- 1 Supplement of
- 2 Assessing the impact of anthropogenic pollution on isoprene-derived secondary organic
- 3 aerosol formation in PM_{2.5} collected from the Birmingham, Alabama ground site during the
- 4 2013 Southern Oxidant and Aerosol Study
- 5 W. Rattanavaraha et al.
- 6 Correspondence to: J. D. Surratt (<u>Surratt@unc.edu</u>)

Category	Variable	Analyze r/Sensor	Time Resolution (Interval, average) (minutes)
Meteorology	Wind Speed/Direction	RMYoung 81000 sonic	5, 60
80	T/RH/BP	Paroscientific Met4A	5, 60
	T/RH	Vaisala	5, 60
	PAR	Licor	5, 60
	Precipitation	ETI-NOAH IV	5, 60
	Aerosol/cloud layers	JenOptik CHM 15k ceilometer	5, 60
	Surface wetness	Vaisala (SWS2)	5, 60
Trace Gases	O ₃	Thermo 49i	5, 60
	СО	Thermo 48i	5, 60
	SO ₂	Thermo 43i	5,60
	NO	Thermo 42i	5, 60
	NO ₂	Photolysis/Thermo 49i	5,60
	HNO ₃	Continuous denuder diff/Thermo 42i	5, 60
	NOy	Cat. reduction/Thermo 42i	5, 60
	NH ₃	Continuous denuder diff/Thermo 42i	5, 60
Continuous PM	PM _{2.5} Mass	TEOM	60
	PMcoarse Mass	Dichotomous TEOM	60
	PM _{2.5} SO ₄	Cat. reduction/Thermo 43i	60
	PM _{2.5} NO ₃	Cat. reduction/Thermo 42i	60
	PM _{2.5} NH ₄	Cat. oxidation/Thermo 42i	60
	PM _{2 5} TC/EC	Sunset	60
	Dry Babs (880 nm)	Radiance Research M903	5,60
	Dry Bsp (530 nm)	Magee 2ch. Aeth	5, 60
	Ambient Bsp (530 nm)	Optec NGN-2a	5, 60
Filter-Based PM	PM _{2.5} Mass	gravimetry	1440, daily
	$PM_{2.5}$ ions	IC	1440, 1 in 3 days
	PM _{2.5} major/minor elements	XRF	1440, daily
	PM _{2.5} water-soluble metals	ICPMS	1440, 1 in 3 days
	PM _{2.5} OC/EC	TOR	1440, 1 in 3 days
	PM _{coarse} Mass	gravimetry	1440, 1 in 3 days
	PM _{coarse} ions	IC	1440, 1 in 3 days
	PM _{coarse} major/minor elements	XRF	1440, 1 in 3 davs
	PM _{coarse} water-soluble metals	ICPMS	1440, 1 in 3 days
Hi-Vol Based PM	PM _{2.5} OC/EC	TOR	23-hr, daily
	$PM_{2.5}$ ions	IC	23-hr, daily
	PM_{25} (other)	Various	11-hr daily

Table S1. Instrumentation and time resolution of collocated measurements at BHM.

Table S2. Correlation (r²) of isoprene-derived SOA tracers and collocated measurements during

regular day sampling (8 am - 7 pm).

SOA tracers	CO	O ₃	NO _x	NOy	SO ₂	NH ₃	SO ₄	NO ₃	NH4	OC	WSOC	рН
MAE/HMML-derived SOA	0.31	0.72	0.04	0.00	0.20	0.34	0.51	0.10	0.53	0.44	0.48	0.01
2-methylglyceric acid	0.14	0.44	0.01	0.00	0.09	0.15	0.19	0.03	0.27	0.09	0.12	0.00
MAE-derived OS	0.28	0.60	0.04	0.00	0.14	0.31	0.66	0.14	0.56	0.58	0.52	0.01
IEPOX-derived SOA tracers	0.09	0.26	0.01	0.01	0.08	0.12	0.41	0.04	0.41	0.31	0.32	0.01
2-methylerythritol	0.04	0.30	0.03	0.00	0.05	0.04	0.31	0.00	0.31	0.24	0.30	0.01
2-methylthreitol	0.02	0.20	0.02	0.00	0.06	0.03	0.21	0.00	0.23	0.13	0.19	0.00
(E)-2-methylbut-3-ene-1,2,4-triol	0.05	0.24	0.02	0.00	0.03	0.05	0.33	0.02	0.32	0.22	0.27	0.00
(Z)-2-methylbut-3-ene-1,2,4-triol	0.10	0.11	0.00	0.01	0.09	0.17	0.34	0.10	0.32	0.24	0.16	0.01
2-methylbut-3-ene-1,2,3-triol	0.11	0.11	0.00	0.01	0.09	0.18	0.36	0.10	0.34	0.25	0.17	0.01
IEPOX-derived OS	0.17	0.41	0.01	0.01	0.08	0.19	0.47	0.07	0.50	0.53	0.59	0.01
IEPOX dimer	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Other isoprene SOA tracers GA sulfate												
$C_2H_3O_6S^-$	0.22	0.20	0.00	0.00	0.07	0.19	0.49	0.20	0.39	0.33	0.21	0.01
Methylglyoxal-derived OS												
$C_3H_5O_6S^-$	0.25	0.40	0.01	0.01	0.11	0.11	0.57	0.05	0.46	0.41	0.47	0.01
Isoprene-derived OSs												
C ₅ H ₇ O ₇ S ⁻	0.13	0.34	0.01	0.01	0.02	0.17	0.35	0.11	0.40	0.21	0.28	0.00
$C_5H_{10}NO_9S^-$	0.02	0.37	0.12	0.06	0.00	0.01	0.48	0.12	0.38	0.18	0.12	0.11
C5H9N2O11S-*	0.25	0.56	0.48	0.40	0.15	0.40	0.52	0.28	0.24	0.57	0.46	0.00
Hydroxyacetone-derived OS												
C2H3O5S	0.42	0.73	0.06	0.16	0.00	0.18	0.55	0.23	0.71	0.57	0.66	0.00
Other tracer												
Levoglucosan	0.26	0.34	0.00	0.00	0.09	0.21	0.44	0.10	0.47	0.22	0.25	0.01

6 The correlations in this table are positive.

Table S3. Correlation (r²) of isoprene-derived SOA tracers and collocated measurements during

intensive 1 sampling (8 am - 11 am).

SOA tracers	CO	O ₃	NO _x	NOy	SO ₂	NH ₃	SO ₄	NO ₃	NH4	OC	WSOC	pН
MAE/HMML-derived SOA tracers	0.00	0.20	0.04	0.16	0.01	0.07	0.35	0.25	0.46	0.47	0.16	0.18
2-methylglyceric acid	0.03	0.22	0.05	0.10	0.00	0.07	0.00	0.43	0.11	0.46	0.07	0.08
MAE-derived OS	0.01	0.09	0.02	0.12	0.01	0.03	0.72	0.06	0.62	0.26	0.08	0.18
IEPOX-derived SOA tracers	0.11	0.04	0.05	0.00	0.06	0.26	0.30	0.00	0.16	0.04	0.02	0.03
2-methylerythritol	0.15	0.01	0.02	0.00	0.16	0.52	0.22	0.03	0.18	0.00	0.00	0.15
2-methylthreitol	0.04	0.00	0.00	0.00	0.10	0.19	0.13	0.02	0.16	0.00	0.02	0.13
(E)-2-methylbut-3-ene-1,2,4-triol	0.12	0.03	0.06	0.01	0.01	0.27	0.23	0.00	0.09	0.11	0.05	0.00
(Z)-2-methylbut-3-ene-1,2,4-triol	0.13	0.02	0.05	0.01	0.03	0.32	0.28	0.00	0.08	0.09	0.05	0.00
2-methylbut-3-ene-1,2,3-triol	0.07	0.02	0.02	0.00	0.02	0.26	0.22	0.01	0.03	0.04	0.28	0.01
IEPOX-derived OS	0.09	0.07	0.07	0.00	0.05	0.19	0.30	0.00	0.17	0.04	0.00	0.02
IEPOX dimer	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Other isoprene SOA tracers GA sulfate												
$C_2H_3O_6S^-$	0.00	0 19	0.03	0.01	0.01	0.03	0.37	0.02	0 44	0.25	0.11	0.00
Methylglyoxal-derived OS	0.00	0.17	0.05	0.01	0.01	0.05	0.57	0.02	0.11	0.20	0.11	0.00
$C_3H_5O_6S^-$	0.05	0.05	0.18	0.28	0.02	0.00	0.01	0.11	0.24	0.09	0.56	0.03
Isoprene-derived OSs												
C5H7O7S ⁻	0.09	0.15	0.00	0.20	0.05	0.02	0.36	0.12	0.25	0.40	0.00	0.02
$C_5H_{10}NO_9S^-$	0.00	0.05	0.02	0.06	0.06	0.04	0.38	0.00	0.23	0.17	0.18	0.37
C5H9N2O11S ^{-*}	0.00	0.00	0.00	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00
Hydroxyacetone-derived OS												
$C_2H_3O_5S^-$	0.25	0.67	0.71	0.65	0.21	0.21	0.03	0.26	0.12	0.50	0.00	0.70
Other tracer												
Levoglucosan	0.03	0.07	0.02	0.00	0.07	0.07	0.08	0.11	0.01	0.03	0.02	0.24
* Found only in 6 of 120 filters												

17 The correlations in this table are positive.

Table S4. Correlation (r²) of isoprene-derived SOA tracers and collocated measurements during intensive 2 sampling (12 pm – 3 pm).

SOA tracers	CO	O ₃	NO _x	NOy	SO ₂	NH ₃	SO ₄	NO ₃	NH4	OC	WSOC	рН
MAE/HMML-derived SOA	0.13	0.42	0.0	0.12	0.04	0.01	0.14	0.05	0.29	0.55	0.19	0.00
2-methylglyceric acid	0.01	0.47	0.25	0.32	0.00	0.04	0.00	0.05	0.04	0.17	0.07	005
MAE-derived OS	0.15	0.20	0.04	0.01	0.06	0.00	0.18	0.15	0.31	0.49	0.24	0.03
IEPOX-derived SOA	0.22	0.00	0.04	0.08	0.00	0.21	0.34	0.32	0.37	0.46	0.81	0.02
2-methylerythritol	0.41	0.00	0.13	0.14	0.01	0.16	0.48	0.24	0.50	0.42	0.77	0.01
2-methylthreitol	0.29	0.00	0.03	0.07	0.00	0.07	0.22	0.41	0.39	0.32	0.70	0.02
(E)-2-methylbut-3-ene-1,2,4-triol	0.17	0.00	0.04	0.07	0.01	0.17	0.30	0.31	0.29	0.44	0.61	0.02
(Z)-2-methylbut-3-ene-1,2,4-triol	0.21	0.00	0.05	0.07	0.01	0.17	0.33	0.29	0.31	0.45	0.64	0.01
2-methylbut-3-ene-1,2,3-triol	0.03	0.02	0.00	0.02	0.03	0.07	0.13	0.21	0.06	0.09	0.62	0.03
IEPOX-derived OS	0.19	0.02	0.11	0.21	0.00	0.32	0.43	0.16	0.39	0.52	0.58	0.00
IEPOX dimer	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Other isoprene SOA tracers GA sulfate												
$C_2H_3O_6S^-$	0.24	0.23	0.00	0.08	0.00	0.06	0.32	0.23	0.46	0.46	0.48	0.00
Methylglyoxal-derived OS												
$C_3H_5O_6S^-$	0.27	0.28	0.01	0.02	0.01	0.06	0.29	0.00	0.29	0.33	0.43	0.03
Isoprene-derived OSs												
C5H7O7S ⁻	0.14	0.02	0.06	0.07	0.03	0.06	0.16	0.00	0.18	0.18	0.09	0.00
$C_5H_{10}NO_9S^-$	0.00	0.15	0.07	0.05	0.21	0.34	0.03	0.05	0.00	0.06	0.00	0.18
C5H9N2O11S ^{-*}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hydroxyacetone-derived OS												
$C_2H_3O_5S^-$	0.09	0.40	0.01	0.01	0.10	0.05	0.04	0.07	0.10	0.07	0.62	0.01
Other tracer												
Levoglucosan	0.03	0.00	0.22	0.13	0.00	0.01	0.03	0.17	0.00	0.02	0.00	0.07

28 The correlations in this table are positive.

29	

Table S5. Correlation (r²) of isoprene-derived SOA tracers and collocated measurements during

intensive 3 sampling (4 pm – 7 pm).

SOA tracers	CO	O ₃	NO _x	NOy	SO ₂	NH ₃	SO ₄	NO ₃	NH4	OC	WSOC	рН
MAE/HMML-derived SOA	0.01	0.47	0.45	0.39	0.47	0.00	0.19	0.10	0.12	0.54	0.23	0.15
tracers 2-methylølyceric acid	0.12	0.37	0.03	0.17	0.25	0.00	0.00	0.05	0.02	0.34	0.50	0.15
MAE-derived OS	0.00	0.37	0.44	0.39	0.41	0.01	0.25	0.09	0.13	0.45	0.04	0.10
IEPOX-derived SOA	0.10	0.15	0.18	0.14	0.50	0.17	0.47	0.00	0.18	0.31	0.24	0.03
2-methylerythritol	0.03	0.34	0.08	0.04	0.58	0.12	0.34	0.01	0.14	0.42	0.22	0.00
2-methylthreitol	0.04	0.32	0.03	0.01	0.43	0.17	0.25	0.03	0.14	0.54	0.21	0.01
(E)-2-methylbut-3-ene-1,2,4-triol	0.00	0.21	0.05	0.02	0.70	0.13	0.33	0.00	0.12	0.38	0.01	0.02
(Z)-2-methylbut-3-ene-1,2,4-triol	0.00	0.21	0.09	0.05	0.77	0.14	0.41	0.00	0.13	0.27	0.01	0.01
2-methylbut-3-ene-1,2,3-triol	0.54	0.00	0.12	0.13	0.00	0.01	0.18	0.04	0.06	0.00	0.33	0.02
IEPOX-derived OS	0.15	0.10	0.17	0.12	0.42	0.16	0.41	0.00	0.15	0.24	0.29	0.03
IEPOX dimer	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Other isoprene SOA tracers GA sulfate												
$C_2H_3O_6S^-$	0.20	0.28	0.43	0.32	0.02	0.00	0.19	0.16	0.30	0.55	0.01	0.21
Methylglyoxal-derived OS	0.20	0.20	0.15	0.52	0.02	0.00	0.19	0.10	0.50	0.55	0.01	0.21
$C_3H_5O_6S^-$	0.26	0.16	0.01	0.01	0.10	0.12	0.57	0.34	0.60	0.03	0.00	0.02
Isoprene-derived OSs												
C ₅ H ₇ O ₇ S ⁻	0.06	0.18	0.19	0.13	0.12	0.14	0.45	0.02	0.35	0.55	0.02	0.00
$C_5H_{10}NO_9S^-$	0.06	0.45	0.00	0.03	0.80	0.05	0.44	0.03	0.18	0.27	0.15	0.00
C5H9N2O11S-*	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hydroxyacetone-derived OS												
C2H3O5S	0.49	0.01	0.10	0.20	0.13	0.05	0.44	0.24	0.11	0.06	0.29	0.10
Other tracer												
Levoglucosan	0.00	0.01	0.02	0.04	0.00	0.06	0.00	0.02	0.00	0.20	0.01	0.04

39 The correlations in this table are positive.

47 **Table S6.** Correlation (r^2) of isoprene-derived SOA tracers and collocated measurements during

48	intensive 4	and regular	nighttime	(8 pm –	7 am next day).
		<u> </u>	<u> </u>	\ I	27

SOA tracers	CO	O ₃	NO _x	NOy	SO ₂	NH ₃	SO ₄	NO ₃	NH4	OC	WSOC	рН
MAE/HMML-derived SOA	0.35	0.08	0.18	0.21	0.17	0.39	0.48	0.15	0.42	0.53	0.15	0.01
tracers 2-methylglyceric acid	0.18	0.00	0.13	0.10	0.12	0.18	0.17	0.05	0.22	0.17	0.01	0.04
MAE-derived OS	0.35	0.14	0.15	0.17	0.11	0.32	0.51	0.17	0.36	0.58	0.20	0.00
IEPOX-derived SOA	0 10	0 10	0.02	0.03	0.08	0 10	0.37	0.02	0.30	0.27	0.15	0.00
tracers	0.10	0.10	0.02	0.05	0.00	0.10	0.07	0.02	0.00	0.27	0.15	0.00
2-methylerythritol	0.02	0.12	0.00	0.00	0.05	0.01	0.23	0.00	0.20	0.14	0.09	0.00
2-methylthreitol	0.06	0.09	0.00	0.01	0.09	0.05	0.38	0.01	0.30	0.21	0.15	0.00
(E)-2-methylbut-3-ene-1,2,4-triol	0.09	0.08	0.02	0.03	0.10	0.10	0.35	0.03	0.28	0.26	0.11	0.00
(Z)-2-methylbut-3-ene-1,2,4-triol	0.07	0.07	0.01	0.02	0.10	0.07	0.32	0.02	0.27	0.22	0.08	0.00
2-methylbut-3-ene-1,2,3-triol	0.02	0.05	0.00	0.01	0.03	0.02	0.18	0.01	0.16	0.15	0.09	0.00
IEPOX-derived OS	0.17	0.10	0.08	0.10	0.01	0.16	0.27	0.03	0.21	0.31	0.14	0.01
IEPOX dimer	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Other isoprene SOA tracers												
GA sulfate												
$C_2H_3O_6S^-$	0.12	0.22	0.02	0.04	0.04	0.14	0.28	0.01	0.15	0.31	0.26	0.01
Methylglyoxal-derived OS												
$C_3H_5O_6S^-$	0.16	0.05	0.03	0.05	0.00	0.18	0.19	0.01	0.17	0.26	0.24	0.00
Isoprene-derived OSs												
C5H7O7S	0.12	0.15	0.01	0.02	0.02	0.09	0.22	0.01	0.11	0.17	0.12	0.00
$C_5H_{10}NO_9S^-$	0.20	0.00	0.11	0.12	0.08	0.21	0.39	0.18	0.33	0.30	0.09	0.00
$C_5H_9N_2O_{11}S^-$ *	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hydroxyacetone-derived OS												
$C_2H_3O_5S^-$	0.89	0.09	0.83	0.89	0.30	0.83	0.00	0.00	0.17	0.40	0.59	0.01
Other tracer												
Levoglucosan	0.23	0.00	0.22	0.24	0.08	0.21	0.13	0.01	0.18	0.25	0.11	0.00

50 The correlations in this table are positive.

Table S7. Regression and correlation (r²) analysis at the 95% confidence interval

	Variable	es		R	egression Stat	istics		
	Y	х	Number of observations	Multiple r	r ²	Adjusted r ²	Standard error	p-value
Nighttime: MAE/HMML-derived SOA vs P[NO ₃]	MAE/HMML - derived SOA	P[NO ₃]	40	0.7532	0.5673	0.5559	12.5098	2.05E-08
Nighttime: IEPOX-derived SOA vs P[NO ₃]	IEPOX-derived SOA	P[NO ₃]	40	0.5086	0.2587	0.2392	393.7399	8.05E-04
Regular day sampling: MAE/HMML-derived SOA vs O ₃	MAE/HMML - derived SOA	O ₃	30	0.8457	0.7153	0.7051	8.9517	4.00E-09
Daytime: 2-methyltetrols vs O ₃	2-methyltetrols	O ₃	64	0.3610	0.1303	0.1163	254.4175	3.39E-03
Intensive 3: MAE/HMML-derived SOA vs O ₃	MAE/HMML - derived SOA	O ₃	15	0.6844	0.4683	0.4274	18.3128	4.89E-03
Intensive 3: 2-methyltetrols vs O ₃	2-methyltetrols	O ₃	15	0.5844	0.3415	0.2908	259.0249	2.22E-02
MAE/HMML-derived SOA vs SO ₄	MAE/HMML - derived SOA	SO_4	117	0.5779	0.3340	0.3282	15.8648	8.96E-12
IEPOX-derived SOA vs SO ₄	IEPOX-derived SOA	SO ₄	117	0.6027	0.3632	0.3577	310.4400	6.51E-13



Figure S1. The locations of the three sampling sites during 2013 SOAS: BHM, CTR, and LRK.
BHM was the focused site in this study.



Figure S2. ¹H NMR (400 MHz, D₂O) of the MAE/HMML-derived OS.



Figure S3. (a) Comparison of organic carbon (OC) and water soluble organic carbon (WSOC),
suggesting that 35% of OC at BHM was WSOC. (b) Comparison of IEPOX- and MAE-derived
SOA tracers with WSOC, indicating that IEPOX- and MAE-derived SOA tracers explained 18
and 0.4% of the WSOC, respectively.



Figure S4. Diurnal variations of (a) meteorology, (b) O_3 and CO, (c) NO_y , NO, NO_2 , and NO_x , and (d) $PM_{2.5}$ constituents at BHM during the 2013 SOAS campaign. High temperature and low RH were observed at 2-4 pm local time. O_3 reached its maximum, while CO dropped to its minimum in early afternoon. NO_x and NO_y were high during early morning hours and declined in the afternoon due to photochemical processes. No significant diurnal variation was observed for NH_3 , SO_2 , SO_4^{2-} , NH_4^+ , and NO_3^- .

111

112



128 was observed.



Figure S6. The box-and-whisker plot (n = 15) of (a) MAE/HMML-SOA, (b) MAE/HMML-OS,
and (c) 2-MG. These demonstrate that the statistical distribution of SOA abundance during each
intensive sampling period. No significant variation amongst intensive samples was observed.



Figure S7. The box-and-whisker plot (n = 15) of (a) IEPOX-derived SOA, (b) IEPOX-OS, (c) 2methyltetrols, and (d) (E)-2-methylbut-3-ene-1,2,4-triol. These demonstrate that the statistical distribution of SOA abundance during each intensive sampling period. No significant variation amongst intensive samples was observed.