

1 ***Supporting Information:***

2 Chemical Composition of Toluene and Cresol Secondary Organic Aerosol: Effect of NO_x Level

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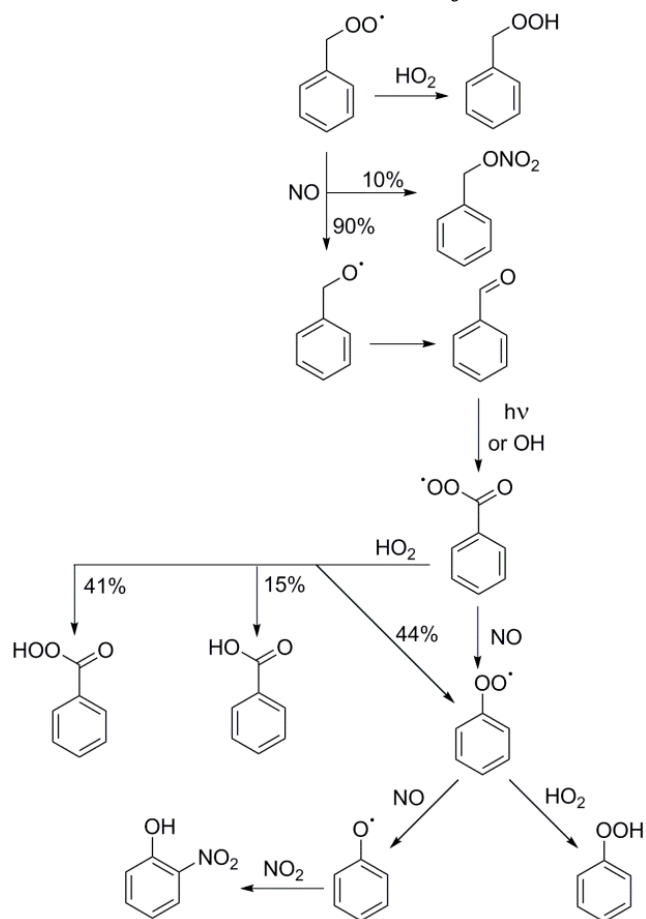
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9 ***Environmental Chamber Experimental Details***

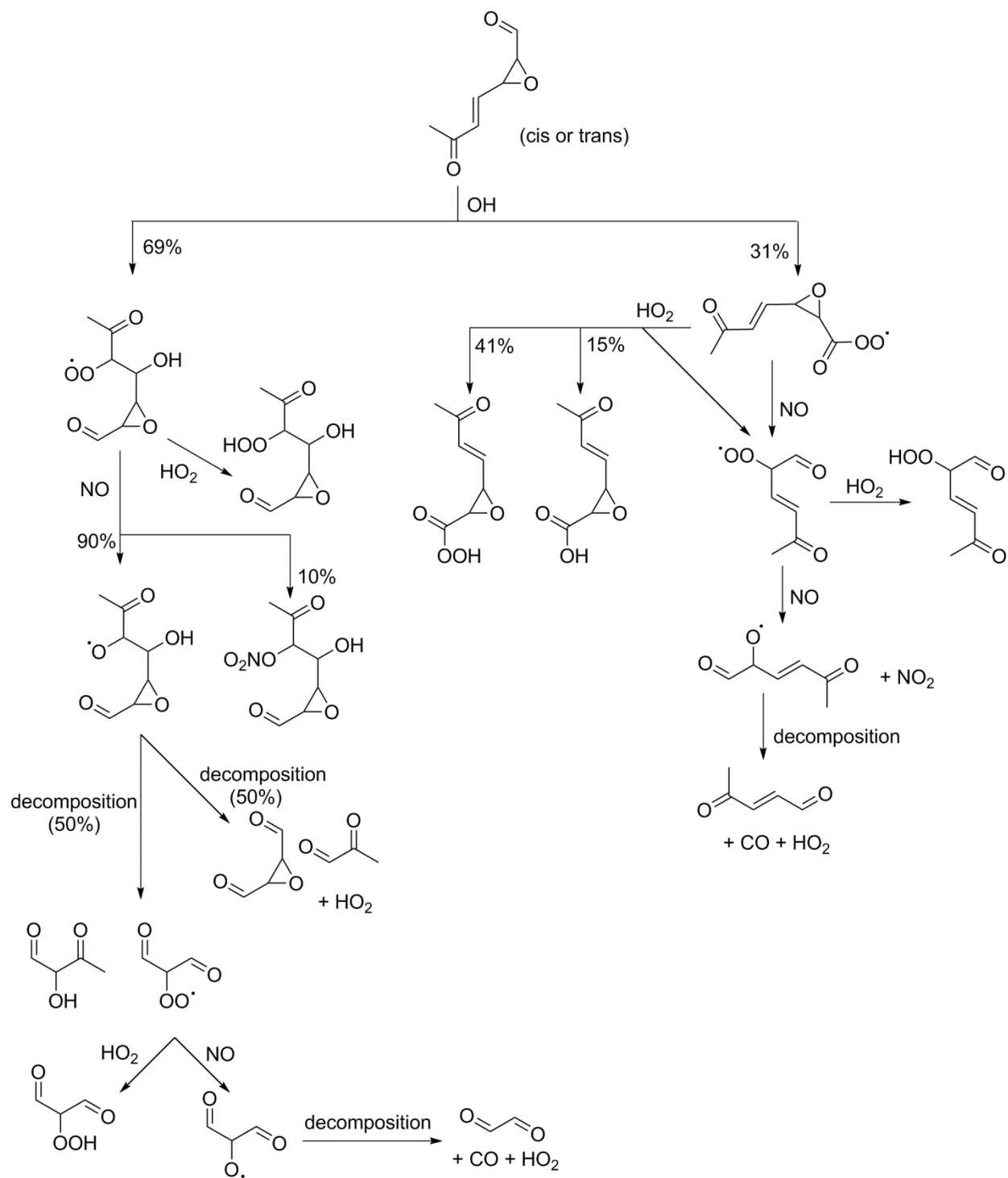
10 Hydroxyl radicals were produced through the photolysis of hydrogen peroxide (50% weight
11 solution, Sigma Aldrich), which was introduced into the environmental chamber using filtered
12 air flowing at 5 L min⁻¹ through a glass trap immersed in a 35 °C water bath over the course of
13 1.5 to 2 h. The environmental chamber black lights' peak wavelength is 350 nm. To minimize
14 self-reaction of peroxy radicals (RO₂+RO₂) and promote the reaction of peroxy radicals with
15 HO₂ radicals (RO₂+HO₂) under low-NO conditions, 220 μL of H₂O₂ solution was injected to
16 reach a concentration of 4 ppm. Under high-NO conditions, 110 μL of H₂O₂ solution was
17 injected to reach a concentration of 2 ppm; less H₂O₂ was necessary to achieve a dominant
18 RO₂+NO regime. For high-NO conditions, an initial injection of 100 ppb was performed prior to
19 the initiation of photooxidation, and a continuous flow of 50 ppb h⁻¹ was used to maintain an
20 RO₂+NO-dominant regime throughout the course of the experiment. Seed aerosol was produced
21 by the atomization of aqueous solutions of inorganic salts. Ammonium sulfate (>99.9%, Sigma
22 Aldrich), sodium chloride (>99%, Sigma Aldrich), sodium sulfate (>99%, Sigma Aldrich), and
23 magnesium sulfate (>99%, Sigma Aldrich) with sulfuric acid (18 M, Sigma Aldrich) were used
24 in seed aerosol preparations. Ammonium sulfate was prepared at a concentration of 0.015 M for

25 the majority of experiments, and at a concentration of 0.06 M for a high seed surface area
26 experiment; the rest of the seed solutions were prepared at concentrations of 0.03 M.

27 **Master Chemical Mechanism for non-Cresol Pathways for Toluene Photooxidation**



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29 **Figure S1.** MCM mechanism for the gas-phase oxidation of the benzyl peroxy radical under low- and
30 high-NO conditions.¹



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32 **Figure S2.** MCM mechanism for the gas-phase oxidation of the toluene-derived epoxy muconaldehyde
 33 under low- and high-NO conditions.¹

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36 **DART-HR-MS Analysis of SOA Collected by Filtration**

37 *Standards & Sampling Material*

38 A mass calibrant and independent quality assurance quality control (QA/QC) compounds
39 were run with each sample set to ensure mass accuracy to within 5 mDa. The mass calibrant
40 used for positive mode was polyethylene glycol (average molecular weight of 600 amu, PEG-
41 600; Acros Organics, Geel, Belgium) which was dissolved in methanol. The independent
42 QA/QC compound used is reserpine, which was purchased from Sigma-Aldrich, which was
43 diluted in methanol. The mass calibrant for negative mode was a mixture of fatty acids including
44 (at approximately 100 μg per fatty acid): hexanoic acid, octanoic acid, decanoic, acid,
45 dodecanoic acid, myristic acid, palmitic acid, stearic acid, eicosanoic acid, docosanoic acid, and
46 tetracosanoic acid; dissolved in 2 mL of hexane. An individual sample of hexadecanoic acid was
47 sampled as a QA/QC compound.

48 Tweezers were used to introduce the samples into the DART gas stream. Before analysis,
49 the tweezers were rinsed with acetone, and were introduced into the gas stream to vaporize any
50 contaminants which may have been present on them.

51 A ~ 1 cm strip was cut from each sample substrate for testing. The cutting was tested in
52 triplicate, with each sampling being from a different are of the substrate.

53 *Development of Mass Calibration Mixtures*

54 In these studies, a solution of PEG-600 (50 μL in 10 mL of methanol) was used to
55 calibrate the mass spectrometer for each run. PEG-600 provided a series of $[\text{M}+\text{H}]^+$ and
56 $[\text{M}+\text{H}_3\text{O}]^+$ ions in positive mode, allowing for tuning peaks in the range of 61-679 Da. In
57 negative mode $[\text{M}+\text{OH}]^-$ peaks were used, providing a tuning range of 75-675 Da. Acceptable
58 calibration was determined if the calibration Mass Center software produced a residual value of

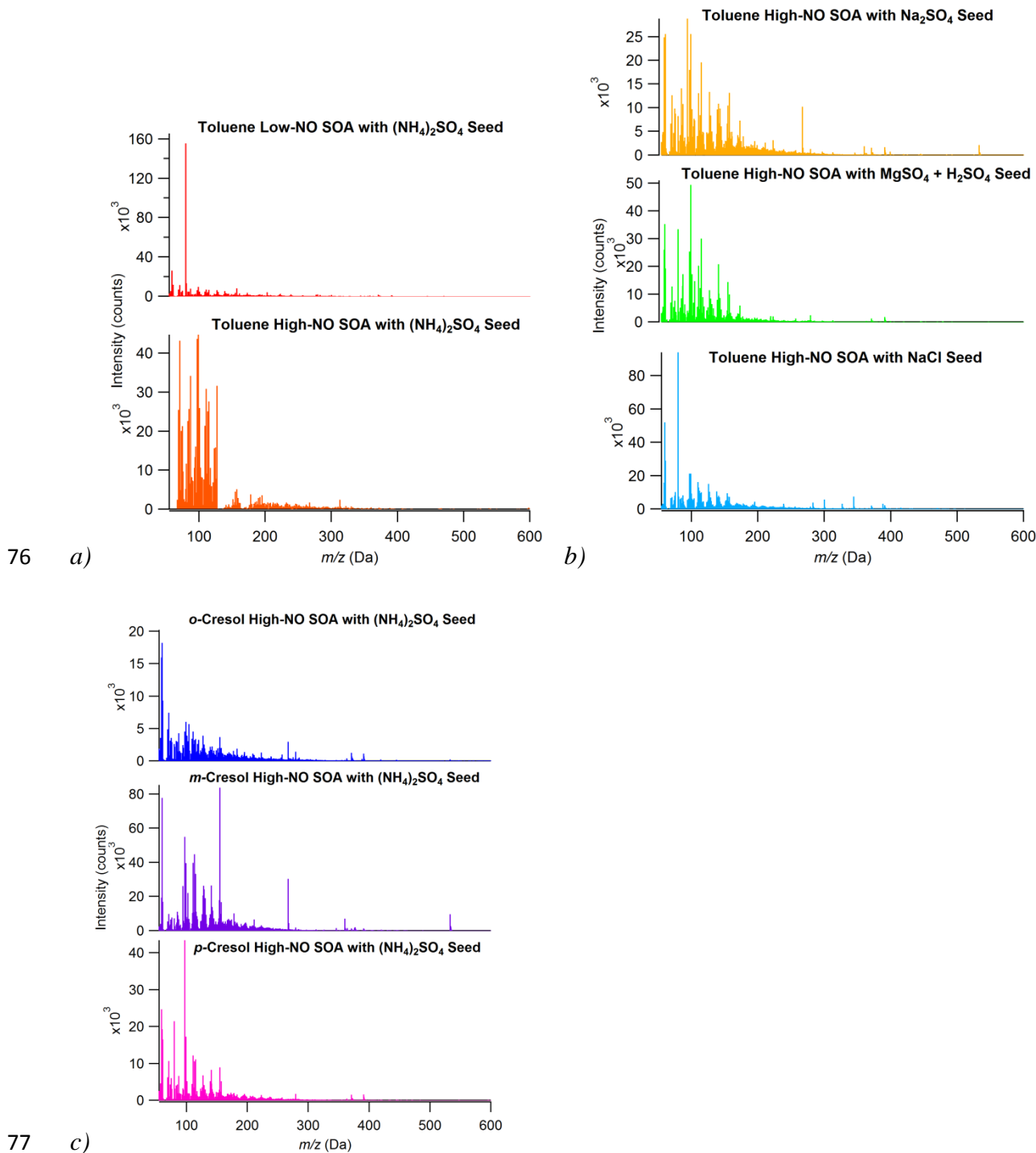
59 $>9 \times 10^{-12}$. To ensure proper calibration, a solution of reserpine (5 mg in 10 mL of methanol) or
60 linoleic acid (20 μ L in 10 mL of methanol) was analyzed subsequent to the PEG-600 in every
61 sample run. Reserpine produces a protonated molecule peak at 609.281 Da in positive mode.
62 Linoleic acid, which produces a deprotonated molecule peak at 279.232 Da was used in negative
63 mode to ensure accurate calibration. Calibration was deemed sufficient if the mass of the above
64 listed peaks fell within ± 0.005 Da of the theoretical value.

65 *Parameters for AccuTOF-DART*

66 The instrument which was used in the study was a JEOL (Tokyo, Japan) AccuTOF™
67 mass spectrometer (JMS-T100LC) coupled with an IonSense (Saugus, MA, USA) DART®
68 source. Ultra-pure helium was used as the ionizing gas with a flow rate of 1.75 L min⁻¹. For all
69 analyses, the DART® source was set to a needle voltage of ± 3.5 kV. Electrode 1 and electrode 2
70 voltages were both set to ± 150 V. Mass spectrometer settings include: an orifice 1 voltage of
71 ± 20 V, orifice 2 voltage of ± 5 V, a ring lens voltage of ± 5 V, a peaks voltage of 1500 V, a mass
72 range of 50 – 1500 m/z at 0.5 seconds per scan. A helium gas stream temperature of 325 °C was
73 also employed.

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75 **DART-HR-MS Mass Spectra for Toluene and o-, m-, and p-Cresol SOA**



78 **Figure S3.** (+)-DART-HR-MS mass spectra for toluene and cresol SOA.

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81 *Measured Chemical Compositions for Toluene and o-, m-, and p-Cresol SOA*82 Table S1: Chemical composition measured by (+)-DART-HR-MS of toluene SOA generated under low-
83 NO conditions with (NH₄)₂SO₄ seed. Abundance is defined as ((C_A/C_{IS})/Σ(C_A/C_{IS})).

<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smiles	P _{vap} (atm)
59.0491	1.21E-12	3	6		1	C _x H _y O ₁	CC(C)=O	3.87E-01
61.0284	4.71E-11	2	4		2	C _x H _y O ₂	CC(O)=O	4.49E-03
71.0491	2.94E-12	4	6		1	C _x H _y O ₁	CC=CC=O	8.30E-02
73.0648	5.62E-13	3	4		2	C _x H _y O ₂	CC(C=O)=O	1.90E-01
75.0441	1.49E-11	3	6		2	C _x H _y O ₂	CC(CO)=O	6.92E-03
80.0495	1.18E-10	5	5	1		C _x H _y N	C1=NC=CC=C1	2.63E-02
85.0284	3.99E-11	4	4		2	C _x H _y O ₂	O=CC=CC=O	3.42E-03
87.0441	2.79E-11	4	6		2	C _x H _y O ₂	O=CCCC=O	6.19E-03
97.0284	1.64E-11	5	4		2	C _x H _y O ₂	O=CC1=CC=CO1	7.54E-03
99.0441	2.02E-10	5	6		2	C _x H _y O ₂	CC(C=CC=O)=O	1.12E-03
101.0597	6.31E-12	5	8		2	C _x H _y O ₂	CC1CCC(O1)=O	2.17E-02
111.0441	7.8E-11	6	6		2	C _x H _y O ₂	O=CC1=CC=C(C)O1	2.46E-03
115.0390	2.89E-07	5	6	3		C _x H _y O ₃	CC(C=CC(O)=O)=O	5.26E-07
123.0441	1.03E-08	7	6	2		C _x H _y O ₂	O=C(C=C1)C=C(C)C1=O	8.12E-06
125.0597	3.64E-08	7	8	2		C _x H _y O ₂	CC1=C(O)C=CC=C1O	2.29E-06
127.0390	3.8E-07	6	6	3		C _x H _y O ₃	O=CC1=C(O)C=C(C)O1	5.26E-07
129.0546	2.22E-07	6	8	3		C _x H _y O ₃	O=CC1=CCC(O1)(O)C	5.26E-07
139.0390	2.67E-07	7	6	3		C _x H _y O ₃	O=C1C(C)=CC(C(O)=C1)=O	5.26E-07
141.0546	1.58E-05	7	8	3		C _x H _y O ₃	CC1=C(O)C=CC(O)=C1O	5.77E-09
143.0339	2.73E-05	6	6	4		C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
155.0339	1.33E-05	7	6	4		C _x H _y O ₄	O=C1C(C)=C(O)C(C(O)=C1)=O	8.26E-09
157.0495	0.007994	7	8	4		C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
173.0445	0.991948	7	8	5		C _x H _y O ₅₊	CC1=C(O)C(O)=C(O)C(O)=C1O	8.99E-14
195.1380	3.06E-07	10	18	2		C _x H _y O ₂	O=C(OCC(C)=O)C1=CC=CC=C1O	2.29E-07

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85 Table S2: Chemical composition measured by (+)-DART-HR-MS of toluene SOA generated under high-
86 NO conditions with (NH₄)₂SO₄ seed. Abundance is defined as ((C_A/C_{IS})/Σ(C_A/C_{IS})). Compounds marked with
87 an asterisk (*) indicate they are also detected in *o*-cresol SOA.

<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smiles	P _{vap} (atm)
69.0692	4.17E-10	4	4		1	C _x H _y O ₁	O1C=CC=C1	2.05E-01
71.0487	1.75E-09	4	6		1	*C _x H _y O ₁	CC=CC=O	8.30E-02
72.0485	1.79E-06	3	5	1	1	C _x H _y NO ₁	C=CC(N)=O	9.20E-06
73.0635	3.55E-10	3	4		2	C _x H _y O ₂	CC(C=O)=O	1.90E-01
75.0433	1.03E-08	3	6		2	*C _x H _y O ₂	CC(CO)=O	6.92E-03
76.0395	1.34E-01	2	5	1	2	C _x H _y NO ₂	NCC(O)=O	2.42E-10
80.0496	6.62E-10	5	5	1		*CHN	C1=NC=CC=C1	2.63E-02
83.0838	1.14E-09	5	6		1	C _x H _y O ₁	CC1=CC=CO1	6.70E-02
85.0297	2.53E-08	4	4		2	*C _x H _y O ₂	O=CC=CC=O	3.42E-03
87.0439	1.86E-08	4	6		2	*C _x H _y O ₂	O=CCCC=O	6.19E-03
89.0581	4.26E-08	4	8		2	*C _x H _y O ₂	O=CCCCO	6.48E-04

91.0540	2.13E-06	3	6	3	C _x H _y O ₃	OC(C(O)=O)C	1.13E-05	
93.0391	2.57E-09	6	4	1	C _x H _y O ₁	C12=C(O2)C=CC=C1	1.39E-02	
95.0815	2.67E-08	6	6	1	C _x H _y O ₁	OC1=CC=CC=C1	2.02E-03	
96.0480	4.19E-05	5	5	1	1	C _x H _y NO ₁	O=C1C=CC=CN1	3.38E-07
97.0327	3.15E-07	5	4	2	C _x H _y O ₂	O=C1C=CC(C1)=O	4.67E-04	
99.0453	1.10E-08	5	6	2	C _x H _y O ₂	CC1=CCC(O1)=O	1.37E-02	
100.0452	8.82E-05	4	5	1	2	C _x H _y NO ₂	O=C(N1)CCC1=O	4.71E-07
101.0576	4.06E-08	4	4	3	C _x H _y O ₃	O=C1CCC(O1)=O	2.15E-03	
102.0896	1.90E-09	4	7	1	2	C _x H _y NO ₂	O=C(OCC)C=N	1.89E-02
103.0428	5.81E-08	4	6	3	C _x H _y O ₃	O=C1C(O)CCO1	4.80E-04	
104.0371	8.01E-10	3	5	1	3	C _x H _y NO ₃	C=CC(ON(=O)=O)	2.60E-02
105.0228	1.23E-05	3	4	4	C _x H _y O ₄	OCC(C(O)=O)=O	2.22E-06	
107.0655	1.41E-08	7	6	1	C _x H _y O ₁	O=CC1=CC=CC=C1	1.83E-03	
109.1014	1.09E-07	7	8	1	C _x H _y O ₁	OC1=C(C)C=CC=C1	6.61E-04	
110.0612	2.73E-08	6	7	1	1	C _x H _y NO ₁	OC1=CC=C(C)N=C1	7.24E-04
111.0475	2.84E-07	6	6	2	C _x H _y O ₂	O=CC=CC=CC=O	3.66E-04	
112.0432	4.35E-08	5	5	1	2	C _x H _y NO ₂	O=C(N1)C=C(C)C1=O	7.03E-04
113.0534	1.72E-07	6	8	2	C _x H _y O ₂	O=CCCC=CC=O	4.92E-04	
114.0581	1.46E-06	5	7	1	2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
115.0418	1.41E-07	6	10	2	C _x H _y O ₂	O=CCCCCC=O	6.62E-04	
117.0570	1.86E-07	5	8	3	C _x H _y O ₃	O=C1C(C)CC(O)O1	1.91E-04	
118.0527	1.73E-09	4	7	1	3	C _x H _y NO ₃	O=C(O)C(O)CC=N	8.50E-03
119.0670	7.35E-07	4	6	4	C _x H _y O ₄	OC(C(O)C=O)C=O	2.68E-05	
123.0470	1.89E-06	7	6	2	C _x H _y O ₂	O=CC1=C(O)C=CC=C1	2.77E-05	
124.0470	6.62E-08	6	5	1	2	C _x H _y NO ₂	O=N(C1=CC=CC=C1)O	2.87E-04
125.0675	2.32E-05	7	8	2	C _x H _y O ₂	CC1=C(O)C=CC=C1O	2.29E-06	
126.0564	2.28E-05	6	7	1	2	C _x H _y NO ₂	OC1=NC(O)=CC(C)=C1	1.15E-06
127.0431	3.29E-03	6	6	3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08	
138.0429	1.49E-04	7	7	1	2	C _x H _y NO ₂	CC1=C(N(O)=O)C=CC=C1	6.57E-09
139.0281	2.72E-05	7	6	3	C _x H _y O ₃	OC1=CC=CC=C1C(O)=O	5.80E-08	
140.0237	1.55E-09	6	5	1	3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
141.0431	3.54E-04	7	8	3	C _x H _y O ₃	OC1=C(O)C(C)=CC=C1O	1.06E-08	
147.0526	4.17E-05	5	6	5	C _x H _y O ₅₊	O=C(O)C(CCC(O)=O)=O	3.95E-08	
154.0417	9.18E-04	7	7	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
155.0286	1.07E-01	7	6	4	C _x H _y O ₄	O=C(O)C1=C(O)C=CC(O)=C1	1.41E-10	
157.0420	7.29E-01	7	8	4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11	
159.0583	3.45E-03	7	10	4	C _x H _y O ₄	CC(C=O)C(O)=C(O)C=CO	2.82E-09	
184.0624	1.99E-02	7	4	1	5	C _x H _y NO ₅₊	OC1=C(C(O)=O)C=C([N+][O-])=O)C=C1	1.24E-10
199.0941	1.30E-03	7	6	2	5	C _x H _y N ₂ O _z	CC1=C(O)C([N+][O-])=O)CC([N+][O-])=O)C1	3.95E-09

88

89 Table S3: Chemical composition measured by (+)-DART-HR-MS of toluene SOA generated under high-
90 NO conditions with Na₂SO₄ seed. Abundance is defined as ((C_A/C_{IS})/Σ(C_A/C_{IS})).

<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smiles	P _{vap} (atm)
61.0295	2.32E-11	2	4		2	C _x H _y O ₂	CC(O)=O	4.49E-03
69.0690	1.45E-13	4	4		1	C _x H _y O ₁	O1C=CC=C1	2.05E-01
70.0295	6.73E-14	3	3	1	1	C _x H _y NO ₁	C1=NC=CO1	1.03E-01
71.0483	7.34E-13	4	6		1	C _x H _y O ₁	CC=CC=O	8.30E-02
72.0465	1.05E-09	3	5	1	1	C _x H _y NO ₁	C=CC(N)=O	9.20E-06
73.0622	1.50E-13	4	8		1	C _x H _y O ₁	C1CCCO1	2.05E-01

74.0586	1.62E-09	3	7	1	1	C _x H _y NO ₁	C1=NCCO1	9.20E-06
75.0435	8.82E-12	3	6		2	C _x H _y O ₂	CCC(O)=O	4.49E-03
76.0392	1.39E-04	2	5	1	2	C _x H _y NO ₂	NCC(O)=O	2.42E-10
80.0493	1.53E-12	5	5	1		CHN	C1=NC=CC=C1	2.00E-02
83.0817	5.12E-13	5	6		1	C _x H _y O ₁	CC1=CC=CO1	6.70E-02
85.0290	1.94E-11	4	4		2	C _x H _y O ₂	O=CC=CC=O	3.42E-03
87.0424	1.08E-11	4	6		2	C _x H _y O ₂	O=CCCC=O	6.19E-03
89.0399	1.90E-09	3	4		3	C _x H _y O ₃	OC(C(O)=O)C	1.13E-05
93.0408	8.61E-13	6	4		1	C _x H _y O ₁	C12=C(O2)C=CC=C1	1.39E-02
95.0667	1.55E-11	6	6		1	C _x H _y O ₁	OC1=CC=CC=C1	2.02E-03
97.0319	2.33E-10	5	4		2	*C _x H _y O ₂	O=C1C=CC(C1)=O	4.67E-04
98.0499	1.18E-11	4	5	2	1	C _x H _y N ₂ O _z	O=C(N1)CCC1=O	2.15E-03
99.0449	8.68E-12	5	6		2	*C _x H _y O ₂	CC1=CCC(O1)=O	1.37E-02
100.0424	7.35E-08	4	5	1	2	*C _x H _y NO ₂	O=C(N1)CCC1=O	4.71E-07
101.0288	2.73E-11	4	4		3	C _x H _y O ₃	O=C1CCC(O1)=O	2.15E-03
102.0563	1.28E-12	4	7	1	2	*C _x H _y NO ₂	O=C(OCC)C=N	1.89E-02
103.0419	5.57E-11	4	6		3	C _x H _y O ₃	O=C1C(O)CCO1	4.80E-04
104.0360	1.19E-12	3	5	1	3	*C _x H _y NO ₃	C=CC(ON(=O)=O)	2.60E-02
105.0208	1.54E-08	3	4		4	C _x H _y O ₄	OCC(C(O)=O)=O	2.22E-06
107.0623	5.40E-12	7	6		1	C _x H _y O ₁	O=CC1=CC=CC=C1	1.83E-03
110.0604	2.01E-11	6	7	1	1	C _x H _y NO ₁	OC1=CC=C(C)N=C1	7.24E-04
111.0463	1.81E-10	6	6		2	*C _x H _y O ₂	O=CC=CC=CC=O	3.66E-04
113.0461	1.24E-10	6	8		2	*C _x H _y O ₂	O=CCCC=CC=O	4.92E-04
114.0550	1.22E-09	5	7	1	2	*C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
115.0409	1.90E-11	5	6		3	C _x H _y O ₃	O=C1C=C(OC)CO1	4.48E-03
117.0539	1.61E-10	5	8		3	C _x H _y O ₃	O=C1C(C)CC(O)O1	1.91E-04
118.0517	2.29E-12	4	7	1	3	*C _x H _y NO ₃	CC=CC(ON(=O)=O)	8.50E-03
121.0767	1.18E-09	7	4		2	C _x H _y O ₂	O=C(C=C1C)C=CC1=O	8.12E-06
123.0461	1.07E-09	7	6		2	*C _x H _y O ₂	O=CC1=C(O)C=CC=C1	2.77E-05
126.0555	2.00E-08	6	7	1	2	*C _x H _y NO ₂	OC1=NC(O)=CC(C)=C1	1.15E-06
127.0423	2.32E-06	6	6		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
128.0388	2.01E-10	5	5	1	3	C _x H _y NO ₃	CC1=CC(N(O)=O)=CO1	1.44E-04
129.0534	1.48E-06	6	8		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
130.0518	9.07E-11	5	7	1	3	C _x H _y NO ₃	CC1OC=C(N(O)=O)C1	2.27E-04
131.0391	7.73E-11	5	6		4	C _x H _y O ₄	O=C1CC(OC)C(O1)=O	3.64E-04
132.0622	3.95E-11	5	9	1	3	C _x H _y NO ₃	CC1OCC(N(O)=O)C1	3.60E-04
133.0524	4.59E-11	5	8		4	C _x H _y O ₄	O=C1CC(OC)C(O1)=O	3.64E-04
138.0557	3.23E-06	7	7	1	2	*C _x H _y NO ₂	CC1=C(N(O)=O)C=CC=C1	6.57E-09
139.0415	5.49E-07	7	6		3	*C _x H _y O ₃	OC1=C(C=O)C(O)=CC=C1	9.59E-08
141.0544	5.51E-06	7	8		3	C _x H _y O ₃	OC1=C(O)C(C)=CC=C1O	1.06E-08
142.0516	3.42E-11	6	7	1	3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
143.0370	1.59E-05	6	6		4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
145.0509	9.26E-06	6	8		4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
146.0484	1.13E-08	5	7	1	4	C _x H _y NO ₄	O=CC(O)C(N=O)CC=O	1.35E-06
147.0545	4.03E-06	8	6	2	1	C _x H _y N ₂ O _z	O=C(C)NC1=CC=CC=C1	3.04E-09
148.0586	2.25E-07	5	9	1	4	C _x H _y NO ₄	O=CC(O)C(N=O)CCO	4.04E-08
149.0337	9.22E-08	7	4	2	2	C _x H _y NO ₂	CC1=CC(N=O)=CC(N=O)=C1	2.01E-07
152.0686	1.23E-09	8	9	1	2	C _x H _y NO ₂	OC1=CC=C(NC(C)=O)C=C1	1.44E-05
153.0611	1.10E-07	7	8	2	2	C _x H _y N ₂ O _z	CC1=CC(N=O)=CC(N=O)=C1	2.01E-07
154.0511	4.70E-06	7	7	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
155.0397	4.21E-04	7	6		4	*C _x H _y O ₄	O=C(O)C1=C(O)C=CC(O)=C1	1.41E-10

157.0504	2.76E-03	7	8	4	*C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11	
158.0487	6.11E-09	6	7	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1	4.33E-06
159.0467	3.90E-09	10	6	2		C _x H _y O ₂	O=C(C1=C2C=CC=C1)C=CC2=O	8.12E-06
160.0607	3.60E-09	6	9	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1	4.33E-06
161.0475	1.93E-06	6	8	5		C _x H _y O ₅₊	O=CC(O)C(O)C(O)=CC=O	1.34E-08
164.0597	2.75E-07	5	9	1	5	C _x H _y NO ₅₊	O=CC(O)C(N(O)=O)CCO	4.04E-08
165.0593	6.84E-10	9	8	3		C _x H _y O ₃	O=CC1=C(OC)C=CC=C1OC	2.10E-05
167.0682	9.11E-10	9	10	3		C _x H _y O ₃	O=CC1=C(OC)C=CC=C1OC	2.10E-05
168.0610	1.52E-09	8	9	1	3	C _x H _y NO ₃	CC1=C(OC)C=CC(N(O)=O)=C1	1.00E-05
169.0591	5.32E-06	7	8	2	3	C _x H _y N ₂ O _z	CC1=C(O)C(N=O)=CC(N=O)=C1	3.95E-09
170.0479	3.85E-07	7	7	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	5.93E-08
171.0431	3.72E-09	11	6	2		C _x H _y O ₂	O=C(C1=C2C=CC(C)=C1)C=CC2=O	8.12E-06
172.0585	1.18E-08	7	9	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	1.42E-06
173.0473	4.21E-01	7	8	5		C _x H _y O ₅₊	CC1=C(O)C(O)=C(O)C(O)=C1O	8.99E-14
174.0686	1.24E-08	7	11	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	1.42E-06
175.0654	1.98E-01	7	10	5		C _x H _y O ₅₊	CC1=C(O)C(O)=C(O)C(O)=C1O	8.99E-14
177.0571	2.56E-09	10	8	3		C _x H _y O ₃	O=CC1=C(OC=C)C=CC=C1OC	6.85E-06
178.0703	4.31E-08	6	11	1	5	C _x H _y NO ₅₊	O=CCC(ON(O)=O)CCCO	4.69E-07
179.0706	1.88E-09	10	10	3		C _x H _y O ₃	O=CC1=C(OC=C)C=CC=C1OC	6.85E-06
180.0679	3.71E-09	9	9	1	3	C _x H _y NO ₃	CC1=C(OC=C)C=CC(N(O)=O)=C1	3.28E-06
181.0651	6.06E-09	8	8	2	3	C _x H _y N ₂ O _z	O=C(C)NC1=CC=C(N(O)=O)C=C1	2.05E-06
183.0784	8.72E-09	8	10	2	3	C _x H _y N ₂ O _z	CC1=CC=C(N(O)=O)C=C1NC=O	2.05E-06
184.0623	1.10E-09	8	9	1	4	C _x H _y NO ₄	CC1=CC=C(ON(O)=O)C=C1OC	1.00E-05
185.0631	8.24E-08	7	8	2	4	C _x H _y N ₂ O _z	CC1=CC(N(O)=O)=CC(N(O)=O)=C1	2.01E-07
186.0504	6.43E-08	6	7	3	4	C _x H _y N ₂ O _z	CC1=NC(N(O)=O)=CC(N(O)=O)=C1	2.01E-07
187.0626	1.52E-01	8	10	5		C _x H _y O ₅₊	CC1=C(O)C(O)=C(O)C(O)=C1OC	8.99E-14
188.0608	1.39E-06	7	9	1	5	C _x H _y NO ₅₊	CC1=C(O)C(ON(O)=O)=CC=C1O	6.57E-09
189.0518	2.83E-06	6	8	2	5	C _x H _y N ₂ O _z	OC1=C(N(O)=O)C=CC(N(O)=O)=C1	9.29E-09
190.0713	1.84E-06	7	11	1	5	C _x H _y NO ₅₊	CC1=C(O)C(ON(O)=O)=CC=C1O	6.57E-09
192.0828	1.81E-06	7	13	1	5	C _x H _y NO ₅₊	CC1=C(O)C(ON(O)=O)=CC=C1O	6.57E-09
193.0737	3.33E-02	7	12	6		C _x H _y O ₅₊	CC(C(C(O)C1O)O)=C(O)C1O	3.18E-13
194.0700	1.10E-04	6	11	1	6	C _x H _y NO ₅₊	OC1=C(O)C(ON(O)=O)=CC=C1O	9.39E-11
196.0650	3.21E-09	9	9	1	4	C _x H _y NO ₄	CC1=CC=C(ON(O)=O)C=C1OC=C	3.28E-06
199.0618	1.91E-01	9	10	5		C _x H _y O ₅₊	CC1=C(O)C(O)=C(O)C(O)=C1OC=C	8.99E-14
202.0709	5.01E-08	8	11	1	5	C _x H _y NO ₅₊	CC1=C(O)C=C(ON(O)=O)C=C1OC	1.52E-07
267.1719	5.15E-06	14	22	2	3	C _x H _y NO ₃	CC(OC(N=O)=CCCC(C)C=O)C=CCCC	9.81E-09

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92 Table S4: Chemical composition measured by (+)-DART-HR-MS of toluene SOA generated under high-
93 NO conditions with NaCl seed. Abundance is defined as $((C_A/C_{IS})/\sum(C_A/C_{IS}))$.

<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smiles	P _{vap} (atm)
71.0486	1.33E-10	4	6	1		C _x H _y O ₁	CC=CC=O	8.30E-02
74.0597	1.01E-06	3	7	1	1	C _x H _y NO ₁	C1=NCCO1	9.20E-06
75.0442	2.41E-09	3	6	2		C _x H _y O ₂	CCC(O)=O	4.49E-03
76.0391	5.36E-02	2	5	1	2	C _x H _y NO ₂	NCC(O)=O	2.42E-10
80.0497	6.17E-09	5	5	1		CHN	C1=NC=CC=C1	2.00E-02
83.0607	6.29E-10	4	6	2		CHN	C1N=CC=NC1	2.00E-02
84.0450	2.61E-10	4	5	1	1	C _x H _y NO ₁	C1=CNC=CO1	3.35E-02
85.0308	3.85E-09	4	4	2		C _x H _y O ₂	O=CC=CC=O	3.42E-03

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86.0582	2.06E-10	4	7	1	1	C _x H _y NO ₁	C1=CNC=CO1	3.35E-02
87.0447	2.06E-09	4	6		2	C _x H _y O ₂	O=CCCC=O	6.19E-03
88.0405	2.93E-02	3	5	1	2	C _x H _y NO ₂	OC(C=CN)=O	2.42E-10
94.0654	3.57E-10	6	7	1		CHN	CC1=NC=CC=C1	2.00E-02
95.0628	4.11E-10	5	6	2		CHN	CC1=NC=CN=C1	2.00E-02
96.0460	6.69E-09	5	5	1	1	C _x H _y NO ₁	OC1=CC=CN=C1	1.32E-03
97.0644	1.92E-08	6	8		1	C _x H _y O ₁	OC1=CC=CC=C1	2.02E-03
98.0612	1.03E-08	5	7	1	1	C _x H _y NO ₁	OC1=CC=CN=C1	1.32E-03
99.0459	2.33E-09	5	6		2	C _x H _y O ₂	CC1=CCC(O1)=O	1.37E-02
100.0420	3.18E-05	4	5	1	2	C _x H _y NO ₂	O=C(N1)CCC1=O	4.71E-07
102.0570	5.40E-10	4	7	1	2	C _x H _y NO ₂	O=C(OCC)C=N	1.89E-02
104.0364	3.44E-10	3	5	1	3	C _x H _y NO ₃	C=CC(ON(=O)=O)	2.60E-02
110.0612	2.92E-08	6	7	1	1	C _x H _y NO ₁	OC1=CC=C(C)N=C1	7.24E-04
112.0424	6.50E-07	5	5	1	2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
113.0574	4.26E-08	6	8		2	C _x H _y O ₂	O=CCCC=CC=O	4.92E-04
114.0567	5.26E-07	5	7	1	2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
117.0574	3.87E-08	5	8		3	C _x H _y O ₃	O=C1C(C)CC(O)O1	1.91E-04
118.0520	9.87E-10	4	7	1	3	C _x H _y NO ₃	CC=CC(ON(=O)=O)	8.50E-03
126.0565	1.82E-05	6	7	1	2	C _x H _y NO ₂	OC1=NC(O)=CC(C)=C1	1.15E-06
129.0563	3.77E-04	6	8		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
130.0528	3.47E-08	5	7	1	3	C _x H _y NO ₃	CC1OC=C(N(O)=O)C1	2.27E-04
138.0563	2.37E-03	7	7	1	2	C _x H _y NO ₂	CC1=C(N(O)=O)C=CC=C1	6.57E-09
139.0474	2.14E-07	6	6	2	2	C _x H _y N ₂ O _z	CC1=NC=CC(N(O)=O)=C1	7.43E-05
141.0580	1.50E-03	7	8		3	C _x H _y O ₃	OC1=C(O)C(C)=CC=C1O	1.06E-08
142.0522	1.24E-08	6	7	1	3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
143.0435	3.93E-06	5	6	2	3	C _x H _y N ₂ O _z	OC1C=C(N(O)=O)C=NC1	2.82E-06
149.0560	1.14E-09	9	8		2	C _x H _y O ₂	O=C(OC=C)C1=CC=CC=C1	6.19E-03
152.0717	6.51E-07	8	9	1	2	C _x H _y NO ₂	OC1=CC=C(NC(C)=O)C=C1	1.44E-05
153.0670	4.77E-05	7	8	2	2	C _x H _y N ₂ O _z	CC1=CC(N=O)=CC(N=O)=C1	2.01E-07
154.0521	2.33E-03	7	7	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
155.0446	2.44E-05	6	6	2	3	C _x H _y N ₂ O _z	OC1=C(C)N=CC(N(O)=O)=C1	7.09E-07
156.0636	1.41E-03	7	9	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
157.0529	6.31E-01	7	8		4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
159.0688	2.68E-01	7	10		4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
168.0675	8.15E-07	8	9	1	3	C _x H _y NO ₃	CC1=C(OC)C=CC(N(O)=O)=C1	1.00E-05
171.0670	9.92E-03	8	10		4	C _x H _y O ₄	CC1=C(C(O)=CC(O)=C1O)OC	8.36E-10
173.0544	9.91E-08	6	8	2	2	C _x H _y N ₂ O _z	CC1=NC=CC(N(O)=O)=C1	7.43E-05
175.0777	1.91E-07	11	10		2	C _x H _y O ₂	O=C(OC=CC=C)C1=CC=CC=C1	3.34E-05
178.0718	1.44E-05	6	11	1	5	C _x H _y NO ₅₊	O=CCC(ON(O)=O)CCCO	4.69E-07

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95 Table S5: Chemical composition measured by (+)-DART-HR-MS of toluene SOA generated under high-
96 NO conditions with MgSO₄ + H₂SO₄ seed. Abundance is defined as ((C_A/C_{IS})/∑(C_A/C_{IS})).

<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smiles	P _{vap} (atm)
61.02876	3.43E-11	2	4		2	C _x H _y O ₂	CC(O)=O	4.49E-03
71.04839	1.51E-12	4	6		1	C _x H _y O ₁	O1C=CC=C1	8.30E-02
73.06233	3.63E-13	3	3		2	C _x H _y O ₂	CC(C=O)=O	1.90E-01
74.0596	5.85E-09	3	7	1	1	C _x H _y NO ₁	C1=NCCO1	9.20E-06
75.04341	9.47E-12	3	6		2	C _x H _y O ₂	CC(CO)=O	6.92E-03
76.03938	1.19E-04	2	5	1	2	C _x H _y NO ₂	NCC(O)=O	2.42E-10

80.0496	1.34E-11	5	5	1	CHN	C1=NC=CC=C1	2.00E-02
83.08333	9.88E-13	5	6	1	C _x H _y O ₁	CC1=CC=CO1	6.70E-02
85.0292	2.84E-11	4	4	2	C _x H _y O ₂	O=CC=CC=O	3.42E-03
86.05703	7.81E-13	4	7	1 1	C _x H _y NO ₁	C1=CNC=CO1	3.35E-02
87.04151	3.74E-11	4	6	2	C _x H _y O ₂	O=CCCC=O	6.19E-03
88.04571	9.27E-05	3	5	1 2	C _x H _y NO ₂	O=C(C)C(N)=O	2.42E-10
89.05108	7.44E-11	4	8	2	C _x H _y O ₂	O=CCCCO	6.48E-04
91.05025	2.63E-09	3	6	3	C _x H _y O ₃	OC(C(O)=O)C	1.13E-05
94.0651	1.68E-11	6	7	1	C _x H _y O ₁	OC1=CC=CC=C1	2.02E-03
95.06317	2.40E-11	6	6	1	C _x H _y O ₁	OC1=CC=CC=C1	2.02E-03
97.03422	6.88E-10	5	4	2	C _x H _y O ₂	O=C1C=CC(C1)=O	4.67E-04
98.05791	3.85E-08	5	7	1 4	C _x H _y NO ₄	O=CC(O)C(N=O)CC=O	1.35E-06
99.04468	3.19E-11	5	6	2	C _x H _y O ₂	CC1=CCC(O1)=O	1.37E-02
100.0442	1.61E-07	4	5	1 2	C _x H _y NO ₂	O=C(N1)CCC1=O	4.71E-07
101.0258	8.45E-11	4	4	3	C _x H _y O ₃	O=C1CCC(O1)=O	2.15E-03
102.0737	2.18E-12	4	7	1 2	C _x H _y NO ₂	O=C(OCC)C=N	1.89E-02
103.0407	1.26E-10	4	6	3	C _x H _y O ₃	O=C1C(O)CCO1	4.80E-04
104.0359	2.18E-12	3	5	1 3	C _x H _y NO ₃	C=CC(ON(=O)=O)	2.60E-02
105.02	5.93E-08	3	4	4	C _x H _y O ₄	OCC(C(O)=O)=O	2.22E-06
107.0572	1.27E-11	7	6	1	C _x H _y O ₁	O=CC1=CC=CC=C1	1.83E-03
109.101	9.78E-11	7	8	1	C _x H _y O ₁	OC1=C(C)C=CC=C1	6.61E-04
111.0455	6.79E-10	6	6	2	C _x H _y NO ₂	O=N(C1=CC=CC=C1)O	2.87E-04
112.0433	6.16E-11	5	5	1 2	C _x H _y NO ₂	O=C(N1)C=C(C)C1=O	7.03E-04
113.0481	3.49E-10	6	8	2	C _x H _y O ₂	O=CCCC=CC=O	4.92E-04
114.0694	3.42E-09	5	7	1 2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
115.0403	3.93E-10	6	10	2	C _x H _y O ₂	O=CCCCCC=O	6.62E-04
117.0548	5.00E-10	5	8	3	C _x H _y O ₃	O=C1C(C)CC(O)O1	1.91E-04
118.0522	3.53E-12	4	7	1 3	C _x H _y NO ₃	CC=CC(ON(=O)=O)	8.50E-03
119.0361	2.08E-09	4	6	4	C _x H _y O ₄	OC(C(O)C=O)C=O	2.68E-05
123.0442	2.00E-09	7	6	2	C _x H _y O ₂	O=CC1=C(O)C=CC=C1	2.77E-05
125.0584	3.20E-08	7	8	2	C _x H _y O ₂	CC1=C(O)C=CC=C1O	2.29E-06
126.0558	2.39E-08	6	7	1 2	C _x H _y NO ₂	OC1=NC(O)=CC(C)=C1	1.15E-06
127.0416	4.51E-06	6	6	3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
128.0372	4.58E-10	5	5	1 3	C _x H _y NO ₃	CC1=CC(N(O)=O)=CO1	1.44E-04
129.054	3.04E-06	6	8	3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
130.0524	1.32E-10	5	7	1 3	C _x H _y NO ₃	CC1OC=C(N(O)=O)C1	2.27E-04
131.0374	1.92E-10	5	6	4	C _x H _y O ₄	O=C1CC(OC)C(O1)=O	3.64E-04
133.0506	1.35E-10	5	8	4	C _x H _y O ₄	O=C1CC(OC)C(O1)=O	3.64E-04
139.0409	9.50E-07	7	6	3	C _x H _y O ₃	OC1=C(C=O)C(O)=CC=C1	9.59E-08
140.0378	5.64E-11	6	5	1 3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
141.0547	1.91E-05	7	8	3	C _x H _y O ₃	OC1=C(O)C(C)=CC=C1O	1.06E-08
142.0519	8.72E-11	6	7	1 3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
143.0382	3.29E-05	6	6	4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
145.0507	1.53E-05	6	8	4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
149.0345	1.95E-07	7	4	2 2	C _x H _y N ₂ O ₂	CC1=C(N=O)C=CC=C1N=O	2.01E-07
154.0507	6.40E-06	7	7	1 3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
155.0365	1.09E-03	7	6	4	C _x H _y O ₄	O=C(O)C1=C(O)C=CC(O)=C1	1.41E-10
157.0503	4.57E-03	7	8	4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
158.0485	9.14E-09	6	7	1 4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1	4.33E-06
159.0442	2.65E-03	7	10	4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
161.0502	2.13E-06	6	8	5	C _x H _y O ₅₊	O=CC(O)C(O)C(O)=CC=O	1.34E-08

167.0706	6.93E-09	9	10	3	C _x H _y O ₃	CC1=C(OC(C)=O)C=CC=C1O	4.72E-06	
169.0593	1.92E-07	7	8	2	3	C _x H _y N ₂ O _z	CC1=CC(N=O)=CC(N=O)=C1	2.01E-07
170.0476	5.90E-07	7	7	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	5.93E-08
171.0454	7.52E-10	6	6	2	4	C _x H _y N ₂ O _z	CC1=NC=CC(N(O)=O)=C1	7.43E-05
172.0564	1.56E-08	7	9	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	1.42E-06
173.0465	7.45E-01	7	8	5	C _x H _y O ₅₊	CC1=C(O)C(O)=C(O)C(O)=C1O	8.99E-14	
175.0647	2.47E-01	7	10	5	C _x H _y O ₅₊	CC1=C(O)C(O)=C(O)C(O)=C1O	8.99E-14	
185.0866	7.10E-05	9	12	4	C _x H _y O ₄	CC1=CC(O)=C(C(O)=C1OCC)O	3.70E-10	

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98 Table S6: Chemical composition measured by (+)-DART-HR-MS of *o*-cresol SOA generated under high-
 99 NO conditions with (NH₄)₂SO₄ seed. Abundance is defined as ((C_A/C_{IS})/Σ(C_A/C_{IS})).

<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smiles	P _{vap} (atm)
59.04897	1.04E-07	3	6		1	C _x H _y O ₁	CC(C)=O	3.87E-01
71.04891	2.65E-07	4	6		1	C _x H _y O ₁	O=CC(C)=C	8.30E-02
73.06351	8.76E-08	4	8		1	C _x H _y O ₁	CC(CC)=O	1.27E-01
75.04392	2.15E-06	3	6		2	C _x H _y O ₂	CCC(O)=O	4.49E-03
80.04964	3.34E-07	5	5	1		CHN	C1=NC=CC=C1	0.02
85.03067	4.04E-06	4	4		2	C _x H _y O ₂	O=CC=CC=O	3.42E-03
87.04418	2.56E-06	4	6		2	C _x H _y O ₂	O=CCCC=O	6.19E-03
89.05853	8.10E-06	4	8		2	C _x H _y O ₂	O=CCCCO	6.48E-04
93.0419	9.58E-06	5	4		2	C _x H _y O ₂	O=C1C=CC(C1)=O	4.67E-04
97.03836	1.07E-05	4	4	2	1	C _x H _y N ₂ O _z	O=C(N1)CCC1=O	2.15E-03
99.04724	1.81E-06	5	6		2	C _x H _y O ₂	CC1=CCC(O1)=O	1.37E-02
100.0428	2.30E-02	4	5	1	2	C _x H _y NO ₂	O=C(N1)CCC1=O	4.71E-07
101.0582	1.21E-06	5	8		2	C _x H _y O ₂	O=C1CCCCO1	1.37E-02
102.0582	6.09E-07	4	7	1	2	C _x H _y NO ₂	O=C(OCC)C=N	1.89E-02
104.036	5.92E-07	3	5	1	3	C _x H _y NO ₃	C=CC(ON(=O)=O)	2.60E-02
107.0699	5.86E-04	4	10		3	C _x H _y O ₃	OCCOCCO	8.37E-06
110.0621	6.62E-06	6	7	1	1	C _x H _y NO ₁	OC1=CC=C(C)N=C1	0.000724
111.048	5.43E-05	6	6		2	C _x H _y O ₂	O=CC=CC=CC=O	3.66E-04
112.0444	2.62E-04	5	5	1	2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
113.0577	2.97E-05	6	8		2	C _x H _y O ₂	O=CCCC=CC=O	4.92E-04
114.0575	3.56E-04	5	7	1	2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
115.0445	2.96E-06	5	6		3	C _x H _y O ₃	O=C1C=C(OC)CO1	4.48E-03
117.0619	2.04E-03	4	8	2	2	C _x H _y N ₂ O _z	ON=C(C)C(C)=NO	3.30E-06
118.0519	8.54E-07	4	7	1	3	C _x H _y NO ₃	CC=CC(ON(=O)=O)	8.50E-03
119.0665	5.11E-06	5	10		3	C _x H _y O ₃	CCOC(C(C)O)=O	9.92E-04
123.0476	3.20E-04	7	6		2	C _x H _y O ₂	O=CC1=C(O)C=CC=C1	2.77E-05
125.0725	4.62E-02	6	8	2	1	C _x H _y N ₂ O _z	CC1=NC(N(O)=O)=CC(N(O)=O)=C1	2.01E-07
126.0569	5.51E-03	6	7	1	2	C _x H _y NO ₂	OC1=NC(O)=CC(C)=C1	1.15E-06
127.0443	6.47E-01	6	6		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
128.0661	4.40E-04	6	9	1	2	C _x H _y NO ₂	N=CCC=C(O)CC=O	2.00E-05
129.0592	3.33E-01	6	8		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
130.0532	2.76E-05	5	7	1	3	C _x H _y NO ₃	CC1OC=C(N(O)=O)C1	2.27E-04
132.0652	1.14E-05	5	9	1	3	C _x H _y NO ₃	CC1OCC(N(O)=O)C1	3.60E-04
136.0604	1.73E-06	4	9	1	4	C _x H _y NO ₄	O=N(O)OCCC(O)C	1.84E-03
138.0569	7.55E-01	7	7	1	2	C _x H _y NO ₂	CC1=C(N(O)=O)C=CC=C1	6.57E-09
139.0457	1.29E-01	7	6		3	C _x H _y O ₃	OC1=C(C=O)C(O)=CC=C1	9.59E-08
140.0655	4.97E-05	7	9	1	2	C _x H _y NO ₂	CC(C=CC1)=CC1N(O)=O	1.49E-04

141.0624	1.01E+00	6	8	2	2	C _x H _y N ₂ O _z	OC1=C(N(O)=O)C=CC(N(O)=O)=C1	9.29E-09
142.0521	8.14E-06	6	7	1	3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
143.0724	3.27E+00	7	10		3	C _x H _y O ₃	CC(C=O)C(O)=C(O)C=CO	2.82E-09
144.0658	5.37E-04	6	9	1	3	C _x H _y NO ₃	OC1CC(N(O)=O)CC=C1	6.86E-06
145.054	2.06E+00	6	8		4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
147.0693	2.70E-02	6	10		4	C _x H _y O ₄	O=CCC(O)C(O)CC=O	1.48E-07
149.0301	5.43E-04	8	4		3	C _x H _y O ₃	O=C1C2=CC=CC=C2C(O1)=O	1.55E-05
152.0727	3.31E-04	8	9	1	2	C _x H _y NO ₂	OC1=CC=C(NC(C)=O)C=C1	1.44E-05
153.0922	2.81E-04	9	12		2	C _x H _y O ₂	CC1=C(OCC)C(O)=CC=C1	3.01E-05
154.055	1.21E+00	7	7	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
155.0409	1.17E+02	7	6		4	C _x H _y O ₄	O=C(O)C1=C(O)C=CC(O)=C1	1.41E-10
156.0622	1.10E+00	7	9	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
157.0534	4.41E+02	7	8		4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
158.052	1.50E-03	6	7	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1	4.33E-06
159.1065	1.32E-05	8	14		3	C _x H _y O ₃	CC(C)C(OC(C(C)C)=O)=O	5.01E-04
160.0636	9.29E-04	6	9	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1	4.33E-06
161.0699	2.03E-03	9	8	2	1	C _x H _y N ₂ O _z	OC1=CC=C(C2=NC=CN2)C=C1	1.89E-06
162.0724	5.26E-01	6	11	1	4	C _x H _y NO ₄	N=CC(O)C(O)C(O)CC=O	7.54E-09
164.065	1.21E-04	9	9	1	2	C _x H _y NO ₂	O=C(C)C1=NC(C(C)=O)=CC=C1	3.06E-05
167.072	3.50E-04	9	10		3	C _x H _y O ₃	O=CC1=C(OC)C=CC=C1OC	2.10E-05
168.0662	5.40E-04	8	9	1	3	C _x H _y NO ₃	CC1=C(OC)C=CC(N(O)=O)=C1	1.00E-05
169.0824	9.86E-04	9	12		3	C _x H _y O ₃	CC1=C(OC)C=C(O)C=C1OC	7.56E-06
171.0693	7.12E+03	7	6		5	C _x H _y O ₅₊	OC1=C(C=O)C(O)=CC(O)=C1O	9.84E-13
172.0635	3.57E-03	7	9	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	1.42E-06
174.0764	2.89E-03	7	11	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	1.42E-06
175.0752	6.61E-04	11	10		2	C _x H _y O ₂	CC1=C(OC=CC(C)=O)C=CC=C1	6.85E-06
178.0689	9.50E-03	6	11	1	5	C _x H _y NO ₅₊	O=CCC(ON(O)=O)CCCO	4.69E-07
179.0758	1.04E-03	10	10		3	C _x H _y O ₃	OC(C1=C(OC)C=CC=C1OC)=C	4.94E-06
180.0687	1.40E-03	9	9	1	3	C _x H _y NO ₃	CC1=C(OC=C)C=CC(N(O)=O)=C1	3.28E-06
185.0965	4.52E-04	13	12		1	C _x H _y O ₁	CC1=CC(OC2=CC=CC=C2)=CC=C1	1.11E-05
187.0794	6.88E-03	12	10		2	C _x H _y O ₂	OC(C=C1)=CC=C1OC2=CC=CC=C2	5.11E-07
189.0916	5.78E-03	12	12		2	C _x H _y O ₂	OC1C=CC(OC2=CC=CC=C2)=CC1	5.11E-07
190.0757	5.01E-01	7	11	1	5	C _x H _y NO ₅₊	CC1=C(O)C(ON(O)=O)=CC=C1O	6.57E-09
193.0865	7.73E-04	11	12		3	C _x H _y O ₃	CC1=C(OCC(CC=O)=O)C=CC=C1	5.72E-06
195.1377	2.02E-04	12	18		2	C _x H _y O ₂	CC(OC1=CC=CC=C1OC(C)C)C	4.38E-05
196.0688	1.27E-03	9	9	1	4	C _x H _y NO ₄	CC1=CC=C(ON(O)=O)C=C1OC=C	3.28E-06
197.074	4.48E-01	12	8	2	1	C _x H _y N ₂ O _z	N=CC1=CC=C(N=C1)C2=CC=C(O)C=C2	1.07E-08
198.0689	1.11E-03	9	11	1	4	C _x H _y NO ₄	CC1=CC=C(C=C1OCC)ON(O)=O	3.28E-06
199.1665	8.32E-05	12	22		2	C _x H _y O ₂	CC(OC1C(OC(C)C)=CCCC1)C	6.94E-05
201.0986	3.15E-01	12	12	2	1	C _x H _y N ₂ O _z	N=CC1=CC=C(N=C1)C2=CC=C(O)C=C2	1.07E-08
205.0858	1.40E-02	12	12		3	C _x H _y O ₃	CC1=C(OCC(C=CC=O)=O)C=CC=C1	3.04E-07
215.1248	1.07E+00	11	18		4	C _x H _y O ₄	CC1CC(O)C=CC1OC(O)CCC=O	3.11E-09
217.137	4.15E-02	13	16	2	1	C _x H _y N ₂ O _z	N=CC1=CC=C(N=C1)C2=CC=C(OC)C=C2	7.57E-08
221.1425	2.19E-02	10	20		5	C _x H _y O ₅₊	O1CCOCCOCCOCCOCC1	1.79E-07
225.078	3.56E+01	11	12		5	C _x H _y O ₅₊	OC1=C(OCC)C(OC=C)=C(C=O)C(O)=C1	1.17E-10
227.1329	5.83E+00	12	18		4	C _x H _y O ₄	CC1=CC(O)C=CC1OC(O)CCCC=O	6.42E-10
231.1549	5.48E+00	12	22		4	C _x H _y O ₄	CC1CC(O)CCC1OC(O)CCCC=O	4.71E-10
233.1337	5.06E+02	11	20		5	C _x H _y O ₅₊	CC1CC(O)CC(O)C1OC(O)CCC=O	4.68E-12
371.3153	5.63E+02	22	42		4	C _x H _y O ₄	CC1CCCCC1OCCCO(O)CCCCOC2CCCCC2C	5.58E-12

101 Table S7: Chemical composition measured by (+)-DART-HR-MS of *m*-cresol SOA generated under
 102 high-NO conditions with (NH₄)₂SO₄ seed. Abundance is defined as ((C_A/C_{IS})/Σ(C_A/C_{IS})).

<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smies	P _{vap} (atm)
71.0487	2.70E-15	4	6		1	C _x H _y O ₁	CC=CC=O	8.30E-02
73.0626	5.43E-16	4	8		1	C _x H _y O ₁	C1CCCO1	2.05E-01
74.0597	1.56E-11	3	7	1	1	C _x H _y NO ₁	C1=NCCO1	9.20E-06
75.0440	1.81E-14	3	6		2	C _x H _y O ₂	CC(CO)=O	6.92E-03
76.0392	6.53E-07	2	5	1	2	C _x H _y NO ₂	NCC(O)=O	2.42E-10
80.0494	7.16E-15	5	5	1		CHN	C1=NC=CC=C1	2.00E-02
84.0450	3.37E-15	4	5	1	1	C _x H _y NO ₁	C1=CNC=CO1	3.35E-02
85.0295	8.64E-14	4	4		2	C _x H _y O ₂	O=CC=CC=O	3.42E-03
86.0598	6.42E-15	4	7	1	1	C _x H _y NO ₁	C1=CNC=CO1	3.35E-02
87.0431	3.81E-14	4	6		2	C _x H _y O ₂	O=CCCC=O	6.19E-03
90.0516	1.03E-13	3	7	1	2	C _x H _y NO ₂	OC1NCOC1	1.18E-03
94.0657	2.70E-14	6	7	1		CHN	CC1=NC=CC=C1	2.00E-02
95.0584	9.68E-15	5	6	2		CHN	CC1=NC=CN=C1	2.00E-02
97.0637	7.92E-13	6	8		1	C _x H _y O ₁	OC1=CC=CC=C1	2.02E-03
98.0617	3.64E-13	5	7	1	1	C _x H _y NO ₁	OC1=CC=CN=C1	1.32E-03
99.0454	6.84E-14	5	6		2	C _x H _y O ₂	CC1=CCC(O1)=O	1.37E-02
102.0563	2.52E-14	4	7	1	2	C _x H _y NO ₂	O=C(OCC)C=N	1.89E-02
104.0366	6.23E-15	3	5	1	3	C _x H _y NO ₃	C=CC(ON(=O)=O)	2.60E-02
105.0209	5.22E-11	3	4		4	C _x H _y O ₄	OCC(C(O)=O)=O	2.22E-06
110.0614	3.04E-13	6	7	1	1	C _x H _y NO ₁	OC1=CC=C(C)N=C1	7.24E-04
111.0462	2.47E-12	6	6		2	C _x H _y O ₂	O=CC=CC=CC=O	3.66E-04
112.0446	4.10E-13	5	5	1	2	C _x H _y NO ₂	O=C(N1)C=C(C)C1=O	7.03E-04
113.0580	2.64E-12	6	8		2	C _x H _y O ₂	O=CCCC=CC=O	4.92E-04
114.0572	1.96E-11	5	7	1	2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
115.0411	1.67E-13	5	6		3	C _x H _y O ₃	O=C1C=C(OC)CO1	4.48E-03
116.0694	1.15E-11	5	9	1	2	C _x H _y NO ₂	O=C(O)C1CCCN1	2.57E-05
117.0567	1.20E-12	5	8		3	C _x H _y O ₃	O=C1C(C)CC(O)O1	1.91E-04
118.0521	1.73E-14	4	7	1	3	C _x H _y NO ₃	CC=CC(ON(=O)=O)	8.50E-03
123.0467	6.09E-12	7	6		2	C _x H _y O ₂	O=CC1=C(O)C=CC=C1	2.77E-05
125.0607	8.60E-11	7	8		2	C _x H _y O ₂	CC1=C(O)C=CC=C1O	2.29E-06
126.0565	1.94E-10	6	7	1	2	C _x H _y NO ₂	OC1=NC(O)=CC(C)=C1	1.15E-06
127.0425	1.74E-08	6	6		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
128.0698	3.72E-10	6	9	1	2	C _x H _y NO ₂	OC(C1)=NC(O)=CC1C	1.82E-06
129.0567	1.76E-08	6	8		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
130.0552	1.17E-12	5	7	1	3	C _x H _y NO ₃	CC1OC=C(N(O)=O)C1	2.27E-04
131.0367	1.33E-12	5	6		4	C _x H _y O ₄	O=C1CC(OC)C(O1)=O	3.64E-04
132.0653	6.15E-13	5	9	1	3	C _x H _y NO ₃	CC1OCC(N(O)=O)C1	3.60E-04
133.0538	3.02E-13	5	8		4	C _x H _y O ₄	O=C1CC(OC)C(O1)=O	3.64E-04
137.0568	7.11E-10	7	8	2	1	C _x H _y N ₂ O _z	CC1=CC(N=O)=CC(N=O)=C1	2.01E-07
138.0561	2.86E-08	7	7	1	2	C _x H _y NO ₂	CC1=C(N(O)=O)C=CC=C1	6.57E-09
139.0450	5.45E-09	7	6		3	C _x H _y O ₃	OC1=CC=CC=C1C(O)=O	5.80E-08
140.0669	2.95E-12	7	9	1	2	C _x H _y NO ₂	CC1=C(CCC=C1)N(O)=O	9.39E-05
141.0555	6.23E-08	7	8		3	C _x H _y O ₃	OC1=C(O)C(C)=CC=C1O	1.06E-08
142.0527	3.79E-13	6	7	1	3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
143.0381	1.05E-07	6	6		4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
144.0652	1.49E-13	6	9	1	3	C _x H _y NO ₃	O=N(O)OC1=CCCC=C1	9.08E-04
145.0524	5.45E-08	6	8		4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09

148.0622	3.35E-09	5	9	1	4	C _x H _y NO ₄	O=CC(O)C(N=O)CCO	4.04E-08
149.0476	1.73E-06	5	8		5	C _x H _y O ₅₊	OC1OC(CO)=C(O)C1O	6.50E-11
151.0858	2.33E-11	8	10	2	1	C _x H _y N ₂ O _z	CC(N=O)=CC=CC=CC=N	6.43E-06
152.0710	9.80E-12	8	9	1	2	C _x H _y NO ₂	OC1=CC=C(NC(C)=O)C=C1	1.44E-05
153.0667	1.37E-09	7	8	2	2	C _x H _y N ₂ O _z	CC1=CC(N=O)=CC(N=O)=C1	2.01E-07
154.0536	7.58E-08	7	7	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
155.0361	1.46E-05	7	6		4	C _x H _y O ₄	O=C(O)C1=C(O)C=CC(O)=C1	1.41E-10
157.0509	1.86E-05	7	8		4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
159.0669	5.58E-08	7	10		4	C _x H _y O ₄	CC(C=O)C(O)=C(O)C=CO	2.82E-09
160.0631	3.10E-11	6	9	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1	4.33E-06
161.0498	9.42E-09	6	8		5	C _x H _y O ₅₊	O=CC(O)C(O)C(O)=CC=O	1.34E-08
162.0737	2.94E-11	6	11	1	4	C _x H _y NO ₄	OC1CCCC(ON(O)=O)C1	4.00E-06
163.0712	8.11E-08	5	10	2	4	C _x H _y N ₂ O _z	COC(C(NC(N)=O)CO)=O	1.33E-09
164.0553	4.88E-09	5	9	1	5	C _x H _y NO ₅₊	O=CC(O)C(N(O)=O)CCO	4.04E-08
165.0657	5.21E-11	8	8	2	2	C _x H _y N ₂ O _z	O=C(C)NC1=CC=C(N(O)=O)C=C1	2.05E-06
167.0714	9.28E-12	9	10		3	C _x H _y O ₃	O=CC1=C(OC)C=CC=C1OC	2.10E-05
168.0673	1.65E-11	8	9	1	3	C _x H _y NO ₃	CC1=C(OC)C=CC(N(O)=O)=C1	1.00E-05
169.0612	8.22E-08	7	8	2	3	C _x H _y N ₂ O _z	CC1=C(N=O)C=C(N=O)C=C1O	3.04E-09
170.0557	1.09E-09	6	7	3	3	C _x H _y N ₂ O _z	CC1=NC(N(O)=O)=CC(N(O)=O)=C1	2.01E-07
171.0610	2.56E-07	8	10		4	C _x H _y O ₄	CC1=C(C(O)=CC(O)=C1O)OC	8.36E-10
172.0642	1.22E-10	7	9	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	1.42E-06
173.0568	1.71E-08	6	8	2	4	C _x H _y N ₂ O _z	OC1=C(N(O)=O)C=CC(N(O)=O)=C1	9.29E-09
174.0765	1.21E-10	7	11	1	4	C _x H _y NO ₄	OC1=CC(ON(O)=O)=CC=C1C	1.42E-06
177.0664	3.25E-10	9	8	2	2	C _x H _y N ₂ O _z	O=C1N=C(N)OC1C2=CC=CC=C2	3.86E-07
178.0682	6.02E-10	6	11	1	5	C _x H _y NO ₅₊	O=CCC(ON(O)=O)CCCO	4.69E-07
179.0709	1.72E-11	10	10		3	C _x H _y O ₃	O=CC1=C(OC=C)C=CC=C1OC	6.85E-06
180.0678	4.63E-11	9	9	1	3	C _x H _y NO ₃	CC1=C(OC=C)C=CC(N(O)=O)=C1	3.28E-06
181.0752	6.52E-10	7	8	2	2	C _x H _y N ₂ O _z	CC1=C(N=O)C=C(N=O)C=C1	2.01E-07
183.0726	8.08E-11	8	10	2	3	C _x H _y N ₂ O _z	CC1=CC=C(N(O)=O)C=C1NC=O	2.05E-06
185.0754	4.00E-07	9	12		4	C _x H _y O ₄	CC1=C(OCC)C(O)=CC(O)=C1O	2.73E-10
190.0737	1.71E-08	7	11	1	5	C _x H _y NO ₅₊	CC1=C(O)C(ON(O)=O)=CC=C1O	6.57E-09
195.0857	9.68E-01	7	14		6	C _x H _y O ₅₊	OC1C(O)C(O)C(O)C(O)C1CO	1.85E-16
197.0738	1.61E-08	12	8	2	1	C _x H _y N ₂ O _z	N=CC1=CC=C(N=C1)C2=CC=C(O)C=C2	1.07E-08
198.0744	4.30E-11	9	11	1	4	C _x H _y NO ₄	CC1=CC=C(ON(O)=O)C=C1OC=C	3.28E-06
207.0737	1.57E-09	10	10	2	3	C _x H _y N ₂ O _z	OC1=C2C=C(OC)C(OC)=CC2=NC=N1	6.61E-08
209.0813	4.07E-06	11	12		4	C _x H _y O ₄	CC1=C(OC=CC=C)C(O)=CC(O)=C1O	2.92E-11
223.0799	3.17E-02	8	14		7	C _x H _y O ₅₊	OC1C(O)C(O)C(O)C(O)C1COC=O	4.14E-15

103

104 Table S8: Chemical composition measured by (+)-DART-HR-MS of *p*-cresol SOA generated under high-
105 NO conditions with (NH₄)₂SO₄ seed. Abundance is defined as ((C_A/C_{IS})/Σ(C_A/C_{IS})).

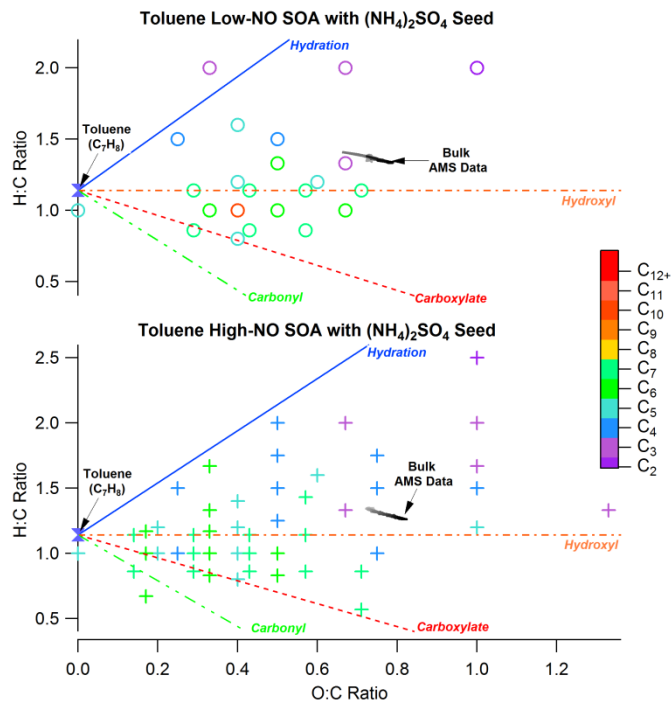
<i>m/z</i> (Da)	Abundance	C	H	N	O	Category	Smiles	P _{vap} (atm)
71.0490	1.75E-13	4	6		1	C _x H _y O ₁	CC=CC=O	8.30E-02
73.0637	3.50E-14	4	8		1	C _x H _y O ₁	C1CCCO1	2.05E-01
75.0440	1.08E-12	3	6		2	C _x H _y O ₂	CC(CO)=O	6.92E-03
80.0499	1.28E-12	5	5	1		CHN	C1=NC=CC=C1	2.00E-02
85.0306	2.65E-12	4	4		2	C _x H _y O ₂	O=CC=CC=O	3.42E-03
87.0443	1.73E-12	4	6		2	C _x H _y O ₂	O=CCCC=O	6.19E-03
94.0656	2.04E-13	6	7	1		CHN	CC1=NC=CC=C1	2.00E-02
97.0654	3.17E-11	6	8		1	C _x H _y O ₁	OC1=CC=CC=C1	2.02E-03

99.0464	1.94E-12	5	6		2	C _x H _y O ₂	CC1=CCC(O1)=O	1.37E-02
101.0584	1.62E-12	5	8		2	C _x H _y O ₂	CC=CCC(O)=O	6.19E-03
110.0618	1.01E-11	6	7	1	1	C _x H _y NO ₁	N=CC=CC=CC=O	3.66E-04
111.0469	5.29E-11	6	6		2	C _x H _y O ₂	O=CC=CC=CC=O	3.66E-04
113.0585	3.87E-11	6	8		2	C _x H _y O ₂	O=CCCC=CC=O	4.92E-04
114.0581	2.80E-10	5	7	1	2	C _x H _y NO ₂	OC(C1=NCCC1)=O	2.57E-05
115.0418	3.60E-12	5	6		3	C _x H _y O ₃	O=C1C=C(OC)CO1	4.48E-03
123.0472	2.32E-10	7	6		2	C _x H _y O ₂	O=CC1=C(O)C=CC=C1	2.77E-05
125.0630	2.77E-09	7	8		2	C _x H _y O ₂	CC1=C(O)C=CC=C1O	2.29E-06
126.0566	4.35E-09	6	7	1	2	C _x H _y NO ₂	OC1=NC(O)=CC(C)=C1	1.15E-06
129.0572	3.91E-11	6	8		3	C _x H _y O ₃	O=C1C(C)CC(O)O1	1.91E-04
138.0559	5.08E-07	7	7	1	2	C _x H _y NO ₂	CC1=C(N(O)=O)C=CC=C1	6.57E-09
141.0562	4.05E-07	7	8		3	C _x H _y O ₃	OC1=C(O)C=CC=C1O	3.24E-08
142.0533	5.07E-12	6	7	1	3	C _x H _y NO ₃	O=N(OC1=CC=CC=C1)O	9.08E-04
143.0420	5.47E-11	5	6	2	3	C _x H _y N ₂ O _z	N=CC(C(O)C(C=O)=N)=O	1.14E-04
145.0531	9.91E-07	6	8		4	C _x H _y O ₄	O=C(O)C=CC=CC(O)=O	3.29E-09
149.0304	2.55E-08	7	4	2	2	C _x H _y N ₂ O _z	CC1=C(N=O)C=CC=C1N=O	2.01E-07
154.0544	7.72E-07	7	7	1	3	C _x H _y NO ₃	CC1=C(O)C(ON(=O)=O)=CC=C1O	6.57E-09
155.0384	1.11E-04	7	6		4	C _x H _y O ₄	O=C(O)C1=C(O)C=CC(O)=C1	1.41E-10
157.0515	4.04E-04	7	8		4	C _x H _y O ₄	CC1=C(O)C(O)=CC(O)=C1O	2.35E-11
159.0630	1.34E-06	7	10		4	C _x H _y O ₄	CC(C=O)C(O)=C(O)C=CO	2.82E-09
167.0660	2.20E-10	9	10		3	C _x H _y O ₃	O=CC1=C(OC)C=CC=C1OC	2.10E-05
171.0619	5.39E-06	8	10		4	C _x H _y O ₄	CC1=C(C(O)=CC(O)=C1O)OC	8.36E-10
173.0514	2.24E-08	6	8	2	4	C _x H _y N ₂ O _z	CC1=NC(N(O)=O)=CC(N(O)=O)=C1	2.01E-07
175.1008	1.53E-06	8	14		4	C _x H _y O ₄	CC(C(OC)C(CC1O)O)=C1O	2.42E-09
178.0700	7.86E-09	6	11	1	5	C _x H _y NO ₅₊	O=CCC(ON(O)=O)CCCO	4.69E-07
179.0726	5.02E-10	10	10		3	C _x H _y O ₃	O=CC1=C(OC=C)C=CC=C1OC	6.85E-06
183.0803	1.89E-09	8	10	2	3	C _x H _y N ₂ O _z	CC1=CC=C(N(O)=O)C=C1NC=O	2.05E-06
191.0814	5.50E-08	10	10	2	2	C _x H _y N ₂ O _z	OC1=C2C=C(OC)C(OC)=CC2=NC=N1	6.61E-08
193.0883	7.05E-10	11	12		3	C _x H _y O ₃	CC1=C(OCC(CC=O)=O)C=CC=C1	5.72E-06
195.1313	1.92E-06	7	8	2	4	C _x H _y N ₂ O _z	CC1=C(N=O)C=C(N=O)C=C1O	3.04E-09
199.0679	5.07E-10	8	10	2	4	C _x H _y N ₂ O _z	CC(N=O)=CC=CC=CC=N	6.43E-06
207.0769	4.86E-08	10	10	2	3	C _x H _y N ₂ O _z	OC1=C2C=C(OC)C(OC)=CC2=NC=N1	6.61E-08
209.0831	1.23E-04	11	12		4	C _x H _y O ₄	CC1=C(OC=CC=C)C(O)=CC(O)=C1O	2.92E-11
223.0787	9.99E-01	8	14		7	C _x H _y O ₅₊	OC1C(O)C(O)C(O)C(O)C1COC=O	4.14E-15

106

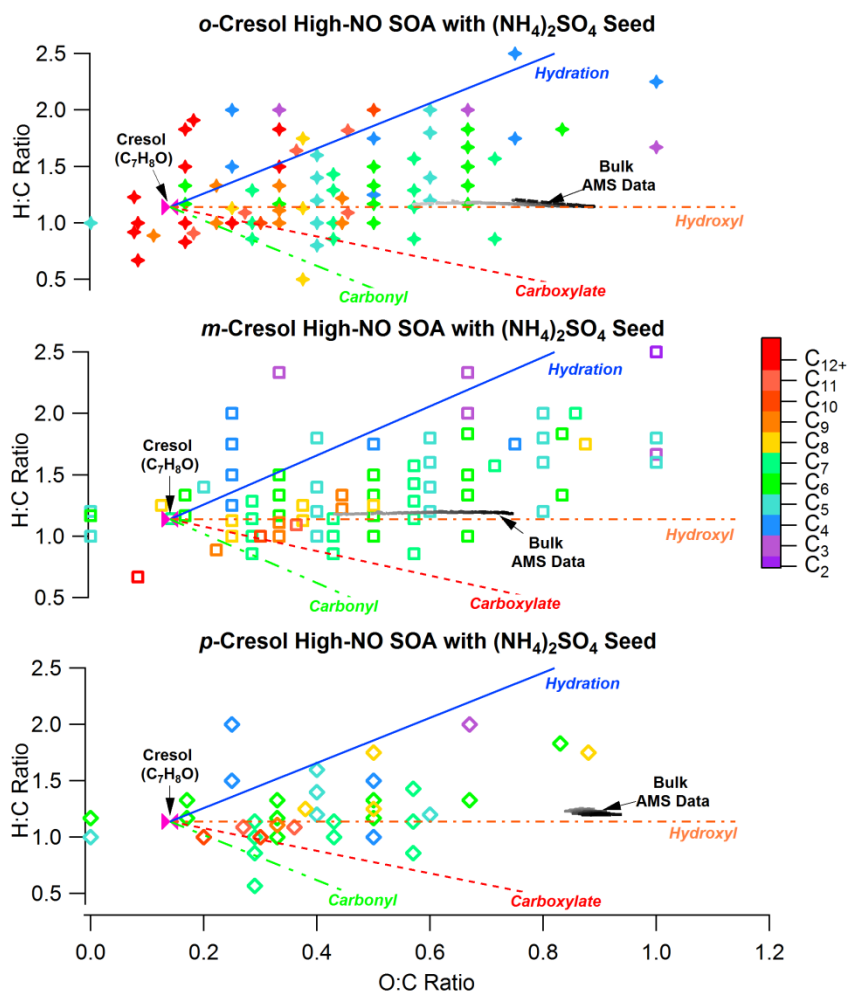
107

108 Annotated van Krevelen Diagrams of DART-HR-MS and HR-AMS Data for Toluene and Cresol
109 SOA



110
111 **Figure S4.** Chemical composition of toluene SOA produced under low- and high-NO conditions
112 with (NH₄)₂SO₄ seed, as measured by offline DART-HR-MS, are displayed in van Krevelen
113 space. Data markers are colored by the molecular formula carbon number and sized by the
114 logarithm of the mixing ratio for each molecular formula. The bulk SOA H:C and O:C elemental
115 ratios derived from HR-AMS measurements are shown in grayscale.

116



117

118 **Figure S5.** Chemical composition of cresol SOA produced under high-NO conditions with
 119 (NH₄)₂SO₄ seed, as measured by offline DART-HR-MS, are displayed in van Krevelen space.
 120 Data markers are colored by the molecular formula carbon number and sized by the logarithm of
 121 the mixing ratio for each molecular formula. The bulk SOA H:C and O:C elemental ratios
 122 derived from HR-AMS measurements are shown in grayscale.

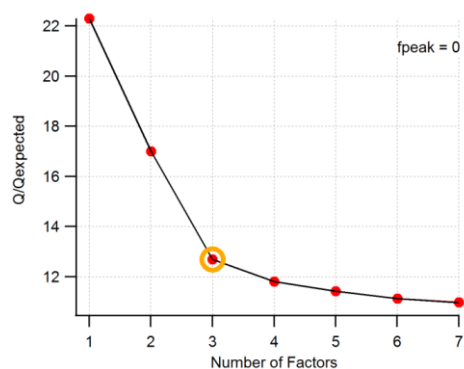
123

124 *PMF Analysis Details*

125 Positive matrix factorization (PMF) was performed on AMS data collected from toluene
 126 and *o*-cresol high-NO experiments. PMF analysis was conducted in two ways. First, each
 127 experiment was analyzed separately to explore the number of factors that could explain the
 128 variations in AMS spectra for a single experimental condition. Second, the data from each

129 experiment was combined into a unified PMF analysis to determine if common factors could be
130 resolved from toluene and o-cresol SOA formation. The results from both analyses were
131 compared to assess the reliability of using PMF on a unified dataset. The same factors were
132 resolved with both methods. The following discussion focuses on the PMF solution for the
133 unified toluene and o-cresol SOA dataset.

134 PMF analysis was performed using the PMF evaluation tool v. 2.04 in Igor Pro V6.36.
135 The organic signal matrix and corresponding errors were calculated via the procedures outlined
136 by Ulbrich et al.² Organic fragments with an average signal-to-noise ratio (SNR) lower than 0.2
137 were removed from analysis. Fragments with an average SNR between 0.2 and 2 were down-
138 weighted by increasing their corresponding errors by a factor of 3 as recommended by Paatero
139 and Hopke.³ The time series of the remaining ion fragments were analyzed for significant trends.
140 Ion fragments with time series trends that did not change significantly from the average
141 background signal ($< 3\sigma$) were removed from analysis. The PMF solution space was explored for
142 seven factors with 1-10 seeds and $-1 < f_{peak} < 1$. The number of factors was chosen to minimize the
143 goodness of fit parameter, $Q/Q_{expected}$.

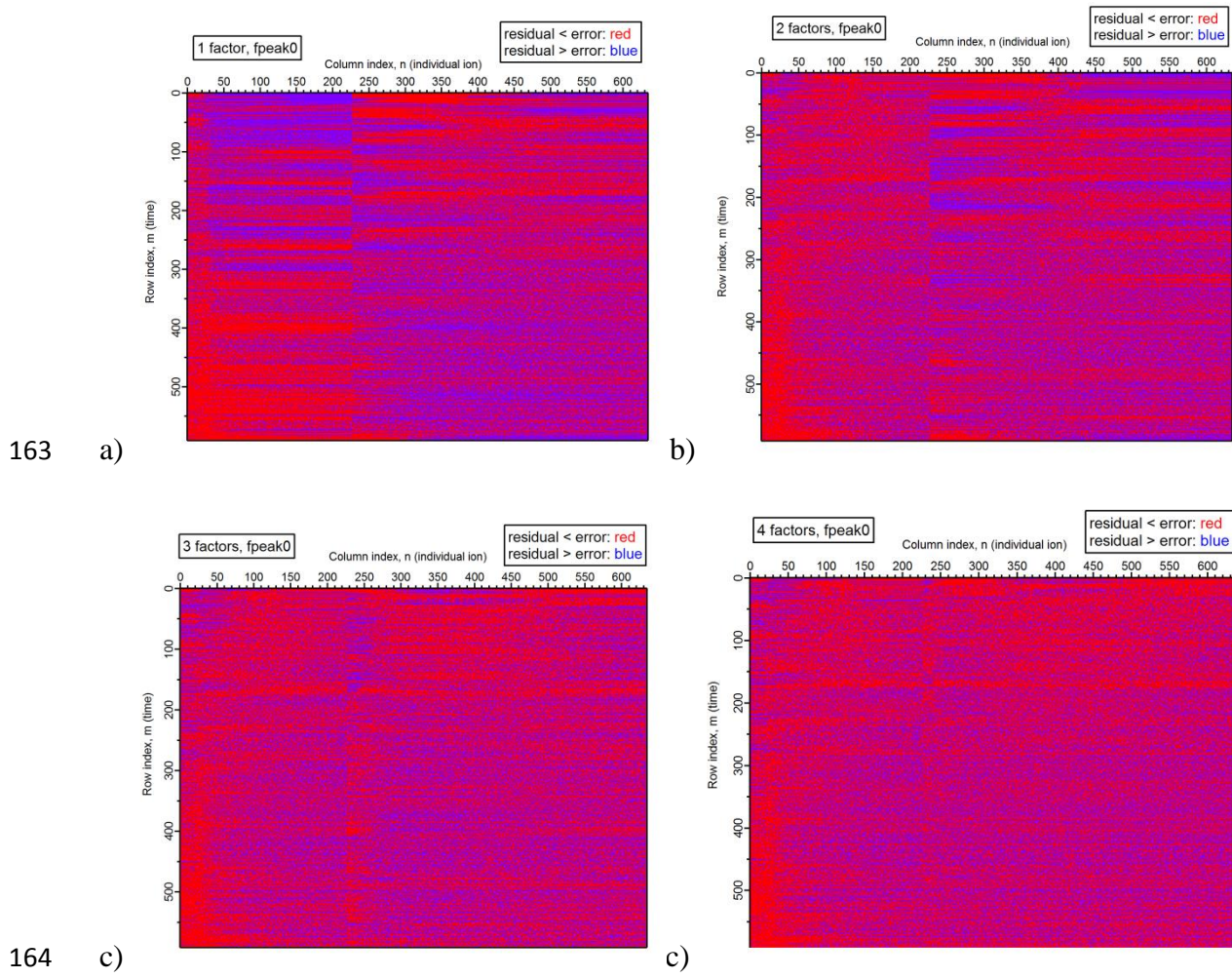


144
145 **Figure S6.** $Q/Q_{expected}$ vs. the number of factors. The chosen solution is highlighted by the yellow
146 circle.

147 Figure S6 demonstrates that solutions with factor spaces > 3 , do not change significantly
148 with respect to $Q/Q_{expected}$. As discussed by Craven et al., a sufficient number of factors is
149 determined when the solution does not drastically improve with an increase in the number of
150 factors fit to the data.⁴

151 Figures S7 and S8 further justify the choice of a 3-factor solution. Figure S8 visualizes
152 the solution optimization by plotting the absolute residual: error ratio as a function of m/z and
153 time. Pixels with a ratio < 1 are colored red whereas those with a ratio > 1 are colored blue. Data
154 are sufficiently fit when no clear structure is observed, or subsequent factors do not improve the
155 randomness of the pixels. A one-factor fit exhibits clear structure in the solution space, indicating
156 that additional factors are needed to explain the variation in the data. This structure disappears
157 when three factors are fit to the data, and no clear improvement is seen when four or more
158 factors are fitted, suggesting that a three-factor solution is sufficient to capture data variation. As
159 discussed by Craven et al., these factors in chamber studies represent time series of groups or
160 fractions of ions that can be connected to different events like gas-particle partitioning and
161 specific generations of gas-phase oxidation.⁴

162



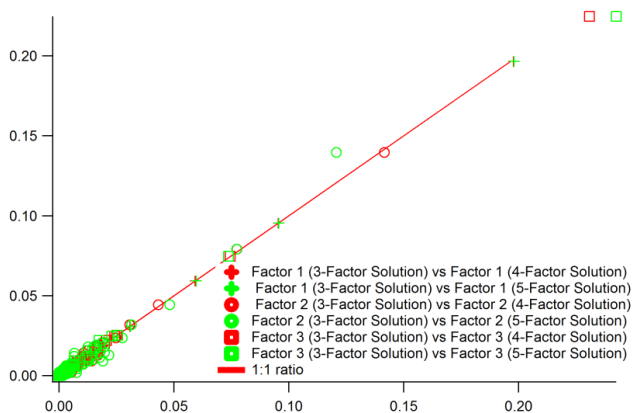
163 a)

b)

164 c)

c)

165 **Figure S7.** Maps for the one (panel a), two (panel b), three (panel c), and four (panel d) factor
 166 solutions. A red dot symbolizes where the $residual_{ij} > error_{ij}$. A blue dot symbolizes where the
 167 $residual_{ij} < -error_{ij}$.

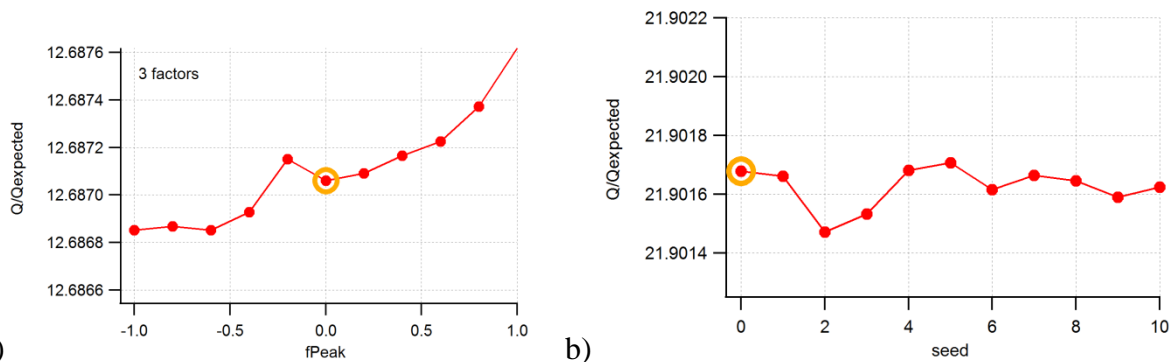


168

169 **Figure S8.** Comparisons of factors 1, 2, and 3 mass spectra between three-factor and four- or five-factor
 170 solutions.

171 Figure S8 reiterates the conclusions drawn from Figure S7. When the mass spectra of a 3-
 172 factor solution are compared to those of 4 and 5-factor solutions, we find that factors 1, 2, and 3
 173 do not change significantly with increasing factor spaces. Thus, the resolved factors are robustly
 174 resolved in higher factor spaces without significant splitting or reallocation of information
 175 amongst factors 1, 2, and 3.

176 For a given number of factors, there could be multiple solutions that yield an equal fit. To
 177 investigate the robustness of the 3-factor solution, one may explore how the solution changes as
 178 a function of seed and f_{peak} .⁴ A detailed discussion about solution robustness in field
 179 measurement data is provided in Coggon et al.⁵ In the solution discussed here, $Q/Q_{expected}$ was
 180 relatively uniform over all explored seed and f_{peak} values (Figure S9).

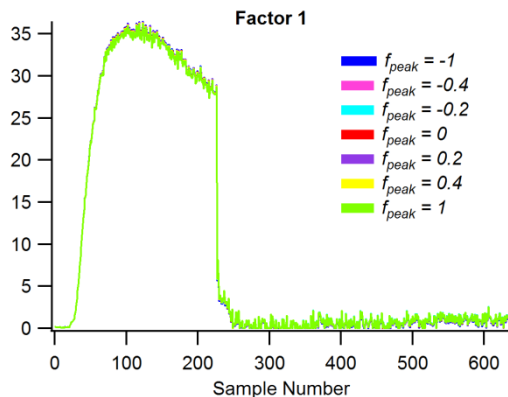


181 a) **Figure S9.** $Q/Q_{expected}$ vs. f_{peak} values (panel a) and vs. seed number (panel b).
 182

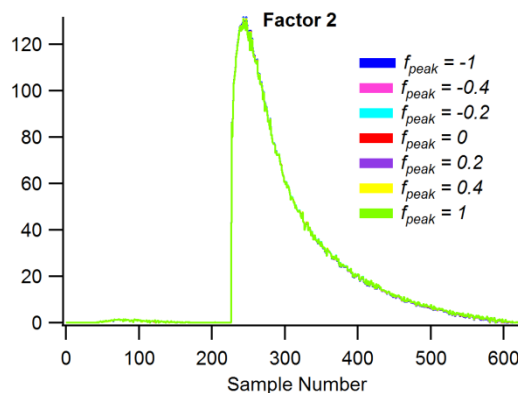
183 This can be further verified by studying how the factor profiles vary as a function of f_{peak} .
 184 In Figure S10, we compare a 3-factor solution at $f_{peak} = 0$, seed = 0 to the same factor space at all
 185 other f_{peak} values. In general, the studied systems change very little with respect to f_{peak} ,
 186 suggesting that the solution at $f_{peak} = 0$, seed = 0 exhibits little rotational ambiguity and thus, it is
 187 sufficiently robust within the range of explored parameters.

188

a)

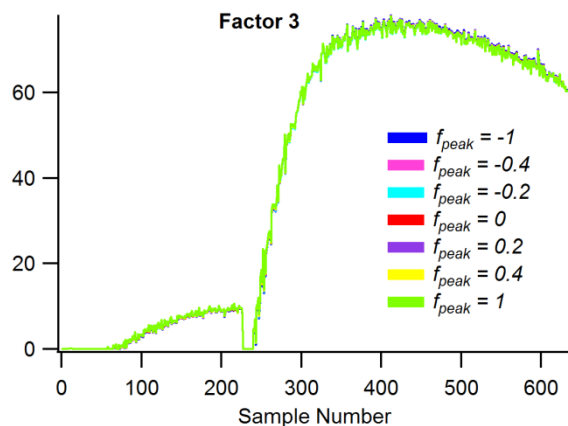


b)



189

c)

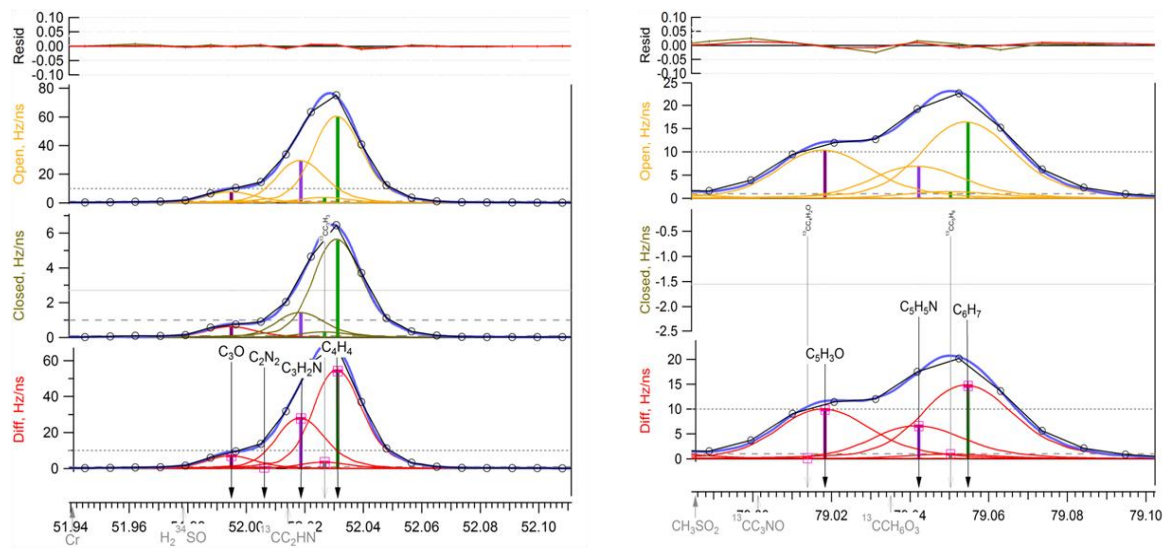


190 **Figure S10.** Factor profiles for a 3-factor solution with varying f_{peak} values. Factor 1 is shown in
 191 panel (a). Factor 2 is shown in panel (b). Factor 3 is shown in panel (c).

192

193 HR-AMS Data Supporting Pyridine Identification

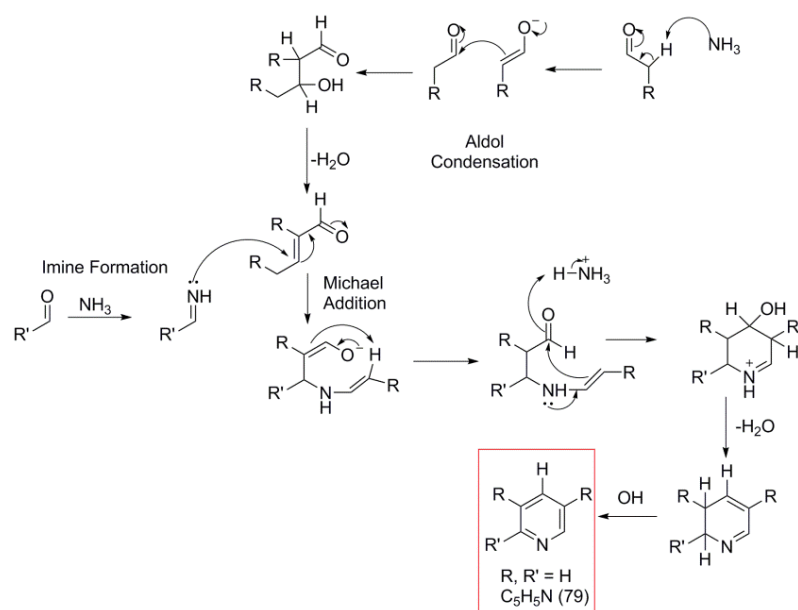
194 Pyridine is in both the ammonium sulfate-seeded and the nucleation case, and it is found in both
 195 DART-HR-MS and HR-AMS measurements. We speculate that ammonia is present in the
 196 chamber in some capacity, perhaps originating from ammonium sulfate deposited on the
 197 chamber walls; we have no means to monitor for ammonia in the gas phase.



198

199 **Figure S11.** High-resolution mass spectra of the molecular ion and major fragment of pyridine,
 200 by HR-AMS.

201 Pyridine forms a molecular ion ($C_5H_5N^+$, m/z 79) and a fragment ion ($C_3H_2N^+$, m/z 52) under EI-
 202 MS conditions; both were found by HR-AMS analysis (Figure S11). The most probable
 203 mechanism for pyridine formation under seeded conditions in a photooxidizing environment is
 204 one analogous to the traditional Chichibabin synthesis (Figure S12).⁶



205

206 **Figure S12.** Variation of Chichibabin synthesis of pyridine, proposed for toluene low-NO SOA
 207 with ammonium sulfate seed aerosol.

208 **Supporting Information References**

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