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Supplement of

Chemical composition of secondary organic aerosol particles formed from mixtures of anthropogenic and biogenic precursors

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Section 1: Supplementary figures

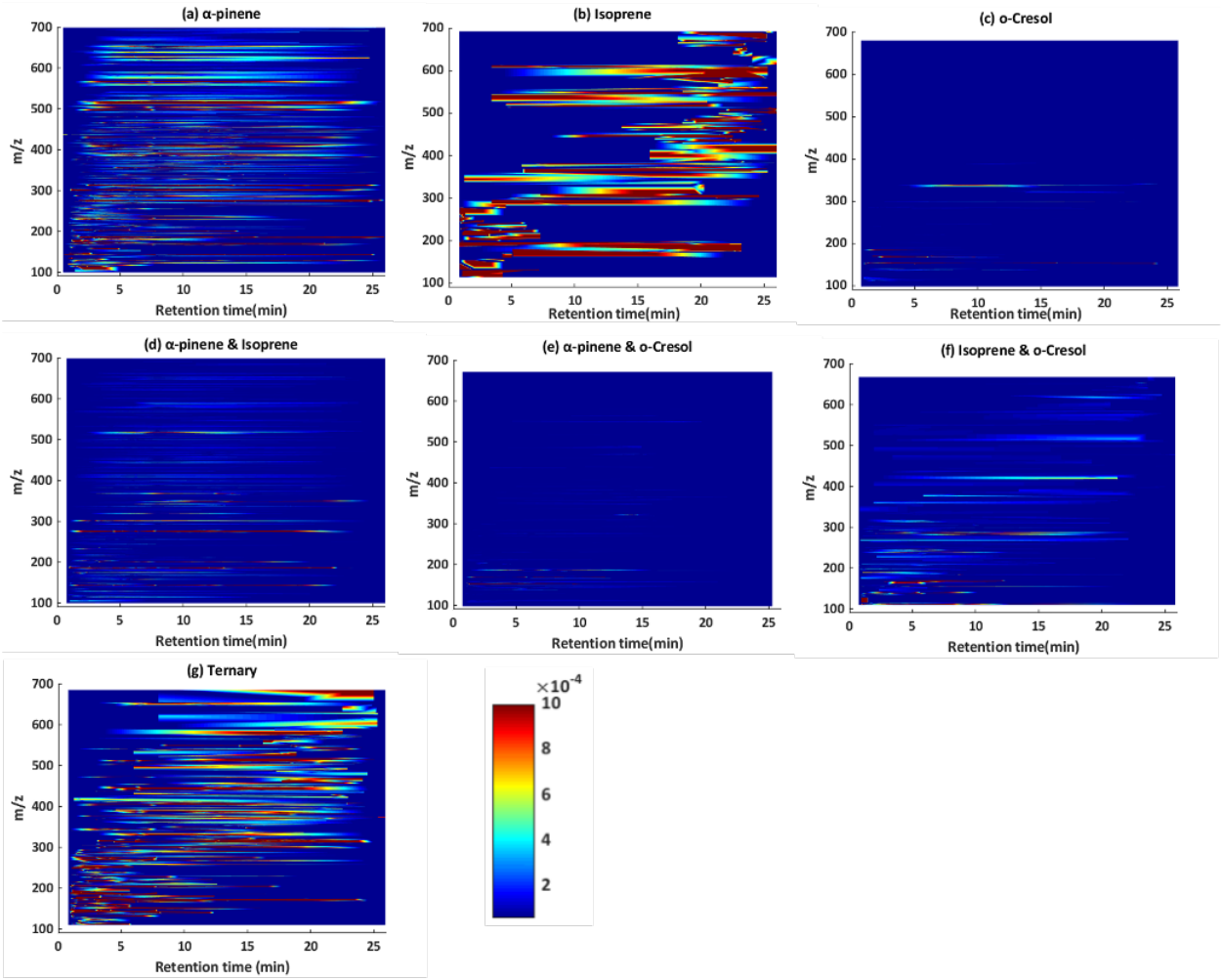

Figure S1: General Mass spectra m/z vs retention time with normalized signal intensity as colour) for compounds detected in Negative ionization mode for single and mixture experiment.

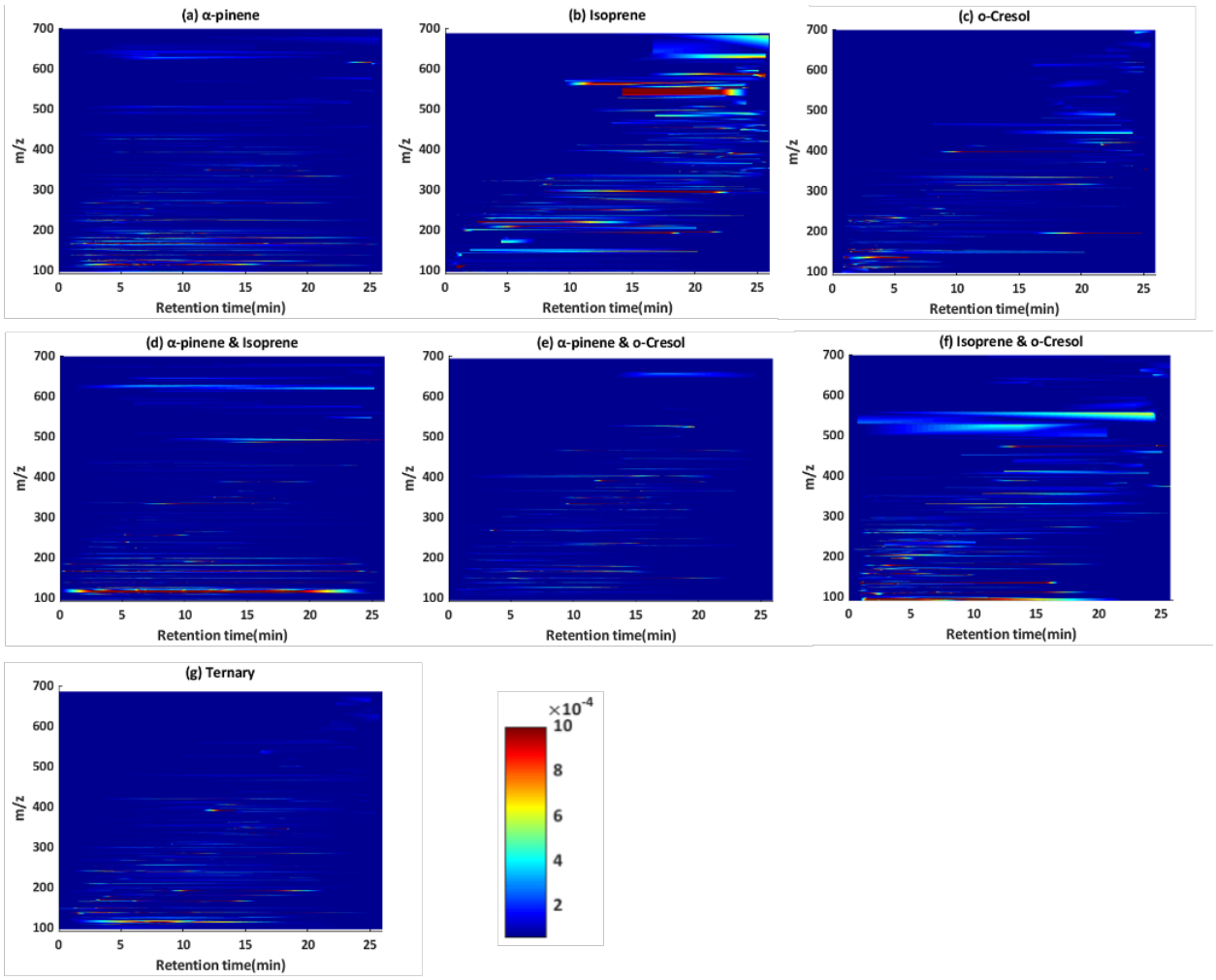

Figure S2: General Mass spectra m/z vs retention time with normalized signal intensity as colour) for compounds detected in Positive ionization mode for single and mixture experiment

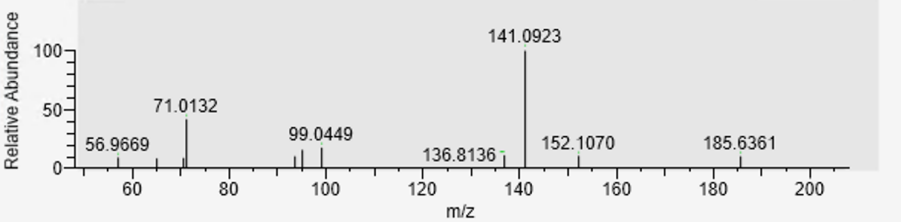

Figure S3:The fragmentation spectra for $C_9H_{14}O_4$ in binary α-pinene/isoprene system.

Section 2: Supplementary Tables

The product ions of deprotonated species of $C_7H_7NO_4$ and $C_7H_7NO_3$ in single o-cresol system, binary α-pinene/o-cresol and Isoprene/o-cresol system will be discussed here in order to illustrate the methodology to assign SOA compound structure. For all of the $C_7H_7NO_4$ isomer, the fragment ion at m/z 138 due to neutral loss of NO group by odd electron cleavage that often happen in ring structures with nitrogen containing group (Hayen et al., 2002; Fu et al., 2006; Pereira et al., 2015). $C_7H_7NO_4$ (i) and (III) also has the combine loss of NO and hydrogen radical (m/z=137), while the 109 m/z fragment corresponding to the combined loss of NO and CO from the deprotonated $C_7H_7NO_4$. For the $C_7H_7NO_3$ compound, the fragment ion m/z=122 has formed as a result of loss of NO from m/z 152, the loss of combined NO and hydrogen radicals resulting forming the 121m/z fragment and the combined loss of CH and NO leading to formation of 109 m/z fragment. These fragmentation ions of deprotonated molecules suggested that the $C_7H_7NO_4$ are the methyl-nitrocatechol and the $C_7H_7NO_3$ is methyl-nitrophenol(Kitanovski et al., 2012).

Table S1: Deprotonated molecular species for $C_7H_7NO_4$ isomers and $C_7H_7NO_3$, obtained from the use of the Orbitrap_LCMS in binary α-pinene/o-cresol and Isoprene/o-cresol system respectively.

Precursors System	Formula	Retention Time (min)	$[M-H]^-$	Fragment ion [m/z]	Loss [Da]	Suspected Fragment ion MF
o-cresol	$C_7H_7NO_4$ (i)	4.46	168	166	2	$C_7H_5NO_4$
				138	30	$C_7H_6O_3$
				122	46	$C_7H_6O_2$
				108	60	$C_6H_4O_2$
	$C_7H_7NO_4$ (ii)	7.40	168	138	30	$C_7H_6O_3$
				137	31	$C_7H_5O_3$
				122	46	$C_7H_6O_2$
				109	59	$C_6H_5O_2$
	$C_7H_7NO_4$ (iii)	8.93	168	138	30	$C_7H_6O_3$
				137	31	$C_7H_5O_3$
				109	59	$C_6H_5O_2$
α-pinene/o-cresol	$C_7H_7NO_4$ (i)	4.52	168	166	2	$C_7H_5NO_4$
				138	30	$C_7H_6O_3$
				108	60	$C_6H_4O_2$
	$C_7H_7NO_4$ (ii)	7.53	168	138	30	$C_7H_6O_3$
				137	31	$C_7H_5O_3$
				109	59	$C_6H_5O_2$
	$C_7H_7NO_4$ (iii)	9.08	168	138	30	$C_7H_6O_3$
				137	31	$C_7H_5O_3$
				109	59	$C_6H_5O_2$
	$C_7H_7NO_3$	10.19	152	122	30	$C_7H_6O_2$
				121	31	$C_7H_5O_2$
				109	43	$C_6H_5O_2$
Isoprene/o-cresol	$C_7H_7NO_4$ (i)	4.52	168	166	2	$C_7H_5NO_4$
				138	30	$C_7H_6O_3$
				137	31	$C_7H_5O_3$
				108	60	$C_6H_4O_2$
	$C_7H_7NO_4$ (ii)	7.53	168	138	30	$C_7H_6O_3$
				137	31	$C_7H_5O_3$
				109	59	$C_6H_5O_2$
	$C_7H_7NO_4$ (iii)	9.14	168	138	30	$C_7H_6O_3$
				137	31	$C_7H_5O_3$
				109	59	$C_6H_5O_2$
	C7H7NO3	10.20	152	122	30	$C_7H_6O_2$
				121	31	$C_7H_5O_2$
				109	43	$C_6H_5O_2$

Table S2: The total normalized peak area and normalized mass concentration attributed to nC>21 molecules that were found in all repeat experiments in selected system. The normalized peak area of nC>21 molecules obtained from the both ionization mode in orbitrap-LCMS, and the particulate mass concentration of each system obtained from HR-TOF-AMS measurement. The normalized mass concentration equals the particulate mass concentration multiply the normalized peak area of nC>21 molecules.

		Negative ionization mode		**Positive ionization mode**	
	Particulate mass concentration at the end of experiment(ug/m^3)	Normalized Peak Area of nC >21 molecules	Normalized mass concentration of nC >21 molecules(ug/m^3)	Normalized Peak Area of nC >21 molecules	Normalized mass concentration of nC >21 molecules(ug/m^3)
a) α-pinene	361	0.008	3.01	0.003	1.34
b) Isoprene	0.4	0.007	0.002	0.040	0.016
d) α-pinene/isoprene	102	0.011	1.15	0.002	0.24
e) α-pinene/o-cresol	150	0.004	0.73	0.019	2.85
f) Isoprene/o-cresol	22	0.0006	0.013	0.006	0.14
g) Ternary	85	0.002	0.16	0.012	1.10

Reference:

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