

Radical conditions are important to SOA formation (Ng, et al., 2007; Li, et al., 2015) and $\text{RO}_2\cdot$ and $\text{HO}_2\cdot$ reaction is a major pathway to SOA formation (Kroll and Seinfeld, 2008;). The relationship of SOA yield to a number of radical parameters were analyzed based the average radical parameters during photooxidation (Table S4). $[\text{HO}_2\cdot]$ shows strong correlation (0.35~0.4) with yield when C_8 and C_9 aromatic hydrocarbons are analyzed either all together or individually. Fig S2 shows the relationship of $[\text{HO}_2\cdot]$ to yield. Fig S2 is colored by substitute number or position and sized with mass loading M_0 . Particle size generally grows larger from left to right demonstrating a positive correlation with M_0 and $[\text{HO}_2\cdot]$ (0.43, p-value=0.00). A similar size circle in each vertical slice illustrates SOA yield differences between isomers at similar $[\text{HO}_2\cdot]$ condition. Two typical slices are boxed to compare isomer SOA yield. The left slice shows that one substitute isomers (turquoise) form more SOA than three substitute ones (mustard) at similar mass loading and radical concentrations. The right slice shows that ortho position isomers (purple) yields are higher than para ones (red). Additionally, a trend showing that ortho position isomers (purple) have higher yield than the meta isomers when $M_0 > 40 \mu\text{g}\cdot\text{m}^{-3}$ (larger size cycle) and $15\text{-}35 \times 10^6 \text{ molecules}\cdot\text{cm}^{-3} [\text{HO}_2\cdot]$. Radical analysis in general further supports the relationship found between SOA yield and precursor molecular structure.

It is further noticed that the low $[\text{HO}_2\cdot]$ and yield correlation is due to the difference in isomer k_{OH} (Table S1). It is found that k_{OH} correlates well with yield especially when only C_9 isomers are considered (-0.451, p-value=0.002). The reverse correlation explains that SOA yield hinges on molecular structure instead of kinetic reaction rate (Li, et al., in preparation). The insignificant correlation between k_{OH} and C_8 isomers is due to a greater impact of molecular structure on SOA formation than k_{OH} .

Table S1 Aromatic hydrocarbon physical properties and rate constant

Compound	Vapor Pressure ^a	Boiling Point ^b	k_{OH}^{c}
Ethylbenzene	9.2	136	0.70
Propylbenzene	3.1	159	0.58
Isopropylbenzene	4.5	152	0.63
<i>m</i> -Xylene	9.0	139	2.31
<i>o</i> -Xylene	6.0	144	1.36
<i>p</i> -Xylene	7.9	138	1.43
<i>m</i> -Ethyltoluene	3.0	158	1.86
<i>o</i> -Ethyltoluene	2.6	164	1.19
<i>p</i> -Ethyltoluene	2.9	162	1.18
1,2,4-Trimethylbenzene	2.1	170	3.25

1,2,3-Trimethylbenzene	1.4	175	3.27
1,3,5-Trimethylbenzene	2.3	165	5.67

Note: a) vapor pressures are referred to Chemispider in unit mmHg at 25 °C; b) boiling points are referred to Chemispider in unit °C; c) OH reaction rate constants used in SAPRC-11 model in unit $10^{-11}\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25 °C ; *Predicted data from on Chemispider.

Table S2 Experiment conditions of additional aromatic hydrocarbon experiments

Precursor	ID	HC/NO ^a	NO ^b	HC ^b	ΔHC^c	Mo ^c	Yield
<i>m</i> -xylene ^{1,3}	104A	10.1	64.4	350	328	21.7	0.07
	104B	29.3	21.4	338	281	20.4	0.07
	129A	15.1	45.5	371	336	21.9	0.07
	149A	13.3	50.2	360	342	52.8	0.15
	164A	12.4	44.0	293	271	16.8	0.06
	164B	12.2	44.1	291	270	14.6	0.05
	217A	36.8	8.90	176	155	9.80	0.06
	217B	35.9	8.70	168	153	7.90	0.05
	219A	63.7	7.00	240	165	9.20	0.06
	219B	67.5	6.60	240	166	9.30	0.06
	288A	63.1	7.00	238	183	9.00	0.05
	290A	31.1	15.3	256	229	9.00	0.04
	293A	29.9	13.7	221	189	9.20	0.05
	368A	17.9	21.0	203	149	6.90	0.05
	485A	17.5	43.3	408	353	37.2	0.11
	485B	16.7	45.0	404	349	40.4	0.12
	488A	15.5	46.2	386	341	29.5	0.09
	492A	13.6	44.3	324	296	29.1	0.10
	492B	13.5	44.8	325	298	29.7	0.10
	566A	14.0	48.3	364	337	48.2	0.14
	566B	13.3	48.0	344	318	48.4	0.15
	758A	47.5	11.4	292	158	13.5	0.09
	820A	30.2	20.7	337	260	17.0	0.07
	1193A	15.5	36.8	71.1	239	13.6	0.06
	1193B	15.2	36.5	69.5	236	11.2	0.05
	1191A	12.6	52.2	82.1	298	15.2	0.05
	1191B	14.6	45.7	83.6	340	14.6	0.04
1516A	27.8	26.7	92.9	357	48.7	0.14	
1950A	14.1	45.5	80.0	327	26.3	0.08	
1950B	14.6	45.9	83.6	345	28.7	0.08	
<i>o</i> -xylene ²	503B	15.5	75.0	626	448	30.0	0.07
	505A	171	48.0	4423	360	32.0	0.09
	508A	17.9	24.3	234	208	12.5	0.06
	517B	30.9	26.8	447	296	32.0	0.11
	522A	8.80	52.0	246	220	7.70	0.04
	522B	41.7	11.0	247	171	15.0	0.09
<i>p</i> -xylene ²	422B	33.1	23.9	426	211	5.90	0.03
	502A	41.0	21.0	464	292	19.0	0.07

	503A	18.0	75.0	728	579	66.0	0.11
	504A	16.3	129	1132	876	103	0.12
	504B	15.8	131	1120	675	52.0	0.08
	515B	18.5	26.0	260	200	8.00	0.04
	519B	29.2	53.0	834	450	36.5	0.08
	525A	45.3	10.2	249	163	8.0	0.05
1, 2, 4-trimethylbenzene	1117A	69.8	10.3	80.0	335	16.8	0.05
	1117B	34.8	20.7	80.0	368	18.2	0.05
	1119A	14.1	49.8	78.0	385	19.6	0.05
	1119B	17.1	41.6	79.0	390	25.5	0.07
	1123A	71.0	10.1	80.0	300	11.2	0.04
	1123B	32.6	22.1	80.0	345	15.4	0.05
	1126A	69.3	10.1	77.5	286	12.6	0.04
	1126B	28.1	24.3	75.9	333	15.4	0.05
	1129B	24.2	15.6	42.0	201	5.60	0.03

Note: 1) Song, et al, 2005; 2) Song, et al, 2007; 3) Li, et al., 2015; a) Unit of HC/NO are ppbC:ppb; b)Unit of NO and HC are ppb; c)Unit of Δ HC and Mo are $\mu\text{g}\cdot\text{m}^{-3}$

Table S3. Two product yield curve fitting parameters for selected compounds

Yield Curve	α_1	$K_{om,1}$ ($\text{m}^3/\mu\text{g}$)	α_2	$K_{om,2}$ ($\text{m}^3/\mu\text{g}$)
Ethylbenzene	0.160	0.039	0.138	0.005
Propylbenzene (i- and n-)	0.117	0.040	0.139	0.005
<i>o</i> -Xylene	0.141	0.025	0.264	0.005
<i>o</i> -Ethyltoluene	0.173	0.024	0.247	0.005
<i>m</i> -Xylene	0.166	0.036	0.083	0.005
<i>m</i> -Ethyltoluene	0.152	0.036	0.085	0.005
<i>p</i> -Xylene	0.168	0.026	0.016	0.005
<i>p</i> -Ethyltoluene	0.144	0.022	0.049	0.005

Table S4 Average radical concentrations during photooxidation

Run ID	RO_2^a	HO_2^a	OH^b	HO_2^*RO^c	HO_2/RO_2	NO/HO_2	OH/HO_2^d	NO_3^a
1142A	17.0	13.78	9.21	474	1.50	4.0E+04	1.5E-01	9.60
1142B	1.38	3.08	5.61	12.6	2.16	3.6E+05	4.8E-01	15.9
1146A	11.3	14.07	4.52	225	1.60	6.9E+02	2.0E-02	4.21
1146B	14.8	14.68	6.91	340	1.42	6.0E+03	5.0E-02	5.92
2084A	12.5	16.99	1.91	257	1.60	1.2E+02	3.7E-03	1.62
2084B	10.1	15.07	1.62	189	1.72	1.4E+02	3.7E-03	1.36
1245A	8.22	10.66	4.17	132	1.49	2.3E+03	3.0E-02	4.75
1246A	8.71	9.03	4.28	194	1.55	2.1E+05	2.3E-01	24.8
1247A	15.6	15.48	5.21	338	1.38	7.6E+02	2.0E-02	3.04
1247B	11.2	10.99	7.56	280	1.62	2.5E+07	2.3E+01	9.12
1253A	23.7	20.12	6.47	726	1.23	2.1E+05	4.3E-01	5.18
1253B	4.24	6.74	5.02	100	2.00	1.1E+05	1.6E-01	28.4
1193A	11.0	12.33	3.14	185	1.34	1.5E+06	1.8E+00	14.0

1193B	8.97	11.59	2.82	141	1.44	3.2E+05	4.2E-01	18.7
1191A	19.1	15.83	5.81	449	1.23	4.5E+05	3.4E-01	32.1
1191B	10.8	12.43	2.36	189	1.46	3.8E+04	5.1E-02	18.5
1516A	18.6	23.1	3.14	465	1.33	1.5E+01	2.0E-03	2.37
1950A	11.7	20.62	4.46	267	1.84	7.2E+01	4.3E-03	38.4
1950B	13.3	22.03	4.64	326	1.74	4.6E+01	3.7E-03	37.1
1315A	17.5	20.7	8.28	495	1.52	1.0E+03	1.8E-02	28.9
1315B	19.8	21.59	5.20	478	1.23	3.5E+01	4.3E-03	3.38
1320A	53.2	21.02	11.9	1432	0.79	3.7E+02	1.7E-02	1.77
1321A	21.0	21.35	5.14	506	1.20	3.1E+01	4.1E-03	2.46
1321B	22.9	19.43	3.58	484	1.02	4.3E+00	2.1E-03	0.72
1308A	12.5	13.89	7.04	308	1.40	2.0E+05	3.9E-01	15.9
1308B	24.0	18.01	5.66	564	1.00	1.0E+03	1.6E-02	3.36
1151A	8.97	14.15	9.27	251	0.00	2.4E+04	8.0E-02	66.7
1151B	23.3	22.14	9.83	788	1.40	5.6E+03	3.6E-02	13.3
1199A	15.1	22.49	4.16	373	1.57	8.1E+01	4.0E-03	24.0
1222B	20.3	27.24	8.11	625	1.15	9.7E+01	4.1E-03	55.5
1226B	24.3	32.15	5.66	885	1.44	3.2E+02	5.8E-03	105
1232A	22.2	30.55	4.57	774	1.52	2.3E+02	4.4E-03	104
1421A	20.0	22.36	3.05	504	1.30	3.7E+00	1.5E-03	2.43
1421B	23.2	27.06	6.33	710	1.30	2.3E+01	3.6E-03	13.7
1179A	12.6	17.6	5.26	294	1.72	3.9E+02	1.0E-02	51.5
1179B	14.0	19.05	5.50	329	1.60	2.2E+02	8.2E-03	51.1
1202A	13.8	17.77	5.94	350	1.57	8.5E+03	3.9E-02	39.6
1215A	25.7	25.73	6.06	981	1.47	3.3E+03	1.8E-02	53.1
1413A	19.1	20.64	3.54	430	1.17	1.7E+01	2.6E-03	3.00
1413B	20.9	22.76	6.96	550	1.24	2.1E+02	8.7E-03	19.4
1194A	23.1	20.6	3.85	675	1.16	5.1E+04	5.9E-02	37.4
1194B	23.5	20.04	4.10	712	1.19	3.9E+04	5.3E-02	26.4
1197A	25.2	20.97	3.60	733	1.13	1.8E+04	4.0E-02	5.61
1197B	24.6	19.92	5.18	782	1.04	1.0E+08	3.7E+01	20.5
1214B	22.3	18.34	7.57	623	1.16	6.4E+03	4.3E-02	14.4
1601A	36.8	31.89	9.25	1489	0.99	9.7E+06	2.1E+01	6.21
1158A	20.1	18.64	1.68	391	1.04	4.2E+00	1.0E-03	1.35
1158B	43.4	21.98	3.49	957	0.72	2.9E-01	1.6E-03	1.28
1162A	19.7	23.94	4.75	523	1.42	7.9E+00	2.4E-03	37.2
1162B	96.9	19.22	5.78	1445	0.44	3.8E-02	3.5E-03	0.33
1117A	13.1	15.79	1.69	220	1.29	1.2E+01	1.5E-03	7.29
1117B	9.83	14.58	2.49	172	1.58	1.9E+02	4.7E-03	34.9
1119A	12.5	18.77	5.29	300	1.66	2.7E+03	1.7E-02	89.0
1119B	12.1	17.26	3.95	296	1.86	2.9E+03	1.7E-02	68.7
1123A	15.9	15.09	1.66	274	1.06	6.8E+01	2.2E-03	2.91
1123B	15.8	18.56	2.54	321	1.22	7.7E+01	3.0E-03	23.2
1126A	17.3	17.63	1.69	324	1.07	1.7E+01	1.5E-03	4.26
1126B	29.9	24.76	7.50	841	1.03	3.2E+01	3.8E-03	33.7
1129B	11.2	15.45	4.29	199	1.58	5.6E+01	4.9E-03	24.0
1153A	14.9	18.64	1.10	292	1.28	1.2E+01	8.3E-04	1.22
1153B	17.5	21.78	1.99	411	0.00	1.6E+01	1.3E-03	3.33
1156A	11.1	19.85	2.08	249	1.97	2.5E+01	1.6E-03	31.8
1156B	9.86	19.63	2.85	218	2.18	6.1E+01	2.8E-03	54.4
1329B	2.51	9.07	4.45	26.0	4.62	2.2E+02	8.0E-03	125

Note: average radical concentrations are calculated by dividing time integrated radical parameters with photooxidation time; average radical concentration throughout photooxidation a) in 10^6 molecules \cdot cm $^{-3}$; b) in 10^8 molecules \cdot cm $^{-3}$; c) in 10^{16} molecules \cdot cm $^{-3}$; d) average radical ratio throughout photooxidation in 10^3

Table S5 Correlation between SOA yields and average radical concentrations

C ₈ & C ₉	RO ₂	HO ₂	OH	HO ₂ *RO	HO ₂ / RO ₂	NO/HO	OH/HO	NO ₃
				2		2	2	
Yield	0.152	0.393	-0.046	0.24	-0.099	-0.046	-0.108	0.093
p-value ^a	0.223	0.001	0.714	0.053	0.428	0.712	0.388	0.457

C ₉	RO ₂	HO ₂	OH	HO ₂ *RO ₂	HO ₂ / RO ₂	NO/HO ₂	OH/HO ₂	NO ₃
Yield	0.189	0.376	0.098	0.303	-0.133	-0.07	-0.141	0.094
p-value ^a	0.208	0.010	0.516	0.040	0.380	0.644	0.349	0.535

C ₈	RO ₂	HO ₂	OH	HO ₂ *RO ₂	HO ₂ / RO ₂	NO/HO ₂	OH/HO ₂	NO ₃
Yield	-0.092	0.353	-0.386	-0.094	0.200	-0.293	-0.318	-0.278
p-value ^a	0.699	0.127	0.093	0.693	0.398	0.209	0.171	0.235

Note: C₈ & C₉ correlation analysis used all the experiments listed in Table S4, C₈ or C₉ correlation analysis only used C₈ or C₉ isomer experiments listed in Table S4. a) P-values range from 0 to 1, 0-reject null hypothesis and 1 accept null hypothesis. Alpha (α) level used is 0.05. If the p-value of a test statistic is less than alpha, the null hypothesis is rejected

Table 3. Correlation among reaction rate (k_{OH}) and SOA chemical composition

	f ₄₄	f ₄₃	f ₅₇	f ₇₁	O/C	H/C	OS _c
K_{OH}	0.631	0.895	-0.33	0.496	-0.544	0.674	-0.67
p-value ^a	0.028	0	0.295	0.101	0.068	0.016	0.01

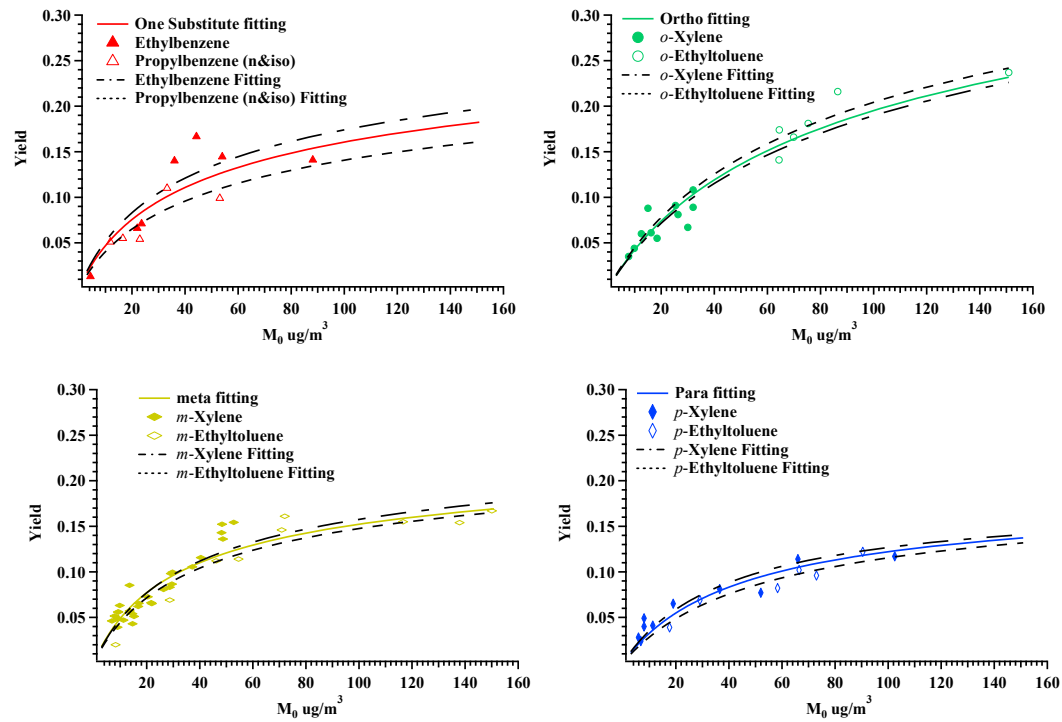


Fig.S1. Aromatic SOA yields as a function of M_0 for single compounds: a) Ethylbenzene (dotted line) vs Propylbenzene (i- and n-)(dashed line); b) *o*-Xylene(dotted line) vs *o*-Ethyltoluene(dashed line); c) *m*-Xylene(dotted line) vs *m*-Ethyltoluene(dashed line); d) *p*-Xylene (dotted line) vs *p*-Ethyltoluene (dashed line) (Note: Song, et al, 2005; Song, et al, 2007; Li, et al., 2015 data are also included)

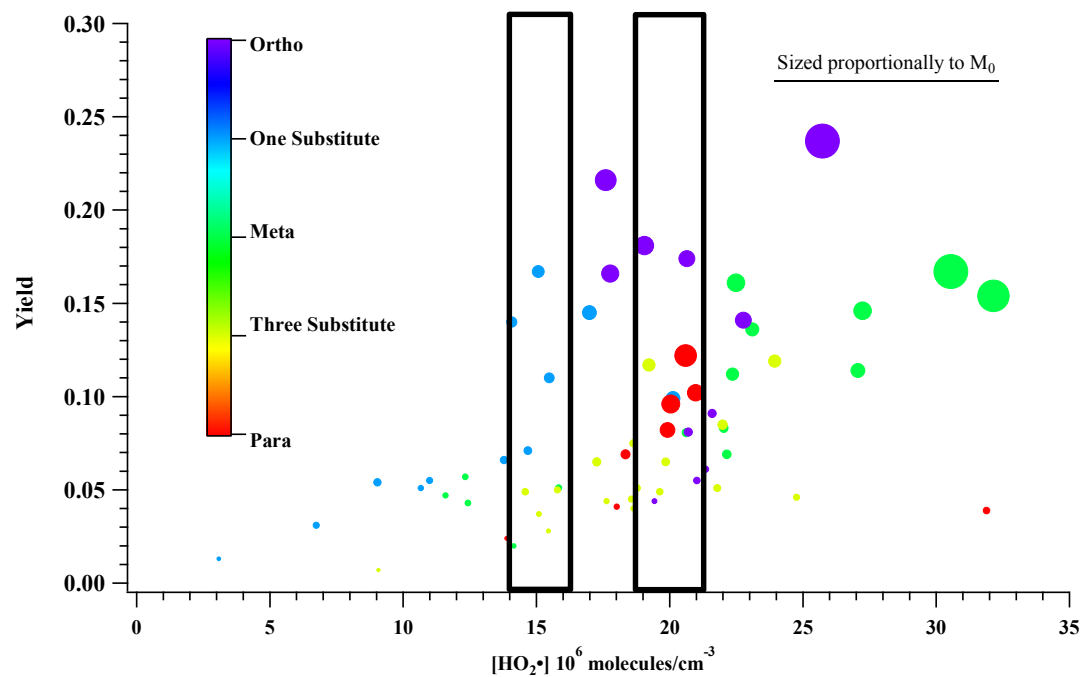
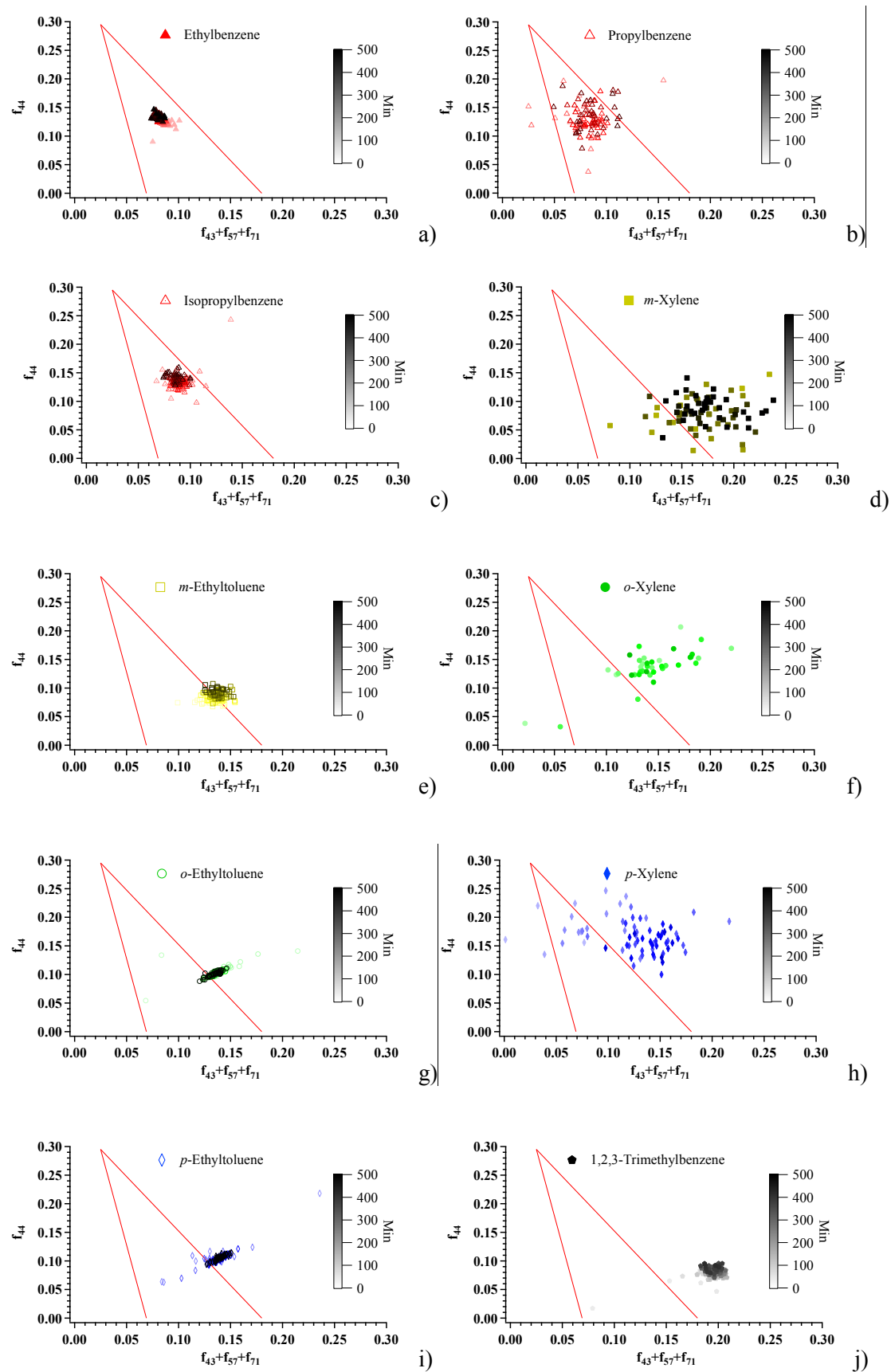


Fig. S2 Relationship between SOA yield and HO₂· radical concentration (Colored with substitute number or position and sized with mass loading M₀)



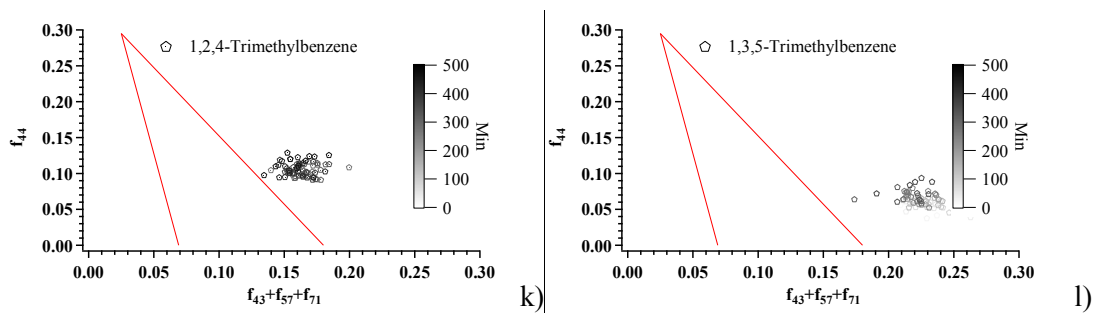
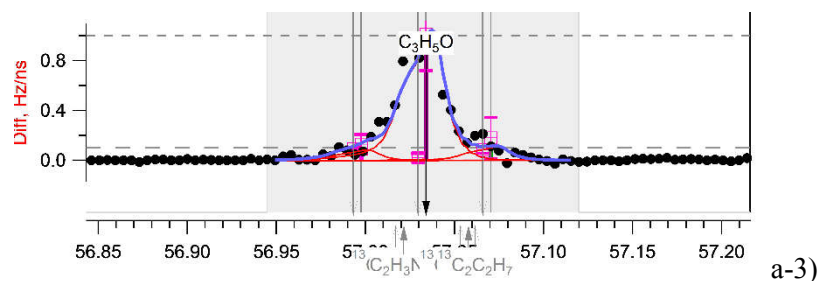
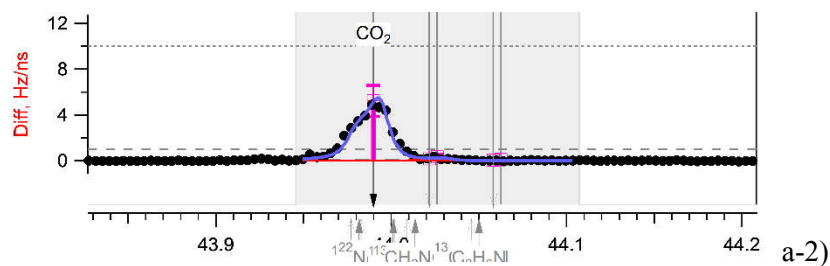
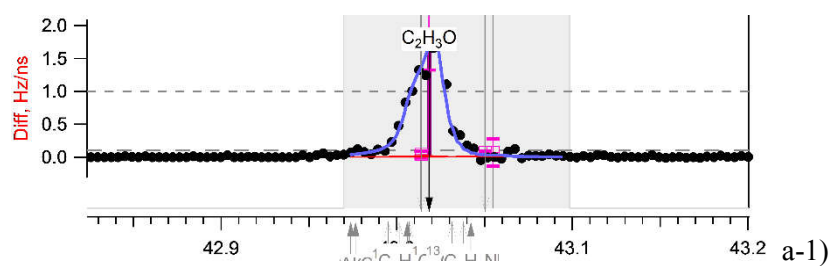
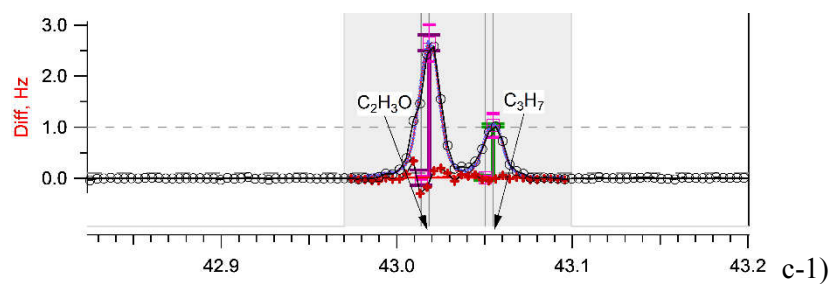
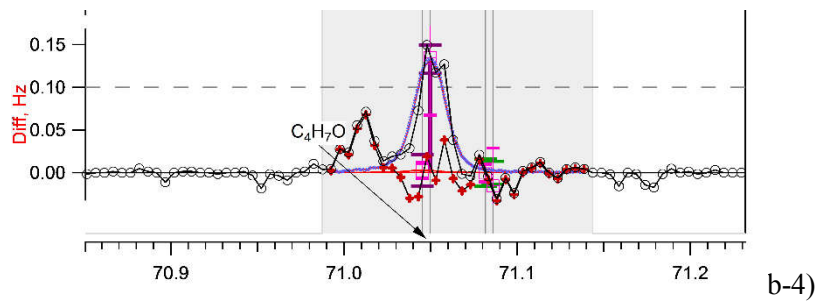
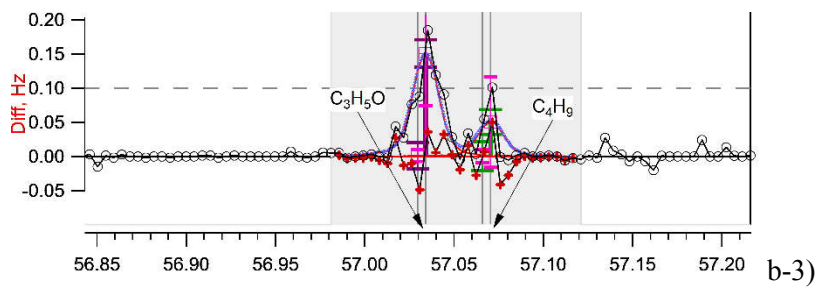
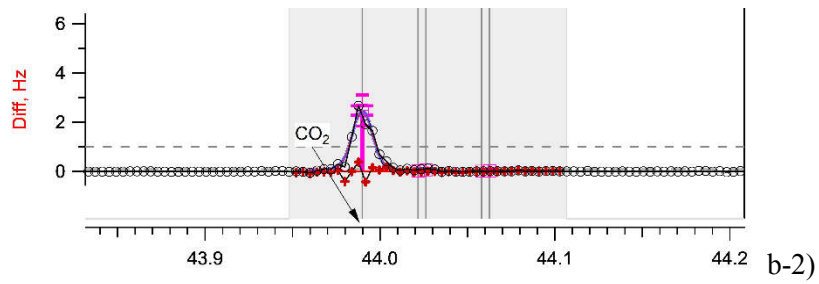
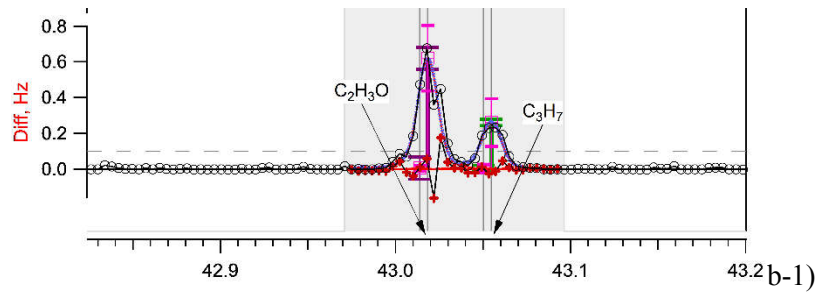
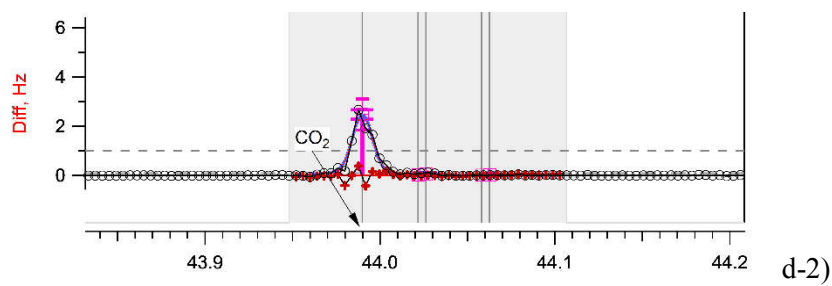
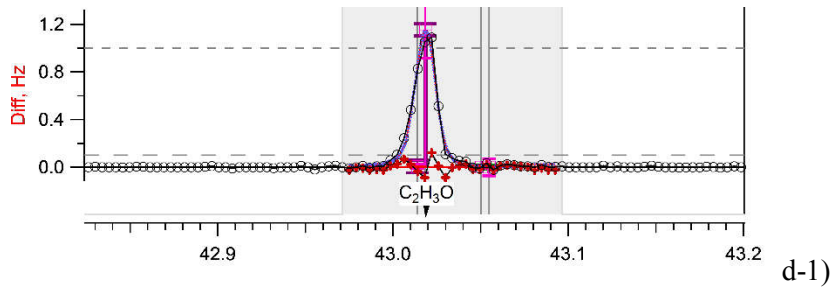
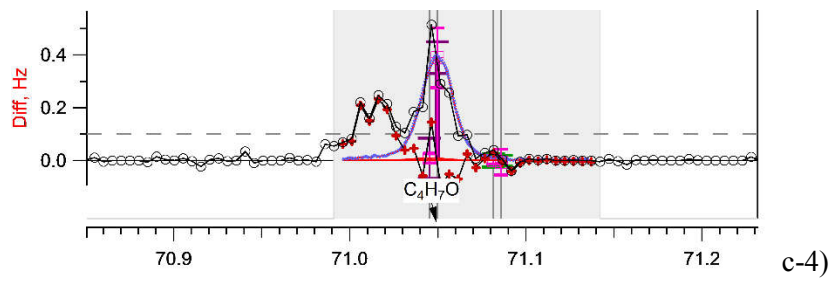
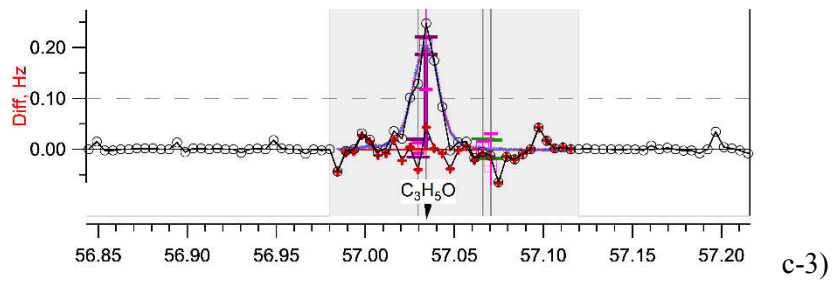
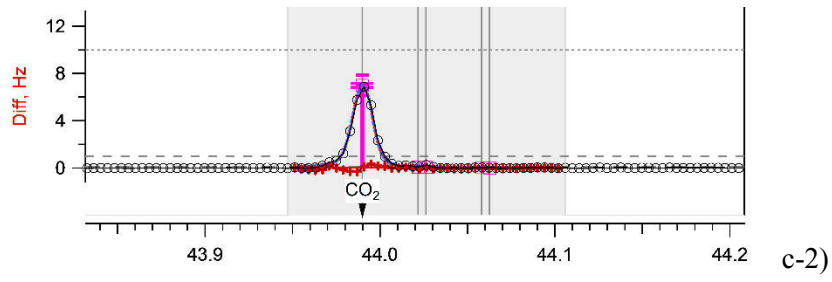
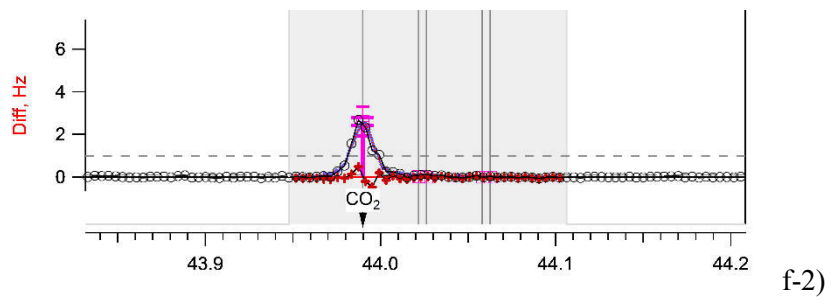
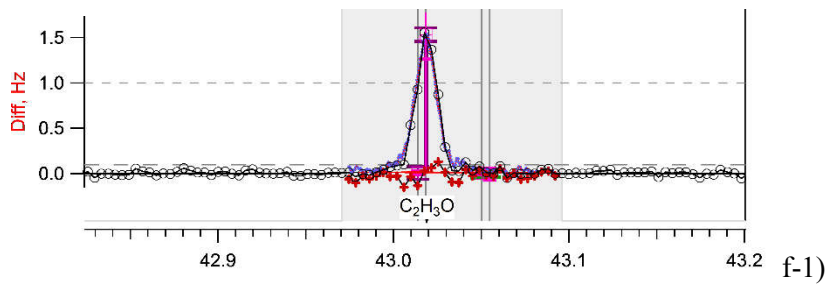
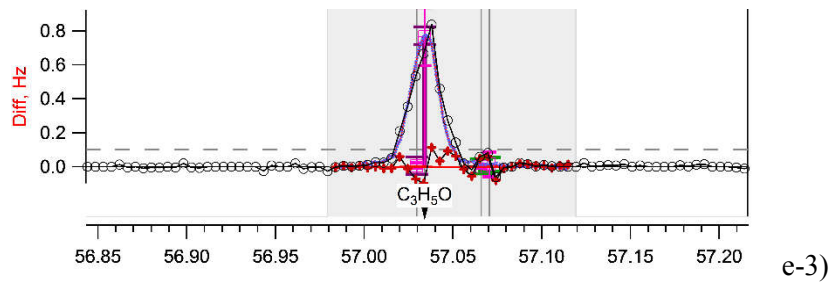
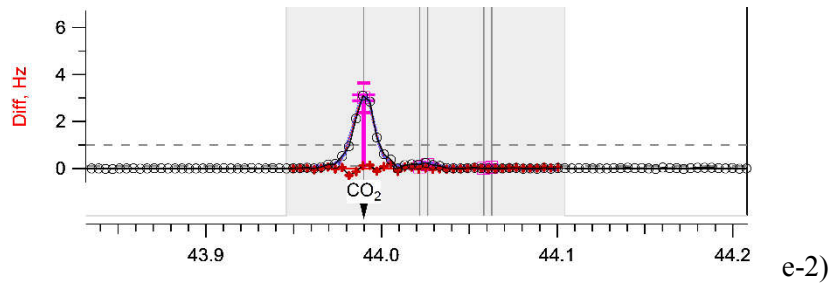
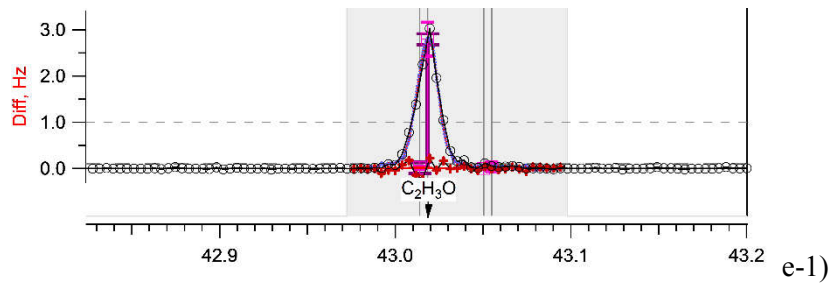


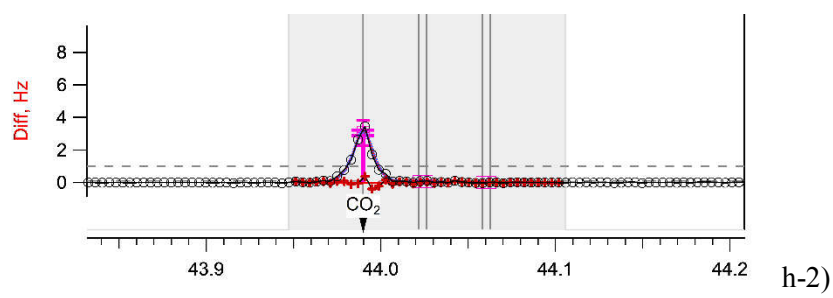
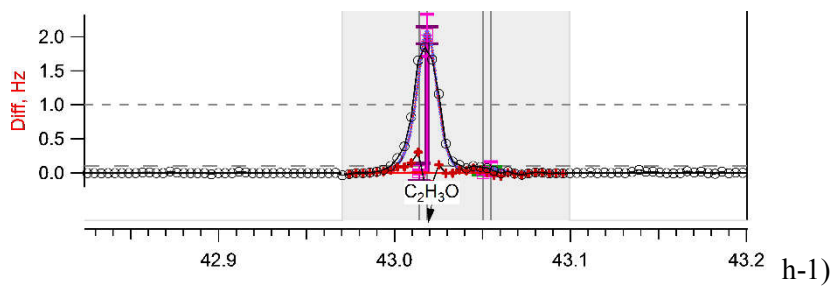
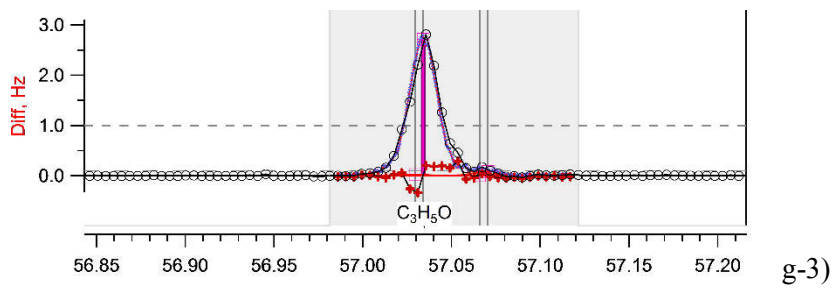
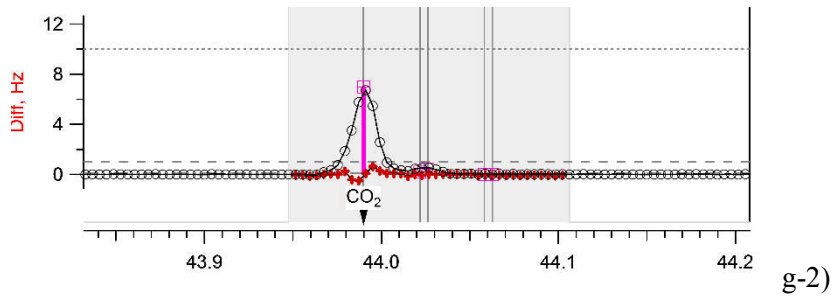
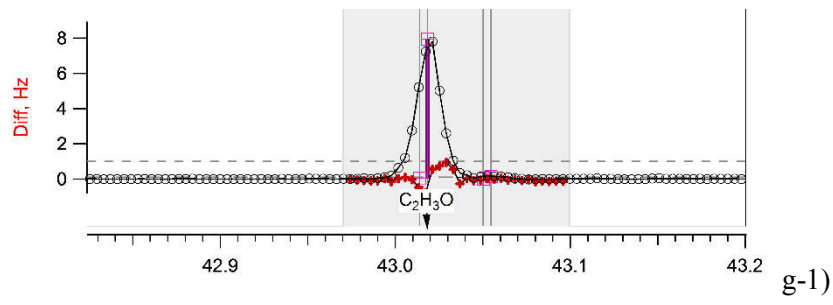
Fig. S3 f_{44} and $f_{43+57+71}$ evolution in SOA formed from different aromatic hydrocarbon photooxidation under low NO_x ; each marker type represents one aromatic hydrocarbon and marker is colored with photooxidation time from light to dark: a) Ethylbenzene 2048A; b) Propylbenzene 1245A; c) Isopropylbenzene 1247A; d) *m*-Xylene 1191A; e) *m*-Ethyltoluene 1199A; f) *o*-Xylene 1320A; g) *o*-Ethyltoluene 1179A; h) *p*-Xylene 1308A; i) *p*-Ethyltoluene 1194A; j) 1,2,3-Trimethylbenzene 1162A; k) 1,2,4-Trimethylbenzene 1119A; l) 1,3,5-Trimethylbenzene 1156A

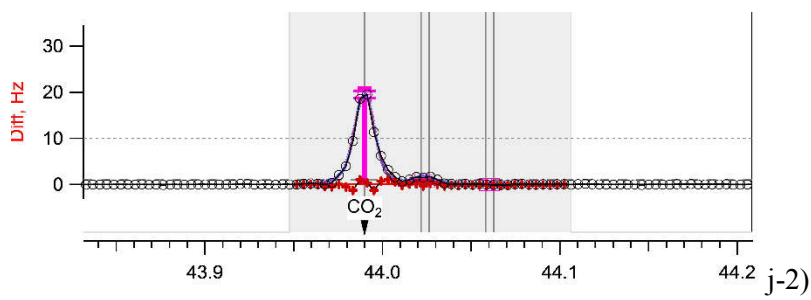
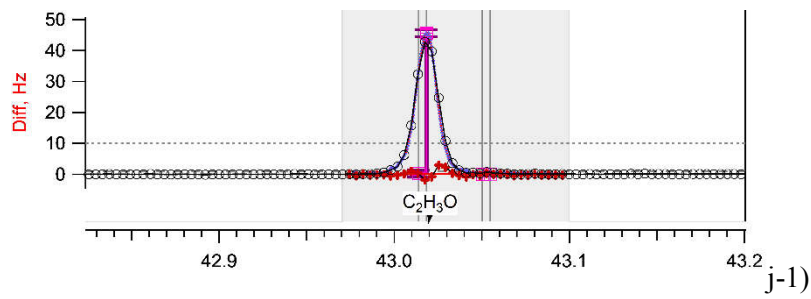
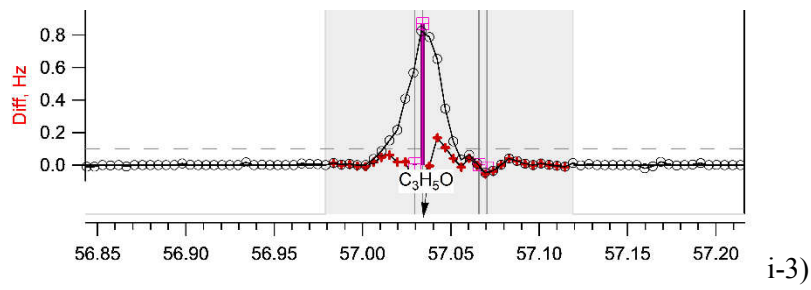
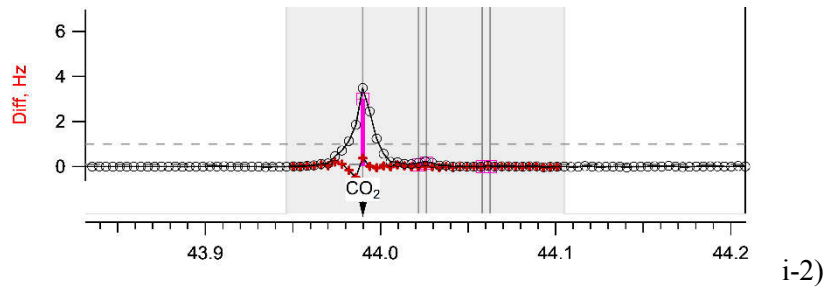
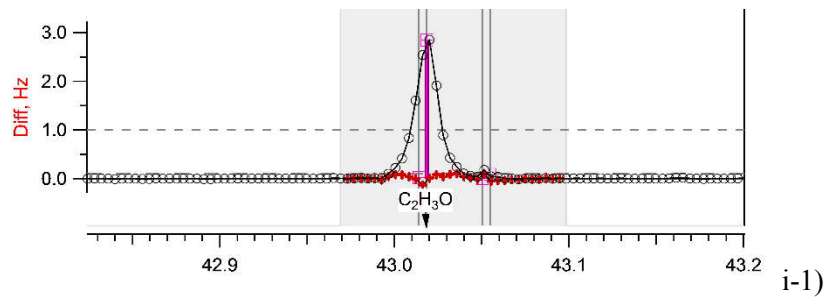


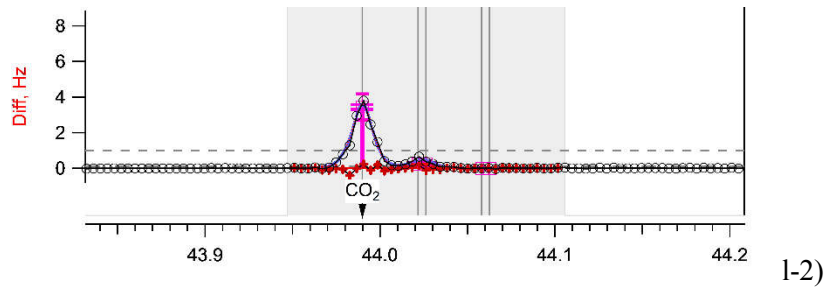
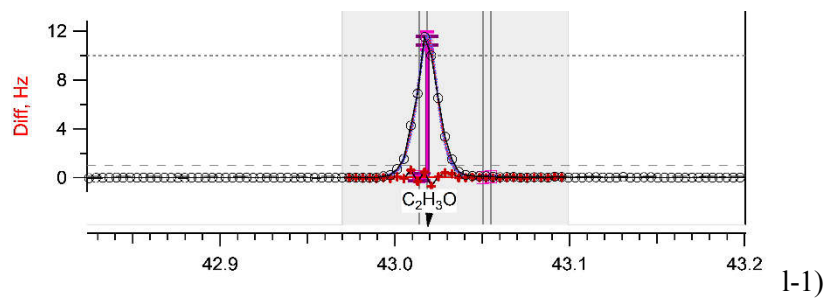
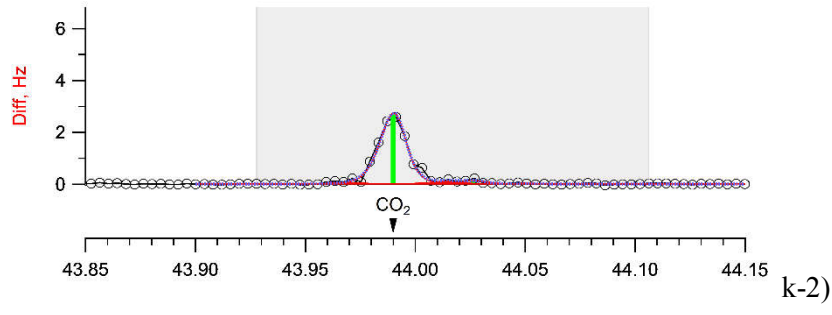
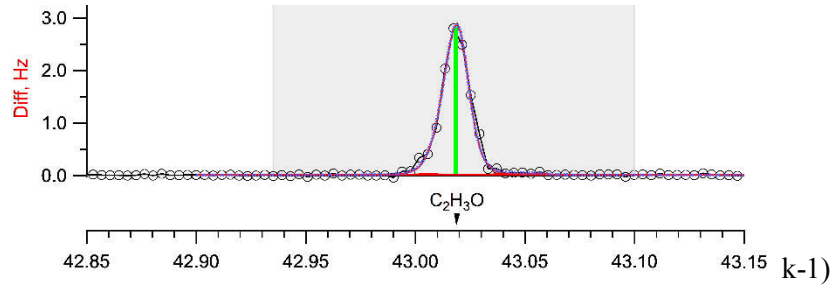
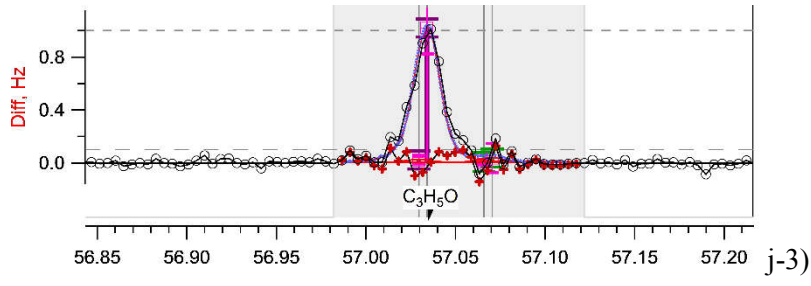












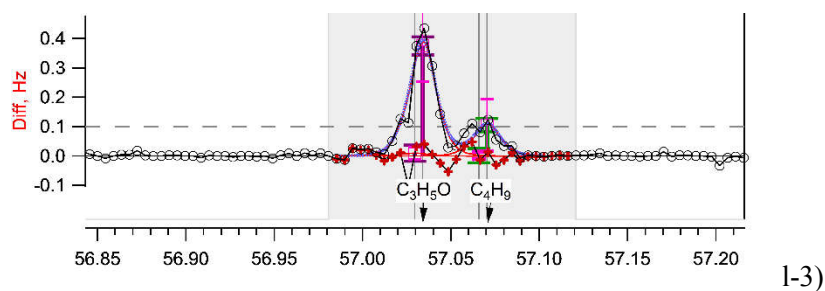


Fig. S4 High-resolution mass spectra of m/z 43, m/z 44, m/z 57 and m/z 71 measured for secondary organic aerosol formed at peak aerosol concentration during aromatic photooxidation a) Ethylbenzene 1146A; b) Propylbenzene 1245A; c) Isopropylbenzene 1247A; d) *m*-Xylene 1191A; e) *m*-Ethyltoluene 1199A; f) *o*-Xylene 1320A; g) *o*-Ethyltoluene 1179A; h) *p*-Xylene 1308A; i) *p*-Ethyltoluene 1194A; j) 1,2,3-Trimethylbenzene 1162A; k) 1,2,4-Trimethylbenzene 1119A; l) 1,3,5-Trimethylbenzene 1156A (m/z 57 only includes $C_3H_5O^+$). * m/z peaks with intensity less than 0.1 are not displayed

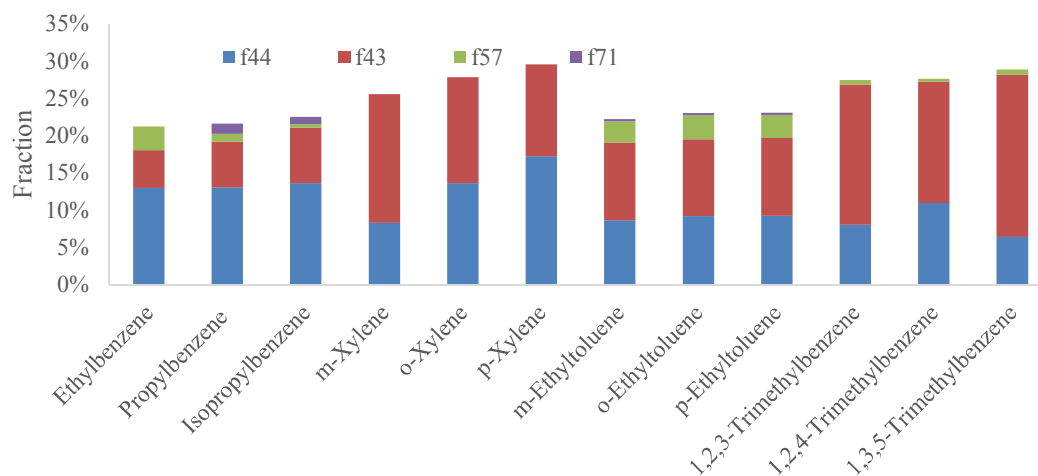
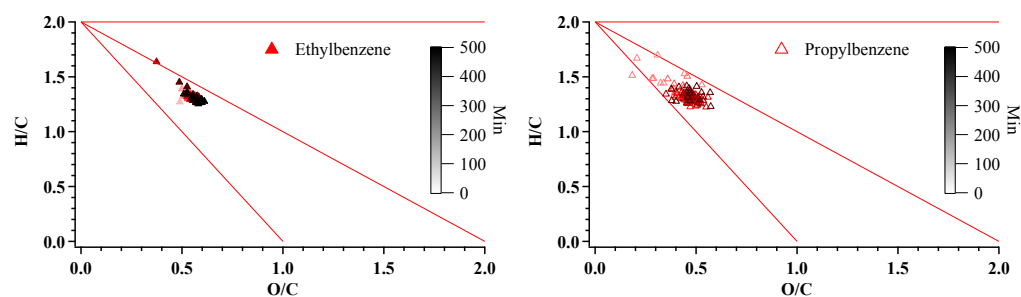


Fig. S5 m/z 43, m/z 44, m/z 57 and m/z 71 fraction in SOA formed from aromatic hydrocarbon photooxidation



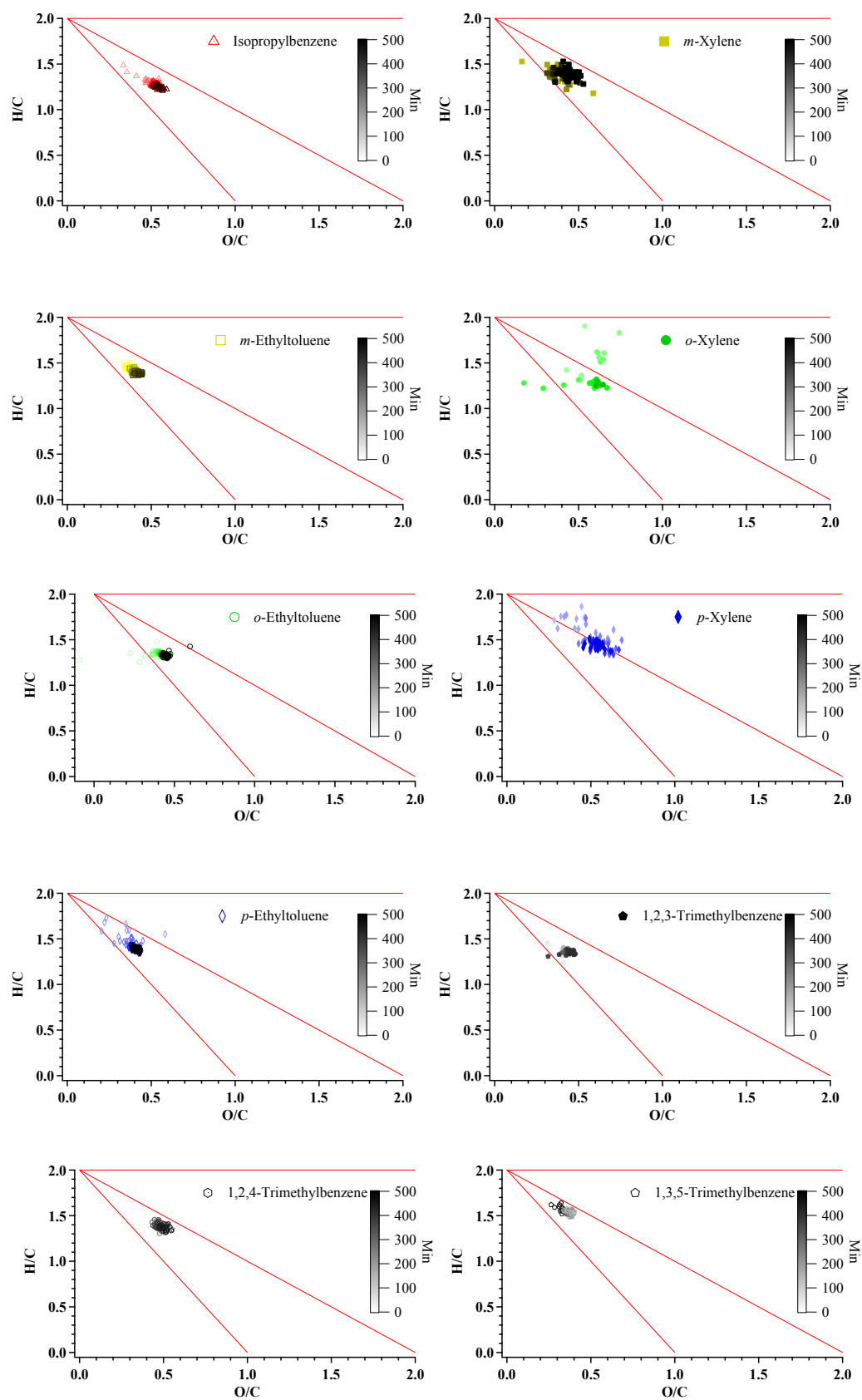


Fig. S6 H/C and O/C evolution in SOA formed from different aromatic hydrocarbon photooxidation under low NO_x ; each marker type represents one aromatic hydrocarbon and

marker is colored with photooxidation time from light to dark: a) Ethylbenzene 1146A; b) Propylbenzene 1245A; c) Isopropylbenzene 1247A; d) *m*-Xylene 1191A; e) *m*-Ethyltoluene 1199A; f) *o*-Xylene 1320A; g) *o*-Ethyltoluene 1179A; h) *p*-Xylene 1308A; i) *p*-Ethyltoluene 1194A; j) 1, 2, 3-Trimethylbenzene 1162A; k) 1, 2, 4-Trimethylbenzene 1119A; l) 1, 3, 5-Trimethylbenzene 1156A.

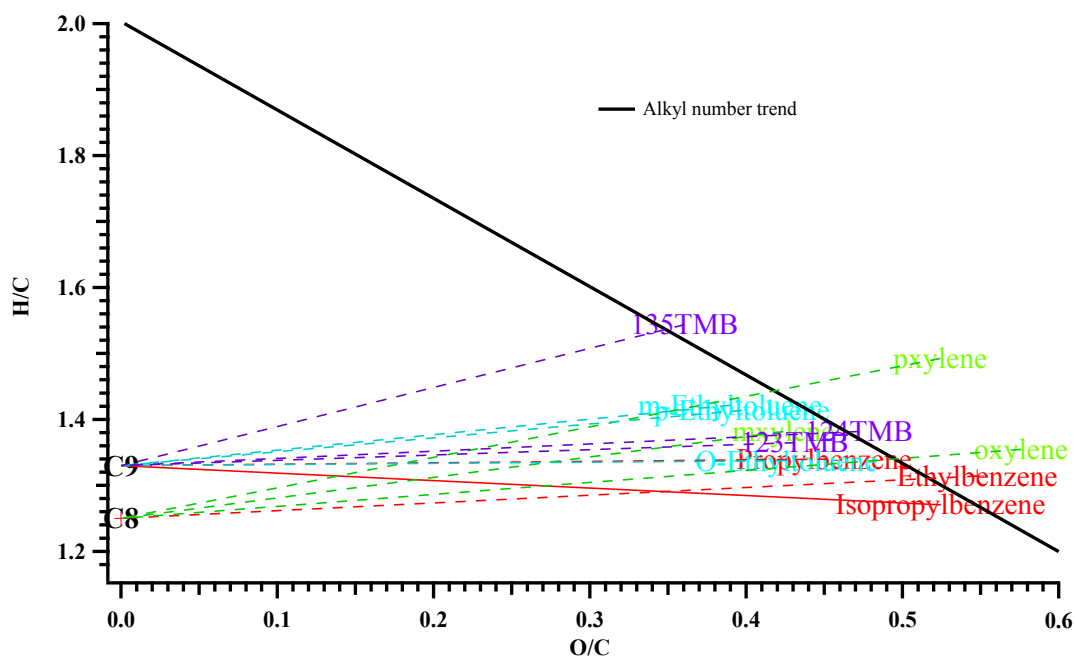


Fig. S7 H/C vs. O/C in SOA formed from different aromatic hydrocarbon photooxidation under low NO_x colored by aromatic isomer type and marked with individual aromatic hydrocarbon species (C8 and C9 on the lower left indicate the location of initial aromatic hydrocarbon precursor; dashed/solid line indicate that changes between precursor and SOA components): Ethylbenzene 2084A; Propylbenzene 1245A; Isopropylbenzene 1247A; *m*-Xylene 1191A; *m*-Ethyltoluene 1199A; *o*-Xylene 1320A; *o*-Ethyltoluene 1179A; *p*-Xylene 1308A; *p*-Ethyltoluene 1194A; 1, 2, 3-Trimethylbenzene (123TMB) 1162A; 1, 2, 4-Trimethylbenzene (124TMB) 1119A; 1, 3, 5-Trimethylbenzene (135TMB) 1156A. Alkyl number trend is the liner fitting in (Li., et al., 2015).

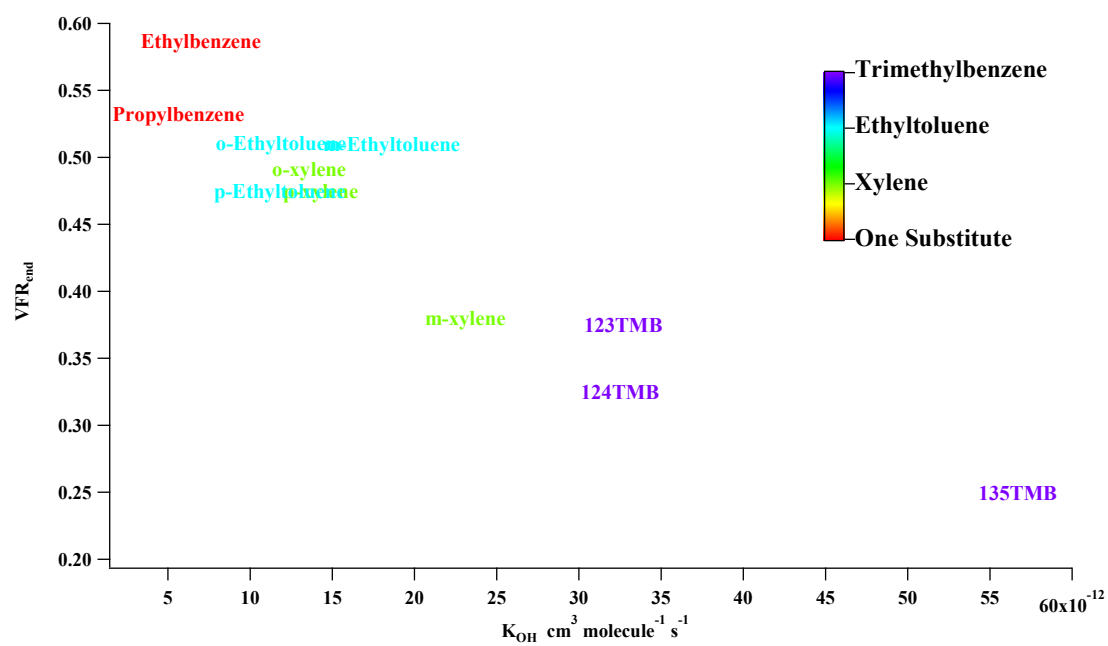


Fig S8 Relationship between VFR and K_{OH} during aromatic hydrocarbon photooxidation under low NO_x