



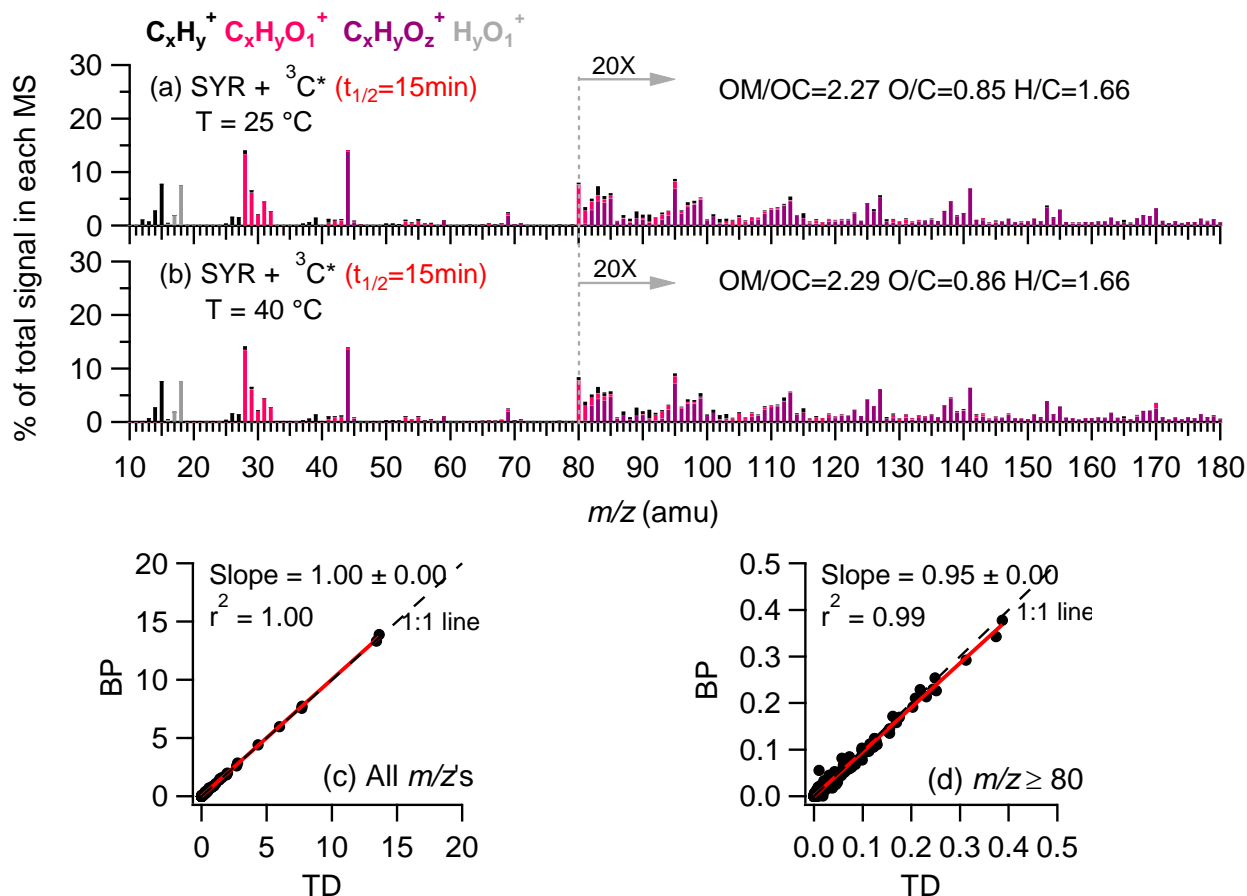
Supplement of

Chemical characterization of SOA formed from aqueous-phase reactions of phenols with the triplet excited state of carbonyl and hydroxyl radical

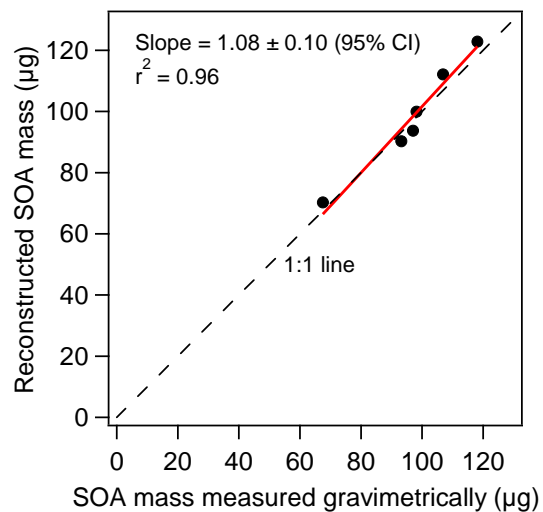
L. Yu et al.

Correspondence to: Q. Zhang (dkwzhang@ucdavis.edu)

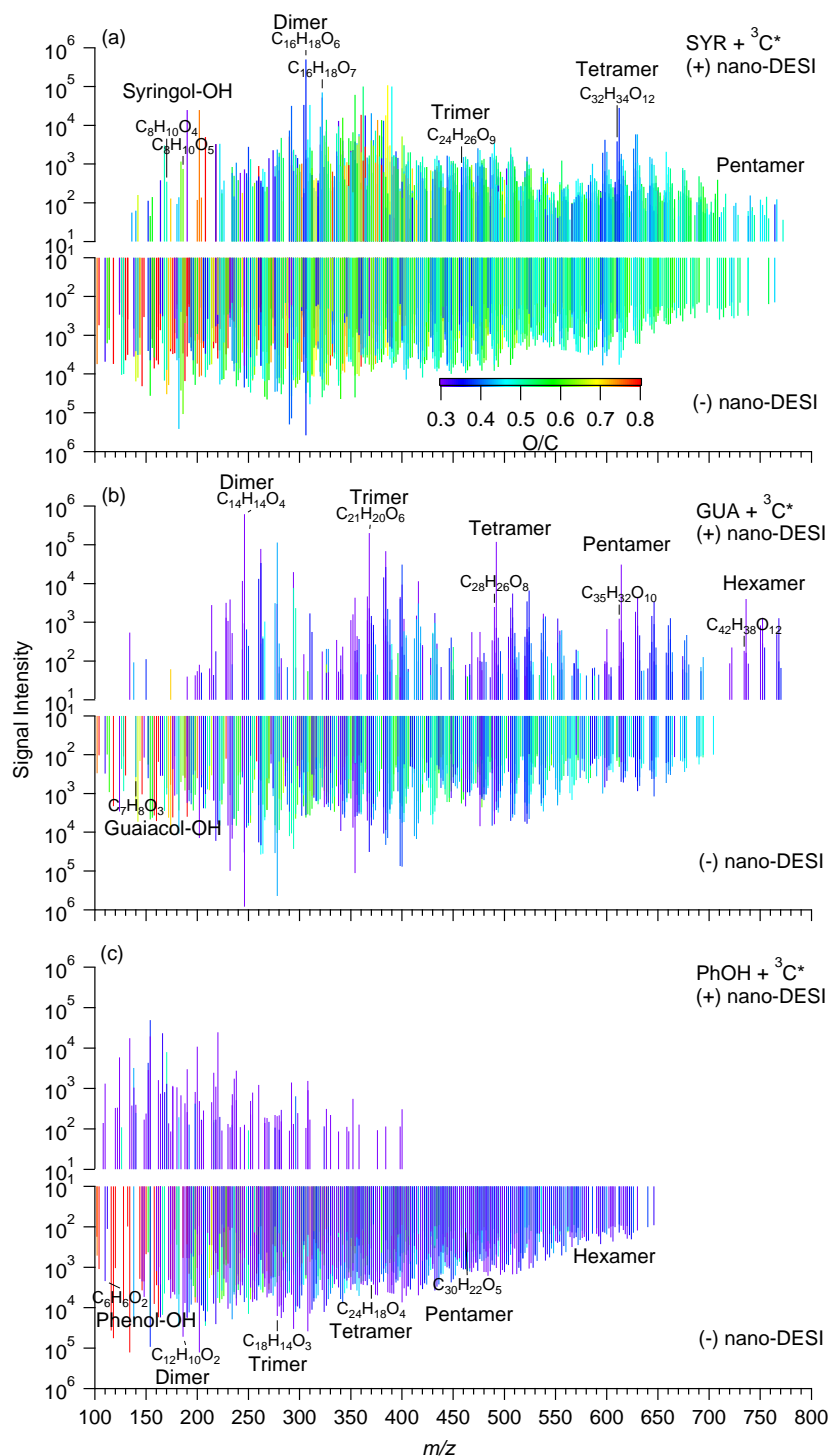
19 **Tables and Figures**
 20



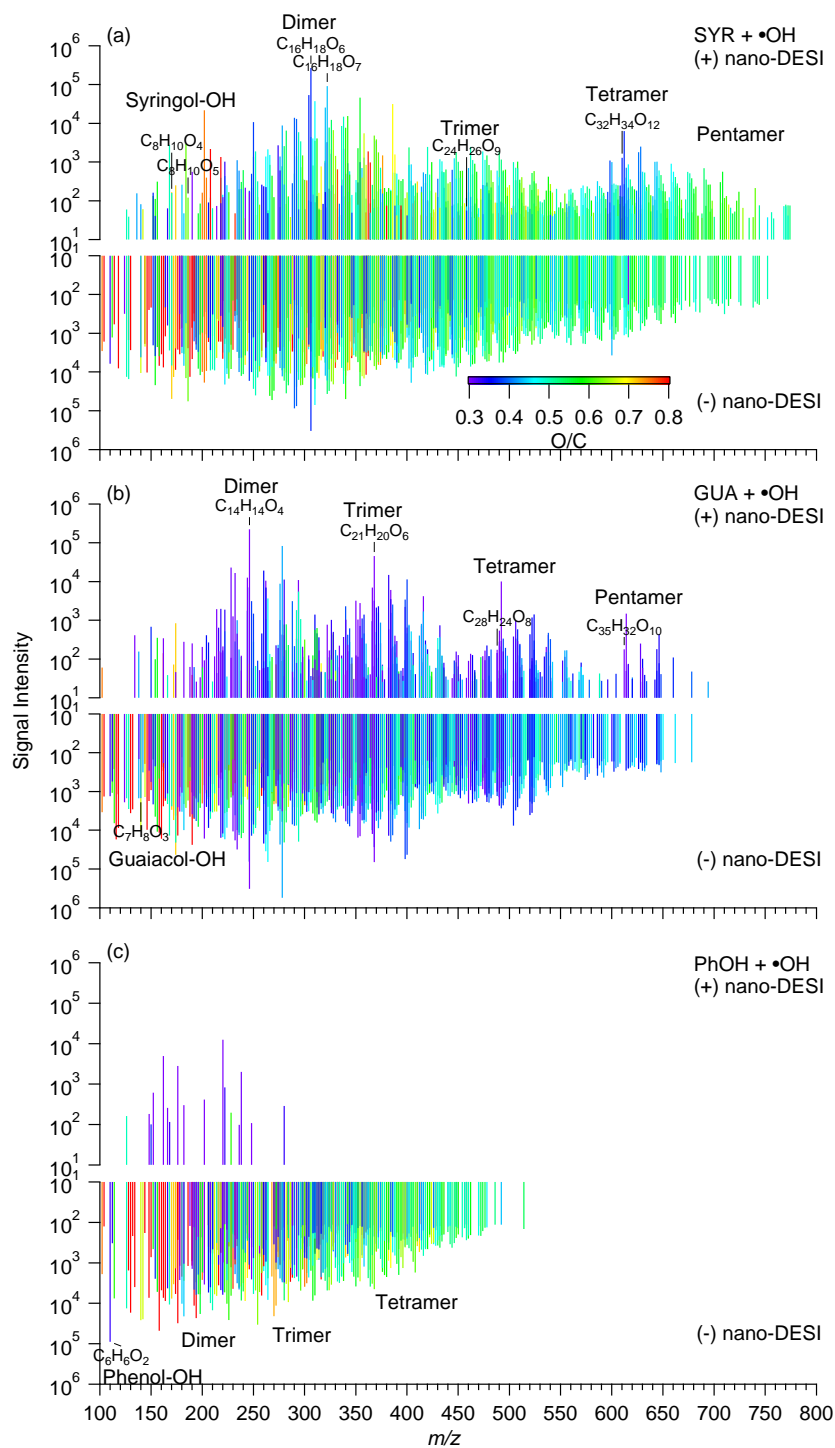
21
 22 **Figure S1.** (a-b) HR-AMS spectra of aqSOA formed from the reactions of syringol (SYR)
 23 with $^3\text{C}^*$ analyzed at room temperature ($T = 25\text{ }^\circ\text{C}$) and after a thermodenuder set at $T = 40\text{ }^\circ\text{C}$.
 24 The peaks are color-coded according to four ion categories: C_xH_y^+ , $\text{C}_x\text{H}_y\text{O}_1^+$, $\text{C}_x\text{H}_y\text{O}_z^+$, and
 25 H_yO_1^+ ($x \geq 1$; $y \geq 0$; $z \geq 2$). The ion signals at $m/z \geq 80$ are enhanced by a factor of 20 for clarity.
 26 The photoreaction time and the elemental ratios of the aqSOA are shown in the legends. (c-d)
 27 Scatter plots that compare the mass spectra of SYR aqSOA initiated with $^3\text{C}^*$ in two different
 28 modes for all m/z 's and $m/z \geq 80$ respectively. The linear regression slopes and correlation
 29 coefficients are shown in the legends.



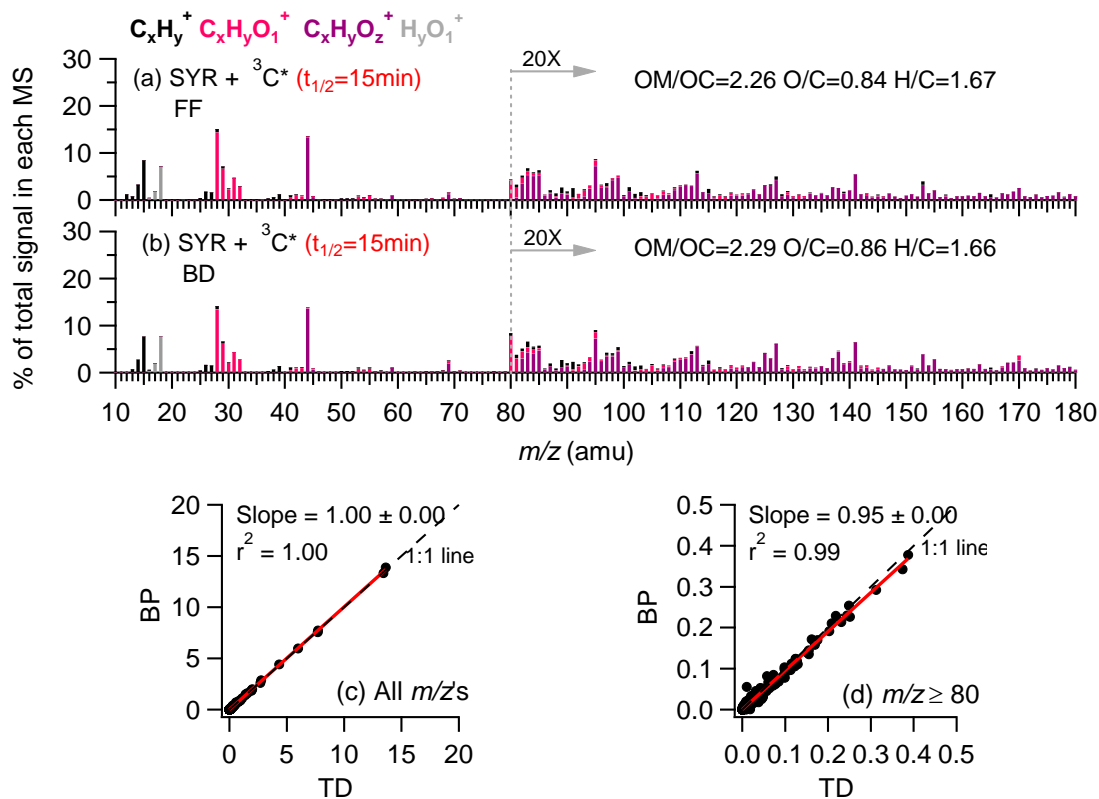
30
 31 **Figure S2.** Comparison of the reconstructed masses of phenolic aqSOA products
 32 (=TOC×OM/OC) versus their masses measured by gravimetric analysis. TOC was measured by
 33 a total carbon analyzer and OM/OC was determined by the HR-AMS. The linear fit was
 34 performed using an orthogonal distance regression (ODR) model.



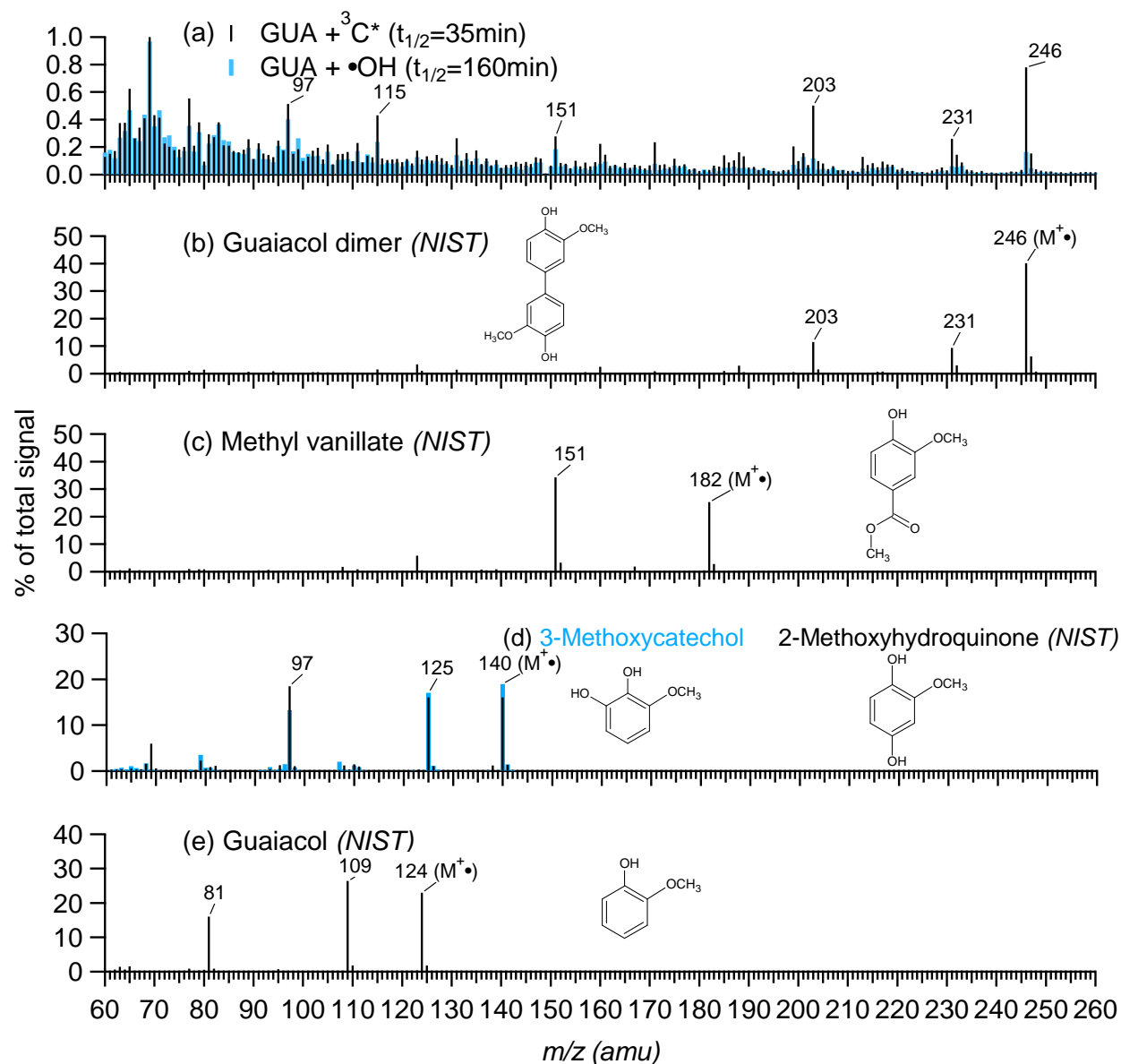
35
 36 **Figure S3.** Nano-DESI spectra of (a) syringol, (b) guaiacol and (c) phenol aqSOA
 37 formed from $^3\text{C}^*$ -mediated oxidation. The top graph in each figure is the positive mode spectrum
 38 and the bottom graph is the negative mode spectrum. Each peak represents the signal of a neutral
 39 molecule, colored by its O/C ratio. Signals corresponding to the hydroxylated monomer and
 40 oligomers are labeled. The mass spectral data and the formula and DBE of individual ions are
 41 provided in Table S2.



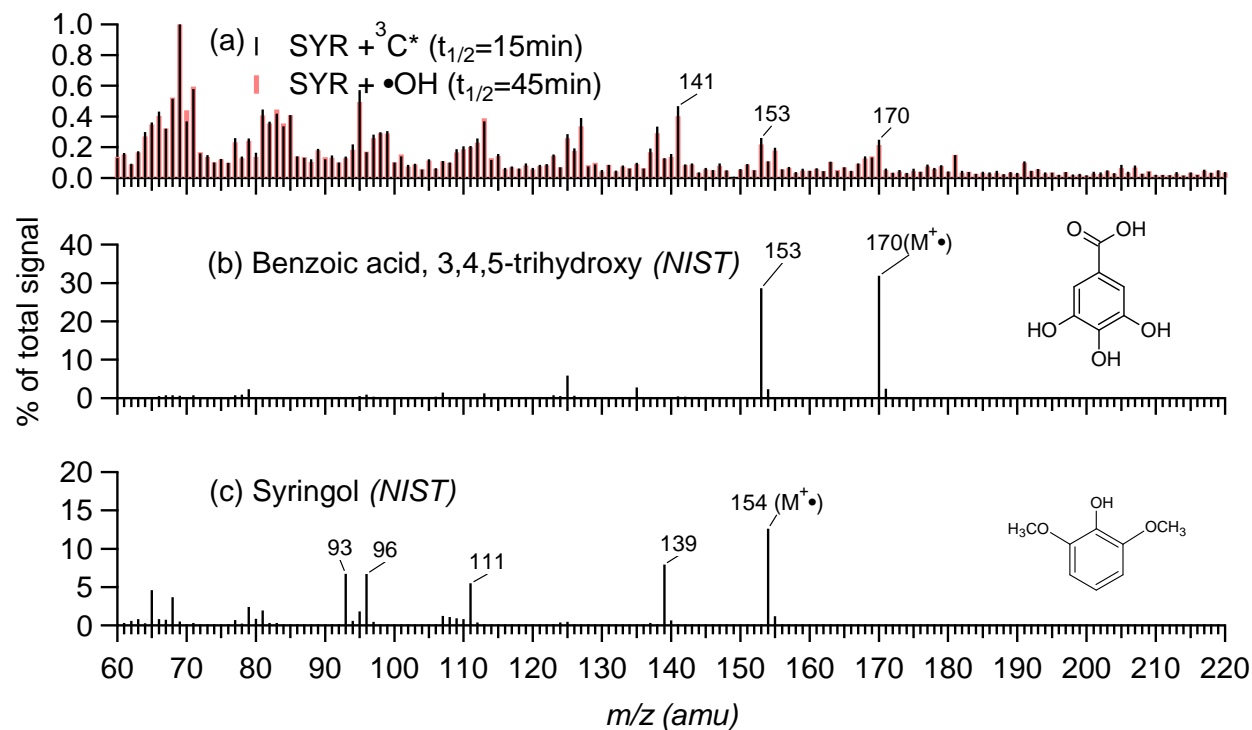
42
 43 **Figure S4.** Nano-DESI spectra of (a) syringol, (b) guaiacol and (c) phenol aqSOA
 44 formed from $\bullet\text{OH}$ -mediated oxidation. The top graph in each figure is the positive mode
 45 spectrum and the bottom graph is the negative mode spectrum. Each peak represents the signal of
 46 a neutral molecule, colored by its O/C ratio. Signals corresponding to the hydroxylated monomer
 47 and oligomers are labeled. The mass spectral data and the formula and DBE of individual ions
 48 are provided in Table S2.



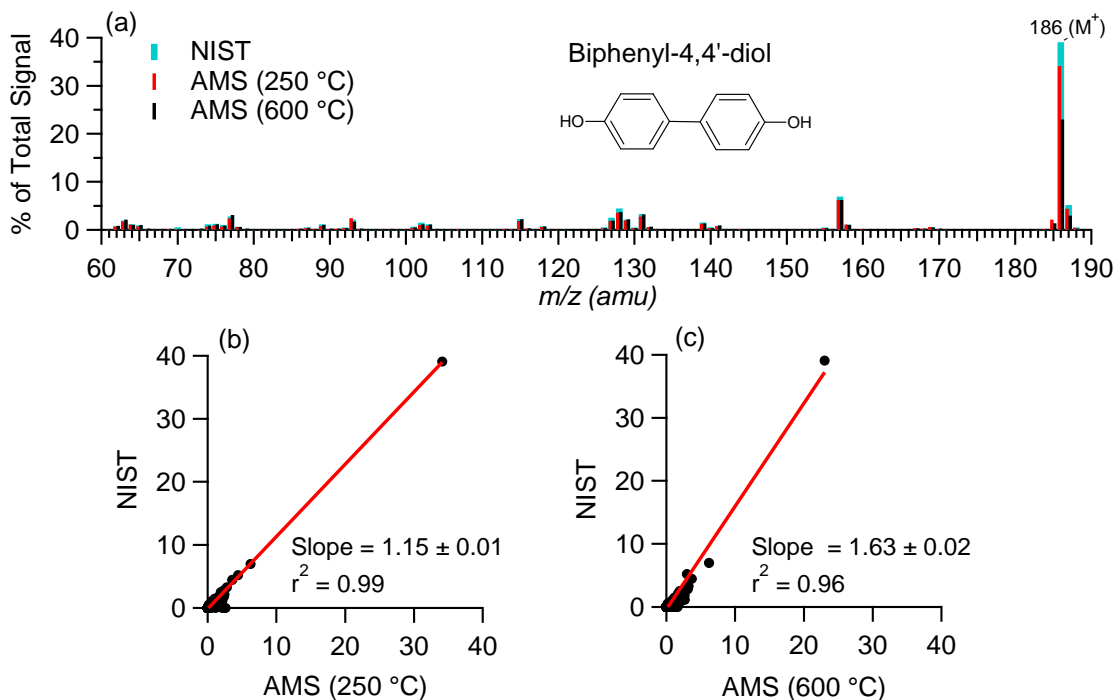
49
 50 **Figure S5.** (a-b) HR-AMS spectra of flash-frozen (FF) and blown-down (BD) samples of
 51 aqSOA formed from the reaction of syringol (SYR) with $^3\text{C}^*$. The peaks are color-coded
 52 according to four ion categories: C_xH_y^+ , $\text{C}_x\text{H}_y\text{O}_1^+$, $\text{C}_x\text{H}_y\text{O}_z^+$, and H_yO_1^+ ($x \geq 1$; $y \geq 0$; $z \geq 2$). The
 53 ion signals at $m/z \geq 80$ are enhanced by a factor of 20 for clarity. The photoreaction time and the
 54 elemental ratios are shown in the legends. (c-d) Scatter plots that compare the mass spectra of FF
 55 and BD samples for all m/z 's and $m/z \geq 80$, respectively. The linear regression slopes and
 56 correlation coefficients are shown in the legends.



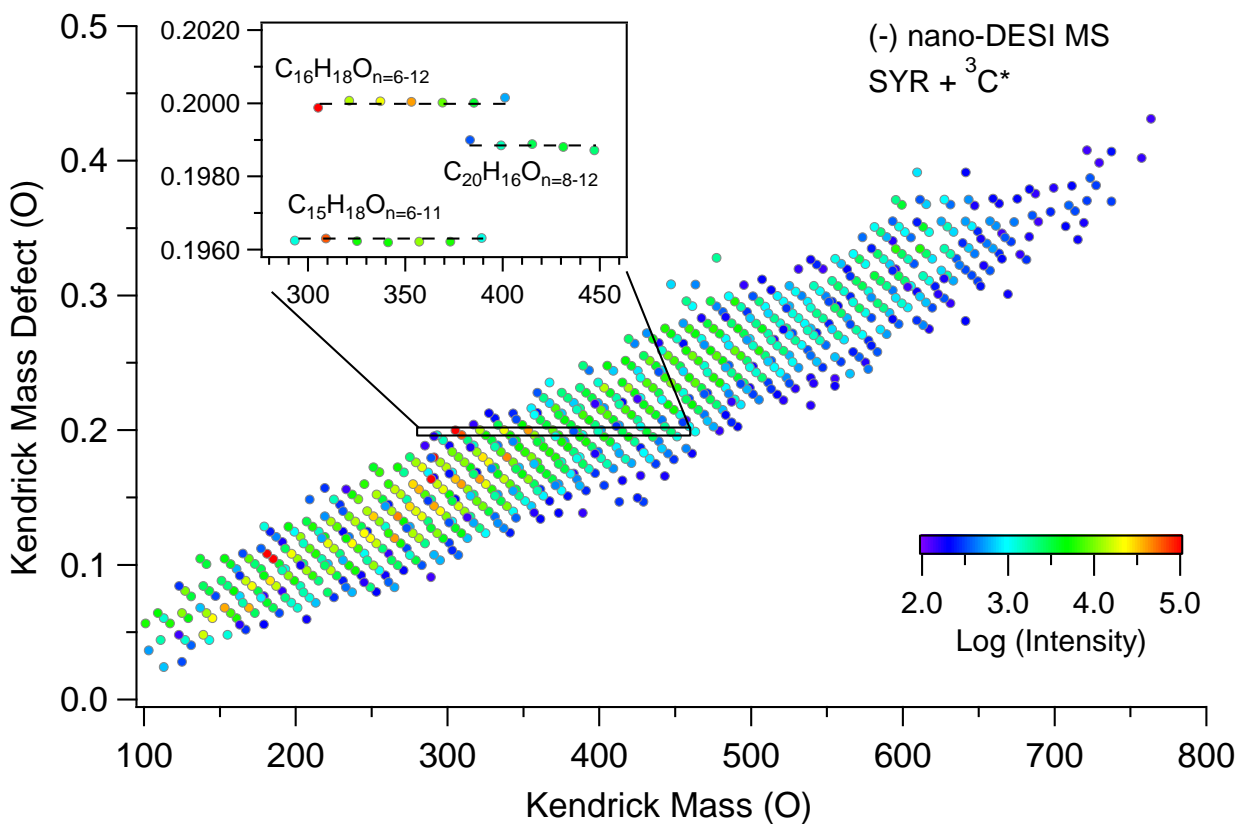
57
 58 **Figure S6.** Comparisons between (a) the HR-AMS mass spectra (in integer m/z) of
 59 guaiacol aqSOA formed via reactions with $^3\text{C}^*$ and $\bullet\text{OH}$, respectively, and the NIST mass
 60 spectra of (b) guaiacol dimer, (c) methyl vanillate, (d) 3-methoxycatechol and 2-
 61 methoxyhydroquinone, and (e) guaiacol. The chemical structures for each compound are shown
 62 and the molecular ions ($\text{M}^+\bullet$) are marked.



63
 64 **Figure S7.** Comparisons between (a) the HR-AMS mass spectra (in integer m/z) of
 65 syringol aqSOA formed via reactions with $^3\text{C}^*$ and $\bullet\text{OH}$, respectively, and the NIST mass
 66 spectra of (b) benzoic acid, 3,4,5-trihydroxy and (c) syringol. The chemical structures for each
 67 compound are shown and the molecular ions ($\text{M}^+\bullet$) are marked.

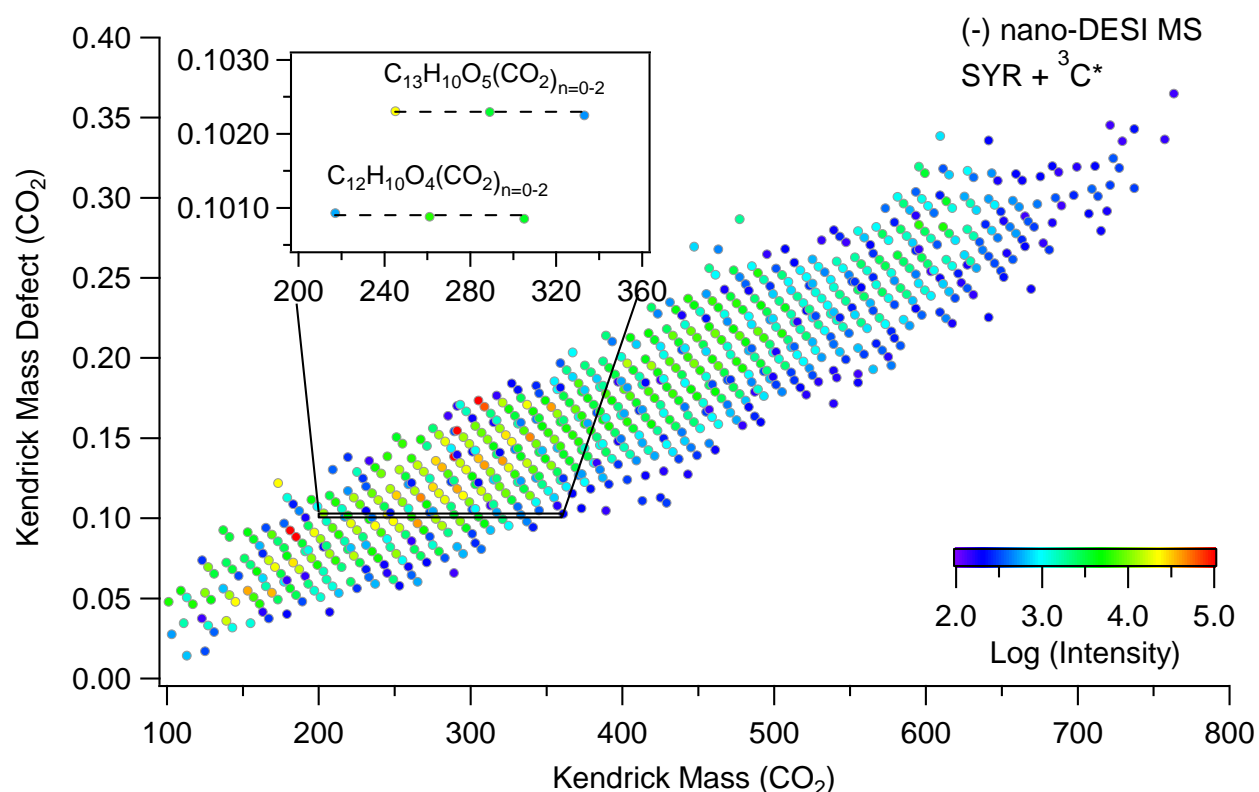


68
 69 **Figure S8.** (a) shows the comparisons of the NIST mass spectrum of biphenyl-4,4'-diol
 70 with the HR-AMS mass spectra acquired at both higher vaporizer temperature (~ 600 °C) and
 71 lower temperature (~ 250 °C). (b-c) show the scatter plots. The linear regression slopes and
 72 correlation coefficients are shown in the legends. Biphenyl-4,4'-diol is an important aqueous
 73 photooxidation product of phenol. The NIST spectrum was compared to the AMS spectra of
 74 biphenyl-4,4'-diol (Sigma Aldrich, > 97%) acquired at both higher vaporizer temperature (~
 75 600 °C) and lower temperature (~ 250 °C) to show the influence of the AMS vaporizer
 76 temperature on the mass spectral pattern. The results show that AMS spectra of biphenyl-4,4'-
 77 diol acquired with both heater temperatures have a good correlation with the NIST spectrum (~
 78 250 °C: $r^2 = 0.99$; ~ 600 °C: $r^2 = 0.96$).



79

80 **Figure S9.** The O Kendrick diagram for syringol aqSOA formed in $^3\text{C}^*$ -mediated
 81 reaction. Homologous series differing in repetitive O units fall on the same horizontal lines with
 82 identical Kendrick mass defects. Data points are colored according to the logarithmic signal
 83 intensity. The inset shows a magnified portion of the Kendrick diagram. Dashed lines serve as
 84 visual guides. Three series of hydroxylated products are shown in the inset, with molecular
 85 formulas indicated in the legend. For example, the $\text{C}_{16}\text{H}_{18}\text{O}_{n=6-12}$ series denotes syringol dimer
 86 with 1-6 additional hydroxyl groups on the rings.



87
 88 **Figure S10.** The CO₂ Kendrick diagram for syringol aqSOA formed from reaction with
 89 ¹³C* at t_{1/2}. Homologous series differing in repetitive CO₂ units fall on the same horizontal lines
 90 with identical Kendrick mass defects. Data points are colored according to the logarithmic signal
 91 intensity. The inset shows a magnified portion of the Kendrick diagram. Dashed lines serve as
 92 visual guides. Two series of carboxylated products are shown in the inset, with molecular
 93 formulas indicated in the legend. For example, the C₁₃H₁₀O₅(CO₂)_{n=0-2} series denotes a syringol
 94 dimer derivative with 1-2 additional carboxyl groups on the rings.
 95

96 **Table S1.** AMS signature ions for the aqSOA of syringol (SYR), guaiacol (GUA), and phenol (PhOH)

	<i>m/z</i>	Ion formula	Possible parent compounds ^a
Syringol aqSOA	170	C ₈ H ₁₀ O ₄ ⁺	SYR-OH
	186	C ₈ H ₁₀ O ₅ ⁺	SYR-2OH ^b
	306	C ₁₆ H ₁₈ O ₆ ⁺	SYR dimer
	322	C ₁₆ H ₁₈ O ₇ ⁺	SYR dimer-OH
Guaiacol aqSOA	140	C ₇ H ₈ O ₃ ⁺	GUA-OH
	156	C ₇ H ₈ O ₄ ⁺	GUA-2OH
	246	C ₁₄ H ₁₄ O ₄ ⁺	GUA dimer
	262	C ₁₄ H ₁₄ O ₅ ⁺	GUA dimer-OH
	278	C ₁₄ H ₁₄ O ₆ ⁺	GUA dimer-2OH
	368	C ₂₁ H ₂₀ O ₆ ⁺	GUA trimer
	384	C ₂₁ H ₂₀ O ₇ ⁺	GUA trimer-OH
Phenol aqSOA	110	C ₆ H ₆ O ₂ ⁺	PhOH-OH
	126	C ₆ H ₆ O ₃ ⁺	PhOH-2OH
	186	C ₁₂ H ₁₀ O ₂ ⁺	PhOH dimer
	202	C ₁₂ H ₁₀ O ₃ ⁺	PhOH dimer-OH
	218	C ₁₂ H ₁₀ O ₄ ⁺	PhOH dimer-2OH
	278	C ₁₈ H ₁₄ O ₃ ⁺	PhOH trimer
	294	C ₁₈ H ₁₄ O ₄ ⁺	PhOH trimer-OH

97

98 ^a Parent compounds are proposed assuming the signature ions identified are molecular ions.

99 ^b 2OH represents 2 additional hydroxyl groups attached to the aromatic ring.

100

101 **Table S2.** Data for the nano-DESI mass spectra of phenolic aqSOA shown in Figure S3 and S4.
102 The formula and DBE of individual ions are provided in Table S2.

Syringol + DMBA aQSOA (Nano-DESI)				Syringol + OH aQSOA (Nano-DESI)				Galualcol + DMBA aQSOA (Nano-DESI)				Galualcol + OH aQSOA (Nano-DESI)				Phenol + DMBA aQSOA (Nano-DESI)				Phenol + OH aQSOA (Nano-DESI)			
Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE
256.0219	1065.69	C11H16O8	7	256.0168	1247.47	C11H14O6	7	256.0168	240.718	C11H18O9	9	248.0321	5888.72	C11H20O6	6	258.0739	160.194	C11H16O8	7	257.0376	2094.65	C11H16O8	7
256.5863	10535.6	C11H16O7	6	268.8209	2686.89	C11H18O8	8	296.5322	4468.39	C13H20O8	8	248.0532	3511.31	C11H20O6	6	258.0892	1009.91	C11H16O8	7	270.0528	349.028	C11H16O8	7
256.9046	6400.74	C11H16O6	5	288.2336	5273.16	C11H18O7	7	296.0896	3380.36	C11H16O7	6	258.1001	3208.56	C11H20O6	6	260.0321	1446.7	C11H16O8	7	272.0321	1446.7	C11H16O8	7
258.0739	3342.09	C11H14O7	5	270.8736	5211.84	C11H18O8	8	298.0477	146.22	C11H16O6	5	250.0147	436.407	C11H16O7	6	260.0321	471.67	C11H16O8	7	272.0321	1144.7	C11H16O8	7
258.0819	192.627	C9H9O9	9	270.8736	5211.84	C11H18O8	8	298.0477	146.22	C11H16O6	5	250.0147	436.407	C11H16O7	6	260.0321	471.67	C11H16O8	7	272.0321	1144.7	C11H16O8	7
260.0131	350.132	C11H16O6	5	270.8736	5211.84	C11H18O8	8	298.0477	146.22	C11H16O6	5	250.0147	436.407	C11H16O7	6	260.0321	471.67	C11H16O8	7	272.0321	1144.7	C11H16O8	7
260.0484	542.118	C11H16O5	4	272.0532	6073.53	C11H18O8	8	300.0270	104.015	C11H16O7	6	252.0270	738.75	C11H16O7	6	262.0481	2775.88	C11H16O5	4	272.0684	982.87	C11H16O5	4
262.0114	394.64	C12H16O7	7	272.0886	3397.83	C11H18O7	7	300.0481	321.712	C12H16O7	7	252.0634	879.33	C11H16O7	6	262.0481	661.627	C11H16O5	4	274.0747	1429.6	C11H16O5	4
262.0235	159.802	C9H9O9	9	274.0938	730	C11H18O9	9	300.0634	693.75	C11H16O6	5	252.0997	262.746	C11H16O5	4	264.0270	421.41	C12H16O7	7	274.0688	719.208	C11H16O5	4
262.0477	635.34	C11H16O6	5	274.0938	730	C11H18O9	9	300.0845	207.501	C11H16O6	5	254.0235	263.56	C11H16O7	6	264.0786	483.37	C11H16O5	4	274.084	232.83	C11H16O5	4
262.0688	254.029	C11H16O6	5	276.0270	571.09	C11H18O9	9	300.0937	419.196	C11H16O6	5	254.0790	248.53	C11H16O6	5	264.0786	3048.11	C11H16O5	4	276.0270	1141.17	C11H16O5	4
262.0841	6134.84	C11H16O5	4	276.0481	937.54	C11H18O9	9	302.0426	983.96	C11H16O7	6	256.0219	336.08	C11H16O6	5	266.0942	1874.01	C11H16O5	4	276.0481	1102.77	C11H16O5	4
264.0270	2650.97	C12H16O7	7	276.0634	786.25	C11H18O9	9	302.0638	135.77	C12H16O7	7	256.0583	316.39	C11H16O7	6	268.0219	1249.18	C11H16O5	4	276.0634	2466.53	C11H16O5	4
264.0474	1923.4	C11H16O6	4	284.0638	404.57	C11H18O9	9	302.0846	273.71	C11H16O6	5	256.0946	209.74	C11H16O6	5	268.0474	280.29	C11H16O5	4	284.0638	280.29	C11H16O5	4
266.0033	584.243	C11H16O6	5	278.0426	9019.18	C11H18O7	7	304.0219	2159.27	C11H16O6	5	258.0376	1288.64	C11H16O6	5	268.0739	554.22	C11H16O5	4	278.0426	2693.69	C11H16O5	4
266.0426	3858.27	C12H16O7	7	278.079	12907.5	C11H18O7	7	304.0583	1117.77	C11H16O6	5	258.0528	808.553	C11H16O6	5	270.0376	3597.11	C11H16O5	4	278.079	3039.62	C11H16O5	4
266.0739	15358.7	C11H16O6	5	280.0219	225.9	C11H18O9	9	304.0946	286.152	C11H16O6	5	258.079	187.11	C11H16O7	6	270.0528	484.45	C11H16O5	4	280.0219	134.76	C11H16O5	4
268.0219	2708.94	C11H16O6	5	280.0583	1629	C11H18O7	7	306.0176	470.68	C11H16O6	5	258.0892	327.621	C11H16O6	5	270.0892	520.66	C11H16O5	4	280.0583	842.54	C11H16O5	4
268.0583	4530.9	C11H16O7	6	280.0946	792.81	C11H18O7	7	306.0739	1768.73	C11H16O7	6	259.0168	141.167	C9H9O9	9	272.0321	191.64	C11H16O5	4	280.0946	882.24	C11H16O5	4
268.0946	5250	C11H16O6	5	282.0736	10337	C12H16O7	7	306.1103	3644.51	C11H16O6	5	260.0219	2104.92	C11H16O6	5	272.0321	181.68	C11H16O5	4	282.0736	3053.01	C11H16O5	4
270.0376	3431.47	C11H16O6	5	282.0739	3544	C11H18O7	7	308.0168	157.87	C11H16O6	5	260.0532	945.919	C11H16O6	5	272.0884	448.12	C11H16O5	4	282.0739	3294.86	C11H16O5	4
270.0739	1429.1	C12H16O7	7	284.0638	404.57	C11H18O9	9	308.0532	3434.69	C11H16O6	5	260.0684	2039.9	C11H16O6	5	274.0321	399.24	C11H16O5	4	284.0638	280.29	C11H16O5	4
272.0168	205.644	C11H16O6	5	284.0532	1780.17	C12H16O7	7	308.0896	275.921	C11H16O7	6	262.0114	153.235	C11H16O7	6	274.0747	503.78	C11H16O5	4	284.0532	156.656	C11H16O5	4
272.0232	4990.89	C11H16O6	5	284.0896	2217	C11H18O7	7	310.0325	862.574	C11H16O6	5	262.0477	3478.4	C11H16O5	4	274.0841	1784.06	C11H16O5	4	284.0896	3278.88	C11H16O5	4
272.0688	1851.51	C11H16O6	5	286.0376	1617.03	C11H18O7	7	310.0688	1104.49	C11H16O6	5	262.079	2184.49	C11H16O5	4	274.0938	1174.06	C11H16O5	4	286.0376	1617.03	C11H16O5	4
274.0232	343.43	C11H16O6	5	286.0688	1086.88	C11H18O7	7	312.0281	1166.01	C11H16O6	5	264.0270	248.14	C11H16O7	6	276.0481	330.39	C11H16O5	4	286.0688	245.6	C11H16O5	4
274.0477	368.48	C11H16O6	5	286.1032	177.178	C11H18O7	7	312.0634	318.93	C11H16O6	5	264.0634	662.14	C11H16O6	5	276.0634	1792.11	C11H16O5	4	286.1032	177.178	C11H16O5	4
274.0688	1632.53	C11H16O5	4	288.0270	176.562	C11H18O7	7	312.0845	2495.76	C11H16O6	5	264.0997	408.402	C11H16O6	5	276.0997	88.0867	C11H16O5	4	288.0270	176.562	C11H16O5	4
276.0270	1370.6	C11H16O6	5	288.0481	2975.89	C11H18O7	7	312.0997	316.884	C11H16O6	5	266.0033	284.261	C11H16O6	5	278.0426	2375.91	C11H16O5	4	288.0481	2975.89	C11H16O5	4
276.0481	76.9841	C11H16O6	5	288.0634	248	C11H18O7	7	314.0474	1494.05	C11H16O6	5	266.0376	317.8	C11H16O6	5	278.0688	439.48	C11H16O5	4	288.0634	248	C11H16O5	4
276.0634	2875.2	C11H16O6	5	288.0845	247.324	C11H18O7	7	314.0638	1085.74	C11H16O6	5	266.0739	1051.17	C11H16O6	5	278.1154	429.35	C11H16O5	4	288.0845	247.324	C11H16O5	4
276.0997	2304.87	C11H16O5	4	290.0426	2196.32	C11H18O7	7	314.079	1283.99	C11H16O6	5	266.0938	1119.8	C11H16O6	5	280.0583	1643.93	C11H16O5	4	288.0997	1972.11	C11H16O5	4
278.0426	278.0426	C11H16O6	5	290.079	2079.76	C11H18O7	7	314.0946	2133.19	C11H16O6	5	266.1154	1189.828	C11H16O6	5	280.0892	638.89	C11H16O5	4	290.079	2079.76	C11H16O5	4
278.0946	2826.11	C11H16O6	5	290.0946	189.766	C11H18O7	7	316.0583	1580.91	C11H16O6	5	268.0426	1030.6	C11H16O6	5	280.0946	144.105	C11H16O5	4	290.0946	189.766	C11H16O5	4
280.0219	3254.81	C12H16O7	7	290.1154	859.966	C11H18O7	7	316.0794	117.467	C11H16O6	5	270.0376	2123.63	C11H16O6	5	282.0736	3069.41	C11H16O5	4	290.1154	859.966	C11H16O5	4
280.0583	1725.91	C11H16O7	6	292.0219	344.062	C11H18O7	7	316.0946	1545.23	C11H16O6	5	270.0528	278.485	C11H16O5	4	282.0892	1797.8	C11H16O5	4	292.0219	344.062	C11H16O5	4
280.0946	1266.97	C11H16O6	5	292.0426	1861.029	C11H18O7	7	318.0168	1896.9	C11H16O6	5	270.0684	1086.1	C11H16O5	4	282.0997	688.89	C11H16O5	4	292.0426	1861.029	C11H16O5	4
280.1154	1266.97	C11H16O6	5	292.0583	1297.17	C11H18O7	7	318.0376	1530.67	C11H16O6	5	272.0321	64.796	C9H9O9	9	282.1103	412.57	C11H16O5	4	292.0583	1297.17	C11H16O5	4
282.0739	3315.45	C11H16O7	6	292.0946	7675.3	C11H18O7	7	320.0168	168.459	C11H18O9	9	272.0321	2058.09	C11H16O5	4	284.1038	271.329	C11H16O5	4	292.0946	7675.3	C11H16O5	4
284.0638	370.061	C11H18O9	9	294.0736	9955.81	C11H18O7	7	320.0376	1413.9	C11H18O9	9	272.0684	731.349	C11H16O5	4	284.1248	192.26	C11H16O5	4	294.0736	9955.81	C11H16O5	4
284.0946	2422.12	C11H16O6	5	294.0946	1420	C11H18O7	7	320.0583	1080.61	C11H18O9	9	274.0321	523.84	C11H16O5	4	284.1458	312.62	C11H16O5	4	294.0946	1420	C11H16O5	4
284.0997	1868.75	C11H16O7	6	294.1103	1366.13	C11H18O7	7	322.0325	661.038	C11H18O9	9	274.0747	3160.86	C11H16O5	4	284.1668	563.122	C11H16O5	4	294.1103	1366.13	C11H16O5	4

346.1052				335.211				386.1001				386.1001				334.0888				346.0481				352.0430				364.8990							
Symring + DMW aSQdL (Pheno-DES)				Symring + DMW aSQdL (Pheno-DES)				Symring + DMW aSQdL (Pheno-DES)				Symring + DMW aSQdL (Pheno-DES)				Symring + DMW aSQdL (Pheno-DES)				Symring + DMW aSQdL (Pheno-DES)				Symring + DMW aSQdL (Pheno-DES)				Symring + DMW aSQdL (Pheno-DES)							
Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE				
348.081	2024.13	C18H12O9	11	360.085	3130.75	C18H16O8	11	388.040	2465.47	C18H12O10	12	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10				
348.092	676.56	C18H12O9	11	360.085	3130.75	C18H16O8	11	388.074	337.57	C18H12O10	12	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
348.094	311.16	C18H12O9	11	360.085	3130.75	C18H16O8	11	388.094	307.22	C18H12O10	12	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
350.030	4203.84	C18H14O9	12	362.074	157.28	C18H16O10	12	390.057	137.19	C18H14O11	12	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
350.011	4903.58	C17H18O9	9	362.074	157.28	C18H16O10	12	390.057	137.19	C18H14O11	12	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
352.030	131.30	C18H12O9	11	362.074	157.28	C18H16O10	12	390.057	137.19	C18H14O11	12	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
352.074	6304.77	C18H16O9	9	362.084	906.11	C18H18O11	6	392.074	876.83	C18H18O11	6	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
354.057	1086.15	C18H14O9	9	362.100	280.58	C18H18O10	9	394.056	185.21	C17H14O11	11	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
354.050	3882.4	C18H18O9	8	364.030	604.52	C18H16O10	11	394.090	212.05	C18H18O10	11	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
356.080	92.88	C18H12O11	9	364.042	371.88	C18H16O11	10	396.081	280.72	C18H12O12	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
356.073	1007.8	C18H18O9	8	364.074	494.21	C17H16O10	10	396.082	110.89	C18H18O10	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
356.107	851.44	C18H16O10	7	364.158	2126.73	C18H16O10	9	396.084	883.58	C18H16O10	9	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
358.025	170.74	C17H10O9	13	366.057	2147.45	C18H14O10	10	398.074	1751.86	C18H10O10	15	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
358.036	729.02	C18H12O11	11	366.058	1398.54	C18H16O11	10	398.074	1751.86	C18H10O10	15	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
358.068	654.20	C18H14O12	12	368.030	213.89	C18H12O11	10	398.101	739.66	C18H12O11	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
358.090	1127.2	C18H18O12	7	368.073	703.82	C18H12O11	10	400.040	2159.84	C18H12O11	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
358.152	392.00	C18H18O11	11	368.110	550.67	C17H20O9	8	400.074	575.43	C18H12O11	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
360.081	1096.83	C17H12O9	12	370.056	3699.77	C18H14O11	9	400.158	7066.7	C17H20O9	12	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
360.092	6432.25	C18H18O11	7	370.090	876.75	C18H12O11	10	402.023	225.49	C18H10O11	14	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
360.085	3284.86	C18H16O11	11	372.081	249.75	C18H12O11	10	402.087	3183.34	C18H14O11	13	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
360.106	230.17	C18H14O10	10	372.092	487.63	C18H16O11	11	402.090	540.63	C18H12O11	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
360.128	305.66	C18H12O11	9	374.042	1398.54	C18H16O11	10	402.114	1752.29	C18H12O11	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
362.074	222.55	C18H12O10	10	372.056	551.92	C18H12O10	7	404.030	748.65	C18H12O11	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
362.085	284.72	C18H14O12	7	374.045	707.86	C18H14O12	8	404.073	1820.2	C18H12O11	10	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
362.078	318.78	C18H12O11	11	374.078	1209.27	C18H12O11	11	404.117	2903.28	C18H12O11	11	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
362.084	2216.39	C18H18O11	6	374.089	662.42	C18H18O11	7	405.036	660.184	C18H14O11	11	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
362.101	3078.37	C18H18O10	8	374.100	3025.9	C18H18O10	11	406.090	764.263	C18H18O10	11	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10
364.030	906.06	C18H16O12	10	376.030	647.08	C17H20O11	12	408.092	201.662	C18H18O11	11	338.052	326.30	C18H12O7	9	346.102	217.45	C18H18O7	10	346.102	217.45	C18H18O7	10	352.053	138.20	C17H14O8	10	352.053	138.20	C17H14O8	10	352.053			

434.1212 8566.18 C21H20D10 11				442.1111 485.234 C19H20D12 9				486.0798 286.245 C23H18D12 15				422.0485 158.87 C18H14D12 12				424.1158 652.102 C23H20D8 14			
Syringol + DMBA aqSO4 (f) Nano-DES				Syringol + OH aqSO4 (f) Nano-DES				Galualcol + DMBA aqSO4 (f) Nano-DES				Galualcol + OH aqSO4 (f) Nano-DES				Phenol + OH aqSO4 (f) Nano-DES			
Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE
436.042	2579.7	C19H16D12	12	442.263	347.03	C23H20D9	13	488.091	237.93	C23H18D12	15	422.068	275.19	C21H14D9	16	426.087	930.45	C21H14D10	15
436.105	7236.18	C19H16D12	11	442.263	275.847	C23H20D9	13	488.074	693.81	C23H18D12	15	422.089	104.21	C21H14D9	16	426.099	1634.33	C21H14D10	15
436.189	138.9	C19H16D12	10	444.052	105.43	C23H20D10	14	488.107	489.64	C23H18D12	15	424.100	645.43	C21H14D9	16	426.113	631.8	C21H14D10	15
438.034	315.23	C18H14D12	12	444.094	384.86	C18H14D12	9	488.107	299.34	C23H20D9	13	424.040	134.219	C21H14D9	16	428.080	277.83	C20H12D11	15
438.078	3731.59	C19H16D12	11	444.105	443.81	C23H20D10	13	488.147	119.53	C23H18D12	15	424.074	100.93	C21H14D9	16	428.032	112.82	C21H14D10	15
438.113	734.142	C19H16D12	10	444.143	443.81	C23H20D10	13	490.127	268.17	C23H18D12	15	424.055	173.209	C21H14D9	16	428.073	1158.99	C21H14D10	15
440.091	435.062	C19H16D12	11	446.045	134.696	C20H14D12	14	490.127	622.06	C23H18D12	15	424.118	585.663	C21H14D9	16	428.086	570.95	C21H14D10	15
440.094	2817.73	C19H16D12	10	446.084	4210.79	C20H14D12	13	492.029	311.258	C23H18D12	15	426.057	712.528	C21H14D9	16	428.107	173.44	C21H14D10	15
442.107	361.214	C23H20D9	14	446.106	141.381	C18H14D12	8	492.062	444.726	C23H18D12	15	426.050	1166.94	C21H14D9	16	428.129	311.55	C21H14D10	15
440.118	184.97	C23H20D9	9	446.122	6079.89	C20H14D12	13	492.066	2468.17	C23H18D12	15	428.080	129.77	C21H14D9	16	430.056	135.83	C21H14D10	15
442.036	718.95	C19H16D12	15	446.064	1478.75	C20H14D12	13	492.120	1625.88	C23H18D12	15	428.074	2188.22	C21H14D9	16	430.068	1098.29	C21H14D10	15
442.074	444.853	C18H14D12	10	448.1005	13116.5	C21H14D12	12	494.045	198.91	C24H18D12	16	428.107	556.856	C21H14D9	16	430.090	676.87	C21H14D10	15
442.090	942.549	C23H20D9	14	448.1369	314.54	C22H14D12	11	494.089	314.51	C23H18D12	15	430.056	1265.76	C21H14D9	16	430.102	625.528	C21H14D10	15
442.113	838.2	C23H20D9	9	450.111	227.43	C21H14D12	11	494.118	2056.31	C23H18D12	15	430.090	350.48	C21H14D9	16	430.105	93.9705	C21H14D10	15
442.163	1303.77	C23H20D9	10	450.162	7545.13	C21H14D12	11	494.1576	869.896	C23H18D12	15	432.062	1486.8	C21H14D9	16	432.045	375.02	C21H14D10	15
444.029	175.917	C21H14D12	15	452.051	652.18	C21H14D12	12	496.064	569.089	C23H18D12	15	432.106	2093.31	C21H14D9	16	432.106	295.084	C21H14D10	15
444.092	1884.46	C21H14D12	11	452.094	989.39	C20H14D12	11	496.105	1285.36	C23H18D12	15	434.045	300.901	C19H14D12	13	432.128	96.3604	C21H14D10	15
444.1056	6184.86	C20H14D12	13	452.138	1322.8	C21H14D12	10	496.169	801.69	C23H18D12	15	434.068	221.607	C21H14D9	16	434.045	97.8255	C21H14D10	15
444.142	5660.09	C21H14D12	12	454.077	1483.46	C19H14D12	11	498.034	120.87	C23H18D12	15	434.089	1923.19	C21H14D9	16	434.049	198.35	C21H14D10	15
446.085	454.023	C20H14D12	14	454.090	296.044	C23H18D12	15	498.078	477.654	C23H18D12	15	434.101	374.712	C21H14D9	16	434.101	3037.67	C21H14D10	15
446.089	508.721	C21H14D12	13	454.111	218.54	C20H14D12	10	498.162	629.125	C23H18D12	15	434.112	410.312	C21H14D9	16	434.074	248.98	C21H14D10	15
446.112	1212	C20H14D12	13	456.091	178.75	C21H14D12	11	500.091	178.75	C21H14D12	11	436.040	189.57	C21H14D9	16	436.005	93.9705	C21H14D10	15
446.042	2118.04	C20H14D12	13	456.094	1467.26	C19H14D12	10	500.094	301.626	C21H14D12	11	436.062	291.864	C21H14D9	16	436.118	356.904	C21H14D10	15
448.1005	9991.63	C21H14D12	12	456.1056	696.196	C23H18D12	15	502.074	124.314	C23H18D12	15	436.074	487.883	C21H14D9	16	438.087	1392.02	C21H14D10	15
448.1169	424.85	C21H14D12	11	456.1267	134.653	C20H14D12	10	504.087	141.805	C23H18D12	15	438.055	694.086	C21H14D9	16	438.059	1513.77	C21H14D10	15
448.172	758.126	C21H14D12	10	458.045	309	C21H14D12	15	504.094	100.375	C23H18D12	15	438.118	754.51	C21H14D9	16	438.103	419.776	C21H14D10	15
450.034	294.29	C19H14D12	14	458.066	146.761	C18H14D12	10	504.140	126.621	C23H18D12	15	438.057	424.346	C21H14D9	16	440.080	150.904	C21H14D10	15
450.078	5394.06	C20H14D12	12	458.089	1600.05	C23H18D12	15	506.033	134.87	C23H18D12	15	438.078	130.056	C21H14D9	16	440.073	1455.99	C21H14D10	15
450.162	6813.26	C21H14D12	11	458.109	372.288	C23H18D12	15	506.089	1600.29	C23H18D12	15	438.095	596.185	C21H14D9	16	440.086	293.611	C21H14D10	15
452.091	160.9	C20H14D12	14	458.129	226.819	C23H18D12	15	506.143	179.203	C23H18D12	15	438.114	309.451	C21H14D9	16	440.099	1076.74	C21H14D10	15
452.104	5806.55	C20H14D12	11	458.156	385.995	C24H20D9	12	506.1576	533.65	C23H18D12	15	440.080	230.925	C21H14D9	16	440.129	270.373	C21H14D10	15
452.158	1427.54	C21H14D12	10	460.062	857.471	C21H14D12	14	508.062	462.458	C23H18D12	15	440.074	1292.91	C21H14D9	16	442.036	415.704	C21H14D10	15
454.077	128.24	C21H14D12	11	460.105	358.25	C23H18D12	15	508.105	190.85	C23H18D12	15	440.107	413.199	C21H14D9	16	442.068	179.885	C21H14D10	15
454.111	2818.21	C20H14D12	10	460.169	1554.89	C23H18D12	15	508.169	3377.8	C23H18D12	15	442.084	168.028	C17H14D12	11	442.090	93.97	C21H14D10	15
456.092	321.513	C21H14D12	15	462.0434	125.84	C20H14D12	14	510.0434	173.89	C24H20D9	12	442.056	380.405	C21H14D9	16	442.102	754.766	C21H14D10	15
456.094	1203.85	C19H14D12	10	462.0798	3140.03	C21H14D12	13	510.0798	1842.96	C23H18D12	15	442.090	1330.9	C21H14D9	16	444.092	498.252	C21H14D10	15
456.1056	171.589	C21H14D12	11	462.1291	127.43	C20H14D12	10	510.162	371.161	C23H18D12	15	442.107	371.161	C21H14D9	16	444.062	1055.89	C21H14D10	15
456.1267	236.153	C20H14D12	9	462.1525	613.763	C23H18D12	15	510.1525	1014.97	C23H18D12	15	444.1056	617.427	C21H14D9	16	444.094	141.071	C21H14D10	15
456.142	531.598	C24H20D9	13	464.051	868.309	C20H14D12	13	512.051	556.781	C23H18D12	15	446.045	238.548	C20H14D12	14	444.128	316.564	C21H14D10	15
458.085	467.69	C21H14D12	15	464.0954	613.07	C21H14D12	12	512.0954	100.62	C23H18D12	15	446.089	1162.66	C21H14D9	16	446.085	100.488	C21H14D10	15
458.096	880.801	C21H14D12	14	464.129	3628.6	C21H14D12	11	514.129	487.279	C23H18D12	15	446.107	212.749	C21H14D9	16	446.091	1076.74	C21H14D10	15
458.049	2576.03	C21H14D12	14	466.077	2357.38	C20H14D12	13	514.077	398.127	C23H18D12	15	446.112	163.84	C21H14D9	16	446.049	326.972	C21H14D10	15
458.1212	5241.35	C21H14D12	13	466.111	6123.48	C21H14D12	11	514.111	326.225	C23H18D12	15	446.064	614.055	C20H14D12	14	446.101	933.868	C21H14D10	15
458.176	2050.56	C24H20D9	12	468.082	210.355	C21H14D12	16	516.084	113.253	C23H18D12	15	448.079	480.871	C24H20D9	12	448.042	129.67	C21H14D10	15
460.062	1004.4	C20H14D12	9	468.109	2339.6	C21H14D12	11	518.109	188.044	C23H18D12	15	448.105	989.427	C21H14D9	16	448.064	283.02	C21H14D10	15
460.083	36.033	C18H14D12	9	468.1056	995.085	C24H20D9	12	518.049	110.702	C23H18D12	15	448.118	684.286	C23H18D12	15	448.118	395.588	C21H14D10	15
460.105	5414.05	C22H14D12	13	468.1267	952.072	C21H14D12	10	520.0642	502.612	C23H18D12	15	450.0587	210.084	C23H18D12	15	450.059	1998.47	C21H14D10	15
460.189	6321.76	C21H14D12	12	468.149	152.787	C20H14D12	16	520.105	1712.12	C23H18D12	15	450.071	690.103	C20H14D12	14	450.103	197.414	C21H14D10	15
462.044	188.507	C21H14D12	14	470.096	388.507	C18H14D12	11	520.169	607.617										

628.1064	351.057	C29H24O16	18	710.1482	321.36	C34H30O17	20
Syringol + DMB aqSOA, ()/Nano-DESI				Syringol + OH aqSOA, ()/Nano-DESI			
Accurate m/z	Intensity	Formula	DBE	Accurate m/z	Intensity	Formula	DBE
628.1216	185.123	C33H24O13	22	712.1639	134.114	C34H32O17	19
628.1428	1643.466	C30H20O15	17	714.1432	197.851	C34H30O18	19
628.1791	1011.34	C31H22O14	16	716.1224	129.902	C32H28O19	19
630.1220	1646.45	C29H26O16	17	724.1639	157.2	C35H32O17	20
630.1584	1579.01	C30H30O15	16	726.1432	194.014	C34H30O18	20
632.1013	161.882	C30H24O17	17	738.1432	219.418	C35H30O18	21
632.1377	1675.86	C29H28O16	16	740.1588	153.187	C35H32O18	20
632.1740	402.636	C30H32O15	15	742.1744	172.899	C35H34O18	19
634.1170	582.978	C28H26O17	16	744.1537	185.446	C34H32O19	19
634.1533	762.367	C29H30O16	15	752.1588	131.46	C36H32O18	21
636.1326	369.607	C28H28O17	15				
638.1271	446.54	C31H26O15	19				
640.1428	280.024	C31H28O15	18				
642.0857	215.204	C29H22O17	19				
642.1220	343.601	C30H26O16	18				
642.1584	561.857	C31H30O15	17				
642.1948	207.624	C32H34O14	16				
644.1377	710.592	C30H30O16	17				
644.1740	523.227	C31H32O15	16				
646.1170	333.188	C29H26O17	17				
646.1533	898.643	C30H30O16	16				
648.1326	451.966	C30H30O17	16				
648.1690	184.88	C30H32O16	15				
650.1119	316.205	C28H26O18	16				
650.1482	271.479	C29H30O17	15				
652.1064	231.82	C31H24O16	20				
652.1428	185.249	C32H28O15	19				
654.1220	175.71	C31H26O16	19				
656.1377	435.857	C31H28O16	18				
658.1370	357.265	C30H30O17	18				
658.1533	519.448	C31H30O16	17				
660.1326	533.503	C30H28O17	17				
660.1690	202.787	C31H32O16	16				
662.1482	508.033	C30H30O17	16				
664.1275	268.992	C29H28O18	16				
664.1639	192.713	C30H32O17	15				
666.1220	228.851	C32H30O16	20				
666.1432	145.731	C29H30O18	15				
668.1377	361.843	C32H28O16	19				
670.0958	197.142	C34H22O15	24				
672.1326	207.637	C31H30O17	18				
674.1482	438.697	C31H30O17	17				
676.1639	204.784	C31H32O17	16				
678.1220	136.815	C33H28O16	21				
682.1170	286.691	C32H30O17	20				
684.1326	182.205	C32H28O17	19				
684.1690	204.781	C33H32O16	18				
686.1482	364.976	C32H30O17	18				
688.1639	156.981	C32H32O17	17				
690.1432	142.517	C31H30O18	17				
698.1482	265.583	C33H30O17	19				
700.1639	169.972	C33H32O17	18				
708.1326	203.728	C34H28O17	21				
710.1482	392.844	C34H30O17	20				
712.1639	215.774	C34H32O17	19				
714.1432	344.287	C33H30O18	19				
716.1324	196.328	C32H28O19	19				
720.1326	175.019	C35H28O17	22				
722.1482	322.225	C35H30O17	21				
722.1846	141.928	C36H30O16	20				
724.1639	367.226	C35H32O17	20				
728.1588	313.28	C34H32O18	19				
730.1744	145.467	C34H34O18	18				
738.1432	313.077	C35H30O18	21				
738.1795	230.472	C36H34O17	20				
768.1694	157.7	C35H34O19	19				
764.1952	141.473	C38H36O17	21				

Guaicol + DMB aqSOA, ()/Nano-DESI			
Accurate m/z	Intensity	Formula	DBE

Guaicol + OH aqSOA, ()/Nano-DESI			
Accurate m/z	Intensity	Formula	DBE

Phenol + DMB aqSOA, ()/Nano-DESI			
Accurate m/z	Intensity	Formula	DBE

Phenol + OH aqSOA, ()/Nano-DESI			
Accurate m/z	Intensity	Formula	DBE