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Supplement of

Spatial variability of organic matter molecular composition and elemental geochemistry in surface sediments of a small boreal Swedish lake

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Supplementary information

Table S1. Identified organic compounds by Py-GC-MS along with their formula, molecular mass (M), retention time (RT), calculated and reference retention index (Kovats retention index, RI[a]), references for the theoretical mass spectra (REF) and how the individual organic compounds have been grouped for the statistical analyses

Name	Formula	M	RT	$RI_{this\ study}$	reference RI[b]		REF	Compounds groups
					$RI_{estimated}$	$RI_{experimental}$		
Carbohydrates								
3-furaldehyde	C5H4O2	96	189.5	N.D.[c]			NIST, [1]	(Alkyl)furans & furanones
2-furaldehyde	C5H4O2	96	204.1	N.D.			NIST, [1]	
2-acetyl-furan	C6H6O2	110	267.2	N.D.			NIST, [1]	
Methyl-3-furaldehyde	C6H6O2	110	269.8	N.D.			NIST, [1]	
2(5H)-furanone	C4H4O2	84	270.5	N.D.			NIST, [1]	
Methyl-2-furaldehyde	C6H6O2	110	276.9	N.D.			NIST, [1]	
Dihydro-methyl-furanone	C5H6O	98	277.8	N.D.			[1]	
5-methyl-2(5H)-Furanone	C5H6O2	98	292.5	907	868	914-917	NIST, [1]	
Methyl-2-furaldehyde	C6H6O2	110	312.8	920	920	924-987	NIST, [1]	
2-Furancarboxylic acid, methyl ester	C6H6O3	126	422.7		909		NIST, [1]	Hydroxyl or carboxy-furans & furanones
2,5-Dimethyl-4-hydroxy-3(2H)-furanone	C6H8O3	128	424.6	1088	1022	1023-1097	NIST	
5-(hydroxymethyl)-2-Furaldehyde	C6H6O3	126	551.9	1236	1163	1176-1236	NIST, [1]	
5,6-dihydro-2H-Pyran-2-one	C5H6O2	98	278.7	N.D.			NIST	Pyrans
4-hydroxy-5,6-dihydro(2H)-pyran-2-one	C5H6O3	114	344.2	941	N.R.[d]	N.R.	[1]	
Dianhydrorhamnose	$C_6H_8O_3$	128	383.4	1041	N.R.	N.R.	[2]	Dianhydrorhamnose
Levoglucosenone	C6H6O3	126	450.1	1119	N.R.	1070	NIST	Levoglucosenone
Levosugars (Levogalactosan)	C6H10O5	162	535.7	1375	N.R.	N.R.	[1]	Anhydrosugars
Ahydrohexose	Unknown		729.0	1450	N.R.	N.R.	[1]	
Levosugars(Levomannosan)	C6H10O5	162	761.5	1447	N.R.	N.R.	[1]	
Levosugars (Levoglucosan)	C6H10O5	162	771.4	1493	1404	1486-1491	[1]	
Chitin derived compounds								
Acetamide	C2H5NO	59	166.3	N.D.			NIST	Chitin derived compounds
3-acetamido-furan	C6H7NO2	125	555.4	1239	N.R.	N.R.	NIST	
3-acetamido-4-pyrone	Unknown	153	656.4	1353	N.R.	N.R.	[3]	
Oxazoline	Unknown		801.9	1548	N.R.	N.R.	[3]	
N-compounds								
Pyridine	C5H5N	79	151.9	N.D.			NIST	(Alkyl)pyridines
2-methyl-pyridine	C6H7N	93	197.6	N.D.			NIST	
3/4-methyl-pyridine	C6H7N	93	234.6	N.D.			NIST	
2-Acetylpyridine	C7H7NO	121	377.2	1034	N.R.	N.R.	NIST	Pyridines_O
3-Acetylpyridine	C7H7NO	121	404.0	1065	N.R.	N.R.	NIST	
2-Methyl-5-acetoxypyridine	C8H9NO2	151	734.1	1457	N.R.	N.R.	NIST	
Pyrrole	C4H5N	67	154.2	N.D.			NIST	(Alkyl)pyrroles
Methyl-pyrrole	C5H7N	81	216.2	N.D.			NIST	
2-formyl-pyrrole	C5H5NO	95	354.2	1008	988	1005-1030	NIST	Pyrroles_O
2-acetyl-pyrrole	C6H7NO	109	402.0	1062	1035	1026-1064	NIST	
2-Formyl-1-methylpyrrole	C6H7NO		459.9	1129	1077	1092-1105	NIST	
2,5-pyrroledione	C4H3NO2	97	335.9	935	N.R.	N.R.	NIST	Pyrroledione & pyrrolidinedione
2,5-pyrrolidinedione	C4H5NO2	99	462.1	1131	934	N.R.	NIST	
Benzeneacetonitrile	C8H7N	117	474.2	1147	1138	1089-1143	NIST	Aromatic N
Benzenepropanenitrile	C9H9N	131	563.9	1248	1238	1186-1242	NIST	
Indole	C8H7N	117	609.9	1293	1174	1260-1303	NIST	Indoles
Methyl-indole	C9H9N	131	686.1	1394	1288	1380-1410	NIST	
Diketodipyrrole	Unknown	186	922.7	1722	N.R.	N.R.	[4]	Diketodipyrrole
Diketopiperazine Pro-Ala	C8H12N2O2	168	938.0	1746	N.R.	N.R.	[5, 6]	Diketopiperazines
Diketopiperazine Pro-Val	C10H16N2O2	196	989.4	1826	N.R.	N.R.	[5, 6]	
Diketopiperazine Pro-Val	C10H16N2O2	196	1005.9	1852	N.R.	N.R.		
Diketopiperazine Cyclo-Leu-Pro	C11H18N2O2	210	1049.0	1922	N.R.	N.R.	NIST	
Diketopiperazine Pro-Pro	C10H14N2O2	194	1067.0	1953	N.R.	N.R.	[5, 6]	
Diketopiperazine Pro-Phe	C14H16N2O2	244	1284.3	2352	N.R.	N.R.	[5, 6]	
Alkylamide1	Unknown		986.8	1821	N.R.	N.R.	NIST	Alkylamides
Alkylamide2	Unknown		1081.1	1977	N.R.	N.R.	NIST	
Alkylamide3	Unknown		1197.6	2185	N.R.	N.R.	NIST	
Alkylamide4	Unknown		1237.3	2260	N.R.	N.R.	NIST	
Alkylamide5	Unknown		1304.2	2392	N.R.	N.R.	NIST	
Alkylamide6	Unknown		1579.6	3020	N.R.	N.R.	NIST	

***n*-alkenes**								
n-C9:1	C9H18	126					NIST	C9-16:1
n-C13:1	C13H26	182	603.4	1286	1204	1187-1289	NIST	
n-C14:1	C14H28	196	684.6	1392	1421	1389-1396	NIST	
n-C16:1	C16H32	224	834.4	1593	1602	1590-1593	NIST	
n-C17:1	C17H34	238	903.6	1693	N.R.	1692-1703	NIST	C17-22:1
n-C18:1	C18H36	252	969.2	1794	1801	1788-1793	NIST	
n-C19:1	C19H38	266	1031.8	1894	1900	1883-1899	NIST	
n-C20:1	C20H40	280	1091.5	1994	N.R.	1889-1994	NIST	
n-C21:1	C21H42	294	1148.5	2096	2117	2060	NIST	
n-C22:1	C22H44	308	1203.2	2195	2198	2192-2195	NIST	
n-C23:1	C23H46	322	1255.5	2295	N.R.	2288-2295	NIST	C23-26:1
n-C24:1	C24H48	336	1305.7	2395	N.R.	2394-2396	NIST	
n-C25:1	C25H50	350	1352.9	2498	N.R.	2483-2496	NIST	
n-C26:1	C26H52	364	1400.5	2596	N.R.	2593-2596	NIST	
n-C27:1	C27H54	350	1445.6	2697	N.R.	2688-2694	NIST	C27-28:1
n-C28:1	C28H56	364	1488.5	2796	N.R.	2794-2797	NIST	
***n*-alkanes**								
n-C10:0	C10H22	142	347.4				NIST	C10-16:0
n-C11:0	C11H24	156	435.0				NIST	
n-C12:0	C12H26	170	515.5				NIST	
n-C13:0	C13H28	184	617.3				NIST	
n-C14:0	C14H30	198	690.7				NIST	
n-C15:0	C15H32	212	767.1				NIST	
n-C16:0	C16H34	226	839.5				NIST	
n-C17:0	C17H36	240	908.1				NIST	C17-22:0
n-C18:0	C18H38	254	973.5				NIST	
n-C19:0	C19H40	268	1035.7				NIST	
n-C20:0	C20H42	282	1095.0				NIST	
n-C21:0	C21H44	296	1150.7				NIST	
n-C22:0	C22H46	310	1206.1				NIST	
n-C23:0	C23H48	324	1258.1				NIST	C23-26:0
n-C24:0	C24H50	338	1308.1				NIST	
n-C25:0	C25H52	352	1355.1				NIST	
n-C26:0	C26H54	366	1402.4				NIST	
n-C27:0	C27H56	380	1447.1				NIST	C27-35:0
n-C28:0	C28H58	394	1490.2				NIST	
n-C29:0	C29H60	408	1530.3				NIST	
n-C30:0	C30H62	422	1571.8				NIST	
n-C31:0	C31H64	436	1610.9				NIST	
n-C32:0	C32H66	450	1648.6				NIST	
n-C33:0	C33H68	464	1685.0				NIST	
n-C35:0	C35H72	492	1723.9				[7]	
Alkan-2-ones								
2-K C13	C13H26O	198	765.4	1498	1449	1476-1498	NIST	2K C13-17
2-K C16	C16H32O	240	975.0	1803	1748	1780-1805	NIST	
2-K C17	C17H34O	254	1038.2	1904	1847	1875-1890	NIST	
2-K C19	C19H38O	282	1155.9	2109	2046	2087-2106	NIST	2K C19-22
2-K C20	C20H40O	396	1210.9	2209	2206	N.R.	NIST	
2-K C21	C21H42O	310	1263.7	2311	2309	N.R.	NIST	
2-K C23	C23H46O	338	1363.0	2517	2513	N.R.	NIST	2K C23-31
2-K C24	C24H48O	352	1410.0	2617	N.R.	N.R.	NIST	
2-K C25	C25H50O	366	1455.1	2719	N.R.	N.R.	NIST	
2-K C26	C26H52O	380	1498.6	2821	N.R.	N.R.	NIST	
2-K C27	C27H54O	394	1540.6	2925	N.R.	N.R.	[7]	
2-K C28	C28H56O	408	1581.3	3024	N.R.	N.R.	[7]	
2-K C29	C29H58O	422	1620.7	3126	N.R.	N.R.	[7]	
2-K C31	C31H62O	450	1696.0	3328	N.R.	N.R.	[7]	
Phenols								
Phenol	C6H6O	94	329.2	931	901	952-1004	NIST	Phenols
2- methyl-phenol	C7H8O	108	396.2	1056	1014	1029-1039	NIST	
3/4- methyl-phenol	C7H8O	108	414.9	1077	1014	1051-1063	NIST	
Dimethyl-phenol	C7H8O	122	418.4	1156	1127	1077-1130	NIST	
Ethyl- phenol	C8H70O	122	497.3	1177	1114	1106-1162	NIST	
Propenyl-phenol	C9H10O	134	646.7	1340	1203	1232-1258	NIST	
Lignins								
Guaiacol **(G)**	C7H8O2	124	428.7	1093	1090	1052-1090	NIST	Guaiacols
Ethyl-guaiacol **(guaiacyl-2C)**	C9H12O2	152	596.2	1279	1303	1243-1287	NIST	

4-vinyl-guaiacol **(guaiacyl -2C)**	C9H10O2	150	625.6	1311	1293	1272-1295	NIST	
4-propenyl-guaiacol **(guaiacyl -3C)**	C10H12O2	164	660.9	1359	1392	1339-1452	NIST	
Vanillin **(guaiacyl -1C or -aldehyde)**	C8H8O3	152	695.9	1407	1392	1350-1447	NIST	
4-alleneguaiacol **(guaiacyl -3C)**	C10H10O2	162	741.0	1466	N.R.	N.R.	[8]	
Acetovanillone **(guaiacyl -2Cor aldehyde)**	C9H10O3	166	763.1	1495	1439	1447-1503	NIST	
Vanillic acid, methyl ester (**guaiacyl -1C or -acid)**	C9H10O4	182	785.5	1525	1470	1463-1525	NIST	
Guaiacylacetone **(guaiacyl -3Cor -aldehyde)**	C10H12O3	180	796.0	1540	1538	1488-1531	NIST	
Syringol **(syringyl)**	C8H10O3	154	655.4	1352	1279	1349-1367	NIST	Syringols
4-vinyl-syringol **(syringy-2C)**	C11H14O4	210	819.5	1572	N.R.	1517-1573	NIST	
4-formyl-syringol **(syringy-1C)**	C9H10O4	182	887.6	1670	1581	1617-1670	NIST	
4-allenesyringol **(syringy-3C)**	C11H12O3	192	901.0	1690	N.R.	N.R.	[8]	
Acetosyringone **(syringy-2C)**	C10H12O4	196	961.1	1781	1628	1740-1744	NIST	
Chlorophylls								
Prist-1-ene	C19H38	266	929.0	1732	N.R.	N.R.	[9]	Pristenes
Prist-2-ene	C19H38	266	936.3	1743	N.R.	N.R.	[9]	
Phytadiene 1	C20H38	278	999.1	1841	N.R.	N.R.	[9]	Phytadienes
Phytadiene 2	C20H38	278	1026.0	1884	N.R.	N.R.	[9]	
Steroids								
Cholest-2-ene	$C_{27}H_{46}$	370	1522.1	2880	2380	N.R.	NIST	Steroids
Cholesta-3,5-diene	$C_{27}H_{44}$	368	1543.4	2932	N.R.	N.R.	NIST	
Stigmasta-5,22-dien-3-ol, acetate	$C_{31}H_{50}O_2$	454	1601.1	3075	2879	N.R.	NIST	
Sitosterol	$C_{29}H_{50}O$	414	1623.4	3133	2731	3173-3220	NIST	
Cholesta-3,5-dien-7-one	$C_{27}H_{42}O$	382	1668.7	3255	2562	N.R.	NIST	
Stigmasta-3,5-dien-7-one	C28H46O	410	1750.1	3462	2696	N.R.	NIST	
Tocopherols								
γ-Tocopherol	C28H48O2	416	1594.1	3057	3036	3055	NIST	Tocopherols
α-Tocopherol	C29H50O2	430	1632.2	3157	3149	3111	NIST	
Hopanoids								
Trinosphopane	unknown		1526.4	2890	N.R.	N.R.	[10]	Hopanoids
Norhopene (triterpene C29)	unknown		1548.9	2945	N.R.	N.R.	[10]	
22,29,30-trisnorhop-17(21)-ene	$C_{27}H_{44}$	368	1553.8	2957	N.R.	N.R.	[11]	
22,29,30-trisnorhop-16(17)-ene	$C_{27}H_{44}$	368	1567.1	2989	N.R.	N.R.	[11]	
Norhopane (C30/C31?)	unknown		1630.7	3153	N.R.	N.R.	[10]	
25-norhopene (C30/C31?)	unknown		1659.0	3229	N.R.	N.R.	[10]	
(Poly)aromatics								
Benzene	C_6H_6	78	113.9	N.D.			NIST	Benzene
Benzaldehyde	C_7H_6O	106	311.2	919	982	925-966	NIST	Benzaldehyde
Acetyl-benzene	C8H8O	120	408.1	1069	1029	1041-1078	NIST	Acetyl-benzene
Styrene	C8H8	104	254.2	N.D.			NIST	Benzenes C2-9
Ethyl-methyl-benzene	C9H12	120	368.2	1024	N.R.	945-973	NIST	
Indene	C9H8	120	389.7	1048	1014	1029-1051	NIST	
Benzene C7	C13H20	176	664.9	1365	1390	1337-1350	NIST	
Benzene C9	C15H24	204	822.1	1576	1555	1552-1586	NIST	
1,2-dihydro-naphthalene	C10H10	130	484.9	1160	1149	1137-1166	NIST	(Poly)aromatics
2,3-dihydro-inden-1-one	C9H8O	132	599.8	1283	1218	1218-1320	NIST	
1~~/2-~~methyl-napthalene	C11H10	142	612.1	1295	1345	1263-1298	NIST	
2~~/1~~methyl-napthalene	C11H10	142	626.7	1313	1345	1267-1298	NIST	
Biphenyl	C12H10	154	680.8	1386	1367	1338-1392	NIST	
Fluorene	C13H10	166	836.9	1596	1494	1549-1611	NIST	
Anthracene	C14H10	178	972.2	1798	1782	1740-1800	NIST	

[a] Kovats retention index (RI) is used to convert retention times into system-independent constants. The RI of a certain chemical compound is its retention time normalized to the retention times of adjacently eluting *n*-alkanes and is determined as follow:

$$\mathrm{RI} = 100 \times [n + \frac{\log(RT\ unknown) - \log(RT\ n)}{\log(RT\ N) - \log(RT\ n)}$$

With, n is the number of carbon in the adjacently eluting smaller *n*-alkane; RT unknown is the retention time of the compound to identify, RT n is the retention time of the adjacently elution smaller *n*-alkane, and RT N is the retention time of the adjacently eluting larger *n*-alkane.

[b] reference RI: the reference RI values were found on the website "NIST Chemistry Webbook" (http://webbook.nist.gov/chemistry/) and/or in the 'NIST/EPA/NIH 2011' library included in the software "NIST MS Search v.2.0"; the reference RI values reported in this table have been either assessed or determined experimentally for non-polar GC column and temperature gradient GC program.;

[c] N.D.: the RI value could not be determined in this study because the adjacently eluting *n*-alkanes needed to calculate the RI could not be identified.

[d] N.R.: no reference RI values were found in the NIST Webbook or library.

References (the complete references are given in the manuscript):

[1] Faix et al. (1991) *Holz als Roh- und Werkstoff*, 49: 213-219; [2] Schellenkens et al. (2009) *Organic geochemistry* 40: 678-691; [3] Gupta and Cody (2011), *in N.S. Gupta (ed.), Chitin, Topics in Geobiology* 34, Springer Science+Busines Media ; [4] Schellenkens et al. (2014) *Organic Geochemistry* 77: 32-42; [5] Chen et al., (2009) *Journal of Food Science*, 74: 100-105; [6] Fabbri et al., (2012) *Journal of Analytical and Applied Pyrolysis*, 95: 145-155; [7] For these long-chain *n*-alkanes and alkan-2-ones, the number of C in the molecule has been determined based on the highest *m/z* present in the mass spectra that corresponds to the molecular mass and on the order of elution; [8] Faix et al. (1990) *Holz als Roh- und Werkstoff*, 48: 281-285; [9] Nguyen et al. (2005) *Organic Geochemistry*, 34: 483-497; [10] Gill (1997) Chapter 16. Analytical techniques in organic chemistry; in: Modern analytical Geochemistry; Taylor & Francis, New York (USA), pp. 243-272; [11] Meredith et al. (2008) *Organic Geochemistry*, 39: 1243-1248

Table S2. Sediment elemental geochemistry variables for the 44 studied sediment samples *(to be continued)*

unit	WD m	BD g cm^{-3}	bSi %	LOI %	[S] mg kg^{-1}	[Br] mg kg^{-1}	[Cu] mg kg^{-1}	[Ni] mg kg^{-1}	[Hg] µg kg^{-1}	[Pb] mg kg^{-1}	[Zn] mg kg^{-1}
N1	3.1	0.057	15	**57**	16620	134	29	**21**	283	151	285
N2	7.4	0.088	6	**58**	18050	127	39	**23**	510	168	320
N3	**1.6**	0.078	14	34	**5570**	**216**	34	**10**	261	170	**43**
N4	7.4	0.056	**22**	37	9700	138	33	17	288	120	121
N5	4	0.073	19	36	9740	174	26	18	187	114	195
N6	7.1	0.061	14	40	9770	176	27	18	291	208	199
N7	4	0.063	11	40	16240	168	34	23	309	236	332
N8	5.3	0.064	15	40	9960	138	28	17	224	175	218
N9	7.7	0.054	11	48	14570	**214**	34	20	288	187	248
N10	2.5	0.080	**21**	27	**4990**	129	37	**10**	290	261	50
N11	3.9	0.068	19	32	17000	134	36	**21**	288	226	254
E1	2	0.061	15	36	15440	119	28	19	235	208	188
E2	6.7	0.087	11	36	11510	129	26	19	242	118	195
E3	3.5	0.075	14	45	8240	177	19	16	198	109	213
E4	6	0.086	13	39	11600	158	27	19	235	152	228
E5	9.4	0.092	9	41	11260	145	29	19	265	138	200
E6	10	0.035	13	42	11350	150	30	20	309	**422**	222
M1	3	0.084	**25**	25	**4840**	146	33	**10**	264	235	49
M2	3.7	0.075	**20**	35	9640	167	22	20	193	120	239
M3	7.9	0.083	8	35	17560	120	36	22	326	206	279
M4	*3.8*	***0.608***	***2***	***3***	***2960***	***11***	***7***	***9***	***34***	***33***	***61***
M5	1.9	**0.127**	**23**	**18**	**5000**	120	**13**	**10**	**117**	135	74
M6	1.8	0.104	16	**10**	**4685**	**71**	**12**	18	141	175	80
S1	5.7	0.083	17	30	6640	104	27	19	181	103	144
S2	6.5	0.091	**23**	27	6600	101	25	14	177	97	111
S3	9.5	0.047	12	35	7410	157	31	14	263	145	104
S4	14	0.035	10	32	6295	133	29	13	242	180	173
S5	3.7	0.101	11	32	8940	91	15	12	177	105	146
S6	12.5	0.043	15	42	6040	172	31	18	196	**58**	104
S9	21	0.040	6	45	12650	175	44	**23**	507	244	299
S10	12.8	0.053	7	40	9230	**187**	49	**21**	370	188	196
S11	14.8	0.058	6	37	12460	159	41	**21**	428	256	308
S12	23.5	0.033	**4**	**50**	20650	**225**	56	**26**	740	279	380
S13	16.5	0.048	12	38	11780	160	45	**22**	491	258	303
S14	9.1	0.046	6	32	18260	119	43	20	385	279	336
S15	*2.9*	***0.737***	***2***	***4***	***2180***	***21***	***11***	***15***	***21***	***10***	***39***
S16	4.2	0.097	**23**	20	5420	90	24	18	162	120	100
S17	18.2	0.047	**4**	41	13980	170	48	25	461	295	**404**
S18	24.5	0.027	5	**51**	**29190**	**212**	**64**	**27**	858	277	**425**
S19	9.5	0.036	9	34	13790	153	39	18	368	224	199
S21	11	0.060	**5**	34	**4950**	153	28	15	187	112	118
S22	19.8	0.057	**5**	40	13950	164	48	**24**	533	299	**415**
S23	3.6	0.024	10	**52**	18370	123	39	20	547	243	255
S24	**24.3**	**0.016**	**4**	**54**	**28840**	175	**75**	**27**	**1152**	273	**445**

The font colors of the sample ID cells correspond to the six clusters identified by the cluster analysis on the elemental geochemistry dataset, for which the sediments M4 and S15 (shown to be outliers) were discarded.
The bold and underlined numbers corresponds to the minimal and maximal value, and the numbers in bold correspond to the values that are below or above 20 % of the maximal and minimal values respectively.

Table S2. *Continuation* Sediment elemental geochemistry variables for the 44 studied sediment samples

	Al	Y	Fe	Fe:Al	Fe:S	[As]	As_{inv}	[P]	[Mn]	**Mn:Fe**	[Co]	[Ca]	[K]	[Mg]	[Na]	$Si_{inorganic}$	[Sr]	[Ti]	[V]	[Zr]
	%	mg kg^{-1}				mg kg^{-1}	$\mu g\ cm^{-2}$	mg kg^{-1}					mg kg^{-1}			%		mg kg^{-1}		
N1	**2.1**	**9**	1.5	0.7	**0.9**	15	9	**760**	149	0.010	11	6230	**2740**	1060	1190	**4**	41	1293	**38**	**44**
N2	**2.2**	15	1.3	0.6	**0.7**	14	13	1230	125	0.010	12	4800	3610	1050	1910	10	45	1648	**36**	70
N3	2.8	25	4.5	1.6	8.1	22	17	1288	397	0.009	8	4530	5490	**990**	2220	9	56	2262	45	**152**
N4	2.6	19	1.8	0.7	1.8	23	13	1839	**94**	0.005	7	**2860**	**2420**	**870**	**440**	7	**27**	1228	51	**39**
N5	2.8	25	2.5	0.9	2.5	19	14	1133	163	0.007	12	3870	3110	**1020**	940	10	39	1676	54	69
N6	2.8	24	2.5	0.9	2.6	20	12	1149	169	0.007	11	3950	3160	1060	860	15	39	1714	54	68
N7	2.7	24	3.6	1.3	2.2	56	36	933	202	0.006	26	4650	4150	1220	1620	13	51	2009	55	105
N8	2.6	20	2.3	0.9	2.3	26	17	1081	175	0.008	13	4850	4110	1240	1360	11	48	2118	53	89
N9	2.7	22	2.5	0.9	1.7	37	20	1285	148	0.006	11	4930	4100	1270	1720	10	51	2219	59	91
N10	**2.3**	25	4.3	1.9	8.7	39	31	1423	**7981**	**0.184**	35	**3050**	3860	1100	1230	9	36	1965	54	76
N11	2.8	28	5.8	2.1	3.4	51	34	1005	240	0.004	27	**3080**	**267**0	**920**	800	9	34	1267	62	81
E1	2.6	26	7.3	2.9	4.7	49	30	**712**	185	0.003	23	5700	3620	1250	1890	10	65	1963	55	129
E2	**2.4**	19	1.8	0.7	1.6	22	19	1183	149	0.008	9	6030	4880	1600	1660	16	61	**2453**	48	119
E3	**2.3**	**7**	**0.9**	**0.4**	1.1	**5**	**3**	**672**	144	0.016	**5**	**7460**	**5070**	1540	1800	7	57	**2357**	**43**	101
E4	2.6	19	1.8	0.7	1.5	22	19	1190	141	0.008	9	5310	4820	1600	1640	14	56	**2541**	54	112
E5	2.9	18	2.0	0.7	1.8	18	17	1396	160	0.008	9	6590	**5370**	**1910**	2180	14	63	**2852**	57	119
E6	2.8	17	1.8	0.6	1.6	14	5	1405	158	0.009	10	6810	**4970**	**1780**	1765	10	60	**2659**	55	99
M1	**2.5**	21	4.0	1.6	8.2	32	27	1381	4288	0.108	22	**3410**	4070	1260	1150	6	38	2188	56	82
M2	**2.5**	17	1.8	0.7	1.9	19	14	688	164	0.009	9	6230	3830	1450	1200	8	53	1679	50	78
M3	3.0	26	3.5	1.2	2.0	48	40	1362	173	0.005	14	5610	**5850**	**1820**	2380	16	69	**2524**	68	**152**
M4	***5.7***	*17*	*3.5*	*0.6*	*11.8*	***<DL***	***<DL***	*989*	*462*	*0.013*	*10*	***31890***	***8660***	***10040***	***11110***	***22***	***218***	***6017***	***91***	***153***
M5	2.8	34	6.5	2.3	12.9	27	**34**	1128	5463	0.085	**62**	5710	4230	**1770**	1710	8	73	**2461**	64	117
M6	**4.3**	**43**	7.4	1.7	**15.8**	18	18	965	5067	0.068	**76**	**8105**	**6140**	**1920**	**3380**	12	**116**	2211	**90**	109
S1	**3.5**	30	3.7	1.0	5.5	29	24	2042	221	0.006	19	4310	4540	1250	1210	11	55	1646	78	89
S2	**3.4**	24	4.5	1.3	6.9	29	26	2001	222	0.005	16	4650	3260	1220	1080	6	41	1642	64	76
S3	2.9	27	3.4	1.2	4.6	27	13	2216	143	0.004	8	4170	4380	1620	1550	13	51	2236	64	104
S4	3.3	29	**11.5**	**3.5**	**18.3**	**57**	20	2013	345	0.003	17	5065	**5560**	**1735**	2695	9	60	**2730**	68	**147**
S5	2.7	16	1.5	0.6	1.7	**7**	7	**655**	176	0.011	7	**9300**	4660	1340	2570	11	**101**	1524	**42**	109
S6	**3.6**	**35**	3.7	1.0	6.1	20	9	**3503**	177	0.005	8	6260	3170	1440	1320	8	46	1677	57	62
S9	**3.5**	28	4.3	1.2	3.4	43	17	2228	195	0.005	13	5300	**5900**	**2030**	2410	14	59	**2844**	79	122
S10	**3.8**	**42**	7.3	1.9	7.9	53	28	2907	208	0.003	18	5160	4430	**1720**	1920	13	56	2079	79	98
S11	**3.7**	33	8.1	2.2	6.5	**69**	**40**	2001	252	0.003	18	6420	**6090**	**2090**	**2920**	14	69	**2870**	77	**160**
S12	**3.4**	25	2.7	0.8	1.3	39	13	2226	182	0.007	12	4960	5130	**1820**	2120	14	53	**2344**	76	92
S13	**3.7**	**36**	**10.2**	2.7	8.6	**71**	**34**	2255	262	0.003	24	6020	**5970**	**2040**	**3030**	6	65	**2859**	**85**	**152**
S14	3.2	32	**11.3**	**3.5**	6.2	**71**	**33**	1744	308	0.003	39	4610	**4980**	1590	2230	**17**	55	**2386**	75	**131**
S15	***5.7***	*22*	*3.3*	*0.6*	*15.1*	***<DL***	***<DL***	*908*	*1657*	*0.050*	*23*	***21190***	***12360***	***4950***	***10280***	***23***	***252***	***2697***	*58*	***162***
S16	**4.0**	30	3.2	0.8	6.0	17	16	1705	275	0.008	22	6150	4710	1490	1810	8	61	2135	59	109
S17	**3.7**	**35**	**9.1**	2.4	6.5	**73**	**34**	2133	389	0.004	35	5380	**5510**	**1990**	**2790**	15	61	**2671**	**80**	**145**
S18	3.3	24	3.4	1.0	1.1	42	11	2303	175	0.005	14	4900	**4930**	**1820**	2040	14	51	2255	77	91
S19	3.0	31	7.4	2.5	5.3	55	20	1690	216	0.003	20	4360	4620	1520	1680	14	54	**2344**	78	126
S21	3.2	26	3.1	1.0	6.2	20	12	2386	170	0.006	10	5420	3810	1510	1230	**21**	53	2109	61	90
S22	**3.6**	**38**	**10.7**	**2.9**	7.7	**73**	**42**	2525	471	0.004	41	5590	**5590**	**2130**	2650	14	64	**2695**	79	**137**
S23	2.7	14	3.6	1.3	2.0	27	7	**711**	134	0.004	10	3920	2970	1110	1270	7	33	**997**	77	48
S24	**3.5**	20	6.9	2.0	2.4	**64**	10	**3769**	157	**0.002**	16	5265	3410	1330	1800	9	44	1491	**101**	53

The font colors of the sample ID cells correspond to the six clusters identified by the cluster analysis on the elemental geochemistry dataset, for which the sediments M4 and S15 (shown to be outliers) were discarded.

The bold and underlined numbers corresponds to the minimal and maximal value, and the numbers in bold correspond to the values that are below or above 20 % of the maximal and minimal values respectively.

Table S3. Average of the sediment elemental geochemistry variables for the whole-lake, the six clusters and the two outliers

Variables (unit)	**Whole-lake[a] (n[b]=42)**	**Near-shore sites**	**North/East basins**		**South basin**		**Shallow central areas**	**Outliers (M4, S15)**
		$Cluster_{geo}$ 4 (n=4)	$Cluster_{geo}$ 1 (n=13)	$Cluster_{geo}$ 6 (n=10)	$Cluster_{geo}$ 2 (n=8)	*$Cluster_{geo}$ 5* (n=3)	$Cluster_{geo}$ 3 (n=4)	
W.D. (m)	*9 ± 7 (74 %)*[c]	*4 ± 2*	*5 ± 3*	*8 ± 3*	*15 ± 4*	*3 ± 1*	*2 ± 1*	*3 ± 1*
B.D. (g cm^{-3})	0.06 ± 0.02 *(38 %)*	0.06 ± 0.03	0.07 ± 0.02	0.07 ± 0.02	0.05 ± 0.01	0.67 ± 0.09	0.100 ± 0.02	0.67 ± 0.09
bSi (%)	12 ± 6 *(31 %)*	12 ± 6	13 ± 3	15 ± 7	7 ± 3	1.8 ± 0.2	21 ± 4	1.8 ± 0.2
OM and organophilic trace elements								
LOI (%)	38 ± 10 *(27 %)*	50 ± 12	39 ± 5	34 ± 7	37 ± 4	52 ± 2	20 ± 8	4 ± 1
S (mg kg^{-1})	11876 ± 5920 *(50 %)*	17510 ± 833	11683 ± 3440	7550 ± 1900	12896 ± 3315	26227 ± 4833	4879 ± 148	2570 ± 552
Br (mg kg^{-1})	149 ± 35 *(23 %)*	130 ± 6	153 ± 36	145 ± 35	154 ± 19	204 ± 26	116 ± 32	16 ± 7
Cu (mg kg^{-1})	34 ± 13 *(37 %)*	36 ± 5	28 ± 6	30 ± 7	42 ± 6	65 ± 10	24 ± 13	9 ± 3
Ni (mg kg^{-1})	19 ± 5 *(23 %)*	21 ± 1	18 ± 4	17 ± 2	21 ± 4	27 ± 1	12 ± 4	12 ± 4
Hg (µg kg^{-1})	337 ± 202 *(60 %)*	407 ± 141	251 ± 47	230 ± 69	427 ± 94	917 ± 212	203 ± 87	28 ± 9
Pb (mg kg^{-1})	192 ± 74 *(39 %)*	199 ± 58	156 ± 58	115 ± 42	300 ± 59	315 ± 7	182 ± 96	24 ± 7
Zn (mg kg^{-1})	219 ± 108 *(49 %)*	279 ± 31	212 ± 68	139 ± 42	305 ± 86	417 ± 33	63 ± 16	50 ± 16
Cu (µg cm^{-2})	*20 ± 6 (30 %)*	*21 ± 11*	*20 ± 6*	19 ± 4	*20 ± 6*	*16 ± 4*	*22 ± 8*	*62 ± 27*
Ni (µg cm^{-2})	*12 ± 4 (35 %)*	*13 ± 6*	*13 ± 4*	11 ± 3	*10 ± 3*	*7 ± 2*	*12 ± 5*	*83 ± 39*
Hg (ng cm^{-2})	*185 ± 65 (35 %)*	*234 ± 146*	*180 ± 45*	146 ± 32	*201 ± 69*	*222 ± 33*	*187 ± 46*	*181 ± 36*
Pb (µg cm^{-2})	*123 ± 60 (48 %)*	*111 ± 46*	*132 ± 53*	83 ± 29	*126 ± 29*	*84 ± 9*	*234 ± 84*	*138 ± 90*
Zn (µg cm^{-2})	*126 ± 60 (47 %)*	*170 ± 90*	*152 ± 54*	92 ± 33	*145 ± 60*	*105 ± 30*	*64 ± 28*	*329 ± 59*
Elements that can be part of or be associated with clays and (oxy)hydroxides								
Al (%)	3.0 ± 0.5 *(18 %)*	2.4 ± 0.3	2.7 ± 0.2	3.3 ± 0.5	3.5 ± 0.3	3.4 ± 0.1	3.0 ± 0.9	5.7 ± 0
Y (mg kg^{-1})	25 ± 8 *(32 %)*	16 ± 8	20 ± 5	28 ± 6	33 ± 3	23 ± 3	31 ± 10	20 ± 3
Fe (%)	4.5 ± 3.0 *(65 %)*	3.1 ± 2.1	2.7 ± 1.7	3.6 ± 1.5	9.1 ± 2.4	4.3 ± 2.2	5.5 ± 1.7	3.4 ± 0.2
Fe:Al	*1.5 ± 0.8 (57 %)*	*1.0 ± 0.5*	*1.0 ± 0.6*	1.1 ± 0.3	*2.5 ± 0.9*	*1.3 ± 0.6*	*1.9 ± 0.3*	*2.0 ± 0.4*
Fe:S	*5.2 ± 4.3 (86 %)*	*1.7 ± 1.2*	*2.5 ± 1.9*	*5.0 ± 0.9*	*8 ± 4*	*1.6 ± 0.7*	*11 ± 4*	*13 ± 2*
As (mg kg^{-1})	35 ± 20 *(56 %)*	27 ± 17	26 ± 16	25 ± 11	64 ± 11	48 ± 14	29 ± 9	< D.L.[d]
As (µg cm^{-2})	*20 ± 11 (52 %)*	*15 ± 13*	*19 ± 11*	17 ± 7	*30 ± 10*	*12 ± 1*	*28 ± 7*	*< D.L.*
P (mg kg^{-1})	1624 ± 741 *(46 %)*	927 ± 240	1065 ± 295	2088 ± 730	2074 ± 275	2766 ± 869	1224 ± 216	949 ± 57
Mn (mg kg^{-1})	729 ± 1690 *(232 %)*	162 ± 53	182 ± 67	184 ± 50	305 ± 93	171 ± 13	5700 ± 1597	1060 ± 845
Mn:Fe	*0.016 ± 0.034 (214 %)*	*0.007 ± 0.002*	*0.008 ± 0.003*	0.006 ± 0.002	*0.004 ± 0.001*	*0.005 ± 0.002*	*0.111 ± 0.051*	*0.08 ± 0.01*
Co(mg kg^{-1})	19 ± 14 *(77 %)*	15 ± 8	12 ± 6	13 ± 5	26 ± 11	14 ± 2	49 ± 24	17 ± 9
Others minerogenic elements								
Ca (mg kg^{-1})	5261 ± 1306 *(25 %)*	4508 ± 1346	6000 ± 1331	4680 ± 1072	5343 ± 683	5042 ± 196	5069 ± 2342	26540 ± 7566
K (mg kg^{-1})	4426 ± 1020 *(23 %)*	2998 ± 428	4686 ± 682	3699 ± 781	5528 ± 504	4490 ± 941	4575 ± 1054	10510 ± 2616
Mg (mg kg^{-1})	1488 ± 354 *(24 %)*	1035 ± 81	1462 ± 274	1320 ± 280	1891 ± 239	1657 ± 283	1513 ± 394	7495 ± 3599
Na (mg kg^{-1})	1794 ± 659 *(37 %)*	1293 ± 460	1847 ± 395	1236 ± 446	2551 ± 437	1987 ± 167	1868 ± 1038	10695 ± 587
$Si_{inorganic}$ (%)	12 ± 4 *(33 %)*	8 ± 3	11 ± 3	11 ± 5	13 ± 3	12 ± 3	9 ± 2	23 ± 1
Sr (mg kg^{-1})	55 ± 16 *(30 %)*	38 ± 6	61 ± 13	47 ± 10	61 ± 5	49 ± 5	66 ± 38	235 ± 24
Ti (mg kg^{-1})	2115 ± 495 *(23 %)*	1301 ± 267	2243 ± 382	1814 ± 314	2675 ± 206	2030 ± 469	2206 ± 203	4357 ± 2348
V (mg kg^{-1})	63 ± 15 *(23 %)*	53 ± 20	53 ± 7	62 ± 10	78 ± 5	85 ± 14	66 ± 16	75 ± 23
Zr (mg kg^{-1})	101 ± 32 *(31 %)*	61 ± 18	112 ± 22	80 ± 22	140 ± 13	79 ± 23	96 ± 20	158 ± 6

[a]whole-lake: averages of all analyzed sediment samples excluding the two outlier samples (sites M4, S15); [b]n: number of sample; [c]the values in parentheses correspond to the relative standard deviation; [d]D.L.: detection limit; The six clusters are presented in Fig. 1b in the manuscript.

Light grey background denotes average values below 10 % of whole-lake average; No background denotes average values close to whole-lake average (±10 %). Dark grey background denotes average values above 10 % of whole-lake average. The variables *in italic* are passive variables in the PCA and cluster analyses.

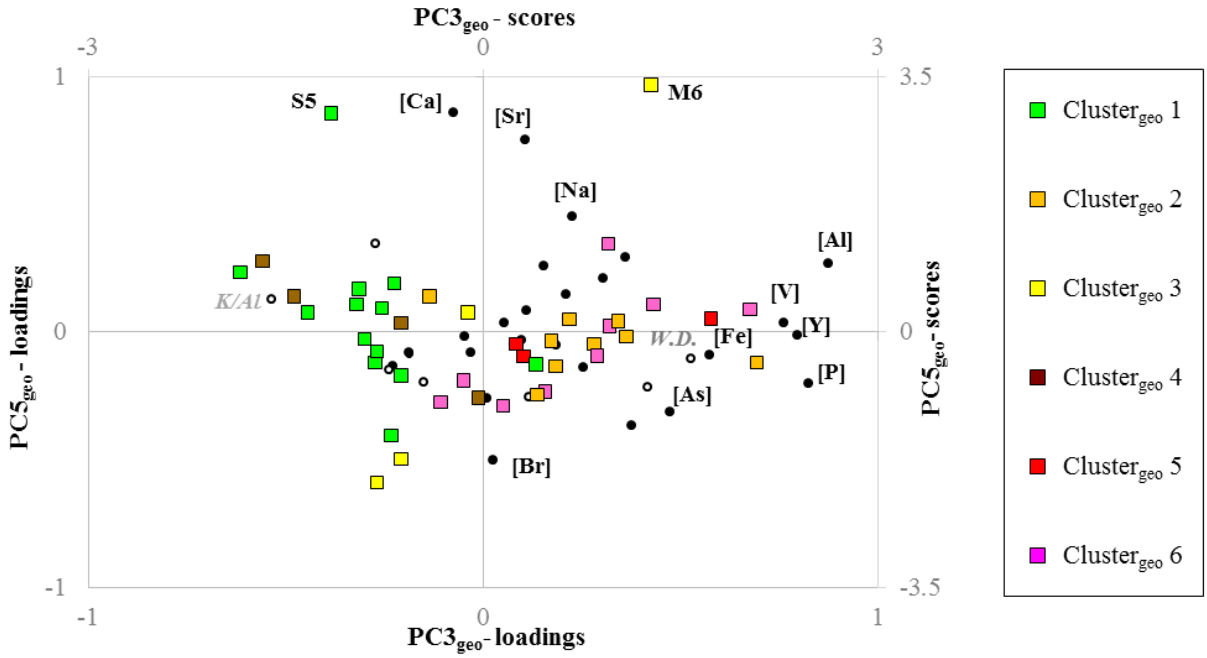

Fig. S1 Combined loading- and score-plots for PCs 3-5 of the elemental geochemistry dataset. For the PC-loadings, filled circles correspond to active variables, and others variables (empty circle and italics letter) were added passively. Sediment samples are colored according to the results of the cluster analysis.

This figure shows that $PC5_{geo}$ (10 % of total variance) separates Ca, Na and Sr on the positive side from Br on the negative side. No reasonable interpretation could be made for this $PC5_{geo}$, which appears to be driven by only two samples which are split into two different clusters by the cluster analysis.

Table S4. Sediment OM molecular composition variables for the 42 sediment samples analysed by Py-GC/MS *(to be continued)*

	Carbohydrates						Chitin-derived compounds	N-compounds									
	(Alkyl)-furans & furanones	Hydroxy- or carboxy-furans & furanones	Pyrans	Dianhydro-rhamnose	Levoglu-cosenone	Anhydro-sugars		(Alkyl)-pyridines	Pyridines_O	(Alkyl)-pyrroles	Pyrroles_O	Pyrroledione & pyrrolidinedione	Aromatic N	Indoles	Diketodi-pyrrole	Diketopi-perazines	Alkyl-amides
N1	**10**	5.1	**4.5**	2.0	2.2	3.1	2.9	**0.42**	0.68	2.1	0.61	1.20	**0.40**	1.40	**1.10**	1.90	0.46
N2	**8**	5.1	3.6	1.3	2.3	3.1	**3.3**	**0.37**	0.69	**2.0**	0.66	1.10	**0.40**	1.40	**1.20**	1.20	0.47
N3	11	5.9	1.7	0.8	**1.5**	2.5	1.2	0.11	0.62	**1.8**	0.86	0.60	0.60	1.20	**0.50**	1.30	0.74
N4	17	4.2	**4.7**	**2.2**	3.1	2.9	**4.0**	**0.40**	**0.91**	2.5	**1.13**	**1.50**	0.60	1.70	0.80	1.80	0.83
N5	13	4.0	3.7	1.7	2.2	6.4	2.9	0.34	0.65	2.2	1.00	**1.40**	0.70	1.40	0.70	1.50	0.61
N6	12	4.1	3.8	1.6	**2.8**	**8.1**	2.2	0.28	0.69	**1.8**	0.79	1.30	0.50	1.30	0.60	1.50	0.70
N7	13	4.0	3.8	1.8	2.3	4.3	2.7	0.31	0.71	**2.0**	0.81	1.20	0.60	1.40	0.70	1.50	0.73
N8	12	4.0	4.1	2.0	2.3	**8.1**	2.7	0.32	0.69	**1.8**	0.82	1.20	0.50	1.30	0.70	1.60	0.63
N9	13	4.6	**4.3**	1.6	**2.6**	2.3	2.5	0.30	0.65	**1.9**	0.75	1.10	0.50	1.30	0.80	1.60	0.74
N10	19	**7.0**	4.1	1.8	**2.7**	2.2	2.5	0.20	**0.85**	2.4	**1.33**	**1.50**	0.80	1.50	0.70	1.50	0.49
N11	16	3.2	2.6	1.5	2.2	2.2	1.9	0.20	**0.73**	2.4	0.96	1.20	0.80	1.50	0.70	1.30	0.69
E1	**10**	3.2	2.2	1.2	1.7	2.0	1.1	0.11	0.57	**1.8**	0.74	0.90	0.70	1.30	0.60	1.10	0.46
E2	**10**	4.2	3.8	1.8	2.3	**8.1**	2.6	0.27	0.70	**1.9**	0.75	1.10	**0.40**	1.30	0.60	1.50	0.73
E3	**9**	5.1	**5.0**	2.1	2.0	4.0	2.5	0.31	0.69	**1.7**	0.67	1.20	**0.30**	1.30	0.80	1.30	0.56
E4	11	4.3	**4.6**	2.0	2.3	6.2	3.2	0.34	**0.81**	2.1	0.82	1.30	0.50	1.40	0.70	1.70	0.74
E5	**10**	4.0	4.0	1.9	2.3	5.6	3.2	0.30	0.70	**2.0**	0.79	**1.40**	0.50	1.40	0.70	1.80	0.80
E6	**10**	4.4	3.8	2.0	1.9	6.8	**3.6**	0.32	0.72	**1.8**	0.87	**1.50**	0.50	1.70	0.70	1.90	0.79
M1	18	**7.5**	3.2	1.3	2.6	2.2	1.4	0.20	0.68	2.6	**1.19**	1.30	0.80	1.40	**0.40**	1.20	0.31
M2	14	4.5	**5.2**	**2.7**	2.2	**8.9**	3.2	0.36	**0.77**	**1.9**	0.91	**1.70**	0.60	1.60	0.70	1.70	0.54
M3	11	3.3	2.6	1.2	2.0	6.2	2.6	0.29	0.71	2.1	0.83	1.10	0.60	1.50	0.80	1.60	0.49
M5	21	**0.8**	**1.2**	**0.3**	**1.5**	**1.0**	**0.2**	**0.06**	**0.17**	2.1	**0.51**	**0.20**	0.60	**0.50**	**0.40**	**0.30**	**0.15**
M6	24	1.6	1.7	0.6	2.3	**1.1**	**0.3**	**0.07**	0.50	2.7	0.77	**0.30**	**1.10**	0.90	1.00	1.00	**0.06**
S1	20	3.2	3.2	1.5	2.5	2.1	2.3	**0.40**	**0.76**	**3.0**	**1.27**	**1.40**	1.00	1.80	0.70	1.20	0.46
S2	**22**	3.2	2.5	1.7	2.1	1.6	1.7	0.33	**0.74**	**3.2**	**1.27**	1.00	**1.10**	1.90	0.60	0.90	0.24
S3	18	4.8	**4.9**	**2.3**	**2.7**	**0.8**	**3.8**	**0.45**	**0.86**	2.7	**1.28**	**1.60**	0.80	1.70	0.80	1.80	0.64
S4	17	3.1	2.2	1.3	1.7	1.8	1.6	0.36	**0.76**	**3.4**	**1.16**	0.80	1.30	1.80	0.70	0.90	0.27
S5	11	5.4	**4.4**	1.9	1.9	**11.0**	1.7	0.34	0.59	**1.7**	0.69	1.30	0.50	1.30	0.90	1.80	0.34
S6	15	3.6	2.9	1.7	1.8	2.5	4.0	0.17	**0.85**	2.7	**1.33**	**1.40**	0.80	1.80	0.80	1.40	0.65
S9	13	4.1	3.2	1.8	1.9	3.2	**3.6**	**0.37**	**0.80**	2.4	0.96	1.10	0.70	1.60	0.90	2.00	0.91
S10	16	3.7	2.5	1.5	2.0	2.7	**3.4**	**0.40**	**0.89**	**3.4**	**1.37**	1.10	0.90	1.70	0.90	1.40	0.58
S11	16	3.7	3.0	1.7	2.5	2.2	2.3	0.31	**0.79**	2.5	**1.19**	0.90	1.00	1.60	0.80	1.20	0.44
S12	12	3.7	3.2	1.5	2.2	1.7	**4.2**	**0.46**	**0.75**	**2.8**	0.90	**1.50**	0.80	1.90	**1.00**	**2.60**	**1.17**
S13	14	3.7	2.3	1.0	1.7	2.0	2.0	0.32	0.65	**2.8**	**1.07**	0.80	1.00	1.60	0.80	1.40	1.08
S14	20	3.6	3.0	1.5	2.6	2.1	1.7	**0.37**	**0.79**	**3.4**	**1.10**	0.90	**1.30**	1.70	0.80	1.30	0.33
S16	**28**	3.9	2.6	2.0	**3.1**	2.2	0.9	0.08	0.48	**3.5**	**1.20**	**1.70**	**1.30**	1.70	0.40	0.80	0.09
S17	14	3.8	2.8	1.5	1.7	2.2	2.6	0.30	**0.81**	2.6	**1.07**	0.80	1.00	1.60	0.80	1.50	0.47
S18	13	3.6	3.2	1.5	2.1	2.9	**3.7**	**0.40**	0.69	**2.8**	0.94	1.30	0.80	1.90	0.90	**2.60**	**1.12**
S19	21	3.8	3.5	1.6	**2.7**	0.9	2.5	0.32	**0.85**	**2.9**	**1.27**	1.30	1.00	1.60	0.70	1.30	0.39
S21	18	3.6	**4.3**	**2.3**	2.1	2.6	**3.4**	**0.37**	**0.85**	2.5	**1.37**	**1.50**	0.90	1.50	0.70	1.40	0.49
S22	14	3.3	2.0	1.3	1.7	1.8	2.1	0.36	0.72	2.7	**1.09**	0.70	1.00	1.60	0.90	1.20	0.38
S23	17	**6.0**	**5.3**	1.6	**2.9**	**8.2**	1.3	0.35	0.57	**1.9**	0.55	1.20	0.70	1.50	0.90	1.40	0.56
S24	11	3.6	2.7	1.8	**1.3**	1.9	**3.4**	**0.37**	**0.86**	**3.1**	0.85	**1.60**	**1.40**	**3.10**	0.90	**2.30**	**1.66**

The font colors of the sample ID cells correspond to the six clusters identified by the cluster analysis on the OM molecular composition dataset.
The bold and underlined numbers corresponds to the minimal and maximal value, and the numbers in bold correspond to the values that are below or above 20 % of the maximal and minimal values respectively.

Table S4. *Continuation* Sediment OM molecular composition variables for the 42 sediment samples analysed by Py-GC/MS *(to be continued)*

	Lignins			Chlorophylls		*n*-alkenes				*n*-alkanes				Alkan-2-ones		
	Phenols	**Syringols**	**Guaiacols**	**Pristenes**	**Phytadienes**	**C9-16:1**	**C17-22:1**	**C23-26:1**	**C27-28:1**	**C13-16:0**	**C17-22:0**	**C23-26:0**	**C27-35:0**	**2K C13-17**	**2K C19-22**	**2K C23-31**
N1	**10.6**	**1.9**	**10.6**	3.7	1.6	**2.0**	5.2	3.9	**1.2**	1.7	3.1	**1.9**	2.3	**0.6**	0.24	1.7
N2	**11.4**	**1.4**	7.7	3.0	1.7	2.3	5.8	3.0	0.9	1.9	3.2	3.2	6.3	**0.6**	0.21	1.5
N3	9.0	0.6	3.6	2.8	1.3	3.8	**7.1**	**4.8**	**1.3**	2.7	4.5	4.1	6.1	1.0	0.40	**3.2**
N4	7.6	0.3	2.3	2.3	**3.5**	2.8	5.1	2.1	0.6	1.9	3.4	2.4	4.1	1.4	0.24	1.0
N5	7.3	0.4	3.0	3.2	1.7	3.5	6.7	3.0	1.0	2.6	4.2	2.7	3.9	1.3	0.35	1.5
N6	7.3	0.4	3.8	3.2	1.9	2.8	6.2	3.4	0.8	1.9	3.5	3.1	6.1	1.1	0.28	1.9
N7	7.6	0.5	3.8	3.2	1.9	3.1	6.5	4.1	**1.2**	2.1	4.0	2.8	4.3	1.1	0.34	**2.6**
N8	7.2	0.4	3.6	3.2	1.6	3.1	6.6	3.4	**1.1**	2.3	3.9	3.0	4.9	1.1	0.33	2.0
N9	8.7	0.6	4.1	3.7	2.0	2.9	6.6	4.0	**1.2**	2.3	4.0	2.8	4.3	0.8	0.36	2.5
N10	9.5	0.2	1.8	1.5	1.5	3.0	5.2	2.1	0.4	2.4	3.1	2.7	3.5	1.0	0.19	0.6
N11	6.6	0.2	2.1	2.5	2.3	3.9	6.7	3.5	**1.4**	2.6	**4.4**	**4.8**	6.6	1.4	0.30	1.0
E1	8.1	0.3	3.5	**4.6**	1.4	**4.0**	**8.9**	**5.4**	**1.3**	2.7	**5.1**	3.9	5.6	1.0	0.35	**3.3**
E2	7.4	0.5	3.7	3.4	1.5	3.1	**7.1**	3.6	**1.2**	2.2	4.1	3.4	5.4	0.9	0.30	2.3
E3	8.8	**1.4**	7.5	3.2	1.5	2.5	6.1	3.8	1.0	1.7	3.5	3.2	6.2	0.6	0.31	2.3
E4	7.3	0.5	3.7	3.2	1.9	2.9	6.6	3.6	1.0	2.0	3.9	2.6	4.8	1.1	0.31	2.3
E5	7.9	0.6	4.1	3.5	1.5	3.0	6.6	3.8	1.0	2.3	4.1	2.8	4.7	1.0	0.36	2.3
E6	8.0	0.7	4.6	3.1	1.8	2.9	6.2	3.6	**1.1**	2.4	3.8	2.4	4.3	1.0	0.40	2.1
M1	8.0	0.2	1.9	2.1	1.3	3.8	6.2	3.0	0.5	2.6	3.5	2.7	3.6	0.9	0.15	0.8
M2	7.0	0.7	4.0	2.2	1.9	2.8	5.4	2.6	0.8	2.1	3.3	2.5	3.5	1.1	0.27	1.2
M3	6.9	0.3	3.3	2.3	2.0	3.1	5.6	2.6	0.6	2.2	3.5	**4.5**	10.1	1.2	0.23	1.3
M5	**4.4**	**0.1**	**1.1**	**0.4**	**0.2**	**4.1**	**3.8**	**0.6**	0.1	2.3	**1.6**	**8.8**	**21.3**	1.6	**0.02**	**0.1**
M6	7.7	0.2	1.5	0.6	1.0	3.8	**4.0**	1.5	0.1	2.4	2.1	**6.7**	11.8	1.6	**0.03**	0.3
S1	8.0	0.3	2.4	2.5	1.8	**4.6**	6.4	2.2	0.3	3.2	**4.6**	2.2	1.9	**1.8**	0.34	0.4
S2	6.9	0.2	2.1	2.7	2.2	**5.1**	6.9	2.1	0.3	**3.7**	**4.6**	2.0	1.4	**1.9**	0.31	0.3
S3	7.8	0.4	2.8	2.6	2.1	3.7	5.8	2.2	0.7	2.8	4.1	**1.5**	1.6	1.6	0.44	0.7
S4	**9.1**	0.3	2.9	3.4	1.5	**4.8**	6.7	2.5	0.4	**4.1**	**4.7**	1.8	1.8	**1.9**	0.38	0.8
S5	**9.6**	**1.8**	**13.5**	2.2	1.2	**2.1**	4.4	2.6	0.7	1.7	2.5	**1.4**	1.4	**0.7**	0.15	0.7
S6	7.9	0.4	2.8	2.9	1.9	**4.6**	6.9	2.5	0.5	**3.7**	**5.4**	**1.8**	1.7	**1.8**	0.53	0.9
S9	8.4	0.4	2.9	2.8	1.9	3.7	6.3	3.1	1.0	2.7	**4.6**	2.5	3.5	1.5	0.44	1.6
S10	8.0	0.3	2.3	2.6	2.1	**4.4**	6.6	2.1	0.6	3.2	**4.6**	**1.6**	1.7	**2.0**	0.47	0.7
S11	8.8	0.3	2.9	3.2	1.6	**4.3**	6.8	2.6	0.7	2.9	**4.5**	**1.9**	2.3	**1.8**	0.40	0.9
S12	8.6	0.4	2.5	2.6	**2.8**	3.4	5.8	2.7	1.0	2.6	4.1	2.2	3.6	1.6	0.34	1.2
S13	9.0	0.3	2.6	2.8	1.4	**4.5**	6.6	2.3	0.6	3.1	4.2	2.9	3.9	**2.0**	**0.82**	1.1
S14	8.5	0.2	2.2	2.9	**3.3**	**4.0**	5.6	2.2	0.4	2.3	3.2	**1.6**	2.4	1.7	0.28	0.6
S16	6.4	0.2	2.1	2.0	1.3	**4.5**	5.8	1.5	**0.1**	3.0	3.4	**1.7**	**1.1**	1.4	0.05	0.1
S17	9.0	0.3	2.7	3.0	2.0	**4.1**	6.6	3.2	0.7	2.8	**4.6**	2.4	3.0	**1.8**	0.44	1.1
S18	8.7	1.2	3.8	2.4	**2.9**	3.1	5.1	2.6	0.9	2.4	3.7	2.2	3.3	1.4	0.30	1.0
S19	8.7	0.2	2.3	2.8	2.4	3.9	5.7	2.3	0.5	2.5	3.9	**1.7**	2.1	1.5	0.27	0.6
S21	7.0	0.4	2.9	2.7	1.5	**4.0**	6.2	2.4	0.5	2.9	**4.7**	2.7	1.9	1.6	0.33	0.7
S22	**9.1**	0.3	2.7	3.1	1.6	**4.5**	7.0	3.3	0.7	3.0	**5.0**	2.9	3.4	**1.9**	0.39	1.0
S23	8.5	1.3	4.6	1.6	2.5	**1.8**	**3.5**	3.5	**1.4**	**1.3**	2.3	3.0	3.6	**0.7**	0.10	1.4
S24	**10.3**	0.5	3.0	2.2	**3.6**	3.4	4.3	2.0	0.6	2.6	3.7	**1.9**	2.7	**2.2**	0.35	1.0

The font colors of the sample ID cells correspond to the six clusters identified by the cluster analysis on the OM molecular composition dataset.
The bold and underlined numbers corresponds to the minimal and maximal value, and the numbers in bold correspond to the values that are below or above 20 % of the maximal and minimal values respectively.

Table S4. *Continuation* Sediment OM molecular composition variables for the 42 sediment samples analysed by Py-GC/MS

	Steroids	Tocopherols	Hopanoids	(Poly)aromatics				
				Benzene	Benzaldehyde	Acetophenone	alkylbenzene C3-9	Polyaromatics
N1	0.91	**1.45**	1.1	**0.4**	**0.31**	**0.57**	**1.4**	**0.9**
N2	1.49	1.00	1.0	0.8	**0.36**	**0.72**	**1.6**	**1.0**
N3	0.99	0.57	1.3	0.9	0.96	1.51	**1.6**	1.4
N4	1.27	0.16	1.2	0.8	0.44	0.76	**1.7**	**1.0**
N5	0.63	0.30	1.4	0.8	0.52	0.94	**1.7**	1.2
N6	1.23	0.42	1.4	0.7	0.42	0.72	**1.5**	**1.0**
N7	1.04	0.42	**1.6**	0.7	0.44	0.82	**1.7**	1.1
N8	0.96	0.42	1.4	0.5	0.43	0.74	1.6	**0.8**
N9	1.50	0.60	1.5	0.7	**0.40**	0.72	1.6	**1.0**
N10	0.32	0.15	0.7	1.8	1.08	**1.98**	1.9	1.6
N11	0.67	0.09	1.3	1.0	0.56	1.01	1.9	1.4
E1	0.90	0.75	**1.5**	0.8	0.61	1.06	1.8	1.5
E2	0.82	0.47	1.3	0.8	0.41	0.75	**1.5**	**1.0**
E3	0.92	0.78	1.3	0.5	**0.35**	0.61	**1.4**	**0.8**
E4	1.03	0.42	1.4	0.8	**0.40**	**0.72**	**1.5**	**1.0**
E5	1.37	0.57	**1.6**	0.8	0.42	0.74	**1.5**	**1.0**
E6	1.39	0.52	**1.5**	0.7	**0.40**	**0.71**	**1.5**	**1.0**
M1	0.28	0.19	0.8	**2.5**	1.33	**2.30**	2.1	1.7
M2	0.47	0.26	1.2	0.7	0.46	0.78	1.8	**1.0**
M3	1.22	0.18	1.3	0.7	**0.40**	0.73	1.8	1.1
M5	**0.03**	**<DL**	**0.2**	0.7	0.64	1.02	1.7	1.5
M6	0.09	**0.01**	**0.2**	0.6	0.78	1.19	1.8	1.3
S1	0.54	0.04	1.3	0.9	0.67	1.16	2.1	**1.7**
S2	0.51	**<DL**	1.4	1.1	0.83	1.41	2.3	**1.7**
S3	1.16	0.09	1.4	0.7	0.63	1.05	2.0	1.3
S4	0.79	0.13	**1.8**	1.1	0.95	1.62	2.7	2.1
S5	0.93	0.48	0.7	**0.5**	0.44	0.68	**1.4**	1.1
S6	1.32	0.12	**1.5**	0.7	0.60	1.05	2.1	1.4
S9	2.14	0.21	**1.6**	0.9	0.53	0.94	1.8	1.3
S10	1.62	0.06	**1.6**	1.1	0.77	1.36	2.2	**1.7**
S11	1.48	0.12	**1.5**	1.1	0.76	1.37	2.4	**1.8**
S12	**3.30**	0.12	**1.6**	1.0	0.43	0.80	2.2	1.2
S13	1.49	0.09	**1.6**	0.9	0.75	1.44	**3.5**	2.0
S14	1.38	0.04	1.4	1.6	0.84	1.45	**2.8**	**1.9**
S16	0.14	**0.01**	0.9	1.7	**1.47**	**2.15**	2.4	**1.8**
S17	2.02	0.08	**1.8**	0.9	0.76	1.35	2.2	**1.8**
S18	**3.53**	0.08	**1.6**	1.2	0.42	0.77	2.1	1.2
S19	1.21	0.03	**1.6**	1.0	0.71	1.29	2.6	**1.7**
S21	0.92	0.09	**1.8**	0.7	0.61	1.03	1.8	1.4
S22	1.51	0.09	**1.8**	1.1	0.76	1.45	2.5	**2.1**
S23	1.18	0.33	0.5	0.6	0.47	0.79	**1.4**	1.0
S24	**4.28**	0.17	**1.9**	0.7	0.67	0.93	2.1	1.2

The font colors of the sample ID cells correspond to the six clusters identified by the cluster analysis on the OM molecular composition dataset. The bold and underlined numbers corresponds to the minimal and maximal value, and the numbers in bold correspond to the values that are below or above 20 % of the maximal and minimal values respectively.

Table S5. Average of the OM molecular composition variables for the whole-lake and the six clusters

		Near-shore sites	North/East basins	South basins		Shallow central areas	
Variables (unit)	**Whole-lake[a] (n[b]=42)**	$Cluster_{OM}$ 5 (n=4)	$Cluster_{OM}$ 1 (n=16)	$Cluster_{OM}$ 3 (n=14)	$Cluster_{OM}$ 2 (n=3)	$Cluster_{OM}$ 4 (n=3)	$Cluster_{OM}$ 6 (n=2)
Carbohydrates							
(Alkyl)-furans & furanones	15 ± 5	12 ± 4	12 ± 2	17 ± 3	11.9 ± 0.7	22 ± 5	23 ± 2
Hydroxy- or carboxy-furans & furanones	4 ± 1	5.4 ± 0.4	4.2 ± 0.7	3.7 ± 0.5	3.7 ± 0.1	6.1 ± 1.9	1.2 ± 0.6
Pyrans	3 ± 1	4.7 ± 0.7	3.6 ± 0.9	3 ± 1	3.0 ± 0.3	3.3 ± 0.8	1.4 ± 0.4
Dianhydrorhamnose	1.6 ± 0.5	1.7 ± 0.3	1.7 ± 0.4	1.7 ± 0.5	1.6 ± 0.2	1.7 ± 0.3	0.5 ± 0.2
Levoglucosenone	2.2 ± 0.4	2.3 ± 0.4	2.2 ± 0.4	2.2 ± 0.4	1.9 ± 0.5	2.8 ± 0.3	1.9 ± 0.5
Anhydrosugars	4 ± 3	6.4 ± 3.9	4.9 ± 2.3	2.4 ± 1.9	2.2 ± 0.6	2.19 ± 0.03	1.02 ± 0.06
Chitin-derived compounds							
Chitin-derived compounds	3 ± 1	2.3 ± 0.9	2.7 ± 0.8	2.6 ± 0.8	3.8 ± 0.4	1.6 ± 0.8	0.23 ± 0.1
N-compounds							
(alkyl)pyridines	0.3 ± 0.1	0.37 ± 0.03	0.28 ± 0.08	0.35 ± 0.06	0.41 ± 0.04	0.16 ± 0.07	0.06 ± 0.01
Pyridines_O	0.7 ± 0.1	0.63 ± 0.06	0.71 ± 0.08	0.79 ± 0.06	0.77 ± 0.09	0.7 ± 0.2	0.3 ± 0.2
(alkyl)pyrroles	2.4 ± 0.5	1.9 ± 0.1	2.0 ± 0.3	2.8 ± 0.4	2.9 ± 0.2	2.8 ± 0.6	2.4 ± 0.4
Pyrroles_O	1.0 ± 0.2	0.63 ± 0.06	0.9 ± 0.1	1.2 ± 0.1	0.90 ± 0.04	1.24 ± 0.08	0.6 ± 0.2
Pyrroledione/ pyrrolidinedione	1.2 ± 0.3	1.2 ± 0.08	1.2 ± 0.2	1.1 ± 0.3	1.5 ± 0.2	1.5 ± 0.2	0.2 ± 0.1
Aromatic N	0.8 ± 0.3	0.5 ± 0.1	0.6 ± 0.1	1.0 ± 0.2	1.0 ± 0.4	1.0 ± 0.3	0.9 ± 0.3
Indoles	1.5 ± 0.4	1.39 ± 0.08	1.4 ± 0.2	1.7 ± 0.1	2.3 ± 0.7	1.5 ± 0.2	0.7 ± 0.3
Diketodipyrrole	0.8 ± 0.2	1.0 ± 0.2	0.7 ± 0.1	0.78 ± 0.08	0.92 ± 0.07	0.5 ± 0.2	0.7 ± 0.4
Proteins	1.5 ± 0.4	1.6 ± 0.3	1.6 ± 0.2	1.3 ± 0.3	2.5 ± 0.2	1.2 ± 0.4	0.6 ± 0.5
Alkylamides	0.6 ± 0.3	0.46 ± 0.09	0.7 ± 0.1	0.5 ± 0.2	1.3 ± 0.3	0.3 ± 0.2	0.11 ± 0.06
Phenols and Lignins							
Phenols	8.2 ± 1.2	10 ± 1	7.7 ± 0.7	8.2 ± 0.8	9.2 ± 0.9	8 ± 1	6 ± 2
Guaiacols	4 ± 2	9 ± 4	4 ± 1	2.7 ± 0.5	3.1 ± 0.7	1.9 ± 0.1	1.3 ± 0.3
Syringols	0.5 ± 0.4	1.6 ± 0.3	0.5 ± 0.3	0.3 ± 0.1	0.7 ± 0.4	0.21 ± 0.01	0.1 ± 0.1
Chlorophylls							
Pristenes	2.7 ± 0.8	2.6 ± 0.9	3.1 ± 0.6	2.8 ± 0.3	2.4 ± 0.2	1.9 ± 0.3	0.5 ± 0.1
Phytadienes	1.9 ± 0.6	1.7 ± 0.6	1.8 ± 0.5	1.9 ± 0.5	3.1 ± 0.4	1.3 ± 0.2	0.6 ± 0.6
***n*-alkenes (Cn:1)**							
C9-16:1	3.5 ± 0.8	2.1 ± 0.2	3.2 ± 0.4	4.2 ± 0.6	3.3 ± 0.2	3.7 ± 0.7	3.9 ± 0.3
C17-C22:1	6 ± 1	5 ± 1	6.6 ± 0.8	6.4 ± 0.5	5.1 ± 0.7	5.7 ± 0.5	3.9 ± 0.2
C23-26_1	2.9 ± 0.9	3.3 ± 0.6	3.6 ± 0.8	2.5 ± 0.4	2.4 ± 0.4	2.2 ± 0.7	1.0 ± 0.6
C27-28:1	0.8 ± 0.4	1.1 ± 0.3	1.1 ± 0.2	0.6 ± 0.1	0.9 ± 0.2	0.3 ± 0.2	0.12 ± 0.02
***n*-alkanes (Cn:0)**							
C13-16:0	2.5 ± 0.6	1.7 ± 0.3	2.3 ± 0.3	3.0 ± 0.5	2.6 ± 0.1	2.7 ± 0.3	2.4 ± 0.1
C17-22:0	3.9 ± 0.8	2.8 ± 0.4	4.0 ± 0.5	4.4 ± 0.6	3.9 ± 0.2	3.3 ± 0.2	1.9 ± 0.4
C23-26:0	3 ± 1	2.4 ± 0.9	3.2 ± 0.8	2.1 ± 0.5	2.1 ± 0.1	2.4 ± 0.6	8 ± 1
C27-35:0	4 ± 4	3 ± 2	5 ± 1	2.3 ± 0.8	3.2 ± 0.4	2.8 ± 1.4	17 ± 7
Alkan-2-ones (2K)							
2K C13-17	1.3 ± 0.4	0.7 ± 0.1	1.1 ± 0.2	1.8 ± 0.2	1.7 ± 0.4	1.1 ± 0.3	1.60 ± 0.02
2K C19-22	0.3 ± 0.1	0.18 ± 0.06	0.33 ± 0.06	0.4 ± 0.1	0.33 ± 0.03	0.13 ± 0.07	0.03 ± 0.01
2K C23-31	1.3 ± 0.8	1.3 ± 0.4	2.1 ± 0.7	0.8 ± 0.3	1.1 ± 0.1	0.5 ± 0.4	0.2 ± 0.2
Steroids							
Steroids	1.2 ± 0.9	1.1 ± 0.3	1.1 ± 0.4	1.2 ± 0.5	3.7 ± 0.5	0.25 ± 0.09	0.06 ± 0.04
Tocopherols							
Tocopherols	0.3 ± 0.3	0.8 ± 0.5	0.4 ± 0.2	0.09 ± 0.06	0.12 ± 0.04	0.11 ± 0.09	0.01 ± 0.01
Hopanoids							
Hopanoids	1.3 ± 0.4	0.8 ± 0.3	1.4 ± 0.1	1.6 ± 0.2	1.7 ± 0.2	0.78 ± 0.09	0.17 ± 0.01
(Poly)aromatics							
Benzene	0.9 ± 0.4	0.6 ± 0.2	0.8 ± 0.1	1.0 ± 0.3	1.0 ± 0.3	2.0 ± 0.4	0.67 ± 0.06
Benzaldehyde	0.6 ± 0.3	0.39 ± 0.07	0.5 ± 0.1	0.7 ± 0.1	0.5 ± 0.1	1.3 ± 0.2	0.71 ± 0.09
Acetylbenzene	1.1 ± 0.4	0.7 ± 0.1	0.8 ± 0.2	1.3 ± 0.2	0.84 ± 0.09	2.2 ± 0.2	1.1 ± 0.1
Alkylbenzenes C3-9	1.9 ± 0.5	1.44 ± 0.09	1.6 ± 0.2	2.4 ± 0.4	2.10 ± 0.04	2.1 ± 0.2	1.71 ± 0.07
Polyaromatics	1.4 ± 0.4	1.01 ± 0.07	1.1 ± 0.2	1.7 ± 0.3	1.21 ± 0.03	1.7 ± 0.1	1.4 ± 0.1

[a]whole-lake: averages of all analyzed sediment samples excluding the two outlier samples (sites M4, S15); [b]n: number of sample; The six clusters are presented in Fig. 1d in the manuscript.

Light grey background denotes average values below 10 % of whole-lake average. No background denotes values close to whole-lake average (±10 %). Dark grey background denotes average values above 10 % of whole-lake average.