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Supplement of

Understanding the anthropogenic influence on formation of biogenic secondary organic aerosols in Denmark via analysis of organosulfates and related oxidation products

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Supplementary Table 1. Statistical results of U Mann-Whitney test performed on daytime and nighttime concentrations of the organic acids, organosulfates and nitrooxy organosulfate detected at HCAB. Statistically different parameters (with p-level < 0.1) are underlined. Parameters with two few measurements (N < 5) were excluded from the test.

Parameter	p-level	Statistically different?	Valid N (Day)	Valid N (Night)
Benzoic acid	0.4233	No	14	13
Adipic acid	0.7338	No	24	24
Pimelic acid	0.4598	No	30	30
<u>Phthalic acid</u>	<u>0.0385</u>	Yes	30	30
Terpenylic acid	0.8245	No	30	30
Suberic acid	0.9176	No	30	30
Pinonic acid	0.6574	No	30	30
Pinic acid	0.2675	No	30	30
Azelaic acid	0.9586	No	26	28
Hydroxy-pinonic acid	N/A	N/A	8	4
MBTCA	0.8592	No	30	30
DTAA	0.7338	No	30	30
Total first generation organic acids	0.3750	No	30	30
Total organic acids	0.6152	No	30	30
OS 154	0.5442	No	30	29
OS 156	0.7901	No	30	30
OS 170	0.3994	No	30	30
OS 182	0.8951	No	25	26
OS 200	0.5154	No	30	30
OS 208	0.9396	No	30	29
<u>OS 210</u>	<u>0.0622</u>	Yes	30	30
OS 212	0.5642	No	30	30
OS 214	0.4333	No	30	30
OS 216	0.6941	No	28	28
OS 248	0.4727	No	27	27
OS 250	0.6574	No	30	30
OS 252	0.5994	No	21	28
OS 254	0.7901	No	30	30
OS 268	0.7338	No	30	30
OS 280	0.4962	No	27	29
OS 298	0.7340	No	13	14
Total organosulfates	0.8360	No	30	30
NOS 295	0.9020	No	18	25
<u>NOS 297</u>	<u>0.0011</u>	Yes	30	30
NOS 311	N/A	N/A	2	4
NOS 313	0.8179	No	23	29
NOS 327	0.6565	No	17	28
NOS 329	0.3691	No	9	10
NOS 331	0.2610	No	19	19
<u>NOS 343</u>	<u>0.0825</u>	Yes	10	13
<u>Total nitrooxy organosulfates</u>	<u>0.0444</u>	Yes	30	30

Supplementary Table 2. Statistical results of U Mann-Whitney test performed on daytime and nighttime concentrations of the organic acids, organosulfates and nitrooxy organosulfate detected at Risø. Statistically different parameters (with p-level < 0.1) are underlined. Parameters with two few measurements (N < 5) were excluded from the test.

Parameter	p-level	Statistically different?	Valid N (Day)	Valid N (Night)
Benzoic acid	0.6275	No	6	6
Adipic acid	0.6501	No	30	30
Pimelic acid	0.8206	No	24	24
Phthalic acid	0.4455	No	24	24
Terpenylic acid	0.3979	No	24	24
Suberic acid	0.5777	No	24	24
Pinonic acid	0.3223	No	24	24
Pinic acid	0.2699	No	22	22
Azelaic acid	0.7164	No	22	23
Hydroxy-pinonic acid	N/A	N/A	0	5
MBTCA	0.6062	No	24	24
DTAA	0.2819	No	24	19
Total first generation organic acids	0.5919	No	24	24
Total organic acids	0.7415	No	24	24
OS 154	0.6501	No	24	24
OS 156	0.7259	No	24	24
OS 170	0.9906	No	21	23
OS 182	0.8984	No	23	24
OS 200	0.8459	No	22	21
OS 208	0.6801	No	24	24
OS 210	0.9015	No	24	24
OS 212	0.9015	No	24	24
OS 214	0.8852	No	24	24
OS 216	0.6949	No	22	19
OS 248	0.9806	No	21	22
OS 250	0.9343	No	24	24
OS 252	0.9496	No	19	23
OS 254	0.5362	No	24	24
OS 268	0.5777	No	24	24
OS 280	0.5637	No	24	24
OS 298	0.2908	No	10	11
Total organosulfates	0.9507	No	24	24
NOS 295	0.9607	No	5	13
<u>NOS 297</u>	<u>0.0011</u>	Yes	24	24
NOS 311	N/A	N/A	3	4
NOS 313	0.8360	No	16	22
NOS 327	0.8257	No	17	21
NOS 329	0.8182	No	11	11
NOS 331	0.1261	No	15	17
NOS 343	N/A	N/A	3	1
<u>Total nitrooxy organosulfates</u>	<u>0.0696</u>	Yes	24	24

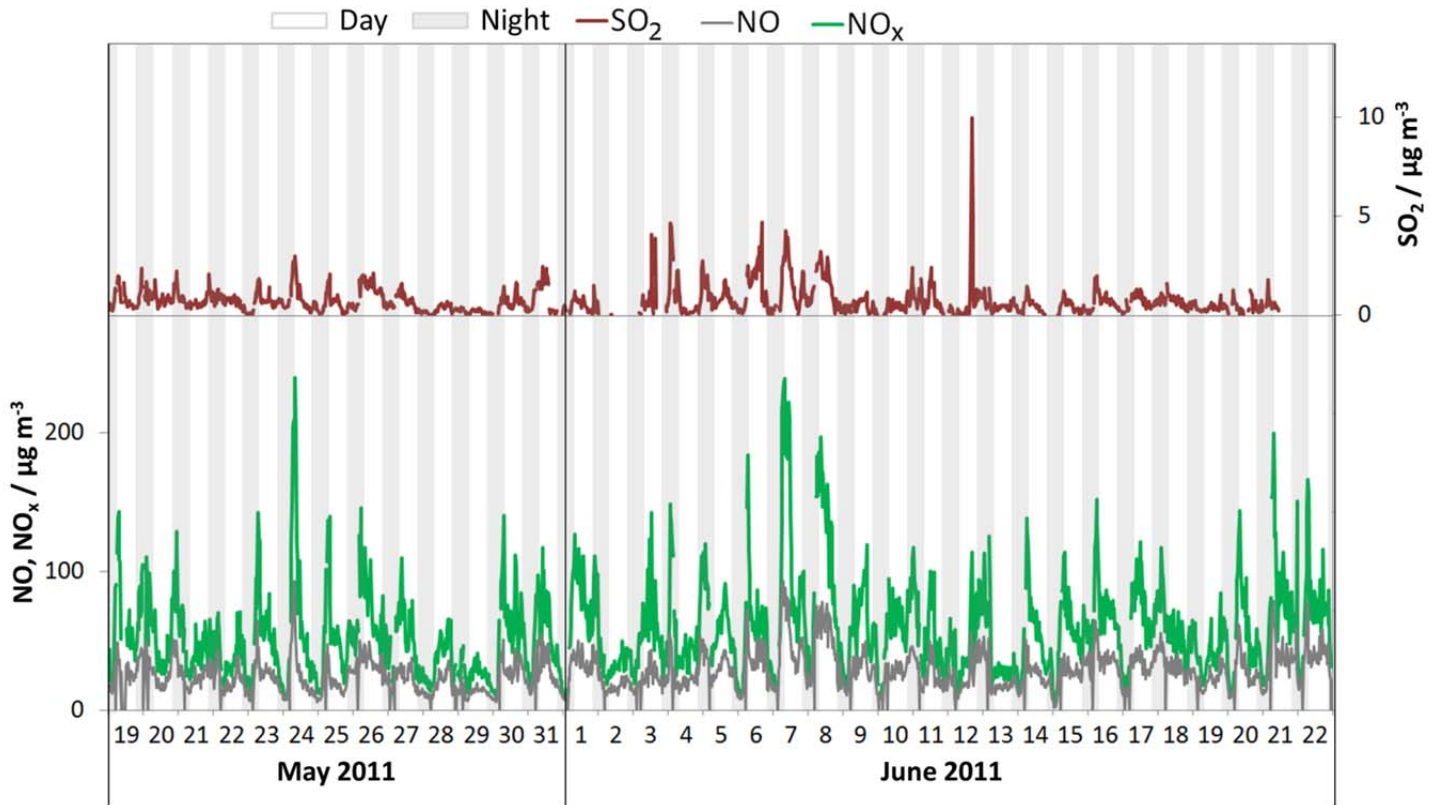
Supplementary Table 3. Relative standard deviations (RSD, %), which were associated with averaging R-square correlation coefficients (between pairs of compounds) at the two sites, were calculated. The species belonging or partly belonging to a common correlating group are marked in blue shade with the corresponding RSD in red (those only partly belonging to the group underlined). RSD values seemed low for the correlating organic acids and OS while larger for the NOs, mostly due to higher correlation coefficients at Risø. The partly-correlating species pinic, pinonic acid and phthalic acid showed relatively larger RSD compared to the other correlating compounds, while another partly-correlating species (OS 248) showed a consistent partly correlating degree at both sites as evident by small RSD values.

Species	Benzoic acid	Adipic acid	Pimelic acid	Phthalic acid	Terpenylic acid	Suberic acid	<u>Pinonic acid</u>	<u>Pinic acid</u>	Azelaic acid	Hydroxyipinonic acid	MBTCA	DTAA	OS 154	OS 156	OS 170	OS 182	OS 200	OS 208	OS 210	OS 212	OS 214	OS 216	<u>OS 248</u>	OS 250	OS 252	OS 254	OS 268	OS 280	OS 298	NOS 295	NOS 297	NOS 313	NOS 327	NOS 329	NOS 331	NOS 343	
Benzoic acid		73	133	82	59	51	138	89	73	123	57	91	25	134	23	135	24	129	129	31	9	109	124	127	18	12	10	94	38	12	43	141	32	2	140		
Adipic acid			6	15	30	57	98	57	7	26	22	28	35	11	33	77	33	129	108	46	46	41	24	126	31	43	35	33	56	79	3	40	72	71	80	141	
Pimelic acid				43	91	8	132	104	20	139	119	122	88	88	67	136	98	111	79	99	89	111	56	141	111	99	95	96	132	58	24	90	109	90	129	141	
<u>Phthalic acid</u>					29	15	<u>80</u>	<u>53</u>	44	116	<u>43</u>	<u>47</u>	<u>39</u>	<u>27</u>	<u>30</u>	119	39	134	22	<u>47</u>	<u>42</u>	<u>50</u>	<u>47</u>	138	<u>35</u>	<u>45</u>	<u>35</u>	<u>37</u>	<u>51</u>	56	61	<u>29</u>	<u>65</u>	<u>42</u>	<u>76</u>	132	
<u>Terpenylic acid</u>						125	<u>16</u>	<u>6</u>	57	120	<u>18</u>	<u>11</u>	<u>12</u>	<u>29</u>	<u>10</u>	138	8	108	138	4	<u>17</u>	<u>9</u>	<u>2</u>	70	<u>11</u>	<u>17</u>	<u>16</u>	<u>5</u>	<u>28</u>	25	56	<u>22</u>	<u>20</u>	<u>9</u>	<u>23</u>	122	
Suberic acid						141	118	13	82	141	141	106	136	83	140	117	140	129	126	121	141	141	63	131	129	128	126	91	141	4	48	110	120	141	140	133	
<u>Pinonic acid</u>								<u>6</u>	74	137	<u>11</u>	<u>24</u>	<u>69</u>	<u>41</u>	<u>55</u>	59	45	89	62	<u>39</u>	<u>37</u>	<u>60</u>	<u>23</u>	74	<u>49</u>	<u>13</u>	<u>16</u>	<u>19</u>	<u>0</u>	33	107	<u>7</u>	<u>41</u>	<u>13</u>	<u>5</u>	120	
<u>Pinic acid</u>									141	131	<u>24</u>	<u>41</u>	<u>61</u>	<u>46</u>	<u>45</u>	141	41	96	123	<u>44</u>	<u>43</u>	<u>74</u>	<u>4</u>	118	<u>40</u>	<u>12</u>	<u>14</u>	<u>9</u>	<u>28</u>	86	88	<u>2</u>	<u>22</u>	<u>4</u>	<u>19</u>	107	
Azelaic acid										56	34	94	126	115	129	131	136	22	124	122	106	131	105	140	106	131	133	138	141	126	112	141	87	130	134	139	
Hydroxyipinonic acid											72	35	130	49	119	46	121	131	141	109	23	16	73	30	45	82	83	82	124	78	0	72	119	3	0	90	
MBTCA												3	4	7	2	116	3	91	131	4	6	11	<u>13</u>	140	2	7	5	5	1	59	89	10	33	5	24	133	
DTAA													3	2	2	108	4	52	137	5	12	8	<u>2</u>	141	3	2	0	7	2	44	102	1	42	15	23	139	
OS 154													10	5	63	3	105	71	5	2	12	<u>8</u>	138	0	18	15	13	8	64	57	9	45	71	45	141		
OS 156														4	15	5	128	141	8	14	3	<u>12</u>	132	25	1	1	9	5	46	89	2	27	32	35	115		
OS 170															120	2	105	28	2	4	9	<u>16</u>	139	16	11	7	2	5	50	42	4	41	55	48	138		
OS 182																102	141	7	95	22	73	57	110	82	86	56	73	22	77	61	31	141	140	86	4		
OS 200																	73	71	0	4	7	<u>16</u>	141	12	6	3	1	7	29	67	4	23	52	32	140		
OS 208																		14	102	107	99	102	18	86	107	108	88	20	70	141	85	101	100	78	123		
OS 210																				116	128	111	126	88	131	133	130	31	130	140	116	56	63	37	120	37	
OS 212																													27	68	4	39	48	31	139		
OS 214																													40	66	4	36	54	37	141		
OS 216																													2	104	11	41	69	45	139		
<u>OS 248</u>																								91	<u>0</u>	<u>4</u>	<u>2</u>	<u>14</u>	<u>11</u>	30	47	<u>3</u>	<u>15</u>	<u>0</u>	<u>14</u>	119	
OS 250																									140	137	138	141	123	138	52	137	5	66	106	47	
OS 252																											3	4	5	13	34	60	10	31	38	14	121
OS 254																												1	2	4	63	82	10	12	6	10	127
OS 268																												4	2	72	81	12	15	6	10	125	
OS 280																													3	26	51	8	8	7	19	126	

Supplementary Table 4. Statistical results of U Mann-Whitney test performed on the organic acids, organosulfates and nitrooxy organosulfate detected at the two sampling sites H.C. Andersen Boulevard (HCAB) and Risø. 14 out of 41 tested parameters are statistically different with p-level < 0.1 (underlined).

Parameter	p-level	Statistically different?	Valid N (HCAB)	Valid N (Risø)
<u>Benzoic acid</u>	<u>0.0014</u>	Yes	11	26
Adipic acid	0.3226	No	37	37
<u>Pimelic acid</u>	<u>0.0016</u>	Yes	37	37
<u>Phthalic acid</u>	<u>0.0029</u>	Yes	37	37
Terpenylic acid	0.7335	No	37	37
<u>Suberic acid</u>	<u>0.0099</u>	Yes	37	37
<u>Pinonic acid</u>	<u>0.0006</u>	Yes	37	37
Pinic acid	0.6352	No	37	36
<u>Azelaic acid</u>	<u>0.0000</u>	Yes	31	34
Hydroxy-pinonic acid	0.3938	No	6	4
MBTCA	0.5131	No	37	37
DTAA	0.1218	No	37	33
<u>Total first generation organic acids</u>	<u>0.0286</u>	Yes	37	37
Total organic acids	0.1108	No	37	37
OS 154	0.7911	No	37	37
OS 156	0.7828	No	37	37
OS 170	0.9551	No	36	36
<u>OS 182</u>	<u>0.0000</u>	Yes	28	36
<u>OS 200</u>	<u>0.0837</u>	Yes	37	35
OS 208	0.4269	No	36	37
<u>OS 210</u>	<u>0.0736</u>	Yes	37	37
OS 212	0.8162	No	37	37
OS 214	0.5061	No	37	37
OS 216	0.6790	No	34	33
<u>OS 248</u>	<u>0.0074</u>	Yes	32	36
OS 250	0.7745	No	37	37
OS 252	0.8474	No	31	32
OS 254	0.7662	No	37	37
OS 268	0.9011	No	37	37
OS 280	0.8415	No	37	37
<u>OS 298</u>	<u>0.0437</u>	Yes	13	16
Total organosulfates	0.7253	No	37	37
NOS 295	0.9138	No	26	15
<u>NOS 297</u>	<u>0.0010</u>	Yes	37	37
NOS 311	0.4142	No	3	8
NOS 313	0.6733	No	31	29
NOS 327	0.1891	No	27	28
NOS 329	0.1565	No	12	17
NOS 331	0.7998	No	21	25
NOS 343	0.1822	No	12	4
<u>Total nitrooxy organosulfates</u>	<u>0.0837</u>	Yes	37	35

Supplementary Figure 1. Temporal variation of concentration of selected gases SO₂, NO, and NO_x (30 min resolution) at HCAB during the campaign period. The x-axis shows a temporal scale from 00 - 24h for each day, with the white and grey shades indicating the intervals for day and night samples, respectively.



Supplementary Figure 2. Temporal variation (30 min resolution) of the local meteorological parameters at the urban background site HCOE, including relative humidity (RH), global radiation (GR) and temperature (T). The x-axis shows a temporal scale from 00 - 24h for each day, with the white and grey shades indicating the intervals for day and night samples, respectively.

