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Dissolved organic matter concentration and composition discontinuity at the peat–pool interface in a boreal peatland

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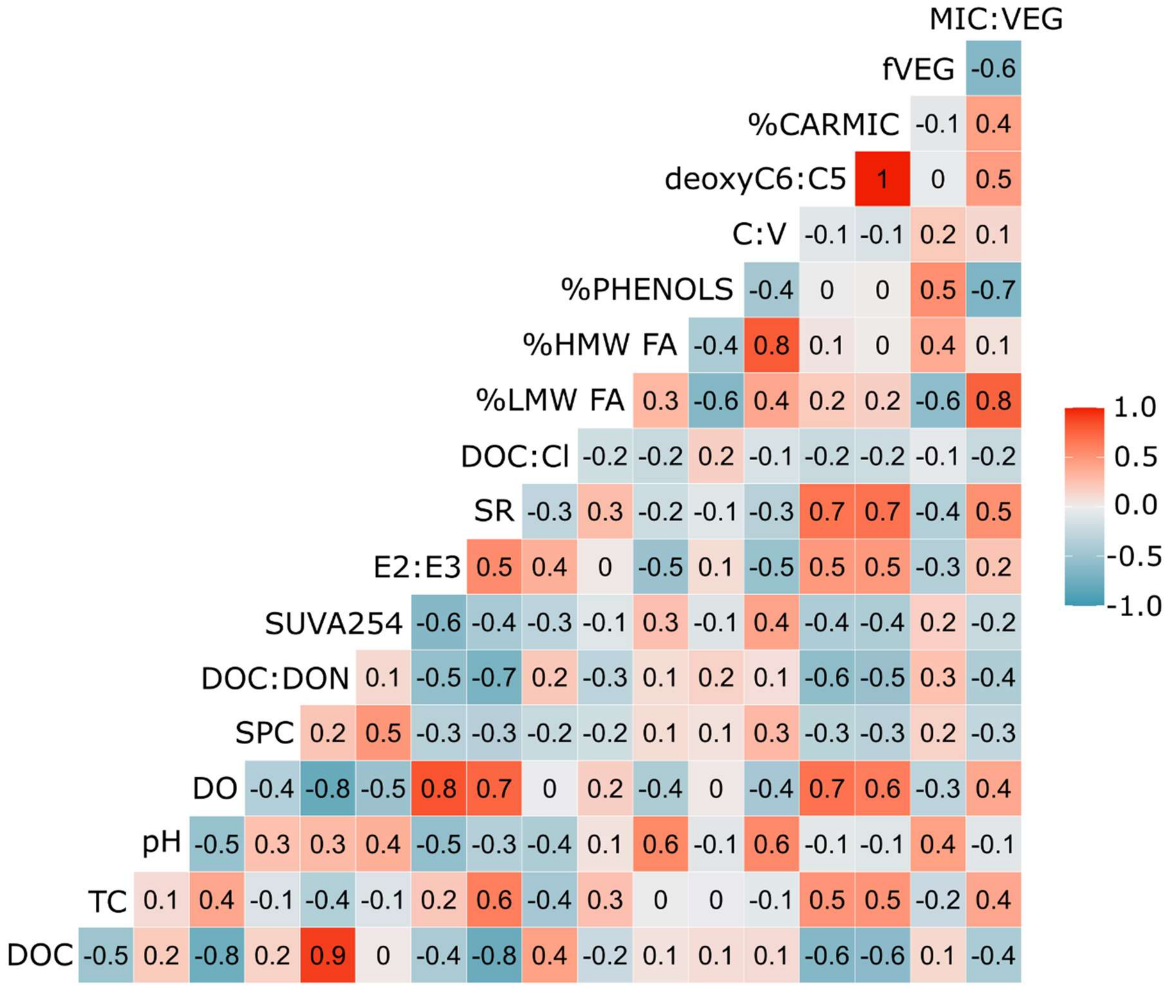


Figure S1. Correlation plot of punctual variables as physico-chemical parameters (water temperature, pH, dissolved oxygen and specific Conductivity), DOC concentrations, DOC:DON ratio. DOC:Cl ratio, absorbance indices ($SUVA_{254}$, E2:E3 ratio and S_R), and molecular index (deoxyC6:C5 ratio, fVEG, C/V ratio), molecular family proportions (%Phenols, %SmallOrganicAcids, %Microbial Carbohydrates, %LowMolecularWeight FattyAcids, %HighMolecularWeight FattyAcids).

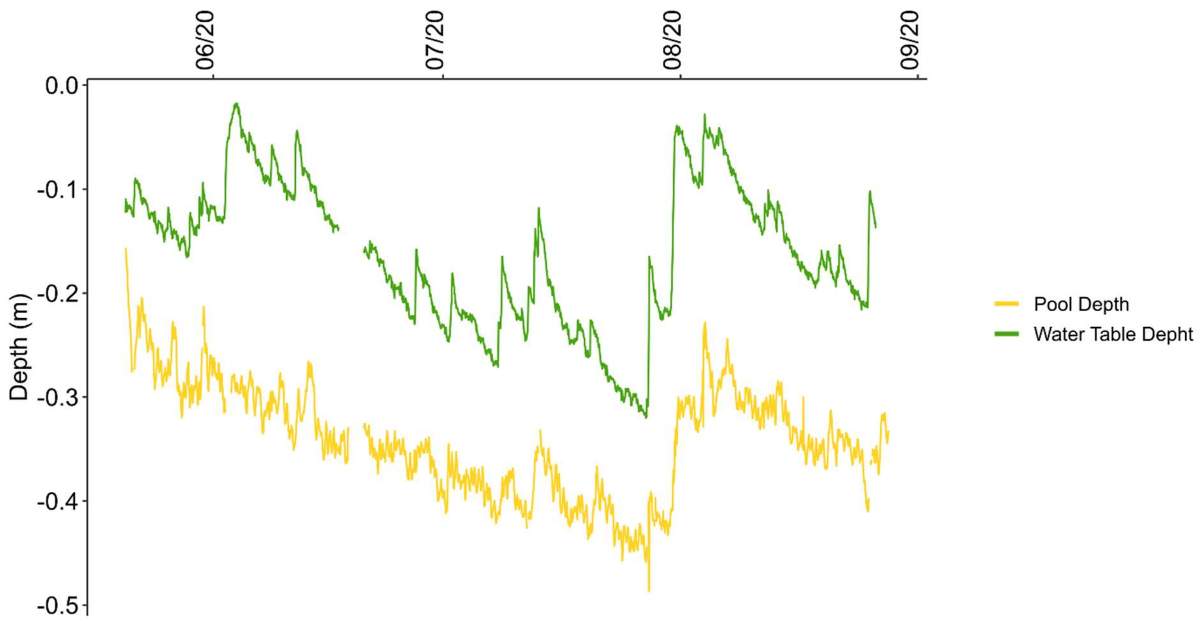


Figure S2. Variation of pool depth as the difference between peat surface at a reference point and water surface and water table depth at the reference point.

Table S1. Synthesis of samples number per analyses per campaigns.

Year	Campaign	Environment	Analyses					
			DOC; DOC:DON	Isotopic	Absorbance	Fluorescence	Molecular	Incubation
2018	June	Porewater	5	1	5			
		Pools	6	2	4			
	July	Porewater	4	2	4		3	
		Pools	6	3	6		3	
	August	Porewater	6		6		3	
		Pools	6		6		3	
	September	Porewater	4	2	4		3	
		Pools	6	3	6		3	
	October	Porewater						
		Pools	6	2	6			
2019	June	Porewater	6	3	6	6	2	x
		Pools	11	3	11	11	2	x
	August	Porewater	6	3	5	5	1	x
		Pools	11	3	11	11	3	x
	September	Porewater	5	5	5	4	3	x
		Pools	11	3	11		2	x
	October	Porewater	5	3	5	5	3	
		Pools	5	3	5	5	3	

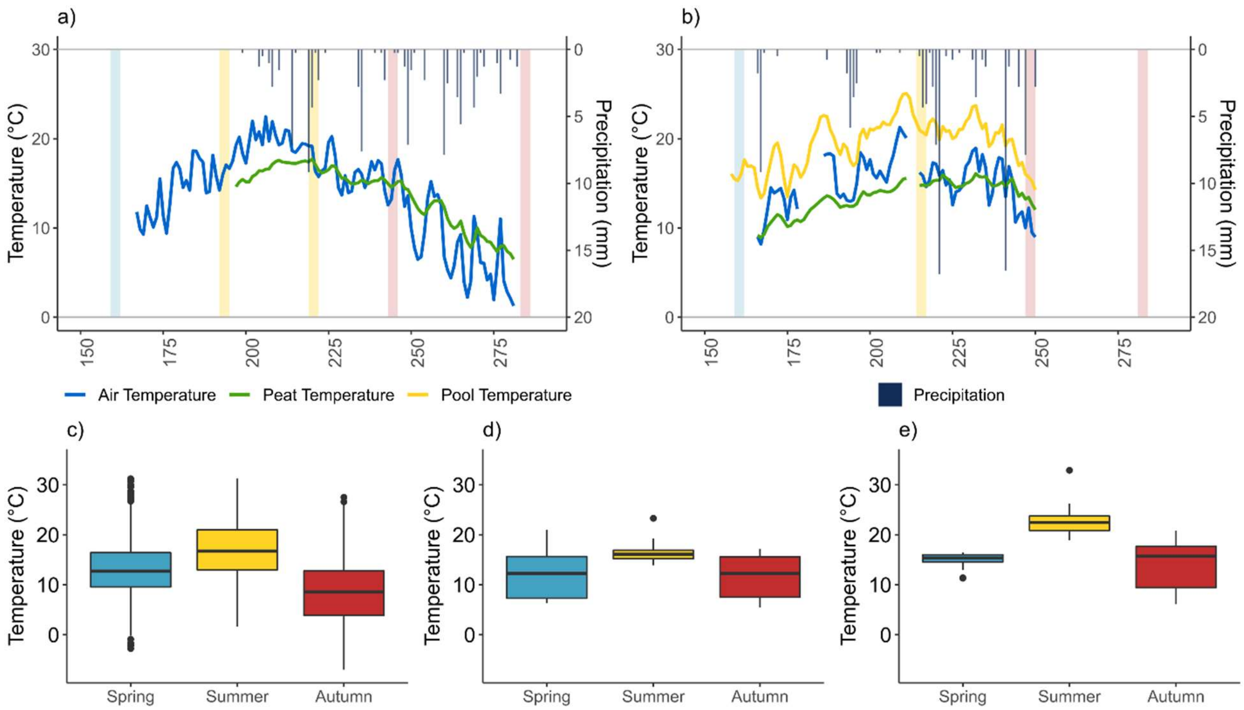
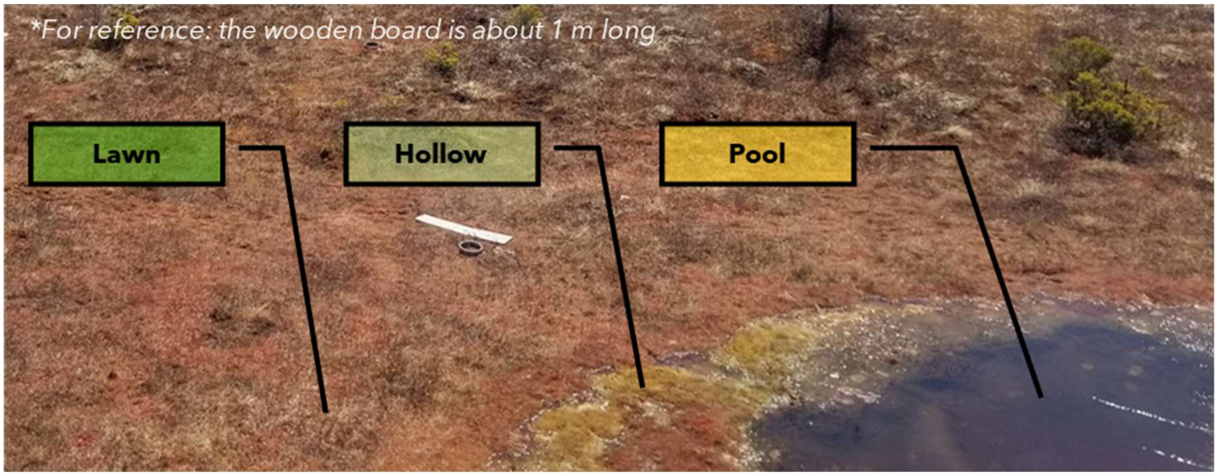


Figure S3. Daily average air, peat temperature and pool temperature (for 2019 exclusively) and precipitation in a) 2018 and b) 2019. Vertical band represented sampling period and color depending on seasons (blue = spring, yellow = summer, red = tumn). Box plot of seasonal c) air temperature, punctual measurements of d) peat porewater and e) pool water temperatures. For boxplot, box represented the lower (25th percentile) and the upper quartile (75th percentile) and median (50th percentile), whiskers represented the interquartile range.

Samples from the two studied years were pooled according to seasons. In this study, seasons were defined based on air and water temperatures measured at the site (Fig. SI.3). Spring was defined from the end of the seasonal thaw that occurred in May to the end of June. Summer included the months of July and August when air and water temperatures were at their warmest. Finally, the autumn season corresponded to the months of September and October when air and water temperature decreased to zero.

a)



b)

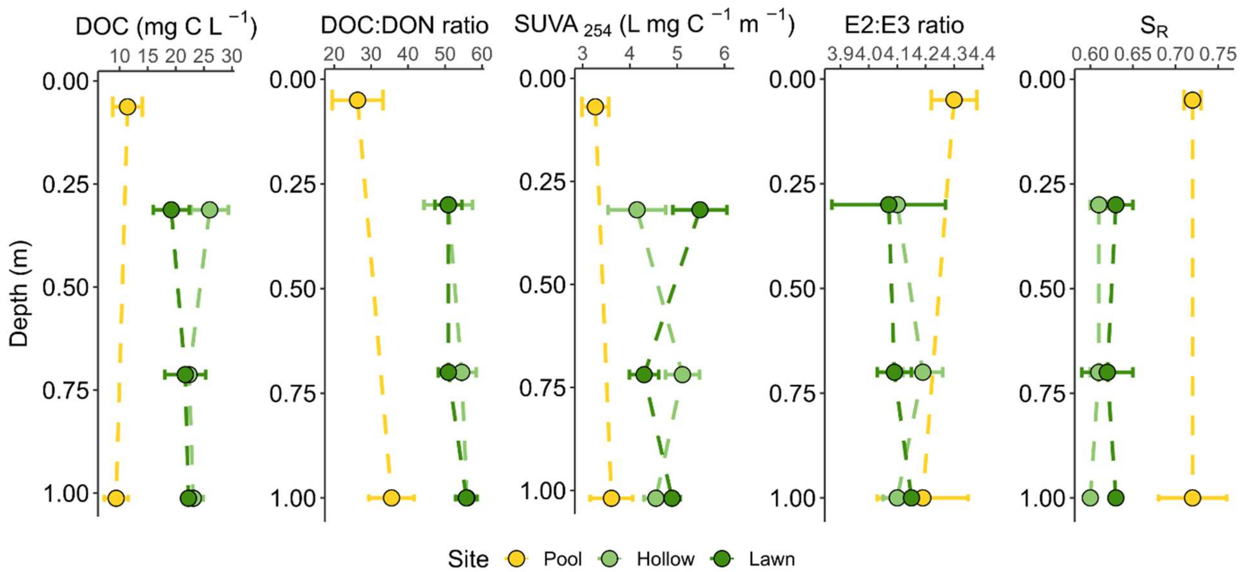


Figure S4. a) Picture of the sampled pool, hollow and lawn. **b)** Variations of DOC concentrations (in mg C L^{-1}), DOC:DON ratio, $SUVA_{254}$ (in L mg C^{-1} cm^{-1}), E2:E3 ratio and spectral slope ratio in two contiguous microforms (one lawn and one hollow) and their adjacent pool (M11 on Fig. 1) at 3 depths in peat porewater (-0.3 m, -0.75 m and -1 m) and at the surface and in depth of the pool. Samples were taken in June, August, and September 2019 using a tubes of 3 mm of diameter inserted into peat and collected into a bottle connected to a manual peristaltic pump. Points represents the average of each variable and error bar the standard deviation. Variables were always significantly different between pool and lawn and pool and hollow, except for E2:E3 ratio, but never significantly different between lawn and hollow.

Table S2. List of compounds analyzed by THM-GC-MS and their related *m/z* and mass specra factor (msf) used for their integration and molecular groups associated with them

Compounds	m/z	msf	Groups
2-butenedioic acid dimethyl ester (fumaric acid)	113	3.3	SOA
Butanedioic acid dimethyl ester (succinic acid)	115	4.5	SOA
heptadienoic acid methyl ester	111	3.9	SOA
2-methylbutanedioic acid dimethyl ester (methylsuccinic acid)	59	2.4	SOA
Pentanedioic acid dimethyl ester (glutaric acid)	59	5.6	SOA
Pentose	129	4	CAR
Desoxyhexose	129	4	CAR
Hexose	129	4	CAR
$C_{8:0}$	74	3	FA
$C_{9:0}$	74	3.6	FA
$C_{10:0}$	74	3	FA
$C_{12:0}$	74	3	LMW FA
$\alpha,\omega C_{9:0}$	74	10.2	FA
$C_{13:0}$	74	4.1	LMW FA
$brC_{14:0}$	74	3.1	LMW FA
$C_{14:0}$	74	3.1	LMW FA
$iC_{15:0}$	74	3.3	LMW FA
$\alpha C_{15:0}$	74	3.3	LMW FA
$C_{15:0}$	74	3.3	LMW FA
$brC_{16:0}$	74	4.9	LMW FA
$C_{16:1}$	74	14.5	LMW FA
$C_{16:1}$	74	14.5	LMW FA
$C_{16:0}$	74	4.9	FA
$iC_{17:0}$	74	3.9	LMW FA
$\alpha C_{17:0}$	74	3.9	LMW FA
$C_{17:1}$	74		LMW FA
$C_{17:0}$	74	3.9	LMW FA
$C_{18:1}$	74	14.6	LMW FA
$C_{18:0}$	74	4.5	FA
$\omega OHC_{16:0}$	74	11.3	HMW FA
$C_{20:0}$	74	4.9	HMW FA
$\omega OHC_{18:0}$	74	17.3	HMW FA
$C_{21:0}$	74	7.5	HMW FA
$\alpha,\omega C_{18:0}$	74	17.7	HMW FA
$C_{22:0}$	74	4.9	HMW FA
$\omega OHC_{20:0}$	74	12.9	HMW FA
$C_{23:0}$	74	8.4	HMW FA
$\alpha,\omega C_{20:0}$	74	10.8	HMW FA
$C_{24:0}$	74	4.4	HMW FA
$\omega OHC_{22:0}$	74	13.5	HMW FA
$C_{25:0}$	74	7.7	HMW FA
$\alpha,\omega C_{22:0}$	74	10.8	HMW FA
$C_{26:0}$	74	4.5	HMW FA
$\omega OHC_{24:0}$	74	13.5	HMW FA
$C_{27:0}$	74	5.1	HMW FA
$\alpha,\omega C_{24:0}$	74	9.7	HMW FA
$C_{28:0}$	74	4.9	HMW FA
benzoic acid methyl ester	105	2.9	PHE
1,2-dimethoxybenzene	138	4.7	PHE
1,4-dimethoxybenzene	138	6	PHE
1,3-dimethoxybenzene	138	3.8	PHE
dimethoxytoluene	152	5.7	PHE
3-methoxybenzaldehyde	136	4.3	PHE

4-methoxybenzaldehyde	136	3.8	PHE
methoxyacetophenone	135	3.5	PHE
3-methoxybenzoic acid methyl ester	135	3.9	PHE
4-methoxybenzoic acid methyl ester	135	2.8	PHE
1,2,3-trimethoxybenzene	168	3.8	PHE
1,2,4-trimethoxybenzene	168	4.3	PHE
1,3,5-trimethoxybenzene	168	3	PHE
trimethoxytoluene	167	7	PHE
1,2,3,4-tetramethoxybenzene	198	3.5	PHE
1,2,3,5-tetramethoxybenzene	198	13.5	PHE
3,4-dimethoxybenzaldehyde (vanilaldehyde)	166	4.2	PHE
3,4-dimethoxyacetophenone (acetovanilone)	165	2.8	PHE
3,5-dimethoxybenzoic acid methyl ester	196	5.1	PHE
3,4-dimethoxybenzoic acid methyl ester (vaniclic acid)	196	5.6	PHE
3,4,5-trimethoxybenzaldehyde (syringealdehyde)	196	6.7	PHE
3-(4-methoxyphenyl)prop-2-enoic acid methyl ester	192	6.7	PHE
3,4,5-trimethoxyacetophenone (acetosyringeone)	195	4.8	PHE
cis-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	194	5.1	PHE
trans-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	194	5.1	PHE
3,4,5-trimethoxybenzoic acid emthyl ester (syringic acid)	226	5.3	PHE
3-(4-methoxyphenyl)but-2-enoic methyl ester	206	8.8	PHE
4-Methoxycarbonylmethoxybenzoic acid methyl ester	193	5.1	PHE
cis-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	224	7.0	PHE
trans-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	224	7.0	PHE
3-(3,4-dimethoxyphenyl)prop-2-enoic acid methyl ester	222	3.7	PHE

Table S3. Results of statistical tests for physico-chemical variables (water temperature, pH, dissolved oxygen and specific conductivity), DOC concentrations, DOC:DON ratio, absorbance indices ($SUVA_{254}$, E2:E3 ratio and S_R) fluorescence indices (FI and β:α index), molecular index (deoxyC6:C5 ratio, fVEG, C/V ratio and Ac:Al(V) ratio) and δ^{13}C-DOC. Statistical tests were based on models for comparison between years of sampling, peat porewater and pools and between seasons of sampling for peat porewater and pools. Significant differences were represented in bold. In the table, statistical test was abbreviating as K-W for Kruskal and Wallis test, WAOV for Welsh analyses of variances and AOV for analyses of variances and environments were abbreviated as P-P for peat porewater and Po for pools. There was no test to compare the effect of years on fluorescent indices considering all data came from samples of the same year of sampling periods.

	~ Year			**~ Env**			**~ Season**						
Variable	**Stat**	**p-value**	**Test**	**Stat**	**p-value**	**Test**	**Env**	**Stat**	**p-value**	**Test**	**SPR/SUM**	**SPR/FAL**	**SUM/FAL**
Water Temperature	1.62	0.203	K-W	14.06	**0.0002**	K-W	P-P	11.36	**0.0003**	WAOV	**0.048**	0.963	**0.00023**
							Po	66.15	**<0.0001**	WAOV	**<0.0001**	0.534	**<0.0001**
pH	15.86	**<0.0001**	K-W	25.24	**<0.0001**	WAOV	P-P	10.9	**0.0003**	WAOV	**0.001**	0.108	**0.0499**
							Po	7.16	**0.002**	AOV	0.752	0.501	**0.00107**
Dissolved Oxygen	1.42	0.233	K-W	89.34	**<0.0001**	K-W	P-P	1.41	0.26	AOV	0.227	0.627	0.618
							Po	12.88	**0.0016**	K-W	0.771	**0.00236**	**0.00835**
Specific Conductivity	0.129	0.719	K-W	45.67	**<0.0001**	K-W	P-P	2.91	0.23	K-W	0.0914	0.408	0.311
							Po	47.1	**<0.0001**	WAOV	**0.0003**	**<0.0001**	**<0.0001**
DOC	0.1	0.751	K-W	27.5	**<0.0001**	WAOV	P-P	14.183	**<0.0001**	AOV	**0.0003**	**0.00003**	0.605
							Po	9.376	**0.0003**	AOV	**0.0431**	**0.000156**	0.138
DOC:DON	4.84	**0.028**	K-W	30.99	**<0.0001**	K-W	P-P	15.3	**<0.0001**	WAOV	**0.015**	**<0.0001**	0.804
							Po	3.93	**0.024**	AOV	**0.0367**	**0.0405**	0.987
δ^{13}C-DOC	0.616	0.432	K-W	0.764	0.382	K-W	P-P	11.706	**0.0006**	AOV	**0.00516**	**0.000555**	0.721
							Po	2.1	0.151	AOV	0.676	0.148	0.546
$SUVA_{254}$	0.986	0.323	AOV	57	**<0.0001**	K-W	P-P	0.11	**0.0173**	K-W	0.0513	0.826	**0.00748**
							Po	16.5	**0.0002**	K-W	0.773	**0.00298**	**0.000606**
E2:E3	1.05	0.306	K-W	312.395	**<0.0001**	AOV	P-P	1.683	0.199	AOV	0.814	0.195	0.43
							Po	29.196	**<0.0001**	AOV	**0.0487**	**<0.0001**	**<0.0001**
S_R	1.68	0.198	WAOV	108	**<0.0001**	WAOV	P-P	2.264	0.118	AOV	0.185	0.994	0.17

							Po	26.6	**<0.0001**	K-W	0.141	**0.0417**	**<0.0001**
Fluorescence Index	*	*	*	19.6	**0.0002**	WAOV	P-P	1.459	0.259	AOV	0.158	0.602	0.0547
							Po	0.353	0.705	AOV	0.726	0.991	0.464
β:α Index	*	*	*	0.898	0.347	AOV	P-P	1.256	0.308	AOV	0.872	0.583	0.313
							Po	5.41	**0.013**	WAOV	**0.015**	0.998	**0.026**
fVEG	5.324	**0.027**	AOV	4.655	**0.038**	AOV	P-P	7.412	**0.006**	AOV	0.918	0.148	**0.00545**
							Po	0.395	0.68	AOV	0.701	0.937	0.804
deoxyC6:C5	4.05	0.054	WAOV	17.3	**<0.0001**	K-W	P-P	1.183	0.333	AOV	0.987	0.562	0.377
							Po	7.38	**0.025**	K-W	**0.0156**	0.364	**0.041**
C:V	0.102	0.749	K-W	8.65	**0.0033**	K-W	P-P	5.129	**0.02**	AOV	0.995	0.187	**0.0217**
							Po	0.542	0.763	K-W	0.48	0.511	0.946
%Phenols	0.474	0.495	AOV	0.38	0.846	AOV	P-P	0.27	0.767	AOV	0.805	0.749	0.991
							Po	0.509	0.611	AOV	0.584	0.719	0.951
%Car	0.452	0.832	K-W	0.0231	0.879	K-W	P-P	0.42	0.675	WAOV	0.635	0.955	0.883
							Po	0.0145	0.993	K-W	0.904	0.930	0.965
%SOA	4.918	**0.033**	AOV	0.016	0.9	AOV	P-P	4.352	**0.032**	AOV	0.92	0.341	**0.0295**
							Po	2.122	0.152	AOV	0.908	0.54	0.137
%LMW FA	0.00831	0.927	K-W	0.208	0.649	K-W	P-P	0.96	0.405	AOV	0.908	0.54	0.137
							Po	2.67	0.263	K-W	0.475	1	0.593
%HMW FA	7.82	**0.00518**	K-W	2.13	0.145	K-W	P-P	0.96	0.405	AOV	0.628	0.991	0.423
							Po	2.67	0.263	K-W	0.475	1	0.593

Table S4. Synthesis of published DOC concentrations (mean ± sd) in peat porewater and pool in northern hemisphere peatlands. All DOC concentrations derived from water sampled during growing season, except for Beer and Blodau (2007) who presented DOC concentrations from sampling in October and December 2005 and Tipping et al. (2010) who presented samples taken weekly, including winters, between 1993 and 2007.

Reference	Peatland type	Location	Biome	Sampled environments	DOC concentrations (mg L^{-1})
Peat Porewater					
This study	Bog	Bouleau peatland (Québec, Canada)	Boreal	6 wells collecting porewater	18.0 ± 8.4
Arsenault et al., 2019	Bog	Grande Plée Bleue (Québec, Canada)	Temperate	10 wells collecting porewater	39.0 ± 9.1
Austnes et al., 2010	Bog	Afon Ddu (Wales)	Temperate	*Sphagnum* porewater (Sph) and 3 porewater samples: one in micro rhizons (MR), one from a lysimeter at 5cm (ZT5) below surface and one from a lysimeter at 10cm bellow surface (ZT10)	Sph : 27-55 MR : 25.5-32 ZT5 : 21.5-33.5 ZT10 : 27-38
Beer and Blodau, 2007	Bog	Mer Bleu Peatland (Ontario, Canada)	Temperate	A multi-level piezometer collecting water from 35 to 165 cm at 10 cm interval and one well collecting peat porewater	Ranged between 10 and 50 mg L-1 and concentrations always higher to 20 mg L-1 in first to 100 cm of peat column
Deshpande et al., 2016	Bog	Sasapimakwananisikw River Valley (Québec, Canada)	Subarctic	Concentration measured from peat solubilized in Milli-Q water from 3 depths at every 2 cores sampled in active layer of peat	Ranged between 13.9 and 28.8
Gandois et al., 2019	Thermokarst bogs	Igarka region (Siberia, Russia)	Subarctic	Water collected by wells in the active layer	Small bogs: 44.1 ± 10.1 Large bogs: 16.7 ± 1.2

Raudina et al., 2017	5 bogs along a longitudinal gradient	Western Siberia Lowlands (Russia)	Artic	Porewater collected in histosols with tension lysimeter	Ranged between 33.7 and 97.9
Tipping et al., 2010	*Sphagnum* peat bog	Cottage Hill Sike (North Pennies, England)	Temperate	Porewater collected weekly with tension lysimeter at 10 and 50 cm depth	20.6 ± 4.1
Pools					
This study	Bog	Bouleau Peatland (Québec, Canada)	Boreal	9 pools	10.5 ± 4.1
Arsenault et al., 2018	Bog	Grande Plée Bleue (Québec, Canada)	Temperate	62 pools	25.8 ± 6.2
Arsenault et al., 2019	Bog	Grande Plée Bleue (Québec, Canada)	Temperate	5 pools	18.3 ± 4.7
Deshpande et al., 2016	Bog	Sasapimakwananisikw River Valley (Québec, Canada)	Subarctic	3 thermokarst lakes	Ranged between 8.5 and 11
Laurion and Mladenov, 2013	Bog	Sirmilik National Park on Bylot Island (Nunavut, Canada)	Arctic	2 pool types: 1. ponds on top of low-centred polygons 2. water from degraded ice wedges	Ranged between 8.5 and 13.1
Laurion et al., 2021	Bog	Sirmilik National Park on Bylot Island (Nunavut, Canada)	Arctic	11 pools from low centred polygons	9.2
Peura et al., 2016	Palsa bog	Whapmagoostui-Kuujjuarapik (Québec, Canada)	Arctic	12 thaw pools (development stage: emerging, developing, and mature pools)	25.8 ± 10.1
Turner et al., 2016	Bog	3 regions: Flow Country (north Scotland), Silver Flowe (southwest Scotland), Northern Ireland	Temperate	66 pools in 6 peatlands	Flow Country: 13.58 ± 4.58 Silver Flowe: 6.7 ± 2.0 Northern Ireland: 14.5 ± 3.1

Table S5. Results of statistical test of the effect of pools surface and depth on DOC concentration, DOC:DON ratio, $SUVA_{254}$, E2:E3 ratio and S_R. Significant differences were represented in bold. In the table, statistical test was abbreviating as K-W for Kruskal and Wallis test, WAOV for Welsh analyses of variances and AOV for analyses of variances.

Variable	Surface			Depth		
	Statistic	p-value	Test	Statistic	p-value	Test
DOC	5.3	0.258	K-W	3.24	0.356	K-W
DOC:DON	0.48	0.75	AOV	1.65	0.266	WAOV
$SUVA_{254}$	3.328	0.039	AOV	4.39	0.02	AOV
E2:E3	0.561	0.694	AOV	0.741	0.543	AOV
S_R	3.89	0.421	K-W	3.69	0.297	K-W