Supporting Information for

Combined application of On-line FIGAERO-CIMS and Off-line LC-MS to Characterize the Chemical Composition of SOA in Smog Chamber Studies

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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 (NO_3^-, $OS_N = +5$) and S (SO_4^{2-}, $OS_S = +6$) are fully oxidized to obtain the lower limit of calculated $\overline{OS_C}$ by Eq. 2: $\overline{OS_C} = 2\times O/C - H/C - 5\times N/C - 6\times S/C$ ($nO \geq 7$). We assumed the N ($-NO_2^-$, $OS_N = +3$) and S (SO_3^{2-}, $OS_S = +4$) are reduced, so the upper limit of $\overline{OS_C}$ was determined by Eq. 3 $\overline{OS_C} = 2\times O/C - H/C - 3\times N/C - 4\times S/C$ ($nO \geq 5$). For the CHOS species, the lower and upper limits of calculated $\overline{OS_C}$ were determined by Eq. 4: $\overline{OS_C} = 2\times O/C - H/C - 6\times S/C$ ($nO \geq 4$) and Eq. 5: $\overline{OS_C} = 2\times O/C - H/C - 4\times S/C$ ($nO \geq 3$), 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.

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

	Unique compounds			**Common compounds**		
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

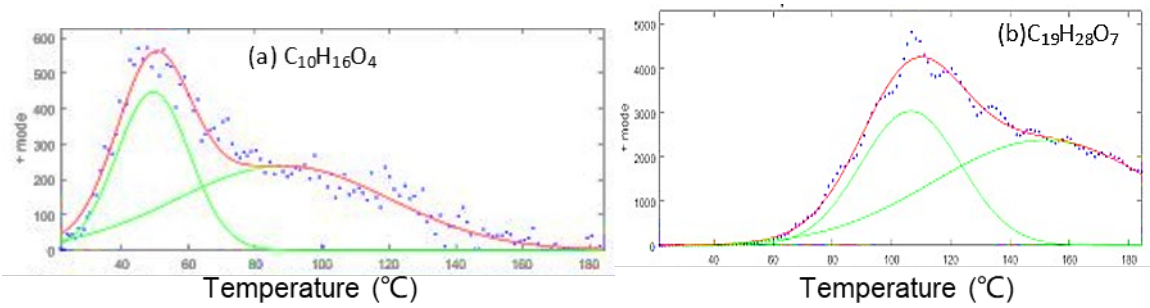


Figure S1. Two examples of an ion having more than a single desorption peak. Here the peaks at the lower desorption temperature were assigned to monomer $C_{10}H_{16}O_4$ (a) and $C_{19}H_{28}O_7$ (b) generated from α-pinene directly and the broader higher temperature peaks being a fragment of another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

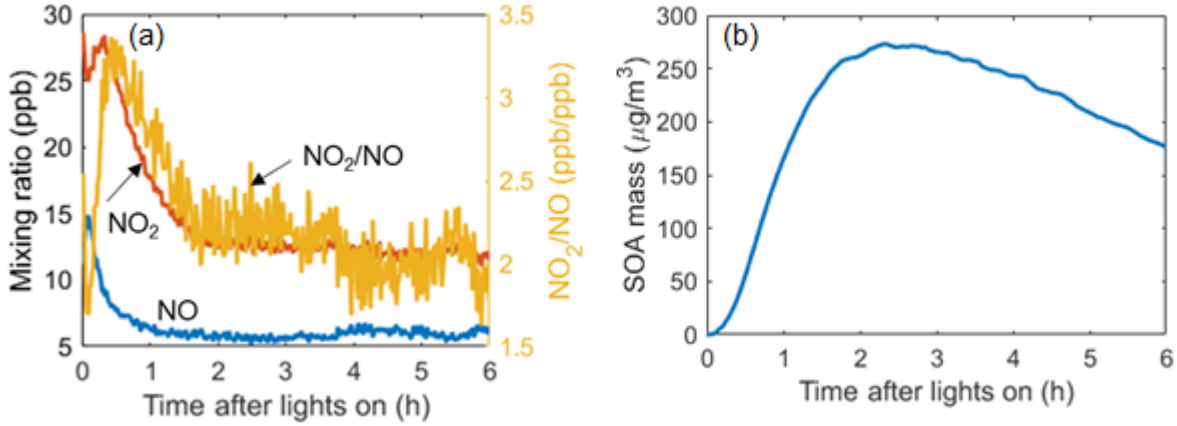


Figure S2. Results from the representative experiment. (a) mixing ratios of NO, NO_2 and NO_2/NO ratio. (b) SOA mass over time.

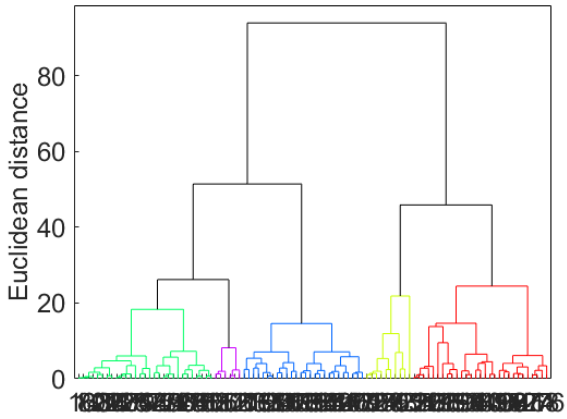


Figure S3. Hierarchical cluster relationship. (Note: the x axis label represents the formula. It is so dense that cannot see them. The formulae are shown in Table S1 in each cluster.)

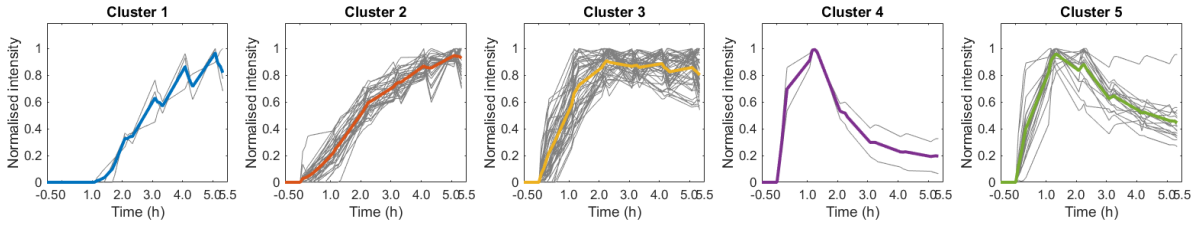


Figure S4. Time series of ions in each cluster in the gas phase.

Table S2. Compounds in the gas phase in each cluster for the representative experiment, ranking by ion's contribution in each cluster.

Cluster 1		**Cluster 3**		**Cluster 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	$C_6H_{10}O_3$	329.960035	$C_8H_{11}O_6$	403.984238	$C_{10}H_{15}NO_8$
312.944719	$C_7H_8NO_5$	298.806598	CH_2O_2		
Cluster 2		214.920516	$C_3H_4O_3$	**Cluster 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	$C_7H_{11}O_5$	234.073953	$C_9H_{14}O_7$	215.091949	$C_{10}H_{15}O_5$
275.936894	$C_4H_7NO_5$	403.012799	$C_{11}H_{18}NO_7$	289.928735	$C_5H_7O_6$
312.993681	$C_9H_{14}O_4$	345.991335	$C_9H_{15}O_6$	387.989324	$C_{10}H_{15}NO_7$
270.983116	$C_7H_{12}O_3$	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	$C_9H_{15}O_7$
242.951816	$C_5H_8O_3$	317.947459	$C_6H_9NO_6$	389.968588	$C_9H_{13}NO_8$
284.998766	$C_8H_{14}O_3$	311.014416	$C_{10}H_{16}O_3$	361.937288	$C_7H_9NO_8$
268.967466	$C_7H_{10}O_3$	327.009331	$C_{10}H_{16}O_4$	385.98625	$C_{11}H_{15}O_7$
199.92085	$C_2H_3NO_2$	296.998766	$C_9H_{14}O_3$	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	$C_9H_{14}O_5$	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	$C_9H_{15}O_5$	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	$C_7H_{12}O_5$	388.984573	$C_9H_{14}N_2O_7$		
331.975685	$C_8H_{13}O_6$	315.009331	$C_9H_{16}O_4$		
212.928675	$C_3H_4NO_2$	345.942374	$C_7H_9NO_7$		

313.952544	$C_7H_9NO_5$	390.004974	$C_{10}H_{17}NO_7$		
272.998766	$C_7H_{14}O_3$	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	$C_6H_{11}O_5$	330.991669	$C_8H_{14}NO_5$		
288.957295	$C_6H_{10}O_5$	341.960035	$C_9H_{11}O_6$		
		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	$C_7H_9O_7$		
		387.005308	$C_{10}H_{16}N_2O_6$		
		338.996755	$C_{10}H_{14}NO_4$		
		370.986584	$C_{10}H_{14}NO_6$		

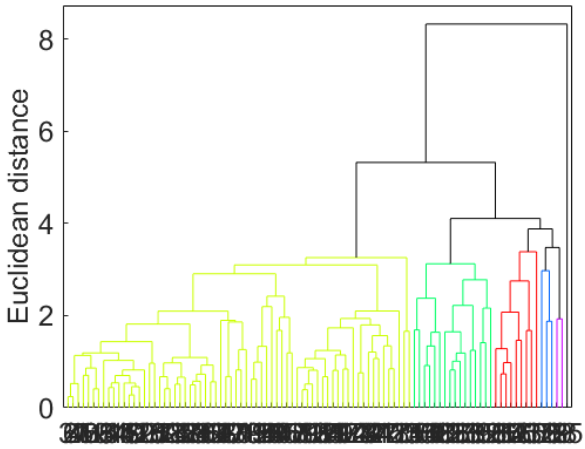


Figure S5. Hierarchical cluster relationship. (Note: the x axis label represents the formula. It is so dense that cannot see them. The formulae are shown in Table S2 in each cluster.)

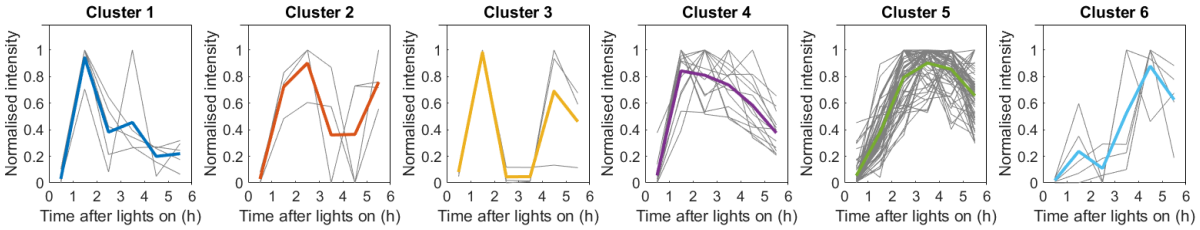


Figure S6. Time series of ions in each cluster in particle phase.

Table S3. Compounds in the particle phase in each cluster for the representative experiment, ranking by ion's contribution in each cluster.

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 2		340.988595	$C_{10}H_{14}O_5$
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	$C_7H_{12}O_5$
MW	**Formula**	300.932143	$C_5H_6N_2O_5$
270.983116	$C_7H_{12}O_3$	256.931081	$C_5H_6O_4$
268.918505	$C_5H_4NO_4$	328.017156	$C_{10}H_{17}O_4$
242.915431	$C_4H_4O_4$	314.001506	$C_9H_{15}O_4$
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	$C_9H_{14}N_2O_7$	214.920516	$C_3H_4O_3$
200.904866	$C_2H_2O_3$	359.994409	$C_9H_{15}NO_6$
316.95221	$C_7H_{10}O_6$	316.988595	$C_8H_{14}O_5$
361.98625	$C_9H_{15}O_7$	495.087975	$C_{19}H_{28}O_7$
341.99642	$C_{10}H_{15}O_5$	373.002234	$C_{10}H_{16}NO_6$
226.920516	$C_4H_4O_3$	372.965849	$C_9H_{12}NO_7$
228.936166	$C_4H_6O_3$	299.014416	$C_9H_{16}O_3$
202.920516	$C_2H_4O_3$	346.99916	$C_9H_{16}O_6$
449.091049	$C_{14}H_{28}NO_7$	342.942708	$C_7H_8N_2O_6$
Cluster 6		332.98351	$C_8H_{14}O_6$
MW	**Formula**	216.936166	$C_3H_6O_3$
314.972945	$C_8H_{12}O_5$	312.944719	$C_7H_8NO_5$
330.991669	$C_8H_{14}NO_5$	283.006926	$C_8H_{14}NO_2$
274.941645	$C_5H_8O_5$	315.009331	$C_9H_{16}O_4$
256.95489	$C_5H_8NO_3$	373.98625	$C_{10}H_{15}O_7$
230.951816	$C_4H_8O_3$	451.070314	$C_{13}H_{26}NO_8$
		370.986584	$C_{10}H_{14}NO_6$
		360.965849	$C_8H_{12}NO_7$
		481.072325	$C_{18}H_{26}O_7$
		302.923984	$C_5H_6NO_6$
		387.005308	$C_{10}H_{16}N_2O_6$
		439.06176	$C_{16}H_{24}O_6$
		345.991335	$C_9H_{15}O_6$
		288.957295	$C_6H_{10}O_5$
		287.00184	$C_7H_{14}NO_3$
		356.947125	$C_9H_{10}O_7$
		427.025375	$C_{14}H_{20}O_7$
		441.028449	$C_{14}H_{20}NO_7$
		467.056675	$C_{17}H_{24}O_7$

		272.949805	$C_5H_8NO_4$
		315.968194	$C_7H_{11}NO_5$
		471.05159	$C_{16}H_{24}O_8$
		355.015479	$C_{10}H_{16}N_2O_4$
		376.0019	$C_{10}H_{17}O_7$
		317.983844	$C_7H_{13}NO_5$
		326.001506	$C_{10}H_{15}O_4$
		399.005308	$C_{11}H_{16}N_2O_6$
		298.006591	$C_9H_{15}O_3$
		303.968194	$C_6H_{11}NO_5$
		327.98077	$C_9H_{13}O_5$
		338.972945	$C_{10}H_{12}O_5$
		369.007319	$C_{11}H_{16}NO_5$
		397.01481	$C_{13}H_{18}O_6$
		296.949805	$C_7H_8NO_4$
		308.998766	$C_{10}H_{14}O_3$

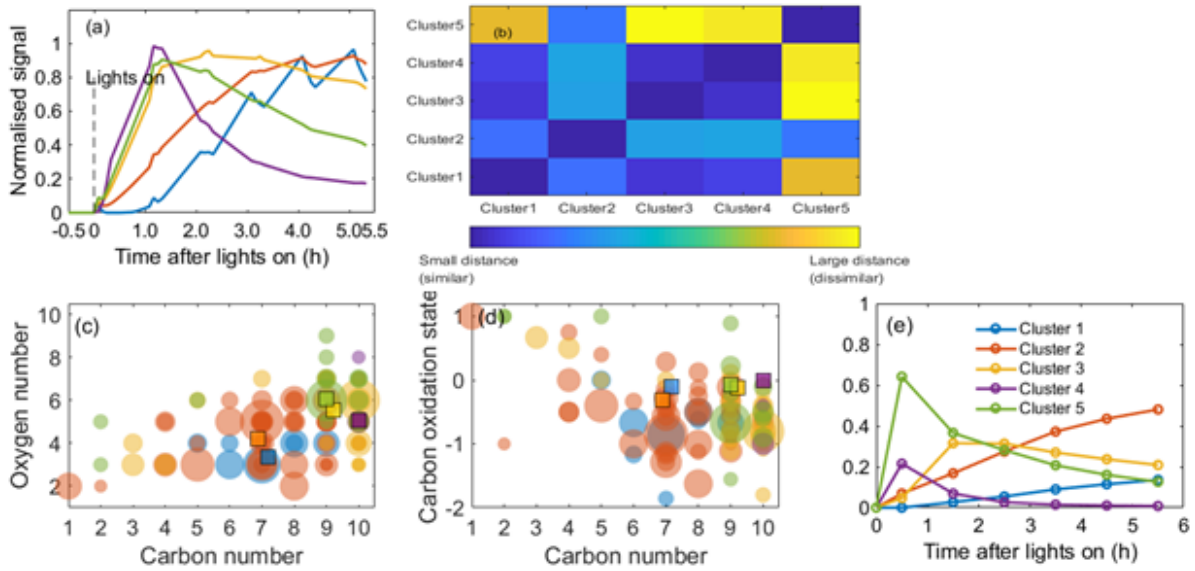


Figure S7. Hierarchical clustering of gas-phase oxidation products for the repeat α-pinene system. (a) Time series of each cluster normalized to the highest ions' intensity between 0 and 1. (b) Matrix showing the relative distance between clusters. (c) Carbon number vs oxygen number for each cluster. (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).

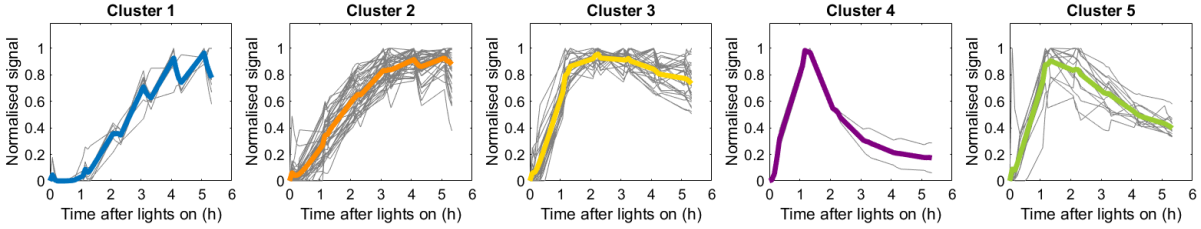


Figure S8. Time series of ions in each cluster in the gas phase for the repeat experiment.

Table S4. Compounds in the gas phase in each cluster for the repeat experiment, ranking by ion's contribution in each cluster.

Cluster 1		**Cluster 2**		**Cluster 3**	
MW	**Formula**	**MW**	**Formula**	**MW**	**Formula**
298.978	$C_8H_{12}O_4$	230.9518	$C_4H_8O_3$	214.9205	$C_3H_4O_3$
270.9831	$C_7H_{12}O_3$	315.9682	$C_7H_{11}NO_5$	232.0821	$C_9H_{14}NO_6$
312.9937	$C_9H_{14}O_4$	298.8066	CH_2O_2	234.074	$C_9H_{14}O_7$
256.9675	$C_6H_{10}O_3$	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	$C_7H_{14}NO_3$	282.9705	$C_7H_{10}NO_3$	373.0022	$C_{10}H_{16}NO_6$
		283.0069	$C_8H_{14}NO_2$	358.9992	$C_{10}H_{16}O_6$
Cluster 4		343.0042	$C_{10}H_{16}O_5$	359.9944	$C_9H_{15}NO_6$
MW	**Formula**	242.9518	$C_5H_8O_3$	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	$C_3H_4O_4$
Cluster 5		268.9675	$C_7H_{10}O_3$	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	$C_9H_{13}NO_6$	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	$C_7H_9NO_7$
215.0919	$C_{10}H_{15}O_5$	329.9964	$C_9H_{15}O_5$	341.96	$C_9H_{11}O_6$
361.9863	$C_9H_{15}O_7$	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	$C_5H_7NO_6$
356.9947	$C_9H_{14}N_2O_5$	316.9886	$C_8H_{14}O_5$	355.0155	$C_{10}H_{16}N_2O_4$
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	$C_9H_{13}O_4$
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	$C_4H_7NO_5$		
		301.9651	$C_7H_{11}O_5$		
		316.9522	$C_7H_{10}O_6$		
		330.9917	$C_8H_{14}NO_5$		
		302.9729	$C_7H_{12}O_5$		
		390.005	$C_{10}H_{17}NO_7$		
		313.9525	$C_7H_9NO_5$		
		256.9311	$C_5H_6O_4$		
		331.9757	$C_8H_{13}O_6$		

		315.0093	$C_9H_{16}O_4$		
		317.9475	$C_6H_9NO_6$		
		326.0015	$C_{10}H_{15}O_4$		
		272.9988	$C_7H_{14}O_3$		
		285.9702	$C_7H_{11}O_4$		
		261.9338	$C_4H_7O_5$		
		346.9992	$C_9H_{16}O_6$		

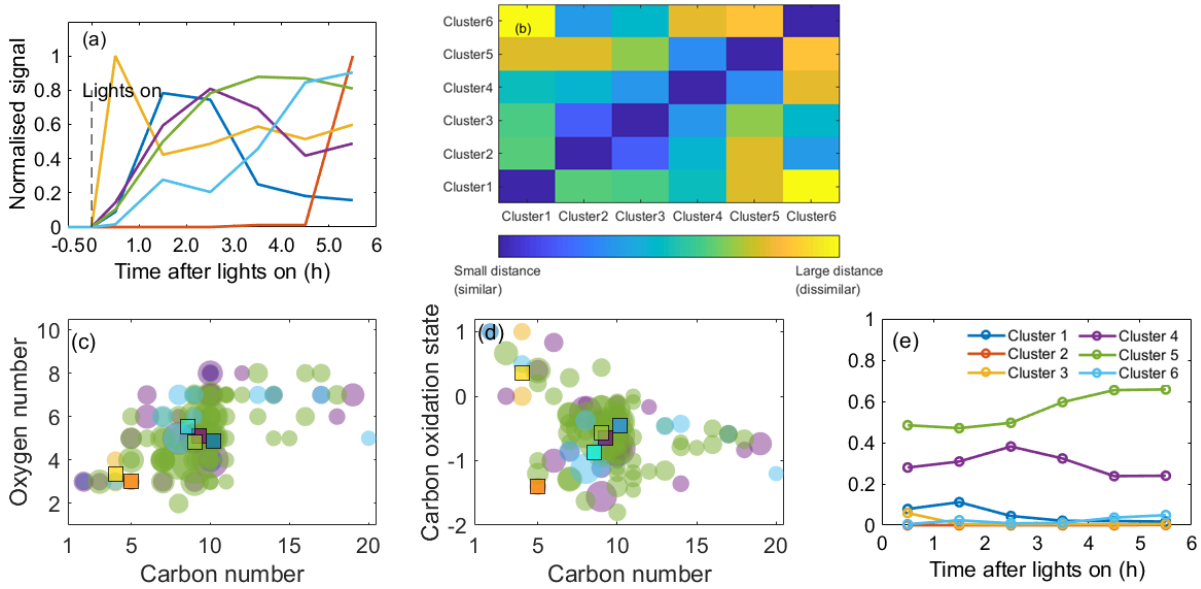


Figure S9. Hierarchical clustering of particle-phase oxidation products for the repeat α-pinene system. (a) Average time series of each cluster normalized to the highest ions' intensity between 0 and 1; (b) Matrix showing the relative distance between clusters. (c) Carbon number vs oxygen number for 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).

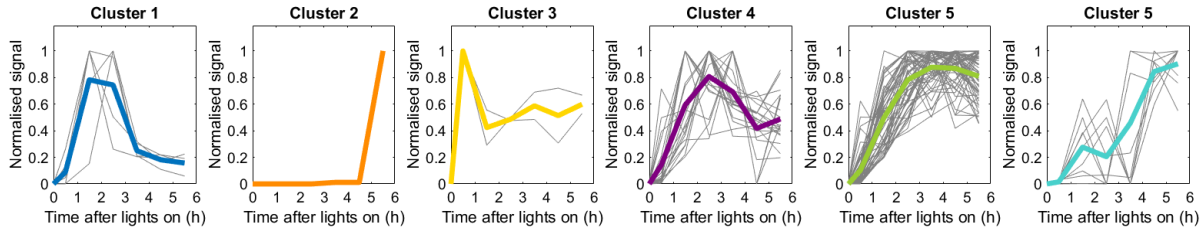


Figure S10. Time series of ions in each cluster in the particle phase for the repeat experiment.

Table S5. Compounds in the particle phase in each cluster for the repeat experiment, ranking by ion's contribution in each cluster.

Cluster 1		**Cluster 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	$C_{10}H_{15}NO_6$
Cluster 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	$C_5H_8NO_3$	390.00497	$C_{10}H_{17}NO_7$	296.99877	$C_9H_{14}O_3$
Cluster 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	$C_5H_8O_5$	302.97295	$C_7H_{12}O_5$
242.91543	$C_4H_4O_4$	299.01442	$C_9H_{16}O_3$	300.98111	$C_7H_{12}NO_4$
Cluster 6		200.90487	$C_2H_2O_3$	214.92052	$C_3H_4O_3$
MW	Formula	270.98312	$C_7H_{12}O_3$	284.96238	$C_7H_{10}O_4$
330.99167	$C_8H_{14}NO_5$	319.9393	$C_6H_9O_7$	316.9886	$C_8H_{14}O_5$
342.94271	$C_7H_8N_2O_6$	216.93617	$C_3H_6O_3$	282.97054	$C_7H_{10}NO_3$
360.96585	$C_8H_{12}NO_7$	449.09105	$C_{14}H_{28}NO_7$	286.97803	$C_7H_{12}O_4$
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	$C_5H_6N_2O_5$
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	$C_4H_4O_3$	331.97569	$C_8H_{13}O_6$	332.98351	$C_8H_{14}O_6$
357.97876	$C_9H_{13}NO_6$			373.00223	$C_{10}H_{16}NO_6$
481.1451	$C_{20}H_{34}O_5$			372.96585	$C_9H_{12}NO_7$
				346.99916	$C_9H_{16}O_6$
				451.07031	$C_{13}H_{26}NO_8$
				312.94472	$C_7H_8NO_5$
				370.98658	$C_{10}H_{14}NO_6$
				283.00693	$C_8H_{14}NO_2$
				481.07233	$C_{18}H_{26}O_7$
				316.95221	$C_7H_{10}O_6$
				439.06176	$C_{16}H_{24}O_6$
				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	$C_5H_6NO_6$
				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	$C_5H_8NO_4$
				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	$C_9H_{15}O_7$
				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	$C_7H_8NO_4$
				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	$C_9H_{13}O_4$

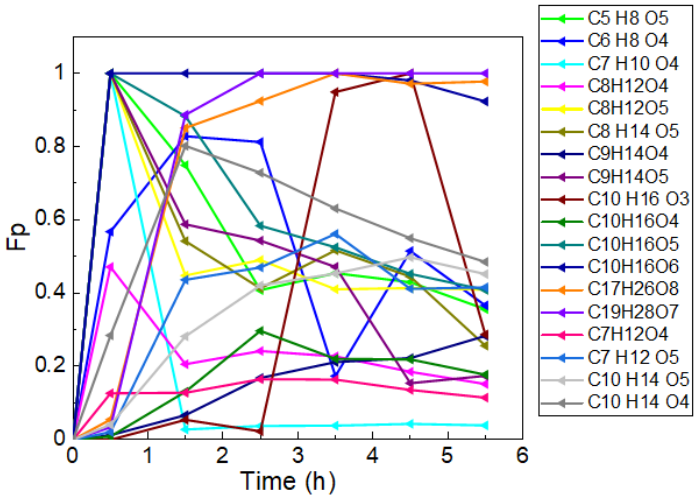
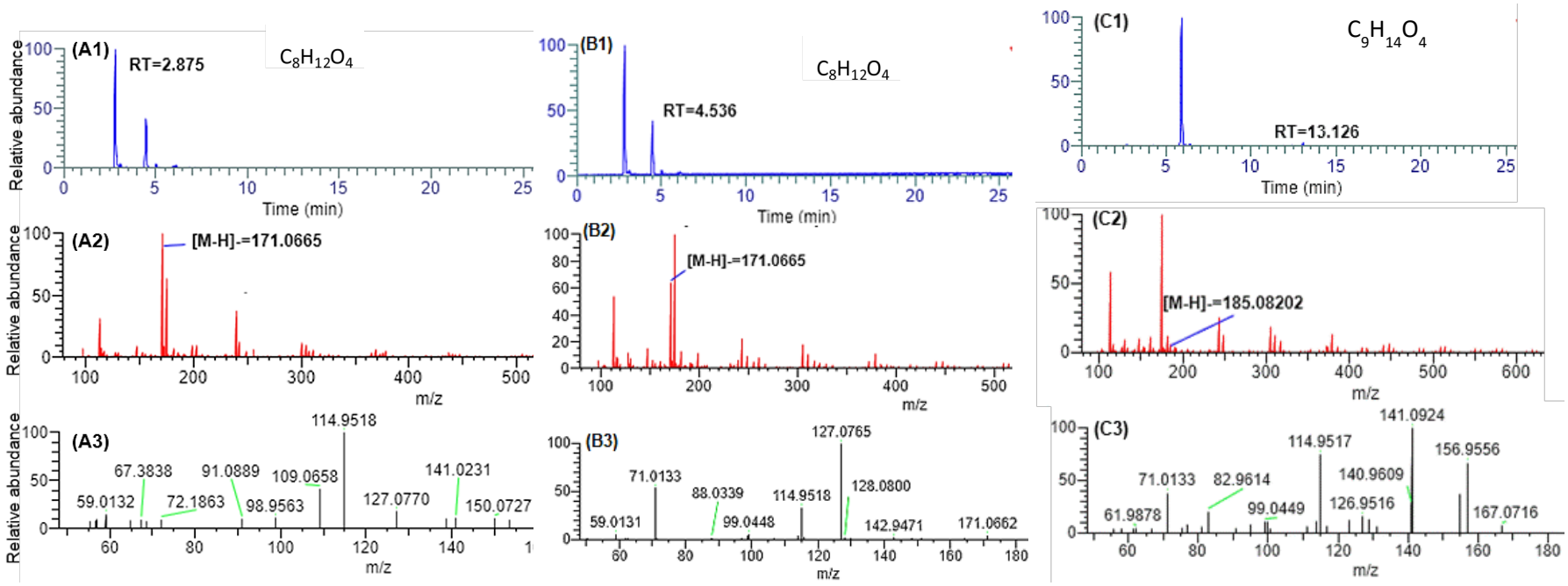
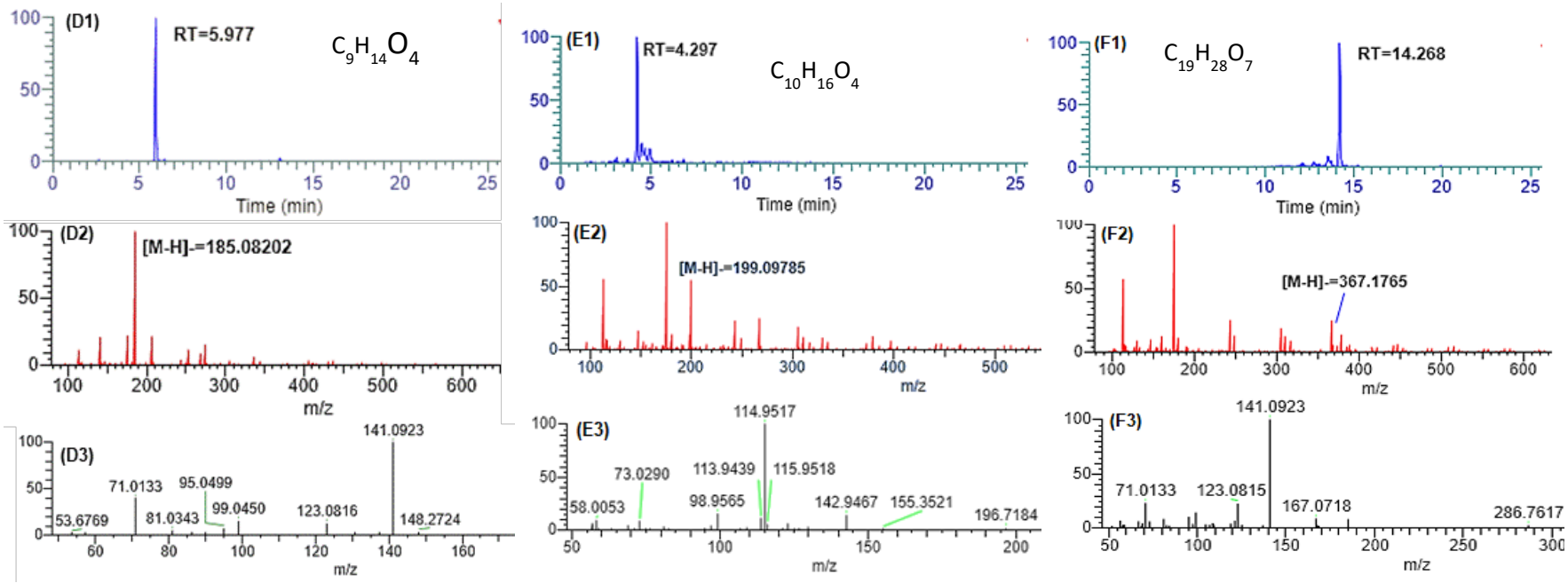
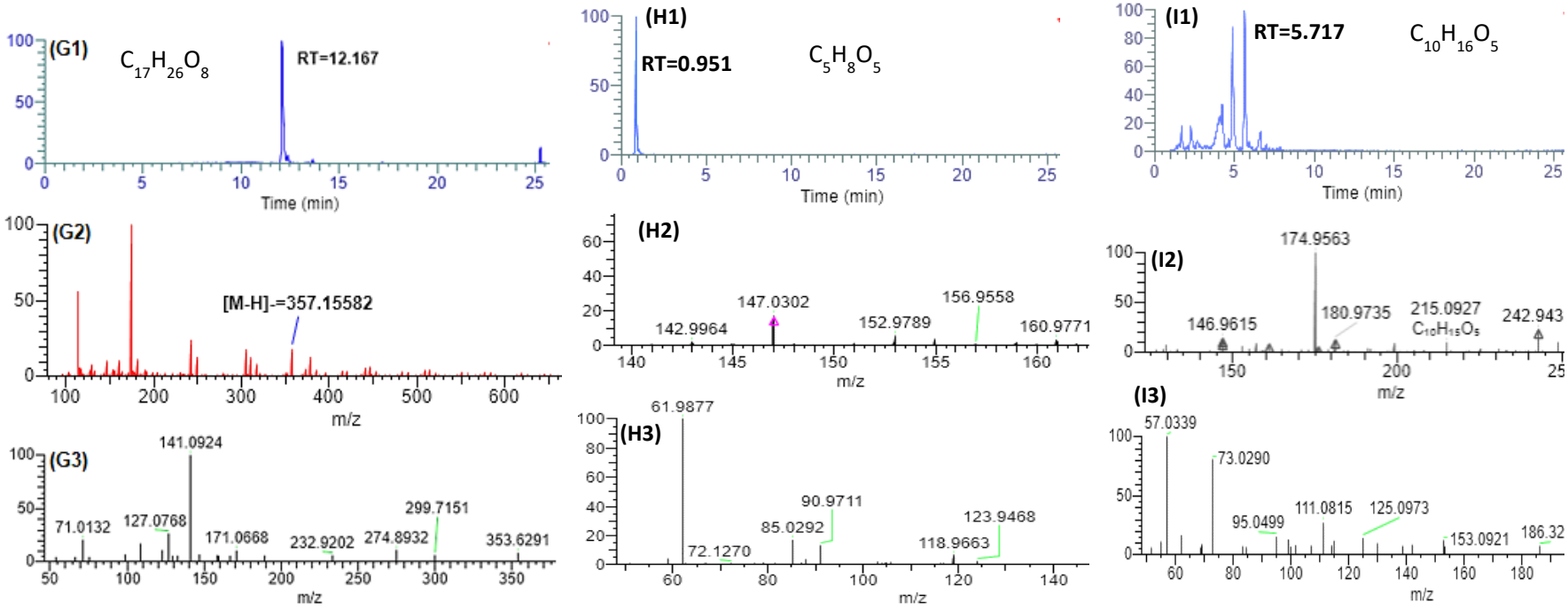
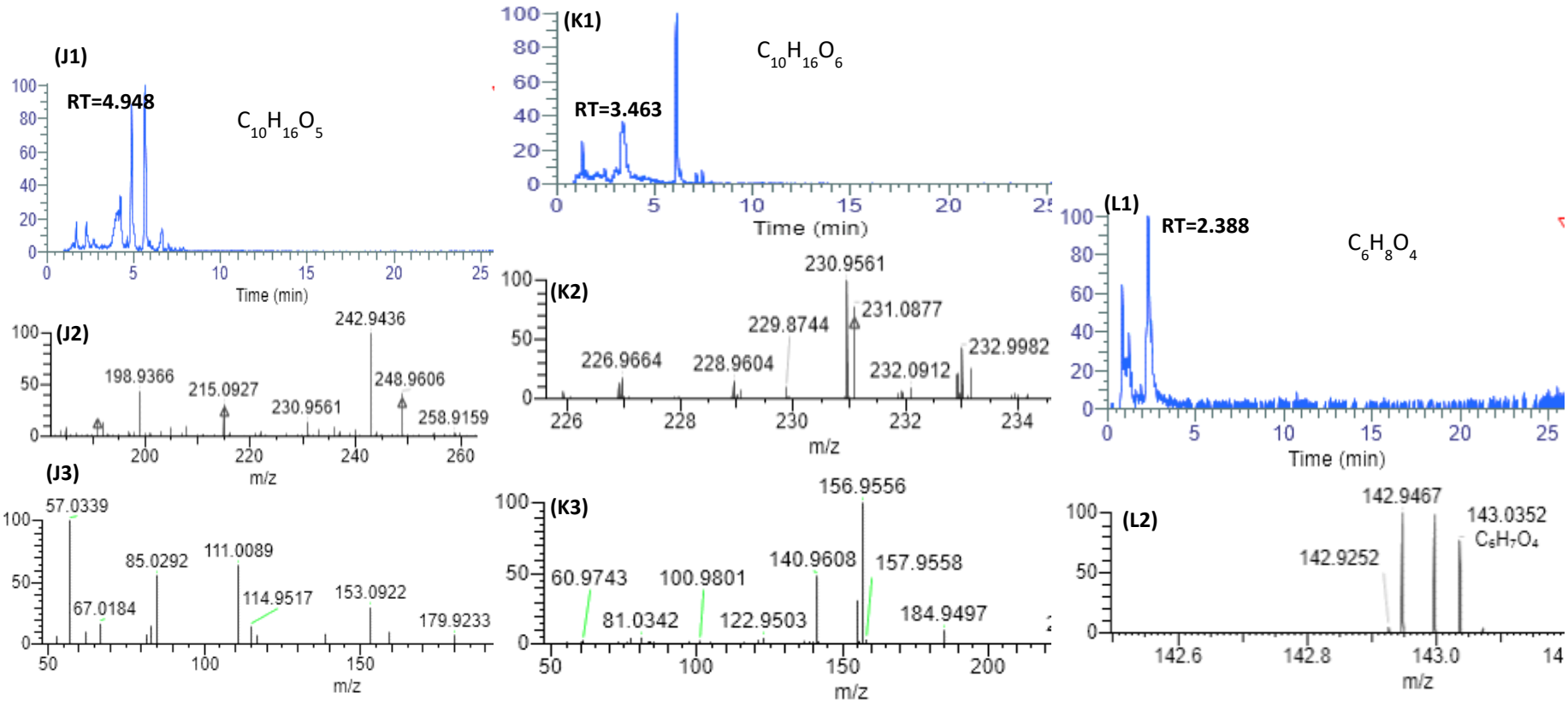


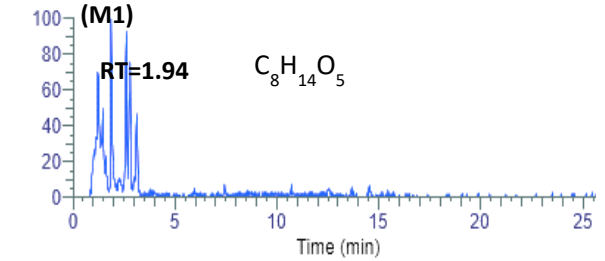
Figure S11. Temporal profiles of particle fractions for the selected identified organic molecules generated from α-pinene photooxidation reactions.

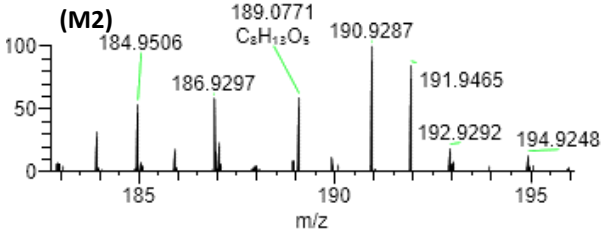

(A1)
RT=2.875
$C_8H_{12}O_4$
Relative abundance
Time (min)
(A2)
[M-H]-=171.0665
m/z
(A3)
114.9518
67.3838
91.0889
109.0658
141.0231
59.0132
72.1863
98.9563
127.0770
150.0727
(B1)
RT=4.536
$C_8H_{12}O_4$
(B2)
[M-H]-=171.0665
(B3)
127.0765
71.0133
88.0339
114.9518
128.0800
59.0131
99.0448
142.9471
171.0662
(C1)
RT=13.126
$C_9H_{14}O_4$
(C2)
[M-H]-=185.08202
(C3)
141.0924
114.9517
156.9556
71.0133
82.9614
140.9609
61.9878
99.0449
126.9516
167.0716

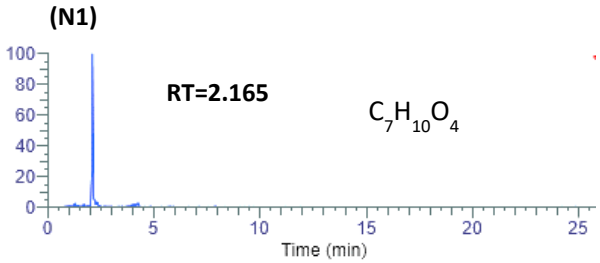

(D1)
RT=5.977
$C_9H_{14}O_4$
Time (min)
(D2)
[M-H]-=185.08202
m/z
(D3)
141.0923
71.0133
95.0499
81.0343
99.0450
123.0816
148.2724
53.6769
m/z
(E1)
RT=4.297
$C_{10}H_{16}O_4$
Time (min)
(E2)
[M-H]-=199.09785
m/z
(E3)
114.9517
73.0290
113.9439
115.9518
58.0053
98.9565
142.9467
155.3521
196.7184
m/z
(F1)
$C_{19}H_{28}O_7$
RT=14.268
Time (min)
(F2)
[M-H]-=367.1765
m/z
(F3)
141.0923
71.0133
123.0815
167.0718
286.7617
m/z

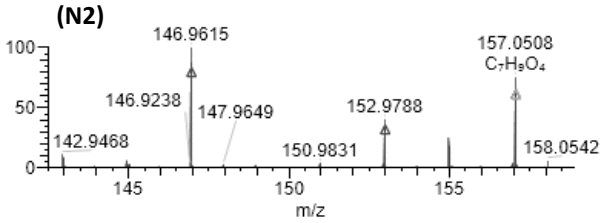

(G1)
$C_{17}H_{26}O_8$
RT=12.167
Time (min)
(G2)
[M-H]-=357.15582
m/z
(G3)
141.0924
71.0132
127.0768
171.0668
232.9202
274.8932
299.7151
353.6291
m/z
(H1)
RT=0.951
$C_5H_8O_5$
Time (min)
(H2)
142.9964
147.0302
152.9789
156.9558
160.9771
m/z
(H3)
61.9877
72.1270
85.0292
90.9711
118.9663
123.9468
m/z
(I1)
RT=5.717
$C_{10}H_{16}O_5$
Time (min)
(I2)
174.9563
146.9615
180.9735
215.0927
$C_{10}H_{15}O_5$
242.943
m/z
(I3)
57.0339
73.0290
95.0499
111.0815
125.0973
153.0921
186.32
m/z

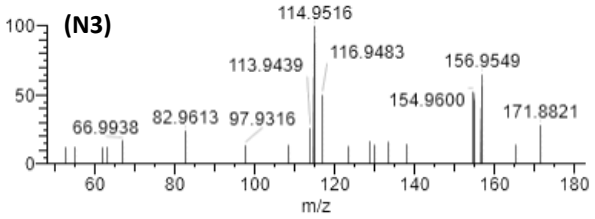

(J1)
RT=4.948
$C_{10}H_{16}O_5$
Time (min)
(J2)
242.9436
198.9366
215.0927
230.9561
248.9606
258.9159
m/z
(J3)
57.0339
85.0292
111.0089
67.0184
114.9517
153.0922
179.9233
m/z
(K1)
RT=3.463
$C_{10}H_{16}O_6$
Time (min)
(K2)
230.9561
231.0877
229.8744
226.9664
228.9604
232.0912
232.9982
m/z
(K3)
156.9556
140.9608
157.9558
60.9743
100.9801
184.9497
81.0342
122.9503
m/z
(L1)
RT=2.388
$C_6H_8O_4$
Time (min)
(L2)
142.9467
143.0352
$C_6H_7O_4$
142.9252
m/z

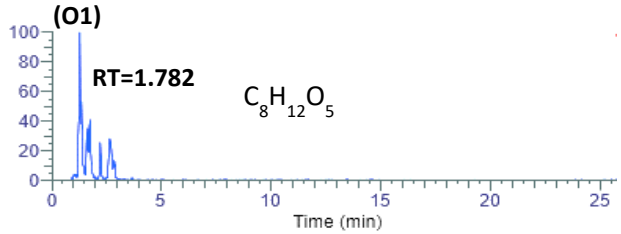

(M1)
RT=1.94
$C_8H_{14}O_5$
Time (min)

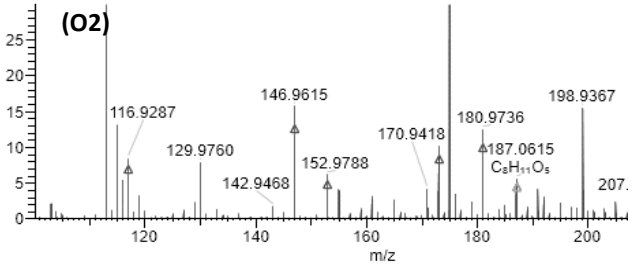

(M2)
184.9506
189.0771
$C_8H_{13}O_5$
190.9287
186.9297
191.9465
192.9292
194.9248
m/z

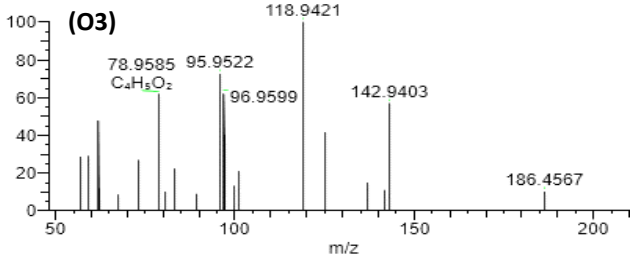

(N1)
RT=2.165
$C_7H_{10}O_4$
Time (min)

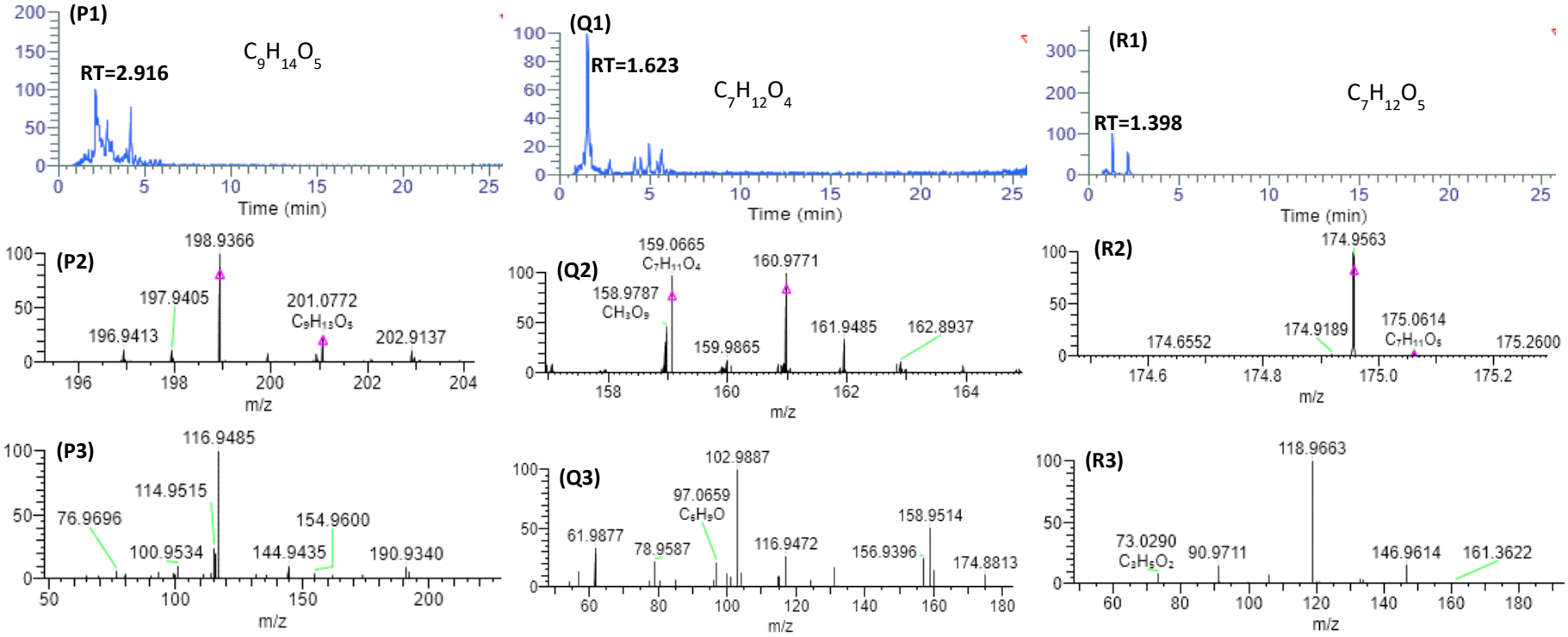

(N2)
146.9615
157.0508
$C_7H_9O_4$
146.9238
147.9649
152.9788
142.9468
150.9831
158.0542
m/z

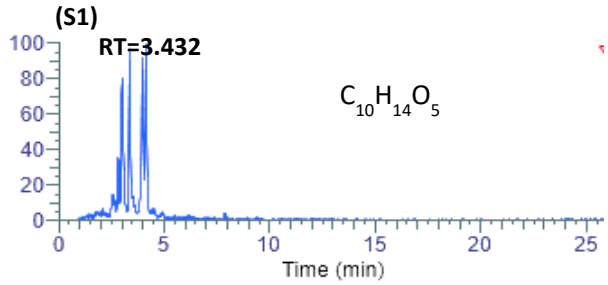

(N3)
114.9516
113.9439
116.9483
156.9549
154.9600
171.8821
66.9938
82.9613
97.9316
m/z

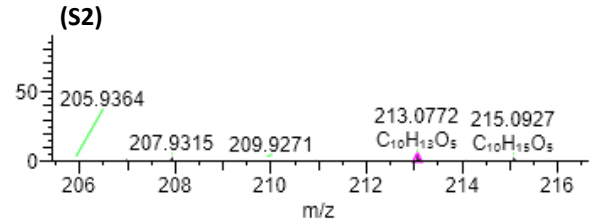

(O1)
RT=1.782
$C_8H_{12}O_5$
Time (min)

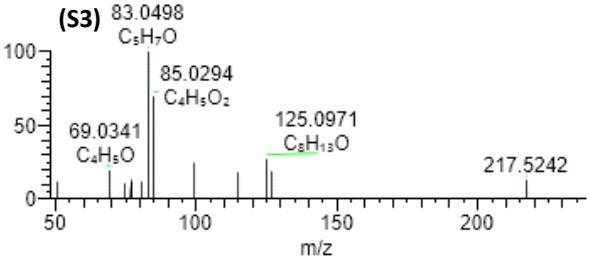

(O2)
116.9287
146.9615
198.9367
129.9760
170.9418
180.9736
152.9788
187.0615
$C_8H_{11}O_5$
142.9468
207.
m/z

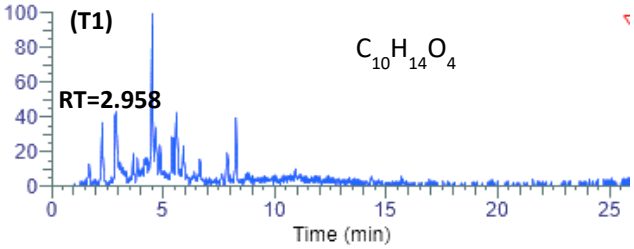

(O3)
118.9421
78.9585
$C_4H_5O_2$
95.9522
96.9599
142.9403
186.4567
m/z

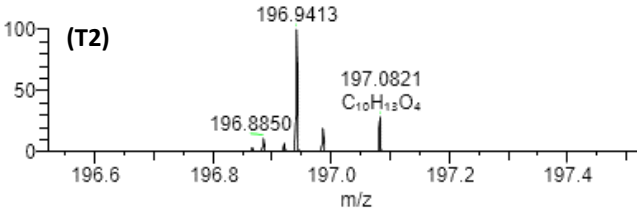

(P1)
$C_9H_{14}O_5$
RT=2.916
Time (min)
(Q1)
$C_7H_{12}O_4$
RT=1.623
Time (min)
(R1)
$C_7H_{12}O_5$
RT=1.398
Time (min)
(P2)
198.9366
197.9405
201.0772
$C_5H_{13}O_5$
196.9413
202.9137
m/z
(Q2)
159.0665
$C_7H_{11}O_4$
158.9787
CH_3O_9
160.9771
159.9865
161.9485
162.8937
m/z
(R2)
174.9563
174.6552
174.9189
175.0614
$C_7H_{11}O_5$
175.2600
m/z
(P3)
116.9485
114.9515
76.9696
154.9600
100.9534
144.9435
190.9340
m/z
(Q3)
102.9887
97.0659
C_6H_9O
61.9877
78.9587
116.9472
158.9514
156.9396
174.8813
m/z
(R3)
118.9663
73.0290
$C_3H_5O_2$
90.9711
146.9614
161.3622
m/z

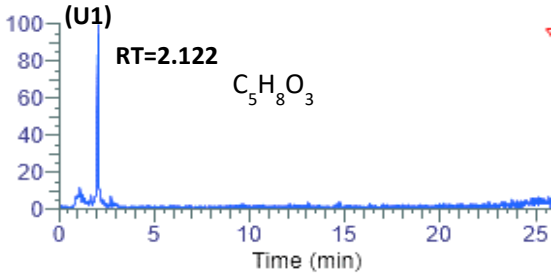

(S1)
RT=3.432
$C_{10}H_{14}O_5$
Time (min)

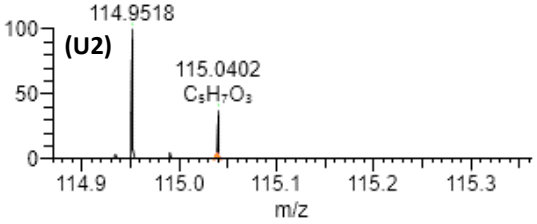

(S2)
205.9364
207.9315
209.9271
213.0772
$C_{10}H_{13}O_5$
215.0927
$C_{10}H_{15}O_5$
m/z

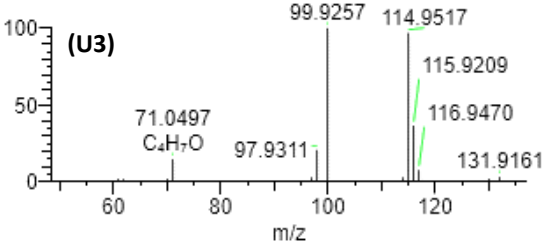

(S3)
83.0498
C_5H_7O
85.0294
$C_4H_5O_2$
69.0341
C_4H_5O
125.0971
$C_8H_{13}O$
217.5242
m/z


(T1)
$C_{10}H_{14}O_4$
RT=2.958
Time (min)


(T2)
196.9413
196.8850
197.0821
$C_{10}H_{13}O_4$
m/z


(U1)
RT=2.122
$C_5H_8O_3$
Time (min)


(U2)
114.9518
115.0402
$C_5H_7O_3$
m/z


(U3)
99.9257
114.9517
115.9209
116.9470
71.0497
C_4H_7O
97.9311
131.9161
m/z

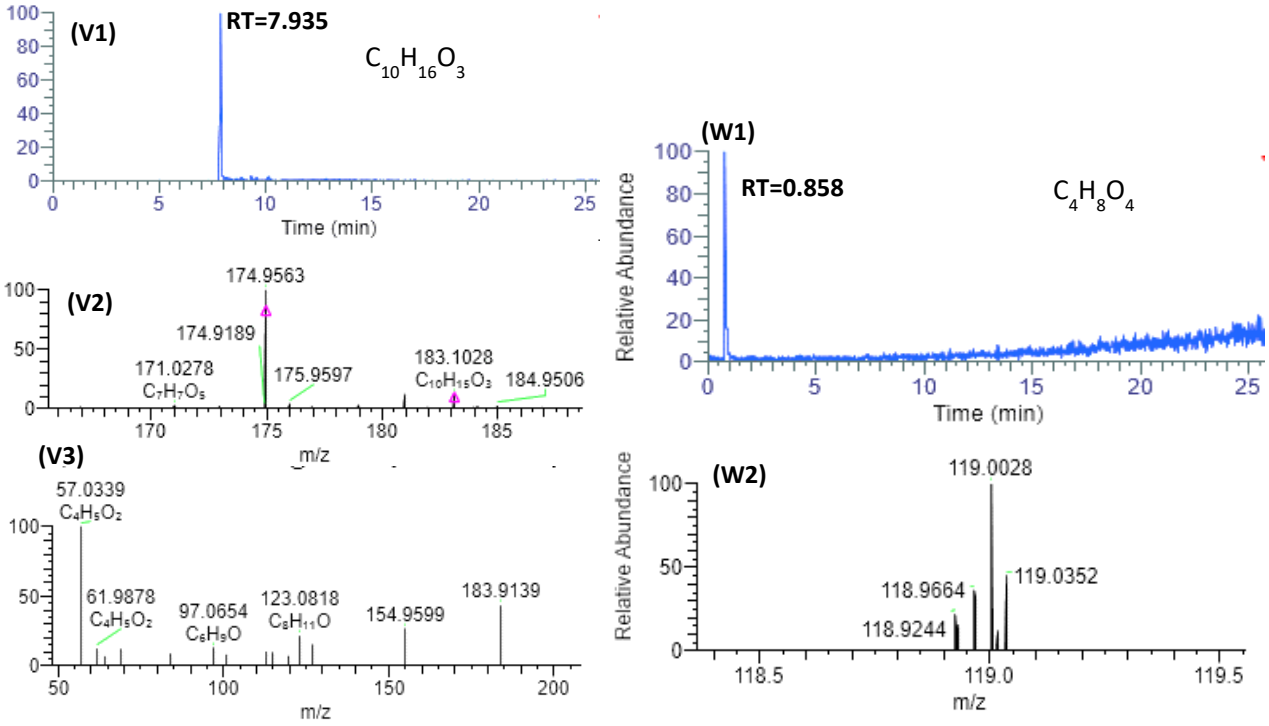


Figure S12 LC-MS chromatographs and mass spectrum of particle phase from a-pinene oxidation products. Subplot (A1-W1): the retention time from liquid chromatograph for each component; subplot (A2-W2): corresponding mass spectra for the peaks in A1-W1. Ions are detected in the negative mode by the loss 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.