Supplement of Atmos. Chem. Phys., 26, 8295–8310, 2026
https://doi.org/10.5194/acp-26-8295-2026-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Measurement report: Ice nucleating particles variability across a megacity

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Table S1. Meteorological parameters for the campaign dates at the southern sampling site (CU).

Date (May, 2022)	Average Temperature (°C)	Relative Humidity (%)	Average Pressure (mb)	Total rain (mm)	Average Radiation (W/m^2)	Average UV Index
12	18.7	50.2	778.5	0.0	175.3	0.9
13	20.4	42.3	777.0	0.0	182.5	0.8
14	20.3	32.1	777.2	0.0	166.8	0.8
15	20.5	32.1	778.0	0.0	172.6	0.8
16	19.0	34.1	778.9	0.0	161.7	0.7
17	21.9	30.8	779.2	0.0	323.3	1.8
18	21.5	31.7	778.4	0.0	190.1	0.7
19	21.9	38.6	776.5	0.0	191.6	0.7
20	22.2	41.3	775.2	0.0	149.6	0.5
Average	**20.7**	**37.0**	**777.7**	**0.0**	**190.4**	**0.9**

Table S2. Meteorological parameters for the campaign dates at the northern sampling site (C5).

Date (May, 2022)	Average Temperature (°C)	Relative Humidity (%)	Average Pressure (mb)	Total rain (mm)	Average Radiation (W/m^2)	Average UV Index
12	19.9	51.8	781.8	0.0	320.3	1.8
13	21.3	45.1	780.5	0.0	296.0	1.6
14	21.9	37.1	780.6	0.0	306.4	1.7
15	21.5	35.6	781.5	0.0	302.4	1.7
16	21.1	35.0	782.2	0.0	301.9	1.6
17	21.7	37.8	782.7	0.0	296.5	1.5
18	22.7	36.6	781.9	0.0	308.4	1.5
19	23.6	40.1	779.8	0.0	300.3	1.5
20	23.7	43.3	778.7	0.0	266.2	1.4
Average	**21.9**	**40.3**	**781.1**	**0.0**	**299.8**	**1.6**

Table S3. Pearson correlation coefficients of oxidized species at the northern site (C5).

North (C5)	NH_4^+	NO_3^-	SO_4^{2-}
NH_4^+	1	0.856	0.976
NO_3^-		1	0.838
SO_4^{2-}			1

Table S4. Pearson correlation coefficients of oxidized species at the southern site (CU).

South (CU)	NH_4^+	NO_3^-	SO_4^{2-}
NH_4^+	1	0.574	0.975
NO_3^-		1	0.543
SO_4^{2-}			1

Table S5. Airborne bacteria isolated at the northern (C5) and southern (CU) sites. Green and red colors indicate the presence of species at both or only at one sampling site, respectively. [1]Onset ice nucleate temperature ranges reported in literature, asterisk indicate temperature ranges based on genera or different species from same genera.

Species	CU	C5	Gram	T_0 range (°C)[1]
Acinetobacter schindleri			**Negative**	-24.8 ± 2.5 (Melchum et al., 2023)*
Arthrobacter gandavensis			**Positive**	Unknown
Bacillus cereus			**Positive**	-6.8 to -18.9 (Mortazavi et al., 2015)*
Bacillus licheniformis			**Positive**	-6.8 to -18.9 (Mortazavi et al., 2015)*
Bacillus megaterium			**Positive**	-17.7 ± 7.9 (Melchum et al., 2023)
Bacillus simplex			**Positive**	-6.8 to -18.9 (Mortazavi et al., 2015)*
Bacillus subtilis			**Positive**	-7 to -9 °C (Failor et al., 2017)
Exiguobacteirum aurantiacum			**Positive**	Unknown
Kocuria rosea			**Positive**	-20.0 ± 1.5 (Mortazavi et al., 2015)*
Microbacterium aerolatum			**Positive**	-21.6 ± 1 (Mortazavi et al., 2015)*
Microbacterium paraoxydans			**Positive**	-21.6 ± 1 (Mortazavi et al., 2015)*
Paenarthrobacter ilicis			**Positive**	Unknown
Pantoea agglomerans			**Negative**	-21.2 ± 5.2 (Melchum et al., 2023)*
Pantoea vagans			**Negative**	-21.2 ± 5.2 (Melchum et al., 2023)*
Pseudarthrobacter chlorophenolicus			**Positive**	Unknown
Pseudarthrobacter oxydans			**Positive**	Unknown
Pseudomonas antarctica			**Negative**	-3.7 to -15.7 (Obata et al., 1999)
Pseudomonas flavescens			**Negative**	-21.6 ± 5.1 (Melchum et al., 2023)*
Pseudomonas xanthomarina			**Negative**	-21.6 ± 5.1 (Melchum et al., 2023)*
Pseudescherichia vulneris			**Negative**	Unknown
Staphylococcus xylosus			**Positive**	-22.3 to -25.4 (Melchum et al., 2023)*

Table S6. Airborne fungi isolated at the northern (C5) and southern (CU) sites. Green and red colors indicate the presence of genera at both or only at one sampling site, respectively. [1]Onset ice nucleate temperature ranges reported in literature.

Genera	CU	C5	T_0 range (°C)[1]
Alternaria			-23.1 ± 2.6 (Melchum et al., 2023)
Aspergillus			-29.0 ± 1.9 (Melchum et al., 2023)
Aureobasidium			Unknown
Cladosporium			-15 °C to -21.8 (Jayaweera and Flanagan, 1982)
Epicoccum			Unknown
Fusarium			-3.5 to -11.2 (Kunert et al., 2019)
Penicillium			
Rhizopus			Unknown

Table S7. Pearson correlation coefficients of bacteria genera concentration between the northern (C5) and southern (CU) sites.

	Pantoea vagans	*Pseudomonas flavescens*	*Bacillus subtilis*	*Kocuria rosea*	*Pantoea agglomerans*	*Exiguobacteirum aurantiacum*	*Bacillus licheniformis*
Pearson coefficient	0.50	0.01	0.12	0.68	0.52	0.33	0.23

Table S8. Pearson correlation coefficients of fungi genera concentration between the northern (C5) and southern (CU) sites.

	Cladosporium	*Aspergillus*	*Penicillium*	*Alternaria*	*Rhizopus*
Pearson coefficient	0.77	0.41	0.15	0.17	0.09

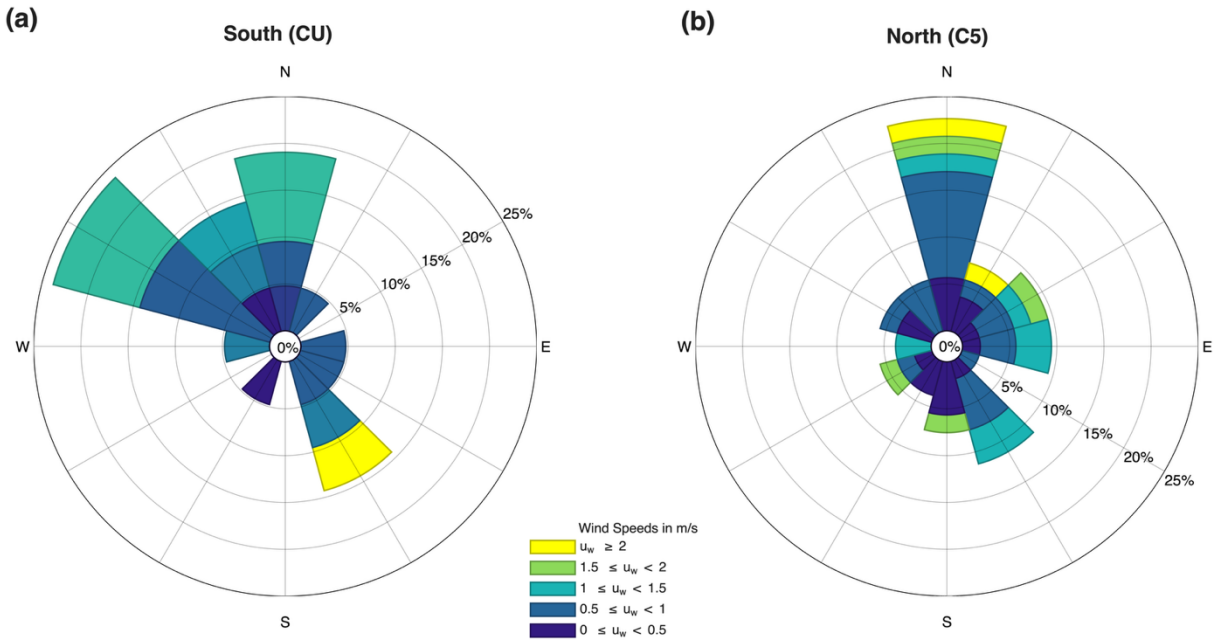

Figure S1. Windrose for ice nucleation sampling periods (May 16th to May 20th, 08:00 h to 13:00 h local time) for **(a)** the southern sampling site (CU) and **(b)** the northern sampling site (C5).

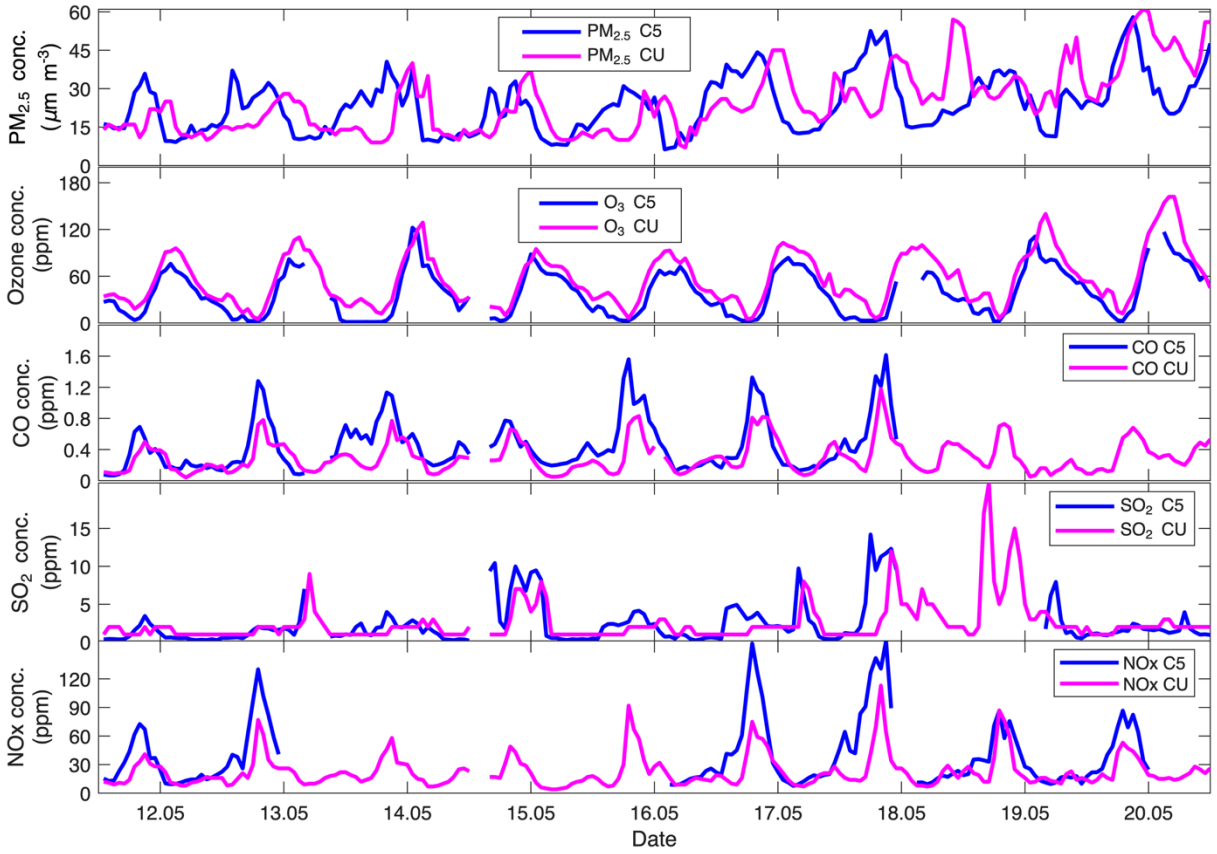

Figure S2. Criteria pollutants concentration time series for the northern (C5, blue) and southern (CU, magenta) sampling sites.

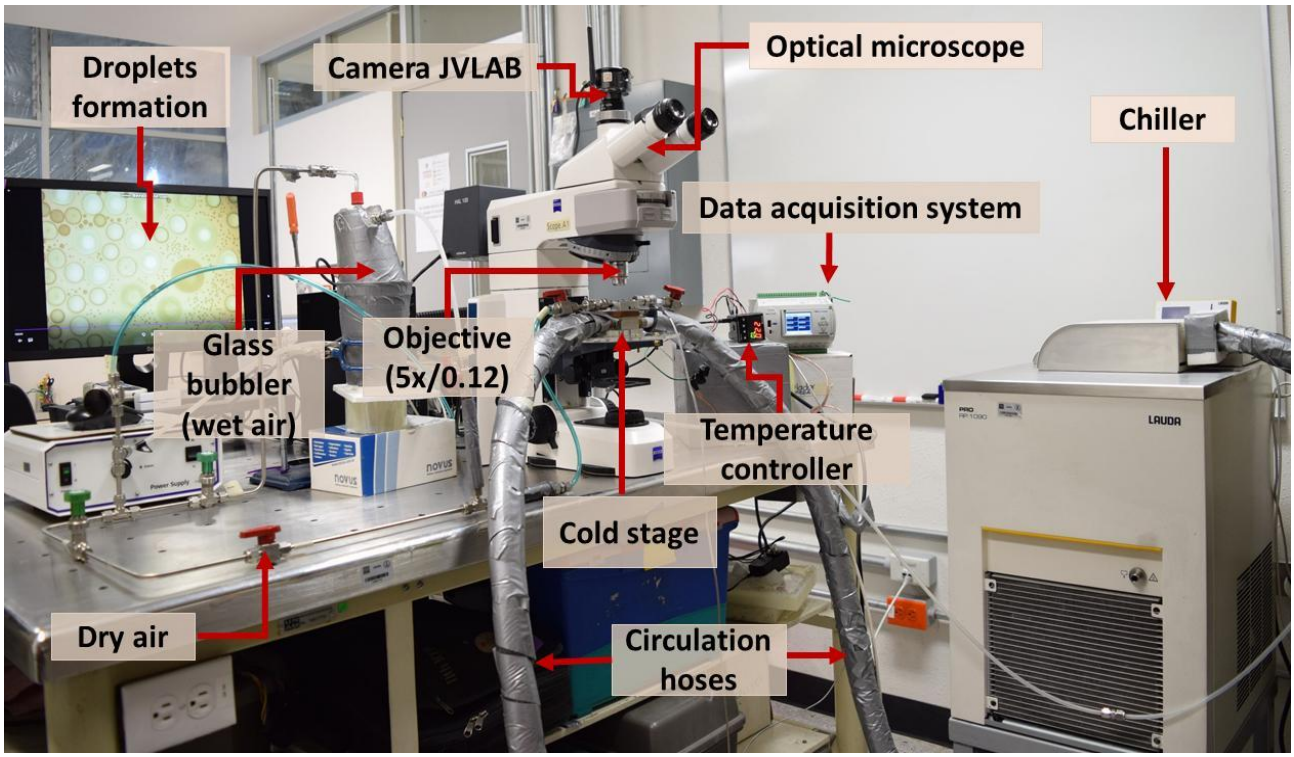

Figure S3. The UNAM-MOUDI-DFT experimental setup with its main components. Reprint of Fig. 3 from Córdoba et al. (2021).

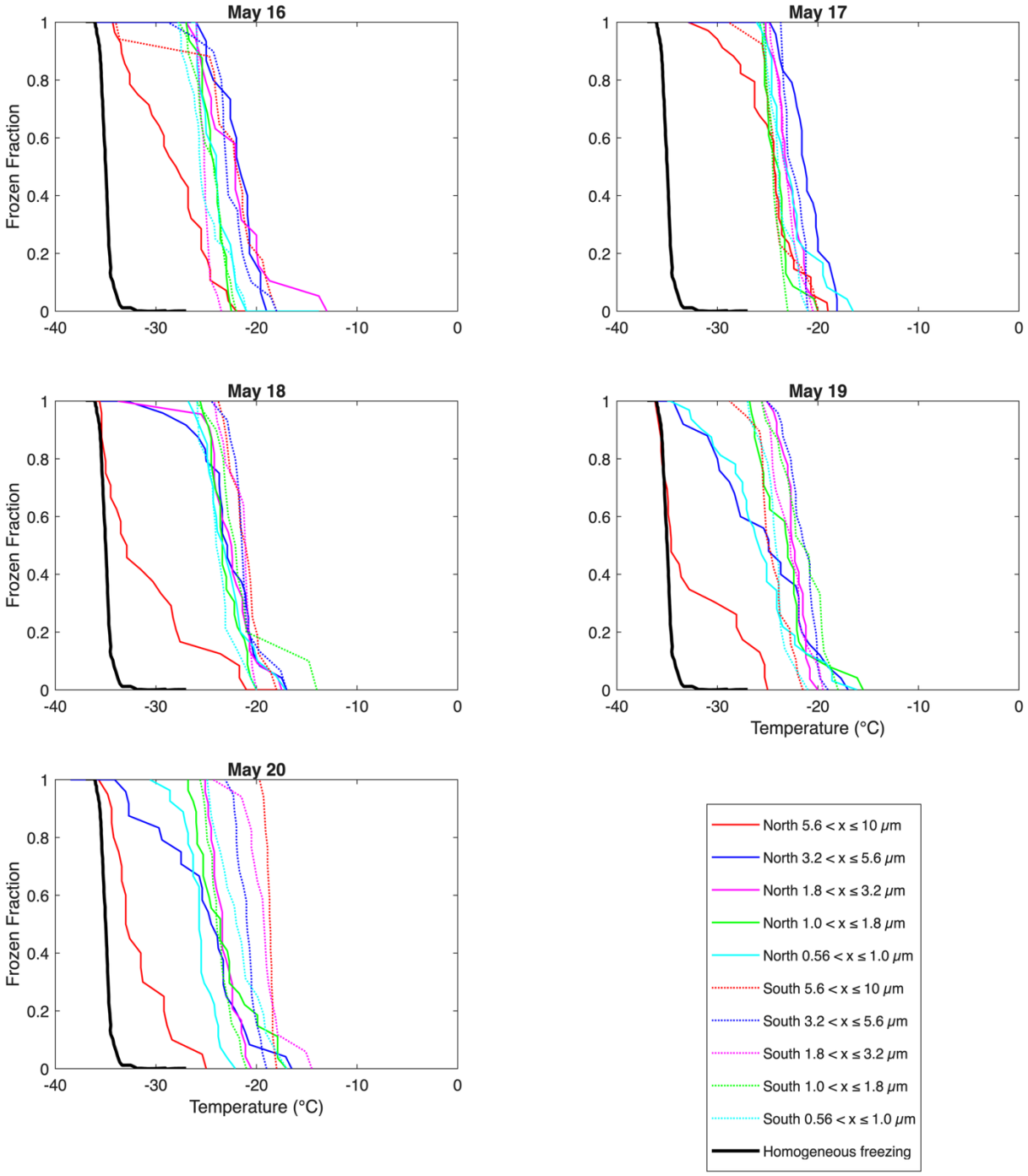

Figure S4. May 16th, 17th, 18th, 19th and 20th frozen fraction curves as a function of temperature for the northern (solid lines) and southern (dotted lines) samples (with aerodynamic diameters between 1.0 µm and 10 µm). The black line shows the average homogeneous freezing curve.

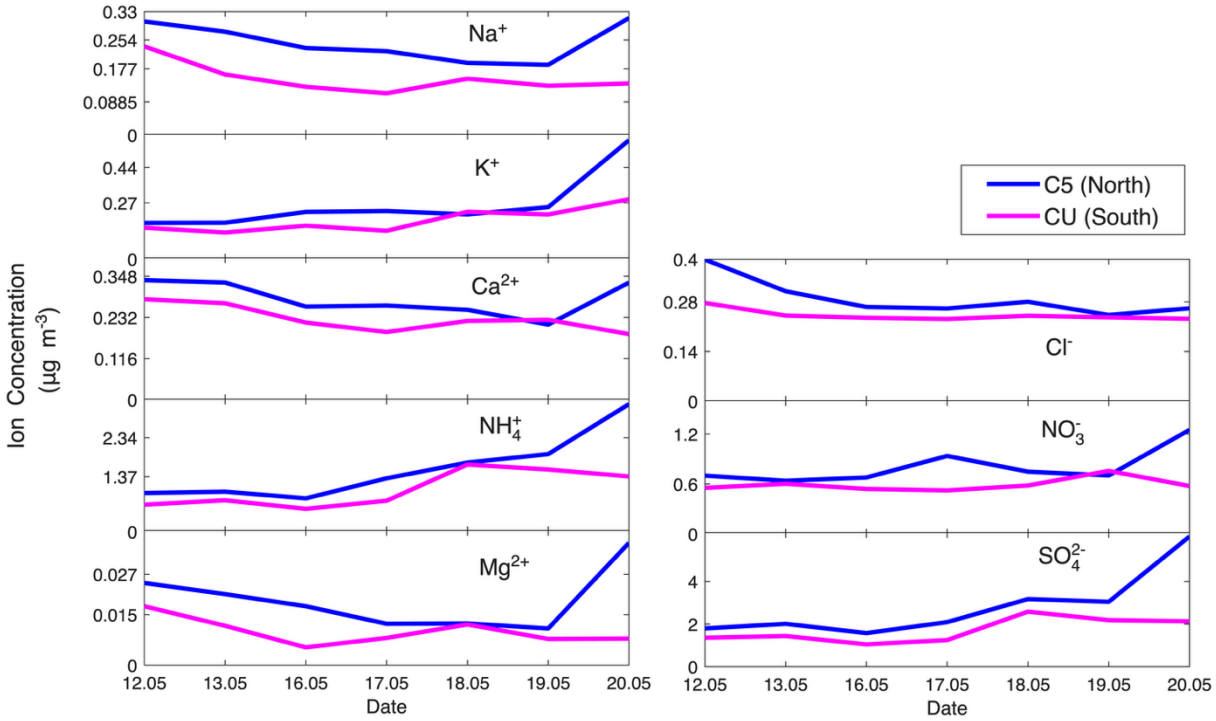

Figure S5. Time series of the cations (left) and anions (right) concentrations measured in the northern (C5, blue) and southern (CU, magenta) sites.

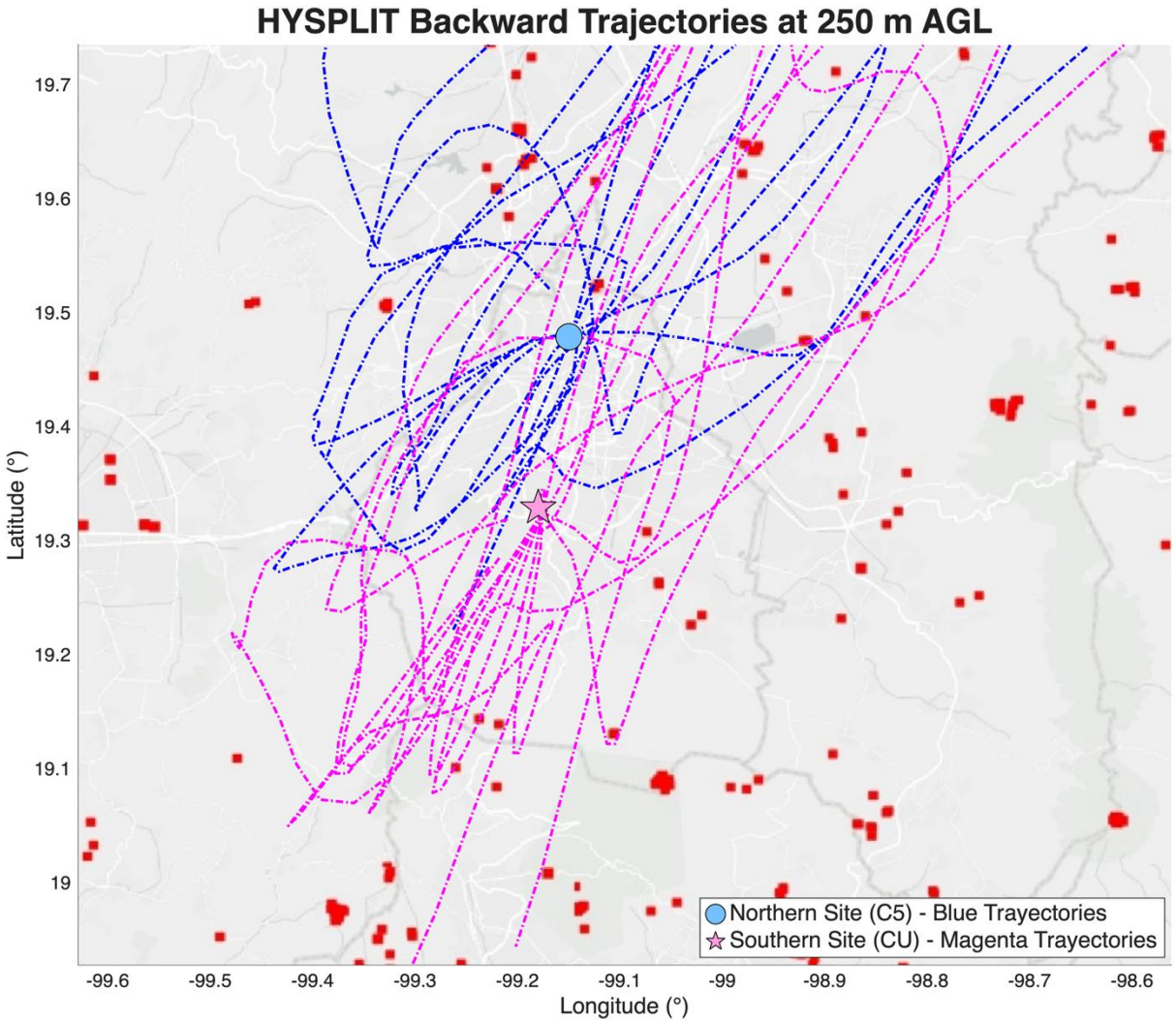

Figure S6. HYSPLIT backward trajectories at 250 m AGL at both MCMA sites overlayed in NASA FIRMS real-time active fire locations for May 12th to 20th. South (CU, blue circle) and north (C5, magenta star) MCMA sample site's locations marked at image.

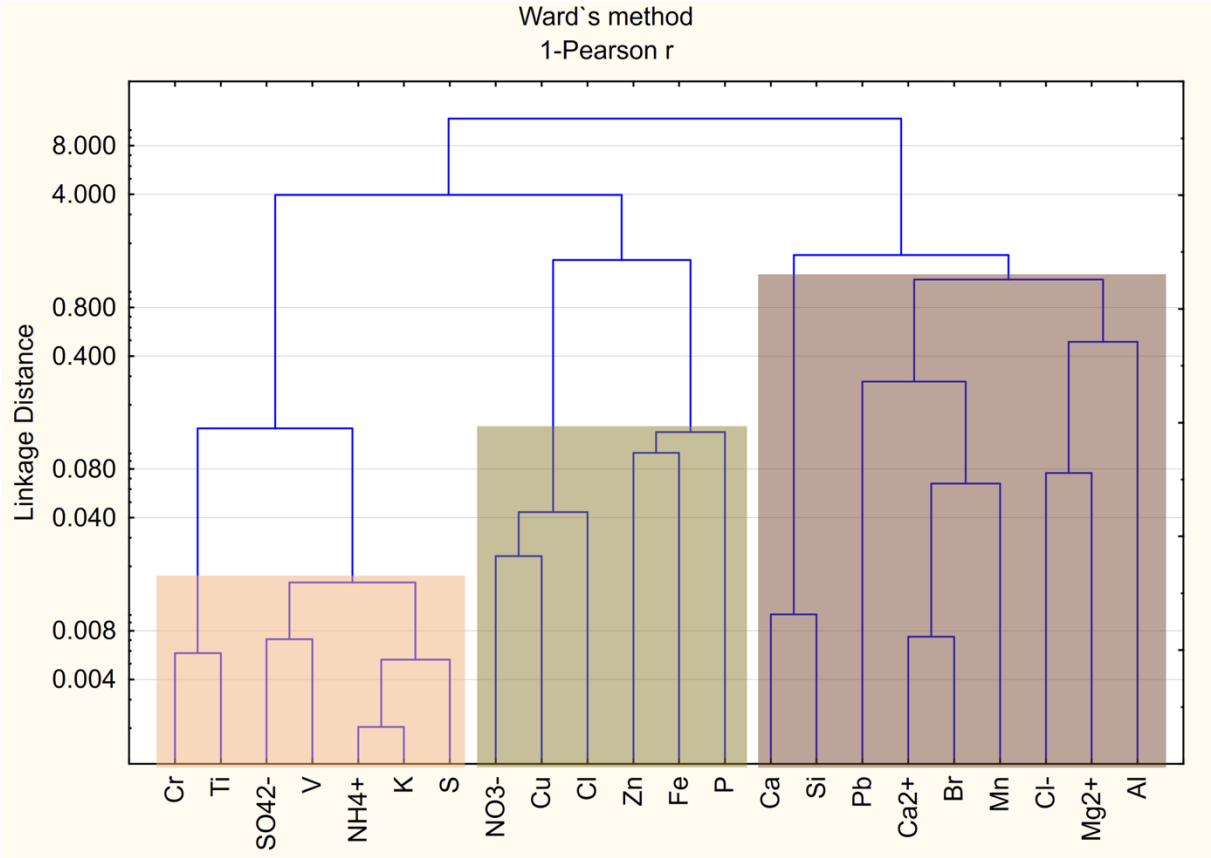

Figure S7. Dendrogram obtained using Ward's method based on Pearson correlation coefficients of every chemical species analyzed in the southern site (CU).

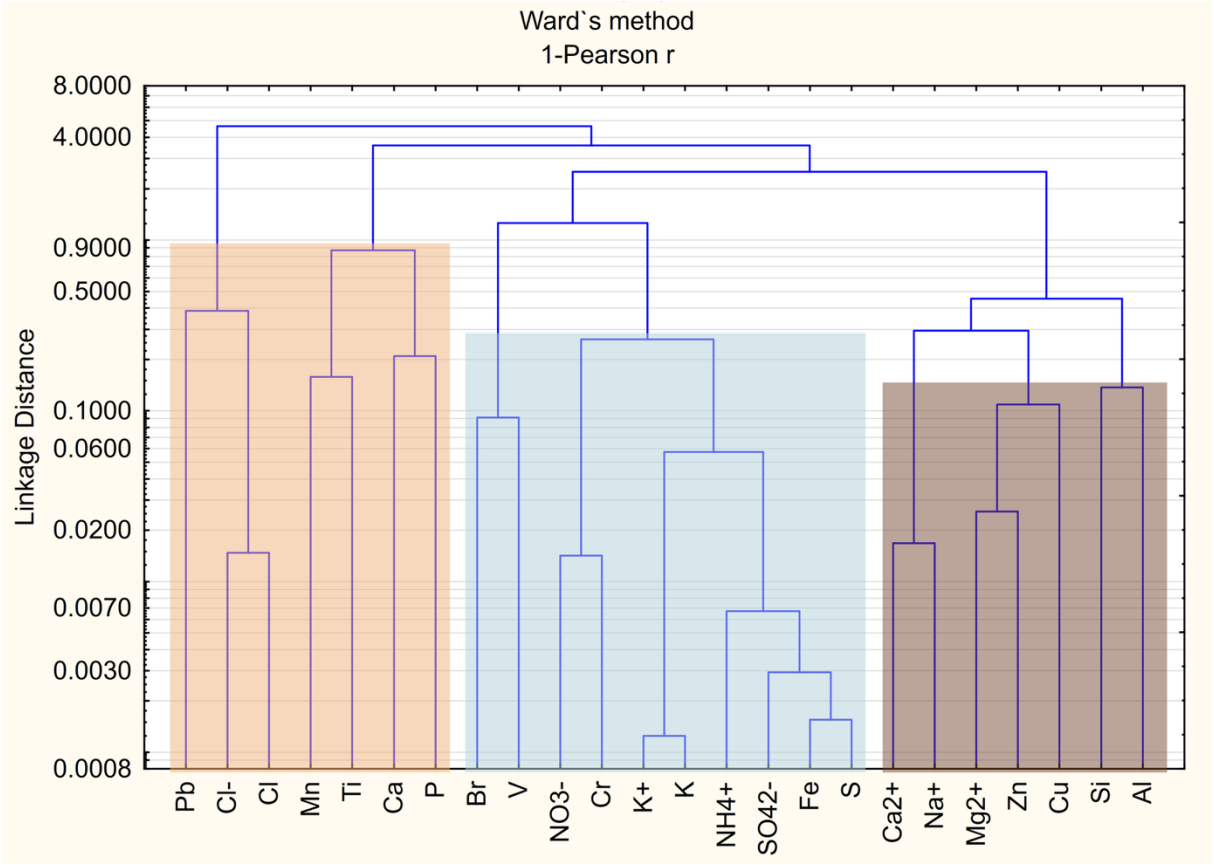

Figure S8. Dendrogram obtained using Ward's method based on Pearson correlation coefficients of every chemical species analyzed in the northern site (C5).

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