

# **Supporting Information (SI) Section**

## **Effect of Solar Radiation on the Optical Properties and Molecular Composition of Laboratory Proxies of Atmospheric Brown Carbon**

Hyun Ji (Julie) Lee,<sup>1</sup> Paige Kuuipo Aiona,<sup>1</sup> Alexander Laskin,<sup>2</sup> Julia Laskin,<sup>3</sup> and Sergey A. Nizkorodov<sup>1,\*</sup>

1. *Department of Chemistry, University of California, Irvine, CA 92697, USA.*

2. *Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352, USA.*

3. *Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA 99352, USA.*

\* Corresponding author phone, fax, and e-mail: 949-824-1262, (949) 824-8571, and nizkorod@uci.edu

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## EXPERIMENTAL METHODS

### SOA Preparation

Photooxidation of NAP was carried out in a 5 m<sup>3</sup> Teflon chamber under dry, high-NO<sub>x</sub> conditions. The chamber was purged overnight with 60 L min<sup>-1</sup> of dry clean air resulting in residual levels of particulate matter, O<sub>3</sub> and NO<sub>y</sub> that were below the detection limits of the corresponding analyzers. Approximately 2–4 ppm (10<sup>-6</sup> by volume) of H<sub>2</sub>O<sub>2</sub> was introduced to the chamber by evaporating 40–80 μL of H<sub>2</sub>O<sub>2</sub> (Sigma-Aldrich, 30% by volume in water). This was followed by adding 450–900 ppb (10<sup>-9</sup> by volume) of NAP by evaporating 25–50 μL of 0.5 g mL<sup>-1</sup> NAP (Fisher, 99% purity) dissolved in dichloromethane (Fisher, 99.9% purity) and 500–800 ppb of NO from a premixed gas-bottle (Praxair, 5000 ppm NO in N<sub>2</sub>). The precursors were thoroughly mixed in the chamber using a fan, which was later turned off once photolysis began to minimize particle wall losses. Photooxidation was driven by 35 UV-B lamps (FS40T12/UVB, Solarc Systems, Inc.) with emission centered at 310 nm. The real-time concentrations of NO/NO<sub>y</sub> and O<sub>3</sub> were monitored by Thermo Scientific 42i-Y and 49i analyzers, respectively. Relative humidity and temperature of the chamber were monitored by a Vaisala HMP233 probe; the temperature typically increased by 3–5 °C during photooxidation. The particle size distribution was monitored with a TSI model 3936 scanning mobility particle sizer (SMPS). Volatile compounds were monitored with a proton-transfer-reaction time-of-flight mass spectrometer, PTR-ToF-MS (IONICON Analytik GmbH, Innsbruck, Austria). The steady-state OH concentration in the chamber was estimated from the rate of decay of NAP, observed by PTR-ToF-MS as its protonated <sup>13</sup>C-isotope at *m/z* 130.16, and the known bimolecular rate constant (2×10<sup>-11</sup> cm<sup>3</sup> molecules<sup>-1</sup> s<sup>-1</sup>) for the NAP + OH reaction.<sup>1</sup> The estimated steady-state concentration of OH was ~5×10<sup>6</sup> molecules cm<sup>-3</sup>.

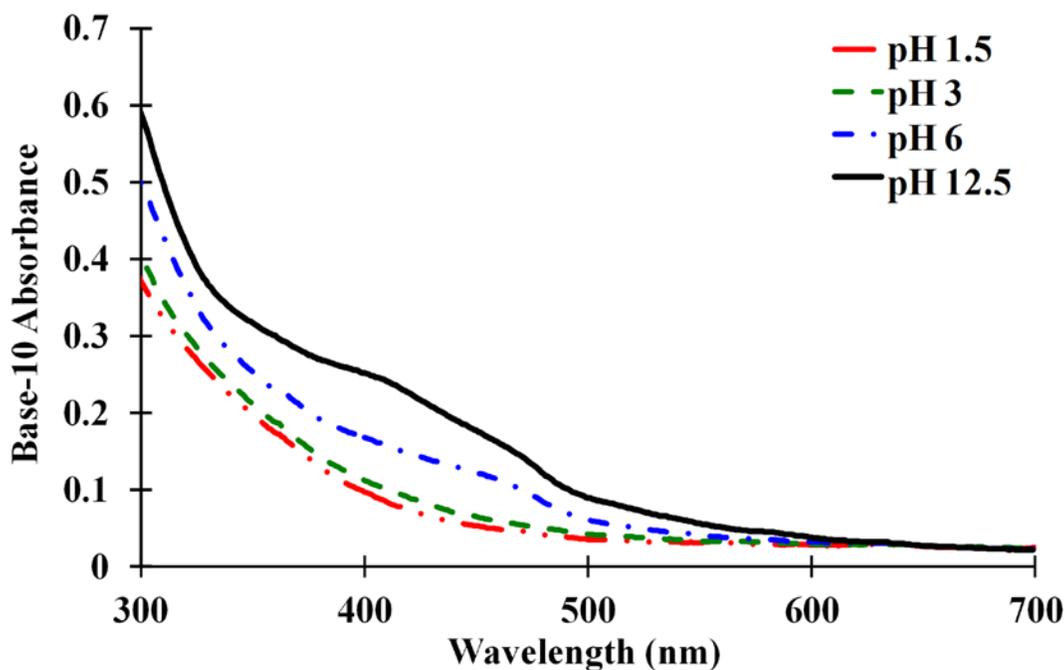
After 3 h of photooxidation, the resulting SOA was collected on two PTFE filters (Millipore 0.2 μm pore size) in parallel at a constant flow rate of about 16 L min<sup>-1</sup> per filter. An activated carbon denuder (Sunset Laboratory) was installed between the chamber and the filters to help remove excess volatiles and O<sub>3</sub>. The amount of SOA collected on each filter was estimated from the SMPS data assuming 100% collection efficiency by the filters and known NAP SOA density of 1.55 g cm<sup>-3</sup>.<sup>2</sup> Typically, 800–1300 μg of SOA material was collected on each filter. The filter samples were either used immediately or were stored in a freezer at -20 °C before photolysis experiments and/or HR-MS analysis.

In addition to the NAP SOA samples, SOA from ozonolysis of LIM (LIM/O<sub>3</sub> SOA) was generated and aged with NH<sub>3</sub> to produce BrC as described in Lee et al.<sup>3</sup> This type of aged SOA has a distinctive, well-characterized absorption spectrum in the visible range,<sup>3-6</sup> making it a convenient model system for studying photochemistry of BrC. We will refer to this material as “aged LIM/O<sub>3</sub> SOA” in the manuscript.

## Optical Properties and Photolysis of Aqueous SOA

SOA was extracted from filters by sonication in 1.8-2 mL of deionized water for 10-15 minutes to achieve a concentration of  $0.58 \pm 0.07 \text{ mg mL}^{-1}$  of dissolved SOA material. The completeness of the extraction was verified by first extracting the filter with water and then extracting the residual material on the filter with acetonitrile. By comparing the UV absorbance of the primary water extract and secondary acetonitrile extract we estimate that water extracted more than 80% of the organic material for both NAP and aged LIM/O<sub>3</sub> SOA. A dual-beam spectrometer (Shimadzu UV-2450) was used to record UV/Vis absorption spectra of the SOA extracts in the 200-700 nm range. Three-dimensional excitation-emission matrix (EEM) spectra of SOA extracts were acquired with a Hitachi F-4500 fluorescence spectrometer as described in Lee et al.<sup>3</sup> The excitation wavelength spanned the 200–500 nm range in 5 nm steps, and the emission was recorded over the 300–600 nm range in 2 nm increments. Deionized water served as the background for the absorption and EEM measurements.

**Figure S1.** Absorption spectra of a NAP SOA sample measured at different pH levels.



We investigated the effect of the solution pH on the absorption spectrum by adding few drops of 0.1 M KOH or HCl to the solution to make it more basic or acidic. We observed that the absorption spectra of the NAP SOA extracts were pH dependent; Fig. S1 shows that the absorbance increased significantly between 400-500 nm with the increase of pH. We attribute the pH dependence to acid-base

equilibria of nitrophenols, which are important products of high-NO<sub>x</sub> photooxidation of aromatics (see Vione et al.<sup>7</sup> and references therein). In addition, ionization of SOA compounds, such as carboxylic acids, may also contribute to the red-shift, as shown by other authors.<sup>8-12</sup> Spectra of nitrophenols are known to experience a significant red-shift upon ionization in solution.<sup>9, 12</sup> For example, 2,4-dinitrophenol does not strongly absorb radiation above 300 nm, while its anion has distinctive absorption bands between 300 and 450 nm. As shown in Fig. S1, an increase in pH above pH = 6 resulted in the appearance of absorption bands between 400-500 nm suggesting that nitrophenols contributed significantly to absorbance by NAP SOA. The measured pH values of the NAP SOA extracts were around 5-6, similar to the pH of cloud droplets.<sup>13, 14</sup> Under these conditions, the degree of ionization of nitrophenols should be relatively small. All the photolysis experiments described in this work have been carried out at pH = 5-6 (obtained when an SOA sample was extracted in water).

The procedure for the photolysis of aqueous SOA extracts was similar to that described by Epstein et al.<sup>15</sup> for photolysis of aqueous methyl hydroperoxide (CH<sub>3</sub>OOH). A standard 1.0 cm quartz cuvette containing the extract was placed in a temperature controlled cuvette holder. A small magnetic stir bar mixed the sample during photolysis. The absorbance at a selected wavelength (300 nm for NAP SOA and 500 nm for the aged LIM/O<sub>3</sub> SOA) was continuously recorded to determine the photolysis rate. In addition, a complete absorption spectrum was periodically taken (the stir bar was stopped during these measurements to avoid noise from solution turbulence). Radiation from a xenon arc lamp in a Newport Optics Photomax housing was reflected with a 90-degree dichroic mirror, filtered with a U-330 band-pass filter (Edmund optics 46-438), and coupled into a 1 m long, 0.95 cm diameter light-guide. The light guide delivered the radiation into the UV/Vis spectrometer and irradiated the cuvette from above. The radiant flux density was determined by photolyzing a 0.1 M solution of azoxybenzene (Fisher Scientific, 98 %) in ethanol in the presence of 0.1 M potassium hydroxide.<sup>15, 16</sup> Azoxybenzene is a convenient actinometer for relatively slow photolysis processes in SOA because its quantum yield is relatively low ( $QY_{azo} \sim 0.020$ ) and does not strongly depend on temperature and concentration.<sup>16</sup> The actinometer measurements were carried out both before and after SOA photolysis. The photolysis rate was determined from the rate of increase in absorbance due to the azoxybenzene's photoisomer, using its known molar extinction coefficient of 7600 L mol<sup>-1</sup> cm<sup>-1</sup> at 458 nm (Figure S2).<sup>16</sup>

### Calculation of the Radiant Flux Density from the Actinometry Measurements

In the experiments described in this paper, the SOA or actinometer solution of volume  $V_{solution}$  is irradiated from the top in a standard  $b = 1.0$  cm cuvette with a collimated beam of radiation with cross-section  $Area$ . The effective, solution-volume-normalized rate with which photons are absorbed by the sample can be described with the following equation,

$$Rate_{absorption} \left( \frac{\text{photons}}{\text{cm}^3 \text{s}} \right) = \frac{Area}{V_{solution}} \int_{\lambda} D_0(\lambda) \left( 1 - 10^{-A_{vertical}(\lambda)} \right) d\lambda \quad (\text{S1})$$

where  $D_0(\lambda)$  is the spectral flux density of the photolyzing radiation (in photons  $\text{cm}^{-2} \text{s}^{-1}$ ), and  $A_{vertical}$  is the base-10 absorbance of the solution over the vertical path length of the photolyzing radiation,  $h_{solution}$ . We measure the absorption spectrum of the solution in a normal way, i.e., perpendicular to the cuvette over path length  $b$ . This gives absorbance  $A(\lambda)$ , which is directly proportional to  $A_{vertical}(\lambda)$  under conditions when the Beer-Lambert law holds.

$$A_{vertical}(\lambda) = \frac{h_{solution} A(\lambda)}{b} \quad (\text{S2})$$

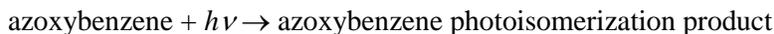
However, for the purposes of actinometry, it is more convenient to make the absorbance of the actinometer reasonably high so that all of the incoming radiation is absorbed by the solution (it is important in this case to mix the solution during photolysis). In this case, eq. S1 simplifies to:

$$Rate_{absorption} = \frac{Area}{V_{solution}} \int_{\lambda} D_0(\lambda) d\lambda \quad (\text{S3})$$

We assume that  $D_0(\lambda)$  is directly proportional to the intensity of the radiation measured with a USB4000 Ocean Optics spectrometer:

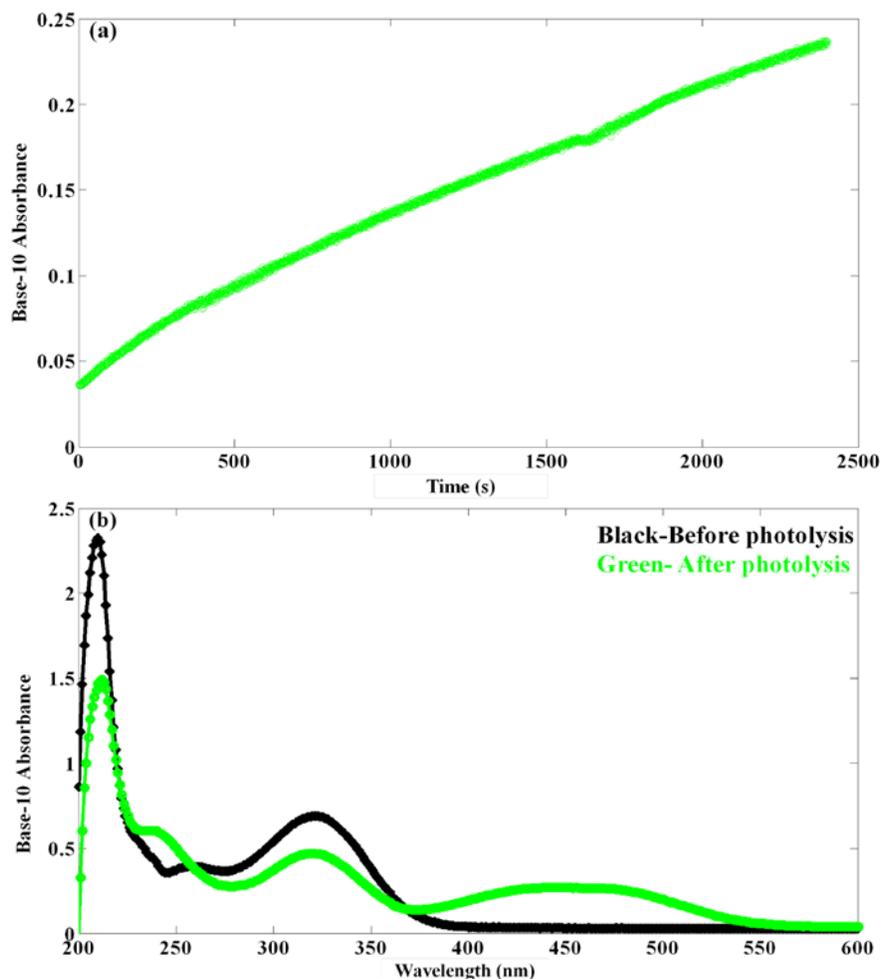
$$D_0(\lambda) = \alpha \times OO(\lambda) \quad (\text{S4})$$

In this formula,  $OO(\lambda)$  is a baseline-corrected dimensionless function of wavelength returned by the USB4000 spectrometer. The constant  $\alpha$ , which has the same units as  $D_0$ , has to be determined for each specific set of experimental conditions. In order to do so, we measure the rate of photolysis of the actinometer from the time-dependent rise in absorbance of the photolysis product of azoxybenzene.



In the strong actinometer absorbance limit, the absorbance by the product,  $A_{product}$ , grows linearly as shown in Fig. S2 (a). This can be converted into the actual photolysis rate using the known molar extinction coefficient of the product,  $\epsilon_{product} = 7600 \text{ L mol}^{-1} \text{cm}^{-1}$  at 458 nm.

**Figure S2.** (a) Absorbance of the product at 458 nm versus time. (b) Absorption spectrum of the actinometer before and after photolysis.



Expressed in molecular units, the photolysis rate is directly proportional to the initial slope in Fig. S2 (a).

$$Rate_{photolysis} \left( \frac{molec}{cm^3 s} \right) = \frac{N_A}{1000} \frac{d[product]}{dt} = \frac{N_A}{1000b\epsilon_{product}} \frac{dA_{product}}{dt} \quad (S5)$$

The ratio of the rate of photolysis from eq. S5 and the rate of absorption from eq. S3 are equal to the quantum yield of azoxybenzene ( $\phi_{azo} \sim 0.020$ ).<sup>16</sup> Combining all the equations together, we obtain eq. S6 to determine constant  $\alpha$ :

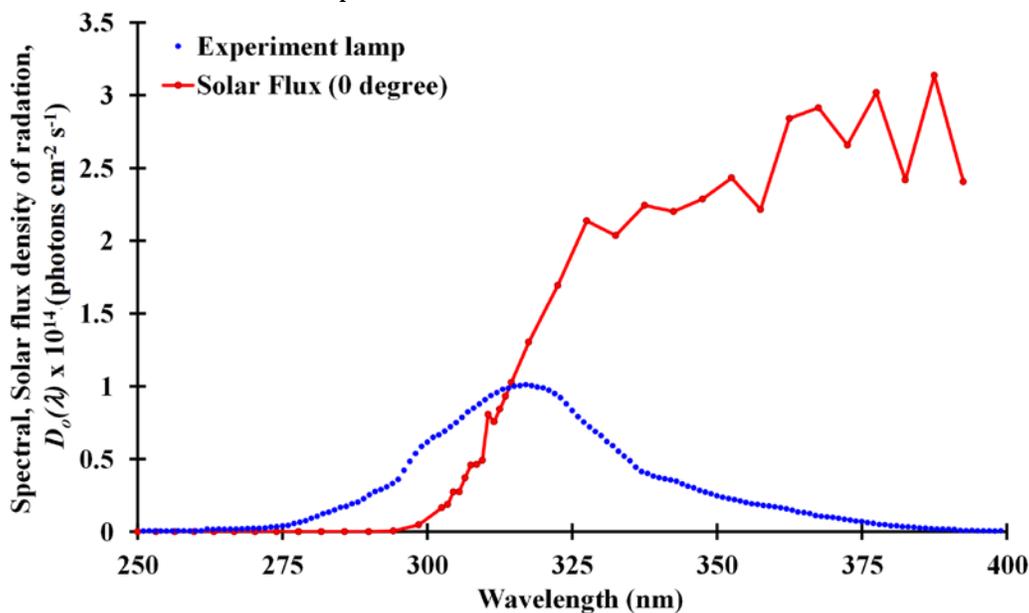
$$a = \frac{\frac{N_A}{1000b\epsilon_{product}} \frac{dA_{product}}{dt}}{\phi_{AZO} \left( \frac{Area}{V_{solution}} \right) \int_{\lambda} OO(\lambda) d\lambda} \quad (S6)$$

Finally, in a case where the entire cross-section of the cuvette is illuminated (which approximately applies to our measurements), all dimension-related terms cancel out, leading to:

$$a = \frac{\frac{N_A}{1000} \varepsilon_{product} dA_{product} dt}{\phi_{AZO} \int_{\lambda} OO(\lambda) d\lambda} \quad (S7)$$

This is the equation we used in calibrating the spectral flux density. A typical result for  $D_o(\lambda)$  is shown in Fig. S3.

**Figure S3.** A typical solar and spectral flux density of radiation,  $D_o(\lambda)$ , from the irradiation source compared to that from a sun in zenith.



### Procedure for Calculating the Effective Photolysis Rate

We calculate the effective rate of NAP SOA photolysis under realistic atmospheric conditions from the experimentally determined rate. Since the wavelength-dependent photolysis quantum yield information is not available from our experiments, we make the following approximations:

1. Photolysis is limited to wavelengths below 400 nm (visible photons are not expected to be energetic enough to result in photolysis). This assumption prevents the overestimation of the atmospheric photolysis rate when convoluting the absorption spectrum of SOA and solar flux.
2. Photolysis quantum yields for the absorbing NAP SOA compounds do not strongly depend on wavelength over the range of the photolysis source (shown in Fig. S3).

These assumptions make it possible to re-scale the experimental photolysis time scale into an effective photolysis time relevant to the atmospheric environment as follows:

$$\frac{J(EXP)}{J(ATM)} = \frac{\int_{250}^{400} D_{lamp}(\lambda) \Phi(\lambda) \sigma_{SOA}(\lambda) d\lambda}{\int_{250}^{400} D_{solar}(\lambda) \Phi(\lambda) \sigma_{SOA}(\lambda) d\lambda} \approx \frac{\int_{250}^{400} D_{lamp}(\lambda) \sigma_{SOA}(\lambda) d\lambda}{\int_{250}^{400} D_{solar}(\lambda) \sigma_{SOA}(\lambda) d\lambda} \quad (S8)$$

In this equation,  $F$  represents the actinic flux from the lamp or from the sun, and  $\sigma$  represents the effective absorption cross section of NAP SOA, which is proportional to the measured absorbance of the NAP SOA solution. The photolysis quantum yields cancel out from this equation because of the second assumption. The spectral flux density of the photolyzing radiation,  $D_{lamp}(\lambda)$ , is obtained using the methods described above (a typical result is shown in Fig. S3). The solar actinic flux,  $D_{solar}(\lambda)$ , was obtained from a TUV calculator provided by NCAR,<sup>17</sup> at one kilometer ground elevation and surface albedo of 0.10 (the result is also shown in Fig. S3).

The effective photolysis time at zero solar zenith angle,  $t(effective)$ , can now be calculated from the experimental photolysis time in the lab,  $t(laboratory)$ , using eq. S9.

$$t(effective) = t(laboratory) * \frac{J(EXP)}{J(ATM)} \quad (S9)$$

For the LIM/O<sub>3</sub> SOA + NH<sub>3</sub> data, the integration range for eq. S8 was from 250–400, due to the optically active region shown in Fig. 3 in the manuscript. The  $J(ratio)$ , ~ 0.56, was slightly higher than NAP SOA, as shown in Table S1.

## Electrospray Ionization High-Resolution Mass Spectrometry (ESI/HR-MS)

Three separate sets of SOA samples were analyzed with a high-resolution ( $m/\Delta m \sim 10^5$  at  $m/z$  450) linear-ion-trap (LTQ) Orbitrap<sup>TM</sup> mass spectrometer (Thermo Corp.) equipped with an electrospray ionization (ESI) source operating in the positive ion mode. In each set of experiments, two identical SOA filter samples were separately extracted to obtain  $0.34 \pm 0.07$  mg mL<sup>-1</sup> SOA solutions in water. One of the solutions was photolyzed while the other was kept in the dark as a control. The exposure was equivalent to about 3-4 h under a solar zenith angle (SZA) of 0°.

After photolysis and immediately prior to analysis, the aqueous solutions were mixed with acetonitrile (Aldrich, HPLC grade) in a 1:1 ratio to improve the ESI source stability. Mass spectra of a blank sample corresponding to a 1:1 mixture of acetonitrile and water, and of a calibration mixture of caffeine MRFA and Ultramark 1621 (LTQ ESI Positive Ion Calibration Solution, Thermo Scientific, Inc.) were also recorded. The combination of the external calibration and an internal re-calibration of each

spectrum with respect to the expected products of NAP oxidation resulted in an estimated peak position accuracy of better than  $\pm 0.0005$  Da over the  $m/z$  100-500 range of interest where more than 95% of the detected peaks were found. The compounds were detected as sodiated  $[M + Na]^+$  and/or protonated  $[M + H]^+$  species. For clarity, the formulas discussed in this paper will correspond to the neutral analytes. The data analysis was carried out as discussed in Nizkorodov et al.<sup>18</sup> Briefly, peaks that appeared in the blank sample and peaks corresponding to  $^{13}C$  isotopes were discarded. The peaks were assigned to formulas  $C_{1-40}H_{2-80}O_{0-35}N_{0-2}Na_{0-1}^+$  with 0.00075  $m/z$  tolerance while constraining the H/C and O/C ratios to 0.4–2.5 and 0–1.0 and only permitting closed-shell ions (no ion-radicals). Most of the peaks could be assigned unambiguously with these constraints. However, for a subset of peaks, either  $N_0$  or  $N_2$  assignments were possible for a single  $m/z$ . In these cases, preference was given to the  $N_0$  assignment based on analysis of the N-atom distribution for the unambiguously assigned peaks.

## RESULTS

### List of Peaks Removed, Formed, and Remaining After Photolysis of Aqueous NAP SOA.

**Table S1.** List of  $m/z$  values, ion formulas, and relative abundances (at  $t = 0$ ) of SOA compounds removed and formed during photolysis. The intensities (in %) are normalized relative to the intensity of the largest peak in each spectrum. Compounds listed on Table 1 of the manuscript are shown in red.

$m/z$	Ion formula					% Abundance		
						Before Photolysis	After Photolysis	After/Before ratio
157.0835	C <sub>6</sub>	H <sub>14</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	5.4	17.0	3.1
157.0260	C <sub>8</sub>	H <sub>6</sub>	O <sub>2</sub>	-	Na <sub>1</sub>	3.6	100.0	28.2
173.0209	C <sub>8</sub>	H <sub>6</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	2.9	18.9	6.6
179.0679	C <sub>8</sub>	H <sub>12</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	15.9		
189.0158	C <sub>8</sub>	H <sub>6</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	4.6		
193.0471	C <sub>8</sub>	H <sub>10</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	8.7		
195.0628	C <sub>8</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	100.0	62.2	0.6
197.0784	C <sub>8</sub>	H <sub>14</sub>	O <sub>4</sub>	-	Na <sub>1</sub>		13.6	
211.0577	C <sub>8</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	20.0	10.1	0.5
169.0260	C <sub>9</sub>	H <sub>6</sub>	O <sub>2</sub>	-	Na <sub>1</sub>	1.5		
171.0417	C <sub>9</sub>	H <sub>8</sub>	O <sub>2</sub>	-	Na <sub>1</sub>	3.9	79.8	20.5
187.0366	C <sub>9</sub>	H <sub>8</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	23.7	47.7	2.0
189.0522	C <sub>9</sub>	H <sub>10</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	1.4		
191.0679	C <sub>9</sub>	H <sub>12</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	4.0		
193.0835	C <sub>9</sub>	H <sub>14</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	18.5	23.5	1.3

201.0158	C <sub>9</sub>	H <sub>6</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	2.2		
203.0315	C <sub>9</sub>	H <sub>8</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	14.1		
205.0471	C <sub>9</sub>	H <sub>10</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	3.5	13.1	3.7
207.0628	C <sub>9</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	16.3	17.9	1.1
210.1101	C <sub>9</sub>	H <sub>17</sub>	O <sub>3</sub>	N <sub>1</sub>	Na <sub>1</sub>	37.7	1.7	0.04
211.0941	C <sub>9</sub>	H <sub>16</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	14.6	17.0	1.2
216.0267	C <sub>9</sub>	H <sub>7</sub>	O <sub>4</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.9	1.8	0.6
221.0420	C <sub>9</sub>	H <sub>10</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	5.4		
223.0577	C <sub>9</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	13.6	12.1	0.9
225.0733	C <sub>9</sub>	H <sub>14</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	40.7	34.2	0.8
227.0890	C <sub>9</sub>	H <sub>16</sub>	O <sub>5</sub>	-	Na <sub>1</sub>		9.4	
239.0526	C <sub>9</sub>	H <sub>12</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	8.1		
241.0683	C <sub>9</sub>	H <sub>14</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	13.3	4.8	0.4
161.0597	C <sub>10</sub>	H <sub>9</sub>	O <sub>2</sub>	-	-	2.1		
177.0546	C <sub>10</sub>	H <sub>9</sub>	O <sub>3</sub>	-	-	4.2		
181.0260	C <sub>10</sub>	H <sub>6</sub>	O <sub>2</sub>	-	Na <sub>1</sub>	1.2		
183.0417	C <sub>10</sub>	H <sub>8</sub>	O <sub>2</sub>	-	Na <sub>1</sub>	2.1		
196.0369	C <sub>10</sub>	H <sub>7</sub>	O <sub>2</sub>	N <sub>1</sub>	Na <sub>1</sub>	6.7		
197.0209	C <sub>10</sub>	H <sub>6</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	6.6		
199.0366	C <sub>10</sub>	H <sub>8</sub>	O <sub>3</sub>	-	Na <sub>1</sub>		26.7	
201.0522	C <sub>10</sub>	H <sub>10</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	8.9	68.9	7.7
205.0835	C <sub>10</sub>	H <sub>14</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	8.3		
207.0992	C <sub>10</sub>	H <sub>16</sub>	O <sub>3</sub>	-	Na <sub>1</sub>	29.2	28.6	1.0
210.0761	C <sub>10</sub>	H <sub>12</sub>	O <sub>4</sub>	N <sub>1</sub>	-	0.9		
212.0318	C <sub>10</sub>	H <sub>7</sub>	O <sub>3</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.5		
213.0158	C <sub>10</sub>	H <sub>6</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	7.9		
214.0475	C <sub>10</sub>	H <sub>9</sub>	O <sub>3</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.0	6.8	3.4
215.0315	C <sub>10</sub>	H <sub>8</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	55.8	10.8	0.2
217.0471	C <sub>10</sub>	H <sub>10</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	49.0	43.7	0.9
219.0628	C <sub>10</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	10.7	23.6	2.2
221.0784	C <sub>10</sub>	H <sub>14</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	33.1	38.7	1.2
223.0941	C <sub>10</sub>	H <sub>16</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	69.1	83.5	1.2
225.1097	C <sub>10</sub>	H <sub>18</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	7.1	8.7	1.2
228.0267	C <sub>10</sub>	H <sub>7</sub>	O <sub>4</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.3		
230.0424	C <sub>10</sub>	H <sub>9</sub>	O <sub>4</sub>	N <sub>1</sub>	Na <sub>1</sub>	15.6	3.6	0.2
231.0264	C <sub>10</sub>	H <sub>8</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	24.9	1.1	0.05
233.0420	C <sub>10</sub>	H <sub>10</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	50.5	17.4	0.3
235.0577	C <sub>10</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	15.4	19.7	1.3
237.0733	C <sub>10</sub>	H <sub>14</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	40.2	19.9	0.5

239.0890	C <sub>10</sub>	H <sub>16</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	60.0	29.1	0.5
241.1046	C <sub>10</sub>	H <sub>18</sub>	O <sub>5</sub>	-	Na <sub>1</sub>		6.1	
244.0216	C <sub>10</sub>	H <sub>7</sub>	O <sub>5</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.6		
246.0373	C <sub>10</sub>	H <sub>9</sub>	O <sub>5</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.3		
251.0526	C <sub>10</sub>	H <sub>12</sub>	O <sub>6</sub>	-	Na <sub>1</sub>		1.3	
253.0683	C <sub>10</sub>	H <sub>14</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	24.1	10.1	0.4
255.0839	C <sub>10</sub>	H <sub>16</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	80.6	8.1	0.1
257.0996	C <sub>10</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>		1.5	
268.0792	C <sub>10</sub>	H <sub>15</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	4.2	2.3	0.6
270.0948	C <sub>10</sub>	H <sub>17</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	0.9		
286.0897	C <sub>10</sub>	H <sub>17</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.4		
228.0631	C <sub>11</sub>	H <sub>11</sub>	O <sub>3</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.0		
229.0471	C <sub>11</sub>	H <sub>10</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	5.7	6.9	1.2
235.0941	C <sub>11</sub>	H <sub>16</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	13.9	4.6	0.3
237.1097	C <sub>11</sub>	H <sub>18</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	4.2	3.8	0.9
245.0420	C <sub>11</sub>	H <sub>10</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	5.1	1.8	0.3
251.0890	C <sub>11</sub>	H <sub>16</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	46.1	34.6	0.8
253.1046	C <sub>11</sub>	H <sub>18</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	9.8	7.1	0.7
255.1203	C <sub>11</sub>	H <sub>20</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	1.3		
267.0839	C <sub>11</sub>	H <sub>16</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	18.4	8.0	0.4
269.0996	C <sub>11</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	7.1	3.0	0.4
285.0945	C <sub>11</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	2.1		
243.0628	C <sub>12</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>		2.8	
245.0784	C <sub>12</sub>	H <sub>14</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	27.7	56.1	2.0
249.1097	C <sub>12</sub>	H <sub>18</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	3.1	3.6	1.2
251.1254	C <sub>12</sub>	H <sub>20</sub>	O <sub>4</sub>	-	Na <sub>1</sub>		4.4	
257.0420	C <sub>12</sub>	H <sub>10</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	2.9		
265.1046	C <sub>12</sub>	H <sub>18</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	17.6	15.7	0.9
267.1203	C <sub>12</sub>	H <sub>20</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.5	3.9	0.9
275.0526	C <sub>12</sub>	H <sub>12</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	2.9		
283.1152	C <sub>12</sub>	H <sub>20</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	3.2	2.2	0.7
297.0945	C <sub>12</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	4.9	1.6	0.3
250.1777	C <sub>13</sub>	H <sub>25</sub>	O <sub>2</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.0	1.0	1.1
261.1097	C <sub>13</sub>	H <sub>18</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	6.6	3.9	0.6
263.1254	C <sub>13</sub>	H <sub>20</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	2.6	2.8	1.1
266.1727	C <sub>13</sub>	H <sub>25</sub>	O <sub>3</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.1		
271.0577	C <sub>13</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.8		
277.1046	C <sub>13</sub>	H <sub>18</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	2.6		
279.1203	C <sub>13</sub>	H <sub>20</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	5.2	4.2	0.8

281.1359	C <sub>13</sub>	H <sub>22</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	2.6		
295.1152	C <sub>13</sub>	H <sub>20</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	6.2	4.0	0.6
297.1309	C <sub>13</sub>	H <sub>22</sub>	O <sub>6</sub>	-	Na <sub>1</sub>		1.6	
305.0632	C <sub>13</sub>	H <sub>14</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	1.3		
277.1410	C <sub>14</sub>	H <sub>22</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	2.7		
285.0733	C <sub>14</sub>	H <sub>14</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	2.5		
289.1046	C <sub>14</sub>	H <sub>18</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	1.0		
291.1203	C <sub>14</sub>	H <sub>20</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	2.6		
293.1359	C <sub>14</sub>	H <sub>22</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.7		
309.1309	C <sub>14</sub>	H <sub>22</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	4.8	3.8	0.8
317.0632	C <sub>14</sub>	H <sub>14</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	2.2		
319.0788	C <sub>14</sub>	H <sub>16</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	2.0		
321.0945	C <sub>14</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	1.4		
349.1833	C <sub>14</sub>	H <sub>30</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	1.1		
299.0890	C <sub>15</sub>	H <sub>16</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.7	3.0	0.6
307.1516	C <sub>15</sub>	H <sub>24</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.9	4.1	0.8
309.1672	C <sub>15</sub>	H <sub>26</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	1.8		
313.0683	C <sub>15</sub>	H <sub>14</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	3.6		
321.1309	C <sub>15</sub>	H <sub>22</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	5.2	4.1	0.8
323.1465	C <sub>15</sub>	H <sub>24</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	8.0	4.5	0.6
325.1622	C <sub>15</sub>	H <sub>26</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	2.3	1.5	0.7
329.0632	C <sub>15</sub>	H <sub>14</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	3.1		
331.0788	C <sub>15</sub>	H <sub>16</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	3.6		
337.1258	C <sub>15</sub>	H <sub>22</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	4.5		
339.1414	C <sub>15</sub>	H <sub>24</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	4.0		
348.1054	C <sub>15</sub>	H <sub>19</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	0.9		
289.0471	C <sub>16</sub>	H <sub>10</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	2.9		
291.0628	C <sub>16</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>		3.9	
301.1410	C <sub>16</sub>	H <sub>22</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	64.4	70.9	1.1
305.0420	C <sub>16</sub>	H <sub>10</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.9	3.7	0.7
307.0577	C <sub>16</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>		1.3	
327.0839	C <sub>16</sub>	H <sub>16</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	8.9	2.7	0.3
329.0996	C <sub>16</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	8.0		
331.1152	C <sub>16</sub>	H <sub>20</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	3.8		
337.1622	C <sub>16</sub>	H <sub>26</sub>	O <sub>6</sub>	-	Na <sub>1</sub>		3.4	
343.0788	C <sub>16</sub>	H <sub>16</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	7.3		
354.0584	C <sub>16</sub>	H <sub>13</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.8		
303.0628	C <sub>17</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	15.8	11.1	0.7
305.0784	C <sub>17</sub>	H <sub>14</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	4.6	3.7	0.8

317.0420	C <sub>17</sub>	H <sub>10</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	11.0		
319.0577	C <sub>17</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	32.4	7.0	0.2
321.0733	C <sub>17</sub>	H <sub>14</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	9.4	2.9	0.3
327.1203	C <sub>17</sub>	H <sub>20</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.3		
335.0526	C <sub>17</sub>	H <sub>12</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	15.1	1.7	0.1
337.0683	C <sub>17</sub>	H <sub>14</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	8.3		
341.0996	C <sub>17</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	12.8		
343.1152	C <sub>17</sub>	H <sub>20</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	14.4		
348.0479	C <sub>17</sub>	H <sub>11</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.2		
353.0632	C <sub>17</sub>	H <sub>14</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	4.7		
357.0945	C <sub>17</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	12.7		
359.1101	C <sub>17</sub>	H <sub>20</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	11.3		
361.1258	C <sub>17</sub>	H <sub>22</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	3.5		
370.0897	C <sub>17</sub>	H <sub>17</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.6		
373.0894	C <sub>17</sub>	H <sub>18</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	7.2		
375.1050	C <sub>17</sub>	H <sub>20</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	5.9		
382.0533	C <sub>17</sub>	H <sub>13</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.2		
389.0843	C <sub>17</sub>	H <sub>18</sub>	O <sub>9</sub>	-	Na <sub>1</sub>	2.9		
315.0628	C <sub>18</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	31.5	3.7	0.1
317.0784	C <sub>18</sub>	H <sub>14</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	8.6	5.0	0.6
330.0737	C <sub>18</sub>	H <sub>13</sub>	O <sub>4</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.5		
331.0577	C <sub>18</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	61.6	3.3	0.1
333.0733	C <sub>18</sub>	H <sub>14</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	28.4	11.8	0.4
335.0890	C <sub>18</sub>	H <sub>16</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	5.2		
344.0529	C <sub>18</sub>	H <sub>11</sub>	O <sub>5</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.2		
346.0686	C <sub>18</sub>	H <sub>13</sub>	O <sub>5</sub>	N <sub>1</sub>	Na <sub>1</sub>		1.9	
347.0526	C <sub>18</sub>	H <sub>12</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	25.6	1.9	0.1
349.0683	C <sub>18</sub>	H <sub>14</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	28.3	4.6	0.2
351.0839	C <sub>18</sub>	H <sub>16</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	8.0	1.9	0.2
352.2458	C <sub>18</sub>	H <sub>35</sub>	O <sub>4</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.1	8.4	7.5
353.0996	C <sub>18</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	6.3		
355.1152	C <sub>18</sub>	H <sub>20</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	21.0	7.8	0.4
357.1309	C <sub>18</sub>	H <sub>22</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	7.9		
362.0635	C <sub>18</sub>	H <sub>13</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	6.9	1.0	0.1
363.0475	C <sub>18</sub>	H <sub>12</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	10.8		
364.0792	C <sub>18</sub>	H <sub>15</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	4.8		
365.0632	C <sub>18</sub>	H <sub>14</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	12.4		
366.0948	C <sub>18</sub>	H <sub>17</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.5		
367.0788	C <sub>18</sub>	H <sub>16</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	6.7		

369.0945	C <sub>18</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	7.5		
371.1101	C <sub>18</sub>	H <sub>20</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	16.5	2.4	0.1
373.1258	C <sub>18</sub>	H <sub>22</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	10.4		
380.0741	C <sub>18</sub>	H <sub>15</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	5.2		
382.0897	C <sub>18</sub>	H <sub>17</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.7		
383.0737	C <sub>18</sub>	H <sub>16</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	4.2		
385.0894	C <sub>18</sub>	H <sub>18</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.2		
387.1050	C <sub>18</sub>	H <sub>20</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	10.3		
389.1207	C <sub>18</sub>	H <sub>22</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.4		
396.0690	C <sub>18</sub>	H <sub>15</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	4.0		
327.0628	C <sub>19</sub>	H <sub>12</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	6.1		
331.0941	C <sub>19</sub>	H <sub>16</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	1.8		
343.0577	C <sub>19</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	11.6		
345.0733	C <sub>19</sub>	H <sub>14</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	17.0		
347.0890	C <sub>19</sub>	H <sub>16</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	11.7	4.8	0.4
349.1046	C <sub>19</sub>	H <sub>18</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	2.8		
358.0686	C <sub>19</sub>	H <sub>13</sub>	O <sub>5</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.4		
359.0526	C <sub>19</sub>	H <sub>12</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	12.9		
360.0842	C <sub>19</sub>	H <sub>15</sub>	O <sub>5</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.6		
361.0683	C <sub>19</sub>	H <sub>14</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	29.9	3.3	0.1
363.0839	C <sub>19</sub>	H <sub>16</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	18.8	3.5	0.2
365.0996	C <sub>19</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>		1.8	
367.1152	C <sub>19</sub>	H <sub>20</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	4.6		
369.1309	C <sub>19</sub>	H <sub>22</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	9.3	2.3	0.2
371.1465	C <sub>19</sub>	H <sub>24</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	3.5		
374.0635	C <sub>19</sub>	H <sub>13</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	5.1		
375.0475	C <sub>19</sub>	H <sub>12</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	6.3		
376.0792	C <sub>19</sub>	H <sub>15</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	5.2		
377.0632	C <sub>19</sub>	H <sub>14</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	22.7	1.2	0.1
379.0788	C <sub>19</sub>	H <sub>16</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	14.7	1.0	0.1
381.0945	C <sub>19</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	6.7	0.9	0.1
383.1101	C <sub>19</sub>	H <sub>20</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	7.9		
385.1258	C <sub>19</sub>	H <sub>22</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	14.0	2.4	0.2
387.1414	C <sub>19</sub>	H <sub>24</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	5.9		
390.0584	C <sub>19</sub>	H <sub>13</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.4		
393.0581	C <sub>19</sub>	H <sub>14</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	8.0		
394.0897	C <sub>19</sub>	H <sub>17</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.8		
395.0737	C <sub>19</sub>	H <sub>16</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.8		
397.0894	C <sub>19</sub>	H <sub>18</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	4.5		

399.1050	C <sub>19</sub>	H <sub>20</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.6		
401.1207	C <sub>19</sub>	H <sub>22</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	9.6		
408.0690	C <sub>19</sub>	H <sub>15</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	5.0		
410.0846	C <sub>19</sub>	H <sub>17</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.6		
426.0796	C <sub>19</sub>	H <sub>17</sub>	O <sub>9</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.2		
355.0577	C <sub>20</sub>	H <sub>12</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	4.6		
359.0890	C <sub>20</sub>	H <sub>16</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	8.5	2.6	0.3
361.1046	C <sub>20</sub>	H <sub>18</sub>	O <sub>5</sub>	-	Na <sub>1</sub>	6.9	6.5	1.0
371.0526	C <sub>20</sub>	H <sub>12</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	5.1		
372.0842	C <sub>20</sub>	H <sub>15</sub>	O <sub>5</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.8		
373.0683	C <sub>20</sub>	H <sub>14</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	22.2		
375.0839	C <sub>20</sub>	H <sub>16</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	25.7	5.1	0.2
377.0996	C <sub>20</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	8.2	2.2	0.3
379.1152	C <sub>20</sub>	H <sub>20</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	3.3	1.3	0.4
385.1622	C <sub>20</sub>	H <sub>26</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	1.2		
388.0792	C <sub>20</sub>	H <sub>15</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	4.0		
389.0632	C <sub>20</sub>	H <sub>14</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	14.1		
390.0948	C <sub>20</sub>	H <sub>17</sub>	O <sub>6</sub>	N <sub>1</sub>	Na <sub>1</sub>	6.2		
391.0788	C <sub>20</sub>	H <sub>16</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	26.6	2.5	0.1
393.0945	C <sub>20</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	10.4	1.2	0.1
395.1101	C <sub>20</sub>	H <sub>20</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	4.3		
402.0584	C <sub>20</sub>	H <sub>13</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	1.9		
404.0741	C <sub>20</sub>	H <sub>15</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	5.6		
405.0581	C <sub>20</sub>	H <sub>14</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.1		
406.0897	C <sub>20</sub>	H <sub>17</sub>	O <sub>7</sub>	N <sub>1</sub>	Na <sub>1</sub>	6.8		
407.0737	C <sub>20</sub>	H <sub>16</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	12.7		
409.0894	C <sub>20</sub>	H <sub>18</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.8		
411.1050	C <sub>20</sub>	H <sub>20</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	3.8		
413.1207	C <sub>20</sub>	H <sub>22</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.2		
415.1363	C <sub>20</sub>	H <sub>24</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	6.6		
420.0690	C <sub>20</sub>	H <sub>15</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	5.3		
422.0846	C <sub>20</sub>	H <sub>17</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	6.3		
423.0687	C <sub>20</sub>	H <sub>16</sub>	O <sub>9</sub>	-	Na <sub>1</sub>	4.2		
424.1003	C <sub>20</sub>	H <sub>19</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	3.3		
426.1159	C <sub>20</sub>	H <sub>21</sub>	O <sub>8</sub>	N <sub>1</sub>	Na <sub>1</sub>	0.9		
438.0796	C <sub>20</sub>	H <sub>17</sub>	O <sub>9</sub>	N <sub>1</sub>	Na <sub>1</sub>	4.5		
441.0792	C <sub>20</sub>	H <sub>18</sub>	O <sub>10</sub>	-	Na <sub>1</sub>	1.4		
454.0745	C <sub>20</sub>	H <sub>17</sub>	O <sub>10</sub>	N <sub>1</sub>	Na <sub>1</sub>	2.2		
389.0996	C <sub>21</sub>	H <sub>18</sub>	O <sub>6</sub>	-	Na <sub>1</sub>	1.3		

403.0788	C <sub>21</sub>	H <sub>16</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	2.4	
405.0945	C <sub>21</sub>	H <sub>18</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	1.8	
407.1101	C <sub>21</sub>	H <sub>20</sub>	O <sub>7</sub>	-	Na <sub>1</sub>	0.8	
427.1363	C <sub>21</sub>	H <sub>24</sub>	O <sub>8</sub>	-	Na <sub>1</sub>	1.8	
437.0843	C <sub>21</sub>	H <sub>18</sub>	O <sub>9</sub>	-	Na <sub>1</sub>	1.2	
413.2662	C <sub>24</sub>	H <sub>38</sub>	O <sub>4</sub>	-	Na <sub>1</sub>	14.9	
505.3347	C <sub>24</sub>	H <sub>50</sub>	O <sub>9</sub>	-	Na <sub>1</sub>		45.6
523.1000	C <sub>28</sub>	H <sub>20</sub>	O <sub>9</sub>	-	Na <sub>1</sub>	2.3	
525.1156	C <sub>28</sub>	H <sub>22</sub>	O <sub>9</sub>	-	Na <sub>1</sub>	1.7	

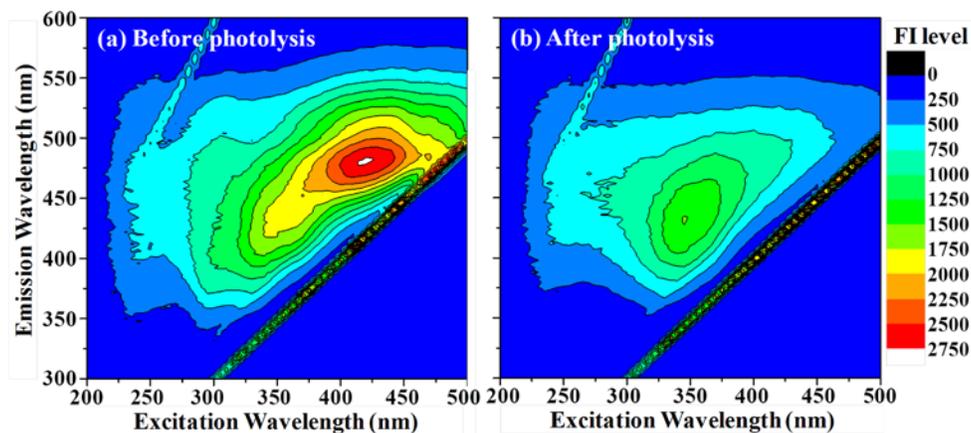
### Distribution of N-Atoms in the Products Before and After Photolysis

**Table S2.** Breakdown of the observed ions by nitrogen content. 0N and 1N refer to compounds containing 0 and 1 nitrogen atoms, respectively. As shown in this table, ~ 13% of the 1N compounds are removed, and ~ 13%, of the 0N compounds are formed by photolysis, suggesting that one of the mechanism of photolysis involves removal of -NO<sub>2</sub> groups from the nitroaromatic compounds or -ONO<sub>2</sub> groups from nitric acid esters.

N-compound	Before Photolysis		After Photolysis		In Both	
	#	%	#	%	#	%
<b>0N</b>	193	79.1	99	91.7	86	91.5
<b>1N</b>	51	20.9	9	8.3	8	8.5
<b>Total</b>	244	100	108	100	94	100

## Fluorescence Measurement Before and After Photolysis of Aqueous Aged LIM/O<sub>3</sub> SOA

**Figure S4.** EEM plot recorded (a) before and (b) after photolysis of solution of aged LIM/O<sub>3</sub> SOA. After 110 minutes of photolysis the fluorescence intensity (FI, color coded as shown on the right) increased somewhat (while the solution absorbance decreased, as shown in Fig. 1).



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