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Relationship between the molecular composition, visible light absorption, and health-related properties of smoldering woodsmoke aerosols

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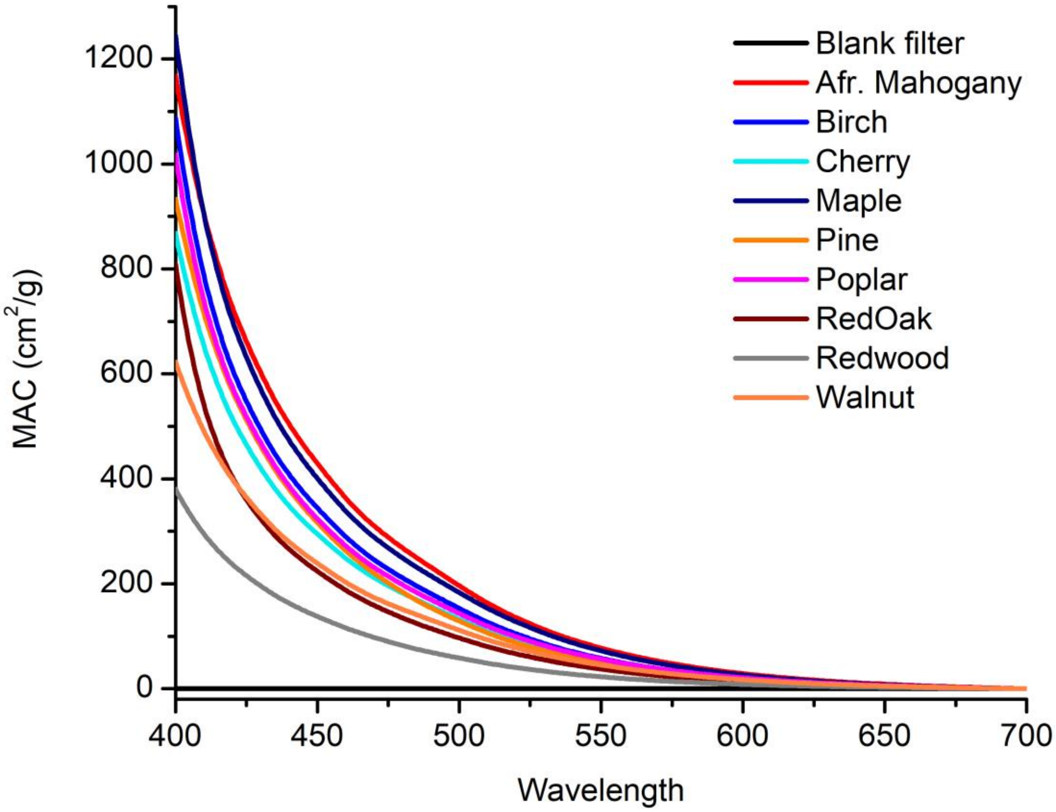

Figure S1: Visible light absorption spectra of WSA extracts.

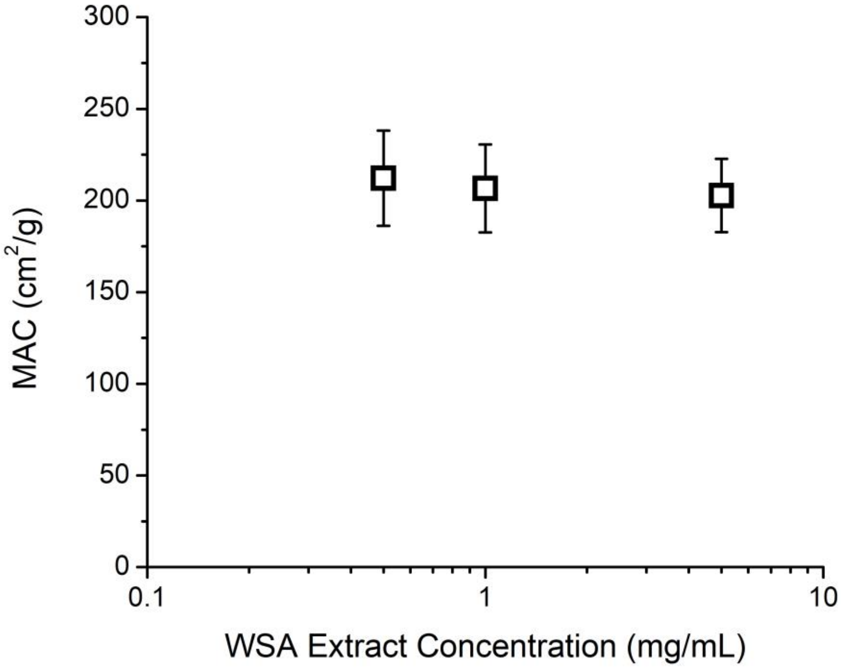

Figure S2: Visible-light mass absorption coefficient of aqueous extract of WSA.

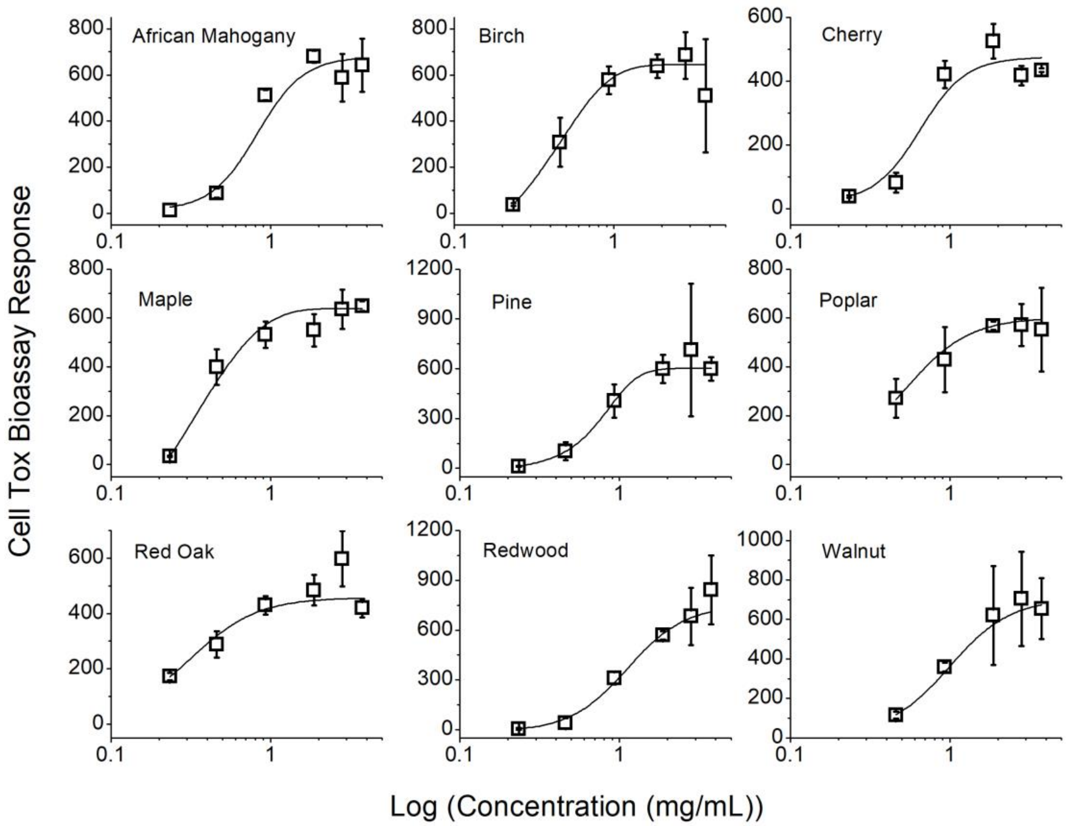

Figure S3: Concentration-response curves for WSA samples in the cell toxicity bioassay. Errors represent standard deviation (±SD) of triplicate determinations. In the case of repeated trials at the same concentration, the error in the average value for n=2 is $(z = 0.5(x+y))$ is propagated as $\sigma_z = 0.5\sqrt{(\sigma_x^2 + \sigma_y^2)}$, where σ_x and σ_y are ±SD%.

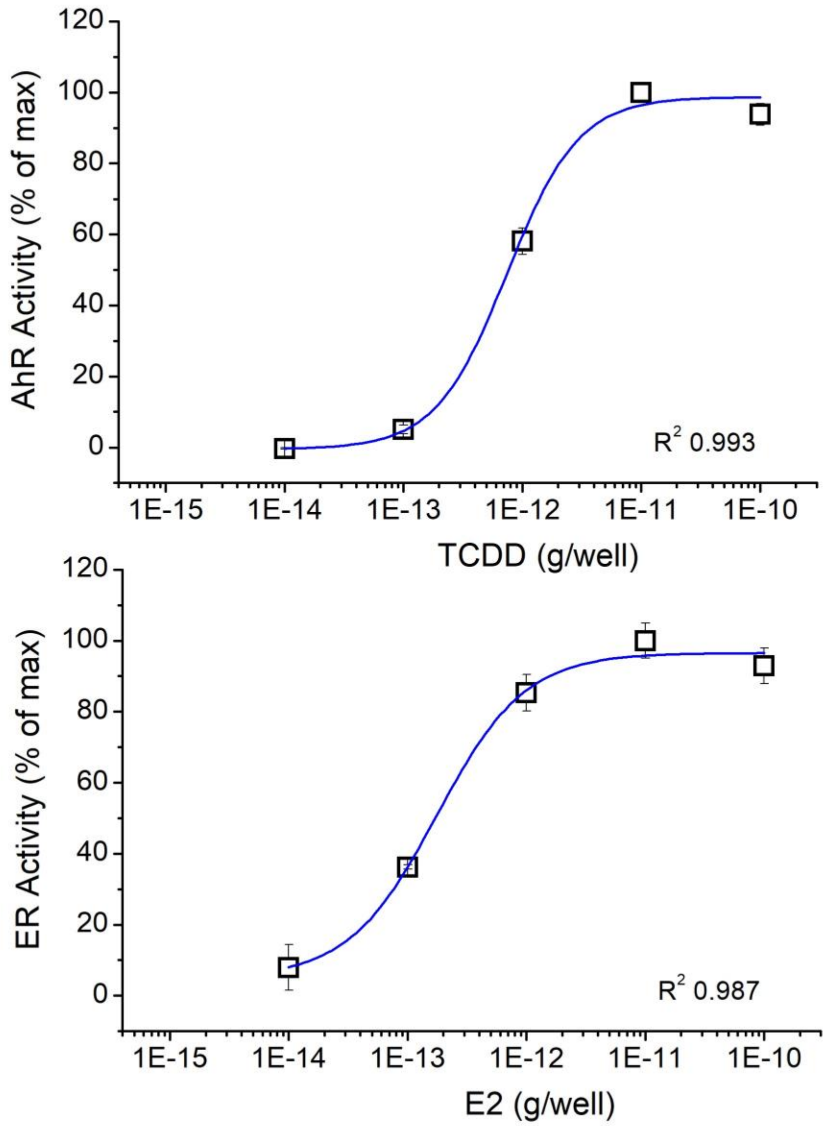

Figure S4: Concentration-response curves for (top) 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD)- and (bottom) 17β-estradiol (E2)-inducible luciferase reporter gene activity in AhR and ER cell bioassays, respectively. Values represent the mean ± SD of triplicate determinations.

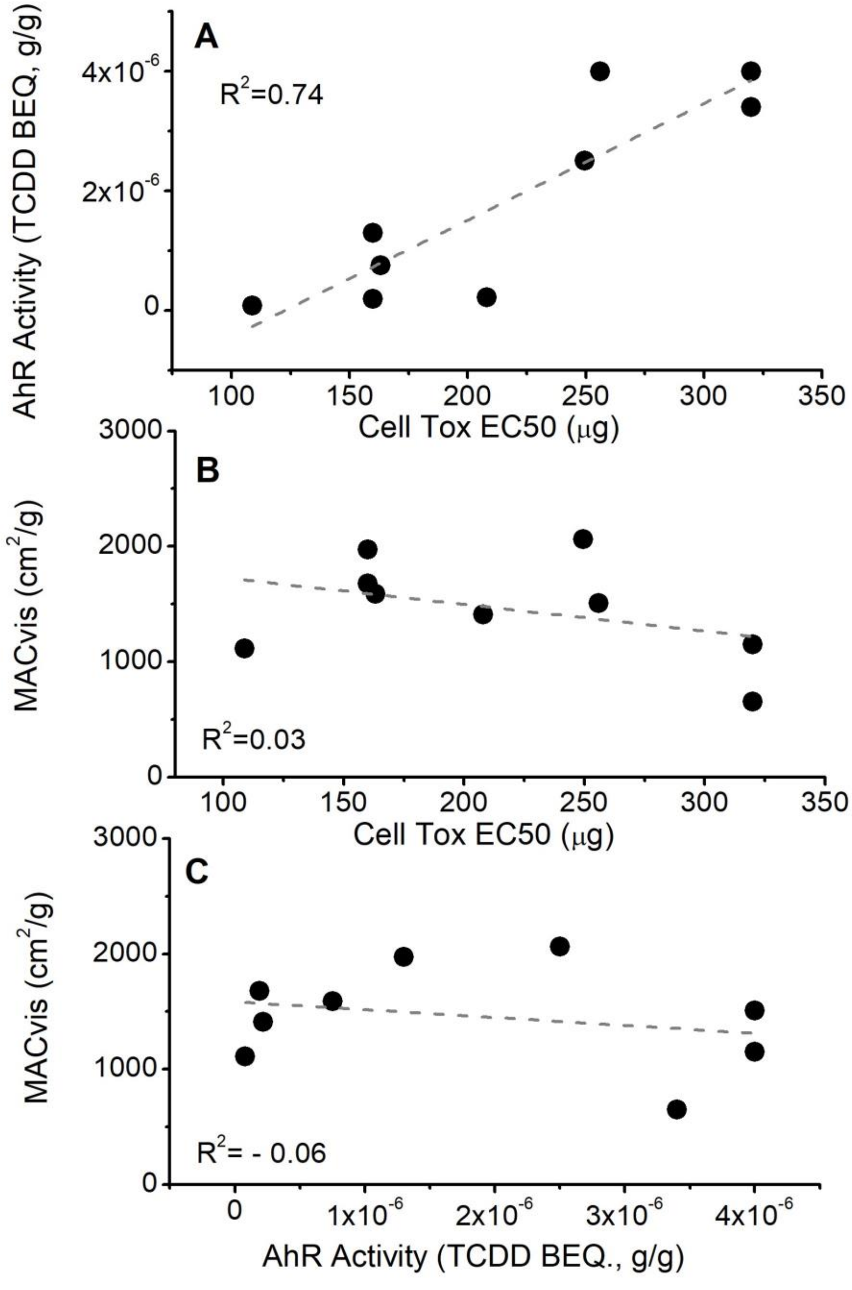

Figure S5: Relationships between visible light absorption and biological activity.

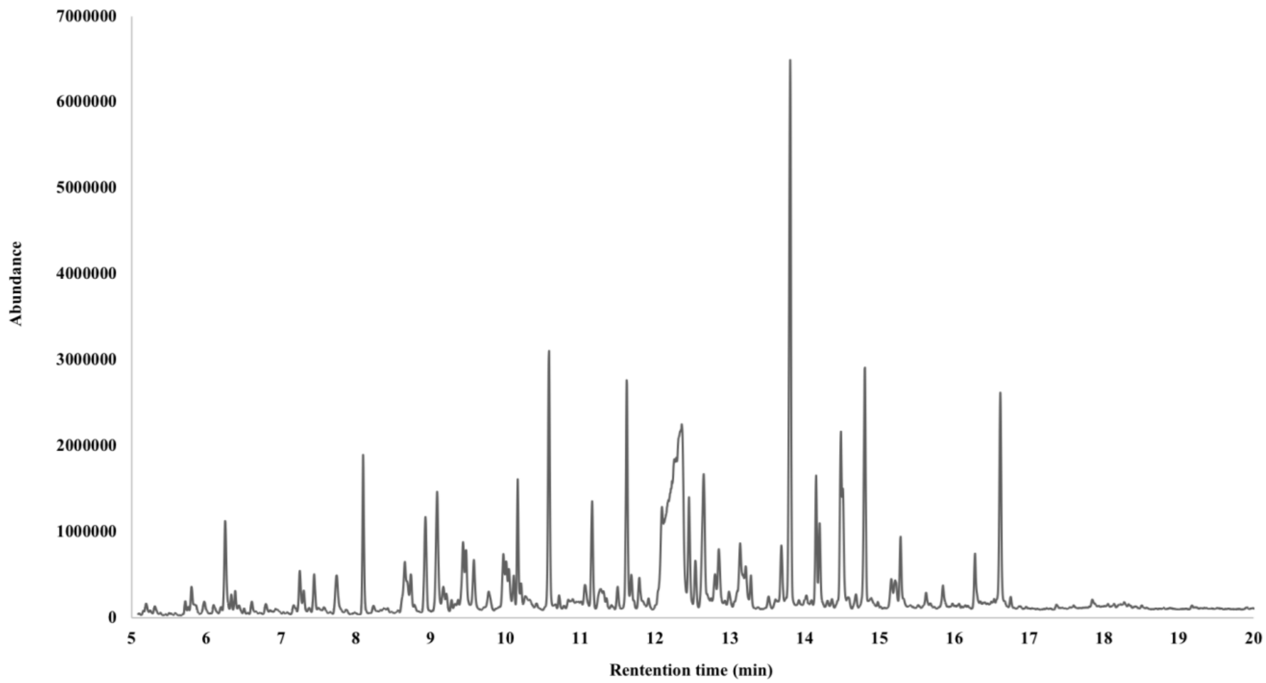

Figure S6: Representative GC-MS chromatogram (shown for Birch WSA). Unresolved peaks at ~12 minutes are from the levoglucosan and other sugar anhydrides.

Table S1: GC-MS analysis of the more volatile less polar chemical constituents of smoldering woodsmoke aerosols for the 9 wood types. Assignments are based on electron-ionization fragmentation and comparison with the NIST GC-MS library.

Compound Name	**Afr. Mahog.**	**Birch**	**Cherry**	**Pine**	**Poplar**	**Red Oak**	**Redwood**	**Walnut**
2-methoxy-4-(1-propenyl)-Phenol	●	●	●	●	●	●	●	●
2-methoxy-Phenol (Guaiacol)		●	●	●	●	●	●	●
4-hydroxy-3-methoxy-Benzoic acid		●	●		●	●		●
4-Isopropyl-1,3-cyclohexanedione		●	●		●	●	●	●
D-Allose		●	●	●			●	●
1-(2,4,6-trihydroxyphenyl)2-Pentanone		●				●		
1-(4-hydroxy-3-methoxyphenyl)-Ethanone	●			●	●	●		
1-(4-hydroxy-3,5-dimethoxyphenyl)-Ethanone	●	●	●		●	●		●
1-butyl-2-propyl-Cyclopentane			●					●
1,2-Benzenediol			●		●	●		
1,2-Cyclopentanedione	●			●				
1,3-bis(1,1-dimethylethyl)-Benzene			●	●	●	●	●	●
1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	●	●	●	●	●	●	●	●
1,6-Anhydro-.beta.-D-glucopyranose(levoglucosan)	●	●					●	
2-hydroxy-3-methyl-2-Cyclopenten-1-one	●	●	●					
2-methoxy-1,4-Benzenediol		●		●	●	●		●
2-methoxy-4-methyl-Phenol	●	●	●	●	●	●	●	●
2-methoxy-4-propyl-Phenol		●		●	●			●
2,3-Dimethoxy-5-aminocinnamonitril			●			●		
2,3,5,8-tetramethyl-Decane	●					●	●	
2,3,6,7-tetramethyl-Octane					●	●	●	
2,5-Furandicarboxaldehyde		●		●				
2,6-dimethoxy-4-(2-propenyl)-Phenol	●	●	●		●	●		●
2,6-dimethoxy-Phenol	●	●	●		●	●		●
2,6,10-trimethyl-Tetradecane		●				●		
3-Allyl-6-methoxyphenol				●			●	
3-Hydroxy-4-methoxybenzoic acid			●	●	●	●	●	

3-methoxy-1,2-Benzenediol	●	●	●	●	●	●	●	●
3-methyl-1,2-Cyclopentanedione		●	●	●				●
3,4-Altrosan	●	●		●	●	●	●	
3,4-dimethoxy-Phenol	●	●	●					
3,5-Dimethoxy-4-hydroxycinnamaldehyde	●	●	●					●
3,5-Dimethoxy-4-hydroxyphenylacetic acid					●			●
4-ethyl-2-methoxy-Phenol	●	●		●	●			●
4-Hydroxy-2-methoxycinnamaldehyde		●		●	●	●	●	
4-hydroxy-3-methoxy-Benzeneacetic acid		●		●		●	●	
4-hydroxy-3-methoxy-methyl ester Benzeneacetic acid		●			●			
4-hydroxy-3,5-dimethoxy-Benzaldehyde (syringaldehyde)	●	●	●	●	●	●	●	●
4-hydroxy-3,5-dimethoxy-Benzoic acid	●	●	●		●			
4-methyl-Phenol	●		●	●				
4,6-dimethyl-Dodecane		●	●		●	●	●	
4,6-dimethyl-Undecane	●		●			●		
5-(hydroxymethyl)-2-Furancarboxaldehyde	●	●	●	●	●	●	●	●
5-Acetoxymethyl-2-furaldehyde		●		●	●			●
5-acetyl-2,4,6,(1H,3H,5H)-Pyrimidinetrione	●	●	●		●			
5-methyl-2-Furancarboxaldehyde	●	●	●	●				●
5-propyl-Tridecane					●	●		
Anhydro-d-mannosan				●				●
Eugenol				●	●	●		
Heptadecane					●	●	●	
Homovanillyl alcohol			●					●
Hydroquinone mono-trimethylsilyl ether			●		●			
Levoglucosenone	●	●	●			●	●	●
n-Hexadecanoic acid	●	●	●	●	●	●	●	●
Octadecanoic acid	●					●		
Pentadecane		●				●		
Phenol	●		●	●				
Tetradecane	●					●	●	
Vanillin	●	●	●	●	●	●	●	

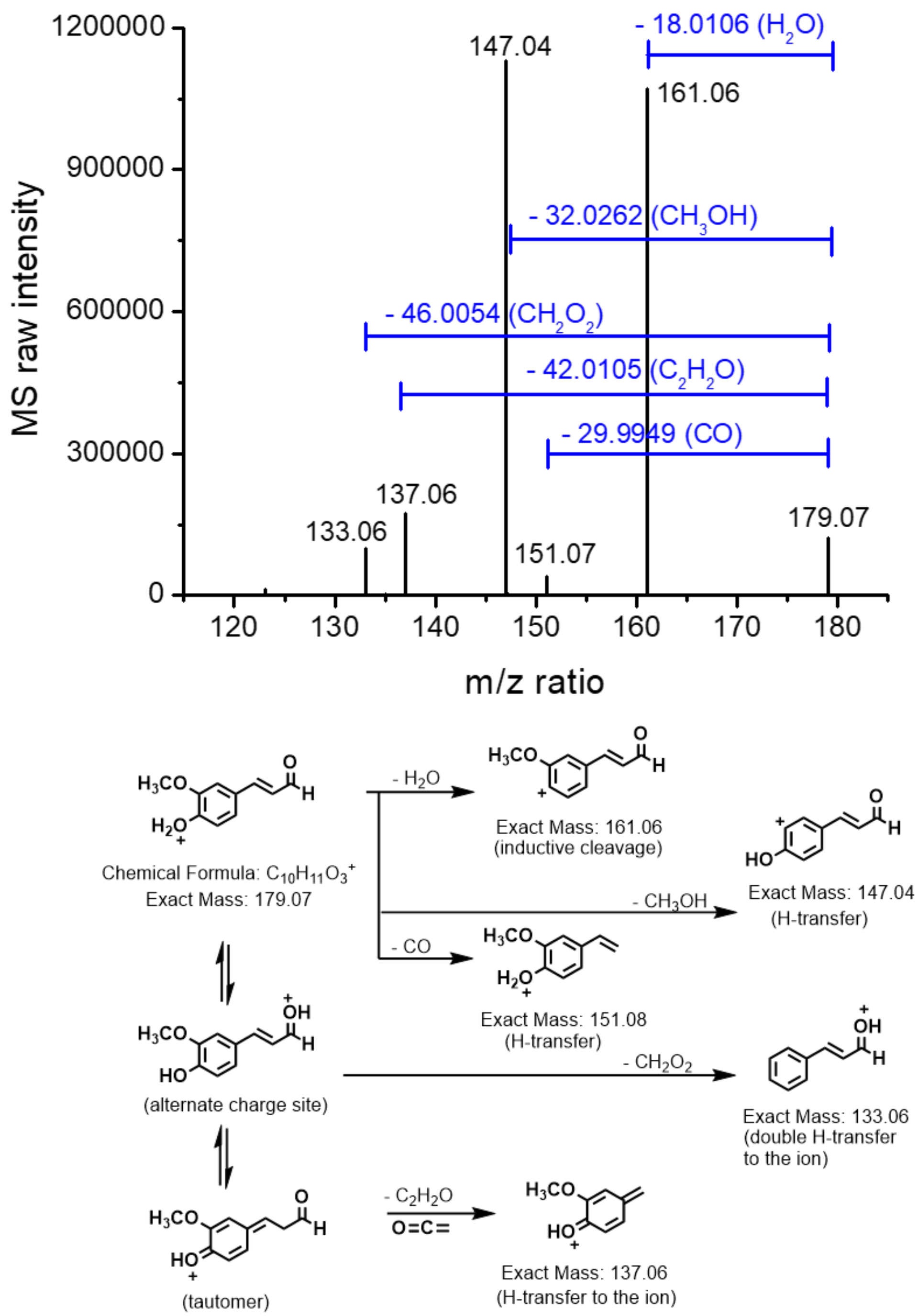

Figure S7: Representative MS^2 spectrum of coniferaldehyde and associated fragmentation mechanisms. H-transfer was the most commonly observed fragmentation mechanism in our CID analyses. CH_2O_2 loss represents the minor contribution of methoxycinammic acid.

Table S2: Positive mode nano-ESI analysis of chemical constituents of smoldering woodsmoke aerosols that are common to most (8 out of 9) wood types. The signal to noise (S/N) ratios are percent normalized to the total S/N of the sample. Neutral molecular formulas have been converted from their protonated or sodiated ionic forms, assigned from the observed m/z.

Obs.	Neutral Formula				Woodsmoke Aerosol Sample (% normalized S/N ratio)								
m/z	C	H	O	N	A. M.	Birch	Cherry	Maple	Pine	Poplar	R. Oak	R.W.	Walnut
127.03	6	6	3	0	1.35	0.81	1.90	0.88	2.12	0.92	0.70	1.82	1.44
127.07	7	10	2	0	0.73	0.23	0.50	0.21	0.36	---	0.17	0.17	0.36
129.05	6	8	3	0	0.48	0.29	0.47	0.28	0.45	0.23	0.10	0.36	0.45
137.05	8	8	2	0	1.00	1.19	1.64	1.20	2.07	0.74	1.14	1.75	1.19
139.07	8	10	2	0	0.20	0.19	0.21	0.18	0.30	0.10	0.09	0.09	0.13
141.05	7	8	3	0	0.42	0.30	0.32	0.31	0.36	0.29	0.16	0.23	0.27
143.03	6	6	4	0	0.29	0.25	2.20	0.26	1.05	0.53	0.32	1.05	1.26
143.07	7	10	3	0	0.44	0.25	0.16	0.24	0.26	0.19	0.13	0.17	0.23
147.04	9	6	2	0	0.16	0.20	0.19	0.22	0.36	0.15	0.18	0.20	0.16
149.05	9	8	2	0	0.21	0.22	0.35	0.25	0.37	0.22	0.18	0.16	0.22
151.03	8	6	3	0	0.40	0.31	0.66	0.38	1.09	0.34	0.50	1.29	0.65
151.07	9	10	2	0	0.77	0.51	0.82	0.77	1.24	0.47	0.29	0.55	0.48
153.05	8	8	3	0	0.59	0.47	0.95	0.58	1.32	0.60	0.39	1.10	0.79
153.09	9	12	2	0	0.26	0.22	0.15	0.18	0.21	0.14	0.09	0.11	0.17
155.07	8	10	3	0	0.70	0.53	1.06	0.65	0.45	0.65	0.61	0.33	0.65
157.04	7	8	4	0	0.30	0.32	0.87	0.14	0.23	0.22	0.19	0.23	0.40
161.05	10	8	2	0	0.31	0.44	0.45	0.52	0.57	0.34	0.34	0.25	0.33
163.03	9	6	3	0	0.61	1.09	0.93	0.35	0.40	0.33	0.80	0.74	0.92
163.07	10	10	2	0	0.59	0.57	0.55	0.74	1.17	0.48	0.40	0.76	0.93
165.05	9	8	3	0	0.34	0.41	0.60	0.38	0.50	0.34	0.26	0.29	0.41
165.09	10	12	2	0	0.51	0.32	0.34	0.38	0.68	0.27	0.21	0.19	0.25
167.07	9	10	3	0	3.32	3.69	3.56	3.59	1.08	2.54	2.99	0.78	2.89
168.06	8	9	3	1	0.09	0.14	0.08	0.14	0.10	0.18	0.36	0.12	0.48
169.04	8	8	4	0	0.22	0.29	0.47	0.31	0.29	0.49	0.45	0.40	0.60
169.08	9	12	3	0	0.85	0.66	0.82	0.75	0.54	0.56	0.45	0.44	0.71
171.06	8	10	4	0	0.17	0.19	0.28	0.15	0.24	0.14	0.13	0.17	0.22
175.07	11	10	2	0	0.40	0.34	0.44	0.34	0.57	0.23	0.13	0.18	0.25
177.05	10	8	3	0	1.44	1.32	2.05	1.19	0.88	1.11	1.08	0.73	1.43
177.09	11	12	2	0	0.45	0.31	0.33	0.42	0.48	0.28	0.17	0.21	0.26
179.07	10	10	3	0	1.68	2.27	1.80	3.19	5.88	1.82	2.93	4.71	2.56
179.10	11	14	2	0	0.19	0.16	0.11	0.20	0.22	0.13	0.08	---	0.11
181.04	9	8	4	0	0.47	0.44	0.74	0.54	0.16	0.52	0.61	0.16	0.56
181.08	10	12	3	0	2.11	1.13	1.90	1.60	0.87	1.11	0.95	0.54	1.24
182.08	9	11	3	1	0.17	0.35	0.09	0.63	0.11	0.16	0.15	0.10	0.53
183.06	9	10	4	0	1.19	1.45	2.22	1.85	0.42	2.23	2.67	1.28	2.99
183.10	10	14	3	0	0.52	0.50	0.36	0.42	0.36	0.34	0.30	0.25	0.30
185.04	6	10	5	0	0.64	0.58	0.60	0.25	0.81	0.43	1.65	4.51	1.73
185.08	9	12	4	0	0.16	0.14	0.16	0.15	0.28	0.07	0.11	0.12	0.16

187.06	8	10	5	0	0.16	0.20	0.19	0.19	0.53	0.12	0.13	0.33	0.23
187.07	12	10	2	0	0.25	0.20	0.18	0.18	0.29	0.14	0.07	0.08	0.14
189.05	11	8	3	0	0.13	0.20	0.31	0.22	0.17	0.14	0.12	0.13	0.21
189.09	12	12	2	0	0.40	0.31	0.40	0.36	0.57	0.22	0.11	0.16	0.27
191.07	11	10	3	0	1.87	1.25	1.45	1.33	1.40	1.07	0.72	0.66	1.22
191.10	12	14	2	0	0.32	0.21	0.15	0.22	0.34	0.16	0.11	0.11	0.17
193.04	10	8	4	0	0.40	0.51	1.01	0.38	0.67	0.36	0.59	0.91	0.65
193.08	11	12	3	0	1.73	1.68	1.34	2.02	1.51	1.30	1.40	0.60	1.40
195.06	10	10	4	0	0.30	0.44	0.62	0.32	0.45	0.39	0.33	0.41	0.49
195.10	11	14	3	0	0.95	1.02	0.55	1.03	0.39	0.80	0.87	0.20	0.53
197.08	10	12	4	0	2.02	2.10	2.68	1.41	0.34	1.49	2.16	0.70	2.08
197.11	11	16	3	0	0.18	0.17	0.12	0.16	0.12	0.14	0.13	---	0.10
198.07	9	11	4	1	0.44	0.71	0.18	1.23	0.31	0.37	0.46	0.27	2.68
199.06	9	10	5	0	0.12	0.16	0.47	0.16	0.10	0.31	0.28	0.13	0.27
201.09	13	12	2	0	0.26	0.17	0.17	0.20	0.29	0.11	0.06	---	0.11
205.04	11	8	4	0	0.12	0.23	0.45	0.12	0.25	0.15	0.16	0.16	---
205.07	8	12	6	0	0.16	0.14	0.08	0.13	0.67	0.11	0.09	0.39	0.23
205.08	10	14	3	0	1.36	0.96	1.16	1.23	1.98	0.70	0.53	1.10	1.03
207.06	11	10	4	0	0.63	0.66	0.97	0.53	0.82	0.47	0.45	0.70	0.83
207.10	12	14	3	0	0.93	0.57	0.79	0.87	0.78	0.49	0.38	0.25	0.56
209.08	11	12	4	0	5.48	9.33	5.77	6.85	0.51	5.72	10.83	0.73	6.78
209.11	12	16	3	0	0.18	0.12	0.10	0.19	0.15	0.13	0.10	---	0.09
211.09	11	14	4	0	3.44	5.35	4.28	4.03	0.43	3.75	6.33	1.22	4.30
212.09	10	13	4	1	0.14	0.24	0.10	0.44	0.18	0.11	0.11	0.10	0.68
213.07	10	12	5	0	0.22	0.31	0.49	0.28	0.17	0.32	0.39	0.14	0.32
215.06	11	12	3	0	0.29	0.20	0.22	---	0.33	0.14	0.11	0.14	0.18
216.08	9	13	5	1	0.09	0.16	---	0.20	0.11	0.07	0.09	0.09	0.53
219.10	13	14	3	0	0.98	0.67	0.49	1.00	1.68	0.61	0.39	0.77	0.68
221.08	12	12	4	0	0.58	0.46	0.67	0.56	0.77	0.46	0.32	0.54	---
221.11	13	16	3	0	0.33	0.27	0.17	0.32	0.26	0.23	0.17	---	0.16
223.06	11	10	5	0	0.29	0.30	0.68	0.34	0.18	0.35	0.79	0.26	---
223.09	12	14	4	0	0.64	0.72	0.71	0.85	0.38	0.73	0.73	0.26	0.62
225.07	11	12	5	0	0.12	0.15	0.26	0.18	0.16	0.17	0.18	0.17	0.21
225.11	12	16	4	0	0.21	0.20	0.16	0.27	0.16	0.25	0.21	0.09	0.15
227.05	5	10	8	2	0.67	0.95	0.38	0.59	1.81	0.55	1.20	2.60	1.68
227.09	11	14	5	0	0.20	0.42	0.30	0.39	0.13	0.46	0.45	0.13	0.29
231.06	11	12	4	0	0.14	0.41	0.18	0.20	---	0.23	0.96	0.13	0.38
231.10	14	14	3	0	0.37	0.27	0.25	0.37	0.60	0.26	0.14	0.17	0.22
233.11	14	16	3	0	0.52	0.30	0.23	0.61	0.78	0.42	0.30	0.28	0.28
235.09	13	14	4	0	0.80	0.67	0.68	0.92	0.75	0.54	0.45	0.36	---
237.07	12	12	5	0	0.16	0.21	---	0.22	0.19	0.23	0.22	0.18	0.23
237.11	13	16	4	0	0.34	0.45	0.26	0.47	0.16	0.39	0.31	0.12	0.24
239.09	12	14	5	0	0.12	0.17	0.15	0.19	0.12	0.13	0.15	0.11	---
245.08	14	12	4	0	0.23	0.16	0.25	0.19	0.42	0.16	0.09	0.31	0.23
245.11	15	16	3	0	0.25	0.15	0.12	0.22	0.40	0.12	---	0.11	0.12
247.09	14	14	4	0	0.46	0.38	0.45	0.65	0.84	0.40	0.26	0.72	0.38
247.13	15	18	3	0	0.21	0.15	0.07	0.21	0.29	0.14	0.07	0.08	---
249.07	13	12	5	0	0.15	0.17	0.28	0.18	0.16	0.18	0.19	0.15	0.20
249.11	14	16	4	0	0.87	0.82	0.68	0.98	0.41	0.73	0.90	0.15	---
251.09	13	14	5	0	0.25	0.20	0.28	0.26	0.16	0.23	0.20	0.11	0.27

251.12	14	18	4	0	0.12	0.13	0.08	0.23	0.10	0.17	0.09	---	0.10
257.08	15	12	4	0	0.17	---	0.16	0.18	0.24	0.14	0.07	0.09	0.15
259.09	15	14	4	0	0.28	0.27	0.25	0.24	0.57	0.15	0.09	0.29	---
261.11	15	16	4	0	0.35	0.28	0.27	0.56	1.34	0.26	0.18	1.05	---
263.09	14	14	5	0	0.39	0.34	0.59	0.39	0.22	0.45	0.39	0.15	0.42
265.10	14	16	5	0	0.27	0.30	0.27	0.52	0.08	0.31	0.22	---	0.31
269.06	7	12	9	2	0.23	0.47	0.15	0.30	0.28	0.25	0.48	0.36	---
271.09	16	14	4	0	0.22	---	0.16	0.16	0.46	0.14	0.10	0.64	0.29
273.11	16	16	4	0	0.25	0.19	0.17	0.25	0.47	0.17	0.08	0.25	---
275.09	15	14	5	0	0.22	0.22	0.40	0.24	0.35	0.24	0.21	0.47	0.26
275.12	16	18	4	0	0.24	0.18	0.15	0.36	1.09	0.18	0.10	0.88	0.20
277.10	15	16	5	0	0.38	0.26	0.46	0.34	0.28	0.29	0.17	0.14	0.35
287.12	17	18	4	0	0.18	---	0.10	0.23	0.51	0.10	0.07	0.25	0.13
289.10	16	16	5	0	0.30	0.30	0.36	0.38	1.08	0.31	0.20	1.92	0.35
291.12	16	18	5	0	0.30	0.28	0.26	---	0.18	0.26	0.19	0.11	0.21
299.07	8	14	10	2	0.10	0.18	---	0.10	0.18	0.11	0.18	0.28	0.14
299.12	18	18	4	0	0.15	0.17	0.13	0.21	0.74	0.18	---	0.51	0.15
301.10	17	16	5	0	0.32	0.25	0.26	0.25	0.69	0.20	0.17	0.60	0.28
303.12	17	18	5	0	0.25	0.19	0.25	0.35	0.49	0.20	0.13	0.47	0.28
305.10	16	16	6	0	0.15	0.12	0.26	0.15	0.09	0.17	0.21	0.11	0.24
305.13	17	20	5	0	0.41	0.21	0.26	0.45	0.12	0.34	0.19	---	0.28
313.08	9	16	10	2	0.09	0.17	---	0.08	0.14	0.10	0.14	0.26	0.16
313.10	18	16	5	0	0.16	0.13	0.18	0.13	0.52	0.12	0.20	0.58	0.18
313.14	19	20	4	0	0.11	0.13	0.08	0.12	0.43	0.14	---	0.21	0.10
315.12	18	18	5	0	0.24	0.18	0.20	0.29	0.55	0.17	0.10	0.47	0.20
317.13	18	20	5	0	0.22	---	0.15	0.36	0.34	0.15	0.09	0.22	0.23
319.11	17	18	6	0	0.23	0.23	0.32	0.34	0.09	0.21	0.17	0.08	0.27
327.12	19	18	5	0	0.15	0.19	0.13	0.22	0.76	0.16	0.24	0.88	0.21
329.10	18	16	6	0	0.10	---	0.12	0.10	0.20	0.12	0.10	0.22	0.11
329.13	19	20	5	0	0.27	0.21	0.17	0.44	0.51	0.28	0.10	0.28	0.32
331.11	18	18	6	0	2.18	1.06	0.98	1.14	0.23	1.14	0.83	0.30	1.19
333.13	18	20	6	0	0.45	0.41	0.78	0.42	0.09	0.25	0.29	---	0.41
341.13	20	20	5	0	0.20	0.15	0.11	0.24	0.85	0.21	0.18	0.58	0.19
343.11	17	20	6	0	0.45	0.27	0.33	0.46	0.26	0.21	0.16	0.19	0.43
345.13	19	20	6	0	0.24	0.23	0.24	0.35	0.19	0.22	0.13	0.12	0.23
353.09	15	16	8	2	0.25	0.25	0.17	0.13	---	0.17	0.44	0.25	0.36
357.13	18	22	6	0	2.75	1.09	1.50	0.79	0.31	---	1.79	0.12	1.86
359.14	20	22	6	0	0.23	0.17	0.14	0.29	0.11	0.12	0.09	---	0.16
369.13	21	20	6	0	0.16	0.14	0.11	0.16	0.10	0.14	0.20	0.08	0.26
383.14	20	24	6	0	0.17	0.19	---	0.16	0.11	0.14	0.16	0.11	0.17

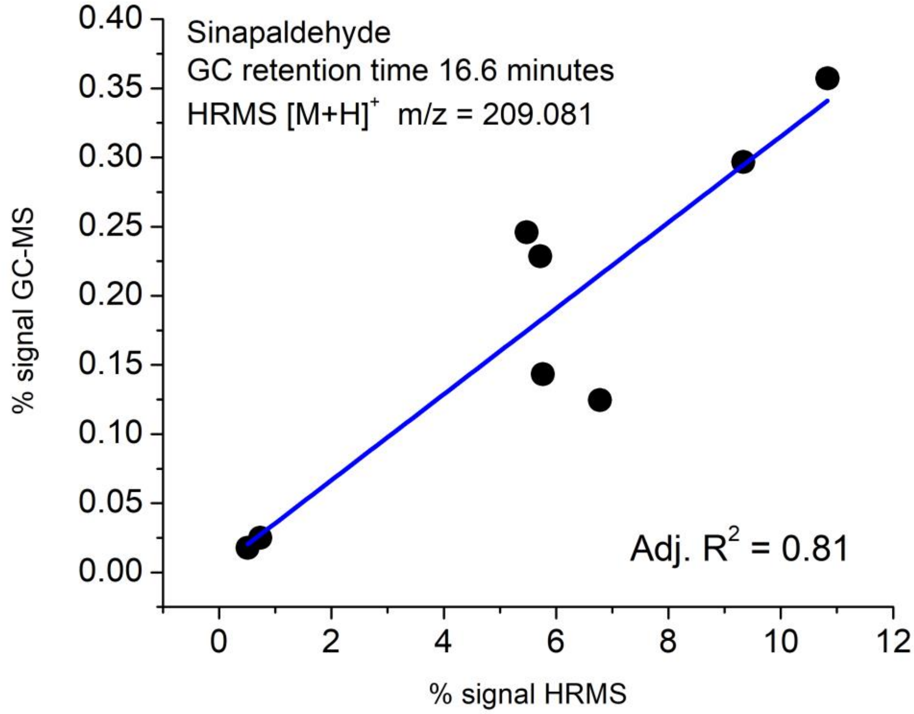

Figure S8: Correlation between sinapaldehyde's HRMS and GC-MS signals. Deviations in the correlation can be due to both GC-MS peak co-elution and HRMS signal competition from the complex mixture analysis and can occur on a sample-to-sample basis.