



Supplement of

Combined application of online FIGAERO-CIMS and offline LC-Orbitrap mass spectrometry (MS) to characterize the chemical composition of secondary organic aerosol (SOA) in smog chamber studies

Mao Du et al.

Correspondence to: Gordon McFiggans (g.mcfiggans@manchester.ac.uk)

The copyright of individual parts of the supplement might differ from the article licence.

1. Discussion about the calculated $\overline{OS_C}$ for CHOS and CHONS species

In this study, we assumed the carbon oxidation states $(\overline{OS_c})$ for the CHOS and CHONS species was determined by Eq. 1: $\overline{OS_c} \approx 2 \times O/C -H/C$ (See assumption column in Table S1). In order to confirm the uncertainty of this assumption to the calculated $\overline{OS_c}$, for the CHONS species, we assumed N (NO₃⁻, OS_N = +5) and S (SO₄²⁻, OS_S = +6) are fully oxidized to obtain the lower limit of calculated $\overline{OS_c}$ by Eq. 2: $\overline{OS_c} = 2 \times O/C -H/C \cdot 5 \times N/C \cdot 6 \times S/C$ (nO ≥ 7). We assumed the N (-NO₂⁻, OS_N = +3) and S (SO₃²⁻, OS_S = +4) are reduced, so the upper limit of $\overline{OS_c}$ was determined by Eq. 3 $\overline{OS_c} = 2 \times O/C - H/C \cdot 3 \times N/C \cdot 4 \times S/C$ (nO ≥ 5). For the CHOS species, the lower and upper limits of calculated $\overline{OS_c}$ were determined by Eq. 4: $\overline{OS_c} = 2 \times O/C - H/C \cdot 6 \times S/C$ (nO ≥ 4) and Eq. 5: $\overline{OS_c} = 2 \times O/C - H/C - 4 \times S/C$ (nO ≥ 3), respectively. The calculated $\overline{OS_c}$ for other compounds without sufficient oxygen numbers was determined by Eq. 1 in the two groups. The calculated $\overline{OS_c}$ was weighted to the normalised peak areas and the results are shown in Table S1. The results suggest that the influence of S or NS on the calculation of $\overline{OS_c}$ is negligible owing to the low fractions of the two species in the oxidation products. Thus, it is reasonable to calculate the $\overline{OS_c}$ for CHOS and CHONS species according to Eq. 1 (as shown in Eq. 3 in the paper) in this study.

	Unique compounds			Commo	n compou	inds
Negative mode						
	Assumption	Upper limit	Lower limit	Assumption	Upper limit	Lower limit
Sum of CHOS and CHONS	-0.037	-0.082	-0.084	-0.018	-0.034	-0.078
The gap between the assumption and upper limit or lower limit		-0.044	-0.046		-0.016	-0.061
Positive mode						
	Assumption	Upper limit	Lower limit	Assumption	Upper limit	Lower limit
Sum of CHOS and CHONS	-0.272	-0.286	-0.304	-0.083	-0.151	-0.177
The gap between the assumption and upper limit or lower limit		-0.014	-0.032		-0.069	-0.094

Table S1. Results of calculated $\overline{OS_C}$ for compounds in the CHOS and CHONS groups.



Figure S1. Two examples of an ion having more than a single desorption peak. Here the peaks at the lower desorption temperature were assigned to monomer $C_{10}H_{16}O_4$ (a) and $C_{19}H_{28}O_7$ (b) generated from α -pinene directly and the broader higher temperature peaks being a fragment of another ion at the same mass.



Figure S2. Results from the representative experiment. (a) mixing ratios of NO, NO₂ and NO₂/NO ratio. (b) SOA mass over time.



Figure S3. Decay rates of α -pinene. The shaded areas represent the variability of the experiments.



Figure S4. Time series of ions in each cluster in the gas phase.

Table S2. Compounds in the gas phase in each cluster for the representative experiment, ranking by ion's contribution in each cluster. All ions are reported as iodide clustered species.

Clus	ter 1	Clu	Cluster 3		ster 4
MW	Formula	MW	Formula	MW	Formula
298.978031	$C_8H_{12}O_4$	371.994409	$C_{10}H_{15}NO_6$	355.999494	$C_{10}H_{15}NO_5$
256.967466	$C_{6}H_{10}O_{3}$	329.960035	$C_8H_{11}O_6$	403.984238	$C_{10}H_{15}NO_8$
312.944719	C ₇ H ₈ NO ₅	298.806598	CH_2O_2		
Clus	ter 2	214.920516	$C_3H_4O_3$	Clu	ster 5
MW	Formula	317.983844	$C_7H_{13}NO_5$	MW	Formula
315.968194	$C_7H_{11}NO_5$	343.975685	$C_9H_{13}O_6$	357.978759	$C_9H_{13}NO_6$
303.968194	$C_6H_{11}NO_5$	343.963109	$C_8H_{11}NO_6$	246.097762	$C_{10}H_{16}NO_6$
283.006926	$C_8H_{14}NO_2$	229.107599	$C_{11}H_{17}O_5$	232.082112	$C_9H_{14}NO_6$
301.96512	C ₇ H ₁₁ O ₅	234.073953	$C_9H_{14}O_7$	215.091949	$C_{10}H_{15}O_5$
275.936894	C ₄ H ₇ NO ₅	403.012799	$C_{11}H_{18}NO_7$	289.928735	C ₅ H ₇ O ₆
312.993681	$C_9H_{14}O_4$	345.991335	$C_9H_{15}O_6$	387.989324	$C_{10}H_{15}NO_{7}$
270.983116	$C_7 H_{12} O_3$	231.923256	$C_3H_5O_4$	373.98625	$C_{10}H_{15}O_7$
282.97054	$C_7H_{10}NO_3$	303.931809	$C_5H_7NO_6$	361.98625	C9H15O7
242.951816	$C_5H_8O_3$	317.947459	C ₆ H ₉ NO ₆	389.968588	$C_9H_{13}NO_8$
284.998766	$C_8H_{14}O_3$	311.014416	$C_{10}H_{16}O_3$	361.937288	C7H9NO8
268.967466	$C_7 H_{10} O_3$	327.009331	$C_{10}H_{16}O_4$	385.98625	$C_{11}H_{15}O_7$
199.92085	$C_2H_3NO_2$	296.998766	$C_{9}H_{14}O_{3}$	341.99642	$C_{10}H_{15}O_5$
299.014416	$C_9H_{16}O_3$	343.004245	$C_{10}H_{16}O_5$	375.952938	$C_8H_{11}NO_8$
324.993681	$C_{10}H_{14}O_4$	328.988595	$C_{9}H_{14}O_{5}$	232.118498	$C_{10}H_{18}NO_5$
228.936166	$C_4H_6O_3$	284.962381	$C_7H_{10}O_4$	388.936954	$C_9H_{10}O_9$
300.981105	$C_7H_{12}NO_4$	359.994409	$C_9H_{15}NO_6$	247.905594	$C_2H_3NO_5$
329.99642	C ₉ H ₁₅ O ₅	340.988595	$C_{10}H_{14}O_5$	340.00458	$C_{10}H_{15}NO_4$
345.019896	$C_{10}H_{18}O_5$	314.972945	$C_8H_{12}O_5$		
286.978031	$C_7H_{12}O_4$	344.012071	$C_{10}H_{17}O_5$		
327.98077	$C_9H_{13}O_5$	358.99916	$C_{10}H_{16}O_{6}$		
230.951816	$C_4H_8O_3$	230.915431	$C_3H_4O_4$		
316.988595	$C_8H_{14}O_5$	308.998766	$C_{10}H_{14}O_{3}$		
258.946731	$C_5H_8O_4$	226.920516	$C_4H_4O_3$		
302.972945	$C_7 H_{12} O_5$	388.984573	$C_{9}H_{14}N_{2}O_{7}$		
331.975685	C ₈ H ₁₃ O ₆	315.009331	$C_9H_{16}O_4$		
212.928675	$C_3H_4NO_2$	345.942374	$C_7H_9NO_7$		

313.952544	C ₇ H ₉ NO ₅	390.004974	$C_{10}H_{17}NO_{7}$	
272.998766	$C_{7}H_{14}O_{3}$	344.98351	$C_9H_{14}O_6$	
272.949805	$C_5H_8NO_4$	356.994743	$C_9H_{14}N_2O_5$	
301.030066	$C_9H_{18}O_3$	314.001506	$C_9H_{15}O_4$	
289.96512	$C_{6}H_{11}O_{5}$	330.991669	$C_8H_{14}NO_5$	
288.957295	$C_{6}H_{10}O_{5}$	341.960035	C ₉ H ₁₁ O ₆	
		355.015479	$C_{10}H_{16}N_2O_4$	
		261.93382	$C_4H_7O_5$	
		373.002234	$C_{10}H_{16}NO_6$	
		376.0019	$C_{10}H_{17}O_7$	
		326.001506	$C_{10}H_{15}O_4$	
		331.9393	C ₇ H ₉ O ₇	
		387.005308	$C_{10}H_{16}N_2O_6$	
		338.996755	$C_{10}H_{14}NO_4$	
		370.986584	$C_{10}H_{14}NO_6$	



Figure S5. Time series of ions in each cluster in particle phase.

Table S3. Compounds in the particle phase in each cluster for the representative experiment, ranking by
ion's contribution in each cluster. All ions are reported as iodide clustered species.

Cluster	1		Cluster 5
MW	Formula	MW	Formula
328.988595	$C_9H_{14}O_5$	312.993681	$C_9H_{14}O_4$
284.962381	$C_7H_{10}O_4$	298.978031	$C_8H_{12}O_4$
258.946731	$C_5H_8O_4$	327.009331	$C_{10}H_{16}O_4$
405.999888	$C_{10}H_{17}NO_8$	358.99916	$C_{10}H_{16}O_{6}$
355.999494	$C_{10}H_{15}NO_5$	371.994409	$C_{10}H_{15}NO_{6}$
Cluster	Cluster 2		$C_{10}H_{14}O_5$
MW	Formula	345.019896	$C_{10}H_{18}O_5$
403.984238	$C_{10}H_{15}NO_8$	356.994743	$C_9H_{14}N_2O_5$
400.997149	$C_{11}H_{16}NO_7$	344.98351	$C_9H_{14}O_6$
319.9393	$C_6H_9O_7$	300.981105	$C_7H_{12}NO_4$
391.996814	$C_{10}H_{17}O_8$	374.994075	$C_{10}H_{16}O_7$
Cluster	3	302.972945	C ₇ H ₁₂ O ₅
MW	Formula	300.932143	$C_5H_6N_2O_5$
270.983116	$C_7 H_{12} O_3$	256.931081	C ₅ H ₆ O ₄
268.918505	C ₅ H ₄ NO ₄	328.017156	$C_{10}H_{17}O_4$
242.915431	$C_4H_4O_4$	314.001506	C9H15O4
Cluster 4		330.942708	$C_6H_8N_2O_6$

MW	Formula	282.97054	$C_7H_{10}NO_3$
343.004245	$C_{10}H_{16}O_5$	469.072325	$C_{17}H_{26}O_7$
324.993681	$C_{10}H_{14}O_4$	387.989324	C ₁₀ H ₁₅ NO ₇
296.998766	$C_9H_{14}O_3$	344.012071	$C_{10}H_{17}O_5$
390.004974	C ₁₀ H ₁₇ NO ₇	299.985856	$C_8H_{13}O_4$
361.01481	$C_{10}H_{18}O_{6}$	286.965455	$C_6H_{10}NO_4$
388.984573	C9H14N2O7	214.920516	C3H4O3
200.904866	C ₂ H ₂ O ₃	359.994409	C ₉ H ₁₅ NO ₆
316.95221	$C_7H_{10}O_6$	316.988595	C ₈ H ₁₄ O ₅
361.98625	CoH15O7	495.087975	C10H28O7
341,99642	C10H15O5	373.002234	C10H16NO6
226.920516	C4H4O3	372.965849	$C_{0}H_{12}NO_{7}$
228.936166	C4H6O3	299.014416	$C_0H_{16}O_3$
202.920516	$C_2H_4O_3$	346.99916	CoH16O5
449.091049	C14H28NO7	342.942708	$C_7H_8N_2O_6$
Cluster	6	332,98351	CsH14O6
MW	Formula	216.936166	C ₃ H ₆ O ₃
314,972945	C ₈ H ₁₂ O ₅	312.944719	C7H8NO5
330.991669	C8H14NO5	283.006926	C ₈ H ₁₄ NO ₂
274,941645	C5H8O5	315.009331	CoH16O4
256.95489	C5H2NO2	373,98625	C10H15O7
230.951816	C ₄ H ₈ O ₂	451.070314	C12H26NO8
200001010	0411803	370.986584	$\frac{C_{13}H_{20}C_{10}}{C_{10}H_{14}NO_{5}}$
		360.965849	$C_{8}H_{12}NO_{7}$
		481 072325	$\frac{C_{19}H_{12}(0)}{C_{19}H_{26}O_{7}}$
		302.923984	CsHeNO6
		387.005308	$C_{10}H_{16}N_{2}O_{6}$
		439.06176	$C_{16}H_{24}O_{6}$
		345 991335	$C_0H_{15}O_6$
		288 957295	C_4H10O5
		287 00184	C7H14NO2
		356 947125	$C_0H_{10}O_7$
		427 025375	C14H20O7
		441 028449	$\frac{C_{14}H_{20}O}{C_{14}H_{20}NO_{7}}$
		467.056675	$\frac{C_{14}T_{20}}{C_{17}}$
		272.949805	CsH8NO4
		315.968194	C ₇ H ₁₁ NO ₅
		471.05159	$C_{16}H_{24}O_8$
		355.015479	$C_{10}H_{16}N_2O_4$
		376.0019	C10H17O7
		317.983844	C7H13NO5
		326.001506	C10H15O4
		399.005308	$C_{11}H_{16}N_2O_6$
		298.006591	C ₉ H ₁₅ O ₃
		303.968194	C ₆ H ₁₁ NO ₅
		327.98077	C ₉ H ₁₃ O ₅
		338.972945	C10H12O5
		369.007319	C ₁₁ H ₁₆ NO ₅
		397.01481	C13H18O6
		296.949805	C ₇ H ₈ NO ₄



Figure S6. Hierarchical clustering of gas-phase oxidation products for the repeat α -pinene system. (a) Time series of each cluster normalized to the highest ions' intensity between 0 and 1. (b) Matrix showing the relative distance between clusters. (c) Carbon number vs oxygen number for each cluster. (d) Carbon number vs oxidation state for each cluster. (e) Time series of the sum of ions' normalized fractions to the total signal in each cluster. Note that the square symbols represent the contribution weighted average carbon numbers, oxygen numbers or and $\overline{OS_C}$ in each cluster. The colors correspond to the ones in (e).



Figure S7. Time series of ions in each cluster in the gas phase for the repeat experiment.

Cluster 1		Ch	uster 2	Cluster 3	
MW	Formula	MW Formula		MW	Formula
298.978	C ₈ H ₁₂ O ₄	230.9518	$C_4H_8O_3$	214.9205	$C_3H_4O_3$
270.9831	C7H12O3	315.9682	C7H11NO5	232.0821	$C_9H_{14}NO_6$
312.9937	$C_9H_{14}O_4$	298.8066	CH ₂ O ₂	234.074	$C_9H_{14}O_7$
256.9675	$C_{6}H_{10}O_{3}$	329.96	$C_8H_{11}O_6$	229.1076	$C_{11}H_{17}O_5$
299.9859	$C_8H_{13}O_4$	343.9631	$C_8H_{11}NO_6$	403.0128	$C_{11}H_{18}NO_7$
345.0199	$C_{10}H_{18}O_5$	317.9838	$C_7H_{13}NO_5$	371.9944	$C_{10}H_{15}NO_6$
286.9655	$C_6H_{10}NO_4$	303.9682	$C_6H_{11}NO_5$	311.0144	$C_{10}H_{16}O_3$
258.9467	$C_5H_8O_4$	296.9988	$C_9H_{14}O_3$	327.0093	$C_{10}H_{16}O_4$
287.0018	C ₇ H ₁₄ NO ₃	282.9705	$C_7H_{10}NO_3$	373.0022	$C_{10}H_{16}NO_6$

Table S4. Compounds in the gas phase in each cluster for the repeat experiment, ranking by ion's contribution in each cluster. All ions are reported as iodide clustered species.

		283.0069	$C_8H_{14}NO_2$	358.9992	$C_{10}H_{16}O_{6}$
Clust	er 4	343.0042	$C_{10}H_{16}O_5$	359.9944	C ₉ H ₁₅ NO ₆
MW	Formula	242.9518	C5H8O3	341.9964	$C_{10}H_{15}O_5$
355.9995	C ₁₀ H ₁₅ NO ₅	343.9757	$C_9H_{13}O_6$	312.0222	$C_{10}H_{17}O_3$
403.9842	C ₁₀ H ₁₅ NO ₈	284.9988	$C_8H_{14}O_3$	230.9154	$C_3H_4O_4$
Clust	er 5	268.9675	$C_7 H_{10} O_3$	340.9886	$C_{10}H_{14}O_5$
MW	Formula	328.9886	$C_9H_{14}O_5$	345.9913	$C_9H_{15}O_6$
357.9788	C ₉ H ₁₃ NO ₆	199.9209	$C_2H_3NO_2$	388.9846	$C_9H_{14}N_2O_7$
246.0978	C ₁₀ H ₁₆ NO ₆	284.9624	$C_7H_{10}O_4$	328.0172	$C_{10}H_{17}O_4$
202.9205	$C_2H_4O_3$	344.0121	$C_{10}H_{17}O_5$	226.9205	$C_4H_4O_3$
358.9628	$C_9H_{12}O_7$	299.0144	$C_9H_{16}O_3$	308.9988	$C_{10}H_{14}O_3$
289.9287	$C_5H_7O_6$	314.9729	$C_8H_{12}O_5$	345.9424	C7H9NO7
215.0919	$C_{10}H_{15}O_5$	329.9964	$C_9H_{15}O_5$	341.96	$C_9H_{11}O_6$
361.9863	C9H15O7	228.9362	$C_4H_6O_3$	372.9658	$C_9H_{12}NO_7$
373.9863	$C_{10}H_{15}O_7$	344.9835	$C_9H_{14}O_6$	303.9318	C ₅ H ₇ NO ₆
356.9947	$C_{9}H_{14}N_{2}O_{5}$	316.9886	$C_8H_{14}O_5$	355.0155	$C_{10}H_{16}N_{2}O_{4} \\$
387.9893	$C_{10}H_{15}NO_7$	300.9811	$C_7H_{12}NO_4$	374.9941	$C_{10}H_{16}O_7$
389.9686	$C_9H_{13}NO_8$	324.9937	$C_{10}H_{14}O_4$	311.9859	$C_{9}H_{13}O_{4}$
388.937	$C_9H_{10}O_9$	314.0015	$C_9H_{15}O_4$	361.0148	$C_{10}H_{18}O_6$
247.9056	$C_2H_3NO_5$	298.0066	$C_9H_{15}O_3$		
385.9863	$C_{11}H_{15}O_7$	312.9447	$C_7H_8NO_5$		
		327.9808	$C_9H_{13}O_5$		
		275.9369	C ₄ H ₇ NO ₅		
		301.9651	$C_7 H_{11} O_5$		
		316.9522	$C_{7}H_{10}O_{6}$		
		330.9917	$C_8H_{14}NO_5$		
		302.9729	$C_7H_{12}O_5$		
		390.005	$C_{10}H_{17}NO_7$		
		313.9525	C7H9NO5		
		256.9311	$C_5H_6O_4$		
		331.9757	$C_8H_{13}O_6$		
		315.0093	$C_{9}H_{16}O_{4}$		
		317.9475	C ₆ H ₉ NO ₆		
		326.0015	$C_{10}H_{15}O_4$		
		272.9988	$C_7 H_{14} O_3$		
		285.9702	$C_7 H_{11} O_4$		
		261.9338	C4H7O5		
		346.9992	$C_9H_{16}O_6$		



Figure S8. Hierarchical clustering of particle-phase oxidation products for the repeat α -pinene system. (a) Average time series of each cluster normalized to the highest ions' intensity between 0 and 1; (b) Matrix showing the relative distance between clusters. (c) Carbon number vs oxygen number for each cluster. (d) Carbon number vs oxidation state for each cluster. (e) Time series of the sum of ions' normalized fractions to the total signal in each cluster. Note that the square symbols represent the contribution weighted average carbon numbers, oxygen numbers or and $\overline{OS_C}$ in each cluster. The colors correspond to the ones in (a).



Figure S9. Time series of ions in each cluster in the particle phase for the repeat experiment.

Table S5. Compounds in the particle phase in each cluster for the repeat experiment, ranking by ion's contribution in each cluster. All ions are reported as iodide clustered species.

Cluster 1		Clus	ster 4	Cluster 5	
MW	Formula	MW	Formula	MW	Formula
324.99368	$C_{10}H_{14}O_4$	327.00933	$C_{10}H_{16}O_4$	312.99368	$C_9H_{14}O_4$
467.05668	$C_{17}H_{24}O_{7}$	314.97295	$C_8H_{12}O_5$	298.97803	$C_8H_{12}O_4$
405.99989	$C_{10}H_{17}NO_8$	356.99474	$C_9H_{14}N_2O_5$	343.00425	$C_{10}H_{16}O_5$
202.92052	$C_2H_4O_3$	328.9886	$C_9H_{14}O_5$	358.99916	$C_{10}H_{16}O_{6}$
355.99949	$C_{10}H_{15}NO_5$	345.0199	$C_{10}H_{18}O_5$	371.99441	$C_{10}H_{15}NO_{6}$
Clus	ster 2	403.98424	$C_{10}H_{15}NO_8$	340.9886	$C_{10}H_{14}O_5$
MW	Formula	330.94271	$C_6H_8N_2O_6$	344.98351	$C_9H_{14}O_6$
256.95489	C ₅ H ₈ NO ₃	390.00497	C10H17NO7	296.99877	$C_9H_{14}O_3$
Clus	ster 1	495.08798	$C_{19}H_{28}O_7$	374.99408	$C_{10}H_{16}O_7$

MW	Formula	387.98932	$C_{10}H_{15}NO_{7}$	256.93108	$C_5H_6O_4$
228.93617	$C_4H_6O_3$	274.94165	C ₅ H ₈ O ₅	302.97295	$C_7 H_{12} O_5$
242.91543	$C_4H_4O_4$	299.01442	$C_9H_{16}O_3$	300.98111	C ₇ H ₁₂ NO ₄
Clus	ster 6	200.90487	$C_2H_2O_3$	214.92052	$C_3H_4O_3$
MW	Formula	270.98312	C ₇ H ₁₂ O ₃	284.96238	$C_7 H_{10} O_4$
330.99167	C ₈ H ₁₄ NO ₅	319.9393	C ₆ H ₉ O ₇	316.9886	$C_8H_{14}O_5$
342.94271	$C_7H_8N_2O_6$	216.93617	C ₃ H ₆ O ₃	282.97054	C ₇ H ₁₀ NO ₃
360.96585	C ₈ H ₁₂ NO ₇	449.09105	$C_{14}H_{28}NO_7$	286.97803	$C_7 H_{12} O_4$
427.02538	$C_{14}H_{20}O_7$	466.08524	C ₁₈ H ₂₇ O ₆	315.00933	$C_9H_{16}O_4$
415.02538	$C_{13}H_{20}O_7$	417.00464	$C_{12}H_{18}O_8$	300.93214	C ₅ H ₆ N ₂ O ₅
388.98457	$C_9H_{14}N_2O_7$	391.99681	$C_{10}H_{17}O_8$	387.00531	$C_{10}H_{16}N_2O_6$
226.92052	C ₄ H ₄ O ₃	331.97569	$C_8H_{13}O_6$	332.98351	$C_8H_{14}O_6$
357.97876	C ₉ H ₁₃ NO ₆			373.00223	$C_{10}H_{16}NO_{6}$
481.1451	C ₂₀ H ₃₄ O ₅			372.96585	C ₉ H ₁₂ NO ₇
				346.99916	$C_9H_{16}O_6$
				451.07031	C13H26NO8
				312.94472	C7H8NO5
				370.98658	C10H14NO6
				283.00693	C8H14NO2
				481.07233	C18H26O7
				316.95221	C7H10O6
				439.06176	C16H24O6
				441.02845	$C_{14}H_{20}NO_7$
				485.06724	$C_{17}H_{26}O_8$
				356.94713	$C_9H_{10}O_7$
				373.98625	$C_{10}H_{15}O_{7}$
				471.05159	C ₁₆ H ₂₄ O ₈
				399.00531	$C_{11}H_{16}N_2O_6$
				302.92398	C ₅ H ₆ NO ₆
				355.01548	$C_{10}H_{16}N_2O_4$
				288.9573	$C_6H_{10}O_5$
				400.99715	$C_{11}H_{16}NO_7$
				272.94981	C ₅ H ₈ NO ₄
				397.01481	$C_{13}H_{18}O_{6}$
				312.02224	$C_{10}H_{17}O_3$
				338.97295	$C_{10}H_{12}O_5$
				376.0019	$C_{10}H_{17}O_7$
				361.98625	C ₉ H ₁₅ O ₇
				340.00458	$C_{10}H_{15}NO_4$
				369.00732	$C_{11}H_{16}NO_5$
				429.01587	$C_{12}H_{18}N_2O_7$
				296.94981	C ₇ H ₈ NO ₄
				341.99642	$C_{10}H_{15}O_5$
				353.01241	$C_{11}H_{16}NO_4$
				409.0512	$C_{15}H_{22}O_5$
				311.98586	$C_9H_{13}O_4$



Figure S10. Temporal profiles of particle fractions for the selected identified organic molecules generated from α -pinene photooxidation reactions.

















Figure S11 LC-MS chromatographs and mass spectrum of particle phase from a-pinene oxidation products. Subplot (A1-W1): the retention time from liquid chromatograph for each component; subplot (A2-W2): corresponding mass spectra for the peaks in A1-W1. Ions are detected in the negative mode by the loss of one hydrogen atom ([M-H]-); subplot (A3-W3): corresponding mass spectra for the product ions produced from the parent ions in A2-W2. Note that mass spectra of products generated from their parent ions for a few compounds cannot be identified likely due to their very low concentrations.