

Supporting Information Section

Secondary Organic Aerosol from Atmospheric Photooxidation of Indole

5 Julia Montoya,¹ Jeremy R. Horne,² Mallory L. Hinks,¹ Lauren T. Fleming,¹ Veronique Perraud,¹ Peng Lin,³ Alexander Laskin,³ Julia Laskin,⁴ Donald Dabdub,² and Sergey A. Nizkorodov¹

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

²Department of Mechanical and Aerospace Engineering, University of California, Irvine, CA 92697, USA

³Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99354, USA

10 ⁴Physical Sciences Division Pacific Northwest National Laboratory, Richland, WA 99354, USA

Correspondence to: Sergey A. Nizkorodov (nizkorod@uci.edu)

S1. Wall loss corrections

The wall loss correction was done by assuming a first-order particle size independent loss of particle mass concentration (PM)

$$\frac{dPM}{dt} = \text{Source}(t) - \text{Loss}(t) = \text{Source}(t) - k_w \times PM, \quad (\text{S1})$$

- 5 where the $\text{Source}(t)$ and $\text{Loss}(t)$ are time dependent production and removal rates for the particles. The effective first-order rate constant $k_w = 0.00090 \text{ min}^{-1}$ was determined in a separate experiment in which indole SOA was produced, the lamps were turned off, and mass concentration of SOA was followed with SMPS for 10 hours without collecting SOA on filters. Using the known k_w , we could determine $\text{Source}(t)$ from the actual measured PM concentration in every experiment.

$$10 \text{ Source}(t) = \frac{dPM}{dt} + k_w \times PM, \quad (\text{S2})$$

The corrected PM concentration (i.e. the hypothetical PM concentration that would be achieved if the wall loss was absent) was calculated from:

$$PM_{\text{corrected}}(t) = PM(t = 0) + \int_0^t \text{Source}(t) dt, \quad (\text{S3})$$

- 15 The integration of data was carried out numerically in Excel. Figure 3 in the main text shows a representative result of the wall loss correction.

S2. PTR-ToF-MS measurements of volatile products of indole photooxidation

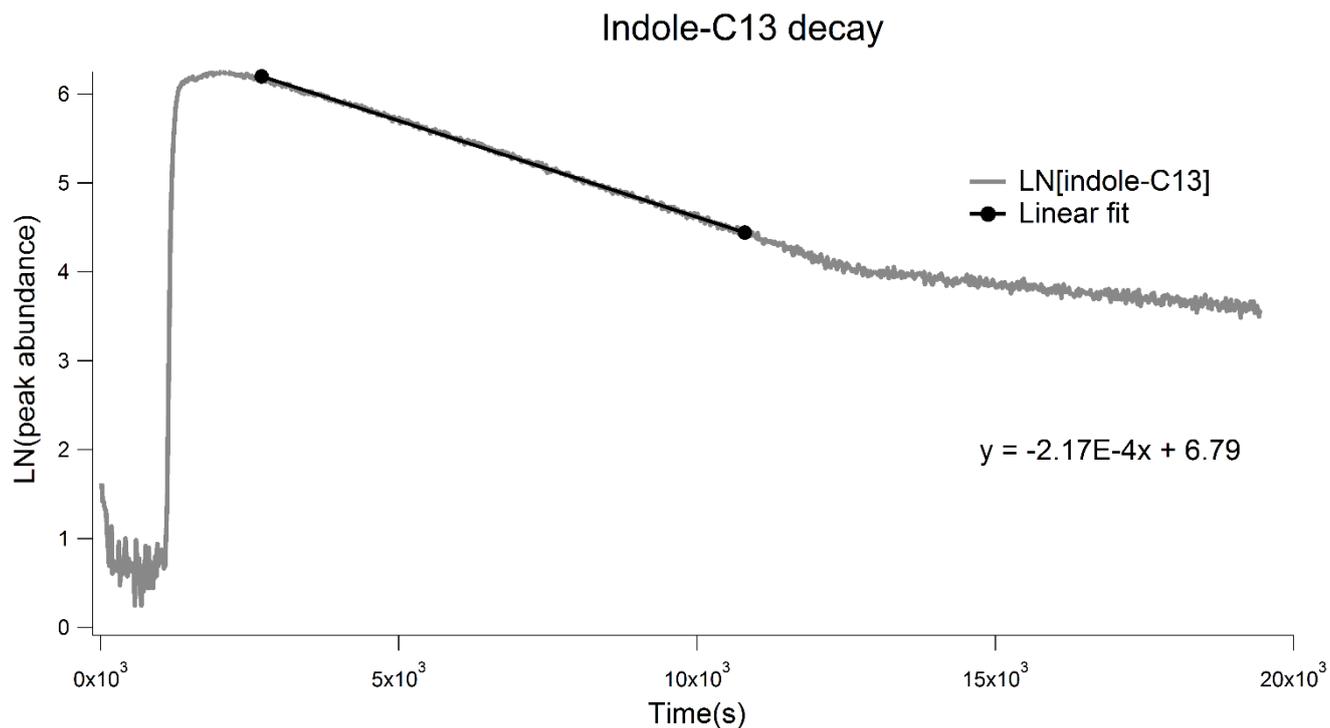


Figure S2.1: Estimating the OH concentration in the chamber from the rate of loss of indole. The slope translates into $[OH] \sim 1.4 \times 10^6 \text{ molec cm}^{-3}$. The break in the time dependence corresponds to switching off the UV lights and simultaneously starting collecting the samples.

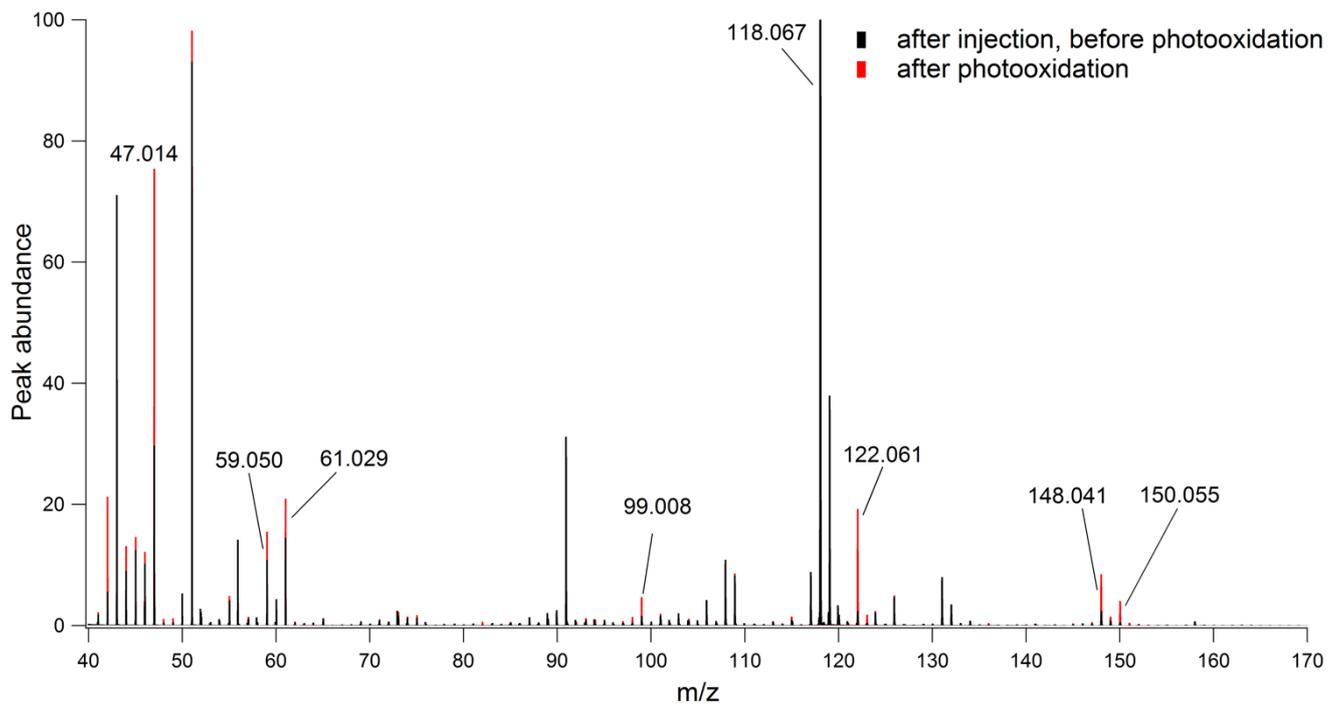


Figure S2.2: Mass spectra of the chamber VOC compounds before and after photooxidation of indole.

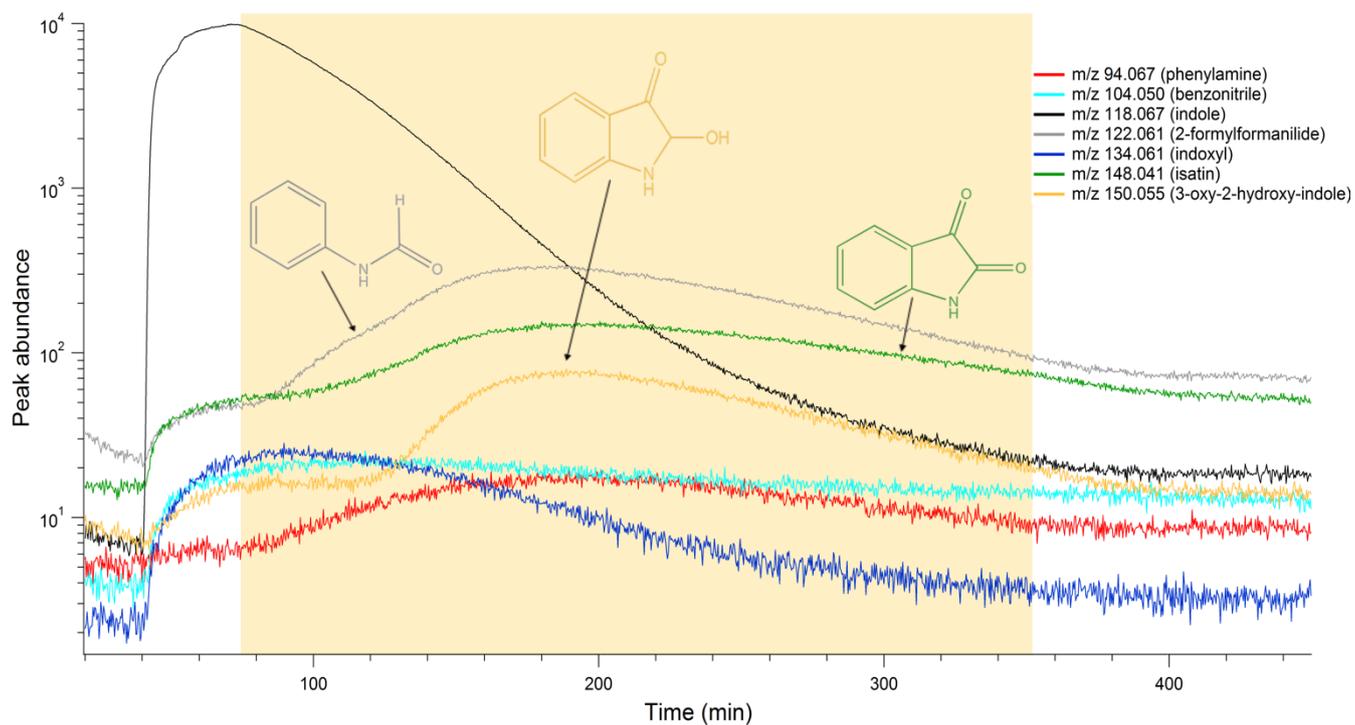


Figure S2.3: Time-dependent signals of ions that were produced and then removed. Shaded region denotes the time when the chamber lamps were on. The unusual time dependence for m/z 150.055 (3-oxy-2-hydroxy-indole, drawn in yellow) and m/z 148.041 (isatin, drawn in green) was reproducible.

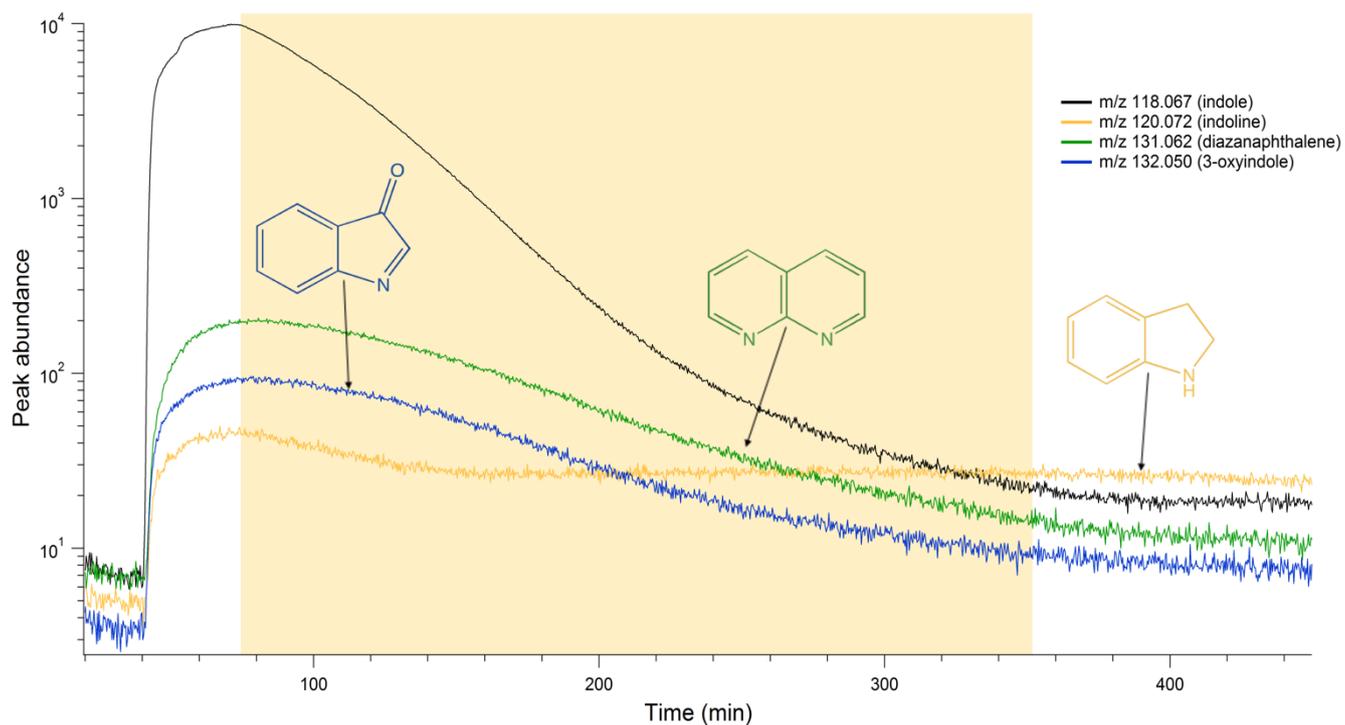


Figure S2.4: Time-dependent signals of ions that were removed during photooxidation. Indoline and diazanaphthalene were likely present in the indole sample as impurities. Shaded region denotes the time when the chamber lamps were on.

5

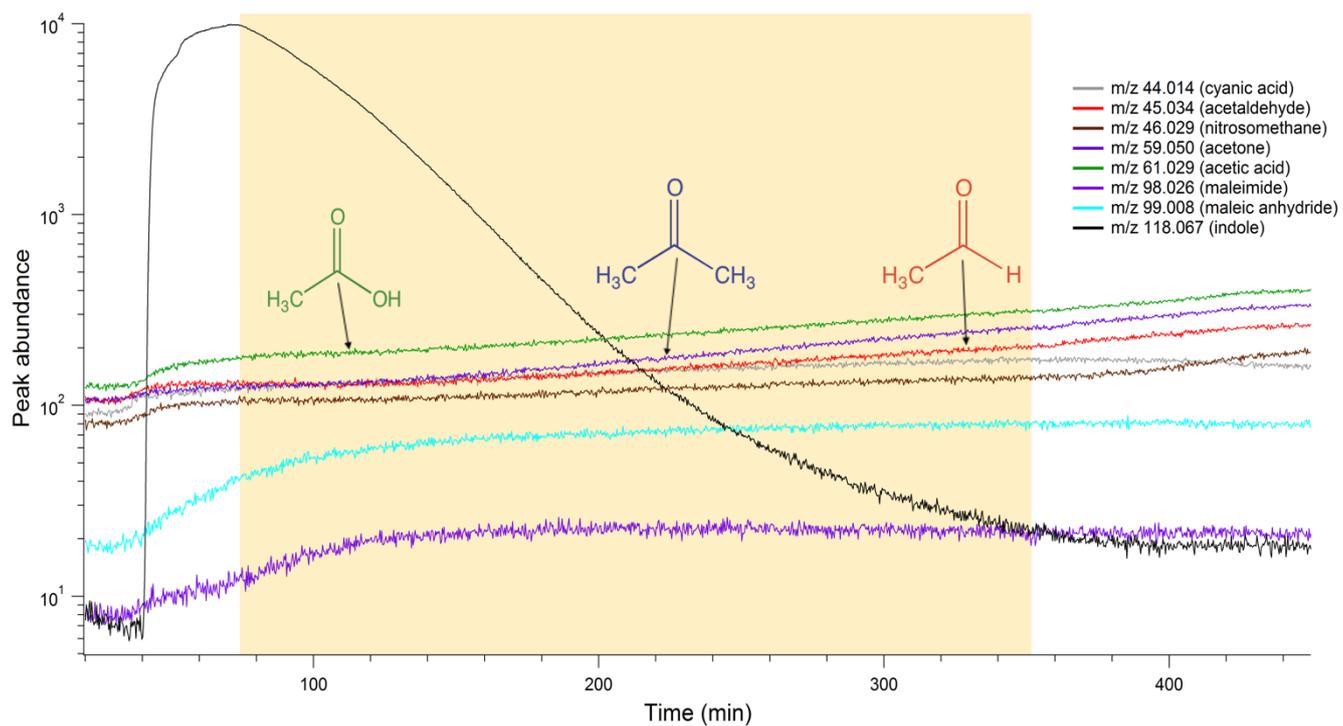


Figure S2.5: Time-dependent signals of ions that increased during photooxidation. Shaded region denotes the time when the chamber lamps were on.

5

Table S2. Summary of assigned PTR-ToF-MS peaks.

Calibrated m/z	Exact m/z	Ion Formula	Neutral Formula	Possible Assignment	Behavior
44.014	44.0131	CH ₂ NO ⁺	HOCN	cyanic acid	produced
45.034	45.0335	C ₂ H ₅ O ⁺	C ₂ H ₄ O	acetaldehyde	produced
46.029	46.0287	CH ₄ NO ⁺	CH ₃ NO	nitrosomethane	produced
47.014	47.0128	CH ₃ O ₂ ⁺	HCOOH	formic acid	produced
59.050	59.0491	C ₃ H ₇ O ⁺	C ₃ H ₆ O	acetone	produced
61.029	61.0284	C ₂ H ₅ O ₂ ⁺	C ₂ H ₄ O ₂	acetic acid	produced
90.950	90.9477	FeO ₂ H ₃ ⁺	H ₂ O·FeO	produced in ion source	removed
94.067	94.0651	C ₆ H ₈ N ⁺	C ₆ H ₇ N	phenylamine (aniline)	produced then removed
98.026	98.0237	C ₄ H ₄ NO ₂ ⁺	C ₄ H ₃ NO ₂	maleimide	produced
99.008	99.0077	C ₄ H ₃ O ₃ ⁺	C ₄ H ₂ O ₃	maleic anhydride	produced
104.050	104.0495	C ₇ H ₆ N ⁺	C ₆ H ₅ CN	benzonitrile	produced then removed
118.067	118.0651	C ₈ H ₈ N ⁺	C ₈ H ₇ N	indole	removed
120.072	120.0808	C ₈ H ₁₀ N ⁺	C ₈ H ₉ N	indoline (impurity)	removed
122.061	122.0600	C ₇ H ₈ NO ⁺	C ₇ H ₇ NO	2-formylformanilide	produced then removed
131.062	131.0604	C ₈ H ₇ N ₂ ⁺	C ₈ N ₆ N ₂	diazanaphthalene (impurity)	removed
132.050	132.0444	C ₈ H ₆ NO ⁺	C ₈ H ₅ NO	3-oxyindole	removed
134.061	134.0600	C ₈ H ₈ NO ⁺	C ₈ H ₇ NO	indoxyl	produced then removed
148.041	148.0393	C ₈ H ₆ NO ₂ ⁺	C ₈ H ₅ NO ₂	isatin	produced then removed
150.055	150.0550	C ₈ H ₈ NO ₂ ⁺	C ₈ H ₇ NO ₂	3-oxy-2-hydroxy-indole	produced then removed

S3. N/C ratio in indole SOA compounds

Reactions that involve oxidation and oligomerization of indole without loss of C or N atoms should conserve the N/C ratio at the value of $1/8$ ($= 0.125$), the initial value in indole. Loss and gain of N atoms should result in a large decrease and increase in the N/C ratio, respectively. Loss and gain of C atoms should result in a small increase and decrease in the N/C ratio, respectively. All of these processes are clearly happening in the photooxidation of indole although the N/C conserving processes are clearly dominant.

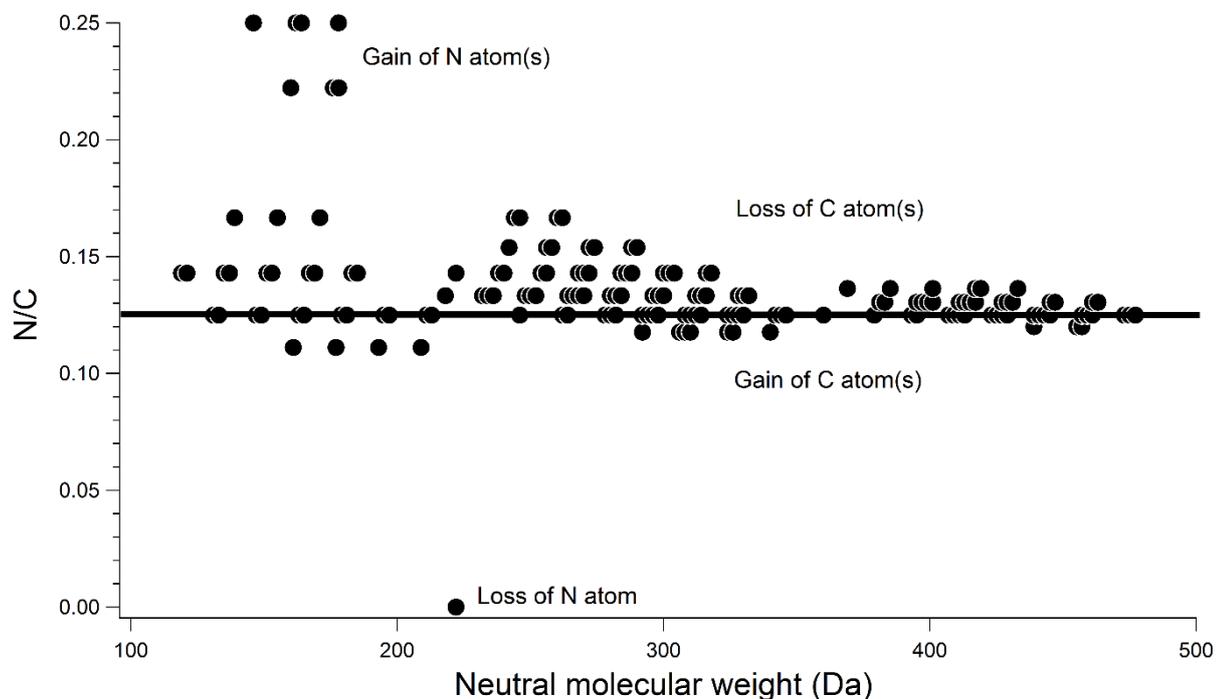


Figure S3: The N/C ratio of indole SOA compounds. The thick horizontal line corresponds to the N/C ratio in indole.

S4. Spatial distribution of gas-phase indole concentrations in SoCAB

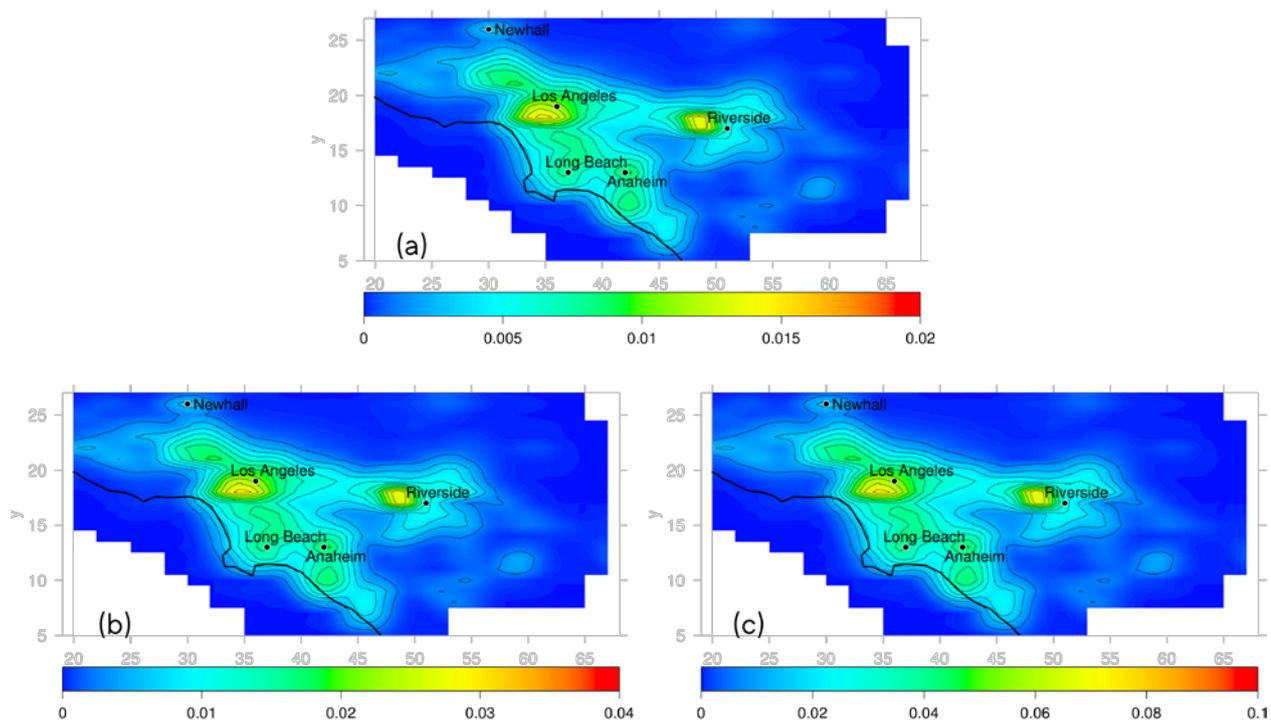


Figure S4: The 24-hour average gas-phase indole concentrations (ppb) in the (a) low emission scenario, (b) medium emissions scenario, and (c) high emission scenario.