



## 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<sup>a</sup>), references for the theoretical mass spectra (REF) and how the individual organic compounds have been grouped for the statistical analyses

Name         Portunal         N         N         Not         Relational         Relational </th <th>Nome</th> <th>Eamula</th> <th>м</th> <th>рт</th> <th>RI<sub>this</sub></th> <th>refere</th> <th>ence RI<sup>b</sup></th> <th>DEE</th> <th>Compounds anouns</th>	Nome	Eamula	м	рт	RI <sub>this</sub>	refere	ence RI <sup>b</sup>	DEE	Compounds anouns
$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	Ivallie	Formula	111	K1	study	RI <sub>estimated</sub>	<b>RI</b> <sub>experimental</sub>	KEF	Compounds groups
3-fundeloyde         CSH402         96         189.5         N.D.*         NIST         III           2-accyb/plum         CGH602         110         267.2         N.D.         NIST. [1]         (Alty)furma & Methyl-5-fundeloyde         CGH602         110         267.2         N.D.         NIST. [1]         (Alty)furma & Methyl-5-fundeloyde         CGH602         110         267.2         N.D.         NIST. [1]         (Alty)furma & Methyl-5-fundeloyde         CGH602         110         27.9         N.D.         NIST. [1]         (Alty)furma & Methyl-5-fundeloyde         CGH602         22.5         907         N68         91.4-917         NIST. [1]         Hydroxyl or         22-fundeloyde         CGH602         128         420         920         924.497         NIST. [1]         Hydroxyl or           22-fundeloyde         CGH602         126         51.9         128         1023         1023         1024.1007         NIST. [1]         Hydroxyl or           22-fundeloyde         CGH603         126         451.9         128         434.1         104         NR         NR         121         Hudoxydrofmance           24-bydroxys-fordingtor/24-promo-         CGH603         126         451.1         118         NR         NR         NR         111	Carbohydrates								
2-fanildebyde         CSH402         96         204.1         N.D.         NIST         II           Methyl-3-fanildebyde         C6H602         110         269.8         N.D.         NIST, [1]         Alkylfurans & fanones           Stadiyl-faranoc         C6H602         110         276.9         N.D.         NIST, [1]         Alkylfurans & fanones           Shighor-methyl-faranoc         CSH602         98         277.8         N.D.         III         Towns           Somethyl-2,5thj-furanoc         CSH602         98         27.5         907         868         914.917         NIST, [1]         Hydroxylf           2-fundidshyle         C6H603         126         422.7         909         NIST, [1]         Hydroxylf or           2-folditydor-2Hydrox-3(2H)-fundios         C6H603         126         422.6         1088         1022         1023         NIST         funances           5-dightydrox-Hydrox-3(2H)-fundios         C6H603         126         451.9         123.6         102         1023         NIST         funances           5-dightydrox-Hydrox-3(2H)-funance         C5H603         14         342.4         040         NR         NR         NIST         funances           5-diditydorox-Hydrox-3(H)-funance </td <td>3-furaldehyde</td> <td>C5H4O2</td> <td>96</td> <td>189.5</td> <td>N.D.<sup>c</sup></td> <td></td> <td></td> <td>NIST, [1]</td> <td></td>	3-furaldehyde	C5H4O2	96	189.5	N.D. <sup>c</sup>			NIST, [1]	
2-accy-brann         C61602         110         267.2         N.D.         NIST, [1]           2(3b) furanose         C41402         84         270.5         N.D.         NIST, [1]         (Alky) furanose           2(3b) furanose         C41402         84         270.5         N.D.         NIST, [1]         (Alky) furanose           Dilydro-methyl-furanone         C51602         98         277.8         N.D.         III         Termanose           Senthyl-S(3r) kacial, methyl ever         C61603         128         422.7         909         NIST, [1]         Hydroxyl or caster (11)         C41603         128         1163         1176-1236         NIST, [1]         Hydroxyl or caster (11)         caboxyl-furanose         5.6         611004         287.7         N.D.         NIST, [1]         Hydroxyl or caster (11)         H	2-furaldehvde	C5H4O2	96	204.1	N.D.			NIST. [1]	
Marthy-3-faradadesyde         C61602         110         29.8         N.D.         NIST, 111         (Alky1)farma & faratoms           S2B-faranone         C416402         84         270.5         N.D.         NIST, 111         (Alky1)farma & faratoms           S18-drive-1/2-drivaldesyde         C61602         110         277.8         N.D.         II1           S-methyl-2-fardidesyde         C61602         110         12.8         920         92-987         NIST, 111           2-brancubox/bit acid, methyl ester         C61603         12.6         42.7         99         NIST, 111         Garbay-forman & formanos           2-brancubox/bit acid, methyl ester         C61603         12.6         42.6         1038         1022         1023-1097         NIST, 111         Garbay-forman & formanos           2-branchyd-hydhory-3(21) Hyran-2one         C51603         12.6         42.6         10.8         1022         1023-1097         NIST, 111         faraaones           2-branchyd-hydhory-3(21) Hyran-2one         C51603         114         4342         941         N.R         N.R         111           Pyrans         Janhydrochamose         C61603         12.6         453.1         117         N.R         111           Lengiglaciseninio	2-acetyl-furan	C6H6O2	110	267.2	ND			NIST [1]	
NSBJ Ammen         C014002         84         270.5         N.D.         NBST. [1]         (Alky)thrmas & faranones           Mehyl-2 (Mindebyde         C61602         110         276.9         N.D.         NBST. [1]         (Alky)thrmas & faranones           Smedyl-2 (Mindebyde         C61602         110         276.9         N.D.         NBST. [1]         (Mindyl-2-farandebyde         C61602         110         312.8         290         924.98         NBST. [1]         Hydroxyl or           2 - Immatryl-Altydroxy-3(2H)-furmance         C61602         126         422.7         900         924.98         NBST. [1]         Hydroxyl or           2 - Immatryl-Altydroxy-3(2H)-furmance         C61602         126         51.9         1236         11063         117.7<126	Methyl-3-furaldehyde	C6H6O2	110	269.8	N D			NIST [1]	
Labory 12 annualization         Coli 602         or         276 or         N.D.         N.B.T.         Inframones           Dibylor-andth-formance         CSI600         98         277.8         N.D.         NET.111           Markin-andth-formance         CSI600         98         292.9         920         924.987         NET.111           Markin-andth-formance         CSI600         110         312.8         920         90         924.987         NET.111           Markin-andth-formance         CSI600         126         422.6         1088         1022         Units         111         Printanones           Schudowymethy-2-fundlehyde         CSI600         126         51.9         123         1163         1176-1236         NIST.111         Furanones           Schudowymethy-2-fundlehyde         CSI600         82         787.8         N.D.         N.R.         111         Prytras           Dambydrohamose         CGI603         126         450.1         1119         N.R.         N.R.         111         Prytras           Levoglacostom         CGI1005         162         761.5         1437         N.R.         N.R.         111         Anhydrosagurs           Levoglacostom         CGI11005	2(5H) furanone	C4H4O2	84	202.0	ND.			NIST, [1]	(Alkyl)furans &
Section-Antimetry of the Critical Stress of the Stress of Stres	Mothyl 2 furaldabyda	C4II402	110	276.0	ND.			NIST, [1]	furanones
	Dihadan mathal famu and	C0H0O2	00	270.9	N.D.			[1]	
Smethyl-2/mithelydek         CoHkoO2         19         392         390         888         91-4317         NIST         Hydroxyl or           2-Furancaboxylic acid, methyl ester         CoHkoO3         126         422.7         909         NIST, [1]         Hydroxyl or           2-Furancaboxylic acid, methyl ester         CoHkoO3         128         424.6         NIST, [1]         Turances           2-Submethyl-Alproxabchylos         CoHkoO3         128         424.6         NIST, [1]         Turances           5-(hydroxy)-5.6 dihydro-2(H) pyran-2-one         CSH603         124         383.4         IVA         N.R.         [1]         Pyrans           Levosignat (Coregulatorsam)         COH1005         162         375.7         N.R.         N.R.         [1]         Anhydrobacooc           Levosignat (Coregulatorsam)         COH1005         162         371.4         1493         1404         1486-1491         [1]         Anhydrosugars           Levosignat (Coregulatorsam)         COH1005         162         771.4         1493         1404         1486-1491         [1]         Anhydrosugars           Levosignatic comanosa         COH7NO3         152         555.4         123         N.R.         N.R.         [3]         compounds	Dinydro-metnyi-iuranone	C5H6U	98	277.8	N.D.	0.60	014 017		
Methyl-2-turnidelyde         CoH602         110         31.2.8         9.00         9.20         9.24         9.24         NIST         Hydroxyl or arboxy-furans &           2.5-Dimatchyl-Mydrox acid, methyl exter         CoH803         126         422.7         909         NIST, 11         Hydroxyl or arboxy-furans &           5.6-diflydro, 2H-lyytan-2-one         CSH602         128         65.4         1176-125         NIST, 11         Fyransone           9.6-diflydro, 2H-lyytan-2-one         CSH603         128         38.3         1041         N.R. 4         N.R.         NIST         Pyrans           Dianhydrothamose         CGH803         128         38.3         1041         N.R. 4         N.R.         NIST         Levoglucosenone           Levoglucoson         CGH1005         162         75.7         17.5         N.R.         N.R.         11           Levoglucoson         CGH1005         162         76.1         1447         N.R.         N.R.         11           Levoglucoson         CGH1005         162         76.1         1447         N.R.         NIST         Acetamido-fuso           Acetamido furan         CGH7N02         125         55.5         1239         N.R.         N.R.         NIST </td <td>5-methyl-2(5H)-Furanone</td> <td>C5H6O2</td> <td>98</td> <td>292.5</td> <td>907</td> <td>868</td> <td>914-917</td> <td>NIST, [1]</td> <td></td>	5-methyl-2(5H)-Furanone	C5H6O2	98	292.5	907	868	914-917	NIST, [1]	
2-Furancarboxylic acd, methyl ester 2-Furancarboxylic acd, methyl ester 2-Sibmethyl-Hydroxy-321F1/nurance 5-thydroxymethyl)-2-Furaldehyde C6H803 124 424.6 1088 1022 1023-1097 NIST cfordhydroxylic acd, MiST, Li 4-hydroxy-5.6-dihydrox2H1-pyran-2-one C5H02 98 278.7 N.D. 4-hydroxy-5.6-dihydrox2H1-pyran-2-one C5H02 98 278.7 N.D. 4-hydroxy-5.6-dihydrox2H1-pyran-2-one C5H02 124 383.4 1041 N.R. N.R. [1] Diandydrorhamose C6H003 126 450.1 1119 N.R. N.R. [1] Levosglacosenone C6H005 162 771.4 1493 1404 1486-1491 [1] Chin derived compands Levosglacosenone C6H005 162 771.4 1493 1404 1486-1491 [1] Chin derived compands N.R. N.R. [1] Anhydrosugars Levosglacosenone C6H7N0 121 555.4 1239 N.R. N.R. NIST - acetamido-4-pyrone Unknown 801.9 1548 N.R. N.R. [3] compounds N-Compands N-Compands N-Compands N-Compands N-Compands 2-methyl-pyrdine C6H7N 93 197.6 N.D. NIST - Anhydrosugars (Alkyl)pyrdine C7H7N0 121 407. 1034 N.R. N.R. NIST - Anhydrosugars 2-nethyl-pyrdine C6H7N 95 151.7 N.R. N.R. NIST - Anhydrosugars 2-nethyl-pyrdine C6H7N 95 151.7 N.R. N.R. NIST - MIST - Acatyhyridine C7H7N0 121 407.2 1034 N.R. N.R. NIST - Acatyhyridine C6H7N 95 354.2 1068 988 1005-1030 NIST - Chilin derived - CH7N 95 354.2 1068 988 1005-1030 NIST - Chilin derived - CH7N 95 354.2 1068 988 1005-1030 NIST - Chilin derived - CH7N 95 354.2 1068 988 1005-1030 NIST - Chilin derived - CH7N 95 354.2 107 1092-1105 NIST - Chilin derived - CH7N 95 354.2 107 1092-1105 NIST - Chilin derived - CH7N 95 354.2 1089 988 1005-1030 NIST - Chilin derived - CH7N 95 354.2 1134 714 1267 0164 NIST - Chilin derived - CH7N 95 354.2 1134 714 128 1089-1143 NIST - Chilin derived - CH7N 95 354.2 11	Methyl-2-furaldehyde	C6H6O2	110	312.8	920	920	924-987	NIST, [1]	
2.5-Dimethyl-4-hydraxy-3(2H)-furanone C6H803 128 424.6 1088 1022 1023-1097 NIST carboxy-furano.es 5.6-ditydoryDHyl-2-Braidebyde C6H803 126 551.9 1236 1136 1176-1236 NIST [1] Granones 5.6-ditydoro2H-Pyran-2-one C5H603 114 344.2 941 N.R. N.R. N.R. [1] Dianhydrorhamnose C6H803 128 383.4 1041 N.R. N.R. [2] Dianhydrorhamnose 1evoglacosanone C6H803 126 450.1 119 N.R. N.R. [2] Dianhydrorhamnose 1evoglacosanone C6H803 126 450.1 119 N.R. N.R. [1] Anhydrohxoc Unknown 729.0 1450 N.R. N.R. [1] Levosagars (Levoglactosan) C6H1005 162 735.7 N.R. N.R. [1] Levosagars (Levoglactosan) C6H1005 162 771.4 1439 1404 [446-149] [1] Levosagars (Levoglactosan) C6H1005 162 771.4 1439 1404 [446-149] [1] Levosagars (Levoglactosan) C6H1005 162 771.4 1439 1404 [446-149] [1] Levosagars (Levoglactosan) C6H1002 125 555.4 1239 N.R. N.R. NIST S-acetamido-furan C6H7N02 125 555.4 1239 N.R. N.R. NIST S-acetamido-furan C6H7N02 125 555.4 1239 N.R. N.R. [3] Chin derived compounds Horomounds	2-Furancarboxylic acid, methyl ester	C6H6O3	126	422.7		909		NIST, [1]	Hydroxyl or
5-(hydroxymethy)-2-Fundlehyde         C6H003         126         51.9         1236         1163         1176.1236         NST         Pyrans           4-hydroxy-5.6-dihydro-ZhP-pyran-2-one         C5H02         98         278.7         N.D.         NST         Pyrans           Levoglacosenone         C6H03         114         344.2         941         N.R.         N.R.         [1]         Pyrans           Levoglacosenone         C6H003         126         450.1         119         N.R.         N.R.         [1]         Anhydrohxmose           Levosgars(Levoglacosan)         C6H1005         162         771.4         493         1404         1486-1491         [1]         Anhydrohxmose           Levosagars(Levoglacosan)         C6H1005         162         771.4         493         1404         1486-1491         [1]         Anhydrohxmose           Levosagars(Levoglacosan)         C6H1005         162         761.5         1447         N.R.         N.R.         NIST         Chitin derived           Sacetamido-furan         C6H7002         125         555.4         1239         N.R.         N.R.         NST         Compounds           Versagire         Unknown         1519         N.D.         NIST	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	C6H8O3	128	424.6	1088	1022	1023-1097	NIST	carboxy-furans &
5.6 dilydro 2H-Pyran-2-one       CSH003       114       344.2       941       N.R.       111       Pyrans         Dianhydrorhannose       C6H903       128       383.4       1041       N.R.       [2]       Dianhydrorhannose         Ursupticosenone       C6H003       126       450.1       1119       N.R.       [1]       Ank       [2]       Dianhydrorhannose         Levosagars (Levoglactosan)       C6H1005       162       761.5       N.R.       N.R.       [1]       Anhydrosugars         Levosagars (Levoglactosan)       C6H1005       162       761.5       1447       N.R.       N.R.       [1]       Anhydrosugars         Levosagars (Levoglacosan)       C6H1005       162       761.5       1447       N.R.       N.R.       [1]       Anhydrosugars         Levosagars (Levoglacosan)       C6H1005       162       761.5       1443       N.R.       N.R.       NIST       Chirin derived         Catamide       C2H5N0       59       166.3       N.D.       NIST       Chirin derived       Chirin derived       Chirin derived       S01.9       N.R.       N.R.       N.R.       N.R.       N.R.       N.R.       N.ST       Chirin derived       Chirin derived       S01.9 <td< td=""><td>5-(hydroxymethyl)-2-Furaldehyde</td><td>C6H6O3</td><td>126</td><td>551.9</td><td>1236</td><td>1163</td><td>1176-1236</td><td>NIST, [1]</td><td>furanones</td></td<>	5-(hydroxymethyl)-2-Furaldehyde	C6H6O3	126	551.9	1236	1163	1176-1236	NIST, [1]	furanones
	5,6-dihydro-2H-Pyran-2-one	C5H6O2	98	278.7	N.D.			NIST	Dyrans
	4-hydroxy-5,6-dihydro(2H)-pyran-2-one	C5H6O3	114	344.2	941	N.R. <sup>d</sup>	N.R.	[1]	1 yraiis
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Dianhydrorhamnose	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub>	128	383.4	1041	N.R.	N.R.	[2]	Dianhydrorhamnose
Levosagars (Levogalactosan)         CH1005         162         35.7         1 375         N.R.         N.R.         [1]           Ahydrohexose         Unknown         729.0         1450         N.R.         N.R.         III         Anhydrosugars           Levosagars (Levoglucosan)         CGH1005         162         761.5         1447         N.R.         N.R.         III           Chtin derived compounds         CGH1005         162         771.4         1493         1404         1486-1491         III           Chtin derived compounds         CGH7NO2         125         555.4         1239         N.R.         N.R.         NIST           Acetamido -fran         CGH7NO2         125         555.4         1239         N.R.         N.R.         ISI         compounds           Necompounds         Unknown         801.9         1548         N.R.         N.R.         ISI         compounds           2-methyl-pyridine         CH71N         93         137.6         N.D.         NIST         (Alkyl)pyridines         O'H7NO         121         474.0         1065         N.R.         N.R.         NIST         Pyridines_O         2-Methyl-pyridine         CH47NO         121         474.0         105	Levoglucosenone	C6H6O3	126	450.1	1119	N.R.	1070	NIST	Levoglucosenone
Ahydrohexose         Unknown         729.0         1450         N.R.         N.R.         I.I.         Anhydrosugars           Levosugars (Levonlucosan)         C6H1005         162         771.4         1443         N.R.         N.R.         I.I.           Levosugars (Levonlucosan)         C6H1005         162         771.4         1443         1444         1486-1491         I.I.           Acetamide         C2H5N0         59         166.3         N.D.         NIST         Chitin derived           Sacetamido-furan         C6H7N0         125         55.4         1239         N.R.         N.R.         NIST         Colitin derived           Sacetamido-furan         C6H7N         93         151.9         N.D.         NIST         Campounds           Verompounds         Unknown         80.1         91.7         10.4         N.R.         NIST         CAlkylypridines           2-methyl-pyridine         C6H7N         93         197.6         N.D.         NIST         CAlkylypridines_O         CAlkylypridine         CH7NO         121         344.0         1065         N.R.         N.R.         NIST           2-Methyl-pyridine         CH17NO         121         377.2         1034         NR         <	Levosugars (Levogalactosan)	C6H10O5	162	535.7	1375	N.R.	N.R.	[1]	8
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Ahydrohexose	Unknown	102	729.0	1450	NR	NR	[1]	
Decomparise         Contrology         Contrology         First         First <thfirst< th="">         First         First<!--</td--><td>Levosugars (Levomannosan)</td><td>C6H10O5</td><td>162</td><td>761.5</td><td>1447</td><td>N P</td><td>N R</td><td>[1]</td><td>Anhydrosugars</td></thfirst<>	Levosugars (Levomannosan)	C6H10O5	162	761.5	1447	N P	N R	[1]	Anhydrosugars
Developing to Prove optimis         Controls         First         <	Levosugars (Levoglucosan)	C6H10O5	162	771.4	1447	1404	1486-1491	[1]	
Califier derived compounds           Acctunide         C2H5NO         59         166.3         N.D.         NIST           3-acetamido-furan         C6H7NO2         125         555.4         1239         N.R.         N.R.         NIST         Chitin derived           3-acetamido-4-pyrone         Unknown         801.9         154.8         N.R.         N.R.         [13]           Neompounds         Verompounds         N.R.         N.R.         N.R.         [13]           2-methyl-pyridine         CSH5N         79         151.9         N.D.         NIST         (Alkyl)pyridines           2-Acetylpyridine         CGH7N         93         234.6         N.D.         NIST         (Alkyl)pyridines_O           2-Acetylpyridine         C7H7NO         121         377.2         1034         N.R.         N.R.         NIST           2-Acetylpyridine         C7H7NO         121         404.0         1065         N.R.         N.R.         NIST           2-Methyl-5-acetoxypyridine         C3H5N         67         154.2         N.D.         NIST         (Alkyl)pyroles           2-formyl-pyrole         C3H5N         67         154.2         N.D.         NIST         (Alkyl)pyroles </td <td>Chitin derived compounds</td> <td>Connoos</td> <td>102</td> <td>//1.4</td> <td>1475</td> <td>1404</td> <td>1400-1471</td> <td>[1]</td> <td></td>	Chitin derived compounds	Connoos	102	//1.4	1475	1404	1400-1471	[1]	
Acetamide         C2H5N0         59         166.3         N.J.         NIST           3-acetamido-furan         C6H7N02         125         55.4         1239         N.R.         N.R.         NIST         Chinin derived           S-acetamido-I-pyrone         Unknown         153         656.4         1333         N.R.         N.R.         [3]         compounds           M-compounds         Nerompounds         NR         NR         NR         [3]         Compounds           2-methyl-pyridine         C6H7N         93         197.6         N.D.         NIST         (Alkyl)pyridines           2-Acetylpyridine         C7H7NO         121         377.2         1034         N.R.         N.R.         NIST           2-Acetylpyridine         C7H7NO         121         374.1         1457         N.R.         N.R.         NIST           2-Methyl-S-acetoxypyridine         C8H9NO2         151         74.1         1457         N.R.         NIST         (Alkyl)pyridies           2-formyl-nethylpyrole         C5H5N         95         354.2         1008         988         1005-1030         NIST           2-formyl-nethylpyrole         C6H7NO         199         162.0         1062         1067 <td>Cintin derived compounds</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	Cintin derived compounds								
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Acetamide	C2H5NO	59	166.3	N.D.			NIST	
3-acctamido-4-pyrone         Unknown         153         656.4         1353         N.R.         N.R.         N.R.         (3]         compounds           M-compounds         543         N.R.	3-acetamido-furan	C6H7NO2	125	555.4	1239	N.R.	N.R.	NIST	Chitin derived
Oxazoline         Unknown         801.9         I548         N.R.         N.R.         [3]           N-compounds	3-acetamido-4-pyrone	Unknown	153	656.4	1353	N.R.	N.R.	[3]	compounds
N-compounds         N.D.         N.D.         NIST           Pyridine         C5H5N         79         151.9         N.D.         NIST           2-methyl-pyridine         C6H7N         93         234.6         N.D.         NIST           2-Acetylpyridine         C7H7NO         121         377.2         1034         N.R.         N.R.         NIST           2-Acetylpyridine         C7H7NO         121         377.2         1034         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         Pyridines_O           2-formyl-pyrrole         C5H7N         81         216.2         N.D.         NIST         CAlkylpyrroles           2-formyl-inenthylpyrrole         C6H7NO         459.9         1205         1026-1064         NIST         Pyrroles_O           2.5-pyrroledione         C4H3NO2         97         335.9         935         N.R.         N.R.         NIST         Aromatic N           2.5-pyrroledione         C4H7N         117         474.2         1143         1153 <td>Oxazoline</td> <td>Unknown</td> <td></td> <td>801.9</td> <td>1548</td> <td>N.R.</td> <td>N.R.</td> <td>[3]</td> <td></td>	Oxazoline	Unknown		801.9	1548	N.R.	N.R.	[3]	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N-compounds							[- ]	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Pyridine	C5H5N	79	151.9	N.D.			NIST	
	2-methyl-pyridine	C6H7N	93	197.6	ND			NIST	(Alkyl)nyridines
2-Acetylpyridine         CHTNO         121         377.2         1034         N.R.         N.R.         NIST           2-Acetylpyridine         CHTNO         121         377.2         1034         N.R.         N.R.         NIST           2-Acetylpyridine         CHTNO         121         374.2         1034         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           2-formyl-pyrrole         C5H7N0         95         354.2         1008         988         1005-1030         NIST           2-acetyl-pyrrole         C6H7NO         109         402.0         1062         1035         1026-1064         NIST         Pyrroles_O           2.5-pyrrolidinedione         C4H3NO2         97         335.9         935         N.R.         N.R.         NIST         Pyrroledione &         2.5-pyrorididinedione         C4H3NO2         97         335.9         935         N.R.         N.R.         NIST         Aromatic N           Benzeneacetonitrile         C8H7N         117	3/4-methyl-pyridine	C6H7N	93	234.6	N D			NIST	(Tink)T)pyrtaines
2-Acetylpyridine         C/H7NO         121         5/1.2         10.57         N.R.         NIST         Pyridines_O           2-Methyl-5-acetoxypyridine         C4H5N         67         154.2         N.D.         NIST         NIST         (Alkyl)pyroles           2-formyl-pyrrole         C5H7N         81         216.2         N.D.         NIST         Virole_0         0	2-Acetylpyridine	C7H7NO	121	377.2	1034	NR	NR	NIST	
Description         CMINO         121         404.0         1000         N.R.         N.ST         Pyrroles_O         C.4H5NO2         97         335.9         935         N.R.         N.R.         NIST         Pyrroledione         C.4H3NO2         97         335.9         935         N.R.         N.R.         NIST         Pyrroledione         C.4H3NO2         9462.1         1131         934         N.R.         NIST         Pyrroledione         C.4H3NO2         127         1474	2 Acetylpyridine	C7H7NO	121	404.0	1054	N.R. N P	N.R.	NIST	Duridines O
2-induty-3-actory pyndame         CorrspNo2         11         74-41         14-37         IN.R.         INST           Methyl-pyrrole         C4H5N         67         154.2         N.D.         NIST         (Alkyl)pyrroles           2-formyl-pyrrole         C5H7N         81         216.2         N.D.         NIST         (Alkyl)pyrroles           2-acetyl-pyrrole         C6H7NO         109         402.0         1062         1035         1026-1064         NIST         Pyrroles_O           2-formyl-l-methylpyrrole         C6H7NO         495.9         1129         1077         1092-1105         NIST           2,5-pyrroledione         C4H3NO2         97         335.9         935         N.R.         N.R.         NIST         Pyrroledione &           2,5-pyrrolidinedione         C4H3NO2         97         335.9         935         N.R.         NIST         pyrroledione &           2,5-pyrrolidinedione         C4H3NO2         97         335.9         134         1082         113         NIST           Benzeneacetonitrile         CSH7N         117         474.2         1147         1138         1088-1143         NIST           Indole         C8H7N         117         60.9         1293	2 Mathyl 5 agetoxymyriding	C/II/NO	121	724.1	1457	N.R. N D	N.R. N D	NIST	I ynulles_0
	2-Methyl-3-acetoxypyhdille	C4115N	67	154.1	14J/	IN.K.	IN.K.	NIST	
Methyl-pyrrole         CSH7N         81         21/2         N.D.         N.D.         N.B.         N.B.           2-formyl-pyrrole         CSH5NO         95         354.2         1008         988         1005-1030         NIST           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 &           2,5-pyrrolidinedione         C4H5NO2         99         462.1         1131         934         N.R.         NIST         pyrroledione           Benzeneacetonitrile         C8H7N         117         474.2         1147         1138         1089-1143         NIST         Aromatic N           Indole         C8H7N         117         609.9         1293         1174         1260-1303         NIST         Indoles           Diketodipyrrole         Unknown         186         938.0         1746         N.R.         N.R.         [5, 6]           Diketopiperazine Pro-Val <td>Pyllole Mathal gamesta</td> <td>C4HJN C5H7N</td> <td>0/</td> <td>134.2</td> <td>N.D.</td> <td></td> <td></td> <td>NIS I</td> <td>(Alkyl)pyrroles</td>	Pyllole Mathal gamesta	C4HJN C5H7N	0/	134.2	N.D.			NIS I	(Alkyl)pyrroles
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Метпут-рупоте		81	210.2	N.D.	000	1005 1020	NIST	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2-formyl-pyrrole	CSH5NO	95	354.2	1008	988	1005-1030	NIST	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2-acetyl-pyrrole	C6H7NO	109	402.0	1062	1035	1026-1064	NIST	Pyrroles_O
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2-Formyl-1-methylpyrrole	C6H7NO		459.9	1129	1077	1092-1105	NIST	
2,5-pyrrolidinedione         C4H5NO2         99         462.1         1131         934         N.R.         NIST         pyrrolidinedione           Benzeneacetonitrile         C8H7N         117         474.2         1147         1138         1089-1143         NIST         Aromatic N           Benzenepropanenitrile         C9H9N         131         563.9         1248         1238         1186-1242         NIST         Aromatic N           Indole         C8H7N         117         609.9         1293         1174         1260-1303         NIST         Indoles         Indoles         C9H9N         131         686.1         1394         1288         1380-1410         NIST         Indoles         Indoles         1164         1184         1288         1380-1410         NIST         Indoles         1164         1184         1288         1380-1410         NIST         Indoles         1160         1184         1288         1380-1410         NIST         Indoles         1164         1184         1288         1380-1410         NIST         Indoles         1160         1181         1288         1380-1410         NIST         Indoles         1160         1283         N.R.         N.R.         1161         1161         1260	2,5-pyrroledione	C4H3NO2	97	335.9	935	N.R.	N.R.	NIST	Pyrroledione &
Benzeneacetonitrile         C8H7N         117         474.2         1147         1138         1089-1143         NIST         Aromatic N           Benzenepropanenitrile         C9H9N         131         563.9         1248         1238         1186-1242         NIST         Aromatic N           Indole         C8H7N         117         609.9         1293         1174         1260-1303         NIST         Indoles           Methyl-indole         C9H9N         131         686.1         1394         1288         1380-1410         NIST         Indoles           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]           Diketopiperazine Pro-Val         C10H16N2O2         196         989.4         1826         N.R.         N.R.         IST           Diketopiperazine Pro-Val         C10H16N2O2         196         1005.9         1852         N.R.         N.R.         IST           Diketopiperazine Pro-Val         C10H16N2O2         194         1067.0         1953         N.R.         N.R. <td>2,5-pyrrolidinedione</td> <td>C4H5NO2</td> <td>99</td> <td>462.1</td> <td>1131</td> <td>934</td> <td>N.R.</td> <td>NIST</td> <td>pyrrolidinedione</td>	2,5-pyrrolidinedione	C4H5NO2	99	462.1	1131	934	N.R.	NIST	pyrrolidinedione
Benzenepropanenitrile         C9H9N         131         563.9         1248         1238         1186-1242         NIST         Attoinate N           Indole         C8H7N         117         609.9         1293         1174         1260-1303         NIST         Indoles           Methyl-indole         C9H9N         131         686.1         1394         1288         1380-1410         NIST         Indoles           Diketodipyrole         Unknown         186         922.7         1722         N.R.         N.R.         [4]         Diketodipyrole           Diketopiperazine Pro-Ala         C8H12N2O2         168         938.0         1746         N.R.         N.R.         [5, 6]           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.         [5, 6]           Diketopiperazine Pro-Val         C10H14N2O2         194         1067.0         1953         N.R.         N.R.         [5, 6]           Diketopiperazine Pro-Pro         C14H16N2O2         244         1284.3         2352         N.R.         N.R.	Benzeneacetonitrile	C8H7N	117	474.2	1147	1138	1089-1143	NIST	Aromatic N
Indole         C8H7N         117         609.9         1293         1174         1260-1303         NIST         Indoles           Methyl-indole         C9H9N         131         686.1         1394         1288         1380-1410         NIST         Indoles           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]           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.         NIST           Diketopiperazine Pro-Val         C10H16N2O2         196         1005.9         1852         N.R.         N.R.         NIST           Diketopiperazine Pro-Pro         C10H14N2O2         194         1067.0         1953         N.R.         N.R.         [5, 6]           Diketopiperazine Pro-Pro         C14H16N2O2         244         1284.3         2352         N.R.         N.R.         NIST      <	Benzenepropanenitrile	C9H9N	131	563.9	1248	1238	1186-1242	NIST	Alomatic IV
Methyl-indole         C9H9N         131         686.1         1394         1288         1380-1410         NIST         Indoles           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]           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.         [5, 6]           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-Pro         C14H16N2O2         244         1284.3         2352         N.R.         N.R.         [5, 6]           Alkylamide1         Unknown         986.8         1821         N.R.         NIST         NIST           Alkylamide3	Indole	C8H7N	117	609.9	1293	1174	1260-1303	NIST	Indolas
DiketodipyrroleUnknown186922.71722N.R.N.R.[4]DiketodipyrroleDiketopiperazine Pro-AlaC8H12N2O2168938.01746N.R.N.R.[5, 6]Diketopiperazine Pro-ValC10H16N2O2196989.41826N.R.N.R.[5, 6]Diketopiperazine Pro-ValC10H16N2O21961005.91852N.R.N.R.[5, 6]Diketopiperazine Pro-ValC10H16N2O21961005.91852N.R.N.R.NISTDiketopiperazine Cyclo-Leu-ProC11H18N2O22101049.01922N.R.N.R.NISTDiketopiperazine Pro-ProC10H14N2O21941067.01953N.R.N.R.[5, 6]Diketopiperazine Pro-ProC14H16N2O22441284.32352N.R.N.R.[5, 6]Alkylamide1Unknown986.81821N.R.N.R.NISTAlkylamide2Unknown1197.62185N.R.N.R.NISTAlkylamide3Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Methyl-indole	C9H9N	131	686.1	1394	1288	1380-1410	NIST	Indoles
Diketopiperazine Pro-Ala         C8H12N2O2         168         938.0         1746         N.R.         N.R.         [5, 6]           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.         [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.         Diketopiperazine Pro-Pro         C10H14N2O2         194         1067.0         1953         N.R.         N.R.         [5, 6]         Diketopiperazines           Diketopiperazine Pro-Pro         C10H14N2O2         194         1067.0         1953         N.R.         N.R.         [5, 6]         Diketopiperazines           Diketopiperazine Pro-Pro         C14H16N2O2         244         1284.3         2352         N.R.         N.R.         [5, 6]         Image: Comparison of Comp	Diketodipyrrole	Unknown	186	922.7	1722	N.R.	N.R.	[4]	Diketodipyrrole
Diketopiperazine Pro-ValC10H16N2O2196989.41826N.R.N.R.[5, 6]Diketopiperazine Pro-ValC10H16N2O21961005.91852N.R.N.R.N.R.Diketopiperazine Cyclo-Leu-ProC11H18N2O22101049.01922N.R.N.R.NISTDiketopiperazine Pro-ProC10H14N2O21941067.01953N.R.N.R.NISTDiketopiperazine Pro-PheC14H16N2O22441284.32352N.R.N.R.[5, 6]Alkylamide1Unknown986.81821N.R.N.R.NISTAlkylamide3Unknown1197.62185N.R.N.R.NISTAlkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Diketopiperazine Pro-Ala	C8H12N2O2	168	938.0	1746	N.R.	N.R.	[5, 6]	
Diketopiperazine Pro-ValC10H16N2O21961005.91852N.R.N.R.DiketopiperazineDiketopiperazine Cyclo-Leu-ProC11H18N2O22101049.01922N.R.N.R.NISTDiketopiperazinesDiketopiperazine Pro-ProC10H14N2O21941067.01953N.R.N.R.N.R.[5, 6]Diketopiperazine Pro-PheC14H16N2O22441284.32352N.R.N.R.[5, 6]Alkylamide1Unknown986.81821N.R.N.R.NISTAlkylamide2Unknown1081.11977N.R.N.R.NISTAlkylamide3Unknown1197.62185N.R.N.R.NISTAlkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Diketopiperazine Pro-Val	C10H16N2O2	196	989.4	1826	N.R.	N.R.	[5, 6]	
Diketopiperazine Cyclo-Leu-ProC11H18N2O2210100001002N.R.N.R.NISTDiketopiperazine Pro-ProC10H14N2O21941067.01953N.R.N.R.N.R.[5, 6]Diketopiperazine Pro-PheC14H16N2O22441284.32352N.R.N.R.[5, 6]Alkylamide1Unknown986.81821N.R.N.R.NISTAlkylamide2Unknown1081.11977N.R.N.R.NISTAlkylamide3Unknown1197.62185N.R.N.R.NISTAlkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Diketopiperazine Pro-Val	C10H16N2O2	196	1005.9	1852	N.R.	N.R.	L- / - J	
Diketopiperazine Pro-ProC10H14N2O21041067.01922N.R.N.R.[5, 6]Diketopiperazine Pro-PheC10H14N2O22441284.32352N.R.N.R.[5, 6]Alkylamide1Unknown986.81821N.R.N.R.NISTAlkylamide2Unknown1081.11977N.R.N.R.NISTAlkylamide3Unknown1197.62185N.R.N.R.NISTAlkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Diketopiperazine Cyclo-Leu-Pro	C11H18N2O2	210	1049.0	1922	NR	NR	NIST	Diketopiperazines
Diketopiperazine Pro-Phe         C14H16N2O2         244         1284.3         2352         N.R.         N.R.         [5, 6]           Alkylamide1         Unknown         986.8         1821         N.R.         N.R.         NIST           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.         NIST	Diketopiperazine Pro-Pro	C10H14N2O2	194	1047.0	1953	N R	N R	[5, 6]	
Diketopiperazine frio-frieC141101/2022441284.32352N.R.N.R.[5, 6]Alkylamide1Unknown986.81821N.R.N.R.NISTAlkylamide2Unknown1081.11977N.R.N.R.NISTAlkylamide3Unknown1197.62185N.R.N.R.NISTAlkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Diketopiperazine Pro Pha	C14H16N2O2	244	128/3	2352	N.R. N P	N.R.	[5, 6]	
Alkylamide1Onknown500.81821N.R.N.R.NISTAlkylamide2Unknown1081.11977N.R.N.R.NISTAlkylamide3Unknown1197.62185N.R.N.R.NISTAlkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Alkylamida1	Unknown	∠ <del>44</del>	086.9	1821	N.R.	N D		
Aikylamide2Onknown1081.11977N.R.N.R.NISTAlkylamide3Unknown1197.62185N.R.N.R.NISTAlkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Alleylamide2			700.0 1001 1	1021	IN.K.	IN.K.	INIS I	
Aikylamide5Unknown1197.62185N.R.N.R.NIS1Alkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Alkylälliluez	UIIKAOWA		1001.1	19//	IN.K.	IN.K.	INIS I	
Alkylamide4Unknown1237.32260N.R.N.R.NISTAlkylamidesAlkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamidesAlkylamide6Unknown1579.63020N.R.N.R.NIST	Aikyiamide3	Unknown		1197.6	2185	N.K.	N.K.	NIST	
Alkylamide5Unknown1304.22392N.R.N.R.NISTAlkylamide6Unknown1579.63020N.R.N.R.NIST	Alkylamide4	Unknown		1237.3	2260	N.R.	N.R.	NIST	Alkylamides
Alkylamide6 Unknown 1579.6 3020 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	

<i>n</i> -alkenes								
n-C9:1	C9H18	126					NIST	
n-C13:1	C13H26	182	603.4	1286	1204	1187-1289	NIST	C9-16·1
n-C14:1	C14H28	196	684.6	1392	1421	1389-1396	NIST	C) 10.1
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	
n-C18:1	C18H36	252	969.2	1/94	1801	1/88-1/93	NIST	
n-C19:1	C19H38	266	1031.8	1894	1900 N D	1883-1899	NIST	C17-22:1
n C21:1	C20H40	200	1091.5	2006	N.K. 2117	2060	NIST	
n-C22:1	C21H42	294	1203.2	2090	2117	2000	NIST	
n-C23:1	C23H46	322	1255.5	2295	N R	2192-2195	NIST	
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	C23-26:1
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	C07 09.1
n-C28:1	C28H56	364	1488.5	2796	N.R.	2794-2797	NIST	C27-28:1
<i>n</i> -alkanes								
n-C10:0	C10H22	142	347.4				NIST	
n-C11:0	C11H24	156	435.0				NIST	
n-C12:0	C12H26	170	515.5				NIST	
n-C13:0	C13H28	184	617.3				NIST	C10-16:0
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	C1/H30	240	908.1				NIS I NIST	
n C10:0	C10H40	234	975.5				NIST	
n-C19.0	C20H42	208	1035.7				NIST	C17-22:0
n-C21:0	C21H44	202	11507				NIST	
n-C22:0	C22H46	310	1206.1				NIST	
n-C23:0	C23H48	324	1258.1				NIST	
n-C24:0	C24H50	338	1308.1				NIST	
n-C25:0	C25H52	352	1355.1				NIST	C23-26:0
n-C26:0	C26H54	366	1402.4				NIST	
n-C27:0	C27H56	380	1447.1				NIST	
n-C28:0	C28H58	394	1490.2				NIST	
n-C29:0	C29H60	408	1530.3				NIST	~~~ ~ ~ ~
n-C30:0	C30H62	422	1571.8				NIST	C27-35:0
n-C31:0	C31H64	436	1610.9				NIST	
n-C32:0	C32H66	450	1648.6				NIST	
n-C35:0	C35H08	404	1085.0				INIS I [7]	
Alkan-2-ones	C35H72	492	1723.9				[/]	
2-K C13	C13H26O	198	765.4	1498	1449	1476-1498	NIST	
2-K C16	C16H32O	240	975.0	1803	1748	1780-1805	NIST	2K C13-17
2-K C17	C17H34O	254	1038.2	1904	1847	1875-1890	NIST	
2-K C19	C19H38O	282	1155.9	2109	2046	2087-2106	NIST	
2-K C20	C20H40O	396	1210.9	2209	2206	N.R.	NIST	2K C19-22
2-K C21	C21H42O	310	1263.7	2311	2309	N.R.	NIST	
2-K C23	C23H46O	338	1363.0	2517	2513	N.R.	NIST	
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	2K C23-31
2-K C27	C27H54O	394	1540.6	2925	N.K.	N.R.	[/]	
2-K C28	C28H56O	408	1581.3	3024	N.K.	N.R.	[/]	
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	CCIECO	0.4	200.0	021	001	052 1004	NICT	
ritefiol	C0H0U	94 109	329.2 306 0	931 1057	901 1014	952-1004 1020-1020	NIST NIST	
2- methyl-phenol	C7H8U	108	390.2 414 0	1030	1014	1029-1039	INIS I NICT	
Dimethyl-phenol	C7H8O	100	414.9 418 1	1156	1117	1077_1120	NIST	Phenols
Ethyl-phenol	C8H700	122	497 3	1177	1127	1106-1162	NIST	
Propenvl-phenol	C9H10O	134	646 7	1340	1203	1232-1258	NIST	
	271100	107	0.10.7	2.0				
Guaiacol (G)	C7H8O2	124	428.7	1093	1090	1052-1090	NIST	<u> </u>
Ethyl-guaiacol (guaiacyl-2C)	C9H12O2	152	596.2	1279	1303	1243-1287	NIST	Guatacols

4-vinyl-guaiacol (guaiacyl -2C) 4-propenyl-guaiacol (guaiacyl -3C) Vanillin (guaiacyl -1C or -aldehyde) 4-alleneguaiacol (guaiacyl -3C) Acetovanillone (guaiacyl -2Cor aldehyde) Vanillic acid, methyl ester (guaiacyl -1C or -acid) Guaiacylacetone (guaiacyl -3Cor - aldehyde)	C9H10O2 C10H12O2 C8H8O3 C10H10O2 C9H10O3 C9H10O4 C10H12O3	150 164 152 162 166 182 180	625.6 660.9 695.9 741.0 763.1 785.5 796.0	1311 1359 1407 1466 1495 1525 1525	1293 1392 1392 N.R. 1439 1470 1538	1272-1295 1339-1452 1350-1447 N.R. 1447-1503 1463-1525 1488-1531	NIST NIST [8] NIST NIST NIST	
Syringol (syringyl) 4-vinyl-syringol (syringy-2C) 4-formyl-syringol (syringy-1C) 4-allenesyringol (syringy-3C) Acetosyringone (syringy-2C)	C8H10O3 C11H14O4 C9H10O4 C11H12O3 C10H12O4	154 210 182 192 196	655.4 819.5 887.6 901.0 961.1	1352 1572 1670 1690 1781	1279 N.R. 1581 N.R. 1628	1349-1367 1517-1573 1617-1670 N.R. 1740-1744	NIST NIST NIST [8] NIST	Syringols
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]	Thistenes
Phytadiene 1	C20H38	278	999.1	1841	N.R.	N.R.	[9]	Phytadianas
Phytadiene 2	C20H38	278	1026.0	1884	N.R.	N.R.	[9]	Thytadicies
Steroids								
Cholest-2-ene	C27H46	370	1522.1	2880	2380	N.R.	NIST	
Cholesta-3,5-diene	C <sub>27</sub> H <sub>44</sub>	368	1543.4	2932	N.R.	N.R.	NIST	
Stigmasta-5,22-dien-3-ol, acetate	C31H50O2	454	1601.1	3075	2879	N.R.	NIST	
Sitosterol	C20H50O	414	1623.4	3133	2731	3173-3220	NIST	Steroids
Choloste 2.5 dian 7 and	C27H42O	200	1629.4	3255	2562	NR	NIST	
Cholesta-3,5-dien-7-one	C2/II420	382	1008./	3233	2502	N.K.	NIGT	
Sugmasta-5,5-dien-7-one	C28H40U	410	1/50.1	3462	2090	N.K.	INIS I	
1 ocopherol	C28H48O2	416	1504.1	2057	2026	2055	MIGT	
a Tocopherol	C20H50O2	410	1632.2	3057	3140	3033	NIST	Tocopherols
Hononoids	027115002	430	1052.2	5157	5147	5111	1151	
Trinosphonane	unknown		1526.4	2890	NR	NR	[10]	
Norhopene (triterpene C29)	unknown		1548.9	2945	N.R.	N.R.	[10]	
22.29.30-trisnorhop-17(21)-ene	C27H44	368	1553.8	2957	N.R.	N.R.	[11]	
22 29 30-trisnorhon-16(17)-ene	C27H44	368	1567.1	2989	N.R.	N.R.	[11]	Hopanoids
Norhonane $(C30/C312)$	unknown	500	1630.7	3153	NR	NR	[10]	
25-norhopene (C30/C31?)	unknown		1659.0	3229	N.R.	N.R.	[10]	
(Poly)aromatics							[-~]	
Benzene	C <sub>6</sub> H <sub>6</sub>	78	113.9	N.D.			NIST	Benzene
Benzaldehyde	C <sub>7</sub> H <sub>6</sub> O	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	
Ethyl-methyl-benzene	C9H12	120	368.2	1024	N.R.	945-973	NIST	
Indene	C9H8	120	389.7	1048	1014	1029-1051	NIST	Benzenes C2-9
Benzene C7	C13H20	176	664.9	1365	1390	1337-1350	NIST	
Benzene C9	C15H24	204	822.1	15/6	1555	1552-1586	NIST	
1,2-unyaro-naphinalene	CIUHIU	130	484.9 500 P	1160	1149	113/-1166	NIST NICT	
2,5-uiiiyui 0-iiiucii-1-0iic 1/2-methyl-nanthalene	C11H10	132	577.0 612 1	1205	1210	1210-1320	NIST	
2/4-methyl-napthalene	C11H10	142	6267	1313	1345	1267-1298	NIST	(Poly)aromatics
Biphenyl	C12H10	154	680.8	1386	1367	1338-1392	NIST	(1 org/aronnarios
Fluorene	C13H10	166	836.9	1596	1494	1549-1611	NIST	
Anthracene	C14H10	178	972.2	1798	1782	1740-1800	NIST	

<sup>a</sup> 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:

$$RI = 100 \text{ x} \left[n + \frac{\log(RT \text{ unknown}) - \log(RT \text{ n})}{\log(RT \text{ N}) - \log(RT \text{ n})}\right]$$

$$\log(RT N) - \log(RT n)$$

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 eluting smaller n-alkane, and RT N is the retention time of the adjacently eluting larger n-alkane.

<sup>b</sup> reference RI: the reference RI values were found on the website "NIST Chemistry Webbook" (<u>http://webbook.nist.gov/chemistry/</u>) 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.;

<sup>c</sup>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.

<sup>d</sup>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

commu	<u>.u)</u>	DD	1.0.	1.01	[0]	(D. 1	[G]]	D.T.		[D] ]	[7]
	WD	BD	bSi	LOI	[S]	[Br]	[Cu]	[N1]	[Hg]	[Pb]	[Zn]
unit	m	g cm <sup>-3</sup>	%	%	mg kg⁻¹	mg kg⁻¹	mg kg⁻'	mg kg⁻¹	µg kg⁻'	mg kg⁻¹	mg kg⁻¹
N1	3.1	0.057	15	57	16620	134	29	21	283	151	285
N2	7.4	0.088	6	<u>58</u>	18050	127	39	23	510	168	320
N3	<u>1.6</u>	0.078	14	34	5570	216	34	<u>10</u>	261	170	<u>43</u>
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	<u>10</u>	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	<u>422</u>	222
M1	3	0.084	25	25	4840	146	33	<u>10</u>	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	<u>10</u>	<u>117</u>	135	74
M6	1.8	0.104	16	<u>10</u>	4685	71	<u>12</u>	18	141	175	80
S1	5.7	0.083	17	30	6640	104	27	19	181	103	144
<b>S</b> 2	6.5	0.091	23	27	6600	101	25	14	177	97	111
<b>S</b> 3	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
<b>S</b> 5	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
<b>S</b> 9	21	0.040	6	45	12650	175	44	23	507	244	299
<b>S</b> 10	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
<b>S</b> 13	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	<u>4</u>	54	28840	175	<u>75</u>	27	<u>1152</u>	273	<u>445</u>

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

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

								$\mathcal{O}$		2							1			
	Al	Y	Fe	Fe:Al	Fe:S	[As]	Asinv	[P]	[Mn]	Mn:Fe	[Co]	[Ca]	[K]	[Mg]	[Na]	$\mathrm{Si}_{\mathrm{inorganic}}$	[Sr]	[Ti]	[V]	[Zr]
	%	mg	kg <sup>-1</sup>			mg kg <sup>-1</sup>	µg cm <sup>-2</sup>	mg	kg <sup>-1</sup>				mg kg <sup>-1</sup>			%		mg k	cg <sup>-1</sup>	
N1	<u>2.1</u>	9	1.5	0.7	0.9	15	9	760	149	0.010	11	6230	2740	1060	1190	<u>4</u>	41	1293	38	44
N2	2.2	15	1.3	0.6	<u>0.7</u>	14	13	1230	125	0.010	12	4800	3610	1050	1910	10	45	1648	<u>36</u>	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	<u>94</u>	0.005	7	<u>2860</u>	<u>2420</u>	<u>870</u>	<u>440</u>	7	27	1228	51	<u>39</u>
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	<u>7981</u>	<u>0.184</u>	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	<b>267</b> 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	<u>0.9</u>	<u>0.4</u>	1.1	<u>5</u>	<u>3</u>	672	144	0.016	<u>5</u>	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
<b>M</b> 1	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< th=""><th><dl< th=""><th>989</th><th>462</th><th>0.013</th><th>10</th><th>31890</th><th>8660</th><th>10040</th><th>11110</th><th>22</th><th>218</th><th>6017</th><th>91</th><th>153</th></dl<></th></dl<>	<dl< th=""><th>989</th><th>462</th><th>0.013</th><th>10</th><th>31890</th><th>8660</th><th>10040</th><th>11110</th><th>22</th><th>218</th><th>6017</th><th>91</th><th>153</th></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	<u>4.3</u>	<u>43</u>	7.4	1.7	15.8	18	18	965	5067	0.068	<u>76</u>	8105	<u>6140</u>	1920	<u>3380</u>	12	<u>116</u>	2211	90	109
<b>S</b> 1	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
<b>S</b> 2	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
<b>S</b> 3	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	<u>11.5</u>	<u>3.5</u>	<u>18.3</u>	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	<u>655</u>	176	0.011	7	<u>9300</u>	4660	1340	2570	11	101	1524	42	109
<b>S</b> 6	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
<b>S</b> 9	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
<b>S</b> 10	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	<u>2870</u>	77	<u>160</u>
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	<u>3.5</u>	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< th=""><th><dl< th=""><th>908</th><th>1657</th><th>0.050</th><th>23</th><th>21190</th><th>12360</th><th>4950</th><th>10280</th><th>23</th><th>252</th><th>2697</th><th>58</th><th>162</th></dl<></th></dl<>	<dl< th=""><th>908</th><th>1657</th><th>0.050</th><th>23</th><th>21190</th><th>12360</th><th>4950</th><th>10280</th><th>23</th><th>252</th><th>2697</th><th>58</th><th>162</th></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	<u>73</u>	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	<u>21</u>	53	2109	61	90
S22	3.6	38	10.7	2.9	7.7	<u>73</u>	<u>42</u>	2525	471	0.004	41	5590	5590	<u>2130</u>	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	<u>997</u>	77	48
S24	3.5	20	6.9	2.0	2.4	64	10	<u>3769</u>	157	<u>0.002</u>	16	5265	3410	1330	1800	9	44	1491	<u>101</u>	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.

Variables (unit)	W/h ala laba <sup>a</sup> (m <sup>b</sup> 42)	Near-shore sites	North/East basins		South basin		Shallow central areas	Outliers
variables (unit)	whole-lake $(\Pi = 42)$	Cluster <sub>geo</sub> 4 (n=4)	Cluster <sub>geo</sub> 1 (n=13)	Cluster <sub>geo</sub> 6 (n=10)	Cluster <sub>geo</sub> 2 (n=8)	Cluster <sub>geo</sub> 5 (n=3)	Cluster <sub>geo</sub> 3 (n=4)	(M4, S15)
W.D. (m)	$9 \pm 7 (74 \%)^c$	4 ± 2	5 ± 3	8 ± 3	15 ± 4	3 ± 1	2 ± 1	3 ± 1
B.D. (g cm <sup>-3</sup> )	0.06 ± 0.02 (38 %)	$0.06\pm0.03$	$0.07\pm0.02$	$0.07\pm0.02$	$0.05\pm0.01$	$0.67 \pm 0.09$	$0.100 \pm 0.02$	$0.67 \pm 0.09$
bSi (%)	12 ± 6 ( <i>31</i> %)	$12 \pm 6$	$13 \pm 3$	$15 \pm 7$	$7 \pm 3$	$1.8 \pm 0.2$	21 ± 4	$1.8 \pm 0.2$
OM and organoph	ilic trace elements							
LOI (%)	38 ± 10 (27 %)	$50 \pm 12$	$39 \pm 5$	$34 \pm 7$	37 ± 4	$52 \pm 2$	20 ± 8	4 ± 1
$S (mg kg^{-1})$	11876 ± 5920 (50 %)	$17510 \pm 833$	$11683 \pm 3440$	$7550 \pm 1900$	$12896 \pm 3315$	$26227 \pm 4833$	$4879 \pm 148$	$2570 \pm 552$
Br (mg kg <sup>-1</sup> )	149 ± 35 (23 %)	$130 \pm 6$	$153 \pm 36$	$145 \pm 35$	$154 \pm 19$	$204 \pm 26$	$116 \pm 32$	$16 \pm 7$
Cu (mg kg <sup>-1</sup> )	34 ± 13 <i>(37 %)</i>	$36 \pm 5$	$28 \pm 6$	$30 \pm 7$	$42 \pm 6$	$65 \pm 10$	24 ± 13	9 ± 3
Ni (mg kg <sup>-1</sup> )	19 ± 5 (23 %)	$21 \pm 1$	$18 \pm 4$	$17 \pm 2$	$21 \pm 4$	$27 \pm 1$	$12 \pm 4$	$12 \pm 4$
Hg ( $\mu$ g kg <sup>-1</sup> )	337 ± 202 (60 %)	$407 \pm 141$	$251 \pm 47$	$230 \pm 69$	$427 \pm 94$	$917 \pm 212$	$203 \pm 87$	$28 \pm 9$
Pb (mg kg <sup>-1</sup> )	192 ± 74 (39 %)	$199 \pm 58$	$156 \pm 58$	$115 \pm 42$	$300 \pm 59$	$315 \pm 7$	$182 \pm 96$	$24 \pm 7$
$Zn (mg kg^{-1})$	219 ± 108 (49 %)	$279 \pm 31$	$212 \pm 68$	$139 \pm 42$	$305 \pm 86$	$417 \pm 33$	63 ± 16	$50 \pm 16$
$Cu(\mu gcm^{-2})$	20 ± 6 (30 %)	$21 \pm 11$	$20 \pm 6$	$19 \pm 4$	20 ± 6	$16 \pm 4$	22 ± 8	62 ± 27
Ni ( $\mu g \ cm^{-2}$ )	12 ± 4 (35 %)	13 ± 6	$13 \pm 4$	$11 \pm 3$	10 ± 3	7 ± 2	12 ± 5	83 ± 39
$Hg (ng \ cm^{-2})$	185 ± 65 (35 %)	234 ± 146	$180 \pm 45$	$146 \pm 32$	201 ± 69	222 ± 33	187 ± 46	181 ± 36
$Pb \ (\mu g \ cm^{-2})$	123 ± 60 (48 %)	$111 \pm 46$	132 ± 53	$83 \pm 29$	126 ± 29	84 ± 9	234 ± 84	138 ± 90
$Zn \ (\mu g \ cm^{-2})$	126 ± 60 (47 %)	170 ± 90	$152 \pm 54$	$92 \pm 33$	$145 \pm 60$	$105 \pm 30$	64 ± 28	<i>329</i> ± <i>59</i>
Elements that can	be part of or be associated	with clays and (oxy)hy	droxides					
Al (%)	3.0 ± 0.5 (18 %)	$2.4 \pm 0.3$	$2.7\pm0.2$	$3.3 \pm 0.5$	$3.5 \pm 0.3$	$3.4 \pm 0.1$	$3.0 \pm 0.9$	$5.7 \pm 0$
$Y (mg kg^{-1})$	25 ± 8 ( <i>32 %</i> )	$16 \pm 8$	$20 \pm 5$	$28 \pm 6$	33 ± 3	$23 \pm 3$	31 ± 10	$20 \pm 3$
Fe (%)	4.5 ± 3.0 (65 %)	$3.1 \pm 2.1$	$2.7 \pm 1.7$	$3.6 \pm 1.5$	$9.1 \pm 2.4$	$4.3 \pm 2.2$	$5.5 \pm 1.7$	$3.4 \pm 0.2$
Fe:Al	1.5 ± 0.8 (57 %)	$1.0 \pm 0.5$	$1.0 \pm 0.6$	$1.1 \pm 0.3$	$2.5 \pm 0.9$	$1.3 \pm 0.6$	$1.9 \pm 0.3$	$2.0 \pm 0.4$
Fe:S	5.2 ± 4.3 (86 %)	$1.7 \pm 1.2$	$2.5 \pm 1.9$	$5.0 \pm 0.9$	8 ± 4	$1.6 \pm 0.7$	11 ± 4	13 ± 2
As (mg kg <sup>-1</sup> )	35 ± 20 (56 %)	$27 \pm 17$	$26 \pm 16$	$25 \pm 11$	$64 \pm 11$	$48 \pm 14$	$29 \pm 9$	< D.L. <sup>d</sup>
As $(\mu g \ cm^{-2})$	20 ± 11 (52 %)	15 ± 13	$19 \pm 11$	$17 \pm 7$	<i>30</i> ± <i>10</i>	$12 \pm 1$	28 ± 7	< <i>D.L</i> .
$P (mg kg^{-1})$	1624 ± 741 (46 %)	$927 \pm 240$	$1065 \pm 295$	$2088 \pm 730$	$2074 \pm 275$	$2766 \pm 869$	$1224 \pm 216$	949 ± 57
Mn (mg kg <sup>-1</sup> )	729 ± 1690 (232 %)	$162 \pm 53$	$182 \pm 67$	$184 \pm 50$	$305 \pm 93$	$171 \pm 13$	$5700 \pm 1597$	$1060 \pm 845$
Mn:Fe	0.016 ± 0.034 (214 %)	$0.007 \pm 0.002$	$0.008 \pm 0.003$	$0.006 \pm 0.002$	$0.004 \pm 0.001$	$0.005 \pm 0.002$	$0.111 \pm 0.051$	$0.08 \pm 0.01$
$Co(mg kg^{-1})$	19 ± 14 (77 %)	$15\pm 8$	$12 \pm 6$	$13 \pm 5$	$26 \pm 11$	$14 \pm 2$	$49 \pm 24$	17 ± 9
Others minerogen	ic elements							
$Ca (mg kg^{-1})$	5261 ± 1306 (25 %)	$4508 \pm 1346$	$6000 \pm 1331$	$4680 \pm 1072$	$5343 \pm 683$	$5042 \pm 196$	$5069 \pm 2342$	$26540 \pm 7566$
$K (mg kg^{-1})$	4426 ± 1020 (23 %)	$2998 \pm 428$	$4686 \pm 682$	$3699 \pm 781$	$5528 \pm 504$	$4490 \pm 941$	$4575 \pm 1054$	$10510 \pm 2616$
Mg (mg kg <sup>-1</sup> )	1488 ± 354 (24 %)	$1035\pm81$	$1462\pm274$	$1320\pm280$	$1891 \pm 239$	$1657\pm283$	$1513 \pm 394$	$7495 \pm 3599$
Na (mg kg <sup>-1</sup> )	1794 ± 659 (37 %)	$1293\pm460$	$1847\pm395$	$1236 \pm 446$	$2551 \pm 437$	$1987 \pm 167$	$1868 \pm 1038$	$10695 \pm 587$
Si <sub>inorganic</sub> (%)	12 ± 4 (33 %)	8 ± 3	$11 \pm 3$	$11 \pm 5$	$13 \pm 3$	$12 \pm 3$	9 ± 2	$23 \pm 1$
$Sr (mg kg^{-1})$	55 ± 16 (30 %)	$38 \pm 6$	$61 \pm 13$	$47 \pm 10$	61 ± 5	$49 \pm 5$	$66 \pm 38$	$235 \pm 24$
Ti (mg kg <sup>-1</sup> )	2115 ± 495 (23 %)	$1301 \pm 267$	$2243\pm382$	$1814 \pm 314$	$2675 \pm 206$	$2030 \pm 469$	$2206\pm203$	$4357 \pm 2348$
V (mg kg <sup>-1</sup> )	63 ± 15 (23 %)	$53 \pm 20$	53 ± 7	$62 \pm 10$	$78 \pm 5$	$85 \pm 14$	$66 \pm 16$	75 ± 23
$Zr (mg kg^{-1})$	101 + 32(31%)	61 + 18	112 + 22	80 + 22	140 + 13	79 + 23	96 + 20	158 + 6

Table S3.	Average of the	sediment elementa	l geochemistr	y variables	for the whole	e-lake, the	e six clusters	and the two ou	utliers
			Q · · · · ·	J		,			

<sup>a</sup>whole-lake: averages of all analyzed sediment samples excluding the two outlier samples (sites M4, S15); <sup>b</sup>n: number of sample; <sup>c</sup>the values in parentheses correspond to the relative standard deviation; <sup>d</sup>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 ( $\pm 10$  %). 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.

			Carbohy	drates			Chitin		-		•	N-compounds					
	(Alkyl)- furans & furanones	Hydroxy- or carboxy-furans & furanones	Pyrans	Dianhydro- rhamnose	Levoglu- cosenone	Anhydro -sugars	derived compounds	(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	<u>8</u>	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	<u>1.20</u>	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	<u>0.91</u>	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	<u>1.7</u>	0.67	1.20	<u>0.30</u>	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	<u>7.5</u>	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	<u>2.7</u>	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	<u>0.8</u>	<u>1.2</u>	<u>0.3</u>	1.5	1.0	0.2	<u>0.06</u>	0.17	2.1	<u>0.51</u>	<u>0.20</u>	0.60	<u>0.50</u>	<u>0.40</u>	<u>0.30</u>	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	<u>0.06</u>
<b>S</b> 1	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
<b>S</b> 2	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
<b>S</b> 3	18	4.8	4.9	2.3	2.7	<u>0.8</u>	3.8	0.45	0.86	2.7	1.28	1.60	0.80	1.70	0.80	1.80	0.64
<b>S</b> 4	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	<u>11.0</u>	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
<b>S</b> 9	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	<u>4.2</u>	<u>0.46</u>	0.75	2.8	0.90	1.50	0.80	1.90	1.00	<u>2.60</u>	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	<u>28</u>	3.9	2.6	2.0	<u>3.1</u>	2.2	0.9	0.08	0.48	<u>3.5</u>	1.20	<u>1.70</u>	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	<u>2.60</u>	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	<u>1.37</u>	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	<u>5.3</u>	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	<u>1.3</u>	1.9	3.4	0.37	0.86	3.1	0.85	1.60	<u>1.40</u>	<u>3.10</u>	0.90	2.30	<u>1.66</u>

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

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.

		Lignins		Chlo	rophylls		<i>n</i> -al	kenes			n-	<i>n</i> -alkanes		Alkan-2-ones		s
	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	<u>0.6</u>	0.24	1.7
N2	<u>11.4</u>	1.4	7.7	3.0	1.7	2.3	5.8	3.0	0.9	1.9	3.2	3.2	6.3	<u>0.6</u>	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	<u>1.4</u>	2.6	4.4	4.8	6.6	1.4	0.30	1.0
E1	8.1	0.3	3.5	<u>4.6</u>	1.4	4.0	<u>8.9</u>	<u>5.4</u>	1.3	2.7	5.1	3.9	5.6	1.0	0.35	<u>3.3</u>
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	<u>4.4</u>	<u>0.1</u>	<u>1.1</u>	<u>0.4</u>	<u>0.2</u>	4.1	3.8	<u>0.6</u>	0.1	2.3	<u>1.6</u>	<u>8.8</u>	<u>21.3</u>	1.6	<u>0.02</u>	<u>0.1</u>
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	<u>5.1</u>	6.9	2.1	0.3	3.7	4.6	2.0	1.4	1.9	0.31	0.3
<b>S</b> 3	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
<u>S4</u>	9.1	0.3	2.9	3.4	1.5	4.8	6.7	2.5	0.4	<u>4.1</u>	4.7	1.8	1.8	1.9	0.38	0.8
S5	9.6	1.8	<u>13.5</u>	2.2	1.2	2.1	4.4	2.6	0.7	1.7	2.5	<u>1.4</u>	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	<u>5.4</u>	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./	2.0	0.47	0.7
S11 012	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
515	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
514	8.5	0.2	2.2	2.9	<b>3.3</b>	4.0	5.0	2.2	0.4	2.3	5.2	1.0	2.4	1./	0.28	0.6
S10	6.4	0.2	2.1	2.0	1.3	4.5	5.8	1.5	$\frac{0.1}{0.7}$	3.0	3.4	1.7	$\frac{1.1}{2.0}$	1.4	0.05	0.1
S17	9.0	0.5	2.1	3.0	2.0	4.1 2.1	0.0 5 1	3.2	0.7	2.8	4.0	2.4	3.0	1.8	0.44	1.1
S18	ð./ 97	1.2	3.8 2.2	2.4	2.9	3.1	5.1 5.7	2.0	0.9	2.4	3.7	2.2	5.5 2.1	1.4	0.30	1.0
\$21	8./ 7.0	0.2	2.3	2.8	2.4	3.9	5.7	2.5	0.5	2.5	5.9 47	1./	2.1	1.5	0.27	0.0
S21 S22	7.0 0.1	0.4	2.9 2.7	2.7	1.3	4.0	0.2	2.4	0.5	2.9	4./	2.7	1.9	1.0	0.35	0.7
\$22	9.1 8.5	0.5	4.1	3.1 1.6	1.0	4.5	7.0	3.3 3.5	0.7	5.0 1 2	<b>5.0</b> 2.3	2.9	3.4 3.6	1.9	0.39	1.0
\$23	10.3	0.5	3.0	2.2	2.5	3.4	<u>3.3</u>	2.0	<u>1.4</u> 0.6	$\frac{1.5}{2.6}$	2.5	3.0 1 Q	5.0 2.7	2.2	0.10	1.4
\$19 \$21 \$22 \$23 \$24	8.7 7.0 9.1 8.5	0.2 0.4 0.3 1.3 0.5	2.3 2.9 2.7 4.6 3.0	2.8 2.7 3.1 1.6 2.2	2.4 1.5 1.6 2.5 3.6	3.9 4.0 4.5 <u>1.8</u> 3.4	5.7 6.2 7.0 <u>3.5</u> 4 3	2.3 2.4 3.3 3.5 2.0	0.5 0.5 0.7 <u>1.4</u> 0.5	2.5 2.9 3.0 <u><b>1.3</b></u> 2.6	3.9 4.7 5.0 2.3 3.7	<b>1.7</b> 2.7 2.9 3.0 <b>1 9</b>	2.1 1.9 3.4 3.6 2.7	1.5 1.6 <b>1.9</b> <b>0.7</b> 2.2	0.27 0.33 0.39 0.10 0.35	0.6 0.7 1.0 1.4

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

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.

	Storoida	Tecophorels	Hononoida			(Poly)aromatics	5	
	Steroius	rocopherois	Hopanolus	Benzene	Benzaldehyde	Acetophenone	alkylbenzene C3-9	Polyaromatics
N1	0.91	<u>1.45</u>	1.1	<u>0.4</u>	<u>0.31</u>	<u>0.57</u>	<u>1.4</u>	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	<u>0.8</u>
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	<u>1.4</u>	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	<u>0.03</u>	<dl< th=""><th>0.2</th><th>0.7</th><th>0.64</th><th>1.02</th><th>1.7</th><th>1.5</th></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
<b>S</b> 1	0.54	0.04	1.3	0.9	0.67	1.16	2.1	1.7
<b>S</b> 2	0.51	<dl< th=""><th>1.4</th><th>1.1</th><th>0.83</th><th>1.41</th><th>2.3</th><th>1.7</th></dl<>	1.4	1.1	0.83	1.41	2.3	1.7
<b>S</b> 3	1.16	0.09	1.4	0.7	0.63	1.05	2.0	1.3
<b>S</b> 4	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
<b>S6</b>	1.32	0.12	1.5	0.7	0.60	1.05	2.1	1.4
<b>S</b> 9	2.14	0.21	1.6	0.9	0.53	0.94	1.8	1.3
<b>S10</b>	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
<b>S13</b>	1.49	0.09	1.6	0.9	0.75	1.44	<u>3.5</u>	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	<u>1.47</u>	2.15	2.4	1.8
S17	2.02	0.08	1.8	0.9	0.76	1.35	2.2	1.8
<b>S18</b>	3.53	0.08	1.6	1.2	0.42	0.77	2.1	1.2
<b>S</b> 19	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	<u>2.1</u>
S23	1.18	0.33	0.5	0.6	0.47	0.79	1.4	1.0
S24	4.28	0.17	<u>1.9</u>	0.7	0.67	0.93	2.1	1.2

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

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.

		Near-shore sites	North/East basins	South	basins	Shallow cer	ntral areas
Variables (unit)	Whole-lake <sup>a</sup> (n <sup>b</sup> =42)	Cluster <sub>OM</sub> 5 (n=4)	Cluster <sub>OM</sub> 1 (n=16)	Cluster <sub>OM</sub> 3 (n=14)	Cluster <sub>OM</sub> 2 (n=3)	Cluster <sub>OM</sub> 4 (n=3)	Cluster <sub>OM</sub> 6 (n=2)
Carbohydrates							
(Alkyl)-furans & furanones	$15 \pm 5$	12 ± 4	$12 \pm 2$	$17 \pm 3$	$11.9 \pm 0.7$	$22 \pm 5$	$23 \pm 2$
Hydroxy- or carboxy-	4 + 1	$54 \pm 04$	$42 \pm 07$	$37 \pm 05$	$37 \pm 01$	61+19	$12 \pm 0.6$
furans & furanones	4 ± 1	J.7 ± 0.7	4.2 ± 0.7	$5.7 \pm 0.5$	5.7 ± 0.1	0.1 ± 1.9	$1.2 \pm 0.0$
Pyrans	$3 \pm 1$	$4.7 \pm 0.7$	$3.6 \pm 0.9$	$3 \pm 1$	$3.0 \pm 0.3$	$3.3 \pm 0.8$	$1.4 \pm 0.4$
Dianhydrorhamnose	$1.6 \pm 0.5$	$1.7 \pm 0.3$	$1.7 \pm 0.4$	$1.7 \pm 0.5$	$1.6 \pm 0.2$	$1.7 \pm 0.3$	$0.5 \pm 0.2$
Levoglucosenone	$2.2 \pm 0.4$	$2.3 \pm 0.4$	$2.2 \pm 0.4$	$2.2 \pm 0.4$	$1.9 \pm 0.5$	$2.8 \pm 0.3$	$1.9 \pm 0.5$
Anhydrosugars	$4 \pm 3$	$6.4 \pm 3.9$	$4.9 \pm 2.3$	$2.4 \pm 1.9$	$2.2 \pm 0.6$	$2.19 \pm 0.03$	$1.02 \pm 0.06$
Chitin-derived compounds							
Chitin-derived compounds	$3 \pm 1$	$2.3 \pm 0.9$	$2.7 \pm 0.8$	$2.6 \pm 0.8$	$3.8 \pm 0.4$	$1.6 \pm 0.8$	$0.23 \pm 0.1$
N-compounds							
(alkyl)pyridines	$0.3 \pm 0.1$	$0.37 \pm 0.03$	$0.28 \pm 0.08$	$0.35 \pm 0.06$	$0.41 \pm 0.04$	$0.16 \pm 0.07$	$0.06 \pm 0.01$
Pyridines_O	$0.7 \pm 0.1$	$0.63 \pm 0.06$	$0.71 \pm 0.08$	$0.79 \pm 0.06$	$0.77 \pm 0.09$	$0.7 \pm 0.2$	$0.3 \pm 0.2$
(alkyl)pyrroles	$2.4 \pm 0.5$	$1.9 \pm 0.1$	$2.0 \pm 0.3$	$2.8 \pm 0.4$	$2.9 \pm 0.2$	$2.8 \pm 0.6$	$2.4 \pm 0.4$
Pyrroles_O	$1.0 \pm 0.2$	$0.63 \pm 0.06$	$0.9 \pm 0.1$	$1.2 \pm 0.1$	$0.90 \pm 0.04$	$1.24 \pm 0.08$	$0.6 \pm 0.2$
Pyrroledione/	$1.2 \pm 0.3$	$1.2 \pm 0.08$	$1.2 \pm 0.2$	$1.1 \pm 0.3$	$1.5 \pm 0.2$	$1.5 \pm 0.2$	$0.2 \pm 0.1$
pyrrolidinedione	0.0.0.0	0.5.01	0 6 0 1	1.0.0.0	10.04	10.00	0.0.0.0
Aromatic N	$0.8 \pm 0.3$	$0.5 \pm 0.1$	$0.6 \pm 0.1$	$1.0 \pm 0.2$	$1.0 \pm 0.4$	$1.0 \pm 0.3$	$0.9 \pm 0.3$
Indoles	$1.5 \pm 0.4$	$1.39 \pm 0.08$	$1.4 \pm 0.2$	$1.7 \pm 0.1$	$2.3 \pm 0.7$	$1.5 \pm 0.2$	$0.7 \pm 0.3$
Diketodipyrrole	$0.8 \pm 0.2$	$1.0 \pm 0.2$	$0.7 \pm 0.1$	$0.78 \pm 0.08$	$0.92 \pm 0.07$	$0.5 \pm 0.2$	$0.7 \pm 0.4$
Proteins	$1.5 \pm 0.4$	$1.6 \pm 0.3$	$1.6 \pm 0.2$	$1.3 \pm 0.3$	$2.5 \pm 0.2$	$1.2 \pm 0.4$	$0.6 \pm 0.5$
Alkylamides	$0.6 \pm 0.3$	$0.46 \pm 0.09$	$0.7 \pm 0.1$	$0.5 \pm 0.2$	$1.3 \pm 0.3$	$0.3 \pm 0.2$	$0.11 \pm 0.06$
Phenois and Lignins	0.0 . 1.0	10 1	77.07	0.0.0	0.0.00	0 1	6.2
Phenols	$8.2 \pm 1.2$	$10 \pm 1$	$7.7 \pm 0.7$	$8.2 \pm 0.8$	$9.2 \pm 0.9$	$8 \pm 1$	$6 \pm 2$
Guaracols	$4 \pm 2$	$9 \pm 4$	$4 \pm 1$	$2.7 \pm 0.5$	$3.1 \pm 0.7$	$1.9 \pm 0.1$	$1.3 \pm 0.3$
Syringois	$0.5 \pm 0.4$	$1.0 \pm 0.3$	$0.5 \pm 0.5$	$0.3 \pm 0.1$	$0.7 \pm 0.4$	$0.21 \pm 0.01$	$0.1 \pm 0.1$
	27.09	26.00	21.06	2.9 . 0.2	24.02	10.02	05.01
Pristenes Distriction of	$2.7 \pm 0.8$	$2.6 \pm 0.9$	$3.1 \pm 0.6$	$2.8 \pm 0.3$	$2.4 \pm 0.2$	$1.9 \pm 0.3$	$0.5 \pm 0.1$
Phytadienes	$1.9 \pm 0.6$	$1.7 \pm 0.6$	$1.8 \pm 0.5$	$1.9 \pm 0.5$	$5.1 \pm 0.4$	$1.3 \pm 0.2$	$0.0 \pm 0.0$
	25.09	$21 \pm 0.2$	$2.2 \pm 0.4$	12+06	22+02	27 + 07	$20 \pm 0.2$
C9-10:1	$5.5 \pm 0.8$	$2.1 \pm 0.2$	$3.2 \pm 0.4$	$4.2 \pm 0.0$	$5.5 \pm 0.2$	$5.7 \pm 0.7$	$3.9 \pm 0.3$
C17-C22:1	$0 \pm 1$	$5 \pm 1$	$0.0 \pm 0.8$	$0.4 \pm 0.5$	$5.1 \pm 0.7$	$5.7 \pm 0.5$	$3.9 \pm 0.2$
C23-20_1 C27_28:1	$2.9 \pm 0.9$	$3.3 \pm 0.0$	$3.0 \pm 0.8$	$2.5 \pm 0.4$	$2.4 \pm 0.4$	$2.2 \pm 0.7$	$1.0 \pm 0.0$
	$0.8 \pm 0.4$	$1.1 \pm 0.5$	$1.1 \pm 0.2$	$0.0 \pm 0.1$	$0.9 \pm 0.2$	$0.5 \pm 0.2$	$0.12 \pm 0.02$
n-arkanes (CII:0)	$25 \pm 0.6$	$1.7 \pm 0.2$	$22 \pm 0.2$	$2.0 \pm 0.5$	$26 \pm 0.1$	$27 \pm 0.2$	$2.4 \pm 0.1$
C13-10:0 C17-22:0	$2.3 \pm 0.0$	$1.7 \pm 0.3$	$2.5 \pm 0.5$	$5.0 \pm 0.5$	$2.0 \pm 0.1$	$2.7 \pm 0.3$	$2.4 \pm 0.1$
C17-22.0 C23-26:0	$3.9 \pm 0.0$ $3 \pm 1$	$2.6 \pm 0.4$ $2.4 \pm 0.9$	$4.0 \pm 0.3$	$4.4 \pm 0.0$	$3.9 \pm 0.2$	$3.3 \pm 0.2$ 2.4 ± 0.6	$1.9 \pm 0.4$
C23-20.0	$3 \pm 1$ $4 \pm 4$	$2.4 \pm 0.9$ 3 + 2	$5.2 \pm 0.0$ 5 + 1	$2.1 \pm 0.3$ 2.3 ± 0.8	$2.1 \pm 0.1$ $3.2 \pm 0.4$	$2.4 \pm 0.0$ 28 + 14	$0 \pm 1$ 17 + 7
$\frac{C27-55.0}{\text{Alken 2 ones (2K)}}$	+ _ +	5 ± 2	$J \pm 1$	$2.3 \pm 0.0$	$5.2 \pm 0.4$	$2.0 \pm 1.4$	1/ 1/
2K C13-17	$13 \pm 0.4$	$0.7 \pm 0.1$	11 + 02	$1.8 \pm 0.2$	$1.7 \pm 0.4$	11 + 03	$1.60 \pm 0.02$
2K C19-22	$1.3 \pm 0.4$ 0.3 ± 0.1	$0.7 \pm 0.1$ 0.18 ± 0.06	$0.33 \pm 0.06$	$1.0 \pm 0.2$ $0.4 \pm 0.1$	$1.7 \pm 0.4$ 0.33 ± 0.03	$1.1 \pm 0.5$ 0.13 ± 0.07	$1.00 \pm 0.02$
2K C23-31	$13 \pm 0.1$	$1.3 \pm 0.00$	$2.1 \pm 0.7$	$0.4 \pm 0.1$ 0.8 ± 0.3	$1.1 \pm 0.03$	$0.15 \pm 0.07$ 0 5 + 0 4	$0.03 \pm 0.01$ 0.2 + 0.2
Steroids	1.5 ± 0.0	1.5 ± 0.4	2.1 ± 0.7	0.0 ± 0.5	1.1 ± 0.1	0.5 ± 0.4	$0.2 \pm 0.2$
Steroids	$12 \pm 09$	$11 \pm 03$	$1.1 \pm 0.4$	$1.2 \pm 0.5$	$37 \pm 05$	$0.25 \pm 0.09$	$0.06 \pm 0.04$
Tocophorols	$1.2 \pm 0.9$	$1.1 \pm 0.3$	1.1 ± 0.4	$1.2 \pm 0.3$	$3.7 \pm 0.3$	$0.25 \pm 0.07$	$0.00 \pm 0.04$
Tocopherols	$0.3 \pm 0.3$	$0.8 \pm 0.5$	$0.4 \pm 0.2$	$0.09 \pm 0.06$	$0.12 \pm 0.04$	$0.11 \pm 0.00$	$0.01 \pm 0.01$
Hopphoids	0.5 ± 0.5	0.0 ± 0.5	0.4 ± 0.2	0.09 ± 0.00	0.12 ± 0.04	0.11 ± 0.09	$0.01 \pm 0.01$
Hopanoida	$1.2 \pm 0.4$	$0.8 \pm 0.2$	$1.4 \pm 0.1$	$16 \pm 0.2$	$1.7 \pm 0.2$	$0.78 \pm 0.00$	$0.17 \pm 0.01$
( <b>Doly</b> ) aromatics	$1.3 \pm 0.4$	$0.0 \pm 0.3$	$1.4 \pm 0.1$	$1.0 \pm 0.2$	$1.7 \pm 0.2$	$0.70 \pm 0.09$	$0.17 \pm 0.01$
	0.0 + 0.4	06.00	$0.9 \pm 0.1$	10+02	10 + 0.2	$20 \pm 0.4$	0.67 + 0.06
Denizene Denzeldebude	$0.9 \pm 0.4$	$0.0 \pm 0.2$	$0.8 \pm 0.1$	$1.0 \pm 0.3$	$1.0 \pm 0.3$	$2.0 \pm 0.4$	$0.07 \pm 0.06$
	$0.0 \pm 0.3$	$0.39 \pm 0.07$	$0.5 \pm 0.1$	$0.7 \pm 0.1$	$0.3 \pm 0.1$	$1.5 \pm 0.2$	$0.71 \pm 0.09$
Allylbonzonos C2 0	$1.1 \pm 0.4$	$0.7 \pm 0.1$	$0.8 \pm 0.2$	$1.5 \pm 0.2$	$0.64 \pm 0.09$	$2.2 \pm 0.2$	$1.1 \pm 0.1$ $1.71 \pm 0.07$
Aikyidenzenes U3-9 Dolvaromatics	$1.9 \pm 0.3$ $1.4 \pm 0.4$	$1.44 \pm 0.09$ 1.01 $\pm 0.07$	$1.0 \pm 0.2$	$2.4 \pm 0.4$	$2.10 \pm 0.04$ 1.21 $\pm 0.02$	$2.1 \pm 0.2$	$1./1 \pm 0.0/$
	1.4 ± 0.4	$1.01 \pm 0.07$	$1.1 \pm 0.2$	$1.7 \pm 0.5$	$1.21 \pm 0.03$	$1.7 \pm 0.1$	$1.4 \pm 0.1$

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

<sup>a</sup>whole-lake: averages of all analyzed sediment samples excluding the two outlier samples (sites M4, S15); <sup>b</sup>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 ( $\pm 10$  %). Dark grey background denotes average values above 10 % of whole-lake average.