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A Unique Spiro-*β*-Triazinedione-*γ*-Hydantoin Type Alkaloid with Antiviral Activitiy against Tobacco Mosaic Virus from *Streptomyces gamaensis*

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Supplementary Information

Contents

Experimental Section 3

Fig. S1. HPLC analysis of hydrolysis reaction. 3

Fig. S2. Two possible modes of ring-cleavage reaction of compound (±)-**1** 4

Fig. S3. Key COSY and HMBC correlations of compound **5** 4

Fig. S4. Packing diagram of the unit cell of compound (±)-**1** 4

Tab. S1. Test dose of compound **1**. 5

Tab. S2. Anti-TMV activity of compound **1** on tomato leaf. 5

Tab. S3. Anti-TMV activity of compound **1** on pepper leaf. 5

Tab. S4. NMR spectral data for compounds **2** and **3** in $CDCl_3$. 6

NMR spectra for compounds 1 and 5 and MS spectra of compounds 1, 4 and 5 7

Fig. S5. HRESIMS spectrum of compound (±)-**1**. 7

Fig. S6. ^{1}H NMR spectrum (400 MHz) of compound (±)-**1** in $CDCl_3$. 8

Fig. S7. ^{13}C NMR spectrum (100 MHz) of compound (±)-**1** in $CDCl_3$. 9

Fig. S8. COSY spectrum of compound (±)-**1** in $CDCl_3$ 10

Fig. S9. HSQC spectrum of compound (±)-**1** in $CDCl_3$ 11

Fig. S10. HMBC spectrum of compound (±)-**1** in $CDCl_3$ 12

Fig. S11. ESIMS spectrum of compound **4**. 13

Fig. S12. HRESIMS spectrum of compound **5**. 14

Fig. S13. ^{1}H NMR spectrum (800 MHz) of compound **5** in $CDCl_3$. 15

Fig. S14. ^{13}C NMR spectrum (200 MHz) of compound **5** in $CDCl_3$. 16

Fig. S15. COSY spectrum of compound **5** in $CDCl_3$ 17

Fig. S16. HSQC spectrum of compound **5** in $CDCl_3$ 18

Fig. S17. HMBC spectrum of compound **5** in $CDCl_3$ 19

Experimental Section

Fig. S1. HPLC analysis (detected at 238 nm) of hydrolysis product of **4**. (a) standard (±)-**1**; (b) hydrolysis reaction of **4**.

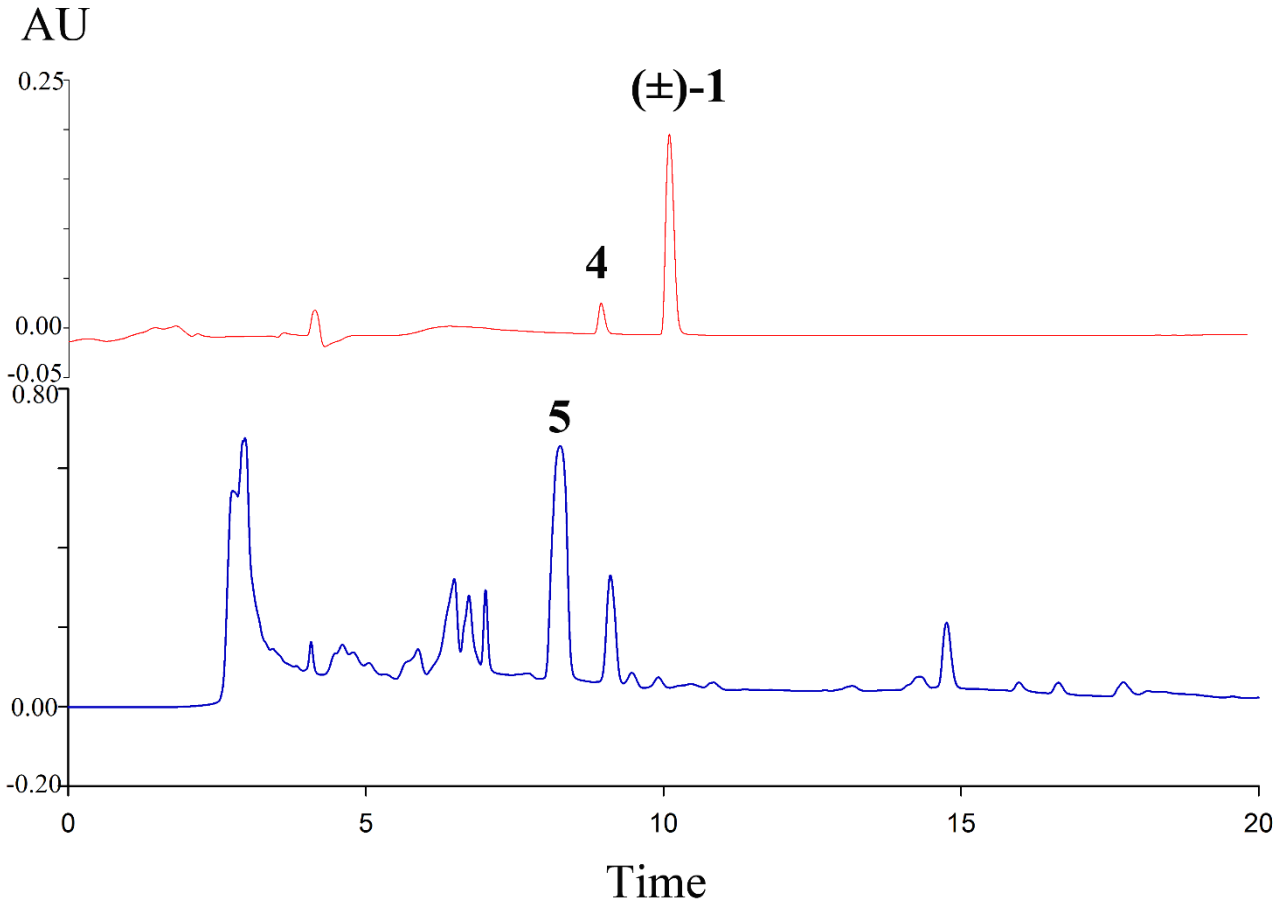


Fig. S2. Two possible modes of ring-cleavage reaction of compound (±)-**1.**

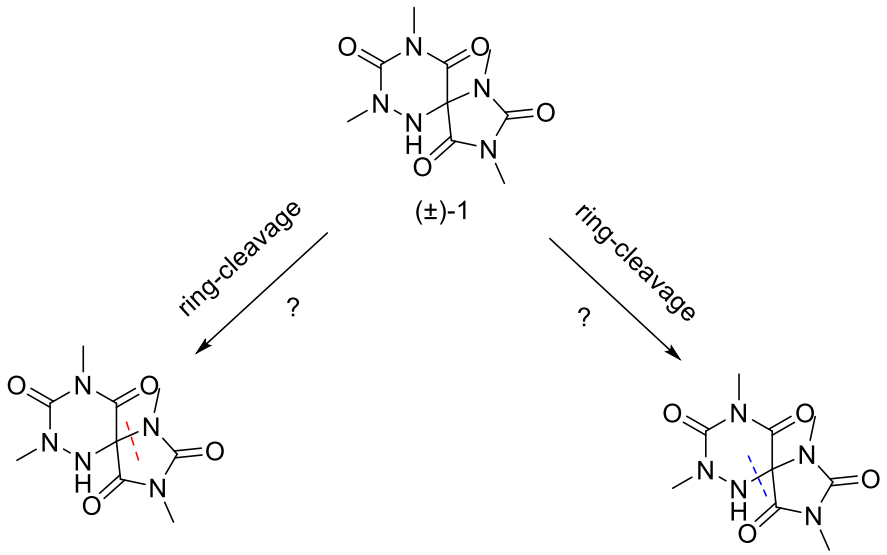


Fig. S3. Key COSY and HMBC correlations of compound **5**.

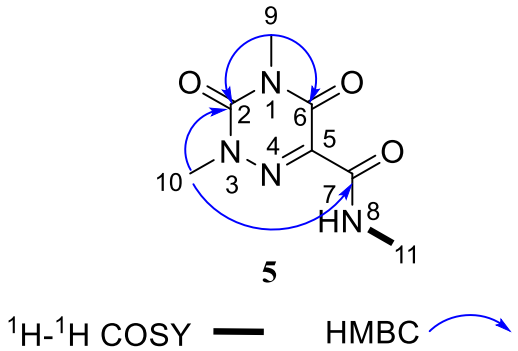
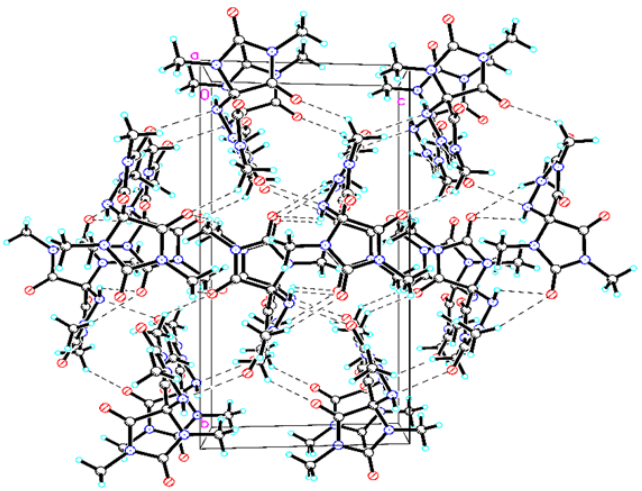


Fig. S4. Packing diagram of the unit cell of compound (±)-**1**.



Tab. S1. Test dose of compound **1** (mg/L).

Group	Compounds	Concentration (mg/L).	Dilution ratio
1	**1**	400	25
2	**1**	300	33.3
3	**1**	200	50
4	**1**	100	100
5	**1**	50	200
6	Ningnanmycin AS (2%)	100	200
7	distilled water		

Tab. S2. Anti-TMV activity of compound **1** on tomato leaf.

Group	Compounds	Concentration (mg/L)	Inhibition rate
1	**1**	400	44.55 ± 3.0
2	**1**	300	59.29 ± 3.2
3	**1**	200	77.45 ± 3.5
4	**1**	100	72.34 ± 2.8
5	**1**	50	52.54 ± 3.8
6	Ningnanmycin AS (2%)	100	57.11 ± 2.8
8	Distilled water		

All results are expressed as mean ± SD; n=3 for all groups.

Tab. S3. Anti-TMV activity of compound **1** on pepper leaf.

Group	Compounds	Concentration (mg/L)	Inhibition rate
1	**1**	400	80.06 ± 2.2
2	**1**	300	73.79 ± 2.5
3	**1**	200	69.98 ± 2.8
4	**1**	100	62.09 ± 3.0
5	**1**	50	61.03 ± 3.1
6	Ningnanmycin AS (2%)	100	67.56 ± 3.0
8	Distilled water		

All results are expressed as mean ± SD; n=3 for all groups.

Tab. S4. NMR spectral data for compounds **2** and **3** in $CDCl_3$.

No	**2**[a]		**3**[a]	
	δ_C, mult.	δ_H (mult, *J* (Hz))	δ_C, mult.	δ_H (mult, *J* (Hz))
1				
2	155.5, C			
3			151.6, C	
4				5.69, brs
4a	151.8, C		55.0, C	
5	158.7, C		166.2, C	
6				
7	155.8, C		149.9, C	
8				
8a	124.6, C		138.6, C	
9	42.5, CH_3	3.91, s	49.6, CH_2	2.95, d (16.3); 3.25, d (16.3)
10	29.5, CH_3	3.52, s	202.7, C	
11	28.9, CH_3	3.41, s	30.8, CH_3	2.15, s
12			37.0, CH_3	3.33, s
13			30.4, CH_3	3.36, s
14			28.8, CH_3	3.30, s

[a]400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR.

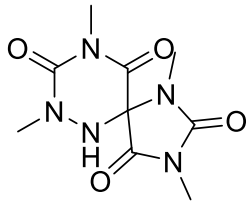
NMR spectra for compounds 1 and 5 and MS for compounds 1, 4 and 5

Fig. S5. HRESIMS spectrum of compound (±)-**1**.

Qualitative Analysis Report

Data Filename	hsx117-3x.d	**Sample Name**	hsx117-3x
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/13/2019 1:54:04 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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



(±)-**1**

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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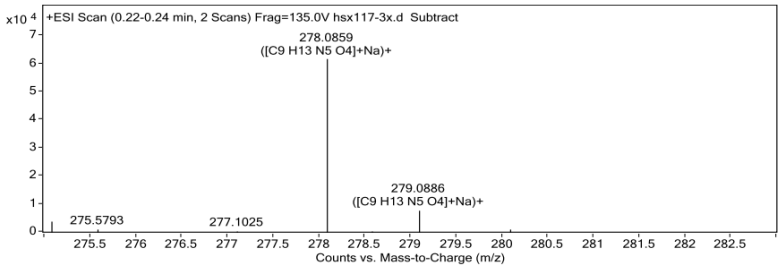

Peak List

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158.025	2	3065.87		
172.0944	1	54698.32		
173.0974	1	6036.86		
221.0653	1	10105.01		
275.0775	2	3787.76		
278.0859	1	61612.49	C9 H13 N5 O4	(M+Na)+
279.0886	1	7852.66	C9 H13 N5 O4	(M+Na)+
294.0594	1	7680.1		
310.1121	1	5096.71		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	10

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C9 H13 N5 O4	255.0968	278.0860	278.0859	0.10	0.36	6.0000

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Agilent Technologies Page 1 of 1 Printed at: 1:56 PM on: 5/13/2019

Fig. S6. ^{1}H NMR spectrum (400 MHz) of compound (±)-**1** in $CDCl_3$.

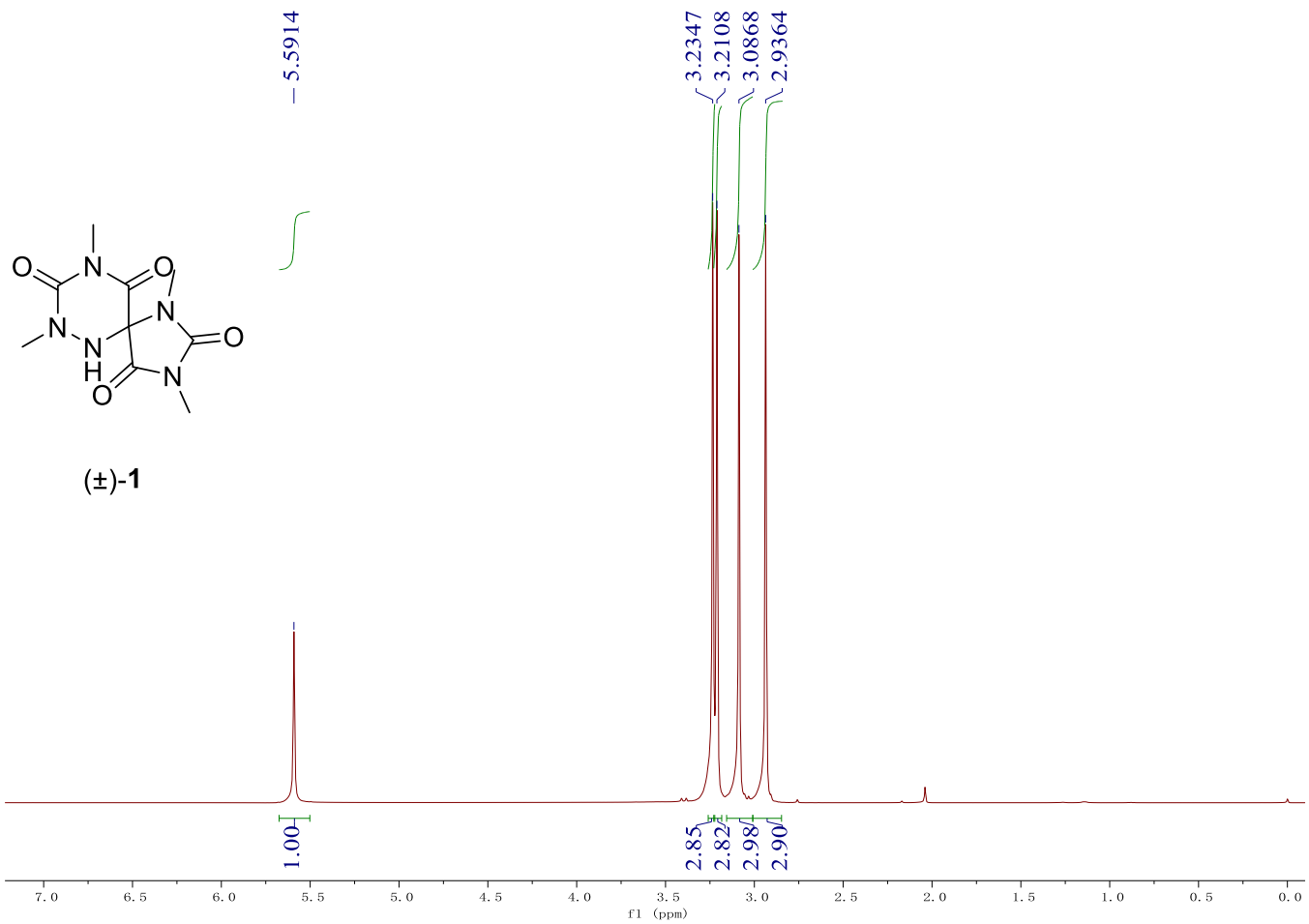

Fig. S7. ^{13}C NMR spectrum (100 MHz) of compound (±)-**1** in $CDCl_3$.

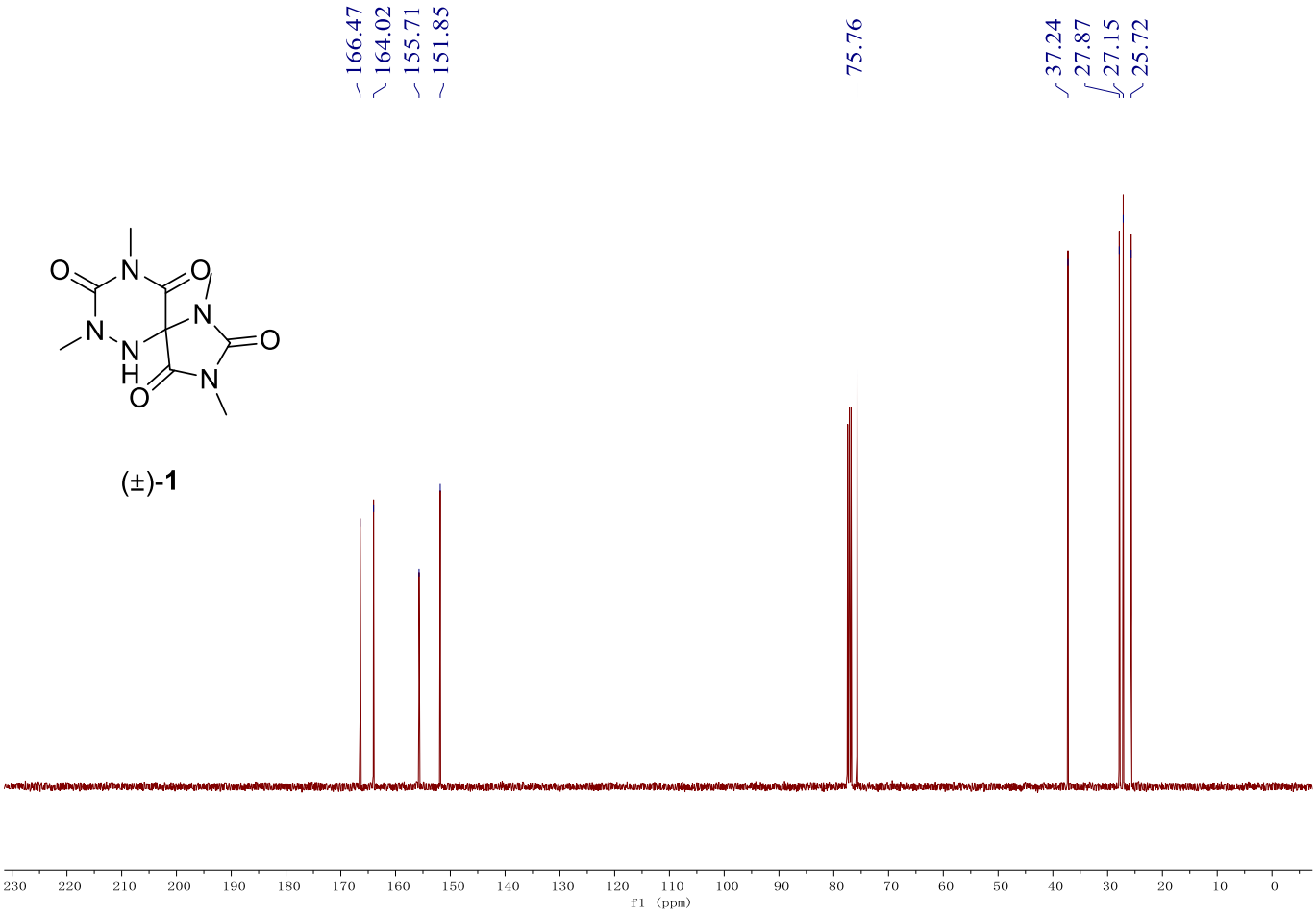

Fig. S8. COSY spectrum of compound (±)-**1** in $CDCl_3$.

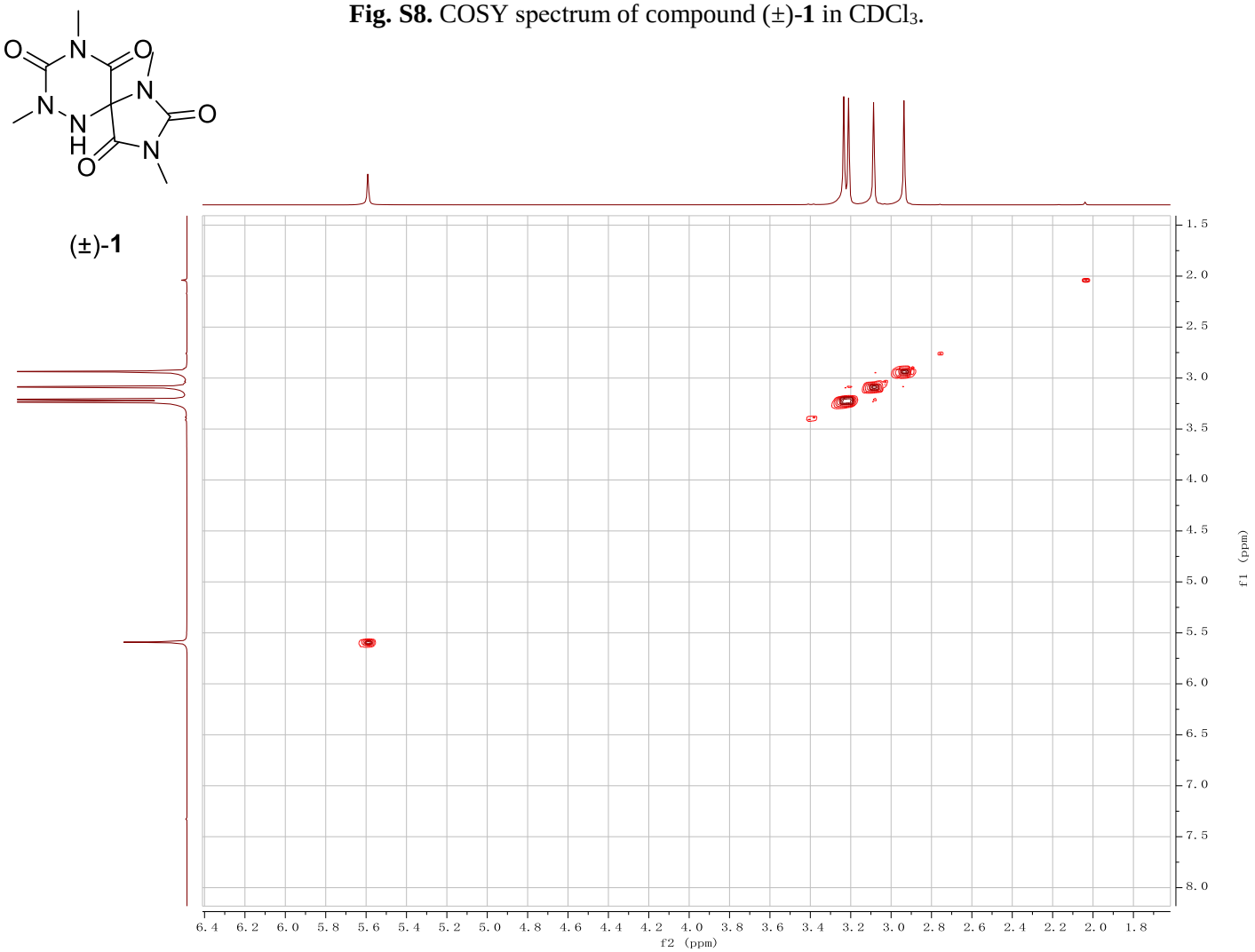

Fig. S9. HSQC spectrum of compound (±)-**1** in $CDCl_3$.

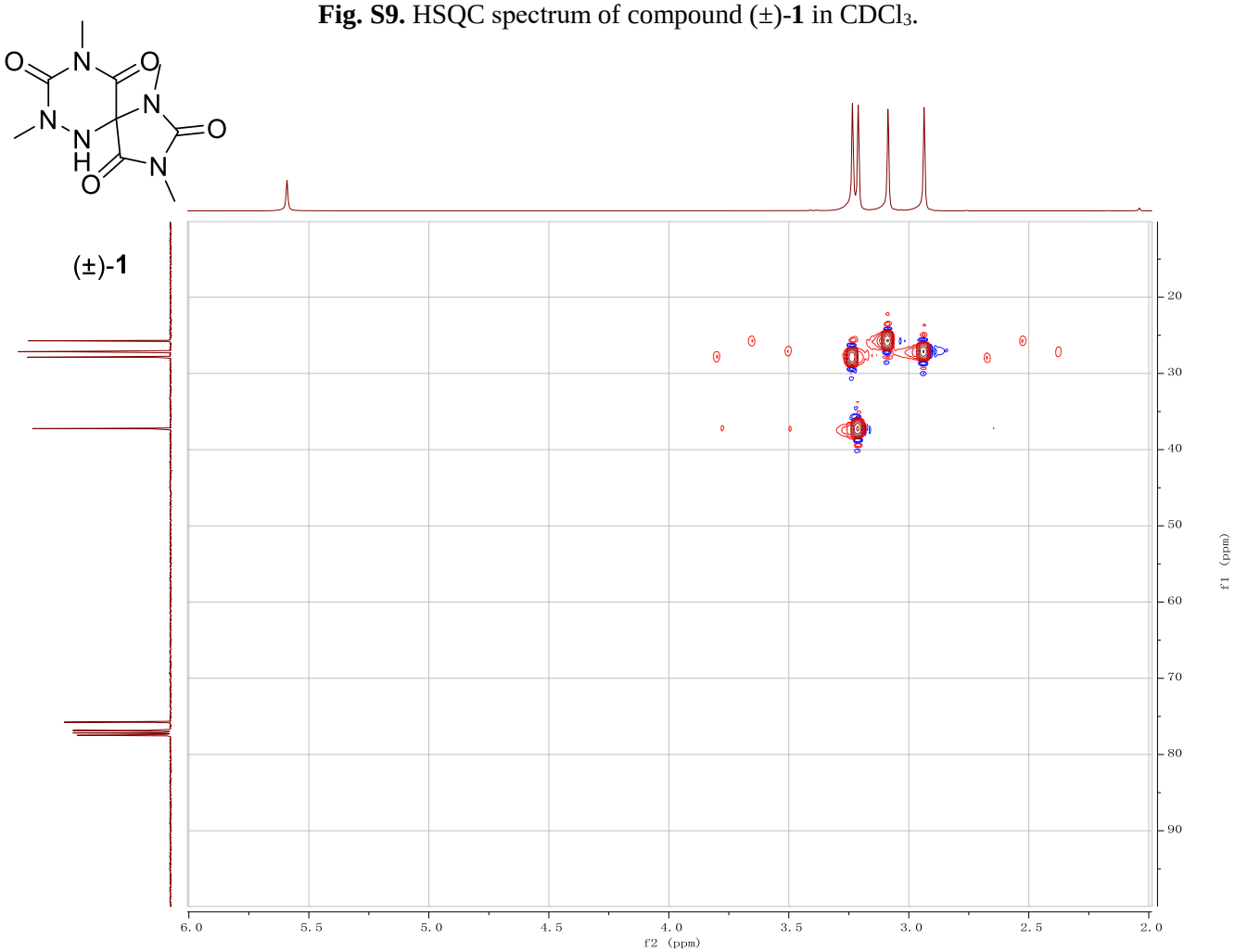

Fig. S10. HMBC spectrum of compound (±)-**1** in $CDCl_3$.

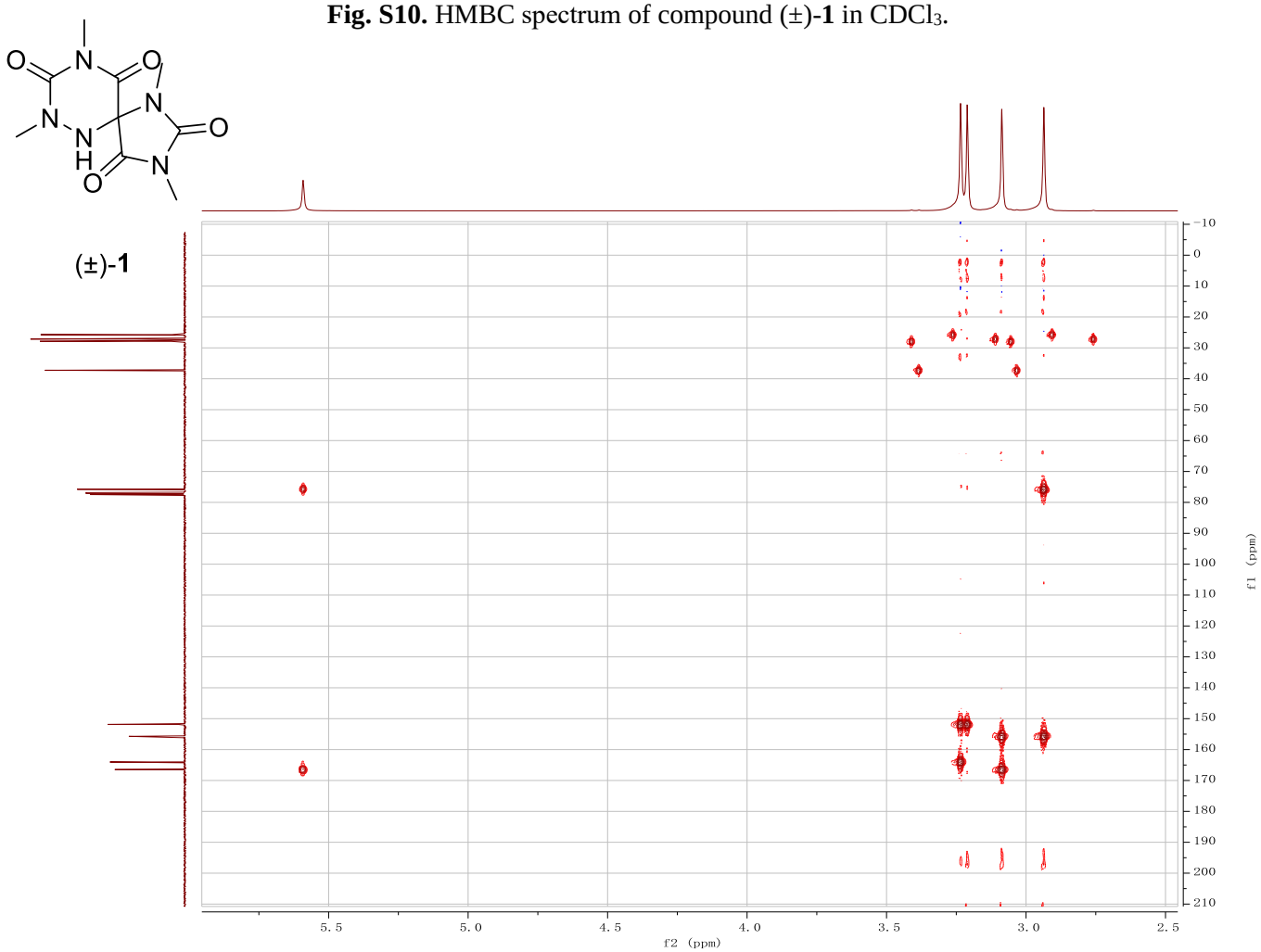

Fig. S11. ESIMS spectrum of compound **4**.

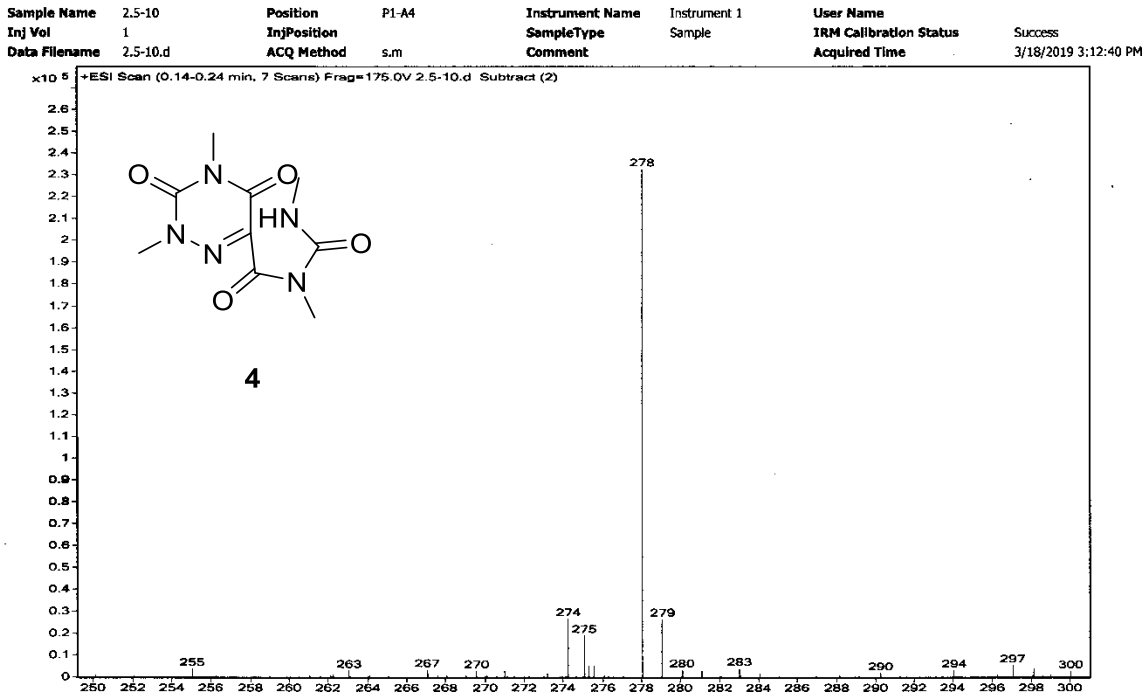

Fig. S12. HRESIMS spectrum of compound **5**.

Qualitative Analysis Report

Data Filename	38.68H.d	**Sample Name**	38.68H
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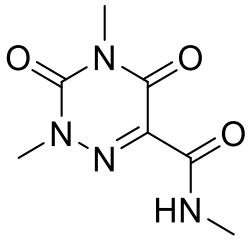
Acq Method	s.m	**Acquired Time**	3/5/2019 3:47:24 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

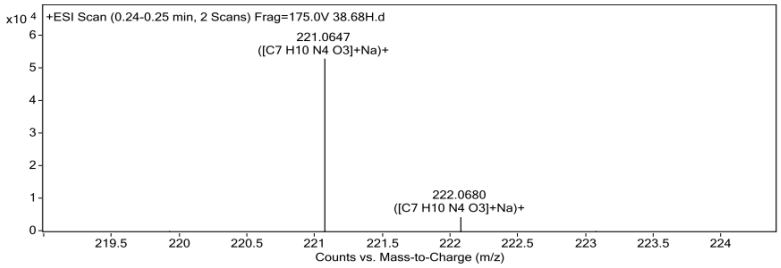
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)



5

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
82.9984	1	17328.5		
98.9759	1	74380.9		
118.9211		4740.67		
136.9312		7124.96		
142.0615	1	28156.26		
170.0562		12915.06		
199.0828	1	26396.69		
221.0647	1	53081.05	C7 H10 N4 O3	(M+Na)+
283.0354	1	7757.64		
297.0514	1	15217.18		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30
N	0	10

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C7 H10 N4 O3	198.0753	221.0645	221.0647	-0.20	-0.90	5.0000

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Agilent Technologies Page 1 of 1 Printed at: 3:22 PM on: 3/26/2019

Fig. S13. ^{1}H NMR spectrum (800 MHz) of compound **5** in $CDCl_3$.

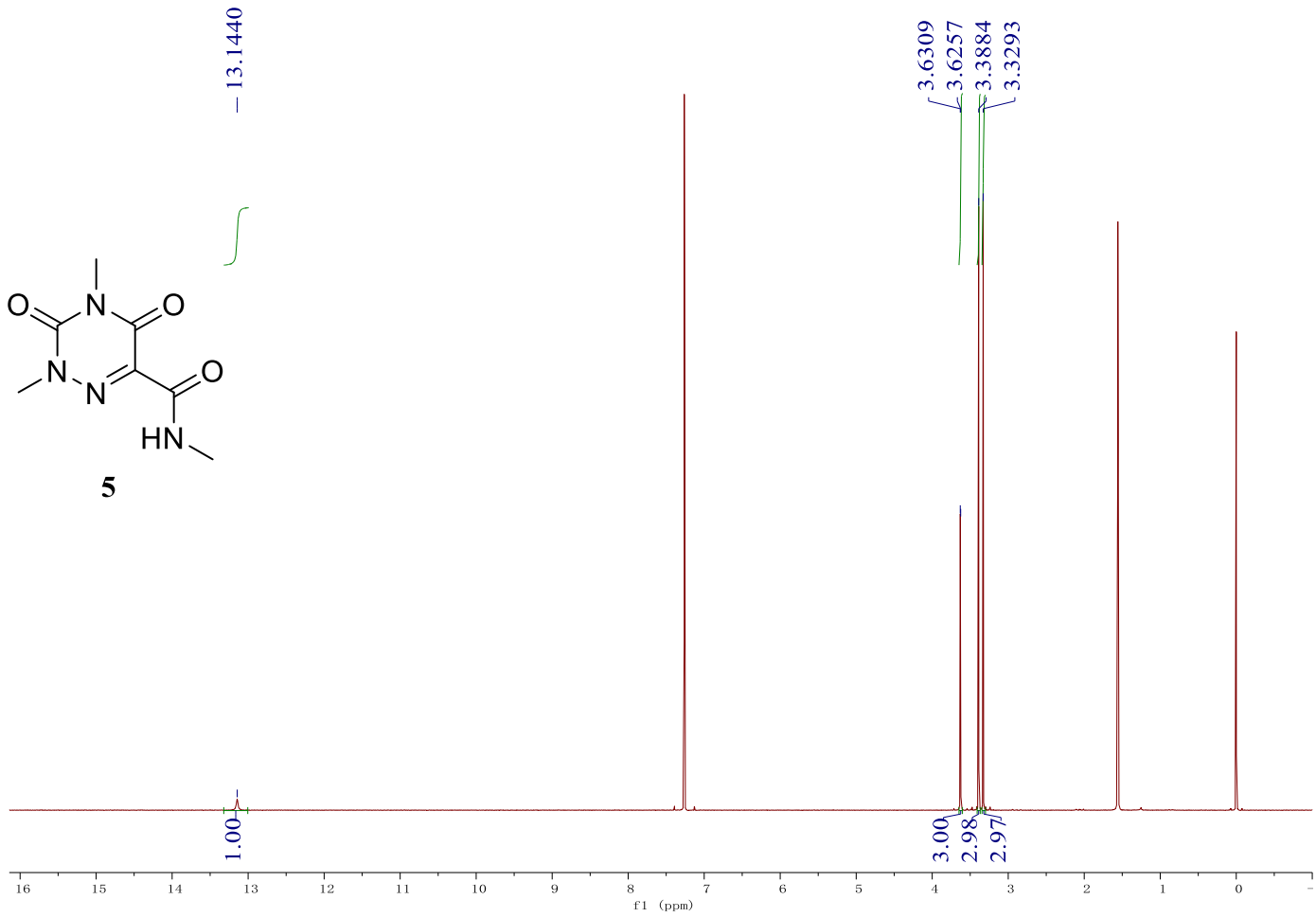
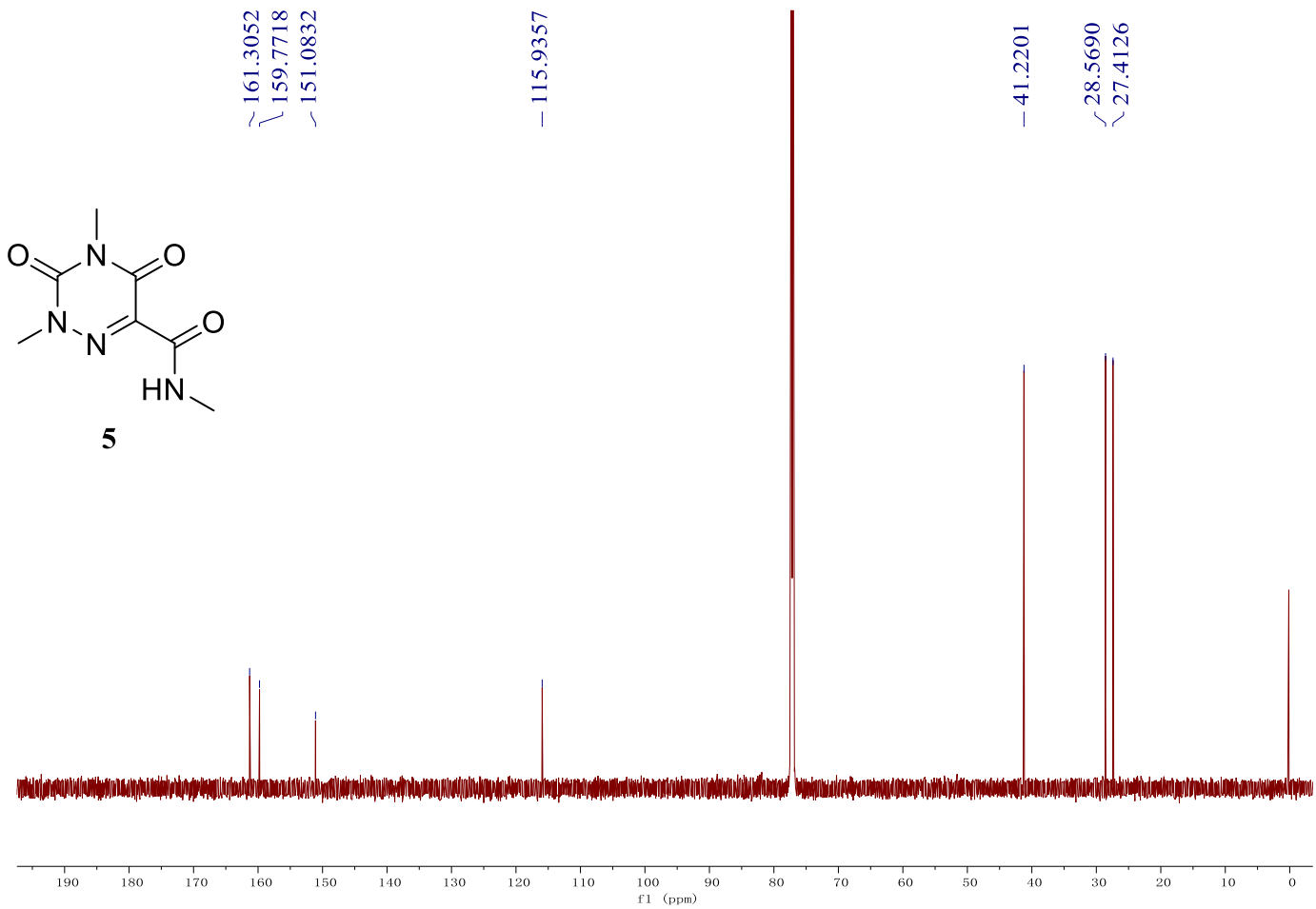
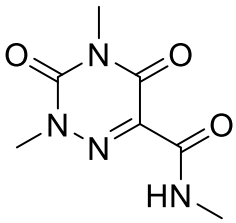


Fig. S14. ^{13}C NMR spectrum (200 MHz) of compound **5** in $CDCl_3$.





5

Fig. S15. COSY spectrum of compound **5** in $CDCl_3$.

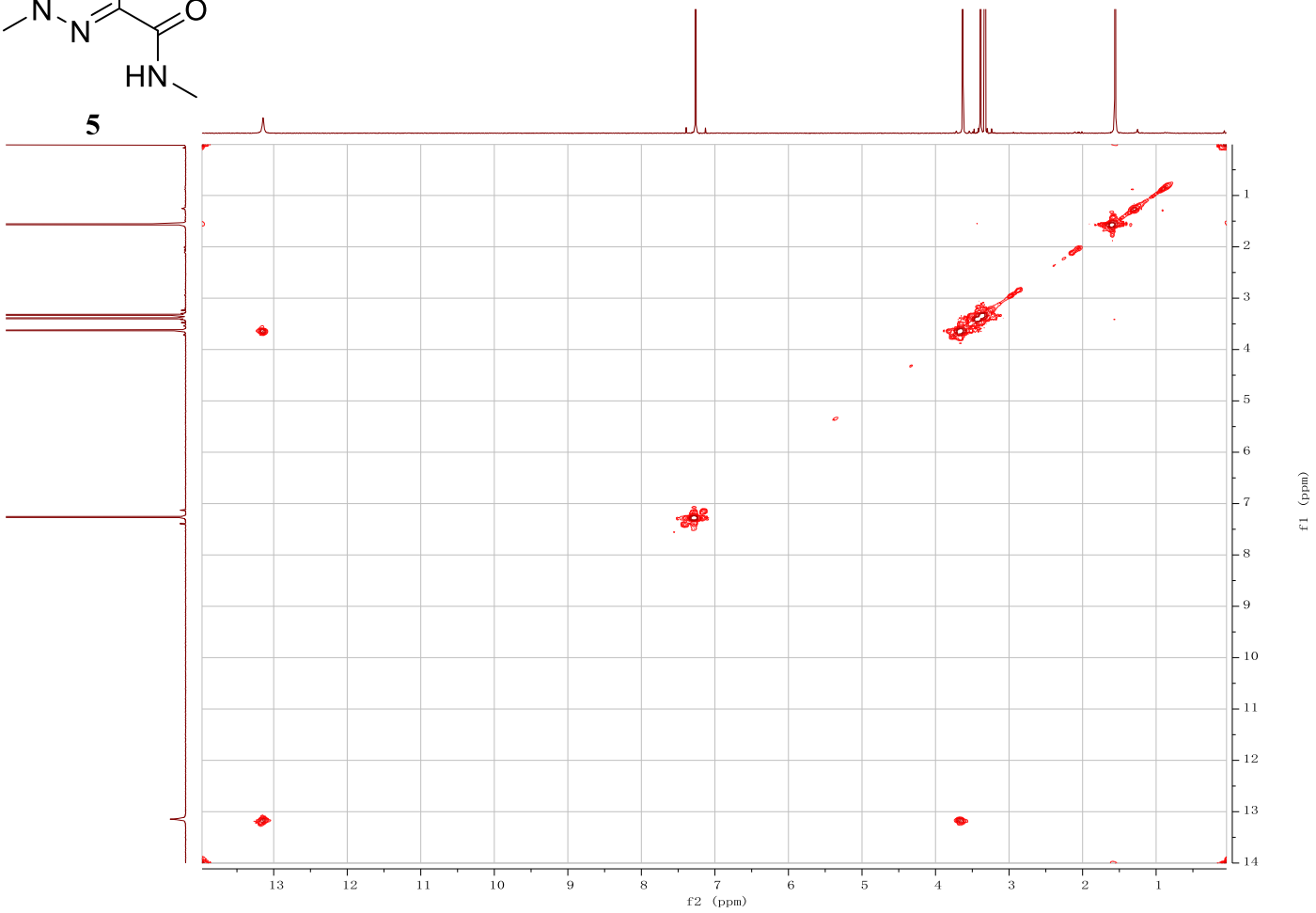
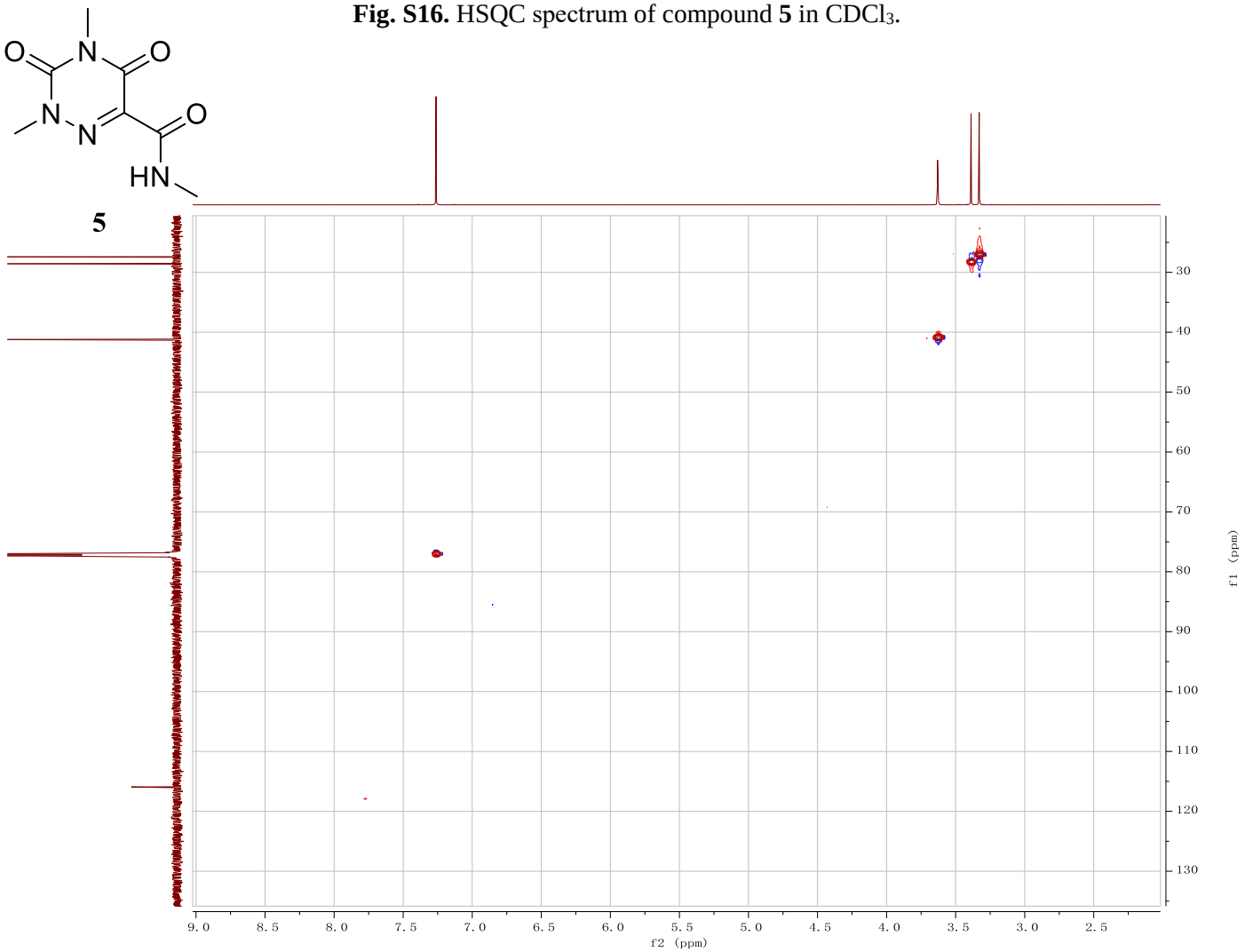
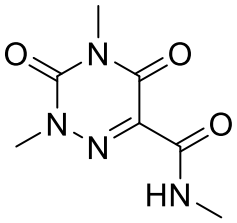


Fig. S16. HSQC spectrum of compound **5** in $CDCl_3$.





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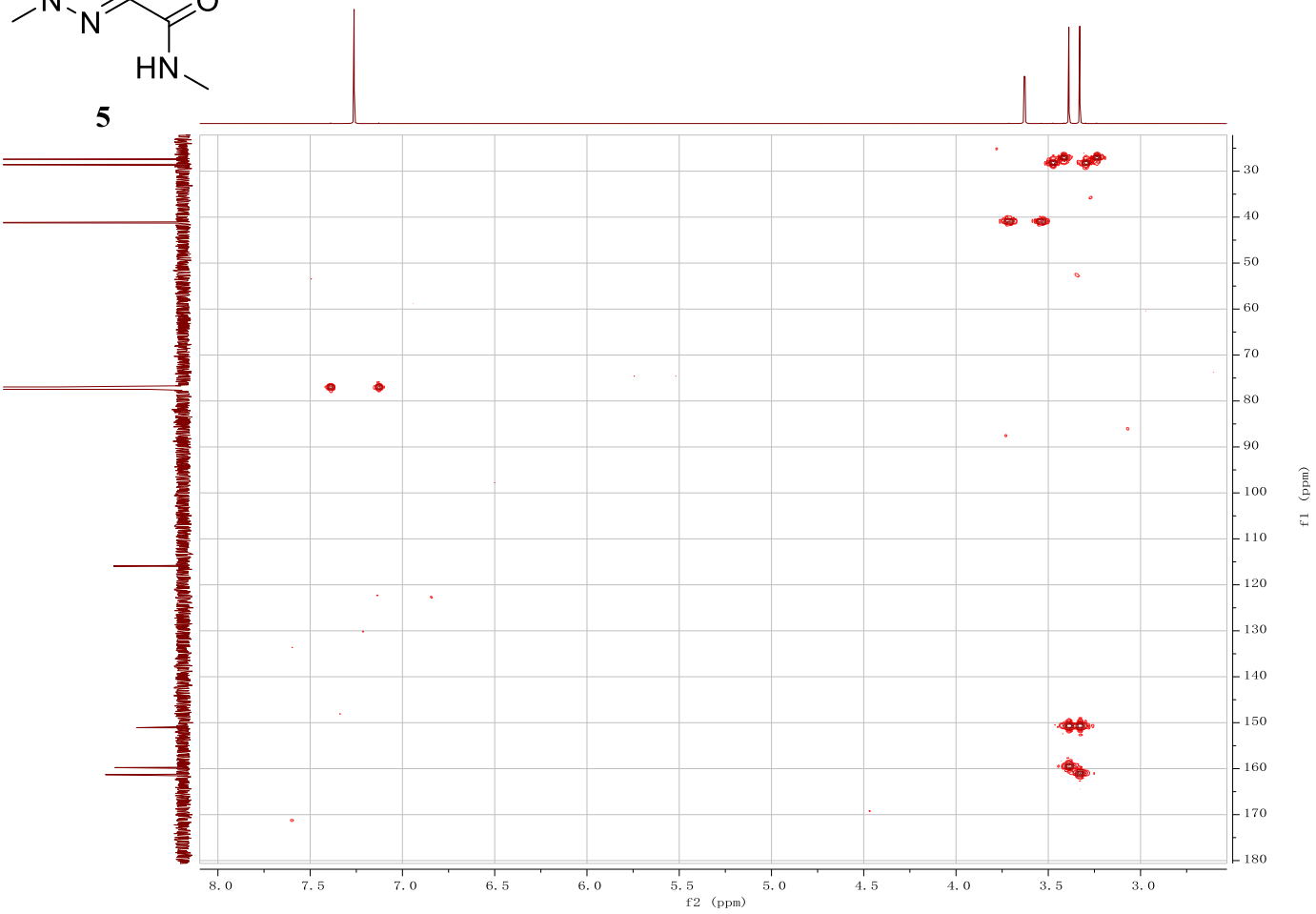
Fig. S17. HMBC spectrum of compound **5** in $CDCl_3$.