

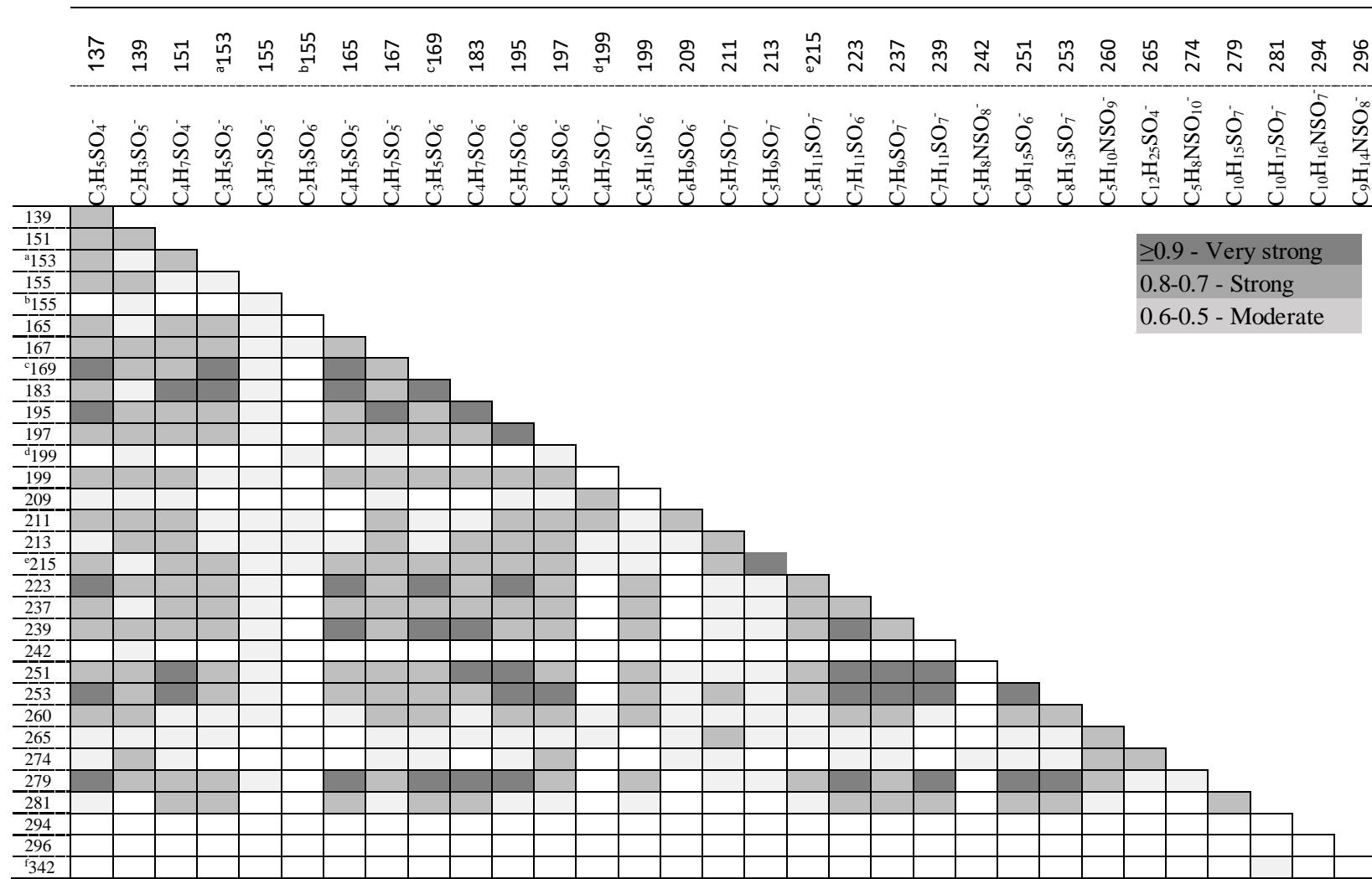
Supplement of

Organosulfates in Atlanta, GA: Anthropogenic influences on biogenic SOA formation

Hettiyadura et al.

Correspondence to: Elizabeth A. Stone (betsy-stone@uiowa.edu)

Table S1. Intercorrelations of organosulfates in Atlanta, GA during August 2015 (n = 26). All shaded cells indicate correlations that are positive and significant at 0.05 level. None of the organosulfates showed negative correlations that are significant at 0.05 level.



^aHydroxyacetone sulfate, ^bglycolic acid sulfate, ^clactic acid sulfate, ^d2-methylglyceric acid sulfate, ^emethyltetrox sulfonate, ^fC₁₀H₁₆NSO₁₀⁻

Table S2. Correlations of organosulfates with biogenic SOA tracers (n=26) in Atlanta, GA during August 2015; IEOPOX-SOA tracers (2-methylthreitol, 2-methylerythritol, cis-2-methyl-1,3,4-trihydroxy-1-butadiene, 3-methyl-2,3,4-trihydroxy-1-butene, and trans-2-methyl-1,3,4-trihydroxy-1-butene), isoprene high-NO_x SOA tracer (2-methylglyceric acid), monoterpene SOA (cis-pinonic acid), and sesquiterpene SOA tracer (β -caryophyllinic acid).

<i>m/z</i>	Chemical formula	2-Methylthreitol	2-Methylerythritol	cis-2-Methyl-1,3,4-trihydroxy-1-butadiene	3-Methyl-2,3,4-trihydroxy-1-butene	trans-2-Methyl-1,3,4-trihydroxy-1-butene	2-Methylglyceric acid	cis-Pinonic acid	β -Caryophyllinic acid
137	C ₃ H ₅ SO ₄ ⁻	.655**	.634**	0.276	0.268	0.279	0.256	0.287	0.296
139	C ₂ H ₅ SO ₅ ⁻	.557**	.472*	0.260	0.286	0.249	0.255	0.258	0.319
151	C ₄ H ₇ SO ₄ ⁻	.705**	.690**	0.388	0.378	0.335	0.353	0.248	0.361
^a 153	C ₃ H ₅ SO ₅ ⁻	.816**	.770**	0.269	0.244	0.278	0.371	0.300	0.379
155	C ₃ H ₇ SO ₅ ⁻	.448*	0.372	0.192	0.216	0.181	0.154	0.122	0.296
^b 155	C ₂ H ₅ SO ₆ ⁻	0.265	0.328	.613**	.585**	.491*	0.197	0.285	.391*
165	C ₄ H ₇ SO ₅ ⁻	.768**	.670**	0.089	0.091	0.134	0.241	0.180	0.190
167	C ₄ H ₉ SO ₅ ⁻	.709**	.727**	.511**	.511**	.515**	.459*	.433*	.514**
^c 169	C ₃ H ₅ SO ₆ ⁻	.725**	.665**	0.236	0.231	0.252	0.259	0.338	0.301
183	C ₄ H ₉ SO ₆ ⁻	.780**	.727**	0.257	0.241	0.238	0.318	0.230	0.308
195	C ₅ H ₉ SO ₆ ⁻	.749**	.708**	0.375	0.381	0.369	.438*	0.336	.439*
197	C ₅ H ₉ SO ₆ ⁻	.670**	.635**	0.361	0.371	0.352	.389*	0.263	.398*
^d 199	C ₄ H ₇ SO ₇ ⁻	.437*	.525**	.524**	.539**	.621**	.608**	0.366	.498**
199	C ₅ H ₁₁ SO ₆ ⁻	.643**	.595**	0.068	0.090	0.166	0.246	0.130	0.093
209	C ₆ H ₉ SO ₆ ⁻	0.339	.402*	.682**	.713**	.658**	.404*	.610**	.474*
211	C ₅ H ₉ SO ₇ ⁻	.633**	.668**	.672**	.678**	.635**	.556**	.490*	.600**
213	C ₅ H ₉ SO ₇ ⁻	.680**	.685**	.646**	.634**	.568**	.475*	.423*	.502**
^e 215	C ₅ H ₁₁ SO ₇ ⁻	.753**	.761**	.553**	.522**	.498**	.446*	0.363	.443*
223	C ₇ H ₁₁ SO ₆ ⁻	.685**	.633**	0.202	0.220	0.262	0.303	0.247	0.307
237	C ₇ H ₉ SO ₇ ⁻	.594**	.549**	0.246	0.243	0.188	0.256	0.186	0.349
239	C ₇ H ₁₁ SO ₇ ⁻	.736**	.668**	0.139	0.140	0.140	0.272	0.136	0.254
242	C ₅ H ₈ NSO ₈ ⁻	0.149	0.053	-0.008	0.016	-0.015	0.163	0.109	0.386
251	C ₉ H ₁₅ SO ₆ ⁻	.687**	.660**	0.288	0.298	0.294	0.348	0.218	0.363
253	C ₈ H ₁₃ SO ₇ ⁻	.618**	.587**	0.255	0.262	0.224	0.236	0.162	0.275
260	C ₅ H ₁₀ NSO ₉ ⁻	.420*	.420*	0.198	0.205	0.205	0.232	0.181	0.265
265	C ₁₂ H ₂₅ SO ₄ ⁻	0.351	0.363	0.379	0.374	0.318	0.344	0.273	.460*
274	C ₅ H ₈ NSO ₁₀ ⁻	0.212	0.173	0.167	0.168	0.081	0.044	0.108	0.213
279	C ₁₀ H ₁₅ SO ₇ ⁻	.682**	.634**	0.200	0.199	0.208	0.239	0.219	0.261
281	C ₁₀ H ₁₇ SO ₇ ⁻	.541**	.495*	-0.019	-0.038	-0.057	0.103	-0.083	0.068
294	C ₁₀ H ₁₆ NSO ₇ ⁻	-0.227	-0.283	-0.189	-0.159	-0.208	-0.047	-0.108	0.017
296	C ₉ H ₁₄ NSO ₈ ⁻	-0.001	-0.059	-0.248	-0.244	-0.302	-0.096	-0.287	0.023
342	C ₁₀ H ₁₆ NSO ₁₀ ⁻	0.030	0.009	-0.235	-0.240	-0.326	-0.106	-0.383	-0.039

*Correlation is significant at the 0.05 level, **Correlation is significant at the 0.01 level, ^ahydroxyacetone sulfate, ^bglycolic acid sulfate, ^clactic acid sulfate, ^d2-methylglyceric acid sulfate, ^emethyltetrol sulfate

Table S3. Correlations of organosulfates with anthropogenic SOA in Atlanta, GA during August 2015

<i>m/z</i>	Chemical formula	Meso-erythrytol	2,3-Dihydroxy-4-oxopentanoic acid	Phthalic acid	Terephthalic acid	Isophthalic acid	4-Methylphthalic acid	4-Nitrophenol	2-Methyl-4-nitrophenol	4-Methyl-2-nitrophenol	4-Nitrocatechol	3-Methyl-6-nitrocatechol	3-Methyl-5-nitrocatechol
n		26	26	26	26	26	26	20	8	18	20	7	25
137	C ₃ H ₅ SO ₄ ⁻	.674**	0.154	0.234	-0.170	0.056	0.202	-0.203	.859**	0.081	.542*	-0.202	0.335
139	C ₂ H ₃ SO ₅ ⁻	.539**	0.254	0.249	-0.144	0.098	0.199	0.115	.806*	0.464	0.387	-0.290	0.129
151	C ₄ H ₇ SO ₄ ⁻	.637**	0.244	0.311	-0.151	0.198	0.268	-0.348	.820*	-0.189	.559*	-0.178	0.341
^a 153	C ₃ H ₅ SO ₅ ⁻	.691**	0.238	0.316	-0.106	0.208	0.298	-.483*	.896**	-0.251	0.417	-0.042	0.328
155	C ₃ H ₇ SO ₅ ⁻	.456*	0.182	0.166	-0.162	-0.003	0.095	0.153	0.673	.527*	.496*	-0.095	0.127
^b 155	C ₂ H ₃ SO ₆ ⁻	.482*	0.376	0.340	0.238	0.254	0.313	.445*	-0.099	.540*	0.173	.927**	0.182
165	C ₄ H ₅ SO ₅ ⁻	.565**	0.133	0.112	-0.201	-0.006	0.081	-0.385	.837**	-0.168	.537*	-0.105	0.369
167	C ₄ H ₇ SO ₅ ⁻	.774**	.403*	.461*	0.076	0.305	.433*	-0.258	.886**	0.072	.508*	-0.373	.413*
^c 169	C ₃ H ₅ SO ₆ ⁻	.663**	0.167	0.216	-0.202	0.069	0.197	-0.327	.815*	-0.066	.502*	-0.394	0.278
183	C ₄ H ₇ SO ₆ ⁻	.634**	0.205	0.241	-0.185	0.125	0.210	-.465*	.847**	-0.223	.544*	-0.264	0.333
195	C ₅ H ₇ SO ₆ ⁻	.719**	0.276	0.370	-0.121	0.203	0.325	-0.165	.899**	0.152	.627**	-0.561	0.277
197	C ₅ H ₉ SO ₆ ⁻	.649**	0.253	0.337	-0.147	0.172	0.278	-0.001	.937**	0.292	.667**	-0.442	0.281
^d 199	C ₄ H ₇ SO ₇ ⁻	.621**	.439*	.552**	0.133	0.349	.493*	.574**	0.425	.650**	0.372	-0.299	0.053
199	C ₅ H ₁₁ SO ₆ ⁻	.542**	0.013	0.056	-0.297	-0.123	0.001	-0.079	0.695	0.177	.588**	-0.263	0.330
209	C ₆ H ₉ SO ₆ ⁻	.666**	0.279	.435*	0.057	0.313	.413*	.534*	0.591	.637**	.487*	-0.576	0.022
211	C ₅ H ₇ SO ₇ ⁻	.750**	.534**	.583**	0.118	.392*	.538**	0.134	.816*	0.378	0.386	-0.369	0.163
213	C ₅ H ₉ SO ₇ ⁻	.693**	.452*	.483*	0.047	0.347	.443*	-0.052	0.658	0.235	0.339	-0.285	0.153
^e 215	C ₅ H ₁₁ SO ₇ ⁻	.710**	.388*	.423*	-0.043	0.292	0.387	-0.282	.737*	0.006	0.395	-0.212	0.218
223	C ₇ H ₁₁ SO ₆ ⁻	.634**	0.138	0.226	-0.222	0.045	0.174	-0.192	.946**	0.085	.716**	-0.367	0.330
237	C ₇ H ₉ SO ₇ ⁻	.516**	0.128	0.253	-0.135	0.190	0.226	-0.291	.816*	-0.103	.609**	-0.112	.419*
239	C ₇ H ₁₁ SO ₇ ⁻	.567**	0.177	0.175	-0.207	0.046	0.131	-0.418	.812*	-0.193	.553*	-0.204	0.389
242	C ₅ H ₈ NSO ₈ ⁻	0.146	0.188	0.292	-0.045	0.242	0.270	0.342	.713*	.694**	-0.010	-0.214	-0.150
251	C ₉ H ₁₅ SO ₆ ⁻	.631**	0.166	0.281	-0.196	0.141	0.229	-0.297	.933**	-0.057	.686**	-0.382	0.367
253	C ₈ H ₁₃ SO ₇ ⁻	.588**	0.173	0.186	-0.174	0.040	0.137	-0.198	.853**	0.037	.689**	-0.172	.406*
260	C ₅ H ₁₀ NSO ₉ ⁻	.498**	0.108	0.231	-0.200	0.062	0.195	-0.010	.923**	0.253	.581**	-0.378	0.246
265	C ₁₂ H ₂₅ SO ₄ ⁻	.426*	.408*	.438*	-0.008	0.292	.409*	0.074	.840**	0.180	.483*	-0.356	0.092

274	C ₅ H ₈ NSO ₁₀ ⁻	0.277	0.125	0.155	-0.100	0.061	0.136	0.018	0.679	0.295	0.289	-0.307	0.152
279	C ₁₀ H ₁₅ SO ₇ ⁻	.632**	0.134	0.168	-0.198	0.024	0.136	-0.263	.830*	0.003	.611**	-0.226	0.356
281	C ₁₀ H ₁₇ SO ₇ ⁻	0.339	-0.031	-0.009	-0.267	-0.048	-0.038	-.535*	.781*	-0.388	.552*	0.054	.437*
294	C ₁₀ H ₁₆ NSO ₇ ⁻	-0.175	-0.078	-0.030	-0.097	0.031	-0.045	.591**	-0.111	0.341	0.201	-0.013	-0.162
296	C ₉ H ₁₄ NSO ₈ ⁻	-0.080	-0.245	-0.092	-0.251	-0.097	-0.130	0.044	0.346	-0.056	.572**	-0.275	0.128
342	C ₁₀ H ₁₆ NSO ₁₀ ⁻	-0.099	0.027	-0.142	0.017	-0.003	-0.151	-0.255	0.161	-0.273	0.129	0.543	.436*

*Correlation is significant at the 0.05 level, **Correlation is significant at the 0.01 level, ^ahydroxyacetone sulfate, ^bglycolic acid sulfate, ^clactic acid sulfate, ^d2-methylglyceric acid sulfate, ^emethyltetrol sulfate

Table S4. Correlations of organosulfates ($n = 26$) with sulfate and nitrate in PM_{2.5}, ozone, NO_x (NO and NO₂), and solar radiation in Atlanta, GA during August 2015.

<i>m/z</i>	Chemical formula	SO ₄ ²⁻	O ₃	NO	NO ₂	Solar radiation
137	C ₃ H ₅ SO ₄ ⁻	.410*	.638**	-.391*	0.002	0.259
139	C ₂ H ₃ SO ₅ ⁻	.544**	.606**	-.518**	-0.214	0.172
151	C ₄ H ₇ SO ₄ ⁻	0.250	.644**	-0.258	0.053	0.283
^a 153	C ₃ H ₅ SO ₅ ⁻	0.178	.527**	-0.238	0.106	0.358
155	C ₃ H ₇ SO ₅ ⁻	.606**	.445*	-.473*	-0.289	0.240
^b 155	C ₂ H ₃ SO ₆ ⁻	0.346	0.267	-0.178	0.132	0.008
165	C ₄ H ₅ SO ₅ ⁻	0.239	.572**	-0.276	-0.062	0.360
167	C ₄ H ₇ SO ₅ ⁻	.484*	.710**	-0.368	0.071	0.254
^c 169	C ₃ H ₅ SO ₆ ⁻	0.361	.600**	-0.362	0.024	0.349
183	C ₄ H ₇ SO ₆ ⁻	0.222	.615**	-0.317	0.037	0.364
195	C ₅ H ₇ SO ₆ ⁻	.389*	.764**	-.522**	0.035	0.371
197	C ₅ H ₉ SO ₆ ⁻	.401*	.802**	-.526**	-0.005	0.371
^d 199	C ₄ H ₇ SO ₇ ⁻	0.213	.533**	-.438*	0.083	0.282
199	C ₅ H ₁₁ SO ₆ ⁻	0.259	.708**	-.478*	-0.229	0.317
209	C ₆ H ₉ SO ₆ ⁻	.422*	.697**	-.475*	0.144	0.326
211	C ₅ H ₇ SO ₇ ⁻	.429*	.616**	-.451*	0.034	0.135
213	C ₅ H ₉ SO ₇ ⁻	0.296	.618**	-.438*	-0.052	0.186
^e 215	C ₅ H ₁₁ SO ₇ ⁻	0.224	.618**	-0.369	0.013	0.271
223	C ₇ H ₁₁ SO ₆ ⁻	.413*	.706**	-.434*	-0.061	.393*
237	C ₇ H ₉ SO ₇ ⁻	0.291	.636**	-0.179	0.138	0.339
239	C ₇ H ₁₁ SO ₇ ⁻	0.284	.570**	-0.296	-0.064	0.279
242	C ₅ H ₈ NSO ₈ ⁻	.486*	0.201	-0.320	-0.121	0.077
251	C ₉ H ₁₅ SO ₆ ⁻	0.350	.705**	-.374	0.052	0.343
253	C ₈ H ₁₃ SO ₇ ⁻	.429*	.621**	-0.329	0.005	0.240
260	C ₅ H ₁₀ NSO ₉ ⁻	.443*	.689**	-.446*	0.068	0.203
265	C ₁₂ H ₂₅ SO ₄ ⁻	0.359	.398*	-0.213	0.242	0.188
274	C ₅ H ₈ NSO ₁₀ ⁻	.498**	.449*	-0.348	0.031	0.016
279	C ₁₀ H ₁₅ SO ₇ ⁻	.392*	.570**	-.356	0.070	0.302
281	C ₁₀ H ₁₇ SO ₇ ⁻	0.065	0.359	0.029	0.154	0.222
294	C ₁₀ H ₁₆ NSO ₇ ⁻	-0.010	-0.055	-0.020	0.213	0.261
296	C ₉ H ₁₄ NSO ₈ ⁻	-0.016	0.101	-0.100	0.242	.418*
342	C ₁₀ H ₁₆ NSO ₁₀ ⁻	-0.023	-0.199	.401*	0.234	0.062

*Correlation is significant at the 0.05 level, **Correlation is significant at the 0.01 level, ^ahydroxyacetone sulfate, ^bglycolic acid sulfate, ^clactic acid sulfate, ^d2-methylglyceric acid sulfate, ^emethyltetrost sulfate