Supplement:

Airborne measurements of particulate organic matter by PTR-MS: a pilot study

Felix Piel[1,2], Markus Müller[1], Tomas Mikoviny[3], Sally Pusede[4], Armin Wisthaler[2,3]

[1]Ionicon Analytik GmbH, Innsbruck, 6020, Austria
[2]Institute for Ion Physics and Applied Physics, University of Innsbruck, Innsbruck, 6020, Austria
[3]Department of Chemistry, University of Oslo, Oslo, 0315, Norway
[4]Department of Environmental Sciences, University of Virginia, Charlottesville, VA 22904-4123, U.S.A.

Correspondence to: Armin Wisthaler (armin.wisthaler@kjemi.uio.no)

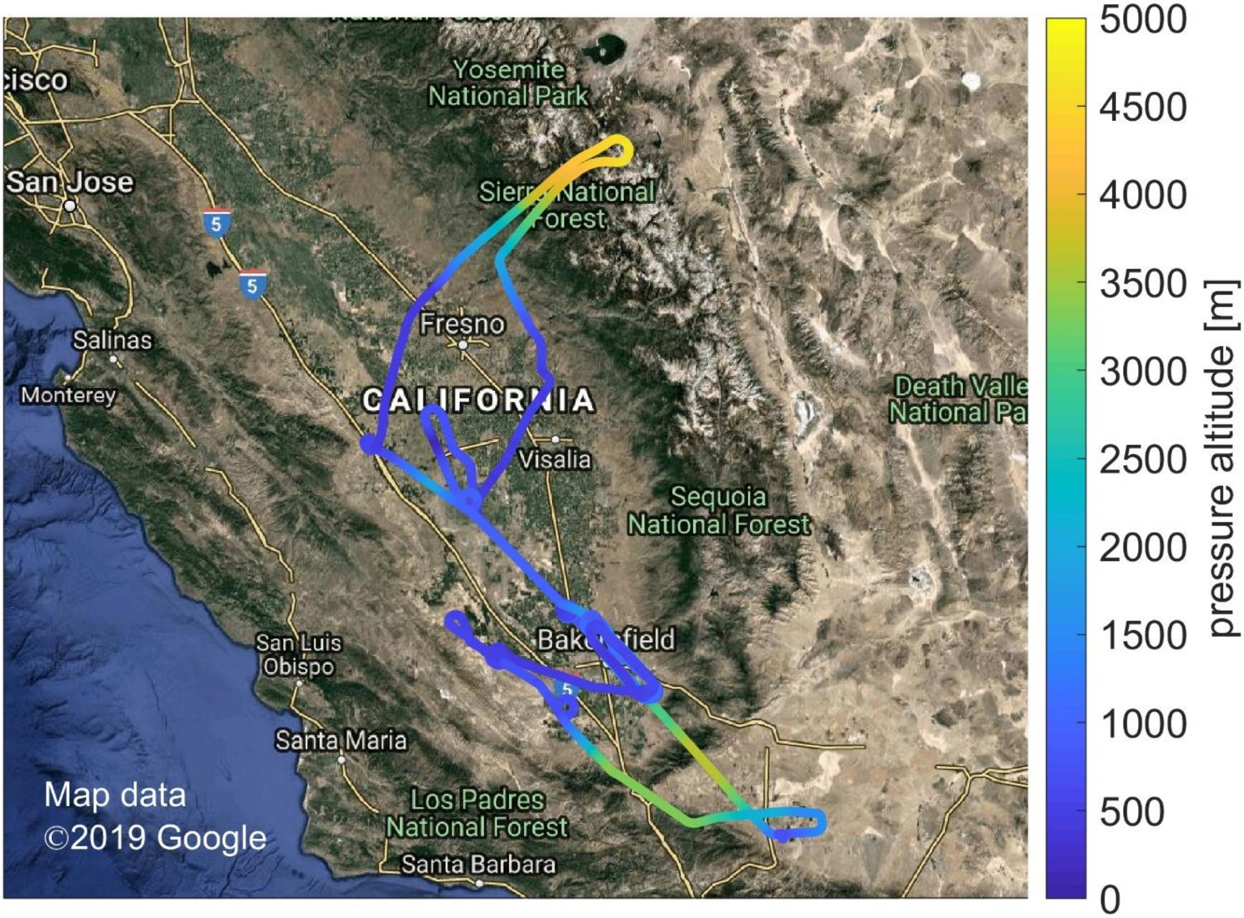

Figure S1. Track of NASA DC-8 flight #1271 carried out on 26 June 2018 between 10:36 and 15:54 hours local time over California. The color coding indicates the pressure altitude.

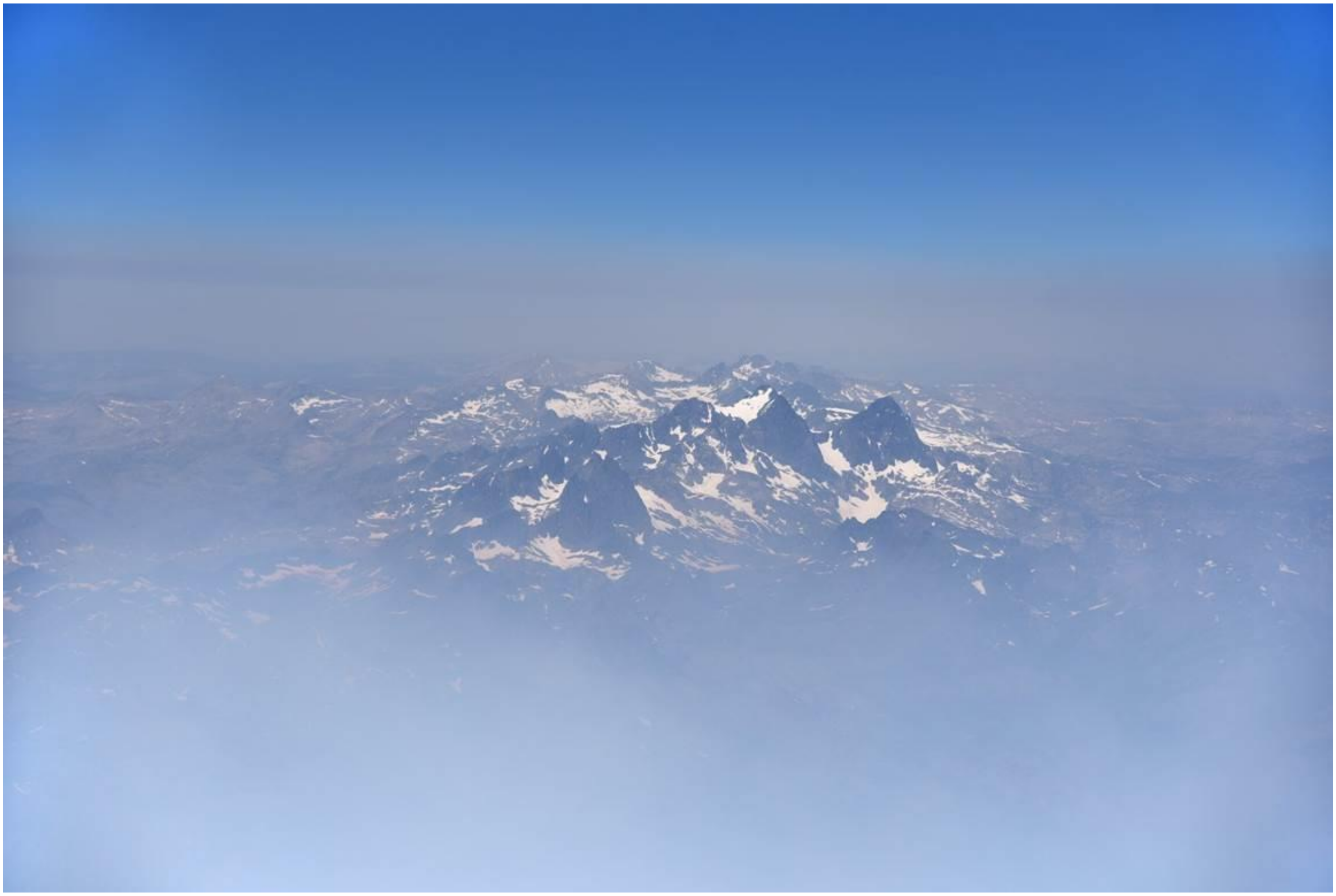

Figure S2. Photo taken from the cockpit when the NASA DC-8 skimmed the plume emanating from the Lions Fire over the Sierra Nevada Mountains in California (Photo credit: Megan Schill/NASA SARP)

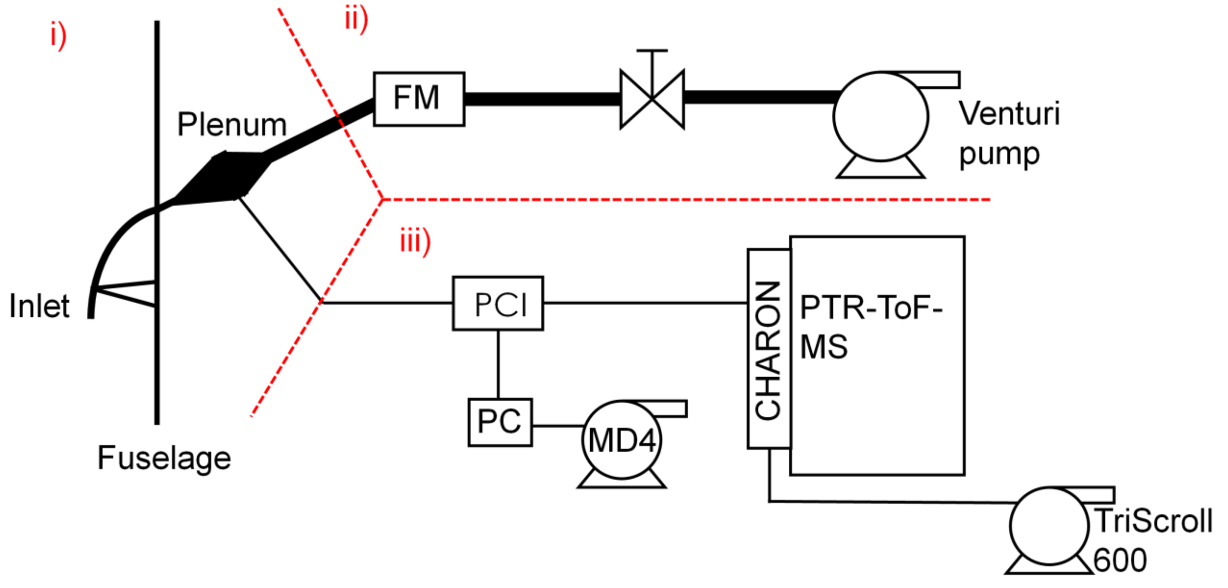

Figure S3. Scheme of the inlet system used for the CHARON PTR-ToF-MS analyzer installed aboard the NASA DC-8.The inlet system consists of i) the UH/LARGE aerosol sampling probe with a plenum for sample distribution, ii) the NOAA/ESRL/CSD flow control system which ensures isokinetic flow conditions and iii) our own pressure-controlled inlet (PCI) from which the CHARON PTR-ToF-MS analyzer takes its sample flow. FM: flow meter; PC: pressure controller, MD4: Vacuubrand MD-4 diaphragm pump; TriScroll 600: Agilent TriScroll 600 scroll pump.

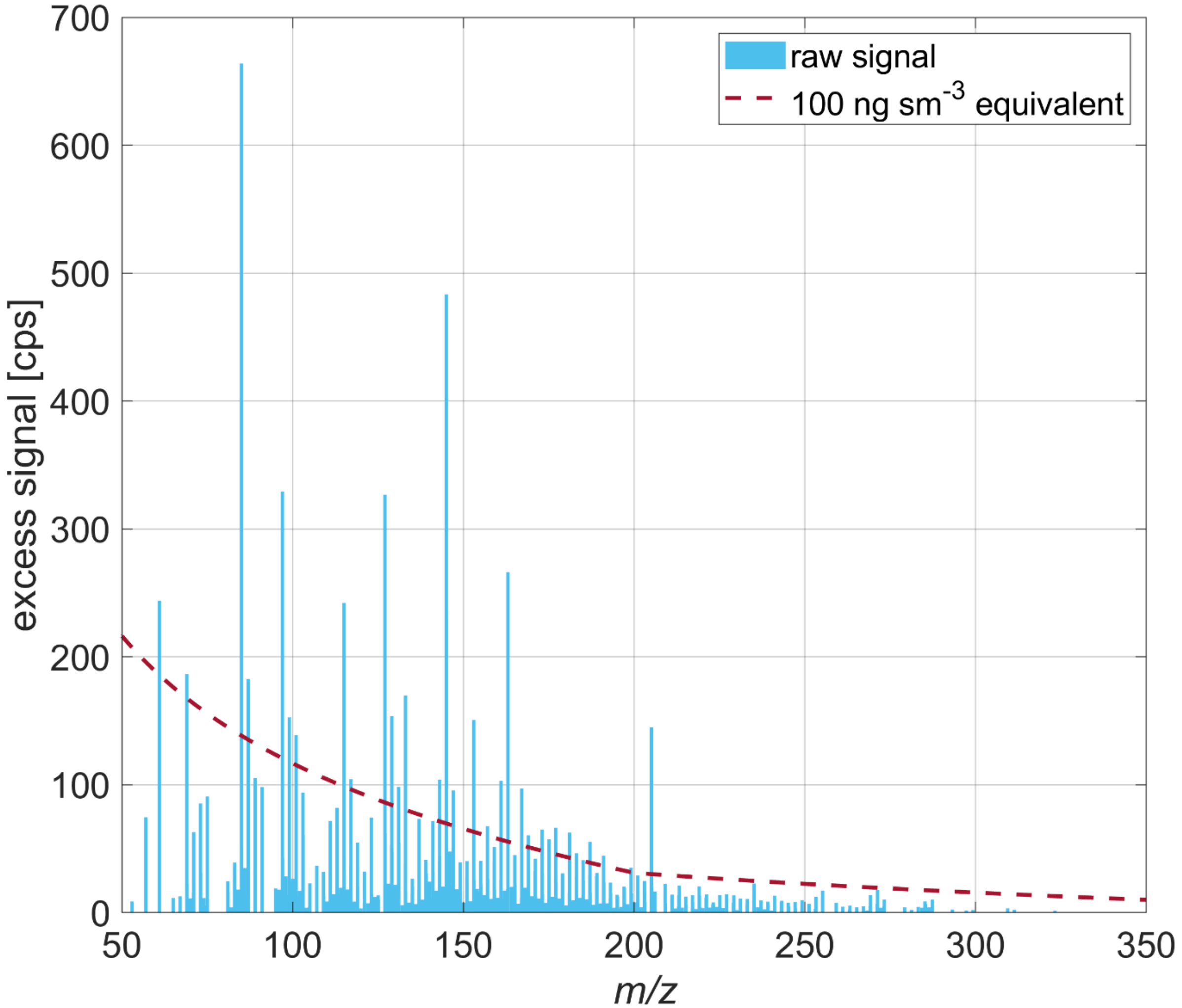

Figure S4. Average mass spectrum recorded by the CHARON PTR-ToF-MS instrument when the Lions Fire plume was sampled on 26 June 2018 between 13:03:50 and 13:04:35 hours local time. The mass spectrum is given in raw counts per second (cps), with only the 90-s pre-plume signal average being subtracted (excess signal). The dashed red line corresponds to a mass loading of 100 ng sm^{-3} at the respective *m/z*, assuming the same signal response factor (sensitivity, in cps ng^{-1} sm^{3}) as for acetone (acetone-equivalents).

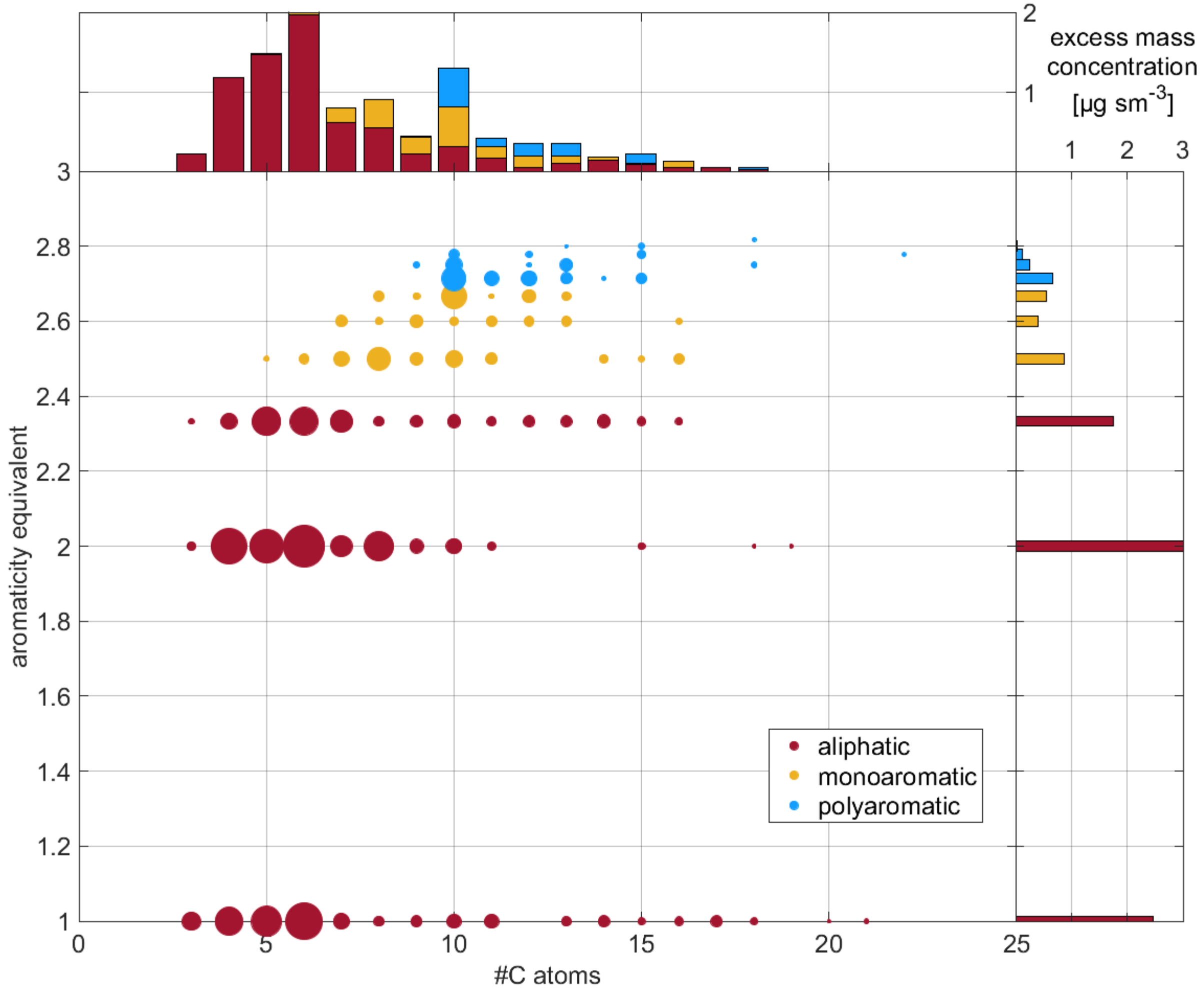

Figure S5. Plot of aromaticity equivalent vs. number of carbon atoms summarizing the qualitative and quantitative organic composition of submicrometer particles detected in the Lions Fire plume. Aliphatic, monoaromatic and polyaromatic species are shown in red, yellow and blue, respectively. Mass distributions as a function of #C atoms and of aromaticity equivalent are shown in the bar graphs above and to the right of the main figure, respectively.

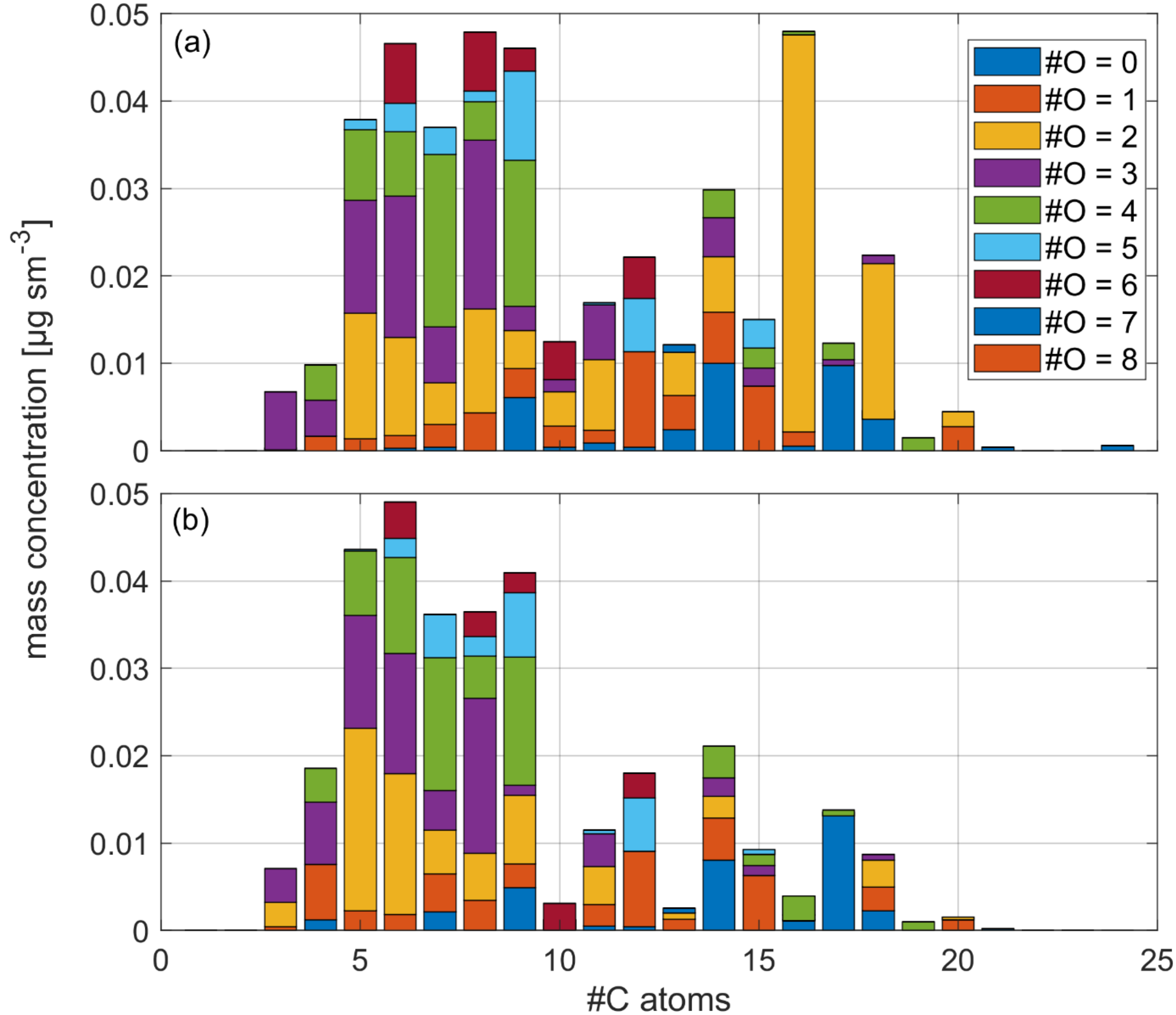

Figure S6. Elementally resolved mass concentration of organic aerosol as measured by CHARON PTR-ToF-MS in the boundary layer of the San Joaquin Valley. The upper panel (a) shows the distribution as recorded between 10:48 and 11:20 hours local time. The lower panel (b) shows the distribution as measured between 14:02 and 15:01 hours local time.

Table ST1. List of *m/z* signals, assigned ion sum formals and potential neutral precursors in biomass burning derived particles

m/z	molecular formula	name	reference
101.024	$C_4H_5O_3^+$	hydroxybutenedial	Yee 2013
101.059	$C_5H_9O_2^+$	methyl methacrylate	Gilman 2015
103.040	$C_4H_7O_3^+$	propanoic acid, 2-oxo-methyl ester	Fitzpatrick 2007
113.026	$C_5H_5O_3^+$	2,5-furandione, 3-methyl	Fitzpatrick 2007
117.059	$C_5H_9O_3^+$	acetoxyacetone	Fitzpatrick 2007
123.046	$C_7H_7O_2^+$	hydroxybenzaldehyde	Schauer 2001
		benzoic acid	Fitzpatrick 2007, Oros and Simoneit 2001, Fine 2002
127.039	$C_6H_7O_3^+$	hydroxymethylfurfural	Schauer 2001
130.049	$C_5H_8NO_3^+$	pyroglutamic acid	Jen 2018
131.033	$C_5H_7O4^+$	methoxy-hydroxy-butenedial	Yee 2013
133.054	$C_5H_9O_4^+$	methylsuccinc acid	Jen 2018
		glutaric acid	Kundu 2010
137.061	$C_8H_9O_2^+$	hydroxyacetophenones	Jen 2018, Fine 2002
137.061	$C_8H_9O_2^+$	phenylacetic acid	Fine 2004
141.060	$C_7H_9O_3^+$	3-methoxycatechol	Yee 2013
145.068	$C_{10}H_9O^+$	1/2-naphtol	Fitzpatrick 2007, Fine 2002
145.124	$C_8H_{17}O_2^+$	n-octanoc acid	Oros and Simoneit 2001
147.061	$C_6H_{11}O_4^+$	adipic acid	Graham 2002, Kundu 2010
151.079	$C_9H_{11}O_2^+$	phenylpropanoic acid	Fine 2002
		p-coumaric alcohol	Jen 2018
		vinylgluaiacol	Fine 2004
153.055	$C_8H_9O_3^+$	vanillin	Lin 2016, Simoneit 2002, Fine 2002
155.032	$C_7H_7O_4^+$	protocatechoic acid	Jen 2018
155.071	$C_8H_{11}O_3^+$	vanillyl alcohol	Oros and Simoneit 2001
		syringol	Fine 2002
159.137	$C_9H_{19}O_2^+$	nonanoic acid	Jen 2018, Oros and Simoneit 2001
161.058	$C_{10}H_9O_2^+$	dihydroxynapthalene	Jen 2018
163.035	$C_9H_7O_3^+$	umbelliferone	Jen 2018
163.061	$C_6H_{11}O_5^+$	levoglucosan	Schauer 2001, Oros and Simoneit 2002, Fine 2002
167.087	$C_{13}H_{11}^+$	fluorene	Fine 2002
169.056	$C_8H_9O_4^+$	vanillic acid	Oros and Simoneit 2001
173.153	$C_{10}H_{21}O_2^+$	n-decanoic acid	Oros and Simoneit 2001
179.087	$C_{14}H_{11}^+$	anthracene	Schauer 2001, Oros and Simoneit 2001
		phenanthrene	Jen 2018, Schauer 2001, Oros and Simoneit 2001
181.086	$C_{10}H_{13}O_3^+$	coniferyl alcohol	Jen 2018, Oros and Simoneit 2001
		guaiacylactone	Schauer 2001, Oros and Simoneit 2001
		propiovanillone	Fine 2002
		dihydroconiferyl alcohol	Jen 2018
		ethylsyringol	Fine 2002
		homovanillyl alcohol	Oros and Simoneit 2001
193.077	$C_7H_{13}O_6^+$	quinic acid	Jen 2018
195.062	$C_{10}H_{11}O_4^+$	methyl caffeate	Jen 2018
197.121	$C_{11}H_{17}O_3^+$	propylsyringol	Fine 2002
205.074	$C_8H_{13}O_6^+$	3-methyl-1,2,3-butanetricarboxylic acid	Wan 2019
209.078	$C_{11}H_{13}O_4^+$	sinapinaldeyde	Fine 2002
253.098	$C_{20}H_{13}^+$	benzopyrene	Oros and Simoneit 2001
253.202	$C_{19}H_{25}^+$	simonellite	Oros and Simoneit 2001
257.248	$C_{16}H_{33}O_2^+$	n-hexadecanoic acid	Schauer 2001, Oros and Simoneit 2001
271.258	$C_{17}H_{35}O_2^+$	n-heptadecanoic acid	Schauer 2001, Oros and Simoneit 2001
		methyl hexadecanoate	Fine 2002
285.279	$C_{18}H_{37}O_2^+$	n-octadecanoic acid	Schauer 2001, Oros and Simoneit 2001
285.279	$C_{18}H_{37}O_2^+$	methyl heptadecanoate	Fine 2002
287.281	$C_{21}H_{35}^+$	pregnene	Oros and Simoneit 2001
309.356	$C_{22}H_{45}^+$	n-docos-1-ene	Oros and Simoneit 2001
311.327	$C_{21}H_{43}O^+$	n-heneicosan-2-one	Oros and Simoneit 2001

References

Fine, P. M., Cass, G. R. and Simoneit, B. R. T.: Chemical Characterization of Fine Particle Emissions from the Fireplace Combustion of Woods Grown in the Southern United States, Environ. Sci. Technol., 36(7), 1442–1451, doi:10.1021/es0108988, 2002.

Fitzpatrick, E. M., Ross, A. B., Bates, J., Andrews, G., Jones, J. M., Phylaktou, H., Pourkashanian, M. and Williams, A.: Emission of Oxygenated Species from the Combustion of Pine Wood and its Relation to Soot Formation, Process. Saf. Environ., 85(5), 430–440, doi:10.1205/psep07020, 2007.

Gilman, J. B., Lerner, B. M., Kuster, W. C., Goldan, P. D., Warneke, C., Veres, P. R., Roberts, J. M., de Gouw, J. A., Burling, I. R. and Yokelson, R. J.: Biomass burning emissions and potential air quality impacts of volatile organic compounds and other trace gases from fuels common in the US, Atmos. Chem. Phys., 15(24), 13915–13938, doi:10.5194/acp-15-13915-2015, 2015.

Graham, B.: Water-soluble organic compounds in biomass burning aerosols over Amazonia1. Characterization by NMR and GC-MS, J. Geophys. Res., 107(D20), doi:10.1029/2001JD000336, 2002.

Jen, C. N., Hatch, L. E., Selimovic, V., Yokelson, R. J., Weber, R., Fernandez, A. E., Kreisberg, N. M., Barsanti, K. C. and Goldstein, A. H.: Speciated and total emission factors of particulate organics from burning western U.S. wildland fuels and their dependence on combustion efficiency, Atmos. Chem. Phys. Discuss., 1–22, doi:10.5194/acp-2018-840, 2018.

Kundu, S., Kawamura, K., Andreae, T. W., Hoffer, A. and Andreae, M. O.: Molecular distributions of dicarboxylic acids, ketocarboxylic acids and α-dicarbonyls in biomass burning aerosols: implications for photochemical production and degradation in smoke layers, Atmos. Chem. Phys., 10(5), 2209–2225, doi:10.5194/acp-10-2209-2010, 2010.

Lin, P., Aiona, P. K., Li, Y., Shiraiwa, M., Laskin, J., Nizkorodov, S. A. and Laskin, A.: Molecular Characterization of Brown Carbon in Biomass Burning Aerosol Particles, Environ. Sci. Technol., 50(21), 11815–11824, doi:10.1021/acs.est.6b03024, 2016.

Oros, D. R. and Simoneit, B. R. T.: Identification and emission factors of molecular tracers in organic aerosols from biomass burning Part 1. Temperate climate conifers, Appl. Geochem., 16(13), 1513–1544, doi:10.1016/S0883-2927(01)00021-X, 2001.

Schauer, J. J., Kleeman, M. J., Cass, G. R. and Simoneit, B. R. T.: Measurement of Emissions from Air Pollution Sources. 3. C_1–C_{29} Organic Compounds from Fireplace Combustion of Wood, Environ. Sci. Technol., 35(9), 1716–1728, doi:10.1021/es001331e, 2001.

Simoneit, B. R. T.: Biomass burning — a review of organic tracers for smoke from incomplete combustion, Appl. Geochem., 17(3), 129–162, doi:10.1016/S0883-2927(01)00061-0, 2002.

Wan, X., Kang, S., Rupakheti, M., Zhang, Q., Tripathee, L., Guo, J., Chen, P., Rupakheti, D., Panday, A. K., Lawrence, M. G., Kawamura, K. and Cong, Z.: Molecular characterization of organic aerosols in the Kathmandu Valley, Nepal: insights into primary and secondary sources, Atmos. Chem. Phys., 19(5), 2725–2747, doi:10.5194/acp-19-2725-2019, 2019.

Yee, L. D., Kautzman, K. E., Loza, C. L., Schilling, K. A., Coggon, M. M., Chhabra, P. S., Chan, M. N., Chan, A. W. H., Hersey, S. P., Crounse, J. D., Wennberg, P. O., Flagan, R. C. and Seinfeld, J. H.: Secondary organic aerosol formation from biomass burning intermediates: phenol and methoxyphenols, Atmos. Chem. Phys., 13(16), 8019–8043, doi:10.5194/acp-13-8019-2013, 2013.