



Supplement of

Molecular transformations of phenolic SOA during photochemical aging in the aqueous phase: competition among oligomerization, functionalization, and fragmentation

L. Yu et al.

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Section S1: Nano-DESI measurement and data analysis

The nano-DESI analyses were performed using a high-resolution LTQ-Orbitrap mass spectrometer (Thermo Electron, Bremen, Germany) with a resolving power ($m/\Delta m$) of 100,000 at $m/z = 400$. The instrument is equipped with a nano-DESI source assembled from two fused-silica capillaries (150 μm o.d./50 μm i.d.) [Roach *et al.*, 2010]. The analysis was performed under the following conditions: spray voltage of 3-5 kV, 0.5-1 mm distance from the tip of the nanospray capillary to the 250 °C heated inlet of the LTQ-Orbitrap, and 0.3-0.9 $\mu\text{L}/\text{min}$ flow rate of acetonitrile : water (7:3 volume) solvent. Both positive and negative mode mass spectra were acquired using the Xcalibur software (Thermo Electron, Inc.).

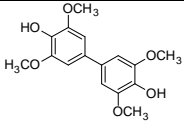
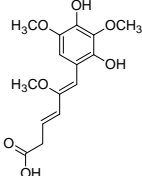
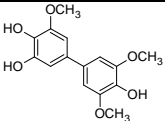
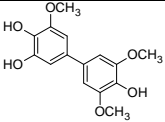
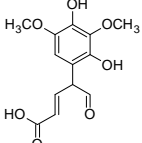
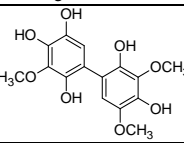
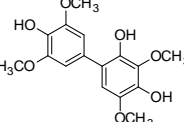
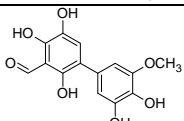
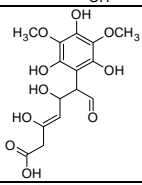
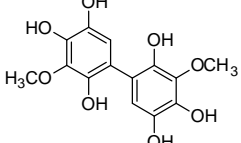
Signals with $S/N > 10$ were picked out using the Decon2LS software developed at the Pacific Northwest National Laboratory (PNNL) [Jaitly *et al.*, 2009]. Data was further processed with Microsoft Excel using a set of built-in macros developed by Roach *et al.* [2011]. The background and sample peaks were first aligned, and the peaks corresponding to ^{13}C isotopes were removed. Peaks in the sample spectra that are at least 10 times bigger than the corresponding peaks in the background spectra were retained for further analysis. Peaks were segregated into different groups using the higher-order mass defect transformation developed by Roach *et al.* [2011]. Molecular formula was assigned with Formula Calculator v. 1.1 (http://www.magnet.fsu.edu/usershub/scientificdivisions/icr/icr_software.html) using the following constraints: $C \geq 0$, $H \geq 0$, $O \geq 0$ for the negative ion mode data and $C \geq 0$, $H \geq 0$, $O \geq 0$, $Na \leq 1$ for the positive ion mode data. Approximately 70% of the peaks can be assigned with molecular formula within these constraints.

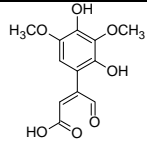
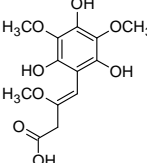
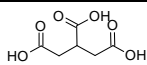
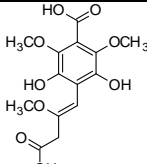
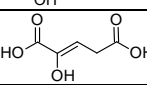
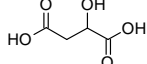
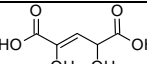
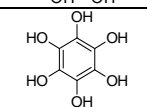
Section S2: HR-AMS measurement and data analysis

In this study, a High Resolution Time-of-Flight Aerosol Mass Spectrometer (Aerodyne Res. Inc., Billerica, MA; thereafter referred to as AMS) was used to characterize the bulk chemical composition and elemental ratios of the low-volatility substances. The working principles of the AMS have been discussed previously [DeCarlo *et al.*, 2006; Canagaratna *et al.*, 2007]. Briefly, the AMS analyzes nonrefractory aerosols that can be evaporated at ~ 600 °C via 70 eV EI mass spectrometry. In this study, the AMS was operated in “V” mode (mass resolutions of ~ 3000) to acquire mass spectra up to m/z 500.

The AMS data were analyzed using the AMS data analysis software (SQUIRREL v1.12 and PIKA v1.53 downloaded from <http://cires.colorado.edu/jimenez-group/ToFAMSResources/ToFSoftware/>). The V-mode data was analyzed to obtain high resolution mass spectra (HRMS), the atomic ratios of oxygen-to-carbon (O/C), hydrogen-to-carbon (H/C) and the organic mass-to-carbon ratio (OM/OC) [Aiken *et al.*, 2008]. The relative humidity measured at the AMS inlet was very low ($< 2\%$), and we assume that contribution from gaseous water molecules was negligible. The H_2O^+ signal of organics was thus determined as the difference between the measured H_2O^+ signal and that produced by sulfates [Allan *et al.*, 2004].

Table S1 Top 10 most abundant compounds identified in SYR aqSOA formed during different stages of the •OH-mediated reactions using (-) nano-DESI MS.

No.	Molecular formula ^a	Proposed structure	C* (µg m ⁻³) at 25 °C, 1 atm ^b	Relative abundance (ranking) ^c		
				P1: 0-2 hrs	P2: 2-4 hrs	P3: 4-6 hrs
1	C ₁₆ H ₁₈ O ₆ (306.1103)		3.2E-03	100 (1)	14 (66)	0.0 (N/A)
2	C ₁₅ H ₁₈ O ₇ (310.1052)		1.7E-05	56 (2)	100 (1)	27 (28)
3	C ₁₅ H ₁₆ O ₆ (292.0946)		3.4E-04	46 (3)	8.6 (109)	0.4 (592)
4	C ₁₅ H ₁₆ O ₉ (340.0794)		3.9E-12	28 (4)	93 (2)	100 (1)
5	C ₁₃ H ₁₄ O ₇ (282.0739)		5.8E-08	19 (5)	48 (5)	29 (21)
6	C ₁₅ H ₁₆ O ₈ (324.0845)		2.8E-09	19 (6)	23 (31)	15 (79)
7	C ₁₆ H ₁₈ O ₇ (322.1052)		1.7E-05	18 (7)	3.7 (261)	0.7 (508)
8	C ₁₄ H ₁₂ O ₇ (292.0583)		4.0E-11	17 (8)	39 (9)	11 (107)
9	C ₁₅ H ₁₈ O ₁₀ (358.0900)		1.5E-13	13 (9)	50 (4)	49 (5)
10	C ₁₄ H ₁₄ O ₈ (310.0688)		9.9E-11	12 (10)	45 (6)	42 (7)

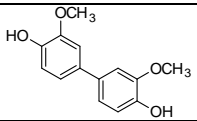
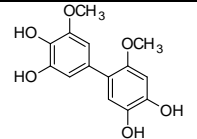
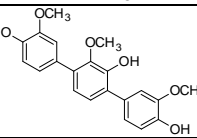
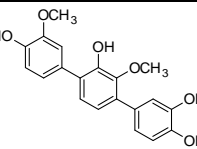
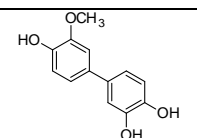
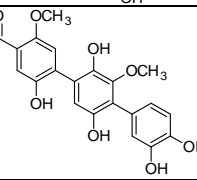
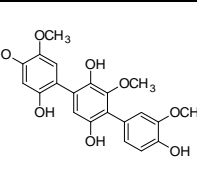
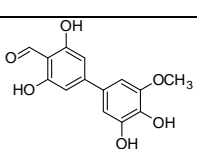
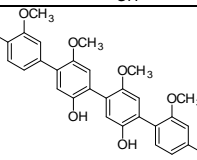
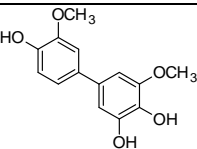
11	C ₁₂ H ₁₂ O ₇ (268.0583)		1.3E-07	11 (13)	43 (7)	37 (11)
12	C ₁₃ H ₁₆ O ₈ (300.0845)		3.4E-07	8.1 (22)	39 (8)	38 (10)
13	C ₆ H ₈ O ₆ (176.0321)		3.1E+04	7.2 (27)	56 (3)	80 (2)
14	C ₁₄ H ₁₆ O ₉ (328.0794)		7.6E-11	6.7 (30)	31 (10)	40 (8)
15	C ₅ H ₆ O ₅ (146.0215)		2.7E+01	4.6 (48)	30 (13)	42 (6)
16	C ₄ H ₆ O ₅ (134.0215)		3.3E+00	4.4 (50)	24 (23)	61 (3)
17	C ₅ H ₆ O ₆ (162.0164)		5.0E-02	4.2 (54)	30 (14)	50 (4)
18	C ₆ H ₆ O ₆ (174.0164)		5.2E-05	3.4 (66)	24 (26)	40 (9)

^a Molecular formulas and proposed structures of the top 10 most abundant compounds identified according to (-) nano-DESI spectra data. The exact molecular weight of each compound is shown in parentheses.

^b Estimated saturation concentrations (C^* , $\mu\text{g m}^{-3}$) of the compounds at 25 °C, 1 atm, determined using the Nannoolal vapor pressure and extrapolation method.

^c Relative abundances (%) of the compounds and, in parentheses, the abundance rank numbers of the compounds according to the nano-DESI mass spectra of in each time period. The rank number is counted in the sorted relative abundance list of all the compounds identified in each time period.

Table S2 Top 10 most abundant compounds identified in GUA aqSOA formed during different stages of the $^{13}\text{C}^*$ -mediated reactions using (-) nano-DESI MS.

No.	Molecular formula ^a	Proposed structure	C^* ($\mu\text{g m}^{-3}$) at 25 °C, 1 atm^{b}	Relative abundance (ranking) ^c		
				P1: 0-2 hrs	P2: 2-4 hrs	P3: 4-6 hrs
1	$\text{C}_{14}\text{H}_{14}\text{O}_4$ (246.0892)		8.8E-01	100 (1)	60 (2)	32 (2)
2	$\text{C}_{14}\text{H}_{14}\text{O}_6$ (278.0790)		2.5E-05	79 (2)	100 (1)	100 (1)
3	$\text{C}_{21}\text{H}_{20}\text{O}_6$ (368.1259)		4.1E-11	65 (3)	34 (3)	16 (6)
4	$\text{C}_{20}\text{H}_{18}\text{O}_6$ (354.1103)		8.0E-09	28 (4)	23 (4)	12 (10)
5	$\text{C}_{13}\text{H}_{12}\text{O}_4$ (232.0735)		8.7E-02	19 (5)	15 (9)	11 (11)
6	$\text{C}_{21}\text{H}_{18}\text{O}_8$ (398.1001)		5.7E-14	16 (6)	22 (5)	20 (3)
7	$\text{C}_{21}\text{H}_{20}\text{O}_8$ (400.1158)		5.0E-13	14 (7)	19 (6)	18 (4)
8	$\text{C}_{14}\text{H}_{12}\text{O}_6$ (276.0634)		3.1E-06	13 (8)	17 (7)	17 (5)
9	$\text{C}_{28}\text{H}_{26}\text{O}_8$ (490.1627)		1.8E-15	10 (9)	4.3 (23)	1.3 (104)
10	$\text{C}_{14}\text{H}_{14}\text{O}_5$ (262.0841)		6.0E-03	9.2 (10)	7.0 (12)	4.7 (23)

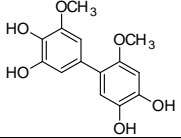
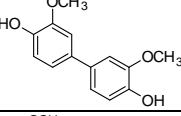
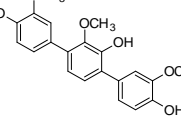
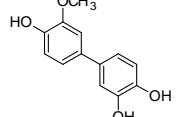
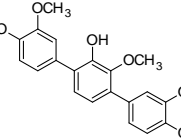
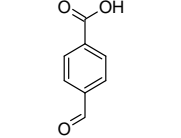
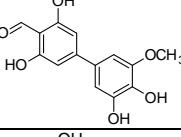
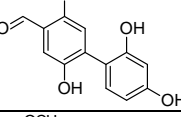
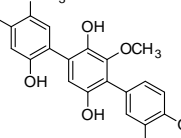
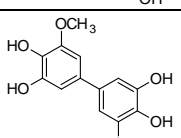
11	$C_{20}H_{16}O_7$ (368.0896)		1.6E-12	9.0 (11)	16 (8)	14 (8)
12	$C_{13}H_{10}O_5$ (246.0528)		4.7E-05	6.9 (12)	13 (10)	15 (7)
13	$C_{13}H_{12}O_6$ (264.0634)		1.1E-06	6.2 (14)	11 (11)	14 (9)

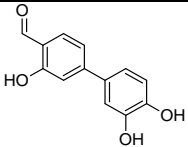
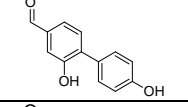
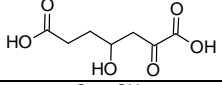
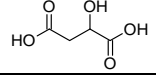
^a Molecular formulas and proposed structures of the top 10 most abundant compounds identified according to (-) nano-DESI spectra data. The exact molecular weight of each compound is shown in parentheses.

^b Estimated saturation concentrations (C^* , $\mu\text{g m}^{-3}$) of the compounds at 25 °C, 1 atm, determined using the Nannoolal vapor pressure and extrapolation method.

^c Relative abundances (%) of the compounds and, in parentheses, the abundance rank numbers of the compounds according to the nano-DESI mass spectra of in each time period. The rank number is counted in the sorted relative abundance list of all the compounds identified in each time period.

Table S3 Top 10 most abundant compounds identified in GUA aqSOA formed during different stages of the •OH-mediated reactions using (-) nano-DESI MS.

No.	Molecular formula ^a	Proposed structure	C* (µg m ⁻³) at 25 °C, 1 atm ^b	Relative abundance (ranking) ^c		
				P1: 0-2 hrs	P2: 2-4 hrs	P3: 4-6 hrs
1	C ₁₄ H ₁₄ O ₆ (278.0790)		2.5E-05	100 (1)	100 (1)	100 (1)
2	C ₁₄ H ₁₄ O ₄ (246.0892)		8.8E-01	52 (2)	37 (2)	18 (3)
3	C ₂₁ H ₂₀ O ₆ (368.1259)		4.1E-11	28 (3)	10 (7)	5.1 (21)
4	C ₁₃ H ₁₂ O ₄ (232.0735)		8.7E-02	23 (4)	15 (5)	12 (8)
5	C ₂₀ H ₁₈ O ₆ (354.1103)		8.0E-09	19 (5)	8.1 (11)	4.9 (22)
6	C ₈ H ₆ O ₃ (150.0317)		5.2E+02	15 (6)	0.0 (N/A)	1.7 (82)
7	C ₁₄ H ₁₂ O ₆ (276.0634)		3.1E-06	13 (7)	17 (3)	17 (4)
8	C ₁₃ H ₁₀ O ₅ (246.0528)		4.7E-05	12 (8)	15 (4)	18 (2)
9	C ₂₁ H ₁₈ O ₈ (398.1001)		5.7E-14	9.9 (9)	8.7 (10)	8.3 (12)
10	C ₁₃ H ₁₂ O ₆ (264.0634)		1.1E-06	9.7 (10)	12 (6)	16 (5)

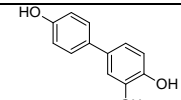
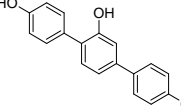
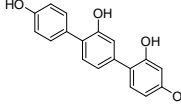
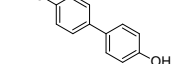
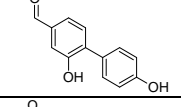
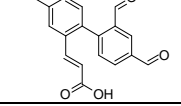
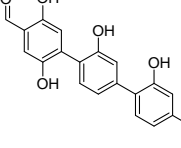
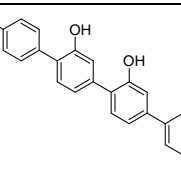
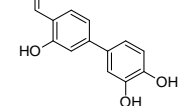
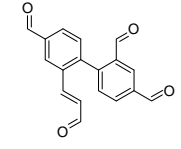
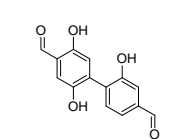
11	C ₁₃ H ₁₀ O ₄ (230.0579)		1.2E-02	6.2 (16)	9.4 (9)	14 (6)
12	C ₁₃ H ₁₀ O ₃ (214.0630)		2.0E+00	5.5 (19)	6.7 (14)	8.7 (10)
13	C ₇ H ₁₀ O ₆ (190.0477)		4.4E-03	3.7 (21)	10 (8)	13 (7)
14	C ₄ H ₆ O ₅ (134.0215)		5.6E+00	0.0 (N/A)	0.0 (N/A)	9.6 (9)

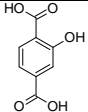
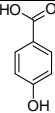
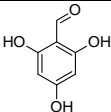
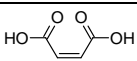
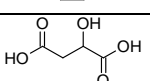
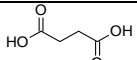
^a Molecular formulas and proposed structures of the top 10 most abundant compounds identified according to (-) nano-DESI spectra data. The exact molecular weight of each compound is shown in parentheses.

^b Estimated saturation concentrations (C^* , $\mu\text{g m}^{-3}$) of the compounds at 25 °C, 1 atm, determined using the Nannoolal vapor pressure and extrapolation method.

^c Relative abundances (%) of the compounds and, in parentheses, the abundance rank numbers of the compounds according to the nano-DESI mass spectra of in each time period. The rank number is counted in the sorted relative abundance list of all the compounds identified in each time period.

Table S4 Top 10 most abundant compounds identified in PhOH aqSOA formed during different stages of the $^3\text{C}^*$ -mediated reactions using (-) nano-DESI MS.

No.	Molecular formula ^a	Proposed structure	C^* ($\mu\text{g m}^{-3}$) at 25 °C, 1 atm ^b	Relative abundance (ranking) ^c		
				P1: 0-5 hrs	P2: 5-9 hrs	P3:19-20 hrs
1	$\text{C}_{12}\text{H}_{10}\text{O}_3$ (202.0630)		9.0E-01	100 (1)	100 (1)	5.7 (18)
2	$\text{C}_{18}\text{H}_{14}\text{O}_3$ (278.9042)		6.5E-04	88 (2)	41 (7)	0.5 (194)
3	$\text{C}_{18}\text{H}_{14}\text{O}_4$ (294.0892)		2.4E-06	45 (3)	40 (8)	1.9 (69)
4	$\text{C}_{12}\text{H}_{10}\text{O}_2$ (186.0680)		9.2E+01	27 (4)	25 (10)	0.6 (175)
5	$\text{C}_{13}\text{H}_{10}\text{O}_3$ (214.0630)		2.0E+00	21 (5)	42 (5)	23 (5)
6	$\text{C}_{18}\text{H}_{12}\text{O}_5$ (308.0684)		4.0E-07	21 (6)	44 (4)	1.8 (80)
7	$\text{C}_{20}\text{H}_{14}\text{O}_6$ (350.0790)		1.1E-10	20 (7)	70 (2)	26 (4)
8	$\text{C}_{24}\text{H}_{18}\text{O}_4$ (370.1204)		9.2E-10	16 (8)	5.9 (45)	0.0 (N/A)
9	$\text{C}_{13}\text{H}_{10}\text{O}_4$ (230.0579)		1.2E-02	16 (9)	42 (6)	34 (2)
10	$\text{C}_{18}\text{H}_{12}\text{O}_4$ (292.0735)		6.0E-04	13 (10)	8.9 (23)	0.1 (377)
11	$\text{C}_{14}\text{H}_{10}\text{O}_5$ (258.0528)		1.0E-04	11 (11)	31 (9)	17 (9)

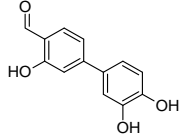
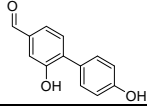
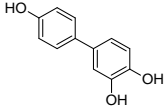
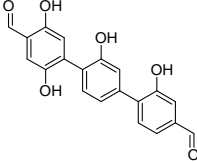
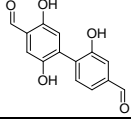
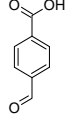
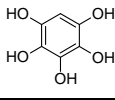
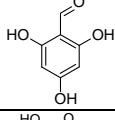
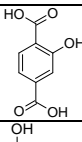
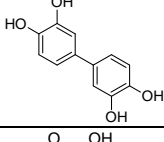
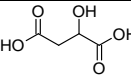
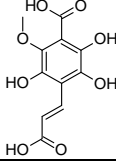
12	C ₈ H ₆ O ₅ (182.0215)		8.8E-02	5.3 (18)	9.4 (21)	8.8 (10)
13	C ₇ H ₆ O ₃ (138.0317)		9.3E+03	4.2 (21)	17 (11)	20 (6)
14	C ₇ H ₆ O ₄ (154.0266)		1.6E+01	2.4 (37)	9.6 (20)	19 (7)
15	C ₄ H ₄ O ₄ (116.0110)		1.1E+03	0.6 (95)	6.5 (37)	18 (8)
16	C ₄ H ₆ O ₅ (134.0215)		5.6E+00	0.0 (N/A)	52 (3)	100 (1)
17	C ₄ H ₆ O ₄ (118.0266)		2.3E+03	0.0 (N/A)	0.0 (N/A)	34 (3)

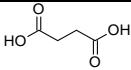
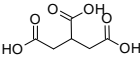
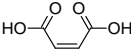
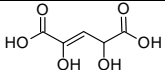
^a Molecular formulas and proposed structures of the top 10 most abundant compounds identified according to (-) nano-DESI spectra data. The exact molecular weight of each compound is shown in parentheses.

^b Estimated saturation concentrations (C^* , $\mu\text{g m}^{-3}$) of the compounds at 25 °C, 1 atm, determined using the Nannoolal vapor pressure and extrapolation method.

^c Relative abundances (%) of the compounds and, in parentheses, the abundance rank numbers of the compounds according to the nano-DESI mass spectra of in each time period. The rank number is counted in the sorted relative abundance list of all the compounds identified in each time period.

Table S5 Top 10 most abundant compounds identified in PhOH aqSOA formed at different stages of the •OH-mediated reactions using (-) nano-DESI MS.

No.	Molecular formula ^a	Proposed structure	C* (µg m ⁻³) at 25 °C, 1 atm ^b	Relative abundance (ranking) ^c		
				P1: 0-6 hrs	P2: 6-12 hrs	P3: 23-24 hrs
1	C ₁₃ H ₁₀ O ₄ (230.0579)		1.2E-02	100 (1)	100 (1)	48 (2)
2	C ₁₃ H ₁₀ O ₃ (214.0630)		2.0E+00	90 (2)	60 (4)	19 (9)
3	C ₁₂ H ₁₀ O ₃ (202.0630)		9.0E-01	48 (3)	24 (8)	2.1 (86)
4	C ₂₀ H ₁₄ O ₆ (350.0790)		1.1E-10	47 (4)	68 (2)	29 (4)
5	C ₁₄ H ₁₀ O ₅ (258.0528)		1.0E-04	39 (5)	34 (5)	15 (12)
6	C ₈ H ₆ O ₃ (150.0317)		8.5E-08	27 (6)	7.3 (32)	2.0 (88)
7	C ₆ H ₆ O ₅ (158.0215)		2.2E-02	19 (7)	27 (7)	19 (8)
8	C ₇ H ₆ O ₄ (154.0266)		1.6E+01	15 (8)	27 (6)	26 (5)
9	C ₈ H ₆ O ₅ (182.0215)		8.8E-02	15 (9)	11 (22)	7.4 (23)
10	C ₁₂ H ₁₀ O ₄ (218.0579)		4.7E-03	14 (10)	19 (10)	4.5 (34)
11	C ₄ H ₆ O ₅ (134.0215)		5.2E+00	0.0 (N/A)	62 (3)	100 (1)
12	C ₁₁ H ₁₀ O ₈ (270.0376)		4.7E-11	0.0 (N/A)	20 (9)	10 (14)

13	C ₄ H ₆ O ₄ (118.0266)		2.3E+03	0.0 (N/A)	0.0 (N/A)	33 (3)
14	C ₆ H ₈ O ₆ (176.0321)		3.1E+04	9.0 (19)	16 (11)	21 (6)
15	C ₄ H ₄ O ₄ (116.0110)		1.1E+03	1.6 (48)	12 (16)	21 (7)
16	C ₅ H ₆ O ₆ (162.0164)		5.0E-02	1.8 (44)	7.1 (35)	16 (10)

^a Molecular formulas and proposed structures of the top 10 most abundant compounds identified according to (-) nano-DESI spectra data. The exact molecular weight of each compound is shown in parentheses.

^b Estimated saturation concentrations (C^* , $\mu\text{g m}^{-3}$) of the compounds at 25 °C, 1 atm, determined using the Nannoolal vapor pressure and extrapolation method.

^c Relative abundances (%) of the compounds and, in parentheses, the abundance rank numbers of the compounds according to the nano-DESI mass spectra of in each time period. The rank number is counted in the sorted relative abundance list of all the compounds identified in each time period.

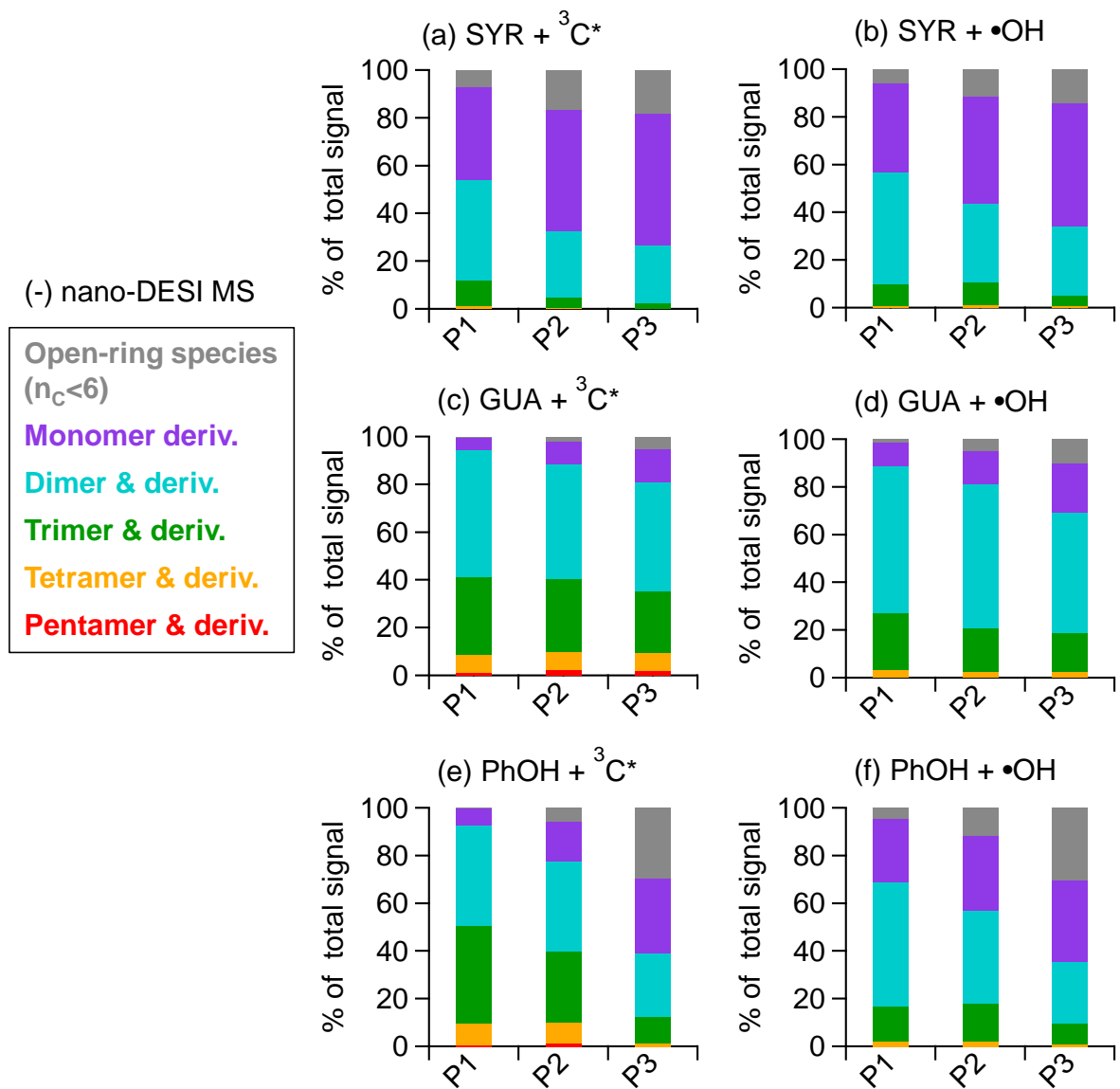


Figure S1. The signal-weighted distributions of (a-b) SYR, (c-d) GUA, and (e-f) PhOH aqSOA formed during three different stages of the $^3\text{C}^*$ - and $\bullet\text{OH}$ -mediated reactions, respectively, based on the degree of oligomerization. The data are from the (-) nano-DESI MS spectra.

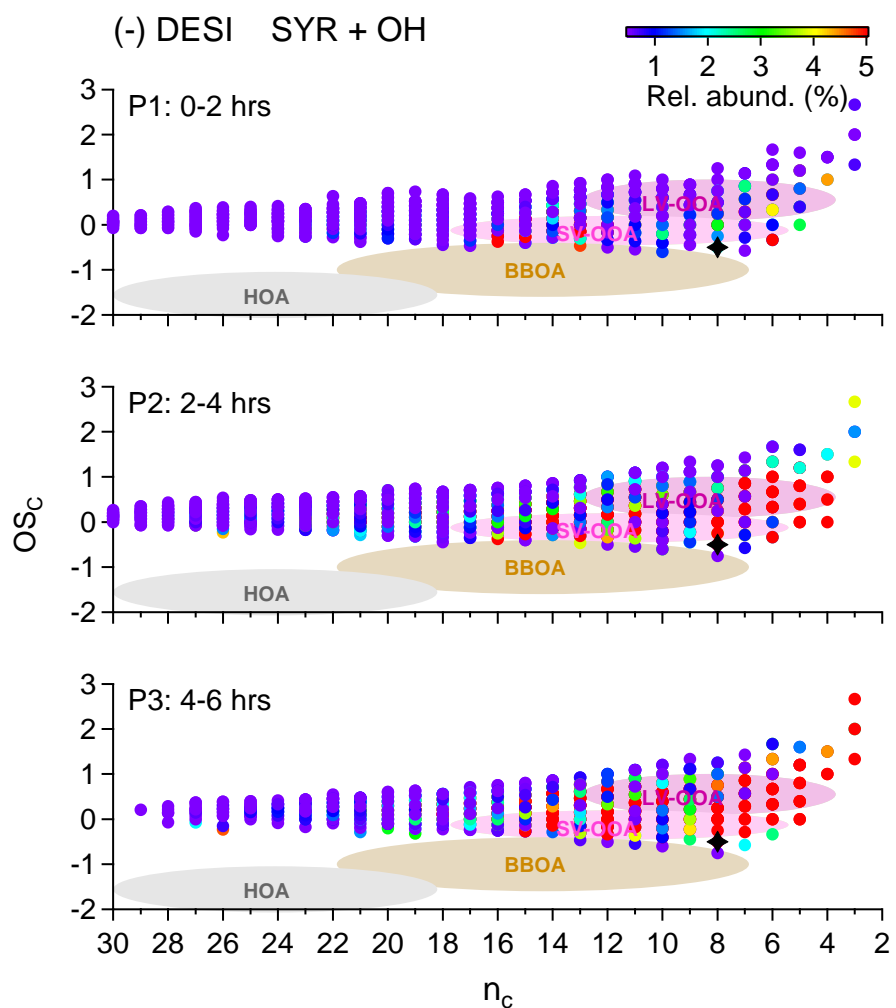


Figure S2. OS_C and n_C of SYR aqSOA formed during different stages of •OH-mediated reactions determined based on (-) nano-DESI MS spectra. Signals are colored by the relative abundance of the molecules. The black star at n_C = 8 represents SYR. The shaded ovals indicate locations of different ambient organic aerosol classes reported in Kroll et al. (2011).

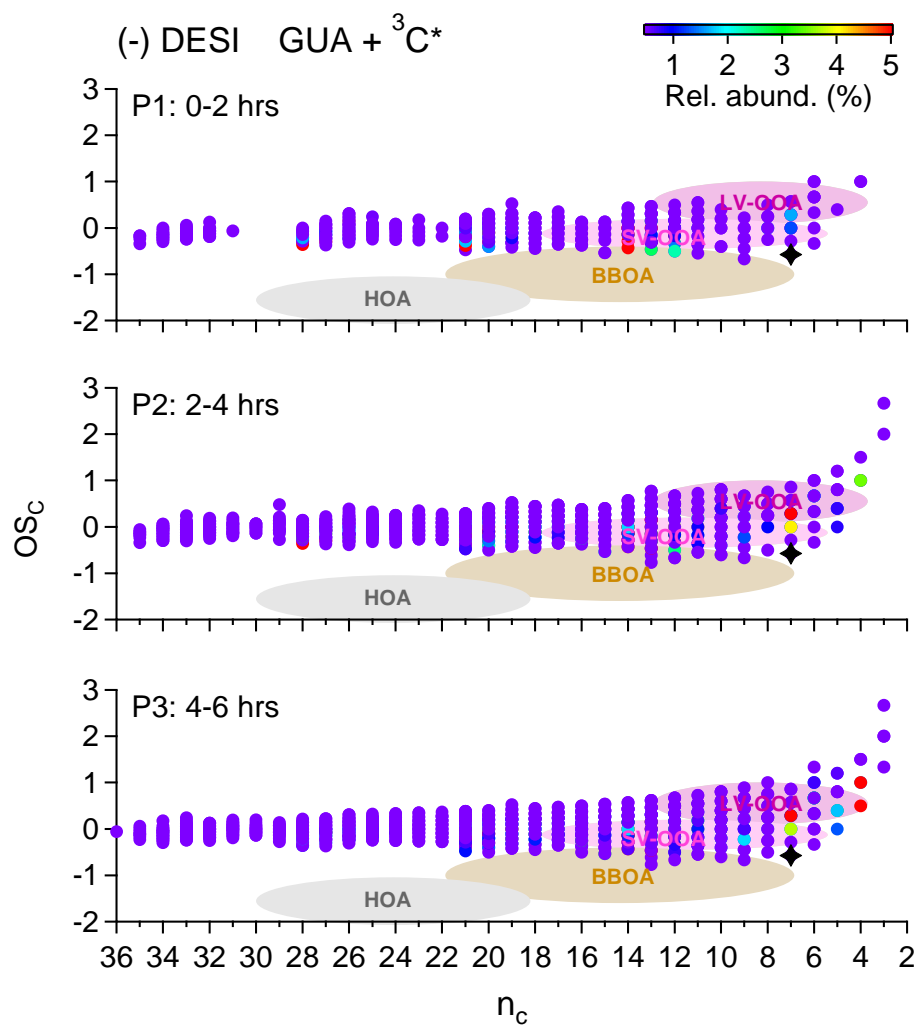


Figure S3. OS_C and n_c of GUA aqSOA formed during different stages of $^3\text{C}^*$ -mediated reactions determined based on (-) nano-DESI MS spectra. Signals are colored by the relative abundance of the molecules. The black star at $n_c = 7$ represents GUA. The shaded ovals indicate locations of different ambient organic aerosol classes reported in Kroll et al. (2011).

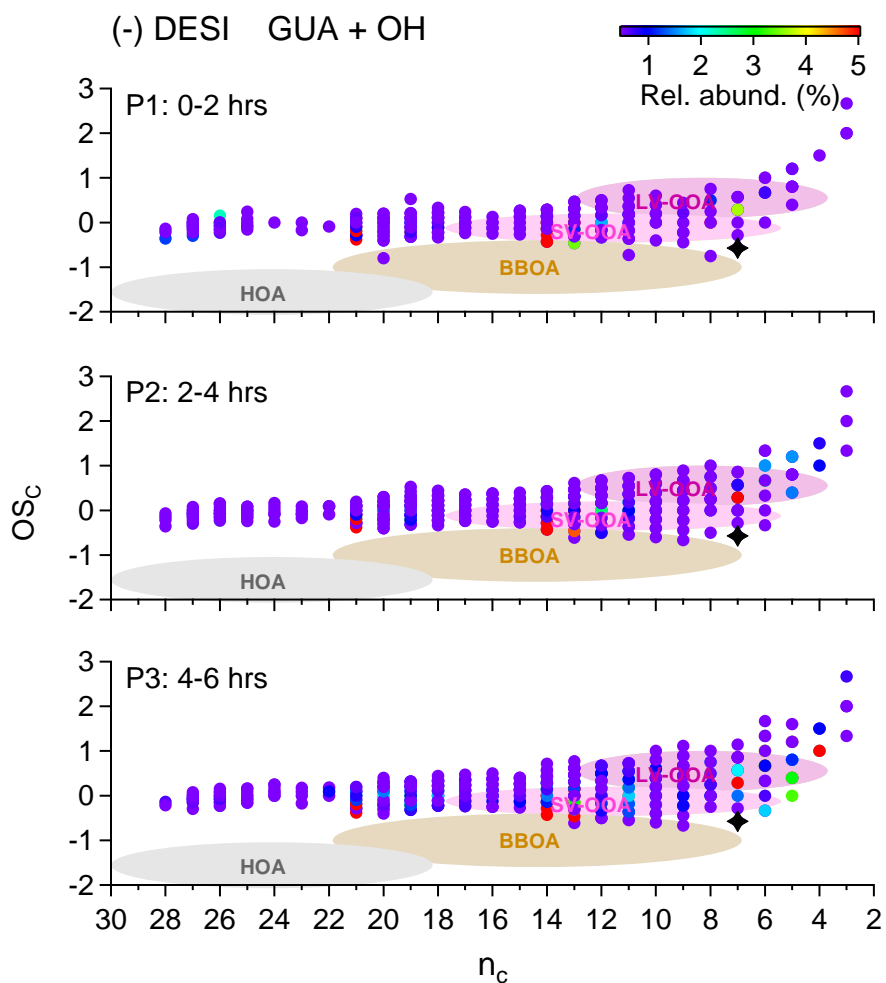


Figure S4. OS_C and n_C of GUA aqSOA formed during different stages of •OH-mediated reactions determined based on (-) nano-DESI MS spectra. Signals are colored by the relative abundance of the molecules. The black star at n_C = 7 represents GUA. The shaded ovals indicate locations of different ambient organic aerosol classes reported in Kroll et al. (2011).

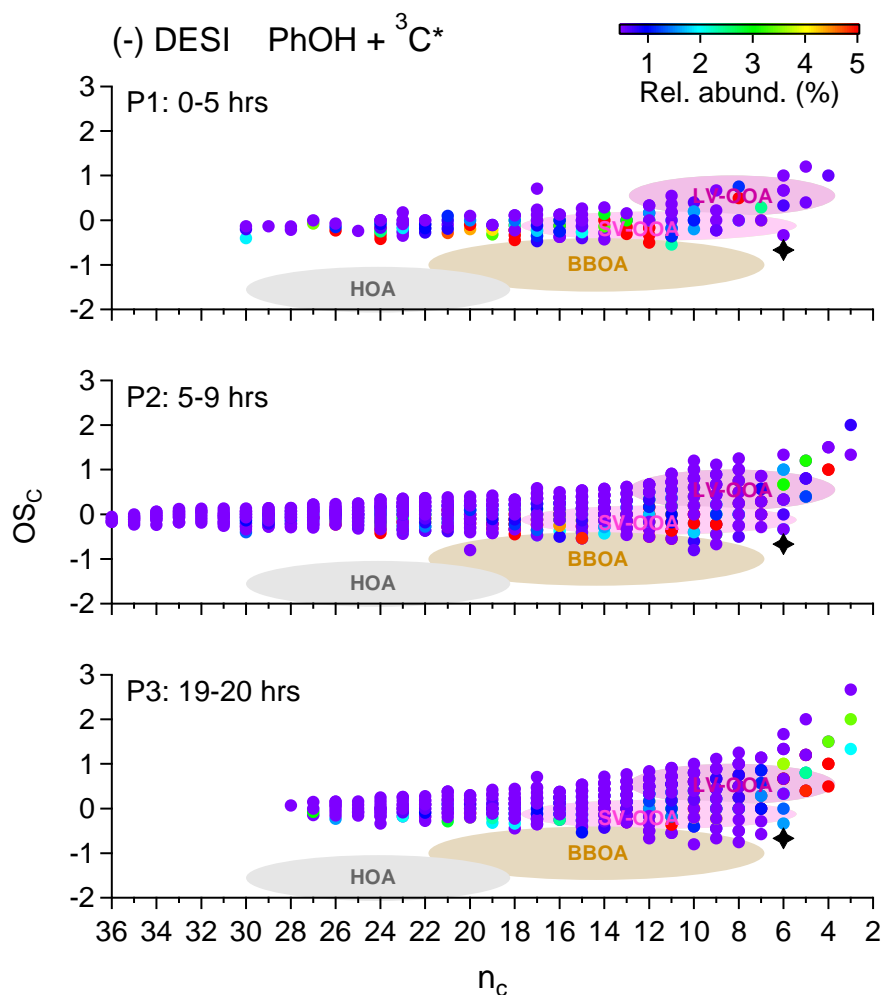


Figure S5. OS_C and n_C of PhOH aqSOA formed during different stages of $^3\text{C}^*$ -mediated reactions determined based on (-) nano-DESI MS spectra. Signals are colored by the relative abundance of the molecules. The black star at $n_C = 6$ represents PhOH. The shaded ovals indicate locations of different ambient organic aerosol classes reported in Kroll et al. (2011).

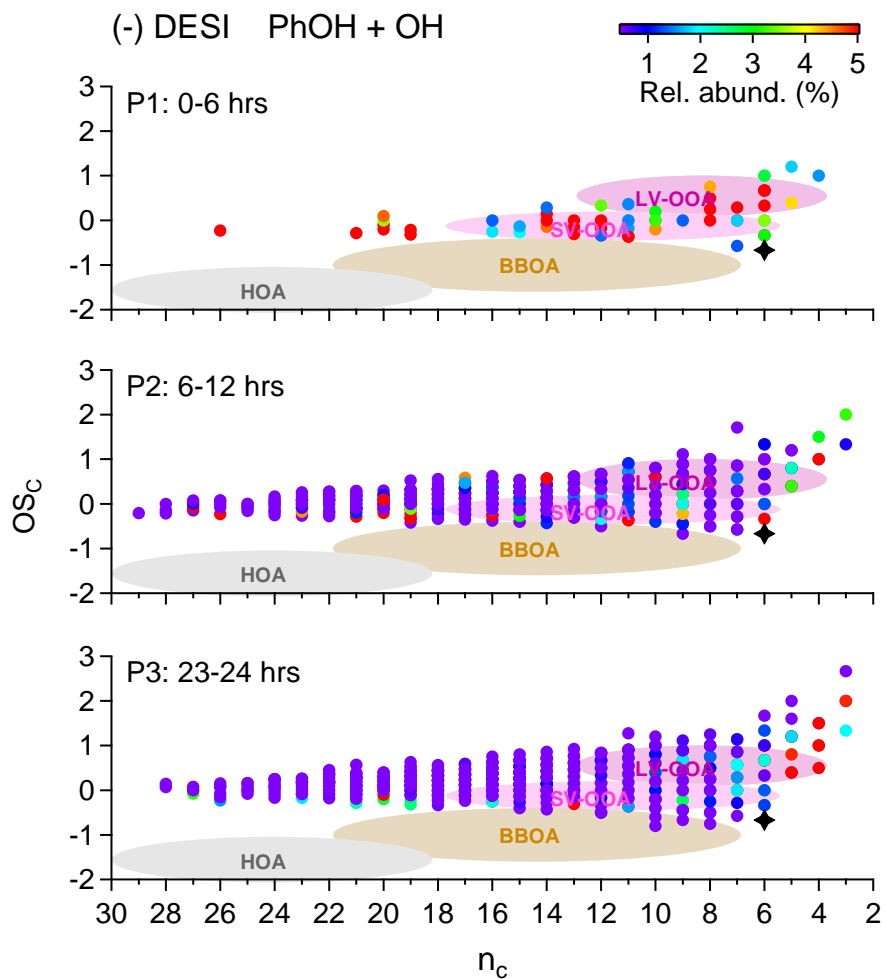


Figure S6. OS_C and n_C of PhOH aqSOA formed during different stages of •OH-mediated reactions determined based on (-) nano-DESI MS spectra. Signals are colored by the relative abundance of the molecules. The black star at n_C = 6 represents PhOH. The shaded ovals indicate locations of different ambient organic aerosol classes reported in Kroll et al. (2011).

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