SUPPORTING INFORMATION

Mutagenic atmospheres resulting from the photooxidation of aromatic hydrocarbon and NO_x mixtures

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No. of figures: 7

Table S1. Additional Experiment Data

Precursor VOC	Total SOA ($\mu g\ m^{-3}$)	Particle OC ($\mu gC\ m^{-3}$)	ΔHC[a] (ppmC)	ΔHC ($\mu gC\ m^{-3}$)	Gas-Phase OC[b] ($\mu C\ m^{-3}$)	SOA Mass Yield	ΔH_{eff}[c] ($kJ\ mol^{-1}$)	Exp No.[d]
benzene	191.8	78.4	2.14	1043	965	0.172	-9.5	763
toluene	165.8	74.5	2.53	1233	1159	0.122	-8.5	756
ethylbenzene	131.2	64.7	2.05	999	935	0.123	-14.6	754
o-xylene	224.0	119.2	3.39	1652	1533	0.127	-22.1	750
m-xylene	105.3	57.8	3.23	1574	1517	0.060	-29.8	751
p-xylene	70.0	37.5	3.31	1613	1576	0.038	-20.5	757
1,2,4-TMB	82.1	51.8	3.13	1526	1474	0.048	-31.3	753
1,3,5-TMB	108.6	72.9	3.00	1462	1390	0.071	-41.9	752
m-cresol	90.0	60.4	0.64	312	252	0.297	-13.3	749
naphthalene	95.8	60.6	0.92	448	388	0.296	-13.6	767
ethylbenzene-3.5	31.9	15.1	0.81	395	380	0.072	*N/A*	759
ethylbenzene-5	37.2	14.1	1.12	546	532	0.062	*N/A*	762
ethylbenzene-7	61.5	24.6	1.56	760	736	0.076	*N/A*	761
ethylbenzene-9	108.9	44.4	1.76	858	814	0.111	*N/A*	760

[a]ΔHC is the difference between Lights OFF and Lights ON Precursor VOC mixing ratios from Table 1.

[b]Gas-Phase OC is the difference between ΔHC and Particle OC not including any residual precursor VOC.

[c]ΔH_{eff} are the effective enthalpies of vaporization for the chamber-generated SOA. For more information, please consult: Offenberg, J. H.; Kleindienst, T. E.; Jaoui, M.; Lewandowski, M.; Edney, E. O., Thermal properties of secondary organic aerosols. *Geophysical Research Letters* **2006,** *33* (3).

[d]Experiment numbers are provided for internal reference.

Table S2. Mutagenicity in *Salmonella* TA100-S9 with Lights On

Precursor VOC	Exposure (h)	rev plate^{-1} [a]		
		Exp 1	Exp 2	
benzene	0	104, 93, 84	94, 92, 106	
	1	112, 139	81, 111	
	2	93, 101	83, 96	
	4	126, 88	118, 101	
	8	138, 126	126, 129	
	16	145, 167	210, 184	
sodium azide[b]		1110, 1145	1161, 1252	
toluene	0	117, 123, 102	107, 98, 131	
	1	130, 130	109, 111	
	2	122, 135	123, 144	
	4	162, 135	123, 158	
	8	195, 241	187, 185	
	16	305, 306		
sodium azide[b]		1193, 1202	1292, 1180	
ethylbenzene	0	121, 112, 119	120, 119, 146	
	1	137, 121	113, 106	
	2	102, 125	126, 159	
	4	155, 139	149, 158	
	8	213, 171	144, 171	
	16	253, 304	305, 314	
sodium azide[b]		1099, 1159	1186, 1153	
				Exp 3
o-xylene	0	149, 137, 119	119, 126, 139	113, 113, 116
	1	139, 134	124, 138	
	2	133, 141	127, 144	
	4	149, 165	181, 193	
	8	251, 250	263, 254	
	16	267, 296		304, 272
sodium azide[b]		801, 809	888	
m-xylene	0	141, 120, 121	106, 105, 128	
	1	144, 159	126, 121	
	2	118, 161	121, 150	
	4	151, 168	146, 144	
	8	218, 223	180, 170	
	16	254, 272	218, 215	
sodium azide[b]		851, 853	880, 824	
p-xylene	0	127, 156, 147	162, 141, 133	
	1	165, 139	178, 169	
	2	138, 153	145, 162	
	4	154, 168	133, 148	
	8	145, 149	196, 193	

	16	192, 204	214, 179
sodium azide[b]		1184, 1182	1196, 1171
1,2,4-TMB	0	118, 129, 124	147, 130, 126
	1	136, 142	150, 120
	2	146, 112	129, 169
	4	157, 144	165, 143
	8	180, 190	189, 187
	16	151, 149[c]	164, 147[c]
sodium azide[b]		599, 670	717, 703
1,3,5-TMB	0	109, 139, 114	112, 118, 111
	1	138, 112	135, 132
	2	171, 141	156, 161
	4	176, 148	151, 173
	8	227, 224	192, 176
	16	203, 195[c]	215, 198[c]
sodium azide[b]		710, 762	692, 680
m-cresol	0	100, 106, 101	116, 110, 117
	1	94, 111	105, 92
	2	111, 115	111, 115
	4	119, 114	120, 99
	8	89, 102	118, 101
sodium azide[b]		509, 463	474, 487
naphthalene	0	84, 106, 115	92, 95, 119
	1	111, 100	83, 92
	2	97, 105	100, 89
	4	94, 88	97, 99
	8	87, 90	78, 89
	16	109, 100[c]	77, 83[c]
sodium azide[b]		910, 889	834, 852
clean air	0	85, 88, 84	76, 80, 98
	1	69, 76	73, 95
	2	61, 94	95, 98
	4	75, 65	90, 100
	8	78, 59	78, 77
	16	54, 58[c]	69, 62[c]
sodium azide[b]		639, 692	744, 708

[a]Three plates were used for DMSO (0 h) controls, and two plates were used for all other exposures.

[b]Positive control at 3 µg/plate.

[c]Data not used in the linear regression because the r^2 value was reduced by inclusion of those data.

Table S3. Mutagenicity in *Salmonella* TA100-S9 with Lights Off

VOC combination	Exposure (h)	rev plate^{-1} [a]	
		Exp 1	Exp 2
benzene + 1,2,4-TMB + *o*-xylene (dark-1)	0	92, 95, 94	85, 72, 74
	1	79, 93	77, 79
	2	97, 95	80, 84
	4	83, 86	80, 73
	8	78, 78	77, 86
	16	54, 47[c]	24, 29[c]
sodium azide[b]		712, 780	515, 511
toluene + *m*-cresol + *m*-xylene (dark-2)	0	103, 101, 91	70, 85, 72
	1	103, 102	74, 62
	2	96, 115	65, 87
	4	90, 72	65, 55
	8	72, 81	40, 60
	16	63, 54[c]	26, 20[c]
sodium azide[b]		720, 745	200, 309
ethylbenzene + 1,3,5-TMB + *p*-xylene (dark-3)	0	70, 105, 109	96,86, 97
	1	86, 105	97, 104
	2	104, 83	99, 97
	4	81, 84	92, 95
	8	101, 111	99, 93
	16	67, 71[c]	61, 69[c]
sodium azide[b]		672, 697	783, 788
benzene + naphthalene (dark-4)	0	84, 79, 91	84, 88, 96
	1	96, 111	95, 73
	2	104, 100	105, 78
	4	79, 87	87, 89
	8	75, 76	77, 80
	16	61, 50[c]	51, 54[c]
sodium azide[b]		861, 858	728, 761
1,2,4-TMB + *o*-xylene (dark-5)	0	88, 104, 102	89, 91, 101
	1	99, 91	98, 120
	2	87, 85	104, 113
	4	103, 101	112, 105
	8	83, 95	96, 111
	16	54, 72[c]	74, 78[c]
sodium azide[b]		868, 818	748, 797

[a]Three plates were used for DMSO (0 h) controls, and two plates were used for all other exposures.

[b]Positive control at 3 µg/plate.

[c]Data not used in the linear regression because the r^2 value was reduced by inclusion of those data.

Table S4. *P*-Values of Correlations between Mutagenic Potencies of Each Experiment[a]

	benzene	toluene	ethylbenzene	*o*-xylene	*m*-xylene	*p*-xylene	1,2,4-TMB
toluene	<0.0001						
ethylbenzene	<0.0001	**0.3442**					
***o*-xylene**	<0.0176	0.0002	<0.0001				
***m*-xylene**	**0.7157**	<0.0001	<0.0001	0.0033			
***p*-xylene**	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001		
1,2,4-TMB	**0.6671**	<0.0001	<0.0001	0.0068	**0.9069**	0.0006	
1,3,5-TMB	0.0208	0.0122	0.0039	**0.6086**	0.0064	<0.0001	0.0118

[a]Correlations (Pearson's r) were the square root of the r^2 values determined by pair-wise comparisons of the mutagenic potencies of the atmospheres using the potency values from Table 1 expressed as rev m^3 mgC^{-1} h^{-1}. Values in **bold** are >0.05, indicating no significant difference between the mutagenic potencies of those two atmospheres with $P < 0.05$.

Table S5. Summary of Results for the Ethylbenzene Variable Residence Time Experiments

	Lights OFF		Lights ON				Mutagenic Potency	
Precursor VOC	**VOC (ppmC)**	**NO (ppbv)**	**VOC (ppmC)**	**NO (ppbv)**	**NO_2 (ppbv)**	**O_3 (ppbv)**	**rev h^{-1} ± SE**	**rev m^3 mgC^{-1} h^{-1} ± SE**
ethylbenzene-3.5	4.02	227	3.21	9	118	47	3.5 ± 0.8	9.2 ± 2.1
ethylbenzene-5	3.63	200	2.51	12	123	41	2.2 ± 0.3	4.1 ± 0.6
ethylbenzene-7	3.64	193	2.08	3	96	96	1.8 ± 0.6	2.4 ± 0.8
ethylbenzene-9	3.76	189	2.00	1	77	142	2.3 ± 0.5	2.8 ± 0.6

Table S6. Mutagenicity in *Salmonella* TA100-S9 with Lights On for Ethylbenzene Residence Time Experiments

Residence time (h)	Exposure (h)	rev plate^{-1} [a]	
		Exp 1	Exp 2
3.5	0	96, 88, 91	124, 153, 112
	1	142, 143	127, 144
	2	136, 144	138, 135
	4	158, 141	119, 125
	8	133, 161	123, 153
	16	178, 181	100, 95[c]
sodium azide[b]		1234, 1179	1232, 1217
5	0	104, 116, 103	106, 111, 104
	1	106, 101	110, 106
	2	128, 112	100, 102
	4	92, 121	98, 115
	8	119, 109	115, 126
	16	151, 141	153, 127
sodium azide[b]		857, 907	984, 910
7	0	98, 103, 105	156, 126, 128
	1	128, 112	134, 116
	2	133, 131	121, 131
	4	117, 150	131, 122
	8	139, 127	130,146
	16	176, 174	131, 117
sodium azide[b]		1154, 1131	1163, 1260
9	0	139, 127, 102	119, 122, 134
	1	147, 116	140, 123
	2	123, 111	114, 133
	4	133, 130	119, 116
	8	151, 117	117, 131
	16	154, 144	156, 198
sodium azide[b]		1180, 1106	1204, 1099

[a]Three plates were used for DMSO (0 h) controls, and two plates were used for all other exposures.

[b]Positive control at 3 µg/plate.

[c]Data not used in the linear regression because the R^2 value was reduced by inclusion of those data.

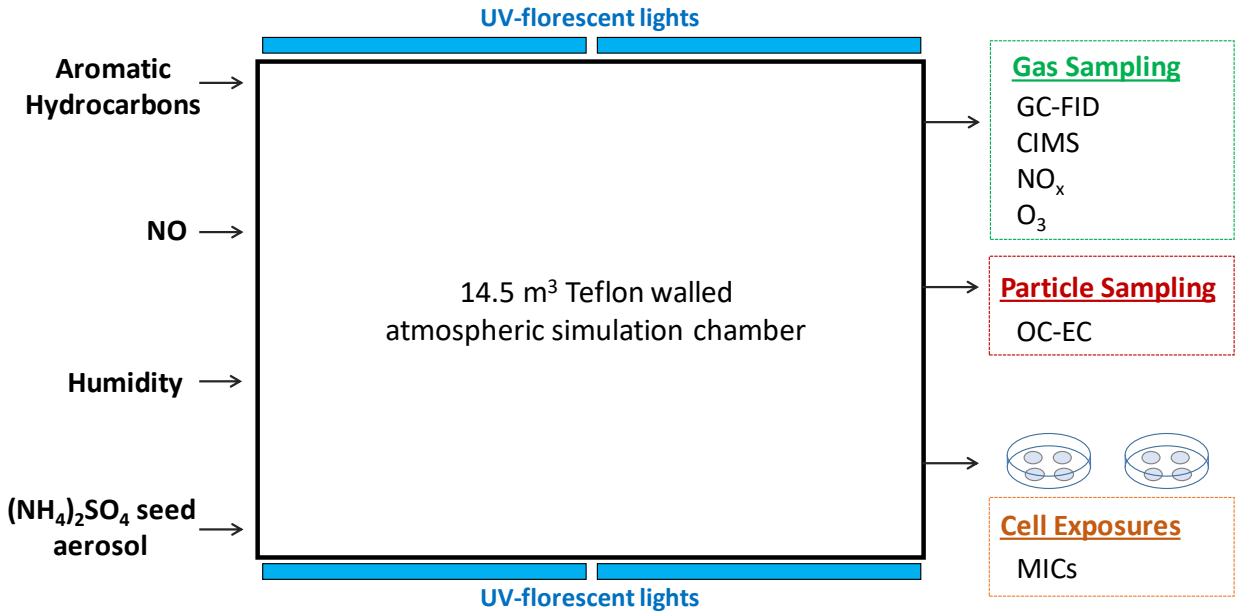

Figure S1. Simplified schematic of atmospheric simulation chamber and experiment setup.

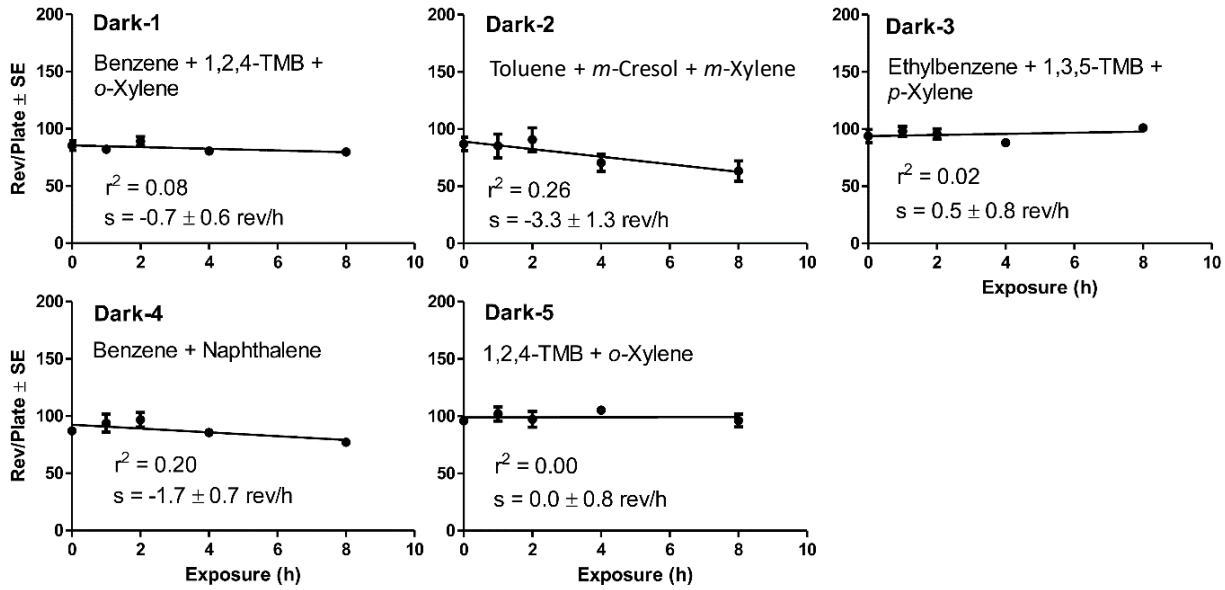

Figure S2. Plots of revertants plate^{-1} versus exposure time for the dark-exposure experiments.

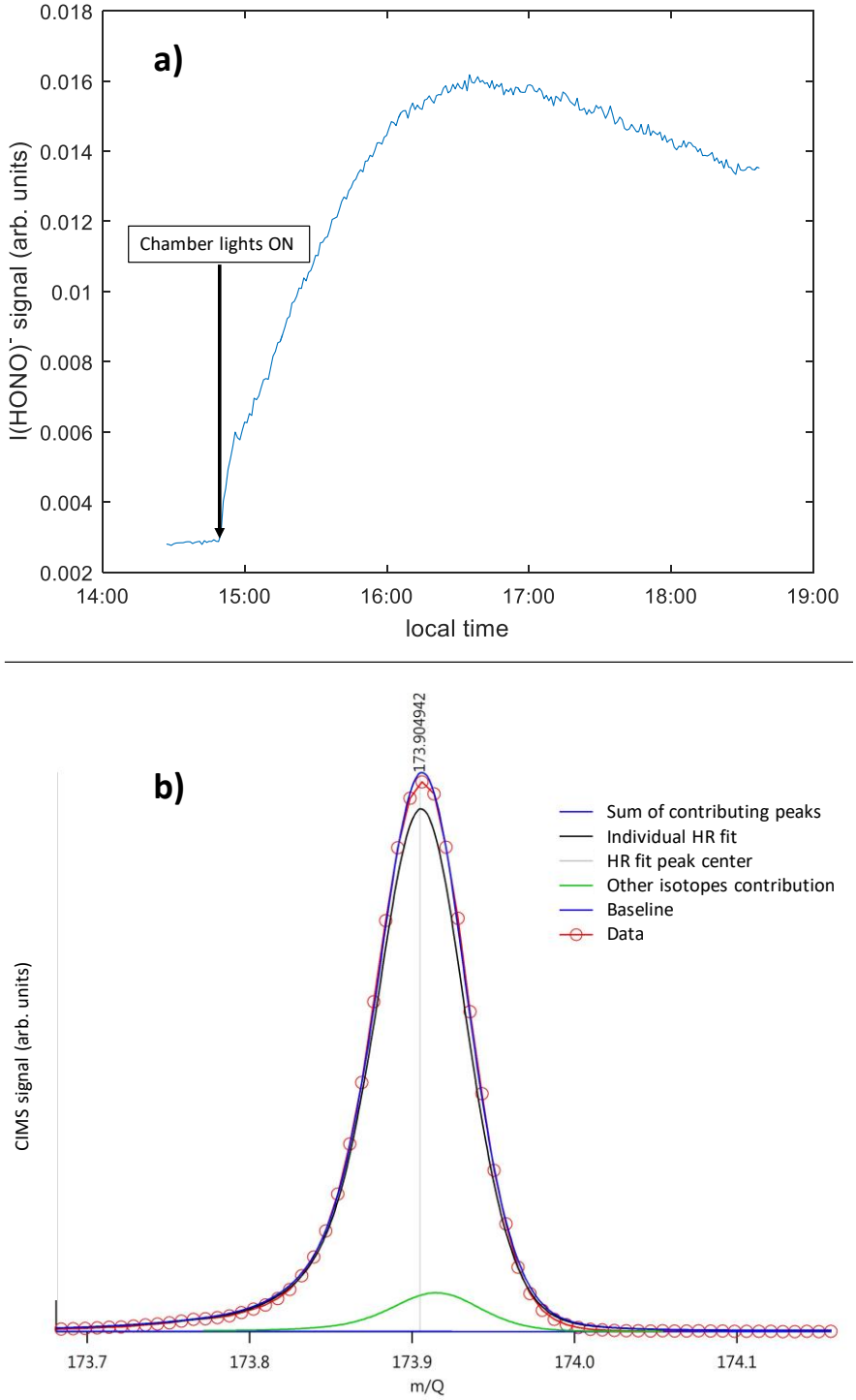

Figure S3. (a) Representative CIMS $I(HONO)^-$ time series during the transition from chamber lights off to lights on. (b) The associated high-resolution (HR) mass spectra peak fit and center for the $I(HONO)^-$ peak assignment.

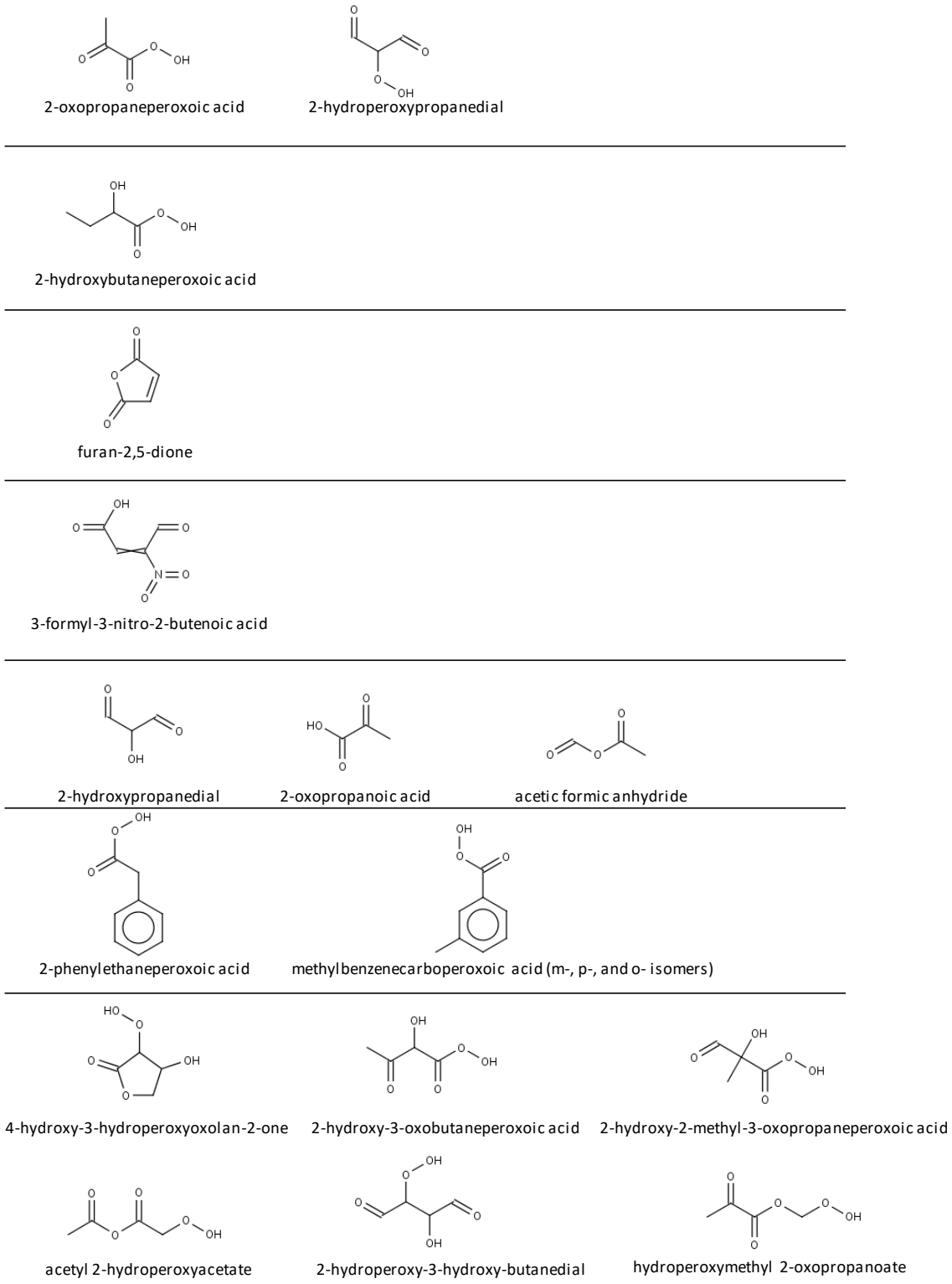

Figure S4. Chemical structures for the potential organic compounds provided in Table 2 of the main text.

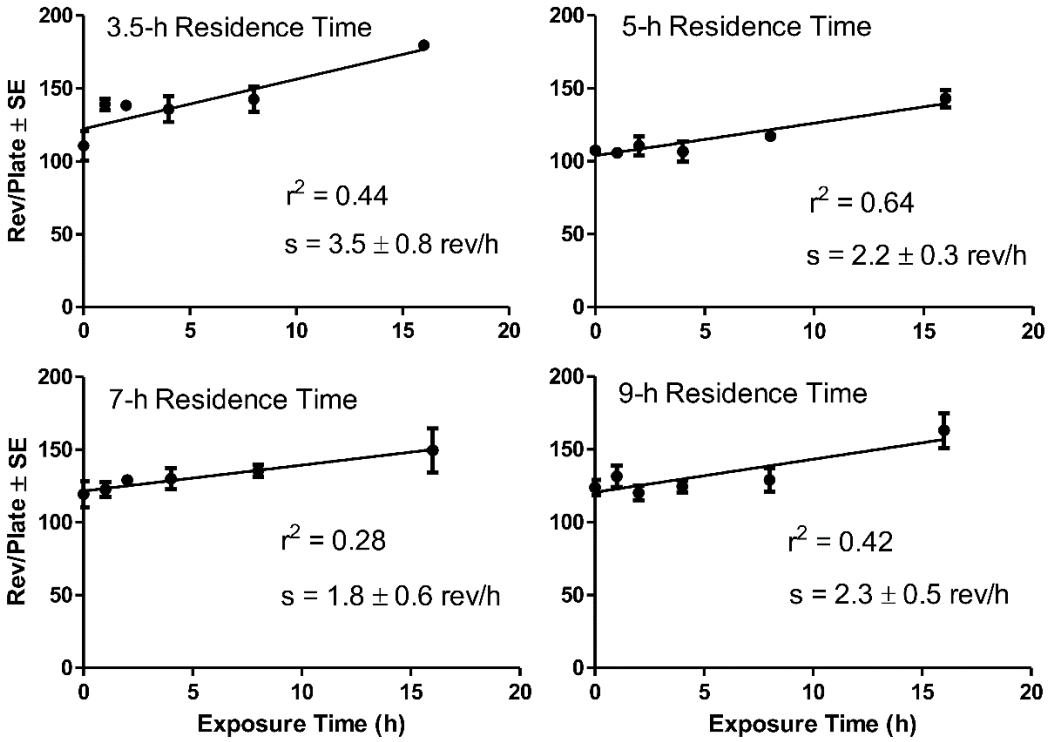

Figure S5. Plots of revertants plate^{-1} versus exposure time for the ethylbenzene variable residence time experiments.

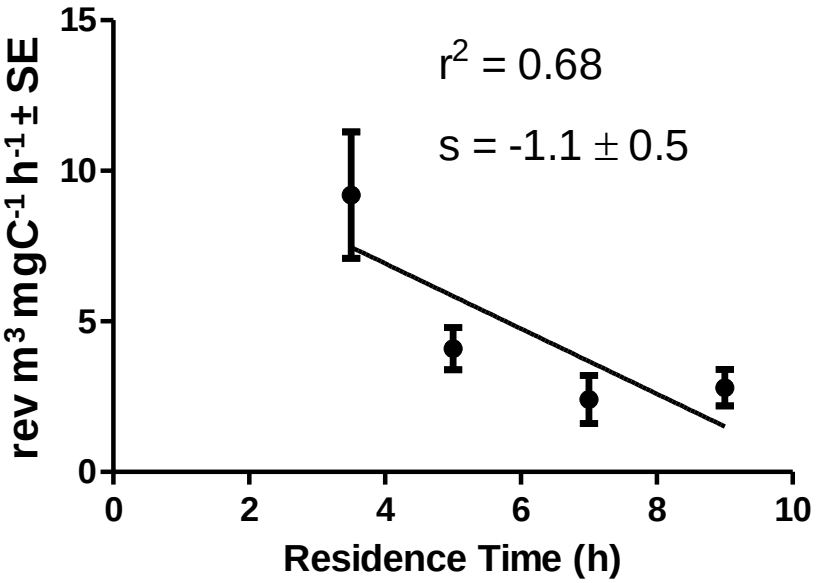

Figure S6. Relationship between residence time and mutagenic potency for the ethylbenzene variable residence time experiments; "s" is the slope.

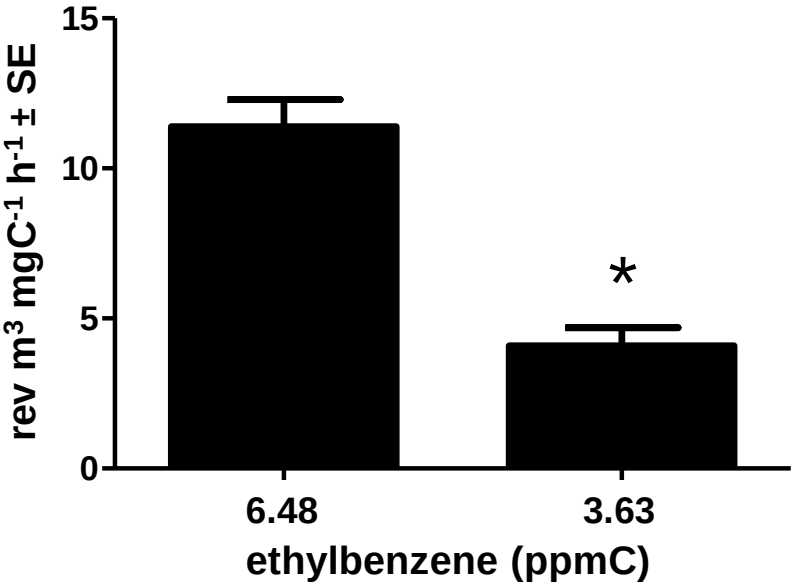

Figure S7. Significant difference ($P < 0.05$) in mutagenic potencies for initial ethylbenzene mixing ratios of 6.48 ppmC with 266 ppbv NO (4.5-h residence time) and 3.63 ppmC with 200 ppbv NO (5-h residence time).