Forensic Toxicology

Spectroscopic characterization and crystal structure of two cathinone derivatives: 1-(4-chlorophenyl)-2-(1-pyrrolidynyl)pentan-1-one (4-chloro-α-PVP) hydrogen sulfate and 1-(4-methylphenyl)-2-(dimethylamino)propan-1-one (4-MDMC) hydrochloride, seized on illicit drug market.

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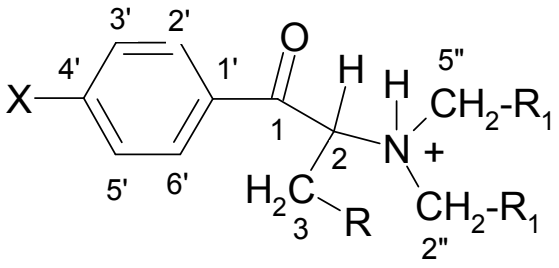
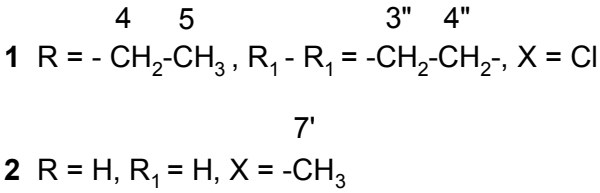
Table S1. NMR data of compounds **1** and **2** in DMSO-d_6 recorded at 400 MHz (^{1}H) and 100.5 MHz (^{13}C), respectively

(structures of compounds **1** and **2** with the numbering of carbon atoms)





Position	Compound **1**		Compound **2**	
	^{1}H NMR	^{13}C NMR	^{1}H NMR	^{13}C NMR
	δ(ppm), J (Hz)	δ(ppm)	δ(ppm), J (Hz)	δ(ppm)
1		196.3		195.2
2	5.30 (q, *J*=7.3, 1H)	68.2	5.49 (bs, 1H)	62.2
3	1.96 (m, 2H)	32.2	1.75 (d, *J*=1.75, 3H)	21.8
4	1.96 (m, 2H)	17.5		
5	0.78 (t, 3H)	14.1		
1’		140.6		131.3
2’/6’	8.12 (d, *J*=8.6, 2H)	129.9	7.87 (d, *J*=8.3, 2H)	128.8
3’/5’	7.71 (d, *J*=8.6, 2H)	131.3	7.31 (d, *J*=8.3, 2H)	130.0
4’		133.3		146.4
7’			2.42 (s, 1H)	15.8
2”	3.61, 3.49 (2bs, 2H)	54.6	3.08, 2.98 (2bs, 6H)	37.9, 42.2
3”	2.04 (m, 2H)	23.2		
4”	1.19, 1.01 (2m, 2H)	23.2		
5”	3.28, 3.05 (2bs, 2H)	52.4		
N-H	10.1 (bs, 1H)		12.5 (bs, 1H)	

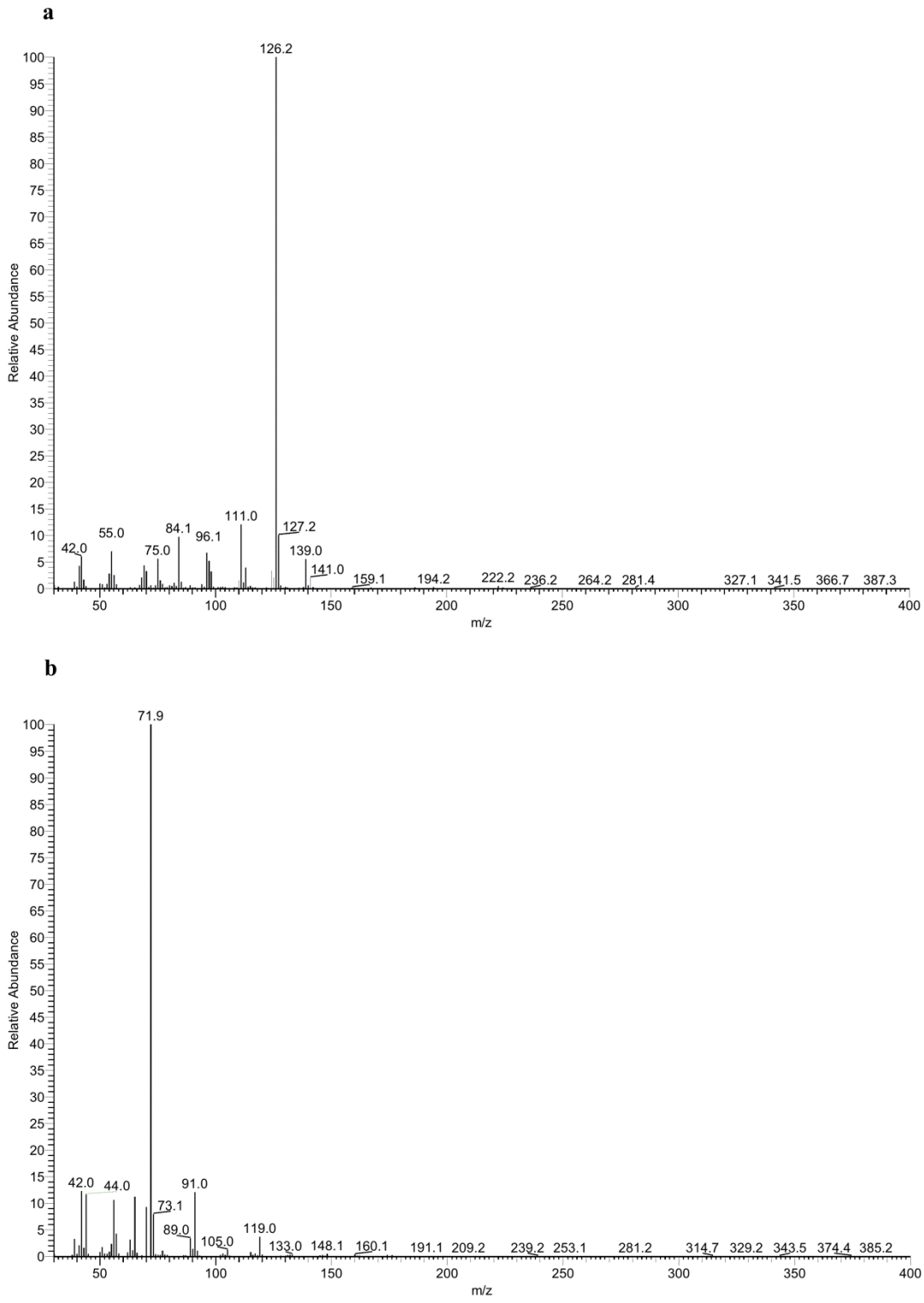


Fig.S1 Electron ionization (EI) mass spectra of: **a** compound **1** and **b** compound **2**

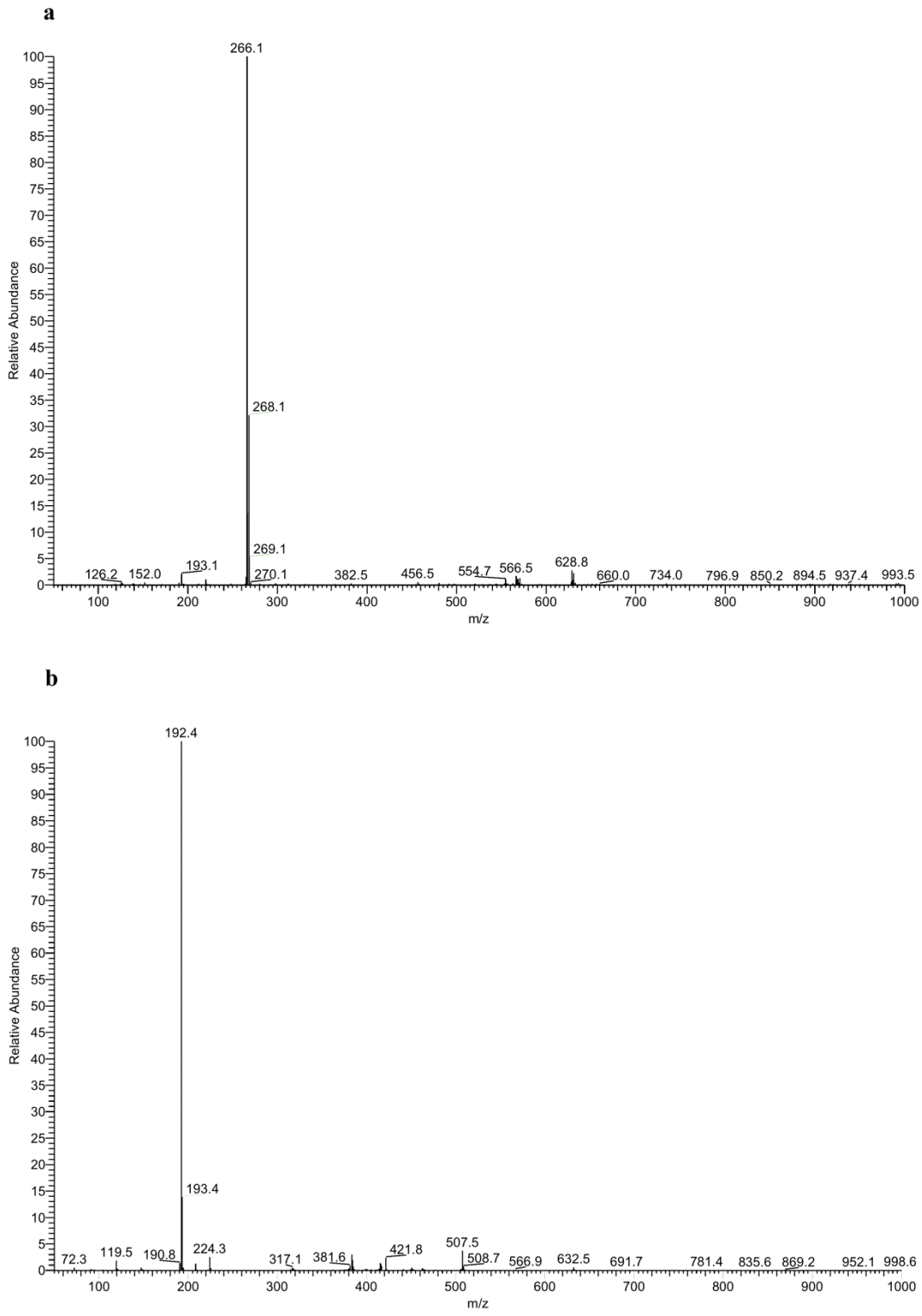


Fig.S2 Electrosprey ionization (ESI) mass spectra of **a** compound **1** and **b** compound **2**

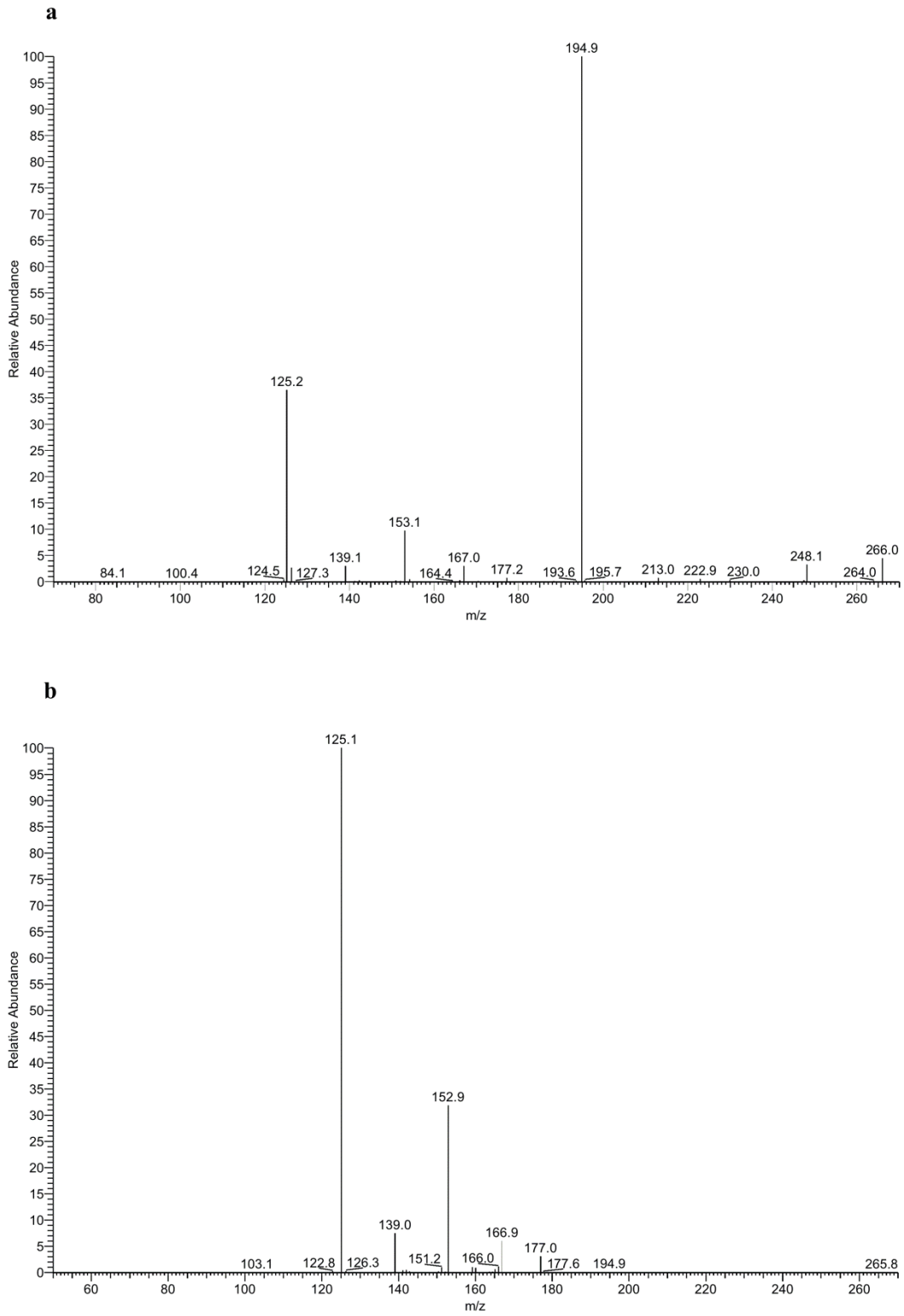


Fig. S3 The ion mass spectra obtained by the ion trap mass spectrometry in the MS^2 (**a**) and MS^3 (**b**) mode for compound **1**. The precursor ions were used for the MS^2 and MS^3 modes: at *m/z* 266 and 195, respectively

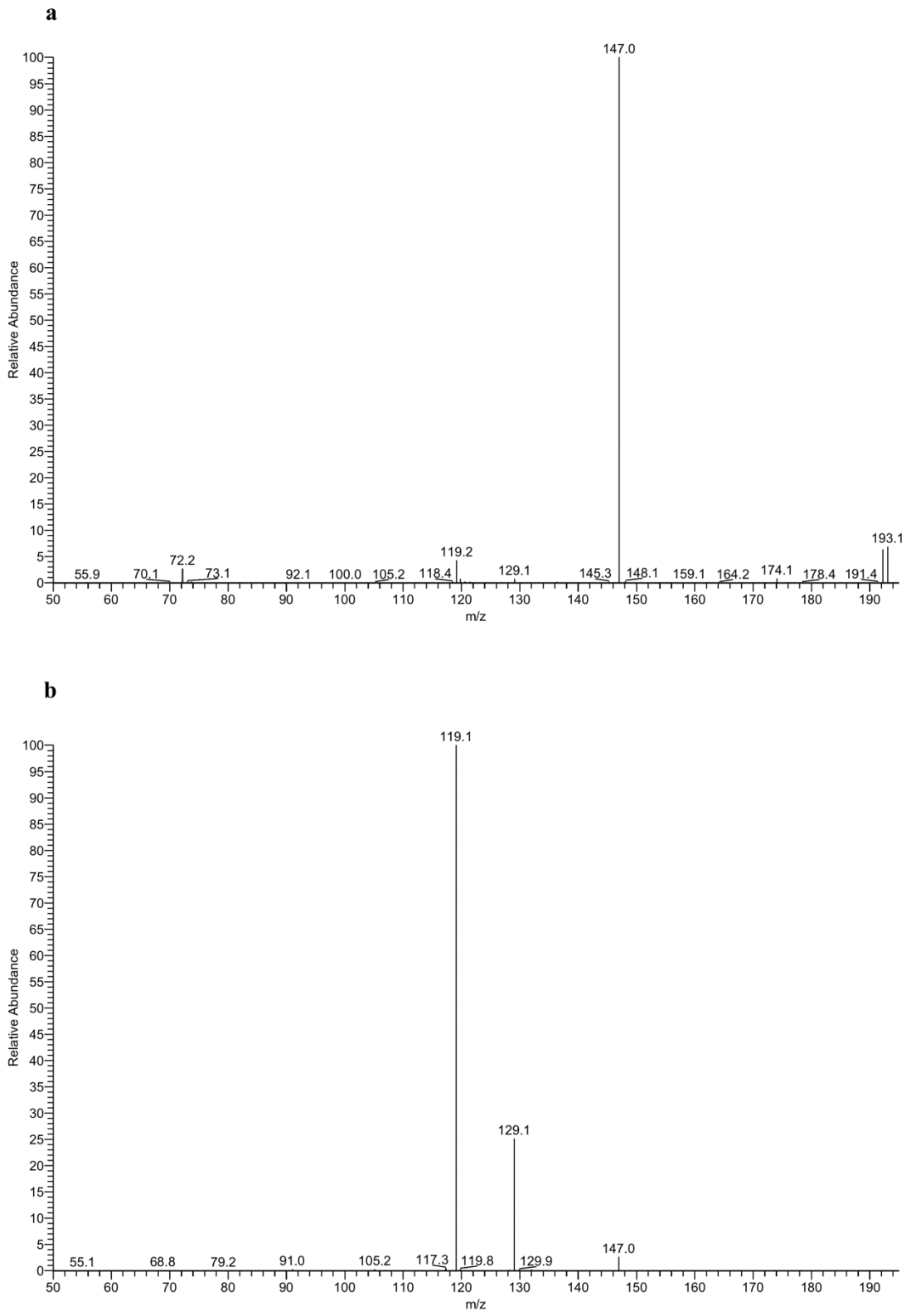


Fig. S4 The ion mass spectra obtained by the ion trap mass spectrometry in the MS^2 (**a**) and MS^3 (**b**) mode for compound **2**. The precursor ions were used for the MS^2 and MS^3 modes: at *m/z* 192 and 147, respectively

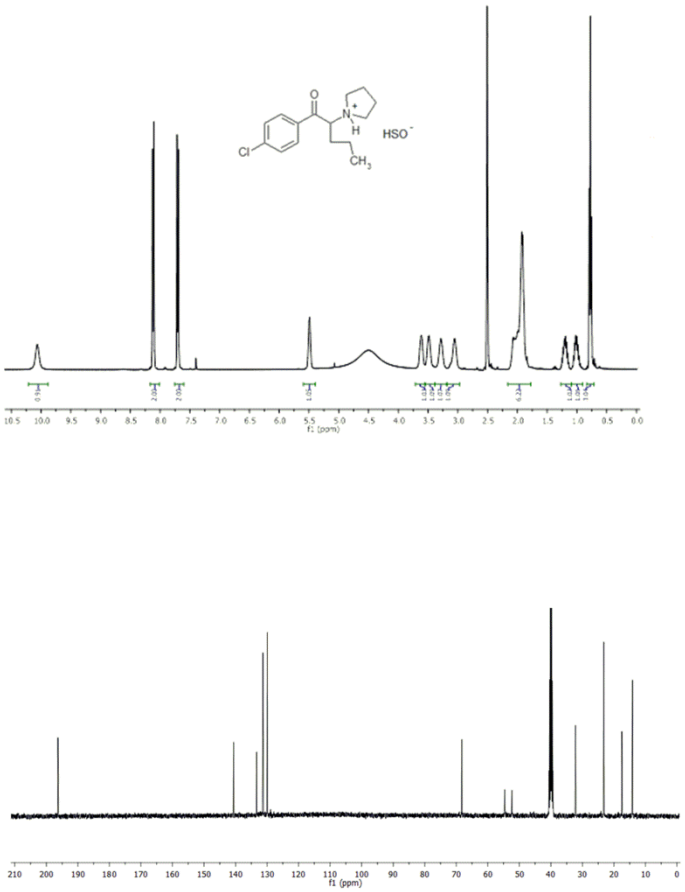


Fig. S5 ^{1}H NMR (*upper*) and ^{13}C NMR (*lower*) spectra of compound **1** in DMSO-d_6

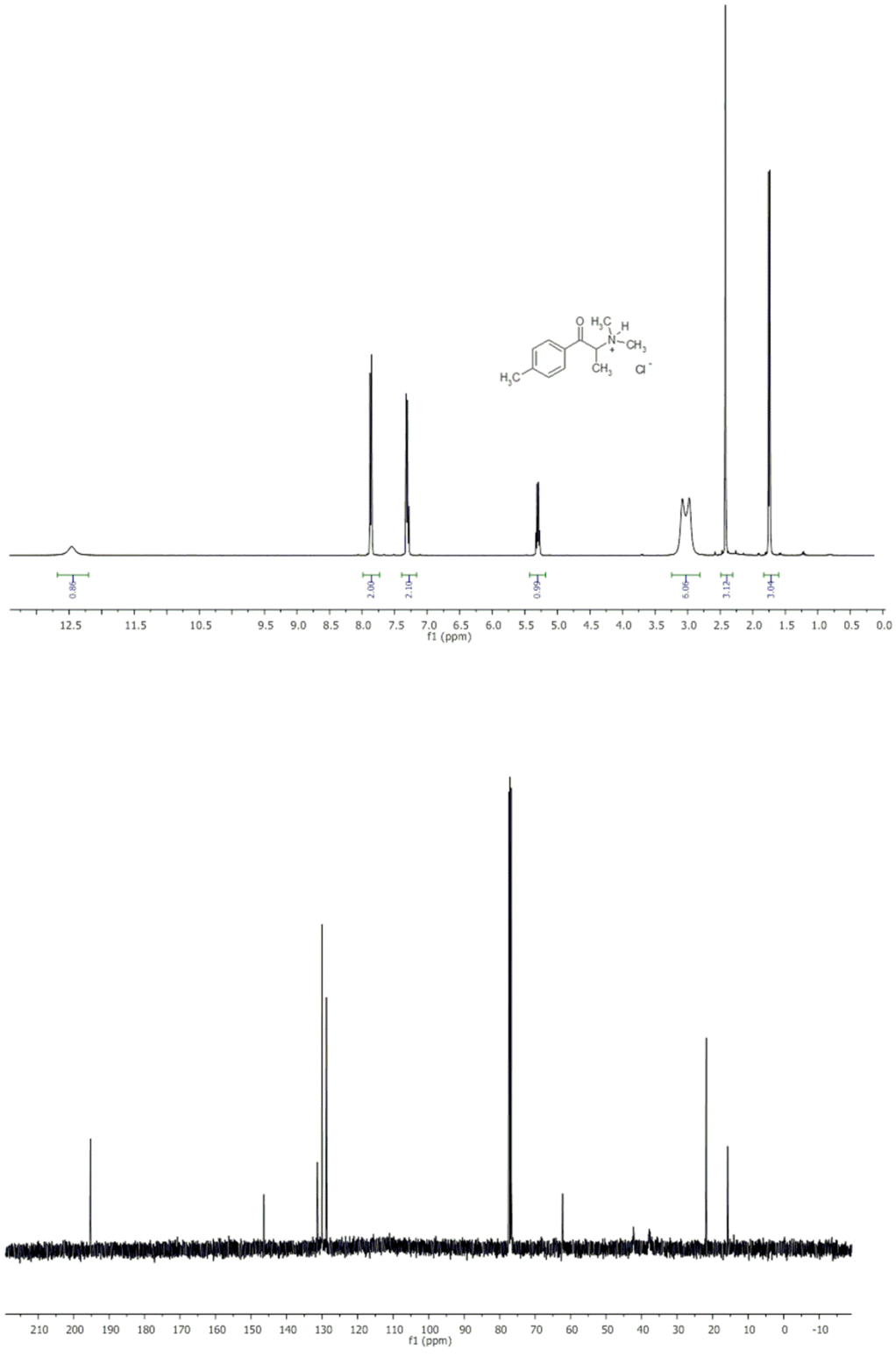


Fig.S6 ^{1}H NMR (*upper*) and ^{13}C NMR (*lower*) spectra of compound **2** in $CDCl_3$

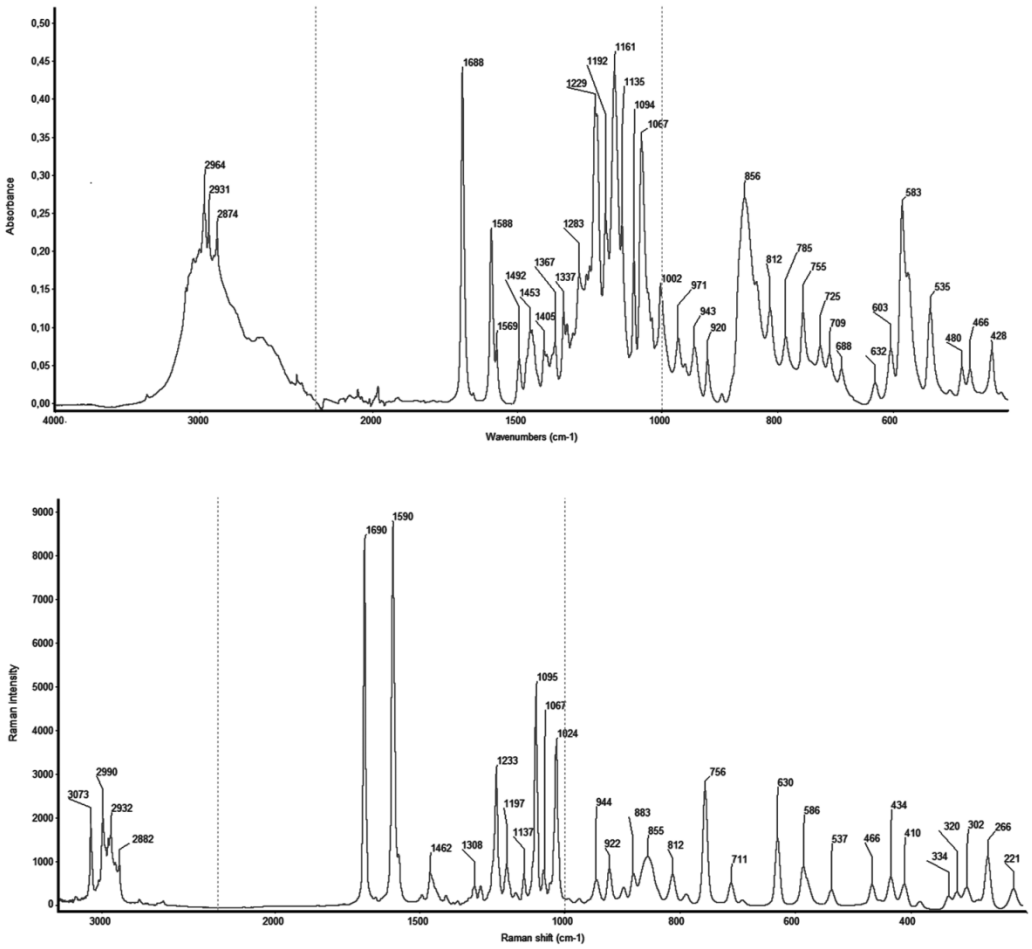


Fig. S7 Infrared (*upper*) and Raman (*lower*) spectra of compound **1** (4-chloro-α -PVP hydrogen sulfate)

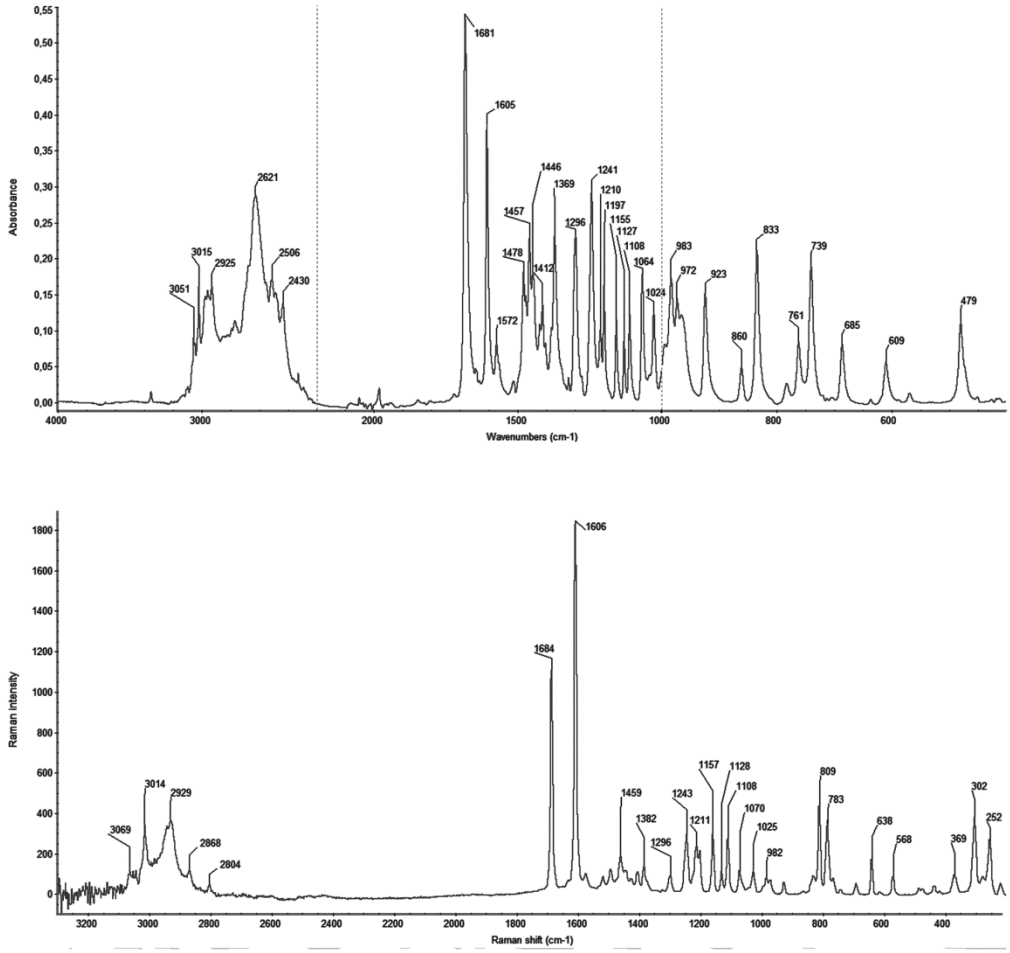


Fig. S8 Infrared (*upper*) and Raman (*lower*) spectra of compound **2** (4-MDMC hydrochloride)