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Quantification of 21 sugars in tropospheric particulate matter by ultra-high-performance liquid chromatography tandem mass spectrometry

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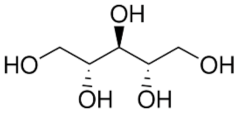
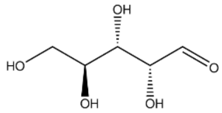
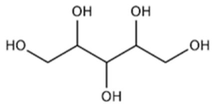
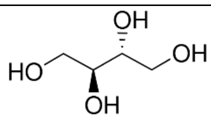
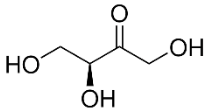
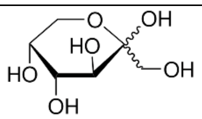
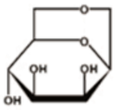
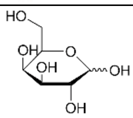
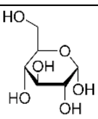
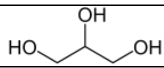
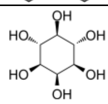
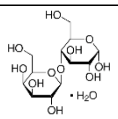
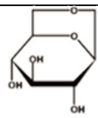
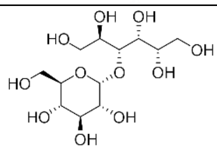
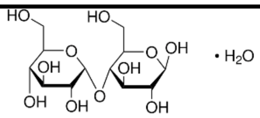
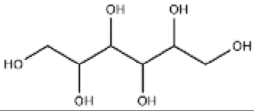
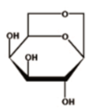
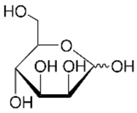
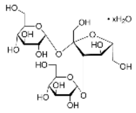
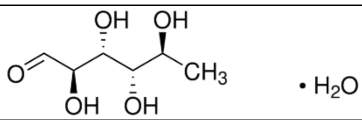
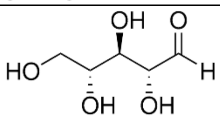
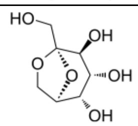
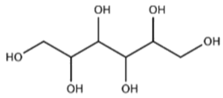
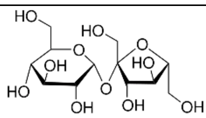
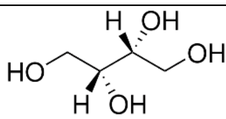
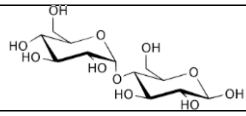
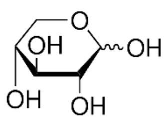
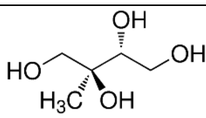
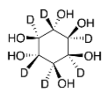
Supplementary data

Table S1: Summary of main sources of sugars in atmospheric aerosol. Many of the links between chemical species and sources proposed in the literature are still tentative and a comprehensive overview is still missing. Modified from Barbaro et al. 2015 and Vincenti et al. 2022.

Compound	Sources	References
ANHYDROSUGARS		
Levoglucosan and its isomers Mannosan and Galactosan	Thermal decomposition of cellulose and hemicellulose including biomass burning	(Kirchgeorg et al., 2014; Simoneit et al., 2004; Simoneit and Elias, 2001; Zennaro et al., 2014)
ALCOHOL-SUGARS	Lichens and bacteria	(Medeiros et al., 2006)
Arabitol	Fungal spores and lichens	(Bauer et al., 2008; Gosselin et al., 2016)
Erythritol	Biomass burning Fungal spores	(Li et al., 2016; Nirmalkar et al., 2019)
Glycerol	Biomass burning Soil	(Zangrando et al., 2016; Zhao et al., 2020)
Inositol	Biomass burning Fungal spores and plant metabolism	(Nirmalkar et al., 2019; Zhu et al., 2015)
Mannitol	Lichen, fungal spores, algae, and higher plants	(Bauer et al., 2008; Gosselin et al., 2016)
2-Methyl-tretol	Plants	(Emygdio et al., 2018)
Trehalose	Fungal spores	(Bauer et al., 2008; Marynowski et al., 2020)
Threitol	Biomass burning and plants	(Emygdio et al., 2018)
Xylitol	Biomass burning Plants, biota	(Nirmalkar et al., 2015, 2019)
SUGARS	Natural biogenic detritus	(Elbert et al., 2006, p.200; Fu et al., 2013; Medeiros et al., 2006; Simoneit et al., 2004; Tominaga et al., 2011)
Arabinose	Biomass burning	(Pietrogrande et al., 2014)
Fructose	Pollen	(Fu et al., 2012; Marynowski et al., 2020; Yttri et al., 2007)
Galactose	Biomass burning	(Pietrogrande et al., 2014)
Glucose	Vascular plants Pollen	(Cowie and Hedges, 1984; Fu et al., 2012; Marynowski et al., 2020; Yttri et al., 2007)
Maltose	Biomass burning Plants	(Ren et al., 2020)
Sucrose	Plant flowering Airbone pollen granules	(Bieleski, 1995; Fu et al., 2012; Pacini, 2000; Yttri et al., 2007)
Trehalose	Yeasts, fungal spores Biomass burning	(Ren et al., 2020) (Nirmalkar et al., 2015)
Xylose	Biomass burning Plants	(Zhao et al., 2020) (Schmidl et al., 2008)
CARBOHYDRATES	Marine organic particles generated by sea spray	(Hawkins and Russell, 2010)

Table S2 : Chemical information of target compounds. S: sugar; SA: sugar alcohol; AS: anhydrosugar; IS: internal standard.

Compound	Type	Molecular mass (g/mol)	Structure	CAS number	Water solubility at 25°C (g/L)
Adonitol	SA	152.15		488-81-3	1000
Arabinose	S	150.13		5328-37-0	1000
Arabitol	SA	152.15		7643-75-6	1000
Erythritol	SA	122.12		149-32-6	1000
Erythrulose	S	120.10		533-50-6	300
Fructose	S	180.16		57-48-7	977
Galactosan	AS	162.14		644-76-8	781
Galactose	S	180.16		59-23-4	1000
Glucose	S	180.16		50-99-7	1000
Glycerol	SA	92.09		56-81-5	1000
Inositol	SA	180.16		87-89-8	1000
Lactose	S	360.31		64044-51-5	1000
Levoglucosan	AS	162.14		498-07-7	781
Maltitol	SA	344.31		585-88-6	1000

Compound	Type	Molecular mass (g/mol)	Structure	CAS number	Water solubility at 25°C (g/L)
Maltose	S	342.30		6363-53-7	1000
Mannitol	SA	182.17		69-65-8	1000
Mannosan	AS	162.14		14168-65-1	781
Mannose	S	180.16		3458-28-4	1000
Melezitose	SA	504.44		207511-10-2	50
Rhamnose	S	182.17		10030-85-0	1000
Ribose	S	150.13		50-69-1	1000
Sedoheptulosan	AS	192.17		469-90-9	816
Sorbitol	SA	182.17		50-70-4	1000
Sucrose	S	342.30		57-50-1	1000
D-Threitol	SA	122.12		2418-52-2	1000
Trehalose	S	342.30		99-20-7	1000
Xylose	S	150.13		58-86-6	1000
2-methyl-D-Erythritol	SA	136.15		58698-37-6	
***myo*-Inositol (1,2,3,4,5,6-D_6, 98%)**	IS	186.19		68922-44-1	-

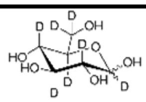
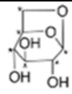
Compound	Type	Molecular mass (g/mol)	Structure	CAS number	Water solubility at 25°C (g/L)
D-Glucose (1,2,3,4,5,6,6-D_7, 97-98%)	IS	187.2		66034-51-3	-
Levoglucosan (Levoglucosan) (U-13C6,98%)	IS	168.1		478518-93-3	-

Table S3 : Results for the 21 sugars for NIST® SRM® 2786 ("Fine Atmospheric Particulate Matter"). N.D: no detected.

Compound	Mean concentration (mg/kg) (n=3)	RSD (%) (n=3)
Adonitol	27.9	14.1
Arabitol	599.7	17.6
Erythrulose	1.3	42.6
Fructose	2.7	30.6
Glucose	151.3	0.3
Glycerol	475.2	48.5
Inositol	60.9	2.2
Lactose	83.5	1.3
Levoglucosan	523.3	2.6
Maltitol	N.D	N.D
Maltose	31.2	1.0
Mannitol	367.5	13.9
Mannose	N.D	N.D
Melezitose	25.9	5.7
Rhamnose	3.7	16.9
Sedoheptulosan	N.D	N.D
Sorbitol	27.5	111.7
Sucrose	547.1	5.0
Trehalose	84.2	5.4
Xylose	N.D	N.D
2-methyl-tetrols	10.8	13.9

Table S4: Jungfraujoch (JFJ) results from 2011 to 2016. Winter: December, January and February; Summer: June, July and August.

Compound	Field blank (n=11) (ng/m^3)	Field LOQ (ng/m^3)	JFJ 2011-2016 concentrations (ng/m^3)				
			Min (n=136)	Max (n=136)	Median (n=136)	Winter mean concentration (n=33)	Summer mean concentration (n=34)
Adonitol	<LOD	<LOD	<LOD	0.04	0.01	0.01	0.02
Arabinose	0.03	0.07	0.04	0.21	0.13	<LOD	0.13
Arabitol	0.01	0.01	<LOD	2.04	0.22	0.03	0.79
Erythrulose	<LOD	<LOD	0.00	0.18	0.03	0.01	0.06
Fructose	0.03	0.03	<Field LOQ	0.58	0.09	0.21	0.17
Galactose	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Glucose	0.14	0.30	<Field LOQ	2.83	0.62	0.24	1.15
Glycerol	3.94	9.40	0.42	69.78	10.14	31.81	2.76
Inositol	<LOD	<LOD	<LOD	0.23	0.04	0.04	0.07
Lactose	<LOD	<LOD	0.01	0.77	0.05	0.03	0.07
Levoglucosan	0.01	0.03	0.04	76.72	1.39	1.44	5.07
Maltitol	<LOD	<LOD	<LOD	0.40	0.08	0.02	0.14
Maltose	0.06	0.08	<LOD	0.39	0.06	0.15	0.11
Mannitol	<LOD	<LOD	<LOD	3.15	0.57	0.07	1.27
Mannose	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Melezitose	<LOD	<LOD	0.01	0.09	0.01	<LOD	0.02
Rhamnose	0.03	0.03	<LOD	0.24	0.04	0.05	0.06
Ribose	<LOD	<LOD	0.08	0.18	0.13	<LOD	0.13
Sedoheptulosan	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Sorbitol	<LOD	<LOD	0.00	0.38	0.11	0.10	0.18
Sucrose	0.78	0.80	0.04	12.37	0.62	0.12	<LOD
Trehalose	<LOD	<LOD	0.07	1.27	0.43	0.16	0.66
Xylose	0.14	0.23	<LOD	<LOD	<LOD	<LOD	<LOD
2-methyl-tetrols	0.06	0.16	0.03	27.31	3.09	0.39	7.06

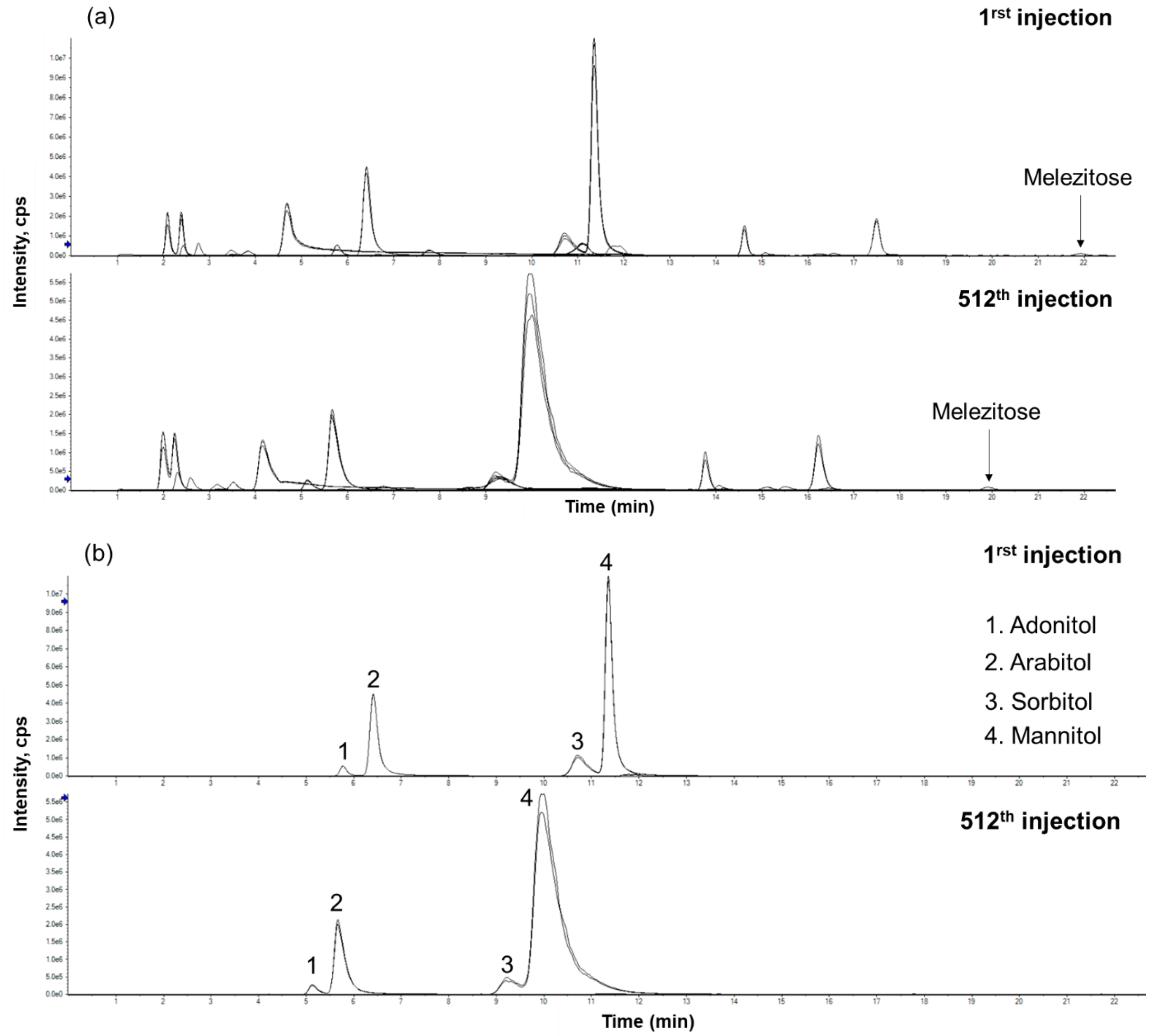


Figure S1: Evolution of sugars separation according to the column ageing. A. Drift of retention time observed between the 1st injection and more than 500 injections (with an average of 0.5 min which can go up to 2.2 min for the case of melezitose). B. Focus on the criteria to put aside an aged column: the compounds adonitol/arabitol and sorbitol/mannitol tend to co-eluate.

REFERENCES

Bauer, H., Claeys, M., Vermeylen, R., Schueller, E., Weinke, G., Berger, A., and Puxbaum, H.: Arabitol and mannitol as tracers for the quantification of airborne fungal spores, Atmospheric Environment, 42, 588–593, https://doi.org/10.1016/j.atmosenv.2007.10.013, 2008.

Bieleski, R. L.: Onset of Phloem Export from Senescent Petals of Daylily, Plant Physiology, 109, 557–565, https://doi.org/10.1104/pp.109.2.557, 1995.

Cowie, G. L. and Hedges, J. I.: Carbohydrate sources in a coastal marine environment, Geochimica et Cosmochimica Acta, 48, 2075–2087, https://doi.org/10.1016/0016-7037(84)90388-0, 1984.

Elbert, W., Taylor, P. E., Andreae, M. O., and Pöschl, U.: Contribution of fungi to primary biogenic aerosols in the atmosphere: active discharge of spores, carbohydrates, and inorganic ions by Asco- and Basidiomycota, https://doi.org/10.5194/acpd-6-11317-2006, 2006.

Emygdio, A. P. M., Andrade, M. de F., Gonçalves, F. L. T., Engling, G., Zanetti, R. H. de S., and Kumar, P.: Biomarkers as indicators of fungal biomass in the atmosphere of São Paulo, Brazil, Science of The Total Environment, 612, 809–821, https://doi.org/10.1016/j.scitotenv.2017.08.153, 2018.

Fu, P., Kawamura, K., Kobayashi, M., and Simoneit, B. R. T.: Seasonal variations of sugars in atmospheric particulate matter from Gosan, Jeju Island: Significant contributions of airborne pollen and Asian dust in spring, Atmospheric Environment, 55, 234–239, https://doi.org/10.1016/j.atmosenv.2012.02.061, 2012.

Fu, P. Q., Kawamura, K., Chen, J., Charrière, B., and Sempéré, R.: Organic molecular composition of marine aerosols over the Arctic Ocean in summer: contributions of primary emission and secondary aerosol formation, Biogeosciences, 10, 653–667, https://doi.org/10.5194/bg-10-653-2013, 2013.

Gosselin, M. I., Rathnayake, C. M., Crawford, I., Pöhlker, C., Fröhlich-Nowoisky, J., Schmer, B., Després, V. R., Engling, G., Gallagher, M., Stone, E., Pöschl, U., and Huffman, J. A.: Fluorescent bioaerosol particle, molecular tracer, and fungal spore concentrations during dry and rainy periods in a semi-arid forest, Atmospheric Chemistry and Physics, 16, 15165–15184, https://doi.org/10.5194/acp-16-15165-2016, 2016.

Hawkins, L. N. and Russell, L. M.: Polysaccharides, Proteins, and Phytoplankton Fragments: Four Chemically Distinct Types of Marine Primary Organic Aerosol Classified by Single Particle Spectromicroscopy, Advances in Meteorology, 2010, 612132, https://doi.org/10.1155/2010/612132, 2010.

Kirchgeorg, T., Schüpbach, S., Kehrwald, N., McWethy, D. B., and Barbante, C.: Method for the determination of specific molecular markers of biomass burning in lake sediments, Organic Geochemistry, 71, 1–6, https://doi.org/10.1016/j.orggeochem.2014.02.014, 2014.

Li, X., Chen, M., Le, H. P., Wang, F., Guo, Z., Iinuma, Y., Chen, J., and Herrmann, H.: Atmospheric outflow of PM2.5 saccharides from megacity Shanghai to East China Sea: Impact of biological and biomass burning sources, Atmospheric Environment, 143, 1–14, https://doi.org/10.1016/j.atmosenv.2016.08.039, 2016.

Marynowski, L., Łupikasza, E., Dąbrowska-Zapart, K., Małarzewski, Ł., Niedźwiedź, T., and Simoneit, B. R. T.: Seasonal and vertical variability of saccharides and other organic tracers of PM10 in relation to weather conditions in an urban environment of Upper Silesia, Poland, Atmospheric Environment, 242, 117849, https://doi.org/10.1016/j.atmosenv.2020.117849, 2020.

Medeiros, P. M., Conte, M. H., Weber, J. C., and Simoneit, B. R. T.: Sugars as source indicators of biogenic organic carbon in aerosols collected above the Howland Experimental Forest, Maine, Atmospheric Environment, 40, 1694–1705, https://doi.org/10.1016/j.atmosenv.2005.11.001, 2006.

Nirmalkar, J., Deshmukh, D. K., Deb, M. K., Tsai, Y. I., and Sopajaree, K.: Mass loading and episodic variation of molecular markers in PM2.5 aerosols over a rural area in eastern central India, Atmospheric Environment, 117, 41–50, https://doi.org/10.1016/j.atmosenv.2015.07.003, 2015.

Nirmalkar, J., Deshmukh, D. K., Deb, M. K., Tsai, Y. I., and Pervez, S.: Characteristics of aerosol during major biomass burning events over eastern central India in winter: A tracer-based approach, Atmospheric Pollution Research, 10, 817–826, https://doi.org/10.1016/j.apr.2018.12.010, 2019.

Pacini, E.: From anther and pollen ripening to pollen presentation, Pl Syst Evol, 222, 19–43, https://doi.org/10.1007/BF00984094, 2000.

Pietrogrande, M. C., Bacco, D., Visentin, M., Ferrari, S., and Casali, P.: Polar organic marker compounds in atmospheric aerosol in the Po Valley during the Supersito campaigns — Part 2: Seasonal variations of sugars, Atmospheric Environment, 97, 215–225, https://doi.org/10.1016/j.atmosenv.2014.07.056, 2014.

Ren, G., Yan, X., Ma, Y., Qiao, L., Chen, Z., Xin, Y., Zhou, M., Shi, Y., Zheng, K., Zhu, S., Huang, C., and Li, L.: Characteristics and source apportionment of PM2.5-bound saccharides and carboxylic acids in Central Shanghai, China, Atmospheric Research, 237, 104817, https://doi.org/10.1016/j.atmosres.2019.104817, 2020.

Schmidl, C., Marr, I. L., Caseiro, A., Kotianová, P., Berner, A., Bauer, H., Kasper-Giebl, A., and Puxbaum, H.: Chemical characterisation of fine particle emissions from wood stove combustion of common woods growing in mid-European Alpine regions, Atmospheric Environment, 42, 126–141, https://doi.org/10.1016/j.atmosenv.2007.09.028, 2008.

Simoneit, B. R. T. and Elias, V. O.: Detecting Organic Tracers from Biomass Burning in the Atmosphere, Marine Pollution Bulletin, 42, 805–810, https://doi.org/10.1016/S0025-326X(01)00094-7, 2001.

Simoneit, B. R. T., Elias, V. O., Kobayashi, M., Kawamura, K., Rushdi, A. I., Medeiros, P. M., Rogge, W. F., and Didyk, B. M.: Sugars--dominant water-soluble organic compounds in soils and characterization as tracers in atmospheric particulate matter, Environ Sci Technol, 38, 5939–5949, https://doi.org/10.1021/es0403099, 2004.

Tominaga, S., Matsumoto, K., Kaneyasu, N., Shigihara, A., Katono, K., and Igawa, M.: Measurements of particulate sugars at urban and forested suburban sites, Atmospheric Environment, 45, 2335–2339, https://doi.org/10.1016/j.atmosenv.2010.09.056, 2011.

Yttri, K. E., Dye, C., and Kiss, G.: Ambient aerosol concentrations of sugars and sugar-alcohols at four different sites in Norway, Atmospheric Chemistry and Physics, 7, 4267–4279, https://doi.org/10.5194/acp-7-4267-2007, 2007.

Zangrando, R., Barbaro, E., Kirchgeorg, T., Vecchiato, M., Scalabrin, E., Radaelli, M., Đorđević, D., Barbante, C., and Gambaro, A.: Five primary sources of organic aerosols in the urban atmosphere of Belgrade (Serbia), Science of The Total Environment, 571, 1441–1453, https://doi.org/10.1016/j.scitotenv.2016.06.188, 2016.

Zennaro, P., Kehrwald, N., McConnell, J. R., Schüpbach, S., Maselli, O. J., Marlon, J., Vallelonga, P., Leuenberger, D., Zangrando, R., Spolaor, A., Borrotti, M., Barbaro, E., Gambaro, A., and Barbante, C.: Fire in ice: two millennia of boreal forest fire history from the Greenland NEEM ice core, Climate of the Past, 10, 1905–1924, https://doi.org/10.5194/cp-10-1905-2014, 2014.

Zhao, Y., Ren, H., Deng, J., Li, L., Hu, W., Ren, L., Yue, S., Fan, Y., Wu, L., Li, J., Sun, Y., Wang, Z., Akimoto, H., Zeng, X., Cheng, Y., Kong, S., Su, H., Cheng, Y., Kawamura, K., and Fu, P.: High daytime abundance of primary organic aerosols over Mt. Emei, Southwest China in summer, Science of The Total Environment, 703, 134475, https://doi.org/10.1016/j.scitotenv.2019.134475, 2020.

Zhu, C., Kawamura, K., and Kunwar, B.: Organic tracers of primary biological aerosol particles at subtropical Okinawa Island in the western North Pacific Rim, Journal of Geophysical Research: Atmospheres, 120, 5504–5523, https://doi.org/10.1002/2015JD023611, 2015.