

*Supplement of*

**A study of volatility by composition, dilution, and heating measurements  
of secondary organic aerosol from 1,3,5-trimethylbenzene**

Kei Sato et al.

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Table S1. Initial concentration condition, mass concentration of produced SOA, geometric mean size of produced SOA, and analytical methods employed in each experimental run.

Run	[HC] <sub>0</sub> ppm	[NO] <sub>0</sub> ppm	[CH <sub>3</sub> ONO] <sub>0</sub> ppm	[SOA] <sup>b</sup> μg m <sup>-3</sup>	Size nm	Measurements <sup>c</sup>	Comment
1	1.48	1.09	0.01	192	395	TD-AMS, LC/MS, PTR-MS	
2	1.48	1.19	0.01	228	558	TD-AMS, LC/MS, PTR-MS	Aging expt. <sup>a</sup>
3	1.50	1.21	0.01	203	364	TD-AMS, EDC (DR = 19.6)	
4	1.53	1.21	0.01	182	391	TD-AMS, EDC (DR = 40.3)	
5	1.52	1.20	0.01	184	391	TD-AMS, EDC (DR = 63.4)	
6	1.49	1.20	0.01	171	393	TD-AMS, EDC (DR = 86.1)	
7	1.51	1.18	0.01	254	408	flow diluter	

<sup>a</sup> SOA formed from the TMB photooxidation was exposed to OH radicals. <sup>b</sup> Calculated from the volume concentration by assuming particle density to 1.40 g·cm<sup>-3</sup> (present study). <sup>c</sup> EDC is external dilution chamber, DR is dilution ratio.

Table S2. Measured mass-to-charge ratio ( $m/z$ ), suggested ion formula, calculated molecular weight (MW), measured total intensities of extracted ion chromatogram (EIC) peaks, calculated O/C ratio, and predicted saturation concentrations for products existing in SOA from TMB.

$m/z$	Ion formula	MW	Total int. of EIC peaks (normal, run 1)	Total int. of EIC peaks (aging, run 2)	O/C	$\log_{10} C^*$ (line fitted to molecular corridor)	$\log_{10} C^*$ (eq. by Li et al., 2016)
185.042	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> Na	162.053	33,796	62,479	0.83	3.77	3.43
193.047	C <sub>8</sub> H <sub>10</sub> O <sub>4</sub> Na	170.058	138,991	134,015	0.50	3.43	4.10
197.042	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub> Na	174.053	57,574	97,423	0.71	3.26	3.28
207.063	C <sub>9</sub> H <sub>12</sub> O <sub>4</sub> Na	184.074	394,346	425,366	0.44	2.83	3.81
209.078	C <sub>9</sub> H <sub>14</sub> O <sub>4</sub> Na	186.089	1,339,087	917,440	0.44	2.75	3.81
213.037	C <sub>7</sub> H <sub>10</sub> O <sub>6</sub> Na	190.048	78,894	66,442	0.86	2.58	2.11
215.053	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> Na	192.063	149,163	212,665	0.86	2.49	2.11
223.058	C <sub>9</sub> H <sub>12</sub> O <sub>5</sub> Na	200.068	337,888	362,721	0.56	2.15	2.85
223.094	C <sub>10</sub> H <sub>16</sub> O <sub>4</sub> Na	200.105	52,609	30,785	0.40	2.15	3.50
225.073	C <sub>9</sub> H <sub>14</sub> O <sub>5</sub> Na	202.084	1,902,497	2,852,655	0.56	2.07	2.85
227.053	C <sub>8</sub> H <sub>12</sub> O <sub>6</sub> Na	204.063	127,216	263,746	0.75	1.98	1.97
239.053	C <sub>9</sub> H <sub>12</sub> O <sub>6</sub> Na	216.063	61,399	99,896	0.67	1.47	1.79
239.089	C <sub>10</sub> H <sub>16</sub> O <sub>5</sub> Na	216.100	614,689	390,379	0.50	1.47	2.59
241.068	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> Na	218.079	1,500,300	1,673,638	0.67	1.39	1.79
243.084	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> Na	220.095	1,081,863	1,371,867	0.67	1.30	1.79
245.078	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub> Na	222.089	1,077,603	1,120,068	0.33	1.22	2.83
253.105	C <sub>11</sub> H <sub>18</sub> O <sub>5</sub> Na	230.115	115,520	114,146	0.45	0.87	2.30
255.084	C <sub>10</sub> H <sub>16</sub> O <sub>6</sub> Na	232.095	142,174	116,783	0.60	0.79	1.58
257.063	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> Na	234.074	127,222	198,565	0.78	0.71	0.66
259.079	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> Na	236.090	180,451	189,460	0.78	0.62	0.66
267.084	C <sub>11</sub> H <sub>16</sub> O <sub>6</sub> Na	244.095	248,734	338,602	0.55	0.28	1.34
267.120	C <sub>12</sub> H <sub>20</sub> O <sub>5</sub> Na	244.131	48,466	40,845	0.42	0.28	2.00
269.100	C <sub>11</sub> H <sub>18</sub> O <sub>6</sub> Na	246.110	232,300	177,791	0.55	0.19	1.34
271.076	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> Na	248.090	1,006,870	1,240,322	0.70	0.11	0.50
273.095	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> Na	250.105	934,881	1,310,159	0.70	0.02	0.50
285.095	C <sub>11</sub> H <sub>18</sub> O <sub>7</sub> Na	262.105	472,668	567,055	0.64	-0.49	0.30
286.053	C <sub>9</sub> H <sub>13</sub> NO <sub>8</sub> Na	263.064	1,116,433	2,098,323	0.89	-0.53	-1.09
287.074	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> Na	264.085	333,899	488,359	0.80	-0.57	-0.65
289.089	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> Na	266.100	153,112	152,395	0.80	-0.66	-0.65
297.095	C <sub>12</sub> H <sub>18</sub> O <sub>7</sub> Na	274.105	392,058	450,345	0.58	-1.00	0.07
309.095	C <sub>13</sub> H <sub>18</sub> O <sub>7</sub> Na	286.105	86,112	147,151	0.54	-1.51	-0.17
319.115	C <sub>15</sub> H <sub>20</sub> O <sub>6</sub> Na	296.126	655,649	411,098	0.40	-1.93	0.17
335.110	C <sub>15</sub> H <sub>20</sub> O <sub>7</sub> Na	312.121	776,371	557,866	0.47	-2.61	-0.72
337.105	C <sub>18</sub> H <sub>18</sub> O <sub>5</sub> Na	314.115	996,703	1,045,977	0.28	-2.70	-0.10

Table S2. Measured mass-to-charge ratio ( $m/z$ ), suggested ion formula, calculated molecular weight (MW), measured total intensities of extracted ion chromatogram (EIC) peaks, calculated O/C ratio, and predicted saturation concentrations for products existing in SOA from TMB (continued).

$m/z$	Ion formula	MW	Total int. of EIC peaks (normal, run 1)	Total int. of EIC peaks (aging, run 2)	O/C	$\log_{10} C^*$ (line fitted to molecular corridor)	$\log_{10} C^*$ (eq. by Li et al., 2016)
339.105	C <sub>14</sub> H <sub>20</sub> O <sub>8</sub> Na	316.116	265,193	336,772	0.57	-2.78	-1.44
351.105	C <sub>15</sub> H <sub>20</sub> O <sub>8</sub> Na	328.116	478,275	419,619	0.53	-3.29	-1.69
363.141	C <sub>17</sub> H <sub>24</sub> O <sub>7</sub> Na	340.152	1,151,661	576,982	0.41	-3.80	-1.33
365.136	C <sub>20</sub> H <sub>22</sub> O <sub>5</sub> Na	342.147	1,827,276	1,925,906	0.25	-3.89	-0.86
367.100	C <sub>15</sub> H <sub>20</sub> O <sub>9</sub> Na	344.111	535,723	258,279	0.60	-3.97	-2.71
369.116	C <sub>15</sub> H <sub>22</sub> O <sub>9</sub> Na	346.126	405,546	425,047	0.60	-4.06	-2.71
377.136	C <sub>21</sub> H <sub>22</sub> O <sub>5</sub> Na	354.147	226,718	163,024	0.24	-4.40	-1.24
379.136	C <sub>17</sub> H <sub>24</sub> O <sub>8</sub> Na	356.147	926,647	423,039	0.47	-4.48	-2.24
381.130	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub> Na	358.142	407,132	317,930	0.30	-4.57	-1.55
383.095	C <sub>15</sub> H <sub>20</sub> O <sub>10</sub> Na	360.106	317,655	130,575	0.67	-4.65	-3.78
383.110	C <sub>19</sub> H <sub>20</sub> O <sub>7</sub> Na	360.121	166,839	222,005	0.37	-4.65	-1.98
391.136	C <sub>18</sub> H <sub>24</sub> O <sub>8</sub> Na	368.147	1,323,695	652,300	0.44	-4.99	-2.53
393.152	C <sub>18</sub> H <sub>26</sub> O <sub>8</sub> Na	370.163	2,818,500	867,842	0.44	-5.08	-2.53
395.131	C <sub>17</sub> H <sub>24</sub> O <sub>9</sub> Na	372.142	611,129	535,442	0.53	-5.16	-3.20
395.168	C <sub>18</sub> H <sub>28</sub> O <sub>8</sub> Na	372.178	214,934	65,202	0.44	-5.16	-2.53
399.126	C <sub>16</sub> H <sub>24</sub> O <sub>10</sub> Na	376.137	274,427	310,964	0.63	-5.33	-3.99
407.135	C <sub>18</sub> H <sub>24</sub> O <sub>9</sub> Na	384.142	694,004	514,558	0.50	-5.67	-3.47
409.147	C <sub>18</sub> H <sub>26</sub> O <sub>9</sub> Na	386.158	2,590,992	1,650,003	0.50	-5.76	-3.47
411.126	C <sub>17</sub> H <sub>24</sub> O <sub>10</sub> Na	388.137	109,514	257,271	0.59	-5.84	-4.21
411.141	C <sub>21</sub> H <sub>24</sub> O <sub>7</sub> Na	388.152	599,344	399,801	0.33	-5.84	-2.67
411.163	C <sub>18</sub> H <sub>28</sub> O <sub>9</sub> Na	388.173	143,870	81,447	0.50	-5.84	-3.47
415.121	C <sub>16</sub> H <sub>24</sub> O <sub>11</sub> Na	392.132	310,719	318,827	0.69	-6.01	-5.08
425.142	C <sub>18</sub> H <sub>26</sub> O <sub>10</sub> Na	402.153	1,153,390	1,172,884	0.56	-6.44	-4.46
427.158	C <sub>18</sub> H <sub>28</sub> O <sub>10</sub> Na	404.168	706,196	562,726	0.56	-6.52	-4.46
441.137	C <sub>18</sub> H <sub>26</sub> O <sub>11</sub> Na	418.148	345,697	529,328	0.61	-7.12	-5.49
441.152	C <sub>22</sub> H <sub>26</sub> O <sub>8</sub> Na	418.163	633,244	273,278	0.36	-7.12	-3.81
443.152	C <sub>18</sub> H <sub>28</sub> O <sub>11</sub> Na	420.163	465,185	374,715	0.61	-7.20	-5.49
457.132	C <sub>18</sub> H <sub>26</sub> O <sub>12</sub> Na	434.142	158,391	226,223	0.67	-7.80	-6.57
459.147	C <sub>18</sub> H <sub>28</sub> O <sub>12</sub> Na	436.158	139,947	307,765	0.67	-7.88	-6.57
472.143	C <sub>18</sub> H <sub>27</sub> NO <sub>12</sub> Na	449.153	1,616,158	1,140,221	0.67	-8.44	-7.02
475.142	C <sub>18</sub> H <sub>28</sub> O <sub>13</sub> Na	452.153	371,298	395,561	0.72	-8.56	-7.68
488.138	C <sub>18</sub> H <sub>27</sub> NO <sub>13</sub> Na	465.148	845,870	776,656	0.72	-9.12	-7.74
504.132	C <sub>18</sub> H <sub>27</sub> NO <sub>14</sub> Na	481.143	271,311	426,529	0.78	-9.80	-8.46

Table S3. SMILES code, SPARC saturation concentration, and molecular weight of measured or suggested products formed from the photooxidation of TMB.

name	SMILES	log(C*/ $\mu\text{g m}^{-3}$ )	MW	ref.
3,5-dimethylbenzaldehyde	<chem>O=CC1=CC(=CC(=C1)C)C</chem>	6.03	134.2	Smith et al., 1999
2,4,6-trimethylphenol	<chem>OC1=C(C=C(C=C1)C)C</chem>	5.14	136.2	Smith et al., 1999
3,5-dimethyl-3(2H)-2-furanone	<chem>O=C1OC(=CC1)C</chem>	6.32	112.1	Smith et al., 1999
3,5-dimethyl-5(2H)-2-furanone	<chem>O=C1OC(C=C1)C</chem>	6.36	112.1	Smith et al., 1999
3-methyl-5-methylidene-5(2H)-2-furanone	<chem>O=C1OC(=C)C=C1C</chem>	5.02	110.1	Smith et al., 1999
2-methyl-4-oxo-2-pentenal	<chem>O=CC(=CC(=O)C)C</chem>	5.78	112.1	Smith et al., 1999
citraconic anhydride	<chem>O=C(O1)C(C)=CC1=O</chem>	3.68	112.1	Smith et al., 1999
methylglyoxal	<chem>O=CC(=O)C</chem>	8.38	72.1	Smith et al., 1999
TM135OXMUC	<chem>O=CC1(OC1C(=CC(=O)C)C)C</chem>	5.31	168.2	MCM v3.3.1
C7M2CO5OOH	<chem>OOC(C(=O)C)C(=CC(=O)C)C</chem>	3.41	172.2	MCM v3.3.1
C7M3CO	<chem>CC(=O)C=C(C)C(=O)C(=O)C</chem>	4.47	154.2	MCM v3.3.1
CH3CO2H	<chem>CC(=O)O</chem>	7.68	60.1	MCM v3.3.1
CH3OOH	<chem>COO</chem>	7.83	48.0	MCM v3.3.1
HCHO	<chem>C=O</chem>	9.86	30.0	MCM v3.3.1
CH3OH	<chem>CO</chem>	8.41	32.0	MCM v3.3.1
CH3NO3	<chem>CON(=O)=O</chem>	8.42	77.0	MCM v3.3.1
CH3O2NO2	<chem>COON(=O)=O</chem>	8.17	93.0	MCM v3.3.1
CH3CO3H	<chem>CC(=O)OO</chem>	7.48	76.1	MCM v3.3.1
PAN	<chem>CC(=O)OON(=O)=O</chem>	6.84	121.0	MCM v3.3.1
MGLYOX	<chem>O=CC(=O)C</chem>	8.38	72.1	MCM v3.3.1
MMALANHY	<chem>O=C1C=C(C)C(=O)O1</chem>	3.68	112.1	MCM v3.3.1
MMALNHYOOH	<chem>CC1(OO)C(O)C(=O)OC1=O</chem>	-0.05	162.1	MCM v3.3.1
CO2H3CO3H	<chem>CC(=O)C(O)C(=O)OO</chem>	4.47	134.1	MCM v3.3.1
HCOCO3H	<chem>OOC(=O)C=O</chem>	6.35	90.0	MCM v3.3.1
HCOCO2H	<chem>O=CC(=O)O</chem>	8.55	74.0	MCM v3.3.1
C4PAN6	<chem>O=N(=O)OOC(=O)C(O)C(=O)C</chem>	3.20	179.1	MCM v3.3.1
MMALNHY2OH	<chem>O=C1OC(=O)C(C)(O)C1O</chem>	0.82	146.1	MCM v3.3.1
C5CODBCO3H	<chem>CC(=CC(=O)C)C(=O)OO</chem>	3.53	144.1	MCM v3.3.1
C4MCODBPAN	<chem>O=N(=O)OOC(=O)C(=CC(=O)C)C</chem>	3.62	189.1	MCM v3.3.1
C5CODBCO2H	<chem>CC(=O)C=C(C)C(=O)O</chem>	4.29	128.1	MCM v3.3.1
CH3COCO2H	<chem>OC(=O)C(=O)C</chem>	7.35	88.1	MCM v3.3.1
C5CO234	<chem>CC(=O)C(=O)C(=O)C</chem>	6.73	114.1	MCM v3.3.1
C5CO234OOH	<chem>CC(=O)C(=O)C(=O)COO</chem>	3.41	146.1	MCM v3.3.1
C5MDICARB	<chem>O=CC(=CC(=O)C)C</chem>	5.78	112.1	MCM v3.3.1
C6CO2OHOOH	<chem>OOC(C)(C=O)C(O)C(=O)C</chem>	3.26	162.1	MCM v3.3.1
C5CO243OH	<chem>CC(=O)C(O)C(=O)C</chem>	5.88	116.1	MCM v3.3.1
C6CO2M2OH	<chem>O=CC(C)(O)C(O)C(=O)C</chem>	3.78	146.1	MCM v3.3.1
C6CO3MOH	<chem>O=CC(C)(O)C(=O)C(=O)C</chem>	5.84	144.1	MCM v3.3.1
C5COHOCO3H	<chem>OOC(=O)C(C)(O)C(=O)C(=O)C</chem>	4.27	176.1	MCM v3.3.1
C4COMOHPAN	<chem>O=N(=O)OOC(=O)C(C)(O)C(=O)C(=O)C</chem>	3.19	221.1	MCM v3.3.1
CHOMOHCO3H	<chem>CC(O)(C=O)C(=O)OO</chem>	5.16	134.1	MCM v3.3.1
MXYFUONE	<chem>CC1OC(=O)C(=C1)C</chem>	6.36	112.1	MCM v3.3.1
NMXYFUOOH	<chem>OOC1(C)C(=O)OC(C)C1ON(=O)=O</chem>	2.34	207.1	MCM v3.3.1
C23O3MCHO	<chem>O=CC(C)OC(=O)C(=O)C</chem>	5.86	144.1	MCM v3.3.1
C23O3MCO2H	<chem>CC(OC(=O)C(=O)C)C(=O)O</chem>	3.17	160.1	MCM v3.3.1
C23O3MCOOH	<chem>CC(OC(=O)C(=O)C)OO</chem>	4.39	148.1	MCM v3.3.1
ACECOCOCH3	<chem>CC(=O)OC(=O)C(=O)C</chem>	5.43	130.1	MCM v3.3.1
ACCOCOMOHH	<chem>OOC(=O)C(=O)OC(=O)C</chem>	2.48	162.1	MCM v3.3.1
CH3CHO	<chem>CC=O</chem>	8.98	44.1	MCM v3.3.1
HCOCH2OOH	<chem>OOC(=O)O</chem>	6.03	76.1	MCM v3.3.1
GLYOX	<chem>O=CC=O</chem>	8.61	58.0	MCM v3.3.1
HOCH2CHO	<chem>OCC=O</chem>	6.87	60.1	MCM v3.3.1
HOCH2CO2H	<chem>OCC(=O)O</chem>	5.17	76.1	MCM v3.3.1
HOCH2CO3H	<chem>OCC(=O)OO</chem>	5.93	92.1	MCM v3.3.1
C23O3MOH	<chem>CC(O)OC(=O)C(=O)C</chem>	5.53	132.1	MCM v3.3.1
C23O3MCO3H	<chem>OOC(=O)C(C)OC(=O)C(=O)C</chem>	4.04	176.1	MCM v3.3.1
C23O3MCPAN	<chem>O=N(=O)OOC(=O)C(C)OC(=O)C(=O)C</chem>	3.87	221.1	MCM v3.3.1
MXYFUOOH	<chem>CC1(OO)C(O)C(C)OC1=O</chem>	1.34	162.1	MCM v3.3.1
CO24C53OOH	<chem>OOC(C(=O)C)C(=O)C</chem>	5.06	132.1	MCM v3.3.1
C7M2CO5OH	<chem>CC(=O)C=C(C)C(O)C(=O)C</chem>	4.12	156.2	MCM v3.3.1

Table S3. SMILES code, SPARC saturation concentration, and molecular weight of measured or suggested products formed from the photooxidation of TMB (continued).

name	SMILES	log(C*/ $\mu\text{g m}^{-3}$ )	MW	ref.
TM135MUO2H	<chem>CC(=O)C=C(C)C1OC1(C)C(=O)O</chem>	1.56	184.2	MCM v3.3.1
TM135MUO3H	<chem>OOC(=O)C1(C)OC1C(=CC(=O)C)C</chem>	3.51	200.2	MCM v3.3.1
TM135MUPAN	<chem>O=N(=O)OOC(=O)C1(C)OC1C(=CC(=O)C)C</chem>	3.32	245.2	MCM v3.3.1
EPXMALKT	<chem>O=CC1(C)OC1C(=O)C</chem>	6.39	128.1	MCM v3.3.1
EPXMKTCO2H	<chem>CC(=O)C1OC1(C)C(=O)O</chem>	3.10	144.1	MCM v3.3.1
EPXMKTCO3H	<chem>CC1(OC1C(=O)C)C(=O)OO</chem>	4.58	160.1	MCM v3.3.1
EPXMKTPAN	<chem>O=N(=O)OOC(=O)C1(C)OC1C(=O)C</chem>	4.41	205.1	MCM v3.3.1
C3MDIALOOH	<chem>OOC(C)(C=O)C=O</chem>	5.68	118.1	MCM v3.3.1
C3MDIALOH	<chem>O=CC(C)(O)C=O</chem>	6.74	102.1	MCM v3.3.1
TM135MUOOH	<chem>OOC(C)(C(O)C(=O)C)C1OC1(C)C=O</chem>	1.58	218.2	MCM v3.3.1
TM135MUNO3	<chem>O=CC1(C)OC1C(C)(ON(=O)=O)C(O)C(=O)C</chem>	2.47	247.2	MCM v3.3.1
TM135MUOH	<chem>O=CC1(C)OC1C(C)(O)C(O)C(=O)C</chem>	2.00	202.2	MCM v3.3.1
TMBOOH	<chem>OOCc1cc(C)cc(C)c1</chem>	4.18	152.2	MCM v3.3.1
TMBCHO	<chem>O=Cc1cc(C)cc(C)c1</chem>	6.03	134.2	MCM v3.3.1
DMPHOOH	<chem>OOc1cc(C)cc(C)c1</chem>	4.55	138.2	MCM v3.3.1
DMPHOHNO2	<chem>Cc1cc(C)c(N(=O)=O)c(O)c1</chem>	4.99	167.2	MCM v3.3.1
MXOHNO2OOH	<chem>OOC1(O)C(=CC2(C)OOC1(N(=O)=O)C2O)C</chem>	-1.59	249.2	MCM v3.3.1
TMBCO2H	<chem>Cc1cc(C)cc(c1)C(=O)O</chem>	3.52	150.2	MCM v3.3.1
TMBCO3H	<chem>OOC(=O)c1cc(C)cc(C)c1</chem>	4.53	166.2	MCM v3.3.1
TMBNO3	<chem>O=N(=O)OCc1cc(C)cc(C)c1</chem>	5.03	181.2	MCM v3.3.1
TMBOH	<chem>OCc1cc(C)cc(C)c1</chem>	4.67	136.2	MCM v3.3.1
TM135BPOOH	<chem>OOC1C(=CC2(C)OOC1(C)C2O)C</chem>	1.56	202.2	MCM v3.3.1
TM135OBPOH	<chem>CC1=CC2(C)OOC(C)(C1=O)C2O</chem>	4.99	184.2	MCM v3.3.1
TM135BPN03	<chem>O=N(=O)OC1C(=CC2(C)OOC1(C)C2O)C</chem>	3.11	231.2	MCM v3.3.1
TM135BP2OH	<chem>CC1=CC2(C)OOC(C)(C1O)C2O</chem>	2.31	186.2	MCM v3.3.1
TM135BZOL	<chem>Cc1cc(C)c(O)c(C)c1</chem>	5.14	136.2	MCM v3.3.1
NTM135LOOH	<chem>OOC1(O)C(=CC2(C)OOC1(C)C2ON(=O)=O)C</chem>	0.99	263.2	MCM v3.3.1
NTM135OLOH	<chem>O=N(=O)OC1C2(C)OOC1(C)C(O)(O)C(=C2)C</chem>	1.20	247.2	MCM v3.3.1
TM135OLOOH	<chem>OOC1(O)C(=CC2(C)OOC1(C)C2O)C</chem>	0.05	218.2	MCM v3.3.1
TM135OLOH	<chem>OC1C2(C)OOC1(C)C(O)(O)C(=C2)C</chem>	-0.03	202.2	MCM v3.3.1
formic acid	<chem>O=CO</chem>	8.15	46.0	Fisseha et al., 2004
acetic acid	<chem>CC(O)=O</chem>	7.68	60.1	Fisseha et al., 2004
pyruvic acid	<chem>CC(C(O)=O)=O</chem>	7.35	88.1	Fisseha et al., 2004
lactic acid	<chem>CC(C(O)=O)O</chem>	5.51	90.1	Fisseha et al., 2004
oxalic acid	<chem>OC(C(O)=O)=O</chem>	5.58	90.0	Fisseha et al., 2004
malonic acid	<chem>OC(CC(O)=O)=O</chem>	1.83	104.1	Fisseha et al., 2004
succinic acid	<chem>OC(CCC(O)=O)=O</chem>	2.86	118.1	Fisseha et al., 2004
methyl maleic acid	<chem>O=C(C(C)=CC(O)=O)O</chem>	2.41	130.1	Fisseha et al., 2004
maleic acid	<chem>O=C(C=CC(O)=O)O</chem>	2.20	116.1	Fisseha et al., 2004
3,5-dimethylbenzoic acid	<chem>CC1=CC(C(O)=O)=CC(C)=C1</chem>	3.52	150.2	Fisseha et al., 2004
citric acid	<chem>OC(CC(O)=O)(C(O)=O)CC(O)=O</chem>	-4.29	192.1	Fisseha et al., 2004
MW88	<chem>CC(C(O)=O)=O</chem>	7.35	88.1	Sato et al., 2012
MW128	<chem>CC(C(O)=O)=CC(C)=O</chem>	4.29	128.1	Sato et al., 2012
MW162	<chem>CC(C(O)C(C)=O)(O)C(O)=O</chem>	1.00	162.1	Sato et al., 2012
MW170	<chem>CC(C(O)=O)=CC(C)=CC(O)=O</chem>	0.35	170.2	Sato et al., 2012
MW174	<chem>CC(C1C(C(O)=O)C)(O1)C(O)=O</chem>	-0.23	174.2	Sato et al., 2012
MW184	<chem>CC(C1C(C)=CC(C)=O)(O1)C(O)=O</chem>	1.56	184.2	Sato et al., 2012
MW186	<chem>CC(C1C(C)=CC(O)=O)(O1)C(O)=O</chem>	-1.04	186.2	Sato et al., 2012
MW190	<chem>CC(C(C(C(O)=O)C)=O)(O)C(O)=O</chem>	-3.75	190.2	Sato et al., 2012
MW192	<chem>CC(C(O)C(C(O)=O)C)(O)C(O)=O</chem>	-1.16	192.2	Sato et al., 2012
MW200	<chem>CC(C1C(C(C(O)=O)C)=O)(O1)C(O)=O</chem>	1.46	200.2	Sato et al., 2012
MW202	<chem>CC(C(O)C(C)=CC(C)=O)(O)C(O)=O</chem>	-0.28	202.2	Sato et al., 2012
MW204	<chem>CC(C1C(C(O)C(O)=O)(O)C)(O1)C(O)=O</chem>	-4.42	220.2	Sato et al., 2012
MW216	<chem>CC(C1C(C(C(O)=O)C)=O)(O)C(O)C(O)=O</chem>	-0.59	216.2	Sato et al., 2012
MW218	<chem>CC(C1C(C(O)C(C)=O)(O)C)(O1)C(O)=O</chem>	-1.49	218.2	Sato et al., 2012
MW232	<chem>CC(C(C(C(C(O)=O)C)=O)(O)C)=O)(O)C(O)=O</chem>	-0.82	232.2	Sato et al., 2012
MW234	<chem>CC(C(O)C(C(C(O)=O)C)=O)(O)C(O)C(O)=O</chem>	-1.50	234.2	Sato et al., 2012
glycolic acid	<chem>OCC(O)=O</chem>	5.17	76.1	Plapran et al., 2014
butanoic acid	<chem>CCCC(O)=O</chem>	6.62	88.1	Plapran et al., 2014
glyoxal 2-mer	<chem>OC(C)(OC(C(C)=O)O1)C1O</chem>	2.05	162.1	Kalberer et al., 2004

Table S3. SMILES code, SPARC saturation concentration, and molecular weight of measured or suggested products formed from the photooxidation of TMB (Continued).

name	SMILES	log(C*/ $\mu\text{g m}^{-3}$ )	MW	ref.
glyoxal 3-mer	<chem>CC1(OC(C(C)=O)O2)C2OC(C(C)=O)O1</chem>	4.56	216.2	Kalberer et al., 2004
glyoxal 4-mer	<chem>CC1(OC(C2(C)OC(O)C(C)(O)O2)O3)C3OC(C(C)=O)O1</chem>	-1.27	306.3	Kalberer et al., 2004
glyoxal 5-mer	<chem>CC1(OC(C2(C)OC(O)C(C)(O)O2)O3)C3OC(C4(C)OC(C)(O)C(O)O4)O1</chem>	-7.53	396.3	Kalberer et al., 2004
glyoxal 5-mer	<chem>CC1(OC(C2(C)OC(OC(C(C)=O)O3)C3(C)O2)O4)C4OC(C(C)=O)O1</chem>	1.55	360.3	Kalberer et al., 2004
glyoxal 6-mer	<chem>CC1(OC(C2(C)OC(OC(C(C)=O)O3)C3(C)O2)O4)C4OC(C5(C)OC(C)(O)C(O)O5)O1</chem>	-4.60	450.4	Kalberer et al., 2004
glyoxal 7-mer	<chem>CC1(OC(C2(C)OC(OC(C(C)=O)O3)C3(C)O2)O4)C4OC(C5(C)OC6(C)C(OC(C(C)=O)O6)O5)O1</chem>	-1.55	504.4	Kalberer et al., 2004
glyoxal 8-mer	<chem>CC1(OC(C2(C)OC(OC(C3(C)OC(O)C(C)(O)O3)O4)C4(C)O2)O5)C5OC(C6(C)OC7(C)C(OC(C(C)=O)O7)O6)O1</chem>	-7.91	594.5	Kalberer et al., 2004
glyoxal 2-mer + benzaldehyde	<chem>CC12C(OC(C(C)=O)O2)OC(C3=CC(C)=CC(C)=C3)O1</chem>	2.37	278.3	Kalberer et al., 2004
glyoxal 3-mer + benzaldehyde	<chem>CC12C(OC(C3(C)OC(O)C(C)(O)O3)O2)OC(C4=CC(C)=CC(C)=C4)O1</chem>	-2.86	368.4	Kalberer et al., 2004
glyoxal 4-mer + benzaldehyde	<chem>CC12C(OC(C3(C)OC4C(C)(OC(C(C)=O)O4)O3)O2)OC(C5=CC(C)=CC(C)=C5)O1</chem>	-0.97	422.4	Kalberer et al., 2004
glyoxal 5-mer + benzaldehyde	<chem>CC12C(OC(C3(C)OC4C(C)(OC(C5(OC(O)C(C)(O)O5)C)O4)O3)O2)OC(C6=CC(C)=CC(C)=C6)O1</chem>	-6.27	512.5	Kalberer et al., 2004
glyoxal 6-mer + benzaldehyde	<chem>CC12C(OC(C3(C)OC4C(C)(OC(C5(OC6C(C)(OC(C(C)=O)O6)O5)C)O4)O3)O2)OC(C7=CC(C)=CC(C)=C7)O1</chem>	-4.18	566.6	Kalberer et al., 2004
glyoxal 2-mer + pyruvic acid	<chem>O=C(C1(OC(OC(C(C)=O)O2)C2(C)O1)C)O</chem>	0.81	232.2	Kalberer et al., 2004
glyoxal 3-mer + pyruvic acid	<chem>O=C(C1(OC(OC(C2(C)OC(O)C(C)(O)O2)O3)C3(C)O1)C)O</chem>	-4.14	322.3	Kalberer et al., 2004
glyoxal 4-mer + pyruvic acid	<chem>O=C(C1(OC(OC(C2(C)OC3C(C)(OC(C(C)=O)O3)O2)O4)C4(C)O1)C)O</chem>	-2.28	376.3	Kalberer et al., 2004
glyoxal 5-mer + pyruvic acid	<chem>O=C(C1(OC(OC(C2(C)OC3C(C)(OC(C4(C)OC(O)C(C)(O)O4)O3)O2)O5)C5(C)O1)C)O</chem>	-7.99	466.4	Kalberer et al., 2004
glyoxal 6-mer + pyruvic acid	<chem>O=C(C1(OC(OC(C2(C)OC3C(C)(OC(C4(C)OC5C(C)(OC(C(C)=O)O5)O4)O3)O2)O6)C6(C)O1)C)O</chem>	-5.52	520.4	Kalberer et al., 2004

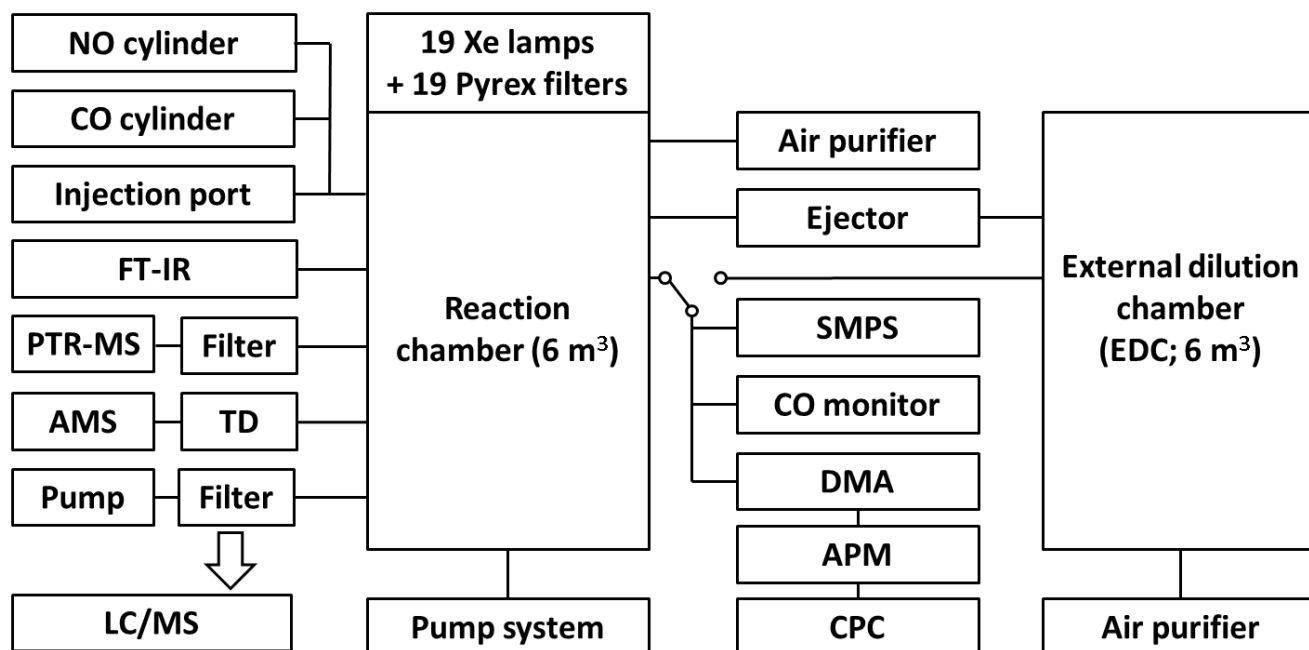


Figure S1. Schematic diagram of the chamber system and analytical instruments used in this study.



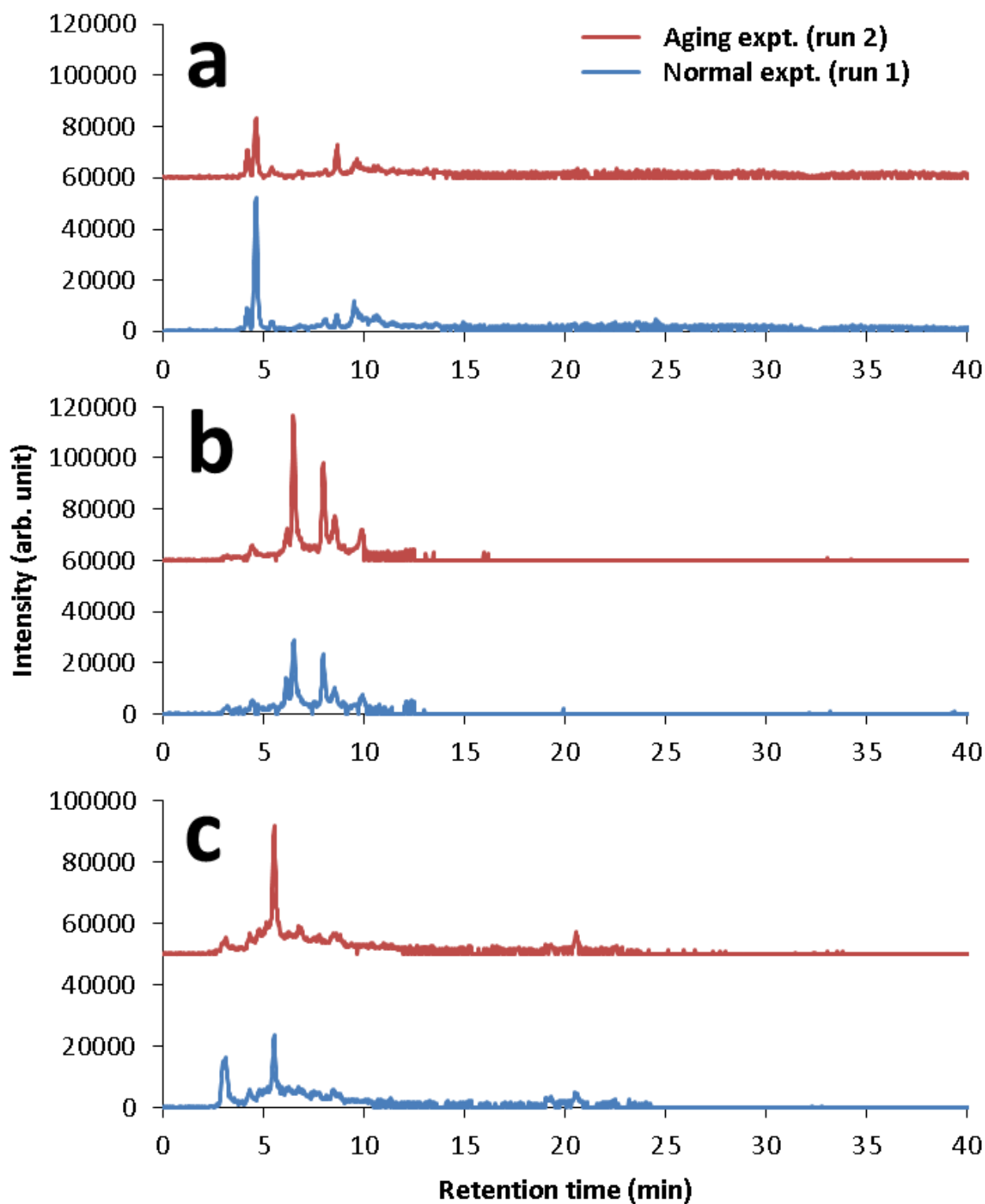


Figure S2. Extracted ion chromatograms observed for (a)  $C_9H_{14}O_4Na^+$ , (b)  $C_9H_{14}O_5Na^+$ , and (c)  $C_9H_{14}O_6Na^+$  by positive-mode LC/MS.

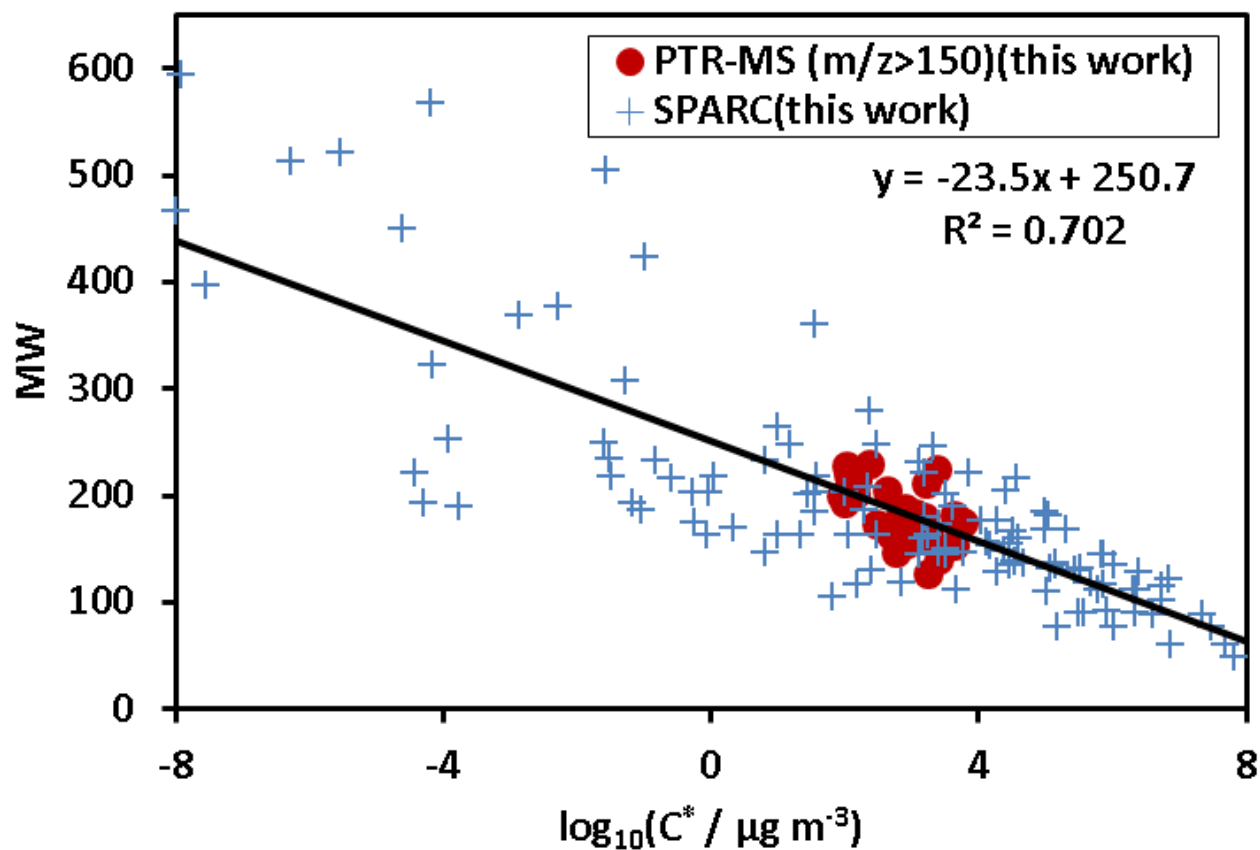


Figure S3. Molecular weight plotted as a function of saturation concentration for products formed from the photooxidation of TMB (molecular corridor).

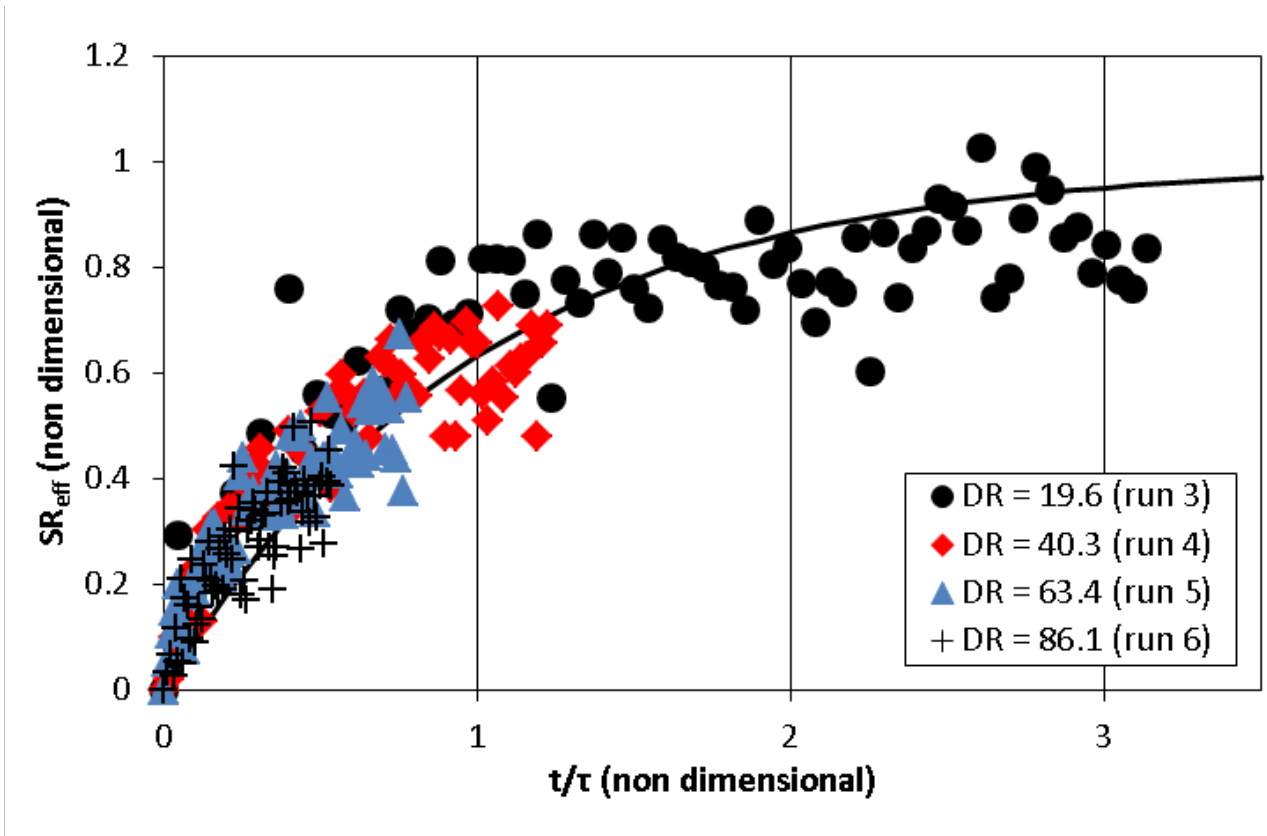


Figure S4. Effective saturation ratio ( $SR_{\text{eff}}$ ) plotted as a function of the ratio of time ( $t$ ) to equilibration timescale ( $\tau$ ).

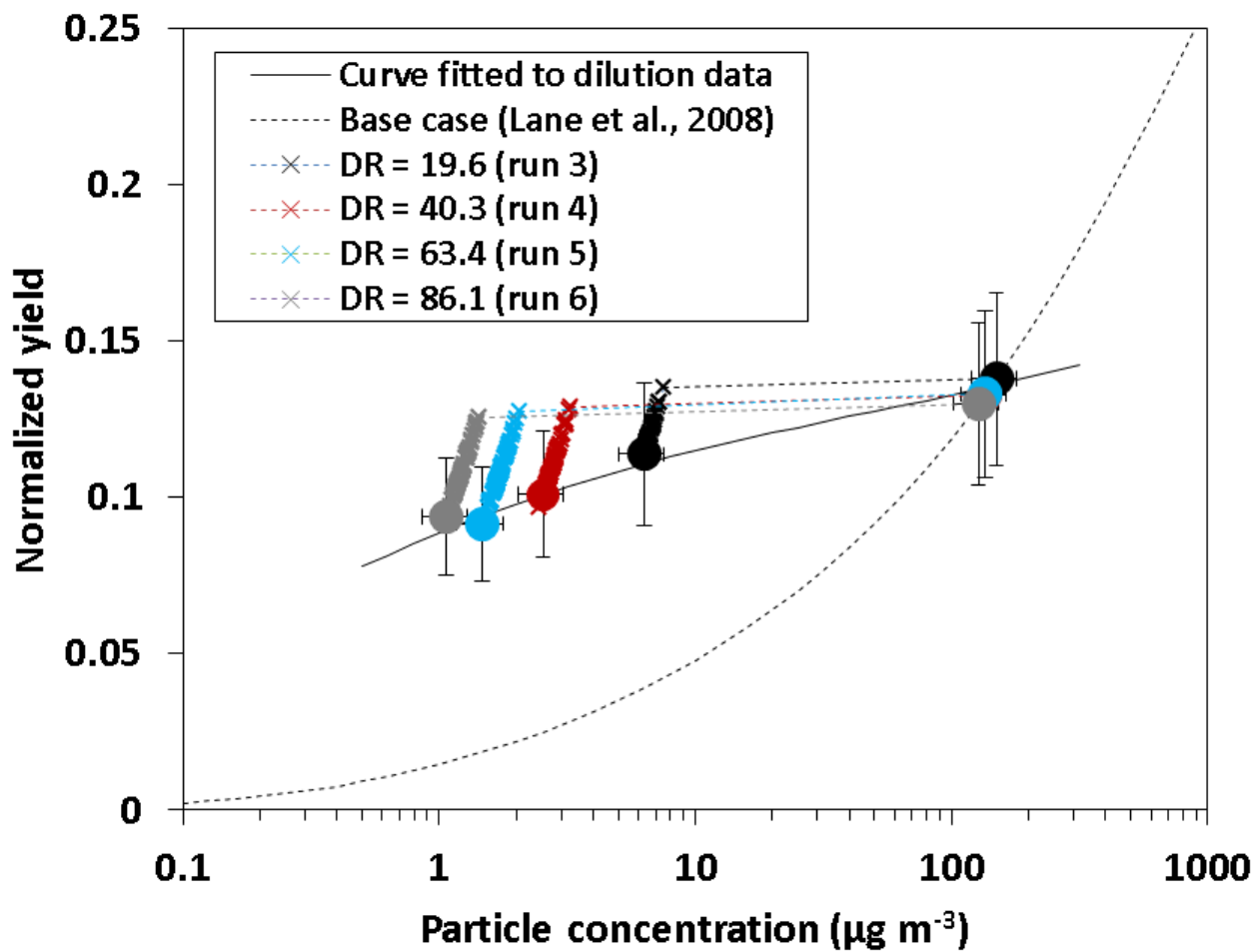


Figure S5. Normalized yield measured during dilution experiments as a function of particle concentration; circle symbols represent data observed before and 300 min after dilution.