

Supporting Information

High-Resolution Electrospray Ionization Mass Spectrometry Analysis of Water Soluble Organic Aerosols Collected with a Particle into Liquid Sampler (PILS)

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Figure S1, limonene SOA negative ESI mode mass spectra for PILS and filter/ACN samples

Figure S2, limonene SOA negative ESI mode correlation for PILS and filter/ACN samples

Figure S3, pine needle BBOA positive ion mode mass spectra collected from filter/ACN, filter/H₂O, and PILS samples

Figure S4, pine needle BBOA positive mode correlations for filter/H₂O vs. filter/ACN and PILS vs. filter/H₂O samples

Table S1, average values calculated for limonene SOA compounds binned according to their O:C ratio

Table S2, average values calculated for BBOA compounds binned according to their O:C ratio

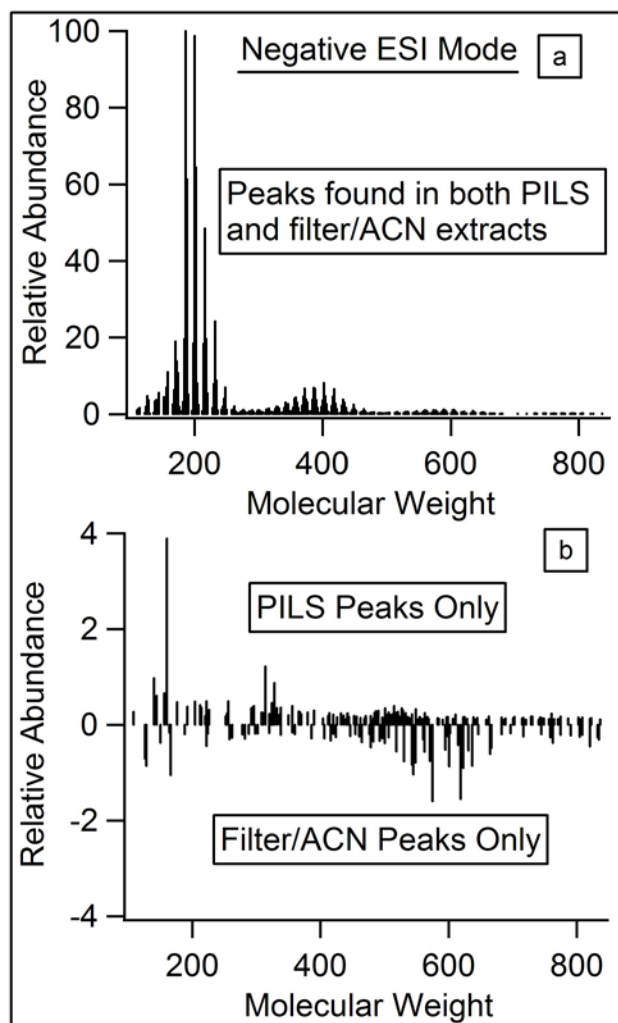


Figure S1. Negative ESI mode mass spectra for limonene SOA. Panel (a) displays peaks due to compounds detected from both PILS and filter/ACN extraction. Panel (b) displays compounds detected only from the PILS extraction (positive peak intensities) and compounds detected only from the filter/ACN extraction (negative peak intensities). The peak intensities are normalized by setting the intensity of the largest peak in each spectrum to 100.

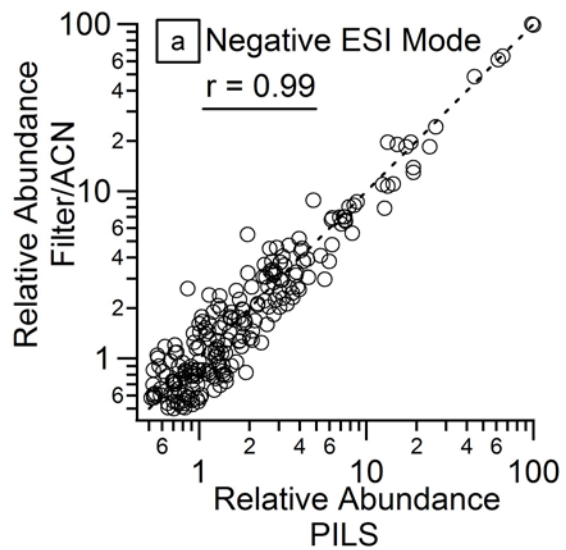


Figure S2. Log-log relative abundance plots generated from the mass spectrum in Figure S1. All intensities correspond to the neutral precursor molecules. As a reference, the dashed lines represent a 1:1 ratio. The r value is the correlation coefficient.

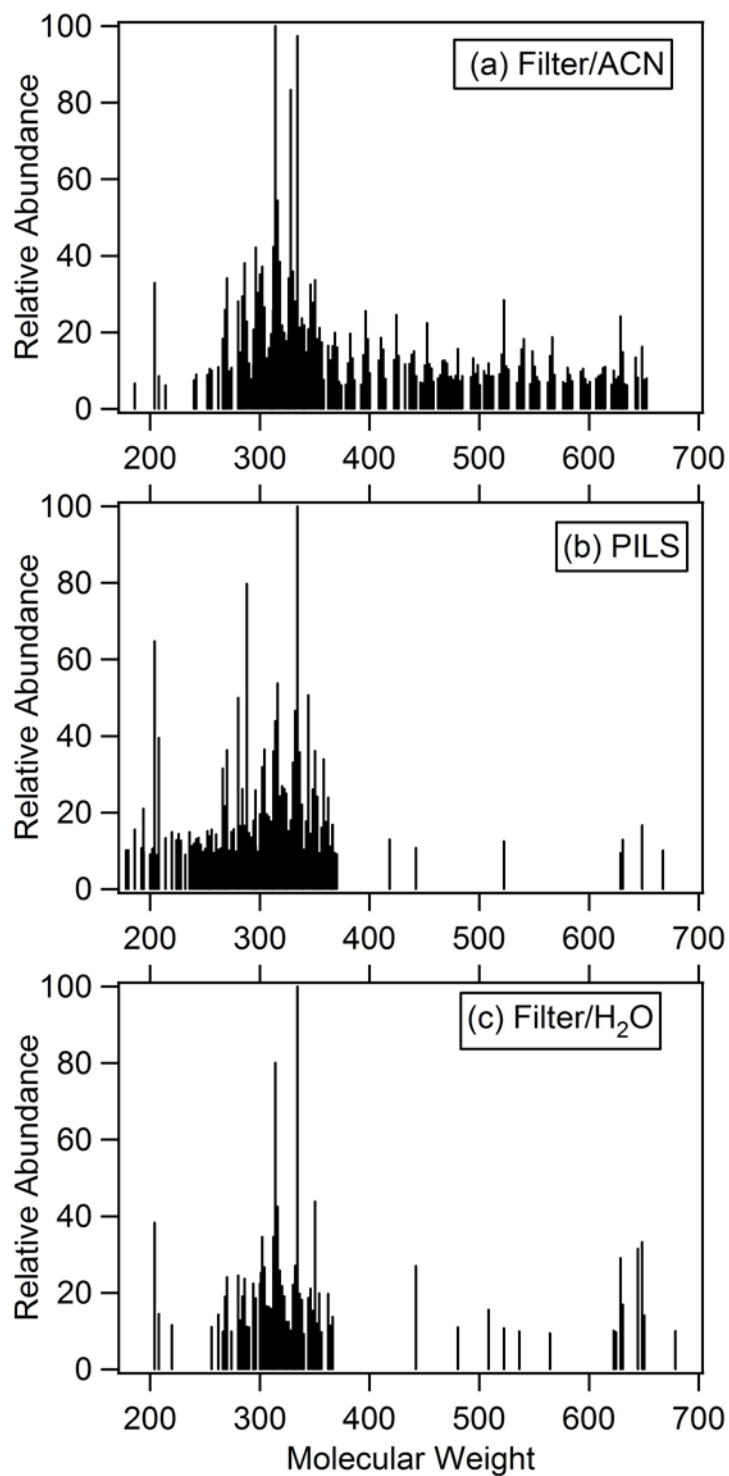


Figure S3. Representative positive mode ESI mass spectra of BBOA collected via (a) filter/ACN extraction, (b) PILS collection, and (c) filter/H₂O extraction.

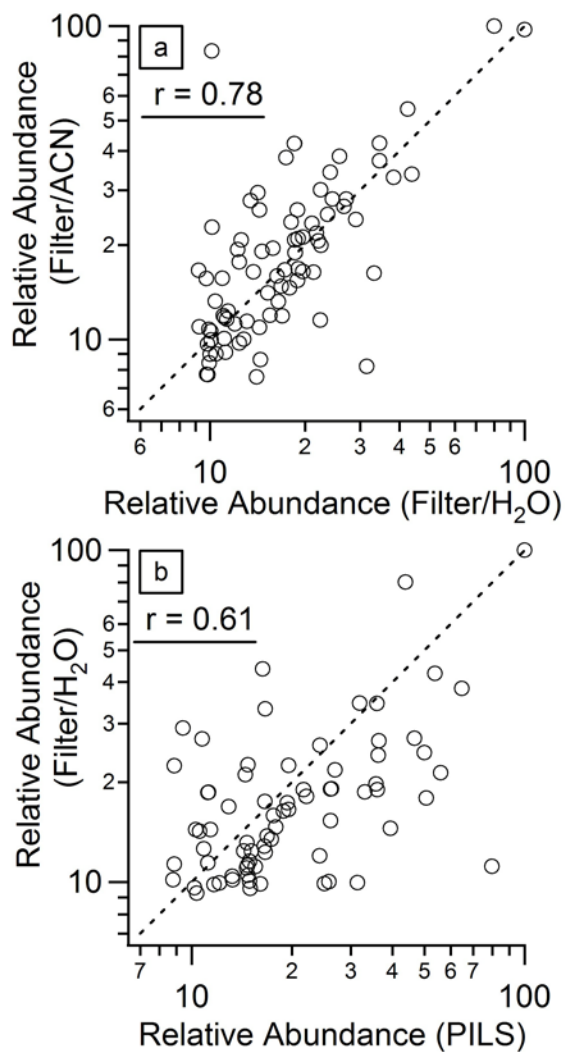


Figure S4. Log-log relative abundance plots generated from positive ESI mode BBOA mass spectra. All mass spectra have been aligned in order to make the abundances correspond to the same compound (m/z). (a) filter/H₂O vs. filter/ACN and (b) PILS vs. filter/H₂O. As a reference, the dashed lines represent a 1:1 ratio. The r -values are the fit correlation coefficients.

Table S1. Limonene SOA compounds binned according to their O:C ratio: 0.0 - 0.3, 0.3 - 0.4, 0.4 – 0.5, 0.5 – 0.6, and 0.6 - 0.9. The total number of peaks and percentage of total peaks, the percentage of total ion signal, and average elemental ratios are calculated for each O:C bin and tabulated.

0.5 ppm Limonene SOA collected with Filter/ACN – Positive ESI Mode							
Compound O:C ratio	# of Peaks	% of Peaks	% Ion Abundance	<O:C>	<H:C>	OM:OC	<DBE>
0-0.3	45	13.2	12.2	0.21	1.38	1.40	4.68
0.3-0.4	92	27.0	35.5	0.33	1.56	1.57	4.06
0.4-0.5	127	37.2	37.9	0.43	1.61	1.70	4.13
0.5-0.6	63	18.5	12.3	0.52	1.62	1.83	3.78
0.6-0.9	355	4	2	0.63	1.65	1.97	2.80
0.5 ppm Limonene SOA collected with Filter/ACN – Negative ESI Mode							
0-0.3	20	3.9	1.8	0.23	1.42	2.91	3.41
0.3-0.4	44	8.5	6.9	0.34	1.50	3.03	3.98
0.4-0.5	156	30.3	34.7	0.43	1.55	3.11	4.06
0.5-0.6	187	36.3	34.6	0.53	1.54	3.10	4.19
0.6-0.9	108	21	22	0.65	1.53	3.09	3.34
0.5 ppm Limonene SOA collected with PILS – Positive ESI Mode							
0-0.3	60	13.7	10.0	0.22	1.37	1.40	5.19
0.3-0.4	128	29.2	35.3	0.33	1.57	1.57	3.82
0.4-0.5	149	34.0	40.6	0.42	1.64	1.70	3.42
0.5-0.6	76	17.4	11.7	0.52	1.64	1.83	3.20
0.6-0.9	25	6	2	0.63	1.67	1.98	2.68
0.5 ppm Limonene SOA collected with PILS – Negative ESI Mode							
0-0.3	21	3.6	2.7	0.23	1.40	2.89	3.58
0.3-0.4	74	12.6	9.7	0.34	1.53	3.07	4.04
0.4-0.5	196	33.3	35.8	0.43	1.56	3.11	3.96
0.5-0.6	193	32.8	31.6	0.53	1.55	3.12	3.90
0.6-0.9	104	18	20	0.65	1.55	3.12	3.16

Table S2. BBOA compounds are binned according to their O:C ratio: 0.0 - 0.3, 0.3 - 0.4, 0.4 – 0.5, 0.5 – 0.6, and 0.6 - 0.9. The total number of peaks and percentage of total peaks, the percentage of total ion signal, and average elemental ratios are calculated for each O:C bin and tabulated. The table is calculated from the list of assigned molecules observed in positive and negative ion mode mass spectra.

BBOA collected with Filter/ACN – Positive ESI Mode							
Compound O:C ratio	# of Peaks	% of Peaks	% Ion Abundance	<O:C>	<H:C>	OM:OC	<DBE>
0-0.3	325	96.2	96.3	0.17	1.62	1.37	5.25
0.3-0.4	8	2.4	2.1	0.32	1.68	1.57	3.59
0.4-0.5	1	0.3	0.1	0.44	1.50	1.71	5.00
0.5-0.6	1	0.3	0.1	0.50	1.50	1.79	5.00
0.6-0.9	3	1	1	0.77	1.62	2.17	2.42
BBOA collected with Filter/H ₂ O – Positive ESI Mode							
0-0.3	82	90.1	89.9	0.19	1.50	1.38	6.24
0.3-0.4	2	2.2	1.4	0.31	1.43	1.54	5.59
0.4-0.5	1	1.1	0.7	0.45	0.73	1.67	8.00
0.5-0.6	0	0.0	0.0	N/A	N/A	N/A	N/A
0.6-0.9	6	7	8	0.80	1.81	2.21	1.78
BBOA collected with PILS – Positive ESI Mode							
0-0.3	121	74.7	75.9	0.21	1.50	1.41	5.63
0.3-0.4	24	14.8	12.1	0.32	1.43	1.55	6.16
0.4-0.5	3	1.9	1.4	0.43	1.11	1.66	6.06
0.5-0.6	3	1.9	1.0	0.53	1.56	1.83	3.98
0.6-0.9	11	7	10	0.78	1.71	2.19	2.31