

Molecular characterization of burned organic matter at different soil depths and its relationship with soil water repellency

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Supplementary Material:

Table S1. Organic compounds released by analytical pyrolysis for 0–2cm burned soil sample.

Retention time (min)	Compound name	O/C	H/C	Relative intensity (%)	Family
2.42	Methylamine, <i>N,N</i> -dimethyl	0.00	3.00	2.22	Peptide
2.93	1,3-Cyclopentadiene, methyl-	0.00	1.33	0.68	Polysaccharide
3.00	Benzene	0.00	1.00	0.56	Aromatic
3.10	1-Heptane	0.00	2.29	1.31	Lipid
3.51	Pyridine	0.00	1.00	1.08	Peptide
3.66	Toluene	0.00	1.14	1.32	Aromatic
3.75	1-Octene	0.00	2.00	0.51	Lipid
3.83	1-Pyrrolidineethanamine	0.00	2.33	0.97	Peptide
4.09	Butanoic acid, 3-methyl-	0.40	2.00	0.29	Lipid
4.16	Furan, 2,5-dimethyl-	0.17	1.33	0.65	Polysaccharide
4.24	Bicyclo(3.3.1.)non-2-ene	0.00	1.56	0.50	Lipid
4.44	Ethylbenzene	0.00	1.25	0.46	Aromatic
4.51	<i>o</i> -Xylene	0.00	1.25	0.81	Aromatic
4.61	2-Nonene	0.00	2.00	0.42	Lipid
4.75	Styrene	0.00	1.00	0.98	Aromatic
4.84	2-Cyclopenten-1-one, 2-methyl	0.17	1.33	0.46	Polysaccharide
5.08	Pyridine, 2,4-dimethyl-	0.00	1.29	0.24	Peptide
5.43	2-Furancarboxaldehyde, 5-methyl-	0.33	1.00	0.37	Polysaccharide
5.47	2-Cyclopenten-1-one, 3-methyl-	0.17	1.33	0.31	Polysaccharide
5.53	Phenol	0.17	1.00	2.02	Aromatic
5.74	Benzene, isocyano-	0.00	0.71	0.45	Aromatic
5.83	Benzene, 1,2,4-trimethyl-	0.00	1.33	0.57	Aromatic
6.08	2-Carene	0.00	1.60	0.19	Lipid
6.17	<i>p</i> -Cymene	0.00	1.40	0.61	Lipid
6.28	Cyclohexene, 4-methylene-1-(1-methyl-ethyl)	0.00	1.80	0.26	Lipid
6.35	2-Cyclopenten-1-one, 2,3-dimethyl	0.14	1.43	0.16	Polysaccharide
6.44	Phenol, 2-methyl-	0.14	1.14	0.60	Aromatic
6.55	Indene	0.00	0.89	0.52	PAH
6.68	<i>p</i> -Cresol	0.14	1.14	1.48	Lignin
6.86	3-Undecene, (Z)-	0.00	2.00	0.42	Lipid
6.98	Phenol, 2-methoxy	0.29	1.14	0.75	Lignin
7.30	3-Phenyl-2-propyn-1-ol	0.00	0.89	0.30	Aromatic
7.66	Phenol, 2,5-dimethyl-	0.13	1.25	0.53	Aromatic
7.80	Octanoic acid	0.25	2.00	0.15	Lipid
7.88	Phenol, 2-ethyl-	0.13	1.25	0.72	Aromatic
7.96	1H-Indene, 1-methyl-	0.00	1.00	0.33	PAH

8.15	1-Dodecene	0.00	2.00	0.29	Lipid
8.27	Phenol, 2,4-dimethyl-	0.13	1.25	0.38	Lipid
8.33	2-Methoxy-4-methylphenol	0.25	1.25	0.13	Lignin
8.42	Azulene	0.00	0.80	0.22	PAH
8.57	2,3-DIHYDRO-BENZOFURAN	0.13	1.00	0.38	Polysaccharide
8.71	Benzofuran, 4,7-dimethyl	0.10	1.00	0.24	Polysaccharide
8.84	1,3-Benzenediol, monoacetate	0.38	1.00	0.20	Aromatic
9.12	Phenol, 2,3,5-trimethyl	0.11	1.33	0.28	Aromatic
9.29	Naphthalene, 1,2-dihydro-3-methyl-	0.00	1.09	0.32	PAH
9.39	1H-Indene, 1,1-dimethyl-	0.00	1.09	0.11	PAH
9.48	1-Tridecene	0.00	2.00	0.49	Lipid
9.58	Tridecane	0.00	2.15	0.22	Lipid
9.66	1H-Inden-1-one, 2,3-dihydro-	0.11	0.89	0.15	PAH
9.78	Indole	0.00	0.88	0.30	Peptide
9.89	Naphthalene, 2-methyl-	0.00	0.91	0.27	PAH
9.97	2-Methoxy-4-vinylphenol	0.22	1.11	0.44	Lignin
10.14	Naphthalene, 2-methyl-	0.00	0.91	0.31	PAH
10.41	Phenol, 2,6-dimethoxy-	0.38	1.25	0.48	Lignin
10.54	Benzaldehyde, 4-propyl	0.10	1.20	0.41	Aromatic
10.65	Benzene, 1-methoxy-4-(1-propenyl)	0.10	1.20	0.20	Lignin
10.72	1H-Indene, 1,1,3-trimethyl	0.00	1.17	0.15	PAH
10.79	4-Tetradecene, (E)-	0.00	2.00	0.37	Lipid
10.88	Tetradecane	0.00	2.14	0.30	Lipid
10.95	Benzene, 1,3-bis(1-methylethyl)	0.00	1.50	0.99	Aromatic
11.14	Vanillin	0.38	1.00	0.21	Lignin
11.20	1,2,3-Trimethylindene	0.00	1.17	0.68	PAH
11.33	Naphthalene, 2,3-dimethyl	0.00	1.00	0.45	PAH
11.41	Benzene, 2-propenyl-	0.00	1.11	0.17	Aromatic
11.53	Naphthalene, 1,3-dimethyl-	0.00	1.00	0.95	PAH
11.74	Phenol, 2-methoxy-6-(1-propenyl)	0.20	1.20	0.32	Lignin
11.80	Aromandendrene	0.00	1.60	1.01	Lipid
11.89	N-Methyl-1-phenylcyclohexylamine	0.00	1.46	0.57	Peptide
12.06	1-Pentadecene	0.00	2.00	0.90	Lipid
12.14	Levoglucozan	0.83	2.00	2.15	Polysaccharide
12.25	Acetovanillone	0.33	1.33	0.88	Lignin
12.47	1H-Cyclopropa(a)naphthalene, 1a,2,3,3a,4,5,6,7b-octahydro-1,1,3a,7- tetramethyl	0.00	1.60	1.47	PAH
12.57	alpha-Gurjunene	0.00	1.60	0.51	Lipid
12.61	Isocaryophyllene	0.00	1.71	0.59	Lipid
12.67	Aromadendrene, dehydro	0.00	1.47	0.35	Lipid
12.72	1-Naphthalenol	0.10	0.80	0.43	PAH
12.82	Benzene, [(tetramethylcyclopropylidene)methyl]	0.00	1.29	0.47	Aromatic
12.95	1,1-Diethylnaphthalene	0.00	1.14	1.15	PAH
13.14	Azulene, 2,4,6-trimethyl-	0.00	1.08	1.18	PAH
13.28	1-Hexadecene	0.00	2.00	0.78	Lipid
13.33	Naphthalene, 2,3,6-trimethyl-	0.00	1.08	0.84	PAH
13.59	Himachala-2,4-diene	0.00	1.60	0.77	Lipid
13.67	9H-Fluorene	0.00	0.77	0.39	PAH
13.88	7-Methyl-1-naphthol	0.09	0.91	0.58	PAH
13.96	1-(6-Methoxynaphthalen-2-yl)ethanone	0.15	0.92	0.45	Lignin
14.03	Cycloisolongifolene, 8,9-dehydro	0.00	1.47	0.52	Lipid

14.15	Benzene, 1,1'-methylenebis(4-methyl)	0.00	1.07	0.76	Aromatic
14.31	7-tert-Butyl-1-naphthol	0.07	1.14	0.56	PAH
14.40	Phenol, 4-(1-methyl-1-phenylethyl)	0.07	1.07	0.55	Aromatic
14.45	1-Heptadecene	0.00	2.00	0.50	Lipid
14.52	Heptadecane	0.00	2.12	0.66	Lipid
14.62	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	0.00	1.20	0.60	PAH
14.73	Phenol, 2,6-dimethoxy-4-(2-propenyl)	0.27	1.27	0.61	Lignin
14.88	3-Undecene, 7-methyl-, (Z)-	0.00	2.00	0.94	Lipid
14.96	1-Octadecene	0.00	2.00	0.33	Lipid
15.13	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)	0.40	1.20	0.56	Lignin
15.20	Tetradecanoic acid	0.14	2.00	0.72	Lipid
15.26	2-Mnethyl-octadecyne	0.00	1.89	0.66	Lipid
15.37	Azulene, 7-ethyl-1,4-dimethyl	0.22	1.13	0.64	PAH
15.55	1-Octadecene	0.00	2.00	0.52	Lipid
15.62	Octadecane	0.00	2.11	0.35	Lipid
15.83	Azulene, 1,4-dimethyl-7-(1-methylethyl)-	0.00	1.20	0.66	PAH
15.89	2-(3'-piperidyl)benzimidazole	0.00	0.75	0.65	Peptide
16.00	Phenanthrene	0.00	0.71	0.61	PAH
16.15	2-Pentadecanone, 6,10,14-trimethyl	0.06	2.00	0.41	Lipid
16.43	9H-Fluorene, 2,3-dimethyl	0.07	0.80	1.00	PAH
16.53	Benzene, 1,2-dimethyl-4-(phenylmethyl)	0.00	1.00	0.61	Aromatic
16.61	1-Nonadecene	0.00	2.00	0.74	Lipid
16.67	Nonadecane	0.00	2.11	0.48	Lipid
16.75	2-Heptadecanone	0.06	2.00	0.65	Lipid
17.06	1,4-Benzenediamine, N-acetyl-N',N'-diethyl	0.08	1.50	0.52	Peptide
17.30	n-Hexadecanoic acid	0.13	2.00	1.25	Lipid
17.50	3-(2,2-dimethylpropylidene)bicyclo(3.3.1)-nonane-2,4-dione	0.14	1.43	1.02	Lipid
17.62	9-Eicosene	0.00	2.00	0.64	Lipid
17.68	Eicosane	0.00	2.10	0.44	Lipid
18.32	2,3,5,6-Detetrahydrocyclohexanone, 2,6-di- <i>t</i> -butyl-4-hydroxymethylene	0.13	1.47	0.71	Lipid
18.58	1-Heneicosene	0.00	2.00	0.93	Lipid
18.64	Heneicosane	0.00	2.10	1.17	Lipid
19.51	1-Docosene	0.00	2.00	2.37	Lipid
19.55	Docosane	0.00	2.09	0.99	Lipid
19.75	Behenic alcohol	0.05	2.09	0.60	Lipid
19.83	3-Pyrrolidino-3-oxo-propylsuccinimide	0.27	1.45	0.52	Peptide
20.39	1-Tricosene	0.00	2.00	1.18	Lipid
20.43	Tricosane	0.00	2.09	0.65	Lipid
21.24	1-Tetracosene	0.00	2.00	2.30	Lipid
21.41	2-Nonadecanone	0.05	2.00	0.67	Lipid
22.08	1-Pentacosene	0.00	2.00	3.07	Lipid
22.30	17-Octadecenoic acid, methyl ester	0.11	1.89	1.77	Lipid
22.85	1-Hexacosene	0.00	2.00	2.55	Lipid
22.97	Hexacosane	0.00	2.08	0.66	Lipid
23.75	1-Heptacosene	0.00	2.00	2.33	Lipid
24.02	Tetracosanoic acid, methyl ester	0.08	2.00	1.07	Lipid
24.65	1-Octacosene	0.00	2.00	1.75	Lipid
25.79	1-Nonacosene	0.00	2.00	0.85	Lipid
25.89	Nonacosane	0.00	2.07	0.71	Lipid

27.06	1-Triacontene	0.00	2.00	0.95	Lipid
28.50	1-Henetriacontene	0.06	2.00	0.58	Lipid
28.85	Anthracene, 9,10-bis(2-methoxyphenyl)	0.07	0.79	0.77	PAH
29.01	17-Androstanone, 1-(3,4-dimethylphenyl)-1-methyl	0.04	1.43	0.36	Sterane
29.19	Clionasterol	0.03	1.72	0.38	Sterane
29.83	Stigmastan-3,5-diene	0.00	1.66	0.88	Sterane

PAH = Polycyclic Aromatic Hydrocarbon

Table S2. Organic compounds released by analytical pyrolysis for 2–5cm burned soil sample

Retention time (min)	Compound name	O/C	H/C	Relative intensity (%)	Family
2.65	Methylamine, <i>N,N</i> -dimethyl-	0.00	3.00	14.95	Peptide
2.70	Furan, 2-methyl	0.20	1.20	4.02	Polysaccharide
3.01	Benzene	0.00	1.00	7.78	Aromatic
3.53	Pyridine	0.00	1.00	3.79	Peptide
3.67	Toluene	0.00	1.14	6.26	Aromatic
4.17	Furfural	0.40	0.80	5.36	Polysaccharide
4.45	Benzene, ethyl	0.00	1.25	0.97	Aromatic
4.52	<i>o</i> -Xylene	0.00	1.25	2.87	Aromatic
4.62	1-Nonene	0.00	2.00	1.16	Lipid
4.75	Benzene, 1,3-dimethyl	0.00	1.25	2.68	Aromatic
5.45	2-Furancarboxaldehyde, 5-methyl-	0.33	1.00	1.00	Polysaccharide
5.48	Benzaldehyde	0.14	0.86	1.16	Lipid
5.54	Phenol	0.17	1.00	2.86	Aromatic
5.74	Benzonitrile	0.00	0.71	1.72	N-comp
5.84	Benzene, 1,2,4-trimethyl-	0.00	1.33	1.52	Aromatic
5.92	Benzofuran	0.13	0.75	1.29	Polysaccharide
6.19	<i>p</i> -Cymene	0.00	1.40	2.60	Aromatic
6.69	Phenol, 3-methyl-	0.14	1.14	0.87	Aromatic
6.72	Ethanone, 1-phenyl-	0.13	1.00	0.71	Aromatic
7.89	Phenol, 3-ethyl-	0.13	1.25	0.90	Aromatic
8.43	Azulene	0.00	0.80	1.49	PAH
9.90	Naphthalene, 1-methyl-	0.00	0.91	1.08	PAH
10.79	1-Tetradecene	0.00	2.00	0.46	Lipid
10.96	Biphenyl	0.00	0.83	0.63	PAH
11.60	Naphthalene, 2,7-dimethyl-	0.00	1.00	0.84	PAH
12.06	1-Pentadecene	0.00	2.00	0.89	Lipid
12.15	Pentadecene	0.00	2.13	0.46	Lipid
12.36	Naphthalene,1,2,3,4-tetrahydro-2,2,5,7-tetramethyl	0.00	1.43	0.48	PAH
12.43	2H-Inden-2-one,1,3-dihydro-1,1,3,3-tetramethyl-	0.08	1.23	0.61	PAH
12.77	1S, <i>Cis</i> -calamenene	0.00	1.47	0.78	Aromatic
12.83	Dibenzofuran	0.08	0.67	0.88	Polysaccharide
13.18	Benzene, nonyl	0.00	1.60	0.85	Aromatic
13.29	7-Hexadecene, (Z)-	0.00	2.00	0.69	Lipid
13.34	Hexadecane	0.00	2.13	1.50	Lipid
14.45	1-Heptadecene	0.00	2.00	0.53	Lipid
14.53	Heptadecane	0.00	2.12	0.58	Lipid
14.63	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	0.00	1.20	1.74	Aromatic

14.88	1-Octadecene	0.00	2.00	0.52	Lipid
15.01	3-Undecene, 2-methyl	0.00	2.00	0.52	Lipid
15.40	1,4,5,8-Tetramethylnaphthalene	0.00	1.14	0.58	PAH
15.51	9H-Fluoren-9-one	0.08	0.62	0.64	PAH
15.56	1-Nonadecene	0.00	2.00	0.60	Lipid
16.01	9H-Fluorene, 9-methylene-	0.00	0.71	0.53	PAH
16.62	1-Eicosene	0.00	2.00	0.40	Lipid
16.67	Eicosane	0.00	2.10	0.36	Lipid
16.75	Hexadecanenitrile	0.00	1.94	0.91	N-comp
17.62	1-Heneicosene	0.00	2.00	0.41	Lipid
17.68	Heneicosane	0.00	2.10	0.11	Lipid
18.59	1-Docosene	0.00	2.00	0.64	Lipid
18.64	Docosane	0.00	2.09	0.49	Lipid
19.51	1-Tricosene	0.00	2.00	3.84	Lipid
19.56	Tricosane	0.00	2.09	0.77	Lipid
19.59	Tricosane	0.00	2.09	1.16	Lipid
20.39	1-Tetracosene	0.00	2.00	0.92	Lipid
20.43	Tetracosane	0.00	2.08	0.59	Lipid
21.24	1-Pentacosene	0.00	2.00	2.45	Lipid
21.31	Pentacosane	0.00	2.08	0.48	Lipid
21.48	13-Methyl-Z-14-nonacosene	0.00	2.00	0.48	Lipid
22.09	1-Hexacosene	0.00	2.00	1.17	Lipid
22.31	Nitrile	0.00	1.94	0.91	N-comp
22.85	1-Heptacosene	0.00	2.00	1.03	Lipid
22.91	Heptacosane	0.00	2.07	0.55	Lipid

PAH = Polycyclic Aromatic Hydrocarbon; N-comp = Nitrogen compounds.