Large differences of highly oxygenated organic molecules (HOMs) and low volatile species in SOA formed from ozonolysis of β-pinene and limonene

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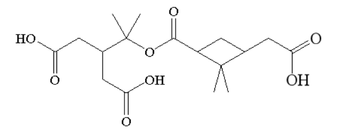
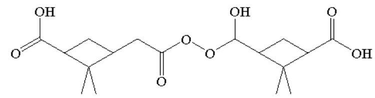
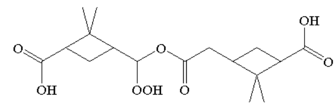
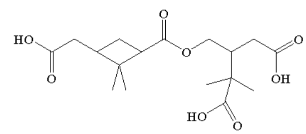
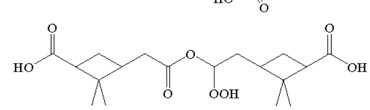
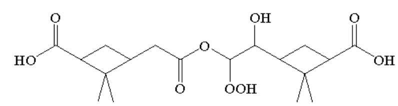
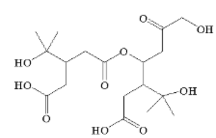
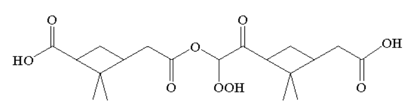
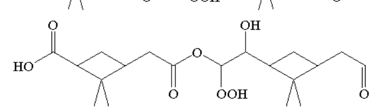
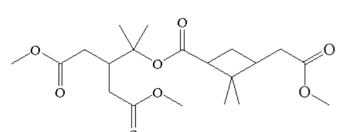
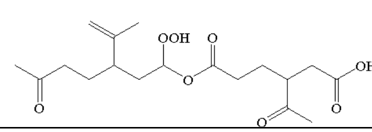
Table S1. The experimental conditions, the collected SOA particles quality of β-pinene and limonene SOA.

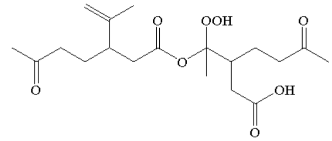
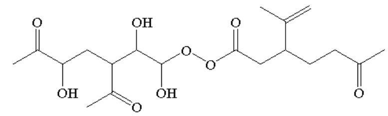
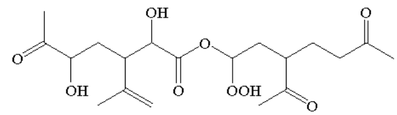
Precursor	Run no.	O_3	$[O_3]$ / ppb	Collection time / h		SOA collected / μg	
				T_1	T_2	m_1	m_2
β-Pinene 1~2 ppm	1	Low O_3	50	0.4	0.4	70	60
	2	Median O_3	315	0.6	0.5	130	110
	3	High O_3	565	0.6	0.8	190	220
Limonene 1~2 ppm	1	Low O_3	50	1.0	1.9	30	30
	2	Median O_3	315	1.2	1.1	220	150
	3	High O_3	565	0.6	1.0	130	230

Table S2. Summary of the top fifteen molecules in relative abundance in SOA particles produced by ozonolysis of β-pinene and limonene at three ozone concentrations. PSOA and LSOA correspond to β-pinene SOA and limonene SOA, respectively. Among them, 50, 315, and 565 represent three ppb levels of the ozone concentration.

	Molecular formula	Molecular weight	Relative abundance (%)					
			PSOA-50O_3	PSOA-315O_3	PSOA-565O_3	LSOA-50O_3	LSOA-315O_3	LSOA-565O_3
Monomer	$C_8H_{12}O_4$	172	3	18	17	5	2	2
	$C_9H_{18}O_2$	158	11	7	1	15	<0.5	<0.5
	$C_9H_{16}O_3$	172	7	48	21	11	1	1
	$C_9H_{14}O_3$	170	19	39	17	53	41	55
	$C_9H_{14}O_4$	186	10	78	57	37	29	22
	$C_{10}H_{16}O_2$	168	9	3	<0.5	14	<0.5	<0.5
	$C_{10}H_{16}O_3$	184	86	95	35	88	52	66
	$C_{10}H_{16}O_4$	200	9	32	19	100	100	100
Dimer	$C_{17}H_{26}O_3$	278	2	1	<0.5	42	2	2
	$C_{17}H_{26}O_4$	294	100	44	8	13	1	2
	$C_{17}H_{26}O_7$	342	4	28	17	20	22	15
	$C_{17}H_{26}O_8$	358	2	21	43	10	15	12
	$C_{18}H_{22}O_4$	302	4	2	1	1	<0.5	<0.5
	$C_{18}H_{26}O_5$	322	2	25	10	5	2	2
	$C_{18}H_{28}O_6$	340	2	34	31	19	16	15
	$C_{18}H_{28}O_7$	356	1	10	15	27	26	22
	$C_{18}H_{30}O_7$	358	1	31	25	7	6	6
	$C_{18}H_{26}O_8$	370	<0.5	1	0	13	19	13
	$C_{18}H_{28}O_8$	372	1	3	5	25	25	19
	$C_{18}H_{30}O_9$	390	2	18	14	3	4	3
	$C_{19}H_{28}O_4$	320	9	12	2	17	7	6
	$C_{19}H_{32}O_4$	324	5	3	1	5	1	<0.5
	$C_{19}H_{30}O_5$	338	3	100	100	74	73	69
	$C_{19}H_{28}O_6$	352	1	15	14	51	36	32
	$C_{19}H_{30}O_6$	354	2	39	32	48	36	28
	$C_{19}H_{28}O_7$	368	<0.5	5	7	48	62	47
	$C_{19}H_{30}O_7$	370	4	78	52	85	35	27
	$C_{19}H_{28}O_8$	384	1	2	2	30	23	18
	$C_{19}H_{30}O_8$	386	1	4	7	21	18	15
	$C_{19}H_{28}O_9$	400	<0.5	<0.5	<0.5	17	24	16
Unclassified	$C_{16}H_{24}O_6$	312	2	26	8	5	5	4
	$C_{23}H_{30}O_3$	354	4	2	1	2	0	<0.5
	$C_{32}H_{42}O_3$	474	12	0	0	0	0	0

Table S3. Dimer HOMs identified by FT-ICR MS analysis of collected particle samples along with observed m/z, proposed molecular formula and molecular structure in SOA produced from ozonolysis of β-pinene and limonene.

Dimer ID	Observed m/z (-)	Molecular formula	Proposed molecular structure	Reference
		β-Pinene SOA		
MW 358	357.155	$C_{17}H_{26}O_8$		Kahnt et al. (2018) Kristensen et al. (2017)
				Müller et al. (2009) Mohr et al. (2017)
				Mohr et al. (2017)
				Mohr et al. (2017)
MW 372	371.171	$C_{18}H_{28}O_8$		Kristensen et al. (2017)
MW 388	387.166	$C_{18}H_{28}O_9$		Kristensen et al. (2017) Kristensen et al. (2016)
MW 406	405.177	$C_{18}H_{30}O_{10}$		Kenseth et al. (2018)
MW 400	399.166	$C_{19}H_{28}O_9$		Kristensen et al. (2017)
MW 386	385.187	$C_{19}H_{30}O_8$		Kristensen et al. (2017)
MW 400	399.202	$C_{20}H_{32}O_8$		Kahnt et al. (2018)
		Limonene SOA		
MW 372	371.171	$C_{18}H_{28}O_8$		Hammes et al. (2019)

MW 386	385.187	$C_{19}H_{30}O_8$		Hammes et al. (2019)
MW 402	401.182	$C_{19}H_{30}O_9$		Kundu et al. (2012)
				Kundu et al. (2012)

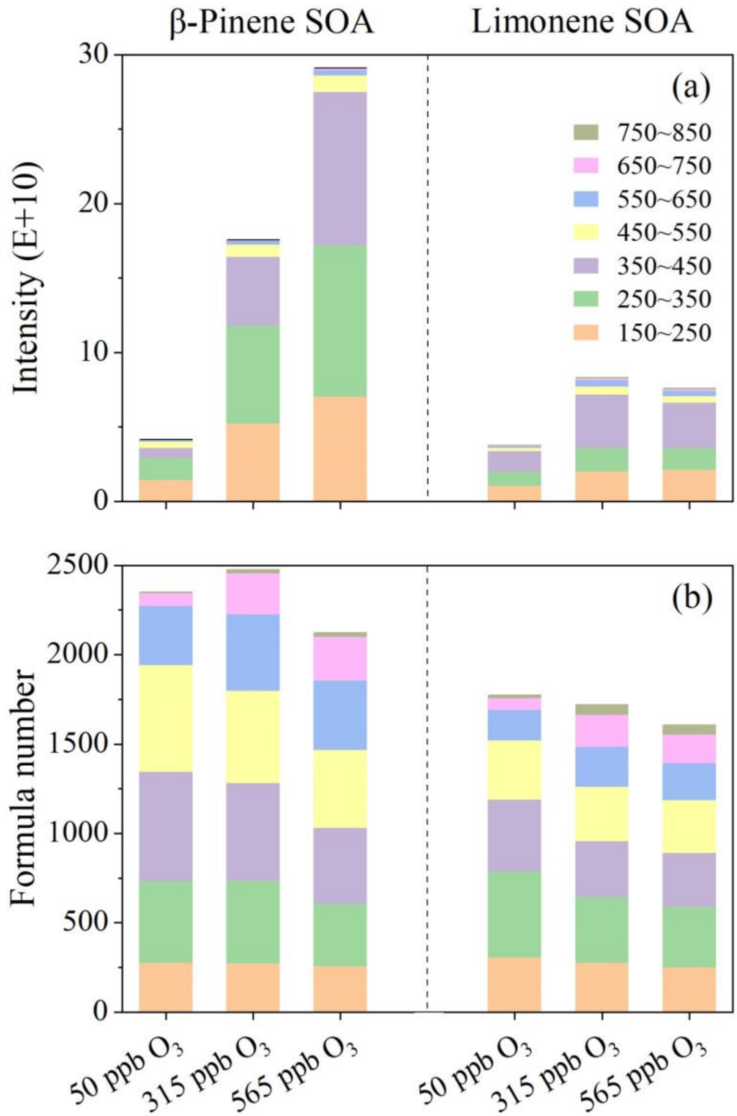
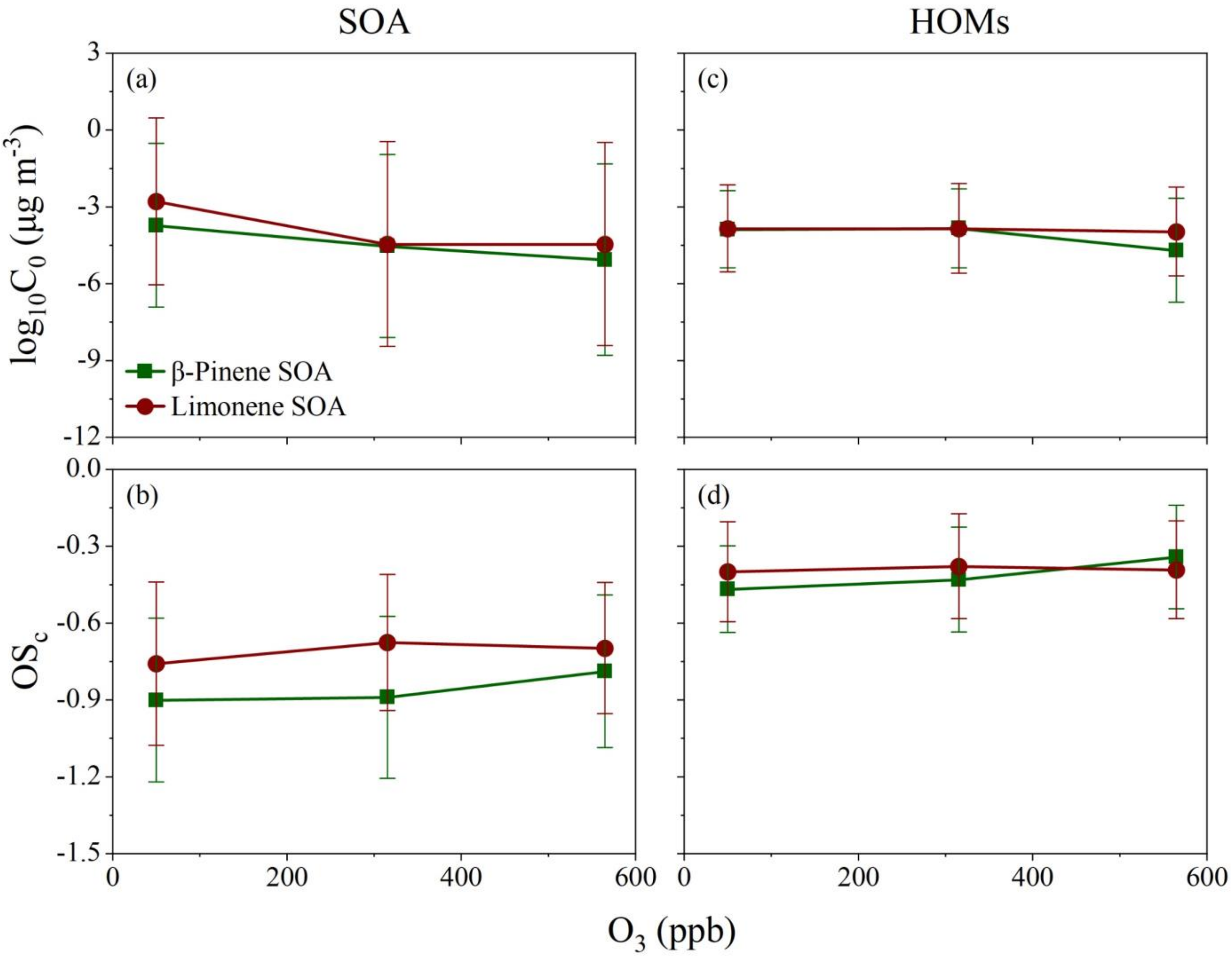


Figure S1. The intensity (a) and formula number (b) of molecular weight distributions for β-pinene and limonene SOA at 50 ppb, 315 ppb and 565 ppb ozone concentrations.



30 **Figure S2.** Average saturation mass concentration (C_0) (a, c) and carbon oxidation state (OS_C) (b, d) for organic compounds from β-pinene SOA (green square) and limonene SOA (red circle) and the corresponding HOMs at different ozone concentrations.

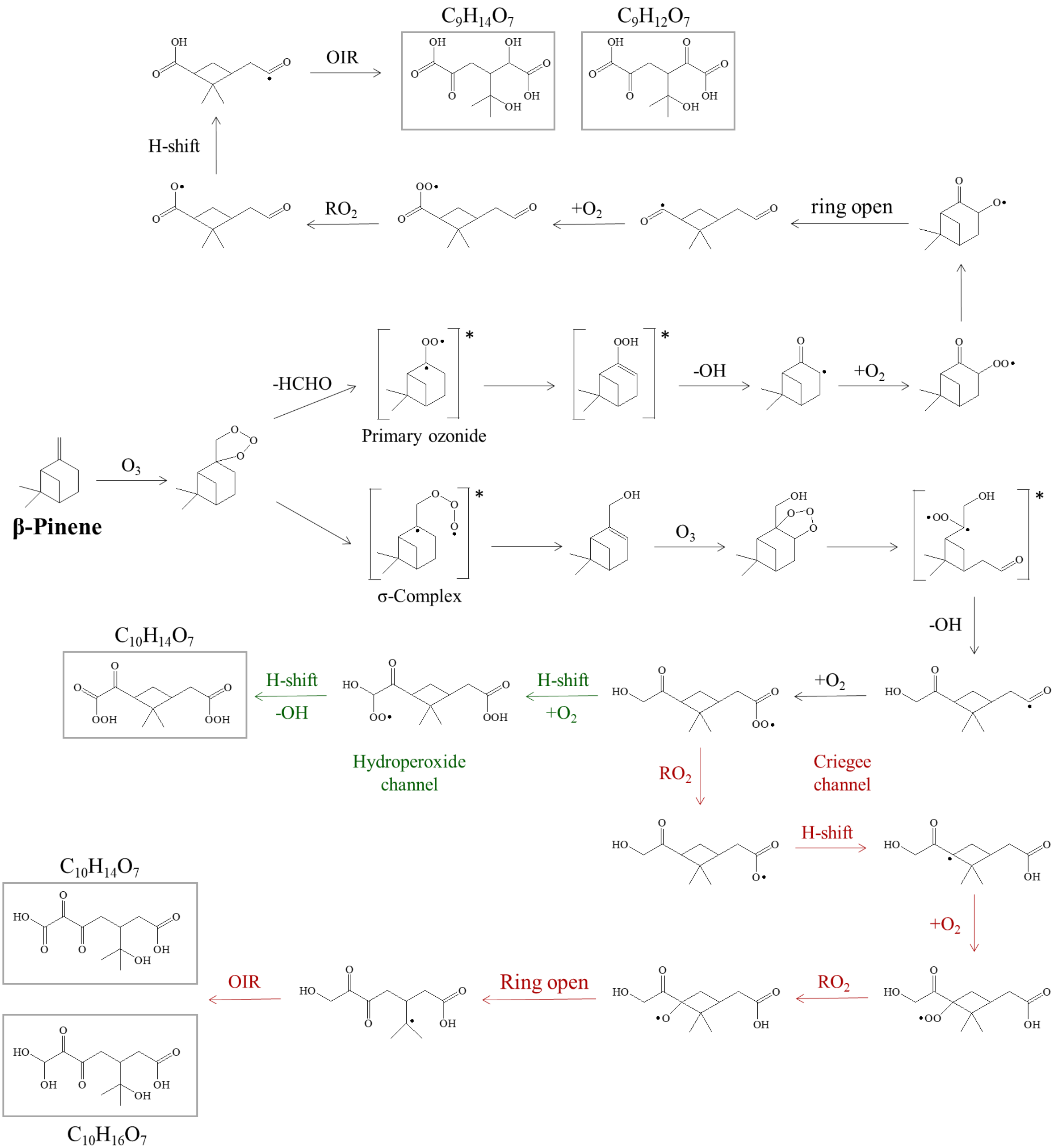


Figure S3. Schematic of the formation of monomer HOMs from the β-pinene ozonolysis via hydroperoxide channel (green) and oxygen-increasing reactions (OIR) (H-shift → O_2 → RO_2) of Criegee channel (red). The organic molecules in the gray rectangle are the possible structures, and the two reaction channels may be intersected, which is not comprehensive.

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