Molecular composition of clouds: a comparison between samples collected at tropical (Réunion Island, France) and mid-north (puy de Dôme, France) latitudes.

Lucas Pailler[1], Laurent Deguillaume[1,2], Hélène Lavanant[3], Isabelle Schmitz[3], Marie Hubert[3], Edith Nicol[4], Mickaël Ribeiro[1], Jean-Marc Pichon[2], Mickaël Vaïtilingom[5], Pamela Dominutti[1,#], Frédéric Burnet[6], Pierre Tulet[7], Maud Leriche[1,8], Angelica Bianco[1,*]

[1] Laboratoire de Météorologie Physique, UMR 6016, CNRS, Université Clermont Auvergne, 63178 Aubière, France.

[2] Observatoire de Physique du Globe de Clermont-Ferrand, UMS 833, CNRS, Université Clermont Auvergne, 63178 Aubière, France.

[3] Univ Rouen Normandie, INSA Rouen Normandie, CNRS, Normandie Univ, COBRA UMR 6014, INC3M FR 3038, F-76000 Rouen, France

[4] Laboratoire de Chimie Moléculaire (LCM), CNRS UMR 9168, Ecole Polytechnique, Institut Polytechnique de Paris, route de Saclay, 91128 Palaiseau cedex, France

[5] Laboratoire de Recherche en Géosciences et Énergies (LaRGE), EA 4539, Université des Antilles, Pointre-à-Pitre, 97110,
France

[6] Centre National de Recherches Météorologiques (CNRM), Université de Toulouse, Météo-France, CNRS, Toulouse, France

[7] Laboratoire d'Aérologie (LAERO), UMR 5560, CNRS, Université Toulouse III, IRD, Toulouse, 31400, France

[8] Centre pour l'étude et la simulation du climat à l'échelle régionale, Département des sciences de la terre et de l'atmosphère (ESCER), Université du Québec à Montréal, Montréal, H2X 3Y7, Canada

[#] now at Institut des Géosciences de l'Environnement (IGE), UMR 5001, CNRS, IRD, Université Grenoble Alpes, Grenoble, 38000, France

Correspondence to: Angelica Bianco (a.bianco@opgc.fr), Laurent Deguillaume (laurent.deguillaume@uca.fr)

The Supplementary information is composed by:

- Formula used in this study
- Five tables
- Six Figures
- References

Formula used in this study:

Determination of Aromaticity index (AI): AI is determined as the ratio between $DBE_{AI(mod)}$ and the number of carbon atoms C, as described by Melendez-Perez et al. (Melendez-Perez et al., 2016)

$$DBE_{AI(mod)} = 1 + \frac{1}{2} \times (2C - H - O - 2S - N)$$

$$AI = \frac{DBE_{AI(mod)}}{C} = \; (1 + \frac{1}{2} \times (2C - H - O - 2S - N))/C$$

And if $DBE_{AI} \leq 0$, then AI = 0. AI measures C-C double bond density and also integrates the contribution of π-bonds by heteroatoms.

CHO Index

$$CHO_{Index} = \frac{2 \times O - H}{C}$$

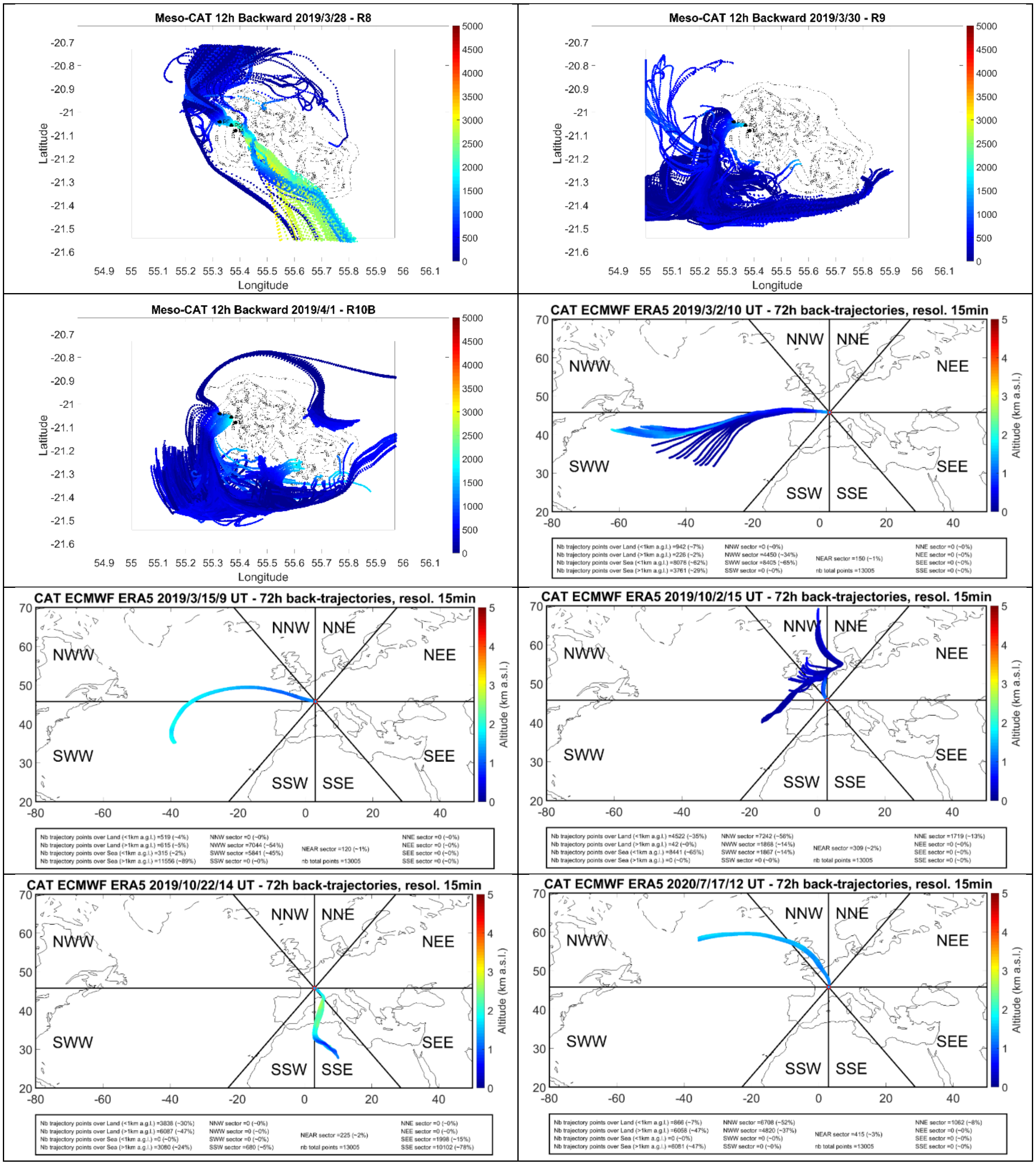
Determination of carbon oxidation state (OSC): the carbon oxidation state (OSC) is an ideal metric to measure the degree of oxidation of organic species in the atmosphere 15 and it is calculated using Equation S3 and S4

$$OSC = \sum\nolimits_i OS_i \times \frac{n_i}{n_c}$$

$$OSC = 2 \times \frac{O}{C} - \frac{H}{C} - 3\frac{N}{C} - 2\frac{S}{C}$$

This parameter was used to investigate the carbon oxidation state in organic aerosol by Kroll et al. (Kroll et al., 2011)

Table S1: Back trajectory plots on 12 h of the air masses corresponding to R8, R9 and R10B, computed with Meso-CAT, resulting from the coupling between high-resolution Meso-NH simulations and the lagrangian tool CAT and back trajectory plots on 72 h of the air masses corresponding to PUY samples using the lagrangian tool CAT.



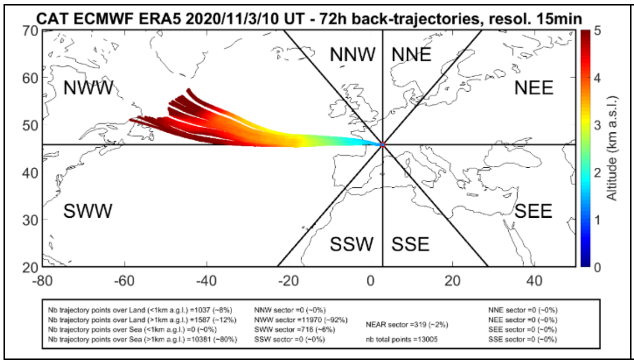
```
Nb trajectory points over Land (<1km a.g.l.) =942 (~7%)      NNW sector =0 (~0%)                                 NNE sector =0 (~0%)
Nb trajectory points over Land (>1km a.g.l.) =226 (~2%)      NWW sector =4450 (~34%)   NEAR sector =150 (~1%)    NEE sector =0 (~0%)
Nb trajectory points over Sea (<1km a.g.l.) =8076 (~62%)     SWW sector =8405 (~65%)                             SEE sector =0 (~0%)
Nb trajectory points over Sea (>1km a.g.l.) =3761 (~29%)     SSW sector =0 (~0%)       nb total points =13005    SSE sector =0 (~0%)
```

```
Nb trajectory points over Land (<1km a.g.l.) =519 (~4%)      NNW sector =0 (~0%)                                 NNE sector =0 (~0%)
Nb trajectory points over Land (>1km a.g.l.) =615 (~5%)      NWW sector =7044 (~54%)   NEAR sector =120 (~1%)    NEE sector =0 (~0%)
Nb trajectory points over Sea (<1km a.g.l.) =315 (~2%)       SWW sector =5841 (~45%)                             SEE sector =0 (~0%)
Nb trajectory points over Sea (>1km a.g.l.) =11556 (~89%)    SSW sector =0 (~0%)       nb total points =13005    SSE sector =0 (~0%)
```

```
Nb trajectory points over Land (<1km a.g.l.) =4522 (~35%)    NNW sector =7242 (~56%)                             NNE sector =1719 (~13%)
Nb trajectory points over Land (>1km a.g.l.) =42 (~0%)       NWW sector =1868 (~14%)   NEAR sector =309 (~2%)    NEE sector =0 (~0%)
Nb trajectory points over Sea (<1km a.g.l.) =8441 (~65%)     SWW sector =1867 (~14%)                             SEE sector =0 (~0%)
Nb trajectory points over Sea (>1km a.g.l.) =0 (~0%)         SSW sector =0 (~0%)       nb total points =13005    SSE sector =0 (~0%)
```

```
Nb trajectory points over Land (<1km a.g.l.) =3838 (~30%)    NNW sector =0 (~0%)                                 NNE sector =0 (~0%)
Nb trajectory points over Land (>1km a.g.l.) =6087 (~47%)    NWW sector =0 (~0%)       NEAR sector =225 (~2%)    NEE sector =0 (~0%)
Nb trajectory points over Sea (<1km a.g.l.) =0 (~0%)         SWW sector =0 (~0%)                                 SEE sector =1998 (~15%)
Nb trajectory points over Sea (>1km a.g.l.) =3080 (~24%)     SSW sector =680 (~5%)     nb total points =13005    SSE sector =10102 (~78%)
```

```
Nb trajectory points over Land (<1km a.g.l.) =866 (~7%)      NNW sector =6708 (~52%)                             NNE sector =1062 (~8%)
Nb trajectory points over Land (>1km a.g.l.) =6058 (~47%)    NWW sector =4820 (~37%)   NEAR sector =415 (~3%)    NEE sector =0 (~0%)
Nb trajectory points over Sea (<1km a.g.l.) =0 (~0%)         SWW sector =0 (~0%)                                 SEE sector =0 (~0%)
Nb trajectory points over Sea (>1km a.g.l.) =6081 (~47%)     SSW sector =0 (~0%)       nb total points =13005    SSE sector =0 (~0%)
```



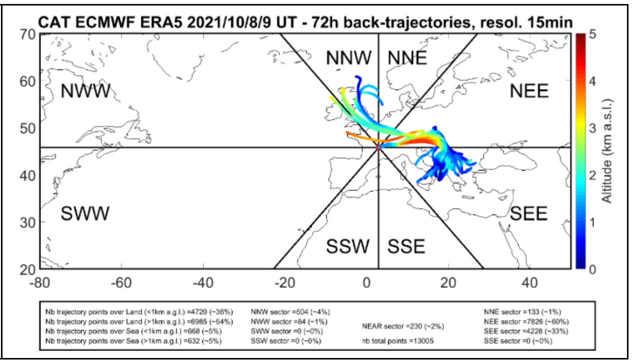


Table S2: Ancillary measurements performed on REU samples and reported in Dominutti et al. 2022.

Sampling characteristics		**R8**	**R9**	**R10B**
DOC [mgC L^{-1}]	TC	9.3	9.3	18.1
	IC	1.5	3.5	1.2
	TOC	7.9	5.8	17.0
Carboxylic acids [µM]	Acetic	31.3	16.8	29.8
	Formic	9.1	10.0	12.2
Dicarboxylic acids [µM]	Oxalic	1.6	0.3	0.4
	Lactic	4.3	0.6	1.0
	Malonic	1.1	0.7	1.7
	Succinic	0.7	0.6	1.3
	Glutaric	0.1	0.1	0.1
Carbonyls [µM]	Formaldehyde	2.9	1.0	0.9
	Acetaldehyde	0.3	0.2	0.3
	Acetone	0.2	0.2	0.6
VOC *[ng mL $^{-1}$]*	Benzene	0.3	0.1	0.2
	Toluene	0.1	0.2	0.1
	Ethylbenzene	0.1	0.2	0.0
	m+p-xylene	0.1	0.0	0.0
	o-xylene	0.0	0.0	0.0

Table S3: Classes of water soluble organic compounds defined by Kroll et al. (2011).

	#C		OSC	
	min	max	min	max
Hydrocarbon-like organic aerosol (HOA)	18	30	-2	-1
Biomass burning organic aerosol (BBOA)	7	22	-1.5	-0.5
Semivolatile oxidized organic aerosol (SV-OOA)	5	17	-0.5	0.5
Low-volatility oxidized organic aerosol (LV-OOA)	4	12	0.2	1

Table S4: Molecular formulas of SOA tracers of isoprene, alpha and beta pinene, limonene, alpha and gamma terpinene, terpinolene, beta caryophyllene in cloud water collected at REU (yellow) and at PUY (blue). The table reports also molecular formula attributed to nitroaromatics, brown carbon, aminoacids and sugars. The intensity of formulas identified in cloud samples is reported in light blue in the corresponding cell. NM: not measured.

Samples	**R8**	**R9**	**R10B**	**02/03/2019**	**15/03/2019**	**02/10/2019**	**22/10/2019**	**17/07/2020**	**03/11/2020**	**08/10/2020**
Organosulfate formation from isoprene										
Surratt et al., 2008										
C4H8O7S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H8O7S	6.1E+06	NM	NM	NM	NM	NM	NM	NM	NM	1.3E+07
C5H11NO8S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H11NO9S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C8H14O10S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.6E+07
C5H10N2O11S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C10H20O10S	NM	NM	NM	NM	NM	NM	NM	NM	NM	2.3E+07
C10H22O10S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C8H13NO12S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H32O13S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Products of isoprene ozonolysis in the presence of sulfate										
Riva et al., 2016 a										
C3H6O5S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C3H6O6S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H10O7S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.6E+07
C5H12O7S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H8O6S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H12O6S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H8O5S	4.0E+06	1.3E+06	NM	NM	NM	NM	NM	NM	NM	5.9E+06
C5H10O5S	4.0E+06	2.1E+06	9.6E+05	4.4E+06	NM	NM	NM	NM	NM	2.8E+07
C5H10O6S	1.1E+07	3.5E+06	1.9E+06	NM	1.1E+07	NM	NM	NM	NM	2.4E+07
C8H10O4S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.1E+07
C6H12O7S	3.6E+06	NM	1.3E+06	NM	NM	NM	NM	NM	NM	3.6E+07
C9H14O6S	5.8E+06	4.1E+06	2.0E+06	NM	5.8E+06	NM	NM	NM	NM	7.1E+07
C9H16O7S	3.8E+07	NM	7.4E+06	5.6E+06	NM	9.3E+06	NM	9.0E+06	7.7E+06	1.7E+07
C10H20O9S	2.8E+06	NM	1.2E+06	NM	NM	NM	NM	NM	NM	2.4E+07

C13H12O10S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H16O12S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Oxidation of isoprene										
Riva et al., 2016 b										
C4H6O3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H6O4	1.2E+06	NM	NM	NM	NM	2.8E+07	NM	NM	NM	NM
C4H8O4	9.7E+05	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H8O5	NM	9.8E+05	1.3E+06	NM	NM	7.3E+06	NM	NM	NM	NM
C5H8O6S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.3E+07
C5H12O8S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C8H14O7S	1.5E+07	6.6E+06	3.6E+06	NM	NM	9.8E+06	NM	4.7E+06	NM	1.5E+08
C7H14O8S	1.6E+06	NM	NM	NM	NM	NM	NM	NM	NM	3.2E+07
C6H14O9S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C8H16O8S	3.6E+06	1.8E+06	2.2E+06	NM	NM	NM	NM	NM	NM	4.6E+07
C10H18O7S	1.9E+07	1.7E+07	5.8E+06	1.5E+07	7.3E+06	NM	NM	NM	NM	2.6E+08
C10H18O8S	2.3E+07	1.4E+07	NM	7.5E+06	1.6E+07	7.3E+06	NM	5.4E+06	NM	1.8E+08
C10H20O8S	9.7E+06	7.2E+06	NM	3.2E+07	6.7E+06	NM	NM	NM	NM	3.4E+07
C10H20O10S	NM	NM	NM	NM	NM	NM	NM	NM	NM	2.3E+07
C10H22O10S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C12H24O11S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.1E+07
C15H28O11S	2.7E+06	2.1E+06	NM	NM	NM	NM	NM	NM	NM	NM
C15H28O12S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H30O12S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H30O13S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C20H40O15S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Organosulfate formation from alpha-pinene										
Surratt et al., 2008										
C7H12O6S	7.8E+06	4.9E+06	1.8E+06	NM	NM	4.6E+06	NM	NM	NM	1.1E+08
C5H8O8S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C8H14O6S	1.8E+07	9.8E+06	4.8E+06	4.9E+06	5.8E+06	1.0E+07	NM	NM	NM	1.5E+08
C10H16O5S	6.1E+06	5.1E+06	NM	1.1E+07	8.0E+06	NM	NM	NM	NM	3.0E+07
C10H18O5S	4.1E+06	4.6E+06	1.3E+06	1.3E+07	6.6E+06	NM	NM	NM	NM	1.3E+08
C10H18O6S	2.3E+07	1.7E+07	6.5E+06	1.5E+07	2.0E+07	NM	NM	NM	NM	1.8E+08
C10H16O7S	1.4E+07	1.2E+07	4.7E+06	7.8E+06	5.2E+06	NM	NM	NM	NM	4.3E+08
C10H18O7S	1.9E+07	1.7E+07	5.8E+06	1.5E+07	7.3E+06	NM	NM	NM	NM	2.6E+08
C10H17NO7S	NM	NM	NM	9.3E+06	7.9E+06	NM	NM	NM	NM	4.5E+08
C10H18O8S	2.3E+07	1.4E+07	NM	7.5E+06	1.6E+07	7.3E+06	NM	5.4E+06	NM	1.8E+08
C10H17NO8S	NM	2.5E+06	NM	NM	NM	NM	NM	NM	NM	1.7E+08
C10H16N2O9S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C10H17NO10S	6.4E+06	6.9E+06	NM	NM	NM	NM	NM	NM	NM	9.3E+08
C10H16N2O10S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.9E+07
Organosulfate formation from beta-pinene										

Surratt et al., 2008										
C10H18O6S	2.3E+07	1.7E+07	6.5E+06	1.5E+07	2.0E+07	NM	NM	NM	NM	1.8E+08
C10H16O6S	9.9E+06	7.1E+06	3.1E+06	1.0E+07	NM	NM	NM	NM	NM	1.2E+08
C10H16O7S	1.4E+07	1.2E+07	4.7E+06	7.8E+06	5.2E+06	NM	NM	NM	NM	4.3E+08
C10H18O7S	1.9E+07	1.7E+07	5.8E+06	1.5E+07	7.3E+06	NM	NM	NM	NM	2.6E+08
C10H20O7S	1.6E+07	1.2E+07	5.9E+06	1.3E+07	NM	NM	NM	NM	NM	6.0E+07
C10H17NO7S	NM	NM	NM	9.3E+06	7.9E+06	NM	NM	NM	NM	4.5E+08
C10H17NO8S	NM	2.5E+06	NM	NM	NM	NM	NM	NM	NM	1.7E+08
C10H17NO9S	NM	2.4E+06	NM	6.6E+06	NM	NM	NM	NM	NM	3.7E+08
C10H17NO10S	6.4E+06	6.9E+06	NM	NM	NM	NM	NM	NM	NM	9.3E+08
Alpha pinene dimer esters										
Kristensen et al., 2016										
C15H26O6	NM	NM	NM	NM	NM	1.5E+07	NM	NM	NM	NM
C16H24O6	NM	NM	NM	1.2E+08	6.5E+07	1.1E+07	6.1E+06	NM	6.7E+06	4.7E+07
C16H26O6	NM	NM	NM	1.6E+08	8.1E+07	1.4E+07	4.6E+06	7.7E+06	NM	5.5E+07
C15H24O7	NM	NM	NM	1.6E+08	1.0E+08	3.3E+07	7.9E+06	1.5E+07	7.5E+06	1.1E+08
C16H24O7	NM	NM	NM	8.8E+07	6.4E+07	2.2E+07	4.6E+06	9.5E+06	5.4E+06	6.5E+07
C16H26O7	NM	NM	NM	1.4E+08	8.4E+07	2.2E+07	5.2E+06	1.1E+07	4.8E+06	7.9E+07
C15H24O8	NM	NM	NM	6.6E+07	5.1E+07	3.5E+07	5.6E+06	1.9E+07	5.1E+06	1.6E+08
C19H28O5	NM	NM	NM	5.3E+07	2.7E+07	NM	NM	NM	NM	1.0E+07
C19H30O5	NM	NM	NM	4.7E+07	2.9E+07	NM	NM	NM	NM	1.1E+07
C18H28O6	NM	NM	NM	9.6E+07	5.5E+07	6.9E+06	NM	NM	4.5E+06	3.9E+07
C17H26O7	NM	NM	NM	1.4E+08	8.0E+07	1.8E+07	6.0E+06	6.9E+06	1.1E+07	6.9E+07
C16H24O8	NM	NM	NM	5.0E+07	4.0E+07	2.8E+07	6.3E+06	1.2E+07	6.7E+06	1.1E+08
C17H28O7	NM	NM	NM	1.5E+08	7.6E+07	1.5E+07	6.0E+06	7.7E+06	6.0E+06	5.3E+07
C19H30O6	1.1E+07	1.2E+07	1.1E+07	5.8E+07	4.2E+07	5.6E+06	NM	NM	NM	1.7E+07
C18H28O7	NM	NM	NM	8.4E+07	5.4E+07	1.2E+07	5.2E+06	NM	6.7E+06	4.6E+07
C17H26O8	NM	NM	NM	1.1E+07	4.5E+07	2.0E+07	NM	9.1E+06	9.6E+06	7.5E+07
C17H28O8	NM	NM	NM	8.6E+07	4.9E+07	1.5E+07	NM	7.2E+06	NM	7.9E+07
C16H26O9	1.3E+07	8.0E+06	5.6E+06	NM	NM	3.0E+07	NM	NM	NM	NM
C19H28O7	NM	NM	NM	8.1E+07	4.9E+07	8.6E+06	NM	NM	7.0E+06	3.8E+07
C19H30O7	NM	NM	NM	7.4E+07	6.1E+07	2.7E+07	6.3E+06	NM	1.6E+07	2.8E+07
C18H28O8	1.7E+07	1.5E+07	9.8E+06	1.1E+07	4.4E+07	1.5E+07	NM	9.8E+06	4.7E+06	5.6E+07
C17H26O9	1.6E+07	9.5E+06	7.3E+06	2.6E+07	2.3E+07	2.0E+07	4.8E+06	9.7E+06	4.9E+06	8.9E+07
C16H26O10	6.9E+06	3.0E+06	2.9E+06	6.9E+06	5.3E+06	8.7E+06	NM	NM	NM	8.4E+07
C19H28O8	1.6E+07	1.4E+07	9.4E+06	5.1E+07	3.2E+07	1.0E+07	NM	NM	5.2E+06	4.5E+07
C19H30O8	1.4E+07	1.5E+07	1.0E+07	7.4E+07	4.0E+07	1.2E+07	4.7E+06	NM	NM	4.5E+07
C18H28O9	1.4E+07	1.0E+07	6.9E+06	5.8E+06	2.4E+07	1.5E+07	5.4E+06	9.4E+06	NM	6.7E+07
C19H28O9	1.3E+07	8.3E+06	6.6E+06	3.0E+07	2.1E+07	1.2E+07	NM	5.6E+06	4.8E+06	4.1E+07
C18H30O10	5.6E+06	3.7E+06	2.5E+06	1.1E+07	7.2E+06	7.1E+06	NM	NM	NM	5.3E+07
Alpha pinene products in aerosol samples										
Kourtchev et al., 2013										

C8H12O5	2.5E+08	1.2E+08	1.6E+08	NM	NM	1.3E+08	NM	NM	NM	NM
C8H12O6	NM	NM	NM	NM	NM	9.7E+07	NM	NM	NM	NM
Organosulfate formation from limonene										
Surratt et al., 2008										
C7H12O7S	NM	NM	NM	NM	NM	4.9E+06	NM	1.2E+07	NM	1.3E+08
C9H14O6S	5.8E+06	4.1E+06	2.0E+06	NM	5.8E+06	NM	NM	NM	NM	7.1E+07
C9H16O6S	1.6E+07	1.1E+07	5.4E+06	9.5E+06	8.6E+06	7.6E+06	NM	6.0E+06	NM	2.1E+08
C9H16O7S	3.8E+07	NM	7.4E+06	5.6E+06	NM	9.3E+06	NM	9.0E+06	7.7E+06	1.7E+07
C10H16O7S	1.4E+07	1.2E+07	4.7E+06	7.8E+06	5.2E+06	NM	NM	NM	NM	4.3E+08
C10H18O7S	1.9E+07	1.7E+07	5.8E+06	1.5E+07	7.3E+06	NM	NM	NM	NM	2.6E+08
C9H15NO8S	NM	1.3E+06	NM	7.0E+06	NM	NM	NM	NM	NM	1.3E+08
C9H15NO9S	5.6E+06	3.9E+06	1.7E+06	NM	NM	NM	NM	NM	NM	1.9E+08
C10H17NO9S	NM	2.4E+06	NM	6.6E+06	NM	NM	NM	NM	NM	3.7E+08
C10H19NO9S	5.6E+06	4.3E+06	NM	9.1E+06	NM	NM	NM	NM	NM	2.7E+08
C9H17NO10S	4.3E+06	4.2E+06	NM	NM	NM	NM	NM	NM	NM	1.0E+08
C10H18N2O11S	NM	NM	NM	NM	NM	NM	NM	NM	NM	3.9E+08
C10H18N2O12S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Limonene products in aerosol samples										
Kourtchev et al., 2013										
C9H14O4	1.4E+08	1.0E+08	7.0E+07	NM	NM	1.0E+08	NM	NM	NM	NM
Oxydation products										
Finessi et al. 2014										
C7H10O4	NM	NM	NM	1.4E+07	1.7E+07	4.7E+07	NM	3.5E+07	7.6E+06	6.4E+08
C8H12O4	NM	NM	NM	NM	NM	1.2E+08	NM	NM	NM	NM
C10H16O4	1.2E+08	8.9E+07	5.4E+07	NM	NM	6.4E+07	NM	NM	NM	NM
C8H12O4	NM	NM	NM	NM	NM	1.2E+08	NM	NM	NM	NM
C9H14O4	1.4E+08	1.0E+08	7.0E+07	NM	NM	1.0E+08	NM	NM	NM	NM
C10H16O3	NM	NM	NM	NM	NM	3.2E+07	NM	NM	NM	NM
C19H18O7	NM	NM	NM	NM	NM	NM	NM	NM	NM	9.7E+06
Organosulfate formation from alpha-terpinene										
Surratt et al., 2008										
C8H14O7S	1.5E+07	6.6E+06	3.6E+06	NM	NM	9.8E+06	NM	4.7E+06	NM	1.5E+08
C10H18O6S	2.3E+07	1.7E+07	6.5E+06	1.5E+07	2.0E+07	NM	NM	NM	NM	1.8E+08
C10H16O7S	1.4E+07	1.2E+07	4.7E+06	7.8E+06	5.2E+06	NM	NM	NM	NM	4.3E+08
C10H18O7S	1.9E+07	1.7E+07	5.8E+06	1.5E+07	7.3E+06	NM	NM	NM	NM	2.6E+08
C9H16O8S	7.6E+06	4.2E+06	3.2E+06	NM	5.7E+06	NM	NM	5.8E+06	NM	1.3E+08
C10H20O7S	1.6E+07	1.2E+07	5.9E+06	1.3E+07	NM	NM	NM	NM	NM	6.0E+07
C10H17NO7S	NM	NM	NM	9.3E+06	7.9E+06	NM	NM	NM	NM	4.5E+08
C10H18O8S	2.3E+07	1.4E+07	NM	7.5E+06	1.6E+07	7.3E+06	NM	5.4E+06	NM	1.8E+08
C10H17NO8S	NM	2.5E+06	NM	NM	NM	NM	NM	NM	NM	1.7E+08
C10H17NO10S	6.4E+06	6.9E+06	NM	NM	NM	NM	NM	NM	NM	9.3E+08
C10H18N2O11S	NM	NM	NM	NM	NM	NM	NM	NM	NM	3.9E+08

Organosulfate formation from gamma-terpinene										
Surratt et al., 2008										
C10H16O7S	1.4E+07	1.2E+07	4.7E+06	7.8E+06	5.2E+06	NM	NM	NM	NM	4.3E+08
C10H17NO8S	NM	2.5E+06	NM	NM	NM	NM	NM	NM	NM	1.7E+08
C10H18N2O11S	NM	NM	NM	NM	NM	NM	NM	NM	NM	3.9E+08
Organosulfate formation from terpinolene										
Surratt et al., 2008										
C9H14O6S	5.8E+06	4.1E+06	2.0E+06	NM	5.8E+06	NM	NM	NM	NM	7.1E+07
C10H18O5S	4.1E+06	4.6E+06	1.3E+06	1.3E+07	6.6E+06	NM	NM	NM	NM	1.3E+08
C10H18O6S	2.3E+07	1.7E+07	6.5E+06	1.5E+07	2.0E+07	NM	NM	NM	NM	1.8E+08
C10H18O7S	1.9E+07	1.7E+07	5.8E+06	1.5E+07	7.3E+06	NM	NM	NM	NM	2.6E+08
C10H20O7S	1.6E+07	1.2E+07	5.9E+06	1.3E+07	NM	NM	NM	NM	NM	6.0E+07
C10H17NO7S	NM	NM	NM	9.3E+06	7.9E+06	NM	NM	NM	NM	4.5E+08
C10H18O8S	2.3E+07	1.4E+07	NM	7.5E+06	1.6E+07	7.3E+06	NM	5.4E+06	NM	1.8E+08
C10H17NO9S	NM	2.4E+06	NM	6.6E+06	NM	NM	NM	NM	NM	3.7E+08
C10H18N2O11S	NM	NM	NM	NM	NM	NM	NM	NM	NM	3.9E+08
Products of β-caryophyllene										
Chan et al., 2011										
C9H14O4	1.4E+08	1.0E+08	7.0E+07	NM	NM	1.0E+08	NM	NM	NM	NM
C10H16O5	2.5E+08	1.5E+08	1.0E+08	NM	NM	1.6E+08	NM	NM	NM	NM
C14H20O4	NM	NM	NM	5.5E+07	2.4E+07	NM	NM	NM	NM	1.7E+07
C15H24O3	NM	NM	NM	3.5E+07	1.7E+07	NM	NM	NM	NM	9.7E+06
C14H22O4	NM	NM	NM	NM	NM	8.6E+06	NM	NM	NM	NM
C13H20O5	NM	NM	NM	3.9E+08	2.1E+08	3.5E+07	1.1E+07	1.6E+07	1.1E+07	1.3E+08
C14H24O4	NM	NM	NM	NM	NM	5.8E+06	NM	NM	NM	NM
C15H22O4	NM	NM	NM	7.1E+07	3.2E+07	NM	NM	NM	NM	1.4E+07
C14H20O5	NM	NM	NM	1.0E+08	6.2E+07	1.7E+07	NM	6.4E+06	5.8E+06	4.8E+07
C15H24O4	NM	NM	NM	NM	NM	5.3E+06	NM	NM	NM	NM
C14H22O5	NM	NM	NM	NM	NM	2.3E+07	NM	NM	NM	NM
C15H26O4	NM	NM	NM	1.3E+08	4.5E+07	NM	NM	NM	NM	1.8E+07
C14H24O5	NM	NM	NM	2.3E+08	1.1E+08	1.4E+07	6.3E+06	6.6E+06	7.3E+06	4.6E+07
C15H24O5	NM	NM	NM	2.6E+08	1.0E+08	1.2E+07	5.7E+06	NM	NM	5.0E+07
C14H22O6	NM	NM	NM	2.0E+08	1.4E+08	4.3E+07	9.4E+06	2.1E+07	1.2E+07	9.2E+07
C15H26O5	NM	NM	NM	2.5E+08	8.6E+07	7.5E+06	NM	NM	NM	3.8E+07
C17H26O4	NM	NM	NM	NM	NM	1.5E+07	NM	NM	NM	NM
C13H28O8	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H22O7	NM	NM	NM	8.2E+07	6.0E+07	3.6E+07	5.7E+06	1.4E+07	7.5E+06	8.9E+07
C16H26O6	NM	NM	NM	1.6E+08	8.1E+07	1.4E+07	4.6E+06	7.7E+06	NM	5.5E+07
C14H24O8	2.2E+07	1.3E+07	1.1E+07	3.1E+07	2.4E+07	1.0E+07	NM	8.7E+06	4.7E+06	1.1E+08
C17H28O6	NM	NM	NM	NM	NM	9.1E+06	NM	NM	NM	NM
C16H26O7	NM	NM	NM	1.4E+08	8.4E+07	2.2E+07	5.2E+06	1.1E+07	4.8E+06	7.9E+07
C17H30O6	NM	NM	NM	NM	NM	5.4E+06	NM	NM	NM	NM

C10H13NO3	9.5E+06	4.0E+06	2.9E+06	7.9E+06	7.2E+06	5.2E+06	NM	NM	NM	1.6E+07
C16H27NO7	8.5E+06	6.1E+06	4.9E+06	2.8E+07	3.3E+07	7.5E+06	NM	4.7E+06	NM	3.7E+07
C15H25NO8	7.2E+06	6.7E+06	5.7E+06	1.3E+07	1.0E+07	7.6E+06	NM	NM	NM	6.4E+07
C14H23NO9	3.8E+06	2.5E+06	1.7E+06	6.0E+06	5.3E+06	1.1E+07	NM	NM	NM	6.6E+07
C15H27NO8	3.8E+06	3.0E+06	3.0E+06	7.8E+06	NM	NM	NM	NM	NM	3.4E+07
C13H22N2O9	2.0E+06	NM	NM	NM	NM	NM	NM	NM	NM	1.9E+07
C15H25NO9	4.1E+06	2.9E+06	2.1E+06	NM	NM	8.6E+06	NM	NM	NM	6.1E+07
C16H29NO8	3.7E+06	2.0E+06	2.1E+06	NM	NM	NM	NM	NM	NM	2.9E+07
C17H29NO8	4.5E+06	4.0E+06	2.3E+06	1.3E+07	1.0E+07	6.9E+06	NM	NM	NM	3.7E+07
C24H38N2O12	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C9H16O6S	1.6E+07	1.1E+07	5.4E+06	9.5E+06	8.6E+06	7.6E+06	NM	6.0E+06	NM	2.1E+08
C14H24O5S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H26O5S	NM	5.7E+06	4.4E+06	NM	NM	NM	NM	NM	NM	NM
C14H23O6S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C14H22O7S	5.0E+06	6.2E+06	2.4E+06	1.4E+07	7.3E+06	NM	NM	NM	NM	1.7E+07
C15H26O6S	1.5E+07	1.8E+07	9.7E+06	3.9E+07	1.2E+07	NM	NM	NM	NM	NM
C15H24O7S	1.4E+07	2.1E+07	9.6E+06	4.6E+07	1.3E+07	NM	NM	NM	NM	1.9E+07
C14H22O8S	8.3E+06	6.7E+06	3.5E+06	1.0E+07	6.0E+06	NM	NM	NM	NM	2.6E+07
C15H26O7S	2.0E+07	3.5E+07	1.3E+07	6.1E+07	2.2E+07	NM	NM	NM	NM	1.8E+07
C14H24O8S	1.3E+07	1.4E+07	6.8E+06	1.9E+07	1.3E+07	NM	NM	NM	NM	2.9E+07
C15H24O8S	1.1E+07	1.3E+07	6.2E+06	2.9E+07	1.1E+07	NM	NM	NM	NM	3.0E+07
C16H28O7S	NM	4.9E+06	NM	1.4E+07	7.2E+06	NM	NM	NM	NM	1.0E+07
C16H28O8S	5.8E+06	7.7E+06	NM	1.7E+07	9.3E+06	NM	NM	NM	NM	1.4E+07
C15H25NO7S	6.3E+06	1.5E+07	5.7E+06	2.2E+07	7.8E+06	NM	NM	NM	NM	6.0E+06
C14H24NO9S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Nitroaromatic compounds										
Zhang et al., 2013										
C6H5NO3	NM	NM	NM	6.4E+06	4.4E+06	5.8E+06	NM	NM	NM	1.3E+07
C8H9NO3	8.5E+06	4.0E+06	NM	5.6E+06	7.5E+06	4.1E+06	NM	NM	NM	1.3E+07
C7H7NO3	1.3E+06	NM	NM	4.8E+06	5.0E+06	4.5E+06	NM	NM	NM	9.8E+06
C7H7NO4	3.1E+06	2.8E+06	1.5E+06	6.7E+06	NM	NM	NM	NM	NM	2.3E+07
C7H6N2O5	NM	NM	NM	NM	NM	NM	NM	NM	NM	4.2E+07
C9H11NO3	1.3E+07	4.6E+06	5.9E+06	2.5E+07	1.8E+07	1.3E+07	5.6E+06	NM	NM	2.6E+07
C10H13NO3	9.5E+06	4.0E+06	2.9E+06	7.9E+06	7.2E+06	5.2E+06	NM	NM	NM	1.6E+07
C11H15NO3	NM	NM	NM	1.5E+07	6.3E+06	NM	NM	NM	NM	9.9E+06
C16H9NO3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H5NO4	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.2E+07
C7H5NO5	9.7E+06	6.2E+06	3.1E+06	NM	6.4E+06	4.3E+06	NM	NM	NM	2.0E+07
C10H7NO3	1.7E+06	1.4E+06	1.1E+06	1.4E+07	1.3E+07	NM	NM	NM	NM	8.5E+06
C12H9NO4	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C14H13NO3	1.5E+06	NM	NM	NM	NM	NM	NM	NM	NM	NM
Brown carbon assigned molecular formula										
Lin et al., 2018										

C8H8O3	2.6E+06	NM	1.8E+06	2.1E+07	3.7E+07	1.0E+07	NM	NM	NM	3.4E+07
C9H6O4	2.4E+06	2.0E+06	NM	NM	NM	NM	NM	NM	NM	2.3E+07
C6H5NO5	1.2E+06	NM	NM	NM	NM	NM	NM	NM	NM	5.7E+06
C8H10O5S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C10H8O4	7.9E+06	5.7E+06	2.8E+06	8.3E+06	7.3E+06	NM	NM	NM	NM	3.5E+07
C9H10O3	2.1E+07	1.6E+07	2.0E+07	NM	NM	5.7E+06	NM	NM	NM	NM
C12H12O4	6.2E+06	5.2E+06	NM	1.8E+07	1.5E+07	NM	NM	NM	NM	2.7E+07
C6H5NO4	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.2E+07
C10H10O3	8.8E+06	7.0E+06	4.5E+06	2.4E+07	1.8E+07	NM	NM	NM	NM	2.6E+07
C11H12O4	1.6E+07	1.2E+07	7.3E+06	3.2E+07	4.2E+07	1.1E+07	6.6E+06	5.7E+06	4.6E+06	3.7E+07
C8H7NO4	NM	3.2E+06	2.3E+06	4.3E+06	NM	NM	NM	NM	NM	1.4E+07
C7H7NO4	3.1E+06	2.8E+06	1.5E+06	6.7E+06	NM	NM	NM	NM	NM	2.3E+07
C8H9NO5	3.7E+06	1.8E+06	1.6E+06	NM	NM	4.4E+06	NM	NM	NM	4.2E+07
C8H9NO4	6.4E+06	3.3E+06	2.2E+06	5.9E+06	6.1E+06	5.0E+06	NM	NM	NM	2.4E+07
C10H11NO5	NM	NM	NM	1.4E+07	1.1E+07	5.9E+06	NM	NM	NM	3.1E+07
C11H13NO5	NM	NM	NM	1.8E+07	1.2E+07	7.6E+06	NM	NM	NM	4.3E+07
C18H16O8	NM	NM	NM	NM	NM	NM	NM	NM	NM	8.8E+06
C10H7NO3	1.7E+06	1.4E+06	1.1E+06	1.4E+07	1.3E+07	NM	NM	NM	NM	8.5E+06
C9H11NO4	1.4E+07	5.4E+06	3.9E+06	5.9E+06	6.9E+06	4.2E+06	NM	NM	NM	5.3E+07
C10H13NO4	1.5E+07	6.5E+06	4.5E+06	1.5E+07	1.1E+07	5.6E+06	NM	NM	NM	4.4E+07
C13H13NO4	3.0E+06	NM	NM	7.6E+06	5.8E+06	NM	NM	NM	NM	5.0E+06
C11H13NO4	NM	NM	NM	2.7E+07	2.0E+07	7.0E+06	NM	NM	NM	3.9E+07
C17H14O4	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H14O4	2.3E+06	2.4E+06	NM	4.7E+06	NM	NM	NM	NM	NM	4.9E+06
C17H10O	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C16H10O	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C19H10O	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C21H12O	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C21H10O2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Brown carbon assigned molecular formula										
Hapsari Budisulistiorini et al., 2017										
C10H10O4	2.8E+07	2.1E+07	1.3E+07	NM	NM	1.1E+07	NM	NM	NM	NM
C9H6O3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C8H8O3	2.6E+06	NM	1.8E+06	2.1E+07	3.7E+07	1.0E+07	NM	NM	NM	3.4E+07
C6H12O4S	NM	NM	1.5E+06	NM	NM	NM	NM	NM	NM	1.6E+07
C10H8O4	7.9E+06	5.7E+06	2.8E+06	8.3E+06	7.3E+06	NM	NM	NM	NM	3.5E+07
C9H8O3	1.4E+07	9.7E+06	5.1E+06	2.5E+07	2.5E+07	NM	NM	NM	NM	2.9E+07
C9H10O4	NM	NM	NM	2.2E+07	2.2E+07	7.3E+06	NM	4.7E+06	NM	5.5E+07
C11H12O5	2.2E+07	1.4E+07	9.7E+06	2.3E+07	1.9E+07	1.2E+07	NM	NM	5.3E+06	6.5E+07
C6H6O3	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.1E+07
C13H16O4	1.1E+07	1.4E+07	1.0E+07	3.5E+07	2.7E+07	5.1E+06	NM	NM	NM	1.6E+07
C13H14O6S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.1E+07
C12H14O7S	NM	NM	NM	5.8E+06	NM	NM	NM	NM	NM	2.2E+07

C18H20O5S	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.3E+07
C23H22O7	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C15H8O5	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H5NO3	NM	NM	NM	6.4E+06	4.4E+06	5.8E+06	NM	NM	NM	1.3E+07
C7H7NO3	1.3E+06	NM	NM	4.8E+06	5.0E+06	4.5E+06	NM	NM	NM	9.8E+06
C6H5NO4	NM	NM	NM	NM	NM	NM	NM	NM	NM	1.2E+07
C7H7NO4	3.1E+06	2.8E+06	1.5E+06	6.7E+06	NM	NM	NM	NM	NM	2.3E+07
C7H8O3	1.8E+06	NM	1.4E+06	NM	NM	NM	NM	NM	NM	NM
C14H18O2S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C9H12O2	1.7E+06	1.4E+06	NM	NM	NM	NM	NM	NM	NM	6.1E+06
C11H10O3	2.1E+06	1.9E+06	1.7E+06	NM	NM	NM	NM	NM	NM	7.2E+06
C10H10O3	8.8E+06	7.0E+06	4.5E+06	2.4E+07	1.8E+07	NM	NM	NM	NM	2.6E+07
C8H10O3S	NM	1.5E+06	NM	NM	4.8E+06	NM	NM	NM	NM	1.6E+07
C12H18O4S	NM	NM	NM	5.8E+06	NM	NM	NM	NM	NM	NM
C12H18O5S	NM	NM	NM	NM	NM	NM	NM	NM	NM	8.4E+06
C17H18O5	2.6E+06	2.9E+06	1.8E+06	5.4E+06	NM	NM	NM	NM	NM	1.0E+07
C10H12O3	8.7E+06	6.3E+06	5.4E+06	2.1E+07	2.7E+07	5.0E+06	NM	NM	NM	2.0E+07
C12H10O2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C11H14O5S	1.1E+07	6.5E+06	5.1E+06	1.4E+07	1.9E+07	5.9E+06	NM	NM	NM	5.1E+07
C15H20O6S	NM	NM	NM	8.4E+06	6.4E+06	NM	NM	NM	NM	NM
C11H14O6S	1.6E+06	NM	NM	NM	NM	NM	NM	NM	NM	2.4E+07
C14H18O4	NM	NM	NM	NM	NM	5.2E+06	NM	NM	NM	NM
C14H14O4	NM	2.5E+06	1.1E+06	5.6E+06	6.1E+06	NM	NM	NM	NM	8.4E+06
C10H18O4S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C10H14O2	9.5E+06	1.6E+07	1.0E+07	5.8E+06	5.3E+06	NM	NM	NM	NM	NM
C16H16O4	1.7E+06	2.1E+06	1.7E+06	NM	NM	NM	NM	NM	NM	NM
C15H23N3O2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Amino acids										
C3H7NO2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H14N4O2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H8N2O3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H7NO4	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C3H7NO2S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H10N2O3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H9NO4	NM	NM	NM	6.3E+06	9.5E+06	4.3E+06	NM	NM	NM	1.3E+07
C2H5NO2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H9N3O2	NM	NM	NM	NM	6.1E+06	NM	NM	NM	NM	NM
C6H13NO2	NM	NM	NM	5.8E+06	4.9E+06	4.4E+06	NM	NM	NM	5.9E+06
C6H13NO2	NM	NM	NM	5.8E+06	4.9E+06	4.4E+06	NM	NM	NM	5.9E+06
C6H14N2O2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H11NO2S	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C9H11NO2	NM	NM	NM	2.8E+07	1.7E+07	4.3E+06	NM	NM	NM	5.7E+07
C5H9NO2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM

C3H7NO3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H9NO3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C11H12N2O2	NM	NM	NM	5.1E+06	NM	NM	NM	NM	NM	8.4E+06
C9H11NO3	1.3E+07	4.6E+06	5.9E+06	2.5E+07	1.8E+07	1.3E+07	5.6E+06	NM	NM	2.6E+07
C5H11NO2	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
Sugars										
C5H12O5	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H10O5	5.7E+06	2.6E+06	3.7E+06	5.5E+06	6.2E+06	NM	NM	NM	NM	8.2E+06
C5H12O5	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H10O4	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H8O4	9.7E+05	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H12O6	NM	NM	NM	1.3E+07	9.6E+06	4.0E+07	NM	1.3E+07	NM	1.2E+07
C6H14O6	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H10O5	6.5E+07	3.0E+07	4.1E+07	NM	NM	3.3E+07	NM	NM	NM	NM
C6H12O6	NM	NM	NM	1.3E+07	9.6E+06	4.0E+07	NM	1.3E+07	NM	1.2E+07
C6H12O6	NM	NM	NM	1.3E+07	9.6E+06	4.0E+07	NM	1.3E+07	NM	1.2E+07
C6H12O6	NM	NM	NM	1.3E+07	9.6E+06	4.0E+07	NM	1.3E+07	NM	1.2E+07
C12H22O11	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H10O5	6.5E+07	3.0E+07	4.1E+07	NM	NM	3.3E+07	NM	NM	NM	NM
C12H24O11	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C12H22O11	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H14O6	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C6H10O5	6.5E+07	3.0E+07	4.1E+07	NM	NM	3.3E+07	NM	NM	NM	NM
C6H12O6	NM	NM	NM	1.3E+07	9.6E+06	4.0E+07	NM	1.3E+07	NM	1.2E+07
C18H32O16	NM	NM	NM	NM	1.4E+07	NM	NM	NM	NM	NM
C6H12O5	2.5E+07	9.9E+06	1.3E+07	1.2E+07	1.4E+07	7.2E+06	NM	6.5E+06	NM	4.7E+07
C5H10O5	5.7E+06	2.6E+06	3.7E+06	5.5E+06	6.2E+06	NM	NM	NM	NM	8.2E+06
C7H12O6	NM	NM	NM	NM	NM	1.9E+07	NM	NM	NM	NM
C6H14O6	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C12H22O11	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C4H10O4	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C12H22O11	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H12O5	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C5H10O5	5.7E+06	2.6E+06	3.7E+06	5.5E+06	6.2E+06	NM	NM	NM	NM	8.2E+06
C5H12O4	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM
C3H8O3	NM	NM	NM	NM	NM	NM	NM	NM	NM	NM

Table S5: Table of loadings, showing the correlation between the first six PCs and the samples (loadings). Color varies from blue (-1) to red (+1), with 0 represented in white.

	PC1	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**
R8	0.51	-0.21	-0.01	-0.03	-0.02	0.01
R9	0.50	-0.24	0.02	-0.14	-0.10	0.09
R10B	0.51	-0.24	0.01	-0.13	-0.12	0.10
02/03/2019	0.06	0.10	0.73	0.33	0.04	0.45
15/03/2019	0.15	0.26	0.57	-0.01	-0.06	-0.47
02/10/2019	0.29	0.04	-0.20	0.64	0.61	-0.28
22/10/2019	0.13	0.40	-0.14	-0.21	0.41	0.62
17/07/2020	0.20	0.46	-0.22	0.24	-0.46	-0.03
03/11/2020	0.20	0.51	-0.17	0.10	-0.30	0.03
08/10/2021	0.15	0.36	0.10	-0.58	0.36	-0.32

Figure S1: a) Comparison of the number of carbons (#C), of hydrogen (#H), of oxygen (#O), of nitrogen (#N) and of sulphur (#S), the DBE, the elemental ratios (oxygen to carbon (O/C), hydrogen to carbon (H/C), nitrogen to carbon (N/C) and sulphur to carbon (S/C)), the carbon oxidation state (OSC), the aromaticity index (AI) and the CHO Index for all the molecular formula presented in samples collected at PUY, in blue, and at REU, in yellow. b), c), d) e) and f) similarly to a), for all the CHO, CHNO, CHOS, CHNOS, and CHOSP compounds, respectively.

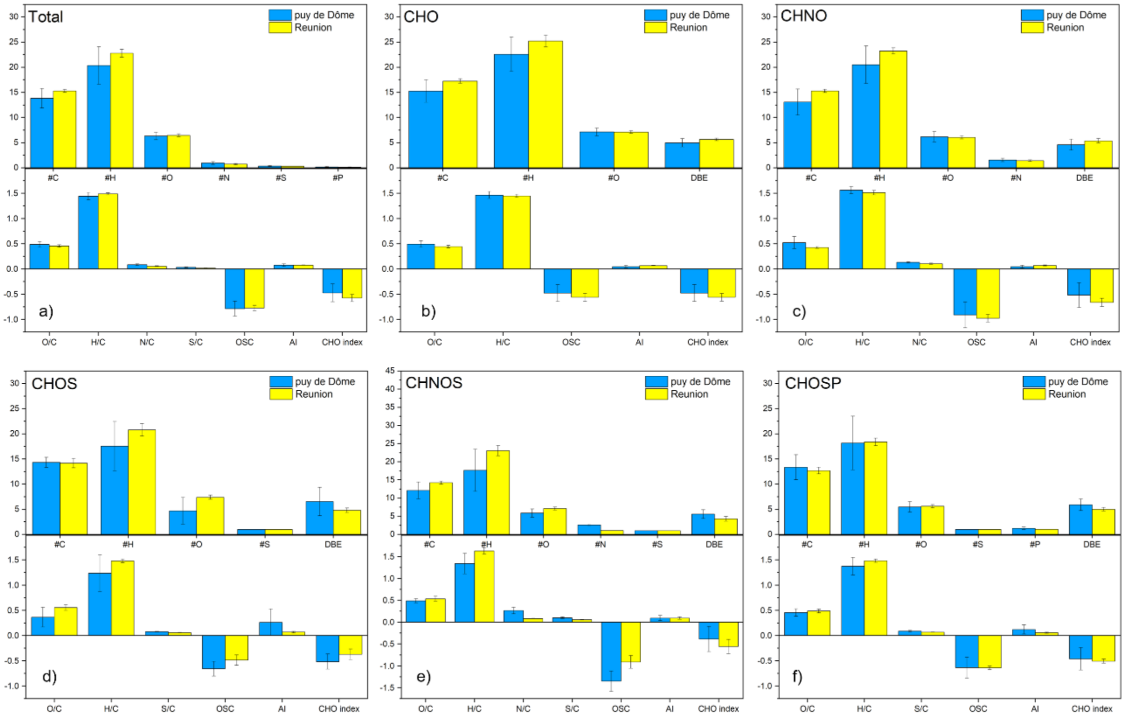


Figure S2: Results of the ANOVA test used to investigate the differences of OSC between PUY and REU samples. The y-axis reports the pair of samples and the color depicts if the difference is significant (red) or not (black).

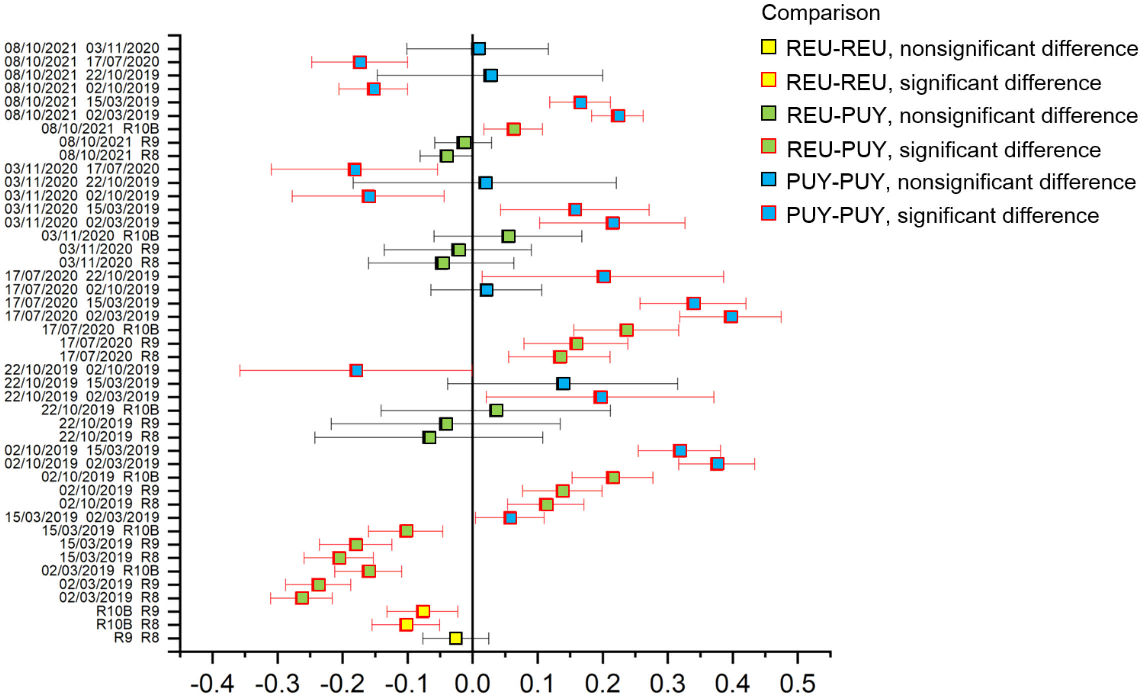


Figure S3: Average OSC for samples collected at PUY (blue) and REU (yellow) for CHO, CHNO, CHOS and CHNOS compounds.

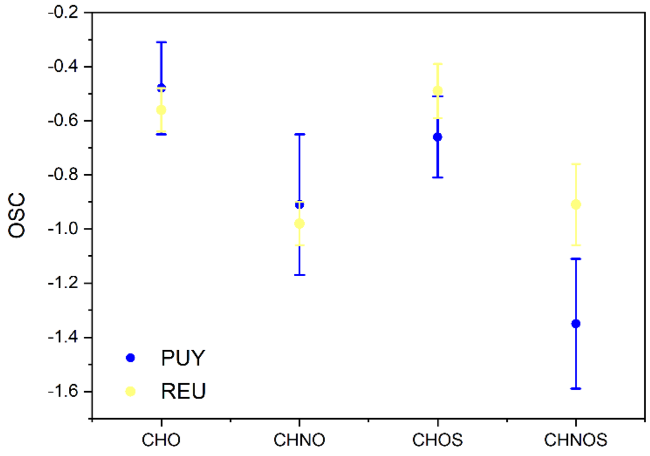


Figure S4: Bubble plot of the OSC – nC space for samples collected at PUY (02/03/2019, 15/03/2019 and 17/07/2020). The intensity of the bubble is proportional to the intensity of the mass signal for all the formulas with the same OSC, normalized by the highest intensity of the mass spectrum.

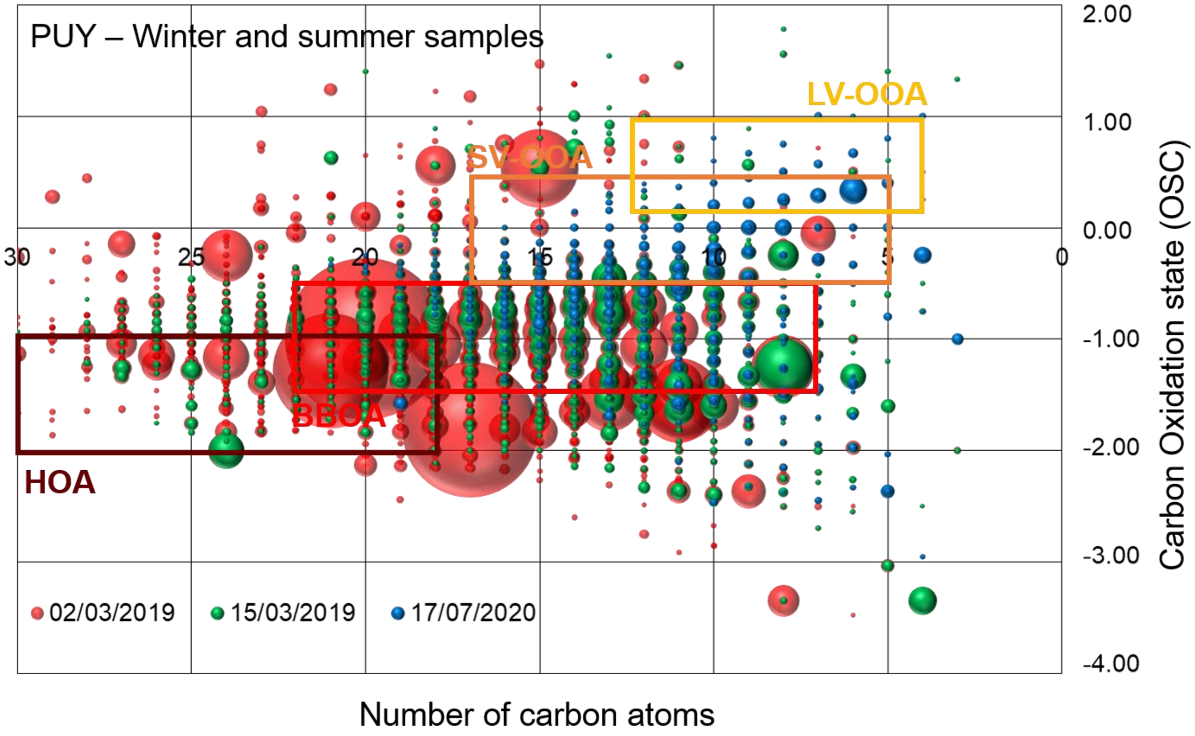


Figure S5: Stacked histogram of the relative contribution (in %) of the Rivas-Ubach categories for samples collected at REU and PUY.

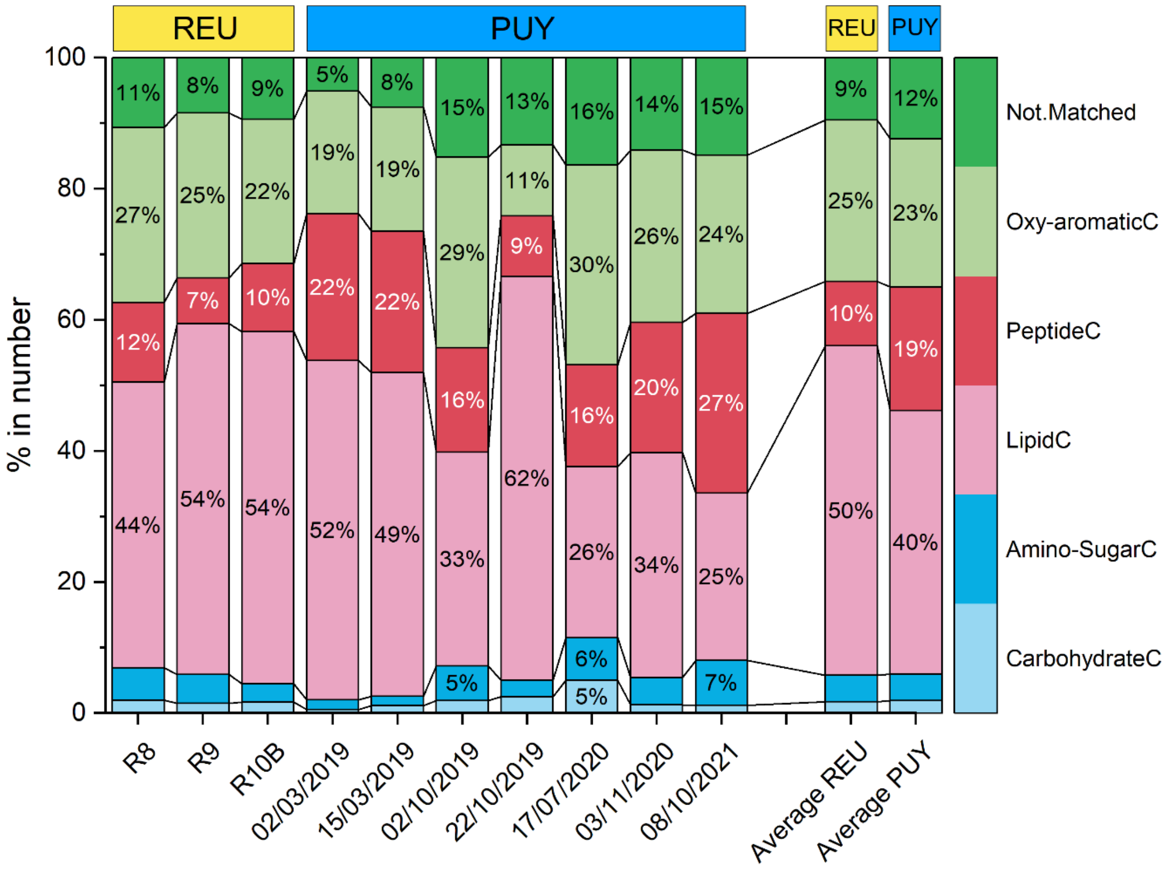
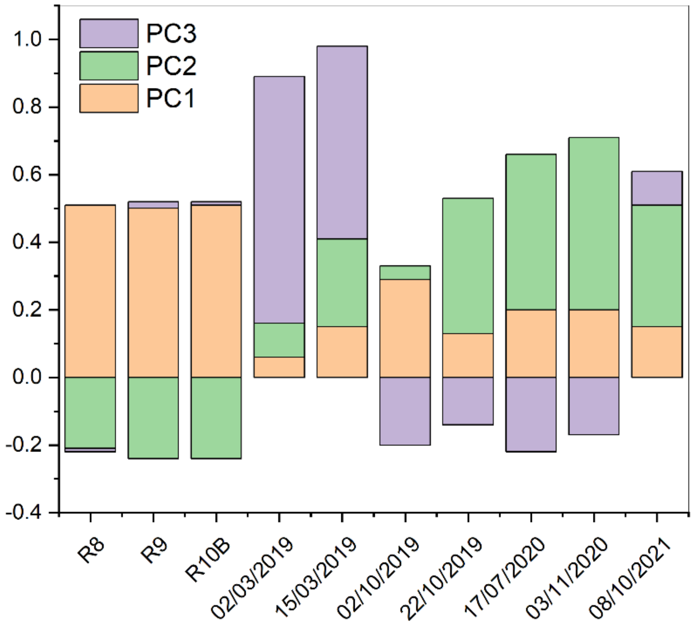


Figure S6: stacked histogram of the first three PCs, explaining 63% of the total variance, to the representation of the loadings.



References

Kroll, J. H., Donahue, N. M., Jimenez, J. L., Kessler, S. H., Canagaratna, M. R., Wilson, K. R., Altieri, K. E., Mazzoleni, L. R., Wozniak, A. S., Bluhm, H., Mysak, E. R., Smith, J. D., Kolb, C. E., and Worsnop, D. R.: Carbon oxidation state as a metric for describing the chemistry of atmospheric organic aerosol, Nature Chemistry, 3, 133–139, https://doi.org/10.1038/nchem.948, 2011.

Melendez-Perez, J. J., Martínez-Mejia, M. J., and Eberlin, M. N.: A reformulated aromaticity index equation under consideration for non-aromatic and non-condensed aromatic cyclic carbonyl compounds, Organic Geochemistry, 95, 29–33, https://doi.org/10.1016/j.orggeochem.2016.02.002, 2016.