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Supplement of

Aerosol mass yields of selected biogenic volatile organic compounds – a theoretical study with nearly explicit gas-phase chemistry

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1 Supplement material

2 **Table 1s(a)**. List of compounds contributing to > 95% of SOA mass yield for α -pinene ozonolysis
 3 at 258K. The names of compounds are given in MCM format. The PRAM compounds are
 4 highlighted in red.

Molecular Weight (g/mol)	Species name	Contribution (%)
430	C20H30O10	0.16
198	C10H14O4	0.17
462	C20H30O12	0.18
214	C10H14O5	0.18
174.19	C810OOH	0.19
178.14	C621OOH	0.19
277	C10H15O8N1	0.19
130.1	H1C23C4CHO	0.2
341	C10H15O12N1	0.21
203.19	C810NO3	0.22
446	C20H30O11	0.22
293	C10H15O9N1	0.24
309	C10H15O10N1	0.24
312	C10H16O11	0.24
206.19	C813OOH	0.25
190.19	C812OOH	0.26
170.21	C89CO2H	0.28
174.19	C811OOH	0.29
188.22	C920OOH	0.29
220.22	C922OOH	0.3
204.22	C921OOH	0.3
310	C10H14O11	0.32
325	C10H15O11N1	0.33
235.19	C813NO3	0.36
294	C10H14O10	0.52
230	C10H14O6	0.55
203.19	C811NO3	0.56
296	C10H16O10	0.58
262	C10H14O8	0.65
280	C10H16O9	0.84
246	C10H14O7	0.88
278	C10H14O9	0.93
264	C10H16O8	1.11
248	C10H16O7	1.12
232	C10H16O6	1.13

216	C10H16O5	1.23
172.22	C96OOH	1.32
200	C10H16O4	1.39
162.14	C614OOH	1.64
191.14	C614NO3	2.49
204.22	C98OOH	2.88
188.22	C97OOH	3.07
174.15	C717OOH	3.43
184.23	PINONIC	4.4
233.22	C98NO3	4.53
200.23	C109OOH	4.75
216.23	C108OOH	5.67
200.23	C107OOH	5.94
245.23	C108NO3	8.97
261.23	C920PAN	9.35
247.2	C811PAN	10.11
203.15	C717NO3	11.29

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7 **Table 1s(b)**. List of compounds contributing to > 95% of SOA mass yield for α -pinene ozonolysis
8 at 293K. The names of compounds are given in MCM format.

Molecular Weight (g/mol)	Species names	Contribution (%)
496	C19H28O15	0.45
174.15	C717OOH	0.53
344	C10H16O13	0.57
446	C20H30O11	0.59
448	C19H28O12	0.62
248	C10H16O7	0.67
200.23	HOPINONIC	0.7
462	C20H30O12	0.7
480	C19H28O14	0.76
186.21	PINIC	0.77
188.22	C920OOH	0.79
510	C20H30O15	0.79
325	C10H15O11N1	0.8
464	C19H28O13	0.82
373	C10H15O14N1	0.9
178.14	C621OOH	1.03
478	C20H30O13	1.1
246	C10H14O7	1.17

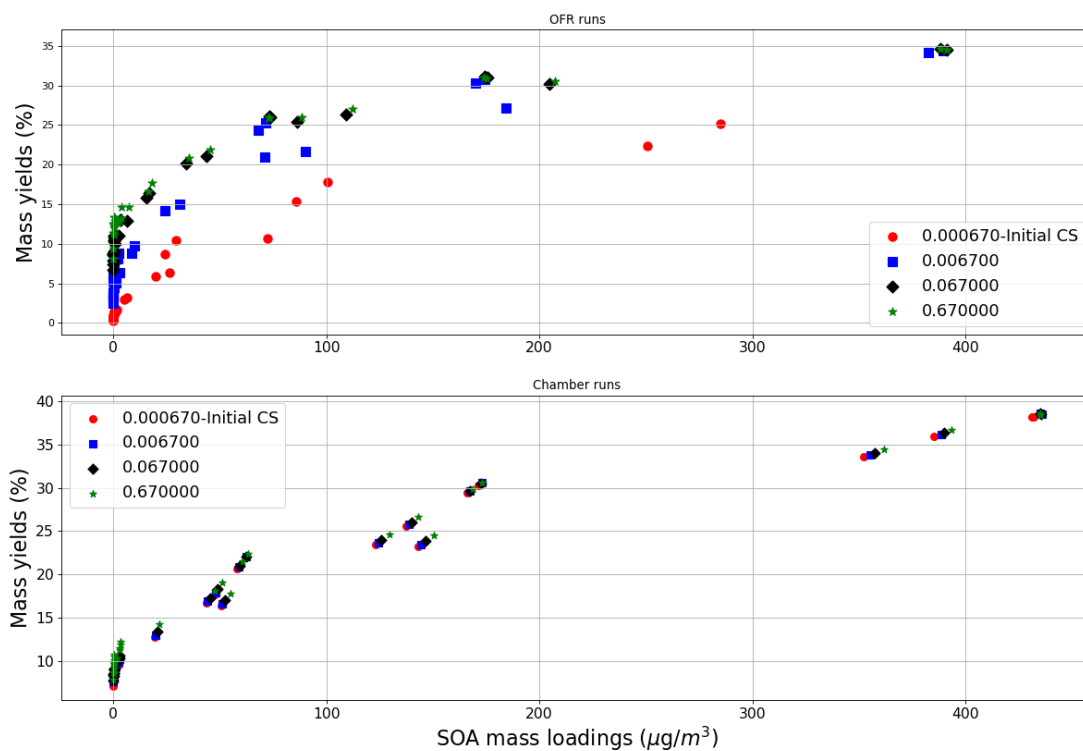
341	C10H15O12N1	1.2
262	C10H14O8	1.26
174.19	C811OOH	1.35
494	C20H30O14	1.39
164.11	C516OOH	1.44
245.23	C108NO3	1.49
162.14	C614OOH	1.6
220.22	C922OOH	1.64
200	C10H16O4	1.65
204.22	C921OOH	1.68
357	C10H15O13N1	1.93
264	C10H16O8	1.97
328	C10H16O12	2.2
280	C10H16O9	2.35
326	C10H14O12	2.41
206.19	C813OOH	2.64
190.19	C812OOH	2.73
312	C10H16O11	2.77
278	C10H14O9	2.86
188.22	C97OOH	3.03
235.19	C813NO3	3.1
296	C10H16O10	3.19
294	C10H14O10	3.63
233.22	C98NO3	3.81
261.23	C920PAN	4.1
247.2	C811PAN	4.57
310	C10H14O11	6.19
216.23	C108OOH	6.24
204.22	C98OOH	7.44

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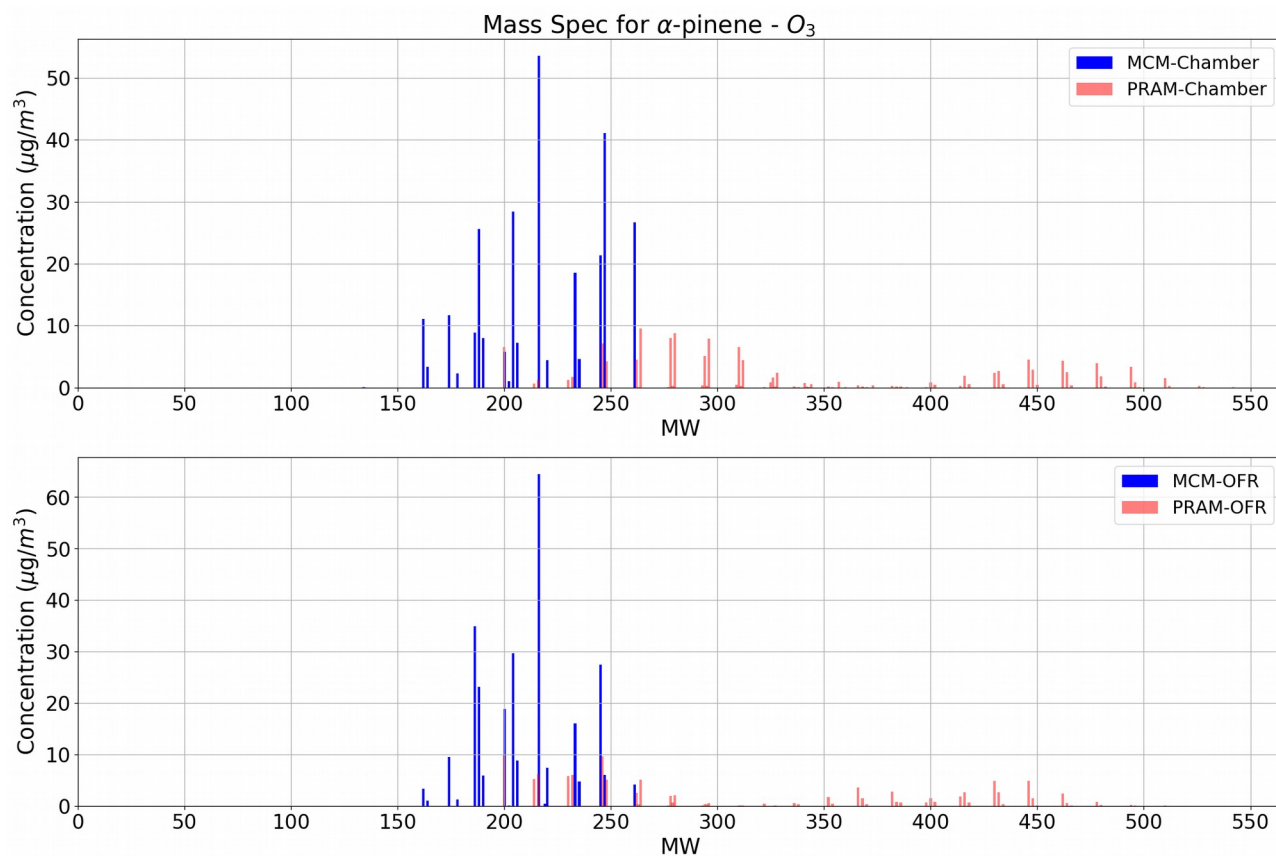
10 **Table 1s(c)**. List of compounds contributing to > 95% of SOA mass yield for α -pinene ozonolysis
 11 at 313K. The names of compounds are given in MCM format.

Molecular Weight (g/mol)	Species names	Contribution (%)
526	C20H30O16	0.54
512	C19H28O16	0.55
450	C18H26O13	0.56
482	C18H26O15	0.6
280	C10H16O9	0.6
294	C10H14O10	0.7
466	C18H26O14	0.79

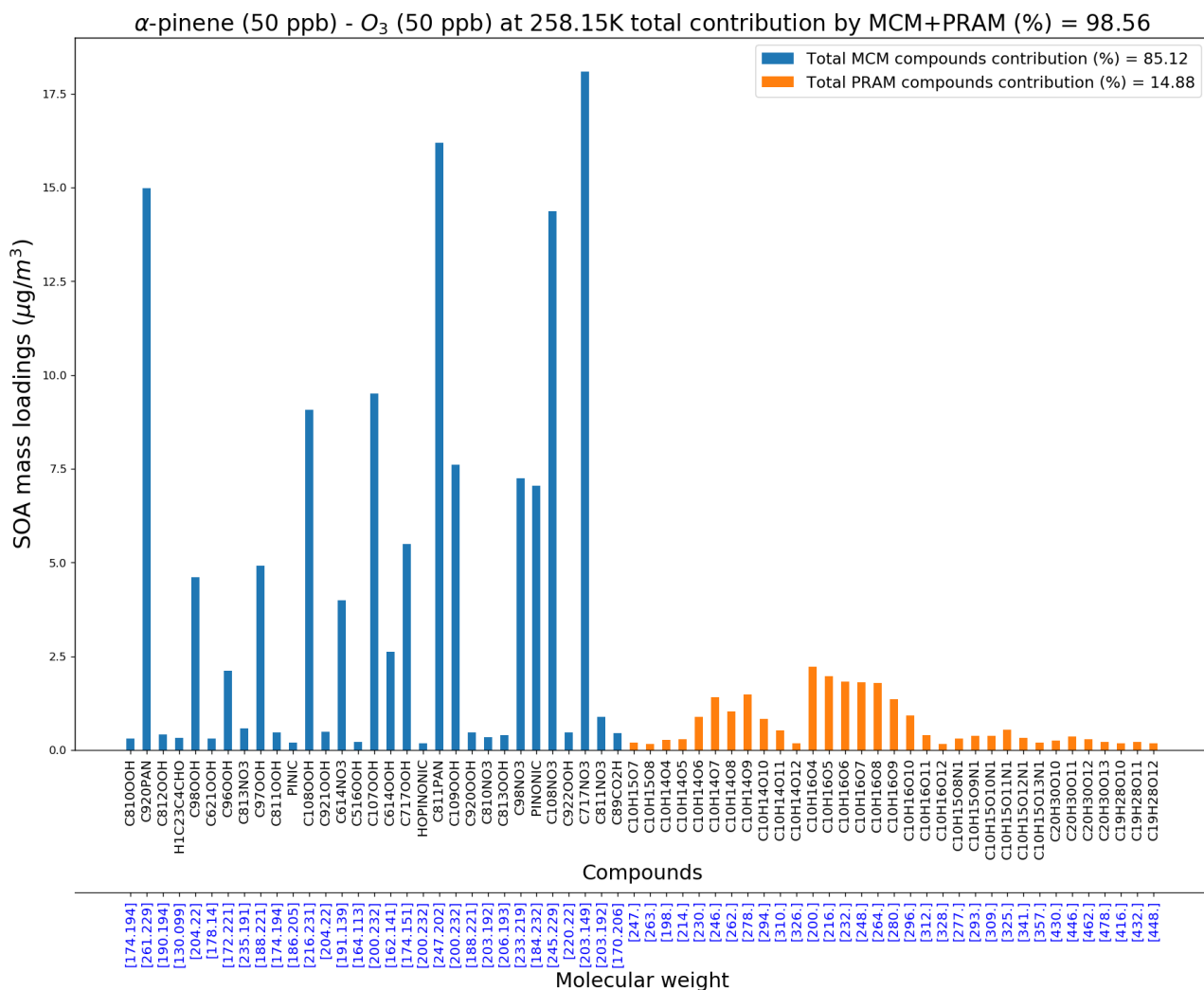
296	C10H16O10	0.9
278	C10H14O9	1
464	C19H28O13	1.2
204.22	C98OOH	1.42
344	C10H16O13	1.51
496	C19H28O15	1.65
480	C19H28O14	1.77
178.14	C621OOH	1.93
373	C10H15O14N1	1.95
510	C20H30O15	2.57
204.22	C921OOH	3.03
494	C20H30O14	3.15
220.22	C922OOH	3.26
164.11	C516OOH	3.85
357	C10H15O13N1	4.63
312	C10H16O11	5.62
326	C10H14O12	6.04
328	C10H16O12	6.56
235.19	C813NO3	6.83
190.19	C812OOH	6.95
206.19	C813OOH	7.46
310	C10H14O11	18.28

α -pinene - O_3 - CS dependence

13 **Figure S1.** SOA mass yields for α -pinene oxidation using O_3 for different CS values. For the OFR runs the yields level
 14 off above a CS value of 0.067 s^{-1} , while chamber simulation show negligible variation with CS. Hence 0.067 s^{-1} is
 15 selected as CS for the OFR simulations while chamber simulations are run with 0.00067 s^{-1} .



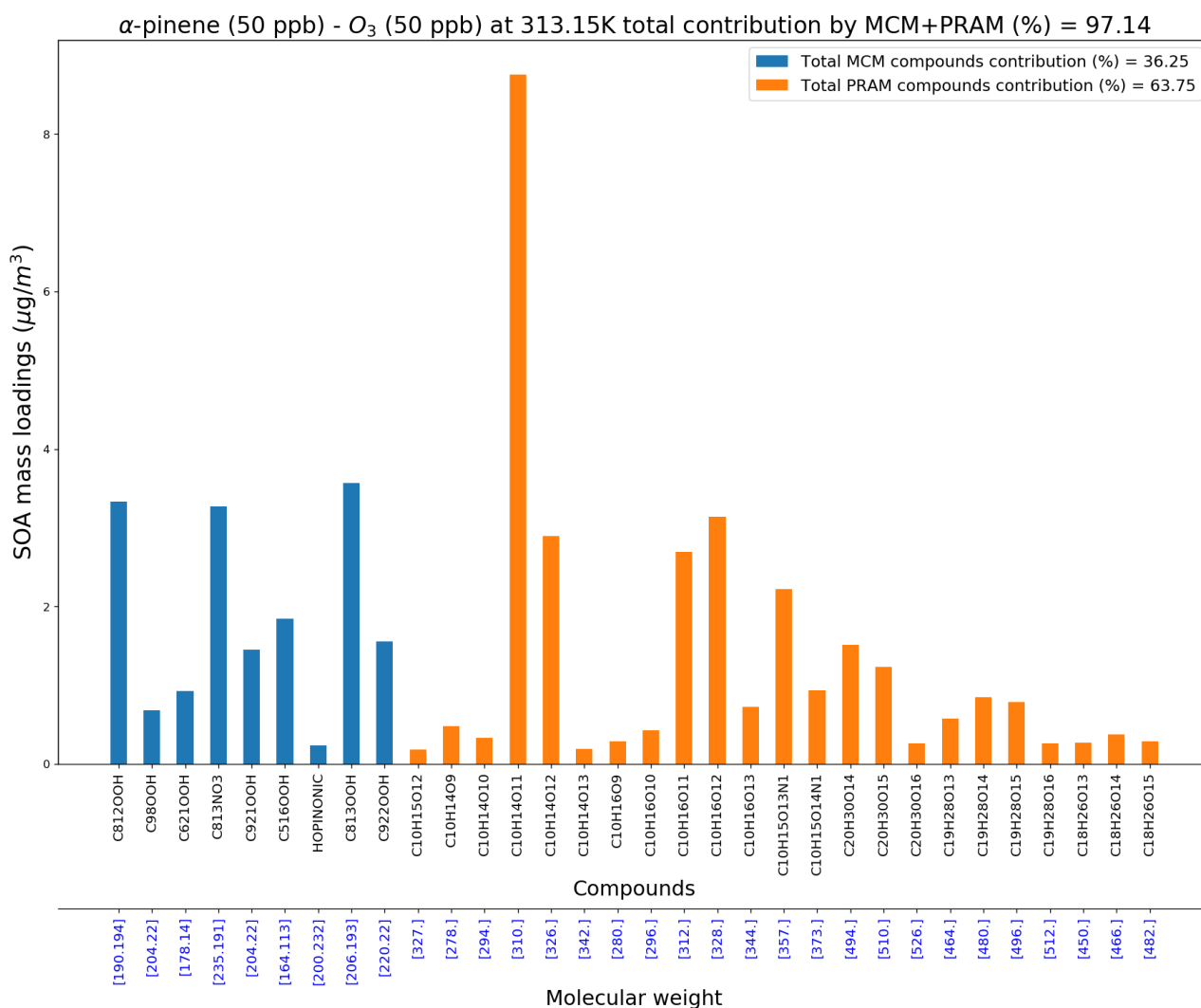
17 **Figure S2.** Mass spectra of SOA formed from α -pinene ozonolysis in the particle phase. The upper panel indicates
18 spectra from chamber simulations while the lower panel represents the spectra from OFR simulations.



20 **Figure S3(a).** MCM and PRAM compounds contributing to > 95% of SOA mass at 258 K and 50ppb O₃ and α -pinene
 21 concentrations. It can be noted that a large fraction of the PRAM species that contribute to the SOA mass at 258 K are
 22 not classified as HOM (i.e. contain at least 6 oxygen atoms), and many of them will not be detected in the gas-phase
 23 using the present state-of-the-art Chemical Ionization-Atmospheric Pressure Interface TOF (CI-APi-TOF) technique.

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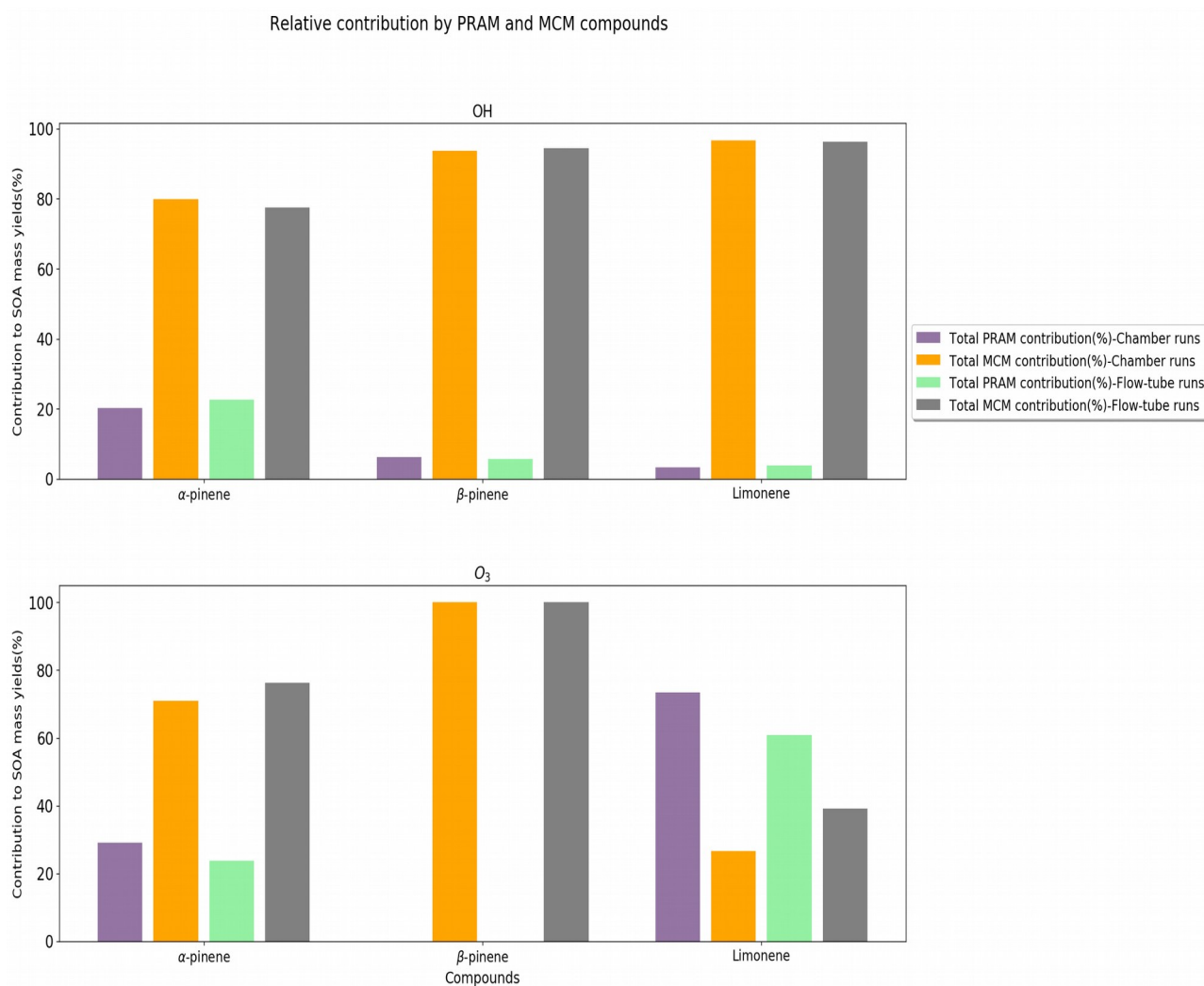


27 **Figure S3(b)**. MCM and PRAM compounds contributing to > 95% of SOA mass at 313.15 K and 50ppb O₃ and α -
 28 pinene concentrations.

29 The importance of using the MCM+PRAM scheme is illustrated in Fig. S4 which shows the relative
 30 contribution by PRAM and MCM compounds for the oxidation of α -pinene, β -pinene and
 31 limonene by OH (upper panel) and O₃ (lower panel) for their respective maximum SOA mass yields
 32 for both chamber and flow tube setup simulations. The present PRAM mechanism does not include
 33 the peroxy radical autooxidation products from β -pinene ozonolysis, products from oxidation of
 34 isoprene and β -caryophyllene and the products from NO₃ oxidation of BVOCs. Therefore, they are
 35 excluded from Fig. S4.

36 The impact of PRAM compounds contribution to limonene ozonolysis, irrespective of chamber or
 37 flow tube setup is considered. It is evident from Fig. S4 (lower panel), which shows that upon using
 38 the standalone MCM mechanism underpredicts the SOA mass yields with PRAM compounds

39 contributing ~ 80% and 60% respectively. For α -pinene ozonolysis, the standalone MCM scheme
 40 under-predicts the modelled mass yields by approximately 25 % and 22.5 % respectively.



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42 **Figure S4.** Relative contribution of HOM and MCM compounds for selected maximum mass yields of α -pinene, β -
 43 pinene and limonene oxidation by OH (upper panel) and O_3 (lower panel) at 293.15 K.

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45 **Summary of experimental data used for comparison**

46 Kristensen et al., (2017) investigated α -pinene ozonolysis SOA mass yields at temperatures of 258
 47 and 293 K. Additionally SOA mass yields from OH oxidation of α -pinene were also investigated.

48 Yields for α -pinene at higher temperatures of 313 K were investigated by Pathak et al., (2007),
 49 wherein they performed experiments using ammonium sulfate seed particles. Shilling et al.,

50 (2008) performed experiments for lower concentrations of α -pinene ozonolysis combinations and

51 hence used to compare yields for loading's $< 10 \mu\text{g m}^{-3}$. Griffin et al., (1999) used smog chambers

52 to investigate the aerosol forming potential of various BVOCs such as β -pinene by ozonolysis and
53 β -caryophyllene by OH oxidation. The SOA mass yields derived from the OH oxidation of
54 isoprene, β -caryophyllene and β -pinene were experimented by Lee et al., (2006b).

55 The SOA mass yields derived from the ozonolysis of α -pinene and limonene using an OFR were
56 compared with the experimental yield from Kang and Root, (2007). The experiments also provided
57 estimates on SOA mass yields underestimation when performed with/without acidic seed particles
58 in the OFR. Yields simulated from the OH oxidation of α -pinene were compared against yields
59 measured by (Bruns et al., 2015) as they had used similar initial BVOC and oxidant concentrations.
60 The simulated yields were also compared with experimental yields from Friedman and Farmer,
61 (2018) due to similar initial oxidant concentrations used.