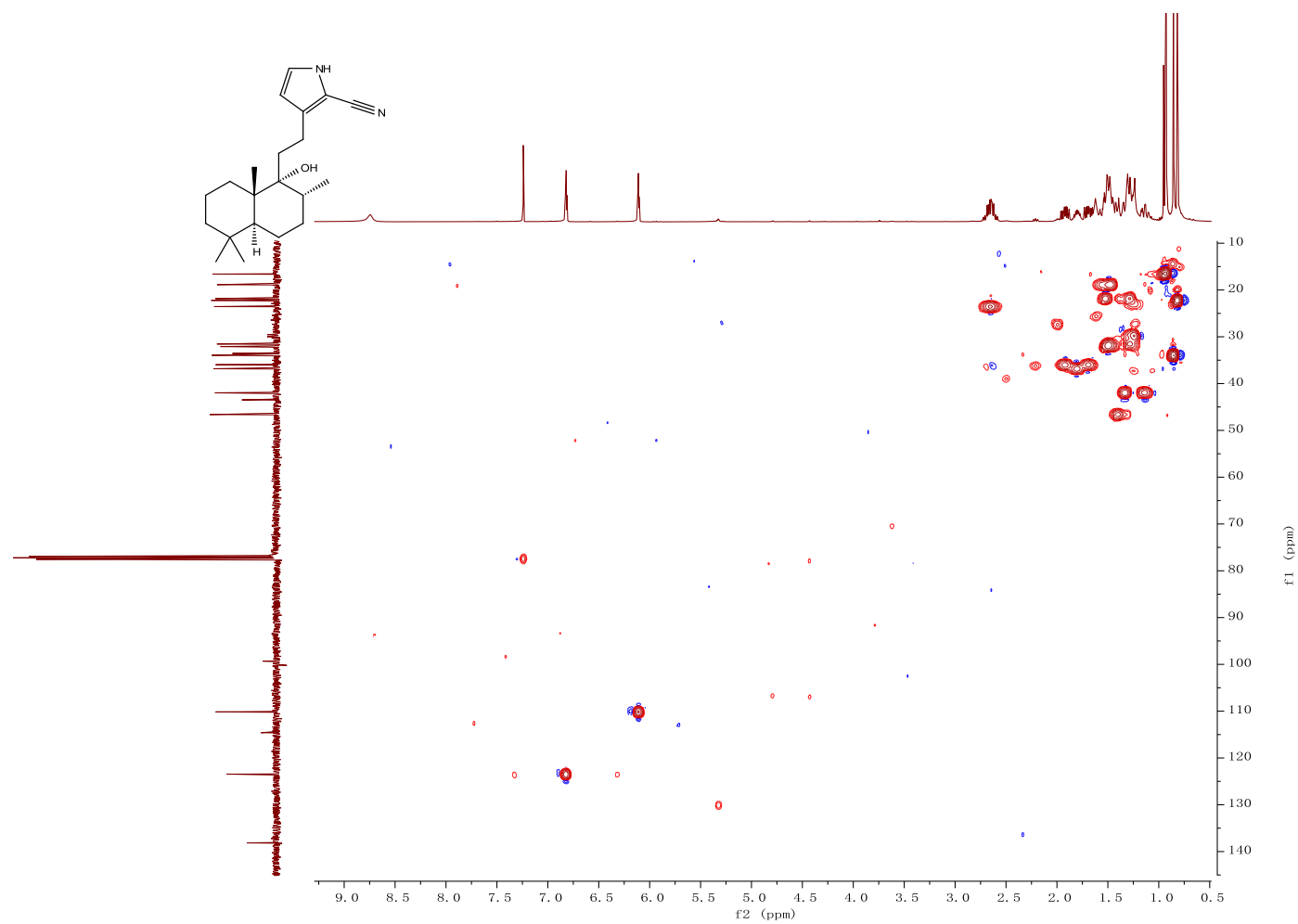


Figure S7. The HSQC Spectrum of Compound **1** in CDCl₃

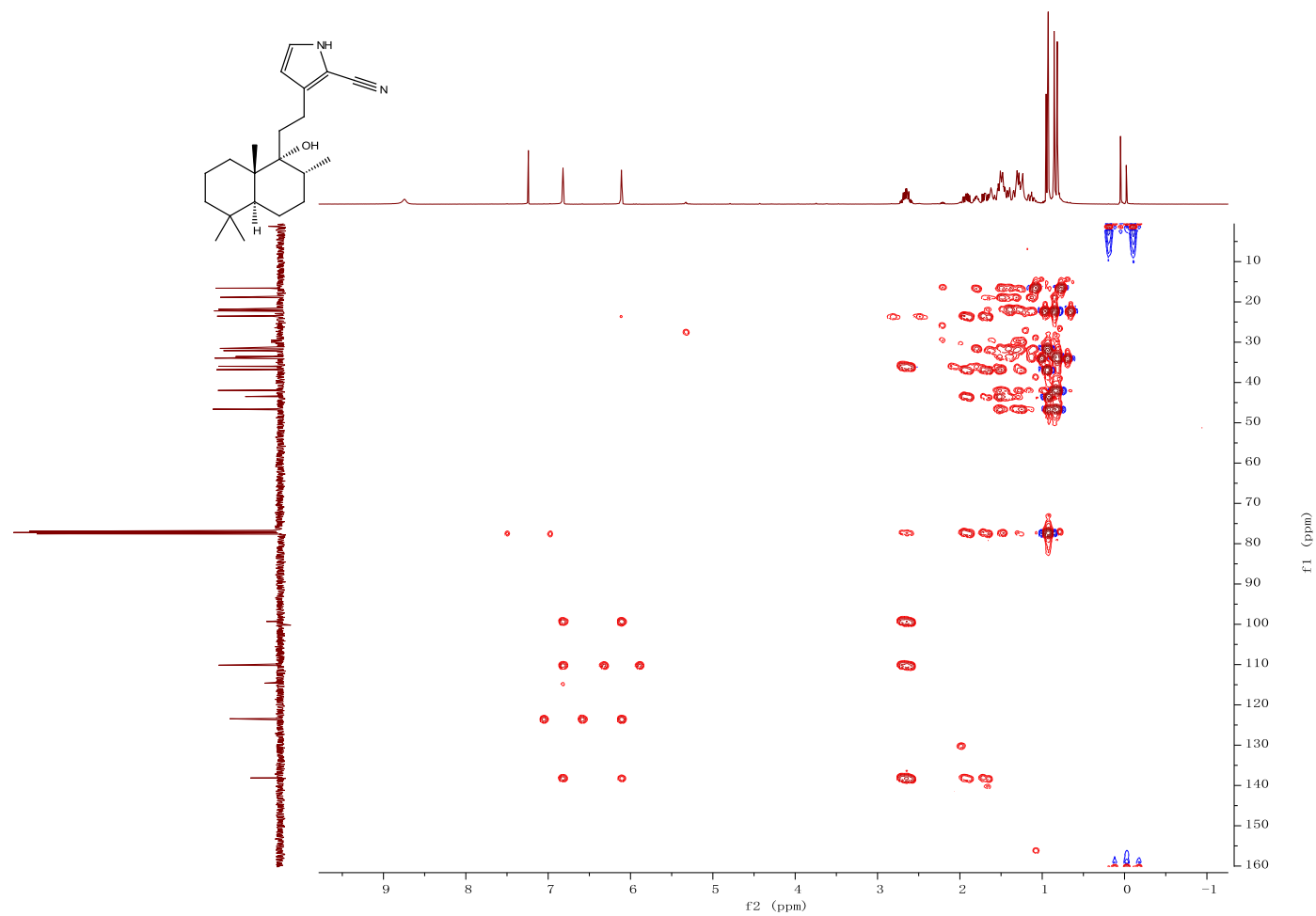


Figure S8. The HMBC Spectrum of Compound **1** in CDCl₃

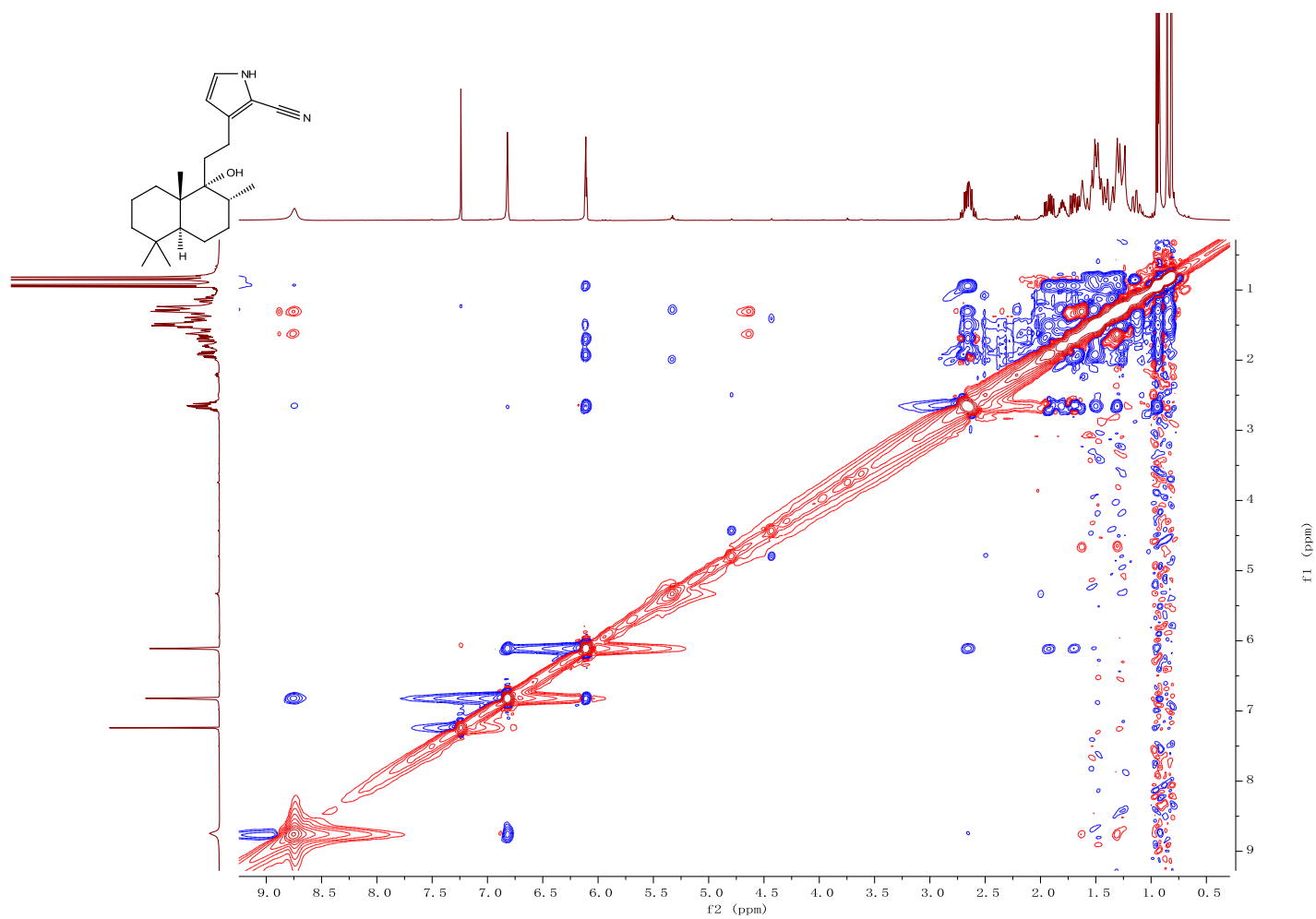


Figure S9. The NOESY Spectrum of Compound **1** in CDCl_3

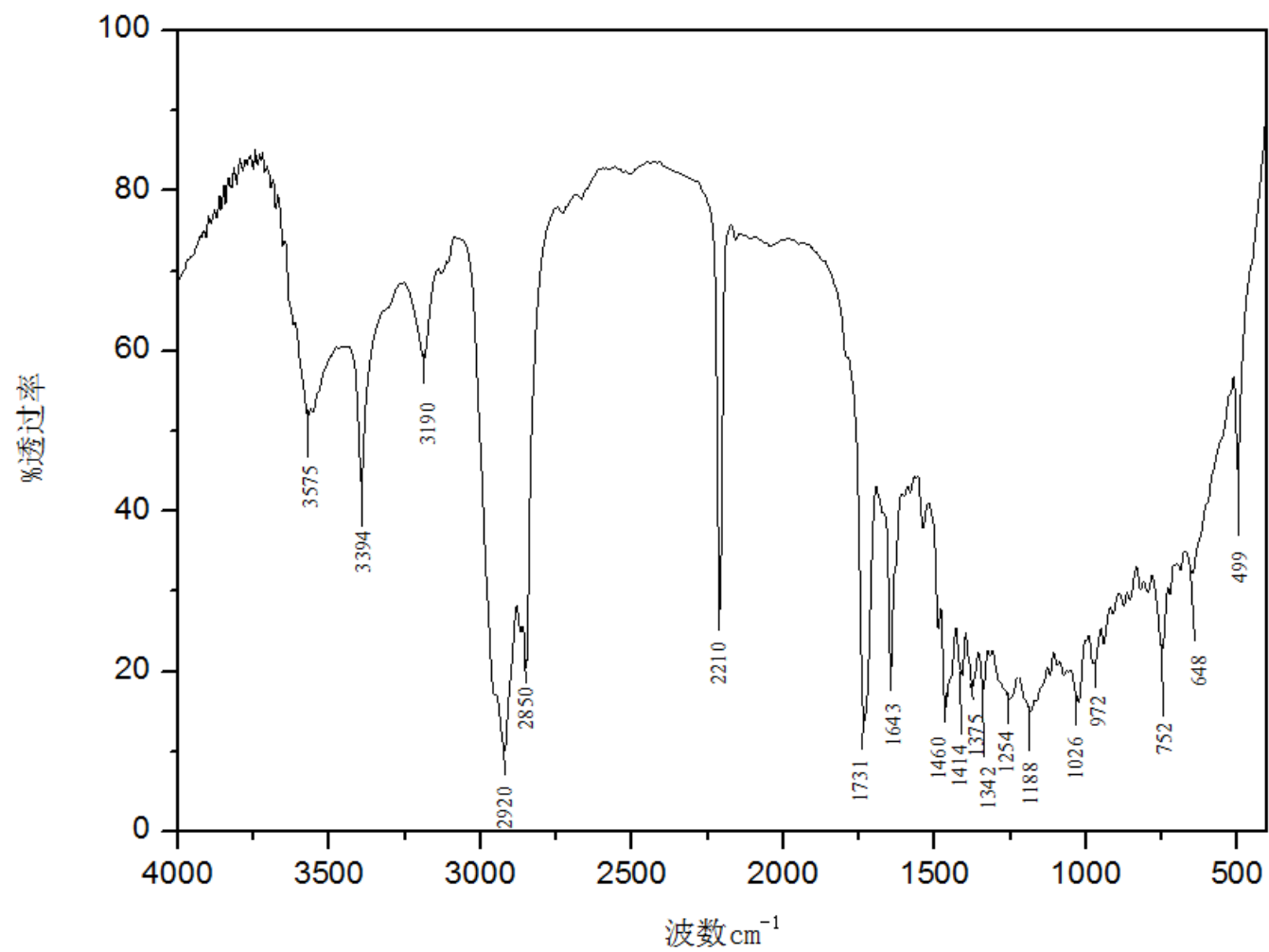


Figure S10. The IR Spectra of Compound 2

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Full ms [316.500 - 333.500] - Range: 328.200 - 328.300⁺

Scan No. 9 of 16⁺

Scan #: 9⁺

RT: 0.33⁺

Data points: 1⁺

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition ⁺
328.2507	100.0	328.2509	-0.6	-0.2	7.0	C ₂₁ H ₃₂ O ₂ N ₂ ⁺

⁺

Instrument: MAT 95XP (Thermo)

D:\DATA-HR\16\090902-mjy-zh-c1

9/9/2016 10:08:48 AM

Mjy-Zh

090902-mjy-zh-c1 #9 RT: 0.33 AV: 1 NL: 1.07E5
T: + e EI Full ms [316.50-333.50]

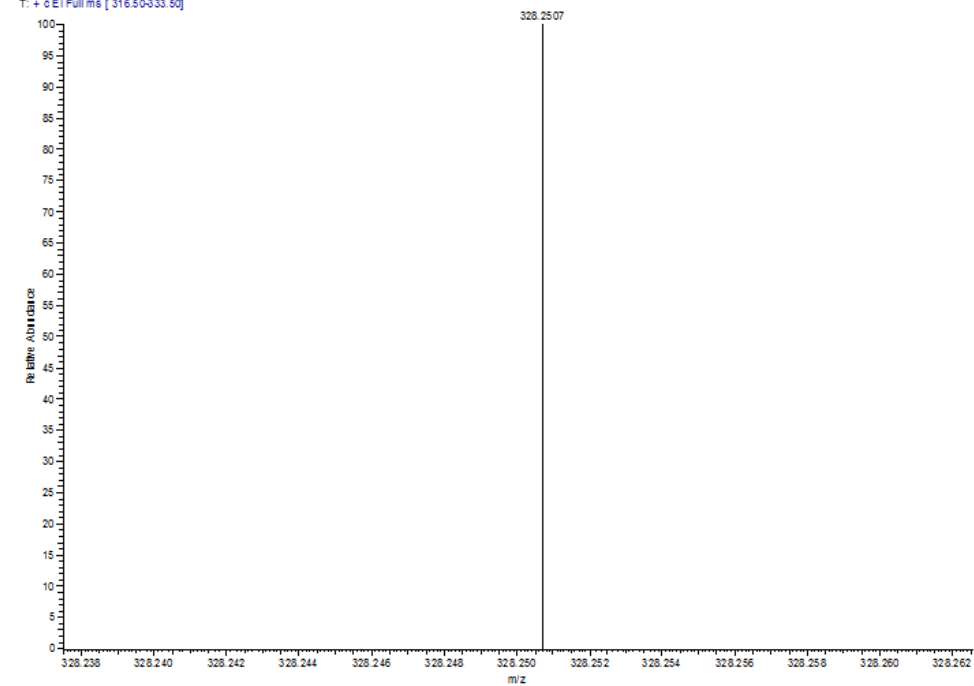


Figure S11. The HREIMS Spectroscopic Data of Compound 2

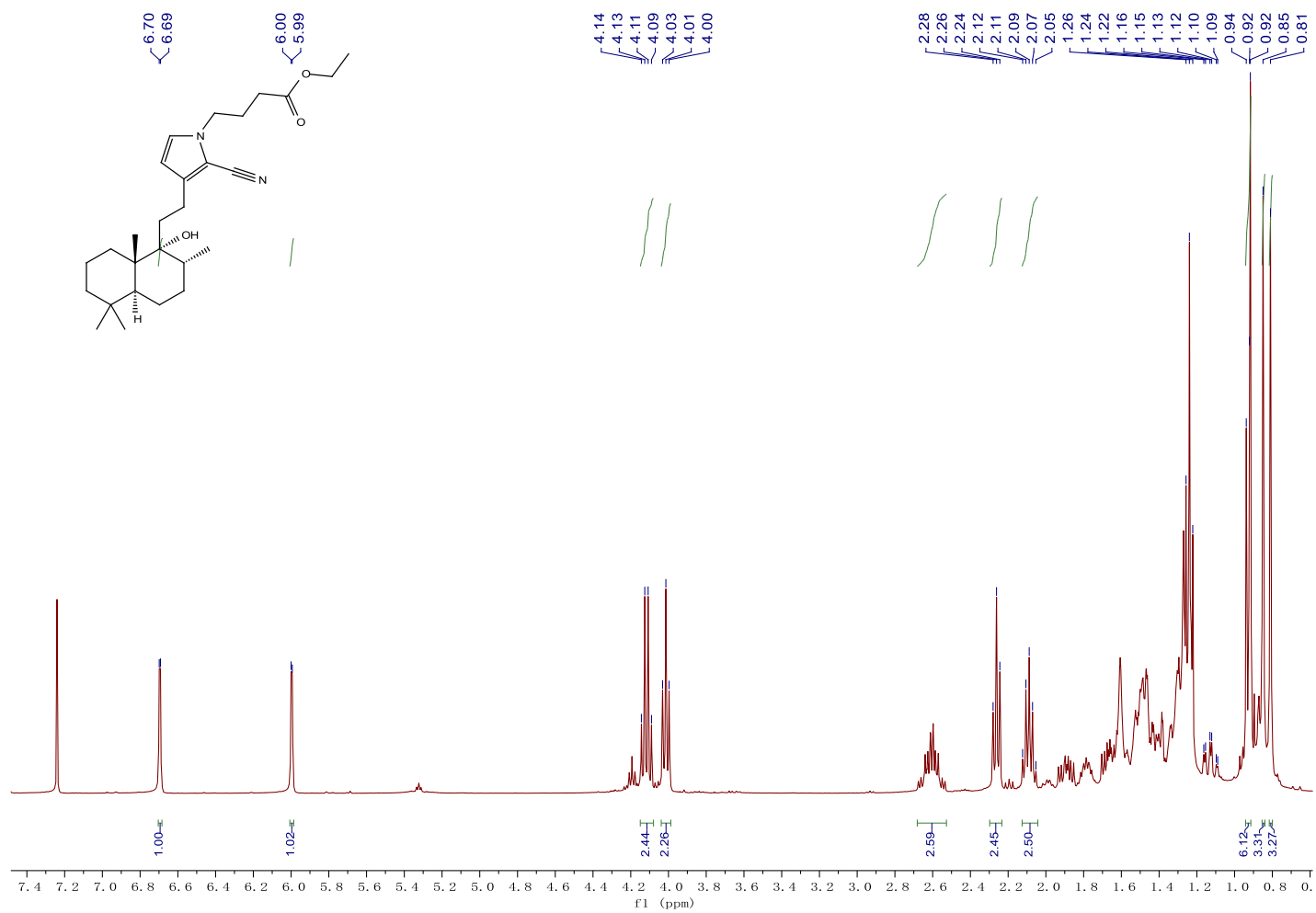


Figure S12. The ^1H NMR Spectrum of Compound **2** in CDCl_3

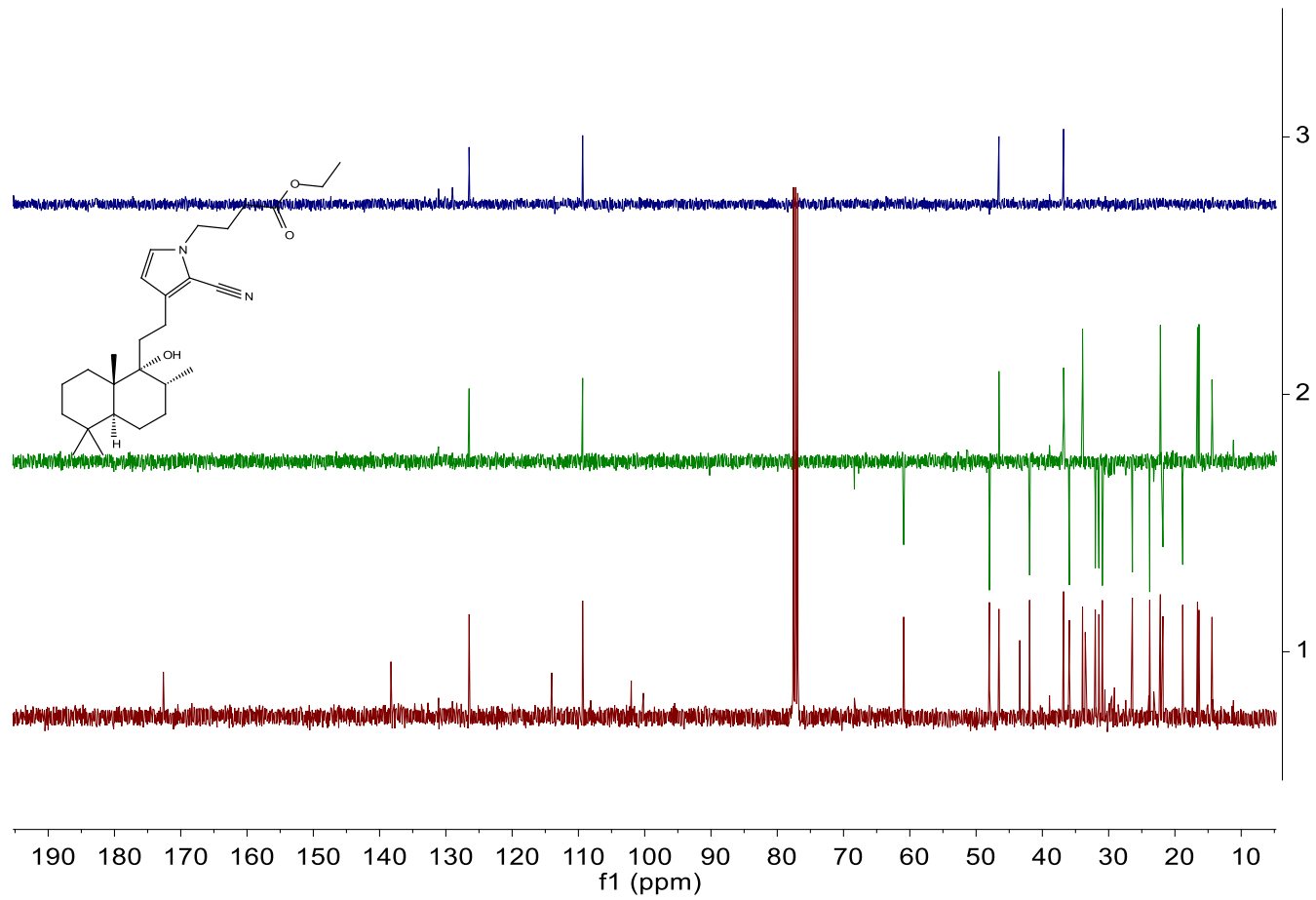


Figure S13. The ^{13}C NMR Spectrum of Compound 2 in CDCl_3

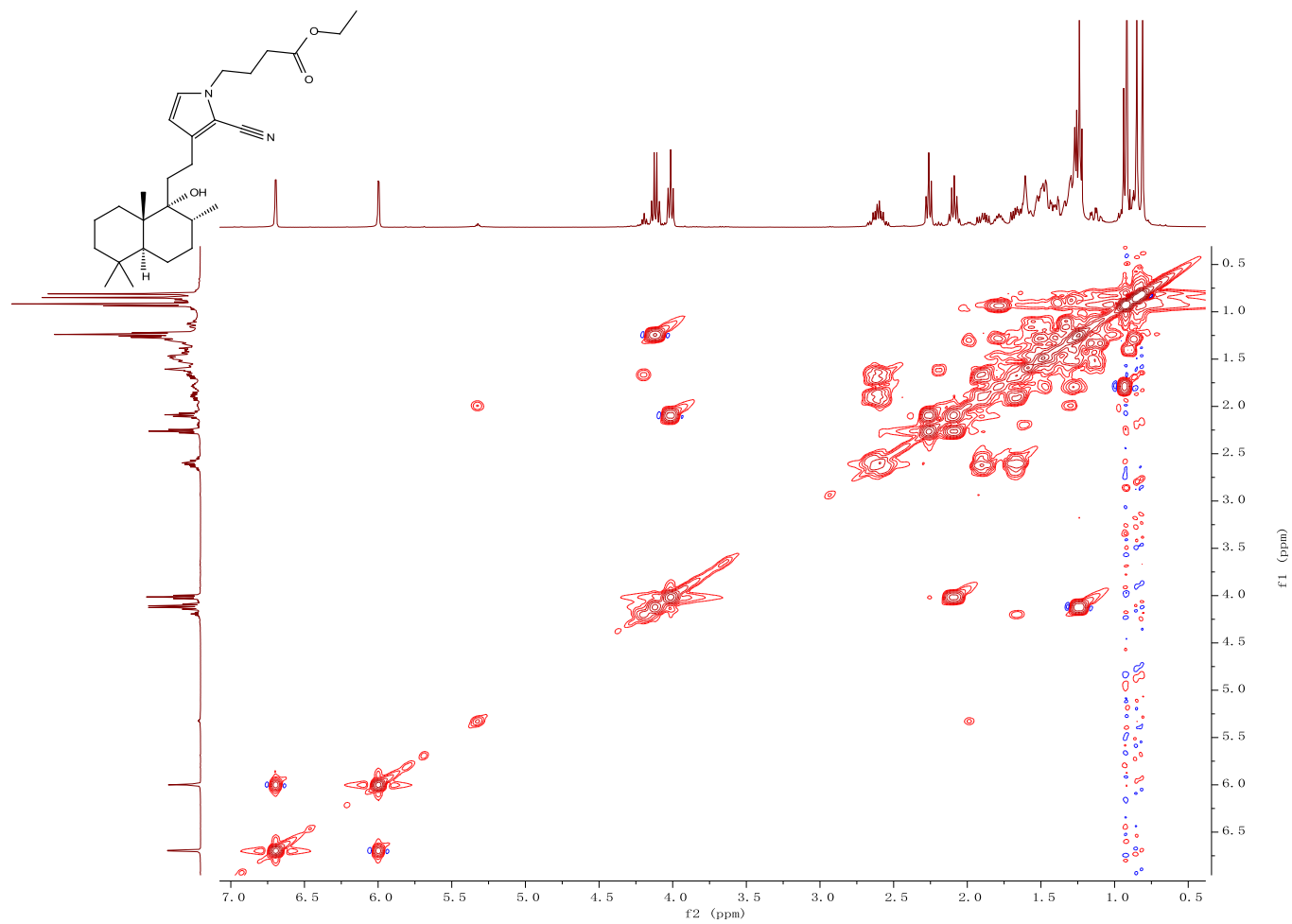


Figure S14. The ^1H - ^1H COSY Spectrum of Compound **2** in CDCl_3

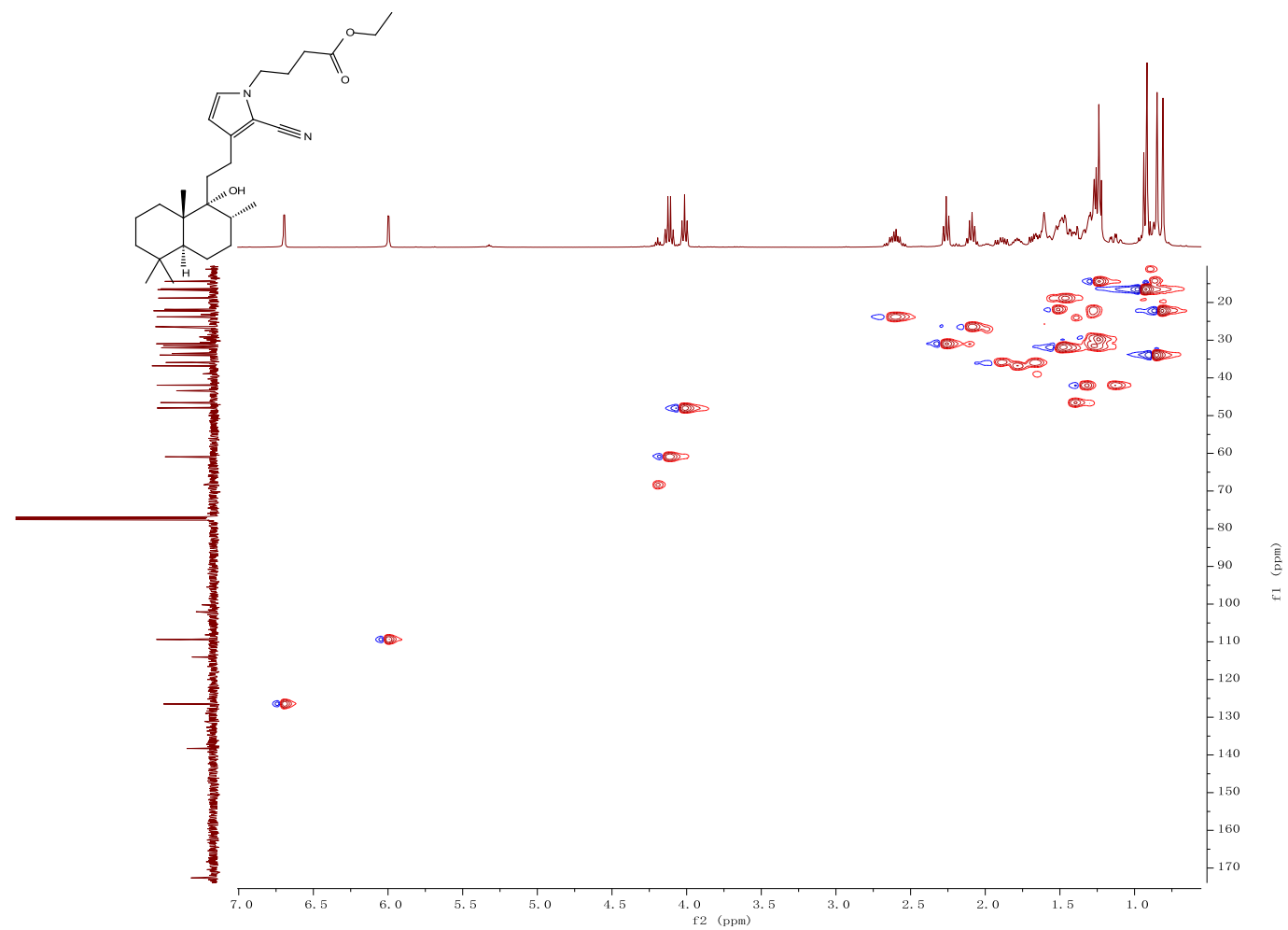


Figure S15. The HSQC Spectrum of Compound **2** in CDCl₃

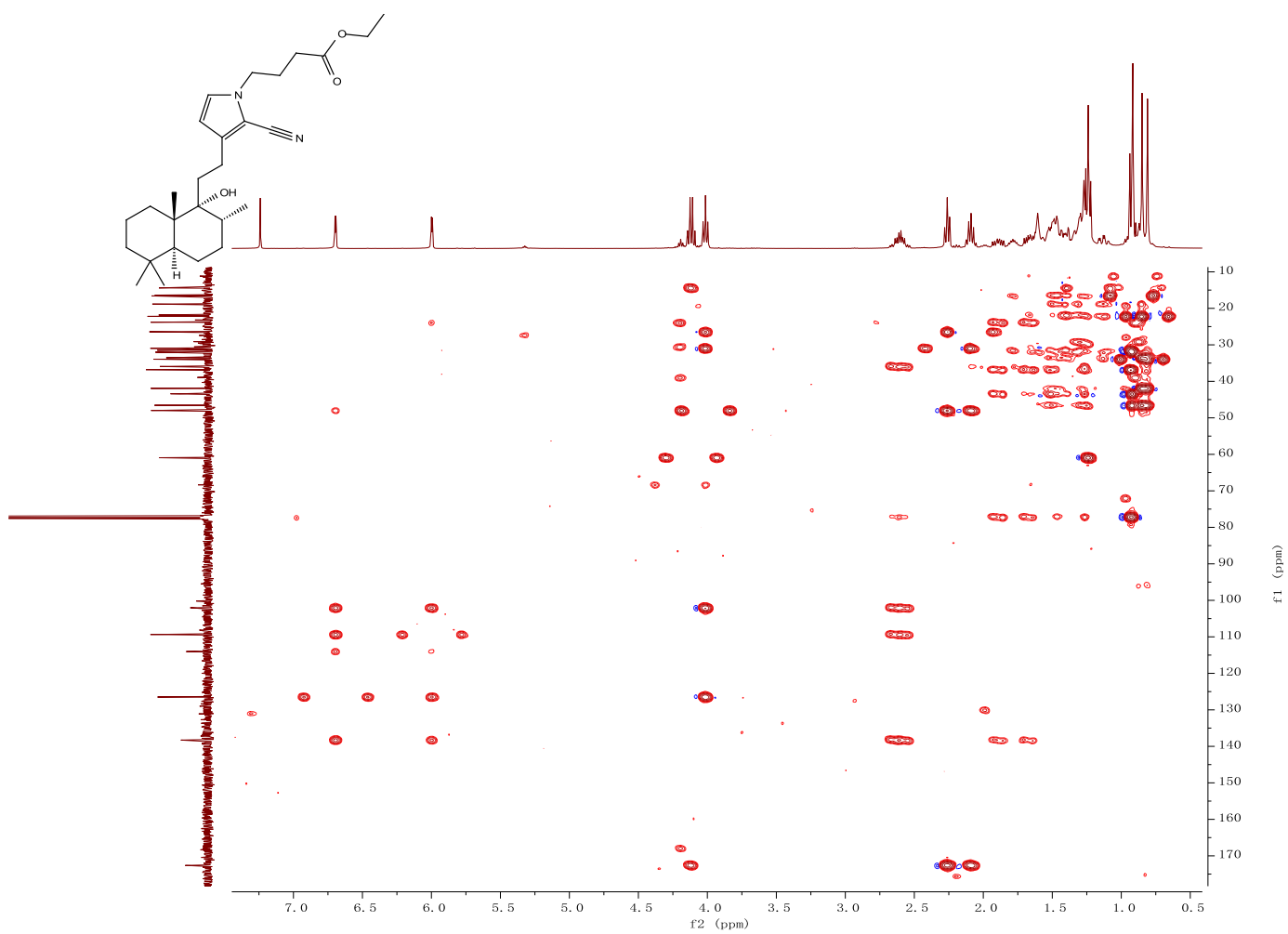


Figure S16. The HMBC Spectrum of Compound **2** in CDCl₃

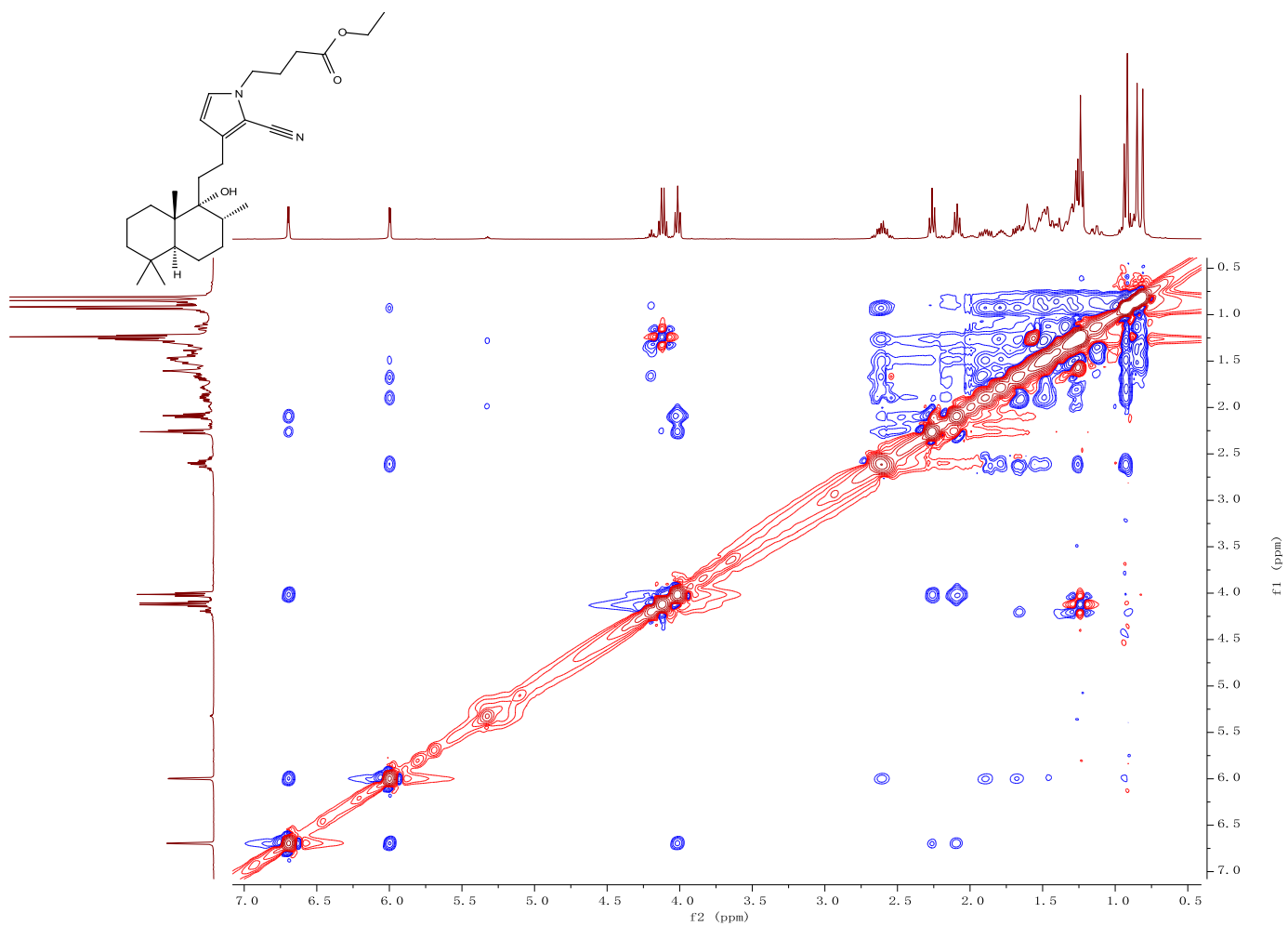


Figure S17. The NOESY Spectrum of Compound **2** in CDCl₃

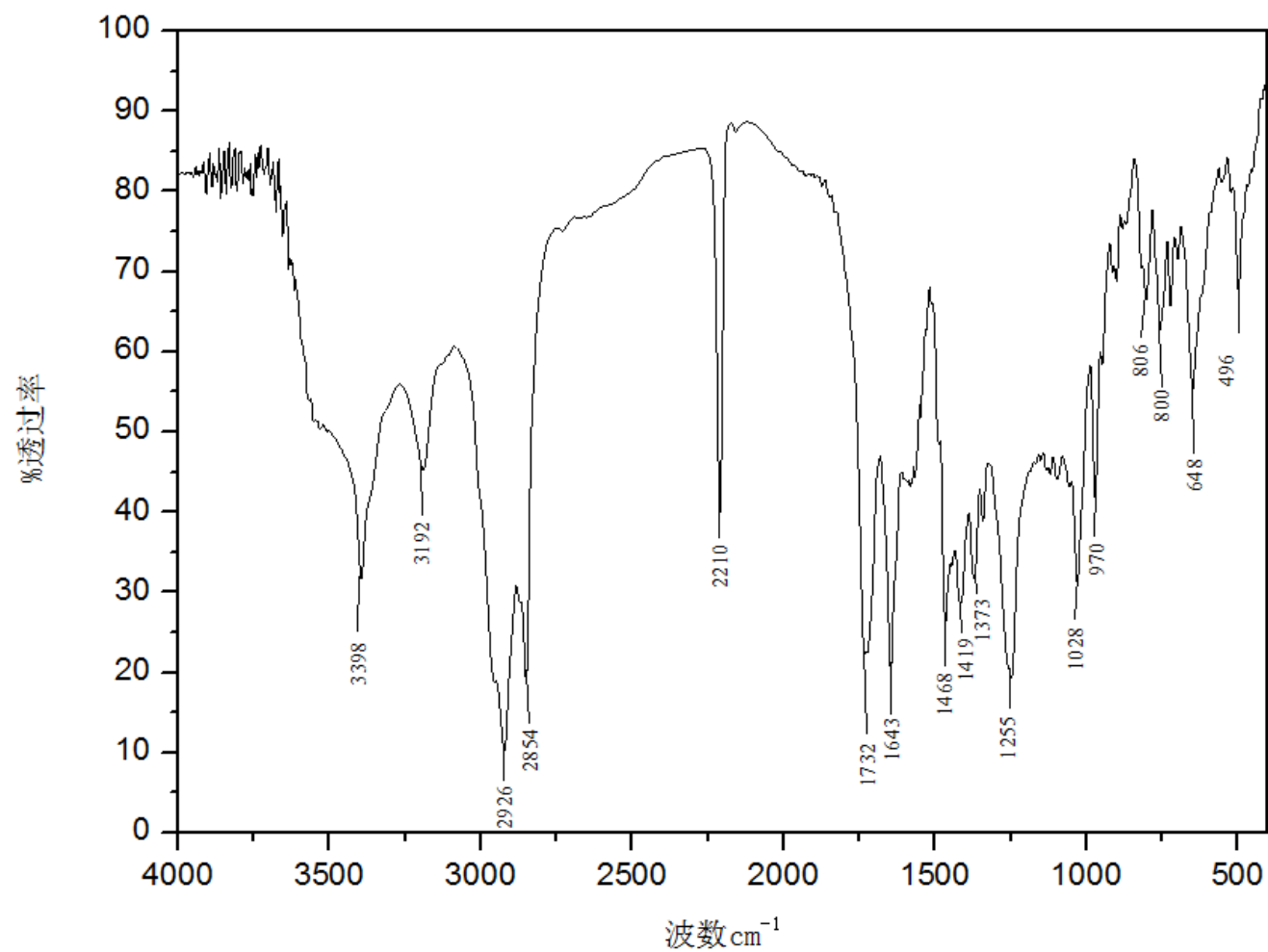


Figure S18. The IR Spectra of Compound 3

Data File: F:\高分辨数据\guojiong\lp\lp-19.Jcd

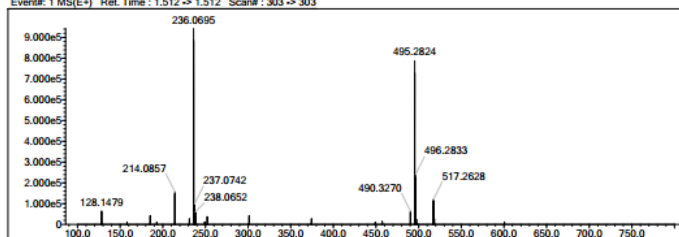
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2H	1	0	0	O	2	0	10	Si	4	0	0	Br	1	0	0	
B	3	0	0	18O	2	0	0	S	2	0	0	I	3	0	0	
C	4	0	70	F	1	0	0	Cl	1	0	0					

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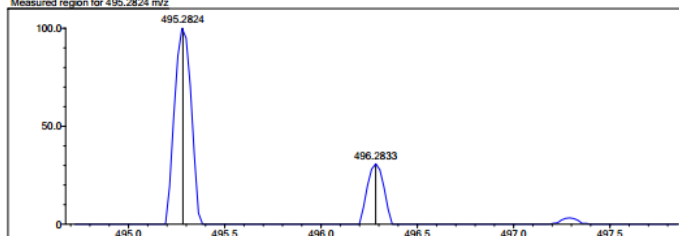
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 MSn Logic Mode: AND

Electron Ion: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

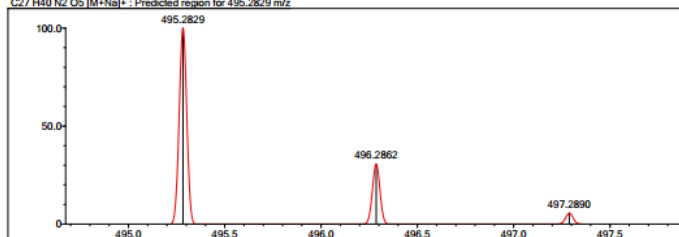
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Measured region for 495.2824 m/z



C27 H40 N2 O5 [M+Na]+ - Predicted region for 495.2829 m/z



Rank	Score	Formula (M)	Ion	Mass. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Isr	DBE
1	79.02	C27 H40 N2 O5	[M+Na]+	495.2824	495.2829	-0.5	-1.01	79.04	9.0

Figure S19. The HRESIMS Spectroscopic Data of Compound 3

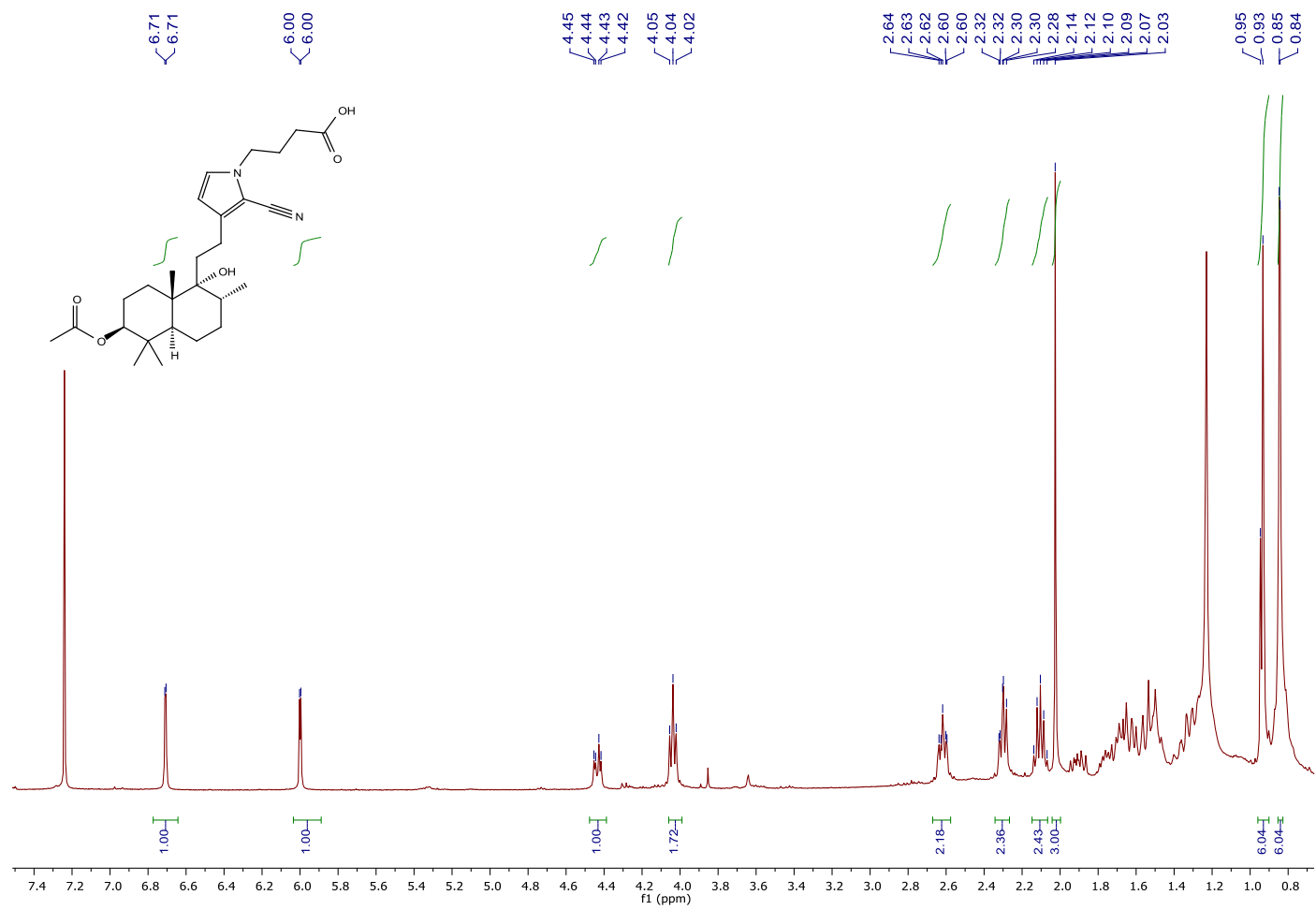


Figure S20. The ^1H NMR Spectrum of Compound **3** in CDCl_3

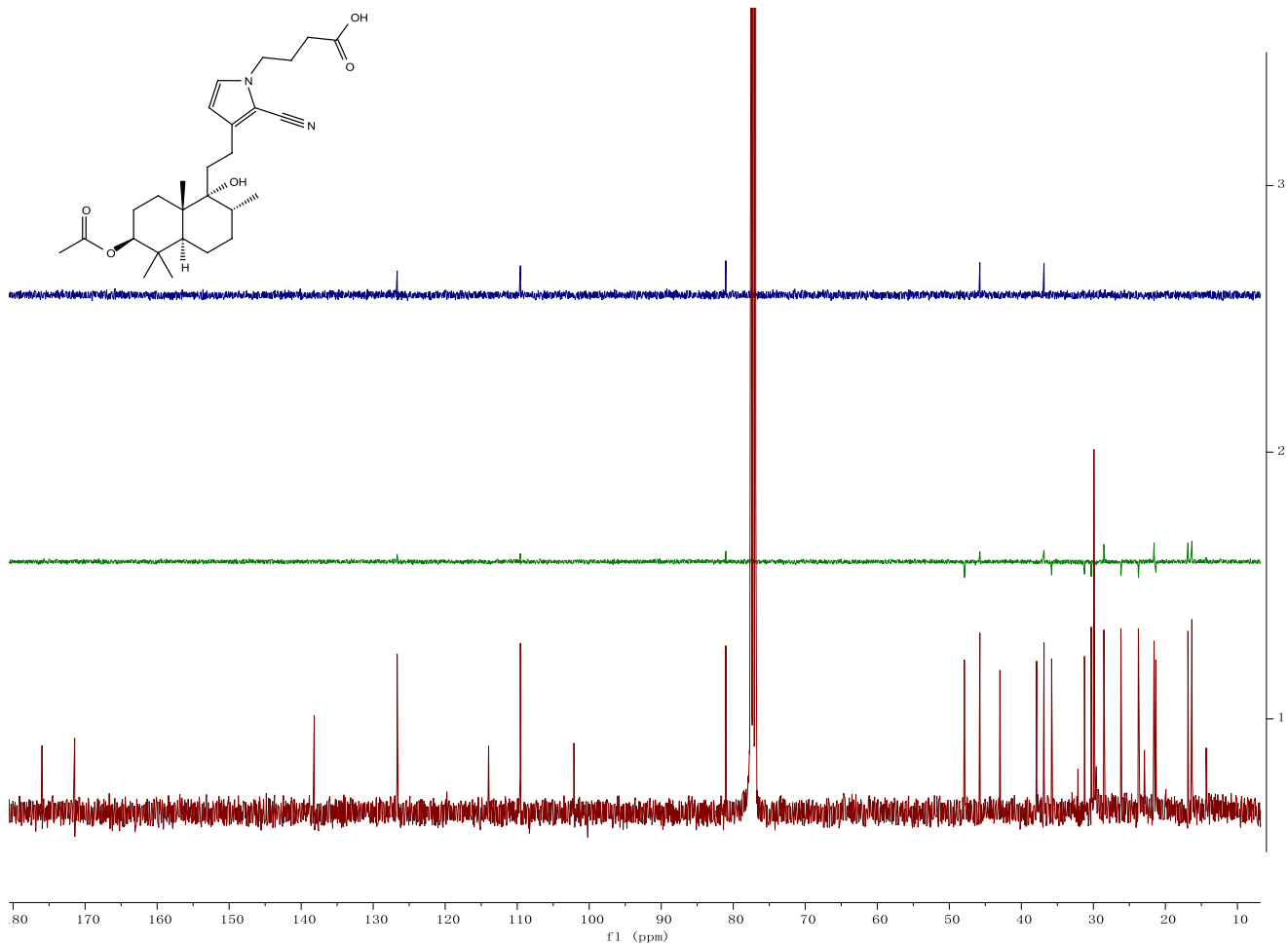


Figure S21. The ^{13}C NMR Spectrum of Compound 3 in CDCl_3

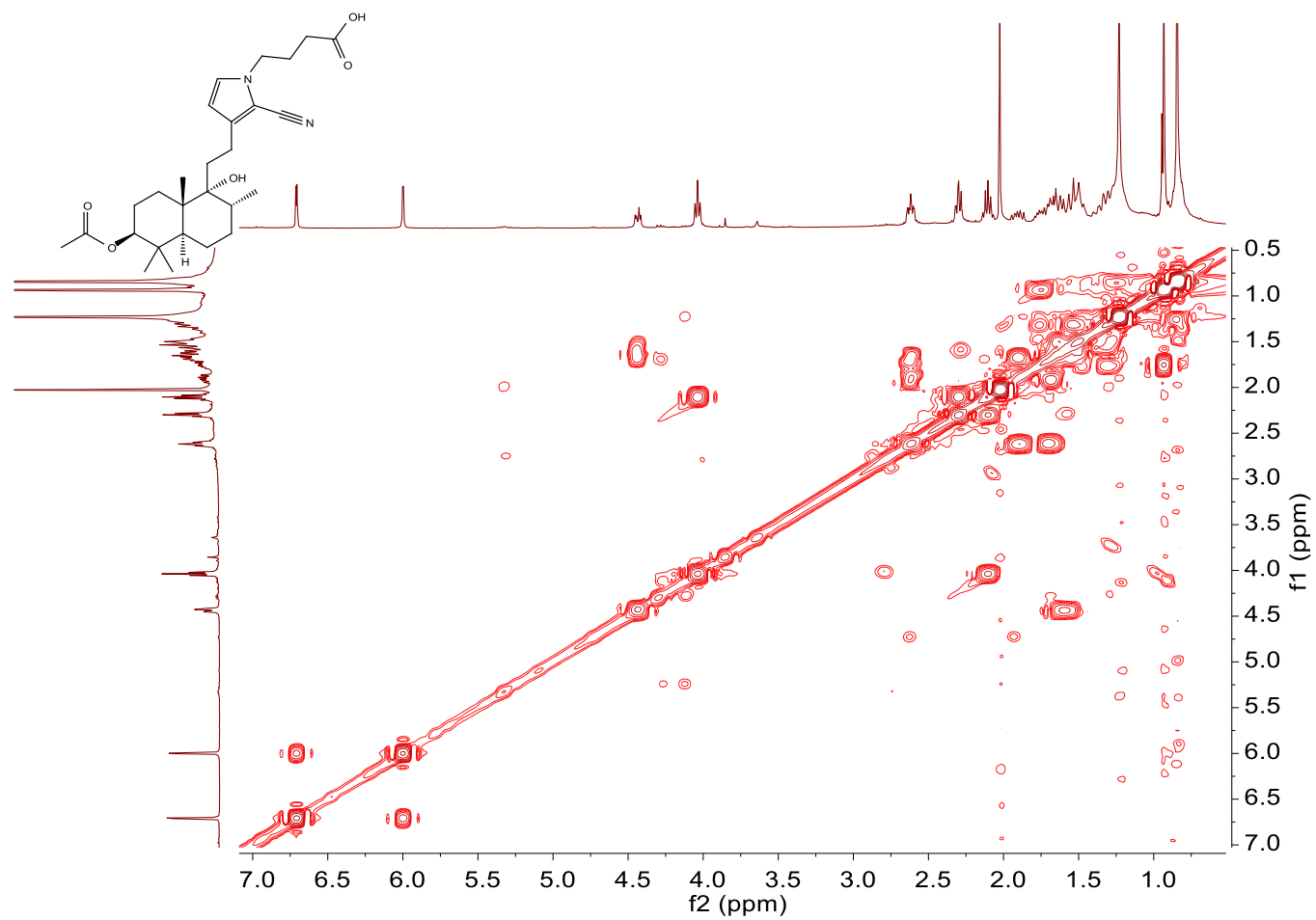


Figure S22. The ^1H - ^1H COSY Spectrum of Compound **3** in CDCl_3

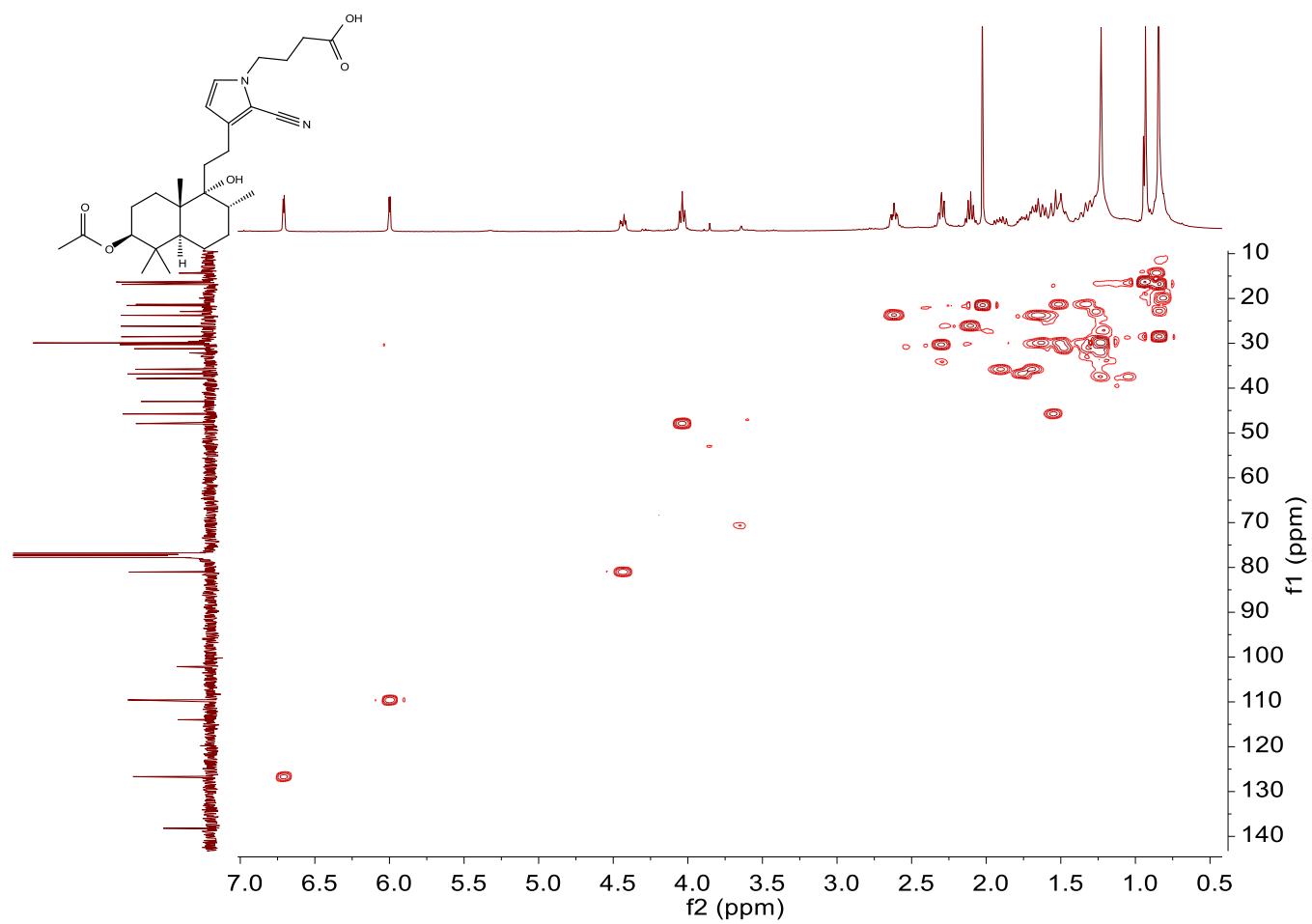


Figure S23. The HSQC Spectrum of Compound **3** in CDCl₃

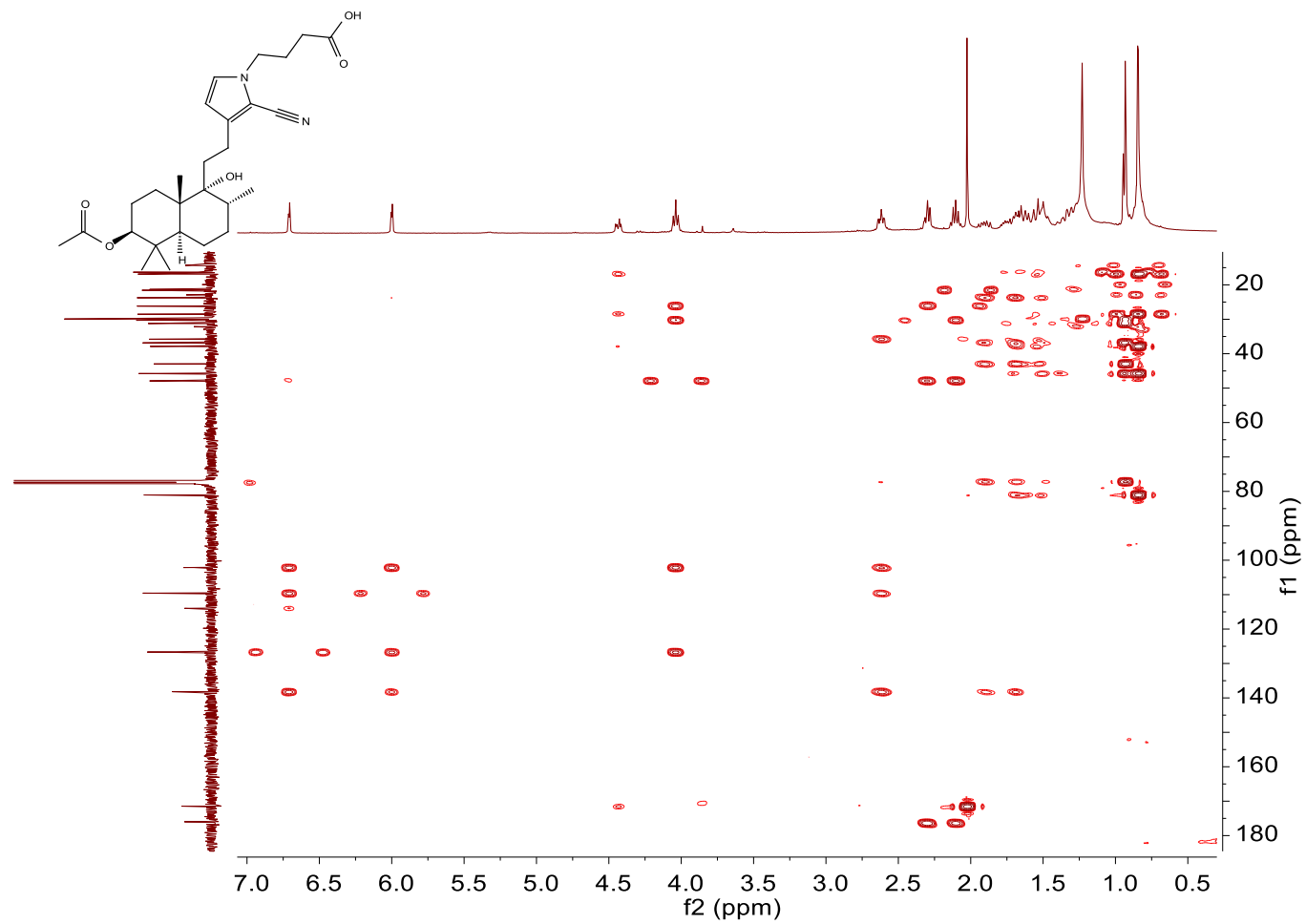


Figure S24. The HMBC Spectrum of Compound **3** in CDCl₃

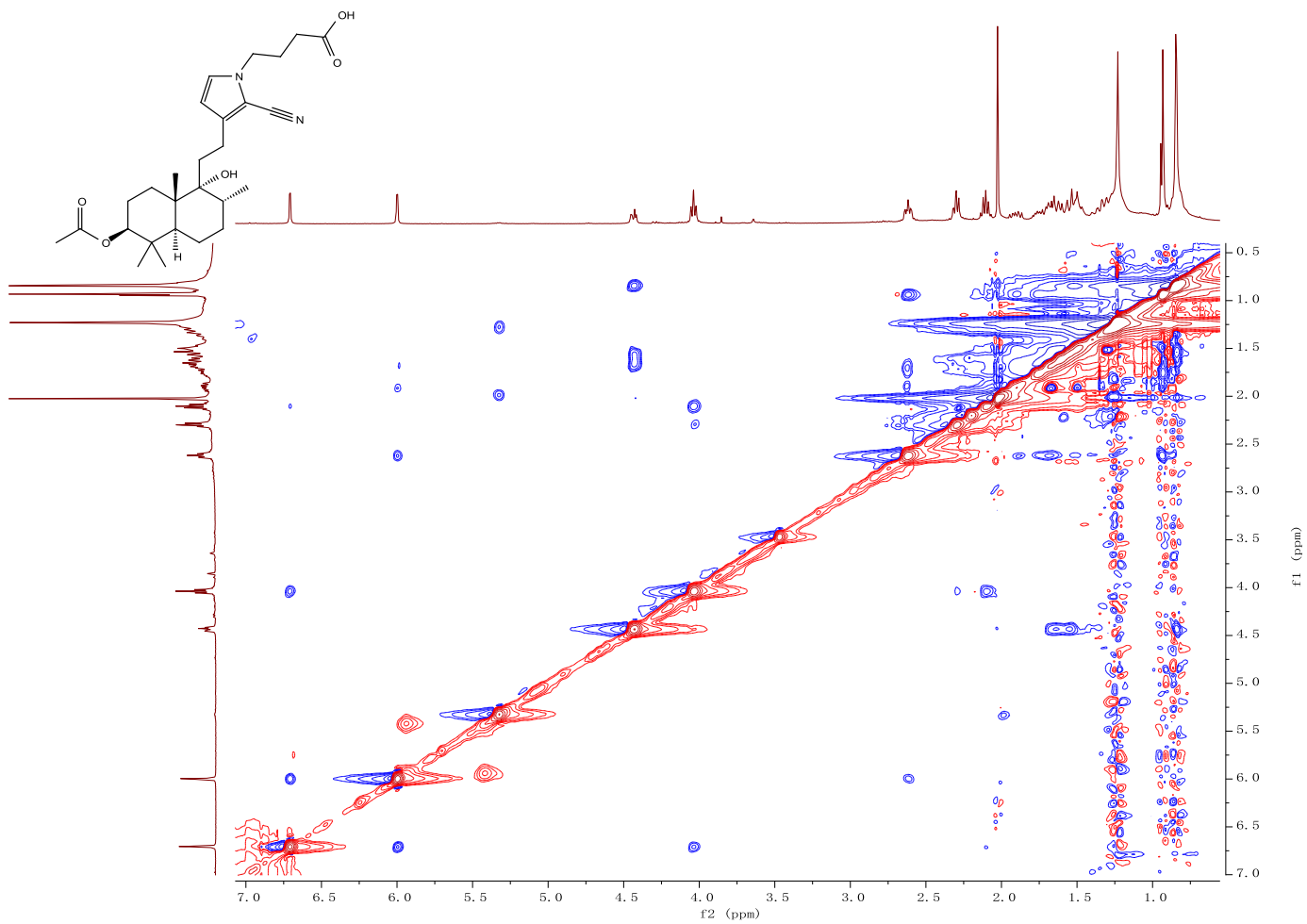


Figure S25. The NOESY Spectrum of Compound 3 in CDCl₃

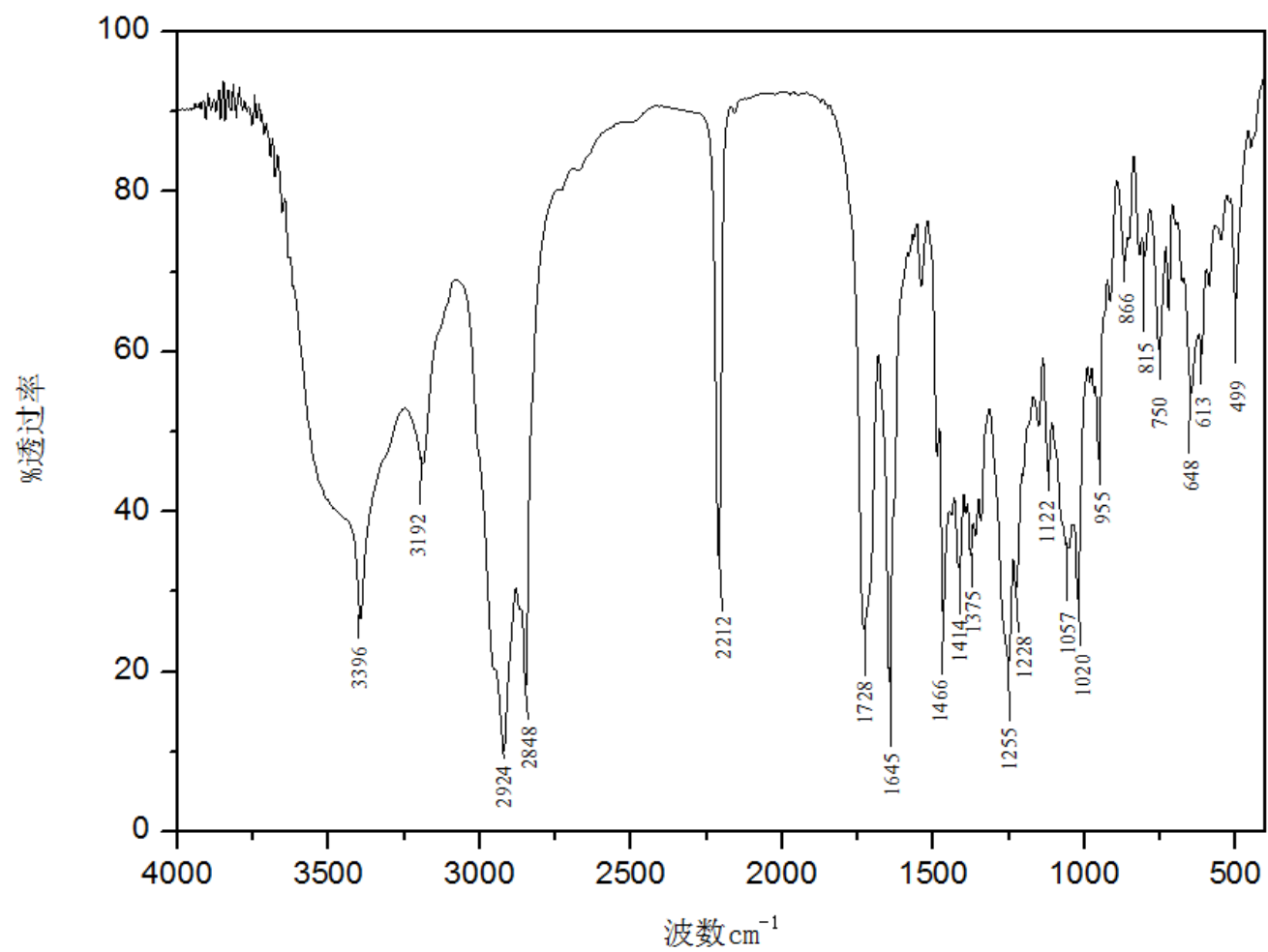


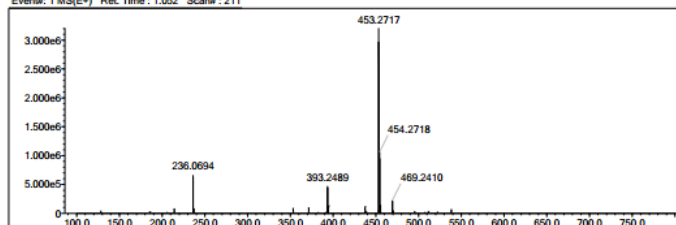
Figure S26. The IR Spectra of Compound 4

Data File: F:\高分辨数据(guajiang)\lp-28.lcd

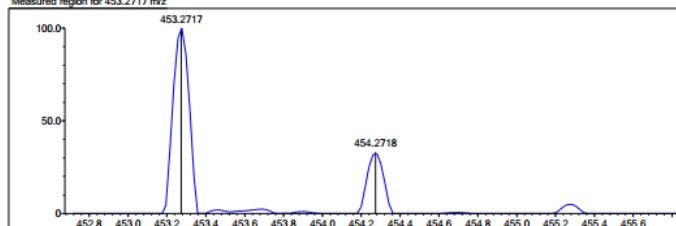
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H	1	0	150	N	3	0	2	Na	1	0	0	K	1	0	0	Na
2H	1	0	0	O	2	0	10	Si	4	0	0	Br	1	0	0	
B	3	0	0	18O	2	0	0	S	2	0	0	I	3	0	0	
C	4	0	70	F	1	0	0	Cl	1	0	0					

Error Margin (ppm): 100
 DBE Range: -0.5 - 1000.0
 Electron Ions: both
 HC Ratio: unlimited
 Apply N Rule: yes
 Use MSn Info: no
 Max Isotopes: all
 Isotope RI (%): 1.00
 Isotope Res: 10000
 MSn Iso RI (%): 75.00
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 Max Results: 500

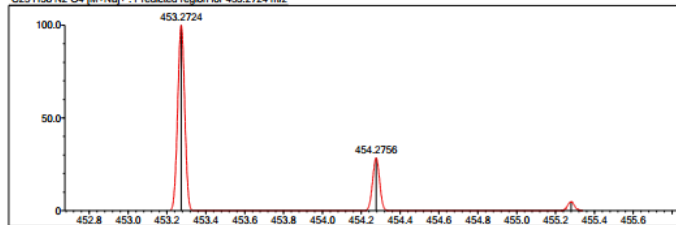
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Measured region for 453.2717 m/z



C25 H38 N2 O4 [M+Na]+ : Predicted region for 453.2724 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	85.61	C25 H38 N2 O4	[M+Na]+	453.2717	453.2724	-0.7	+1.54	86.78	8.0

Figure S27. The HRESIMS Spectroscopic Data of Compound 4

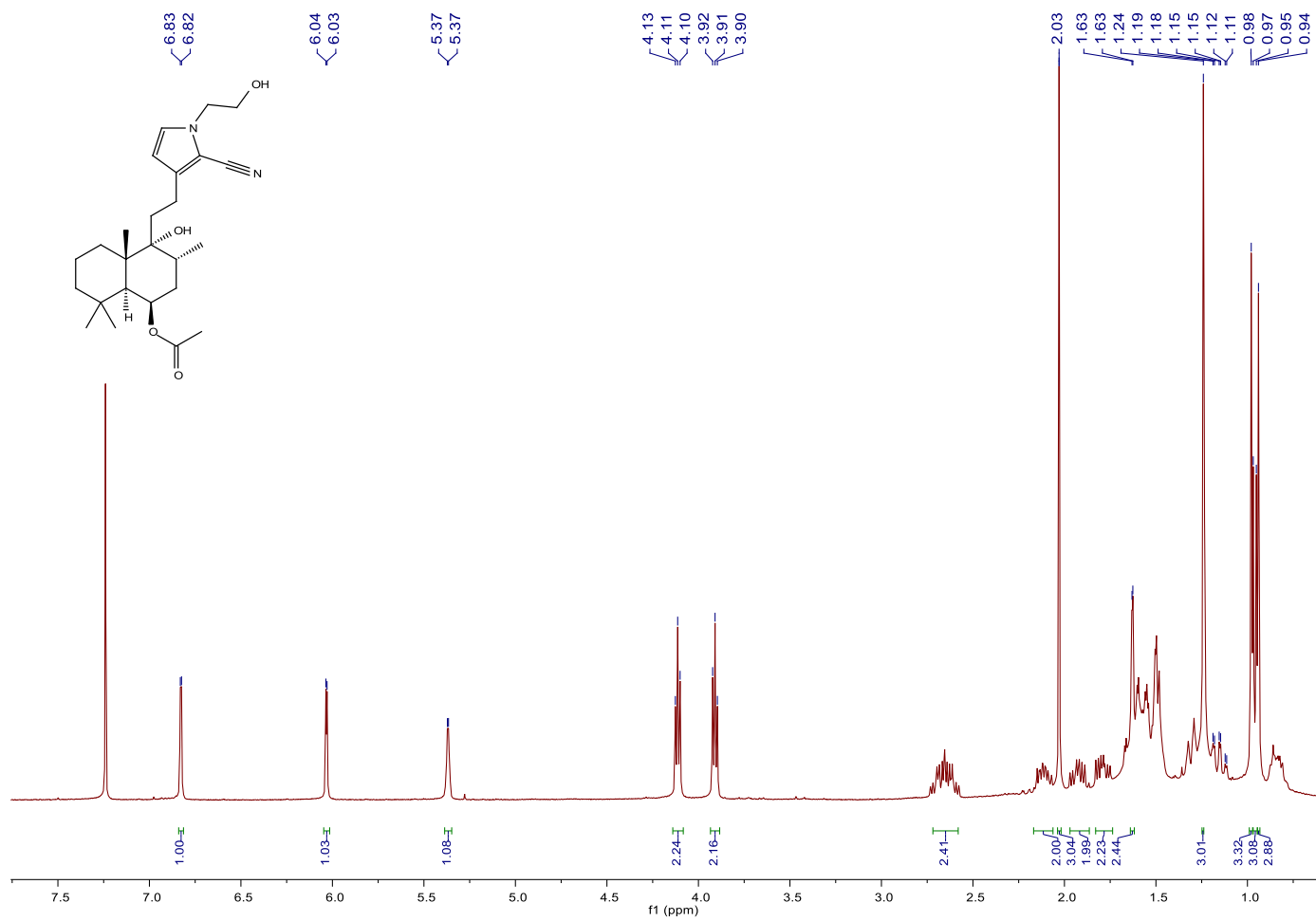


Figure S28. The ¹H NMR Spectrum of Compound 4 in CDCl₃

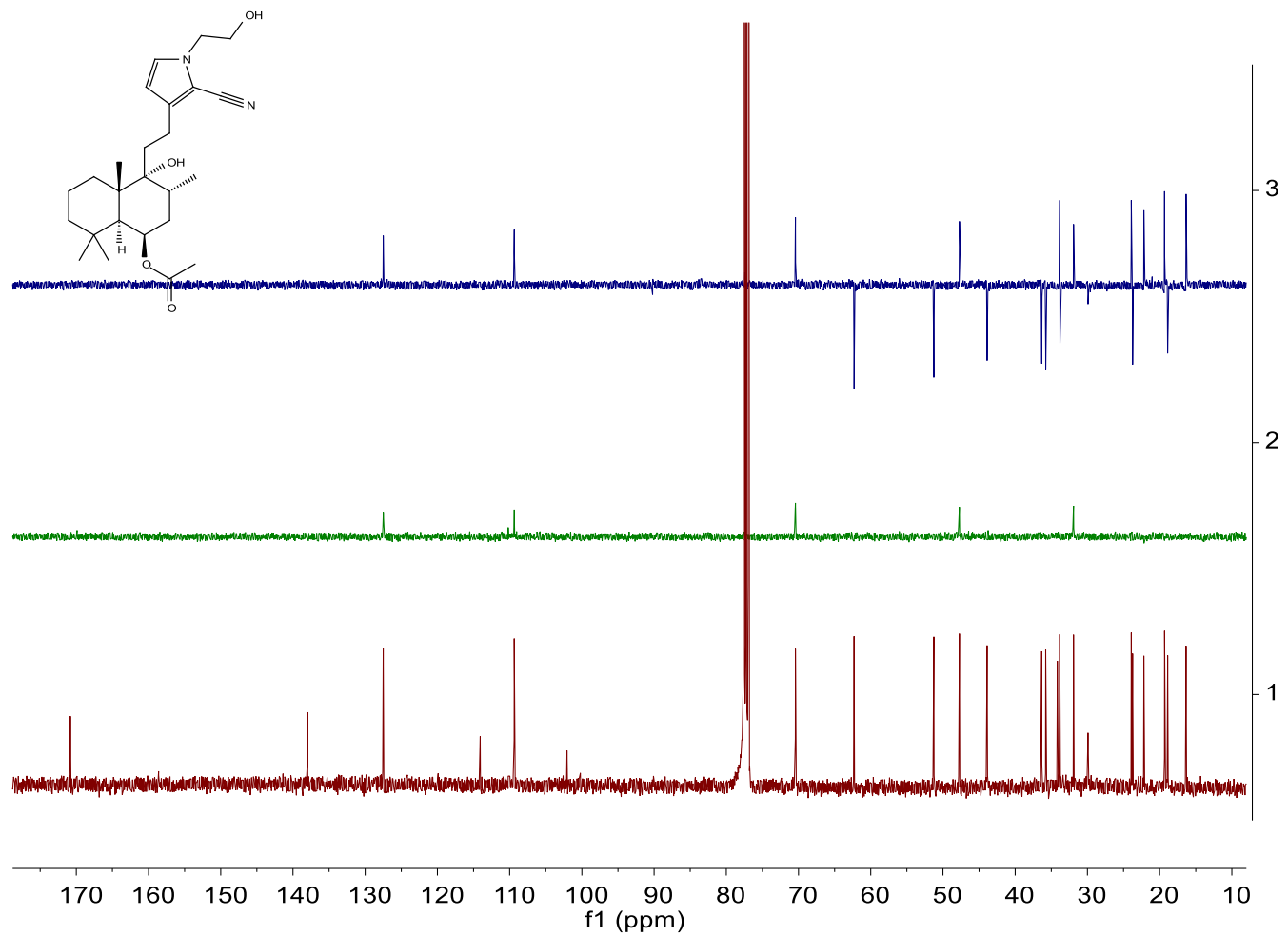


Figure S29. The ^{13}C NMR Spectrum of Compound 4 in CDCl_3

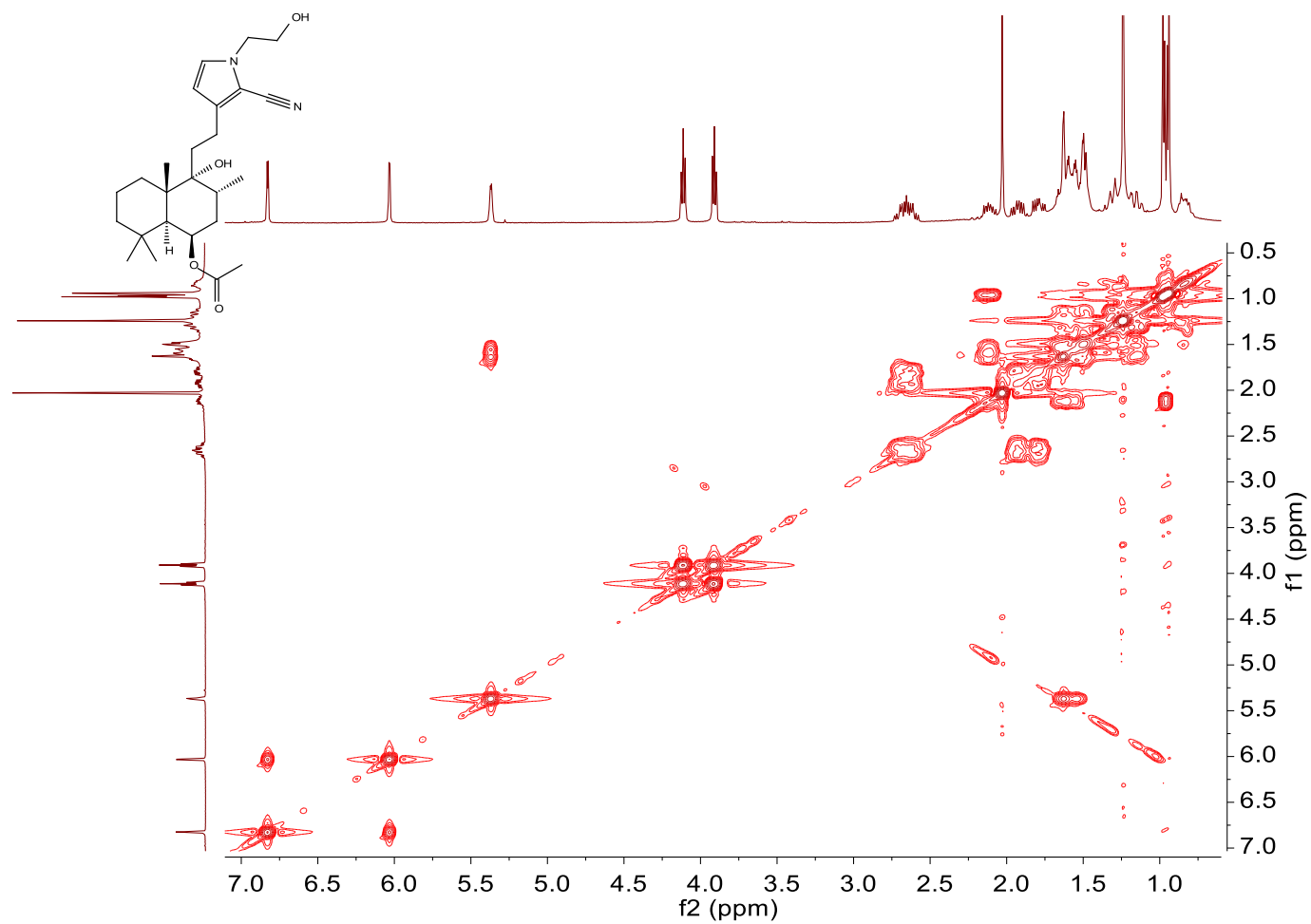


Figure S30. The ^1H - ^1H COSY Spectrum of Compound **4** in CDCl_3

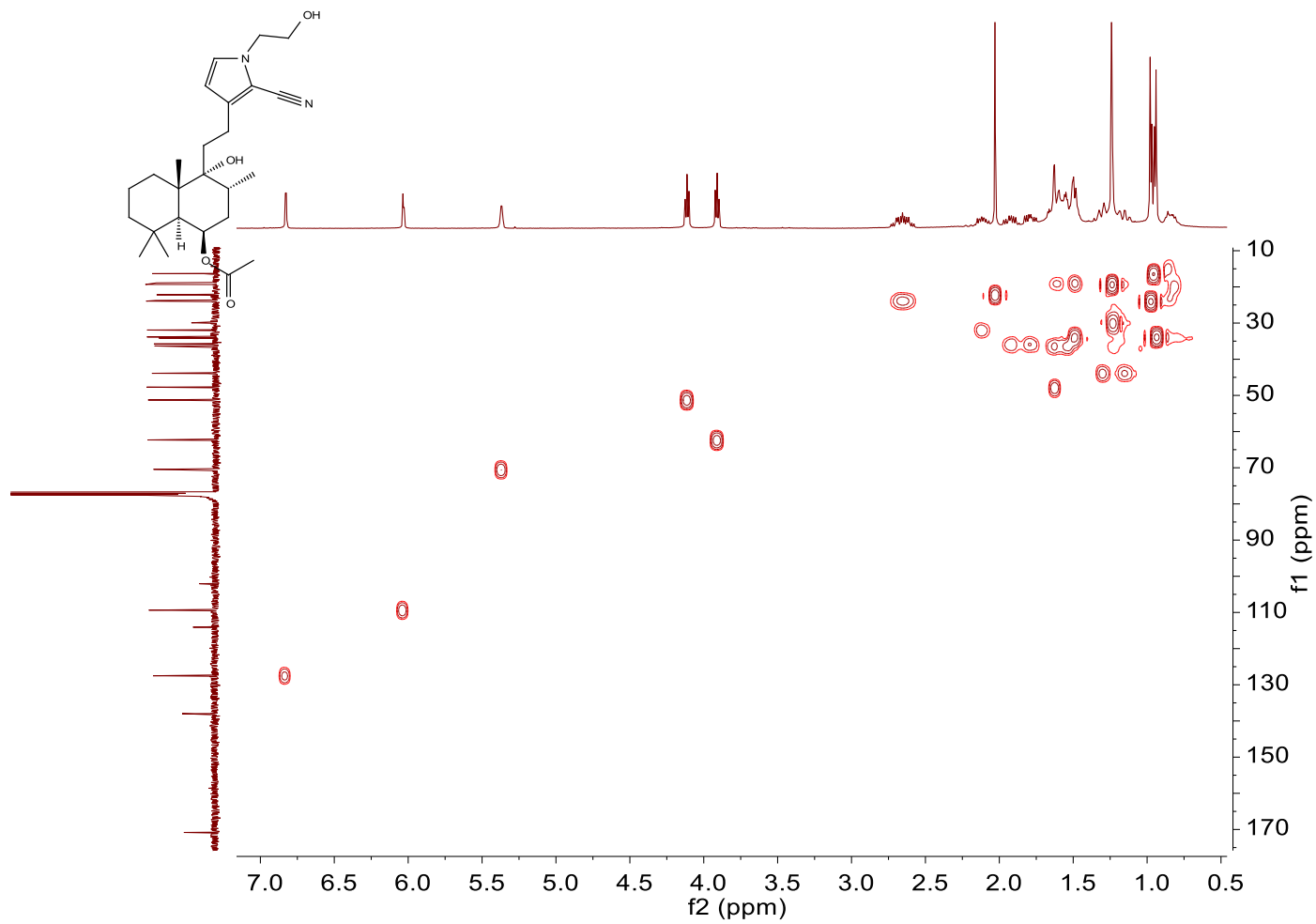


Figure S31. The HSQC Spectrum of Compound **4** in CDCl₃

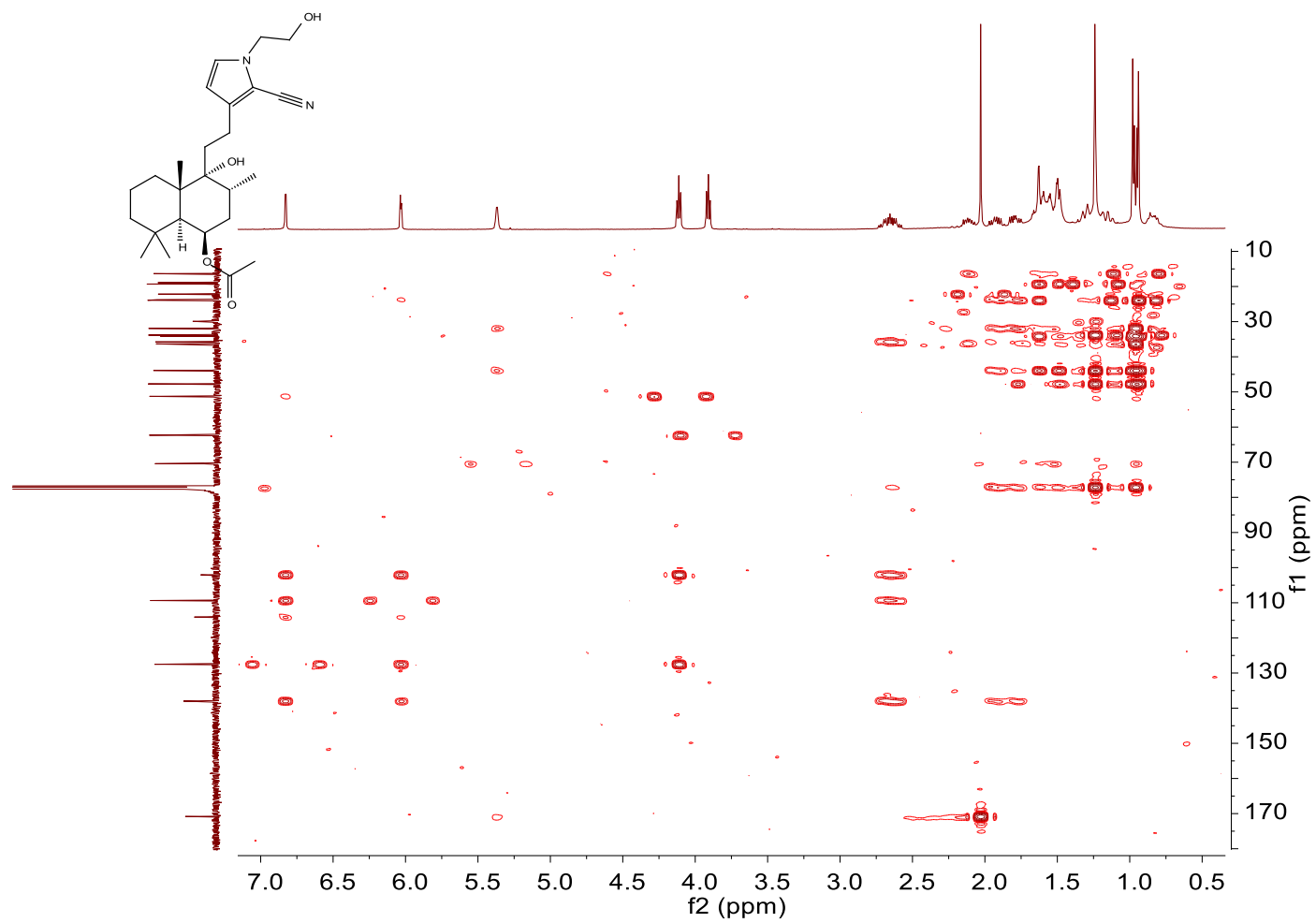


Figure S32. The HMBC Spectrum of Compound **4** in CDCl_3

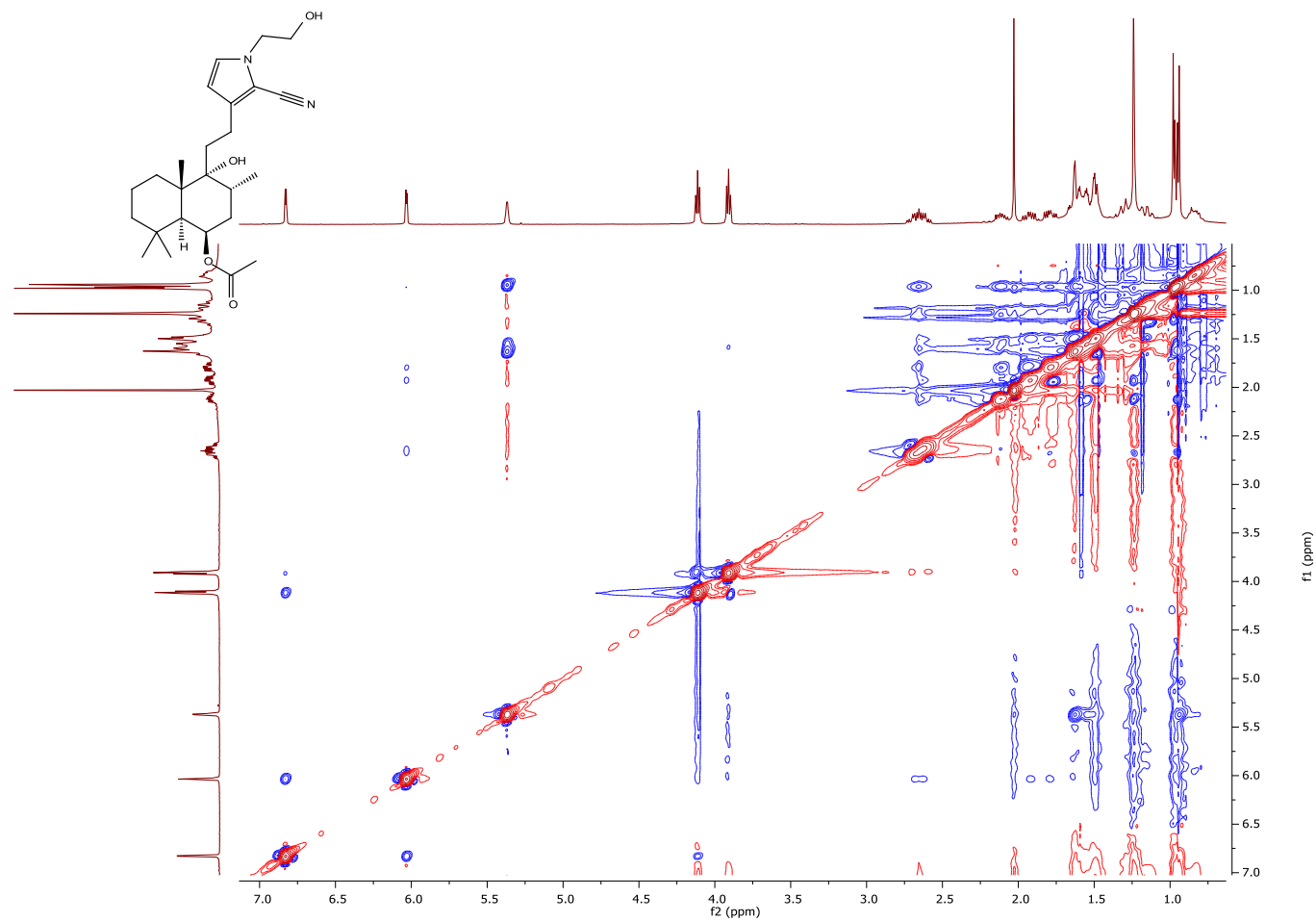


Figure S33. The NOESY Spectrum of Compound 4 in CDCl₃

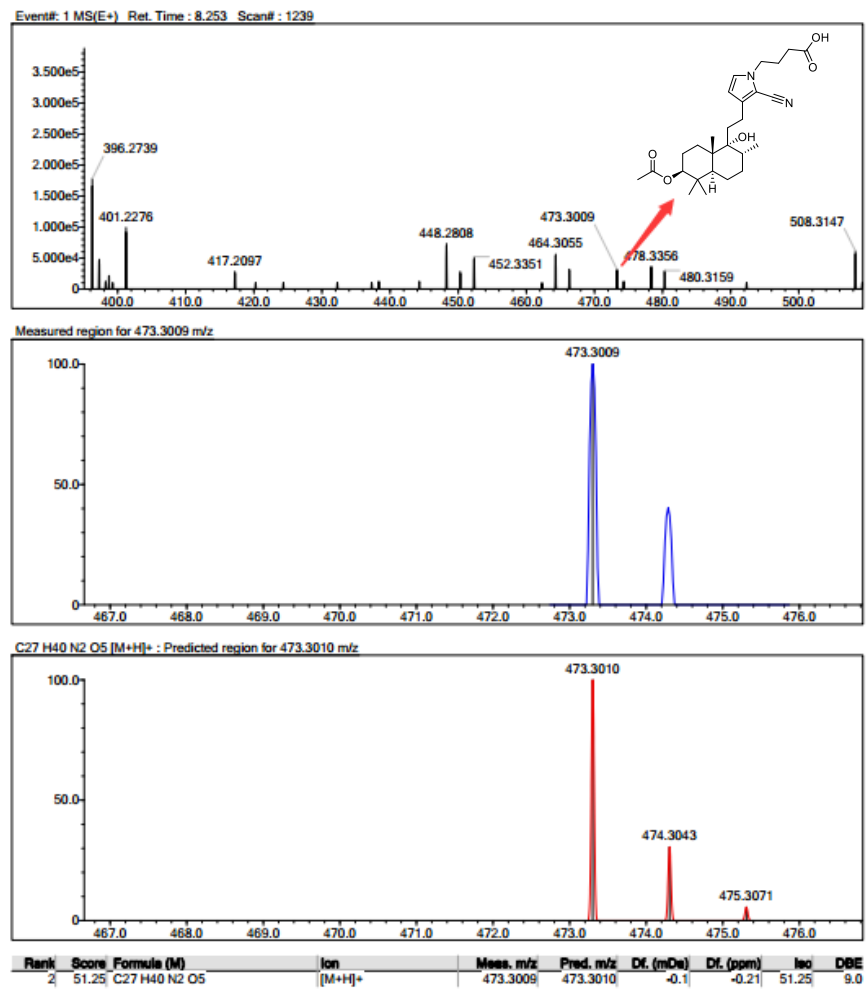


Figure S34. LC-HRESIMS for methanol extract of *Vitex trifolia*

Table S1. Cytotoxicity of Compounds **1–4**^a

compound	IC ₅₀ (μM) ± SD	
	CNE1	CNE2
1	8.7± 0.9	>10
2	>50	>50
3	>50	>50
4	>50	>50
cisplatin ^b	4.6±0.1	8.5±0.1

^a Cytotoxicity was expressed as the mean values of three experiments ± SD;

^b Cisplatin was tested as positive control