Supplementary section

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

No	Compound 1 (DMSO-d_6)		Thymine (DMSO-d_6) [31]	
	δ_H (ppm), J (Hz)	δ_C (ppm)	δ_H (ppm), J (Hz)	δ_C (ppm)
2		151.9		153.9
4		165.4		168.3
5		108.0		110.9
6	7.21 (1H, *s*)	138.3	7.28	139.8
5-CH_3	1.69 (3H, *s*)	12.0	1.75	12.1

The compound (**1**) was obtained as a white amorphous powder. *^{1}H-NMR (DMSO-d6, 500 MHz) δH: 7.21 (1H, s), 1.69 (3H, s). ^{13}C-NMR (DMSO-d6, 125 MHz) δC:* 165.4, 151.9, 138.3, 108.0, 12.0. HR-ESI-MS spectrum: $[M-H]^-$ 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-d_6)			Hexahydropyrrolo [1,2-a]pyrazine-1,4-dione (D_2O) [32]
	δ_H (ppm), J (Hz) (500 MHz)	δ_C (ppm) (125 MHz)	HMBC ($H \rightarrow C$)	δ_H (ppm), J (Hz) (400 MHz)
1	-	169.7		
2	3.52 (1H, *dd*, 16.5, 4.6)	46.1		3.77 (1H, *d*, 17.3)
	3.98 (1H, *dd*, 16.6, 1.8)		C1, C4	4.04 (1H, *d*, 2.7)
3	8.04 (1H, *s*)	-	C2, C5	
4	-	164.3		
5	4.11 (1H, *t*, 7.41)	58.3	C1, C4, C6, C8	4.22 (1H, *s*)
6	1.82 (1H, *m*)	28.1		1.96 (1H, *s*)
	2.13 (1H, *m*)		C5, C7, C8	2.23 (1H, *s*)
7	1.82 (2H, *m*)	22.2	C5, C6, C8	1.84 (2H, *d*, 5.6)
8	3.36 (2H, *m*)	44.9	C1, C5, C6, C7	3.44 (2H, *dd*, 8.7, 4.8)

The compound (**2**) was obtained as a white amorphous powder. *^{1}H-NMR (DMSO-d6, 500 MHz) δH:* 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*). *^{13}C-NMR (DMSO-d6, 125 MHz) δC:* 169.7, 164.3, 58.3, 46.1, 44.9, 28.1, 22.2. HR-ESI-MS spectrum: $[M+H]^+$ at *m/z* 155.0815. The NMR and mass spectra data are presented in the supplementary section (Figure S4 – Figure S8).

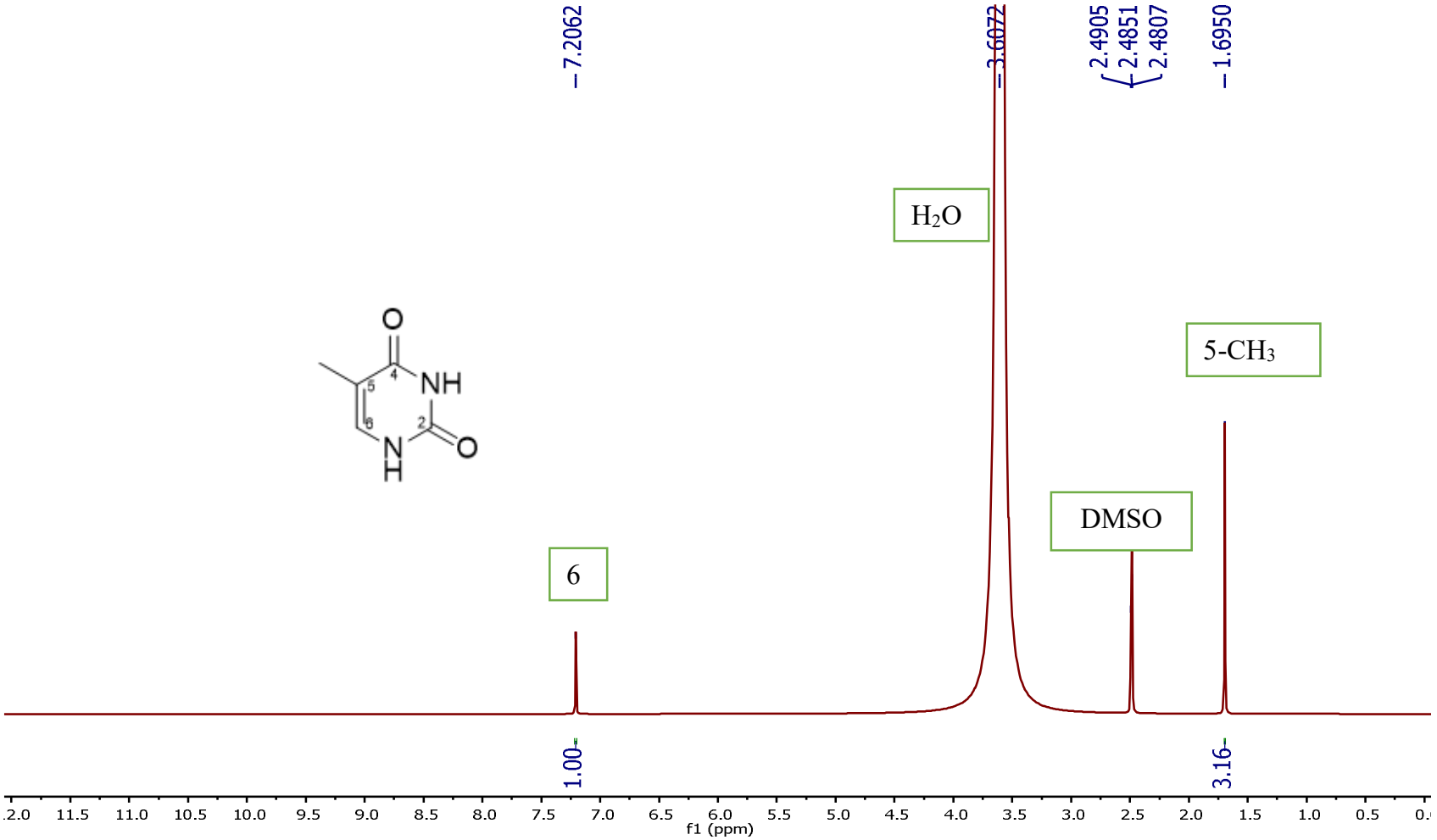

Figure S1. ^{1}H NMR spectrum of compound **1** (thyamine), measured in DMSO-d6 at 500 MHz.

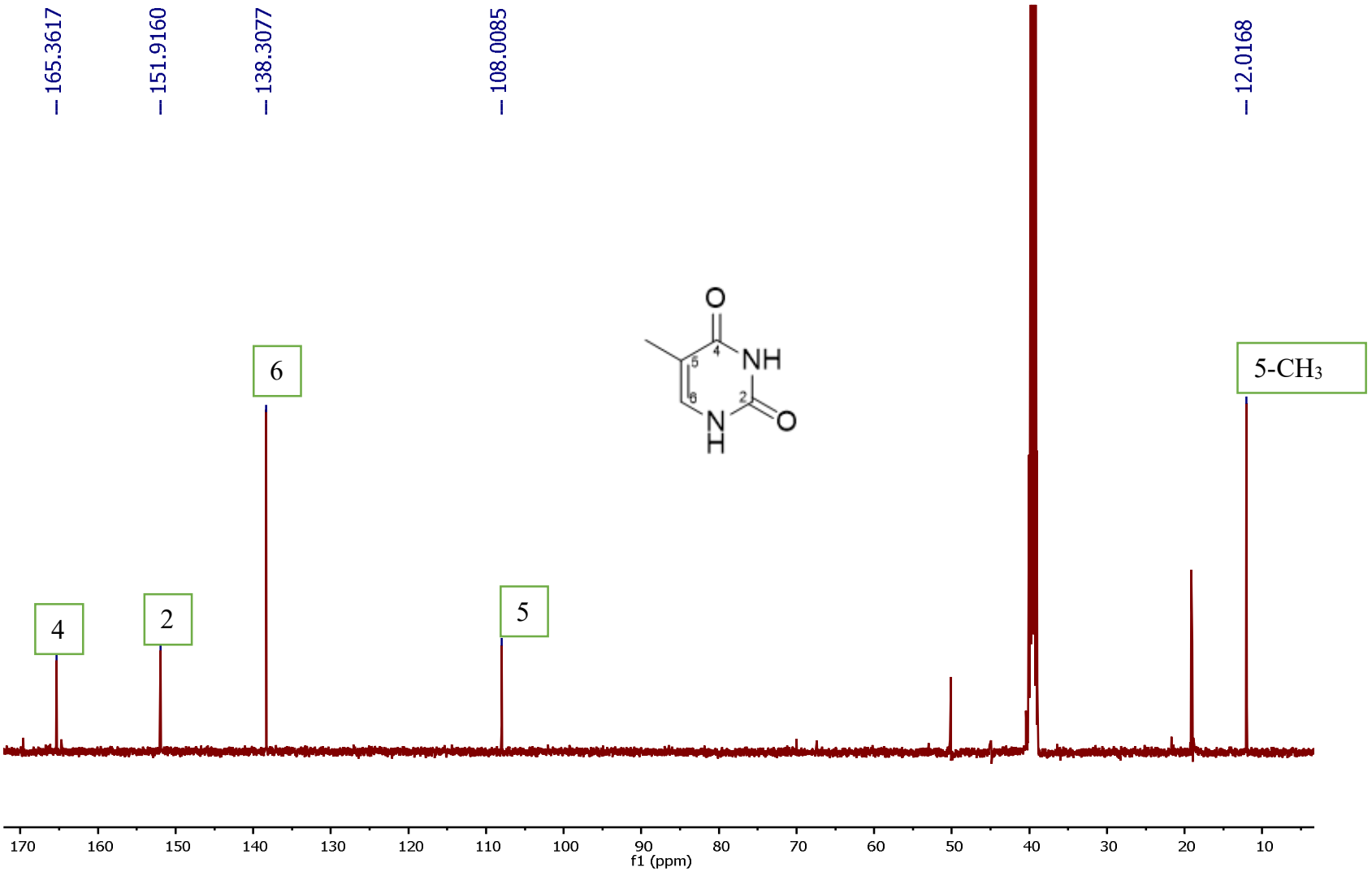

Figure S2. ^{13}C NMR spectrum of compound **1** (thyamine), measured in DMSO-d6 at 125 MHz.

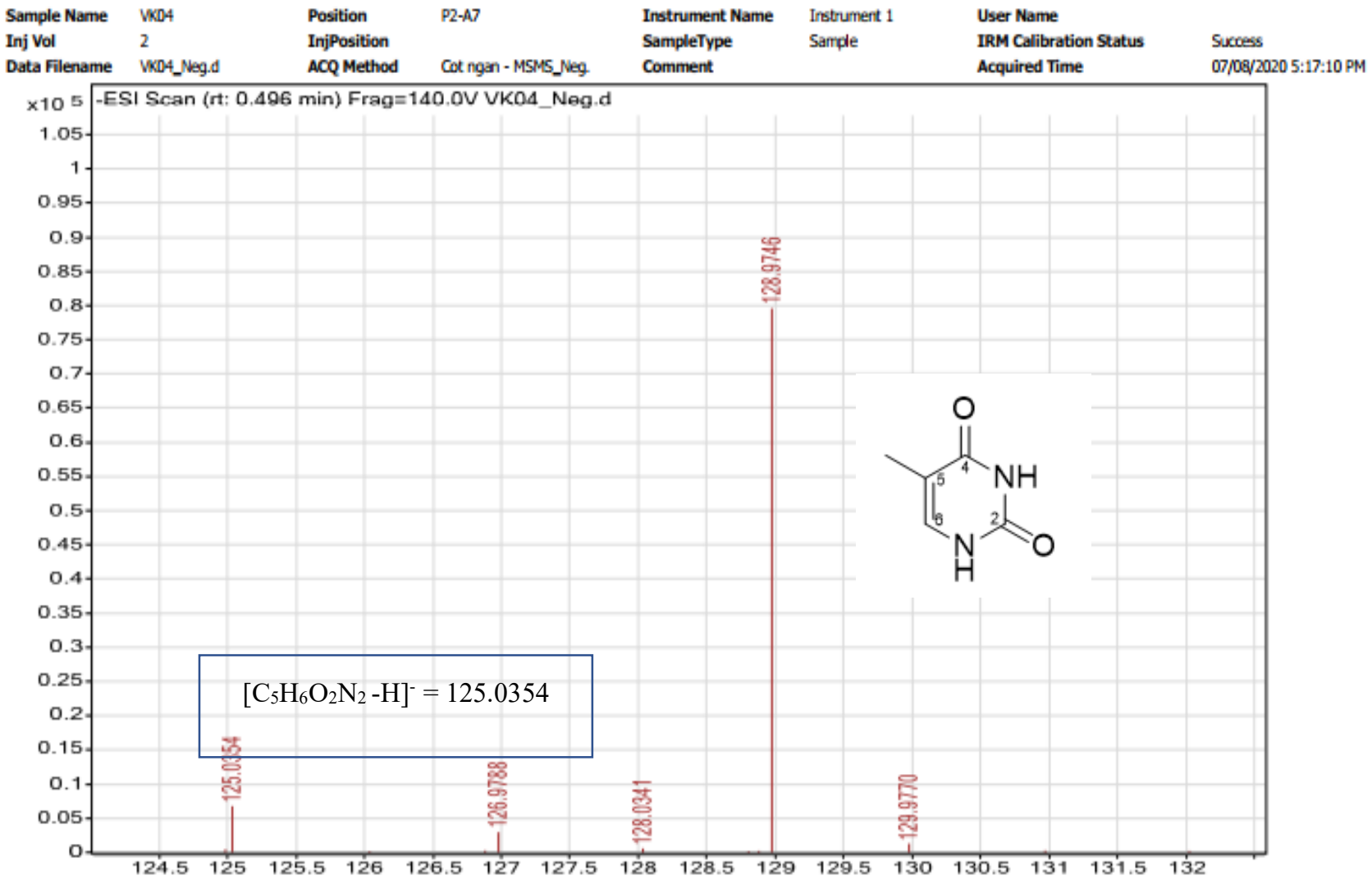

Figure S3. HR-ESI-MS spectrum of compound **1** (thyamine): $[M-H]^-$ at *m/z* 125.0354

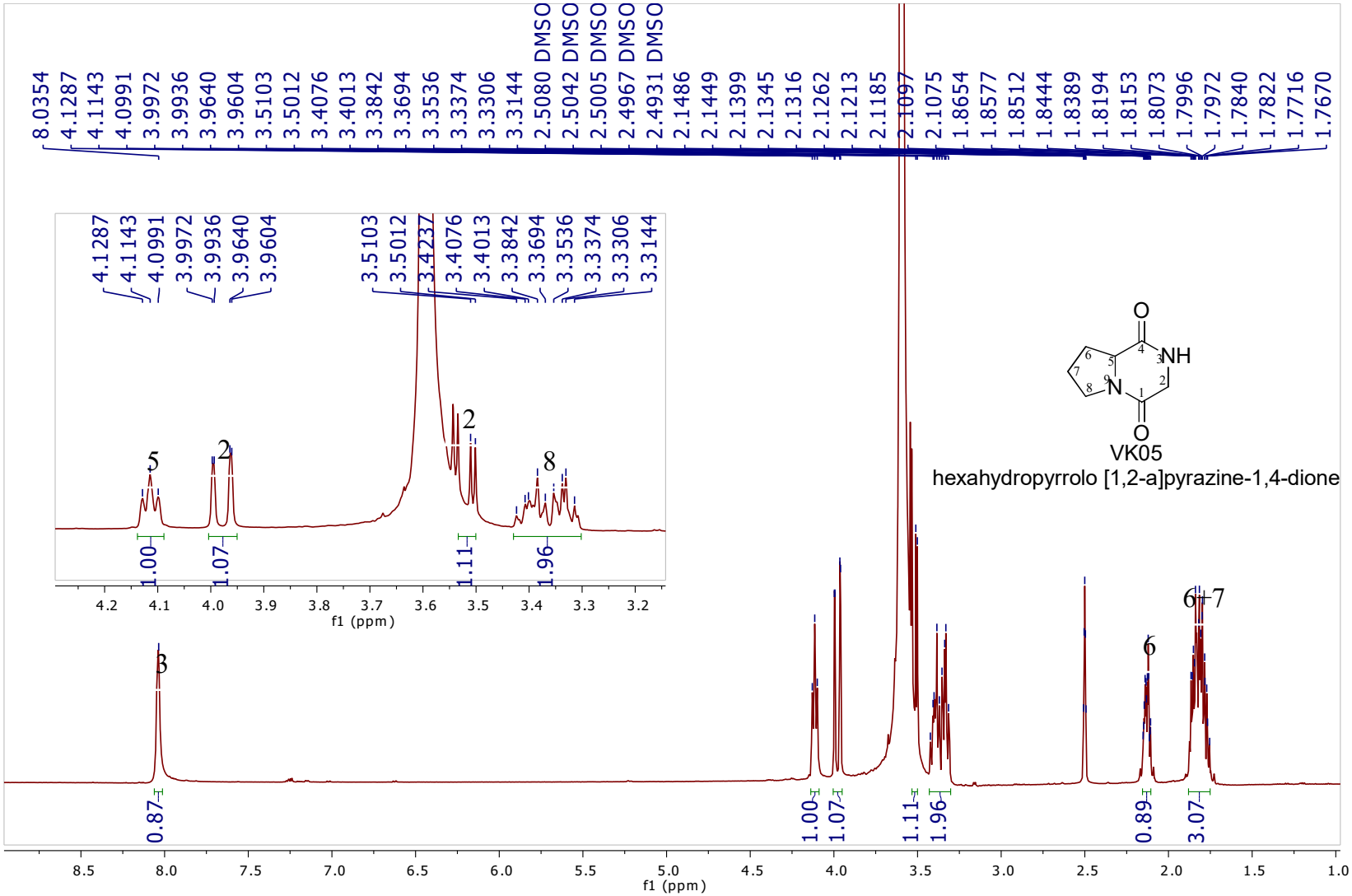

Figure S4. [1]H NMR spectrum of compound **2** (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione), measured in DMSO-d6 at 500 MHz.

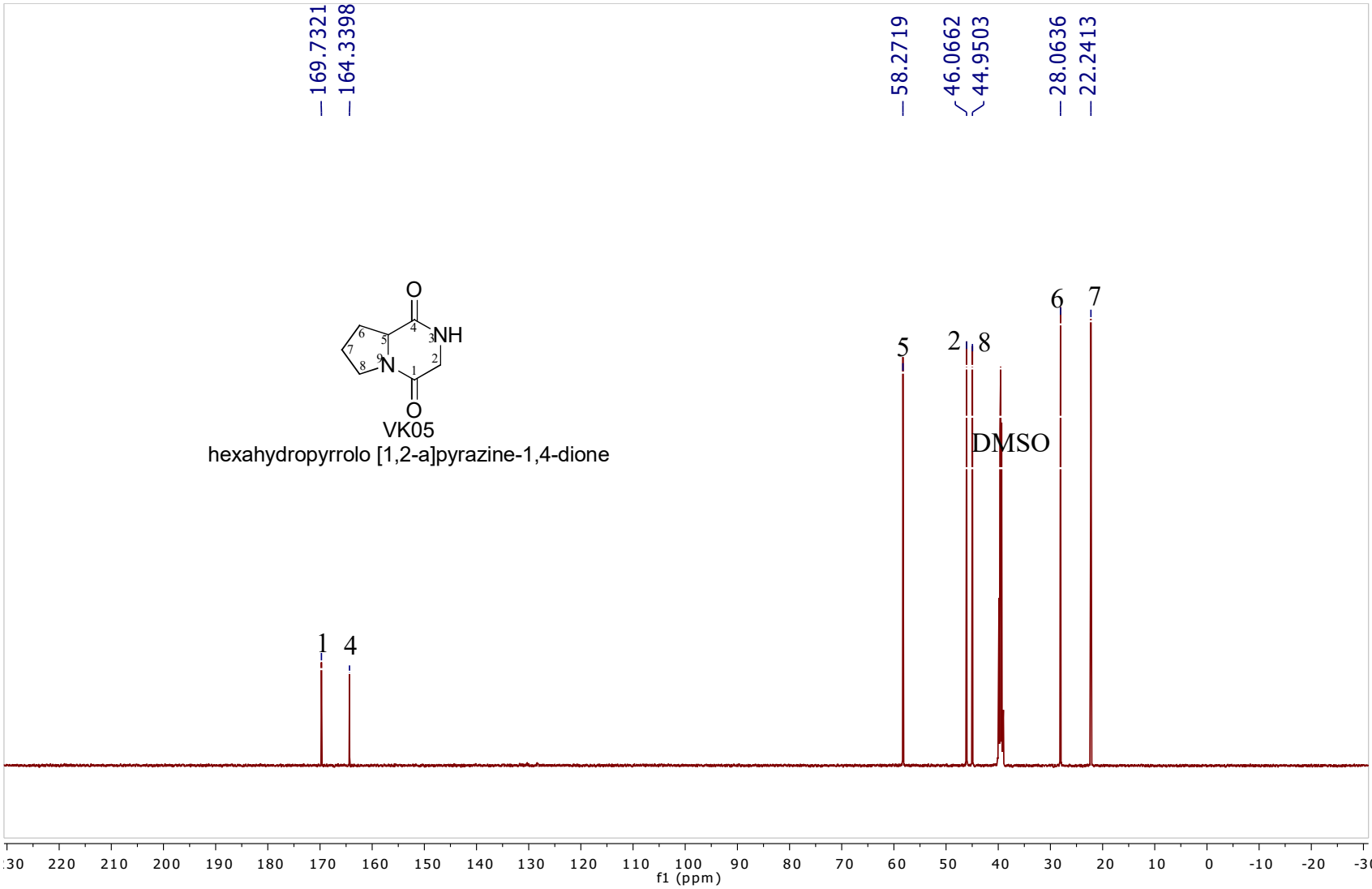

Figure S5. ^{13}C NMR spectrum of compound **2** (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione), measured in DMSO-d6 at 125 MHz.

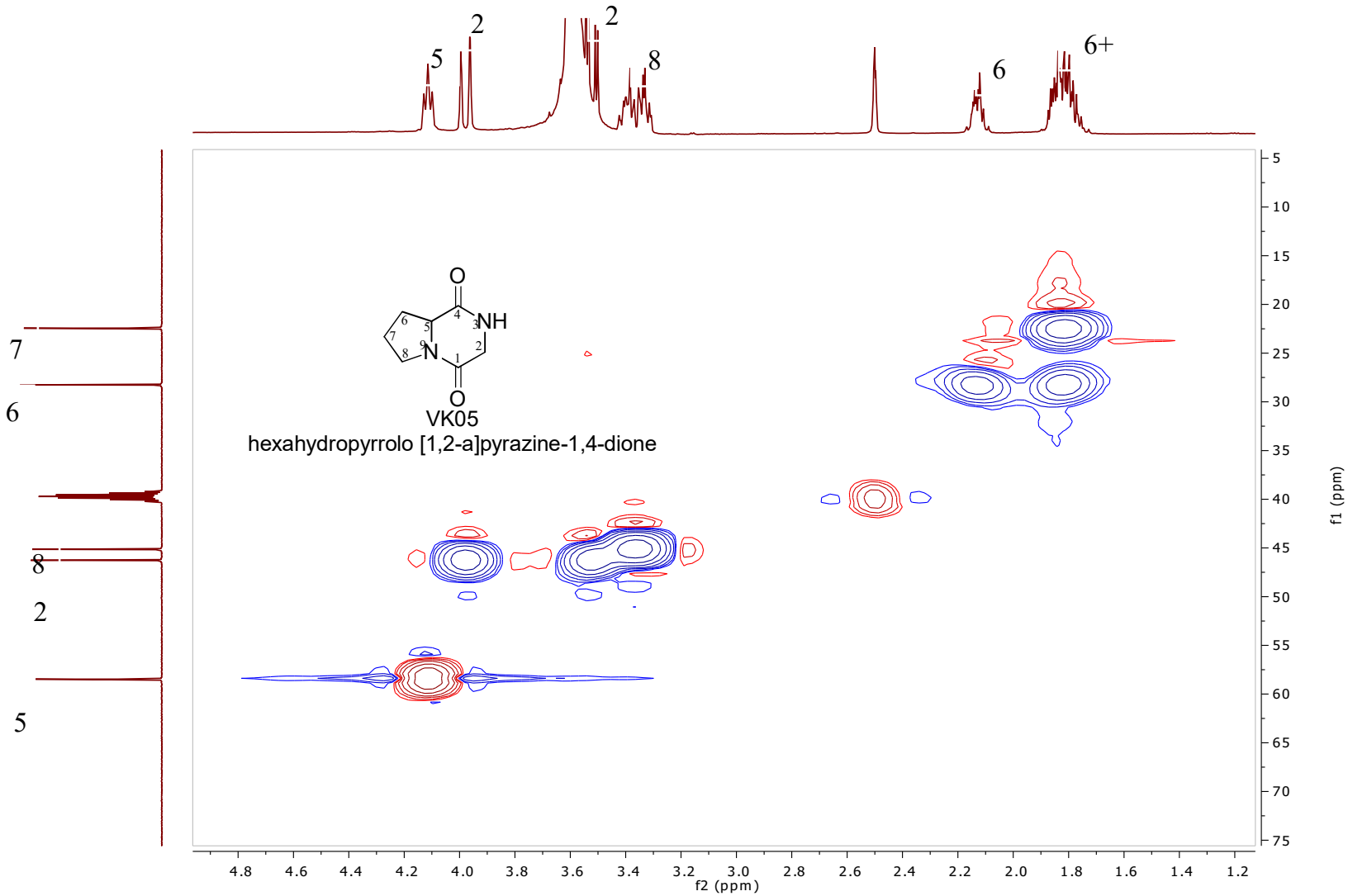

Figure S6. HSQC spectrum of compound **2** (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione)

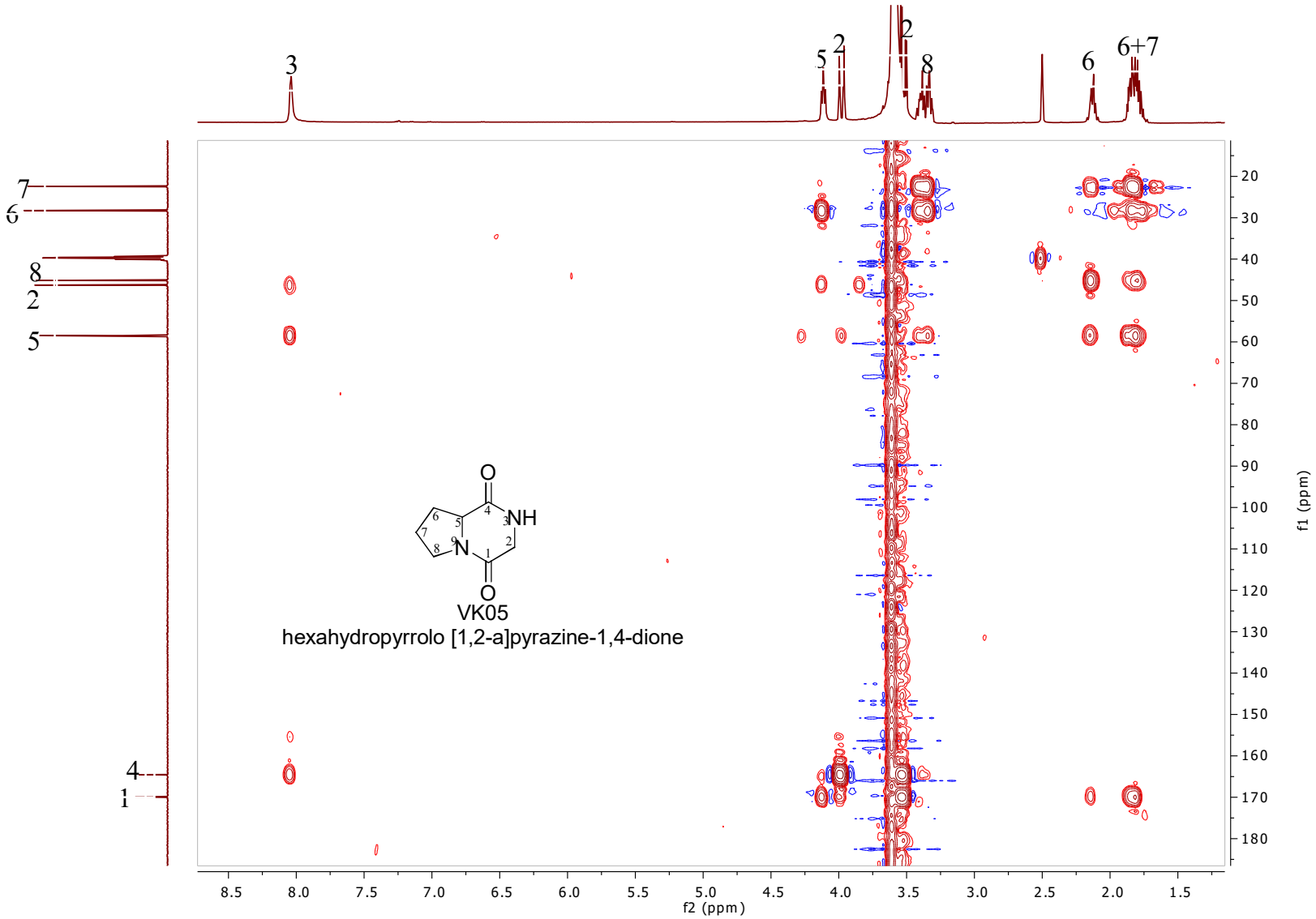

Figure S7. HSQC spectrum of compound **2** (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione)

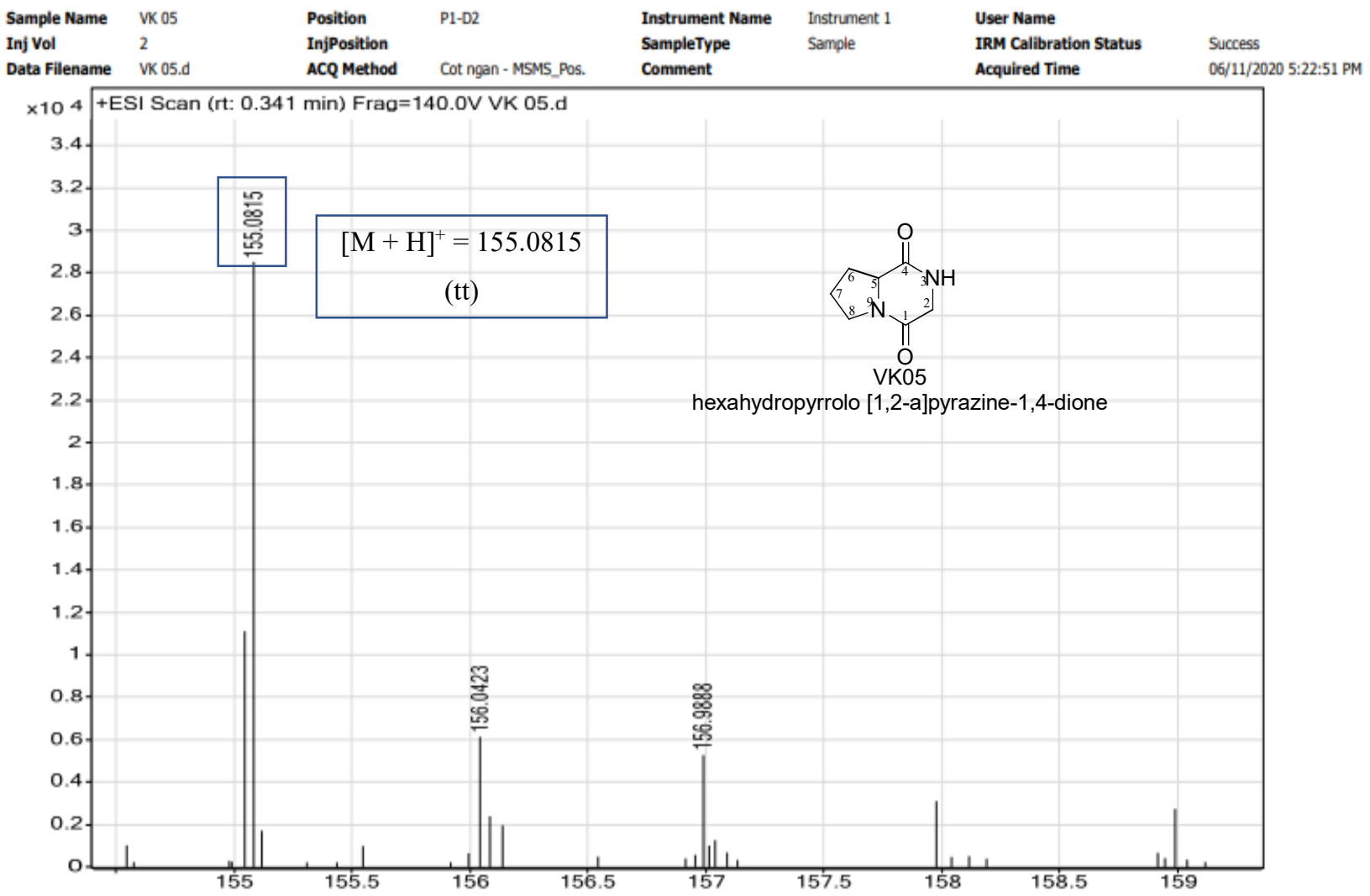

Figure S8. HR-ESI-MS spectrum of compound **2** (hexahydropyrrolo [1,2-a] pyrazine-1,4-dione)