



Supplement of

Investigating the role of ammonia in enhancing secondary organic aerosol formation from the co-photooxidation of anthropogenic and biogenic VOCs

Yongxin Yan et al.

Correspondence to: Junling Li (lijl@craes.org.cn) and Hong Li (lihong@craes.org.cn)

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Table S1. Summary of the initial conditions and results of the conducted experiments.

Number	Date	α -pinene (ppb)	n-heptylcyclohexane (ppb)	NH ₃ (ppb)	NO (ppb)	NO ₂ (ppb)	NO _x (ppb)	Δ VOC/NO _x (ppbC ppb ⁻¹)	JNO ₂ ($\times 10^{-3}$ s ⁻¹)	T (°C)	RH (%)	O ₃ (ppb)	Mass ($\mu\text{g m}^{-3}$)
MIX-1	20231020	43.7	30.4	--	63.5	92.7	156.2	5.3	4.4	34.8	--	121.6	3.5
MIX-2	20231022	63.9	31.7	--	57.7	84.7	142.4	7.4	4.0	38.5	--	235.1	2.6
MIX-3	20231110	66.0	39.1	--	41.5	95.6	137.1	8.5	4.0	25.7	8.6	108.5	51.6
MIX-4	20231206	84.9	87.3	--	40.7	91.7	132.4	15.0	2.1	21.1	7.0	89.5	20.4
MIX-N1	20231103	63.6	38.9	748.5	48.6	94.5	143.1	8.0	3.9	34.0	12.2	136.9	140.7
MIX-N2	20231115	86.3	84.8	748.5	41.4	94.9	136.3	14.4	0.9	14.4	14.4	52.9	125.5
MIX-N3	20231231	86.7	90.1	748.5	33.9	94.6	128.5	15.9	3.1	23.2	11.7	90.2	187.4
MIX-N4	20240103	83.8	81.7	133.7	37.5	80.1	117.6	16.2	3.1	26.0	8.7	98.6	133.5
MIX-N5	20240116	78.3	96.2	74.85	35.1	91.2	126.3	16.1	2.1	19.3	11.8	79.0	165.0
AL-1	20231026	--	36.6	--	59.0	96.1	155.1	3.1	3.9	40.7	6.4	32.2	0.8
AL-2	20231204	--	88.6	--	42.6	80.5	123.1	9.4	2.2	17.1	9.3	7.8	5.6
AL-N1	20231028	--	57.3	748.5	61.2	95.8	157.0	4.7	2.7	36.4	6.4	13.2	17.5
AL-N2	20231113	--	34.5	748.5	42.6	95.4	138.0	3.3	3.5	24.3	14.0	10.9	98.2
AL-N3	20240108	--	93.4	74.85	36.4	80.7	117.1	10.4	2.0	19.0	9.9	10.1	58.2
AL-N4	20240131	--	69.5	214	26.6	63.3	89.9	10.1	2.4	16.3	12.3	17.4	52.6
AP-1	20231024	62.0	--	--	58.1	80.8	138.9	4.5	3.4	39.0	--	202.1	4.5
AP-2	20231201	69.9	--	--	44.9	78.7	123.6	5.7	3.3	24.1	8.8	85.1	16.6
AP-N1	20231101	65.6	--	748.5	48.3	91.3	139.6	4.7	3.1	36.5	12.8	147.9	93.4
AP-N2	20231128	81.2	--	748.5	43.1	85.0	128.1	6.3	3.4	22.4	10.2	69.4	173.4

AP-N3	20240112	79.8	--	74.85	40.8	89.5	130.3	6.1	1.9	21.2	13.9	71.5	172.7
AP-N4	20240126	49.5	--	74.85	49.9	76.3	126.2	3.9	3.3	25.2	11.3	83.6	122.1
AP-N5	20240129	57.6	--	214	48.1	71.7	119.8	4.8	1.5	19.9	13.5	48.3	90.9

The mass here was the measured value with the SMPS; the density of the formed SOA derived from n-heptylcyclohexane was assumed to be 1.1 g cm⁻³; the density of the formed SOA derived from α -pinene was assumed to be 1.4 g cm⁻³; the density of the formed SOA derived from the mixed VOCs was assumed to be 1.25 g cm⁻³.

Table S2. Total count of detected compounds detected across all SOA samples in positive (+) and negative (-) ionization mode, the signal relative intensity of which were greater than 0.05. A relative intensity of 1 was assigned to the most intense peak that was non-impurity in each sample group.

Mode	Phase	Total count of detected compounds	
Positive (+)	Former	343	414
	Latter	305	573
Negative (-)	Former	149	182
	Latter	168	

Table S3. Identified molecular formulas and DBE of SOA in nitrate-containing experiments.

m/z	Molecular formula	Latter (+)			Former (+)			Latter (-)			Former (-)			DBE
		MIX-N	AL-N	AP-N	MIX-N	AL-N	AP-N	MIX-N	AL-N	AP-N	MIX-N	AL-N	AP-N	
113.06	C ₆ H ₁₀ O ₂							√	√	√	√	√	√	2
129.05	C ₆ H ₈ O ₃	√	√	√	√	√	√		√			√		3
141.09	C ₈ H ₁₄ O ₂							√	√	√	√	√	√	2
141.10	C ₇ H ₁₄ N ₂ O							√	√	√	√	√		2
143.11	C ₇ H ₁₆ N ₂ O							√	√		√	√	√	1
151.11	C ₁₀ H ₁₄ O	√		√	√		√							4
153.09	C ₉ H ₁₂ O ₂	√	√	√	√	√	√							4
157.05	C ₇ H ₈ O ₄							√	√	√	√	√	√	4
157.06	C ₆ H ₈ N ₂ O ₃							√	√	√	√	√	√	4
157.12	C ₉ H ₁₈ O ₂							√	√	√	√	√	√	1
157.13	C ₈ H ₁₈ N ₂ O							√	√	√	√	√	√	1
167.11	C ₇ H ₁₆ N ₂ O	√	√	√	√		√							1
169.08	C ₇ H ₁₄ O ₃							√		√	√		√	1
169.09	C ₆ H ₁₄ N ₂ O ₂		√	√		√	√	√	√	√	√	√	√	1
169.12	C ₁₀ H ₁₈ O ₂							√		√	√		√	2
171.06	C ₆ H ₁₂ O ₄							√		√	√		√	1
171.07	C ₅ H ₁₂ N ₂ O ₃		√	√		√	√	√	√	√	√	√	√	1
171.10	C ₉ H ₁₄ O ₃		√	√		√	√	√	√	√	√		√	3
173.08	C ₈ H ₁₂ O ₄	√	√		√				√					3
174.11	C ₈ H ₁₅ NO ₃	√	√	√		√	√							2
179.07	C ₈ H ₁₂ O ₃	√	√	√	√	√	√							3
183.09	C ₈ H ₁₆ O ₃							√		√	√		√	1
183.10	C ₁₀ H ₁₄ O ₃		√			√		√	√	√	√	√	√	4

183.11	C ₇ H ₁₆ N ₂ O ₂	√		√			√	√	√	√	√	√	√	1
183.13	C ₁₁ H ₂₀ O ₂							√		√	√		√	2
183.14	C ₁₀ H ₂₀ N ₂ O							√		√	√		√	2
184.13	C ₁₀ H ₁₉ NO ₂							√		√	√		√	2
185.08	C ₉ H ₁₂ O ₄		√			√		√	√	√	√		√	4
185.09	C ₆ H ₁₄ N ₂ O ₃							√	√	√	√		√	1
185.11	C ₁₀ H ₁₈ O ₃							√		√	√		√	2
185.12	C ₉ H ₁₆ N ₂ O ₂	√		√	√		√	√		√	√		√	3
187.10	C ₈ H ₁₆ N ₂ O ₃							√	√	√	√	√	√	2
199.10	C ₇ H ₁₆ N ₂ O ₃		√			√		√	√	√	√		√	1
208.11	C ₈ H ₁₇ NO ₅	√	√	√	√	√	√							1
209.09	C ₈ H ₁₄ N ₂ O ₃	√	√	√	√	√	√							3
211.18	C ₁₂ H ₂₂ N ₂ O	√	√		√	√			√			√		3
221.09	C ₉ H ₁₄ N ₂ O ₃	√	√	√	√	√	√							4
223.10	C ₇ H ₁₄ N ₂ O ₆	√	√	√	√	√	√							2
233.16	C ₁₀ H ₂₀ N ₂ O ₄	√	√	√	√	√	√							2
235.18	C ₁₄ H ₂₂ N ₂ O	√	√		√	√								5
238.12	C ₉ H ₁₉ NO ₆				√									1
240.10	C ₈ H ₁₇ NO ₇	√	√	√	√	√	√							1
253.03	C ₆ H ₈ N ₂ O ₉	√			√									4
255.10	C ₉ H ₁₈ O ₈	√			√									1
255.24	C ₁₅ H ₃₂ N ₂ O							√	√	√	√	√	√	1
267.04	C ₅ H ₁₂ N ₂ O ₉	√		√	√	√								1
280.17	C ₁₂ H ₂₅ NO ₆	√			√									1
281.06	C ₈ H ₁₂ N ₂ O ₉	√	√		√	√								4
283.10	C ₁₀ H ₁₈ O ₉	√	√	√	√	√	√							2
283.27	C ₁₇ H ₃₆ N ₂ O							√	√		√	√		1

333.22	C ₁₇ H ₃₂ O ₆	√		√	√		√							2
345.22	C ₁₈ H ₃₂ O ₆	√		√	√		√							3
358.22	C ₁₈ H ₃₁ NO ₆	√			√		√							4
359.04	C ₈ H ₁₆ O ₁₄	√			√									1
363.20	C ₁₇ H ₃₀ O ₈	√		√	√		√							3
364.23	C ₁₇ H ₃₅ NO ₇							√			√		√	1
367.23	C ₁₇ H ₃₆ O ₈							√		√	√		√	0
367.24	C ₁₉ H ₃₆ O ₅							√		√	√		√	2
372.23	C ₁₉ H ₃₃ NO ₆	√			√		√							4
373.06	C ₁₁ H ₁₆ O ₁₄	√			√									4
373.23	C ₁₆ H ₃₄ N ₂ O ₆	√			√									1
376.23	C ₁₈ H ₃₃ NO ₇	√			√		√							3
377.21	C ₁₈ H ₃₂ O ₈	√		√	√		√							3
388.23	C ₁₇ H ₃₅ NO ₇	√		√	√		√							1
389.21	C ₁₇ H ₃₄ O ₈							√		√	√		√	1
390.24	C ₁₉ H ₃₅ NO ₇	√		√			√							3
401.26	C ₂₀ H ₃₆ N ₂ O ₆	√			√		√							4
413.21	C ₁₉ H ₃₄ O ₈	√		√	√		√							3
522.40	C ₂₇ H ₅₅ NO ₈	√			√									1
525.36	C ₂₆ H ₅₂ O ₁₀	√			√		√							1

The DBE here was the abbreviation of ring and double-bond equivalent. "√" signified the detection of the substance in the respective experiment.

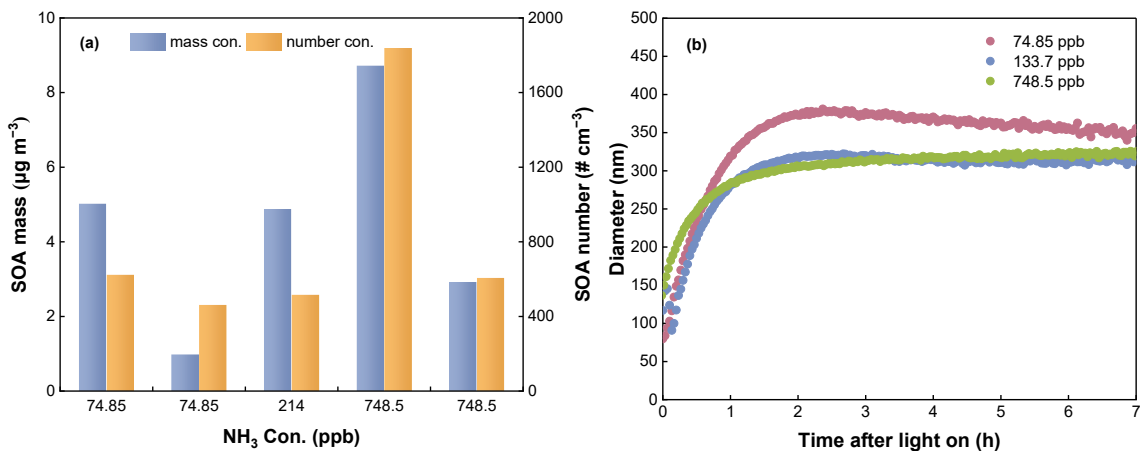


Figure S1. (a) Number and mass concentration of particulate matter formed by photochemical reaction of NH_3+NO_x . (b) The particle size distribution at varying NH_3 concentration.

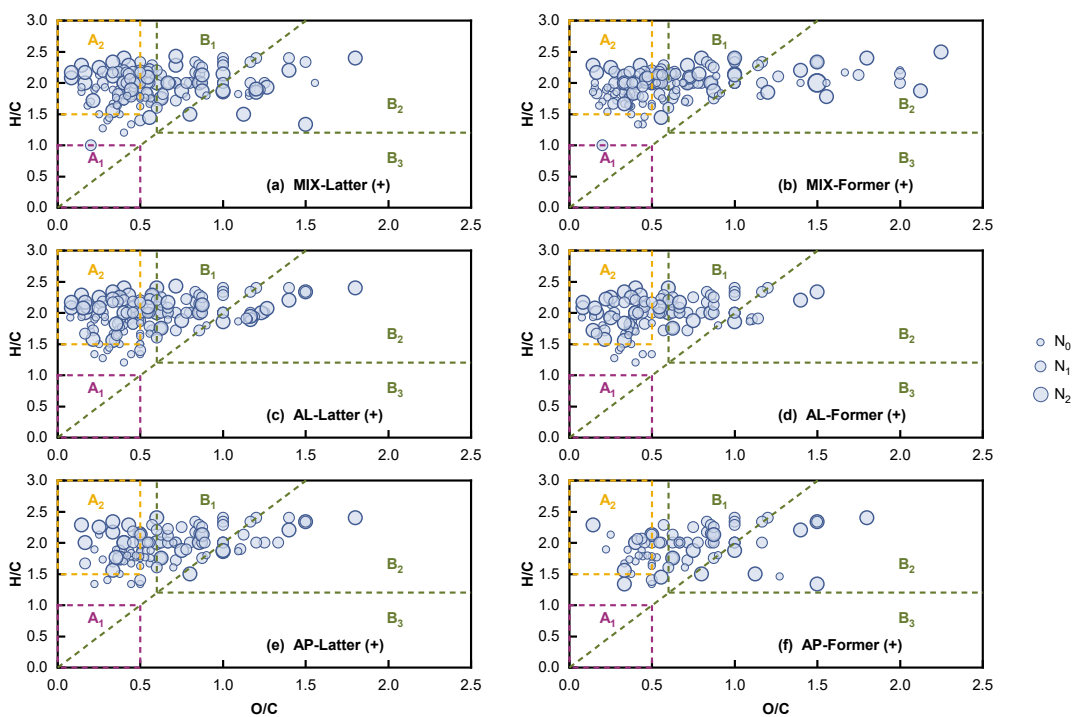


Figure S2. Van Krevelen diagram of compounds detected in the MIX experiment, AL experiment and AP experiment under positive mode.

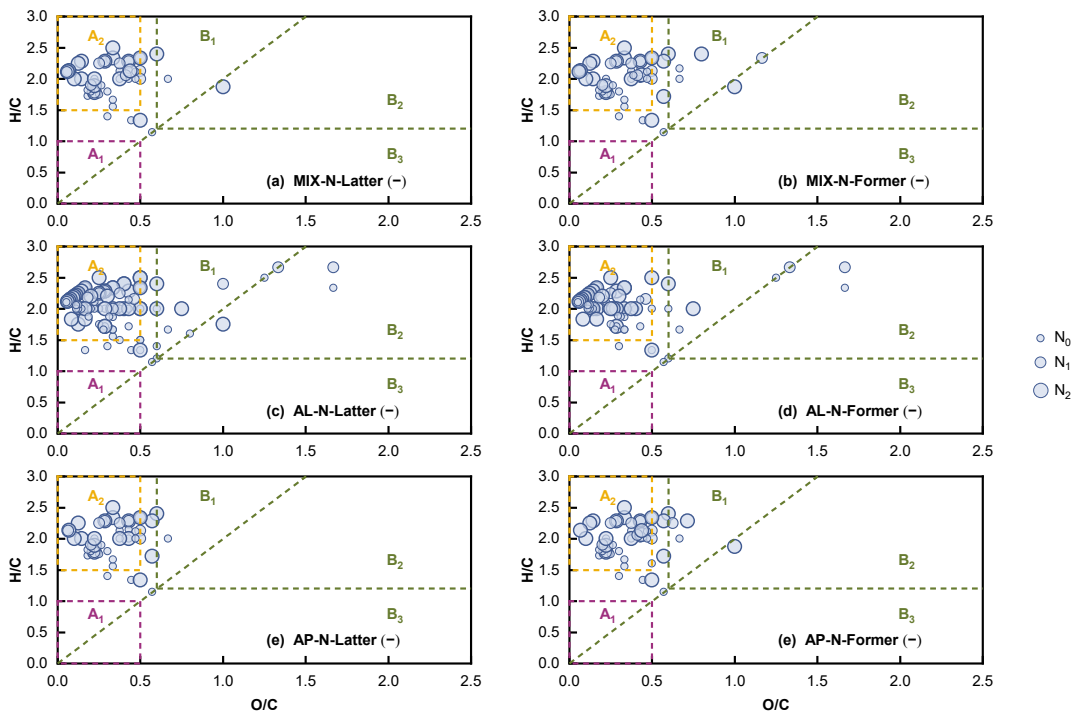


Figure S3. Van Krevelen diagram of compounds detected in the MIX-N experiment, AL-N experiment and AP-N experiment under negative mode.

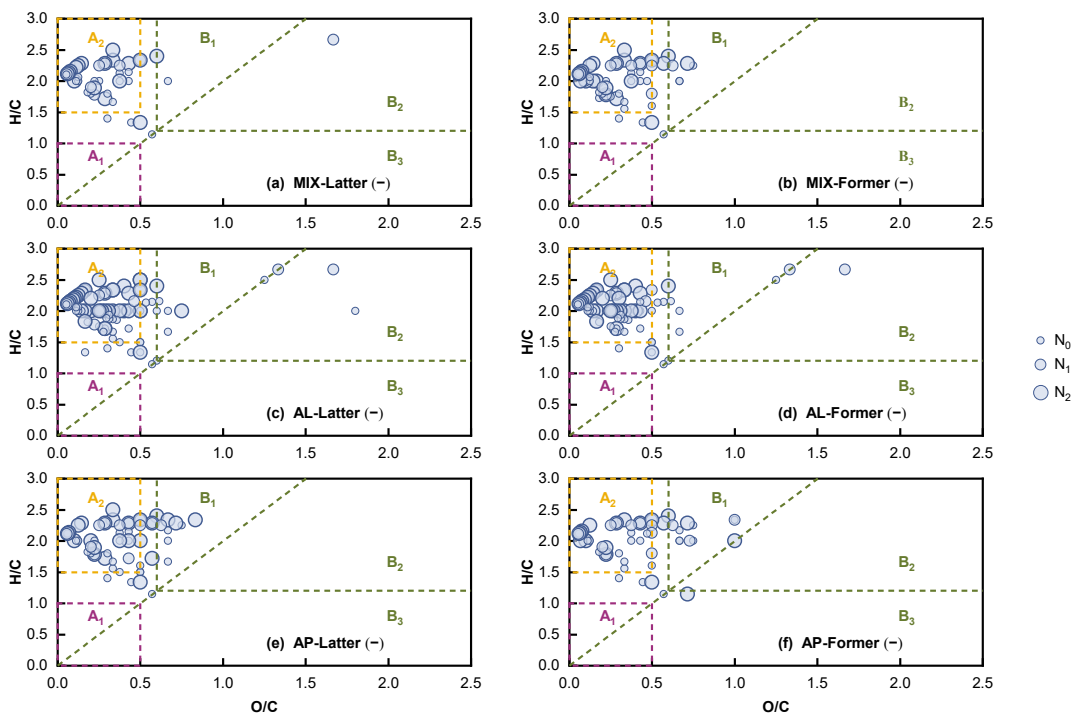


Figure S4. Van Krevelen diagram of compounds detected in the MIX experiment, AL experiment and AP experiment under negative mode.

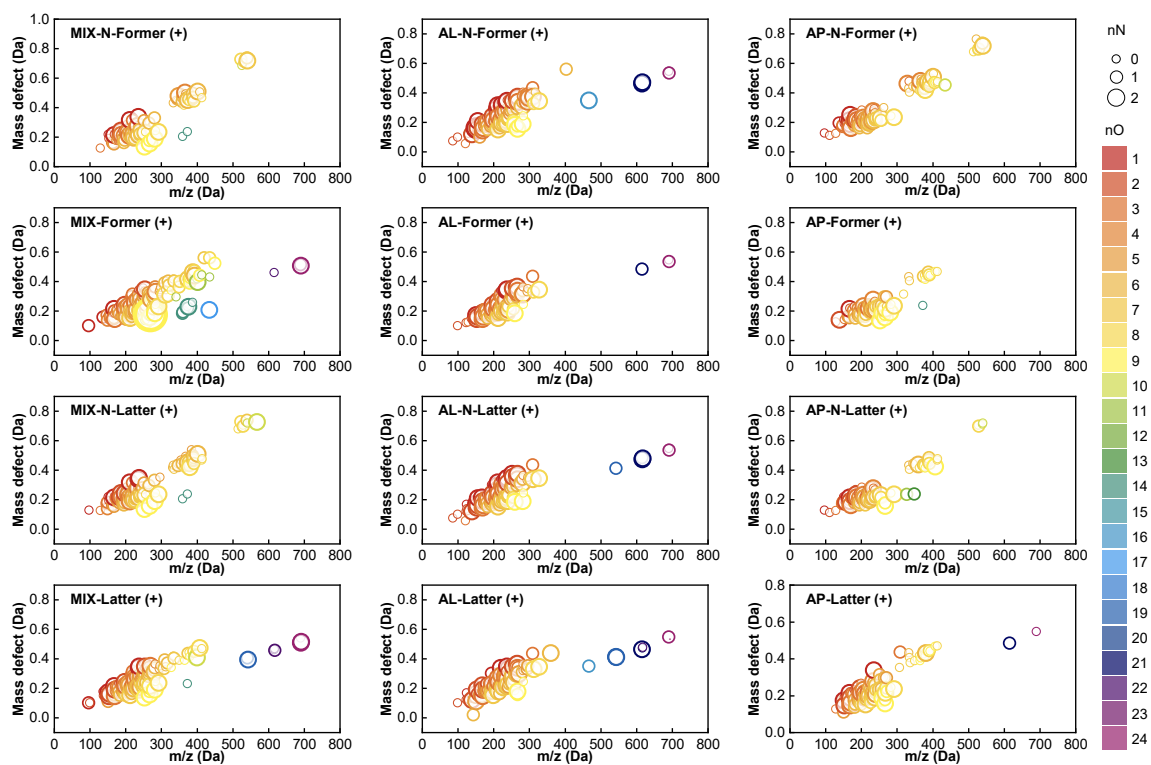


Figure S5. Mass defect vs mass to charge ratio of multifunctional organic compounds in secondary organic aerosols derived from single / mixed experiments of n-heptylcyclohexane and α -pinene under positive and negative mode (Each circle denotes a unique oxidative molecule, colored based on its oxygen content, with the circle's size reflecting the molecule's nitrogen count).

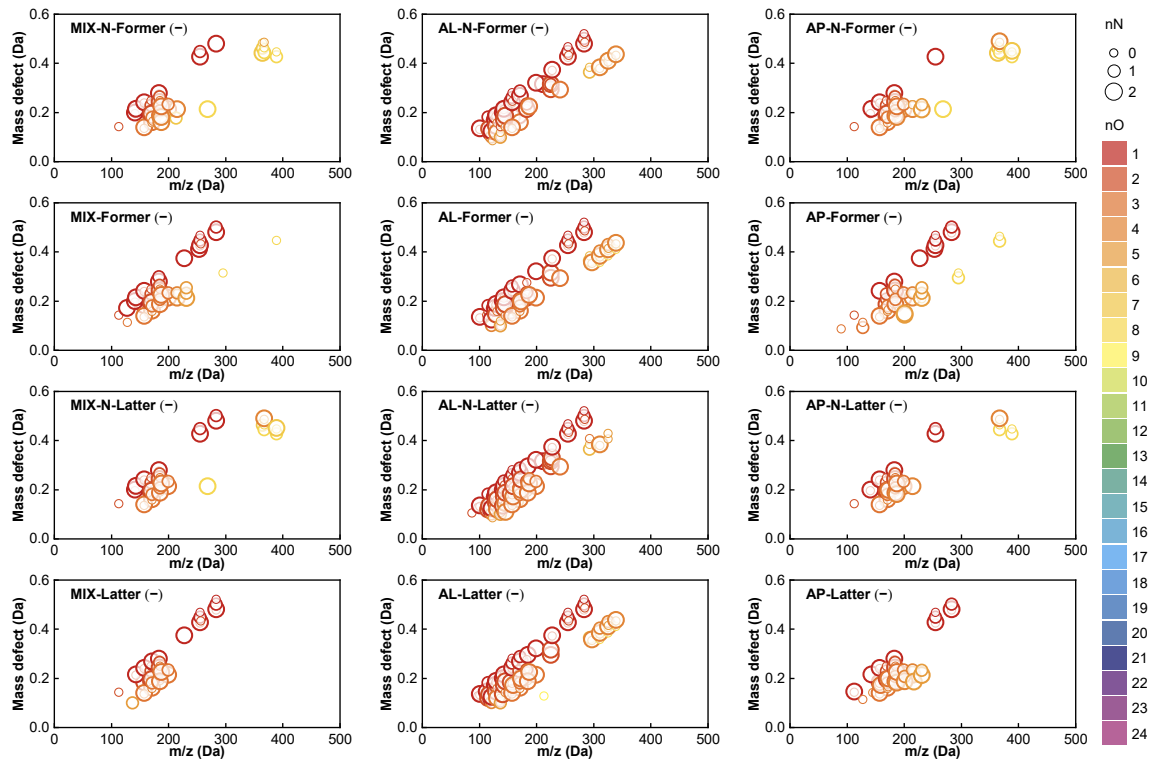


Figure S6. Mass defect vs mass to charge ratio of multifunctional organic compounds in secondary organic aerosols derived from single / mixed experiments of n-heptylcyclohexane and α -pinene under positive and negative mode (Each circle denotes a unique oxidative molecule, colored based on its oxygen content, with the circle's size reflecting the molecule's nitrogen count).