Supplement of Atmos. Chem. Phys., 18, 5799–5819, 2018
https://doi.org/10.5194/acp-18-5799-2018-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Organic aerosol in the summertime southeastern United States: components and their link to volatility distribution, oxidation state and hygroscopicity

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Table S1. Volatility distribution, average volatility and vaporization enthalpy for each PMF factor and for the total OA.

OA Type	**Saturation Concentration C^* (μg m^{-3})**				**ΔH_{vap} (kJ mol^{-1})**
	10^{-1}	1	10	Average C^*	
			a_m=1		
MO-OOA	0.44	0.14	0.42	0.95±0.31	89±10
LO-OOA	0.27	0.19	0.54	1.88±0.32	58±13
Isoprene-OA	0.41	0.16	0.43	1.05±0.30	63±15
BBOA	0.47	0.29	0.24	0.59±0.22	55±11
Total OA	0.54	0.19	0.27	0.55±0.29	86±9
			a_m=0.1		
MO-OOA	0.23	0.17	0.60	2.36±3.33	100
LO-OOA	0.52	0.18	0.30	0.59±3.17	98±6
Isoprene-OA	0.60	0.10	0.30	0.49±3.53	96±8
BBOA	0.64	0.19	0.17	0.34±2.48	86±9
Total OA	0.65	0.09	0.25	0.40±3.53	100
			a_m=0.01		
MO-OOA	0.46	0.11	0.43	0.92±3.74	150
LO-OOA	0.40	0.06	0.54	1.41±3.32	121±25
Isoprene-OA	0.32	0.12	0.56	1.72±2.93	113±22
BBOA	0.32	0.35	0.32	1.00±2.47	100
Total OA	0.40	0.19	0.41	1.00±3.16	100
			a_m=1, CE_{TD}=0.9*CE_{BP}		
MO-OOA	0.41	0.24	0.35	0.86±2.97	86±9
LO-OOA	0.42	0.29	0.28	0.73±3.69	63±15
Isoprene-OA	0.39	0.25	0.36	0.95±2.70	54±10
BBOA	0.52	0.46	0.02	0.32±1.89	54±10
Total OA	0.19	0.19	0.62	2.64±4.5	58±13

Table S2: Volatility distribution and average volatility for specific vaporization enthalpies for each PMF factor and for the total OA.

OA Type	**Saturation Concentration C^* (μg m^{-3})**			
	10^{-1}	1	10	Average C^*
		ΔH_{vap}=50 kJ mol^{-1}		
MO-OOA	0.00	0.05	0.95	9.00±3.96
LO-OOA	0.25	0.05	0.70	2.80±3.15
Isoprene-OA	0.35	0.05	0.60	1.78±3.15
BBOA	0.65	0.05	0.30	0.45±3.15
Total OA	0.05	0.05	0.9	7.08±3.15
		ΔH_{vap}=80 kJ mol^{-1}		
MO-OOA	0.35	0.15	0.50	1.41±3.15
LO-OOA	0.64	0.16	0.20	0.26±3.15
Isoprene-OA	0.75	0.05	0.20	0.28±3.15
BBOA	0.87	0.03	0.10	0.17±3.17
Total	0.45	0.25	0.3	0.71±3.15
		ΔH_{vap}=100 kJ mol^{-1}		
MO-OOA	0.60	0.04	0.36	0.58±3.95
LO-OOA	0.90	0.04	0.06	0.14±3.96
Isoprene-OA	0.95	0	0.05	0.13±3.54
BBOA	0.96	0.04	0.00	0.11±3.15
Total OA	0.76	0.04	0.2	0.27±3.16

Table S3. Saturation vapor pressure (P^o) and saturation concentration (C^*) (at 298 K) for various acids.

Organic acid	P^o(298K) (Pa*10^{-5})	C^*(298K) (μg m^{-3})
Adipic acid		
Bilde et al. (2003)	0.73 (0.4)	0.43
Riipinen et al. (2007)	0.78 (0.43)	0.46
Saleh et al. (2009)	0.52 (0.3)	0.31
Yaws et al. (2003)	0.78 (0.43)	0.46
Azelaic acid		
Bilde et al. (2003)	0.44 (0.18)	0.34
Yaws et al. (2003)	0.81 (0.3)	0.62
Malonic acid		
Bilde et al. (2003)	8.35 (1.78)	3.5
Hyvärinen et al. (2006)	7.45 (1.58)	3.1
Suberic acid		
Bilde et al. (2003)	0.05 (0.14)	0.036
Pimelic acid		
Saleh et al. (2008)	7.2 (1.7)	4.65
Oxalic acid		
Booth et al. (2010)	2150 (860)	780
Glutaric acid		
Bilde and Pandis (2001)	75 (37)	39.9
Bilde (2003)	88 (44)	46.8
Succinic acid		
Bilde 2003	3.93	1.9
Hyvärinen et al. 2006	4.97	2.4
Saleh 2009	4.31	2.1
Yaws 2003	4.77	2.3
Levoglucosan		
May et al. (2012)		13 (2)
Pinonic acid		
Bilde (2001)	7	5.19
Salo et al. (2010)	0.42 (0.15)	0.312

Table S4. Hygroscopicity values (κ) for the same acids as in Table S4. Values in parenthesis represent standard deviations.

Organic acid	κ
Adipic acid	
Cerully et al. (2014)	0.022 (0.002)
Kuwata et al. (2013)	0.002 (0.001)
Rissman et al. (2007)	0.059 (+0.021; -0.014)
Huff Hartz et al. (2006)	0.03 (+0.002; -0.001)
Broekhuizen et al. (2004)	0.096 (n/a)
Raymond and Pandis (2002)	0.02 (+0.018; -0.008)
Prenni et al. (2001)	0.014 (n/a)
Corrigan and Novakov (1999)	0.03 (n/a)
Cruz and Pandis (1997)	0.099 (+0.048; -0.029)
Azelaic acid	
Cerully et al. (2014)	0.061 (0.007)
Kuwata et al. (2013)	0.03 (0.01)
Huff Hartz et al. (2006)	0.022 (+0.018; -0.009)
Malonic acid	
Cerully et al. (2014)	0.281 (0.034)
Kumar et al. (2003)	0.227 (0.028)
Prenni et al. (2001)	0.237 (n/a)
Suberic acid	
Cerully et al. (2014)	0.007 (0.000)
Kuwata et al. (2013)	0.001 (n/a)
Pimelic acid	
Cerully et al. (2014)	0.213 (0.016)
Kuwata et al. (2013)	0.15 (0.01)
Frosch et al. (2010)	0.15 (0.04)
Huff Hartz et al. (2006)	0.14 (+0.109; -0.054)
Oxalic acid	
Sullivan et al. (2009)	0.5 (0.05)
Glutaric acid	
Reymond and Pandis (2002)	0.195 (0.082)
Koehler et al. (2006)	0.2 (0.08)
Succinic acid	
Cerruly 2014	0.285 (0.029)
Hori (2003)	0.231 (0.065)
Prenni (2001)	0.310
Corrigan and Novakov (1999)	0.225
Levoglucosan	
Svenningsson et al. (2006)	0.208 (0.015)
Koehler et al. (2006)	0.165 (0.015)
Pinonic acid	
Raymond and Pandis (2002)	0.106 (0.09)

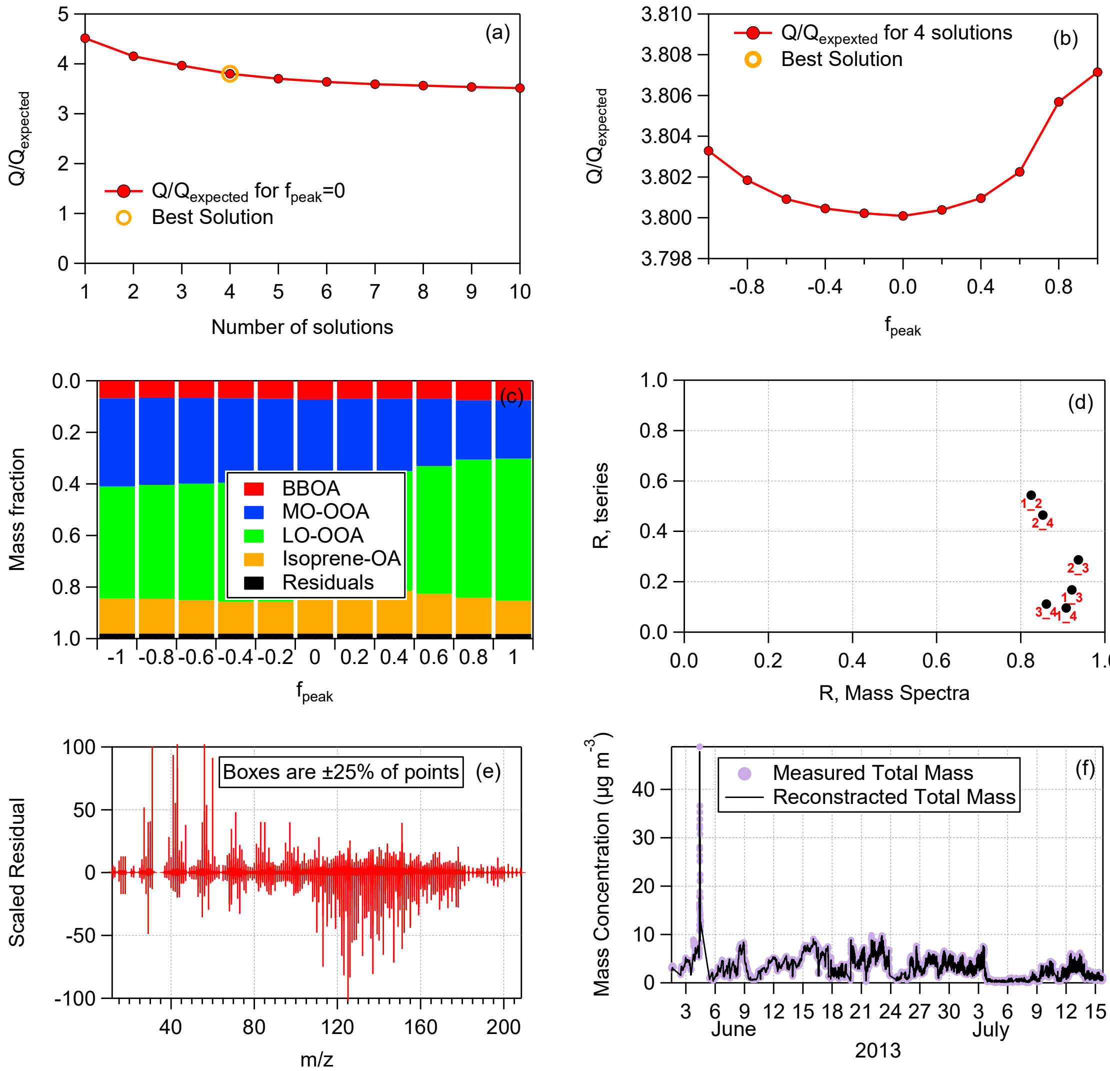

Figure S1. Diagnostic plots of the PMF analysis: (a) $Q/Q_{expected}$ versus the number of the examined factors, (b) $Q/Q_{expected}$ versus the f_{peak} for the optimum solution (4 factors), (c) mass fraction of PMF factors versus the f_{peak}, (d) correlations of time series and mass spectra among the 4 PMF factors, (e) distribution of scaled residuals for each *m/z* and (f) time series of the measured and the reconstructed organic mass.

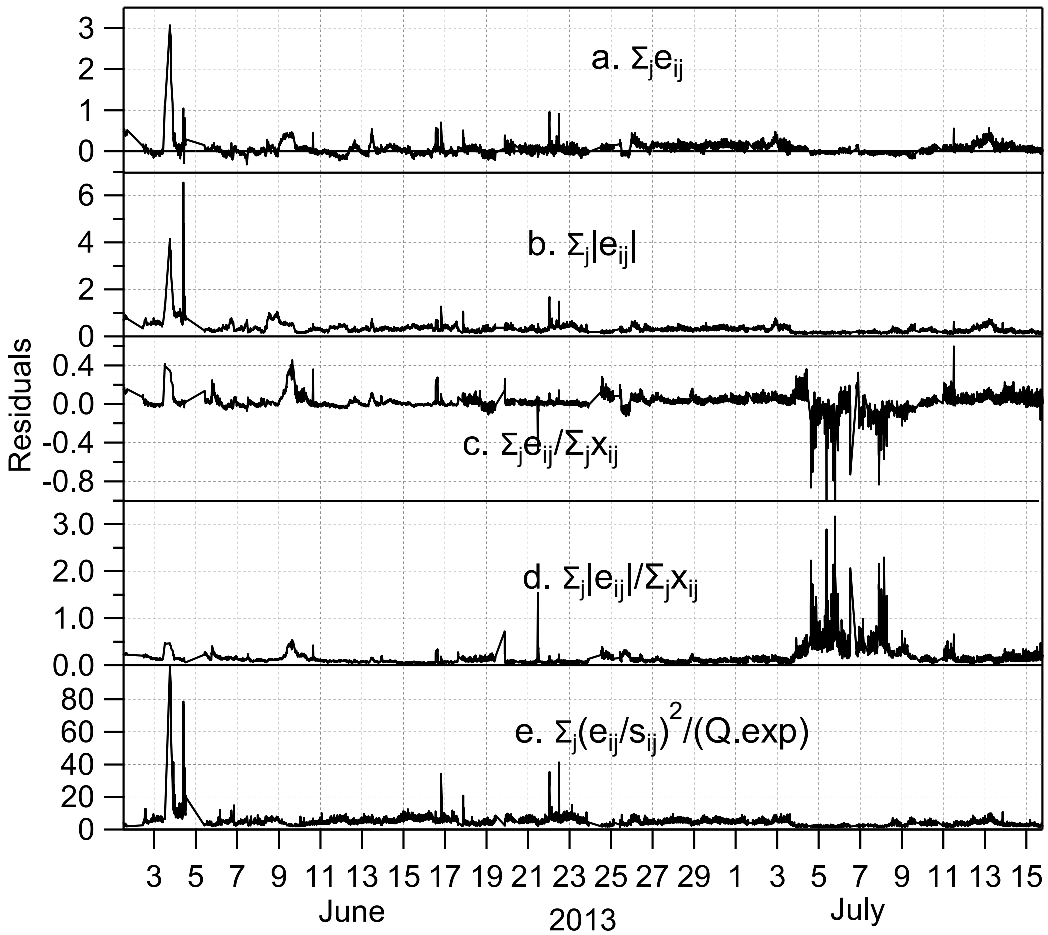

Figure S2. Model residuals **E= X-GF** calculated using the PMF evaluation tool, PET (Ulbrich et al., 2009).

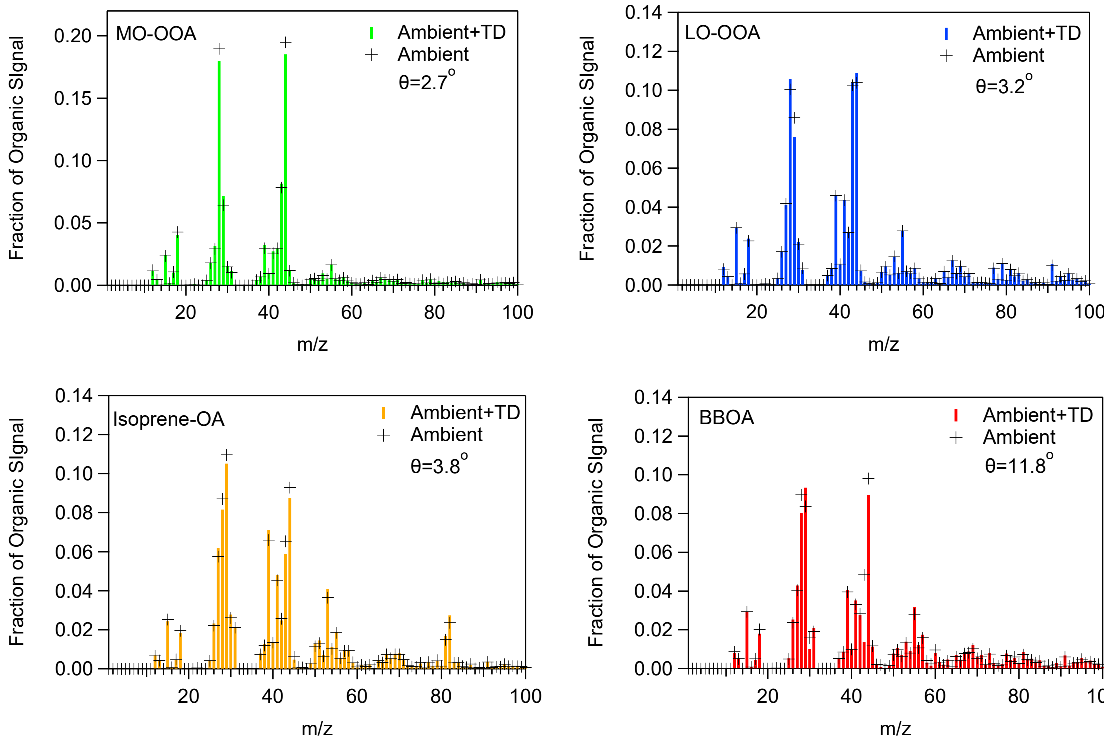

Figure S3. Comparison between the ambient PMF factors (crosses) as reported by Xu et al. (2015) and ambient plus TD OA PMF factors (bars) found in this work.

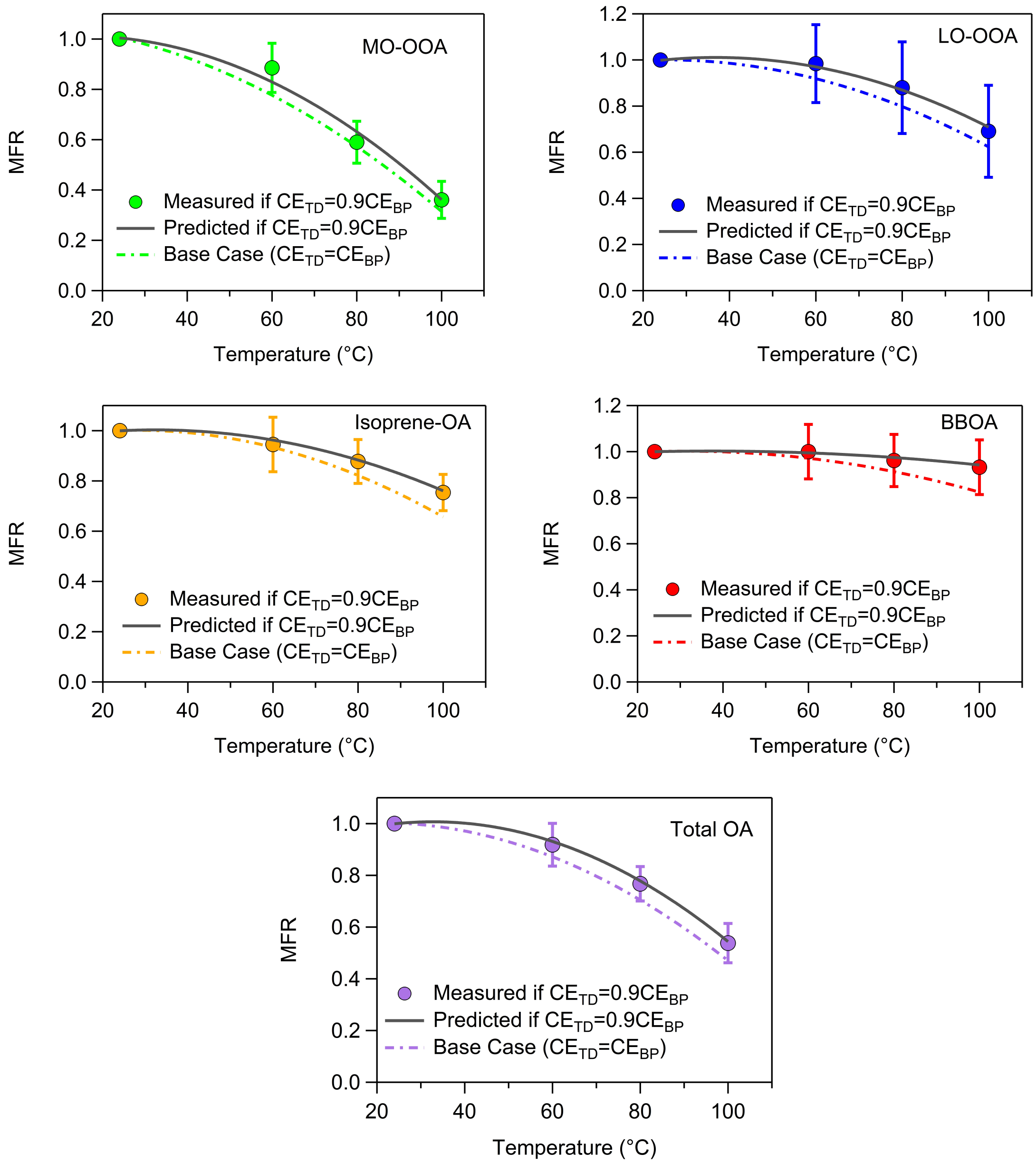

Figure S4. MFRs of the loss-corrected PMF OA factors and total OA for a lower TD CE. The circles denote the measurements with the one standard deviation of the mean for a 10% lower TD CE, the grey solid lines stand for the optimum solution if CE TD was 10% lower and the dash lines correspond to the predicted base case.

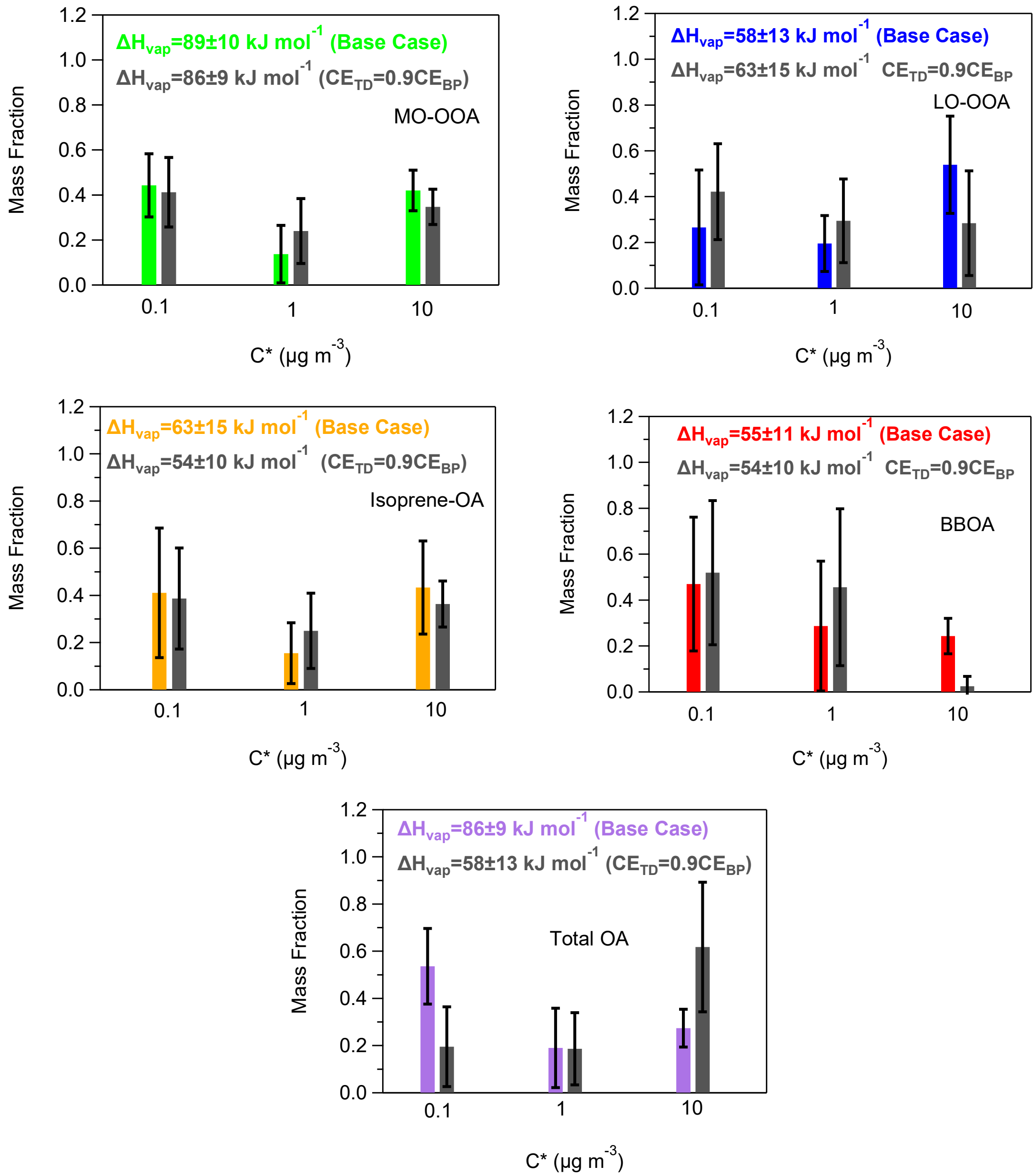

Figure S5. Predicted volatility distributions of the OA PMF factors and total OA for a lower TD CE. The error bars are estimated using the approach of Karnezi et al. (2014). The grey solid bars represent the results for a 10% lower TD CE. The green, blue, orange, red and purple bars stand for the base case solutions of MO-OOA, LO-OOA, Isoprene-OA, BBOA and total OA.

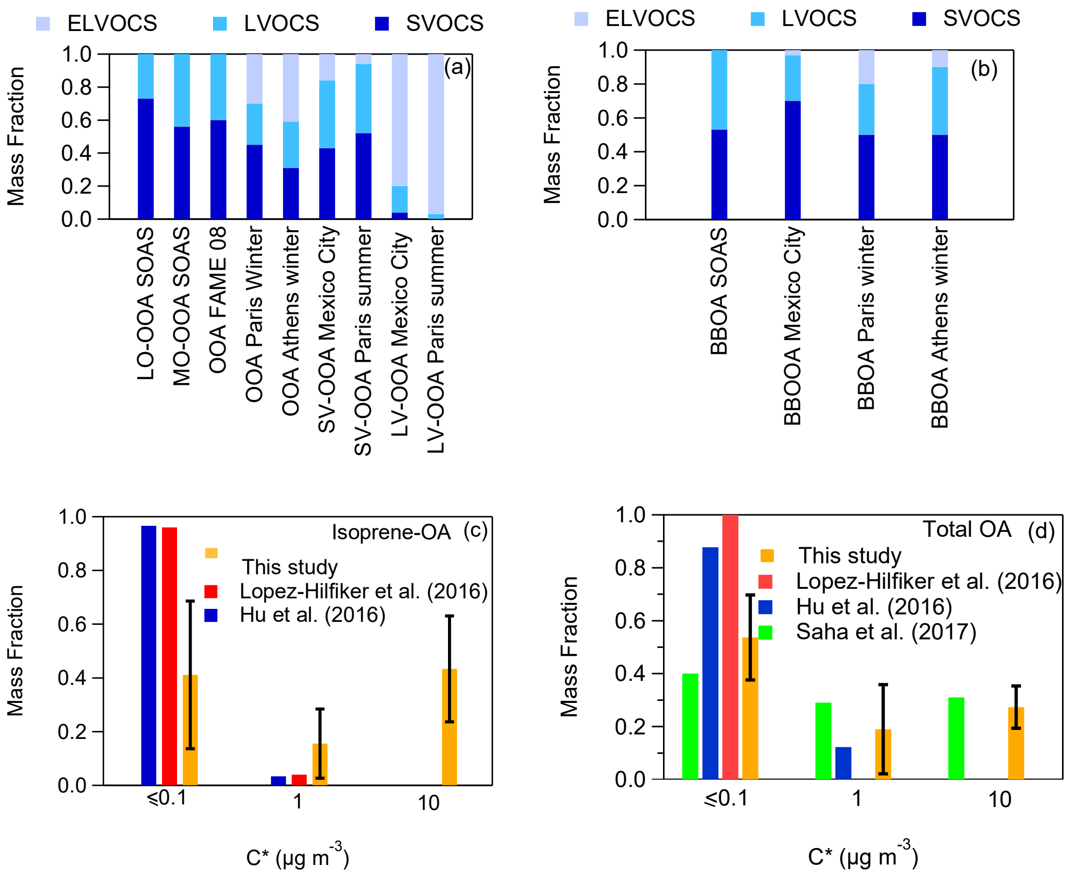

Figure S6. (a) and (b) Comparison between volatility compositions of OA for various studies: MILAGRO (Mexico City), MEGAPOLI (Paris winter and summer), Athens winter and FAME-08 (Finokalia, Crete). (c) and (d) Comparison between volatility distributions of Isoprene-OA and total OA estimated by other groups in Centreville during SOAS.

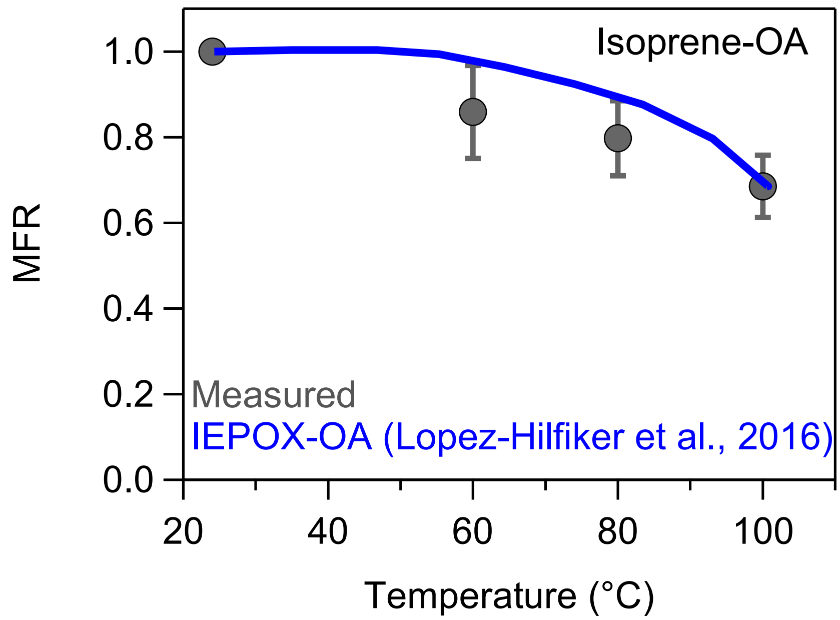

Figure S7. MFRs of the loss-corrected Isoprene-OA factor. The circles correspond to the measurements with the one standard deviation of the mean. The blue line is the predicted solution using as input the volatility distribution of IEPOX SOA of Lopez-Hilfiker et al. (2016).

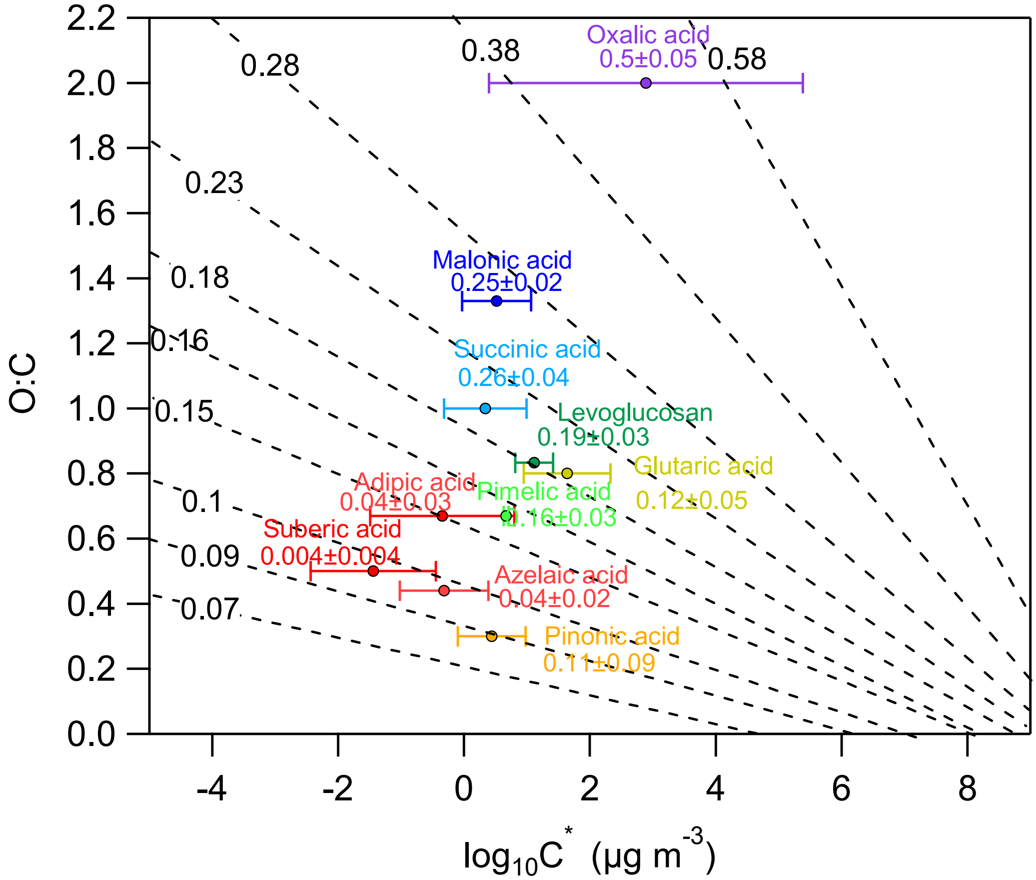

Figure S8. O:C ratios versus the average volatility as $\log_{10}C^*$. The black isolines correspond to the theoretically intrinsic κ suggested by Nakao et al. (2017). The circles stand for the volatility and hygroscopicity measurements of known compounds based on Tables S3 and S4.

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