Assessment of air quality in Leipzig, Germany: Detailed source apportionment of size-resolved aerosol particles and comparison with the year 2000

D. van Pinxteren[1], K.W. Fomba[1], G. Spindler[1], K. Müller[1], L. Poulain[1], Y. Iinuma[1], G. Löschau[2], A. Hausmann[2], and H. Herrmann[1]

1) Leibniz Institute for Tropospheric Research (TROPOS), Atmospheric Chemistry Department (ACD), Permoserstr. 15, 04318 Leipzig, Germany

2) Saxon State Agency for Environment, Agriculture and Geology (LfULG), Pillnitzer Platz 3, 01326 Dresden

Electronic Supplementary Information

Table S1: List of chemical species included in PMF calculations, their assigned category in the PMF software ("strong" if not indicated, "weak" means downweighted by increasing uncertainty, "bad" means excluded from analysis), and their typical source categories.

Species	Category in EPA PMF	Typical sources
Mass	"weak" on all stages	Total variable
Ammonium		NH_3, combustion processes, agriculture
Nitrate		NO_x, combustion processes
Sulfate		SO_2, combustion processes, photochemistry
WSOC		biomass combustion, photochemistry
WISC		combustion processes, primary biological material
Sodium	"weak" on stage 5; "bad" on stages 1,2,3	sea salt, crustal material
Magnesium	"bad" on stages 1,2,3	sea salt, crustal material
Chloride	"weak" on stage 3; "bad" on stage 1	sea salt, combustion processes
Oxalate		photochemistry
Levoglucosan		biomass combustion
Arabitol	"bad" on stages1,2,3	primary biological material (fungal spores)
n-Alkanes C22-C34		primary biological material (e.g. plant waxes), combustion processes
Fluoranthene (FLU)	"bad" on stage 5	combustion processes
Pyrene (PYR)	"bad" on stage 5	
Retene (RET)	"bad" on stage 5	
Benzo[b]naphtho(1,2-d)thiophene (BNTHIO)	"bad" on stage 5	
Cyclopenta(cd)pyrene (CCPYR)	"bad" on stage 5	
Benzo(k)fluoranthene (BkFLU)		
Benzo(e)pyrene (BePYR)		
Benzo(a)pyrene (BaPYR)		
Benzo(ghi)perylene (BghiPER)	"bad" on stage 5	
17alpha(H),21beta(H)-30-Norhopane (NHOP)	"bad" on stages 4,5	combustion processes (diesel fuel and coal)
17alpha(H),21beta(H)-Hopane (abHOP)	"weak" on stages 4,5	
17alpha(H),21beta(H)-22S-Homohopane (ab22SHHOP)	"bad" on stages 4,5	
17alpha(H),21beta(H)-22R-Homohopane (ab22RHOP)	"bad" on stages 4,5	
K		combustion processes, crustal material, industrial emissions
Ca		
Ti		
Mn		
Fe		
Cu		
Zn		
As		
Se	"bad" on stage 5	
Ba		
Pb		
Ni	"bad" on stages1,3	
Cr		
Sr	"bad" on stages1,2,3	
Sn	"weak" on stages 1,2,4	

Table S2: Sampling dates during summer 2013 (Nr. 1-21) and winters 2013/14 (Nr. 22-31) and 2014/15 (Nr. 32-42), with corresponding daily mean meteorological data at LMI, TRO, and MEL, and sector of air mass origin (W: West, E: East, --:other)

Nr.	Date	Day of Week	Temp. [°C]			Rel. Humid. [%]			Glob. Rad. [W m^{-2}]			Wind Speed. [m s^{-1}]			Precip. [mm]			Sector.
			LMI	TRO	MEL	LMI	TRO	MEL	LMI	TRO	MEL	LMI	TRO	MEL	LMI	TRO	MEL	
1	06/08/2013	Tue	25.4	24.4	23.9	66	70	77	195	193	216	1.2	1.7	1.7	11	8.6	0.1	W
2	11/08/2013	Sun	18.6	17.9	16.3	56	59	73	180	183	221	2	2.2	3.1	0	0	0.2	W
3	16/08/2013	Fri	22.7	21.3	20	46	52	59	248	248	279	1.1	1.7	1.6	0	0	0	W
4	18/08/2013	Sun	22.7	21.9	20.4	56	60	71	118	121	149	1.9	2.2	3.1	0.09	0	0	W
5	20/08/2013	Tue	18	17.1	16.4	65	69	76	162	159	192	1.8	2.9	3.2	0	0	1	W
6	23/08/2013	Fri	18.5	17.3	16	68	72	82	75	74	107	0.84	1.3	1.3	2.4	1	0	--
7	25/08/2013	Sun	20.3	19.5	19.4	54	57	57	157	165	217	1.6	2.5	4.2	0	0	0	E
8	27/08/2013	Tue	18.1	17	15.2	57	61	72	173	186	174	1.5	2.2	2.5	0	0	0	E
9	29/08/2013	Thu	20	NA	16.2	58	NA	73	187	NA	210	0.9	NA	1.3	0	NA	0	E
10	01/09/2013	Sun	15.5	15	14.5	61	64	68	110	114	140	2.2	2.6	4	0	0	0	W
11	04/09/2013	Wed	20	19.2	17.9	79	85	90	101	100	100	0.74	0.96	1.2	0.09	0.6	0.2	W
12	06/09/2013	Fri	21.8	20.9	19.5	59	63	68	204	206	232	1.1	2.2	2.8	0	0	0	E
13	08/09/2013	Sun	19.7	19.2	19.1	65	67	70	80	86	140	1.4	2.1	2.8	0.29	0	0.4	E
14	11/09/2013	Wed	13.5	12.7	12.4	80	82	86	42	46	70	1.4	2.6	3.3	3.5	2.3	0.2	W
15	14/09/2013	Sat	17.1	16.4	15.4	77	80	85	124	150	187	1.5	1.9	2.4	0.15	0	0	W
16	17/09/2013	Tue	11.9	11.4	10.6	70	73	79	135	160	175	2.4	2.7	3.5	0	0.1	0	W
17	19/09/2013	Thu	12.3	11.7	11.1	75	77	83	78	83	104	2.1	2.4	3.6	0.86	0.3	0	W
18	23/09/2013	Mon	16.6	16.3	16	77	79	85	41	42	33	2.5	3	5.3	0	0	0	W
19	25/09/2013	Wed	14.3	13	12	80	86	92	57	52	50	1	1.6	2	0	0	0	W
20	27/09/2013	Fri	10.5	9.1	6.98	75	82	90	119	129	146	0.73	0.83	1.2	0	0	0	--
21	01/10/2013	Tue	9.04	8.21	7.03	67	72	77	93	162	161	1.4	2.2	3	0	0	0	E
22	14/12/2013	Sat	2.6	2.2	1.5	88	91	94	16	28	39	2.7	2.9	4.2	1.1	0	0.1	W
23	17/12/2013	Tue	7.5	6.7	4.5	57	61	74	24	29	30	0.9	1.4	2.3	0.1	0	0	W
24	08/01/2014	Wed	10.8	10.4	9.4	73	75	82	26	37	42	2	2.7	4.3	0.4	0.3	0.3	W
25	15/01/2014	Wed	4.8	3.9	3.1	86	91	100	21	20	16	1.2	1.4	1.6	0.1	0	0.9	W
26	23/01/2014	Thu	-2.9	-3.6	-4.4	92	100	100	11	10	20	2.3	2.2	4.1	0.7	0.2	0	E
27	25/01/2014	Sat	-9	-9.8	-11.2	85	91	89	25	27	45	2.2	2.4	3.7	0.2	0	0	E
28	29/01/2014	Wed	-3.7	-4.3	-5.4	85	90	90	19	20	23	3	2.9	4.5	0	0	0	E
29	06/02/2014	Thu	6.7	6.2	5.4	70	73	79	38	65	75	2	2.8	4	0.03	0	0	W
30	17/02/2014	Mon	6.7	7.6	4.3	71	67	85	64	137	108	1.4	2.1	2.3	0	0	0	W
31	24/02/2014	Mon	7.9	6.7	5	58	63	70	94	123	136	1.2	1.9	2.2	0	0	0	--
32	01/12/2014	Mon	-0.8	-2.0	-2.0	78	78	82	18	11	19	4.2	3.9	6.2	NA	0	0	E
33	03/12/2014[a]	Wed	-0.8	-1.9	-1.3	88	92	90	5	5	8	1.8	2	3.2	NA	0	0	E
34	21/01/2015	Wed	0.7	-0.5	0.0	81	86	87	28	55	51	1.7	1.7	1.9	NA	0	0	W
35	30/01/2015	Fri	2.5	1.4	1.3	86	89	92	31	34	26	3	3.2	4.5	NA	2.3	1	W
36	10/02/2015	Tue	5.8	4.5	4.5	83	87	91	14	16	22	1.4	1.9	2.2	NA	0	0	W
37	13/02/2015	Fri	2.6	1.2	0.2	76	80	87	42	111	112	1	1.9	1.6	NA	0	0	--
38	15/02/2015	Sun	2.6	1.3	1.6	79	83	85	36	51	48	1.4	1.5	2.6	NA	0	0	E
39	19/02/2015	Thu	2.3	1.3	1.1	78	80	85	65	114	115	2.2	2.5	3.8	NA	0	0	--
40	24/02/2015	Tue	5.7	4.7	4	71	72	81	76	93	89	1.8	2.5	3.3	NA	0	0	W
41	26/02/2015	Thu	5.4	3.2	1.7	63	68	78	101	139	141	0.84	1.7	1.3	NA	0	0	W
42	16/03/2015	Mon	9.6	8.7	8.9	66	66	72	118	124	112	3.3	3.3	4.5	NA	0	0.1	E

a Sampling in MEL from 09:10–09:10 CET due to technical issues

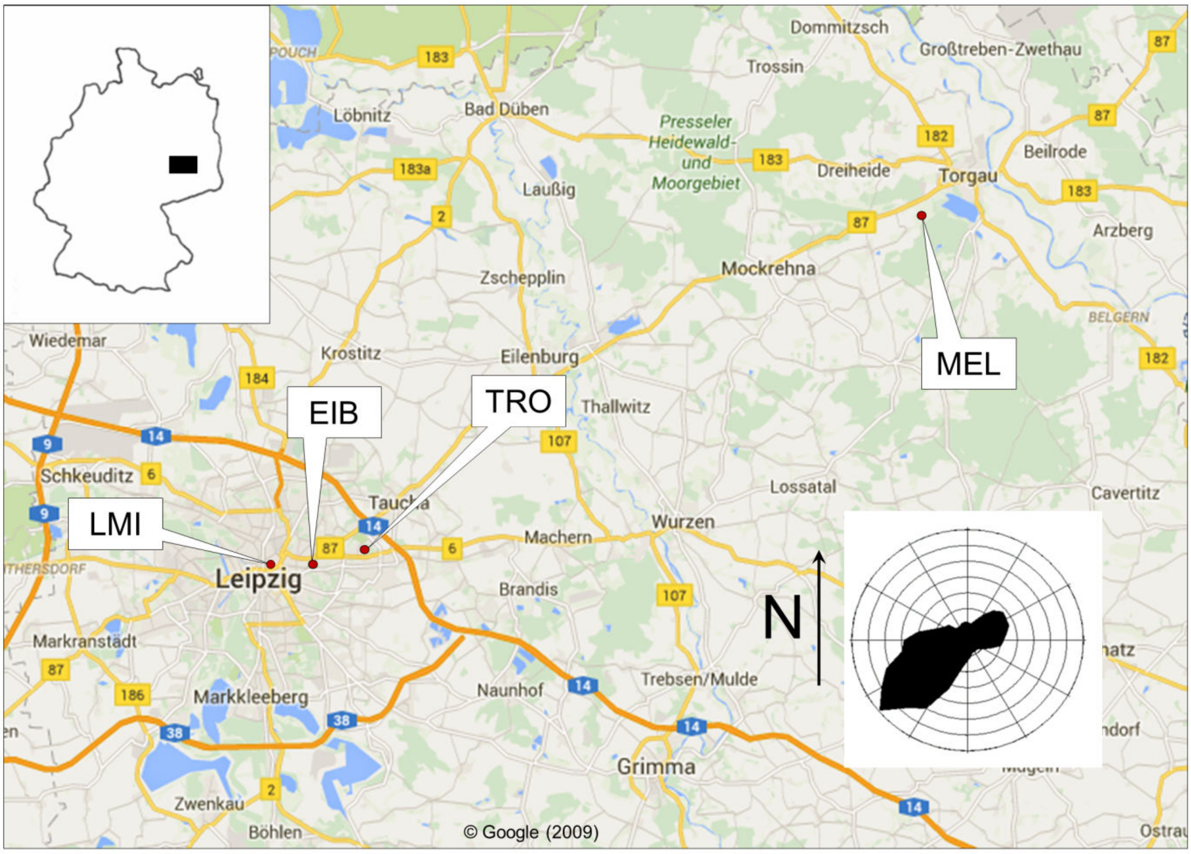

Figure S1: Location of the area of investigation in Germany with the sampling places in Leipzig LMI (traffic hotspot, EIB (kerbside and residential site) and TRO (urban background) and in Melpitz (MEL) in the regional background. The wind rose in 10°-steps indicates main wind directions at Melpitz (2010 to 2014).

Figure S2: Mean mass fractions of regional, urban and traffic increments from Lenschow approach for $PM_{1.2}$, $PM_{3.5}$, and PM_{10} (sum of 3, 4, and 5 impactor stages) in 2 seasons and 2 main air mass inflow sectors. "All" refers to all data per season and/or sector (for sector including non-categorized samples). Numbers printed in black above the bars indicate mean particle mass concentrations at the LMI kerbside site, while numbers in white indicate the respective mass fractions.

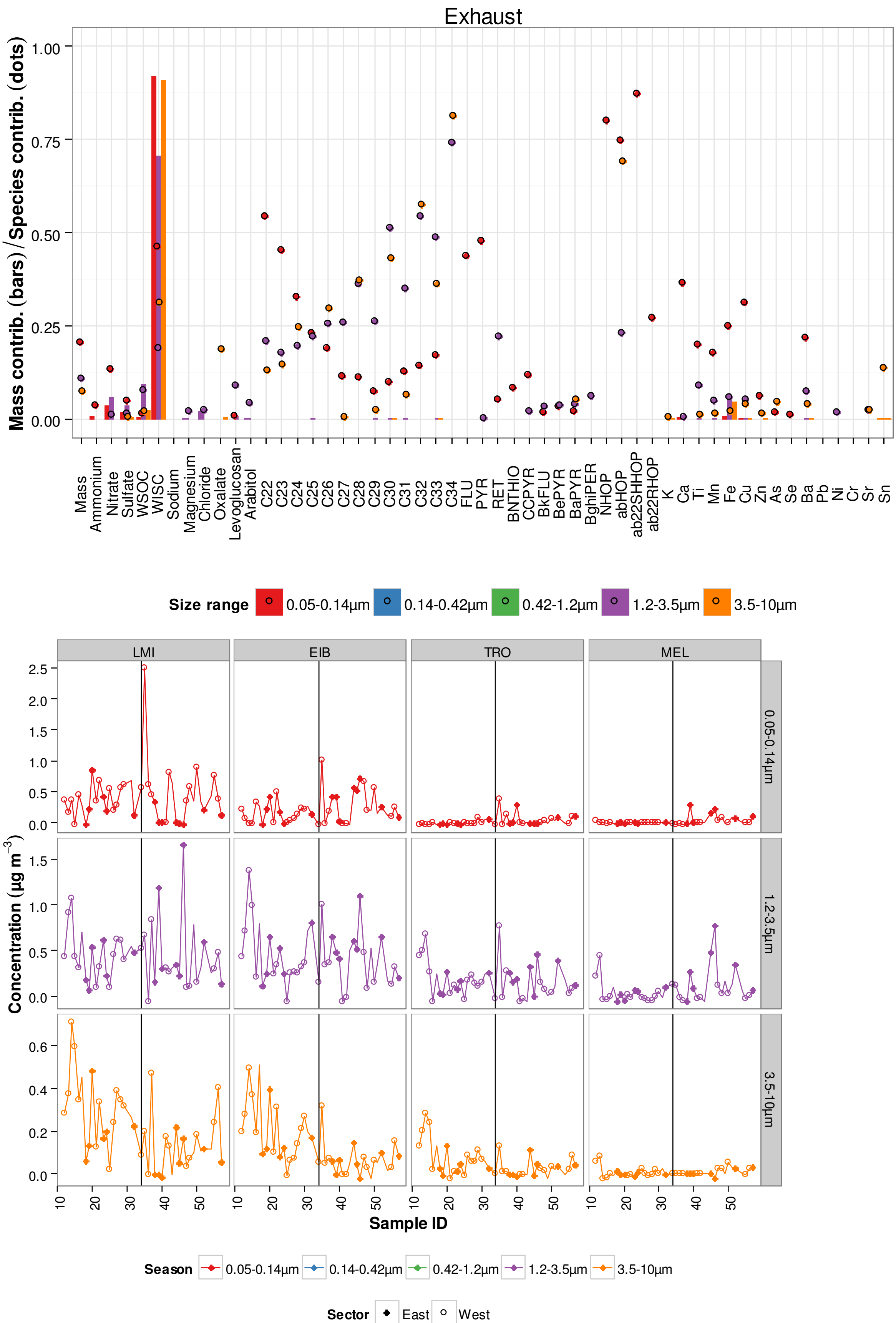

Figure S3: Chemical profile (top) of PMF factor "Traffic Exhaust", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

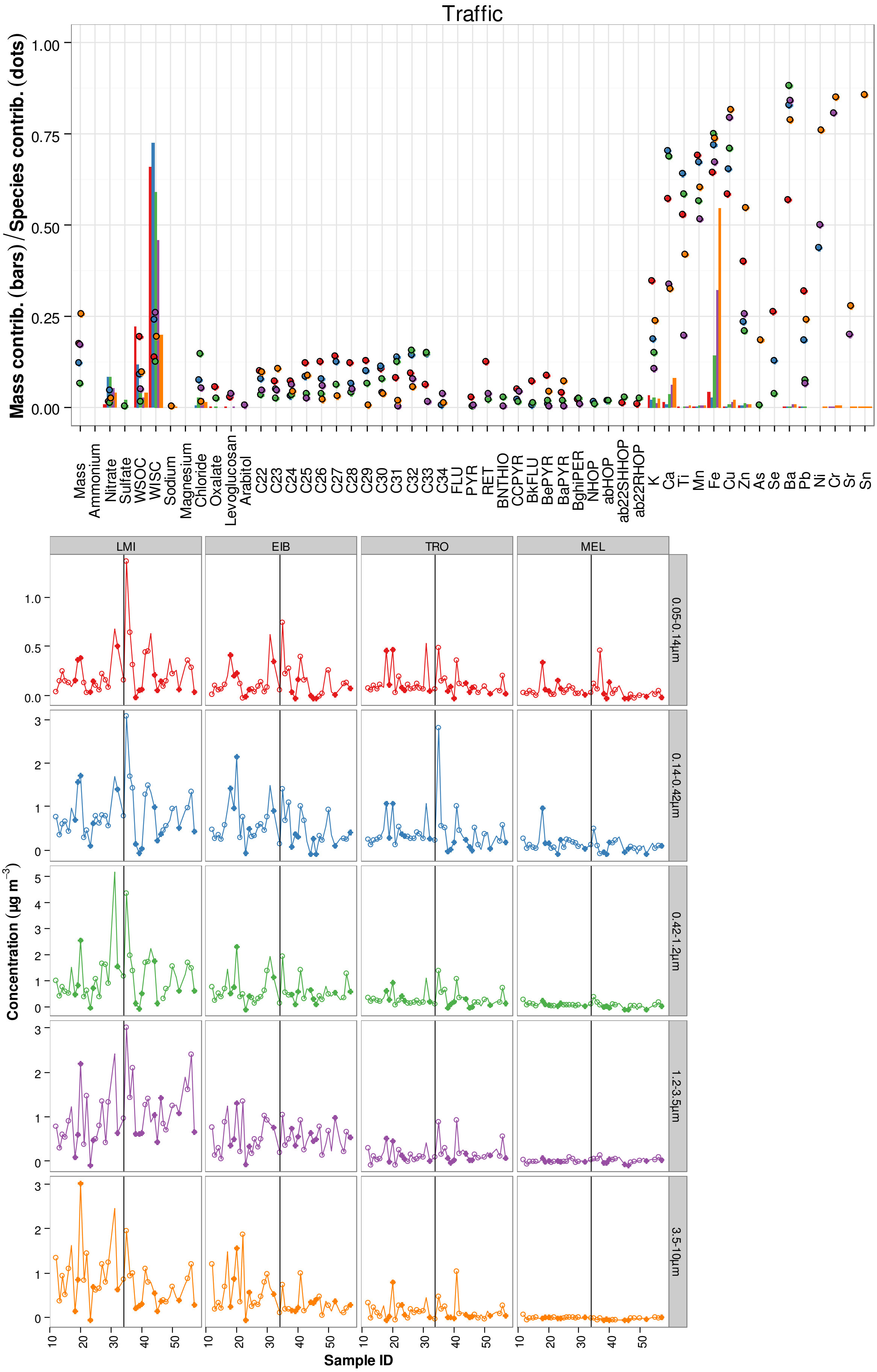

Figure S4: Chemical profile (top) of PMF factor "General Traffic", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in. Legends as in previous Figure.

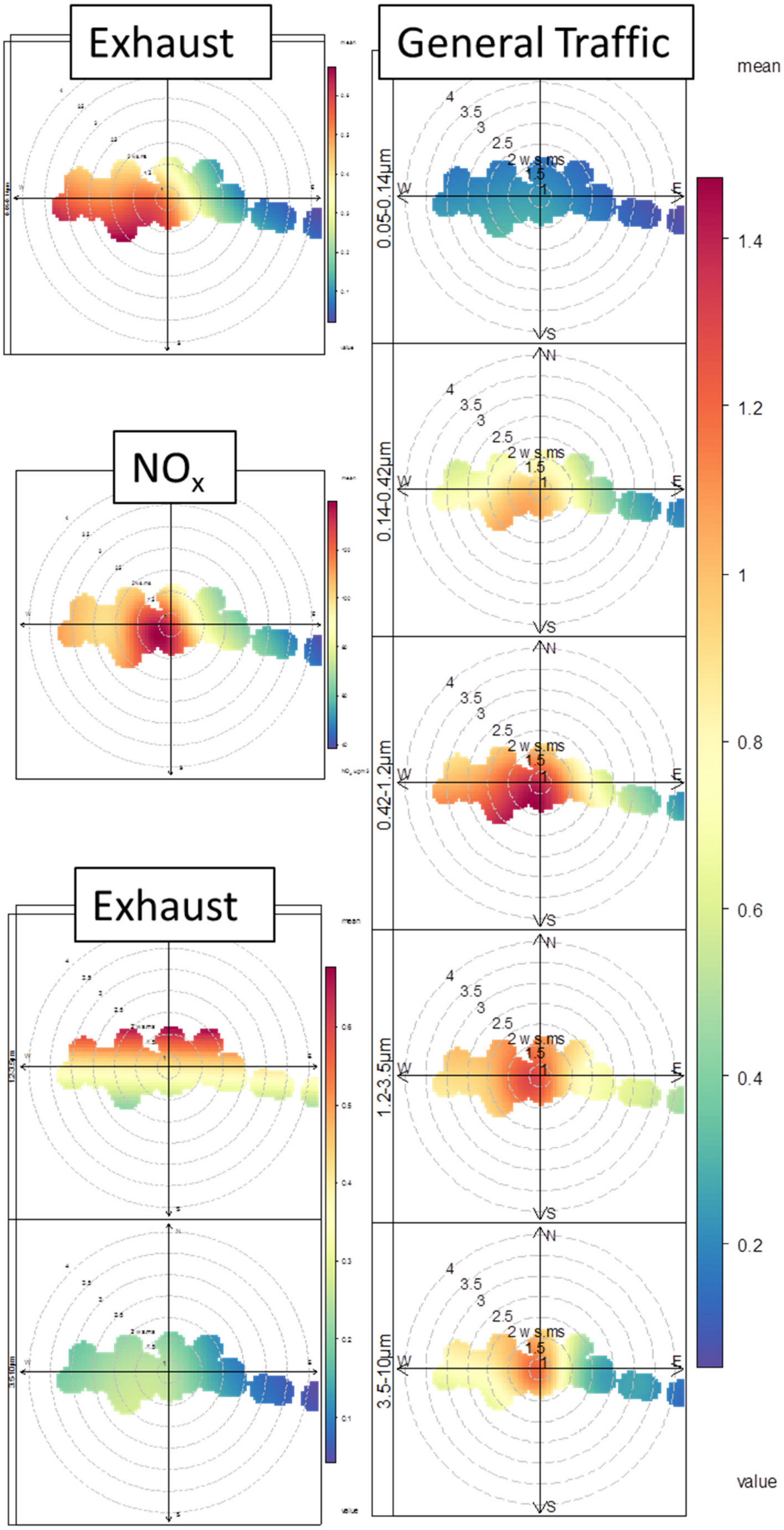

Figure S5: Polar plots of exhaust emissions (left column top and bottom), general traffic emissions (right column), and NO_x during sampling days (left column middle) at LMI traffic site, showing local wind direction (and wind speed in m s^{-1}) dependency of traffic emission transport to the sampling inlet.

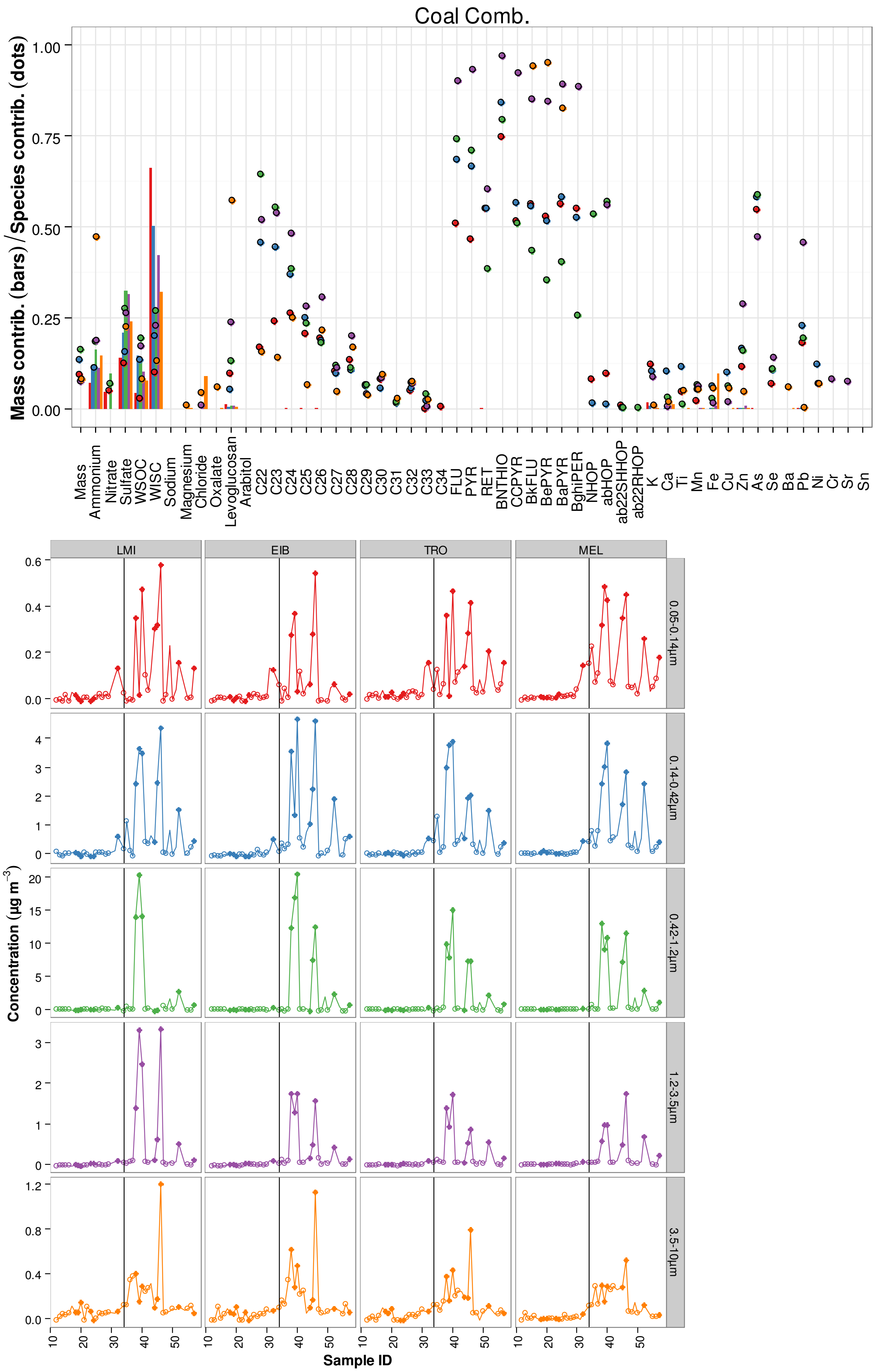

Figure S6: Chemical profile (top) of PMF factor "Coal Combustion", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in. Legends as in previous Figures.

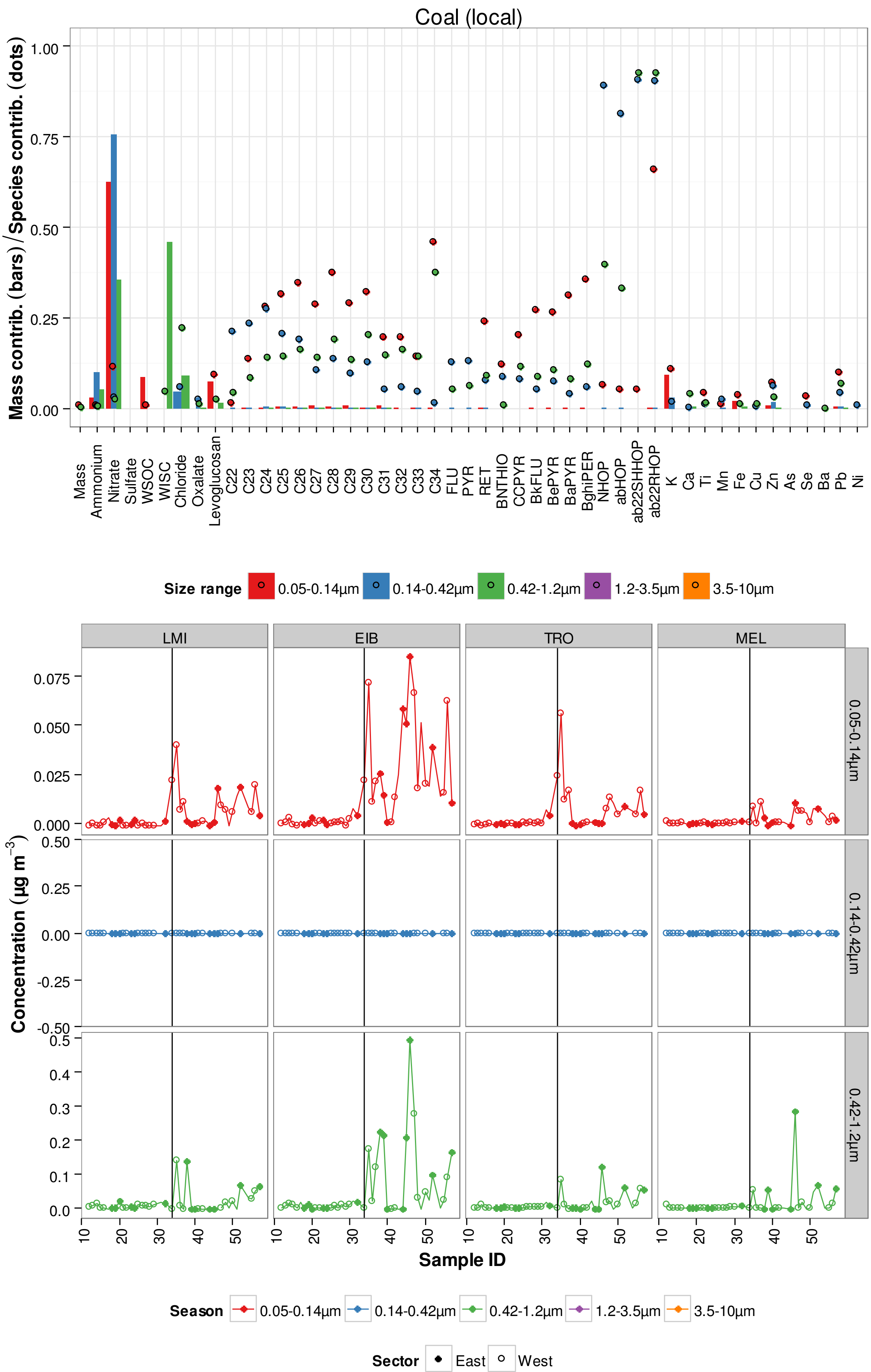

Figure S7: Chemical profile (top) of PMF factor "Local Coal Combustion", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in. No mass assigned by PMF model in 0.14–0.42 µm size range.

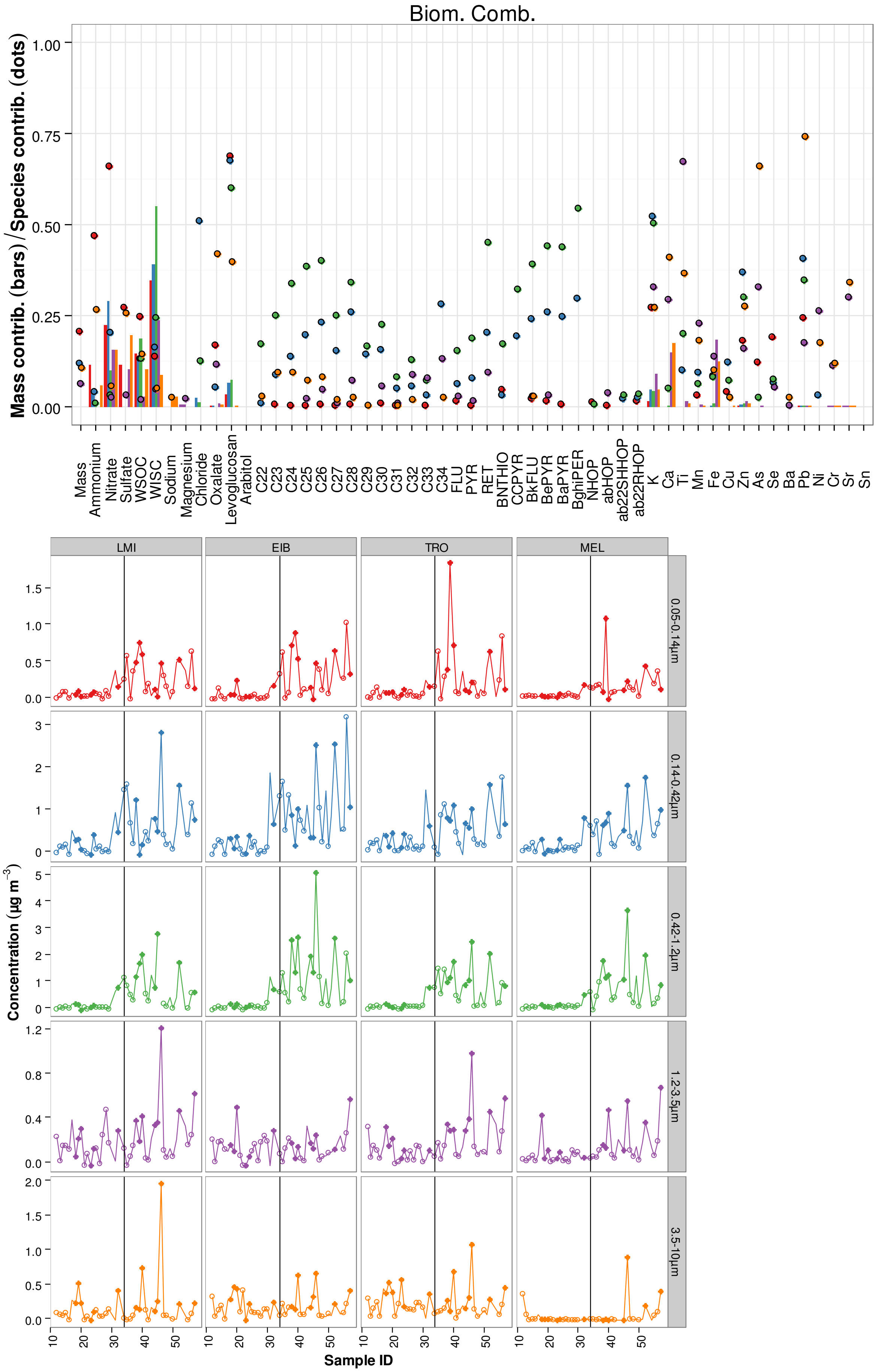

Figure S8: Chemical profile (top) of PMF factor "Biomass Combustion", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in. Legends as in previous Figures.

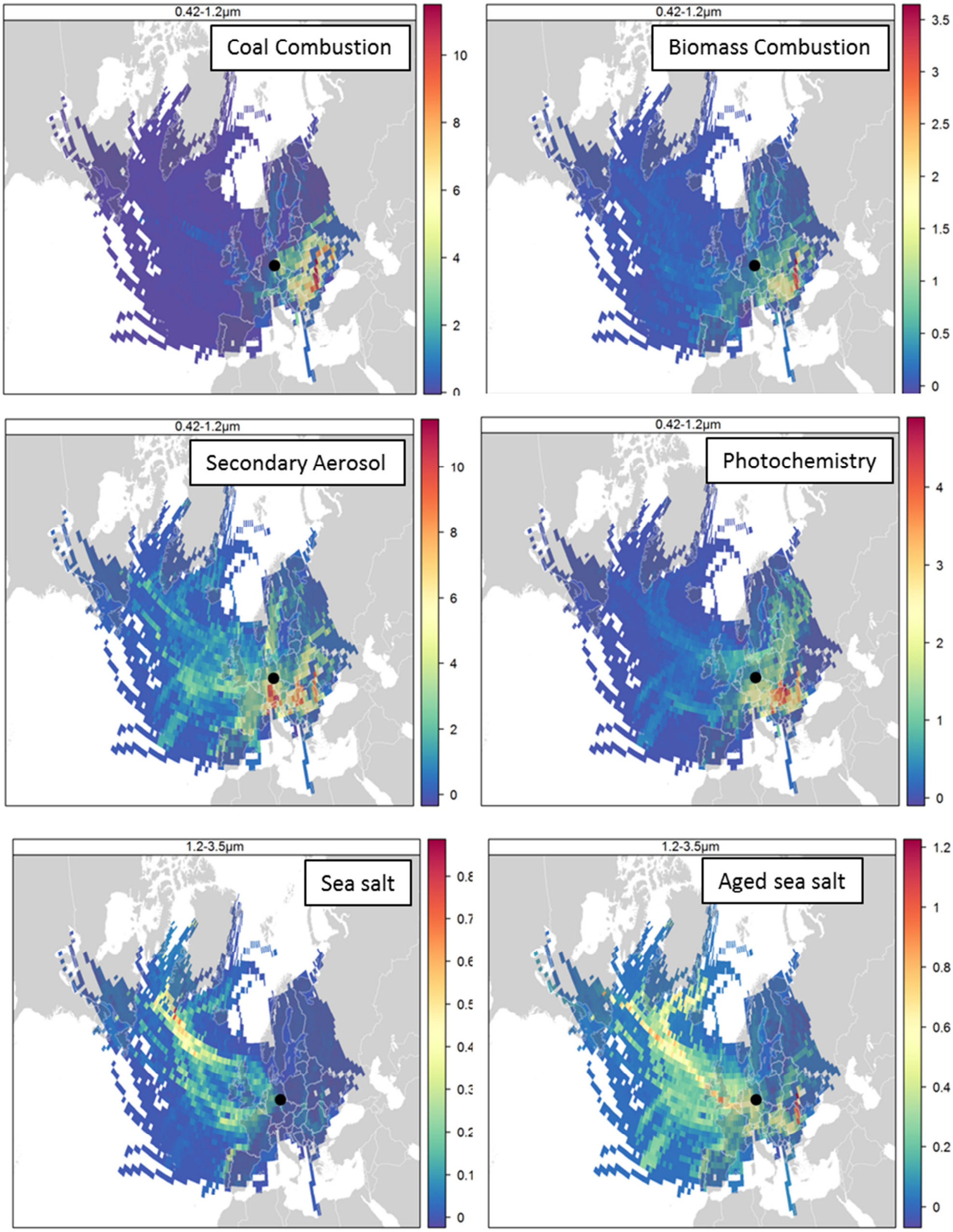

Figure S9: Concentration-weighted trajectory plots for 6 regional sources, shown for 0.42-1.2 µm size range for combustion and secondary sources, and 1.2-3.5 µm size range for sea salt related sources. Factor concentrations from regional background site in Melpitz used for plotting.

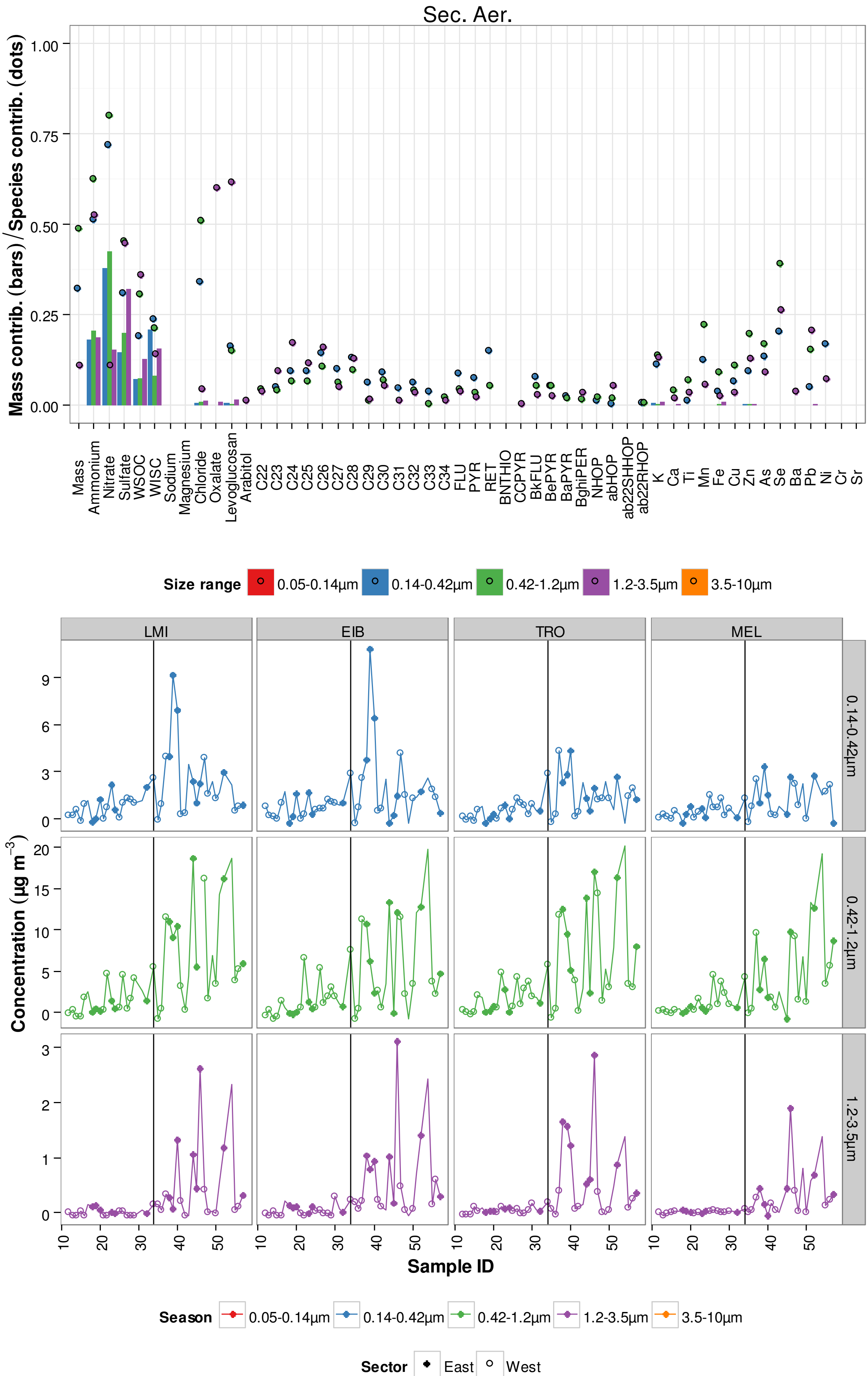

Figure S10: Chemical profile (top) of PMF factor "Secondary Aerosol", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

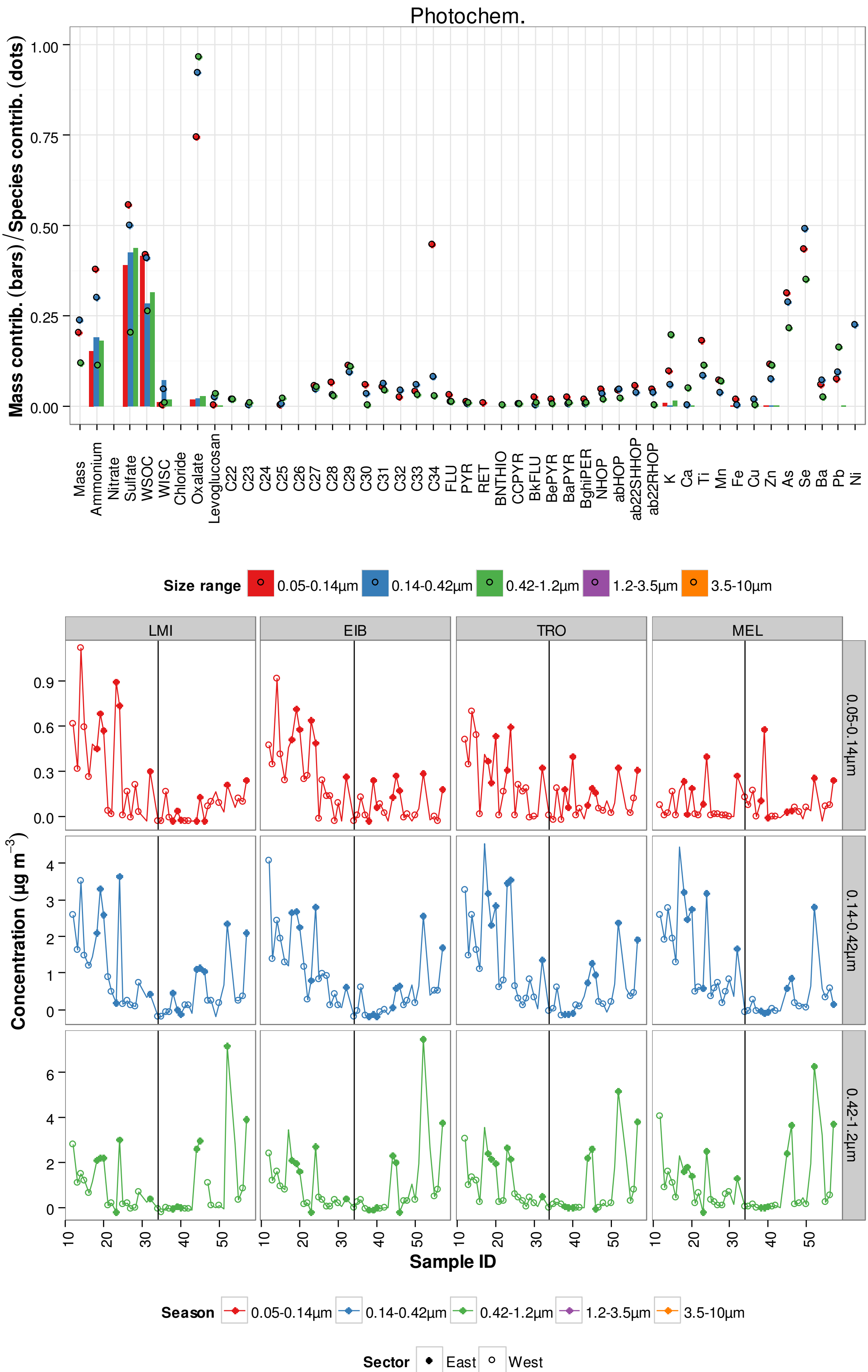

Figure S11: Chemical profile (top) of PMF factor "Photochemistry", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

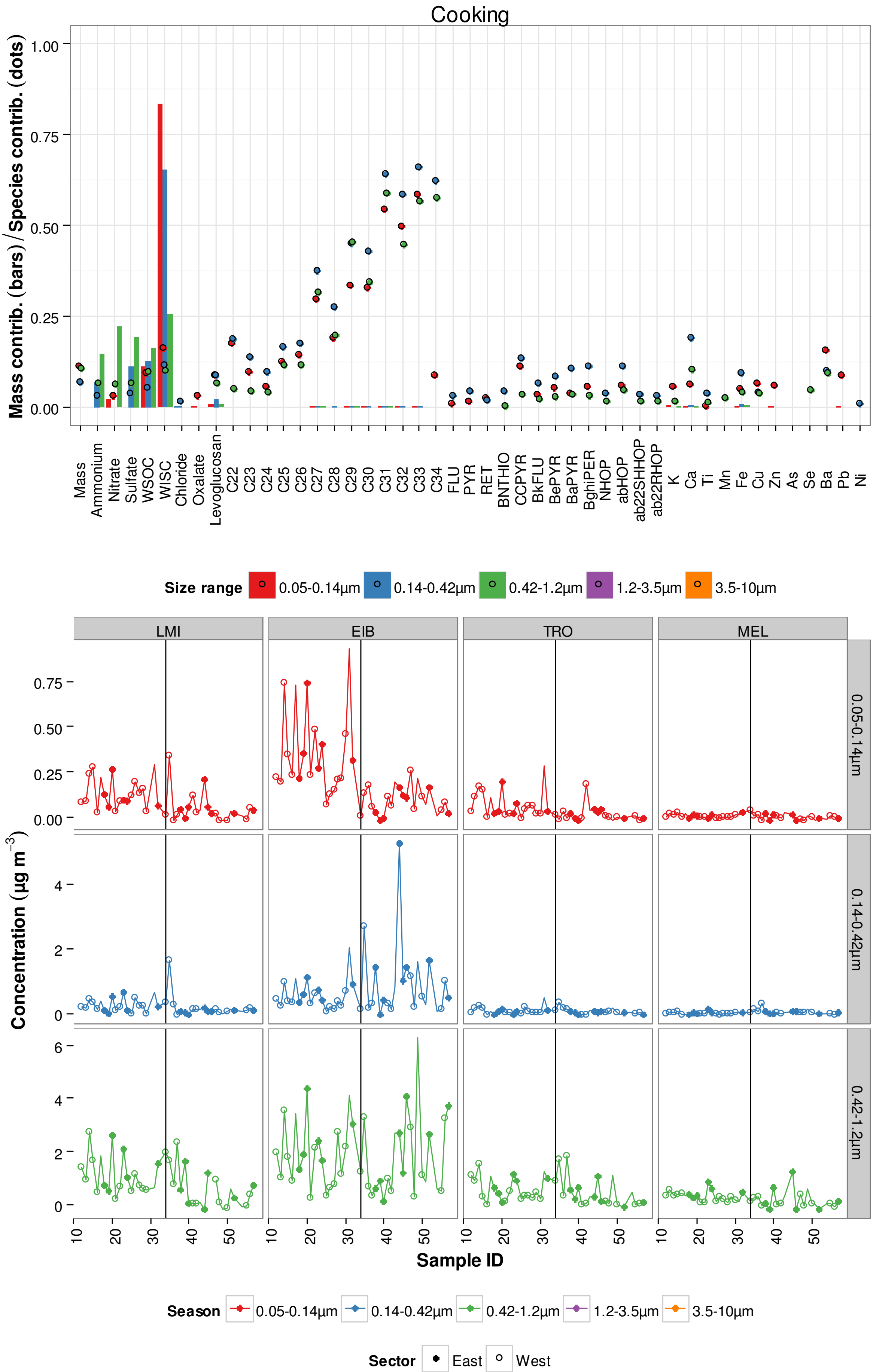

Figure S12: Chemical profile (top) of PMF factor "Cooking", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

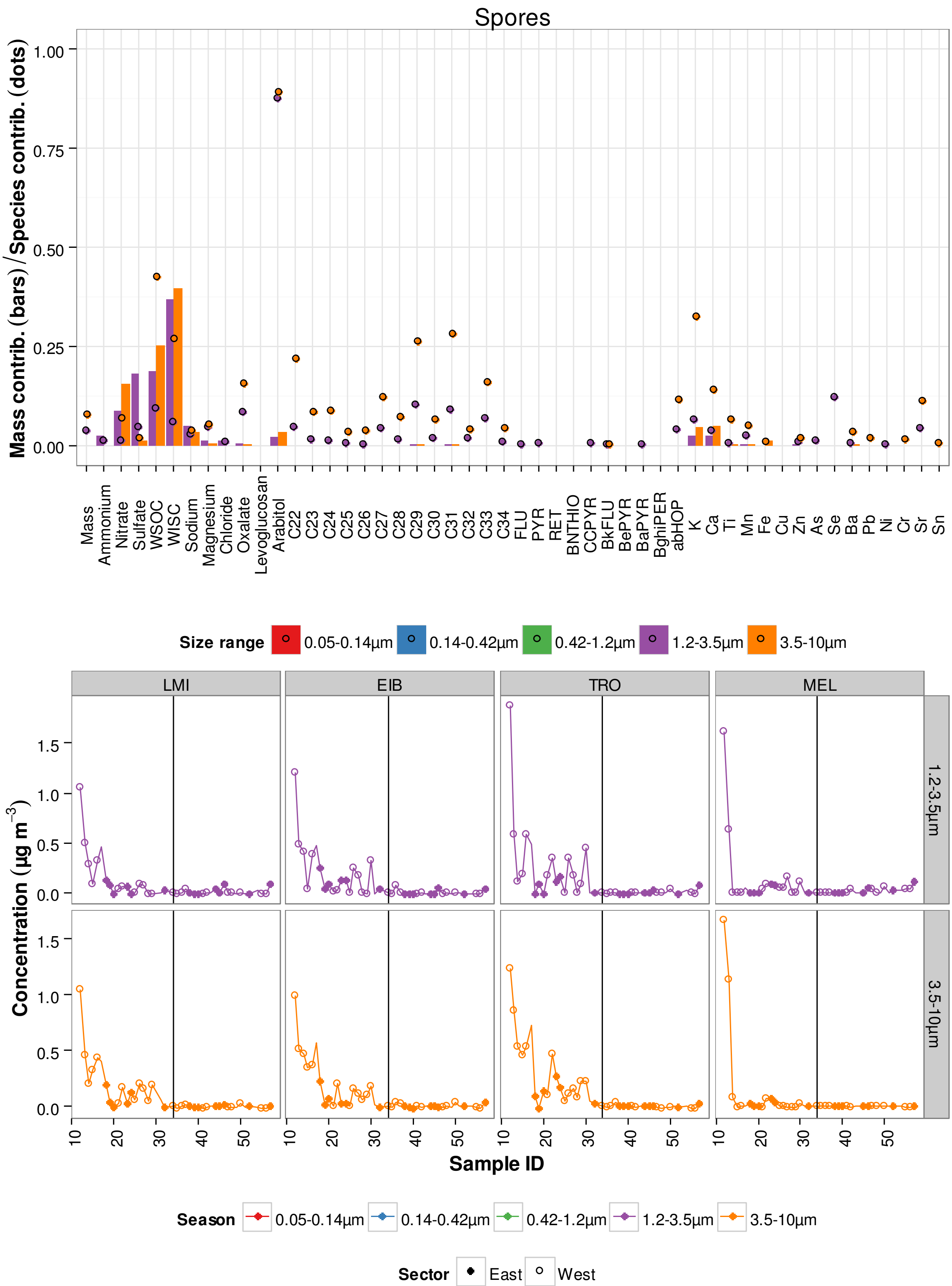

Figure S13: Chemical profile (top) of PMF factor "Fungal Spores", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

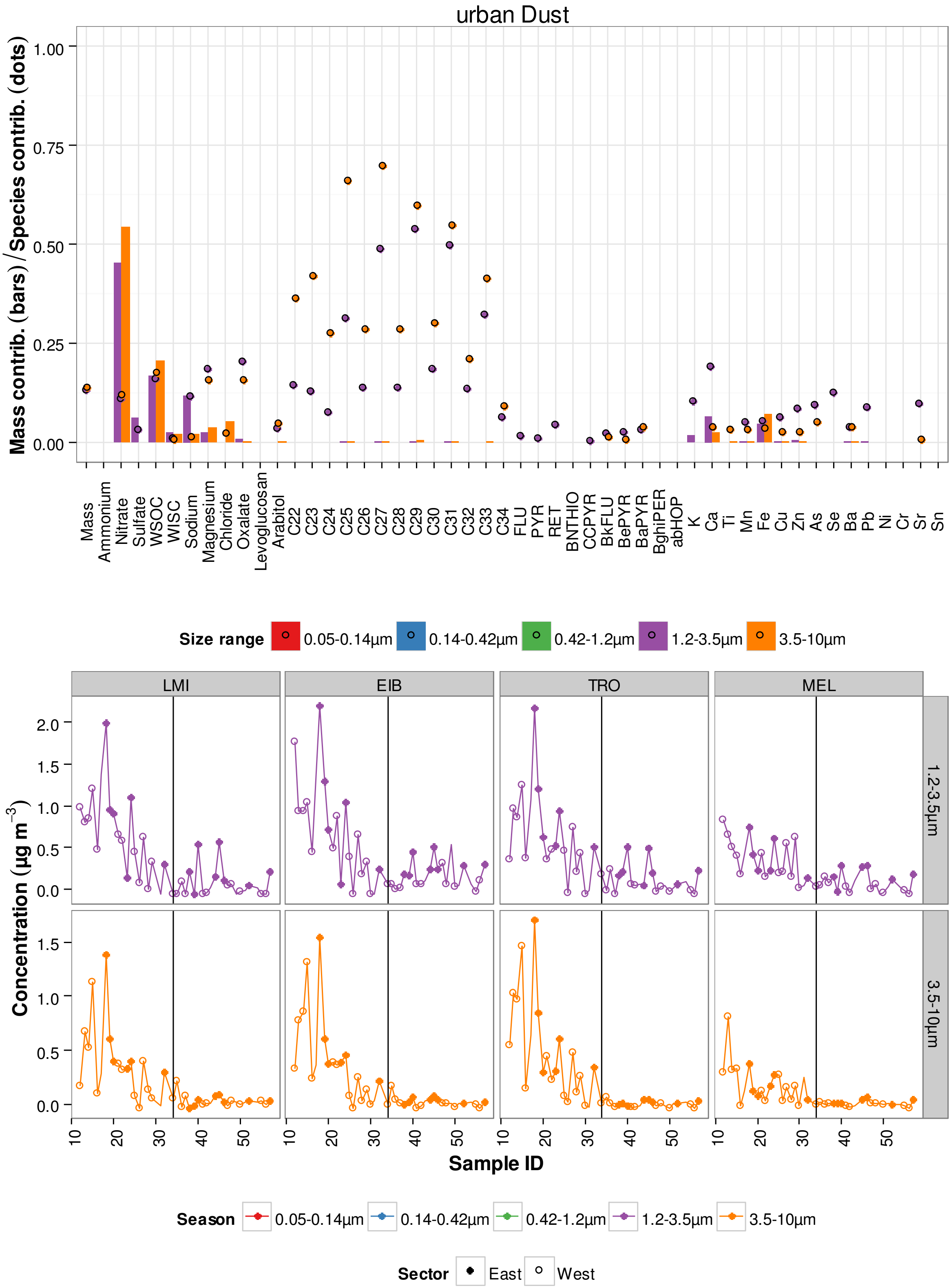

Figure S14: Chemical profile (top) of PMF factor “Urban Dust”, indicating mass and species contributions of particle constituents, as well as “time series” of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

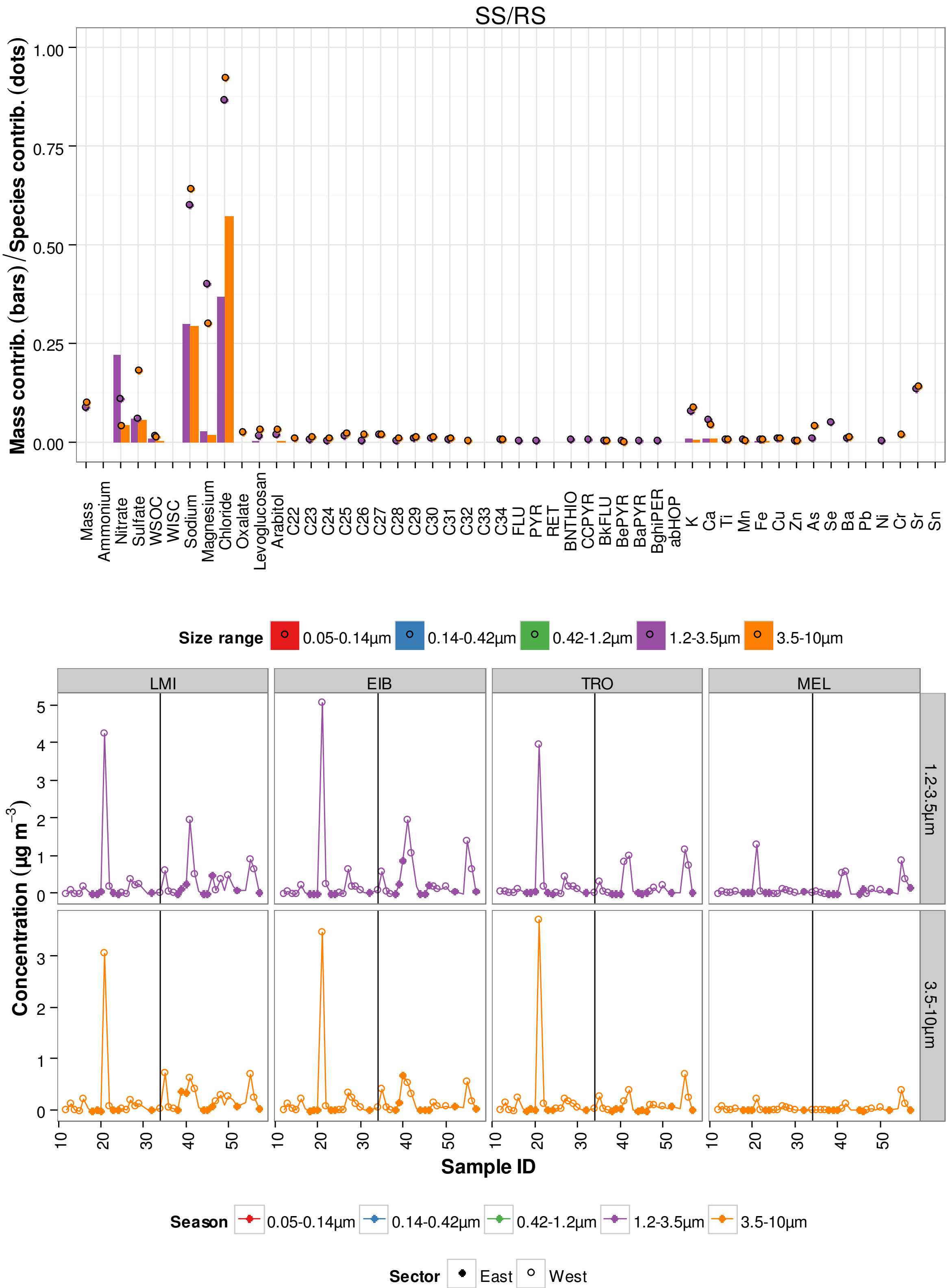

Figure S15: Chemical profile (top) of PMF factor “Sea and Road Salt”, indicating mass and species contributions of particle constituents, as well as “time series” of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

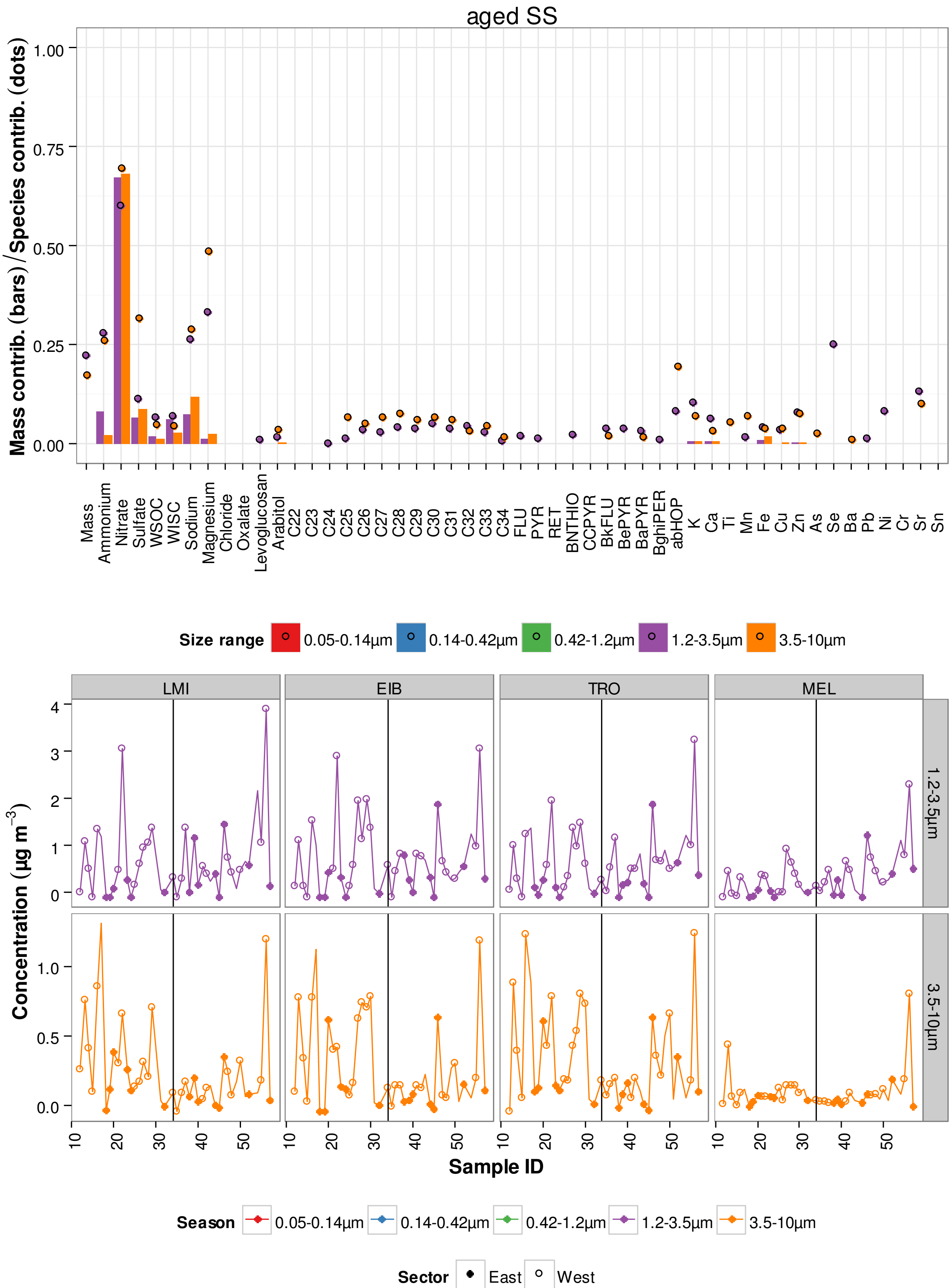

Figure S16: Chemical profile (top) of PMF factor "Aged Sea Salt", indicating mass and species contributions of particle constituents, as well as "time series" of particle mass concentrations (bottom) for all particle size ranges the source was resolved in.

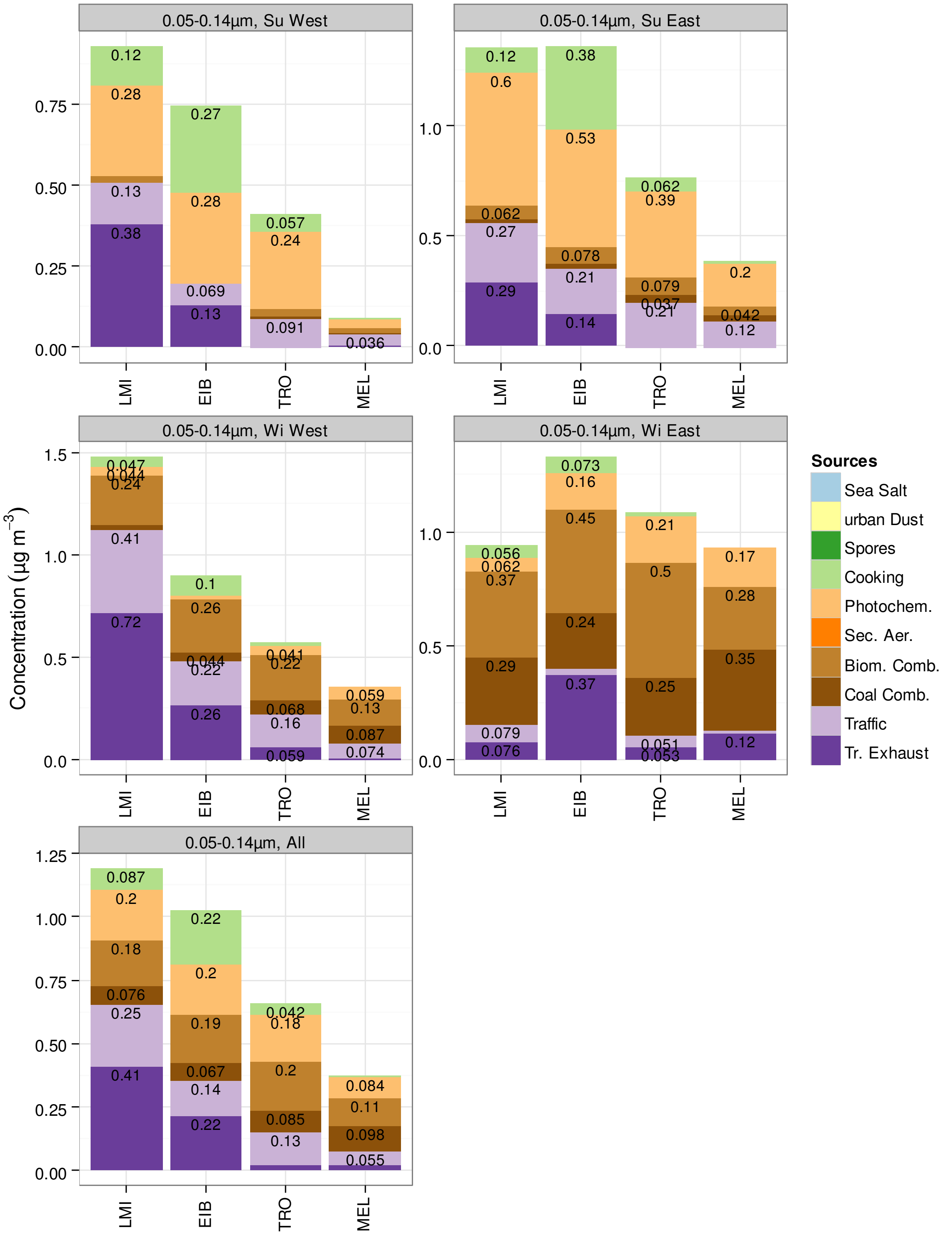

Figure S17: Mean source contributions to particle mass concentrations for 0.05–0.14 µm size range in summer (Su) and winter (Wi) as well as during western and eastern air mass inflow and as total average for all samples ("All").

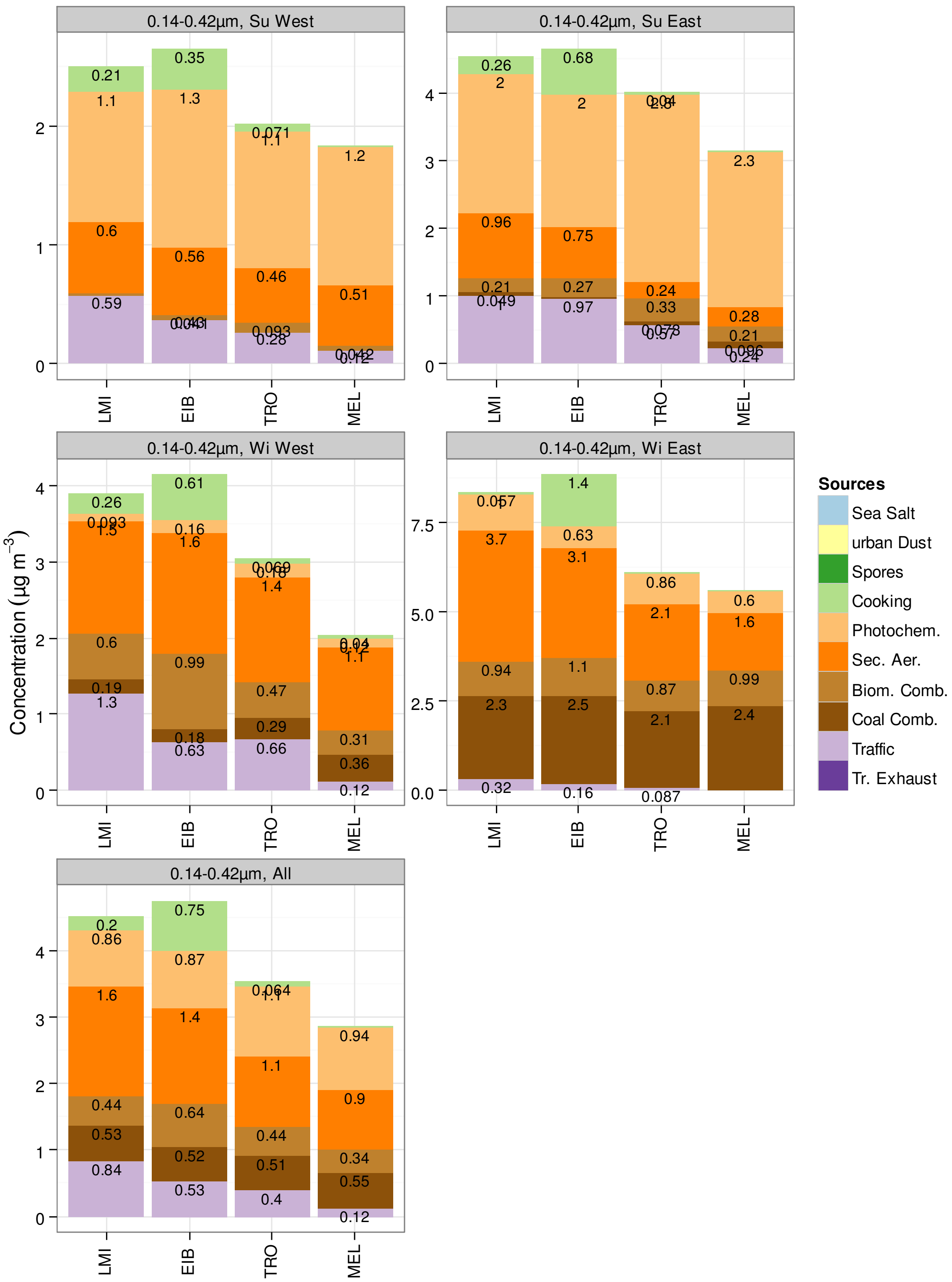

Figure S18: Mean source contributions to particle mass concentrations for 0.14–0.42 µm size range in summer (Su) and winter (Wi) as well as during western and eastern air mass inflow and as total average for all samples ("All").

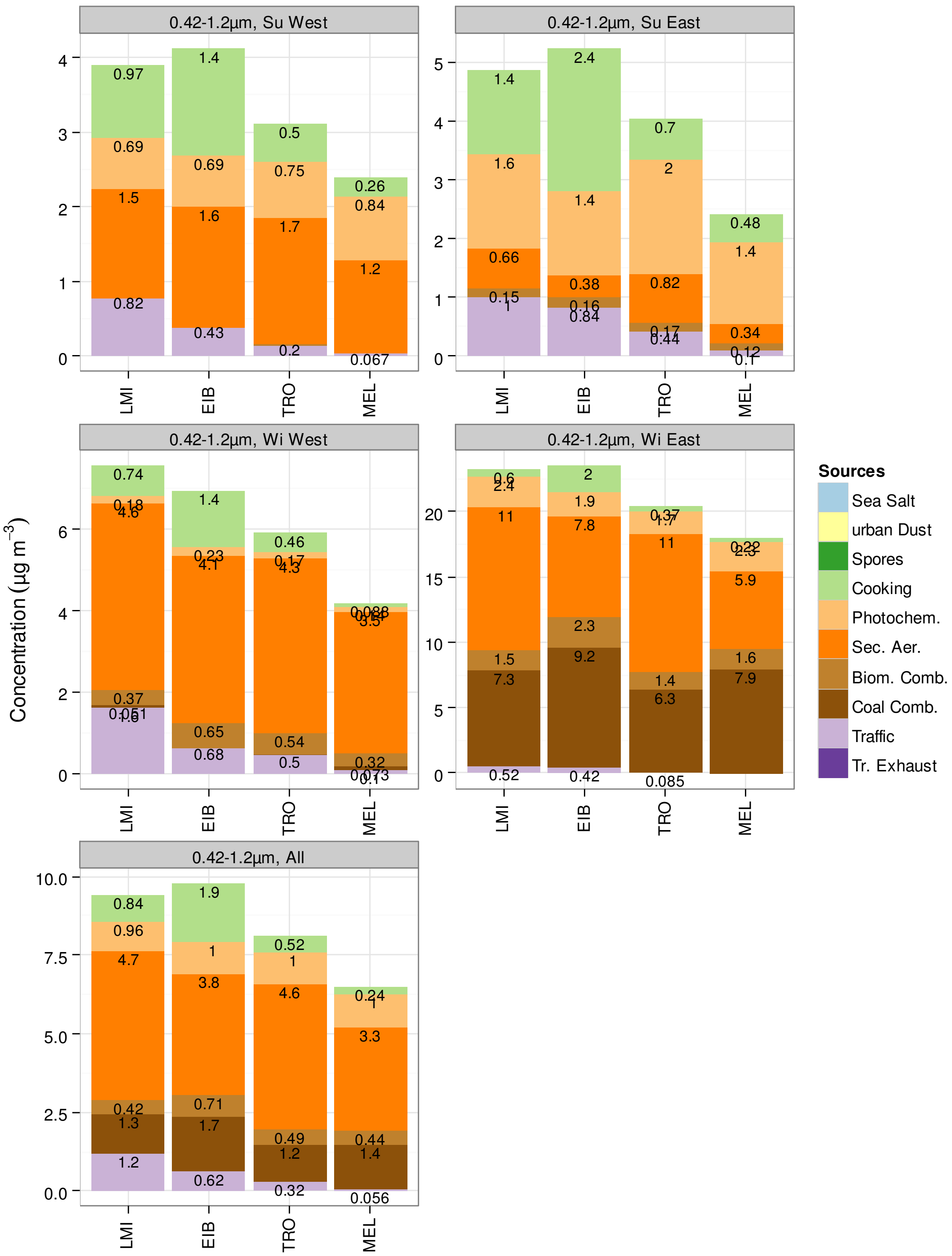

Figure S19: Mean source contributions to particle mass concentrations for 0.42–1.2 µm size range in summer (Su) and winter (Wi) as well as during western and eastern air mass inflow and as total average for all samples ("All").

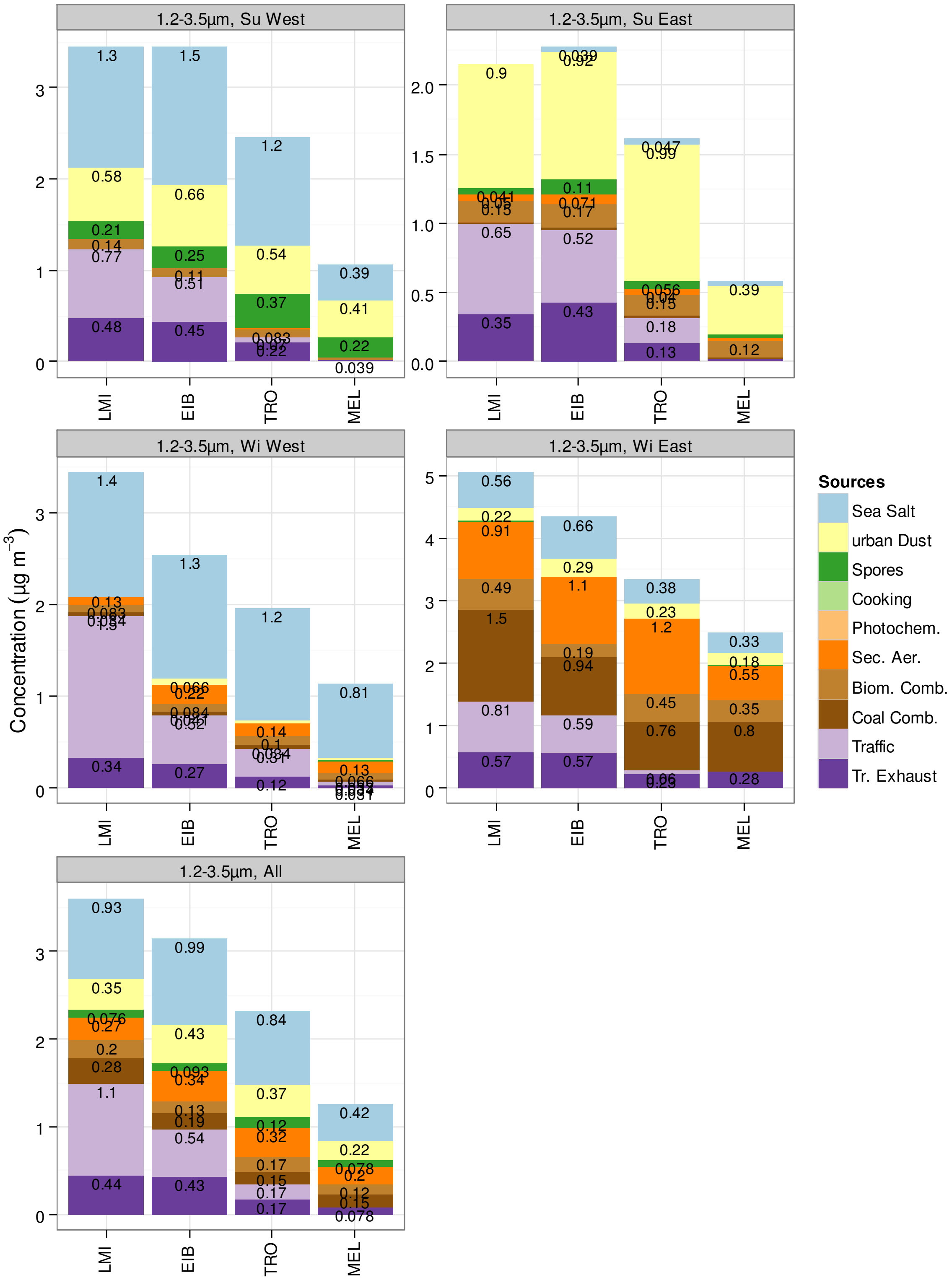

Figure S20: Mean source contributions to particle mass concentrations for 1.2–3.5 µm size range in summer (Su) and winter (Wi) as well as during western and eastern air mass inflow and as total average for all samples ("All").

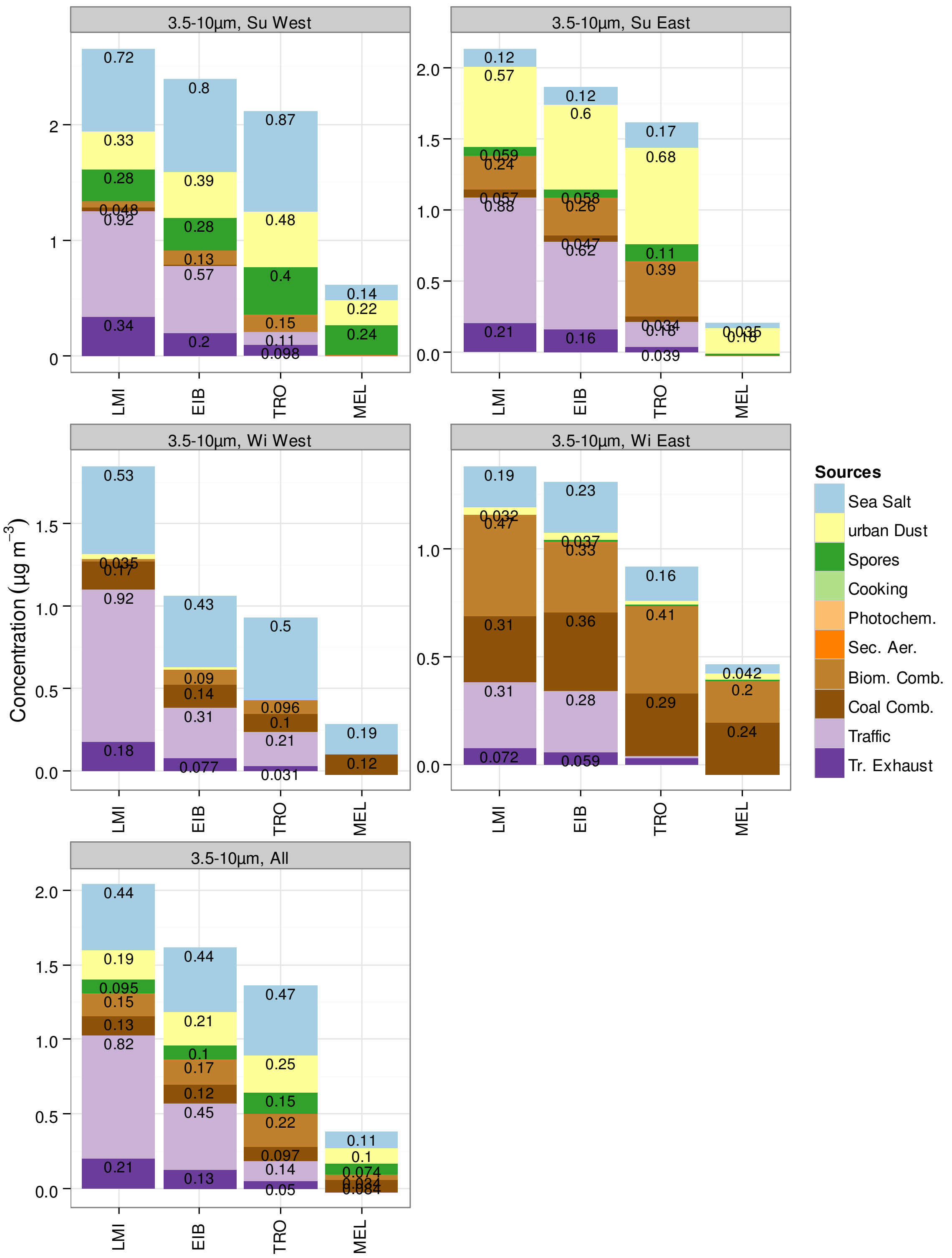

Figure S21: Mean source contributions to particle mass concentrations for 3.5–10 µm size range in summer (Su) and winter (Wi) as well as during western and eastern air mass inflow and as total average for all samples ("All").

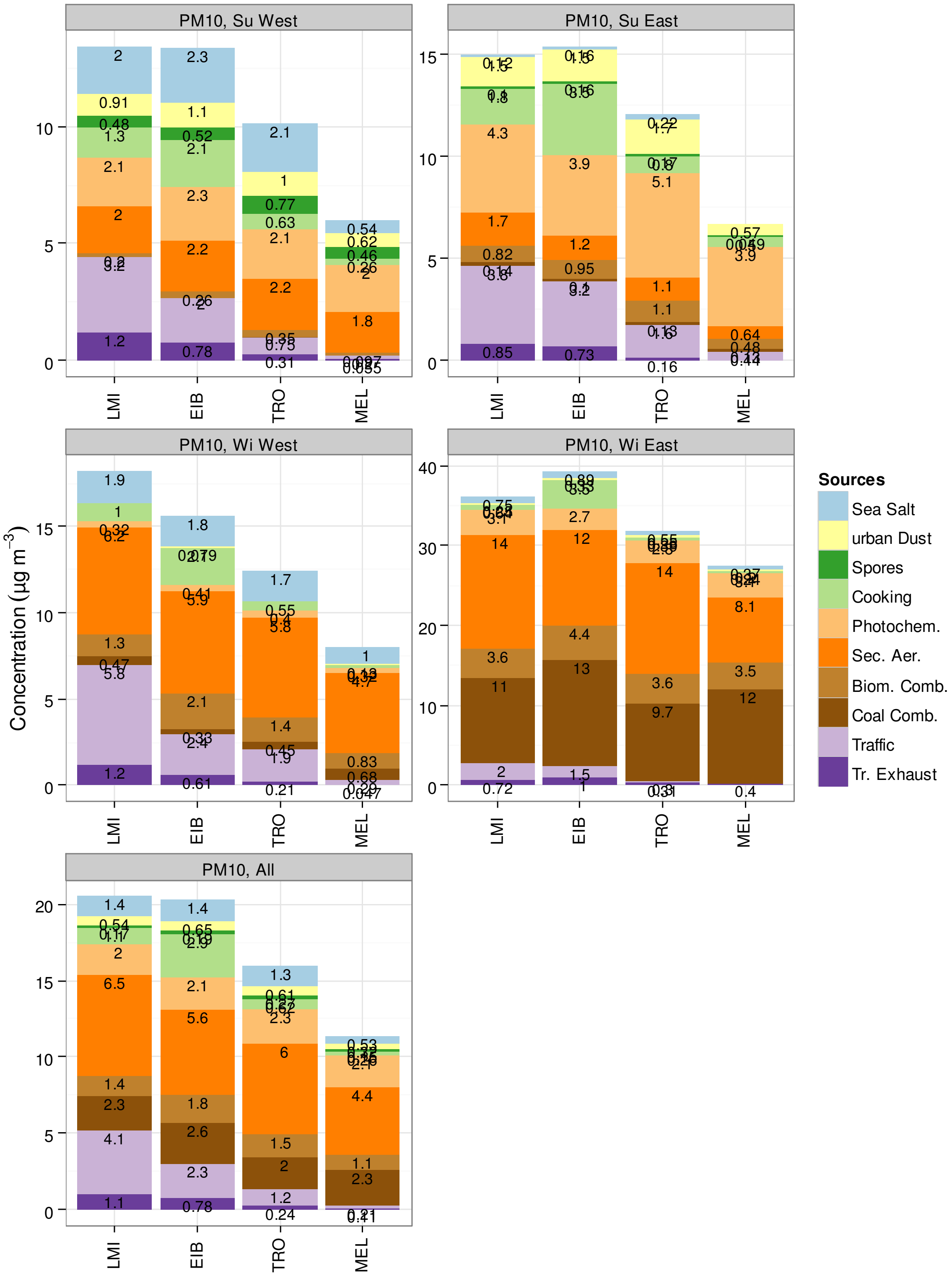

Figure S22: Mean source contributions to particle mass concentrations for PM_{10} (sum of impactor stages) in summer (Su) and winter (Wi) as well as during western and eastern air mass inflow and as total average for all samples ("All").

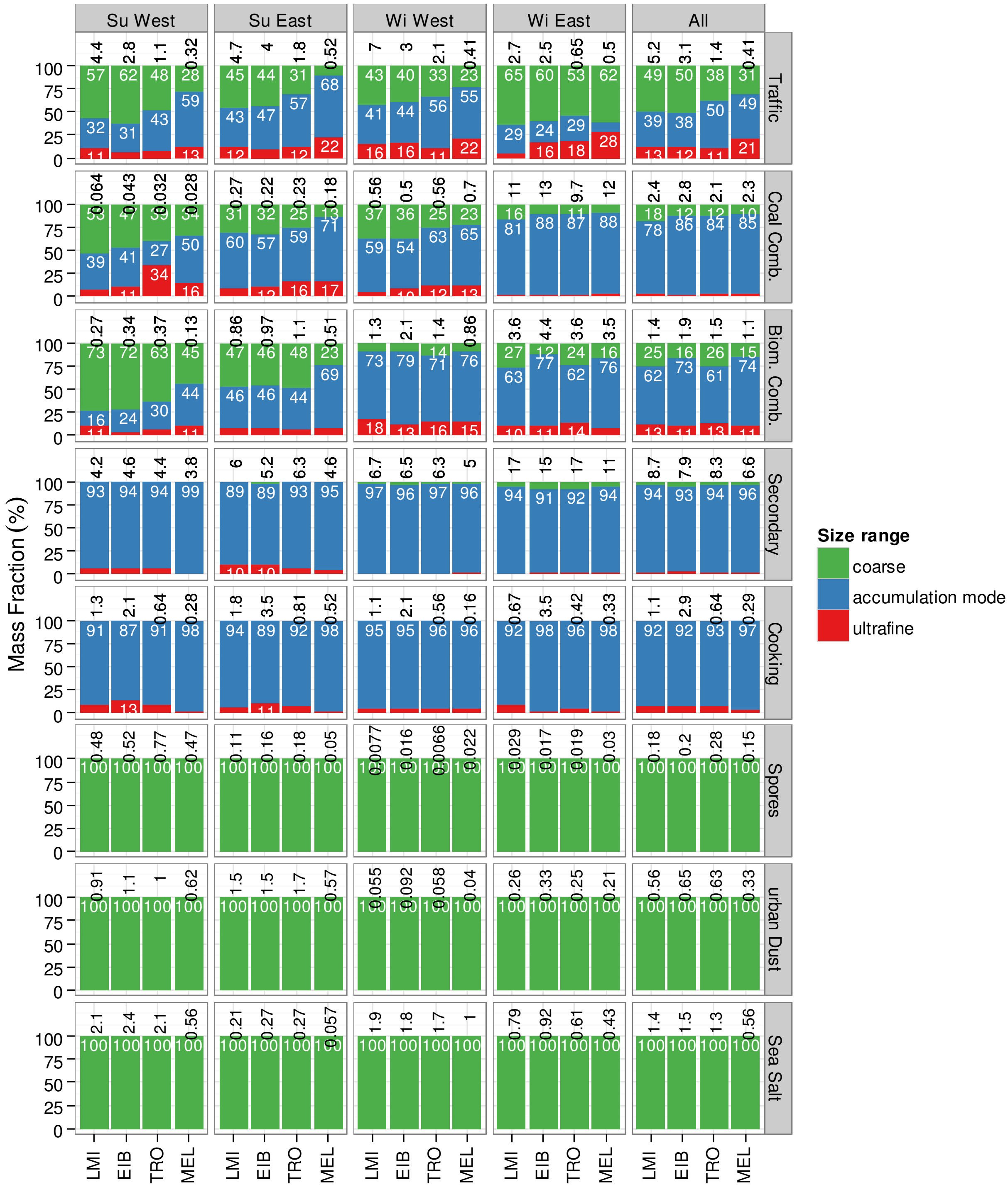

Figure S23: Mean source contributions summarised into ultrafine (impactor stage 1), accumulation mode (impactor stages 2 and 3) and coarse particles (impactor stages 4 and 5). Total source concentrations (µg m-3) are printed in black on top, while stacked bars indicate fractions in respective size ranges. Note that 2 traffic, 2 coal combustion, 2 secondary and 2 sea salt related sources were combined for this plot).

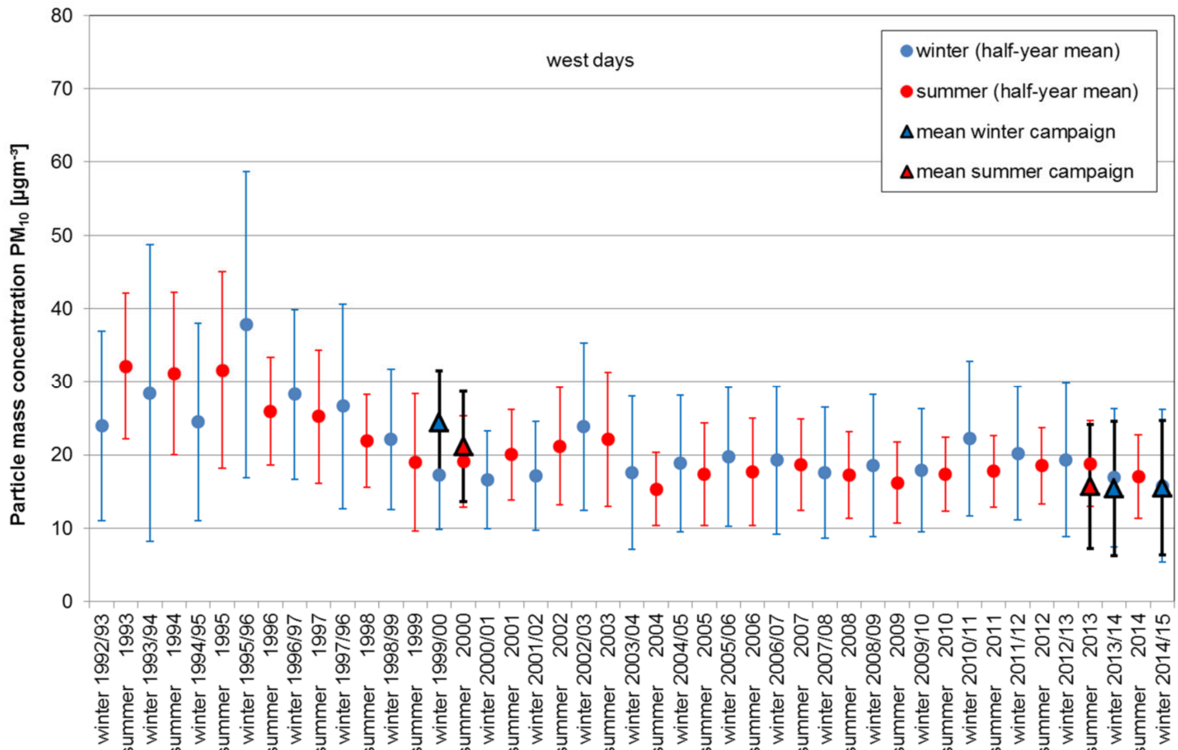

Figure S24: Mean PM_{10} particle mass concentration at Melpitz for the summer (May – October) and winter (November – April) half years (red and blue points) compared with the means for all days in the campaigns in winter 1999/2000, summer 2000, summer 2013, winter 2013/14 and winter2014/15 (red and blue triangles). The error bars are the standard deviation of daily particle mass concentration.

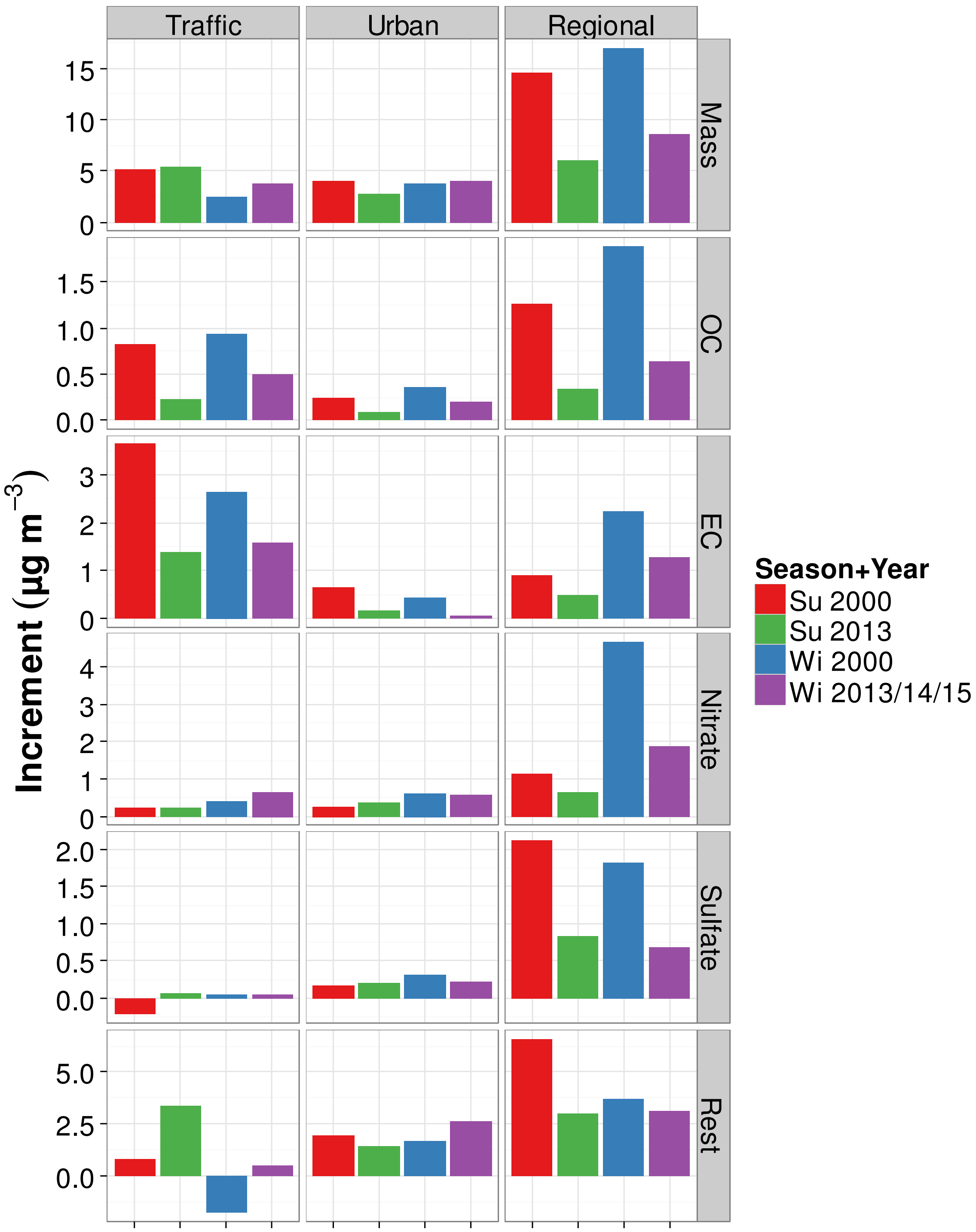

Figure S25: Mean PM3.5 concentrations at Melpitz ("Regional" column) and urban and traffic increments (Lenschow approach) of particle mass and constituents in summer and winter durint the year 2000 and the present study.