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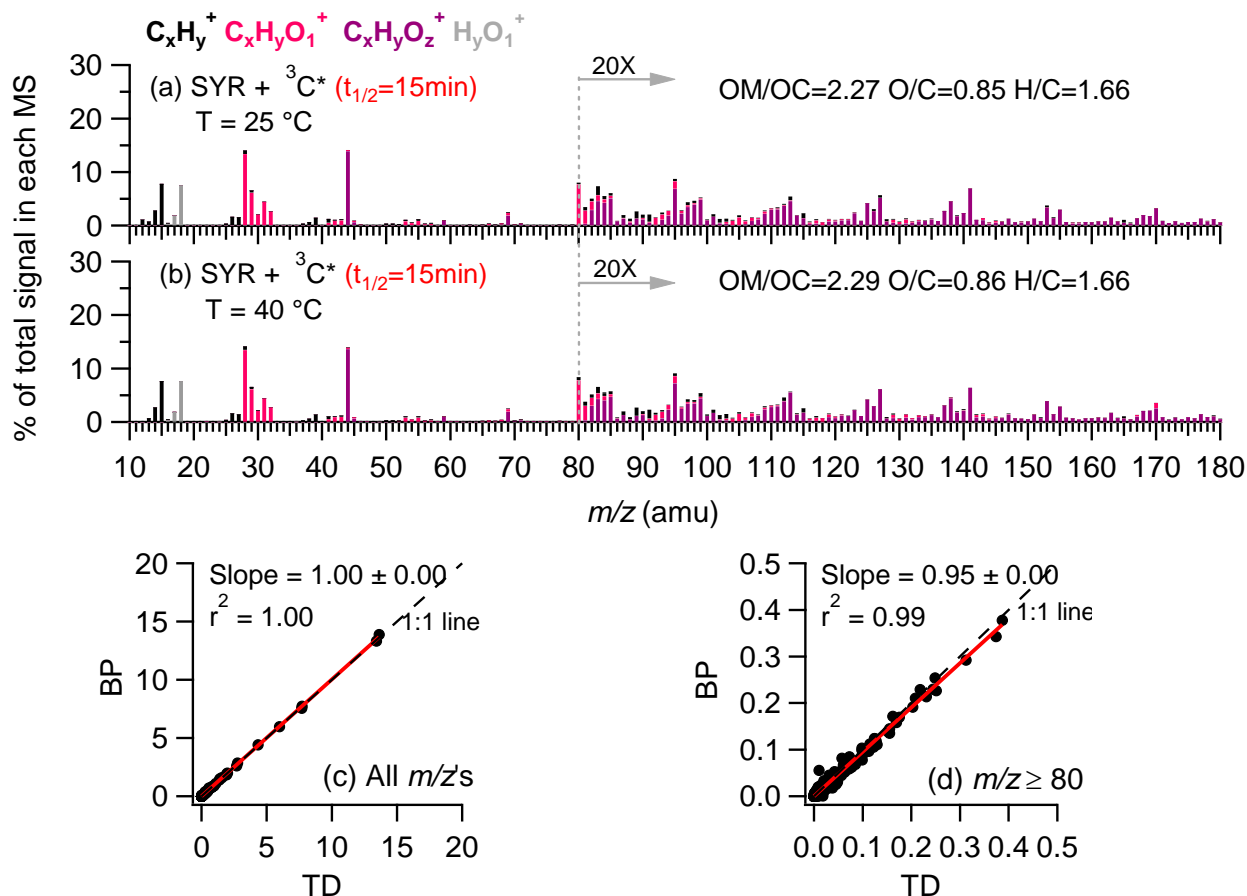
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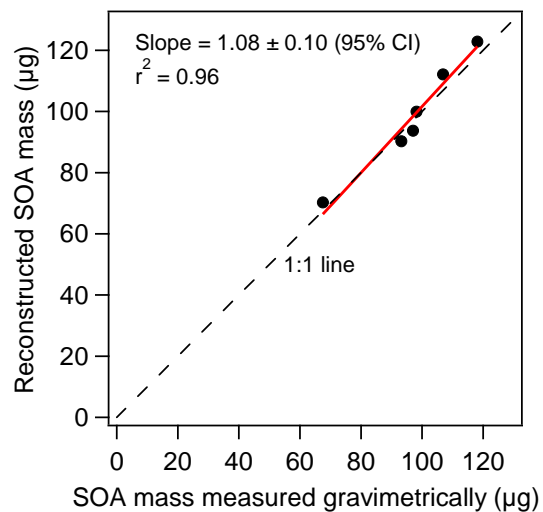
Chemical characterization of SOA formed from aqueous-phase reactions of phenols with the triplet excited state of carbonyl and hydroxyl radical

L. Yu et al.

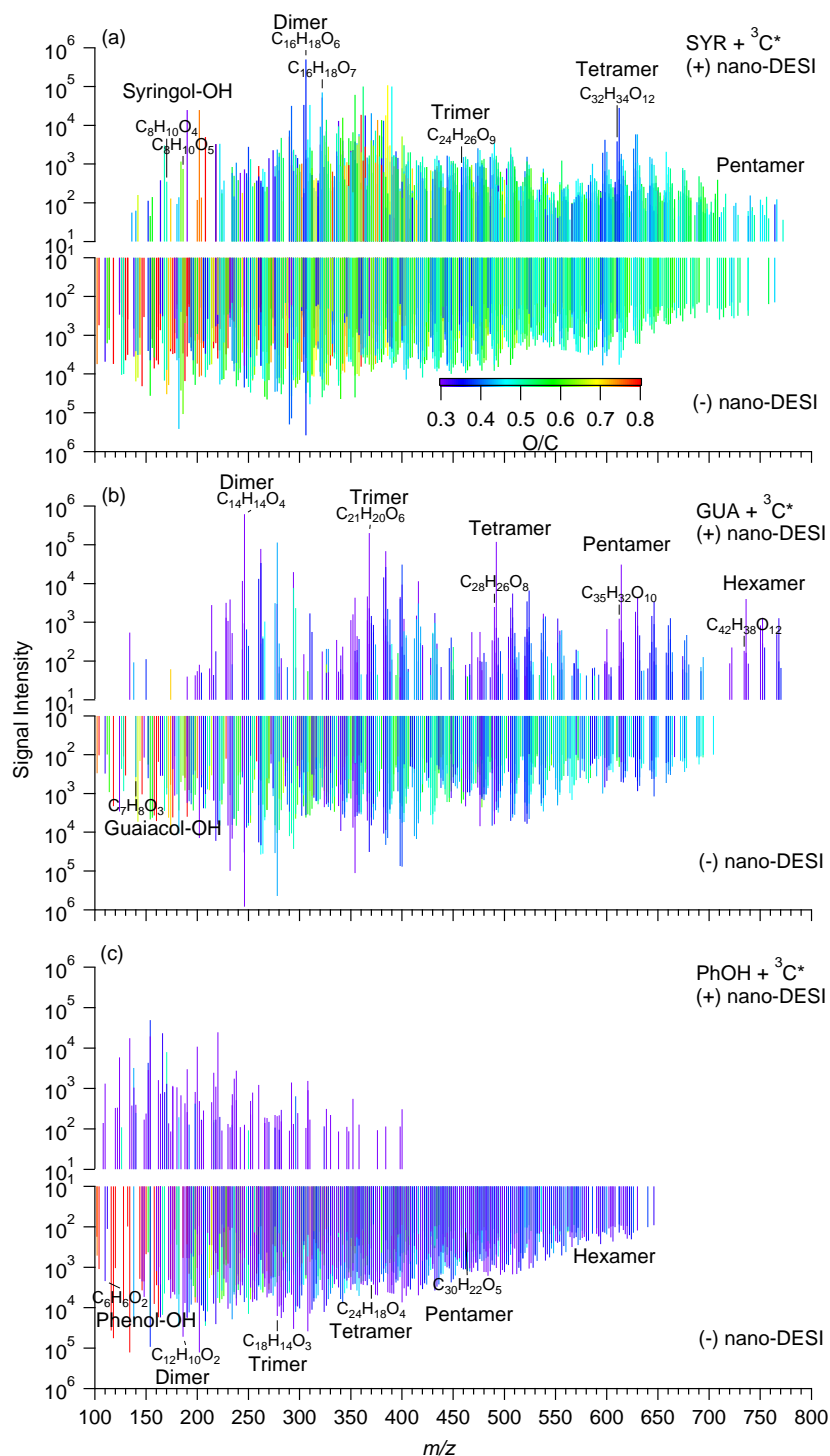
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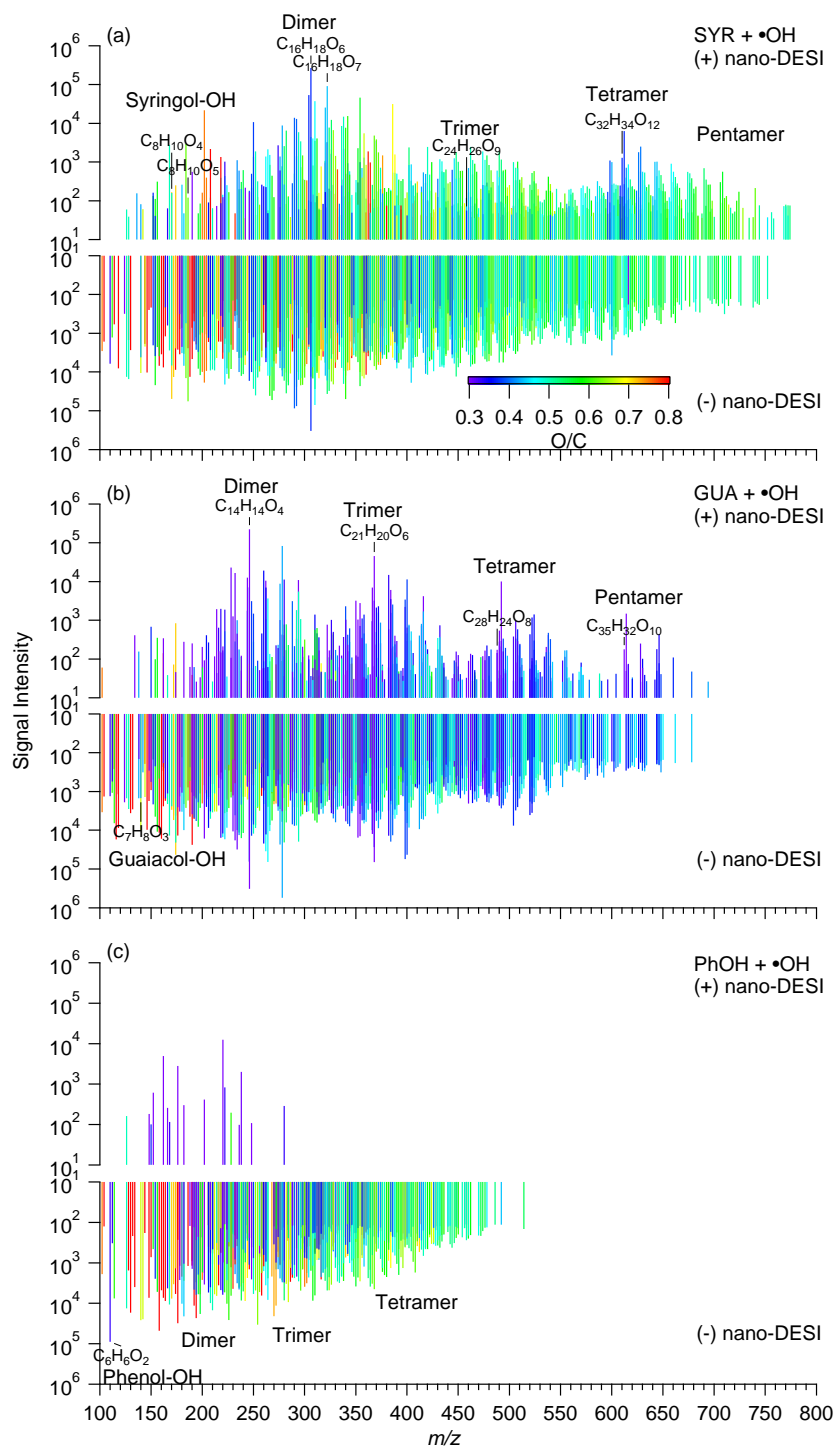
21
22 **Figure S1.** (a-b) HR-AMS spectra of aqSOA formed from the reactions of syringol (SYR)
23 with $^3\text{C}^*$ analyzed at room temperature ($T = 25\text{ }^\circ\text{C}$) and after a thermodenuder set at $T = 40\text{ }^\circ\text{C}$.
24 The peaks are color-coded according to four ion categories: 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.



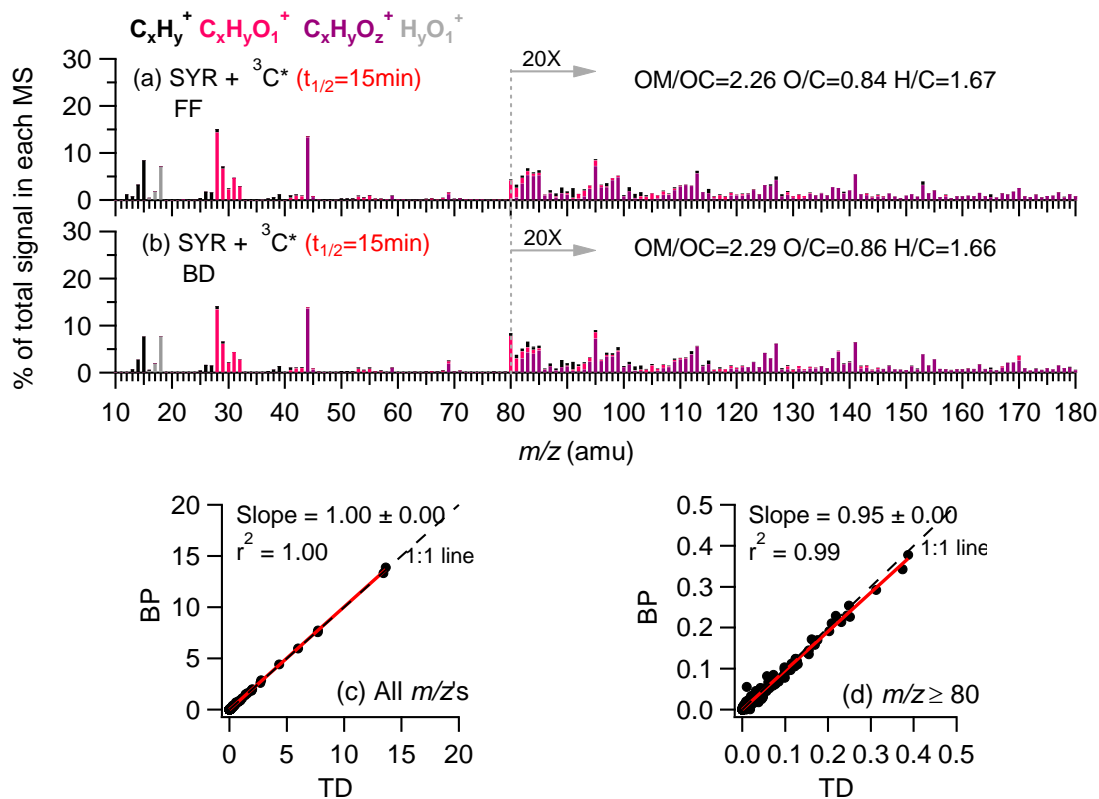
30
31 **Figure S2.** Comparison of the reconstructed masses of phenolic aqSOA products
32 (=TOC×OM/OC) versus their masses measured by gravimetric analysis. TOC was measured by
33 a total carbon analyzer and OM/OC was determined by the HR-AMS. The linear fit was
34 performed using an orthogonal distance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



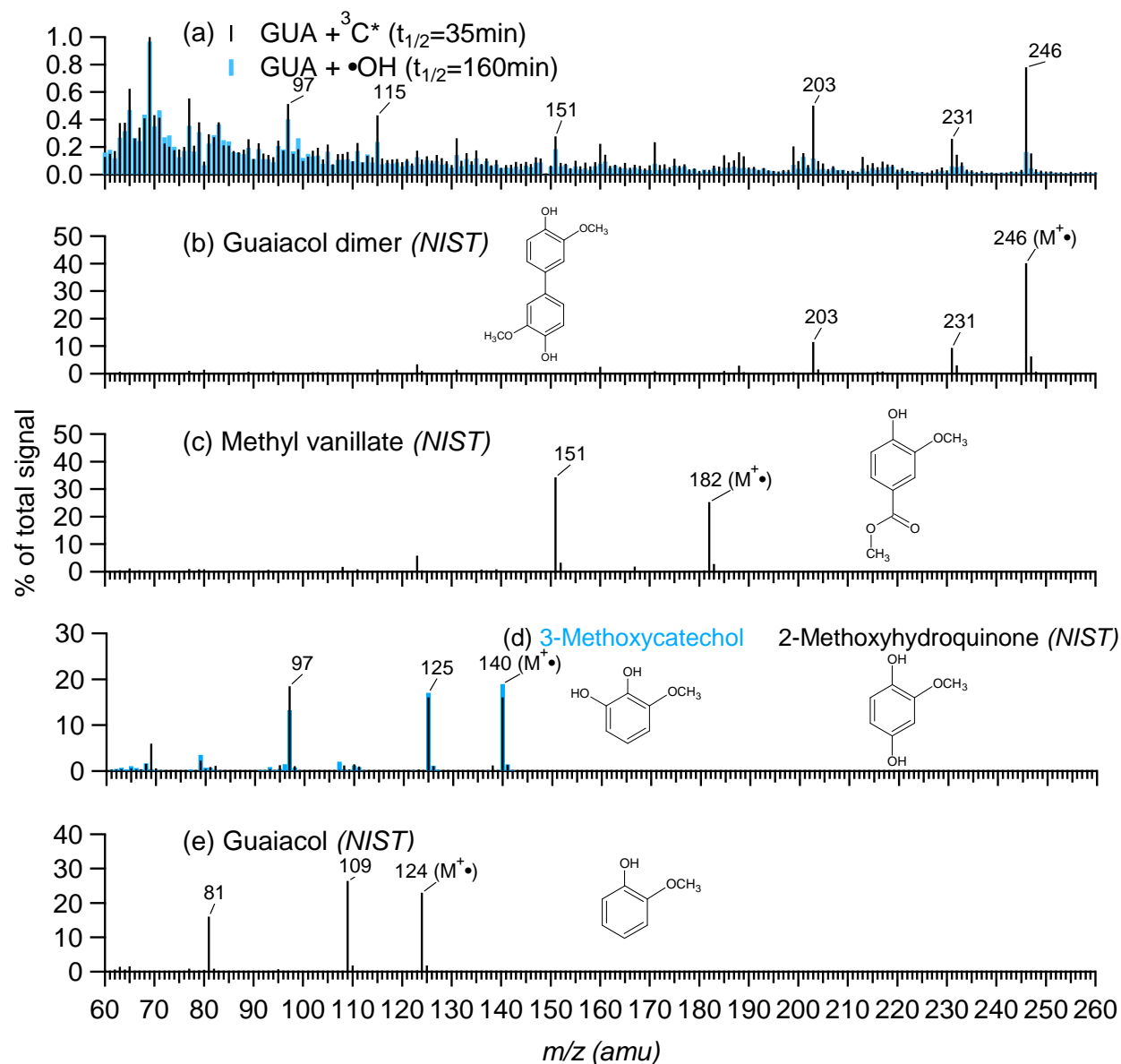
35
 36 **Figure S3.** Nano-DESI spectra of (a) syringol, (b) guaiacol and (c) phenol aqSOA
 37 formed from $^3\text{C}^*$ -mediated oxidation. The top graph in each figure is the positive mode spectrum
 38 and the bottom graph is the negative mode spectrum. Each peak represents the signal of a neutral
 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.



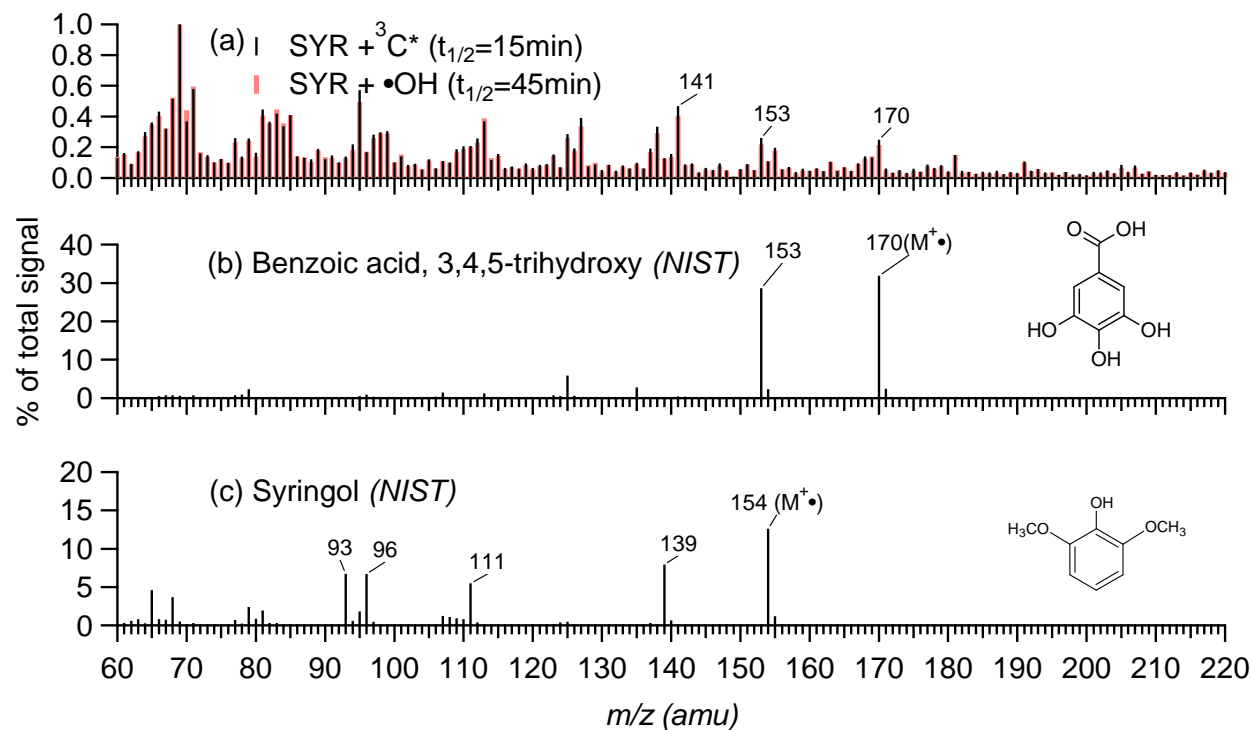
42
 43 **Figure S4.** Nano-DESI spectra of (a) syringol, (b) guaiacol and (c) phenol aqSOA
 44 formed from $\bullet\text{OH}$ -mediated oxidation. The top graph in each figure is the positive mode
 45 spectrum and the bottom graph is the negative mode spectrum. Each peak represents the signal of
 46 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.



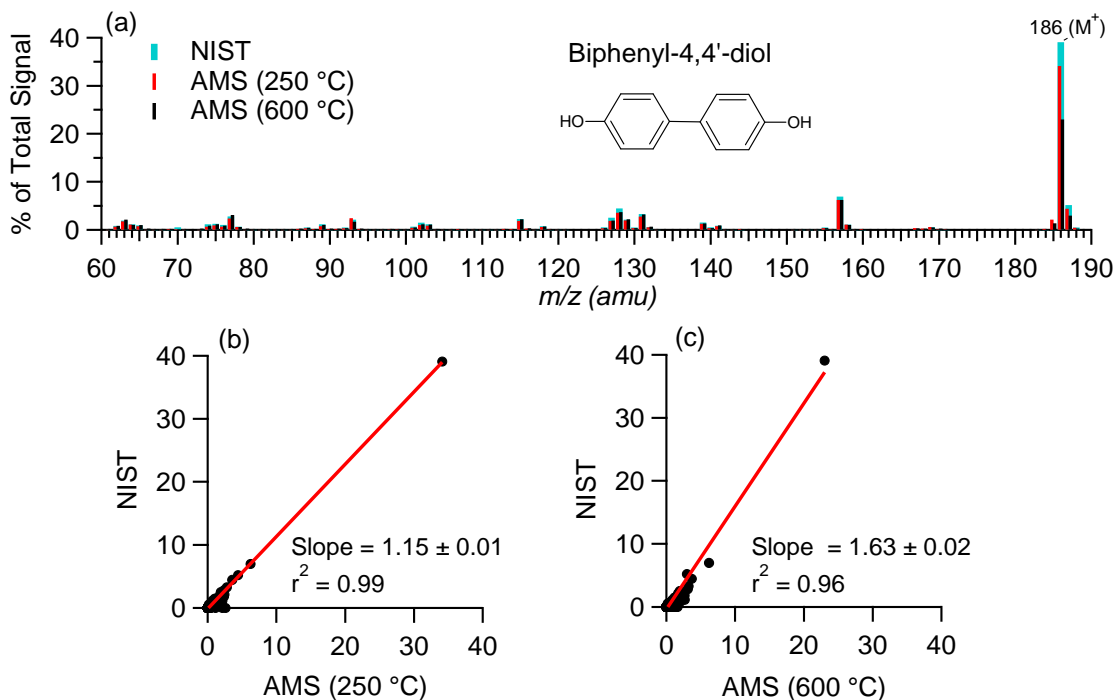
49
 50 **Figure S5.** (a-b) HR-AMS spectra of flash-frozen (FF) and blown-down (BD) samples of
 51 aqSOA formed from the reaction of syringol (SYR) with $^3C^*$. The peaks are color-coded
 52 according to four ion categories: $C_xH_y^+$, $C_xH_yO_1^+$, $C_xH_yO_z^+$, and $H_yO_1^+$ ($x \geq 1$; $y \geq 0$; $z \geq 2$). 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.



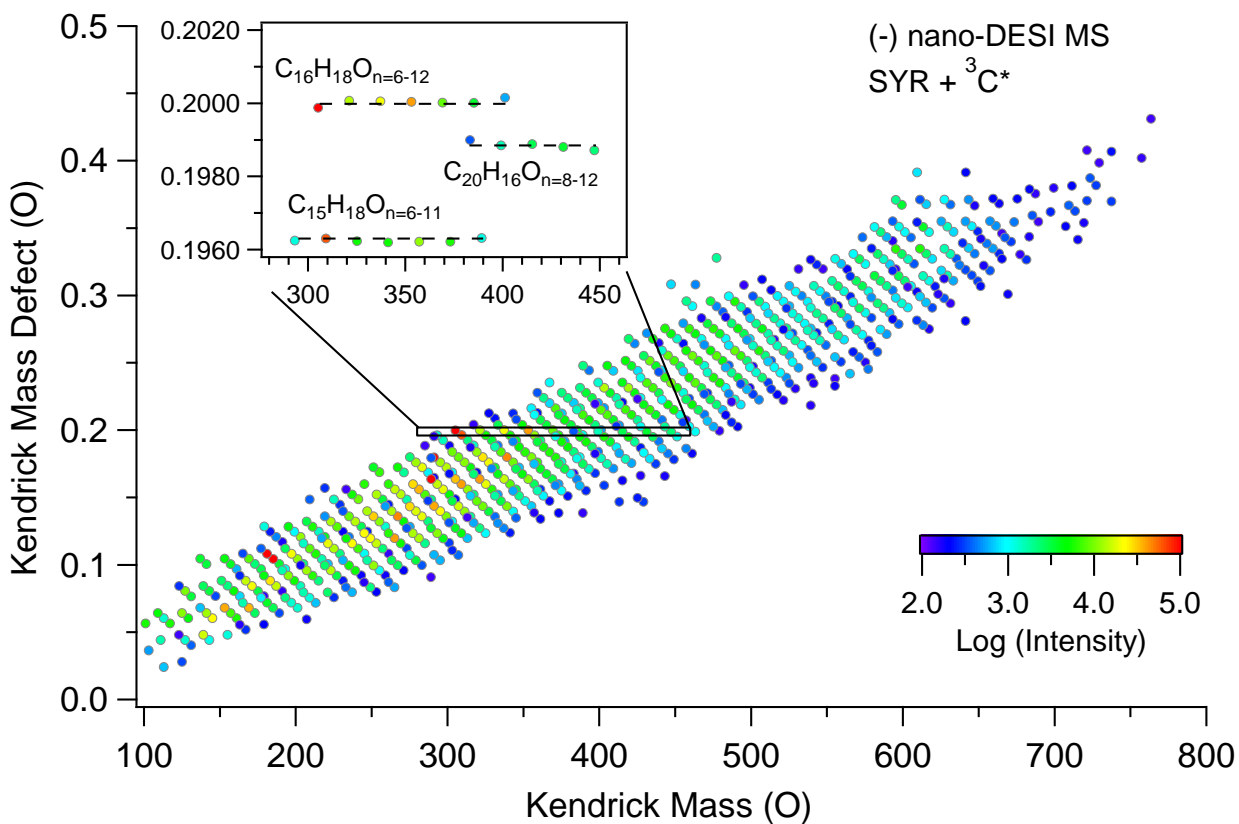
57
 58 **Figure S6.** Comparisons between (a) the HR-AMS mass spectra (in integer m/z) of
 59 guaiacol aqSOA formed via reactions with $^3\text{C}^*$ and $\bullet\text{OH}$, respectively, and the NIST mass
 60 spectra of (b) guaiacol dimer, (c) methyl vanillate, (d) 3-methoxycatechol and 2-
 61 methoxyhydroquinone,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

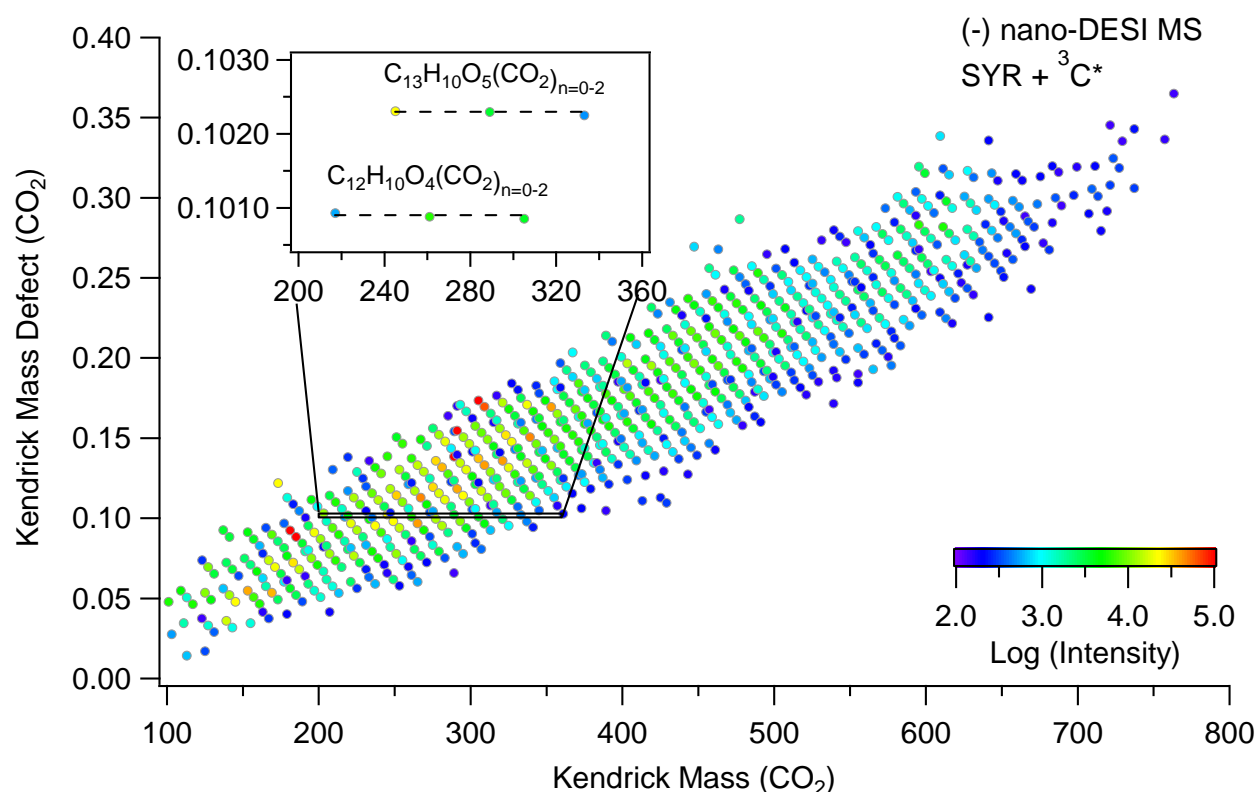


68
 69 **Figure S8.** (a) shows the comparisons of the NIST mass spectrum of biphenyl-4,4'-diol
 70 with the HR-AMS mass spectra acquired at both higher vaporizer temperature (~ 600 °C) and
 71 lower temperature (~ 250 °C). (b-c) show the scatter plots. The linear regression slopes and
 72 correlation 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 ³C* 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 + DMG aqSO ₄ (Nano-DESI)				Syringol + OH aqSO ₄ (Nano-DESI)				Galualcol + DMG aqSO ₄ (Nano-DESI)				Galualcol + OH aqSO ₄ (Nano-DESI)				Phenol + DMG aqSO ₄ (Nano-DESI)				Phenol + OH aqSO ₄ (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	Accurate m/z	Intensity	Formula	DBE
256.019	1065.69	C ₁₁ H ₁₆ O ₈	7	266.079	1247.47	C ₁₃ H ₁₈ O ₈	7	296.018	240.718	C ₁₄ H ₂₀ O ₈	7	248.031	588.72	C ₁₁ H ₁₆ O ₈	7	258.079	160.194	C ₁₁ H ₁₆ O ₈	7	270.037	2094.65	C ₁₃ H ₁₈ O ₈	7	270.037	2094.65	C ₁₃ H ₁₈ O ₈	7
256.583	10535.6	C ₁₁ H ₁₆ O ₇	6	268.029	2688.89	C ₁₃ H ₁₈ O ₇	6	296.532	4468.39	C ₁₄ H ₂₀ O ₇	6	248.032	351.311	C ₁₁ H ₁₆ O ₇	6	258.082	1009.91	C ₁₁ H ₁₆ O ₇	6	270.038	3492.08	C ₁₃ H ₁₈ O ₇	6	270.038	3492.08	C ₁₃ H ₁₈ O ₇	6
256.946	6400.74	C ₁₁ H ₁₆ O ₆	5	272.036	5273.36	C ₁₃ H ₁₈ O ₆	5	296.886	3380.36	C ₁₄ H ₂₀ O ₆	5	248.033	480.265	C ₁₁ H ₁₆ O ₆	5	258.091	2028.76	C ₁₁ H ₁₆ O ₆	5	270.039	1446.2	C ₁₃ H ₁₈ O ₆	5	270.039	1446.2	C ₁₃ H ₁₈ O ₆	5
258.079	3342.09	C ₁₁ H ₁₆ O ₅	4	276.043	3812.07	C ₁₃ H ₁₈ O ₅	4	297.447	1462.22	C ₁₄ H ₂₀ O ₅	4	250.047	1215.8	C ₁₁ H ₁₆ O ₅	4	260.084	2775.88	C ₁₁ H ₁₆ O ₅	4	272.044	982.87	C ₁₃ H ₁₈ O ₅	4	272.044	982.87	C ₁₃ H ₁₈ O ₅	4
258.613	192.67	C ₁₁ H ₁₆ O ₄	3	277.079	3017.4	C ₁₃ H ₁₈ O ₄	3	298.088	1937.93	C ₁₄ H ₂₀ O ₄	3	250.088	694.774	C ₁₁ H ₁₆ O ₄	3	260.108	100.398	C ₁₁ H ₁₆ O ₄	3	272.086	147.864	C ₁₃ H ₁₈ O ₄	3	272.086	147.864	C ₁₃ H ₁₈ O ₄	3
260.033	350.13	C ₁₁ H ₁₆ O ₃	2	278.118	2391.45	C ₁₃ H ₁₈ O ₃	2	300.041	1214.11	C ₁₄ H ₂₀ O ₃	2	250.118	1391.45	C ₁₁ H ₁₆ O ₃	2	260.138	100.398	C ₁₁ H ₁₆ O ₃	2	274.094	232.83	C ₁₃ H ₁₈ O ₃	2	274.094	232.83	C ₁₃ H ₁₈ O ₃	2
260.684	542.118	C ₁₁ H ₁₆ O ₂	1	279.157	1673.53	C ₁₃ H ₁₈ O ₂	1	300.070	1044.05	C ₁₄ H ₂₀ O ₂	1	250.157	786.75	C ₁₁ H ₁₆ O ₂	1	260.157	100.398	C ₁₁ H ₁₆ O ₂	1	274.123	533.309	C ₁₃ H ₁₈ O ₂	1	274.123	533.309	C ₁₃ H ₁₈ O ₂	1
262.014	394.64	C ₁₁ H ₁₆ O	0	279.696	1397.83	C ₁₃ H ₁₈ O	0	300.081	321.712	C ₁₄ H ₂₀ O	0	250.186	879.33	C ₁₁ H ₁₆ O	0	260.186	100.398	C ₁₁ H ₁₆ O	0	274.152	142.6	C ₁₃ H ₁₈ O	0	274.152	142.6	C ₁₃ H ₁₈ O	0
262.025	159.802	C ₁₁ H ₁₆ O	0	279.735	730	C ₁₃ H ₁₈ O	0	300.084	693.75	C ₁₄ H ₂₀ O	0	250.199	262.746	C ₁₁ H ₁₆ O	0	260.199	100.398	C ₁₁ H ₁₆ O	0	274.165	719.208	C ₁₃ H ₁₈ O	0	274.165	719.208	C ₁₃ H ₁₈ O	0
262.877	635.34	C ₁₁ H ₁₆ O	0	279.848	2191.67	C ₁₃ H ₁₈ O	0	300.085	2071.01	C ₁₄ H ₂₀ O	0	250.208	263.56	C ₁₁ H ₁₆ O	0	260.208	100.398	C ₁₁ H ₁₆ O	0	274.176	1183.1	C ₁₃ H ₁₈ O	0	274.176	1183.1	C ₁₃ H ₁₈ O	0
262.888	254.209	C ₁₁ H ₁₆ O	0	279.910	571.09	C ₁₃ H ₁₈ O	0	300.093	419.36	C ₁₄ H ₂₀ O	0	250.219	248.3	C ₁₁ H ₁₆ O	0	260.219	100.398	C ₁₁ H ₁₆ O	0	274.187	1141.17	C ₁₃ H ₁₈ O	0	274.187	1141.17	C ₁₃ H ₁₈ O	0
262.981	613.84	C ₁₁ H ₁₆ O	0	279.981	937.54	C ₁₃ H ₁₈ O	0	300.242	983.96	C ₁₄ H ₂₀ O	0	250.219	336.08	C ₁₁ H ₁₆ O	0	260.219	100.398	C ₁₁ H ₁₆ O	0	274.187	1102.77	C ₁₃ H ₁₈ O	0	274.187	1102.77	C ₁₃ H ₁₈ O	0
264.020	265.97	C ₁₁ H ₁₆ O	0	279.984	786.25	C ₁₃ H ₁₈ O	0	300.268	135.77	C ₁₄ H ₂₀ O	0	250.268	316.39	C ₁₁ H ₁₆ O	0	260.268	100.398	C ₁₁ H ₁₆ O	0	274.187	2466.53	C ₁₃ H ₁₈ O	0	274.187	2466.53	C ₁₃ H ₁₈ O	0
264.024	1393.4	C ₁₁ H ₁₆ O	0	279.989	404.57	C ₁₃ H ₁₈ O	0	300.299	273.71	C ₁₄ H ₂₀ O	0	250.299	273.71	C ₁₁ H ₁₆ O	0	260.299	100.398	C ₁₁ H ₁₆ O	0	274.187	280.29	C ₁₃ H ₁₈ O	0	274.187	280.29	C ₁₃ H ₁₈ O	0
266.003	584.243	C ₁₁ H ₁₆ O	0	279.992	9019.18	C ₁₃ H ₁₈ O	0	304.0219	2159.27	C ₁₄ H ₂₀ O	0	250.376	1288.64	C ₁₁ H ₁₆ O	0	260.376	100.398	C ₁₁ H ₁₆ O	0	274.187	2693.69	C ₁₃ H ₁₈ O	0	274.187	2693.69	C ₁₃ H ₁₈ O	0
266.046	3858.27	C ₁₁ H ₁₆ O	0	279.997	12907.5	C ₁₃ H ₁₈ O	0	304.0583	1117.77	C ₁₄ H ₂₀ O	0	250.378	808.553	C ₁₁ H ₁₆ O	0	260.378	100.398	C ₁₁ H ₁₆ O	0	274.187	3039.62	C ₁₃ H ₁₈ O	0	274.187	3039.62	C ₁₃ H ₁₈ O	0
266.790	15358.7	C ₁₁ H ₁₆ O	0	280.025	225.9	C ₁₃ H ₁₈ O	0	304.0946	286.152	C ₁₄ H ₂₀ O	0	250.479	187.11	C ₁₁ H ₁₆ O	0	260.479	100.398	C ₁₁ H ₁₆ O	0	274.187	134.76	C ₁₃ H ₁₈ O	0	274.187	134.76	C ₁₃ H ₁₈ O	0
268.019	2708.94	C ₁₁ H ₁₆ O	0	280.049	1639	C ₁₃ H ₁₈ O	0	306.0176	4170.68	C ₁₄ H ₂₀ O	0	250.589	227.621	C ₁₁ H ₁₆ O	0	260.589	100.398	C ₁₁ H ₁₆ O	0	274.187	280.65	C ₁₃ H ₁₈ O	0	274.187	280.65	C ₁₃ H ₁₈ O	0
268.083	4530.9	C ₁₁ H ₁₆ O	0	280.096	792.81	C ₁₃ H ₁₈ O	0	306.0739	1768.73	C ₁₄ H ₂₀ O	0	250.618	141.167	C ₁₁ H ₁₆ O	0	260.618	100.398	C ₁₁ H ₁₆ O	0	274.187	882.24	C ₁₃ H ₁₈ O	0	274.187	882.24	C ₁₃ H ₁₈ O	0
268.094	5250	C ₁₁ H ₁₆ O	0	280.176	10337	C ₁₃ H ₁₈ O	0	306.1103	3644.51	C ₁₄ H ₂₀ O	0	250.618	141.167	C ₁₁ H ₁₆ O	0	260.618	100.398	C ₁₁ H ₁₆ O	0	274.187	3053.01	C ₁₃ H ₁₈ O	0	274.187	3053.01	C ₁₃ H ₁₈ O	0
270.076	3431.47	C ₁₁ H ₁₆ O	0	280.279	3544	C ₁₃ H ₁₈ O	0	308.0168	157.837	C ₁₄ H ₂₀ O	0	250.632	945.919	C ₁₁ H ₁₆ O	0	260.632	100.398	C ₁₁ H ₁₆ O	0	274.187	329.46	C ₁₃ H ₁₈ O	0	274.187	329.46	C ₁₃ H ₁₈ O	0
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272.032	4990.89	C ₁₁ H ₁₆ O	0	280.386	22177	C ₁₃ H ₁₈ O	0	310.0325	862.574	C ₁₄ H ₂₀ O	0	250.677	3478.4	C ₁₁ H ₁₆ O	0	260.677	100.398	C ₁₁ H ₁₆ O	0	274.187	1784.06	C ₁₃ H ₁₈ O	0	274.187	1784.06	C ₁₃ H ₁₈ O	0
272.066	1851.51	C ₁₁ H ₁₆ O	0	280.409	1617.03	C ₁₃ H ₁₈ O	0	310.0449	310.449	C ₁₄ H ₂₀ O	0	250.677	3478.4	C ₁₁ H ₁₆ O	0	260.677	100.398	C ₁₁ H ₁₆ O	0	274.187	1784.06	C ₁₃ H ₁₈ O	0	274.187	1784.06	C ₁₃ H ₁₈ O	0
274.025	343.43	C ₁₁ H ₁₆ O	0	280.486	1086.88	C ₁₃ H ₁₈ O	0	312.0481	1166.01	C ₁₄ H ₂₀ O	0	250.677	3478.4	C ₁₁ H ₁₆ O	0	260.677	100.398	C ₁₁ H ₁₆ O	0	274.187	280.65	C ₁₃ H ₁₈ O	0	274.187	280.65	C ₁₃ H ₁₈ O	0
274.047	368.48	C ₁₁ H ₁₆ O	0	280.486	177.178	C ₁₃ H ₁₈ O	0	312.0634	318.93	C ₁₄ H ₂₀ O	0	250.677	3478.4	C ₁₁ H ₁₆ O	0	260.677	100.398	C ₁₁ H ₁₆ O	0	274.187	280.65	C ₁₃ H ₁₈ O	0	274.187	280.65	C ₁₃ H ₁₈ O	0
274.088	1632.53	C ₁₁ H ₁₆ O	0	280.520	176.562	C ₁₃ H ₁₈ O	0	312.0845	2495.76	C ₁₄ H ₂₀ O	0	250.697	408.02	C ₁₁ H ₁₆ O	0	260.697	100.398	C ₁₁ H ₁₆ O	0	274.187	882.24	C ₁₃ H ₁₈ O	0	274.187	882.24	C ₁₃ H ₁₈ O	0
276.020	1370.06	C ₁₁ H ₁₆ O	0	280.581	2975.89	C ₁₃ H ₁₈ O	0	312.0997	316.864	C ₁₄ H ₂₀ O	0	250.697	284.261	C ₁₁ H ₁₆ O	0	260.697	100.398	C ₁₁ H ₁₆ O	0	274.187	882.24	C ₁₃ H ₁₈ O	0	274.187	882.24	C ₁₃ H ₁₈ O	0
276.081	76.8481	C ₁₁ H ₁₆ O	0	280.581	248	C ₁₃ H ₁₈ O	0	314.0419	314.0419	C ₁₄ H ₂₀ O	0	250.697	284.261	C ₁₁ H ₁₆ O	0	260.697	100.398	C ₁₁ H ₁₆ O	0	274.187	882.24	C ₁₃ H ₁₈ O	0	274.187	882		

346.1052				335.211				386.1001				386.1001				334.0888				346.0481				352.0430							
Syringol + DMBA aSOA (Pheno-DESI)				Syringol + DMBA aSOA (Pheno-DESI)				Guaiacol + DMBA aSOA (Pheno-DESI)				Guaiacol + DMBA aSOA (Pheno-DESI)				OH aSOA (Pheno-DESI)				Phenol + DMBA aSOA (Pheno-DESI)				Phenol + OH aSOA (Pheno-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	Accurate m/z	Intensity	Formula	DBE				
348.081	2024.13	C16H12O9	11	360.085	3130.75	C18H16O8	11	388.040	2465.47	C18H12O10	12	334.1052	326.302	C17H14O9	9	346.1052	217.245	C18H16O8	10	352.0583	138.29	C17H14O9	10	352.0583	138.29	C17H14O9	10	352.0583	138.29	C17H14O9	10
348.092	676.566	C16H12O9	11	360.085	3130.75	C18H16O8	11	388.074	337.57	C18H12O10	12	334.1052	100.875	C17H14O9	9	346.1052	134.883	C18H16O8	10	352.0583	249.238	C17H14O9	10	352.0583	249.238	C17H14O9	10	352.0583	249.238	C17H14O9	10
348.094	317.116	C16H12O9	11	360.085	3130.75	C18H16O8	11	388.093	307.227	C18H12O10	12	334.1052	139.665	C17H14O9	9	346.1052	134.883	C18H16O8	10	352.0583	249.238	C17H14O9	10	352.0583	249.238	C17H14O9	10	352.0583	249.238	C17H14O9	10
350.038	4203.84	C16H14O8	10	362.074	157.283	C16H16O10	10	390.057	1357.19	C18H14O10	12	336.085	2132.36	C16H16O10	8	348.034	1088.88	C16H12O10	10	354.0587	288.8	C15H14O10	9	354.0587	288.8	C15H14O10	9	354.0587	288.8	C15H14O10	9
350.101	4903.58	C17H18O8	9	362.074	426.156	C16H14O10	10	390.057	1913.47	C18H14O10	12	336.085	170.117	C16H16O10	10	348.045	1200.12	C17H16O10	10	354.0587	203.55	C15H14O10	9	354.0587	203.55	C15H14O10	9	354.0587	203.55	C15H14O10	9
351.330	141.13	C16H14O8	10	362.074	157.283	C16H16O10	10	390.057	1357.19	C18H14O10	12	336.085	2132.36	C16H16O10	10	348.045	1200.12	C17H16O10	10	354.0587	203.55	C15H14O10	9	354.0587	203.55	C15H14O10	9	354.0587	203.55	C15H14O10	9
352.074	6304.77	C16H16O9	9	362.084	906.111	C14H18O11	6	392.074	876.883	C18H16O10	12	338.074	2744.87	C19H14O6	13	350.074	302.763	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
354.0587	1086.15	C15H14O10	9	362.100	2804.58	C18H16O10	10	394.056	185.211	C17H14O11	11	398.101	250.87	C18H16O10	8	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
354.059	3882.4	C15H16O10	9	364.030	604.521	C16H12O10	11	394.090	212.045	C18H16O10	12	398.154	587.036	C18H16O10	10	350.074	364.2	C16H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
355.080	92.888	C16H12O11	9	364.042	371.808	C18H16O10	10	396.081	280.702	C18H16O10	12	401.114	175.299	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
355.074	1007.8	C16H16O10	8	364.074	494.521	C17H16O10	10	396.082	110.859	C18H16O10	10	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
356.107	851.444	C16H20O8	7	364.158	2126.73	C18H16O10	10	396.085	883.58	C18H16O10	10	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
358.025	170.764	C17H10O9	13	366.057	2147.45	C16H14O10	10	398.074	1751.86	C19H16O10	15	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
358.036	729.02	C16H12O11	11	366.058	1398.54	C18H16O10	10	398.074	1751.86	C19H16O10	15	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
358.068	654.209	C18H14O8	12	368.030	213.089	C15H12O11	10	398.101	2139.63	C19H16O10	15	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
358.090	1127.2	C15H18O10	7	368.073	703.82	C18H16O10	10	400.040	2159.84	C19H16O10	14	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
358.152	392.502	C18H16O10	11	368.110	550.637	C17H20O9	8	400.074	575.43	C19H16O10	14	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
360.081	1096.83	C17H12O9	12	370.056	3699.77	C15H14O10	9	400.158	7086.7	C19H16O10	12	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
360.092	6432.25	C18H16O10	7	370.090	876.75	C16H16O10	10	402.023	225.491	C18H16O10	10	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
360.085	3284.86	C18H16O10	11	372.081	245.76	C18H16O10	10	402.023	225.491	C18H16O10	10	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
360.156	220.147	C15H16O10	10	372.092	497.63	C15H16O10	10	402.023	225.491	C18H16O10	10	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
360.128	305.66	C16H12O11	9	374.042	1398.54	C18H16O10	10	402.023	225.491	C18H16O10	10	402.023	225.491	C18H16O10	10	350.074	194.396	C15H16O10	9	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10	354.0587	172.77	C15H16O10	10
362.074	222.155	C16H16O10	10	372.056	551.92	C16H16O10	10	404.080	748.65	C18H16O10	11	404.080	748.65	C18H16O10	11	346.088	36.29	C17H14O9	11	358.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
362.085	284.72	C15H14O10	7	374.045	707.836	C18H16O10	10	404.080	748.65	C18H16O10	11	404.080	748.65	C18H16O10	11	346.088	36.29	C17H14O9	11	358.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
362.078	81.28	C17H14O10	11	374.045	707.836	C18H16O10	10	404.080	748.65	C18H16O10	11	404.080	748.65	C18H16O10	11	346.088	36.29	C17H14O9	11	358.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
362.084	2216.39	C14H18O11	6	374.049	662.42	C15H18O11	7	406.056	660.184	C18H16O10	11	406.056	660.184	C18H16O10	11	346.088	36.29	C17H14O9	11	358.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
362.101	3078.37	C18H16O10	8	374.100	3062.9	C18H16O10	11	406.090	764.263	C18H16O10	11	406.090	764.263	C18H16O10	11	348.081	345.97	C16H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
364.040	906.056	C16H16O10	10	376.040	647.085	C17H12O10	12	408.062	201.662	C18H16O10	11	408.062	201.662	C18H16O10	11	348.085	238.68	C17H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
364.074	558.35	C17H16O10	10	376.049	327.19	C16H16O10	10	408.085	197.881	C18H16O10	11	408.085	197.881	C18H16O10	11	350.074	292.58	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
364.158	554.158	C16H16O10	10	376.074	438.409	C18H16O10	10	410.089	438.409	C18H16O10	11	410.089	438.409	C18H16O10	11	350.074	292.58	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10	360.081	1859.65	C18H16O10	10
366.057	378.99	C16H16O10	10	376.105	1206.22	C15H16O10	10	410.089	438.409	C18H16O10	11	410.089	438.409	C18H16O10	11	350.074															

434.1212 8566.18 C21H2010 11				442.1111 485.234 C19H2012 9				486.0798 286.245 C23H18012 15				422.0485 158.87 C18H14012 12				424.1158 652.102 C23H2008 14			
Symyx® - DMW aqSO4 (f) Nano-DES				Symyx® - OH aqSO4 (f) Nano-DES				Guaiacol - DMW aqSO4 (f) Nano-DES				Guaiacol - 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	C19H16012	12	442.263	347.053	C23H2209 13		488.0591	237.931	C23H18012	15	422.0638	275.719	C21H1409 16		426.0887	930.45	C21H14010 15	
436.1005	7236.18	C21H2010	11	442.263	347.053	C23H2209 13		488.0743	693.841	C23H18012	15	422.0869	104.271	C21H14011 11		426.0950	1634.33	C21H14009 14	
436.1389	189.97	C21H2010	11	444.0592	105.44	C23H2010 12		488.1001	483.954	C23H18012	15	423.1001	645.453	C21H14011 11		426.1187	643.818	C21H14009 14	
438.0434	315.23	C18H14013	12	444.0904	384.861	C18H14013 12		488.1107	299.34	C27H2009 17		424.0430	134.219	C21H14010 10		428.0380	277.883	C20H12011 11	
438.0798	3731.59	C19H18012	11	444.1056	443.896	C22H2010 13		488.1470	119.353	C28H2408 17		424.0774	1002.93	C21H14010 10		428.0532	112.582	C21H14008 14	
438.1163	734.1430	C21H2010	11	444.1430	384.861	C22H2010 13		488.1576	268.87	C28H2408 17		424.0930	129.727	C21H14011 11		428.0686	1158.99	C21H14010 10	
440.0591	435.062	C19H18012	11	446.0485	134.696	C20H14012 14		490.1627	622.06	C28H2408 17		424.1158	585.663	C23H2008 14		428.0896	570.995	C25H1607 18	
440.0954	2817.73	C19H18012	11	446.0849	4210.79	C21H14011 11		492.0329	131.258	C28H2408 17		426.0587	712.528	C21H14010 10		428.1107	173.144	C20H14009 14	
442.1037	361.214	C23H2009 13		446.1060	141.381	C18H14013 12		492.0692	444.726	C25H1607 18		426.0950	1166.94	C21H14010 10		428.1259	311.355	C26H2006 17	
440.1318	184.987	C21H2010	11	446.1272	6079.89	C22H2010 13		492.1260	268.87	C26H2010 13		428.0380	129.727	C21H14011 11		430.0536	135.833	C20H14011 11	
442.0536	718.935	C21H14011 11		446.0642	1478.75	C21H14012 12		492.1420	1625.88	C27H2409 17		428.0743	2188.22	C21H14010 10		430.0688	1098.29	C21H14008 14	
442.0747	444.853	C18H14013 12		448.1005	1311.65	C21H14011 11		494.0485	198.91	C24H14012 12		428.1107	556.856	C21H14010 10		430.0900	676.847	C21H14010 10	
442.0900	942.549	C22H18012 12		448.1369	314.54	C22H2010 13		494.0849	314.54	C25H1607 18		430.0536	1265.76	C21H14011 11		430.1052	625.528	C25H1807 17	
442.1163	838.24	C23H2010 13		450.0904	122.43	C21H14011 11		494.1128	2056.31	C27H2409 17		430.0900	626.468	C21H14010 10		432.0262	338.57	C20H14011 11	
442.1263	1303.77	C23H2010 13		450.1162	7545.13	C21H14011 11		494.1576	869.896	C27H2409 17		432.0262	1486.8	C20H14011 11		432.0485	375.02	C24H1608 17	
444.0239	175.917	C21H2010 11		452.0591	652.18	C21H14012 12		496.0642	569.089	C28H2408 17		432.1056	2093.31	C21H14010 10		432.1056	295.084	C21H14010 10	
444.0292	189.046	C21H2010 11		452.0954	989.39	C20H14012 14		496.1005	1285.36	C25H1607 18		434.0485	300.901	C19H14013 13		432.1208	96.3604	C25H2007 16	
444.1056	6184.86	C21H2010 11		452.1338	1322.8	C21H14011 11		496.1369	800.249	C26H2010 13		434.0638	221.607	C21H14009 14		434.0485	97.8255	C20H14012 12	
444.1420	5660.09	C21H2010 11		454.0747	1483.46	C19H18012 11		498.0434	120.87	C23H18012 15		434.0849	1923.19	C21H14011 11		434.0849	198.395	C20H14011 11	
446.0485	454.023	C20H14012 14		454.0904	296.044	C23H18012 15		498.0798	477.654	C24H14012 12		434.1001	374.712	C21H14010 10		434.1001	3037.67	C24H1808 17	
446.0849	508.721	C21H18013 13		454.1111	2184.54	C20H14012 14		498.1162	429.125	C24H14012 12		434.1212	410.312	C21H14010 10		434.0974	248.98	C21H14009 14	
446.1212	1383	C21H2010 11		456.0904	1467.26	C19H18012 11		500.0904	178.75	C21H14011 11		436.0485	189.57	C21H14010 10		434.1005	93.9075	C20H14011 11	
448.042	2118.04	C20H14012 14		456.0904	1467.26	C19H18012 11		500.0904	301.626	C21H14011 11		436.0642	291.864	C21H14010 10		436.1158	536.904	C24H2008 15	
448.1005	9991.63	C21H2010 11		456.1056	696.196	C23H2010 14		502.0747	124.314	C23H18012 15		436.0794	487.883	C21H14010 10		438.0587	1392.02	C21H14010 10	
448.1369	424.845	C21H2010 11		456.1267	134.653	C21H14012 12		504.0849	141.807	C21H14011 11		438.0587	694.086	C21H14011 11		438.0590	1513.77	C21H14009 14	
448.1732	758.236	C21H2010 11		458.0485	309	C21H14012 12		504.0904	100.375	C23H2010 14		438.1158	754.51	C24H2008 15		438.1103	419.776	C21H14010 10	
450.0434	294.29	C19H18012 11		458.0696	346.763	C18H14014 10		504.1420	176.621	C21H14011 11		438.0587	424.346	C21H14010 10		440.0380	150.904	C21H14011 11	
450.0798	5394.06	C20H18012 12		458.0849	1600.05	C22H18012 12		506.0333	134.847	C21H14011 11		438.0798	130.056	C21H14010 10		440.0743	1455.99	C22H18012 12	
450.1162	6813.26	C21H2010 11		458.1060	372.288	C21H14012 12		506.0849	1600.29	C21H14011 11		438.0900	596.185	C21H14010 10		440.0896	293.611	C21H14009 14	
452.0591	612.691	C21H2010 11		458.1369	226.879	C21H14012 12		506.1162	179.203	C21H14011 11		438.1144	309.451	C21H14010 10		440.1259	470.373	C21H14008 14	
452.0954	5806.55	C21H2010 11		458.1576	385.995	C24H2009 15		506.1576	533.65	C21H14011 11		440.0380	230.925	C21H14011 11		440.1259	270.373	C21H14008 14	
452.1318	1427.54	C21H2010 11		460.0642	857.471	C21H14012 12		508.0642	462.458	C25H1607 18		440.0743	1292.91	C21H14010 10		442.0336	415.704	C21H14011 11	
454.0747	1228.24	C21H2010 11		460.1005	358.25	C21H14012 12		508.1162	189.203	C21H14011 11		440.1107	413.199	C21H14010 10		442.0485	179.885	C21H14010 10	
454.1111	2818.21	C21H2010 11		460.1369	1554.89	C23H2010 14		508.1369	3377.8	C21H14011 11		442.0384	168.028	C17H14014 10		442.0900	939.57	C23H18012 15	
456.0692	321.513	C22H16013 13		462.0434	125.84	C20H14012 14		510.0434	173.839	C21H14011 11		442.0536	380.405	C21H14011 11		442.1052	754.746	C26H1807 18	
456.0904	1203.85	C19H18012 11		462.0798	3140.03	C21H14012 12		510.0798	1842.96	C21H14012 12		442.0900	1330.9	C21H14010 10		444.0692	498.252	C21H14011 11	
456.1056	171.598	C21H2010 11		462.1005	122.43	C21H14012 12		510.1162	331.161	C21H14011 11		442.1107	413.199	C21H14010 10		444.0849	1055.89	C21H14011 11	
456.1267	236.153	C20H14012 14		462.1525	613.763	C21H14010 10		510.1525	1014.97	C21H14011 11		444.1056	617.427	C21H14010 10		444.1056	141.071	C22H2010 13	
456.1420	531.598	C24H2009 15		464.0591	868.309	C20H14012 14		512.0591	556.781	C21H14011 11		446.0485	238.548	C20H14012 12		444.1208	316.564	C26H2007 16	
458.0485	467.69	C21H14012 12		464.0954	613.07	C21H14012 12		512.0954	1002.62	C21H14011 11		446.0849	1162.66	C21H14011 11		446.0485	100.488	C20H14012 12	
458.0849	801.801	C21H14012 12		464.1369	2628.67	C21H14012 12		514.1111	487.279	C21H14011 11		446.1107	212.749	C21H14010 10		446.0692	1076.74	C21H14011 11	
458.0904	2576.03	C21H14012 12		464.0747	2357.38	C20H14012 14		514.0747	398.127	C21H14011 11		446.1212	163.84	C21H14010 10		446.0849	326.972	C21H14011 11	
458.1212	5241.35	C21H2010 11		466.1111	6123.48	C21H14012 12		514.1111	326.225	C21H14011 11		448.0642	614.055	C20H14012 12		446.1001	933.868	C23H1808 17	
458.1576	2050.56	C24H2009 15		468.0849	2100.55	C21H14012 12		516.0849	113.253	C21H14011 11		448.0798	480.871	C24H2009 15		448.0485	293.611	C21H14009 14	
460.0642	1004.4	C18H14014 10		468.1060	2339.64	C21H14012 12		518.0485	188.044	C21H14011 11		448.1005	989.427	C21H14010 10		448.1158	395.588	C21H14010 10	
460.0849	326.033	C18H14014 10		468.1056	958.205	C24H2009 15		518.0849	110.702	C21H14011 11		448.1158	684.286	C23H2008 14		448.1158	395.588	C21H14010 10	
460.1005	5414.05	C21H2010 11		468.1267	952.072	C21H14012 12		520.0642	502.612	C21H14011 11		450.0587	210.084	C21H14010 10		450.0590	1998.47	C24H1808 17	
460.1369	6321.76	C21H2010 11		468.1576	182.787	C21H14012 12		520.1005	1712.12	C21H14									

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	231.92	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	196.415	C32H28O16	21				
682.1170	286.691	C32H30O17	20				
684.1326	182.205	C32H28O17	19				
684.1690	204.781	C33H32O16	18				
686.1482	364.976	C32H30O17	19				
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	C36H30O18	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