

Supplementary material

Long-term watershed management is an effective strategy to reduce organic matter export and disinfection by-products (DBPs) precursors in source water

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Factor analysis on duff water extracts

For the duff water extracts, the first two factors of F1 and F2 explained 33.2% and 23.0% of the total variance (Figure S1). The samples at managed watershed had the scores of F1 < 0 and F2 < 0 (except one sample), while the samples at unmanaged watershed had F1 > 0 and F2 > 0. According to the location of sample scores, it is useful to have the interpretations of F1<0 & F2<0 and F1>0 & F2>0, respectively. For the interpretation of F1<0 & F2<0, we observed 2 out of 3 identified LgC (2/3 LgC), 1/3 PhC, 11/30 Carb, and 10/32 Ntg had F1 loadings < -0.50 or F2 loadings < -0.50. For the interpretation of F1>0 & F2>0, we observed 1/3 PhC, 11/30 Carb, 1/1 Un, 17/32 Ntg, 4/6 ArH, and 1/1 PAH had F1 loadings > 0.50 or F2 loadings > 0.50. Furans and levoglucosenone, as the markers of polysaccharides (cellulose and hemicellulose) (Buurman et al., 2008; Conti et al., 2014), was found in two regions of F1 loadings < -0.50 or F2 loadings < -0.5 (Ca4, Ca6, Ca7) and F1 loading > 0.50 or F2 loadings > 0.50 (Ca2, Ca3, Ca5, Ca8, Ca13). 2-cyclopentene-1-methanol (Ca9) with F1 loading > 0.5 is the compound based on cyclopentenone, as the known pyrolysates of polysaccharide (Dignac et al., 2006). Carb with alkene(s) or alkyne(s) and without aromatic ring(s) were only found in the region of F1 loadings < -0.50 or F2 loadings < -0.5 (Ca1, Ca15, Ca16, Ca19). Pyrrole (Nt7, Nt8, Nt22), pyrazole (Nt3, Nt10, Nt17), indazole (Nt23, Nt26) were found only in the region of F1 loading > 0.50 or F2 loadings > 0.50. Therefore, the region of F1 loading > 0.50 or F2 loadings > 0.50 (unmanaged watershed) could be interpreted as aromatic carbon/nitrogen, while the region of F1 loadings < -0.50 or F2 loadings < -0.5 (managed watershed) as unsaturated carbohydrates.

Factor analysis on litter water extracts

The first two factors of F1 and F2 explained 32.3% and 22.8% of the total variance (Figure S2). The samples at managed watershed had the scores of F2 > 0 (except one sample), while the samples at unmanaged watershed had F2 < 0. For the F1 interpretation, we observed 10/31 Carb, 1/1 Un, 11/30 Ntg, 8/10 ArH, and 2/2 PAH had F1 loadings > 0.50 and 3/5 LgC, 1/4 PhC, 3/31 Carb, 3/30 Ntg, and 1/10 ArH had F1 loading < -0.50. The positive F1 could be interpreted as aromatic hydrocarbons, while negative F1 as lignin compounds. For the F2 interpretation, we observed 1/5 LgC, 12/31 Carb, 1/1 Sa, 1/1 Un, 6/30 Ntg, and 1/10 ArH had F2 loadings > 0.50 and 5/31 Carb, 7/30 Ntg, and 1/10 ArH had F2 loading < -0.50. Pyrrole (Nt22), pyrazole (Nt3, Nt17), indazole (Nt23) had F2 loadings < -0.50, suggesting native F2 (unmanaged watershed) could be interpreted as aromatic nitrogen.

Table S1. Identified and quantified pyrolyrates from the water extracts of litter and duff samples at managed and unmanaged watersheds.

ID	Compounds	CAS	MajorP
Ar1	1,3-Cyclopentadiene	542-92-7	66,65,39
Ar2	Benzene	71-43-2	78
Ar3	Toluene	108-88-3	91,92
Ar4	Ethylbenzene	100-41-4	91
Ar5	p-Xylene	106-42-3	91,106
Ar6	Benzene, 1,2,4-trimethyl-	95-63-6	105,120
Ar7	Benzene, 1,3,5-trimethyl-	108-67-8	105,120
Ar8	1-Phenyl-1-butene	824-90-8	117,132,115
Ar9	Benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	119
Ar10	Benzene, 4-ethyl-1,2-dimethyl-	934-80-5	119
Ca1	3-Penten-1-ol	39161-19-8	55,68,56,41,29,43,31,39,27
Ca2	Furan, 3-methyl-	930-27-8	82,53,81,39,54,51
Ca3	Furfural	98-01-1	96,95,39,29
Ca4	Levogluconone	37112-31-5	98,96,39,53,68,97,42,41,70,29
Ca5	Furan, 2-ethyl-	3208-16-0	81,96
Ca6	Furan, 2,5-dimethyl-	625-86-5	96,95,43,53,81
Ca7	2-Furancarboxaldehyde, 5-methyl-	620-02-0	110,109,53
Ca8	Ethanone, 1-(2-furanyl)-	1192-62-7	95,39,110
Ca9	2-Cyclopentene-1-methanol	13668-59-2	67
Ca10	2-Cyclopentylethanol	766-00-7	67,68,41,55
Ca11	2(3H,4H)-Cyclopenta[b]furanone, 3a,6a-dihydro-	-	79,80
Ca12	1,3,4-Hexatriene, 3-methoxy-	53783-88-3	28,45,77,39,41,79,95,51,67,29
Ca13	Furan, 2-ethyl-5-methyl-	1703-52-2	95
Ca14	5-Octyn-3-ol	53723-18-5	67,68,41,59,31,39,53,29,27
Ca15	cis-2-Ethyl-2-hexen-1-ol	-	41,27,55,57,39,43,29,85,81
Ca16	1-Methoxymethoxy-hexa-2,4-diene	-	45,81,41
Ca17	2,6-Nonadienal, (E,Z)-	557-48-2	41,70,69
Ca18	2H-Pyran, 2-(3-butynyloxy)tetrahydro-	40365-61-5	40,55,85,39,84,41,53,56,83
Ca19	6-Nonynoic acid	56630-31-0	41,39,79,67,27,45,94,53
Ca20	Phenol, 2-methoxy-, acetate	613-70-7	124,109,43
Ca21	2,6-Nonadien-1-ol	7786-44-9	41,69,27,39,68
Ca22	Benzofuran, 2-methyl-	4265-25-2	131,132
Ca23	2-Pentanol, 1-(2-methylenecyclopropyl)-4-methyl-	-	69,68,43,41,45,67
Ca24	3,5-Heptadienal, 2-ethylidene-6-methyl-	99172-18-6	107,91,79,150,41,77,135,39,105,27
Ca25	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-	7764-50-3	67,95,41,68,81,82,55,39,69,109
Ca26	Benzofuran, 4,7-dimethyl-	28715-26-6	146,145
Ca27	Hexane, 1-(2,2-dimethoxyethoxy)-	17597-95-4	75,43,47
Ca28	4-Oxo-4-(para-tolyl)-butyric acid	4619-20-9	119,91
Ca29	Methyl 3-hydroxy-decanoate	-	103,71
Ca30	1-Acetoxy-p-menth-3-one	58315-85-8	82,110,43,41,95,85,39,109,55,44
Ca31	Geranyl vinyl ether	-	69,41
Ca32	9-Methoxycalamene	-	157,200,217,142

Ca33	2,9-Heptadecadiene-4,6-diyn-8-ol, (Z,E)-	50816-77-8	91,41,159,43,117,55,131,145,115,29
Lg1	2-Furanmethanol	98-00-0	98,41,81,97,39,53,42,27
Lg2	Maltol	118-71-8	126,71
Lg3	Benzaldehyde, 3-hydroxy-4-methoxy-	621-59-0	151,152
Lg4	2,4-Dimethoxyphenol	13330-65-9	154,139,111,79,155,53,96,52
Lg5	2-Methoxy-4-vinylphenol	7786-61-0	135,150,107,77
Nt1	Methanamine, N-methoxy-	1117-97-1	46,61,28
Nt2	2-Propenamide	79-06-1	27,44,71,55,26
Nt3	5-Amino-3-methylpyrazole	31230-17-8	97
Nt4	Glycylsarcosine	29816-01-1	128,30,42,44,43,71
Nt5	2-Butynamide, N-methyl-	63798-30-1	67,97,96,39
Nt6	Pyridine	110-86-1	79,52,51,50
Nt7	1H-Pyrrole, 1-methyl-	96-54-8	81,80,39,42,53
Nt8	1H-Pyrrole, 2-methyl-	636-41-9	80,81
Nt9	2-Pyrrolidinone, 1-methyl-	872-50-4	99,44,42,98,28,41
Nt10	Pyrazole-4-carboxaldehyde, 1-methyl-	25016-11-9	109,110
Nt11	1-Pentene, 5-nitro-	23542-51-0	41,39,67
Nt12	3-Methylpyridazine	1632-76-4	94,39,40,65
Nt13	5-Vinyl-pyrazole	-	94
Nt14	2-Pyrroline, 1,2-dimethyl-	5370-57-0	94,96,45,97,95,42,29,40,27,69
Nt15	Acetic acid, 2-(2-pyrrolidinylideneamino)-	-	41,97,98,69,55,68,42
Nt16	1H-Imidazole, 2,4,5-trimethyl-	822-90-2	42,95,109,54,110,41,68
Nt17	1H-Pyrazole, 1,3,5-trimethyl-	1072-91-9	110,109
Nt18	3,4,5-Trimethylpyrazole	5519-42-6	109,110,95
Nt19	Pyridine, 3-methyl-	108-99-6	93,66,92
Nt20	Piperidine, 1,3-dimethyl-	695-35-2	112,43,58,42,113
Nt21	Benzonitrile	100-47-0	103,76
Nt22	1H-Pyrrole-2-acetonitrile, 1-methyl-	24437-41-0	120,119,94
Nt23	1H-Indazole, 3-methyl-	-	132,131
Nt24	Acetylhydrazide, 2-hydroxy-N2-(3-pyridylmethylene)-	-	105,63,51,39,120
Nt25	4-Methyl-6-propyloxyhexahydropyrimidin-2-thione	-	128,113,43,86,129,44,130,71,41,42
Nt26	1H-Indazole, 5,7-dimethyl-	43067-41-0	146,145,131
Nt27	2,2-Diallylpyrrolidine	40162-97-8	110
Nt28	Formamide, N-methyl-N-4-[1-(pyrrolidinyl)-2-butynyl]-	18327-40-7	70,42,108,55,41,43,120,110,121
Nt29	Uridine, 5-methyl-	1463-10-1	126,127,55,73,57,133
Nt30	Ethyl 3-(3-pyridyl)propenoate	28447-17-8	132,104,51,133
Nt31	3,4-Dimethoxy-dl-phenylalanine	33522-62-2	151
Nt32	1-[2-Pyridyl]-2,2-dimethyl-2-morpholino ethanol	-	128
Nt33	Propanamide, N-(2-fluorophenyl)-3-(4-morpholy)-	284679-89-6	114
Nt34	Phenethylamine, N-hexyl-	24997-83-9	44,114,43
PA1	Naphthalene, 1,3-dimethyl-	575-41-7	156,141
PA2	Naphthalene, 1,6,7-trimethyl-	2245-38-7	170,155
Ph1	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	112,69,55
Ph2	Hydroquinone	123-31-9	110
Ph3	Phenol	108-95-2	94,66
Ph4	Phenol, 3-methyl-	108-39-4	108,107,79,39
Sa1	Cyclopentane, 1,1'-ethylidenebis-	4413-21-2	97,55,41,68
Un1	4-t-Pentylcyclohexene	51874-62-5	71,70,67,43,81,41

Table S2. Concentrations of identified and quantified pyrolysates and their loadings on factor analysis.

ID	Litter in WS77		Litter in WS80		Litter		Duff in WS77		Duff in WS80		Duff	
	n	mean(sd)	n	mean(sd)	F1	F2	n	mean(sd)	n	mean(sd)	F1	F2
Ar1	4	1.06(0.16)	5	1.66(0.30)	0.71	-0.23	4	0.94(0.22)	5	1.07(0.41)	0.43	0.50
Ar2	4	2.38(0.43)	5	2.90(0.97)	0.94	-0.03	4	2.68(0.86)	5	2.18(0.83)	0.39	0.01
Ar3	5	6.77(3.50)	5	10.81(3.50)	0.95	-0.15	5	7.34(3.51)	5	10.16(2.21)	0.71	0.39
Ar4	4	0.89(0.30)	5	0.99(0.38)	0.94	0.09	3	0.61(0.05)	5	1.01(0.28)	0.04	0.95
Ar5	5	4.22(2.17)	5	6.40(1.68)	0.96	-0.07	5	3.21(1.62)	5	5.11(1.22)	0.78	0.46
Ar6	1	1.39(-)	0	-	0.25	0.52	0	-	0	-	-	-
Ar7	5	1.15(0.50)	5	1.56(0.41)	0.83	-0.04	4	0.32(0.09)	5	0.86(0.45)	0.25	0.71
Ar8	4	0.42(0.16)	0	-	-0.70	0.32	0	-	0	-	-	-
Ar9	0	-	1	0.39(-)	0.16	-0.15	0	-	0	-	-	-
Ar10	0	-	3	0.28(0.07)	0.56	-0.59	0	-	0	-	-	-
Ca1	2	0.98(0.92)	0	-	0.25	0.61	1	0.60(-)	0	-	-0.15	-0.52
Ca2	5	8.37(1.60)	5	11.51(2.26)	0.55	-0.58	5	10.36(3.11)	5	12.71(0.51)	1.00	0.10
Ca3	3	0.74(0.10)	5	6.12(2.35)	0.66	-0.72	5	2.20(2.58)	5	7.95(1.51)	0.79	0.59
Ca4	0	-	0	-	-	-	3	1.20(0.90)	0	-	-0.67	-0.18
Ca5	4	0.90(0.16)	5	1.24(0.27)	0.93	-0.15	4	0.74(0.08)	5	1.31(0.07)	-0.07	0.87
Ca6	5	4.74(1.68)	5	1.26(0.30)	-0.06	0.93	5	4.10(1.73)	5	1.05(0.29)	-0.80	-0.44
Ca7	5	6.70(3.87)	1	1.41(-)	-0.86	0.29	4	9.02(0.56)	4	2.62(1.38)	-0.93	-0.37
Ca8	5	3.39(0.85)	5	4.44(0.98)	0.35	-0.60	5	3.30(1.08)	5	4.05(0.97)	0.71	0.12
Ca9	0	-	2	1.32(0.09)	0.51	-0.47	1	1.31(-)	3	1.96(0.99)	0.66	0.31
Ca10	4	0.95(0.40)	0	-	0.06	0.93	1	1.19(-)	0	-	-0.45	-0.15
Ca11	4	0.85(0.32)	5	1.21(0.30)	0.96	-0.14	2	0.54(0.15)	5	0.80(0.49)	0.19	0.80
Ca12	2	0.29(0.10)	0	-	0.17	0.63	2	0.12(0.05)	0	-	-0.49	-0.40
Ca13	4	0.87(0.23)	5	1.11(0.31)	0.97	-0.06	5	0.86(0.28)	5	1.33(0.18)	0.80	0.49
Ca14	5	5.30(2.07)	4	7.23(1.27)	0.25	0.29	5	6.93(2.43)	5	7.90(0.95)	0.87	0.03
Ca15	1	0.55(-)	0	-	-0.01	0.41	3	0.74(0.14)	0	-	-0.59	-0.37
Ca16	0	-	0	-	-	-	3	0.22(0.10)	0	-	-0.46	-0.53
Ca17	4	0.31(0.07)	4	0.40(0.10)	0.80	0.15	2	0.28(0.02)	3	0.27(0.12)	-0.26	0.37
Ca18	4	1.23(0.21)	0	-	-0.08	0.93	4	1.94(0.25)	0	-	-0.83	-0.48
Ca19	3	0.50(0.13)	0	-	0.09	0.84	2	0.49(0.03)	0	-	-0.65	-0.15
Ca20	5	3.60(1.19)	0	-	-0.46	0.74	4	1.46(1.10)	0	-	-0.50	-0.59
Ca21	0	-	5	0.35(0.15)	0.54	-0.73	0	-	2	0.38(0.26)	0.35	0.42
Ca22	4	0.83(0.13)	0	-	0.03	1.00	4	0.57(0.07)	0	-	-0.86	-0.43
Ca23	3	0.34(0.13)	0	-	-0.15	0.67	0	-	0	-	-	-
Ca24	4	0.94(0.20)	4	1.08(0.37)	0.38	0.21	4	0.42(0.09)	4	0.86(0.44)	0.09	0.57
Ca25	2	0.38(0.08)	0	-	-0.09	0.50	0	-	0	-	-	-
Ca26	4	0.72(0.15)	5	0.81(0.17)	0.98	0.11	3	0.44(0.03)	5	0.81(0.10)	0.04	1.00
Ca27	2	0.41(0.05)	0	-	0.00	0.62	2	0.38(0.00)	0	-	-0.45	-0.50
Ca28	0	-	4	0.52(0.08)	0.62	-0.66	0	-	4	0.45(0.09)	0.42	0.67
Ca29	0	-	1	0.40(-)	0.37	-0.38	0	-	1	0.38(-)	0.30	0.27
Ca30	2	1.37(1.82)	0	-	-0.84	-0.25	2	0.71(0.21)	0	-	-0.49	-0.43
Ca31	2	0.13(0.02)	0	-	-0.14	0.56	1	0.12(-)	0	-	-0.34	-0.06
Ca32	3	0.40(0.27)	0	-	-0.90	-0.04	0	-	0	-	-	-
Ca33	0	-	2	0.29(0.00)	0.03	-0.39	0	-	2	0.22(0.05)	0.13	0.23
Lg1	2	0.86(0.08)	0	-	0.17	0.70	0	-	0	-	-	-
Lg2	2	0.93(0.28)	0	-	-0.58	0.08	3	1.01(0.26)	0	-	-0.77	-0.15
Lg3	3	0.86(0.82)	0	-	-0.91	-0.12	2	0.47(0.07)	0	-	-0.43	-0.53
Lg4	0	-	2	1.37(1.43)	0.42	-0.42	0	-	3	0.99(0.86)	0.19	0.47
Lg5	1	1.75(-)	0	-	-0.83	-0.26	0	-	0	-	-	-
Nt1	2	0.18(0.05)	0	-	0.05	0.55	3	0.53(0.23)	0	-	-0.70	-0.31
Nt2	3	1.41(0.35)	4	1.52(0.30)	0.57	0.02	4	1.21(0.30)	5	1.27(0.45)	-0.42	0.65
Nt3	0	-	4	1.28(0.39)	0.38	-0.54	1	0.86(-)	2	1.38(0.25)	0.64	0.25
Nt4	0	-	5	0.46(0.11)	0.59	-0.76	0	-	4	0.44(0.08)	0.39	0.66
Nt5	1	1.37(-)	0	-	-0.20	0.32	4	1.25(0.20)	0	-	-0.83	-0.43
Nt6	0	-	0	-	-	-	1	0.55(-)	0	-	-0.40	-0.05
Nt7	1	0.52(-)	1	1.47(-)	0.36	-0.22	1	0.52(-)	2	0.80(0.24)	0.03	0.53
Nt8	0	-	2	0.75(0.16)	0.51	-0.48	0	-	4	0.99(0.35)	0.37	0.76
Nt9	0	-	0	-	-	-	3	0.83(0.13)	0	-	-0.63	-0.48
Nt10	4	1.49(0.45)	4	4.72(1.19)	0.29	-0.38	5	3.34(1.85)	5	3.50(0.70)	0.91	-0.29
Nt11	0	-	0	-	-	-	1	0.09(-)	0	-	0.66	-0.59

Nt12	4	0.76(0.13)	5	1.18(0.24)	0.77	-0.27	5	0.78(0.26)	5	1.02(0.28)	0.83	0.19
Nt13	0	-	2	0.34(0.12)	0.50	-0.48	0	-	2	0.29(0.23)	0.20	0.50
Nt14	5	24.04(12.55)	4	12.59(8.46)	-0.88	0.20	5	24.22(7.71)	5	7.92(7.77)	-0.58	-0.74
Nt15	0	-	1	1.04(-)	-0.10	-0.26	0	-	2	0.52(0.11)	0.11	0.33
Nt16	2	0.29(0.03)	3	1.27(0.53)	0.15	-0.57	1	0.68(-)	5	0.62(0.29)	0.79	0.33
Nt17	0	-	4	0.54(0.15)	0.63	-0.66	0	-	4	0.42(0.12)	0.35	0.56
Nt18	2	0.46(0.21)	0	-	0.14	0.64	0	-	0	-	-	-
Nt19	0	-	4	0.65(0.39)	0.54	-0.61	4	0.55(0.37)	5	1.40(0.55)	0.60	0.66
Nt20	0	-	0	-	-	-	2	0.82(0.55)	0	-	-0.47	-0.08
Nt21	0	-	1	0.47(-)	0.31	-0.25	0	-	3	0.46(0.09)	0.20	0.65
Nt22	1	1.53(-)	5	3.19(1.90)	0.60	-0.56	0	-	4	1.78(0.94)	0.34	0.64
Nt23	0	-	5	0.99(0.26)	0.58	-0.77	1	0.53(-)	5	1.11(0.26)	0.57	0.60
Nt24	3	1.13(0.53)	0	-	-0.18	0.58	3	0.87(0.10)	0	-	-0.80	-0.17
Nt25	0	-	3	1.40(0.69)	0.04	-0.39	1	1.19(-)	5	1.46(0.22)	0.77	0.57
Nt26	4	0.61(0.14)	5	0.73(0.19)	0.90	0.07	1	0.69(-)	5	0.58(0.09)	0.90	0.42
Nt27	2	0.39(0.00)	0	-	0.04	0.64	3	0.44(0.08)	0	-	-0.62	-0.52
Nt28	1	1.15(-)	0	-	-0.20	0.32	1	1.37(-)	0	-	-0.34	-0.06
Nt29	3	1.36(0.45)	4	1.12(0.12)	0.07	0.20	4	1.25(0.67)	3	1.48(0.37)	0.38	-0.28
Nt30	4	0.47(0.15)	5	0.56(0.12)	0.94	0.03	5	0.42(0.12)	5	0.56(0.08)	0.75	0.44
Nt31	4	0.53(0.39)	0	-	-0.93	0.05	2	0.29(0.03)	0	-	-0.60	-0.16
Nt32	2	0.49(0.08)	0	-	-0.14	0.56	4	0.53(0.07)	0	-	-0.84	-0.44
Nt33	4	1.95(0.87)	0	-	-0.87	0.23	4	2.69(0.84)	0	-	-0.75	-0.49
Nt34	3	0.37(0.22)	0	-	-0.22	0.58	0	-	0	-	-	-
PA1	5	0.61(0.34)	5	0.75(0.31)	0.74	0.12	1	0.22(-)	4	0.41(0.27)	0.58	0.50
PA2	4	0.27(0.08)	5	0.31(0.11)	0.74	0.08	0	-	0	-	-	-
Ph1	4	1.08(0.67)	3	1.16(0.72)	-0.25	0.02	4	1.50(0.50)	3	1.34(0.52)	-0.62	-0.17
Ph2	1	1.60(-)	0	-	-0.83	-0.26	0	-	0	-	-	-
Ph3	3	4.05(1.38)	4	5.97(5.61)	-0.23	-0.35	1	2.37(-)	3	7.42(4.18)	0.06	0.41
Ph4	5	2.79(0.72)	5	3.33(1.23)	-0.03	-0.13	5	2.27(0.98)	5	5.32(3.01)	0.18	0.51
Sa1	3	1.29(0.24)	0	-	0.14	0.83	0	-	0	-	-	-
Un1	2	1.06(0.37)	4	1.11(0.10)	0.64	-0.14	5	0.79(0.26)	5	0.71(0.11)	0.70	-0.47

-: not available; The F1 or F2 loading with the absolute value ≥ 0.50 was bold.

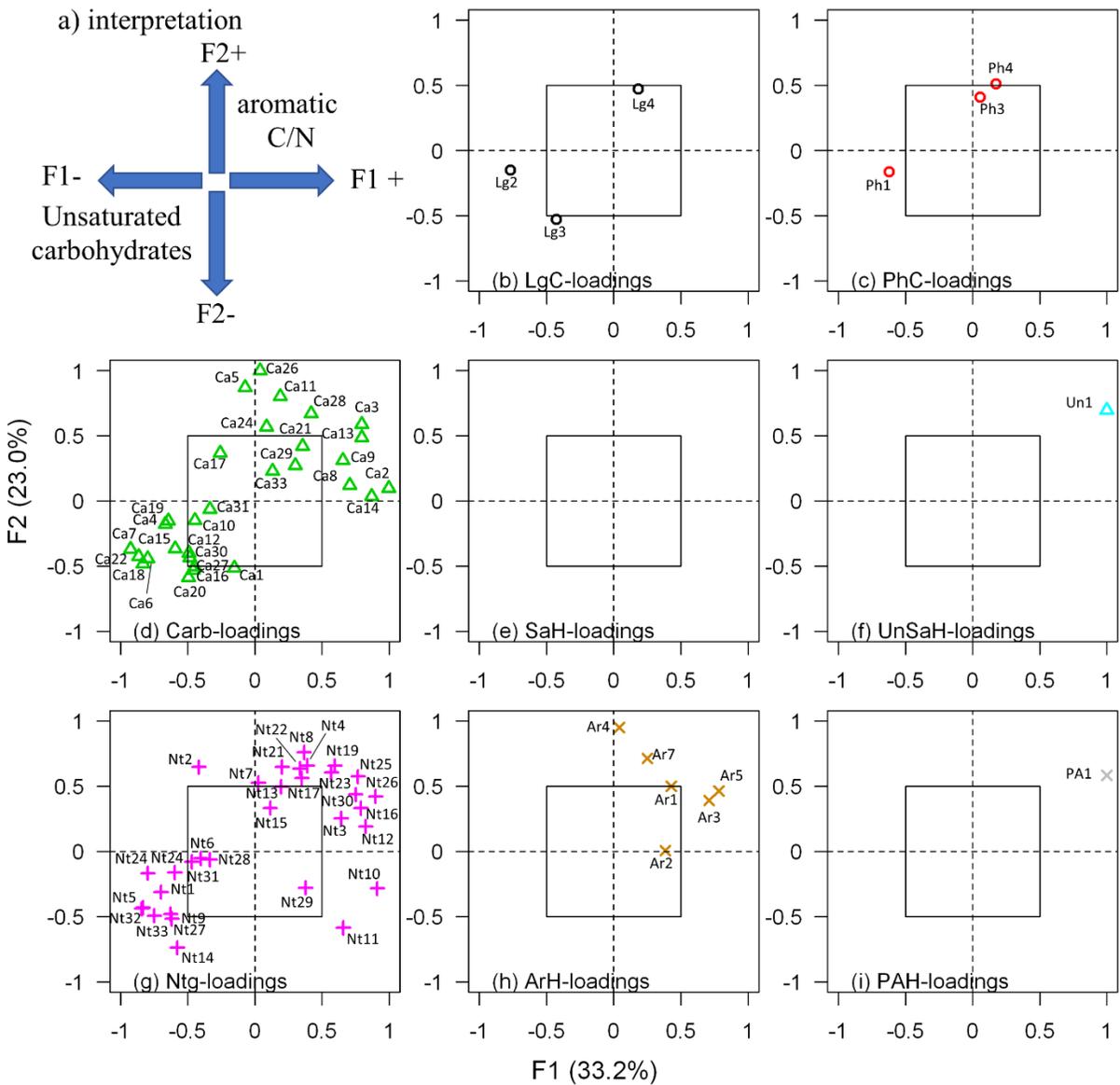


Figure S1. Loadings of chemical classes in factor analysis on the pyrolysates of the duff samples. LgC: lignin compounds; PhC: phenol compounds; Carb: carbohydrates; SaH: saturated hydrocarbons; UnSaH: unsaturated hydrocarbons; Ntg: nitrogen-containing compounds; ArH: aromatic hydrocarbons; and PAH: polyaromatic hydrocarbons.

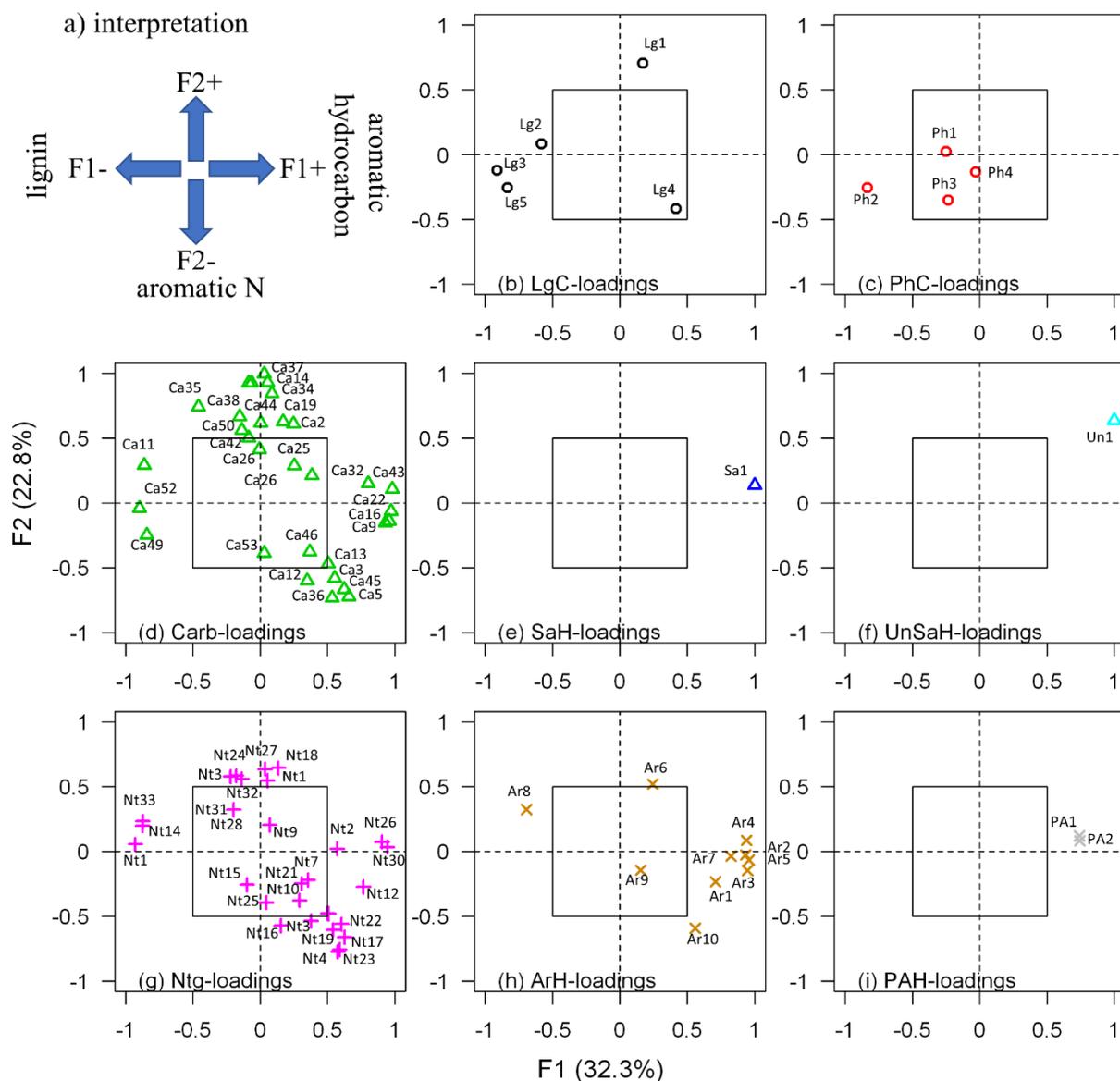


Figure S2. Loadings of chemical classes in factor analysis on the pyrolysates of the litter samples. LgC: lignin compounds; PhC: phenol compounds; Carb: carbohydrates; SaH: saturated hydrocarbons; UnSaH: unsaturated hydrocarbons; Ntg: nitrogen-containing compounds; ArH: aromatic hydrocarbons; and PAH: polyaromatic hydrocarbons.