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Positive matrix factorization of organic aerosol: insights from a chemical transport model

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SI-1 Model evaluation metrics

The normalized mean bias (NMB), the normalized mean error (NME), the mean bias (MB), the mean absolute gross error (MAGE) are used for the evaluation of the prediction of PMCAMx-SR

$$NMB = \frac{\sum_{i=1}^{n}(P_i - O_i)}{\sum_{i=1}^{n} O_i} \qquad NME = \frac{\sum_{i=1}^{n}|P_i - O_i|}{\sum_{i=1}^{n} O_i}$$

$$MAGE = \frac{\sum_{i=1}^{n}|P_i - O_i|}{n} \qquad MB = \frac{\sum_{i=1}^{n}(P_i - O_i)}{n}$$

where P_i represents the concentration of each PMF factor for data point i, O_i is the PMCAMx-SR predicted value for specific components and n is the total number of data points.

Table S1. List of PMCAMx-SR OA components used in the PMCAMx-SR PMF analysis.

Number	**Component**	**Volatility (C*)** ($\mu g\ m^{-3}$)
1	POA	0.01
2	POA	0.1
3	POA	1
4	POA	10
5	POA	100
6	SOA-sv and SOA-iv	0.01
7	SOA-sv and SOA-iv	0.1
8	SOA-sv and SOA-iv	1
9	SOA-sv and SOA-iv	10
10	SOA-sv and SOA-iv	100
11	bSOA	1
12	bSOA	10
13	bSOA	100
14	aSOA	1
15	aSOA	10
16	aSOA	100
17	bbPOA	0.01
18	bbPOA	0.1
19	bbPOA	1
20	bbPOA	10
21	bbPOA	100
22	bbSOA	0.01
23	bbSOA	0.1
24	bbSOA	1
25	bbSOA	10
26	bbSOA	100
27	LRT	0.01

Table S2. OA components used to perform PMF analysis taking into account the age of OA components.

Number	Component	Volatility (C*) ($\mu g\ m^{-3}$)	Age
1	POA	0.01-100	fresh
2	bSOA	1-100	first generation
3	SOA-sv and SOA-iv	0.01	first generation
4	SOA-sv and SOA-iv	0.1	first generation
5	SOA-sv and SOA-iv	1	first generation
6	SOA-sv and SOA-iv	10	first generation
7	SOA-sv and SOA-iv	100	first generation
8	aSOA	1	first generation
9	aSOA	10	first generation
10	aSOA	100	first generation
11	LRT	0.01	highly aged
12	SOA-sv and SOA-iv	0.01	second or higher generation
13	SOA-sv and SOA-iv	0.1	second or higher generation
14	SOA-sv and SOA-iv	1	second or higher generation
15	SOA-sv and SOA-iv	10	second or higher generation
16	SOA-sv and SOA-iv	100	second or higher generation
17	aSOA	1	second or higher generation
18	aSOA	10	second or higher generation
19	aSOA	100	second or higher generation

Table S3. Evaluation the PMF predictions* for the bbPOA factor against the PMCAMx-SR fresh bbPOA predictions in selected locations.

Location	Mean bbPOA factor ($\mu g\ m^{-3}$)	Mean bbPOA ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	NB (%)	NME (%)
St.Petersburg	5	5.2	-0.2	0.3	-3	5
Catania	1.1	1.1	0.06	0.1	5	11
Majden	0.9	0.8	0.1	0.2	13	24

* Number of data points: 696

Table S4. Evaluation the PMF predictions* for the POA factor against the PMCAMx-SR fresh bbPOA predictions in selected locations.

POA	Mean POA factor ($\mu g\ m^{-3}$)	Mean POA ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	NMB (%)	NME (%)
St.Petersburg	1.1	0.9	0.3	0.4	25	34
Majkow Duzy	3.2	3.4	-0.1	0.3	-5	10

* Number of data points: 696

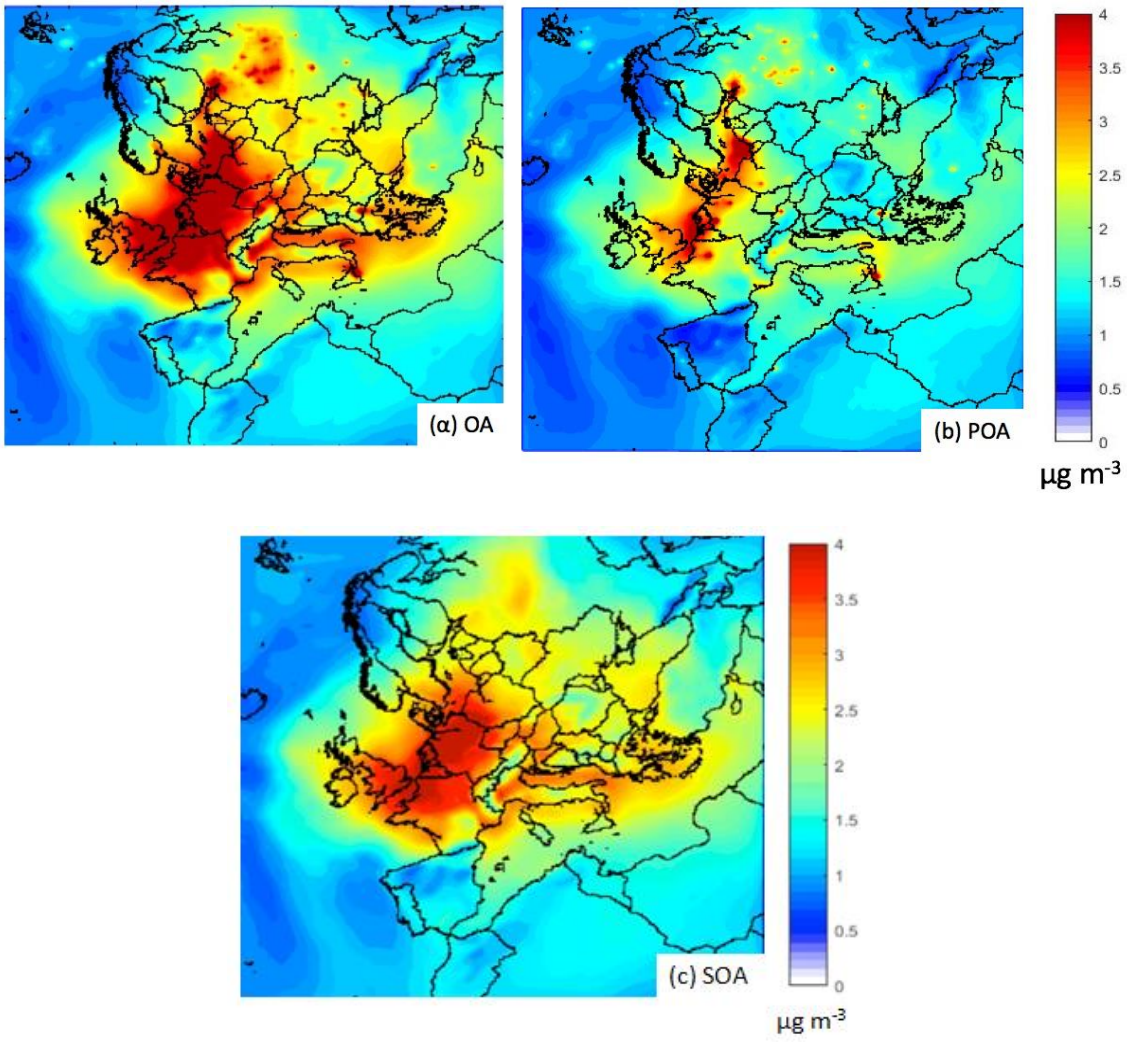

Figure S1. PMCAMx-SR predicted ground – level concentrations of PM_1: (a) OA, (b) POA, and (c) SOA during May 2008.

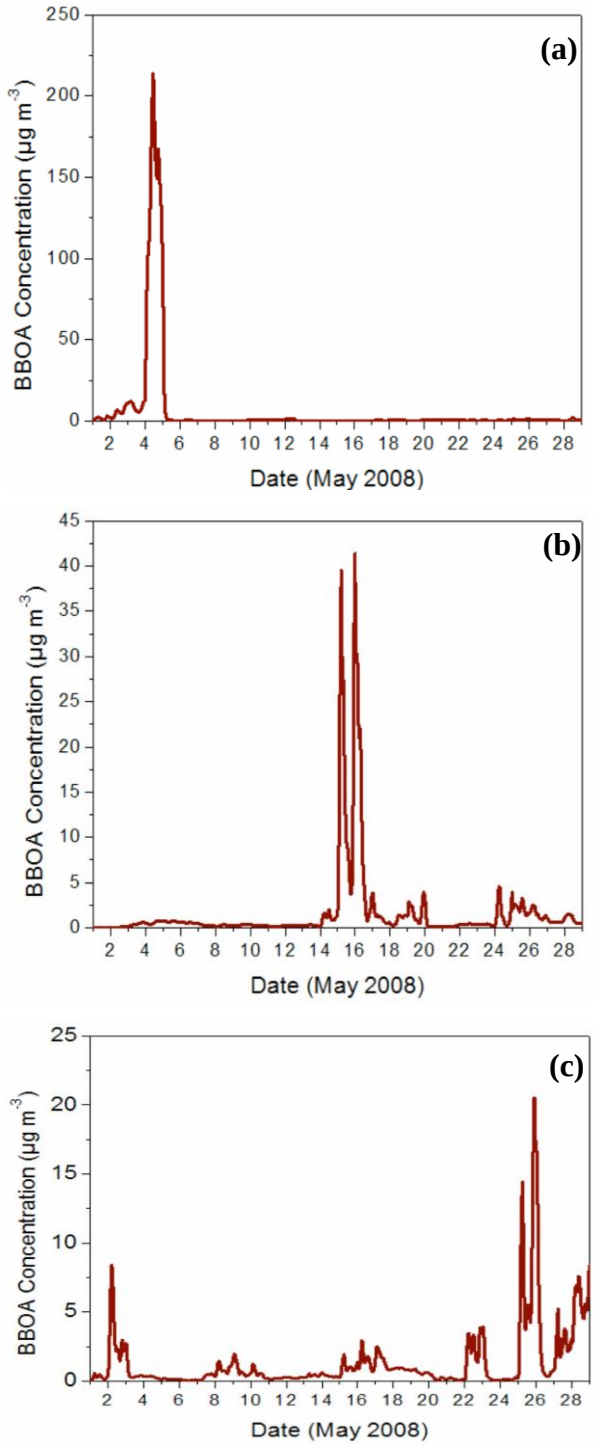

Figure S2. Time series of predicted biomass burning OA by PMCAMx-SR during May 2008: (a) St. Petersburg (Russia), (b) Catania (Italy) and (c) Majden (FYROM).

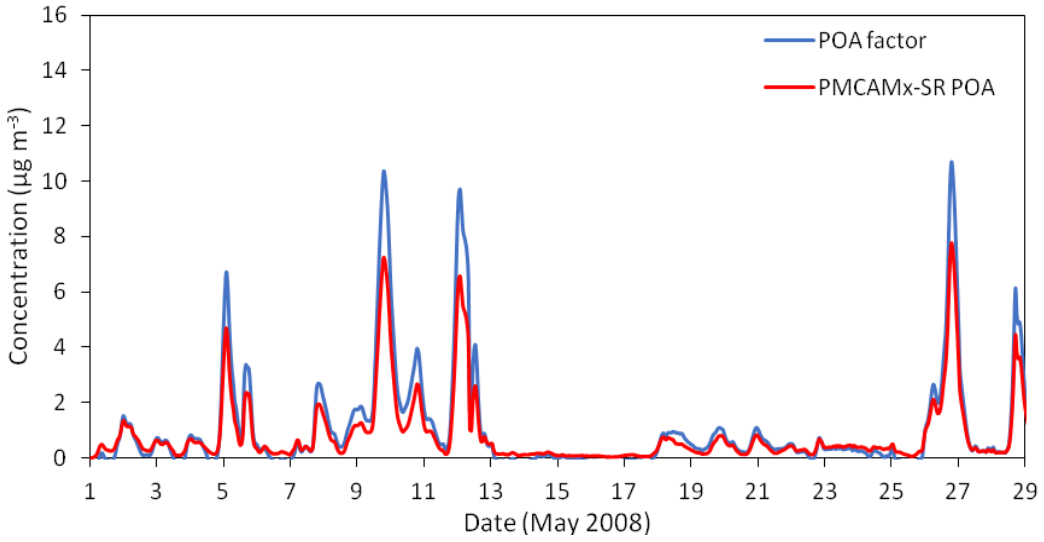

Figure S3. Time series of POA factor (blue line) and PMCAMx-SR POA (red line) in St. Petersburg during May 2008.

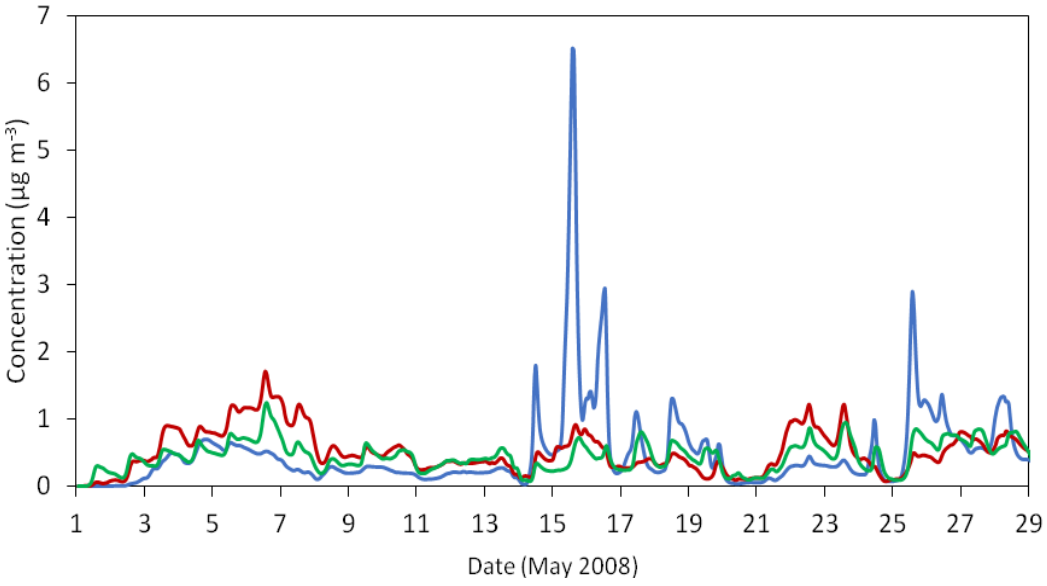

Figure S4. Time series of bbSOA (blue line), aSOA (red line) and SOA-sv and SOA-iv (green line) in Catania during May 2008.

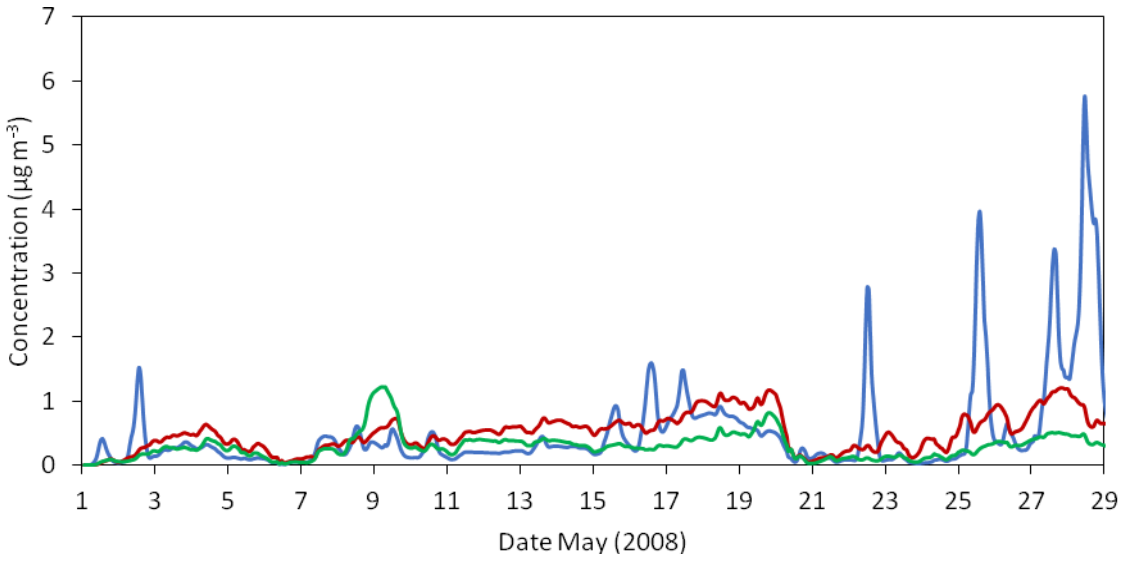

Figure S5. Time series of bbSOA (blue line), aSOA (red line) and bSOA (green line) in Majden during May 2008.

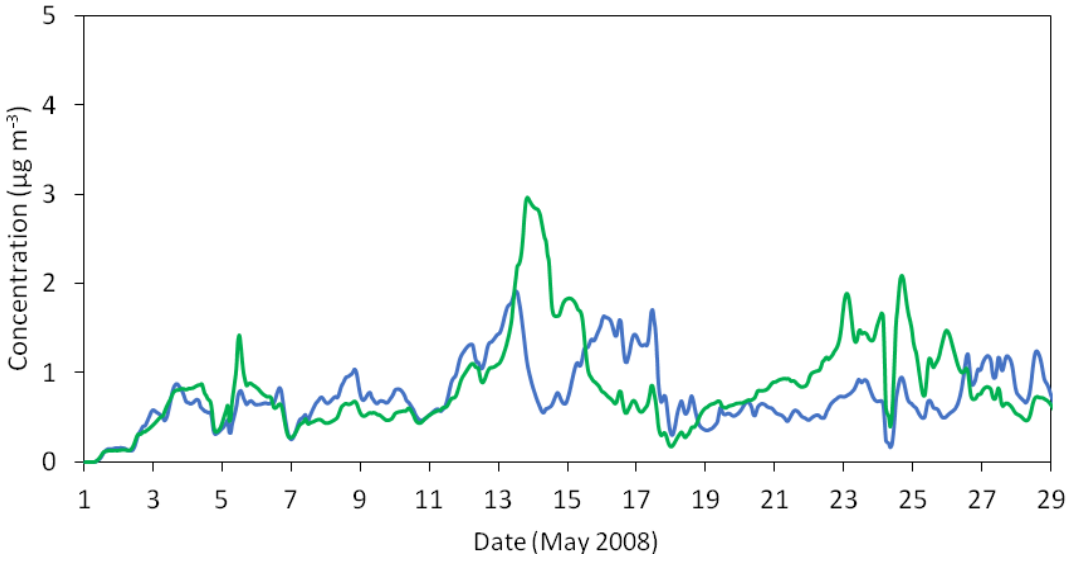

Figure S6. Time series of aSOA (blue line) and SOA-sv and SOA-iv (green line) in Melpitz during May 2008.

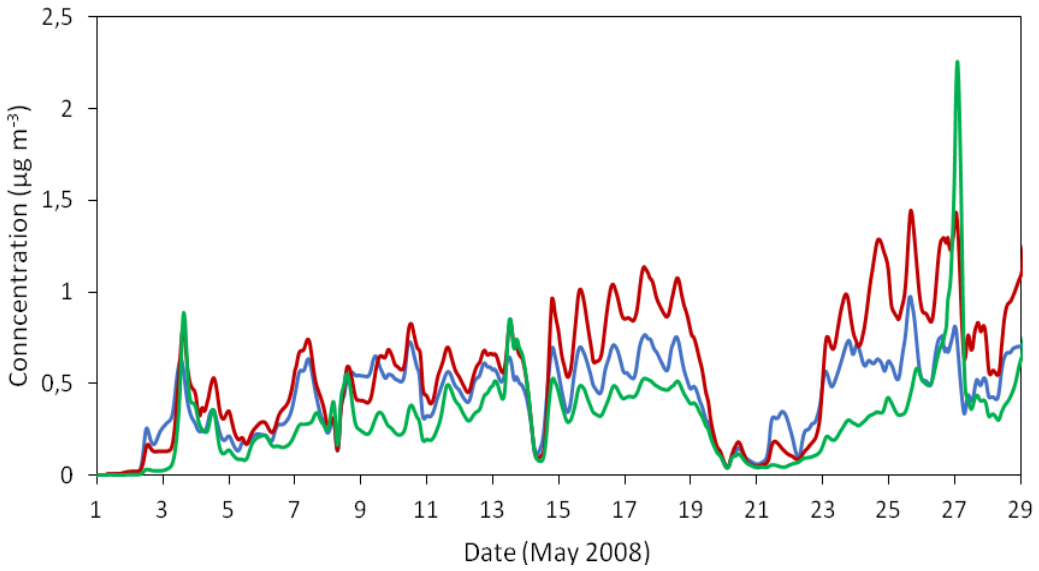

Figure S7. Time series of SOA-sv and SOA-iv (blue line), aSOA (red line) and bbSOA (green line) in Finokalia during May 2008.

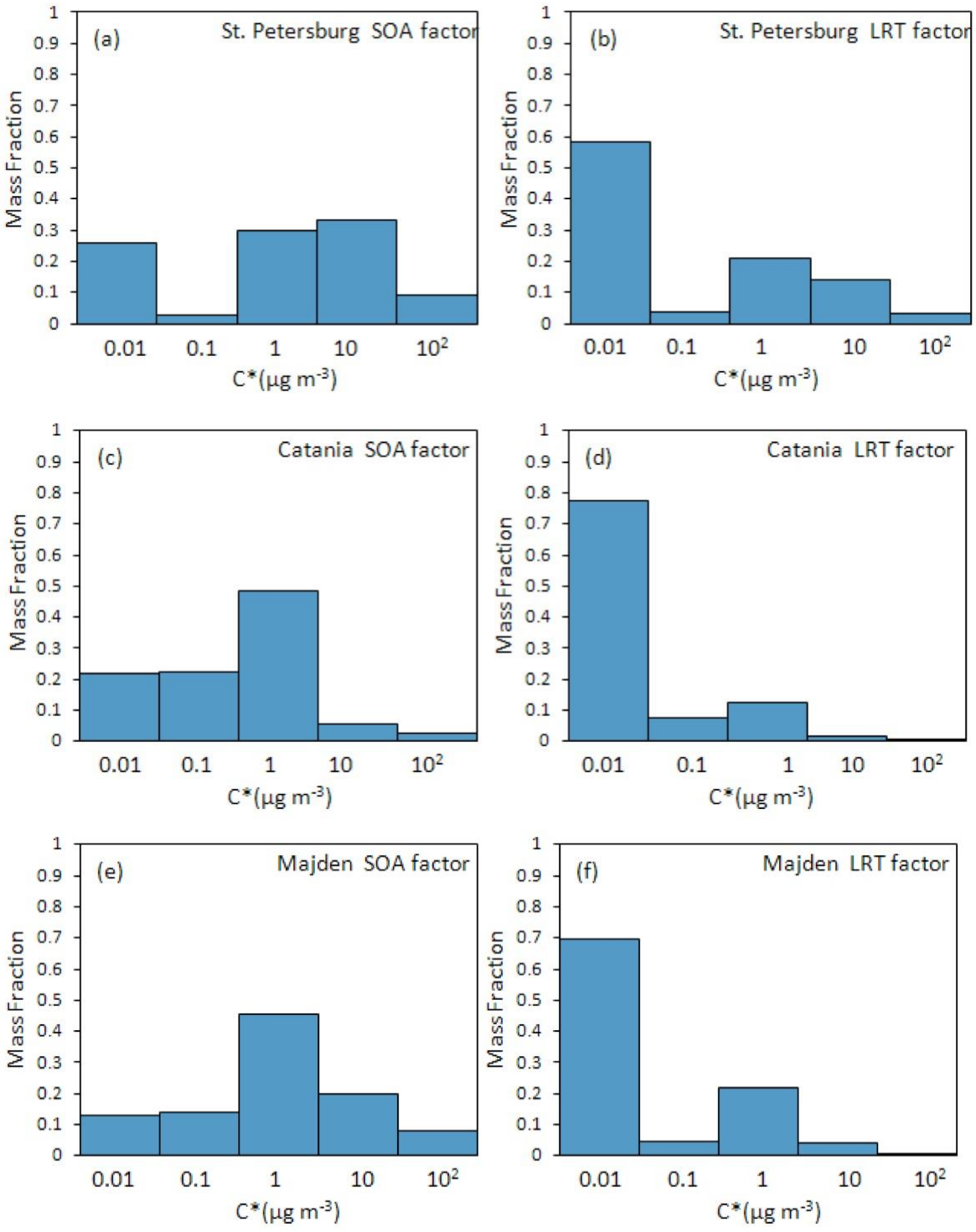

Figure S8. Volatility distributions of each factor in: (a)-(b) St. Petersburg, (c)-(d) Catania, and (e)-(f) Majden.

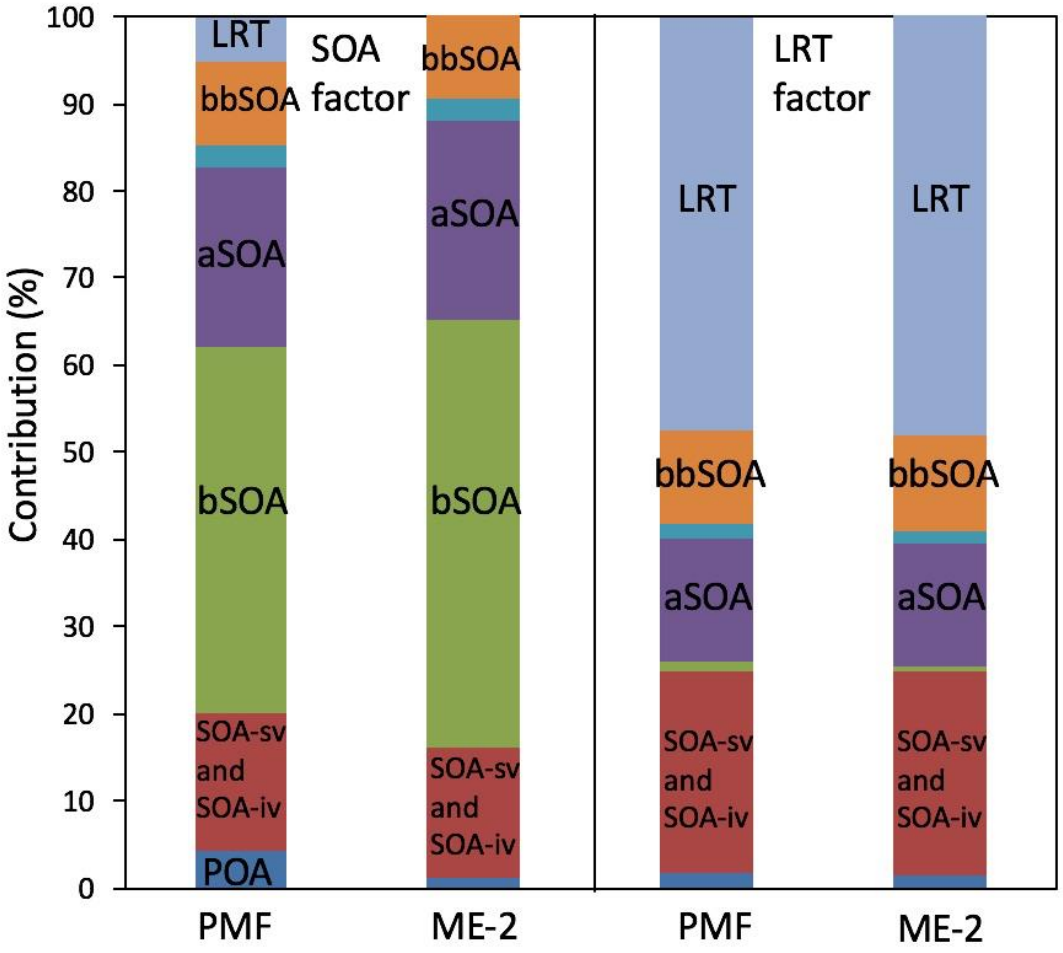

Figure S9. Contribution of each OA component to the SOA and LRT factors based on the PMF and ME-2 analysis of PMCAMx-SR predicted OA in Melpitz.

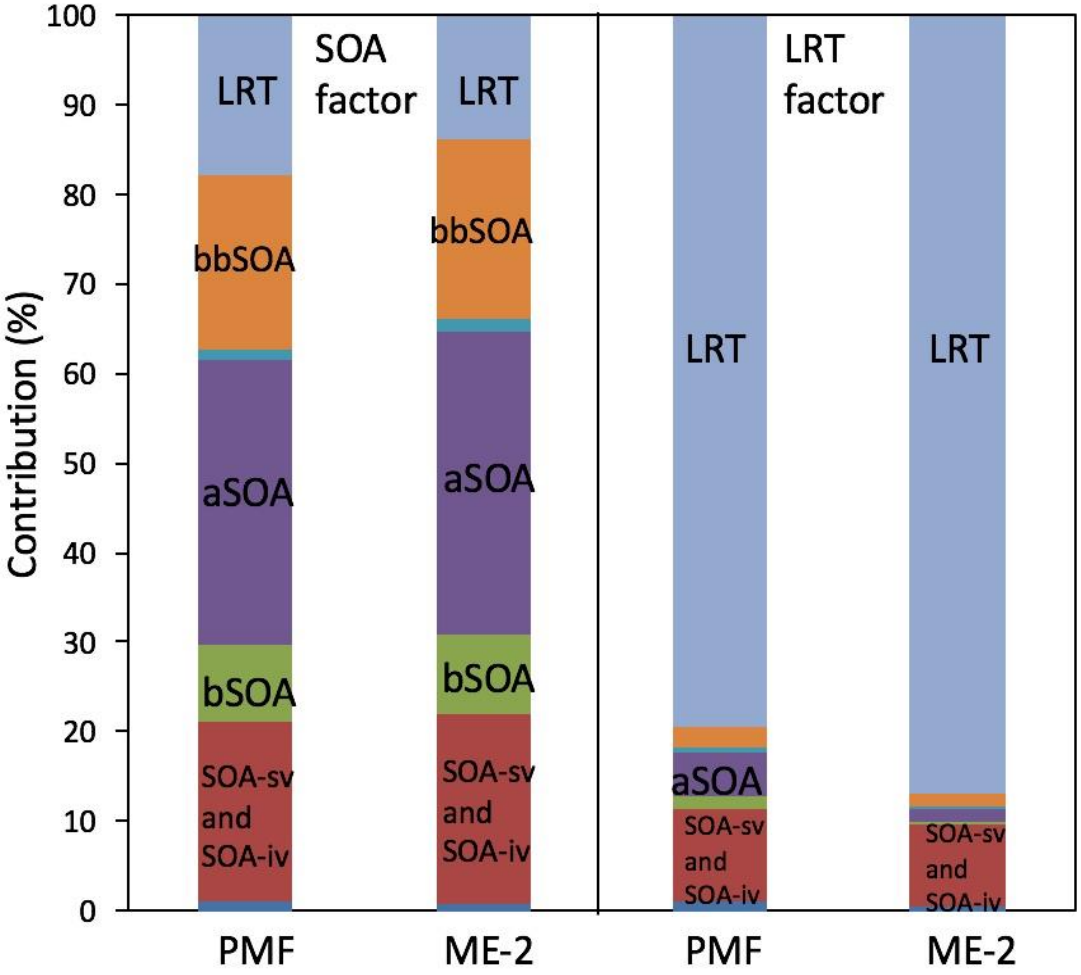

Figure S10. Contribution of each OA component to the SOA and LRT factors based on the PMF and ME-2 analysis of PMCAMx-SR predicted OA in Finokalia.

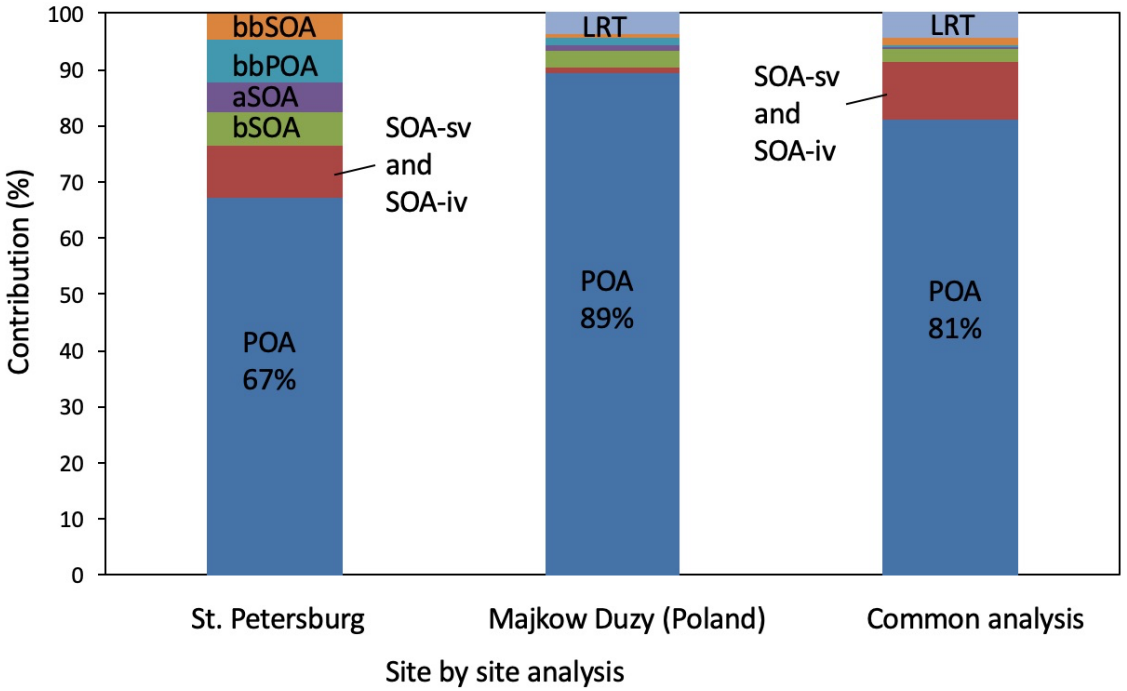

Figure S11. Comparison of the composition of POA factor in St. Petersburg, Majkow Duzy (Poland) and common analysis (all sites analyzed together).

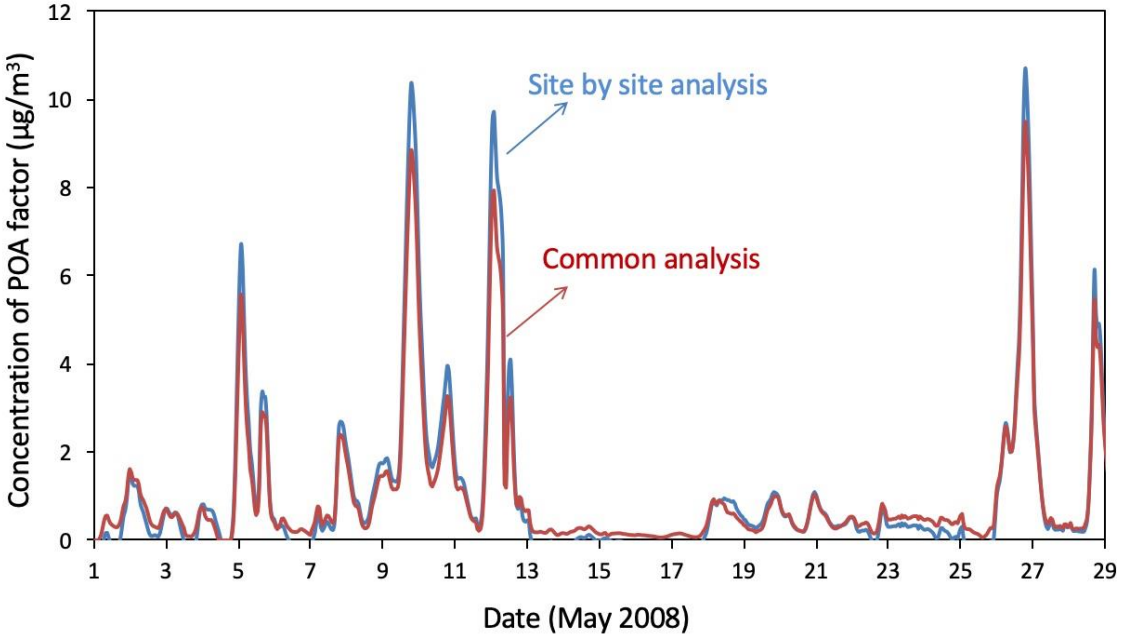

Figure S12. Time series of POA factor in St. Petersburg from site by site analysis (blue line) and common analysis (red lines).

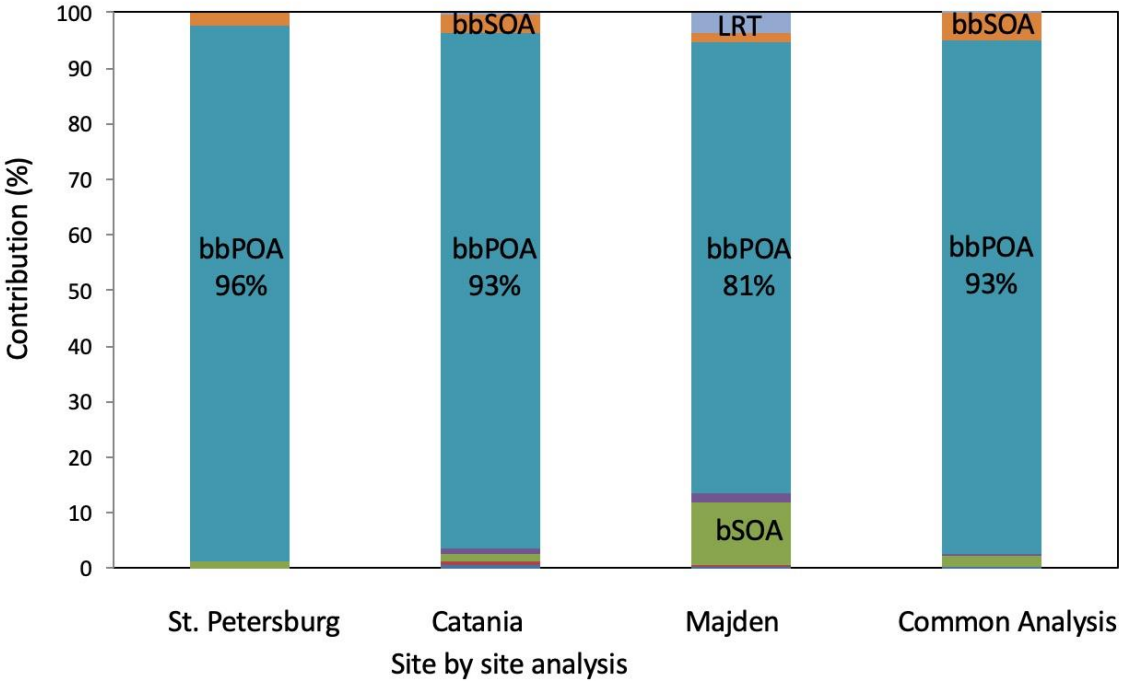

Figure S13. Comparison of the composition of bbPOA factor in St. Petersburg, Catania, Majden and common analysis (all sites analyzed together).

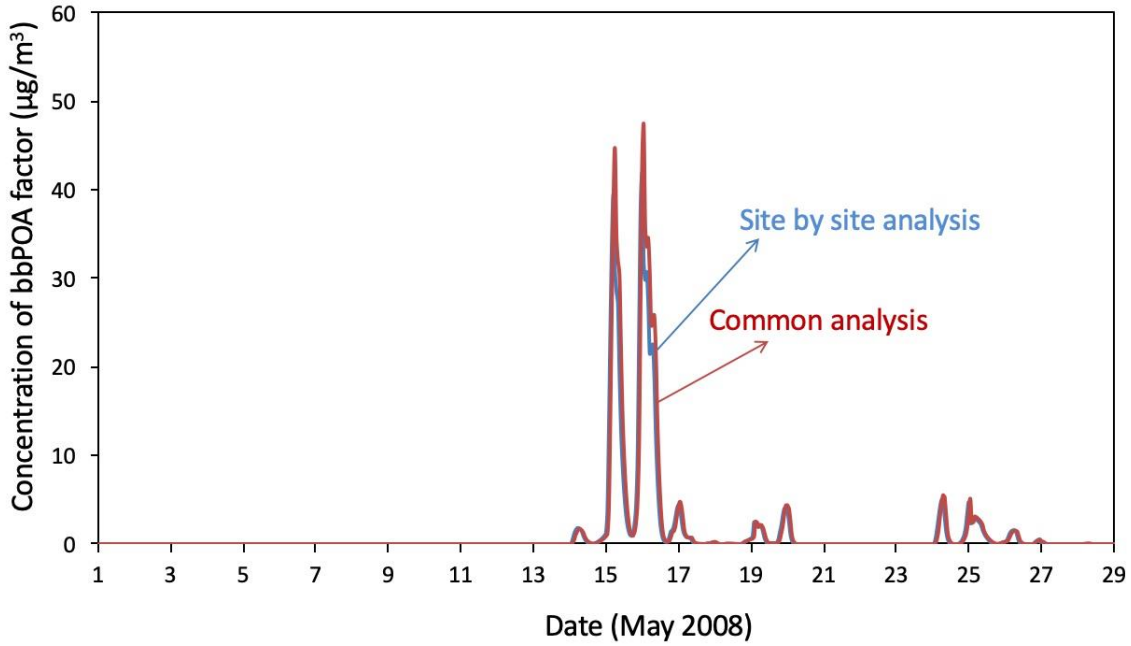

Figure S14. Time series of bbPOA factor in St. Petersburg from site by site analysis (blue line) and common analysis (red lines).

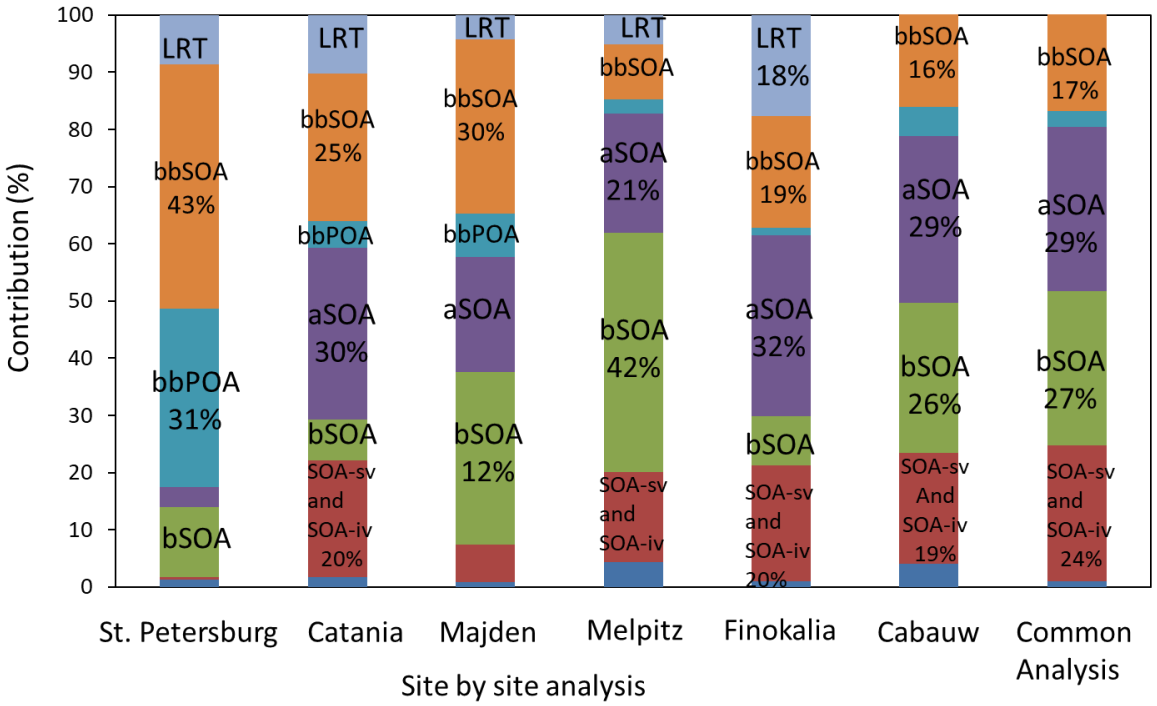

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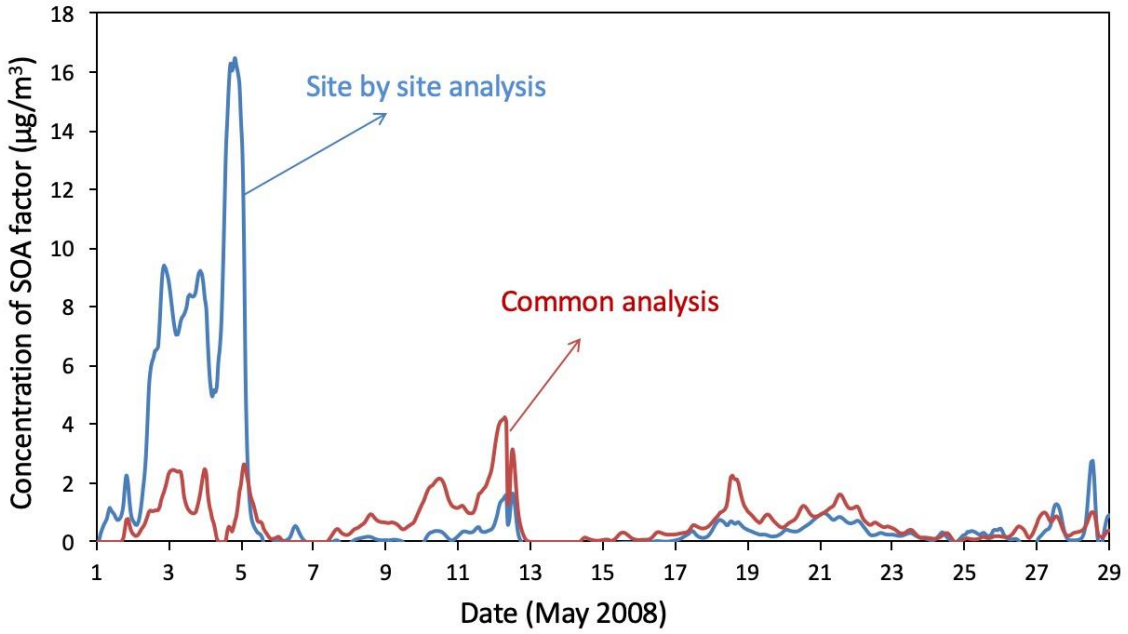
Figure S15. Comparison of the composition of SOA factor in St. Petersburg, Catania, Majden, Melpitz, Finokalia and common analysis (all sites analyzed together).



120 **Figure S16.** Time series of SOA factor in St. Petersburg from site by site analysis (blue line) and common analysis (red lines).

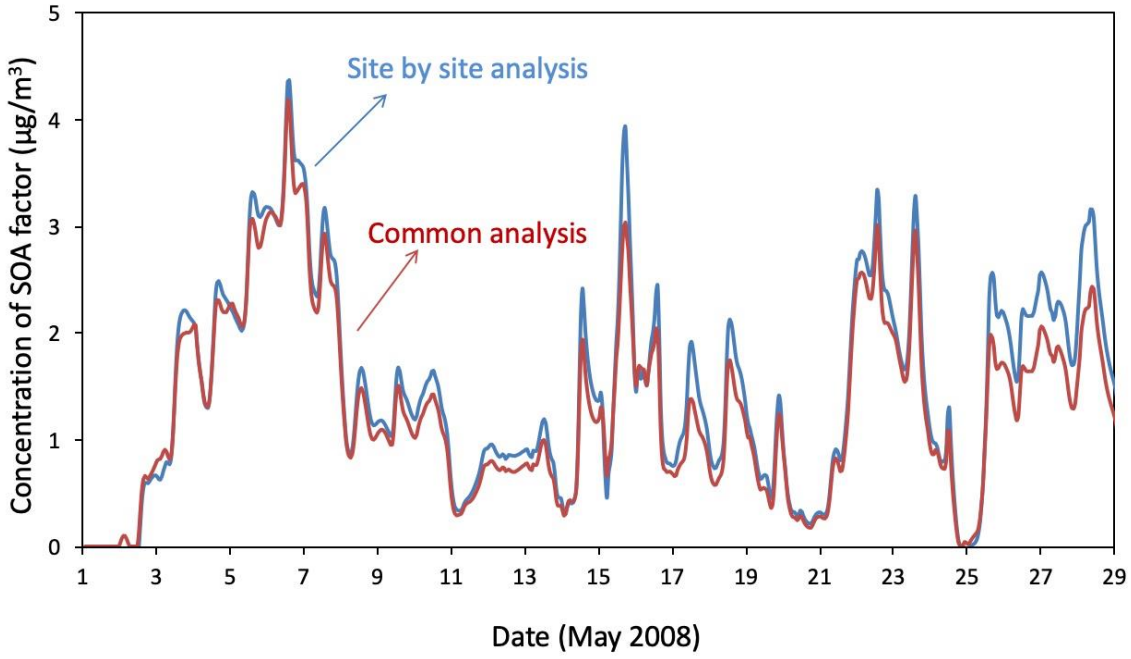


Figure S17. Time series of SOA factor in Catania from site by site analysis (blue line) and common analysis (red lines).

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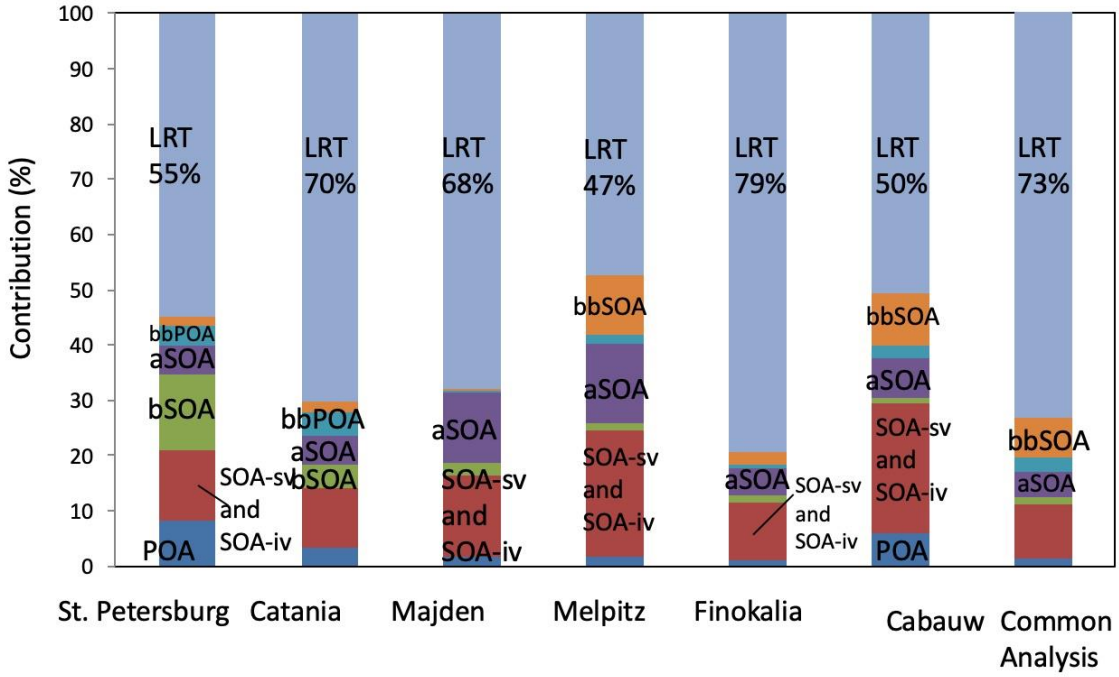
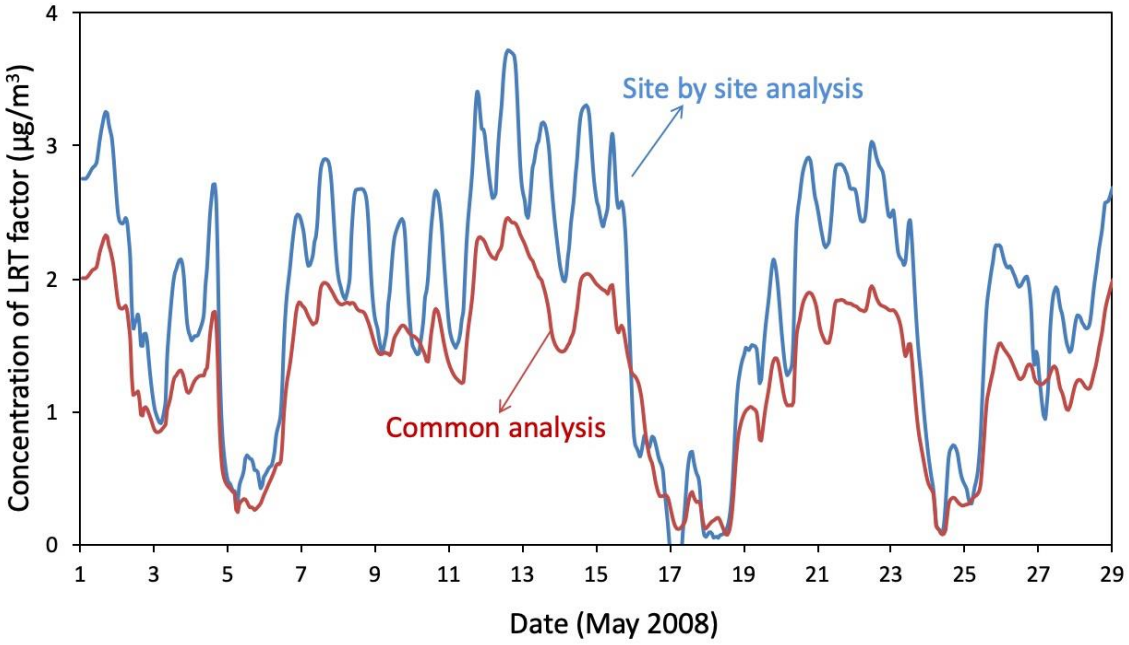


Figure S18. Comparison of the composition of LRT factor in St. Petersburg, Catania, Majden, Melpitz, Finokalia, Cabauw and common analysis (all sites analyzed together).



130 **Figure S19.** Time series of LRT factor in Melpitz from site by site analysis (blue line) and common analysis (red lines).