Supporting Information

Rec. Nat. Prod. 14:3 (2020) 196-200

Two New 2(1*H*)-Pyrazinone Derivatives from the Plant Endophyte *Streptomyces* sp. KIB-H1992

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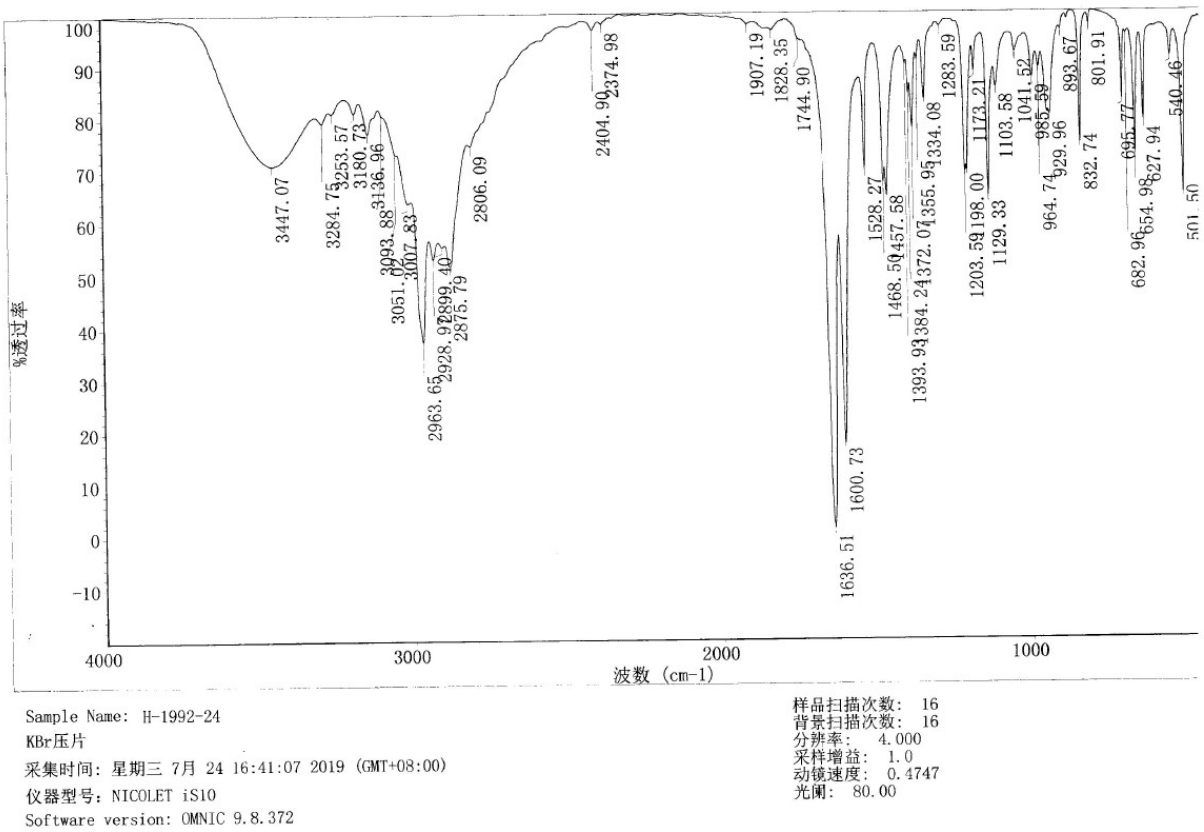


Figure S1: IR Spectrum of Compound **1**.

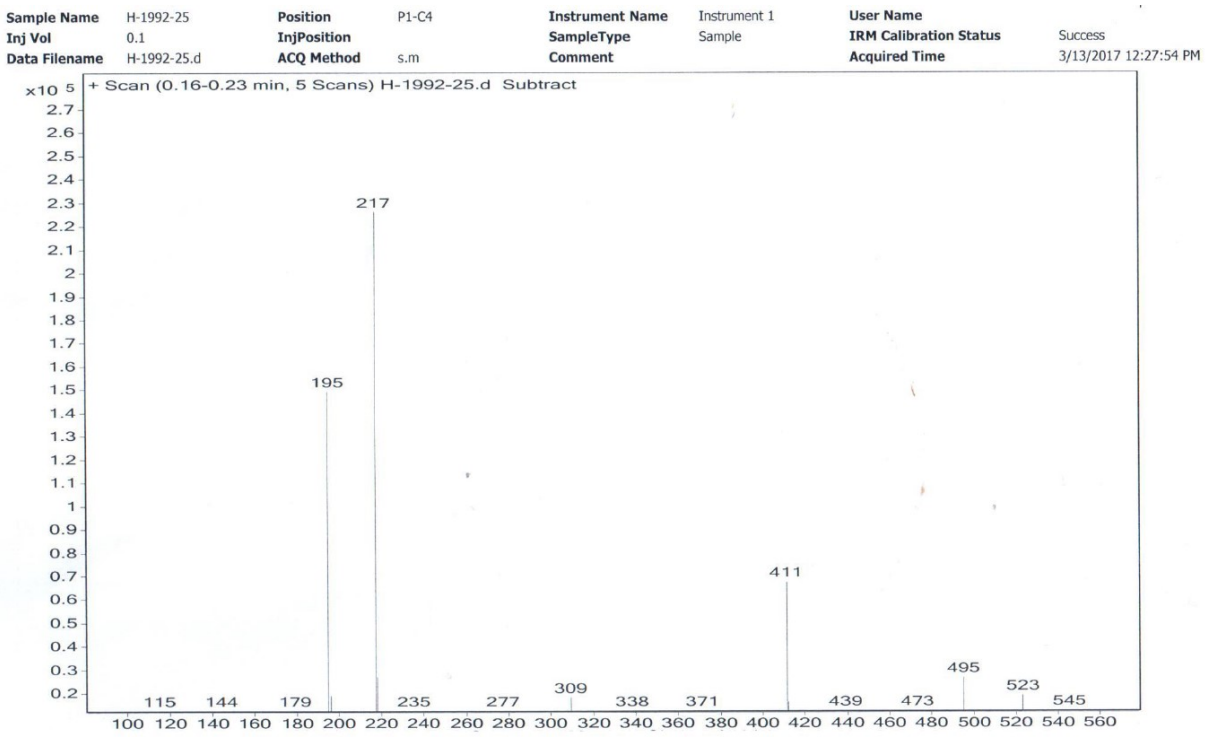


Figure S2: ESI-MS Spectrum of Compound **1**.

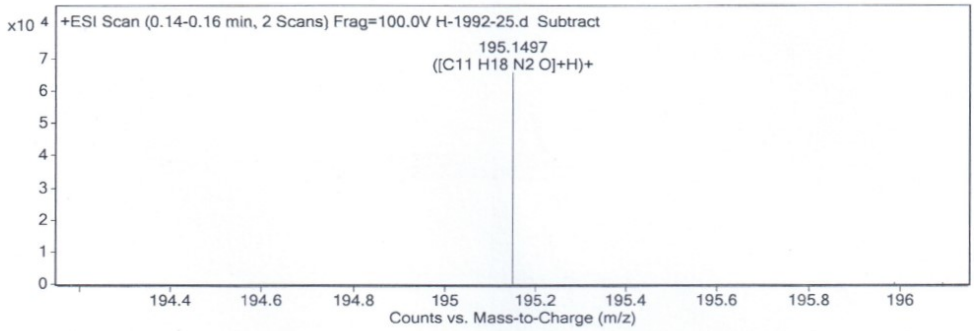
Qualitative Analysis Report

Data Filename	H-1992-25.d	**Sample Name**	H-1992-25
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	4/25/2018 2:04:47 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
158.0788	2	6185.94		
195.1497	1	65888.23	C11 H18 N2 O	(M+H)+
196.1526	1	8972.76	C11 H18 N2 O	(M+H)+
217.1317	1	103980.96		
218.1351	1	12963.37		
233.1051	1	25164.96		
411.2747	1	35706.78		
412.2771	1	8893.81		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C11 H18 N2 O	194.1419	195.1492	195.1497	-0.50	-2.56	4.0000

Figure S3: HR-ESI-MS Spectrum of Compound **1**.

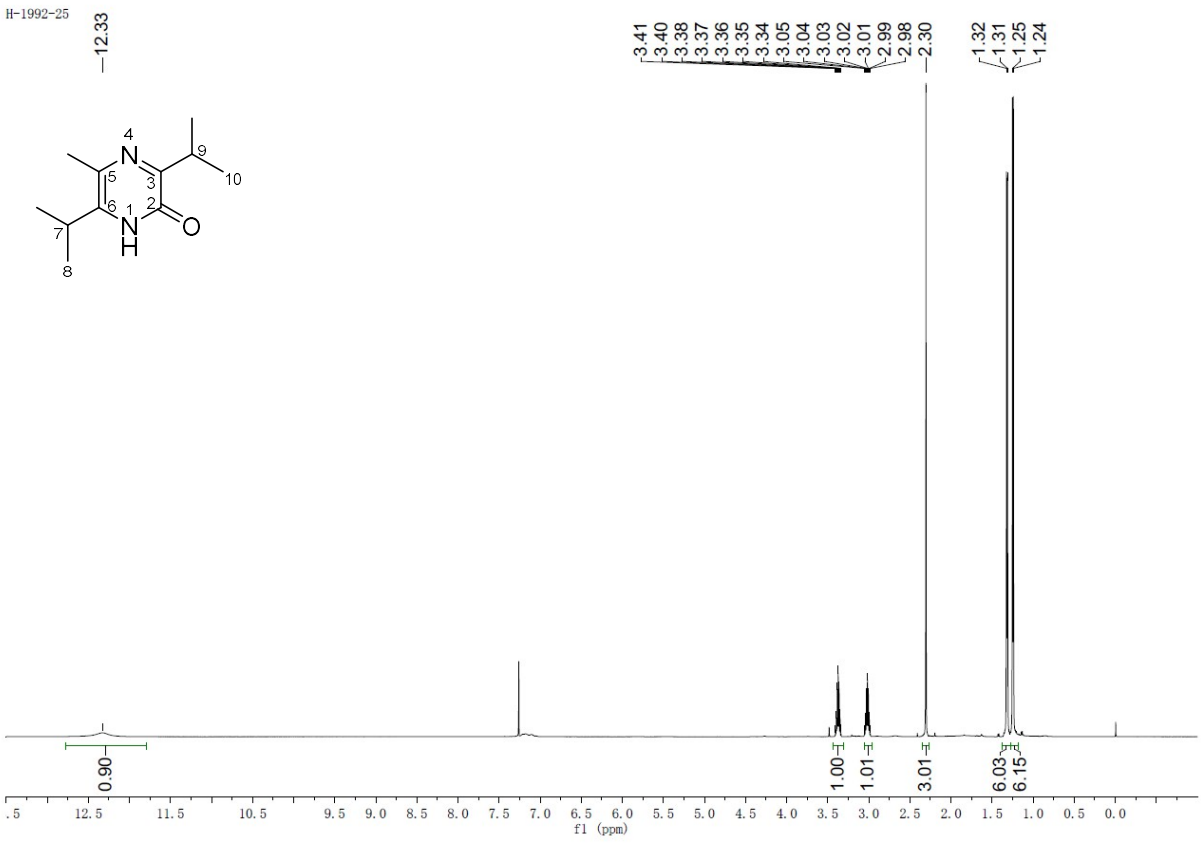


Figure S4: ^{1}H NMR spectrum of compound **1** (in $CDCl_3$, 600 MHz)

^{1}H NMR (600 MHz, $CDCl_3$): δ_H 12.33 (1H, brs, NH), 3.37 (1H, hept, J = 6.6 Hz, H-9), 3.02 (1H, hept, J = 7.2 Hz, H-7), 2.30 (3H, s, CH_3-5), 1.32 (6H, d, J = 7.2 Hz, H-8), 1.24 (6H, d, J = 6.6 Hz, H-10).

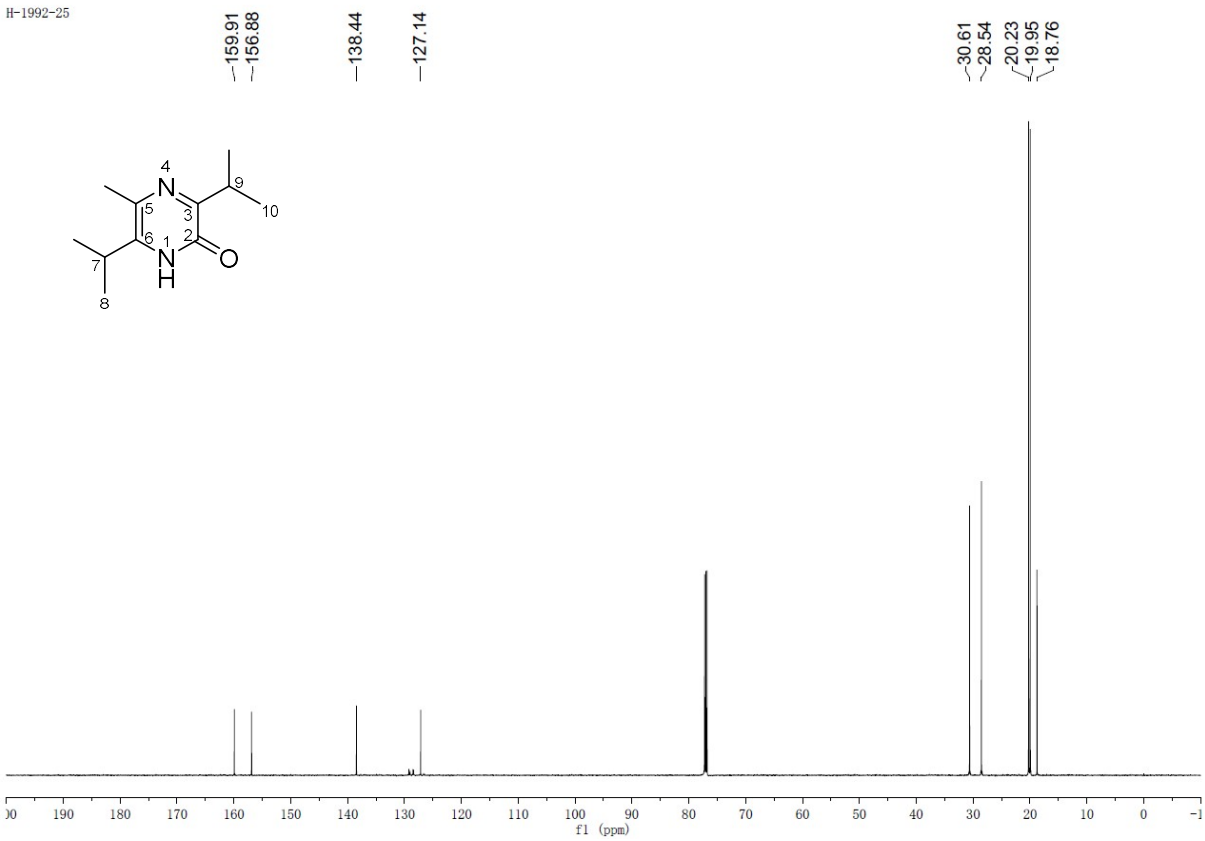


Figure S5: ^{13}C NMR spectrum of compound **1** (in $CDCl_3$, 150 MHz)

^{13}C NMR (150 MHz, $CDCl_3$): δ_C 159.9 (C-3), 156.7 (C-2), 138.4 (C-6), 127.1 (C-5), 30.6 (C-9), 28.5 (C-7), 20.2 (C-8), 19.9 (C-10), 18.8 (CH_3-5).

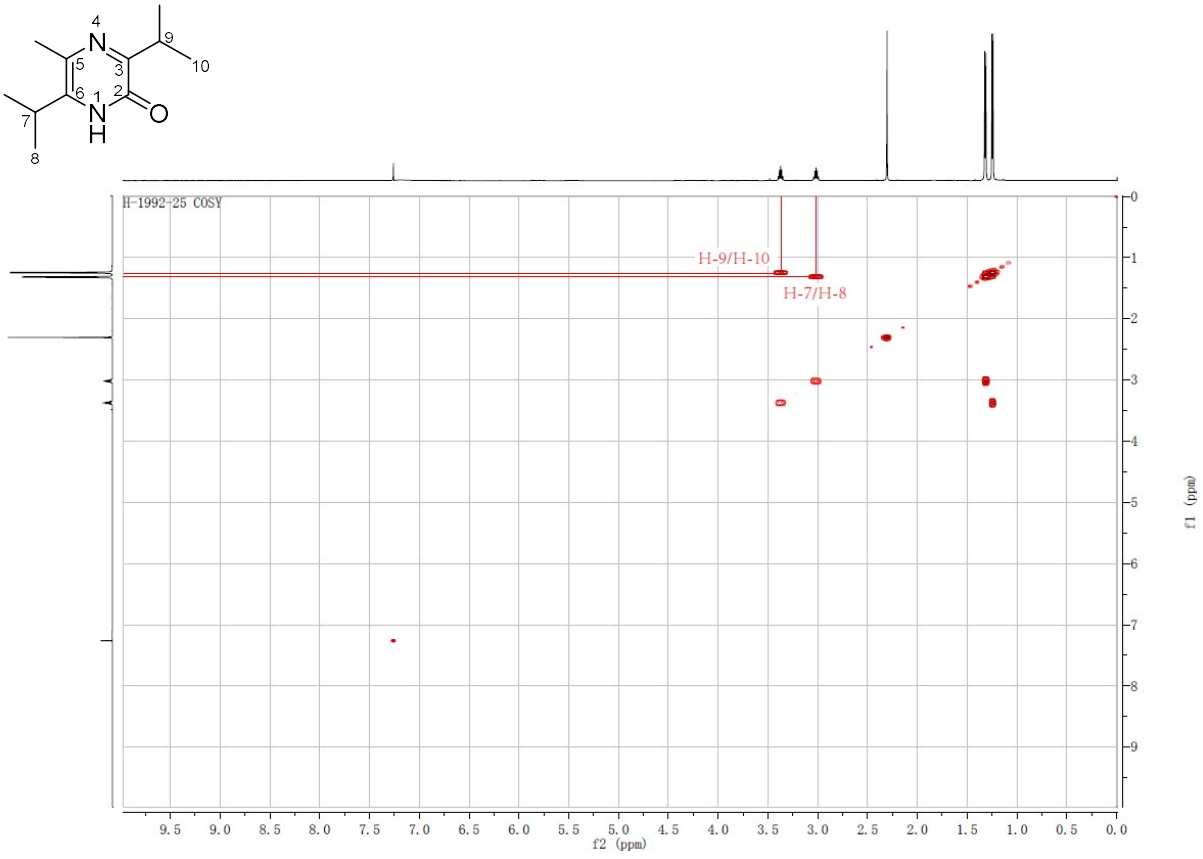


Figure S6: H-H COSY spectrum of compound **1** (in $CDCl_3$)

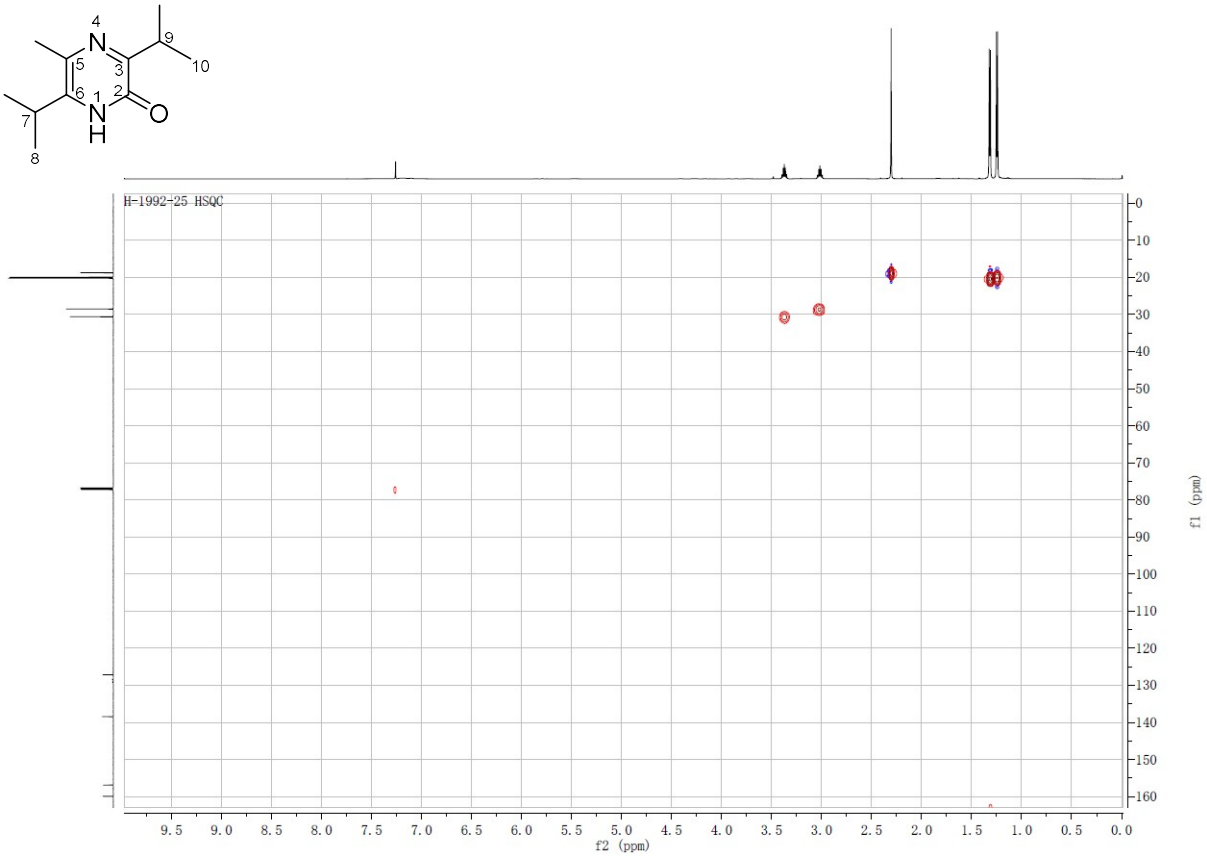


Figure S7: HSQC spectrum of compound **1** (in $CDCl_3$)

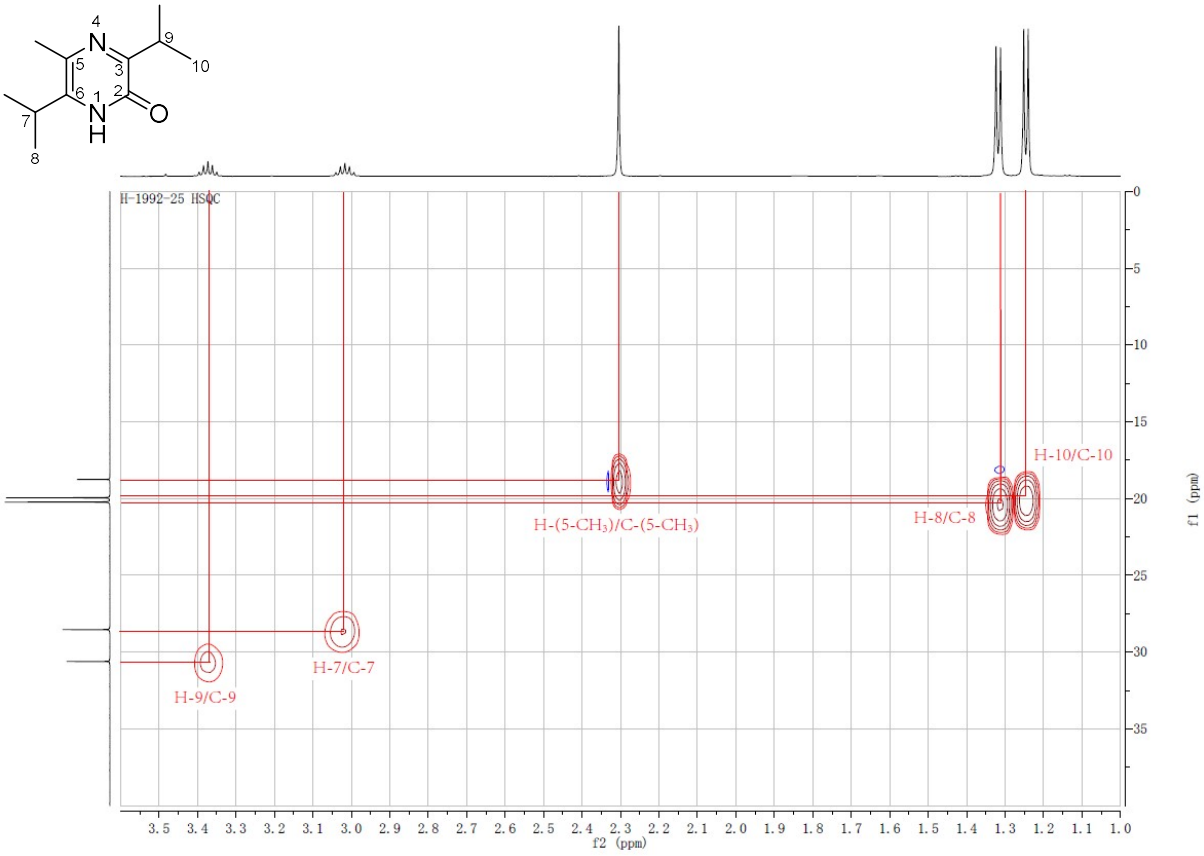


Figure S8: HSQC spectrum of compound **1** (^{1}H NMR from 1.00 to 3.60 ppm, ^{13}C NMR from 0 to 40 ppm)

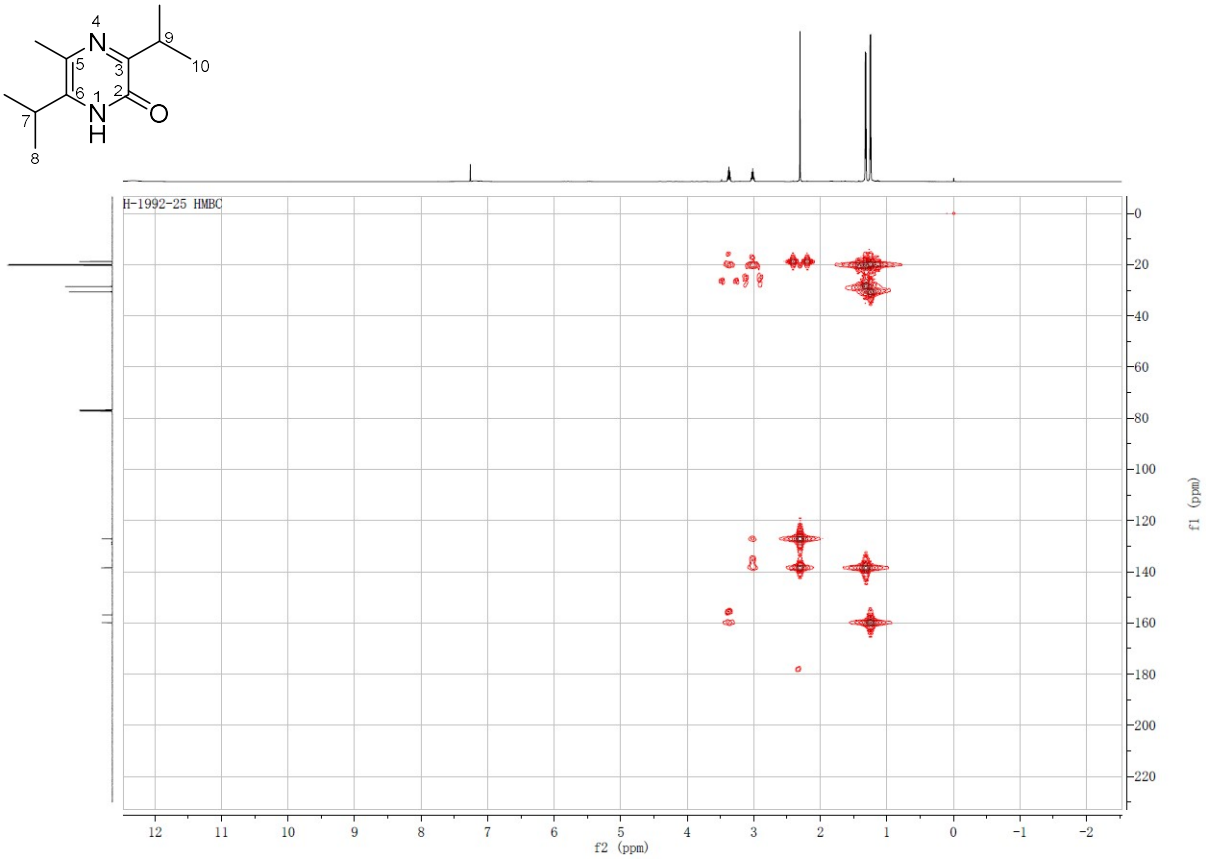


Figure S9: HMBC spectrum of compound **1** (in $CDCl_3$)

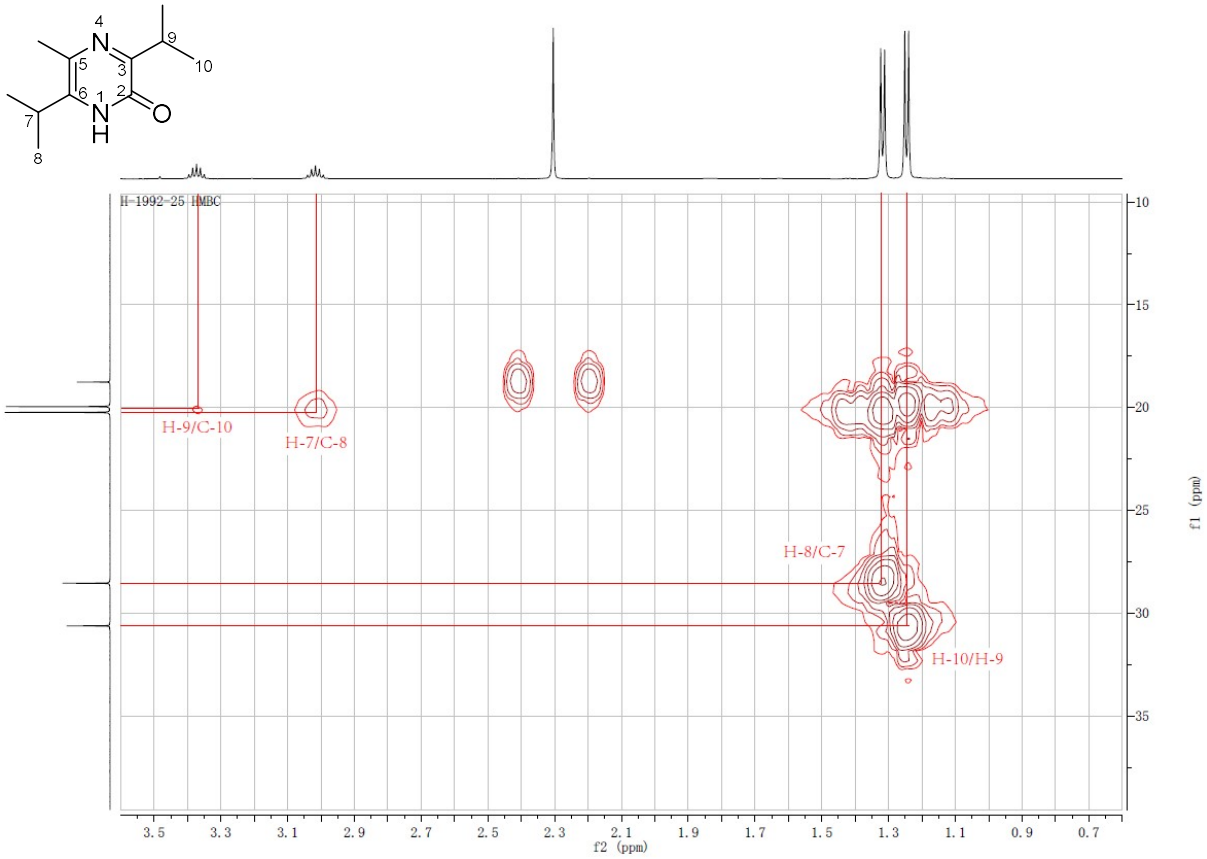


Figure S10: HMBC spectrum of compound **1** (^{1}H NMR from 0.6 to 3.60 ppm, ^{13}C NMR from 10 to 40 ppm)

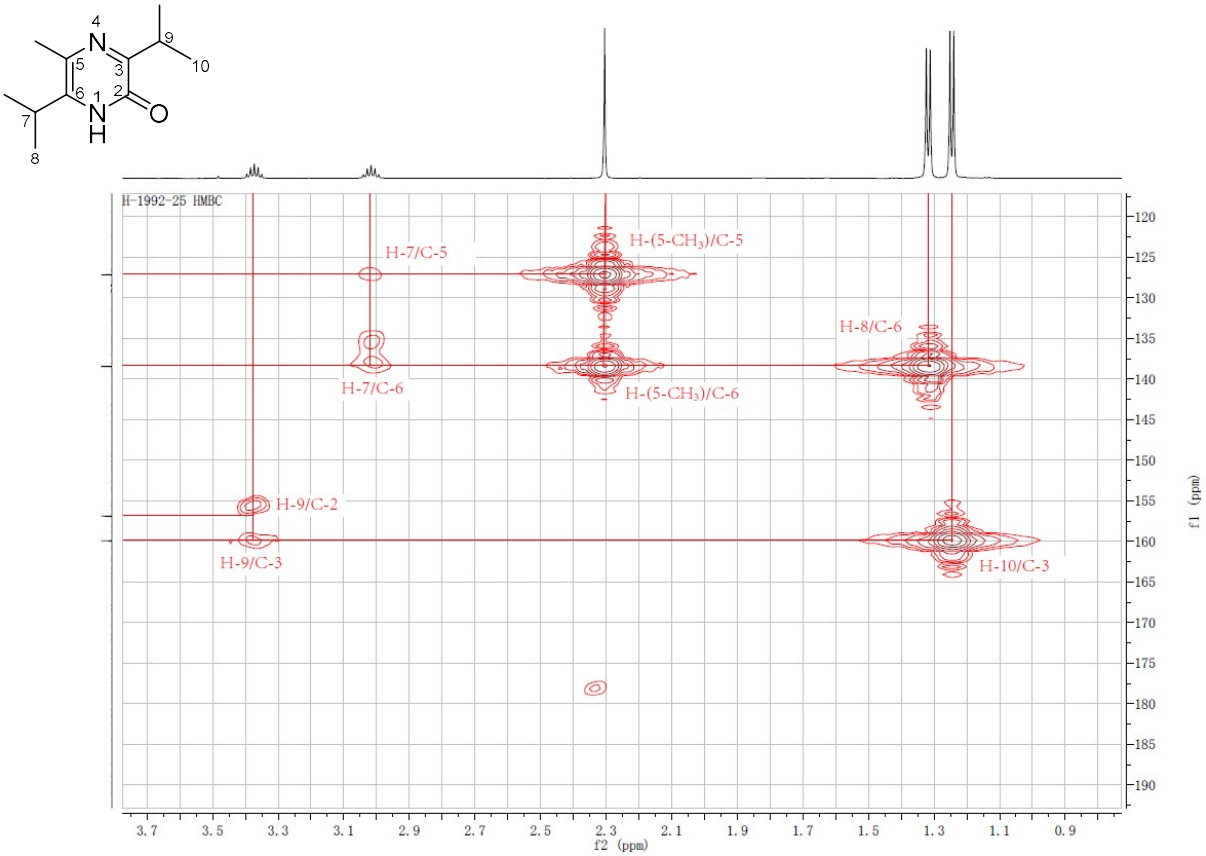


Figure S11: HMBC spectrum of compound **1** (^{1}H NMR from 0.0 to 3.75 ppm, ^{13}C NMR from 115 to 195 ppm)

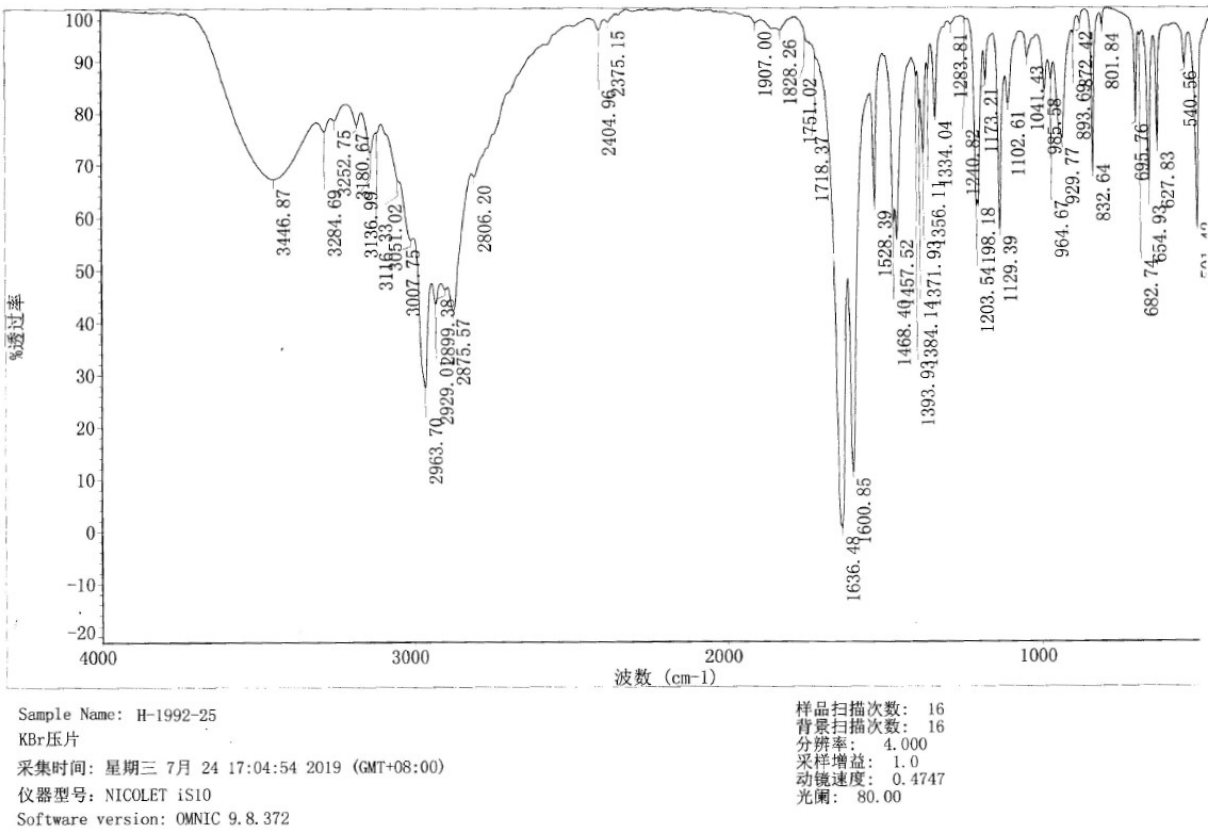


Figure S12: IR Spectrum of Compound **2**.

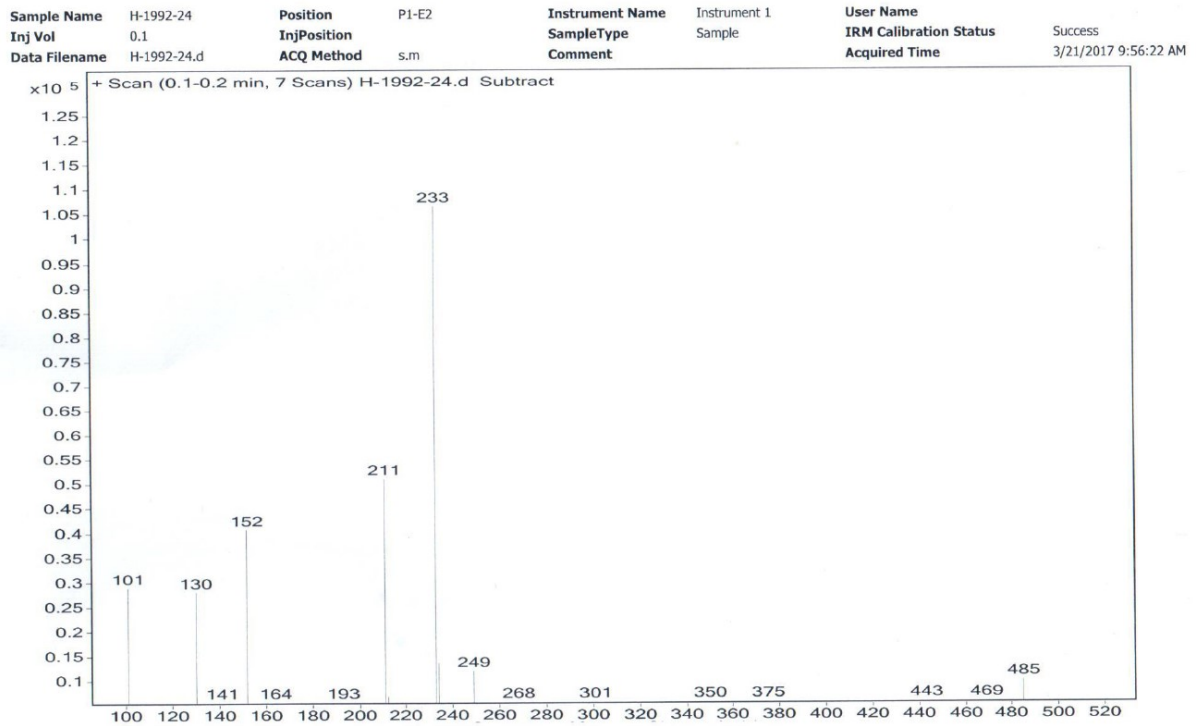


Figure S13: ESI-MS Spectrum of Compound **2**.

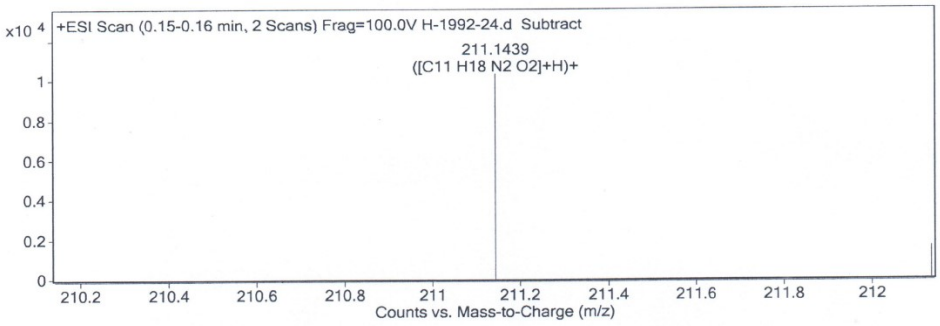
Qualitative Analysis Report

Data Filename	H-1992-24.d	**Sample Name**	H-1992-24
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	4/25/2018 11:38:56 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
60.082		3105.94		
148.0898		2910.95		
211.1439		10342.82	C11 H18 N2 O2	(M+H)+
233.1262	1	15062.13		
249.0991	1	3410.26		
437.1945	1	4734.09		
453.1687	1	10771.16		
483.2524	1	3488.22		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C11 H18 N2 O2	210.1368	211.1441	211.1439	0.20	0.95	4.0000

Figure S14: HR-ESI-MS Spectrum of Compound **2**.

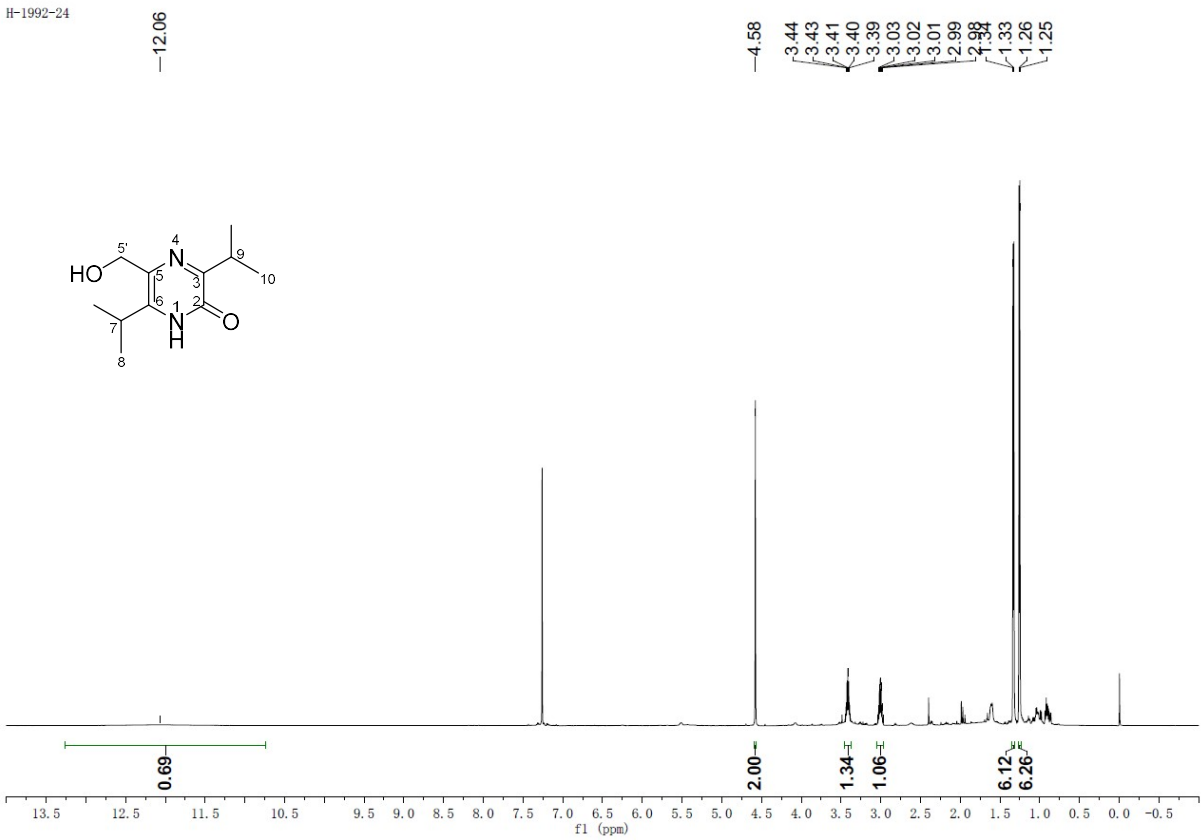


Figure S15: ^{1}H NMR spectrum of compound **2** (in $CDCl_3$, 600 MHz)

^{1}H NMR (600 MHz, $CDCl_3$): δ_H 12.06 12.06 (1H, brs, NH), 4.58 (2H, s, H-5'), 3.41 (1H, hept, J = 6.6 Hz, H-9), 3.01 (1H, hept, J = 7.2 Hz, H-7), 1.33 (6H, d, J = 7.2 Hz, H-8), 1.26 (6H, d, J = 6.6 Hz, H-10).

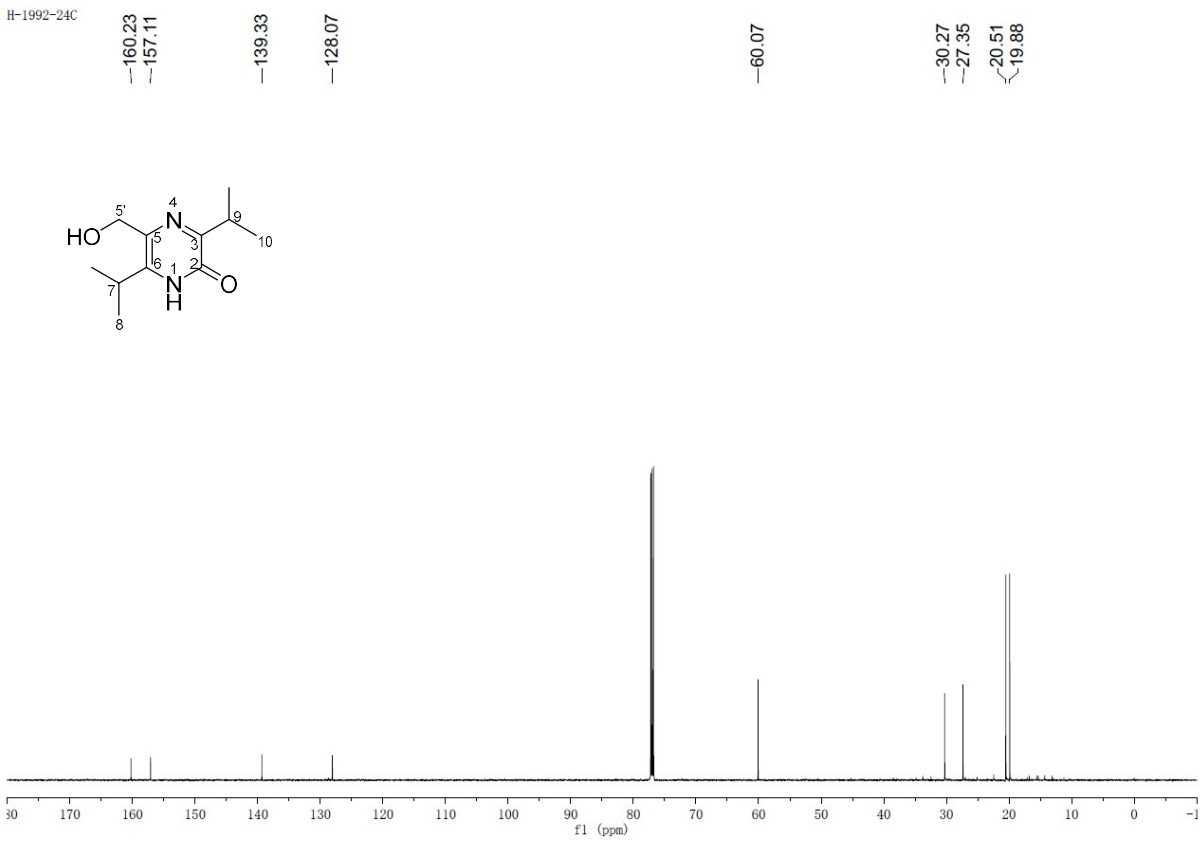


Figure S16: ^{13}C NMR spectrum of compound **2** (in $CDCl_3$, 150 MHz)

^{13}C NMR (150 MHz, $CDCl_3$): δ_C 160.2 (C-3), 157.1 (C-2), 139.3 (C-6), 128.1 (C-5), 60.1 (C-5'), 30.3 (C-9), 27.4 (C-7), 20.5 (C-8), 19.9 (C-10).

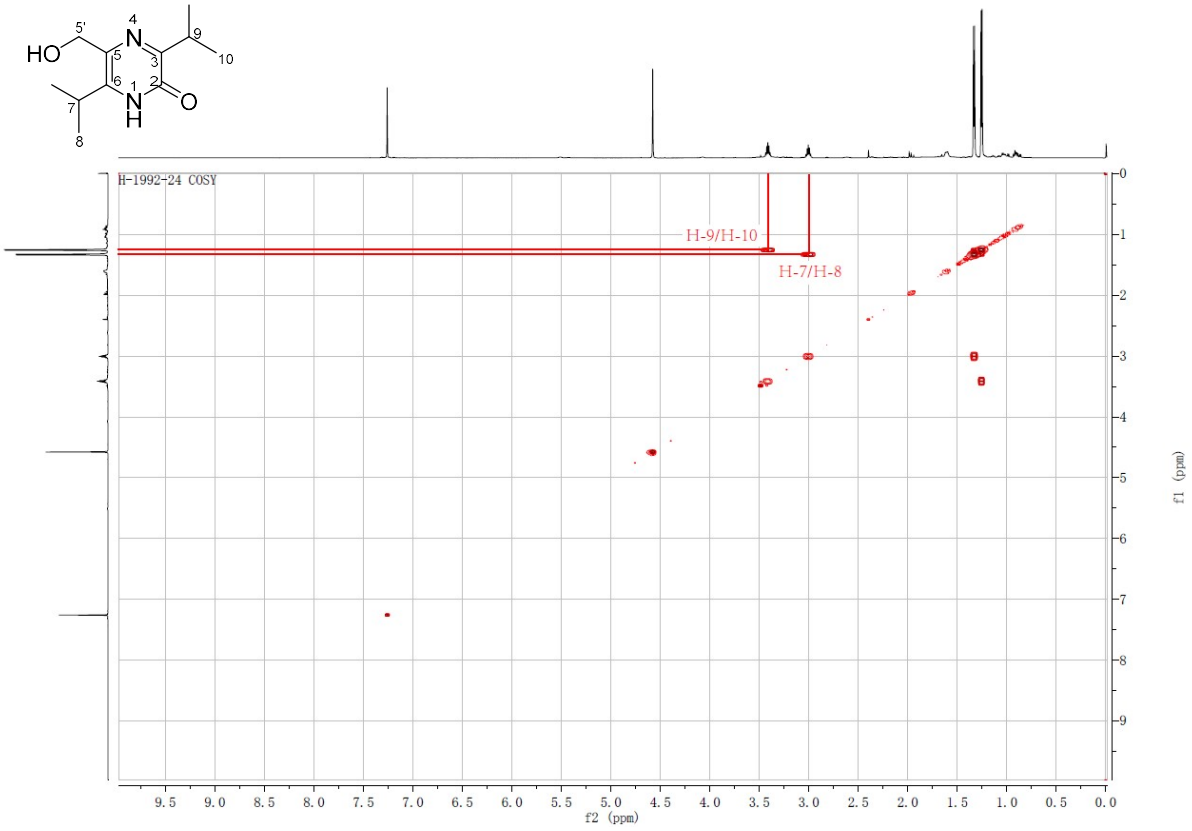


Figure S17: H-H COSY spectrum of compound **2** (in $CDCl_3$)

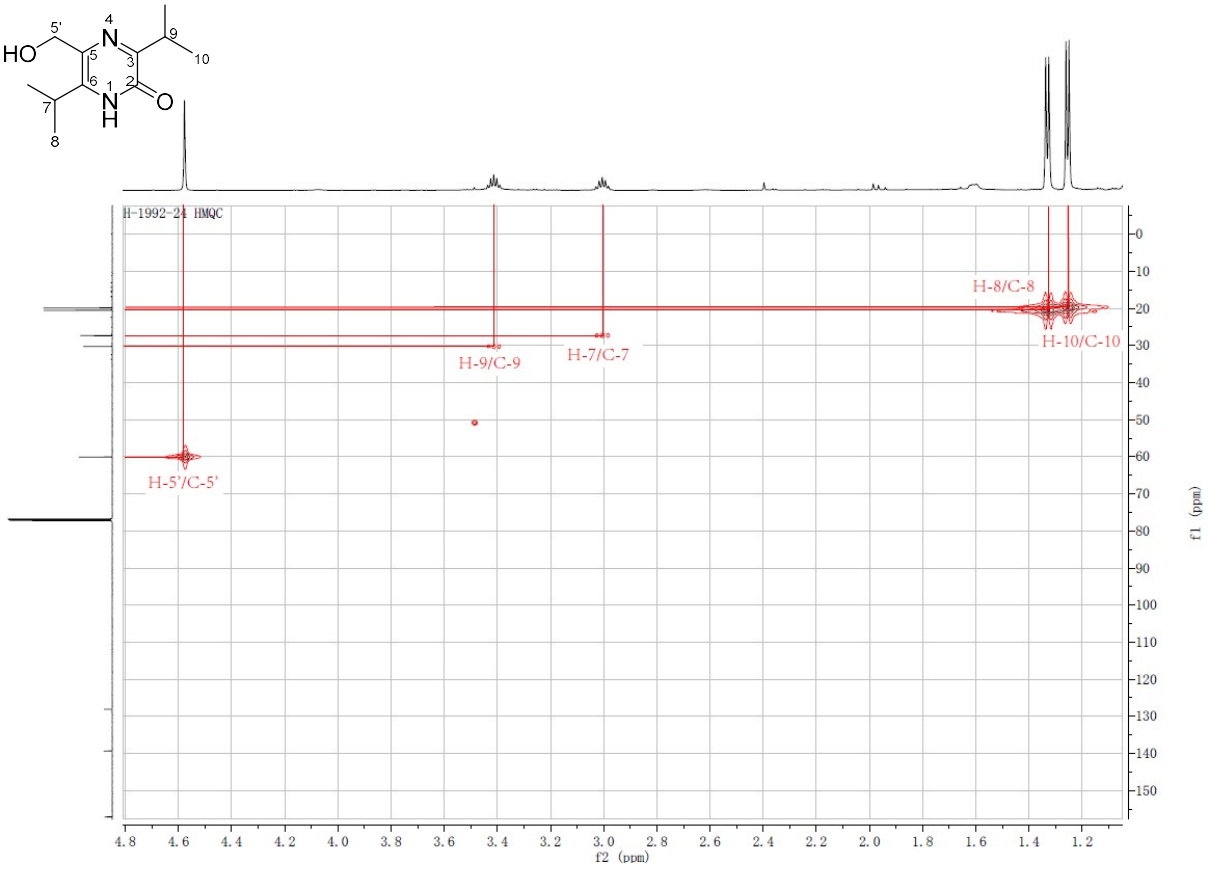


Figure S18: HSQC spectrum of compound **2** (in $CDCl_3$)

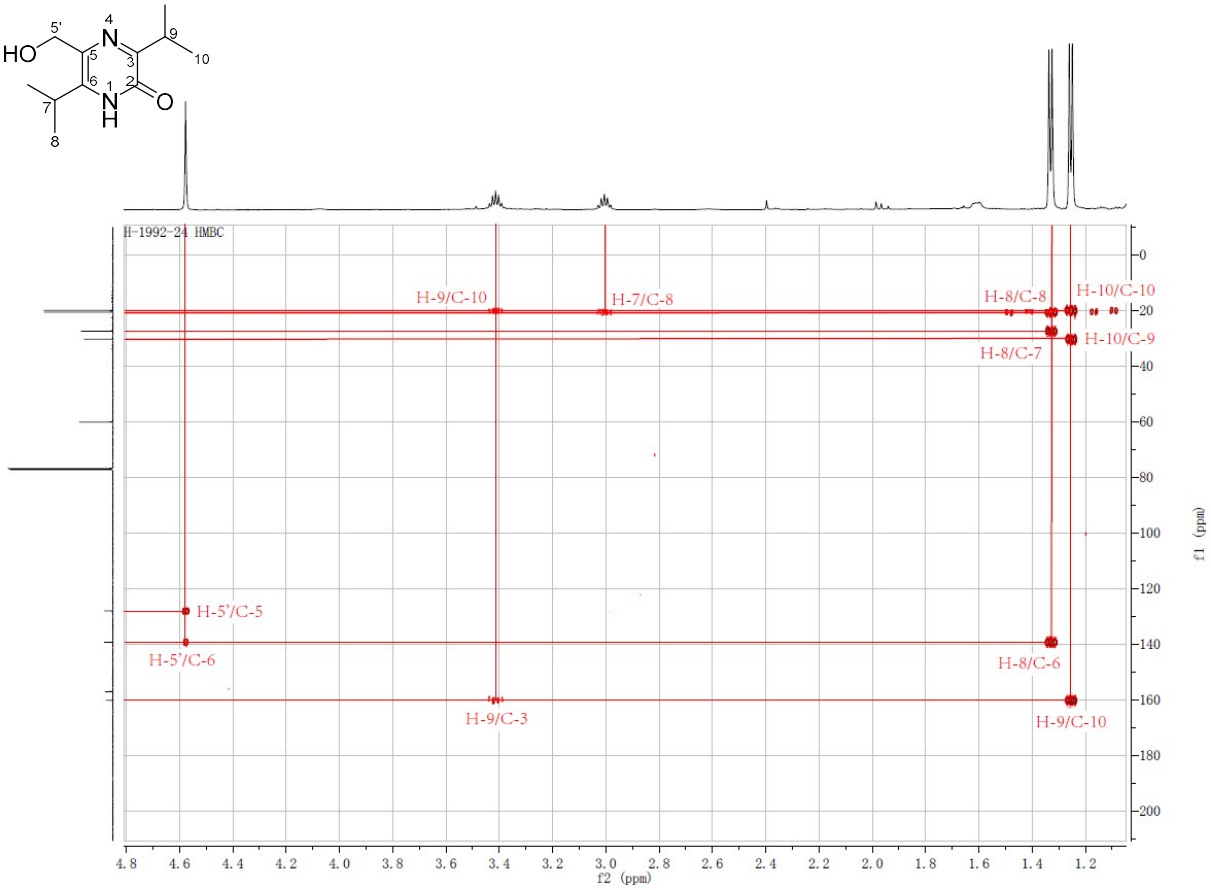
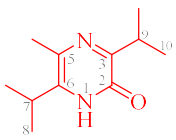


Figure S19: HMBC spectrum of compound **2** (in $CDCl_3$)

The NMR Data comparison of compound **1** with compounds **3-4** in *Tetrahedron* **1995**, *51*, 7361-7372 and compound **5** in *J. Nat. Prod.* **2014**, *77,* 2545-2552.



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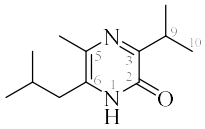
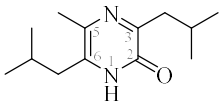


3-isobutyl-6-isopropyl-5-methylpyrazin-2(1H)-one (**3**)



3,6-diisobutyl-5-methylpyrazin-2(1H)-one (**4**)

Sorazinone B (5)

Table S1. ^{1}H and ^{13}C NMR data of compound **1**, **3-5** in $CDCl_3$.

Position	1		3		4		5	
	δc (ppm)	δ_H (ppm, *J* in Hz)	δc (ppm)	δ_H (ppm, *J* in Hz)	δc (ppm)	δ_H (ppm, *J* in Hz)	δc (ppm)	δ_H (ppm, *J* in Hz)
1		12.33 (1H, brs)		13.4 (lH, brs)		13.2 (lH, brs)		11.06 (lH, brs)
2	156.7		159.8		157.8		156.6	
3	159.9		157.2		155.7		154.7	
5	127.1		129.5		129.5		130.5	
5-Me/5'	18.8	2.30 (3H, s)	18.9	2.28 (3H, s)	18.7	2.29 (3H, s)	19.1	2.26 (3H, s)
6	138.4		133.7		134.1		136.1	
9	30.6	3.37 (1H, hept, *J* = 6.6 Hz)	30.6	3.37 (lH, heptet, *J* =6.9 Hz)				
10	19.9	1.24 (6H, d, *J* = 6.6 Hz)	20.0	1.25 (6H, d, *J* = 6.9 Hz)				