

S-1. Identified compounds from UHPLC–(–)ESI–UHRMS analysis of filter samples

Table S-1: List of CHO-containing compounds that were identified by UHPLC–(–)ESI–UHRMS analysis of the filter samples.

formula for [M–H] [–]	<i>m/z</i> for [M–H] [–]	measured <i>m/z</i>	Δm / ppm	Number of Oxygen	Number of Carbon	O:C
C ₄ H ₅ O ₅	133.0142	133.0141	-1.1	5	4	1.3
C ₆ H ₇ O ₄	143.0350	143.0349	-0.6	4	6	0.7
C ₆ H ₉ O ₄	145.0506	145.0506	-0.2	4	6	0.7
C ₆ H ₉ O ₅	161.0455	161.0454	-0.9	5	6	0.8
C ₆ H ₁₃ O ₆	181.0718	181.0718	0.2	6	6	1.0
C ₆ H ₇ O ₇	191.0197	191.0197	-0.1	7	6	1.2
C ₇ H ₉ O ₃	141.0557	141.0557	-0.1	3	7	0.4
C ₇ H ₉ O ₄	157.0506	157.0505	-0.9	4	7	0.6
C ₇ H ₁₁ O ₄	159.0663	159.0661	-1.2	4	7	0.6
C ₇ H ₉ O ₅	173.0455	173.0453	-1.4	5	7	0.7
C ₇ H ₁₁ O ₅	175.0612	175.0611	-0.6	5	7	0.7
C ₇ H ₇ O ₆	187.0248	187.0247	-0.6	6	7	0.9
C ₇ H ₉ O ₆	189.0405	189.0403	-0.9	6	7	0.9
C ₈ H ₁₃ O ₃	157.0870	157.0871	0.5	3	8	0.4
C ₈ H ₁₁ O ₄	171.0663	171.0662	-0.5	4	8	0.5
C ₈ H ₁₁ O ₅	187.0612	187.061	-1.1	5	8	0.6
C ₈ H ₁₃ O ₅ *	189.0768	189.0767	-0.8	5	8	0.6
C ₈ H ₉ O ₆	201.0405	201.0403	-0.8	6	8	0.8
C ₈ H ₁₁ O ₆ *	203.0561	203.0561	-0.1	6	8	0.8
C ₉ H ₇ O ₄	179.0350	179.0351	0.7	4	9	0.4
C ₉ H ₁₃ O ₄	185.0819	185.0818	-0.7	4	9	0.4
C ₉ H ₁₁ O ₅	199.0612	199.0612	0.0	5	9	0.6
C ₉ H ₁₃ O ₅	201.0768	201.0768	-0.2	5	9	0.6
C ₉ H ₁₅ O ₅	203.0925	203.0925	0.0	5	9	0.6
C ₉ H ₉ O ₆	213.0405	213.0405	0.2	6	9	0.7
C ₉ H ₁₁ O ₆	215.0561	215.0555	-2.9	6	9	0.7
C ₉ H ₁₃ O ₆	217.0718	217.0716	-0.8	6	9	0.7
C ₉ H ₉ O ₇	229.0354	229.0348	-2.5	7	9	0.8
C ₉ H ₁₁ O ₇	231.0510	231.0505	-2.3	7	9	0.8
C ₁₀ H ₁₅ O ₃	183.1027	183.1026	-0.4	3	10	0.3
C ₁₀ H ₁₃ O ₅	213.0768	213.0768	-0.2	5	10	0.5
C ₁₀ H ₁₅ O ₅	215.0925	215.0924	-0.5	5	10	0.5
C ₁₀ H ₁₃ O ₆	229.0718	229.0715	-1.2	6	10	0.6

C ₁₀ H ₁₅ O ₆	231.0874	231.0872	-0.9	6	10	0.6
C ₁₀ H ₁₁ O ₇	243.0510	243.0506	-1.8	7	10	0.7
C ₁₀ H ₁₅ O ₇	247.0823	247.0822	-0.5	7	10	0.7
C ₁₁ H ₁₅ O ₆	243.0874	243.0873	-0.5	6	11	0.5
C ₁₁ H ₁₇ O ₆ *	245.1031	245.103	-0.3	6	11	0.5
C ₁₂ H ₁₉ O ₅	243.1238	243.1237	-0.4	5	12	0.4
C ₁₂ H ₂₁ O ₅	245.1394	245.1392	-1.0	5	12	0.4
C ₁₃ H ₁₉ O ₅	255.1238	255.1239	0.4	5	13	0.4
C ₁₃ H ₁₉ O ₆	271.1187	271.1188	0.3	6	13	0.5
C ₁₄ H ₂₁ O ₅ *	269.1394	269.1394	-0.2	5	14	0.4
C ₁₇ H ₂₅ O ₈	357.1555	357.1559	1.1	8	17	0.5

*isobaric compounds detected

Table S-2: List of CHONS-containing compounds that were identified by UHPLC–(–)ESI–UHRMS analysis of the filter samples.

formula for [M–H] [–]	m/z for [M–H] [–]	measured m/z	$\Delta m /$ ppm	Number of Oxygen	Number of Carbon	O:C
C ₅ H ₁₀ O ₉ NS	260.0082	260.0079	-1.1	9	5	1.8
C ₅ H ₉ O ₁₁ N ₂ S	304.9933	304.9932	-0.2	11	5	2.2
C ₆ H ₁₀ O ₉ NS	272.0082	272.0081	-0.3	9	6	1.5
C ₇ H ₁₀ O ₉ NS	284.0082	284.0080	-0.6	9	7	1.3
C ₇ H ₁₀ O ₁₀ NS	300.0031	300.0029	-0.6	10	7	1.4
C ₁₀ H ₁₆ O ₇ NS	294.0653	294.0657	1.4	7	10	0.7
C ₁₀ H ₁₄ O ₈ NS	308.0446	308.0448	0.8	8	10	0.8
C ₁₀ H ₁₆ O ₈ NS	310.0602	310.0605	0.9	8	10	0.8
C ₁₀ H ₁₆ O ₉ NS	326.0551	326.0551	-0.1	9	10	0.9
C ₁₀ H ₁₆ O ₁₀ NS	342.0500	342.0497	-1.0	10	10	1.0
C ₁₀ H ₁₈ O ₁₀ NS	344.0657	344.0655	-0.6	10	10	1.0
C ₁₀ H ₁₇ O ₁₁ N ₂ S	373.0559	373.0558	-0.2	11	10	1.1
C ₁₀ H ₁₅ O ₁₂ N ₂ S	387.0351	387.0350	-0.3	12	10	1.2

Table S-3: List of CHON-containing compounds that were identified by UHPLC–(–)ESI–UHRMS analysis of the filter samples.

formula for [M–H] [–]	m/z for [M–H] [–]	measured m/z	$\Delta m /$ ppm	Number of Oxygen	Number of Carbon	O:C
C ₇ H ₄ O ₅ N	182.0095	182.0096	0.6	5	7	0.7
C ₇ H ₃ O ₇ N ₂	226.9946	226.9947	0.5	7	7	1.0
C ₁₀ H ₁₆ O ₈ N	278.0881	278.0882	0.2	8	10	0.8
C ₁₁ H ₁₈ O ₉ N	308.0987	308.0988	0.3	9	11	0.8

Table S-4: List of CHOS-containing compounds that were identified by UHPLC–(–)ESI–UHRMS analysis of the filter samples.

formula for [M–H][–]	<i>m/z</i> for [M–H][–]	measured <i>m/z</i>	Δm / ppm	Number of Oxygen	Number of Carbon	O:C
C ₂ H ₃ O ₆ S	154.9656	154.9656	0.1	6	2	3.0
C ₃ H ₅ O ₆ S	168.9812	168.9812	-0.2	6	3	2.0
C ₄ H ₇ O ₆ S	182.9969	182.9967	-1.0	6	4	1.5
C ₅ H ₉ O ₆ S	197.0125	197.0124	-0.7	6	5	1.2
C ₅ H ₁₁ O ₆ S	199.0282	199.0280	-0.9	6	5	1.2
C ₅ H ₇ O ₇ S	210.9918	210.9916	-0.9	7	5	1.4
C ₅ H ₉ O ₇ S	213.0074	213.0075	0.2	7	5	1.4
C ₅ H ₁₁ O ₇ S	215.0231	215.0229	-0.9	7	5	1.4
C ₅ H ₇ O ₈ S	226.9867	226.9865	-0.9	8	5	1.6
C ₆ H ₁₁ O ₆ S	211.0282	211.0280	-0.9	6	6	1.0
C ₇ H ₁₁ O ₆ S	223.0282	223.0280	-0.8	6	7	0.9
C ₇ H ₁₁ O ₇ S	239.0231	239.0231	0.0	7	7	1.0
C ₇ H ₁₃ O ₇ S	241.0387	241.0385	-1.0	7	7	1.0
C ₇ H ₇ O ₈ S	250.9867	250.9868	0.3	8	7	1.1
C ₇ H ₉ O ₈ S	253.0024	253.0028	1.7	8	7	1.1
C ₈ H ₁₃ O ₇ S	253.0387	253.0384	-1.4	7	8	0.9
C ₈ H ₁₁ O ₉ S	283.0129	283.0127	-0.8	9	8	1.1
C ₈ H ₁₃ O ₉ S	285.0286	285.0284	-0.6	9	8	1.1
C ₈ H ₁₃ O ₁₀ S	301.0235	301.0231	-1.3	10	8	1.3
C ₉ H ₁₅ O ₆ S	251.0595	251.0593	-0.7	6	9	0.7
C ₉ H ₁₅ O ₇ S	267.0544	267.0540	-1.5	7	9	0.8
C ₉ H ₁₃ O ₈ S	281.0337	281.0334	-0.9	8	9	0.9
C ₉ H ₁₃ O ₉ S	297.0286	297.0282	-1.3	9	9	1.0
C ₁₀ H ₁₇ O ₅ S	249.0802	249.0801	-0.5	5	10	0.5
C ₁₀ H ₁₅ O ₇ S	279.0544	279.0544	0.0	7	10	0.7
C ₁₀ H ₁₇ O ₇ S	281.0700	281.0698	-0.9	7	10	0.7
C ₁₀ H ₁₇ O ₈ S	297.0650	297.0646	-1.2	8	10	0.8
C ₁₀ H ₁₅ O ₉ S	311.0442	311.0440	-0.7	9	10	0.9
C ₁₀ H ₁₇ O ₉ S	313.0599	313.0596	-0.9	9	10	0.9
C ₁₀ H ₁₅ O ₁₀ S	327.0391	327.0387	-1.4	10	10	1.0
C ₁₀ H ₁₃ O ₁₁ S	341.0184	341.0183	-0.3	11	10	1.1
C ₁₁ H ₁₉ O ₇ S	295.0857	295.0858	0.3	7	11	0.6

S-2. Trajectory calculations for the campaign period

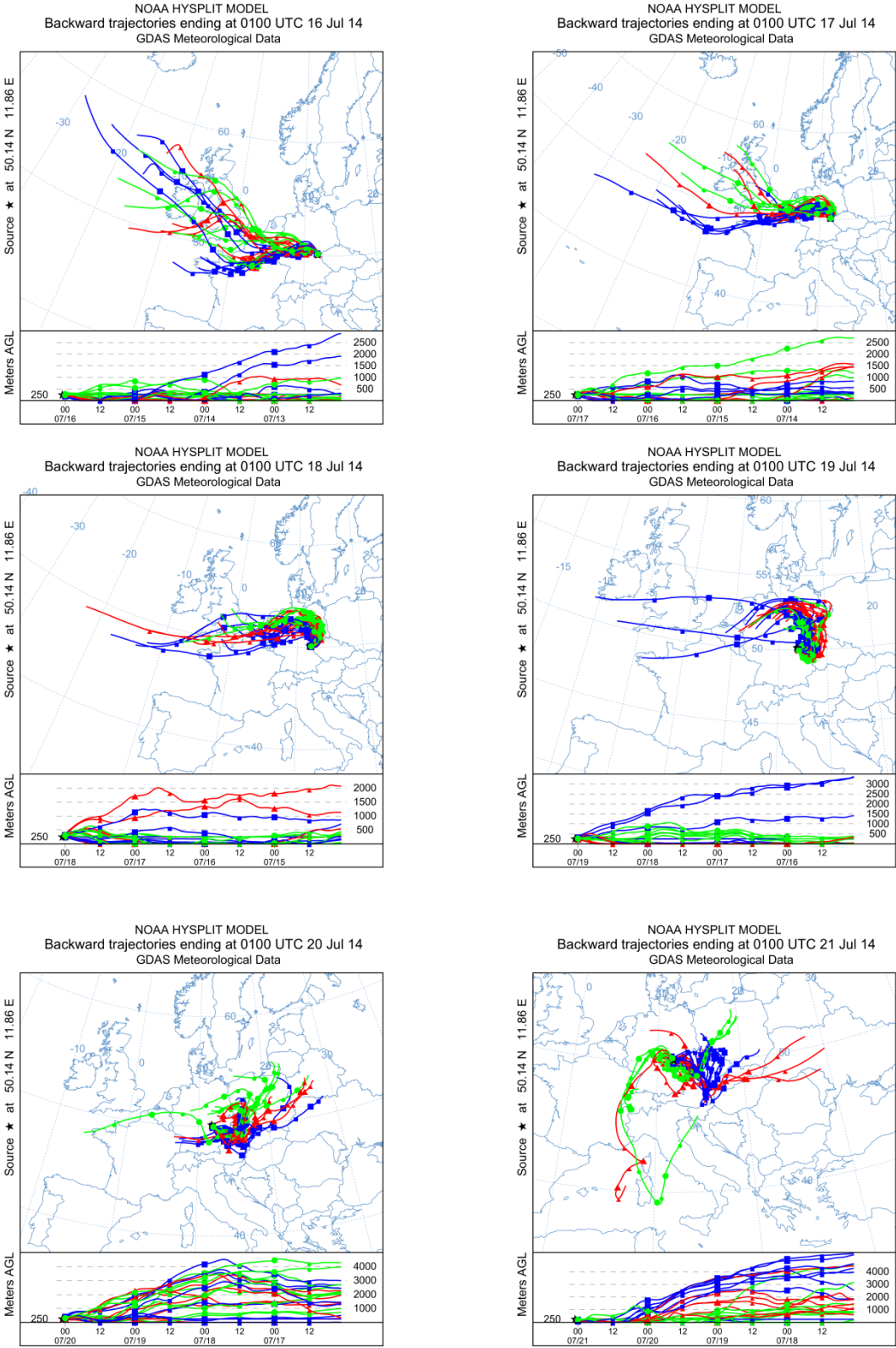


Figure S-1: 96 hours backward HYSPLIT trajectory calculations for the 16th-21st of July (each at 12 midnight CET) (Draxler and Rolph).

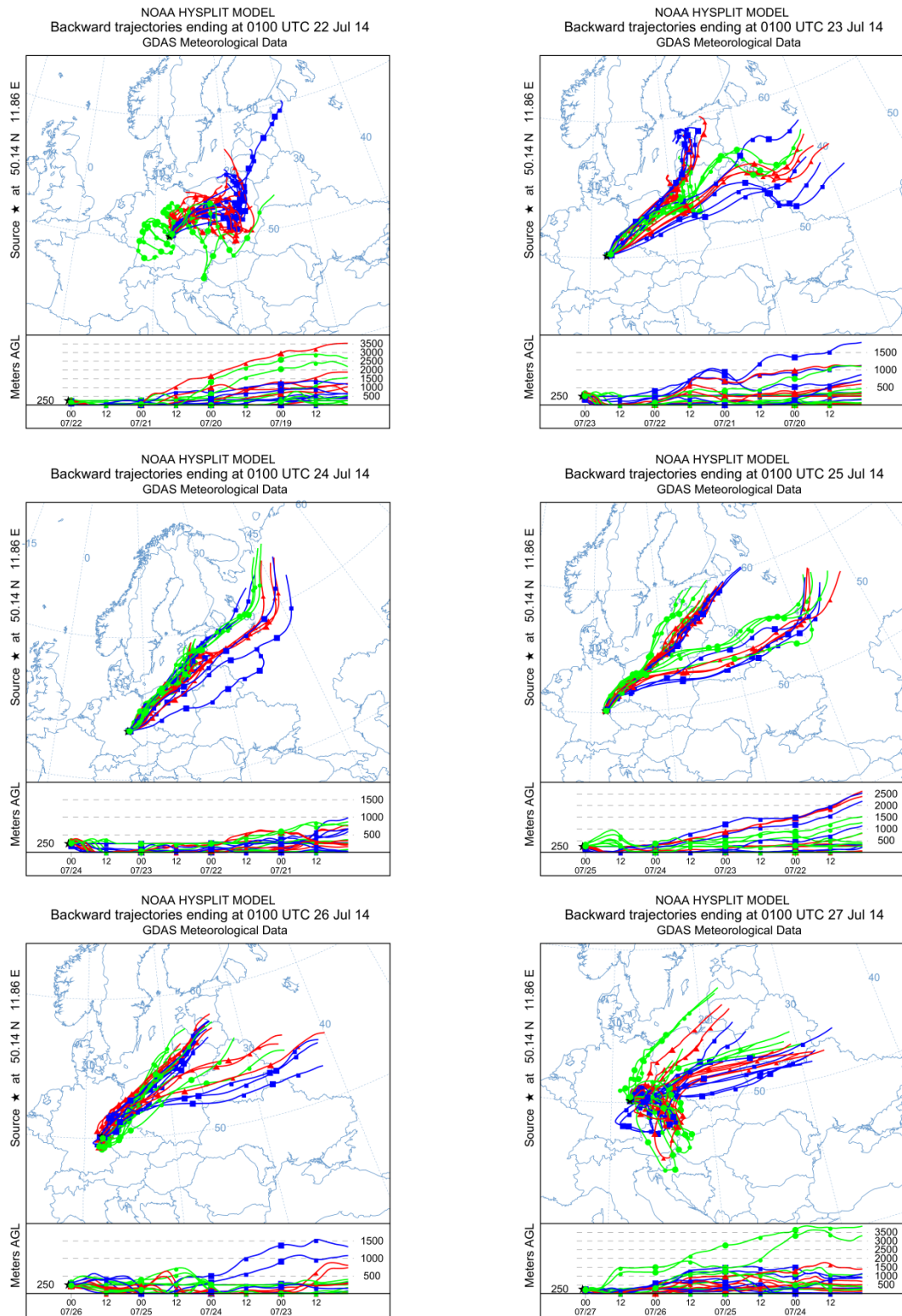


Figure S-2: 96 hours backward HYSPLIT trajectory calculations for the 22nd–27th of July (each at 12 midnight CET) (Draxler and Rolph).

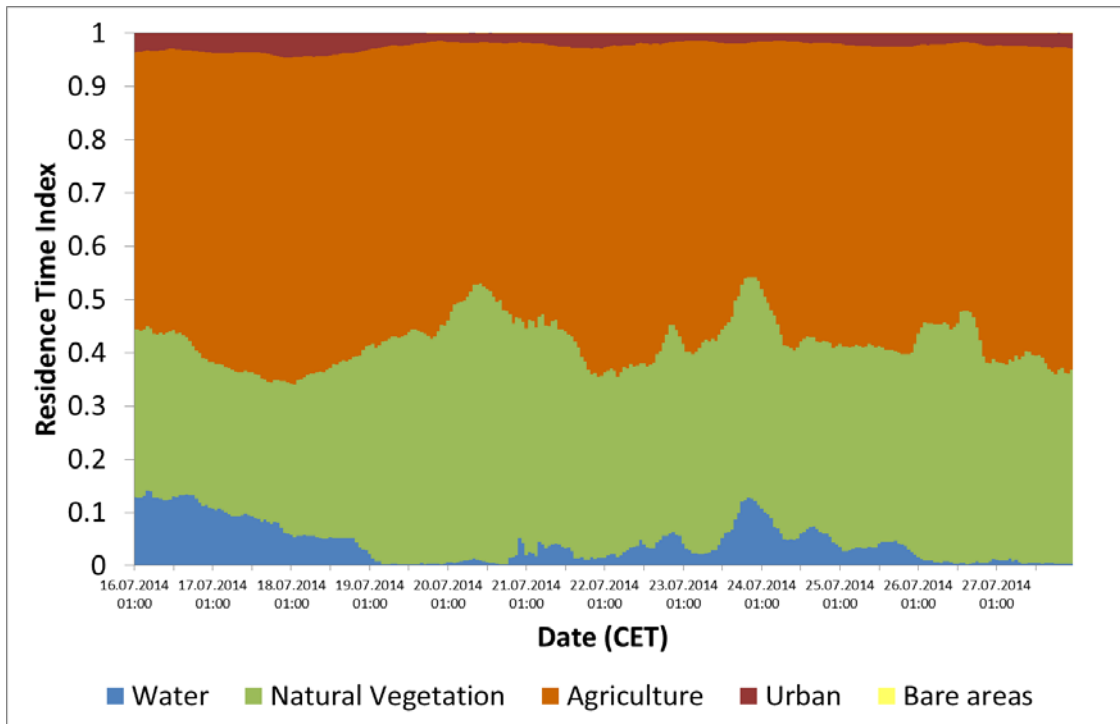


Figure S-3: Residence times for 96 hours backward trajectories arriving at the site intersected with satellite-derived global landcover data to give indications of influences of main land cover classes. A detailed description of the calculation method can be found elsewhere (van Pinxteren et al., 2010).

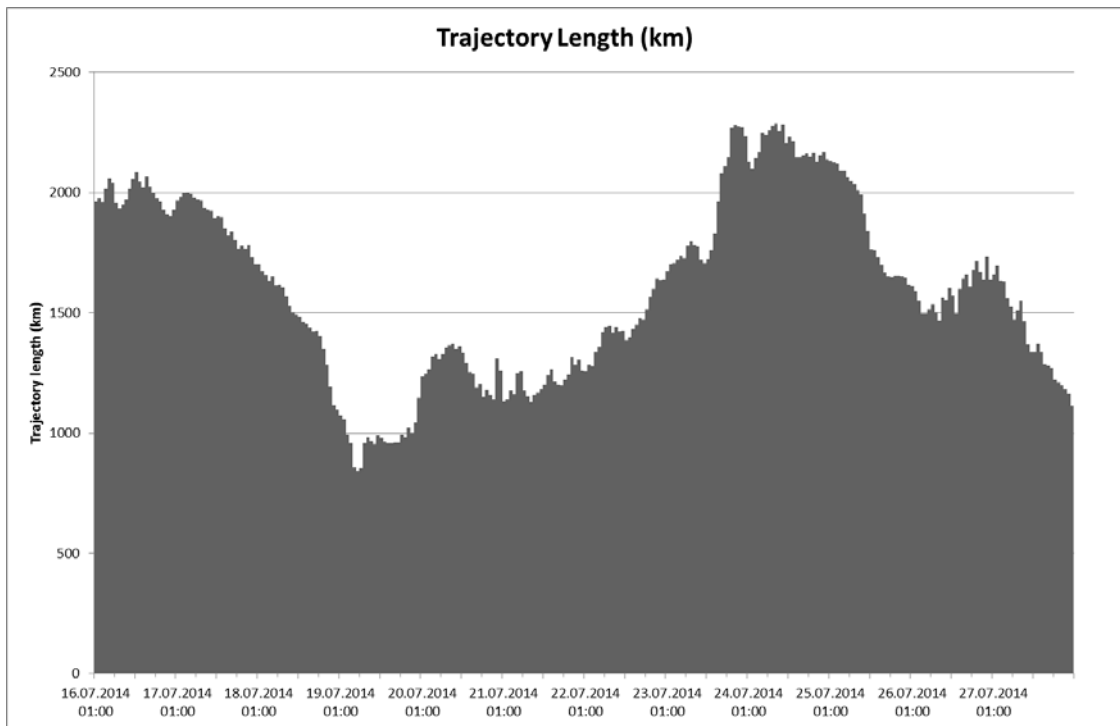


Figure S-4: Trajectory lengths for 96 hours backward trajectories arriving at the site. For details see van Pinxteren et al. (2010).

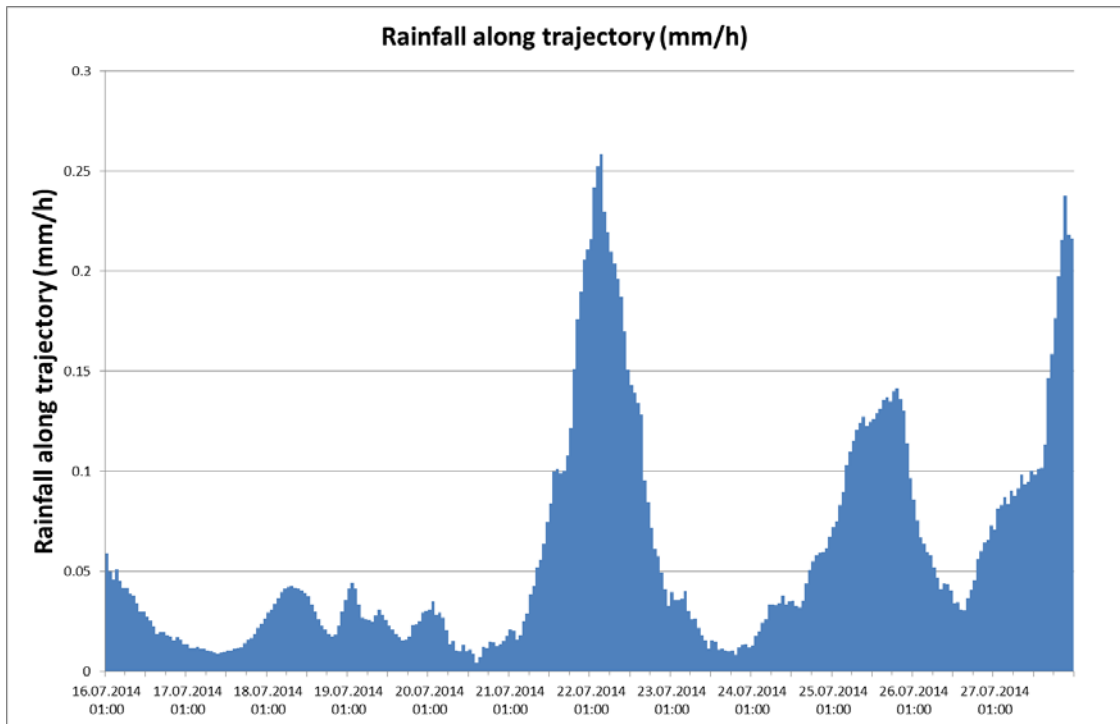


Figure S-5: Rainfall along the calculated 96 hours backward trajectories arriving at the site. For details see van Pinxteren et al. (2010).

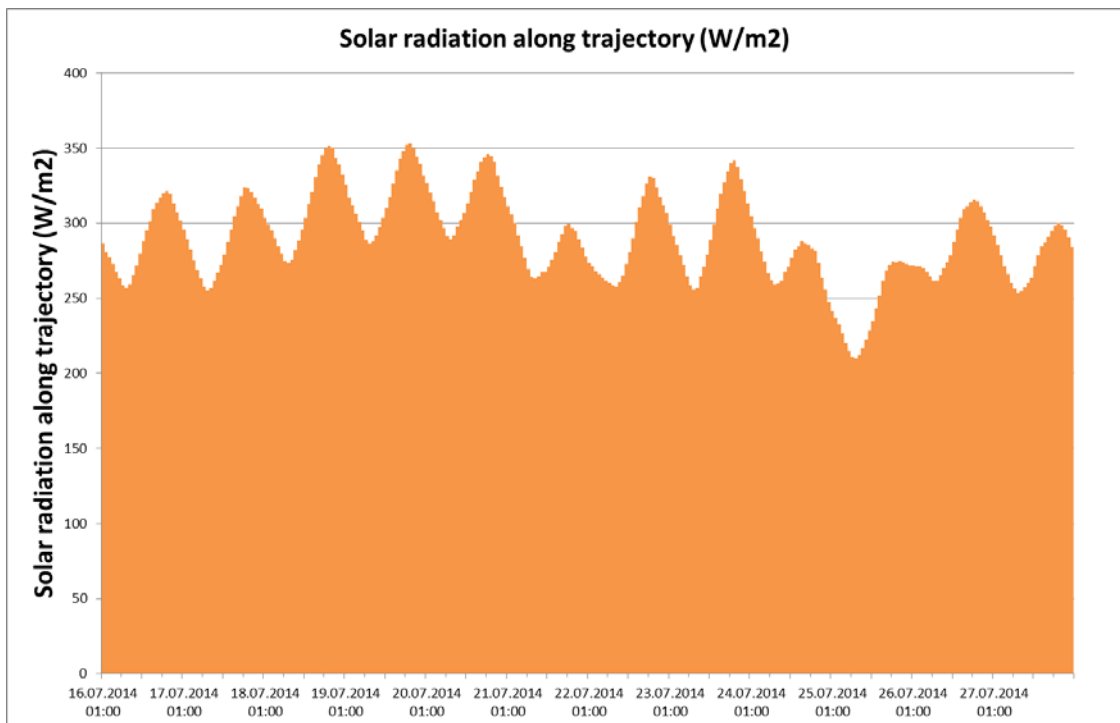


Figure S-6: Solar radiation along the calculated 96 hours backward trajectories arriving at the site. For details see van Pinxteren et al. (2010).

S-3. Supplementary mass spectrometric data

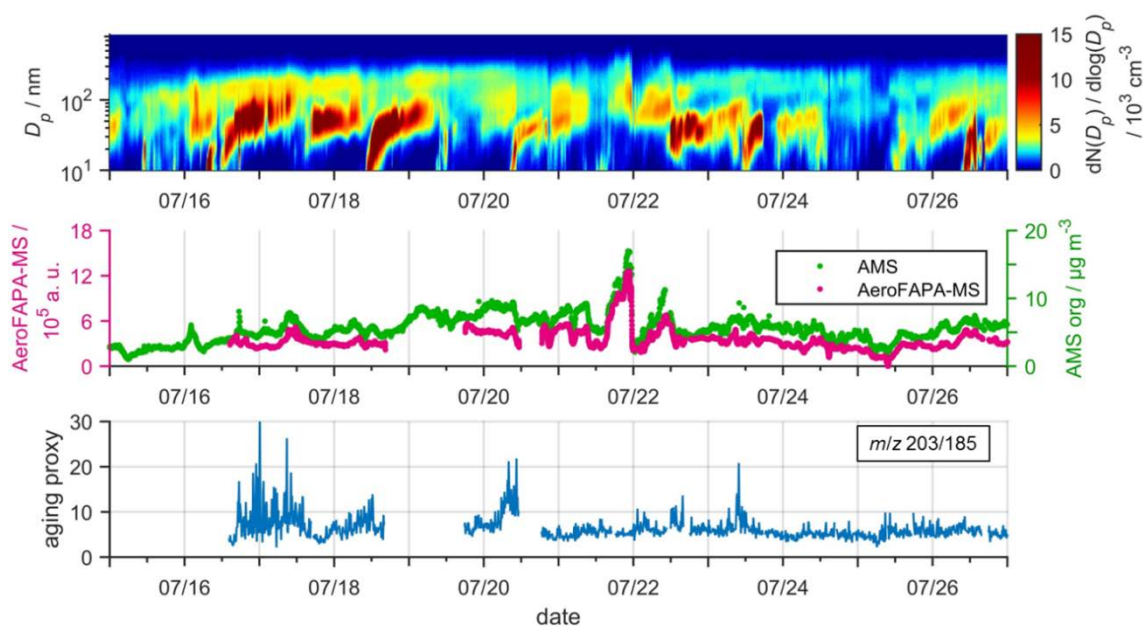


Figure S-7: Top panel: Number size distribution of aerosol particles which was measured by an SMPS. Middle panel: Time traces of the total ion current of the AeroFAPA-MS (magenta) and the organic aerosol mass measured by an AMS (green). Bottom panel: Ratio of m/z 203/185 as aging proxy for SOA particles at the site.

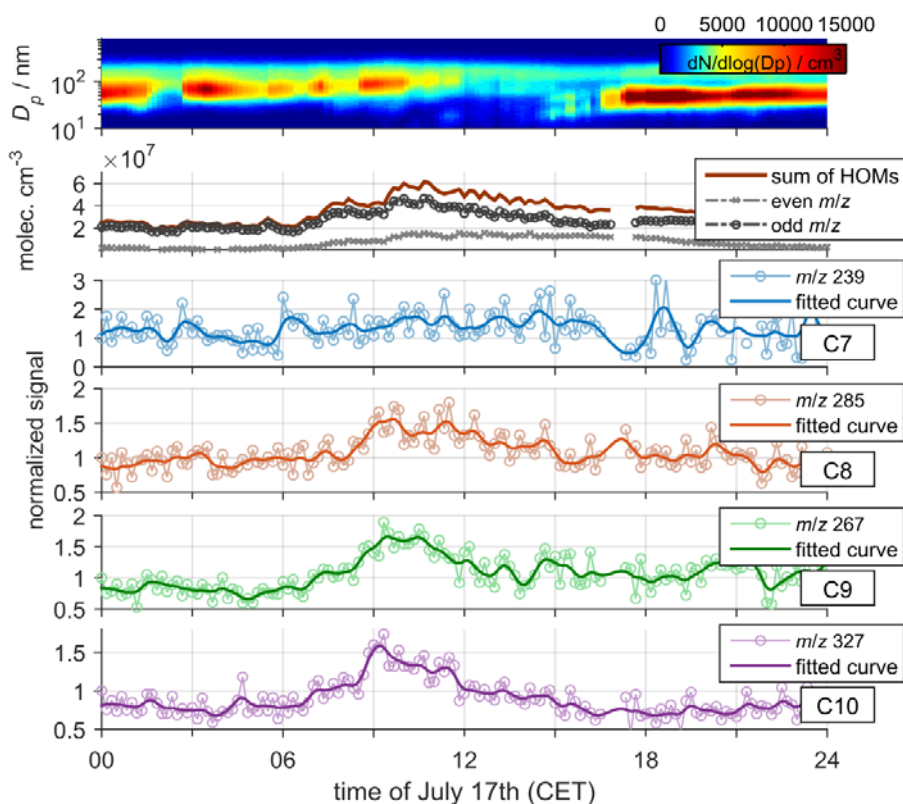


Figure S-8: Time traces for C7–C10 HOOS, gas-phase HOMs and particle number size distribution during July 17th. HOM concentration is dominated by ions with odd m/z ratios ($[M+NO_3]^-$), indicating the presence of peroxyradicals (RO_2^*), organonitrates ($RONO_2$) and peroxy nitrates (RO_2NO_2). While the larger HOOS are following the trend of the HOM signals with odd m/z ratios, the C7 HOOS differ from this behavior, supporting the assumption that these species are not directly formed but by decomposition of the larger HOOS.

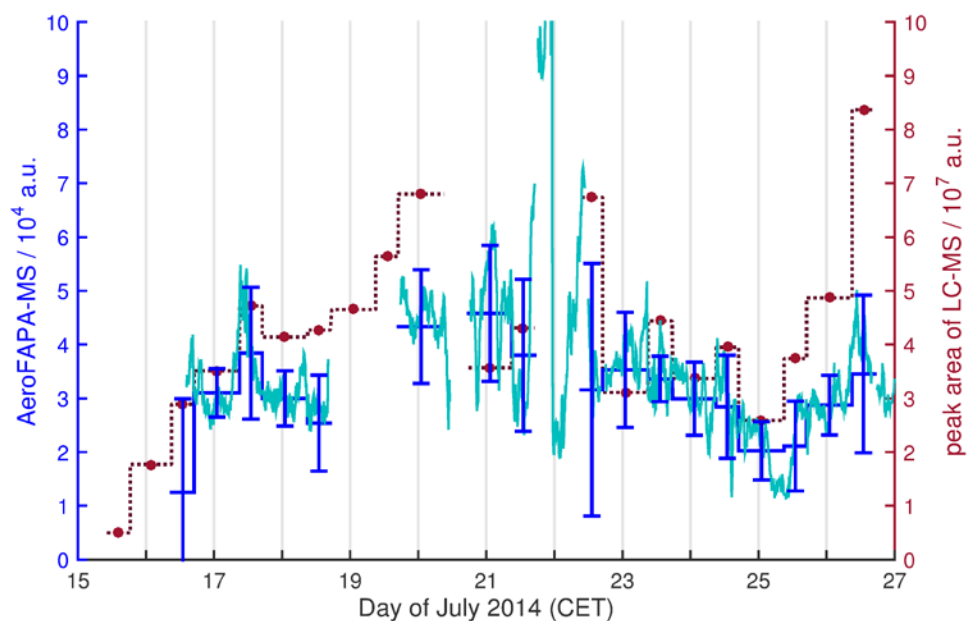


Figure S-9: Comparison of the signals for the sum of HOOS detected by AeroFAPA-MS (light blue), and by LC-MS (red). The signals of the AeroFAPA-MS are averaged for the filter sampling times (dark blue); error bars depict one standard deviation.

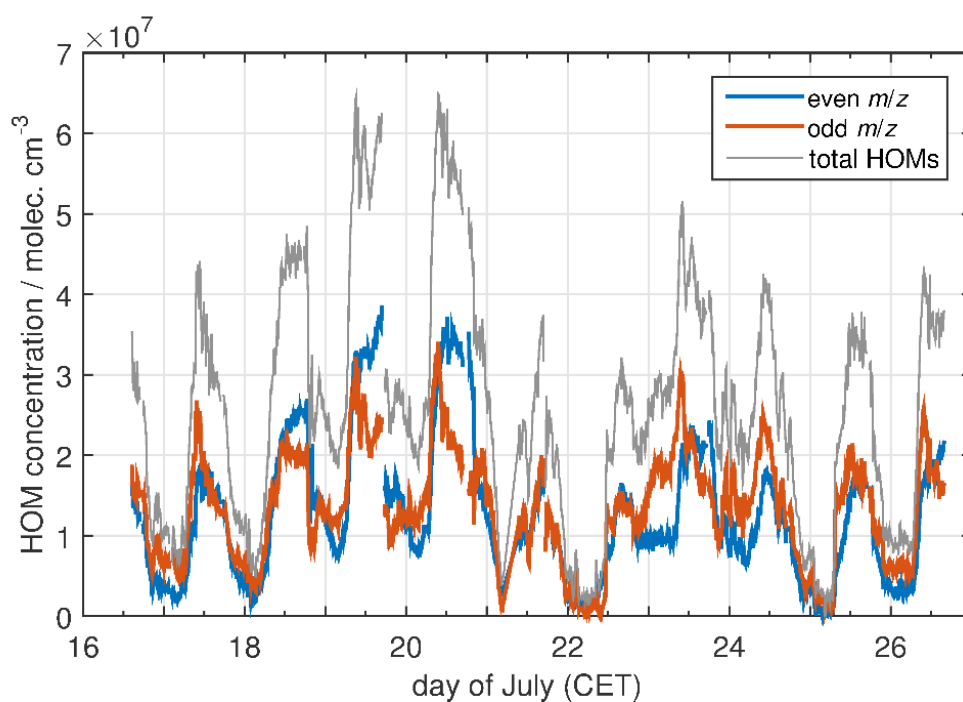


Figure S-10: Concentrations of gas-phase HOMs measured by the CI-APiToF-MS over the entire campaign period.

Table S-5: Signals and assignments for gas-phase HOMs detected by CI-APiTOF-MS.

formula assignment	classification	molecular weight	m/z for $[M+NO_3]^-$	reference
C ₇ H ₁₀ O ₄	HOM	158	220	Ehn <i>et al.</i> , 2014
C ₁₀ H ₁₅ O ₆	RO ₂ radical	231	293	Jokinen <i>et al.</i> , 2014
–	–	232	294	
–	–	233	295	
–	–	235	297	
C ₈ H ₁₂ O ₈	HOM	236	298	Ehn <i>et al.</i> , 2014
–	–	245	307	
C ₁₀ H ₁₄ O ₇	HOM	246	308	Ehn <i>et al.</i> , 2014
–	–	247	309	
C ₉ H ₁₂ O ₈ / C ₁₀ H ₁₆ O ₇	HOM	248	310	Ehn <i>et al.</i> , 2014
C ₁₀ H ₁₇ O ₇	RO ₂ radical	249	311	Jokinen <i>et al.</i> , 2014
C ₁₀ H ₁₅ O ₈	RO ₂ radical	263	325	Jokinen <i>et al.</i> , 2014
C ₁₀ H ₁₆ O ₈ / C ₉ H ₁₂ O ₉	HOM	264	326	Ehn <i>et al.</i> , 2014
–	–	265	327	
–	–	267	329	
–	RO ₂ NO ₂ (m/z 293+NO ₂)	277	339	Jokinen <i>et al.</i> , 2014
C ₁₀ H ₁₄ O ₉	HOM	278	340	Ehn <i>et al.</i> , 2014
C ₁₀ H ₁₆ O ₉	HOM	280	342	Ehn <i>et al.</i> , 2014
–	RONO ₂ (m/z 325+NO)	293	355	Jokinen <i>et al.</i> , 2014
C ₁₀ H ₁₅ O ₁₀	RO ₂ radical	295	357	Jokinen <i>et al.</i> , 2014
C ₁₀ H ₁₆ O ₁₀	HOM	296	358	Ehn <i>et al.</i> , 2014
–	–	308	370	
C ₁₀ H ₁₄ O ₁₁	HOM	310	372	Ehn <i>et al.</i> , 2014
C ₁₀ H ₁₆ O ₁₁	HOM	312	374	Ehn <i>et al.</i> , 2014

References

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