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Monasnicotinic acid, a novel pyridine alkaloid of the fungus *Aspergillus cavernicola*: isolation and structure elucidation

Tatiana V. Antipova, Kirill V. Zaitsev, Alexander Ya. Zherebker, Victor A. Tafeenko, Boris P. Baskunov, Valentina P. Zhelifonova, Natalya E. Ivanushkina, Alexey S. Kononikhin, Eugene N. Nikolaev and Anatoly G. Kozlovsky

Content

Experimental

UV/vis spectra were registered in MeOH on UV-160A spectrophotometer “Shimadzu”. IR spectra were registered on Nicolet iS5 Fourier Transform IR-spectrometer in KBr. Polarimetry was performed on a Atago AP-300 automatic polarimeter. Mass spectra (EI-MS, 70 eV) were recorded on a quadropoule mass spectrometer FINNIGAN MAT INCOS 50 with direct insertion; all assignments were made with reference to the most abundant isotopes. High-resolution mass-spectra were acquired using a commercial 7 Tesla LTQ FT ultra mass spectrometer equipped with an Ion Max electrospray ion source (Thermo Electron Corp., Bremen Germany) located at the facilities of the Institute of Biochemical Physics of the Russian Academy of Sciences. The substance (200 mg/L in methanol) were injected at a flow rate of 60 μL/h. The mass-spectra were acquired in negative or positive electrospray (ESI) ion modes by accumulation of at least 30 scans. Mass-spectra were externally calibrated on standard compounds (Tunemix, Agilent). For in-ESI source H/D exchange (HDX) experiments a copper plate was installed just beneath the ESI cone and a droplet of D_2O was placed on it. As a result the atmosphere of D_2O was formed, and the injected ions were subjected to H/D exchange. HDX mass-spectra were registered at 200 or 400 ^{0}C at desolvating capillary. ^{1}H NMR (400.130 MHz) and ^{13}C NMR (100.613 MHz) spectra were recorded in $CDCl_3$ with a Agilent 400MR spectrometer at 298 K. Chemical shifts are given in ppm relative to internal Me_4Si.

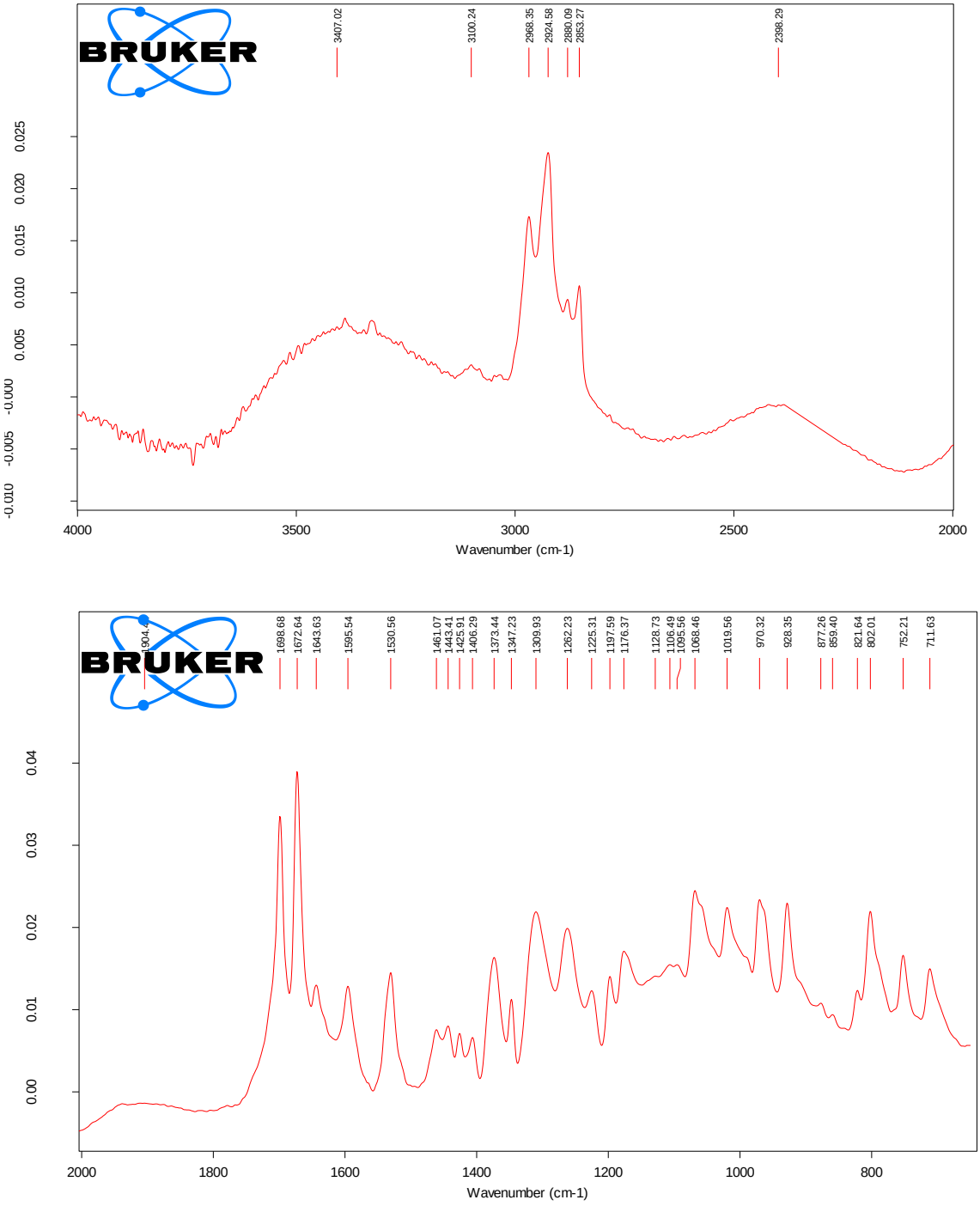

Figure S1 IR spectra of monasnicotinic acid (KBr).

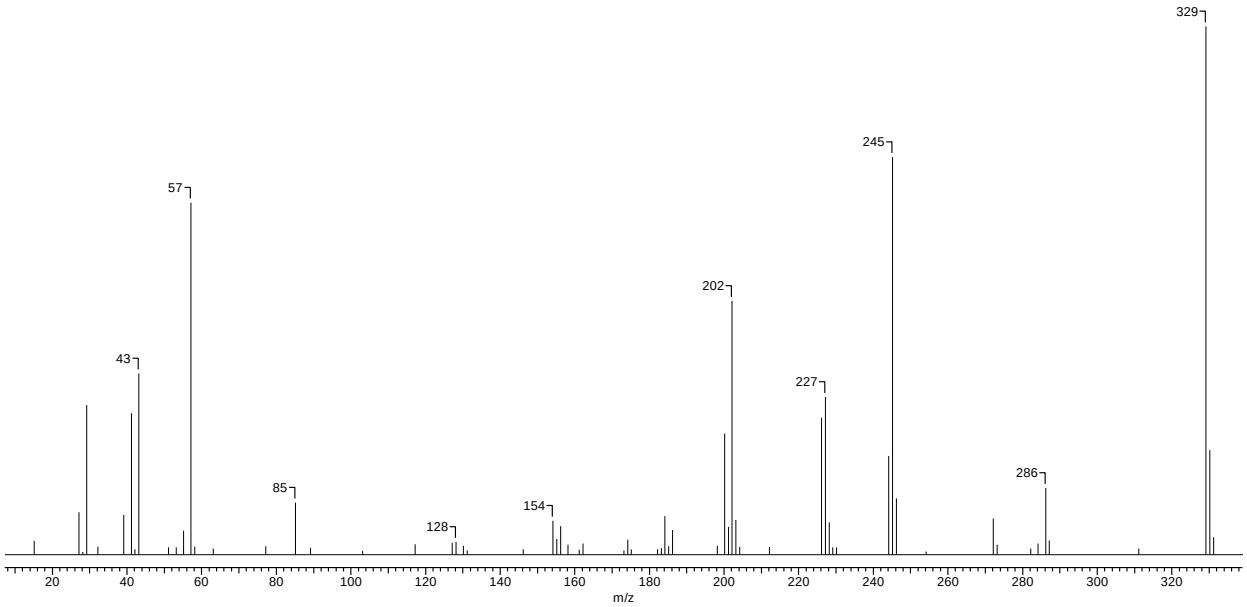

Figure S2 EI MS spectra of monasnicotinic acid (70 eV).

Table S1 ^{1}H and ^{13}C NMR data of the **1** ($CDCl_3$, rt).

	δ_H, ppm	δ_C, ppm
2		160.37
3	7.26, s	123.24
4		146.04
5		120.77
6	9.32, s	152.00
7	6.50, m	127.86
8	6.19, m	135.86
9	2.09, dd	15.86
10	8.15, s	140.63
11		137.15
12	3.36, dd	39.53
13		211.99
14	2.55, m	48.30
15	1.68, 1.38, 2m	25.84
16	0.84, t	11.53
17	1.07, d	15.49
18		198.77
19	2.49, s	25.48
20		168.42
OH-20	4.93, br s	

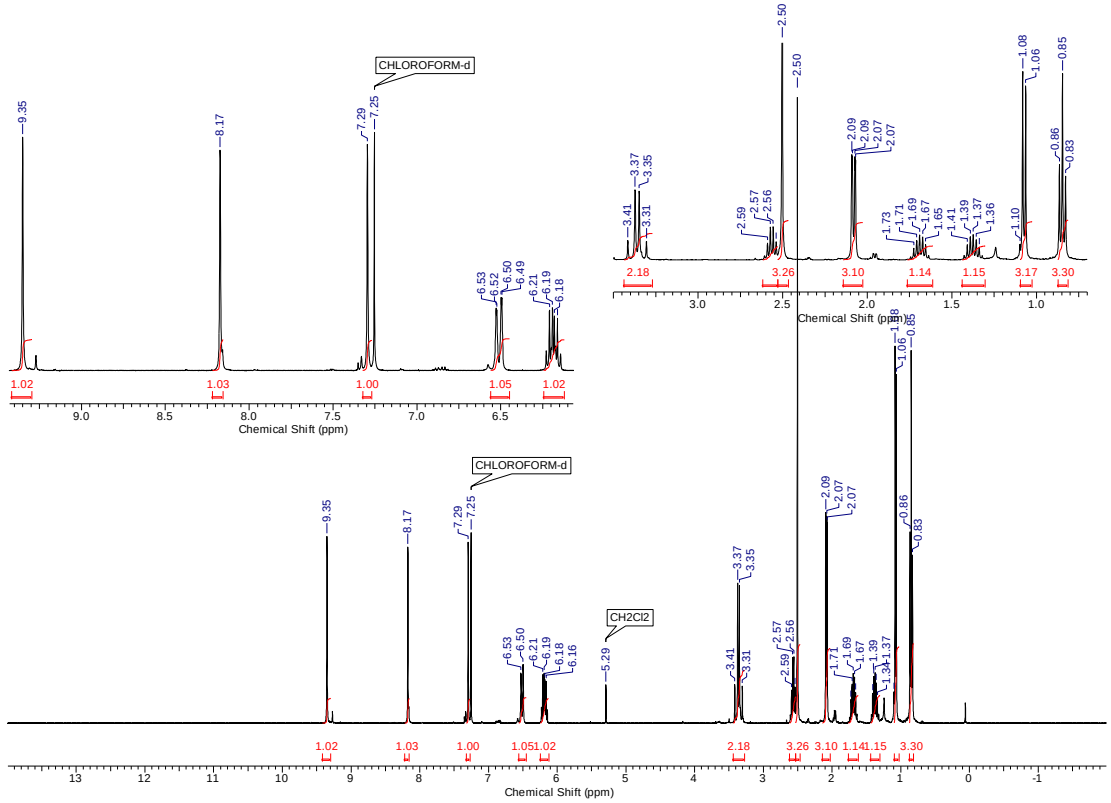

Figure S3 ^{1}H NMR spectrum of monasnicotinic acid ($CDCl_3$, rt).

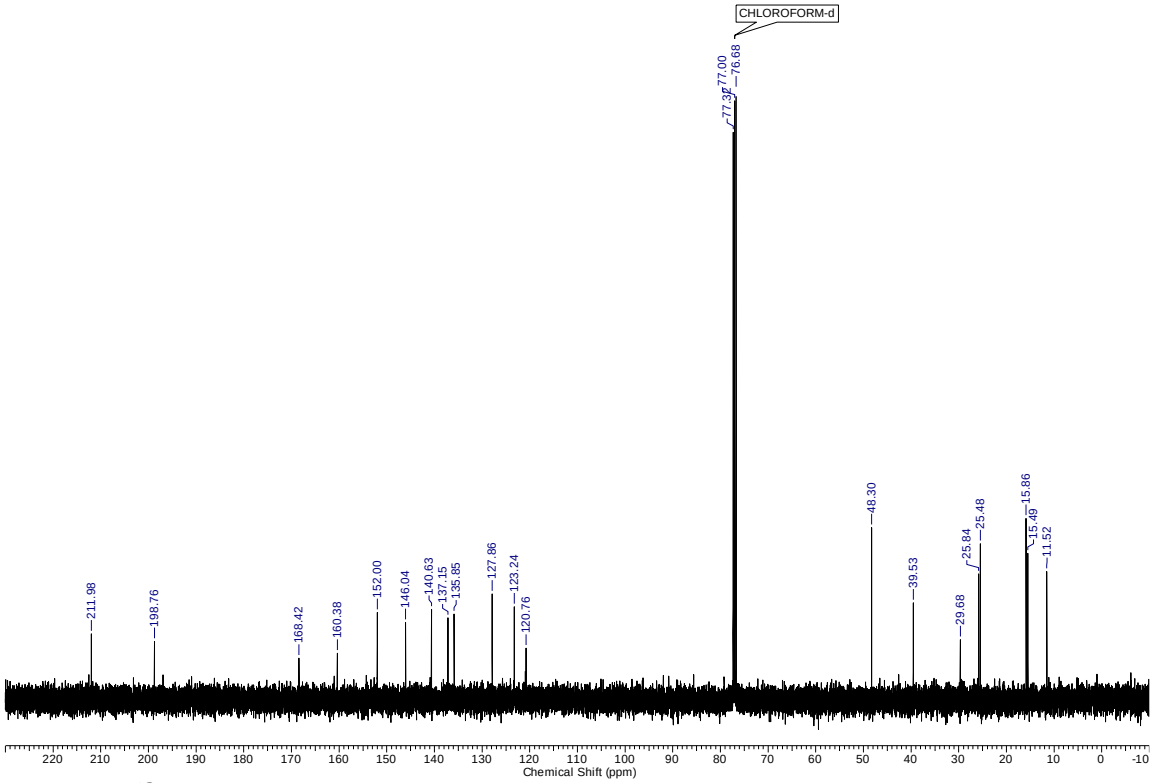

Figure S4 ^{13}C NMR spectrum of monasnicotinic acid ($CDCl_3$, rt).

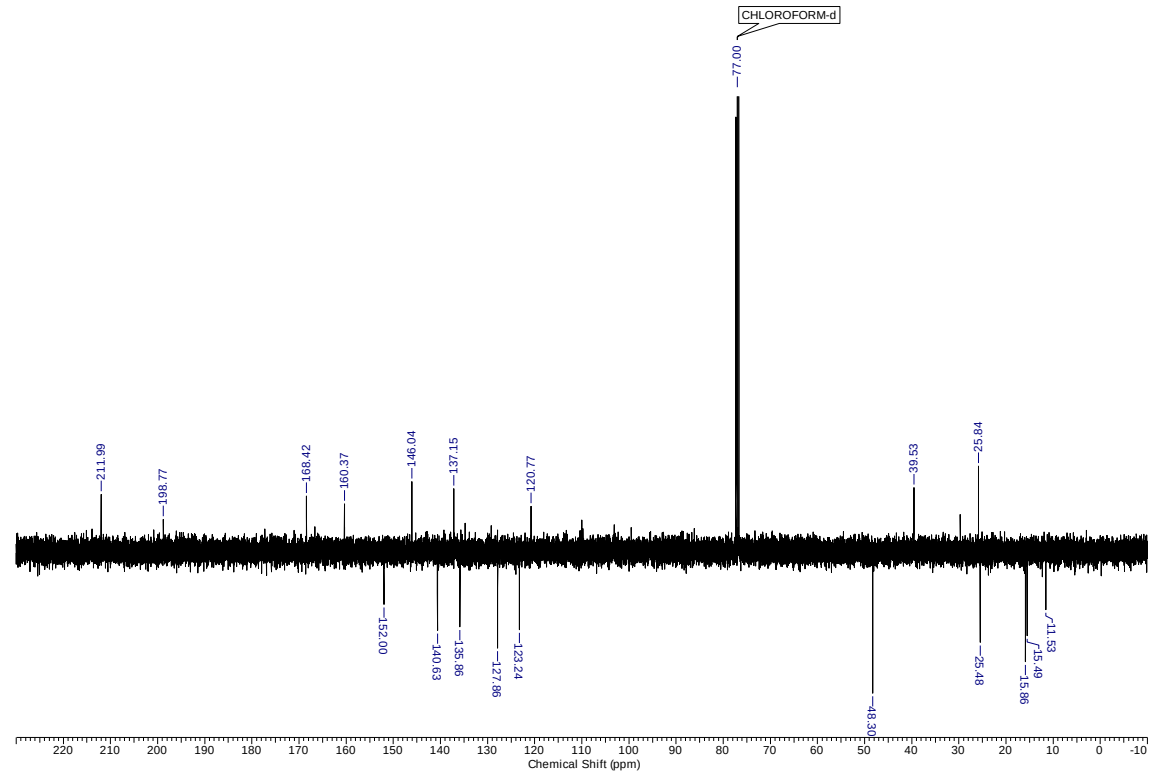

Figure S5 ^{13}C APT NMR spectrum of monasnicotinic acid ($CDCl_3$, rt).

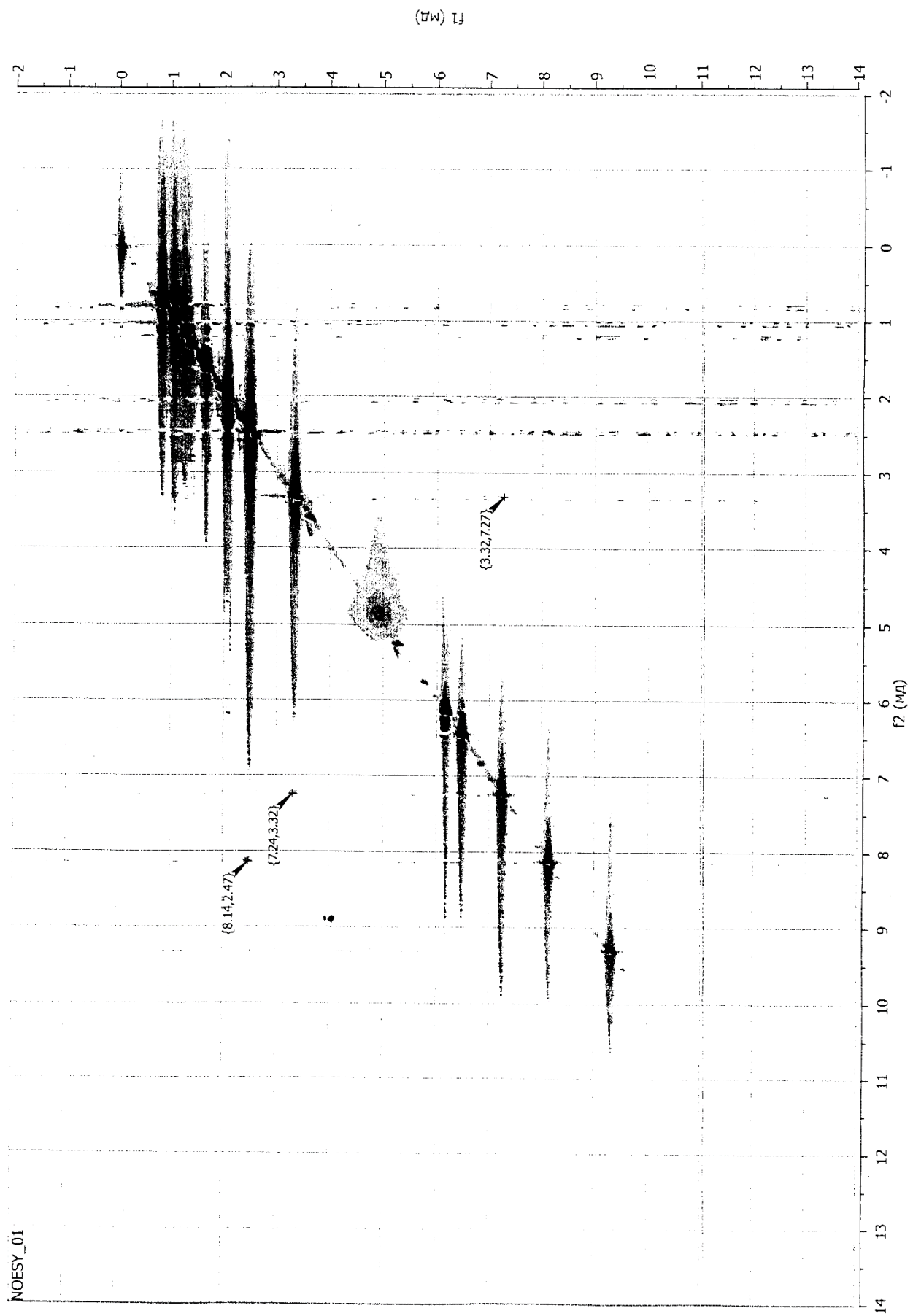

Figure S6 NOESY NMR spectrum of monasnicotinic acid ($CDCl_3$, rt).

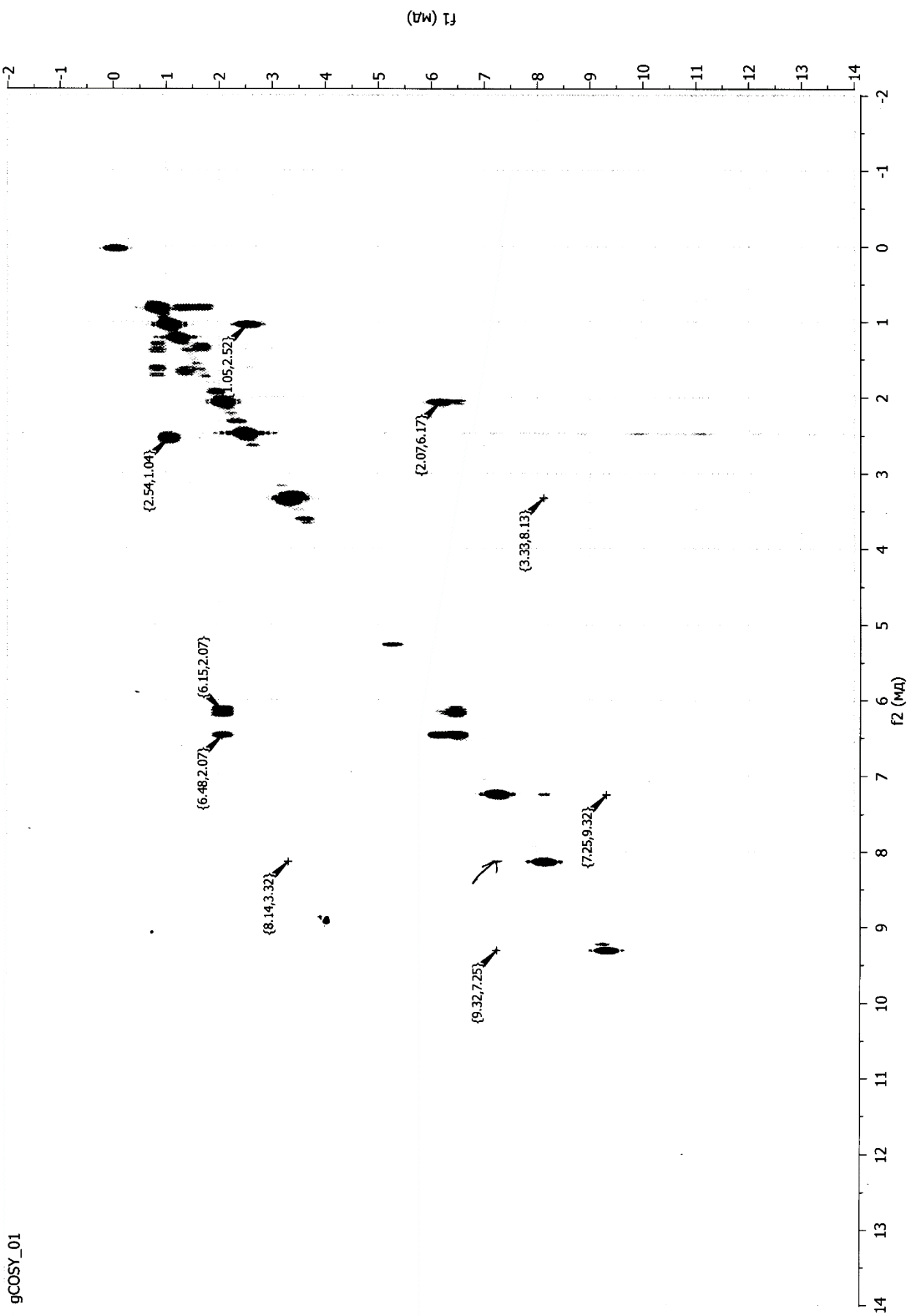

Figure S7 COSY NMR spectrum of monasnicotinic acid ($CDCl_3$, rt).

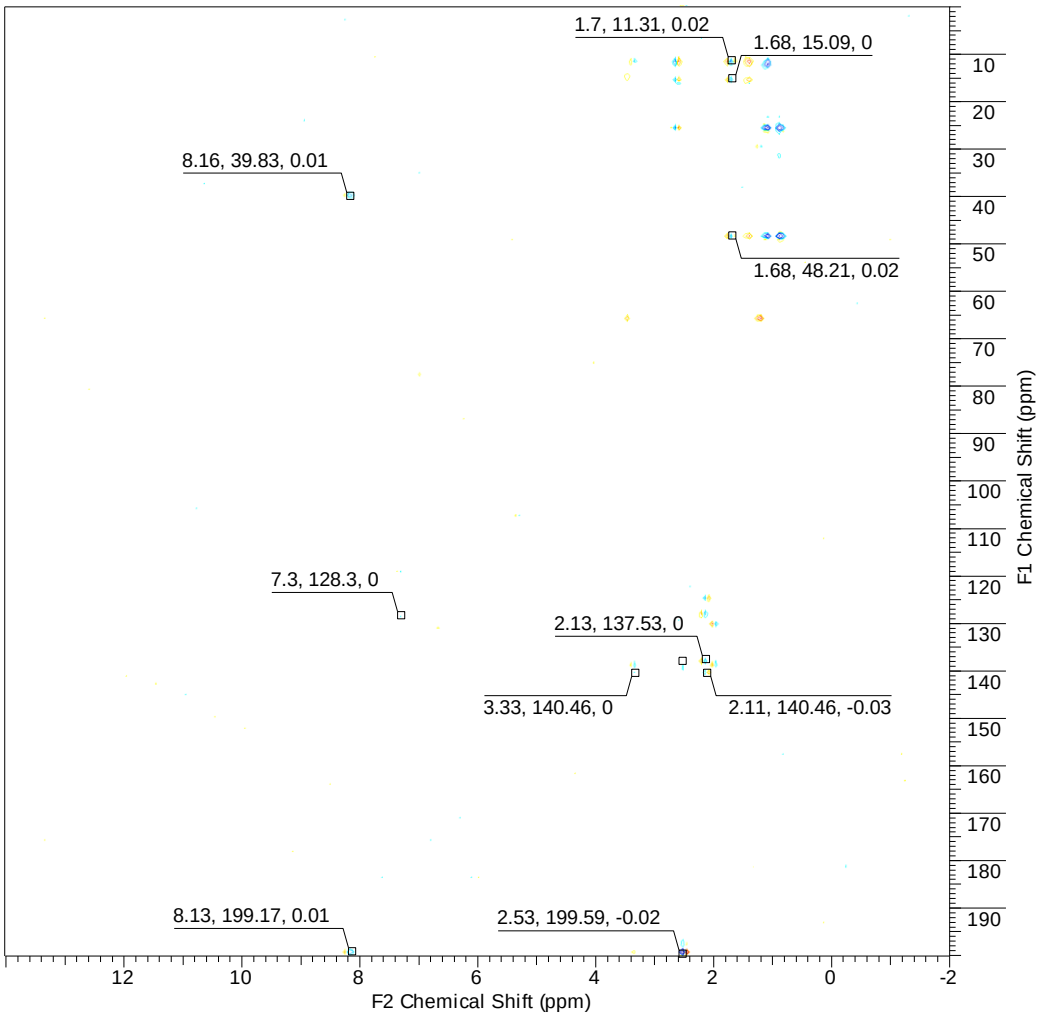

Figure S8 Correlation spectrum of monasnicotinic acid ($CDCl_3$, rt).

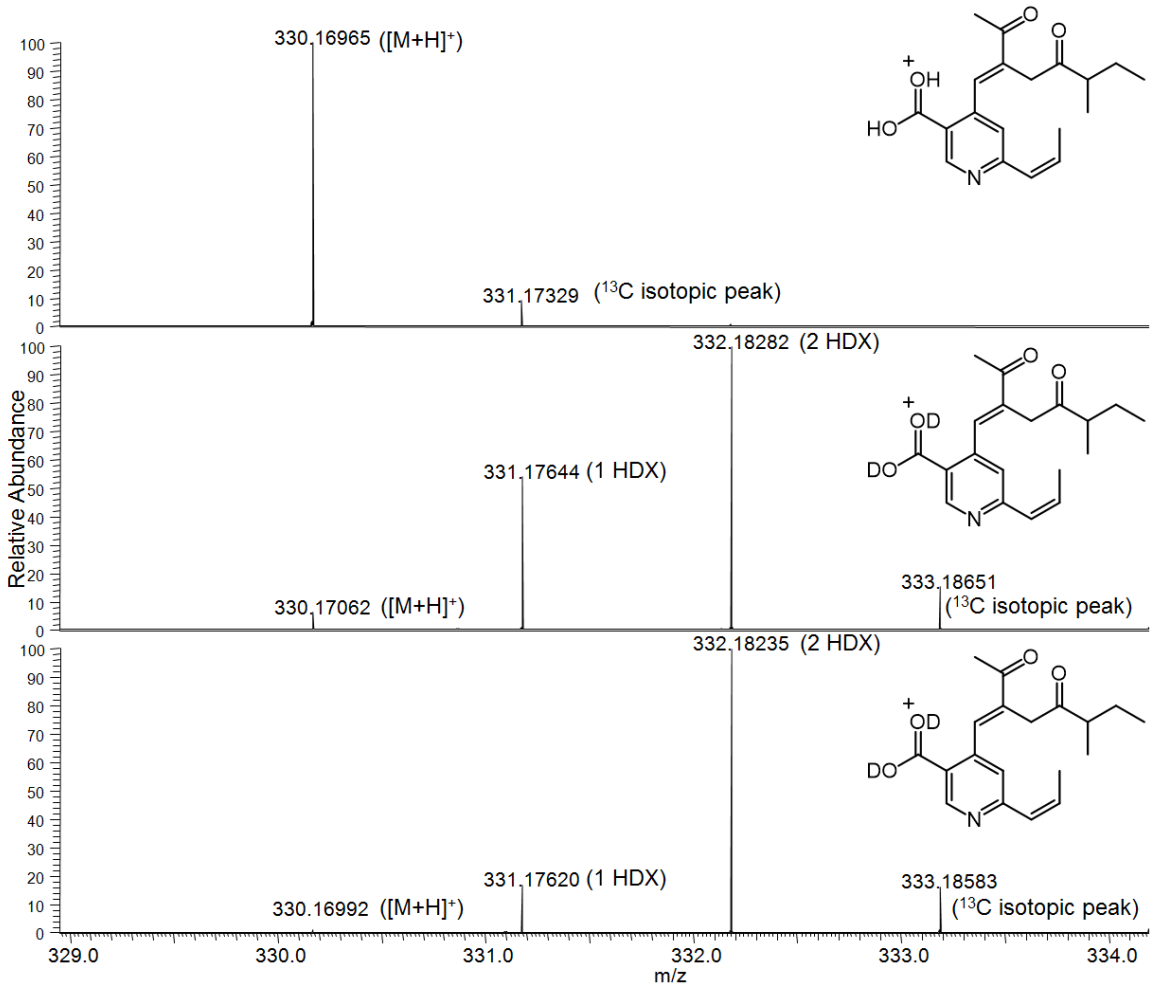

Figure S9 FTICR mass spectra of monasnicotinic acid in positive ESI mode and HDX mass spectra at 200°C and 400°C of the desolvating capillary.

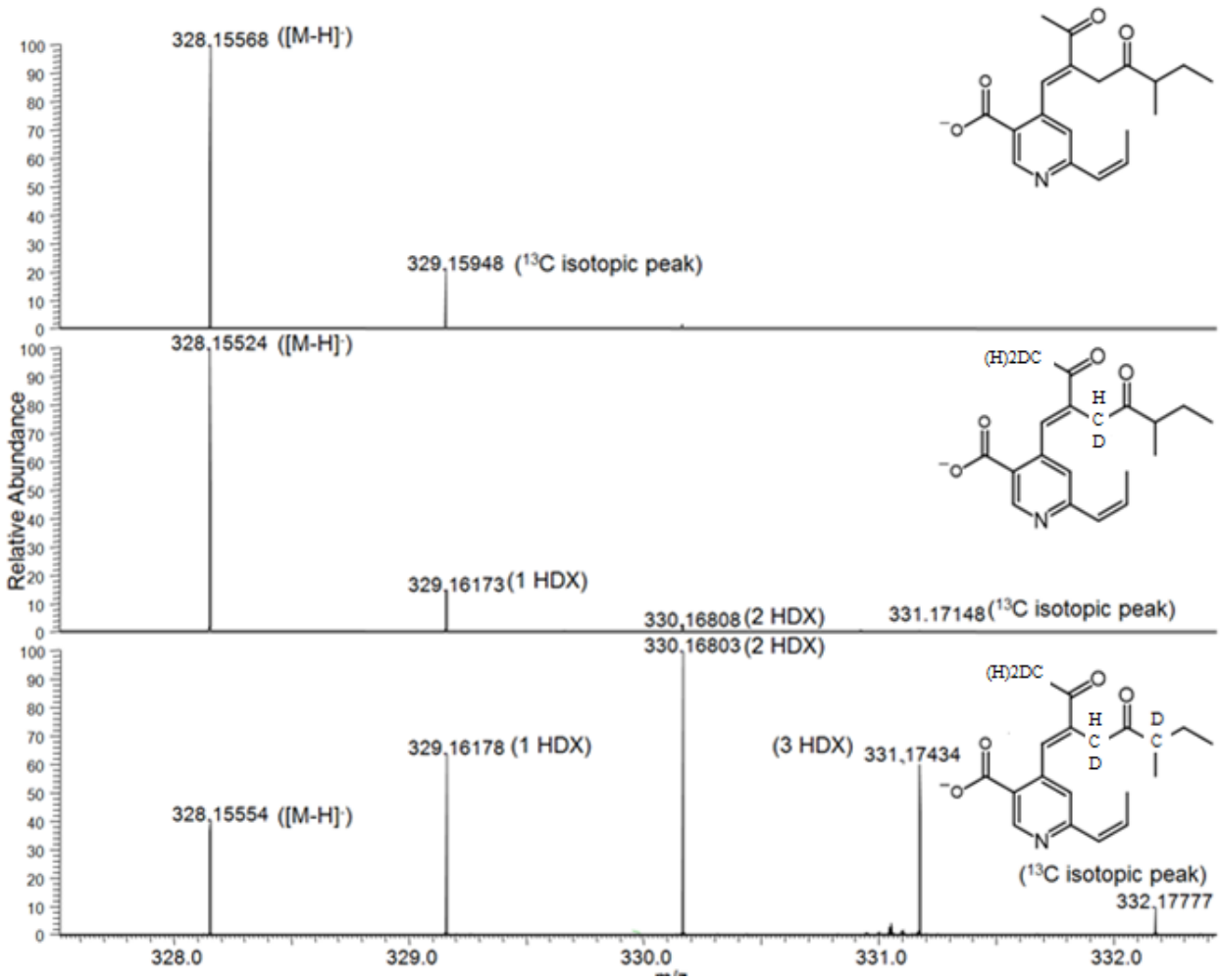

Figure S10 FTICR mass spectra of monasnicotinic acid in negative ESI mode and mass spectra of HDX at 200°C and 400°C of the desolvating capillary.