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Supplement of

Seasonal lake surface water temperature trends reflected by heterocyst glycolipid based molecular thermometers

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Supplementary Table 1. Physical and biological data obtained from surface waters of Lake Schreventeich at time of sampling. n.d. = not determined

Date	SWT (°C)	Oxygen Concentration (mg L ⁻¹)	pH	Biomass (mg L ⁻¹)
29/07/2013	24.0	n.d.	7.62	10.0
30/07/2013	23.0	n.d.	n.d.	n.d.
31/07/2013	23.2	7.6	7.56	12.0
01/08/2013	22.0	n.d.	n.d.	n.d.
02/08/2013	24.0	7.1	7.41	24.0
06/08/2013	23.0	n.d.	n.d.	n.d.
07/08/2013	23.0	6.5	7.18	22.0
09/08/2013	22.8	5.9	7.62	16.0
12/08/2013	19.8	5.2	7.36	22.0
14/08/2013	19.0	5.7	7.58	20.0
15/08/2013	19.5	n.d.	n.d.	n.d.
16/08/2013	20.0	6.8	7.79	21.5
20/08/2013	19.0	n.d.	n.d.	n.d.
21/08/2013	19.0	5.7	7.65	18.3
22/08/2013	19.8	n.d.	n.d.	n.d.
23/08/2013	20.0	6.5	7.67	20.4
30/08/2013	18.3	5.9	7.60	21.8
03/09/2013	17.0	3.7	7.41	17.1
06/09/2013	18.0	7.2	7.42	40.0
10/09/2013	16.0	3.6	7.35	50.0
16/09/2013	14.2	3.8	7.37	34.0
20/09/2013	13.0	4.3	7.32	25.5
24/09/2013	14.0	4.0	7.48	30.0
27/09/2013	13.0	4.8	7.50	32.5
01/10/2013	11.5	4.2	7.41	17.5
04/10/2013	11.5	4.1	7.45	22.5
10/10/2013	11.5	3.6	7.48	17.5
14/10/2013	11.0	3.4	7.50	17.5
18/10/2013	10.5	3.0	7.43	25.0
23/10/2013	13.0	3.2	7.41	30.0
25/10/2013	11.0	2.5	7.24	27.5

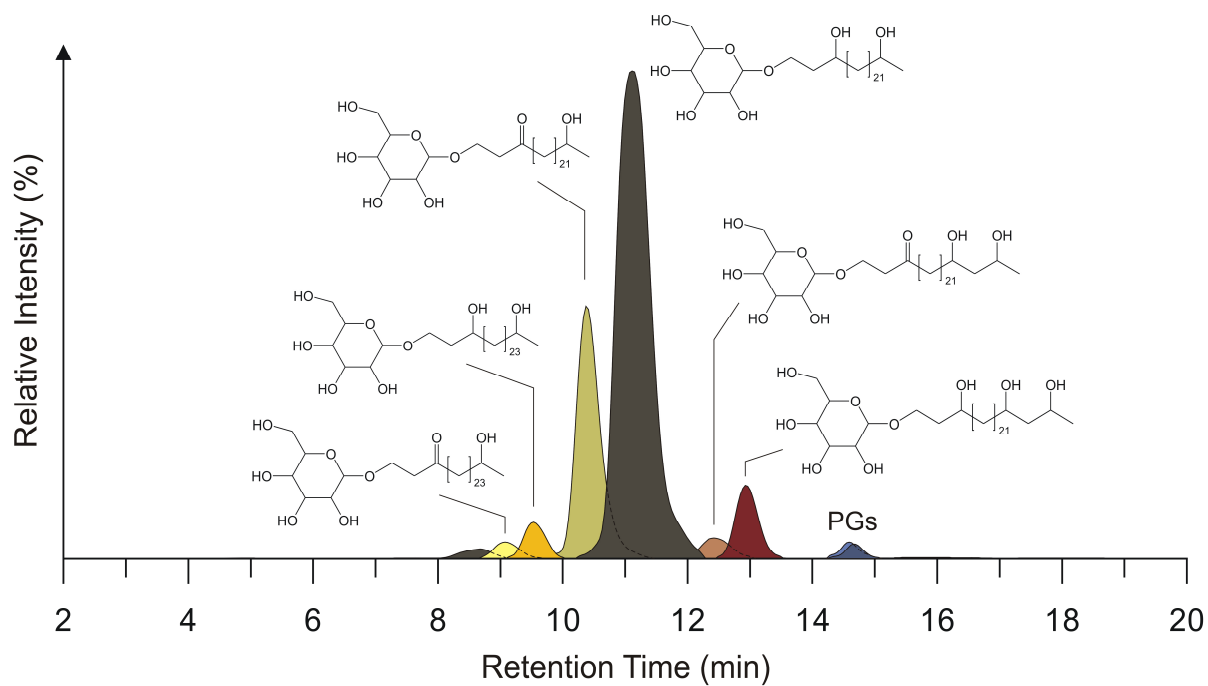
Supplementary Table 2. Fractional abundances (*f*) of heterocyst glycolipids detected in water column filtrates and surface sediments of lake Schreventeich. n.d. = not detected

Date	<i>f</i> HG ₂₆ diol	<i>f</i> HG ₂₆ keto-ol	<i>f</i> HG ₂₈ diol	<i>f</i> HG ₂₈ keto-ol	<i>f</i> HG ₂₈ triol	<i>f</i> HG ₂₈ keto-ol
16/08/2013	0.894	0.106	n.d.	n.d.	n.d.	n.d.
21/08/2013	0.652	0.095	n.d.	n.d.	0.178	0.074
23/08/2013	0.677	0.091	n.d.	n.d.	0.178	0.055
03/09/2013	0.716	0.144	0.022	0.010	0.082	0.027
06/09/2013	0.772	0.137	0.017	0.004	0.056	0.013
10/09/2013	0.662	0.195	0.023	0.011	0.082	0.028
20/09/2013	0.657	0.238	0.022	0.012	0.046	0.026
24/09/2013	0.597	0.232	0.030	0.027	0.074	0.040
27/09/2013	0.630	0.212	0.025	0.020	0.070	0.044
01/10/2013	0.588	0.249	0.026	0.028	0.061	0.048
04/10/2013	0.563	0.232	0.029	0.029	0.082	0.065
10/10/2013	0.508	0.253	0.046	0.064	0.062	0.066
14/10/2013	0.466	0.242	0.054	0.072	0.081	0.085
18/10/2013	0.584	0.225	0.048	0.035	0.064	0.044
23/10/2013	0.563	0.222	0.040	0.022	0.087	0.066
Average	0.635	0.192	0.025	0.022	0.080	0.045
Surface sediment	0.589	0.156	0.087	0.064	0.067	0.038

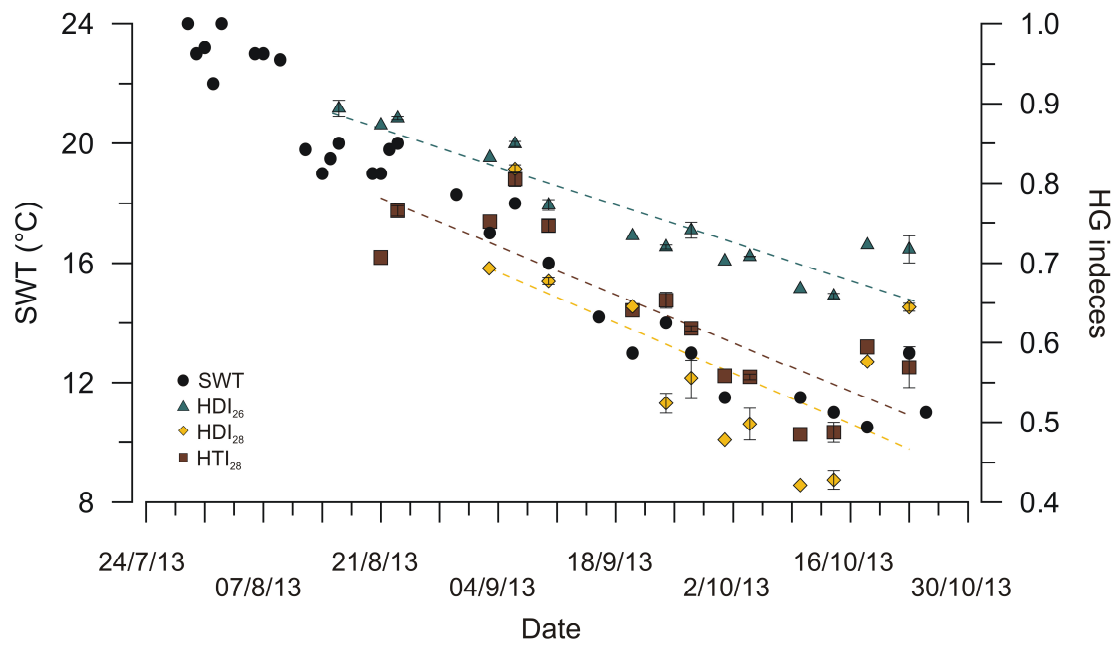
Supplementary Table 3. Variation of the HDI₂₆, HDI₂₈ and HTI₂₈ in water column filtrates and surface sediments of Lake Schreventeich together with surface water temperatures (SWT) calculated from the different HG indices as well as residual SWT (reconstructed SWT – measured SWT).

Date	HDI ₂₆	SWT ^a (°C)	Residual SWT (°C)	HDI ₂₈	SWT ^b (°C)	Residual SWT (°C)	HTI ₂₈	SWT ^c (°C)	Residual SWT (°C)
16/08/2013	0.894	20.35	0.35	-	-	-	-	-	-
21/08/2013	0.873	19.40	0.40	-	-	-	0.707	16.60	-2.40
23/08/2013	0.882	19.80	-0.20	-	-	-	0.765	18.59	-1.41
03/09/2013	0.833	17.61	0.61	0.691	16.08	-0.92	0.752	18.15	1.15
06/09/2013	0.849	18.35	0.35	0.818	19.22	1.22	0.805	20.01	2.01
10/09/2013	0.773	14.93	-1.07	0.678	15.75	-0.25	0.748	18.02	2.02
20/09/2013	0.734	13.20	0.20	0.646	14.95	1.95	0.641	14.29	1.29
24/09/2013	0.720	12.59	-1.41	0.524	11.95	-2.05	0.653	14.72	0.72
27/09/2013	0.748	13.83	0.83	0.556	12.75	-0.25	0.615	13.41	0.41
01/10/2013	0.703	11.80	0.30	0.478	10.82	-0.68	0.559	11.43	-0.07
04/10/2013	0.708	12.05	0.55	0.499	11.33	-0.17	0.558	11.41	-0.09
10/10/2013	0.668	10.25	-1.25	0.421	9.41	-2.09	0.485	8.88	-2.62
14/10/2013	0.659	9.85	-1.15	0.427	9.55	-1.45	0.486	8.92	-2.08
18/10/2013	0.722	12.69	2.19	0.577	13.25	2.75	0.595	12.70	2.20
23/10/2013	0.717	12.45	-0.55	0.648	15.01	2.01	0.570	11.85	-1.15
Average	0.765	14.61	-	0.58	13.34	-	0.639	14.21	-
Surface sediment	0.791	15.75	-	0.575	13.21	-	0.637	14.16	-

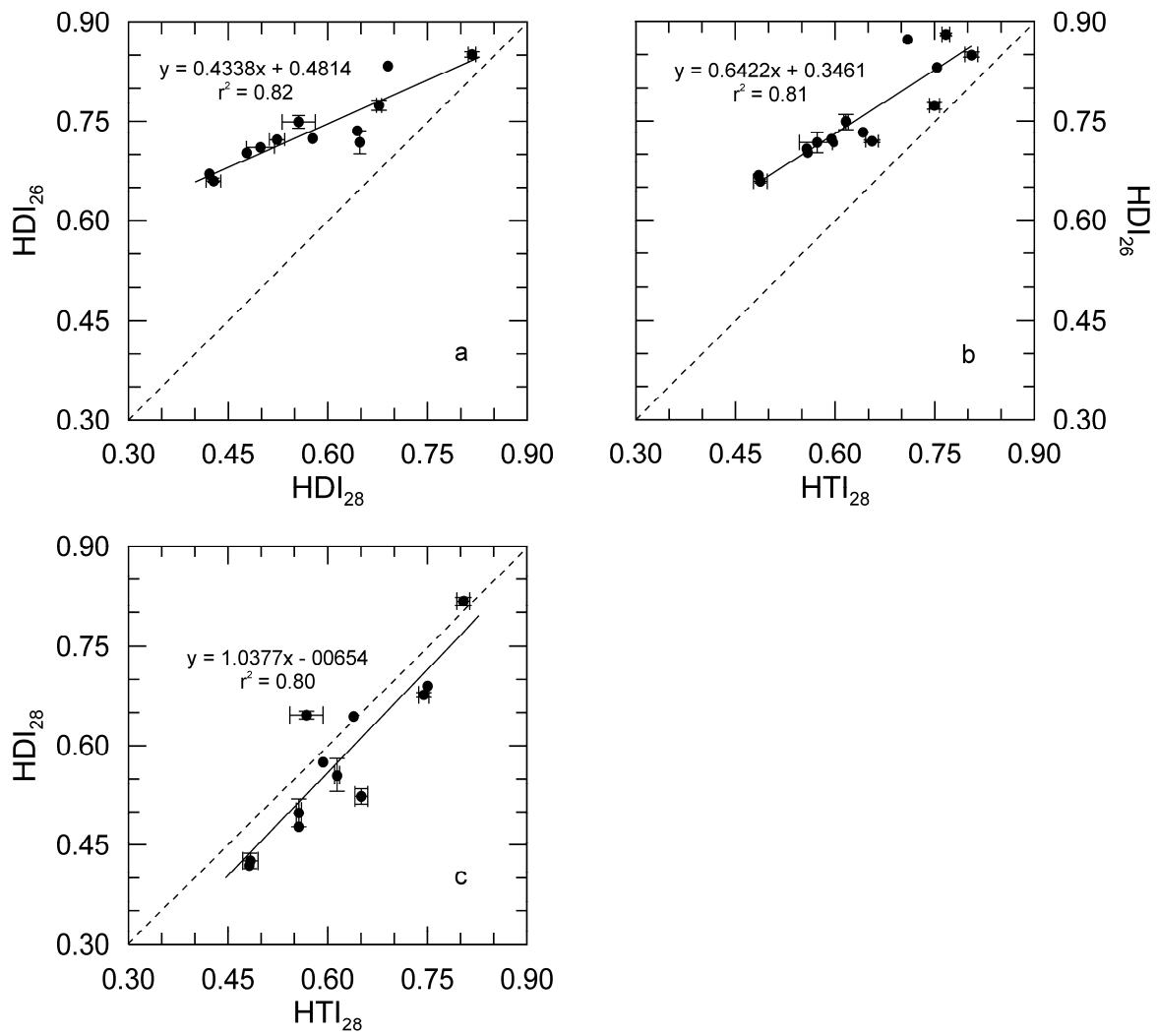
^a HDI₂₆ = 0.0224 × SWT + 0.4381; ^b HDI₂₈ = 0.0405 × SWT + 0.0401; ^c HTI₂₈ = 0.0288 × SWT + 0.2292



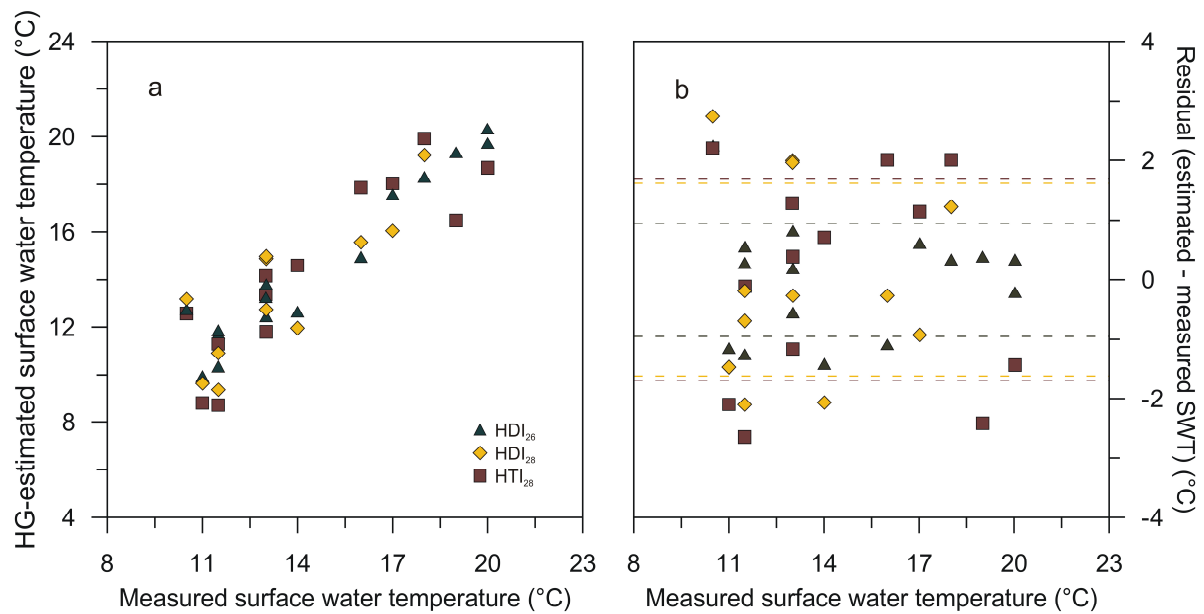
Supplementary Figure 1. Composite HPLC/MS chromatogram showing the distribution of heterocyst glycolipids in a water column filtrate of Lake Schreventeich collected in early September. Note that mass traces of the HG₂₆ diol and HG₂₆ keto-ol contained additional signals at around 14.5 min, which resulted from the in-source fragmentation of different species of the glycerophospholipid phosphatidylglycerol (PG).



Supplementary Figure 2. Comparison of measured surface water temperatures (SWT) with the variation of calculated HG indices (e.g. HDI₂₆, HDI₂₈ and HTI₂₈) in Lake Schreventeich over time.



Supplementary Figure 3. Correlations between the different HG indices determined in this study. (a) HDI₂₆ vs. HDI₂₈, (b) HDI₂₆ vs. HTI₂₈ and (c) HDI₂₈ vs. HTI₂₈. Dashed lines represent 1:1 lines. Note that all correlations are statistically significant with p -values < 0.001 .



Supplementary Figure 4. (a) HG-calculated surface water temperatures vs. measured surface water temperatures (SWT). (b) Residual SWT (estimated SWT using the HG temperature calibrations – measured SWT). Coloured dashed lines denote the standard deviations of the residuals of each HG index.