

# Supplementary Materials: Characterization of Products from the Aqueous-Phase Photochemical Oxidation of Benzene-Diols *Atmosphere* 2021, 12

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**Table S1.** Summary of experimental conditions and relevant analyses.

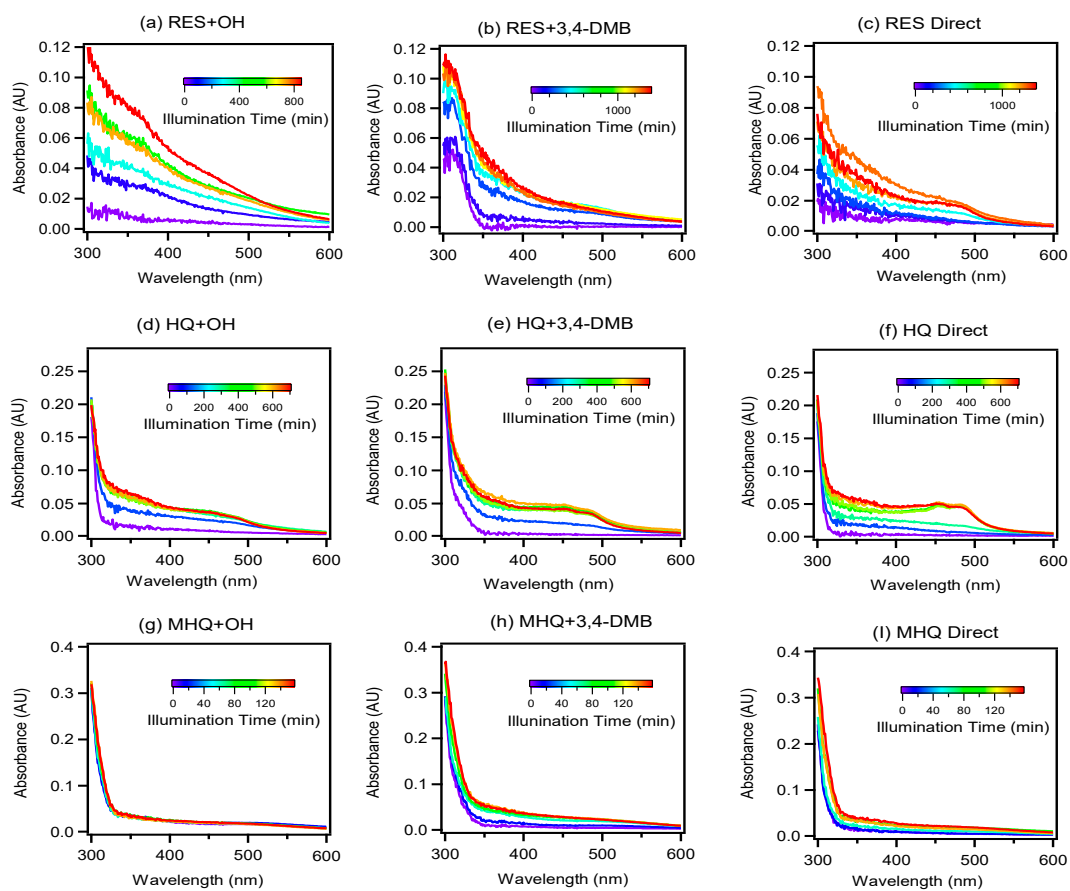
Precursor	Oxidant <sup>a</sup>	SP-AMS <sup>b</sup>	HPLC <sup>c</sup>	UV-Vis <sup>d</sup>	TOC <sup>e</sup>	DTT <sup>f</sup>
<b>RES</b>	·OH	√	√	√	√	√
C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	<sup>3</sup> C*	√	√	√	√	√
MW:110.11	/		√	√	√	√
<b>HQ</b>	·OH	√	√	√	√	√
C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	<sup>3</sup> C*	√	√	√	√	√
MW:110.11	/		√	√	√	√
<b>MHQ</b>	·OH	√	√	√	√	√
C <sub>7</sub> H <sub>8</sub> O <sub>3</sub>	<sup>3</sup> C*	√	√	√	√	√
MW:140.14	/		√	√	√	√

<sup>a</sup> There are three types of oxidants: ·OH from photolysis of H<sub>2</sub>O<sub>2</sub>, <sup>3</sup>C\* from photolysis of 3,4-DMB and ‘/’ means no oxidant; <sup>b</sup> Only experiments contains ammonium sulfate (i.e. in ·OH and <sup>3</sup>C\* oxidation group) are measured by SP-AMS; <sup>c</sup> HPLC with UV-vis detector for kinetic study; <sup>d</sup> UV-Vis and <sup>e</sup> TOC are used to examine the light absorption of aqueous-phase products; <sup>f</sup> DTT assay for oxidative potential analysis.

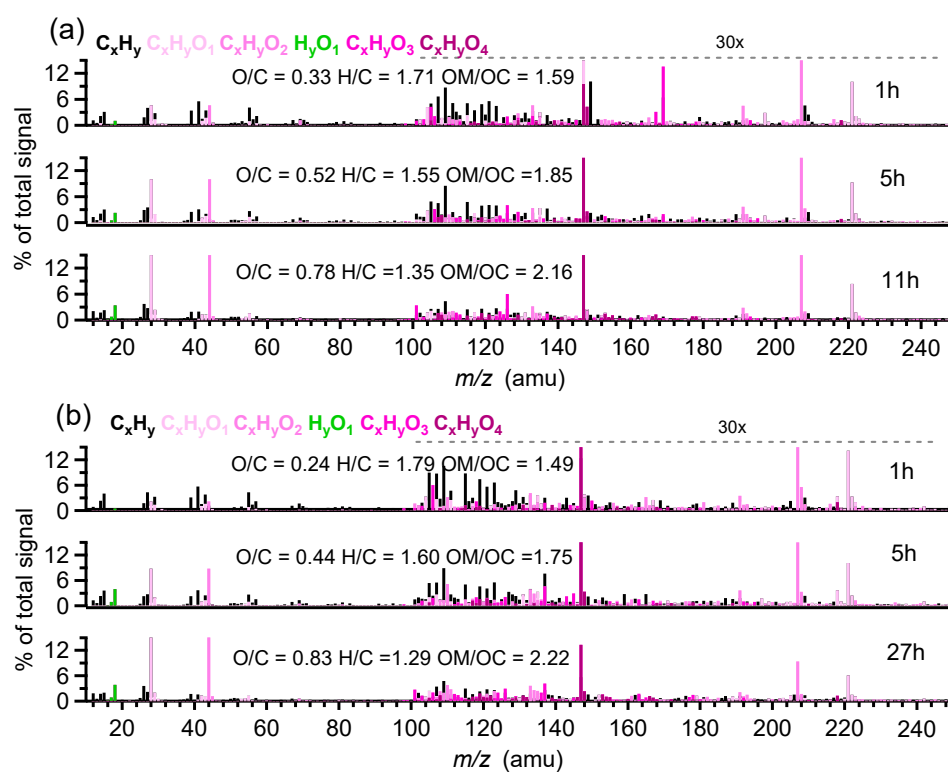
**Table S2.** Summary of the kinetic parameters of the benzene-diols precursors.

Precursor	oxidant	t <sub>1/2</sub> (min) <sup>a</sup>	Rate constant k <sub>d</sub> (h <sup>-1</sup> ) <sup>b</sup>
RES	·OH	763	0.067
	<sup>3</sup> C*	1697	0.023
	/	1825	0.022
HQ	·OH	967	0.050
	<sup>3</sup> C*	1384	0.033
	/	1208	0.035
MHQ	·OH	154	0.26
	<sup>3</sup> C*	159	0.24
	/	197	0.23

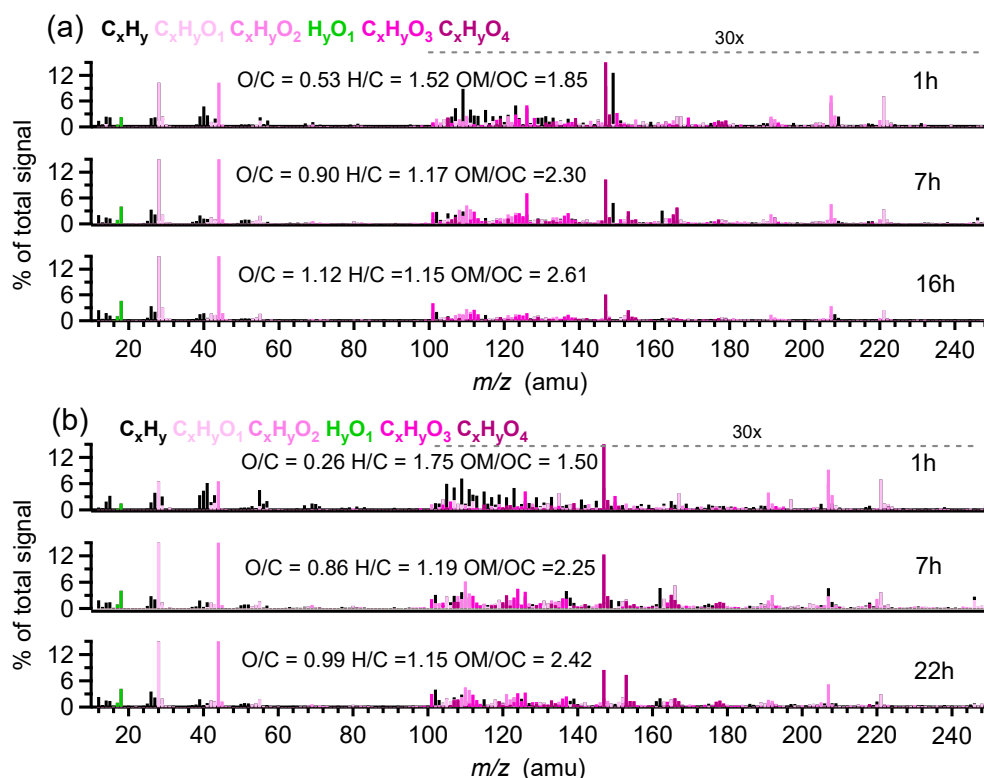
<sup>a</sup> t<sub>1/2</sub> means the time when approximately half of the precursor was consumed; <sup>b</sup> rate constant for precursor loss determined by Eq.1.



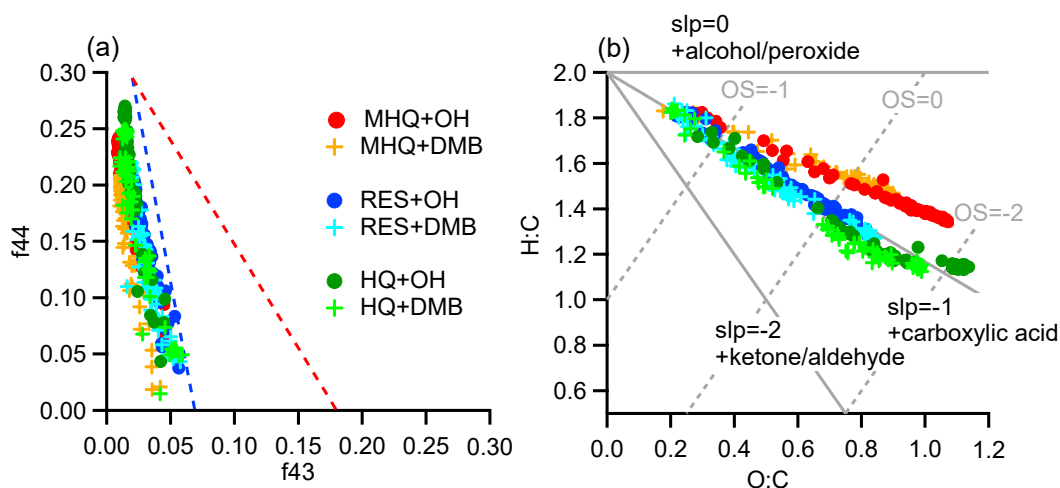
**Figure S1.** Time-dependent UV-Vis light absorption spectra of the reacted solutions obtained at different times during the oxidation experiments



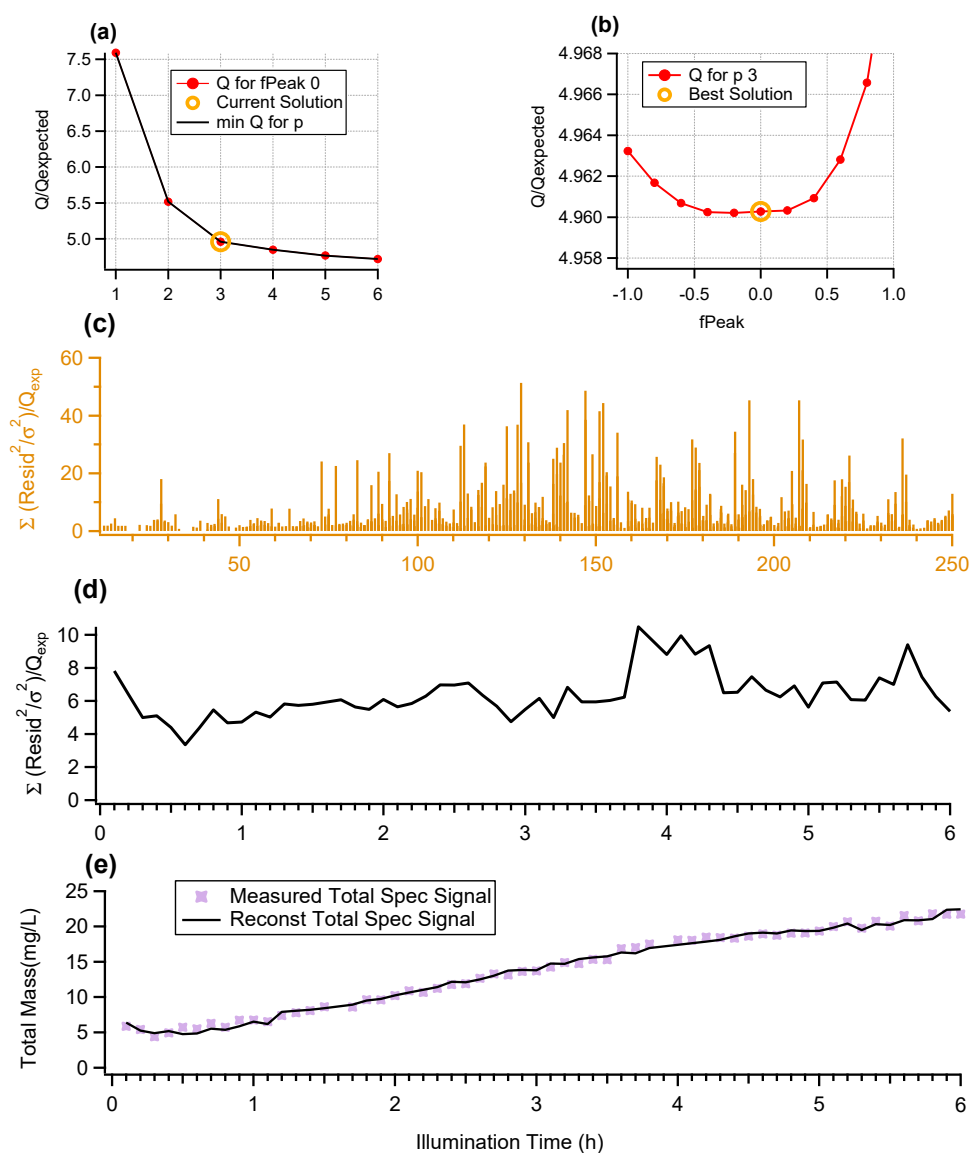
**Figure 2.** Mass spectra of (a) RES+OH and (b) RES+3,4-DMB at different reaction times. The H/C, O/C ratios and OSc values are also shown. The colored sticks represent 6 ion families:  $C_xH_y$ ,  $C_xH_yO_1$ ,  $C_xH_yO_2$ ,  $H_yO_1$ ,  $C_xH_yO_3$  and  $C_xH_yO_4$ . The ion signals at  $m/z > 100$  are amplified 30 times for clarity.



**Figure S3.** Mass spectra of (a) HQ+OH and (b) HQ+3,4-DMB at different reaction times. The H/C, O/C ratios and OSc values are also shown. The colored sticks represent 6 ion families:  $C_xH_y$ ,  $C_xH_yO_1$ ,  $C_xH_yO_2$ ,  $H_yO_1$ ,  $C_xH_yO_3$  and  $C_xH_yO_4$ . The ion signals at  $m/z > 100$  are amplified 30 times for clarity.



**Figure S4.** Evolution profiles of aqueous-phase SOA: (a)  $f_{44}$  (mass ratio of ion signal at  $m/z$  44 to total organic signal) vs.  $f_{43}$  (mass ratio of ion signal at  $m/z$  43 to total organic signal). (b) Van Krevelen (VK) diagram based on AMS data, in which lines with slopes of 0, -1 and -2 represent the reaction pathways with additions of alcohol/peroxide, carboxylic acid, and ketone/aldehyde functional group, respectively. Dashed lines are OSc values.



**Figure S5.** Three- factor solution for PMF analysis of OH<sup>-</sup> mediated oxidations of MHQ: (a)  $Q/Q_{\text{exp}}$  as a function of number of factors ( $p$ ) selected for PMF. For the beat solution(3-factor), (b)  $Q/Q_{\text{exp}}$  as a function of  $f_{\text{Peak}}$ , (c) the  $Q/Q_{\text{exp}}$  values for each ion, (d) the  $Q/Q_{\text{exp}}$  for each point in time, (e) time series of the measured and the reconstructed organic mass loading.