[Paleoceanography and Paleoclimatology]

Supporting Information for

Southward displacement of the Subtropical Gyre circulation system during North Atlantic cold spells

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Data Set S2. M78/1-235-1 *G. ruber (p)* and *G. truncatulinoides* stable oxygen isotope, Mg/Ca and calculated temperature data [see below].

Introduction

This supplementary file addresses information on the possible sample contamination monitored by Al/Ca, Mn/Ca, Fe/Ca ratios, a potential diagenetic overprint of the sample material, an overview about the data points that were treated as outliers inclusive a short discussion. We discuss a potential habitat change of *G. truncatulinoides* and show the raw data of both analyzed sediment cores.

Text S1 Assessment of sample contamination

Together with Mg and Ca concentrations we analyzed furthermore Al, Ba, Co, Fe, Li, Mn, Ni, Sr, Ti and Zn e.g. to monitor contamination by diagenetic overgrowth and insufficient removal of siliciclastic material during the cleaning procedure.

In sediment core M78/1-235-1 we obtained for *G. truncatulinoides* tests Fe/Ca ratios that exceed the value of 0.1 mmol/mol (mean: 0.41 ± 0.41 mmol/mol, n = 238) given as critical for possible sample contamination by Fe-oxide coatings (Barker et al., 2003). Mn/Ca ratios which are commonly higher than the critical value of 0.1 mmol/mol (mean: 0.12 ± 0.03 mmol/mol, n = 238) were obtained. We do not assume that our record is contaminated by Mn-Fe-Oxide coatings which influence our measured Mg/Ca values, due to no statistically significant correlation between Mg/Ca versus Fe/Ca (R^2 = 0.04) and Mg/Ca versus Mn/Ca (R^2 = 0.02) which infers that the Mg/Ca values are not biased by Fe-Mn coatings (Fig. S1). Furthermore concentrations of Fe and Mn were an order of magnitude smaller than Mg values. Most samples with obvious elevated Fe/Ca ratios (<0.4 mmol/mol) appear in the range between 1.95-2.6 mmol/mol Mg/Ca (15.5 - 19.3°C) matching with modern average water temperatures of living *G. truncatulinoides* individuals by plankton net samples (Jetzen, 2017; Schmunker and Schiebel, 2002) in the Caribbean Sea and Golf of Mexico, whereas highest observed Mg/Ca ratios of 2.6-3.4 mmol/mol exhibit slightly increased Fe/Ca ratios (0.2 mmol/mol) and are in good agreement with observed temperatures. Al/Ca ratios higher than 0.1 mmol/mol can be indicative for insufficient clay removal during the cleaning procedure (Barker et al., 2003). *G. truncatulinoides* yield out obvious increased Al/Ca ratios (mean: 0.16 ± 0.21 mmol/mol, n = 238) though there is no significant correlation between Al/Ca and Mg/Ca (R^2 = 0.03). After the clay removal sample preparation step we did not observe a remaining milky solution pointing out that clay removal was sufficient and clay is not a source of sample contamination in our study. When cracking especially the *G. truncatulinoides* test, for the following cleaning procedure, we observed golden to silver colored crystalline particles at the inner chamber walls and linked them to pyrite (FeS_2) which can be formed in sea sediments by sulfate-reducing bacteria. It is dissolvable in nitric acid which we used to dissolve sample material for measuring the trace metal concentrations. We tried to remove all particles with a brush but cannot be sure all particles have been removed. This can explain the elevated Fe/Ca ratios without influencing the Mg/Ca ratios of the sample material.

Diagenetically overgrown foraminifera tests by microcrystalline Ca carbonates, due to carbonate dissolution and reprecipitation, can yield to abnormal high Mg/Ca ratios (>6 mmol/mol) accompanied by reduced Sr/Ca ratios (<1.3 mmol/mol) and elevated $\delta^{18}O$ values, attributed to the chemical composition of the overgrowths (Regenberg et al., 2007). We did not observe unusual low Sr/Ca ratios for *G. truncatulinoides*. The $\delta^{18}O$ for both species are comparable to other records in the Caribbean and Gulf of Mexico (Fig. S2). Therefore we exclude diagenetic overgrowth as a source for the elevated $SST_{Mg/Ca}$.

Sediment core SO164-03-4 exhibit no significant Fe/Ca (mean: 0.01 ± 0.02 mmol/mol, n=121), Mn/Ca (mean: 0.07 ± 0.027 mmol/mol, n = 121) and Al/Ca values (mean: 0.03 ± 0.04 mmol/mol, n = 121) for *G. truncatulinoides* (Fig. S1). For *G. ruber* values of Al/Ca (mean: 0.03 ± 0.07 mmol/mol, n = 48), Fe/Ca (mean: 0.01 ± 0.02 mmol/mol, n = 48) and Mn/Ca (mean: 0.03 ± 0.02 mmol/mol, n = 48) do not exceed critical values given by Barker et al. (2003).

Furthermore we eliminated Mg/Ca ratios from the record when we obtained extremely high values of Al/Ca (>2 mmol/mol) and/or Fe/Ca (>1 mmol/mol) although they obviously fit into the record. We tested our Mg/Ca ratios with a Grubbs' test to detect outliers and removed values when they were reported with $P<0.05$ as a significant outlier taking the nearest 20 samples into account (Fig. S4).

Text S2 Comparison of subsurface temperature calibrations for *G. truncatulinoides*

Quite a few $Mg/Ca_{G.truncatulinoides}$ based subsurface temperature calibrations are currently available, which all have their strengths and weaknesses (Fig. S5). We finally decided to present and apply the most reasonable calibration, which is the species and morphotype specific Cléroux et al. (2008) calibration, established from widely distributed sample material of the Atlantic Ocean. This calibration provides Holocene $subSST_{Mg/Ca}$ consistent with the modern subsurface temperature of ~15.5°C at ~200 m water depth at Tobago Basin core 235 and ~20.4°C Beata Ridge core 03 (Fig. 3). Most calibrations yield $subSST_{Mg/Ca}$ being either too warm or too cool (Fig. S5, exemplarily for Tobago Basin core 235). The resulting downcore $subSST_{Mg/Ca}$ reconstructions are close to those derived from the McKenna and Prell (2004) calibration, which was not applied as it is based on electron-probe Mg/Ca analyses on Indian Ocean sample material. Thus, the sample material was not oxidative either nor reductive cleaned.

Text S3 Propagated error for $\delta^{18}O_{sw-ifv}$ calculations

We performed error propagation based on the uncertainty of the paleotemperature and $\delta^{18}O_{calcite}$ to $\delta^{18}O_{sw}$ conversion equations and the reproducibility of the $\delta^{18}O$ and Mg/Ca measurements to assess the error of the $\delta^{18}O_{ivf-sw}$ calculations. As mentioned in the main text, the obtained unusually high 2σ-error for *G. truncatulinoides* at both sites is based on the comparatively large uncertainty (±1.4°C) of the Mg/Ca temperature calibration ($Mg/Ca_{G.\ truncatulinoides}$ [mmol/mol] = 0.62 (±0.16) exp(0.074 (±0.017) SST [°C]) of Cléroux et al. (2008). Notably, the error of each term of the calibration is relatively high. To check if our calculated $\delta^{18}O_{ivf-sw}$ displays significant changes in past sub-surface seawater salinity, we calculated them by applying another temperature calibration equation exemplarily for Tobago Basin core 235 (Fig. 5S). For that purpose we used the temperature calibration equation $Mg/Ca_{G.truncatulinoides}$ [mmol/mol]= 0.355 (±0.053) exp(0.098 (±0.008) T [°C]) of McKenna and Prell (2004). The resulting calculated subsurface temperatures are quite similar to that of the Cléroux et al. (2008) calibration (Fig. S5). Subsequently we proceed as described in chapter 3.3. The calculated $\delta^{18}O_{ivf-sw}$ shows an identical pattern as when applying the Cléroux et al. (2008) subsurface temperature calibration. However, the resulting $\delta^{18}O_{ivf-sw}$ amplitude variations are similar but offset by ~ 0.2-0.4‰ (Fig. S5). The propagated 2σ-error (±0.49‰ for Beata Ridge core 03 (not shown); ±0.52‰ for Tobago Basin core 235 (in orange) is two times lower than by using the Cléroux et al. (2008) calibration equation (±1.16‰). Based on this test we clearly show that the error associated with each term of the Cléroux et al. (2008) calibration equation (±0.16 and ±0.017) is reasonable for the extraordinary high calculated 2σ-error when applying this equation for the subsurface temperature reconstruction. Thus, we assume that the calculated salinity gradients between Tobago Basin core 235 and Beata Ridge core 03 are significant.

Text S4 Error estimation for calculating the vertical gradient at Beata Ridge core 03

We propagated the error for thermocline reconstruction at Beata Ridge core 03 by using the reproducibility of Mg/Ca measurements. The calculated errors for $SST_{Mg/Ca}$ and $subSST_{Mg/Ca}$ are ±0.62°C and ±0.92°C, respectively. Thus, our calculated error is lower than the predicted 2σ-error for Mg/Ca analyses of ±1.2°C given by Nürnberg et al. (2000). The resulting 2σ-error for the vertical gradient is ±2.2°C (Fig. S6). The calculated vertical gradient at Beata Ridge core 03 ranges between ~5°C and ~10.9°C but most of the variability is within error. The propagated error for raw Mg/Ca ratios is ±0.5 mmol/mol (±0.24 mmol/mol for *G. ruber* and ±0.18 mmol/mol for *G. truncatulinoides*), while the values range between 2.8 mmol/mol and 0.88 mmol/mol. This implies a range of ~2 mmol/mol and that most of the calculated variations are outside the calculated error. We hence conclude that our calculated thermocline changes are significant at this point.

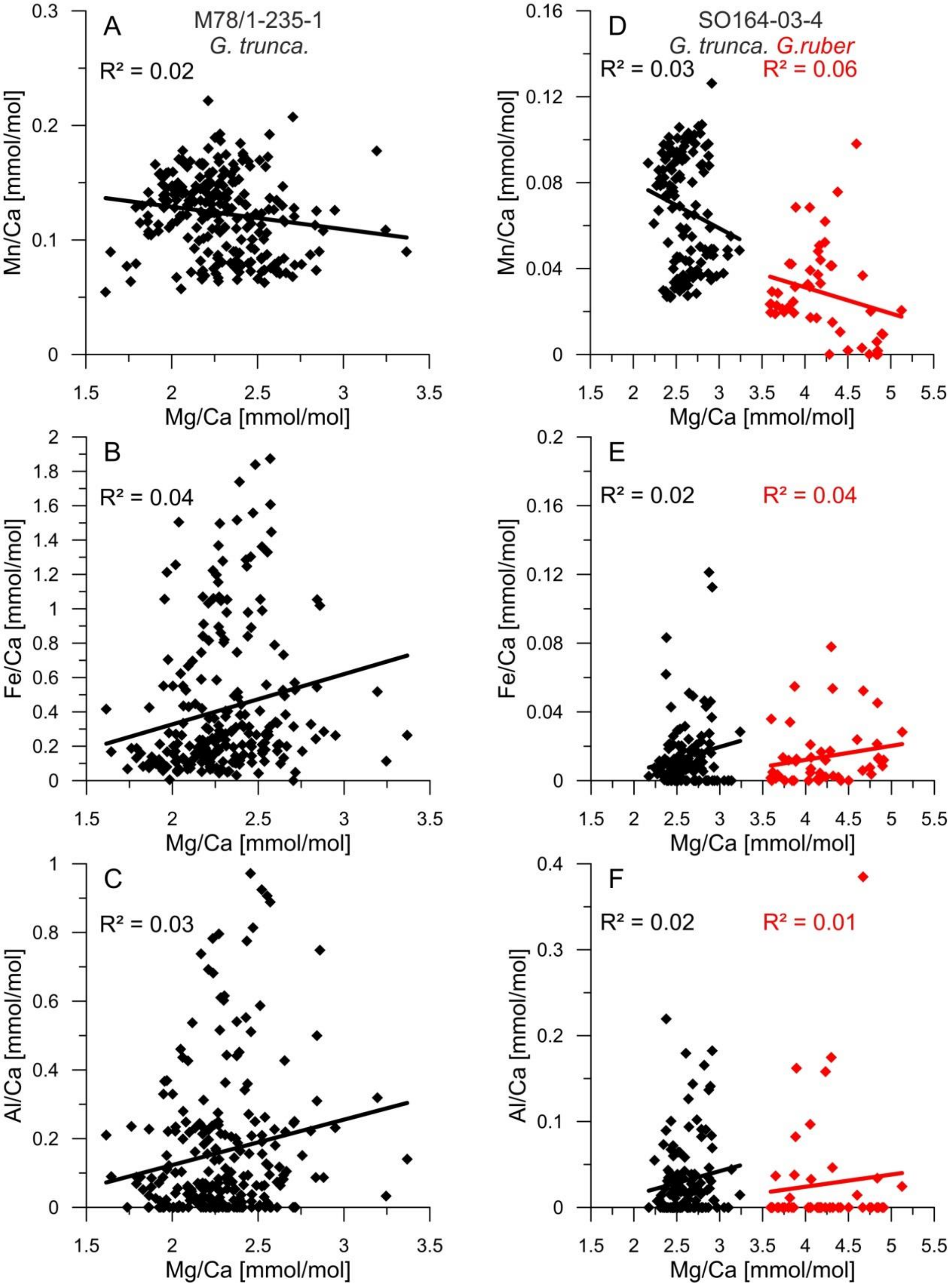

Figure S1. Planktonic Foraminiferal Mg/Ca in relation to contaminant phases Fe/Ca (top), Mn/Ca (middle) and Al/Ca (base) from clay and Mn-Fe-oxides. Black diamonds represent data from *G. truncatulinoides* and red diamonds from *G. ruber*. Correlation coefficients (R^2) are indicated. Data are from sediment cores M78/1-235-1 (A, B, C) and SO164-03-4 (D, E, F).

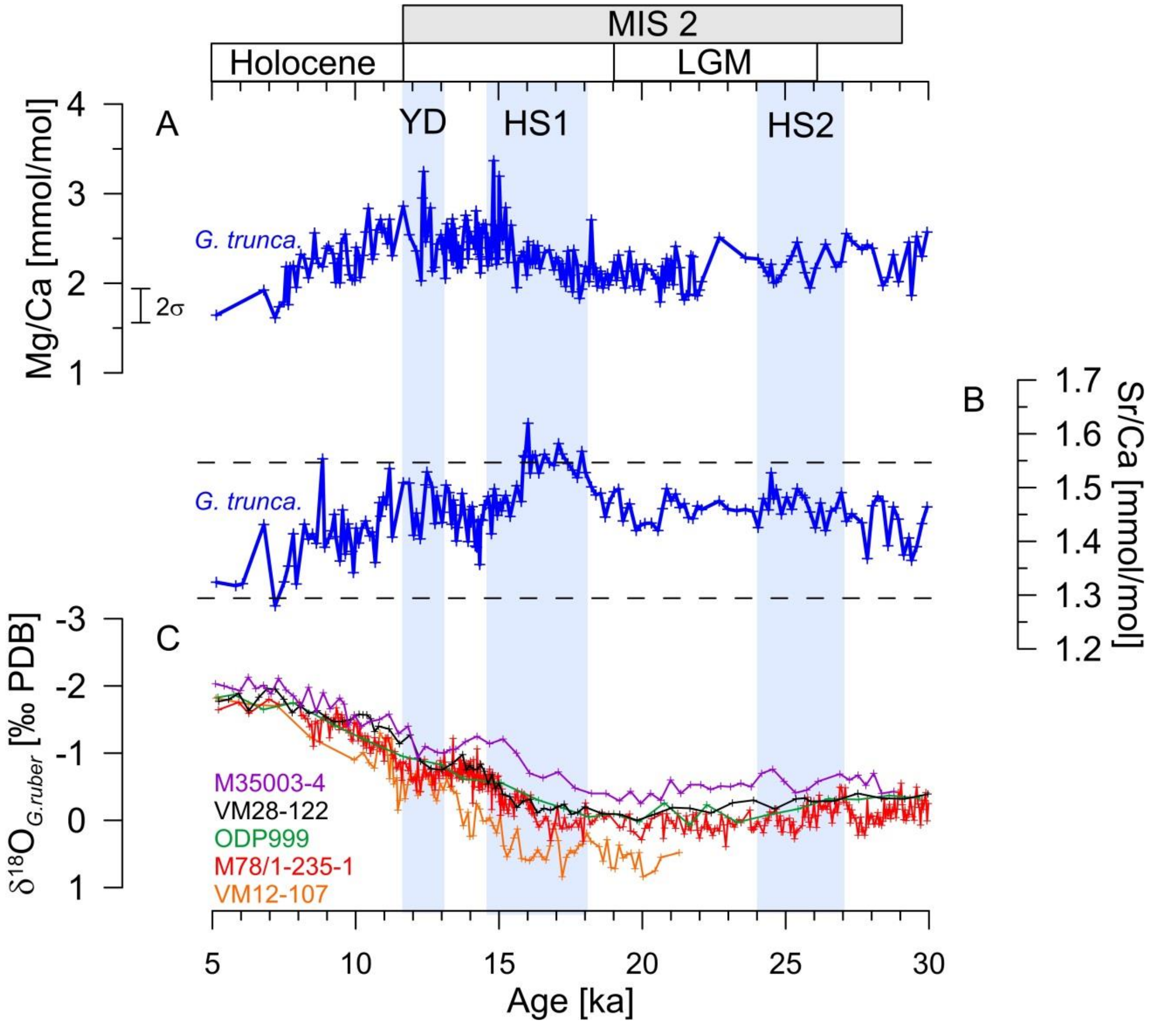

Figure S2. Evaluation of potential diagenetic overprint of foraminiferal calcite from sediment core M78/1-235-1. A) Mg/Ca ratios for *G. truncatulinoides*. B) Sr/Ca ratios for *G. truncatulinoides*. No extremely high Sr/Ca ratios pointing to potential diagenetic overgrowths (c.f. Regenberg et al., 2007) were obtained. Dashed black line marks critical Sr/Ca ratio given by Regenberg et al. (2007). C) δ^{18}O values of *G. ruber (p)* selected from core M78/1-235-1 are within the range of other surface δ^{18}O records from the Caribbean (VM12-107, Schmidt et al., 2012; VM28-122 and ODP999, Schmidt et al., 2004; M35003-4, Rühlemann et al. 1999), implying that diagenetic alteration is negligible. Blue shadings mark Younger Dryas (YD) and Heinrich Stadials (HS2 and HS1). LGM = Last Glacial Maximum, MIS2 = Marine Isotope Stage 2.

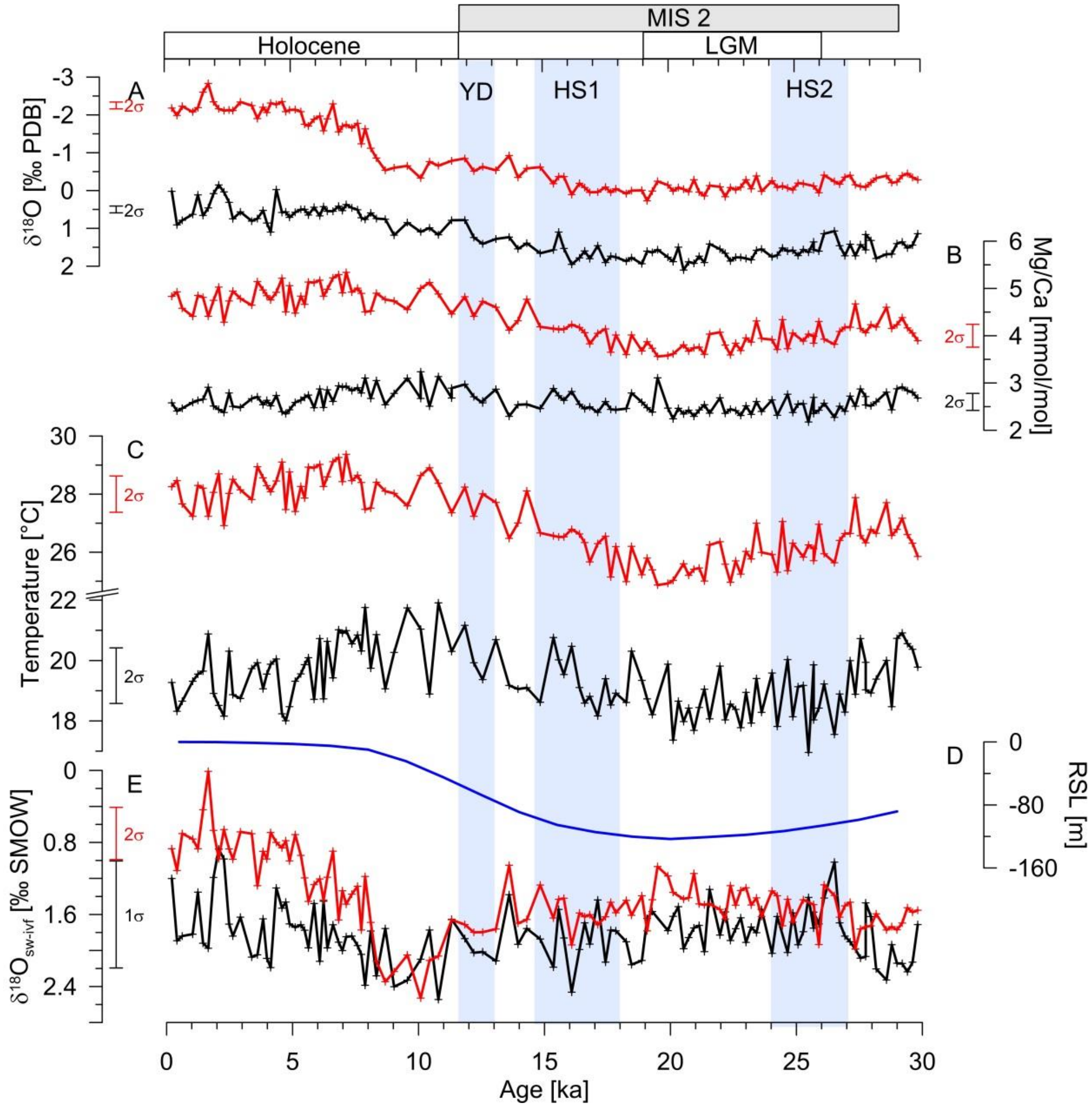

Figure S3. Planktonic foraminiferal isotope and trace metal data of sediment core SO164-03-4, and calculated ocean temperature, and salinity approximations ($\delta^{18}O_{sw}$). Data of *G. ruber* in red and *G. truncatulinoides* in black. A) $\delta^{18}O$ records; B) Mg/Ca ratios; C) $SST_{Mg/Ca}$ and $subSST_{Mg/Ca}$ calculated from equations of Anand et al. (2003) and Cléroux et al. (2008); D) relative changes of the sea level (Waelbroeck et al., 2002) used to calculate (E) relative changes of $\delta^{18}O_{sw}$ as approximation for SSS and subSSS using the equation by Thunell et al. (1999) corrected for ice volume changes (Waelbroeck et al. (2002). Blue shadings mark Younger Dryas (YD) and Heinrich Stadials (HS2 and HS1). LGM = Last Glacial Maximum, MIS2 = Marine Isotope Stage 2.

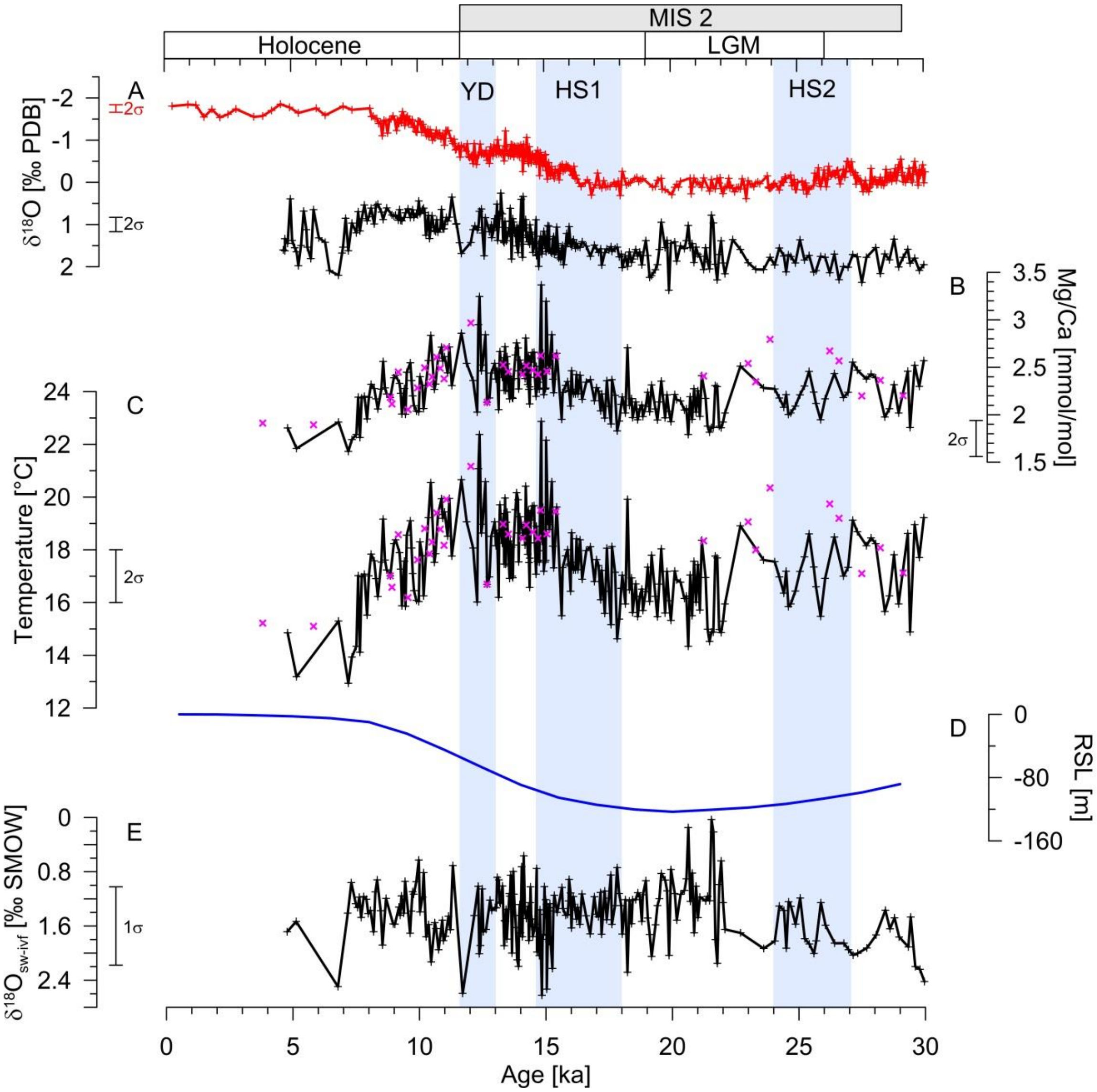

Figure S4. Planktonic foraminiferal isotope and trace metal data of sediment core M78/1-235-1, and calculated ocean temperature, and salinity approximations ($\delta^{18}O_{sw}$). Data of *G. ruber* (p) in red and *G. truncatulinoides* in black. Purple crosses indicate measurements we decide to eliminate from the dataset due to elevated Al/Ca and Fe/Ca ratios as well as values which were defined as outliers by using the Grubbs test. A) $\delta^{18}O$ records; B) Mg/Ca ratios; C) subSST$_{Mg/Ca}$ calculated with the equation of Cléroux et al. (2008); D) changes of the relative sea level (Waelbroeck et al., 2002); (E) relative changes of $\delta^{18}O_{sw}$ as approximation for subSSS using the equation by Thunell et al. (1999) corrected for ice volume changes (Waelbroeck et al. (2002). Blue shadings mark Younger Dryas (YD) and Heinrich Stadials (HS2 and HS1). LGM = Last Glacial Maximum, MIS2 = Marine Isotope Stage 2.

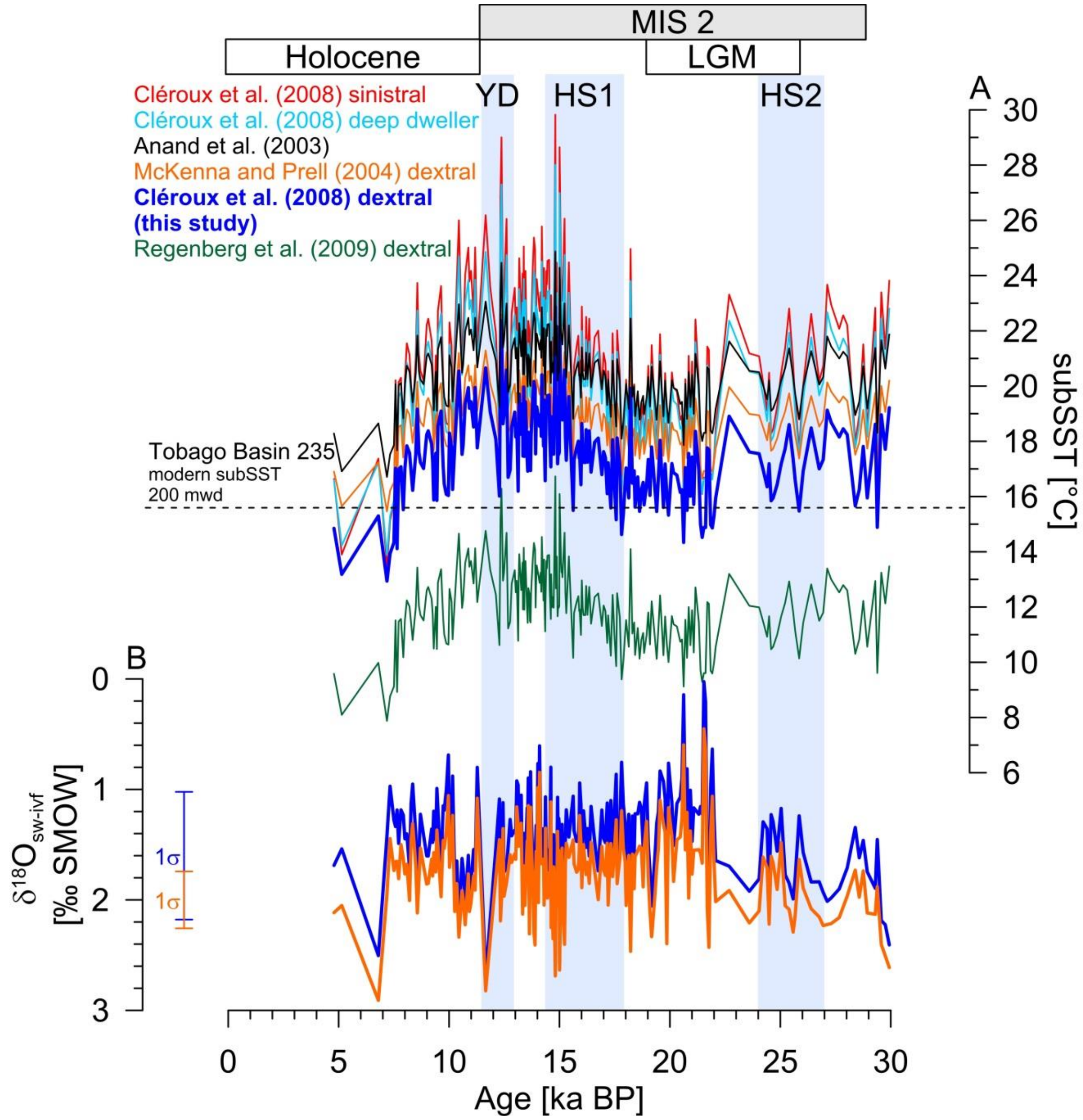

Figure S5: Comparison of Mg/Ca-temperature calibrations available for *G. truncatulinoides*. A) The calibration of Cléroux et al. (2008) for *G. truncatulinoides* dextral morphotype was considered best applicable (thick blue). The calibration of McKenna and Prell (2004) shows slightly higher temperatures(~0.5-1°C) (orange). Calibrations from Cléroux et al. (2008) and Anand et al. (2003) provide unrealistic high subSST$_{Mg/Ca}$ up to 30°C, while the Regenberg et al. (2009) calibration underestimates modern temperatures by ~8°C. B) Relative subsurface salinity changes approximated from δ^{18}O$_{sw-ivf}$ at Tobago Basin core 235 ~~by~~ using the McKenna and Prell (2004) (orange) and Cléroux et al. (2008) (blue) temperature calibrations for *G. truncatulinoides.* Blue shadings mark Younger Dryas (YD) and Heinrich Stadials (HS2 and HS1). LGM = Last Glacial Maximum, MIS2 = Marine Isotope Stage 2.

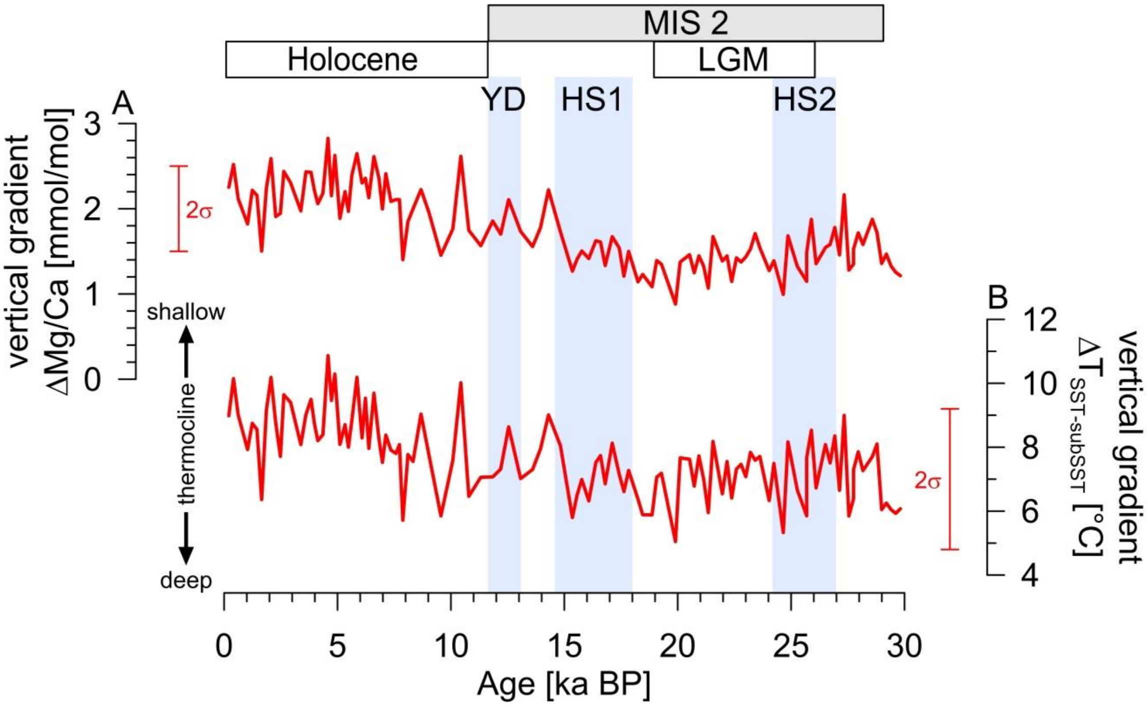

Figure S6: Vertical gradient at Beata Ridge core 03 between surface and subsurface. A) Vertical Mg/Ca gradient ($\mathrm{Mg/Ca_{suface}} - \mathrm{Mg/Ca_{subsurface}}$). B) Vertical temperature gradient ($\Delta T_{SST\text{-}subSST}$) between sea surface and subsurface indicating thermocline depth variations at Beata Ridge core 03. Red error bars show propagated 2σ-errors for each plot. Blue shadings mark Younger Dryas (YD) and Heinrich Stadials (HS2 and HS1). LGM = Last Glacial Maximum, MIS2 = Marine Isotope Stage 2.

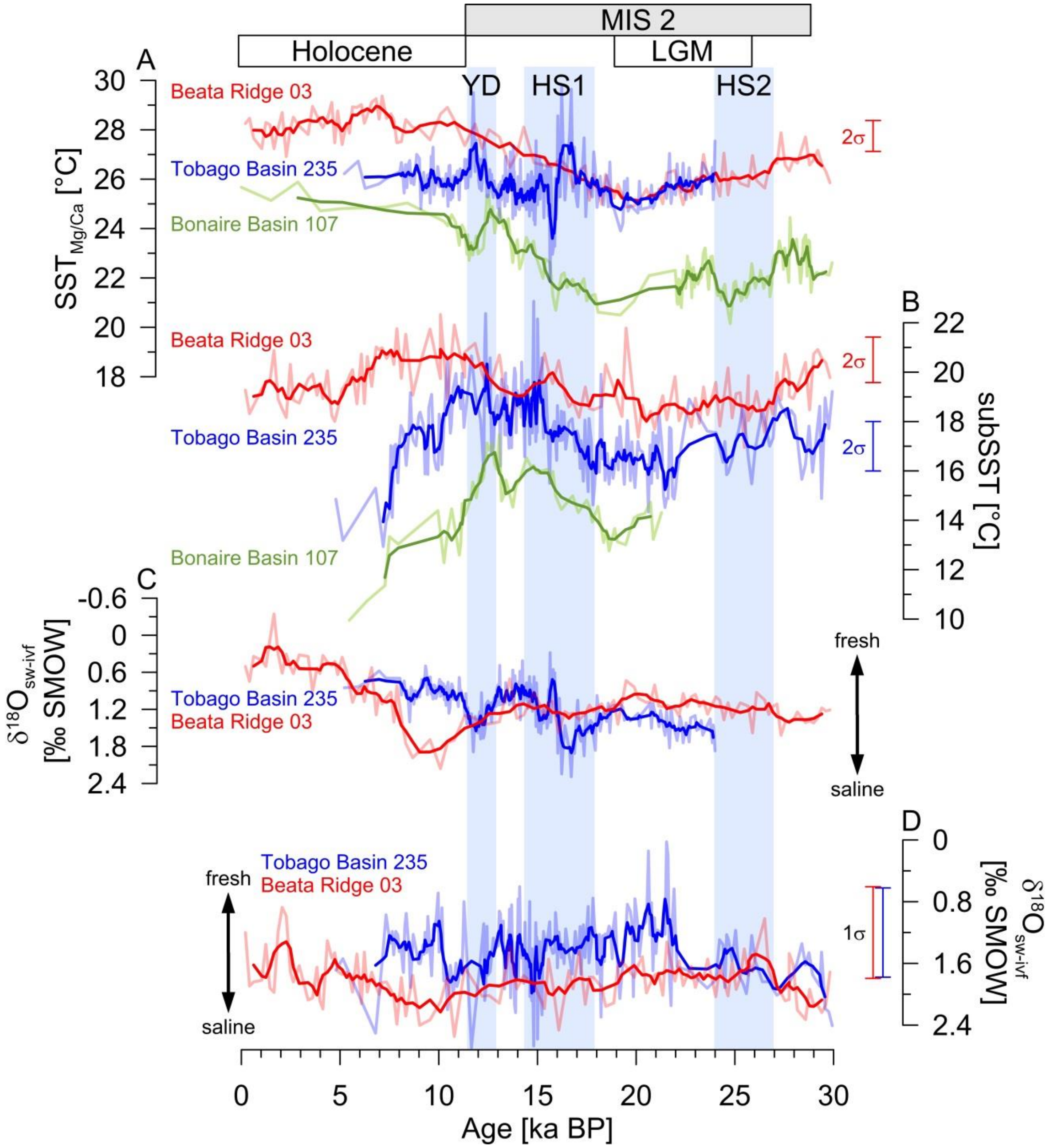

Figure 3: Sea surface temperature (SST$_{Mg/Ca}$), subsurface temperature (subSST$_{Mg/Ca}$), sea surface and sea subsurface δ^{18}O$_{sw-ivf}$ (salinity) development in the tropical W Atlantic from 30-0 ka BP. A) SST$_{Mg/Ca}$ record of Beata Ridge core 03 (*G. ruber*) (red = 5 pt-running average, light red = raw data), Tobago Basin 235 (*G. ruber pink*) (blue = 5 pt-running average, light blue = raw data) in comparison to the SST$_{Mg/Ca}$ (*G. ruber*) record of Bonaire Basin core 107 (dark green = 5 pt-running average, light green = raw data; Parker et al., 2015; Schmidt et al., 2012). B) subSST$_{Mg/Ca}$ development at Tobago Basin core 235(dark blue = 5 pt-running average, light blue = raw data for *G. truncatulinoides*), at Beata Ridge core 03 (red = 5 pt-running average, light red = raw data for *G. truncatulinoides*) and at Bonaire Basin core 107 (Schmidt et al., 2012; dark green = 5 pt-running average, light green = raw data for *G. crassaformis*).C) Relative ses surface salinity changes approximated from calculated δ^{18}O$_{sw-ivf}$ for Beata Ridge core 03 (red = 5 pt-running average, light red = raw data for *G. ruber*) and Tobago Basin core 235 (dark

blue = 5 pt-running average, light blue = raw data for *G. ruber pink*). D) Relative subsurface salinity changes approximated from calculated $\delta^{18}O_{sw-ivf}$ for Beata Ridge core 03 (red = 5 pt-running average, light red = raw data for *G. truncatulinoides*) and Tobago Basin core 235 (dark blue = 5 pt-running average, light blue = raw data for *G. truncatulinoides*). Blue shadings mark Younger Dryas (YD) and Heinrich Stadials (HS2 and HS1). LGM = Last Glacial Maximum, MIS 2 = Marine Isotope Stage 2

Data Set S1. SO164-03-4 *G. ruber* and *G. truncatulinoides* stable oxygen isotope, Mg/Ca and calculated temperature data.

Data Set S2. M78/1-235-1 *G. ruber (p)* and *G. truncatulinoides* stable oxygen isotope, Mg/Ca and calculated temperature data.