Two new antimicrobial monoterpenoid indole alkaloids from the roots of *Rauvolfia yunnanensis*

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Supporting Information

Contents of supporting information

Quantum chemical ECD calculations

The theoretical calculations were achieved using Gaussian 09[1]. After established the 3D structure by ROESY spectra, the conformational analysis using CONFLEX software at MMFF94s force field within 7 Kcal/mol was carried out. The resulting conformers were subjected to geometry optimization and energy calculation using Density Functional Theory (DFT) at the B3LYP/6-31+G(d) level in gas phase. The theoretical calcaulation of ECD was using Time Dependent DFT at B3LYP/6-31G (d, p) level in MeOH with PCM model[2]. The ECD spectra were combined after Boltzmann weighting according to their population contribution[3].

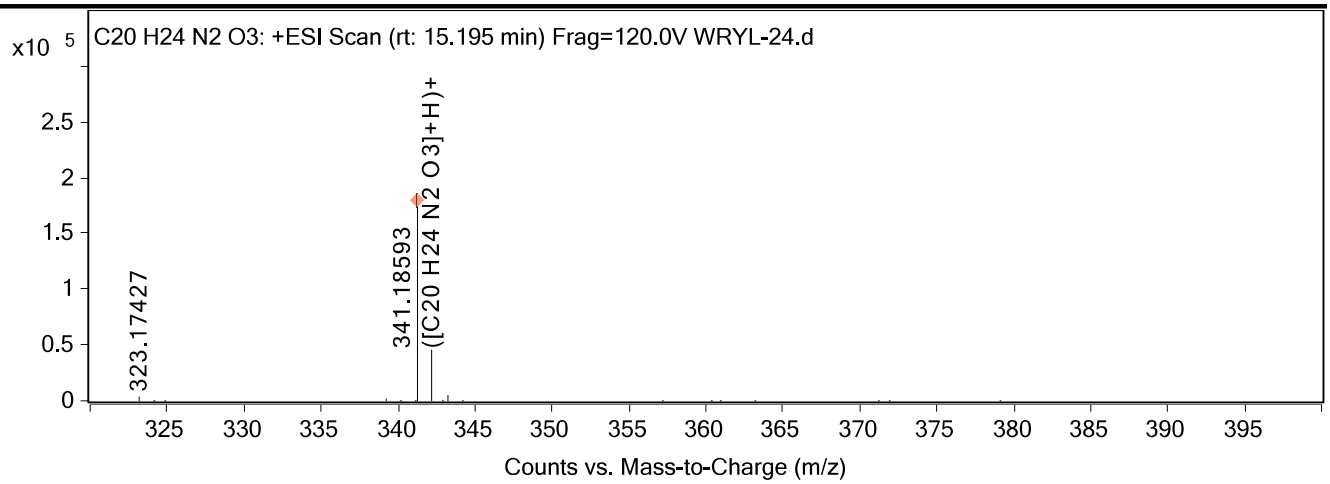
Reference

[1] Gaussian 09, Revision A.02, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, G.A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B.G. Janesko, R. Gomperts, B. Mennucci, H.P. Hratchian, J.V. Ortiz, A.F. Izmaylov, J.L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V.G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J.A. Montgomery, Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, J.M. Millam, M. Klene, C. Adamo, R. Cammi, J.W. Ochterski, R.L. Martin, K. Morokuma, O. Farkas, J.B. Foresman, and D.J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[2] T. Yanai, D.P. Tew, and N.C. Handy, *Chem. Phys. Lett.* **393**, 51 (2004).

[3] Y.L. Si, G.C. Yang, M.G. Hu, and M. Wang, *Chem. Phys. Lett.* **502**, 266 (2011).

Qualitative Analysis Report



Peak List

m/z	z	Abund	Formula	Ion
78.02226		2242.11		
98.97487		8475.12		
111.04233		1955.3		
113.9632		2900.15		
114.94736		2730.69		
122.09617		3228.41		
132.97272		1984.9		
137.05473		1955.19		
138.0913		3749.74		
140.00043		1961.22		
141.03974		2308.5		
143.0007		4887.41		
155.97354		2943.16		
157.01637		13911.72		
158.0021		1894.58		
173.01088		5388.2		
187.02707		8958.53		
281.16362		6980.27		
323.17427		3744.34		
341.18593	1	186861.44	C20 H24 N2 O3	(M+H)+
342.18799	1	44768.03	C20 H24 N2 O3	(M+H)+
343.19036	1	5163.6	C20 H24 N2 O3	(M+H)+

Formula Calculator Element Limits

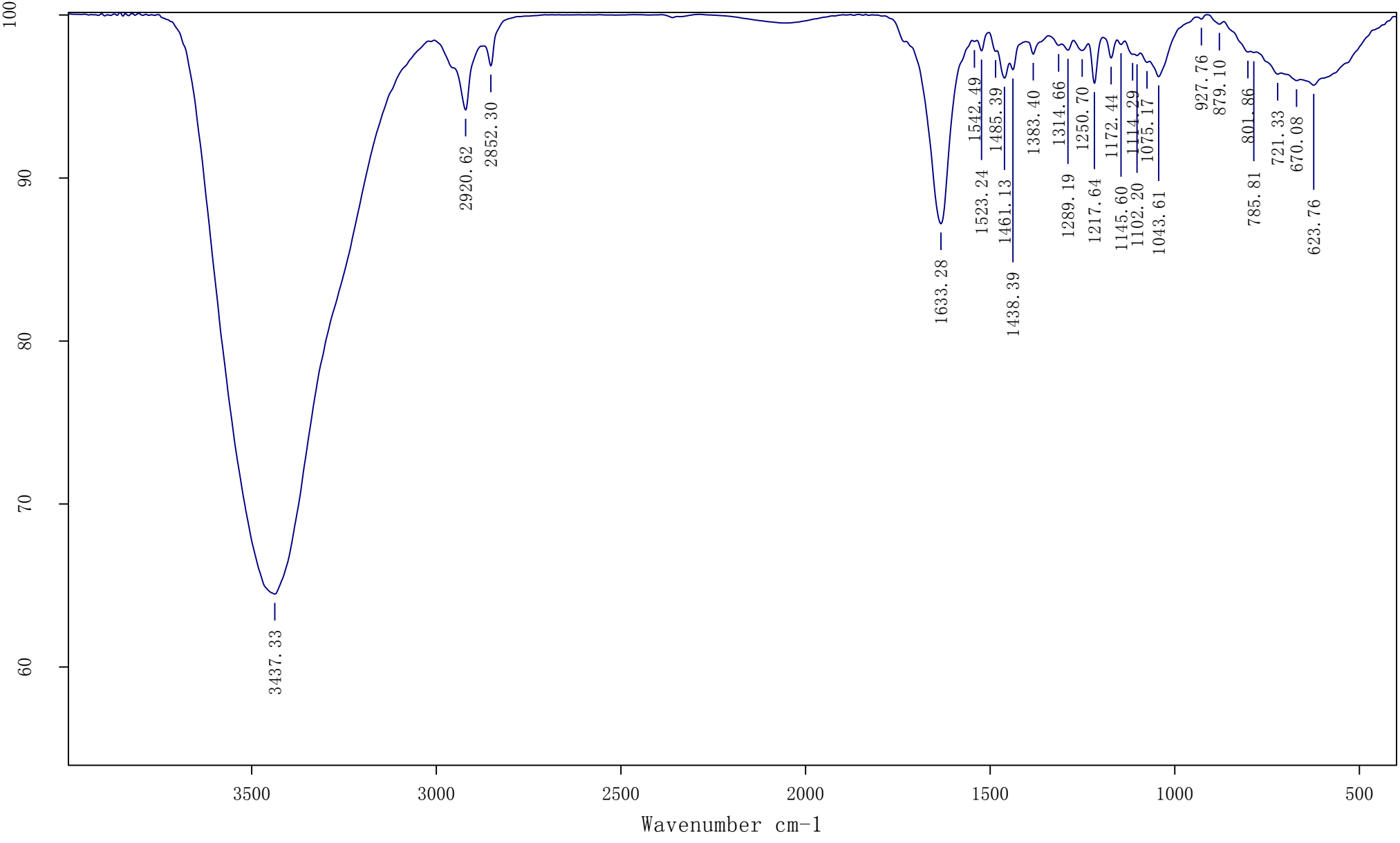
Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5
S	0	0
Cl	0	0
P	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H24 N2 O3	True	340.17841	340.17869	0.83	C20 H25 N2 O3	97.7

--- End Of Report ---

Figure S1. HRESIMS spectrum of 3-hydroxylochnerine (**1**)



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Date of Measurement: 2021/11/26

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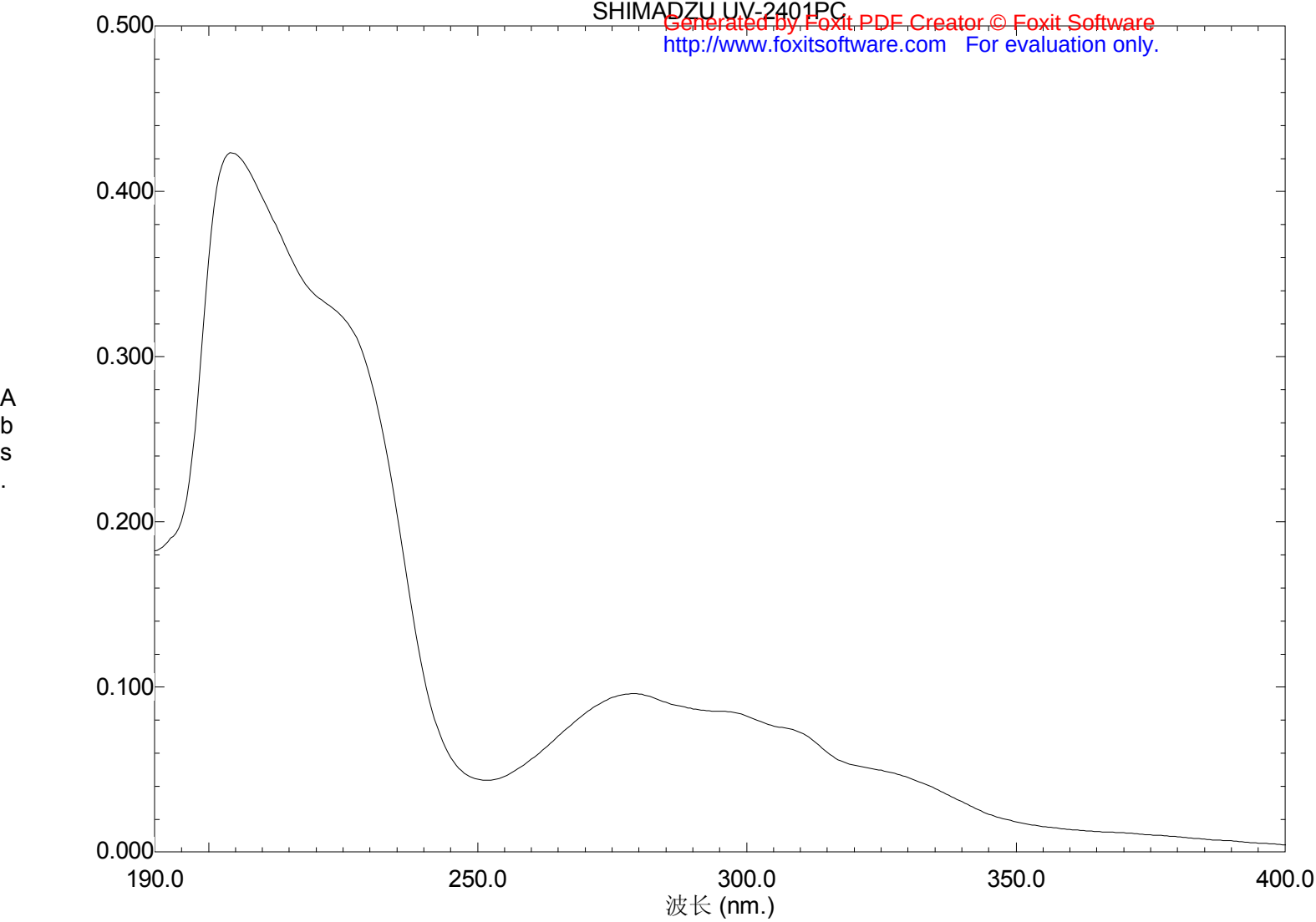
Number of Background Scans: 16
Number of Sample Scans: 16

Beamsplitter Setting: KBr
Source Setting: MIR
Instrument Type: BRUKER VERTEX 70
Soft Version: OPUS8.1

Figure S2. IR spectrum of 3-hydroxylochnerine (**1**)



文件名: WRY42

WRY42 ————

样品浓度：0.0086毫克/毫升
溶剂：甲醇

创建于: 10:22 21-12-09
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.5

否.	波长 (nm.)	Abs.
1	204.50	0.4231
2	221.50	0.3330
3	278.50	0.0957
4	295.50	0.0851
5	322.00	0.0513

Figure S3. UV spectrum of 3-hydroxylochnerine (**1**)

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 01-DEC-2021

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	34.71	0.41	1.18	35.29	34.12

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp
1	WRY-42	02:10:53 PM	35.29	SR	0.060	589	100.00	0.170	19.4
2	WRY-42	02:10:59 PM	34.71	SR	0.059	589	100.00	0.170	19.4
3	WRY-42	02:11:06 PM	34.71	SR	0.059	589	100.00	0.170	19.4
4	WRY-42	02:11:12 PM	34.71	SR	0.059	589	100.00	0.170	19.4
5	WRY-42	02:11:18 PM	34.12	SR	0.058	589	100.00	0.170	19.4

Figure S4. Specific rotation of 3-hydroxylochnerine (**1**)

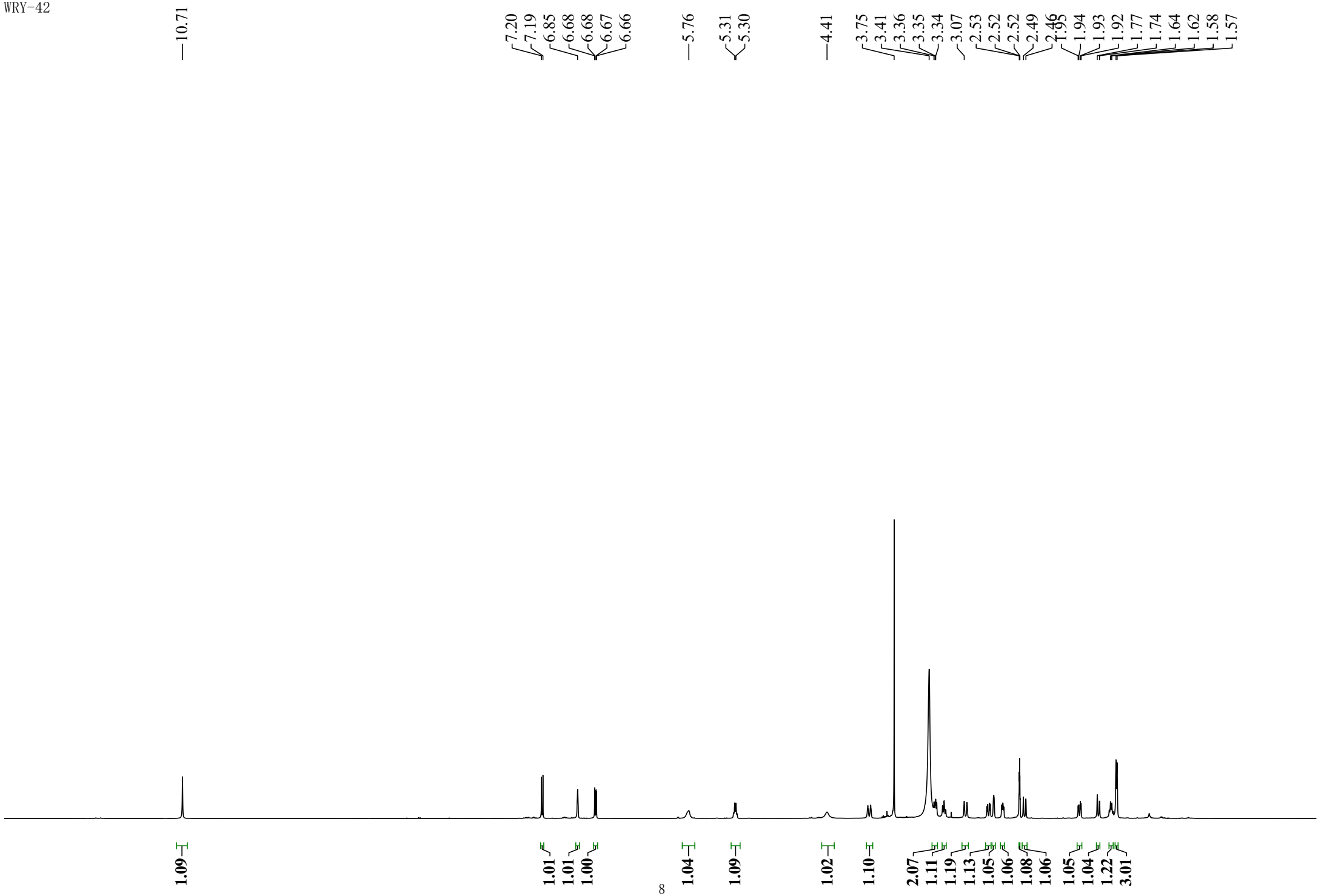


Figure S5 ^{1}H-NMR spectrum of 3-hydroxylochnerine (**1**)

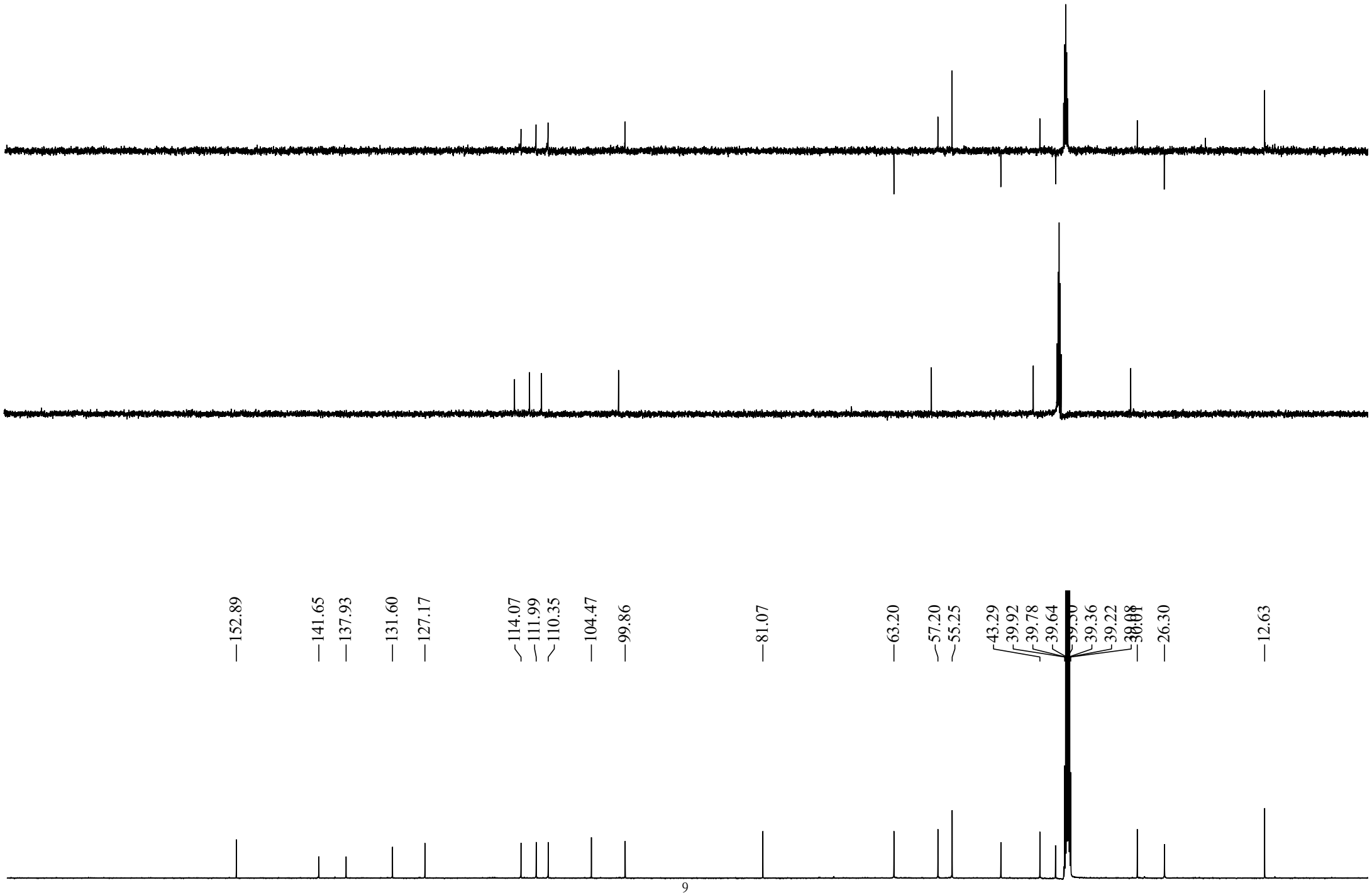


Figure S6 ^{13}C-NMR spectrum of 3-hydroxylochnerine (**1**)

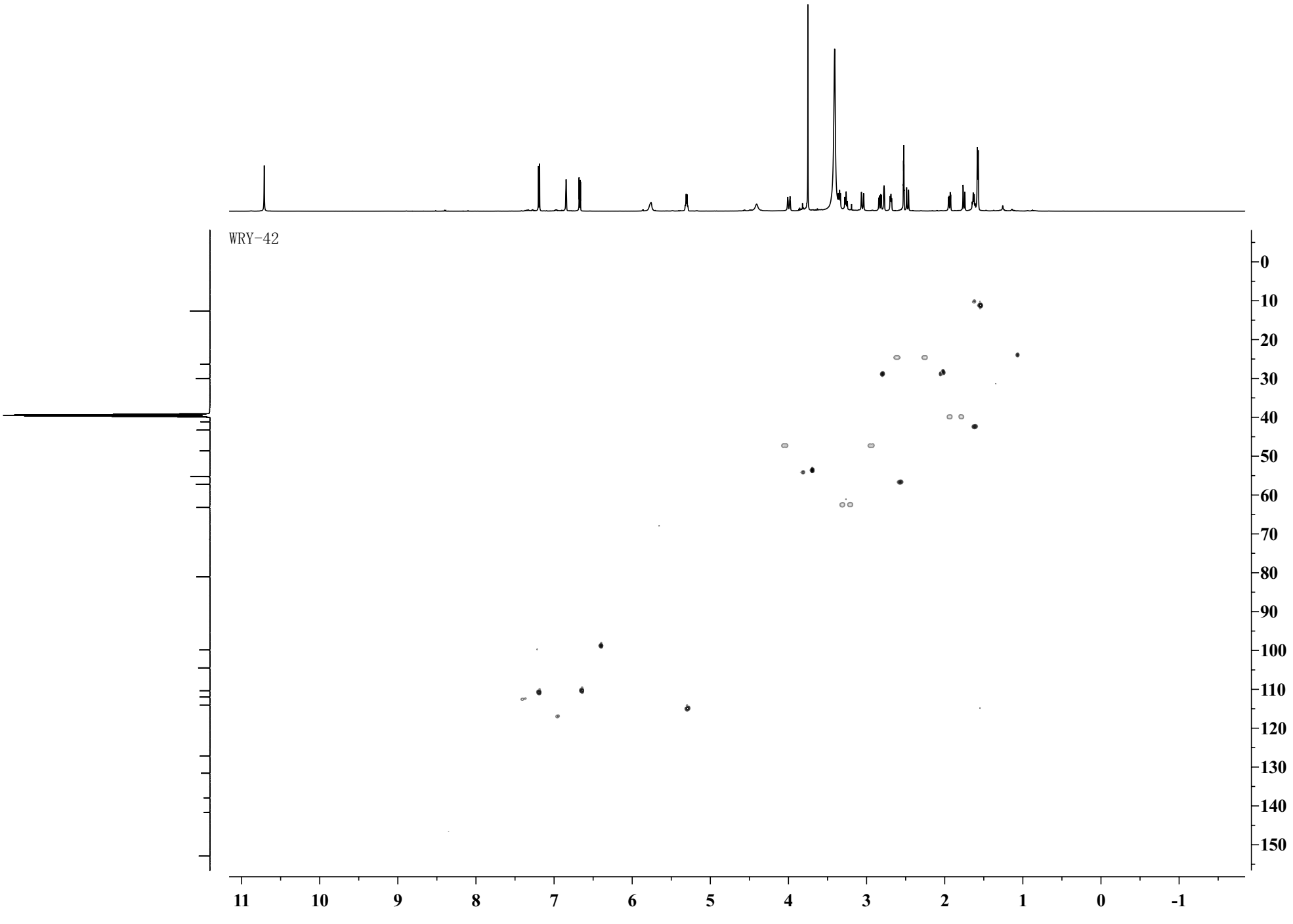


Figure S7 HSQC spectrum of 3-hydroxylochnerine (**1**)

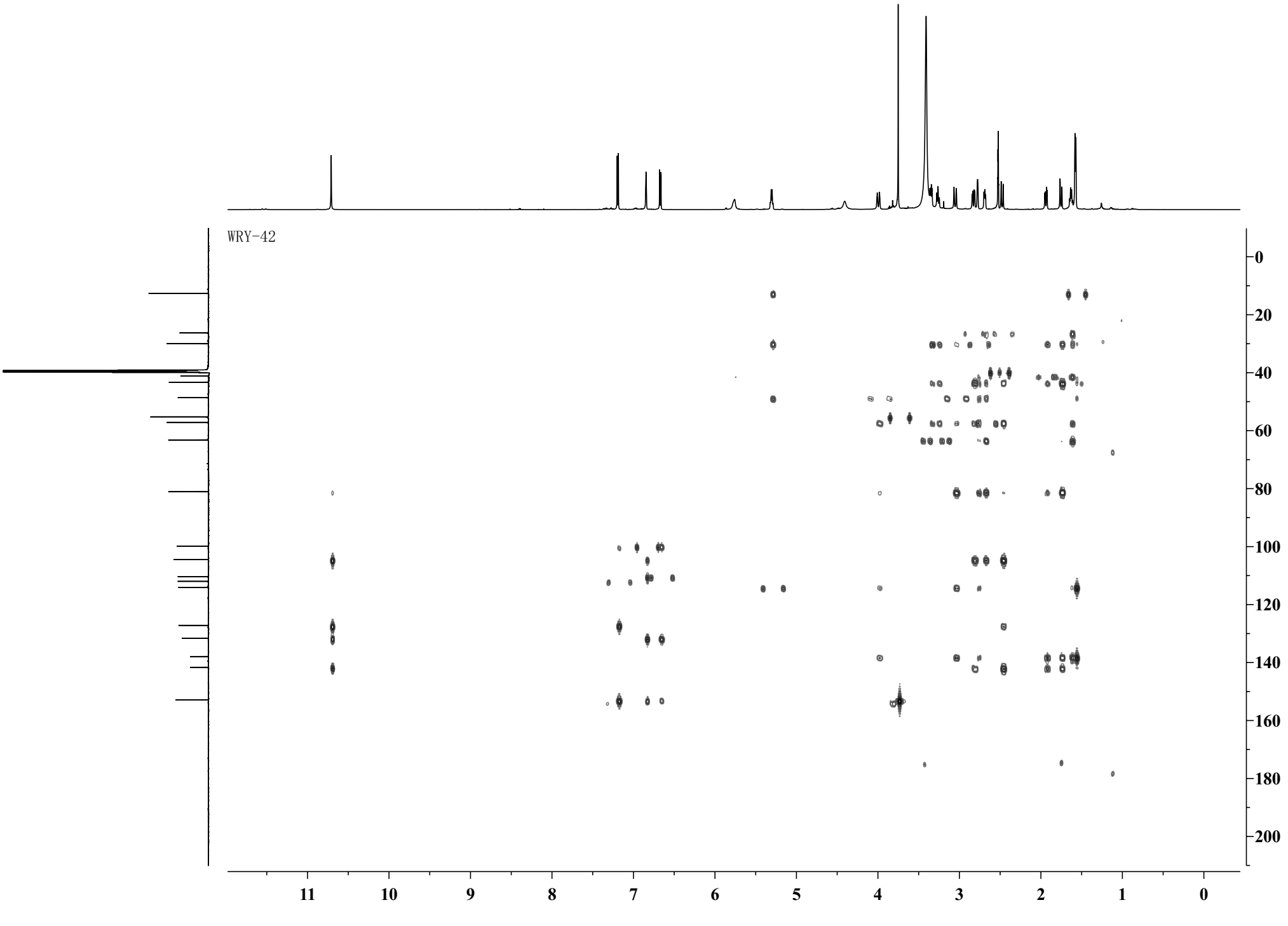


Figure S8 HMBC spectrum of 3-hydroxylochnerine (**1**)

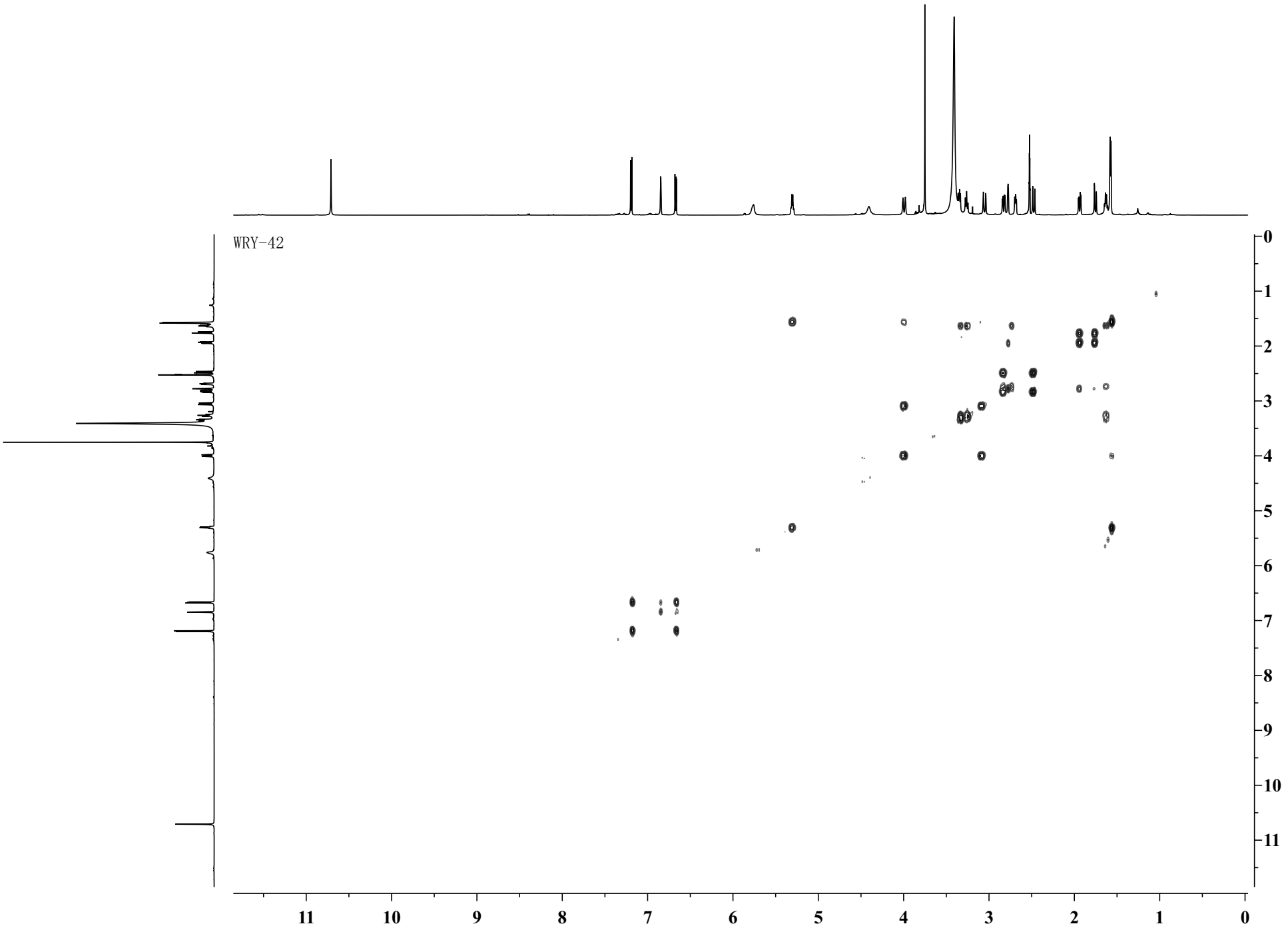


Figure S9 ^{1}H-^{1}H COSY spectrum of 3-hydroxylochnerine (**1**)

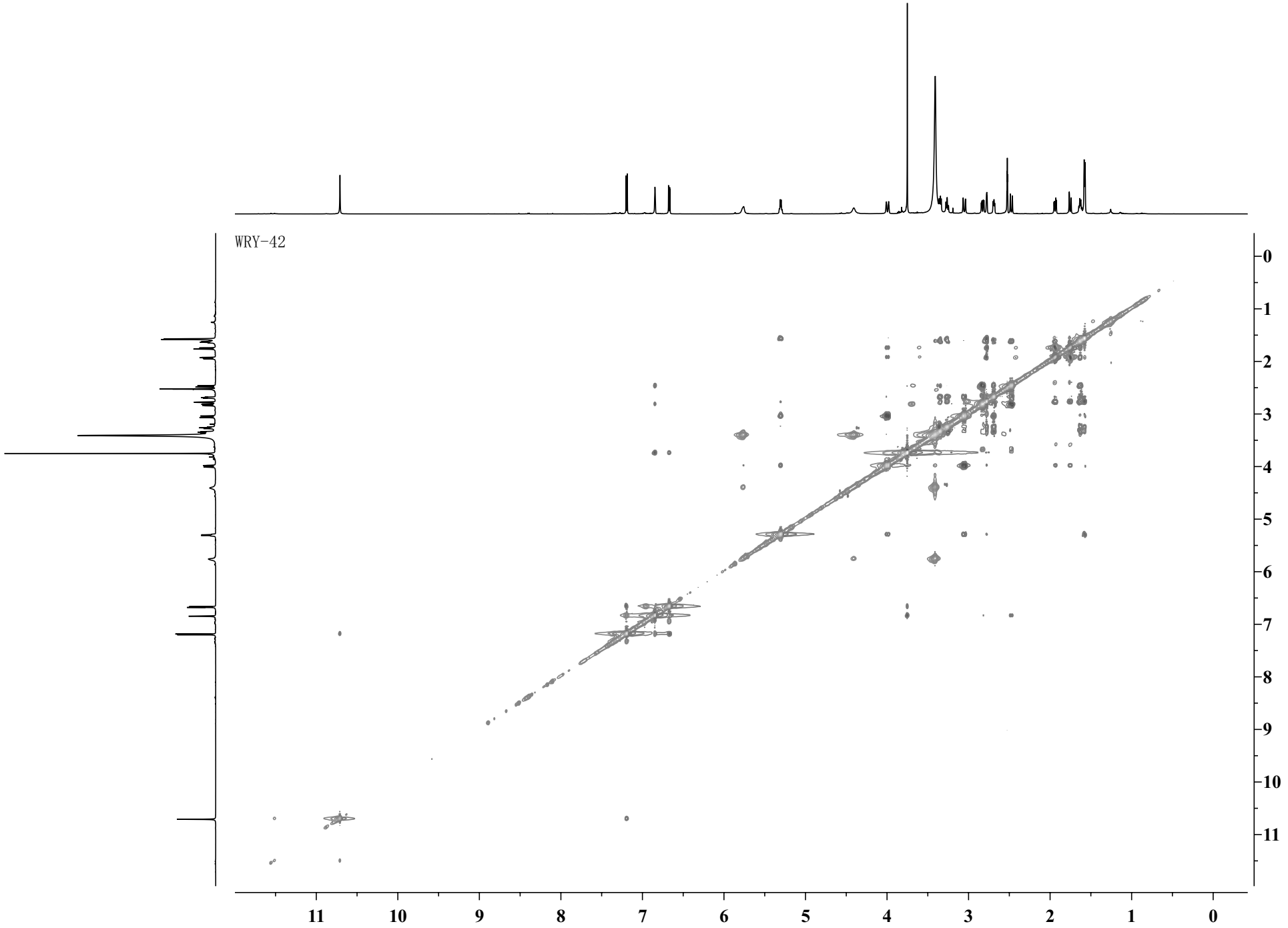


Figure S10 ROESY spectrum of 3-hydroxylochnerine (**1**)

Data File: E:\DATA\2021\0830\wry30.lcd

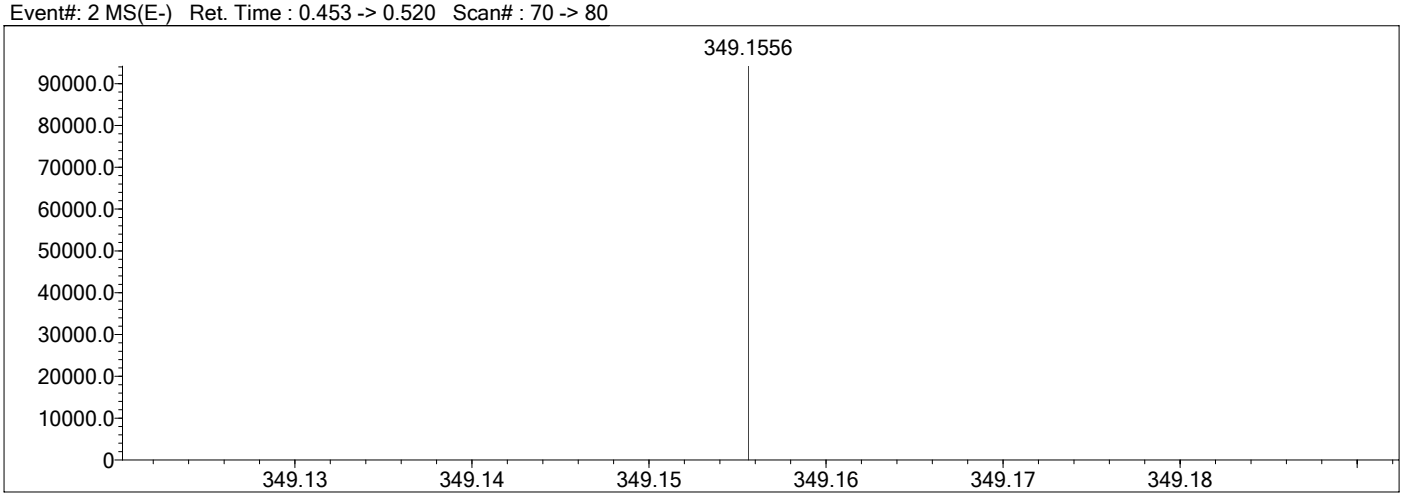
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	150	O	2	0	30	P	3	0	0	Se	2	0	0	H
2H	1	0	0	F	1	0	0	S	2	0	0	Br	1	0	0	HCOO
B	3	0	0	Na	1	0	0	Cl	1	0	0	Pd	2	0	0	
C	4	5	100	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
N	3	0	10	Si	4	0	0	Cu	2	0	0	I	3	0	0	

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

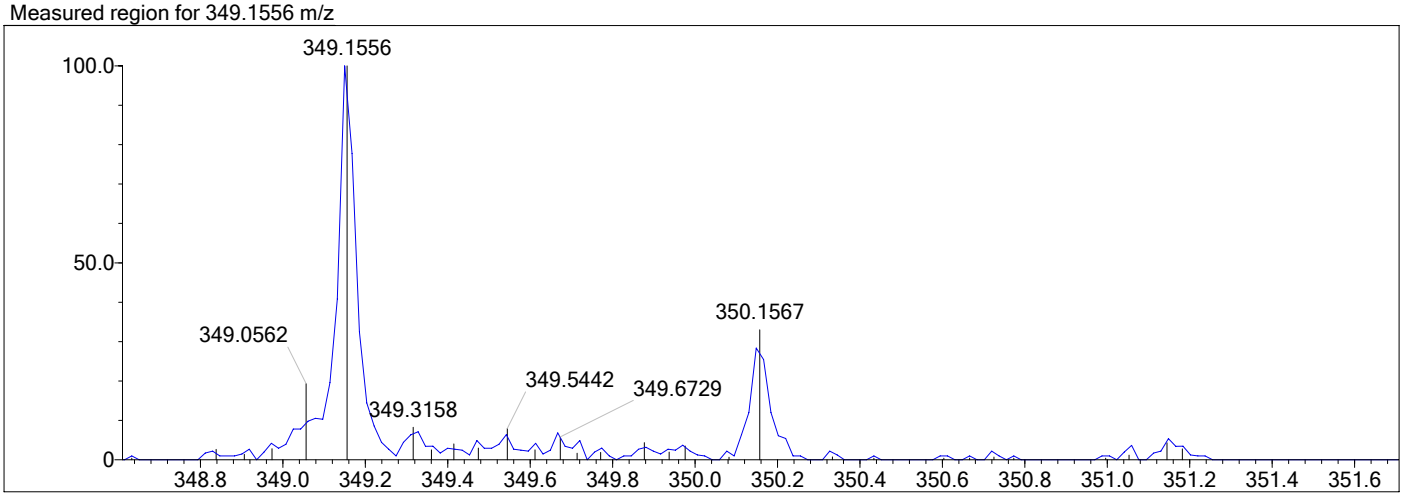
DBE Range: not fixed
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 20

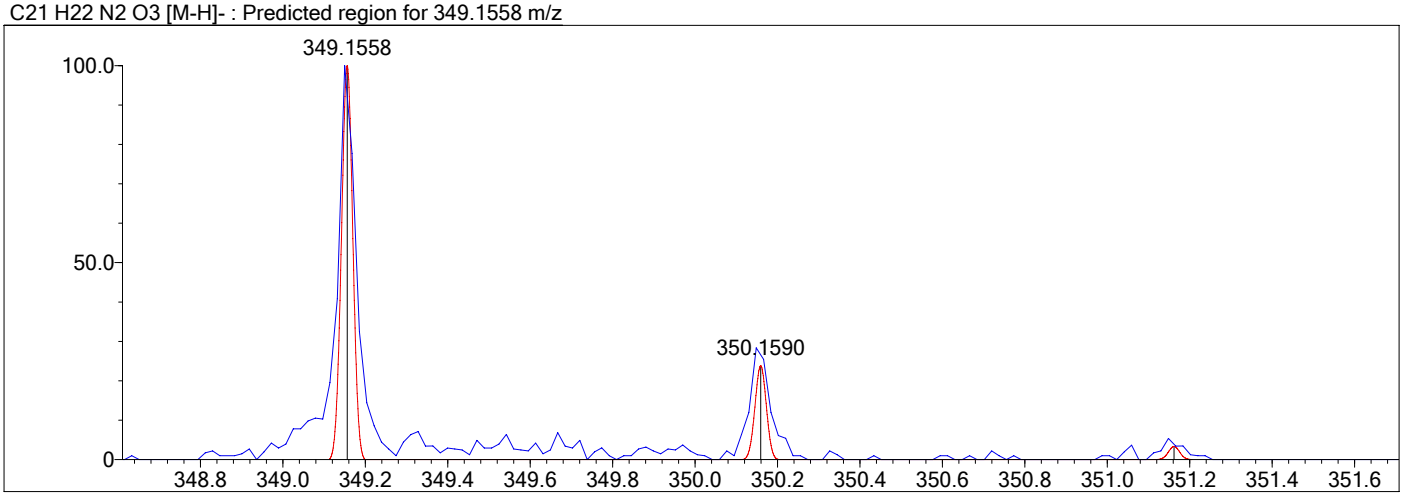
Event#: 2 MS(E-) Ret. Time : 0.453 -> 0.520 Scan# : 70 -> 80



Measured region for 349.1556 m/z

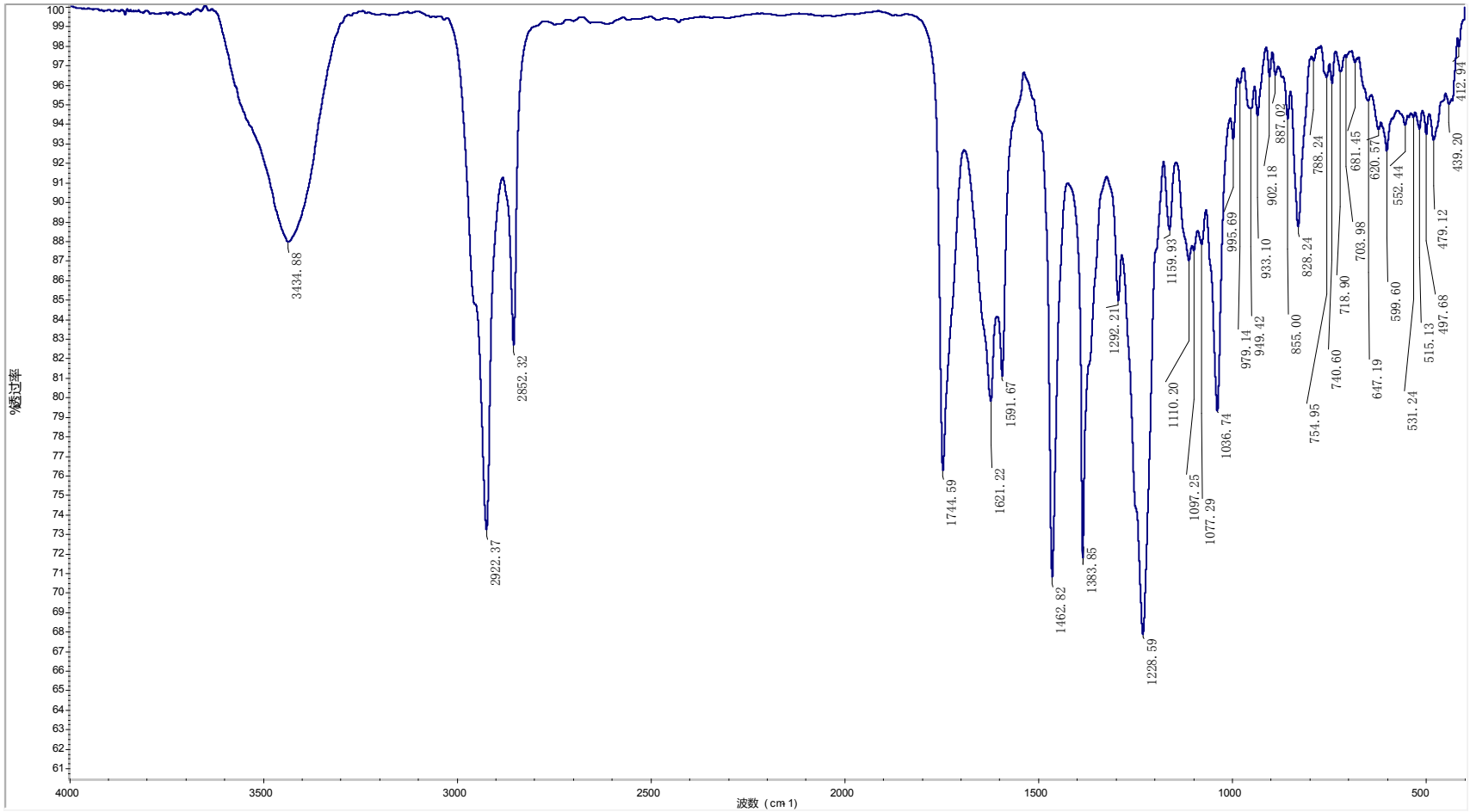


C21 H22 N2 O3 [M-H]- : Predicted region for 349.1558 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C21 H22 N2 O3	[M-H]-	349.1556	349.1558	-0.2	-0.57	12.0

Figure S11. HRESIMS spectrum of 10-hydroxyvinorine (**2**)



Sample Name: wry30
KBr压片
采集时间: 星期三 9月 01 10:44:29 2021 (GMT+08:00)
仪器型号：NICOLET iS10
Software version: OMNIC 9.8.372

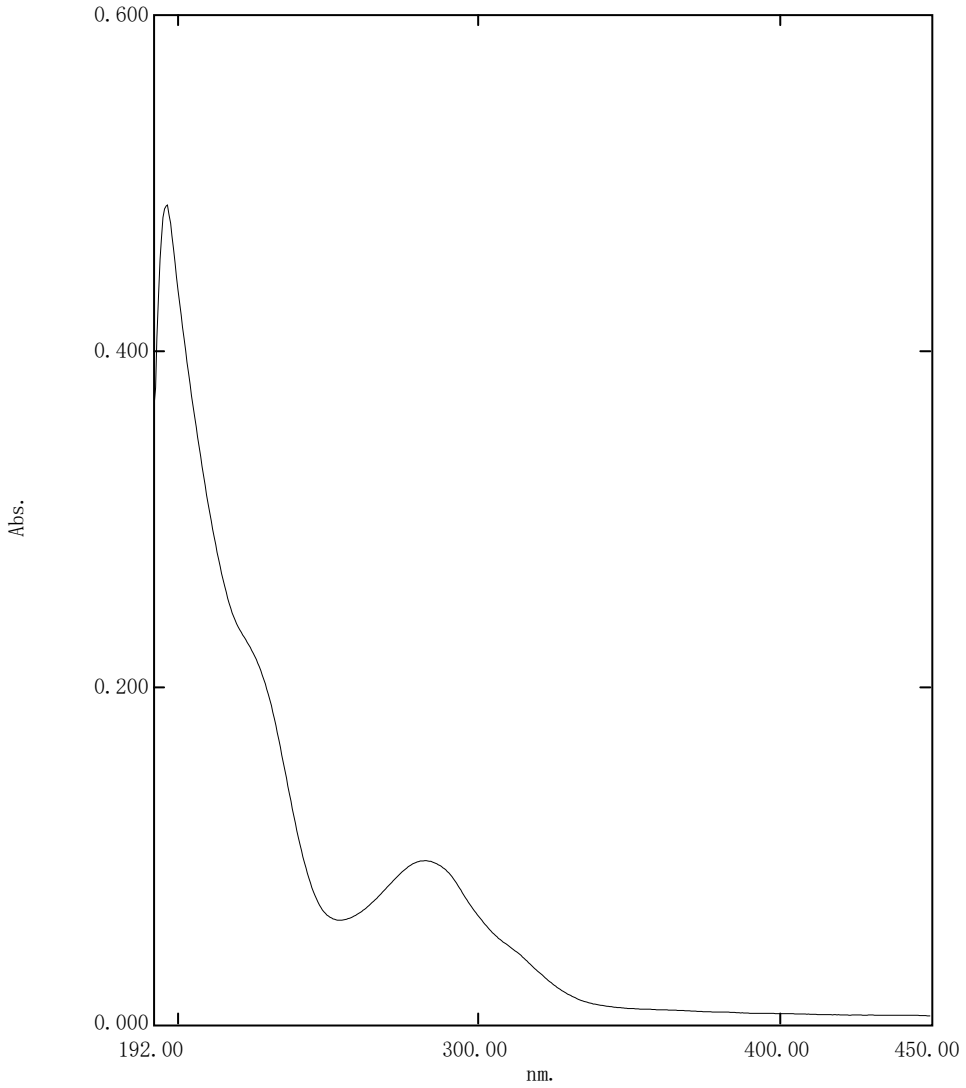
样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 80.00

Figure S12. IR spectrum of 10-hydroxyvinorine (**2**)

光谱峰值检测报告

2021/10/19 15:40:03

数据集: WRY30 - RawData



[测定属性]
波长范围(nm): 190.00 到 600.00
扫描速度: 中速
采样间隔: 0.5
自动采样间隔: 停用
扫描模式: 单个

[仪器属性]
仪器类型: UV-2700 系列
测定方式: 吸收值
狭缝宽: 5.0 nm
积分时间: 0.1 秒
光源转换波长: 323.0 nm
检测器单元: 直接
S/R 转换: 标准
阶梯校正: OFF

[附件属性]
附件: 无

[数据处理参数]
阈值: 0.0010000
点: 4
内插: 停用
平均: 停用

[样品准备属性]
重量:
体积:
稀释:
光程长: 10mm
附加信息: 样品浓度：0.0114毫克/毫升
溶剂：甲醇

No.	P/V	波长(nm)	Abs.	描述
1	↑	282.00	0.097	
2	↑	196.50	0.487	
3	↓	254.00	0.061	

Figure S13. UV spectrum of 10-hydroxyvinorine (**2**)

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 09-OCT-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	16.76	1.14	6.80	18.00	15.33

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	WRY30	02:38:03 PM	18.00	SR	0.0216	589	100.00	0.120	24.5
2	WRY30	02:38:11 PM	17.83	SR	0.0214	589	100.00	0.120	24.5
3	WRY30	02:38:20 PM	16.58	SR	0.0199	589	100.00	0.120	24.5
4	WRY30	02:38:28 PM	16.08	SR	0.0193	589	100.00	0.120	24.5
5	WRY30	02:38:36 PM	15.33	SR	0.0184	589	100.00	0.120	24.5

Figure S14. Specific rotation of 10-hydroxyvinorine (**2**)

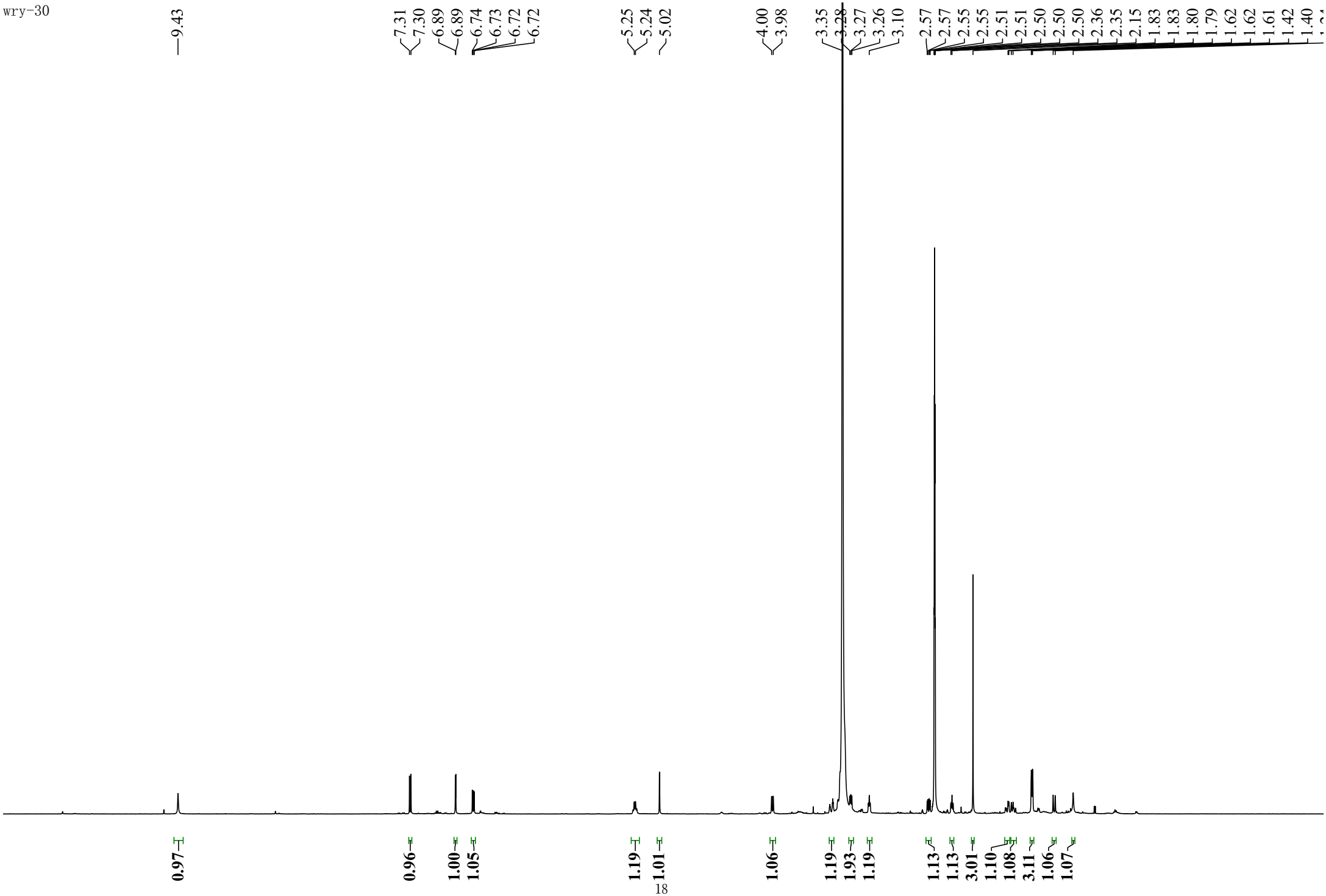


Figure S15 ^{1}H-NMR spectrum of 10-hydroxyvinorine (**2**)

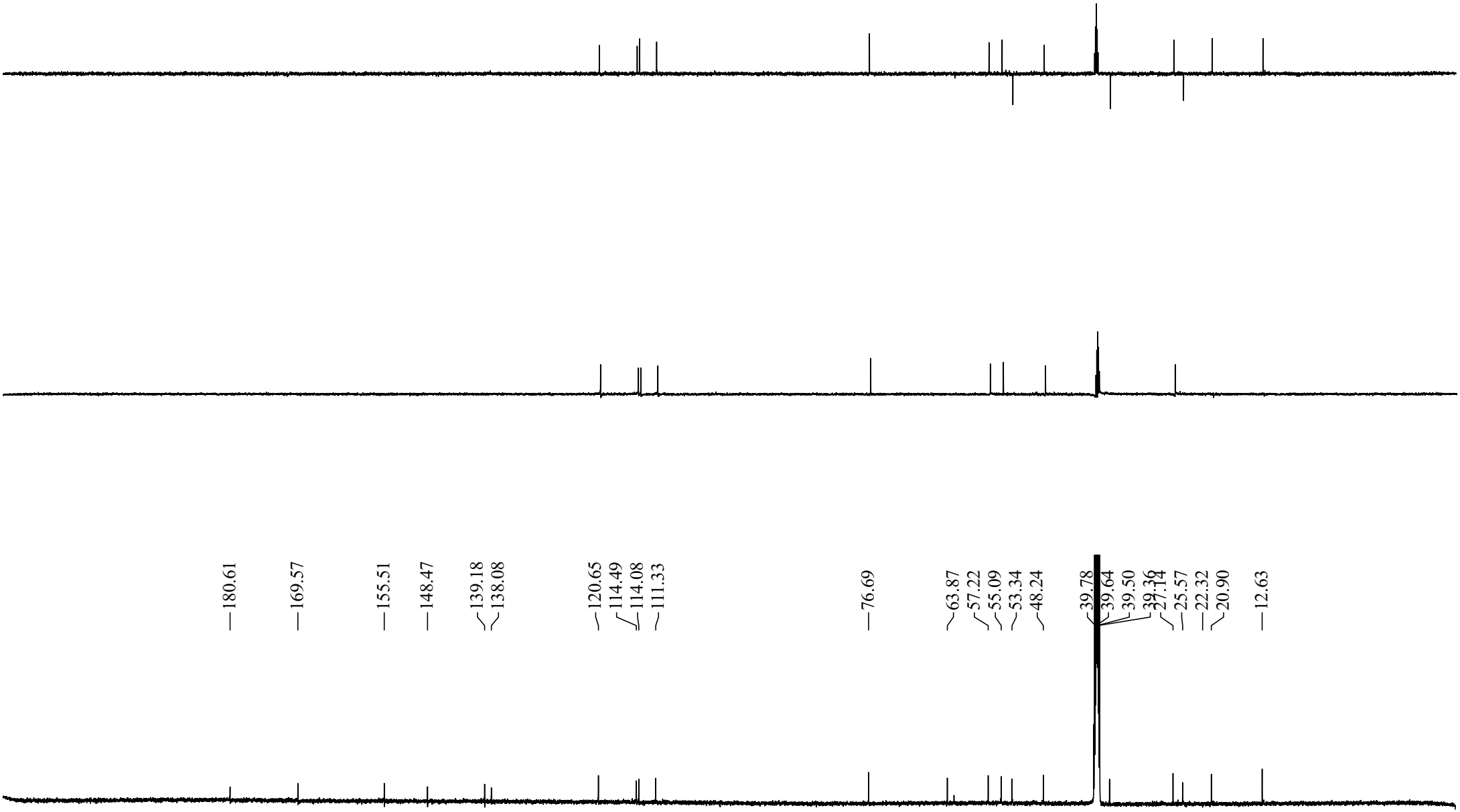


Figure S16 ^{13}C-NMR spectrum of 10-hydroxyvinorine (**2**)

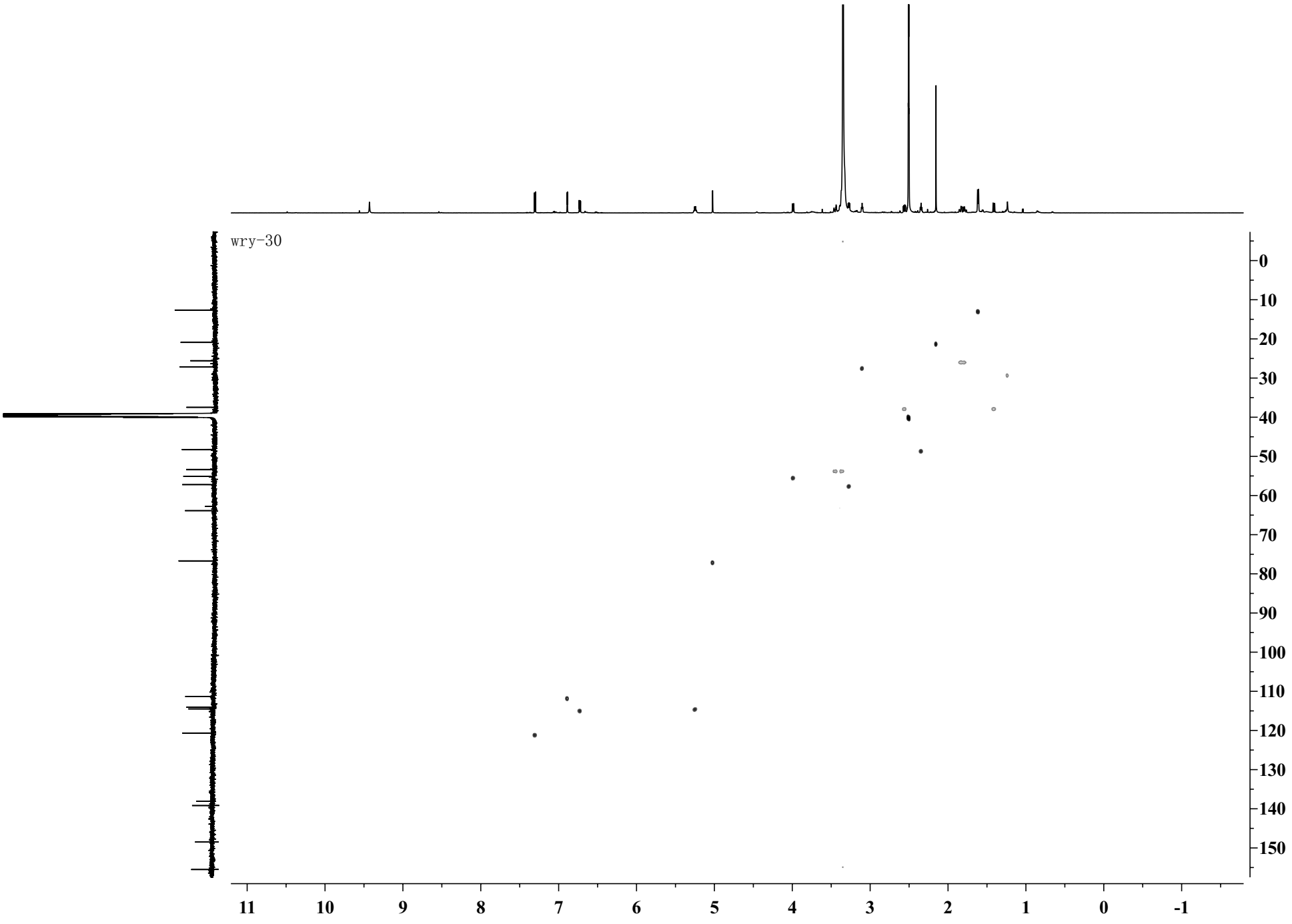


Figure S17 HSQC spectrum of 10-hydroxyvinorine (**2**)

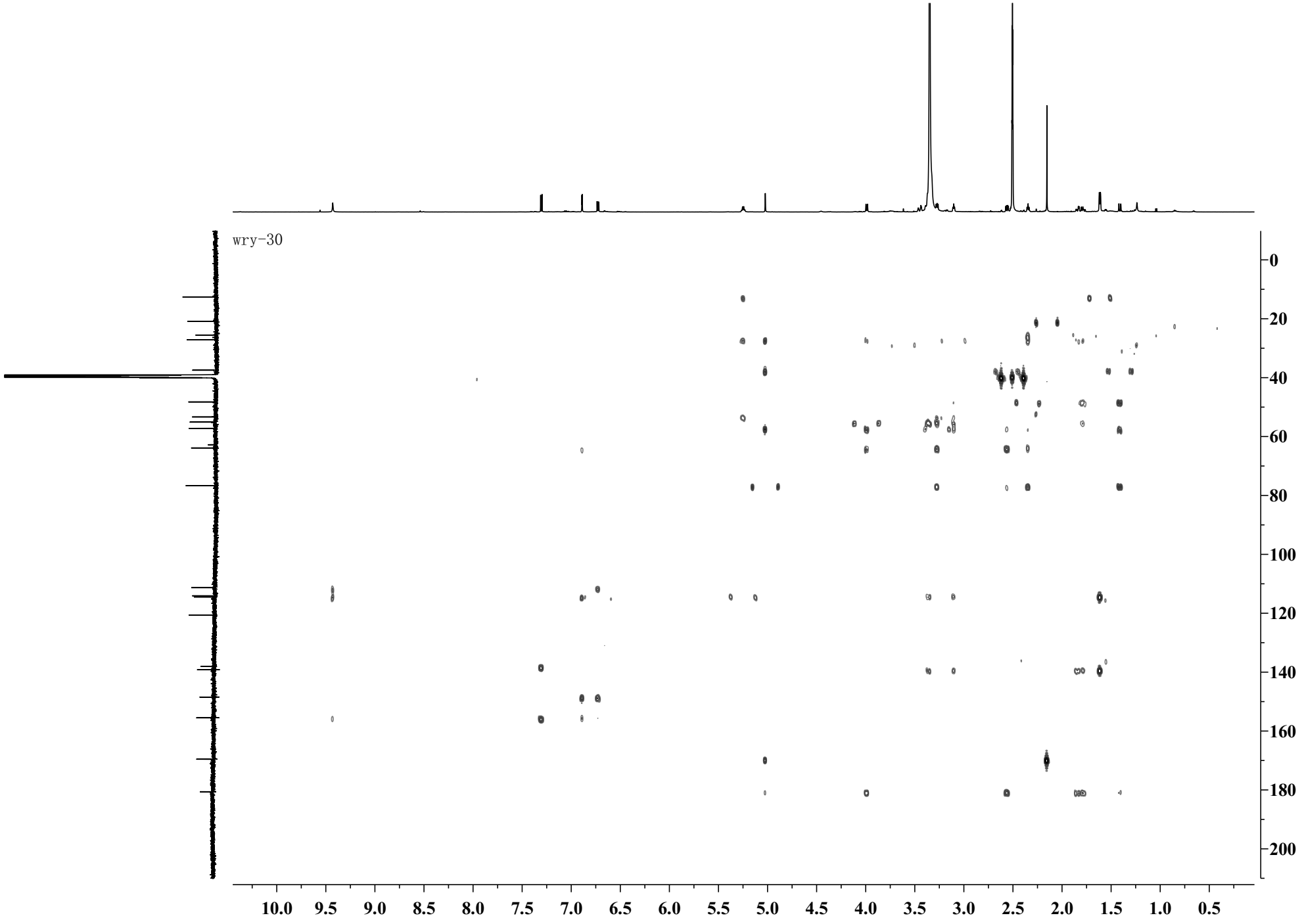


Figure S18 HMBC spectrum of 10-hydroxyvinorine (**2**)

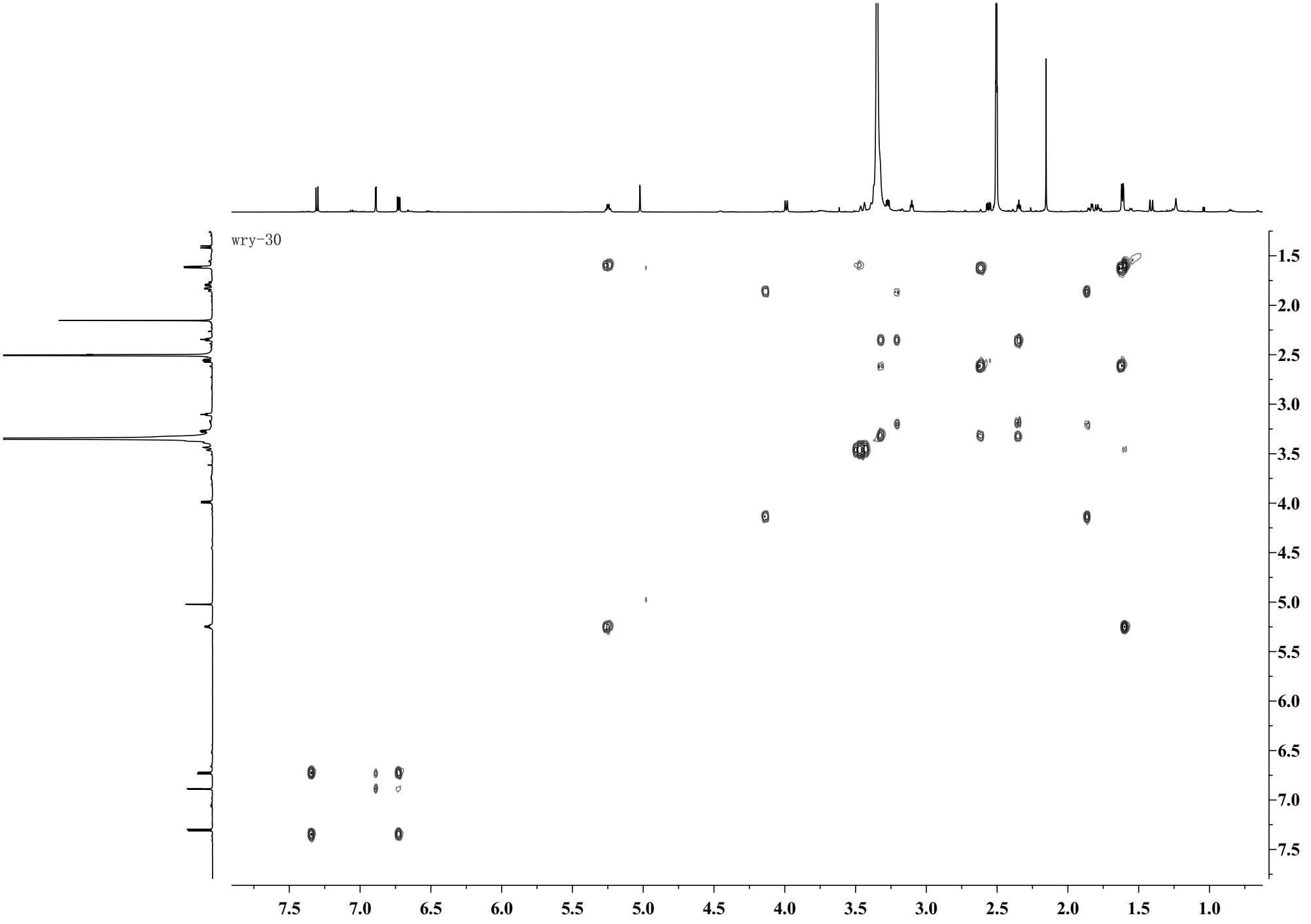


Figure S19 ^{1}H-^{1}H COSY spectrum of 10-hydroxyvinorine (**2**)

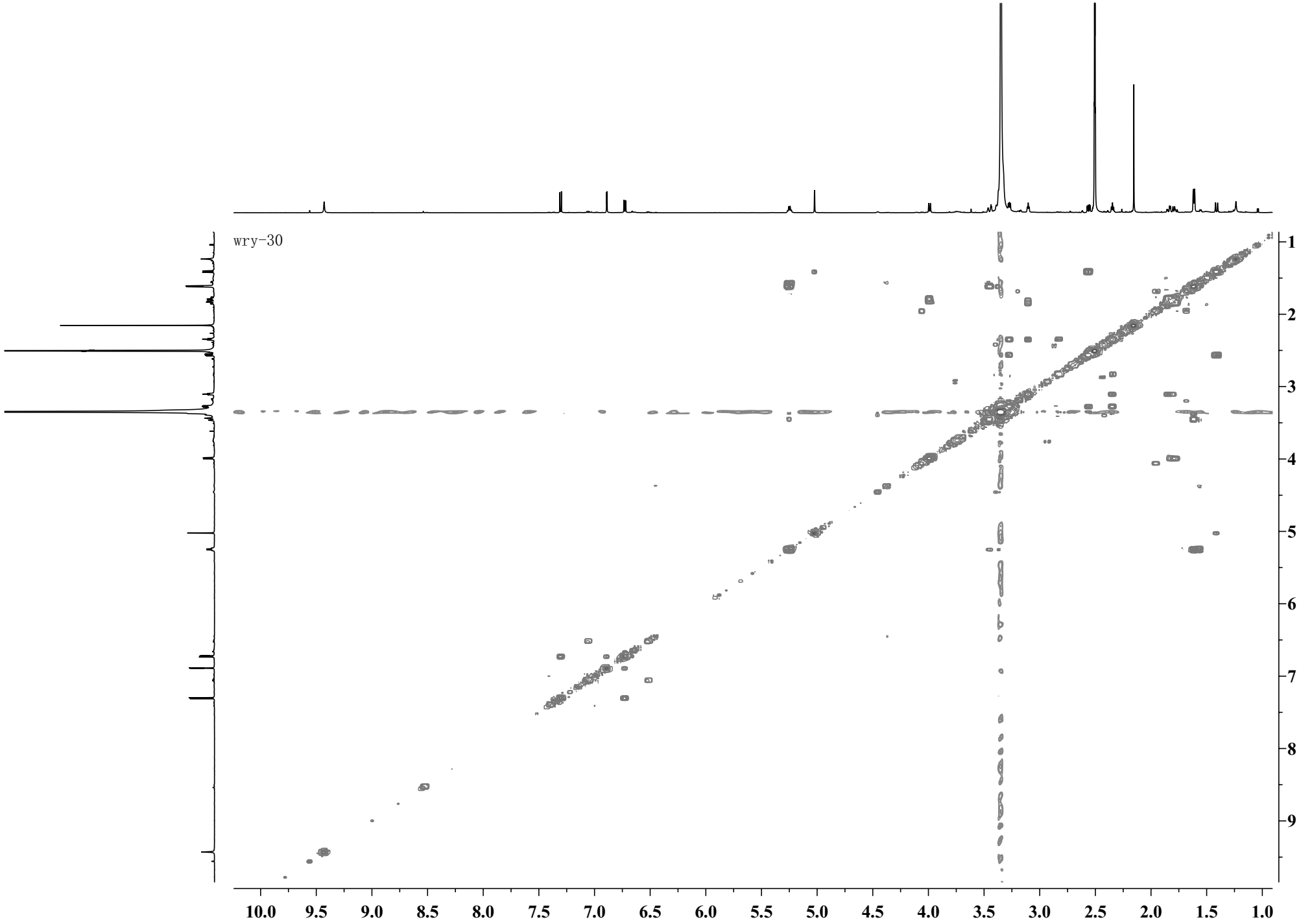


Figure S20 ROESY spectrum of 10-hydroxyvinorine (**2**)