

Supporting Information

Analysis of Volatile Organic Compound Mixtures Using Radio-Frequency Ionization/Mass Spectrometry

Abayomi D. Olaitan^a, Behrooz Zekavat^a, Birendra Dhungana^a, William C. Hockaday^b, C. Kevin Chambliss^a, Touradj Solouki*^a

^aDepartment of Chemistry and Biochemistry, Baylor University, Waco, TX 76798, USA.

^bDepartment of Geology, Baylor University, Waco, TX 76798, USA.

*Address reprint requests to: Professor Touradj Solouki, Department of Chemistry and Biochemistry, Baylor University, Waco, TX 76798, USA.
Telephone: 254-710-2678, Fax: 254-710-4272, E-mail: Touradj_Solouki@baylor.edu

Table S1. A list of experimental (observed, column 1) and theoretical (exact, column 2) m/z values, mass measurement errors (column 3), assigned chemical compositions (column 4), and double bond equivalents (DBEs, column 5) for ionic species observed in RFI/FT-ICR mass spectra of pine shavings (PS) bio-oil aqueous (column 6) and oily (column 7) phases, corn stover (CS) bio-oil aqueous (column 8) and oily phases (column 9), and a commercial gasoline sample (RON = 87, column 10).

Obs. m/z	Exact m/z	Error (ppm)	Chemical Composition	DBE*	PS (Aqueous)	PS (Oily)	CS (Aqueous)	CS (Oily)	Gasoline
29.03845	29.03858	-4.48	C ₂ H ₅ ⁺	0.5	x	x	x	x	✓
31.01788	31.01784	1.40	CH ₃ O ⁺	0.5	✓	x	x	✓	✓
32.02585	32.02567	5.62	CH ₄ O ^{•+}	0.0	✓	x	x	x	x
33.03342	33.03349	-2.12	CH ₅ O ⁺	-0.5	✓	x	✓	x	x
39.02291	39.02293	-0.56	C ₃ H ₃ ⁺	2.5	✓	✓	✓	✓	✓
41.03858	41.03858	0.00	C ₃ H ₅ ⁺	1.5	✓	x	x	x	✓
42.03388	42.03383	1.07	C ₂ H ₄ N ⁺	1.5	✓	x	✓	x	x
42.04622	42.04640	-4.28	C ₃ H ₆ ^{•+}	1.0	x	x	x	x	✓
43.01783	43.01784	-0.23	C ₂ H ₃ O ⁺	1.5	✓	✓	✓	✓	✓
43.05420	43.05423	-0.70	C ₃ H ₇ ⁺	0.5	x	x	x	x	✓
45.03356	45.03349	1.48	C ₂ H ₅ O ⁺	0.5	✓	x	✓	x	✓
47.04911	47.04914	-0.57	C ₂ H ₇ O ⁺	-0.5	✓	x	✓	x	✓
53.03858	53.03858	0.00	C ₄ H ₅ ⁺	2.5	✓	✓	x	✓	✓
55.01807	55.01784	4.18	C ₃ H ₃ O ⁺	2.5	x	✓	x	✓	x
55.05438	55.05423	2.79	C ₄ H ₇ ⁺	1.5	✓	x	✓	x	✓
56.04961	56.04948	2.32	C ₃ H ₆ N ⁺	1.5	✓	x	x	x	x
56.06207	56.06205	0.36	C ₄ H ₈ ^{•+}	1.0	x	x	x	x	✓
57.03347	57.03349	-0.35	C ₃ H ₅ O ⁺	1.5	✓	✓	✓	✓	x
57.06953	57.06988	-6.13	C ₄ H ₉ ⁺	0.5	x	x	x	x	✓
58.04103	58.04132	-4.99	C ₃ H ₆ O ^{•+}	1.0	✓	x	x	x	x
59.04925	59.04914	1.86	C ₃ H ₇ O ⁺	0.5	✓	✓	✓	✓	✓
60.05553	60.05562	-1.58	CH ₆ N ₃ ⁺	0.5	✓	x	✓	x	x
61.02839	61.02841	-0.33	C ₂ H ₅ O ₂ ⁺	0.5	✓	x	✓	x	x
65.03835	65.03858	-3.54	C ₅ H ₅ ⁺	3.5	x	✓	x	x	✓
67.05431	67.05423	1.12	C ₅ H ₇ ⁺	2.5	✓	✓	x	✓	✓
69.03354	69.03349	0.65	C ₄ H ₅ O ⁺	2.5	✓	✓	✓	✓	x
69.07000	69.06988	1.66	C ₅ H ₉ ⁺	1.5	✓	✓	x	✓	✓
70.06476	70.06513	-5.28	C ₄ H ₈ N ⁺	1.5	✓	x	x	x	x
70.07781	70.07770	1.57	C ₅ H ₁₀ ^{•+}	1.0	x	x	x	x	✓
71.04921	71.04914	1.02	C ₄ H ₇ O ⁺	1.5	✓	✓	✓	✓	x
71.08507	71.08553	-6.47	C ₅ H ₁₁ ⁺	0.5	x	x	x	x	✓
72.05640	72.05697	-7.91	C ₄ H ₈ O ^{•+}	1.0	x	✓	x	x	x
73.02817	73.02841	-3.29	C ₃ H ₅ O ₂ ⁺	1.5	✓	x	x	x	x
73.06480	73.06479	0.17	C ₄ H ₆ O ⁺	0.5	✓	✓	✓	✓	x
75.04416	75.04406	1.37	C ₃ H ₇ O ₂ ⁺	0.5	✓	✓	✓	✓	x
76.05194	76.05188	0.79	C ₃ H ₈ O ₂ ^{•+}	0.0	x	x	x	✓	x
77.03954	77.03858	12.46	C ₆ H ₅ ⁺	4.5	x	x	x	x	✓
78.04685	78.04640	5.70	C ₆ H ₆ ^{•+}	4.0	x	✓	x	x	✓
79.05421	79.05423	-0.25	C ₆ H ₇ ⁺	3.5	x	x	x	x	✓
80.05020	80.04948	8.99	C ₅ H ₆ N ⁺	3.5	x	✓	x	x	x
81.03311	81.03349	-4.72	C ₅ H ₅ O ⁺	3.5	✓	✓	✓	✓	x
81.07004	81.06988	2.01	C ₆ H ₉ ⁺	2.5	x	✓	x	✓	✓
82.04153	82.04132	2.56	C ₅ H ₆ O ^{•+}	3.0	✓	✓	x	✓	x
82.07691	82.07770	-9.63	C ₆ H ₁₀ ^{•+}	2.0	x	x	x	x	✓
83.04922	83.04914	0.96	C ₅ H ₇ O ⁺	2.5	✓	✓	✓	✓	x
83.08574	83.08553	2.57	C ₆ H ₁₁ ⁺	1.5	x	✓	x	✓	✓

84.05565	84.05562	0.31	C ₃ H ₆ N ₃ ⁺	2.5	✓	✓	✓	x	x
84.09315	84.09335	-2.38	C ₆ H ₁₂ ^{•+}	1.0	x	x	x	x	✓
85.06482	85.06479	0.38	C ₅ H ₉ O ⁺	1.5	✓	✓	✓	✓	x
85.10117	85.10118	-0.12	C ₆ H ₁₃ ⁺	0.5	x	x	x	x	✓
86.07247	86.07262	-1.80	C ₅ H ₁₀ O ^{•+}	1.0	✓	✓	✓	✓	x
87.04378	87.04406	-3.27	C ₄ H ₇ O ₂ ⁺	1.5	✓	x	✓	x	x
87.08049	87.08044	0.52	C ₅ H ₁₁ O ⁺	0.5	✓	✓	✓	✓	x
88.05179	88.05188	-1.02	C ₄ H ₈ O ₂ ^{•+}	1.0	✓	x	x	x	x
89.05975	89.05971	0.48	C ₄ H ₉ O ₂ ⁺	0.5	✓	✓	✓	✓	x
90.06753	90.06753	0.00	C ₄ H ₁₀ O ₂ ^{•+}	0.0	✓	x	x	x	x
91.01752	91.01784	-3.52	C ₆ H ₃ O ⁺	5.5	x	✓	x	x	x
91.05442	91.05423	2.11	C ₇ H ₇ ⁺	4.5	✓	✓	x	✓	✓
92.06177	92.06205	-3.08	C ₇ H ₈ ^{•+}	4.0	✓	x	x	✓	✓
93.06992	93.06988	0.43	C ₇ H ₉ ⁺	3.5	✓	x	x	x	✓
94.07770	94.07770	0.00	C ₇ H ₁₀ ^{•+}	3.0	x	✓	x	x	x
95.01248	95.01276	-2.95	C ₅ H ₃ O ₂ ⁺	4.5	✓	x	x	x	x
95.04933	95.04914	1.95	C ₆ H ₇ O ⁺	3.5	x	✓	x	✓	x
95.08561	95.08553	0.88	C ₇ H ₁₁ ⁺	2.5	x	✓	x	✓	✓
96.02062	96.02058	0.36	C ₅ H ₄ O ₂ ^{•+}	4.0	✓	x	x	✓	x
96.05745	96.05697	4.96	C ₆ H ₈ O ^{•+}	3.0	✓	✓	x	✓	x
96.09339	96.09335	0.42	C ₇ H ₁₂ ^{•+}	2.0	x	x	x	x	✓
97.02821	97.02841	-2.04	C ₅ H ₅ O ₂ ⁺	3.5	✓	✓	✓	✓	x
97.06481	97.06479	0.23	C ₆ H ₉ O ⁺	2.5	✓	✓	✓	✓	x
97.10136	97.10118	1.82	C ₇ H ₁₃ ⁺	1.5	x	✓	x	✓	✓
98.03574	98.03623	-4.99	C ₅ H ₆ O ₂ ^{•+}	3.0	✓	x	✓	x	x
98.07276	98.07262	1.43	C ₆ H ₁₀ O ^{•+}	2.0	x	✓	x	x	x
98.10910	98.10900	1.02	C ₇ H ₁₄ ^{•+}	1.0	x	x	x	x	✓
99.08055	99.08044	1.06	C ₆ H ₁₁ O ⁺	1.5	✓	✓	✓	✓	x
99.11701	99.11683	1.82	C ₇ H ₁₅ ⁺	0.5	x	x	x	x	✓
101.02337	101.02332	0.49	C ₄ H ₅ O ₃ ⁺	2.5	x	✓	x	x	x
101.02940	101.02937	0.29	C ₄ H ₇ NS ^{•+}	2.0	✓	x	x	x	x
101.05989	101.05971	1.78	C ₅ H ₉ O ₂ ⁺	1.5	✓	✓	✓	✓	x
101.09603	101.09609	-0.59	C ₆ H ₁₃ O ⁺	0.5	✓	✓	✓	✓	x
102.04530	102.04640	-10.78	C ₈ H ₆ ^{•+}	6.0	x	✓	x	x	x
103.05416	103.05420	-0.68	C ₈ H ₇ ⁺	5.5	x	x	x	x	✓
103.07570	103.07536	3.29	C ₅ H ₁₁ O ₂ ⁺	0.5	✓	✓	✓	✓	x
105.06473	105.06585	-10.66	C ₃ H ₉ N ₂ O ₂ ⁺	0.5	✓	x	x	x	x
105.06952	105.06988	-3.43	C ₈ H ₉ ⁺	4.5	x	✓	x	✓	✓
106.07799	106.07770	2.87	C ₈ H ₁₀ ^{•+}	4.0	x	✓	x	✓	✓
107.08609	107.08553	5.23	C ₈ H ₁₁ ⁺	3.5	✓	x	x	x	✓
109.06458	109.06479	-1.93	C ₇ H ₉ O ⁺	3.5	x	✓	x	✓	x
109.10101	109.10118	-1.56	C ₈ H ₁₃ ⁺	2.5	x	✓	x	✓	✓
110.03700	110.03623	6.99	C ₆ H ₆ O ₂ ^{•+}	4.0	✓	x	x	x	x
110.07303	110.07262	3.73	C ₇ H ₁₀ O ^{•+}	3.0	x	✓	x	✓	x
110.10908	110.10900	0.73	C ₈ H ₁₄ ^{•+}	2.0	x	x	x	x	✓
111.03171	111.03148	2.07	C ₅ H ₅ NO ₂ ^{•+}	4.0	x	✓	x	x	x
111.04376	111.04406	-2.70	C ₆ H ₇ O ₂ ⁺	3.5	✓	x	✓	✓	x

111.08029	111.08044	-1.35	C ₇ H ₁₁ O ⁺	2.5	✓	✓	✓	✓	x
111.11730	111.11683	4.23	C ₈ H ₁₅ ⁺	1.5	x	x	x	✓	✓
112.08590	112.08692	-9.10	C ₅ H ₁₀ N ₃ ⁺	2.5	x	✓	x	x	x
112.12526	112.12465	5.44	C ₈ H ₁₆ ^{•+}	1.0	x	x	x	x	✓
113.09500	113.09475	2.21	C ₅ H ₁₁ N ₃ ^{•+}	2.0	✓	x	x	x	x
113.09606	113.09609	0.27	C ₇ H ₁₃ O ⁺	1.5	x	✓	✓	✓	x
113.13210	113.13248	-3.36	C ₈ H ₁₇ ⁺	0.5	x	x	x	x	✓
115.07575	115.07536	3.39	C ₆ H ₁₁ O ₂ ⁺	1.5	✓	✓	✓	✓	x
117.05500	117.05462	3.25	C ₅ H ₉ O ₃ ⁺	1.5	✓	x	✓	x	x
117.06976	117.06988	-1.03	C ₉ H ₉ ⁺	5.5	x	x	x	x	✓
117.09071	117.09101	-2.56	C ₆ H ₁₃ O ₂ ⁺	0.5	x	x	✓	✓	x
119.08556	119.08553	0.25	C ₉ H ₁₁ ⁺	4.5	x	✓	x	✓	✓
120.09302	120.09335	-2.75	C ₉ H ₁₂ ^{•+}	4.0	x	x	x	✓	✓
121.10200	121.10118	6.77	C ₉ H ₁₃ ⁺	3.5	✓	x	x	✓	✓
123.07989	123.08044	-4.47	C ₈ H ₁₁ O ⁺	3.5	✓	x	x	✓	x
123.11756	123.11683	5.93	C ₉ H ₁₅ ⁺	2.5	x	x	x	x	✓
124.12455	124.12465	-0.81	C ₉ H ₁₆ ^{•+}	2.0	x	x	x	x	✓
125.05876	125.05836	3.20	C ₅ H ₇ N ₃ O ^{•+}	4.0	✓	x	x	x	x
125.09587	125.09609	-1.76	C ₈ H ₁₃ O ⁺	2.5	✓	✓	✓	✓	x
125.13245	125.13248	-0.24	C ₉ H ₁₇ ⁺	1.5	x	x	x	x	✓
128.06166	128.06205	-3.05	C ₁₀ H ₈ ^{•+}	7.0	✓	✓	✓	✓	x
129.07010	129.06988	1.70	C ₁₀ H ₉ ⁺	6.5	✓	x	✓	x	x
129.08906	129.08966	-4.65	C ₅ H ₁₁ N ₃ O ^{•+}	2.0	x	✓	x	x	x
130.07504	130.07368	10.46	C ₅ H ₁₀ N ₂ O ₂ ^{•+}	2.0	✓	x	x	x	x
131.07266	131.07295	-2.21	C ₉ H ₉ N ^{•+}	6.0	✓	x	x	x	x
131.08543	131.08553	-0.76	C ₁₀ H ₁₁ ⁺	5.5	x	x	x	x	✓
132.04204	132.04171	2.49	C ₅ H ₈ O ₄ ^{•+}	2.0	x	✓	x	x	x
133.04911	133.04954	-3.23	C ₅ H ₉ O ₄ ⁺	1.5	x	✓	x	x	x
133.10139	133.10118	1.58	C ₁₀ H ₁₃ ⁺	4.5	x	x	x	x	✓
134.10900	134.10900	0.00	C ₁₀ H ₁₄ ^{•+}	4.0	x	x	x	x	✓
135.11672	135.11683	-0.81	C ₁₀ H ₁₅ ⁺	3.5	x	x	x	x	✓
137.13272	137.13248	1.75	C ₁₀ H ₁₇ ⁺	2.5	x	✓	x	✓	x
138.10314	138.10392	-5.65	C ₉ H ₁₄ O ^{•+}	3.0	x	✓	x	x	x
139.11227	139.11174	3.81	C ₉ H ₁₅ O ⁺	2.5	x	✓	x	x	x
143.05134	143.05117	1.19	C ₅ H ₉ N ₃ S ^{•+}	3.0	x	✓	x	x	x
155.10667	155.10666	0.06	C ₉ H ₁₅ O ₂ ⁺	2.5	x	✓	x	x	x
163.14786	163.14813	-1.65	C ₁₂ H ₁₉ ⁺	3.5	x	x	x	✓	x
171.13787	171.13796	-0.53	C ₉ H ₁₄ O ₃ ^{•+}	1.5	x	✓	x	✓	x

* Double Bond Equivalent (DDE) = (Number of Carbon Atoms) - (Number of Hydrogen Atoms / 2) + (Number of Nitrogen Atoms / 2) + 1.

✓: Present

x: Not Present

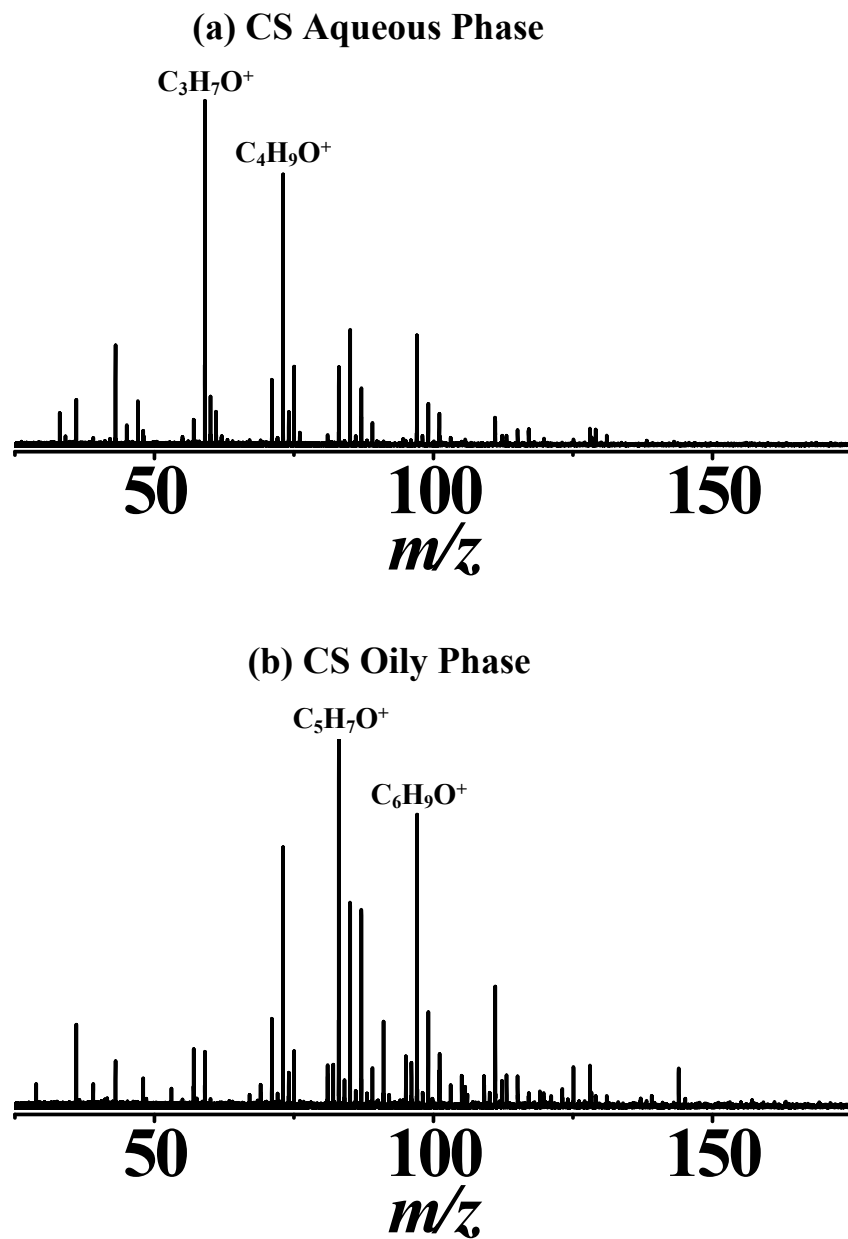


Figure S1. RFI/FT-ICR mass spectra of VOCs from (a) aqueous and (b) oily phases of corn stover (CS) slow pyrolysis bio-oil. The two most abundant peaks in each mass spectrum are labeled. For each mass spectrum, 5 FT-ICR MS time-domain transients of 128 k data points were summed prior to Fourier transformation.