

## Supplementary section

**Table S1.** The comparison of the NMR data of compound **1** to those of the reported compound [31]

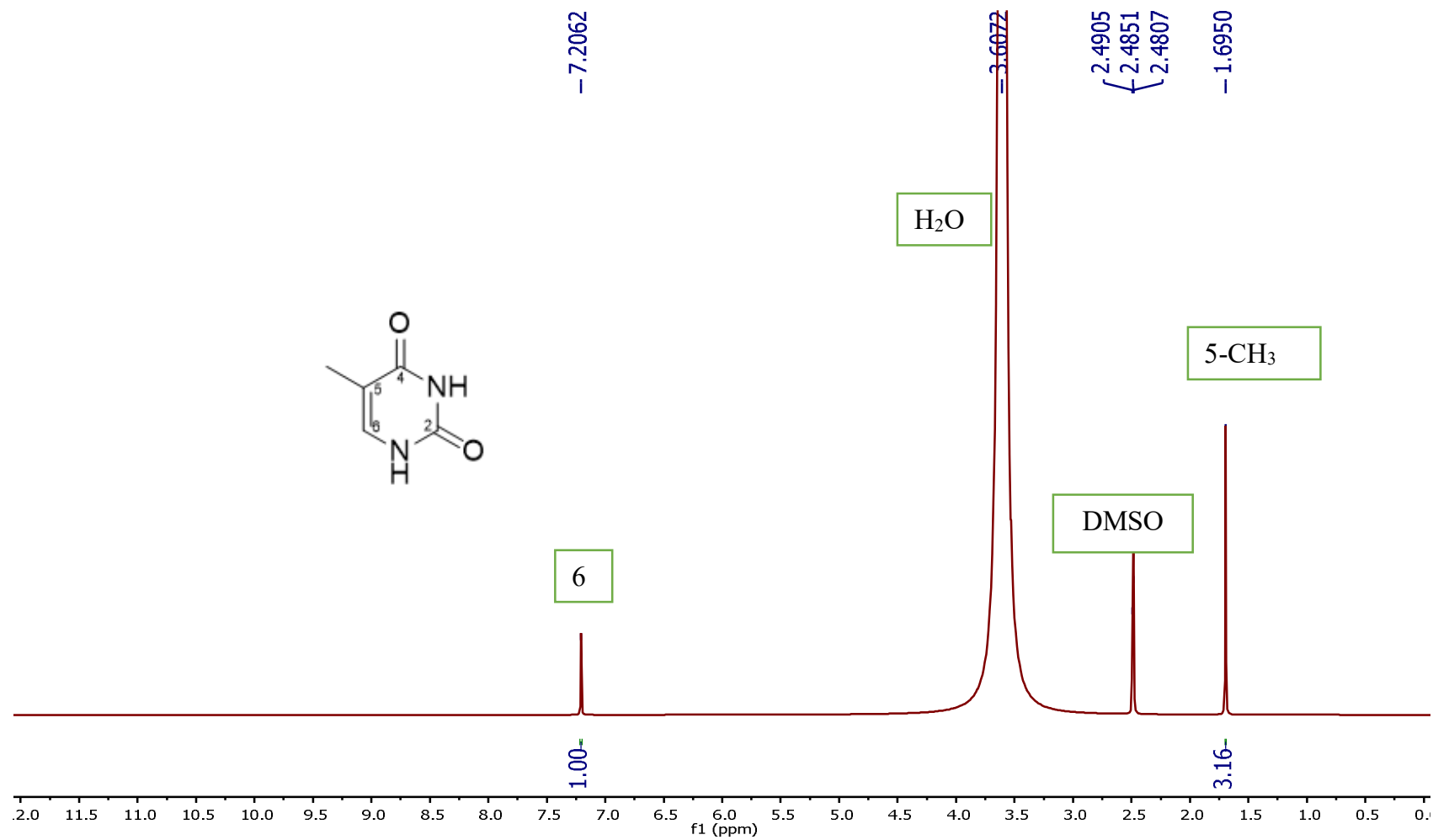
No	Compound <b>1</b> (DMSO- <i>d</i> <sub>6</sub> )		Thymine (DMSO- <i>d</i> <sub>6</sub> ) [31]	
	$\delta_{\text{H}}$ (ppm), <i>J</i> (Hz)	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm), <i>J</i> (Hz)	$\delta_{\text{C}}$ (ppm)
2		151.9		153.9
4		165.4		168.3
5		108.0		110.9
6	7.21 (1H, <i>s</i> )	138.3	7.28	139.8
5-CH <sub>3</sub>	1.69 (3H, <i>s</i> )	12.0	1.75	12.1

The compound (**1**) was obtained as a white amorphous powder. <sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>, 500 MHz)  $\delta_{\text{H}}$ : 7.21 (1H, *s*), 1.69 (3H, *s*). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>, 125 MHz)  $\delta_{\text{C}}$ : 165.4, 151.9, 138.3, 108.0, 12.0. HR-ESI-MS spectrum: [M-H]<sup>-</sup> at *m/z* 125.0354. The NMR and mass spectra are presented in the supplementary section (Figure S1 – Figure S3).

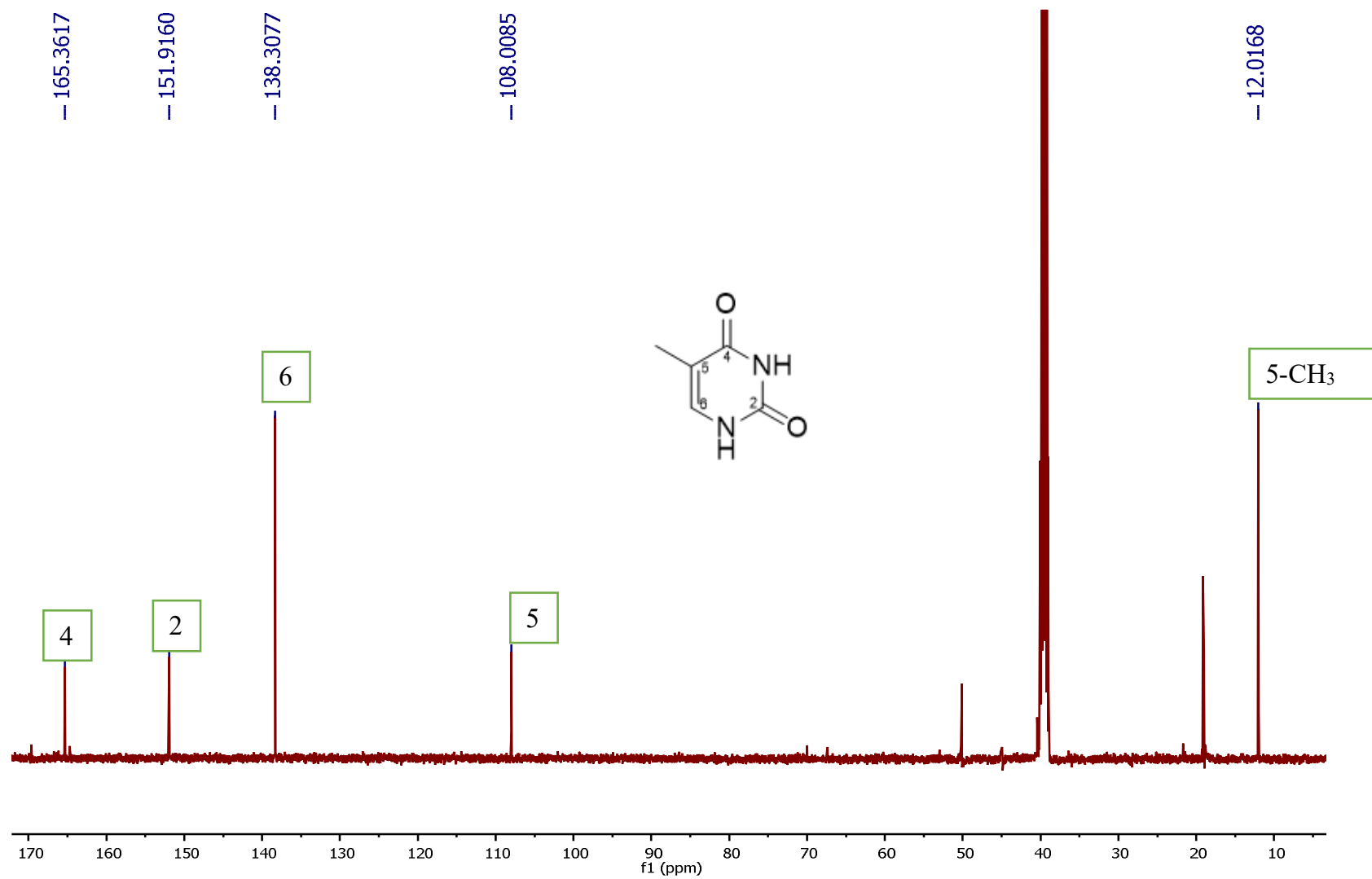
**Table S2.** The comparison of the NMR data of compound **2** to those of the reported compound [32]

No	VK05 (DMSO- <i>d</i> <sub>6</sub> )			Hexahydropyrrolo [1,2- <i>a</i> ]pyrazine-1,4-dione (D <sub>2</sub> O) [32]
	$\delta_{\text{H}}$ (ppm), <i>J</i> (Hz) (500 MHz)	$\delta_{\text{C}}$ (ppm) (125 MHz)	HMBC ( <i>H</i> → <i>C</i> )	$\delta_{\text{H}}$ (ppm), <i>J</i> (Hz) (400 MHz)
1	-	169.7		
2	3.52 (1H, <i>dd</i> , 16.5, 4.6)	46.1	C1, C4	3.77 (1H, <i>d</i> , 17.3)
	3.98 (1H, <i>dd</i> , 16.6, 1.8)			4.04 (1H, <i>d</i> , 2.7)
3	8.04 (1H, <i>s</i> )	-	C2, C5	
4	-	164.3		
5	4.11 (1H, <i>t</i> , 7.41)	58.3	C1, C4, C6, C8	4.22 (1H, <i>s</i> )
6	1.82 (1H, <i>m</i> )	28.1	C5, C7, C8	1.96 (1H, <i>s</i> )
	2.13 (1H, <i>m</i> )			2.23 (1H, <i>s</i> )
7	1.82 (2H, <i>m</i> )	22.2	C5, C6, C8	1.84 (2H, <i>d</i> , 5.6)
8	3.36 (2H, <i>m</i> )	44.9	C1, C5, C6, C7	3.44 (2H, <i>dd</i> , 8.7, 4.8)

The compound (**2**) was obtained as a white amorphous powder. <sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>, 500 MHz)  $\delta_{\text{H}}$ : 8.04 (1H, *s*), 4.11 (1H, *t*, 7.41), 3.98 (1H, *dd*, 16.6, 1.8), 3.52 (1H, *dd*, 16.5, 4.6), 3.36 (2H, *m*), 2.13 (1H, *m*), 1.82 (1H, *m*), 1.82 (2H, *m*). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>, 125 MHz)  $\delta_{\text{C}}$ : 169.7, 164.3, 58.3, 46.1, 44.9, 28.1, 22.2. HR-ESI-MS spectrum: [M+H]<sup>+</sup> at *m/z* 155.0815. The NMR and mass spectra data are presented in the supplementary section (Figure S4 – Figure S8).

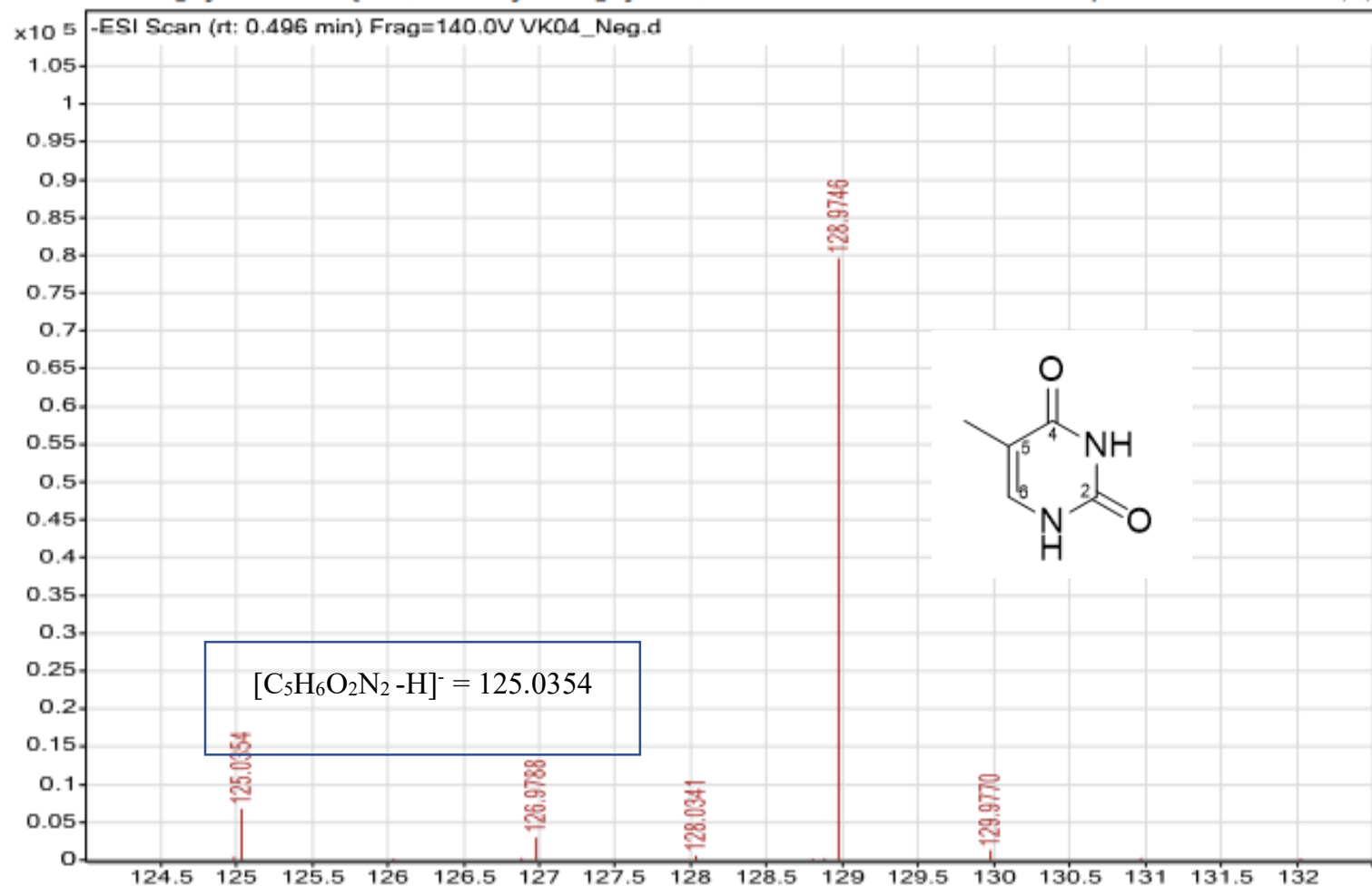


**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** (thiamine), measured in  $\text{DMSO-d}_6$  at 500 MHz.

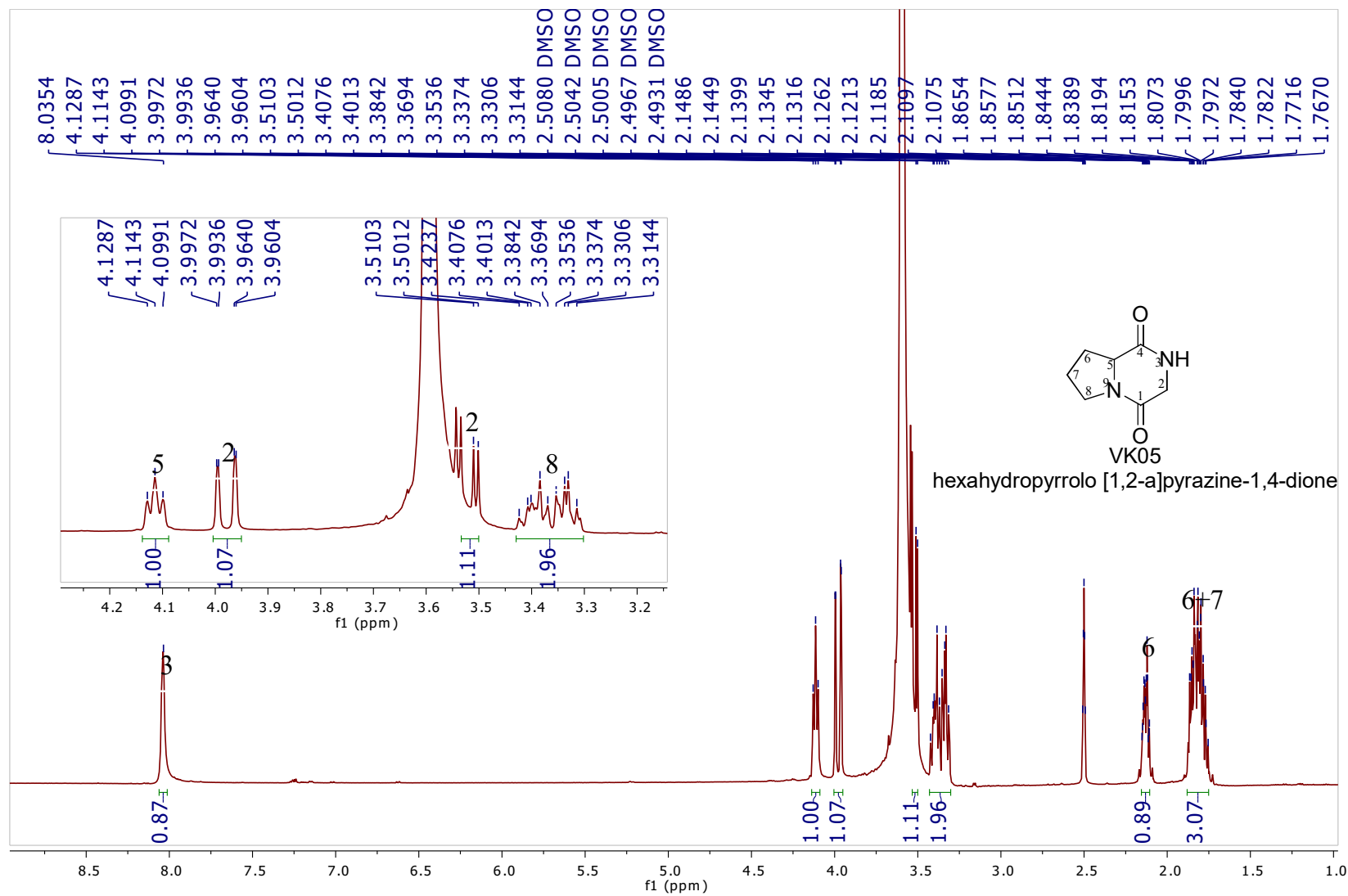


**Figure S2.**  $^{13}\text{C}$  NMR spectrum of compound 1 (thiamine), measured in DMSO- $d_6$  at 125 MHz.

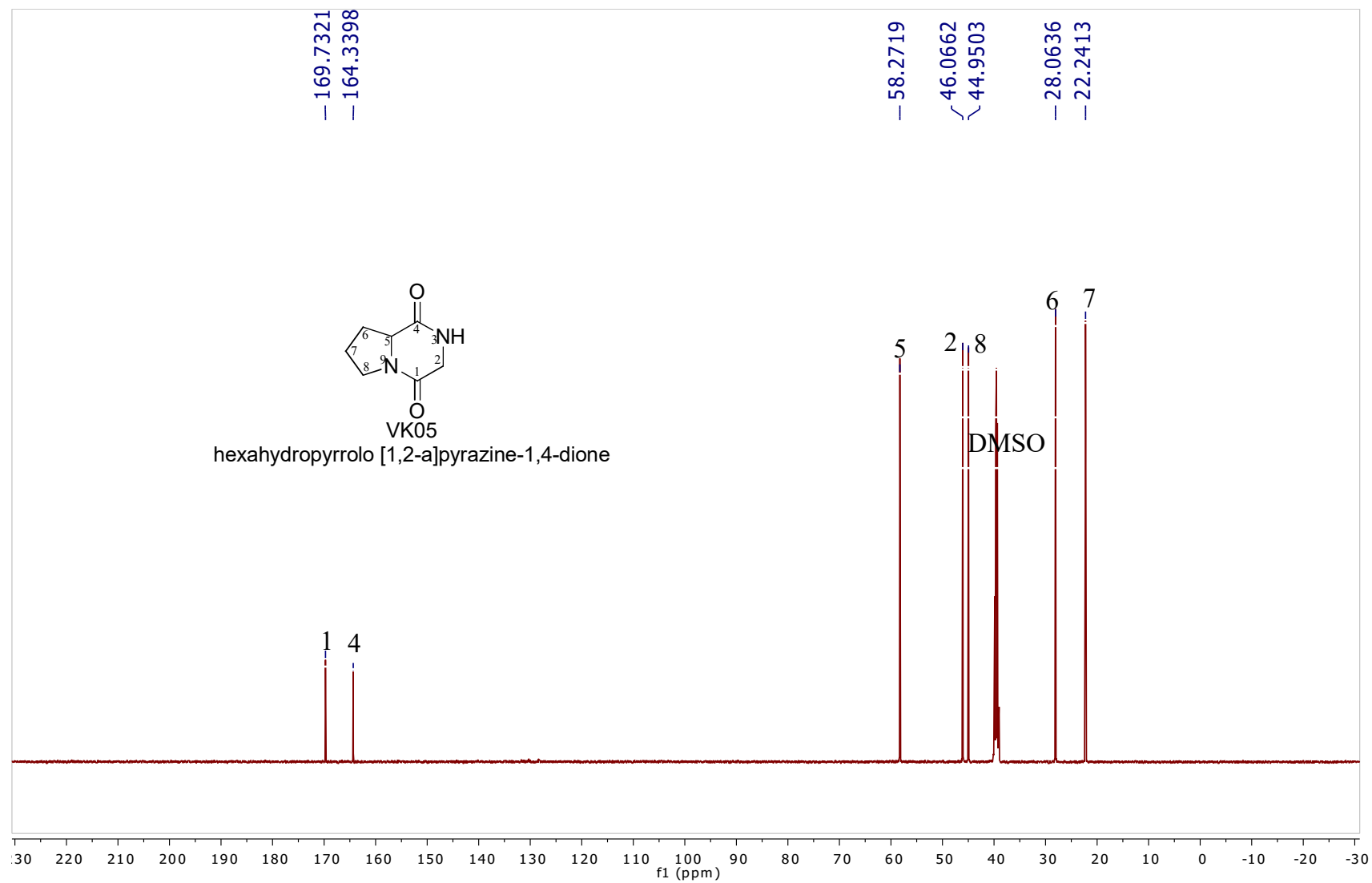
Sample Name	VK04	Position	P2-A7	Instrument Name	Instrument 1	User Name	
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	VK04_Neg.d	ACQ Method	Cot ngan - MSMS_Neg.	Comment		Acquired Time	07/08/2020 5:17:10 PM



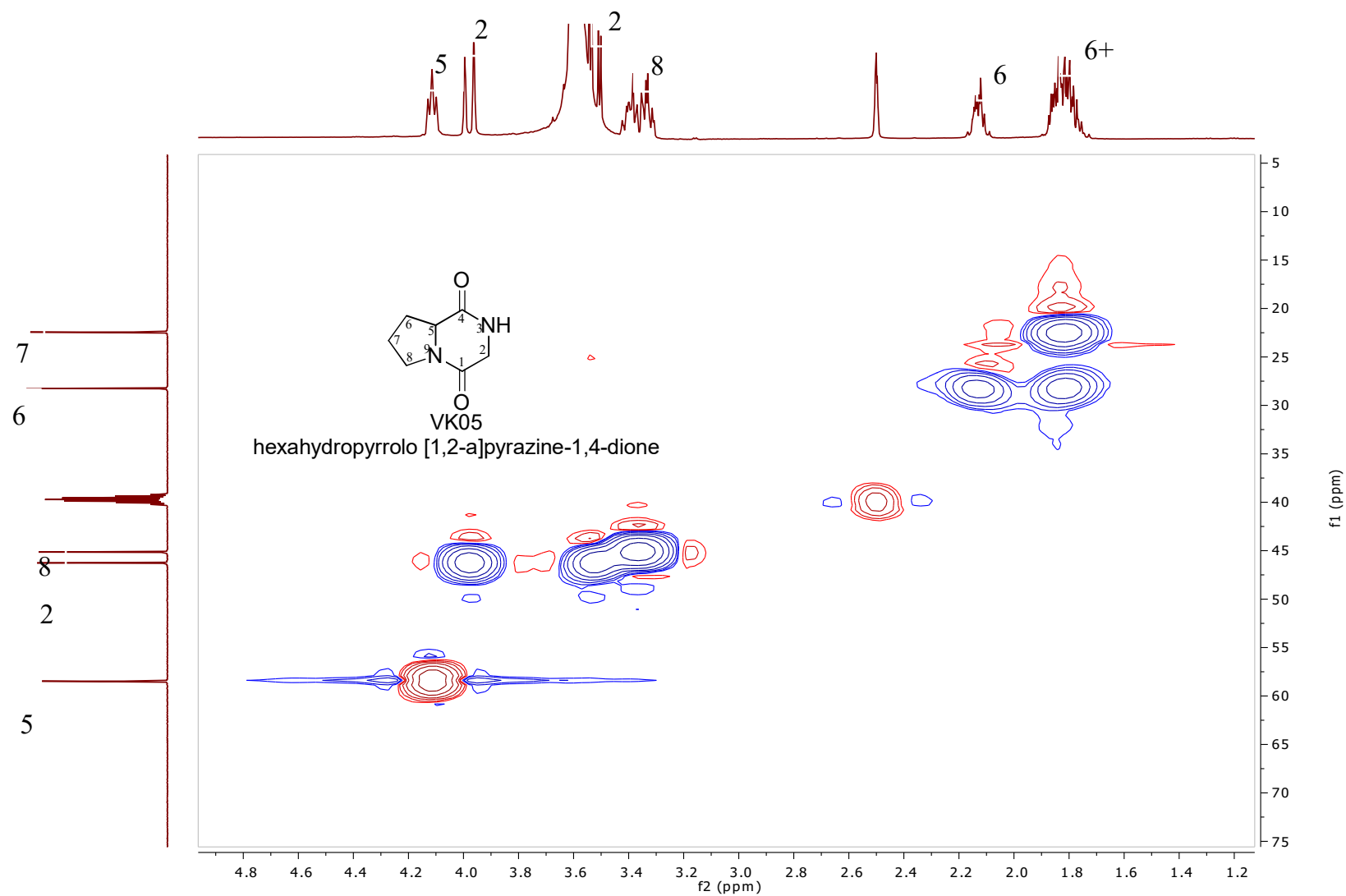
**Figure S3.** HR-ESI-MS spectrum of compound 1 (thiamine):  $[M-H]^-$  at  $m/z$  125.0354



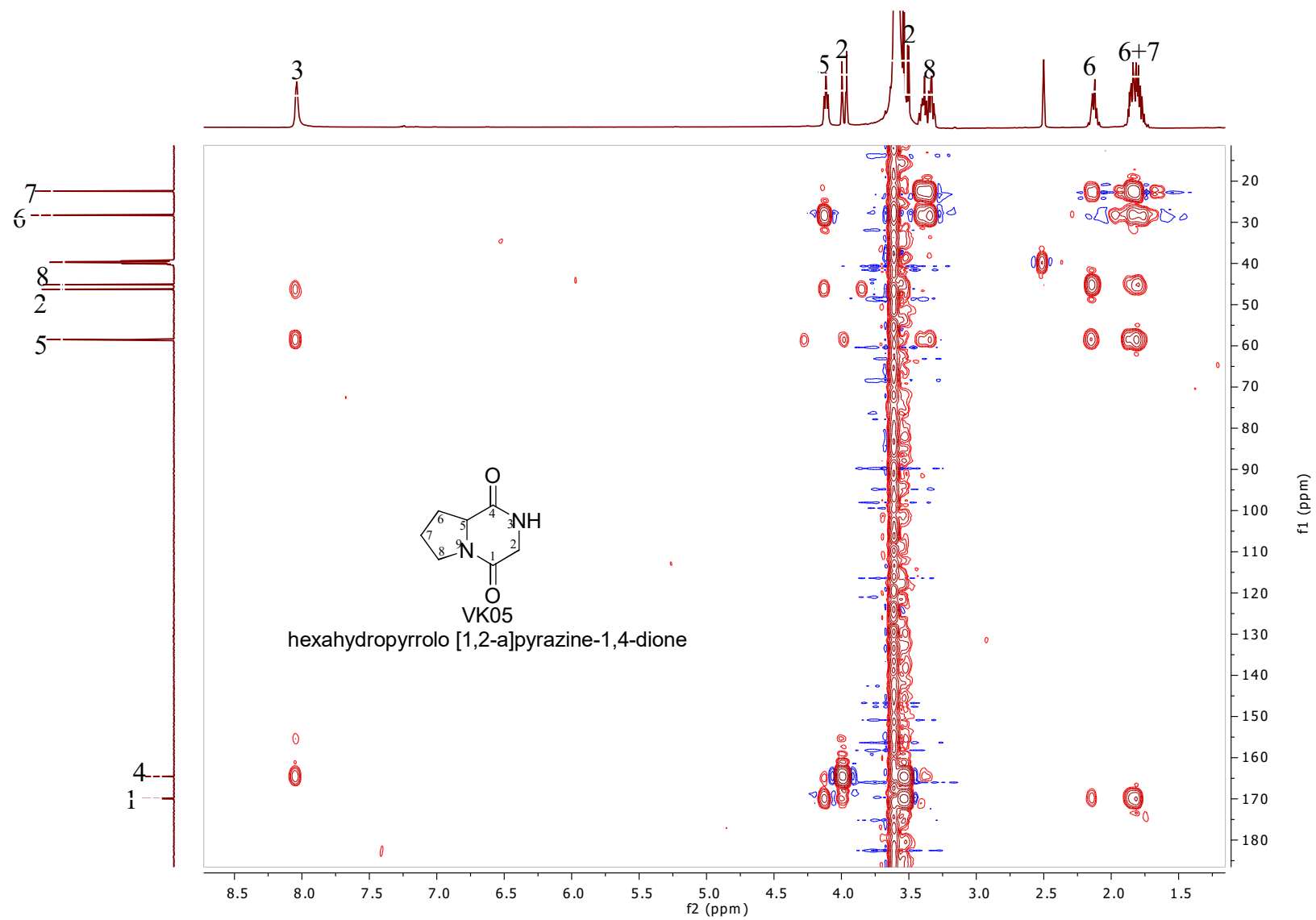
**Figure S4.**  $^1\text{H}$  NMR spectrum of compound **2** (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione), measured in DMSO- $d_6$  at 500 MHz.



**Figure S5.** <sup>13</sup>C NMR spectrum of compound 2 (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione), measured in DMSO-d<sub>6</sub> at 125 MHz.



**Figure S6.** HSQC spectrum of compound 2 (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione)



**Figure S7.** HSQC spectrum of compound 2 (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione)



Sample Name	VK 05	Position	P1-D2	Instrument Name	Instrument 1	User Name	
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	Success
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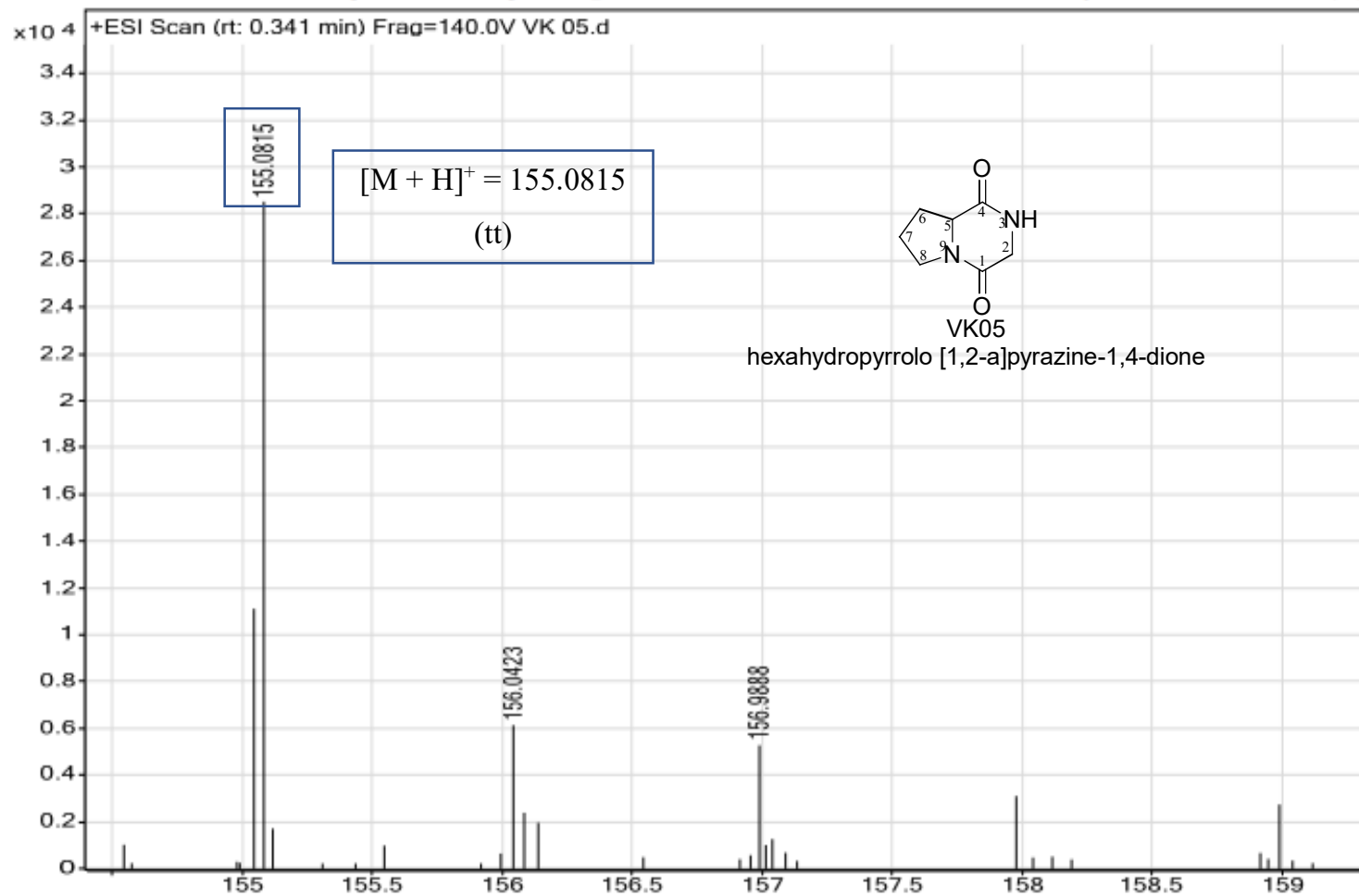


Figure S8. HR-ESI-MS spectrum of compound 2 (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione)