Chapter 2

Refining *C. wuellerstorfi* and *H. elegans* Mg/Ca temperature calibrations

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Abstract

We present core top Mg/Ca, Sr/Ca and $\delta^{18}O$ measurements for *Cibicidoides wuellerstorfi* and *Hoeglundina elegans* from the Timor Sea and the Makassar Strait, which span a bottom water temperature (BWT) range from 2 to 18 °C. In both species Mg/Ca ratios are positively and significantly correlated with BWT, while $\delta^{18}O$ measurements are significantly anti-correlated with BWT. Comparison of calcification temperatures derived from Mg/Ca ratios and $\delta^{18}O$ measurements yield comparable results and closely match CTD-measured temperatures. We integrate our results with previously published data sets from the Atlantic, Indian and Pacific Oceans and provide temperature calibration equations over the temperature range from 2 to 12 °C for *H. elegans* and from 0 to 10 °C for *C. wuellerstorfi.* We found geographical differences in the relation of benthic Mg/Ca ratios to BWT: *C. wuellerstorfi* shows Mg/Ca sensitivity to BWT of 19% increase in Mg/Ca per °C for the Atlantic Ocean and of 15% per °C for the Indian and Pacific Oceans. *Hoeglundina elegans* shows Mg/Ca sensitivity to BWT of 16% increase in Mg/Ca per °C for the Atlantic Ocean and of 14% per °C for the Indian and Pacific Oceans. *Cibicidoides wuellerstorfi* Sr/Ca variability appears to be driven by carbonate ion saturation, whereas *H. elegans* Sr/Ca variability is closely linked to BWT in the compiled data sets from the Atlantic, Indian and Pacific Oceans.

2.1. Introduction

The recognition that substitution of magnesium for calcium in both planktonic and benthic foraminiferal tests occurs as a temperature-controlled process [*Savin and Douglas*, 1973; *Bender at al.*, 1975] led to the development of Mg/Ca ratios as a proxy for paleotemperature reconstructions [e.g.: *Russell et al.*, 1994; *Nürnberg et al.*,

1996; *Rosenthal et al*., 1997; *Rathburn and De Deckker* 1997; *Lea et al.*, 1999; *Reichart et al.*, 2003; *Regenberg et al.,* 2009]. However, the degree of Mg^{2+} substitution in benthic foraminiferal tests varies from species to species, depending on biological controls during the biomineralization process (vital effects) [*Erez* 2003; *Bentov and Erez,* 2005 and 2006; *de Nooijer et al.*, 2014]. Therefore, species-specific Mg/Ca calibrations are needed to reliably reconstruct BWT variability over time [*Rosenthal et al.,* 1997; *Lear et al.,* 2002; *Elderfield et al*., 2006; *Healey et al.*, 2008; *Raitzsch et al.*, 2008].

The relationship between benthic Mg/Ca ratios and BWT remains controversial. Previously published benthic Mg/Ca-BWT calibrations, covering a wide BWT range (from -1 to 18 °C), were based on multiple species of the genus *Cibicidoides*, such as *C. wuellerstorfi, C. pachyderma, C. compressa, C. kullenbergi* and *wuellerstorfi*-like *Cibicidoides* [*Lear et al.*, 2002; *Martin et al*., 2002; *Elderfield et al.*, 2006]. In these studies, the colder part of the *Cibicidoides* spp. BWT calibration was characterized by Mg/Ca measurements of *C. wuellerstorfi*, as this species was the most abundant below 5 °C. In contrast, the warmer part of the calibration represented the relationship between *C. pachyderma* Mg/Ca ratios and BWT, as this species was dominant above 5 °C [*Lear et al*., 2002; *Martin et al.*, 2002; *Elderfield et al.*, 2006]. As samples from lower BWT fell along a steeper trend than that described by the *Cibicidoides* spp. calibration, *Martin et al.* [2002] and *Elderfield et al.* [2006] suggested that other factors (e.g., dissolution, carbonate ion effect) may exert a second-order control on Mg/Ca variability at low BWT.

To resolve this issue, recent studies focused on species-specific calibrations, based on *C. wuellerstorfi* Mg/Ca ratios covering the colder part of the BWT calibration range (<6 °C) [*Healey et al*., 2008; *Raitzsch et al*., 2008; *Yu and Elderfield*

2008; *Tisserand et al.*, 2013]. These studies found that the slope of the *C. wuellerstorfi* Mg/Ca-BWT relationship is steeper than previously published *Cibicidoides* spp. calibrations. However, this difference was considered too large to be exclusively ascribed to species-specific vital effects on Mg^{2+} uptake into foraminiferal tests. It was, thus, suggested that low carbonate ion saturation inhibits Mg^{2+} uptake into *C. wuellerstorfi* tests (carbonate ion effect) [*Elderfield et al*., 2006; *Healey et al*., 2008; *Raitzsch et al*., 2008; *Yu and Elderfield* 2008; *Tisserand et al.*, 2013]. In addition, four published *Hoeglundina elegans* Mg/Ca temperature calibrations, covering a temperature range between 2 and 19 °C, reported very different rates of Mg/Ca increase in relation to BWT: ~3% per 1°C increase in BWT [*Rosenthal et al.*, 2006; *Bryan and Marchitto* 2008], ~7% [*Rosenthal et al.*, 2006] and ~16% per °C [*Ní Fhlaithearta et al.*, 2010]. This also led to the suggestion that changes in bottom water carbonate ion saturation ($\Delta[CO_3^{2-}]$), rather than BWT, might control Mg/Ca variability in *H. elegans* [*Rosenthal et al.*, 2006, *Bryan and Marchitto* 2008].

The carbonate ion effect is thought to become significant in bottom waters, where $\Delta[CO_3^{2-}]_{calcite}$ <25 μmol kg^{-1} or temperature is lower than 3 °C for *C. wuellerstorfi* [*Elderfield et al*., 2006; *Healey et al*., 2008; *Raitzsch et al*., 2008; *Yu and Elderfield* 2008] and where $\Delta[CO_3^{2-}]_{aragonite}$ <15 μmol kg^{-1} for *H. elegans* [*Rosenthal et al*., 2006]. *Elderfield et al.* [2006] first quantified the effect of $\Delta[CO_3^{2-}]_{calcite}$ in *C. wuellerstorfi* Mg/Ca ratios and proposed Mg/Ca sensitivity to $\Delta[CO_3^{2-}]_{calcite}$ of 0.0086 mmol mol^{-1} per μmol kg^{-1}. *Healey et al*. [2008] reported a similar value, while *Raitzsch et al*. [2008] and *Yu and Elderfield* [2008] proposed a value of ~0.01 mmol mol^{-1} per μmol kg^{-1}. At present, it is unclear to what extent Mg/Ca ratios in *C. wuellerstorfi* and *H. elegans* can be reliably used for paleotemperature

reconstructions, as it remains a challenge to distinguish between temperature and carbonate ion effect on benthic Mg/Ca ratios. In a recent study, *Yu et al.* [2014] found that $\Delta[CO_3^{2-}]_{calcite}$ exerts a significant control on modern *C. wuellerstorfi* Sr/Ca ratios and used this relationship to track past changes in deep water carbonate ion saturation. Paired measurements of Mg/Ca and Sr/Ca ratios in the same foraminiferal samples can, thus, provide a valuable tool to better evaluate the relationship between carbonate ion saturation and element to calcium ratios in benthic foraminifera.

We present new *C. wuellerstorfi* and *H. elegans* Mg/Ca, $\delta^{18}O$, and Sr/Ca measurements from core tops retrieved from the Timor Sea and the Makassar Strait (Indonesia), which span BWT between 2 and 18 °C, $\Delta[CO_3^{2-}]_{calcite}$ between 14 and 41 μmol kg^{-1} and $\Delta[CO_3^{2-}]_{aragonite}$ between -23 and 100 μmol kg^{-1} (Fig. 2.1 and Tab. 2.1). In this region, *C. wuellerstorfi* is found in relatively shallow waters depths (~300–1000 m), thus in warmer BWT than the deeper/bathyal and abyssal specimens previously studied. These new Mg/Ca measurements provide an opportunity to expand the data sets of previously published calibrations for *C. wuellerstorfi* and *H. elegans* and to discuss regional differences in benthic Mg/Ca ratios in relation to BWT. New Sr/Ca ratios contribute to improve our understanding of changes in deep water $\Delta[CO_3^{2-}]$ and to better define the geochemical characteristics of different ocean basins.

2.2. Material and Methods

2.2.1 Sampling strategy

We analyzed Mg/Ca, Sr/Ca and $\delta^{18}O$ in the benthic foraminifera *C. wuellerstorfi* and *H. elegans* in 19 core tops (0 – 1 cm slice) from multicores retrieved

in the Timor Sea during the Sonne-185 "VITAL" Cruise [*Kuhnt et al*., 2005] and in 16 core tops (0 – 1 cm slice) from the Makassar Strait collected during the Sonne-217 "MAJA" Cruise [*Kuhnt et al*., 2011] (Fig. 2.1 and Tab. 2.1). *Cibicidoides wuellerstorfi* is an epifaunal species, which lives in middle to lower bathyal and abyssal depths [*Holbourn et al*., 2013] and has been commonly used to reconstruct BWT [*Lear et al.*, 2002; *Elderfield et al.*, 2006]. *Hoeglundina elegans* lives at or close to the sediment-water interface and has an aragonitic, glassy test that is less susceptible to diagenetic overgrowth than calcitic specimens [*Boyle et al.*, 1995; *Schönfeld*, 2001; *Fontanier et al*., 2002; *Reichart et al.*, 2003; *Rosenthal et al*., 2006].

Table 2.1. Core Top Locations

Core	Latitude, S	Longitude, E	Water Depth, m	BWT, °C
		Timor Sea		
18454	9° 46.201'	131° 14.105'	131	18.3
18503	15° 18.861'	121° 05.007'	354	9.95
18489	13° 03.016'	122° 56.016'	431	9.01
18488	12° 53.529'	122° 45.353'	555	7.82
18493	13° 25.160'	122° 05.061'	599	7.23
18469	9° 14.395'	129° 38.549'	704	6.25
18501	15° 08.503'	120° 47.010'	742	6.13
18468	9° 11.982'	129° 31.939'	803	5.80
18467	9° 10.429'	129° 27.928'	899	4.99
18466	9° 09.383'	129° 25.008'	1004	4.62
18465	9° 08.683'	129° 23.405'	1082	4.61
18500	14° 58.833'	120° 41.852'	1167	4.1
18464	9° 07.264'	129° 19.286'	1203	4.26
18463	9° 06.231'	129° 16.682'	1311	4.18
18499	14° 54.500'	120° 33.989'	1383	3.51
18462	9° 05.324'	129° 14.220'	1422	4.26
18478	11° 00.974'	120° 05.016'	1769	3.56
18506	15° 18.652'	119° 30.089'	2410	2.17
18507	13° 50.993'	120° 00.008'	2450	2.00
		Makassar Strait		
18534	7°30.618'	116°15.804'	563	6.90
18518	4°31.490'	118°56.510'	620	6.43
18532	5°55.849'	116°49.300'	629	6.60
18517	1°32.210'	117°33.792'	699	6.14
18545	5°5.315'	118°43.333'	707	6.07
18541	6°46.302'	119°23.928'	739	5.75
18536	7°28.130'	118°13.948'	836	5.65
18530	5°14.459'	117°20.348'	876	5.31
18537	7°35.595'	118°14.644'	929	5.38
18522	1°24.120'N	119°4.758'	974	4.67
18531	5°10.129'	117°27.918'	1086	4.50
18540	6°52.405'	119°34.997'	1200	4.09
18526	3°36.860'	118°10.058'	1538	3.95
18527	3°57.844'	117°49.161'	1615	3.61
18528	4°45.331'	117°53.369'	1785	3.47
18525	2°32.754'	118°38.128'	1822	3.52

Conductivity-temperature-depth (CTD) casts were deployed at the multicore locations during the two cruises to measure *in situ* temperature (Tab. 2.1).

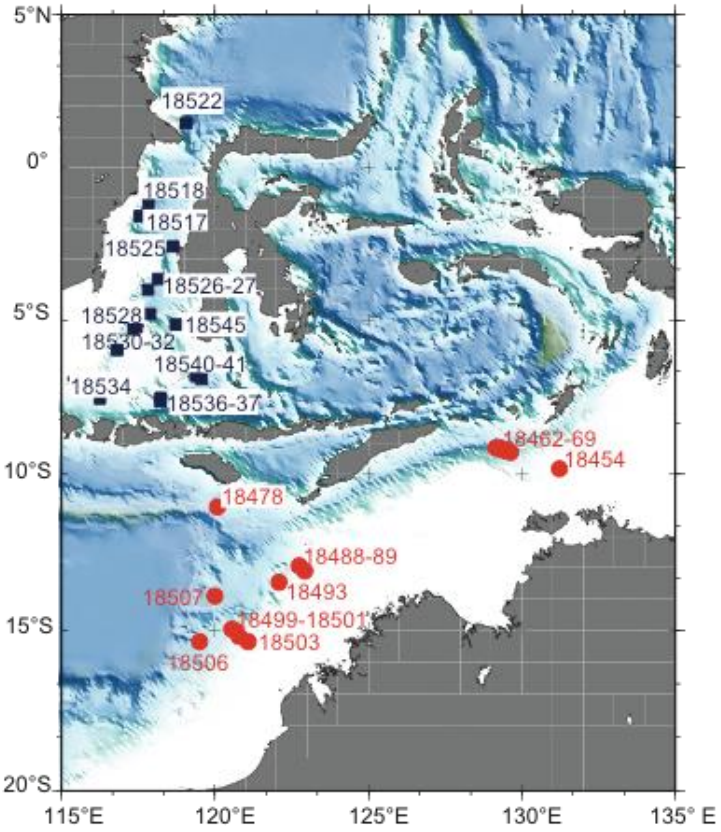

Fig. 2.1. a) Bathymetric chart with location of multicores referred to in this work. Red circles indicate multicores retrieved from the Timor Sea in a water depth range from 130 to 2500 m, blue squares indicate multicores retrieved from the Makassar Strait in a water depth range from 350 to 1800 m.

Five multicore stations in the Timor Sea and eight in the Makassar Strait were not paired with CTD measurements; therefore we derived *in situ* temperature by linear interpolation from the closest stations available. Timor Sea core top samples from water depths between 130 and 2500 m correspond to CTD-derived BWT between 2 and 18 °C; Makassar samples from water depths between 550 and 1800 m correspond to CTD-derived BWT between 3.5 and 7 °C (Tab. 2.1 and Fig. 2.1). Most core top samples were retrieved in areas where sedimentation rates are higher than ~10 cm per kyr [*Kuhnt et al.*, 2005, 2011]. Additionally, all core top samples contained rose-Bengal stained specimens of benthic foraminifers indicative of well-preserved sediment surfaces.

Water samples were collected at different water depths in six stations in the Timor Strait and in 17 stations in the Makassar Strait using a CTD-Rosette. Aliquots

of seawater from the CTD-Rosette were sampled for seawater stable oxygen isotope ($\delta^{18}O_{sw}$) measurements (Auxiliary Tabs. 2.1 and 2.2). When water samples were not available, $\delta^{18}O_{sw}$ values were estimated by linear interpolation from the next CTD station that reached deeper water depth.

2.2.2 Mg/Ca and Sr/Ca measurements of benthic foraminiferal tests

Between 5 and 30 tests of *H. elegans* and *C. wuellerstorfi* were selected for Mg/Ca, Sr/Ca and $\delta^{18}O$ analysis from the > 250 μm size fraction. All tests were checked under the microscope for cement encrustations and infillings before being broken into large fragments. After crushing, foraminiferal samples were split into sub-samples for Mg/Ca and Sr/Ca analyses (2/3 of the total sample) and $\delta^{18}O$ analyses (remaining 1/3). Mg/Ca and Sr/Ca samples were cleaned of the contaminant phases using the cleaning procedure with reductive step detailed in *Martin and Lea* [2002], without the alkaline chelation step. Samples were analyzed by ICP-OES (Inductively Coupled Plasma-Optical Emission Spectrometer) using a Spectro Ciros SOP instrument with cooled cyclonic spraychamber and microconcentric nebulization (200 μl min^{-1}) at the Institute of Geosciences, University of Kiel. Intensity ratio calibration followed the method of *de Villiers et al.* [2002] and internal analytical precision was 0.1 – 0.2% RSD. For external normalization and drift control, the certified reference material ECRM 752-1 (limestone) was measured after every sixth foraminiferal sample. The differences between the expected Mg/Ca ratio of 3.821 mmol mol^{-1} and Sr/Ca of 0.18 mmol mol^{-1} [*Greaves et al.*, 2008; not centrifuged] and the measured values were used to correct foraminiferal Mg/Ca and Sr/Ca ratios incrementally for offset and instrument drift.

In samples containing sufficient numbers of specimens, duplicates were measured (Auxiliary Tabs. 2.1 and 2.2). Twenty-two paired analyses of *H. elegans* Mg/Ca ratios gave a reproducibility of ±0.10 mmol mol^{-1} (standard deviation) corresponding to an overall average precision of 5.6% (pooled relative standard deviation). Foraminiferal Fe/Ca, Al/Ca and Mn/Ca ratios were additionally checked to monitor cleaning efficacy and no correlation with Mg/Ca ratios was found. Four *C. wuellerstorfi* samples from the Timor Sea and four *H. elegans* samples from the Makassar Strait, which showed Al/Ca ratios higher than 1 mmol mol^{-1}, indicative of sample contamination, were not included in the calibration study (Auxiliary Tabs. 2.1 and 2.2). Additionally, one *H. elegans* Mg/Ca measurement from the Makassar Strait (sample 18534; Mg/Ca = 2.45 mmol mol^{-1}), was discarded as it substantially diverged from its replicates (~1.6 mmol mol^{-1}, equivalent to ~7 °C), pointing to a problem either during cleaning or measuring the sample (Auxiliary Tab. 2.2).

2.2.3 $\delta^{18}O$ analyses in *H. elegans* tests and $\delta^{18}O_{sw}$ measurements

Foraminiferal samples for stable isotopes analysis were cleaned in absolute ethanol in an ultrasonic bath, dried at 40 °C and measured with a Finnigan MAT 253 mass spectrometer at the Leibniz Laboratory for Radiometric Dating and Isotope Research (Leibniz Laboratory), University of Kiel. The instrument is coupled on-line to a Carbo-Kiel Device (Type IV) for automated CO_2 preparation from carbonate samples for isotopic analysis. On the basis of the performance of international and lab-internal standard carbonates, the precision is better than ±0.09‰. Results were calibrated using the NIST (National Institute of Standard and Technology, Gaithersburg, Maryland) carbonate isotope standard and NBS (National Bureau of Standard) 19 and in addition NBS 20, and are reported on the Vienna PeeDee

Belemnite (V-PDB) scale. We integrated the new *C. wuellerstorfi* $\delta^{18}O$ measurements with previously published measurements from the same Timor Sea core top samples [*Holbourn et al.*, 2011].

$\delta^{18}O_{sw}$ was measured at the Leibniz Laboratory, University of Kiel, on a Thermo Finnigan DeltaPlusXL mass spectrometer connected to a Gasbench II device. The oxygen isotopic composition of water is analyzed by a so-called carbon dioxide-water equilibration method: not water, but carbon dioxide equilibrated with water is actually measured in the mass spectrometer. $\delta^{18}O_{sw}$ was measured relative to Vienna Standard Mean Ocean Water (V-SMOW) and internal lab standard. Measurements reproducibility is ±0.06‰ (standard deviation) based on multiple analyses performed on the same water samples.

Since the isotopic fractionation between seawater and $CaCO_3$ is a temperature dependent process, calcite $\delta^{18}O$ and $\delta^{18}O_{sw}$ can be used as a temperature proxy [e.g.: *Urey*, 1947; *Shackleton*, 1974]. However, as benthic $\delta^{18}O$ was measured relative to the V-PDB standard, and $\delta^{18}O_{sw}$ was referenced to V-SMOW, it was necessary to convert the V-SMOW scale to the V-PDB scale before generating a temperature calibration. We used the correction factor of 0.27‰ following *Hut* [1987].

2.2.4 Carbonate ion concentration and saturation

The degree of carbonate ion saturation ($\Delta[CO_3^{2-}]$) is the key parameter when evaluating carbonate ion control on benthic Mg/Ca ratios [*Rosenthal et al*., 2006; *Elderfield et al.*, 2006]. We used carbonate ion saturation with respect to aragonite ($\Delta[CO_3^{2-}]_{aragonite}$) to assess the carbonate ion effect on *H. elegans* Mg/Ca ratios and carbonate ion saturation with respect to calcite ($\Delta[CO_3^{2-}]_{calcite}$) to evaluate the

carbonate ion effect on *C. wuellerstorfi* Mg/Ca ratios. To estimate carbonate ion concentration ($[CO_3^{2-}]_{in\ situ}$), $\Delta[CO_3^{2-}]_{aragonite}$ and $\Delta[CO_3^{2-}]_{calcite}$ in the Timor Sea and Makassar Strait core tops, we used data from *Rosenthal et al*. [2006]. These authors measured total dissolved inorganic carbon and total alkalinity in water samples collected in the Makassar Strait and entered these parameters together with temperature and salinity measurements from the CTD into the co2sys program [*Lewis and Wallace*, 1998] to obtain $[CO_3^{2-}]_{in\ situ}$. For this study, we re-calculated carbonate ion saturation ($[CO_3^{2-}]_{saturation}$) after *Jansen et al.* [2002] for aragonite and calcite. The degree of saturation with respect to aragonite and calcite was then calculated using the following equation and the appropriate $[CO_3^{2-}]_{saturation}$ value:

$$\Delta[CO_3^{2-}] = [CO_3^{2-}]_{in\ situ} - [CO_3^{2-}]_{saturation} \quad (1)$$

For previous studies, we used published carbonate ion concentration and saturation data [*Elderfield et al.*, 2006; *Raitzsch et al*., 2008; *Yu and Elderfield* 2008; *Tisserand et al.*, 2013; *Kubota et al*., 2015]. When not available, we used data from the nearest GEOSECS stations for each core location following the approach described above [i.e. in *Martin et al*., 2002, and *Lear et al.*, 2002; *Reichart et al.*, 2003; *Healey et al.*, 2008]. For the *H. elegans* samples of *Reichart et al*. [2003] from the Bay of Biscay, it was not possible to estimate $\Delta[CO_3^{2-}]_{aragonite}$ as there is no GEOSECS station in close proximity.

2.2.5 Compilation of benthic Mg/Ca measurements from different ocean basins

Combination of our data with previously published *C. wuellerstorfi* and *H. elegans* Mg/Ca ratios is complicated by the usage of different cleaning techniques (i.e., oxidative vs. reductive cleaning) or instruments (i.e., ICP-OES, ICP-MS and

Laser Ablation ICP-MS) in previous studies, which may lead to systematic offsets (Tab. 2.2). The *C. wuellerstorfi* Mg/Ca measurements of *Tisserand et al.* [2013] did not include a reductive step in the cleaning procedure, whereas the measurements of *Reichart et al.* [2003] and *Raitzsch et al.* [2008] were performed with laser ablation. All other studies [*Martin et al.*, 2002; *Lear et al*., 2002; *Elderfield et al*., 2006; *Rosenthal et al.*, 2006; *Yu and Elderfield* 2008; *Kubota et al*., 2015] used a cleaning protocol similar to ours, including a reductive step.

Table 2.2. Published Mg/Ca temperature calibrations referred to in this study

Reference	Species	Cleaning Method	Calibration equation	Temperature range (°C)
Martin et al. [2002]	*Cibicidoides* spp.	Reductive	Mg/Ca = 1.22 exp(0.109 BWT)	-1.1 - 18
Lear et al. [2002]	*Cibicidoides* spp.	Reductive	Mg/Ca = 0.867 exp(0.109 BWT)	0.8 - 18.4
Elderfield et al. [2006]	*Cibicidoides* spp.	Reductive	Mg/Ca=0.90 exp(0.11 BWT)	-1.1 - 18
Raitzsch et al. [2008]	*C. wuellerstorfi*	Laser Ablation	Mg/Ca = 0.83 exp(0.145 BWT)	0.39 - 3.88
Healey et al. [2008]	*C. wuellerstorfi*	Reductive	Mg/Ca = 0.78 exp(0.23 BWT)	0.8 - 3.8
Yu and Elderfield [2008]	*C. wuellerstorfi*	Reductive	Mg/Ca = 0.59 exp(0.28 BWT) without carbonate ion saturation correction	0.98 - 4.26
Tisserand et al. [2013]	*C. wuellerstorfi*	Oxidative	Mg/Ca = 0.82 exp(0.19 BWT)	0 - 6
Reichart et al. [2003]	*H. elegans*	Laser Ablation	Mg/Ca = 0.39 exp (0.16 BWT)	2.5 - 13
Rosenthal et al. [2006]	*H. elegans*	Reductive	Mg/Ca = 0.96+0.0034 BWT (Atlantic)	4.2 - 18.4
Rosenthal et al. [2006]	*H. elegans*	Reductive	Mg/Ca = 0.248+0.0071 BWT (Pacific; without carbonate ion saturation correction)	1.7 - 17
Bryan and Marchitto [2008]	*H. elegans*	Reductive	Mg/Ca = 1.01+0.030 BWT	1.7 - 19
Ni Fhlaithearta et al. [2010]	*H. elegans*	Laser Ablation	Mg/C a= 0.39 exp(0.156 BWT)	2 - 16

Elderfield et al. [2006] proposed an offset of 0.2 mmol mol^{-1} between paired *C. wuellerstorfi* samples from the same core top measured with oxidative and reductive cleaning, which we used as a correction factor ($Mg/Ca_{Tisserand} - 0.2$) for the dataset of *Tisserand et al.* [2013]. No offset is apparent, when Mg/Ca measurements obtained with laser ablation [*Reichart et al.*, 2003; *Raitzsch et al.*, 2008] are plotted together with Mg/Ca ratios measured with wet chemistry (Figs. 2.5a and 2.6a). As the calibration equations of *Martin et al.* [2002], *Lear et al*. [2002] and *Elderfield et al*. [2006] were based on Mg/Ca measurements performed in multiple species of the genus *Cibicidoides*, we selected the *C. wuellerstorfi* measurements from their studies to generate new species-specific *C. wuellerstorfi* Mg/Ca temperature calibrations.

Hoeglundina elegans samples retrieved from Little Bahama Banks [*Rosenthal et al*., 2006] are not included in this calibration study, as *Curry and Marchitto* [2008] found that foraminiferal samples are diagenetically overprinted by high-Mg overgrowth in these shallow, carbonate-rich sediments, resulting in anomalously high Mg/Ca ratios.

2.3. Results

2.3.1 Benthic Mg/Ca-temperature relationships for the Timor Sea and Makassar Strait

Core top Mg/Ca ratios in *C. wuellerstorfi* range from 0.90 to 4.15 mmol mol^{-1}, corresponding to CTD-measured BWT from 2 to 10°C (Auxiliary Tab. 2.1). Mg/Ca ratios in *H. elegans* vary between 0.33 and 1.84 mmol mol^{-1}, corresponding to CTD-measured BWT from 2 to 18°C (Auxiliary Tab. 2.2). In both species, Mg/Ca ratios decrease with increasing water depth (Figs. 2a and 3a), showing good agreement with *in situ* BWT measurements (Figs. 2b and c, 3b and c). Linear and exponential regressions show positive correlation between benthic Mg/Ca ratios and BWT, described by the following equations (Figs. 2d and 3d):

Cibicidoides wuellerstorfi

$$Mg/Ca = (0.57 \pm 0.21) + (0.23 \pm 0.04)\ BWT \quad (2)$$

($R^2 = 0.56$; n = 30; $p<0.0001$)

$$Mg/Ca = (0.91 \pm 0.10)\ exp^{(0.12 \pm 0.02)\ BWT} \quad (3)$$

($R^2 = 0.65$; n = 30; $p<0.0001$)

Hoeglundina elegans:

$$Mg/Ca = (0.36 \pm 0.04) + (0.07 \pm 0.006)\ BWT \quad (4)$$

(R^2 = 0.65; n = 74; p<0.0001)

$$Mg/Ca = (0.47 \pm 0.06)\ exp^{(0.08 \pm 0.009)\ BWT} \quad (5)$$

(R^2 = 0.56; n = 74; p<0.0001)

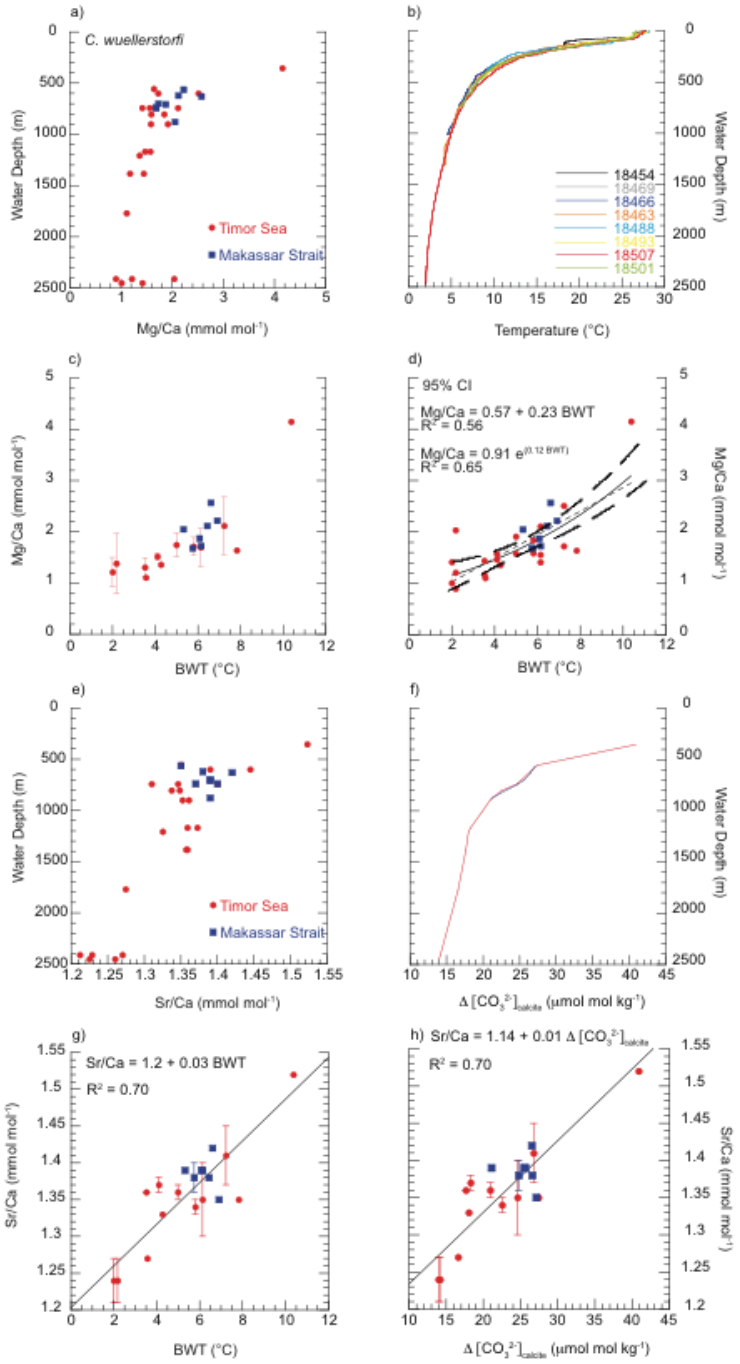

Fig. 2.2. a) *Cibicidoides wuellerstorfi* Mg/Ca versus water depth. **b)** CTD-measured temperature profiles. **c)** *Cibicidoides wuellerstorfi* Mg/Ca ratios versus CTD-derived bottom water temperatures; replicate samples were averaged and error bars represent their standard deviation. **d)** Calibration of *C. wuellerstorfi* Mg/Ca ratios versus CTD-derived BWT; solid line represents exponential fit, finely dashed line represents linear fit, black dashed lines mark the 95% confidence interval. **e)** *Cibicidoides wuellerstorfi* Sr/Ca versus water depth. **f)** Carbonate ion saturation profile with respect to calcite. **g)** *Cibicidoides wuellerstorfi* Sr/Ca ratios versus CTD-derived BWT. **h)** *Cibicidoides wuellerstorfi* Sr/Ca ratios versus $\Delta[CO_3^{2-}]_{calcite}$.

2.3.2 Benthic Sr/Ca-temperature and Sr/Ca-$\Delta[CO_3^{2-}]$ relationships for the Timor Sea and Makassar Strait

Core top Sr/Ca ratios in *C. wuellerstorfi* range from 1.21 to 1.52 mmol mol^{-1}, corresponding to $\Delta[CO_3^{2-}]_{calcite}$ values between 14 and 41 μmol kg^{-1} (Figs. 2e and f). Sr/Ca ratios in *H. elegans* vary between 0.44 to 3.26 mmol mol^{-1}, corresponding to $\Delta[CO_3^{2-}]_{aragonite}$ values between -23 and 100 μmol kg^{-1} (Figs. 3e and f). In both species, Sr/Ca ratios decrease with increasing water depth (Figs. 2e and 3e). Linear regressions best describe relationships between benthic Sr/Ca ratios and BWT (Figs. 2g and 3g) and between benthic Sr/Ca ratios and $\Delta[CO_3^{2-}]$ (Figs. 2h and 3h):

Cibicidoides wuellerstorfi

$$Sr/Ca = (1.2 \pm 0.02) + (0.03 \pm 0.003)\ BWT \quad (6)$$

($R^2 = 0.70$; n = 30; $p<0.0001$)

$$Sr/Ca = (1.14 \pm 0.03) + (0.01 \pm 0.001)\ \Delta[CO_3^{2-}]_{calcite} \quad (7)$$

($R^2 = 0.70$; n = 30; $p<0.0001$)

Hoeglundina elegans:

$$Sr/Ca = (0.19 \pm 0.07) + (0.19 \pm 0.01)\ BWT \quad (8)$$

($R^2 = 0.82$; n = 74; $p<0.0001$)

$$Sr/Ca = (1.4 \pm 0.04) + (0.023 \pm 0.002)\ \Delta[CO_3^{2-}]_{aragonite} \quad (9)$$

($R^2 = 0.64$; n = 74; $p=0.06$)

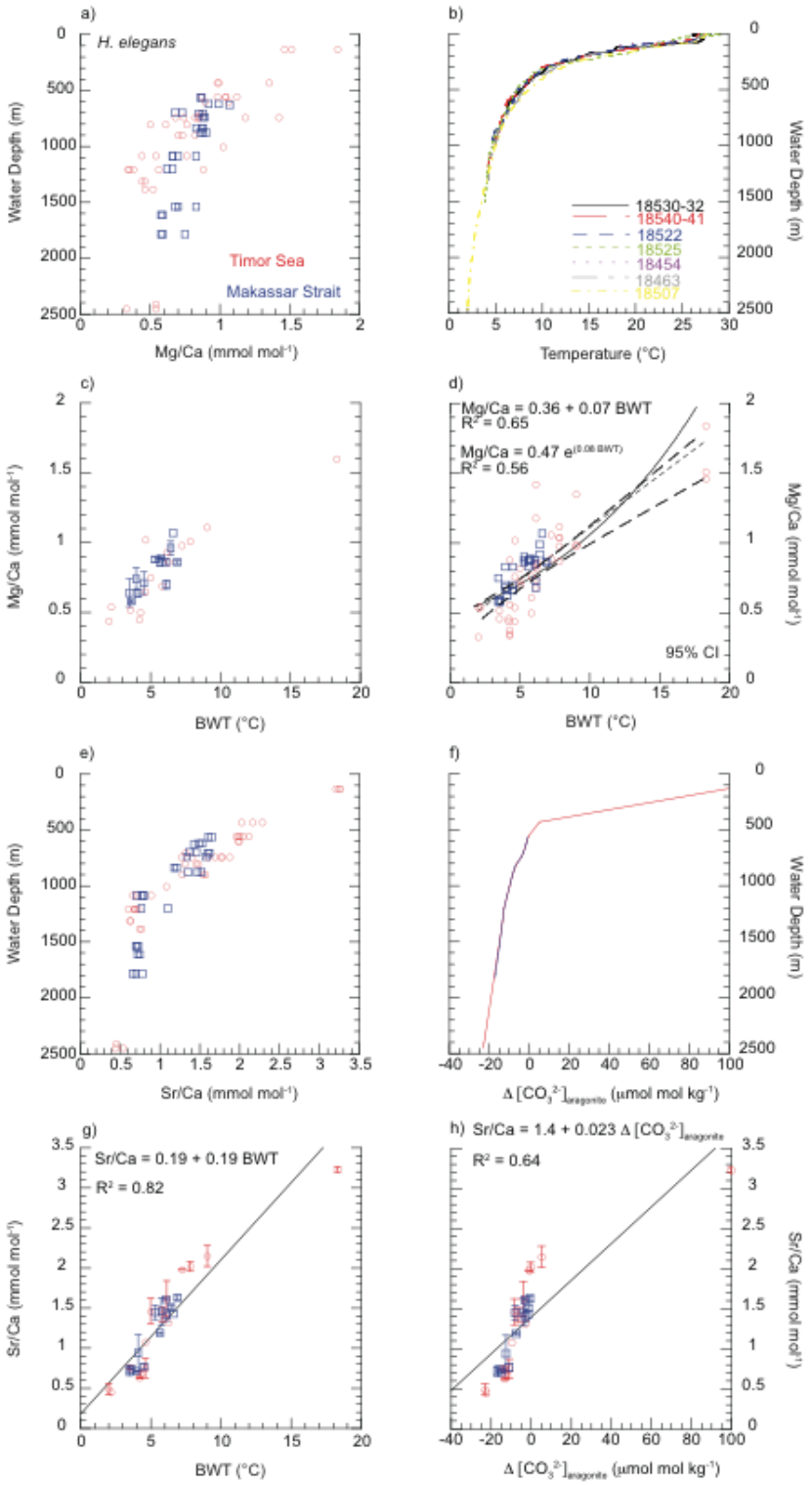

Fig. 2.3. a) *Hoeglundina elegans* Mg/Ca versus water depth. **b)** CTD-measured temperature profiles. **c)** *Hoeglundina elegans* Mg/Ca ratios versus CTD-derived BWT; replicate samples were averaged and error bars represent their standard deviation. **d)** Calibration of *H. elegans* Mg/Ca ratios versus CTD-derived BWT; solid line represents exponential fit, finely dashed line represents linear fit, thicker dashed lines mark the 95% confidence interval. **e)** *Hoeglundina elegans* Sr/Ca versus water depth. **f)** Carbonate ion saturation profile with respect to aragonite. **g)** *Hoeglundina elegans* Sr/Ca ratios versus CTD-derived BWT. **h)** *Hoeglundina elegans* Sr/Ca ratios versus $\Delta[CO_3^{2-}]_{aragonite}$.

2.3.3 Benthic $\delta^{18}O$ – temperature relationship for the Timor Sea and Makassar Strait

In the Timor Sea, *C. wuellerstorfi* $\delta^{18}O$ values range between 0.67 and 2.74‰, while *H. elegans* $\delta^{18}O$ values vary between -0.20 and 4.21‰, both exhibiting consistent increases with water depth (Figs. 4a and d). In the Makassar Strait, *C. wuellerstorfi* $\delta^{18}O$ values fluctuate between 1.77 and 2.20‰ and *H. elegans* $\delta^{18}O$ values between 2.88 and 3.60‰ (Figs. 4a and d). Benthic $\delta^{18}O$ is strongly anti-correlated with CTD-measured BWT (R^2 >0.8) (Figs. 4b and e) and linear regressions best describe the relationship between BWT and benthic $\delta^{18}O$ measurements corrected for $\delta^{18}O_{sw}$ ($\delta^{18}O - \delta^{18}O_{sw} + 0.27$) (Figs. 4c and f):

C. wuellerstorfi

$$(\delta^{18}O_{C.wuellerstorfi} - \delta^{18}O_{sw} + 0.27) = (3.6 \pm 0.07) - (0.22 \pm 0.013)\ BWT \quad (10)$$

($R^2 = 0.84$; n = 57; $p<0.0001$)

H. elegans

$$(\delta^{18}O_{H.elegans} - \delta^{18}O_{sw} + 0.27) = (5.2 \pm 0.1) - (0.26 \pm 0.016)\ BWT \quad (11)$$

($R^2 = 0.89$; n = 35; $p=0.004$)

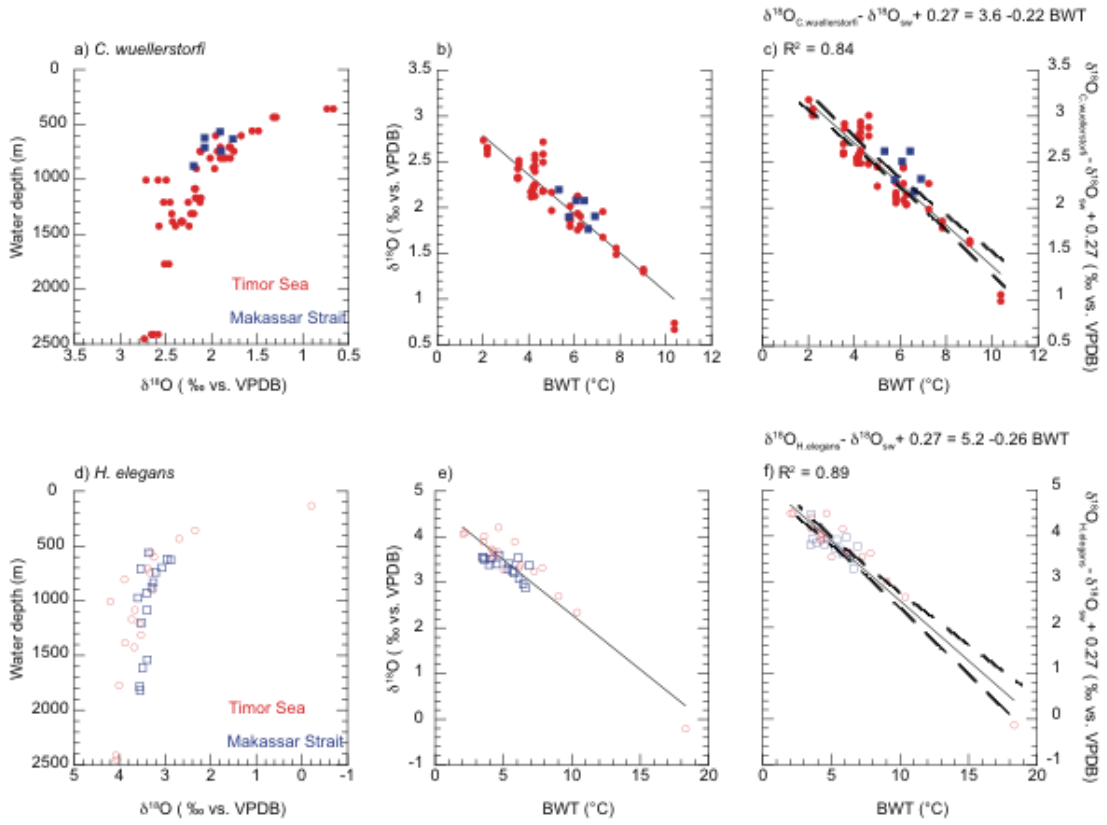

Fig. 2.4. a) *Cibicidoides wuellerstorfi* $\delta^{18}O$ versus water depth. **b)** *Cibicidoides wuellerstorfi* $\delta^{18}O$ versus BWT. **c)** Corrected *C. wuellerstorfi* $\delta^{18}O$ versus BWT. Dashed lines represent 95% confidence interval. **d)** *Hoeglundina elegans* $\delta^{18}O$ versus water depth. **b)** *Hoeglundina elegans* $\delta^{18}O$ versus BWT. **c)** Corrected *H. elegans* $\delta^{18}O$ versus BWT. Dashed lines mark the 95% confidence interval.

2.4. Discussion

2.4.1 *Cibicidoides wuellerstorfi*

2.4.1.1 Comparison to published data

We plotted published *C. wuellerstorfi* Mg/Ca ratios from BWT ranging between -1 and 16 °C together with new Mg/Ca data from the Timor Sea and Makassar Strait covering the 2 to 10 °C temperature range (compiled dataset) (Fig. 2.5a). Core top samples include samples from the Atlantic Ocean [*Lear et al.*, 2002; *Martin et al.*, 2002; *Elderfield et al.*, 2006; *Healey et al.*, 2008; *Raitzsch et al.*, 2008; *Yu and Elderfield* 2008], samples from the Brazilian margin, where $\Delta[CO_3^{2-}]_{calcite}$ is

almost constant [*Tisserand et al*., 2013], samples from the Norwegian Sea, where BWT changes are minimal [*Elderfield et al.,* 2006; *Yu and Elderfield* 2008], samples from the Pacific Ocean [*Lear et al.,* 2002; *Martin et al*., 2002; *Elderfield et al.,* 2006; *Yu and Elderfield* 2008; *Kubota et al*., 2015] and from the Indian Ocean [*Elderfield et al.,* 2006; *Healey et al.*, 2008; *Yu and Elderfield* 2008] (Supplementary Fig. 2.1). Previous works showed that Mg/Ca variability in samples from the Norwegian Sea is not driven by temperature [*Elderfield et al*., 2006; *Yu and Elderfield,* 2008], as relatively high Mg/Ca ratios correspond to almost uniform and generally low BWT (Fig. 2.5a). *Kubota et al*. [2015] reported Mg depletion in samples where $\Delta[CO_3^{2-}]_{calcite} > 80$ μmol kg^{-1} (Figs. 5a and d), as benthic foraminifera tend to uptake less Mg^{2+} when calcifying in highly supersaturated conditions [*Marchitto et al*., 2007; *Bryan and Marchitto*, 2008]. We did not include these data, as the aim of this study is to provide Mg/Ca temperature calibrations, where BWT is the main driver of Mg/Ca variability and $\Delta[CO_3^{2-}]_{calcite}$ exerts a minimal influence on Mg/Ca ratios. Our Timor Sea and Makassar Strait *C. wuellerstorfi* Mg/Ca ratios are interspersed with measurements from the Pacific and Indian Oceans (Fig. 2.5a), in contrast to samples from the Atlantic Ocean which show higher Mg/Ca ratios over the same BWT range (Fig. 2.5a), suggesting a possible geographical trend in the distribution of Mg/Ca ratios in relation to BWT.

To further investigate inter-basinal differences, we divided the compiled dataset between Atlantic and Indian + Pacific (Ind+Pac) samples and recalculated the relationship between *C. wuellerstorfi* Mg/Ca ratios and BWT. We obtained Mg/Ca sensitivity to BWT of 0.19 ± 0.009 mmol mol^{-1} per °C for the Atlantic Ocean and of 0.15 ± 0.01 mmol mol^{-1} per °C for the Ind+Pac samples (Fig. 2.5b and c). Post-depositional alteration can be likely excluded as only pristine foraminiferal tests were

selected for Mg/Ca analyses. The different sensitivities may be related to differences in seasonality of primary production and food supply [*Reygondeau et al*., 2013, *Burkett et al.*, 2015], considering that 99 out of 180 Atlantic samples come from high latitudes (north of 30 °N, and south of 30 °S), whereas only 32 out of 128 Ind+Pac samples come from high latitudes (Auxiliary Material Fig. 2.1). Another consideration is that *C. wuellerstorfi* has a characteristic upper depth limit at ~1000 m in the Atlantic [*Altenbach et al.,* 1999], whereas it commonly occurs between 1000 and 300 m in the South China Sea, eastern Indian Ocean and Pacific Ocean [*Kuhnt et al*., 1999; *Kubota et al*., 2015]. This difference in depth distribution may be related to food availability and microhabitat for the epifaunal, suspension-feeding *C. wuellerstorfi*. At shallower water depths and in areas with reduced bottom currents such as the South China Sea and eastern Indian Ocean, *C. wuellerstorfi* may live and calcify more commonly within a layer of phytodetritus fluff above the sediment surface [*Kuhnt et al*., 1999], which is characterized by lower pH and lower carbonate ion concentrations than clear ocean bottom waters.

2.4.1.2 Carbonate ion effect on *C. wuellerstorfi* Mg/Ca ratios

Several authors suggested that the carbonate ion effect instead of BWT is the main driver of *C. wuellerstorfi* Mg/Ca variability at temperatures below 3 °C [*Martin et al.,* 2002; *Elderfield et al.*, 2006; *Yu and Elderfield*, 2008] and recommended separation of temperature and $\Delta[CO_3^{2-}]_{calcite}$ signals. *Elderfield et al.* [2006, ref. Fig. 6] found that above 3 °C the sensitivity of $\Delta[CO_3^{2-}]_{calcite}$ to BWT is ~3 μmol kg^{-1} per °C, whereas below 3 °C the sensitivity is ten times higher. Thus, these authors identified a threshold at 3 °C, below which *C. wuellerstorfi* Mg/Ca ratios are controlled by $\Delta[CO_3^{2-}]_{calcite}$ and not BWT. In our compiled dataset, we found $\Delta[CO_3^{2-}]_{calcite}$

sensitivity to BWT of ~15 μmol kg^{-1} per °C for the Atlantic Ocean, and of ~19 μmol kg^{-1} per °C for the Ind+Pac data below 3 °C (Fig. 2.5d). This agrees with previous studies that described waters of the Indian and Pacific Oceans as more corrosive than Atlantic Ocean waters [e.g.: *Yu et al.*, 2014]. We found no correlation between $\Delta[CO_3^{2-}]_{calcite}$ and BWT in the Atlantic Ocean above 3 °C, and $\Delta[CO_3^{2-}]_{calcite}$ sensitivity to BWT of ~4 μmol kg^{-1} per °C for the Ind+Pac dataset for the BWT range from 3 to 10 °C (Fig. 2.5d), confirming that the carbonate ion effect on *C. wuellerstorfi* Mg/Ca ratios is negligible for the selected data. Samples from the Norwegian Sea and from highly supersaturated waters ($\Delta[CO_3^{2-}]_{calcite}$>80 μmol kg^{-1}) fall on different trends (Fig. 2.5d) confirming that BWT is not the main driver of Mg/Ca variability for these samples [*Elderfield et al*., 2006; *Yu and Elderfield*, 2008; *Kubota et al*., 2015]. We thus excluded these samples from the discussion of the relationship between Mg/Ca and BWT.

To further investigate the relationship between *C. wuellerstorfi* Mg/Ca ratios and $\Delta[CO_3^{2-}]_{calcite}$, we attempted to separate the effect of $\Delta[CO_3^{2-}]_{calcite}$ on Mg/Ca ratios from the temperature signal following the approach detailed in *Elderfield et al.* [2006]. This requires a temperature calibration where *C. wuellerstorfi* Mg/Ca variability is only driven by BWT, which is the case for the compiled dataset between 3 and 10 °C (Fig. 2.5d). We therefore recalculated the relationship between *C. wuellerstorfi* Mg/Ca ratios and BWT (3 - 10 °C) and obtained the following equations (Figs. 5b and c):

Atlantic Ocean

$$Mg/Ca = (0.73 \pm 0.06)\ exp^{(0.21 \pm 0.01\ BWT)} \quad (12)$$

($R^2 = 0.73$; n = 67; $p<0.0001$)

Ind+Pac samples

$$Mg/Ca = (0.72 \pm 0.13) \exp^{(0.145 \pm 0.02\ BWT)} \quad (13)$$

($R^2 = 0.62$; n = 35; $p<0.0001$)

We estimated Mg/Ca ratios using published BWT and exponential equations (12) and (13) and calculated the difference between measured and estimated Mg/Ca ratios ($\Delta Mg/Ca = Mg/Ca_{measured} - Mg/Ca_{estimated}$) to subtract the temperature component from the measured Mg/Ca ratios over the BWT range from 0 to 3°C (Fig. 2.5e) and from 3 to 10 °C (Fig. 2.5f). ΔMg/Ca represents the Mg/Ca component that is not explained by temperature. In the selected Atlantic Ocean dataset, low correlation (R^2 <0.2) between ΔMg/Ca and $\Delta[CO_3^{2-}]_{calcite}$ suggests that the carbonate ion effect on *C. wuellerstorfi* Mg/Ca ratios is negligible over the temperature range from 0 to 6 °C (Figs. 5e and f). This likely reflects the fact that 130 out of 180 samples come from waters where $\Delta[CO_3^{2-}]_{calcite}$ >25 µmol kg^{-1}, the threshold proposed by *Yu and Elderfield* [2008] above which Mg/Ca variability is driven by BWT and 175 out of 180 samples come from supersaturated waters with respect to calcite ($\Delta[CO_3^{2-}]_{calcite}$ >0 µmol kg^{-1}) (Figs. 5e and f).

We extended the temperature range of equation (12) down to 0 °C, and obtained the following exponential equation (Fig. 2.5b):

Atlantic Ocean

$$Mg/Ca = (0.80 \pm 0.03) \exp^{(0.19 \pm 0.009\ BWT)} \quad (14)$$

($R^2 = 0.74$; n = 180; $p<0.0001$)

The consistent distribution of *C. wuellerstorfi* Mg/Ca ratios along calibration equation (14) and high correlation coefficient ($R^2 = 0.74$) also suggest that temperature rather than $\Delta[CO_3^{2-}]_{calcite}$ controls *C. wuellerstorfi* Mg/Ca variability in the selected Atlantic Ocean dataset (0 to 6 °C) (Fig. 2.5b). Additionally equation (12) lies within the 95% confidence interval of equation (14) (Fig. 2.5b).

In the selected Indian and Pacific dataset, only 11 out of 128 samples come from waters where $\Delta[CO_3^{2-}]_{calcite}$ is >25 µmol kg^{-1} and 80 out of 128 samples come from supersaturated waters with respect to calcite ($\Delta[CO_3^{2-}]_{calcite}$ >0 µmol kg^{-1}) (Figs. 5e and f). Low correlation (R^2 <0.2) between ΔMg/Ca and $\Delta[CO_3^{2-}]_{calcite}$ is found from 0 to 3°C (Fig. 2.5e) and from 3 to 10 °C (Fig. 2.5f). The standard deviation of the difference between the calculated and measured temperature is relatively high (±1.5 °C) for equation (13) used to calculate ΔMg/Ca and it may account for the relatively high scatter of the data (Figs. 5e and f). Therefore, it remains unclear to what extent the carbonate ion effect influences *C. wuellerstorfi* Mg/Ca ratios for the Indian and Pacific dataset.

We extended the temperature range of equation (13) down to 0 °C, and obtained the following exponential equation (Fig. 2.5c):

Ind+Pac samples

$$Mg/Ca = (0.71 \pm 0.04)\ exp^{(0.15 \pm 0.01\ BWT)} \quad (15)$$

($R^2 = 0.68$; n = 128; p<0.0001)

The consistent distribution of *C. wuellerstorfi* Mg/Ca ratios along calibration equation (15) and good correlation (R^2 = 0.68) suggest that temperature rather than $\Delta[CO_3^{2-}]_{calcite}$ controls *C. wuellerstorfi* Mg/Ca variability in the selected Ind+Pac dataset (0 to 10 °C) (Fig. 2.5c). Additionally equation (15) lies within the 95% confidence interval of equation (13) (Fig. 2.5c).

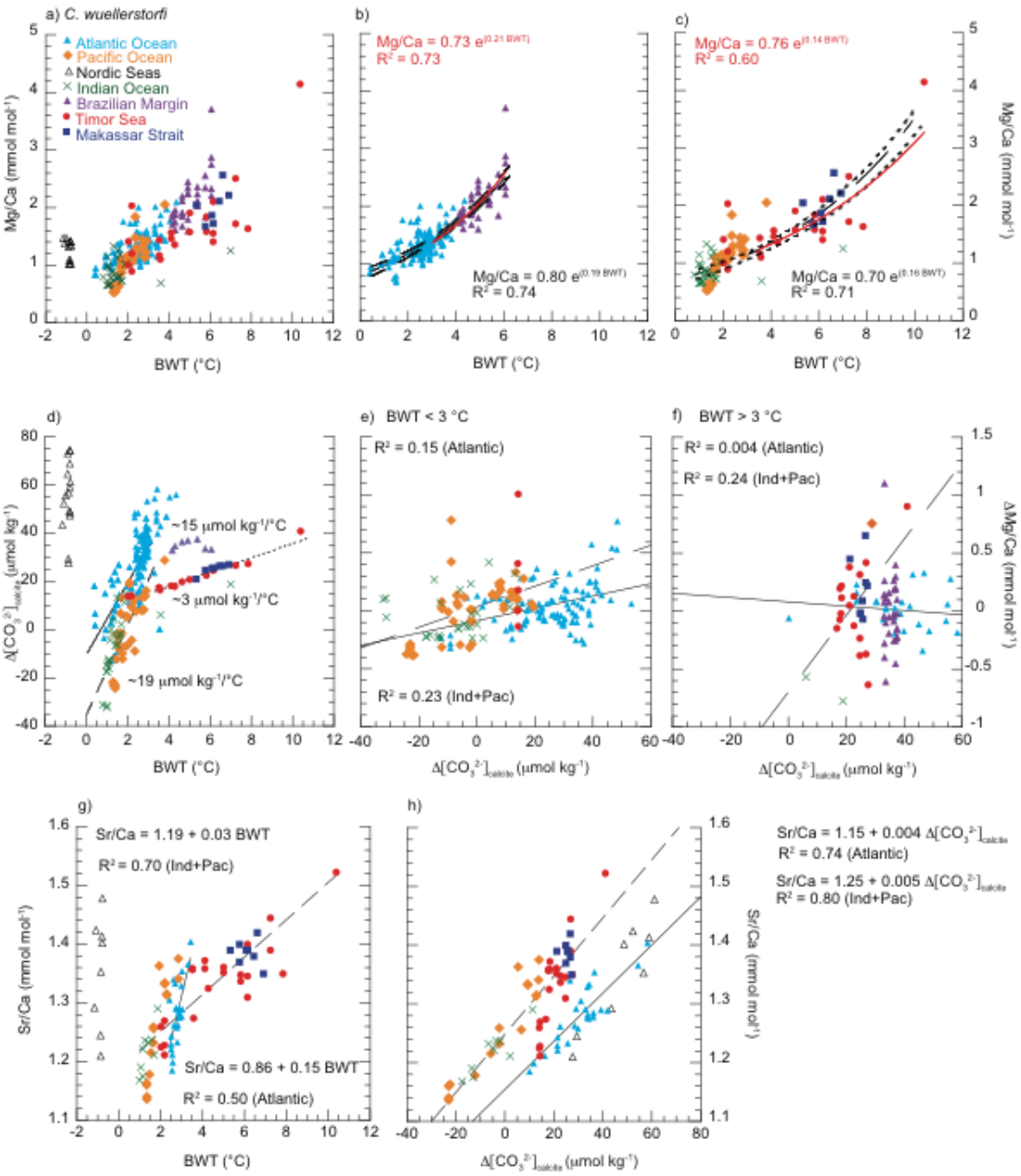

Fig. 2.5. a) Comparison between published and new *C. wuellerstorfi* Mg/Ca measurements, spanning the BWT range from -1 to 10 °C. An offset is evident between samples from the Atlantic Ocean, and samples from the Indian and Pacific Oceans. **b)** *Cibicidoides wuellerstorfi* Mg/Ca ratios versus BWT for the Atlantic Ocean. Solid black curve represents *C. wuellerstorfi* Mg/Ca temperature calibration for the BWT range from 0 to 6 °C; dashed black lines mark the 95% confidence interval. Red curve represents the temperature equation for the BWT range from 3 to 6 °C. **c)** *Cibicidoides wuellerstorfi* Mg/Ca ratios versus BWT for the Indian and Pacific Oceans. Black dashed curve represents the *C. wuellerstorfi* Mg/Ca temperature calibration for the BWT range from 1 to 10 °C; finely dashed lines mark the 95% confidence interval. Red curve represents the temperature equation for the BWT range from 3 to 10 °C. **d** $\Delta[CO_3^{2-}]_{calcite}$ sensitivity to BWT. Solid black line represents the relationship for the Atlantic Ocean below 3 °C; dashed black line represents the relationship for the Ind+Pac data below 3 °C; finely dashed black line represents the relationship for the Ind+Pac data above 3 °C **e)** *Cibicidoides wuellerstorfi* Mg/Ca sensitivity to $\Delta[CO_3^{2-}]_{calcite}$ below 3 °C. No correlation indicates negligible carbonate ion effect on *C. wuellerstorfi* Mg/Ca ratios for the selected data sets. **f)** *Cibicidoides wuellerstorfi* Mg/Ca sensitivity to $\Delta[CO_3^{2-}]_{calcite}$ above 3 °C. No correlation indicates negligible carbonate ion effect on *C. wuellerstorfi* Mg/Ca ratios for the selected data sets. **g)** *Cibicidoides wuellerstorfi* Sr/Ca sensitivity to BWT. **h)** *Cibicidoides wuellerstorfi* Sr/Ca sensitivity to $\Delta[CO_3^{2-}]_{calcite}$.

2.4.1.3 Controls on *C. wuellerstorfi* Sr/Ca variability

We plotted published *C. wuellerstorfi* Sr/Ca ratios [*Yu et al.,* 2014] together with new Sr/Ca measurements versus BWT (Fig. 2.5g). Once again, Sr/Ca ratios of samples from the Nordic seas, which lie on a different trend compared to samples from the Atlantic and Ind+Pac regions (Fig. 2.5g), were excluded. The relationship between *C. wuellerstorfi* Sr/Ca ratios and BWT is best described by the following linear equations (Fig 5g):

Atlantic Ocean

$$Sr/Ca = (0.86 \pm 0.09) + (0.15 \pm 0.03)\ BWT \quad (16)$$

($R^2 = 0.5$; n = 26; $p<0.0001$)

Ind+Pac samples

$$Sr/Ca = (1.19 \pm 0.01) + (0.03 \pm 0.003)\ BWT \quad (17)$$

($R^2 = 0.7$; n = 59; $p<0.0001$)

We found a correlation between Sr/Ca and temperature of $R^2 = 0.5$ in the Atlantic data set and of 0.7 in the Ind+Pac data set. In the Atlantic Ocean *C. wuellerstorfi* Sr/Ca sensitivity to BWT is ~0.15 mmol mol^{-1} per °C, whereas in the Ind+Pac samples sensitivity is ~0.03 mmol mol^{-1} per °C (Fig. 2.5g). Interestingly, a change in the slope of the relationship between *C. wuellerstorfi* Sr/Ca ratios and BWT is evident at ~3 °C in the Ind+Pac data (Fig. 2.5g). At BWT lower than 3 °C, Sr/Ca ratios fall on a steeper trend than at higher temperatures, possibly reflecting a carbonate ion effect on *C. wuellerstorfi* Sr/Ca ratios in deeper waters. Due to the limited number of Sr/Ca measurements above 3 °C in the Atlantic Ocean, we cannot evaluate whether a similar trend occurs in this basin (Fig. 2.5g). On account of the low sensitivity, we speculate that the influence of BWT on *C. wuellerstorfi* Sr/Ca variability is negligible above 3 °C in the Atlantic and Ind+Pac regions. In contrast,

below 3 °C, the higher Sr/Ca sensitivity to temperature may reflect a carbonate ion effect on *C. wuellerstorfi* Sr/Ca ratios (Fig. 2.5g).

We next plotted published *C. wuellerstorfi* Sr/Ca ratios [*Yu et al.*, 2014] together with our Sr/Ca measurements against $\Delta[CO_3^{2-}]_{calcite}$ to evaluate the carbonate ion effect on *C. wuellerstorfi* Sr/Ca variability (Fig. 2.5h). Our Sr/Ca measurements from the Timor Sea and Makassar Strait are interspersed with the Ind+Pac Sr/Ca ratios, whereas a clear offset is shown between Atlantic and Ind+Pac samples (Fig. 2.5h), in agreement with *Yu et al.* [2014]. The following linear equations best describe the relationship between Sr/Ca ratios and $\Delta[CO_3^{2-}]_{calcite}$ (Fig. 2.5h):

Atlantic Ocean:

$$Sr/Ca = (1.15 \pm 0.016) + (0.004 \pm 0.0005)\ \Delta[CO_3^{2-}]_{calcite} \quad (18)$$

($R^2 = 0.74$; n = 26; $p<0.0001$)

Ind+Pac samples:

$$Sr/Ca = (1.25 \pm 0.007) + (0.005 \pm 0.0003)\ \Delta[CO_3^{2-}]_{calcite} \quad (19)$$

($R^2 = 0.80$; n = 59; $p<0.0001$)

The high correlation (R^2 >0.74) between *C. wuellerstorfi* Sr/Ca ratios and $\Delta[CO_3^{2-}]_{calcite}$ for both ocean basins and no discernible change in the slope of this relationship between saturated and undersaturated ($\Delta[CO_3^{2-}]_{calcite}$ <0 μmol kg^{-1}) waters (Fig. 2.5h) suggest that $\Delta[CO_3^{2-}]_{calcite}$ exerts the main control on Sr/Ca variability. These results support the findings of *Yu et al.* [2014], who suggested using this ratio as an auxiliary proxy to monitor past changes in $\Delta[CO_3^{2-}]_{calcite}$ in deeper waters, given that seawater Sr/Ca remained stable over time. *Dawber and Tripati* [2012] also found a significant and positive correlation between *Oridorsalis umbonatus* Sr/Ca and $\Delta[CO_3^{2-}]_{calcite}$ and suggested that this dependence may be related to the carbonate ion effect on the amount of calcium remaining in the "internal biomineralization pool"

after calcite precipitation, and consequently on the fractionation of Sr (Rayleigh fractionation, *Erez* [2003]; *de Nooijer et al*. [2014]).

2.4.2 *Hoeglundina elegans*

2.4.2.1 Comparison to published data

Our *H. elegans* Mg/Ca measurements from the Timor Sea and Makassar Strait are interspersed with published measurements of *Rosenthal et al.* [2006] from Hawaii and the Makassar Strait and of *Reichart et al.* [2003] from the Arabian Sea (Indo+Pacific samples) (Fig. 2.6a). In contrast, samples from the Bay of Biscay (Atlantic Ocean) show higher Mg/Ca ratios for the same BWT range (Fig. 2.6a), pointing to a geographical trend, as we noted for *C. wuellerstorfi* Mg/Ca ratios. By dividing the compiled dataset between samples from the Atlantic and Indo+Pacific Oceans, we obtained the following exponential equations (Fig. 2.6b and c):

Atlantic Ocean

$$Mg/Ca = (0.4 \pm 0.18)\ exp^{(0.16 \pm 0.02\ BWT)} \quad (20)$$

($R^2 = 0.83$; n = 9; $p<0.0001$)

Indo+Pacific Ocean

$$Mg/Ca = (0.405 \pm 0.05)\ exp^{(0.09 \pm 0.007\ BWT)} \quad (21)$$

($R^2 = 0.51$; n = 138; $p<0.0001$)

Interestingly, the three Indo+Pacific samples from shallow locations (samples MC047 from Hawaii, MC037 from Indonesia, and 18454 from the Timor Sea) depart from the main trend towards lower Mg/Ca ratios, despite the high BWT (>15 °C) of ambient waters (Fig. 2.6c). In contrast, samples from the Bay of Biscay, covering a

temperature range between 2.5 and 13 °C, do not show Mg^{2+} depletion at higher temperatures (Fig. 2.6b).

2.4.2.2 Carbonate ion effect on *H. elegans* Mg/Ca ratios

Rosenthal et al. [2006] found a threshold at 15 μmol kg^{-1} below which *H. elegans* Mg/Ca variability appears to depend on the combined effects of temperature and $\Delta[CO_3^{2-}]_{aragonite}$. Following the approach in section 4.1.2 and detailed in *Elderfield et al.* [2006], we plotted BWT against $\Delta[CO_3^{2-}]_{aragonite}$ and found $\Delta[CO_3^{2-}]_{aragonite}$ sensitivity to BWT of ~5 μmol kg^{-1} $°C^{-1}$ below 15 μmol kg^{-1}, and of ~9 μmol kg^{-1} $°C^{-1}$ above 15 μmol kg^{-1} for the Indo+Pacific Ocean (Fig. 2.6d), which differs from *Rosenthal et al.* [2006]. The sensitivity of $\Delta[CO_3^{2-}]_{aragonite}$ to BWT of 5-9 μmol kg^{-1} $°C^{-1}$ is lower than the sensitivity of $\Delta[CO_3^{2-}]_{calcite}$ to BWT of ~30 μmol kg^{-1} $°C^{-1}$ (below 3 °C) identified by *Elderfield et al.* [2006], as the threshold below which the carbonate ion effect on *C. wuellerstorfi* Mg/Ca ratios becomes significant. No $\Delta[CO_3^{2-}]_{aragonite}$ measurements are available for the Atlantic Ocean dataset.

As for *C. wuellerstorfi* (section 4.1.2), we attempted to separate the effects of temperature and carbonate ion saturation on *H. elegans* Mg/Ca ratios, following *Elderfield et al.* [2006]. In equation (20), the consistent distribution of *H. elegans* Mg/Ca ratios along the calibration equation together with the high correlation coefficient (R^2 >0.8) suggest that temperature rather than carbonate ion saturation is the main control on Mg/Ca variability (Fig. 2.6b). However, we do not have $\Delta[CO_3^{2-}]_{aragonite}$ estimates for the Atlantic Ocean, and cannot quantify the carbonate ion effect on *H. elegans* Mg/Ca ratios for this region. For the Indo+Pacific dataset (equation (21)), the three samples showing Mg depletion at higher BWT (>15 °C) (Fig. 2.6c)

come from highly supersaturated waters where $\Delta[CO_3^{2-}]_{aragonite}$ > 70 μmol kg^{-1} (Fig. 2.6d) and, as for *C. wuellerstorfi*, were not included in the following discussion as the aim of this study is to provide Mg/Ca temperature calibrations where BWT is the main driver of Mg/Ca variability and $\Delta[CO_3^{2-}]_{aragonite}$ exerts a minimal influence on Mg/Ca ratios. We also did not consider 20 samples corresponding to BWT <3 °C, as the carbonate ion effect on *H. elegans* Mg/Ca ratios below 3 °C is unclear. We therefore recalculated equation (21) for the BWT range from 3 to 12 °C and obtained the following exponential equation (Fig. 2.6c):

Indo+Pacific Ocean

$$Mg/Ca = (0.43 \pm 0.07) \exp^{(0.1 \pm 0.01\ BWT)} \quad (22)$$

(R^2 = 0.42; n = 110; p<0.0001)

We calculated ΔMg/Ca based on published BWT and equation (22) over the whole temperature range from 2 to 12 °C and found low correlation (R^2 < 0.2) between ΔMg/Ca and $\Delta[CO_3^{2-}]_{aragonite}$ below or above 15 μmol kg^{-1} (Fig. 2.6e), or below or above 3 °C (Fig. 2.6f). This may reflect that $\Delta[CO_3^{2-}]_{aragonite}$ sensitivity to BWT is generally low (Fig. 2.6d) and/or may be biased by the fact that below 3 °C *H. elegans* Mg/Ca measurements are scarce (Fig. 2.6c). However, the standard deviation of the difference between the calculated and measured temperature is relatively high (±2.2 °C) for equation (22) used to calculate ΔMg/Ca.

When we extend the temperature range of equation (22) down to 2 °C, we obtain the following exponential equation (Fig. 2.6c):

Indo+Pacific

$$Mg/Ca = (0.31 \pm 0.06) \exp^{(0.14 \pm 0.01\ BWT)} \quad (23)$$

(R^2 = 0.61; n = 130; p<0.0001)

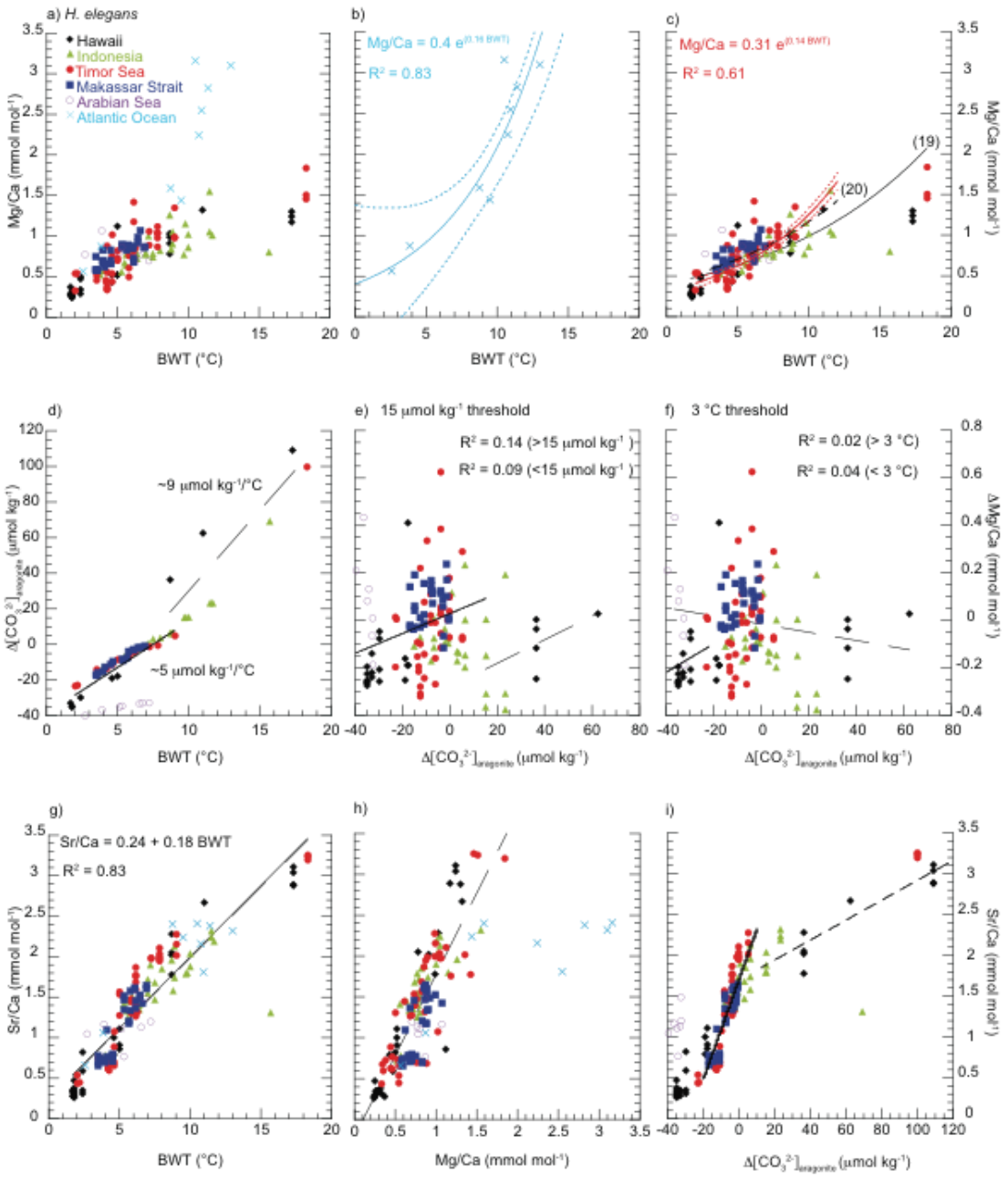

Fig. 2.6. a) Comparison between published and new *H. elegans* Mg/Ca measurements, spanning the BWT range from 2 to 18 °C. An offset is evident between samples from the Atlantic Ocean and samples from the Indian and Pacific Oceans. **b)** Calibration of *H. elegans* Mg/Ca ratios versus BWT for the Atlantic Ocean (solid blue curve). Dashed lines mark the 95% confidence interval. **c)** *Hoeglundina elegans* Mg/Ca ratios versus BWT for the Indian and Pacific Oceans. Red curve represents *H. elegans* Mg/Ca temperature calibration for the BWT range from 2 to 12 °C; dashed red lines mark the 95% confidence interval. Black and dashed black curves represent equations (19) and (20), respectively. **d)** $\Delta[CO_3^{2-}]_{aragonite}$ sensitivity to BWT. Solid black line represents the relationship for the Indo-Pacific data below 15 µmol kg^{-1}; dashed black line represents the relationship for the Indo-Pacific data above 15 µmol kg^{-1}. No data are available for the Atlantic Ocean. **e)** *Hoeglundina elegans* Mg/Ca sensitivity to $\Delta[CO_3^{2-}]_{aragonite}$. No correlation above or below 15 µmol kg^{-1} indicates negligible carbonate ion effect on *H. elegans* Mg/Ca ratios for the selected dataset. **f)** *Hoeglundina elegans* Mg/Ca sensitivity to $\Delta[CO_3^{2-}]_{aragonite}$. No correlation above or below 3 °C indicates negligible carbonate ion effect on *H. elegans* Mg/Ca ratios for the selected dataset. **g)** *Hoeglundina elegans* Sr/Ca sensitivity to BWT; solid black line represents the relationship between Sr/Ca ratios and BWT for the compiled set of data, while the dashed black line represents the same relationship for the Indo-Pacific samples only. **h)** *Hoeglundina elegans* Sr/Ca versus Mg/Ca ratios. Variations in Mg/Ca and Sr/Ca ratios are positively correlated in the Indo-Pacific Ocean (dashed line), suggesting that BWT controls both Mg and Sr uptake in *H. elegans* tests. It is unclear why Sr/Ca ratios in the Atlantic Ocean do not increase with increasing Mg/Ca ratios at higher BWT. **i)** *Hoeglundina elegans* Sr/Ca sensitivity to $\Delta[CO_3^{2-}]_{aragonite}$.

The consistent distribution of *H. elegans* Mg/Ca ratios along calibration equation (23) and significant correlation (R^2 = 0.61; p<0.0001) suggest temperature exerts a main control on *H. elegans* Mg/Ca variability (Fig. 2.6c). Applying equation (22) or (23) to estimate BWT leads to similar results, with a small offset of ±0.65 °C, above 3 °C. However, the offset between BWT estimates increases up to 3 °C below 3 °C.

2.4.2.3 Controls on *H. elegans* Sr/Ca variability

We calculated the relationship between *H. elegans* Sr/Ca ratios and BWT for the compiled dataset without discriminating between sample provenance (on account of the limited number of measurements in the Atlantic Ocean) and obtained the following linear equation (Fig 6g):

Compiled dataset

$$Sr/Ca = (0.24 \pm 0.05) + (0.18 \pm 0.007)\ BWT \quad (24)$$

(R^2 = 0.83; n = 147; p<0.0001)

We found high correlation (R^2 >0.8) between Sr/Ca and BWT, most likely due to the aragonitic mineralogy of *H. elegans* tests, since Sr^{2+} has a better fit in the aragonitic lattice than in the calcitic one [e.g.: *Rosenthal et al.,* 2006]. Additionally, no change in the slope of the relationship between *H. elegans* Sr/Ca ratios and BWT over the temperature range from 2 to 18 °C (Fig. 2.6g) suggests that BWT drives Sr/Ca variability in *H. elegans* tests. Only the shallow sample from Indonesia (MC037, *Rosenthal et al.* [2006]) departs from the main trend. Furthermore, *H. elegans* Mg/Ca and Sr/Ca ratios are positively and significantly correlated (R^2 = 0.74) for the Indo+Pacific samples, suggesting that BWT controls the variability of both parameters (Fig. 2.6h). In contrast, in the Atlantic Ocean, Mg/Ca and Sr/Ca ratios are positively correlated at lower BWT, fitting together with the Indo+Pacific samples,

whereas at higher BWT *H. elegans* Sr/Ca ratios do not increase with Mg/Ca ratios (Fig. 2.6h). The reason for this discrepancy is unclear and more measurements from the Atlantic Ocean are needed to better define the relationship between *H. elegans* Mg/Ca, Sr/Ca and BWT. We additionally examined the relationship between $\Delta[CO_3^{2-}]_{aragonite}$ and *H. elegans* Sr/Ca ratios (Fig. 2.6i). Changes in the slope of this relationship suggest that $\Delta[CO_3^{2-}]_{aragonite}$ does not drive *H. elegans* Sr/Ca variability (Fig. 2.6i). Below -20 μmol kg^{-1}, we found no correlation between *H. elegans* Sr/Ca ratios and $\Delta[CO_3^{2-}]_{aragonite}$, although different sensitivities of *H. elegans* Sr/Ca ratios to $\Delta[CO_3^{2-}]_{aragonite}$ are found between -20 and 15 μmol kg^{-1} and above 15 μmol kg^{-1} (Fig. 2.6i).

2.4.3 Robustness of paleotemperature proxies: benthic $\delta^{18}O$ versus benthic Mg/Ca ratios

To test the reliability of Mg/Ca temperature equations, we compared calcification temperatures derived from Mg/Ca ratios with those derived from $\delta^{18}O$ measurements. These two independent methods yielded comparable results, providing good approximations of CTD-measured temperatures (Fig. 2.7a and b). For *C. wuellerstorfi*, the difference between CTD-measured and $\delta^{18}O$-derived temperature (equation (10)) (ΔT = CTD-measured BWT – $\delta^{18}O$-derived temperature) shows a standard error of ± 0.83 °C in the Timor Sea and Makassar Strait. In contrast, the difference between CTD-measured and Mg/Ca-based temperatures shows a standard error of ± 0.77 °C for the Atlantic Ocean (equation (14)), and of ± 1.5 °C for the Ind+Pac area (equation (15)) (Fig. 2.7a). The higher standard error found for Ind+Pac BWT estimates probably relates to the scarcity of Mg/Ca measurements above 2 °C,

as 58 Mg/Ca samples were measured for the temperature range from 0.8 to 2 °C and 70 cover the whole range from 2 to 10 °C (Fig. 2.5c).

For *H. elegans*, the difference between CTD-measured and $\delta^{18}O$-derived temperatures (equation (11)) shows a standard error of ± 1 °C, whereas the difference with Mg/Ca-based temperatures shows a standard error of ± 1.1 °C for the Atlantic Ocean (equation (20)), and a standard error of ± 1.9 °C for the Indo+Pacific Ocean (equation (23)) (Fig. 2.7b). The higher standard error found for Indo+Pacific BWT estimates is most likely due to the high number of Mg/Ca measurements and their associated natural variability (n = 130) compared to the limited number of samples for the Atlantic Ocean (n = 9), and the Timor Sea and Makassar Strait (n = 35).

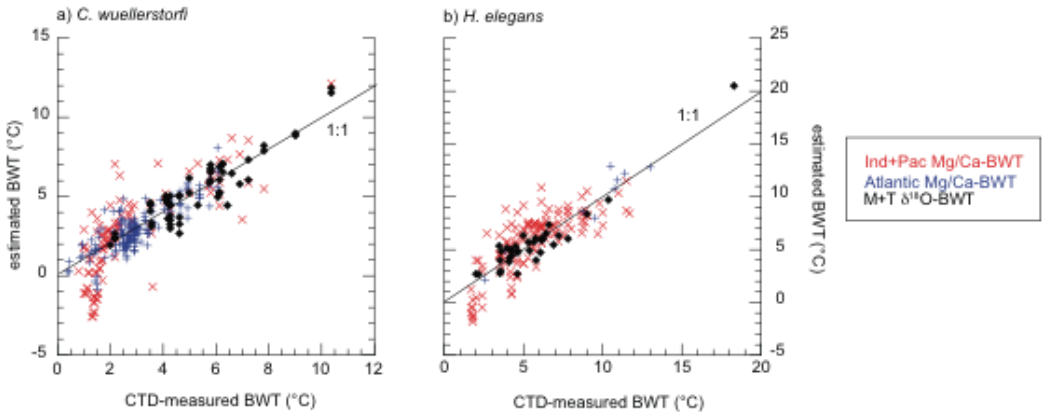

Fig. 2.7. a) CTD-measured BWT versus BWT estimates based on *C. wuellerstorfi* Mg/Ca ratios (red crosses Ind+Pac data, blue crosses Atlantic data), and $\delta^{18}O$ measurements (black diamonds). **b)** CTD-measured BWT versus BWT estimates based on *H. elegans* Mg/Ca ratios (red crosses Indo-Pacific data, blue crosses Atlantic data), and $\delta^{18}O$ measurements (black diamonds).

2.5. Conclusion

Compiling new *C. wuellerstorfi* Mg/Ca measurements with published data, we extended the Mg/Ca temperature calibration for this species to 10 °C. Exponential equations (14) and (15) best describe the relationship between temperature and *C. wuellerstorfi* Mg/Ca ratios for the Atlantic Ocean and for the Indian and Pacific

Oceans, respectively. Our study indicates that temperature rather than $\Delta[CO_3^{2-}]_{calcite}$ controls *C. wuellerstorfi* Mg/Ca variability in the selected Atlantic Ocean dataset (0 to 6 °C) and Ind+Pac dataset (0 to 10 °C). *Cibicidoides wuellerstorfi* Sr/Ca ratios show high potential to record past changes in carbonate ion saturation, as $\Delta[CO_3^{2-}]_{calcite}$ appears to drive *C. wuellerstorfi* Sr/Ca variability. Distinct *C. wuellerstorfi* Sr/Ca-$\Delta[CO_3^{2-}]_{calcite}$ relationships are found for the different ocean basins, which may be due to the higher "corrosiveness" of Indian and Pacific waters.

Combining new *H. elegans* Mg/Ca measurements with published data, we provided temperature calibration equations over the temperature range from 2 to 12 °C. Exponential equations (20) and (23) best describe the relationship between *H. elegans* Mg/Ca ratios and BWT for the Atlantic Ocean and the Indo+Pacific Ocean, respectively. In highly supersaturated waters with respect to aragonite ($\Delta[CO_3^{2-}]_{aragonite}$ > 70 μmol kg^{-1}), Mg/Ca depletion in *H. elegans* tests was observed. *Hoeglundina elegans* Sr/Ca variability appears to be driven by BWT, most likely because of the aragonitic mineralogy of this benthic foraminiferal species, since Sr^{2+} has a better fit in the aragonitic lattice than in the calcitic one. No geographical trend in the distribution of Sr/Ca ratios in relation to BWT is apparent between the Atlantic and Indo+Pacific Oceans, possibly because Sr/Ca ratios in the Atlantic Ocean do not increase with increasing Mg/Ca ratios at higher BWT.

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Appendix. Taxonomic Information

Cibicidoides wuellerstorfi (Schwager), 1866

Original Designation: *Anomalina wuellerstorfi* Schwager, 1866, p. 258, pl.7, figs. 105-107.

Hoeglundina elegans (d'Orbigny), 1826

Original designation: *Rotalia (Turbinulina) elegans* d'Orbigny, 1826, p. 276, Model No. 54, illustrated in Parker et al., 1871, pl. 12, fig. 142.

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2.6 Auxiliary Material

Auxiliary Table 2.1. *C. wuellerstorfi* results

Station	Water Depth, m	BWT, °C	$\Delta[CO_3]_{calcite}$ µmol kg^{-1}	$\delta^{18}O_{sw}$ vs SMOW	*C. wuellerstorfi* Mg/Ca, mmol mol^{-1}	*C. wuellerstorfi* Sr/Ca, mmol mol^{-1}	*C. wuellerstorfi* $\delta^{18}O$ vs VPDB	*C. wuellerstorfi* $\delta^{18}O - \delta^{18}O_{sw}$ vs VPDB
				Timor Sea				
18503	354	10.37	40.89	-0.05	4.15	1.52	0.67	0.99
18503	354	10.37	40.89	-0.05			0.74	1.06
18489	431	9.01	32.31	-0.05			1.3	1.62
18489	431	9.01	32.31	-0.05			1.33	1.65
18488	555	7.82	27.40	-0.03	1.64	1.35	1.49	1.79
18488	555	7.82	27.40	-0.03	3.96	1.33	1.56	1.86
18493	599	7.23	26.75	-0.04	2.51	1.44	1.68	1.99
18493	599	7.23	26.75	-0.04	1.72	1.39	1.96	2.27
18469	704	6.25	25.42	0.03			1.91	2.15
18469	704	6.25	25.42	0.03			1.81	2.05
18469	704	6.25	25.42	0.03			1.8	2.04
18501	742	6.13	24.59	-0.06	2.11	1.35	2.12	2.44
18501	742	6.13	24.59	-0.06	1.56	1.40	2.13	2.45
18501	742	6.13	24.59	-0.06	1.41	1.31	1.94	2.27
18501	742	6.13	24.59	-0.06	2.23	1.43	1.76	2.09
18468	803	5.80	22.52	0.01	1.84	1.35	2.02	2.28
18468	803	5.80	22.52	0.01	1.59	1.34	1.8	2.06
18468	803	5.80	22.52	0.01			1.91	2.17
18468	803	5.80	22.52	0.01			1.88	2.14
18468	803	5.80	22.52	0.01			1.85	2.11
18467	899	4.99	20.93	0.00	1.91	1.35	2.17	2.45
18467	899	4.99	20.93	0.00	1.58	1.36	1.97	2.24

Auxiliary Table 2.1. (continued)

Station	Water Depth, m	BWT, °C	$\Delta[CO_3]_{calcite}$ µmol kg^{-1}	$\delta^{18}O_{sw}$ vs SMOW	*C. wuellerstorfi* Mg/Ca, mmol mol^{-1}	*C. wuellerstorfi* Sr/Ca, mmol mol^{-1}	*C. wuellerstorfi* $\delta^{18}O$ vs VPDB	*C. wuellerstorfi* $\delta^{18}O$ - $\delta^{18}O_{sw}$ vs VPDB
18466	1004	4.62	19.91	-0.02	2.20	1.41	2.5	2.79
18466	1004	4.62	19.91	-0.02			2.72	3.01
18466	1004	4.62	19.91	-0.02			2.59	2.88
18465	1082	4.61	19.13	-0.03			2.19	2.49
18465	1082	4.61	19.13	-0.03			2.18	2.48
18500	1167	4.10	18.28	-0.10	1.57	1.37	2.17	2.54
18500	1167	4.10	18.28	-0.10	1.47	1.36	2.18	2.55
18500	1167	4.10	18.28	-0.10			2.12	2.49
18464	1206	4.26	18.02	-0.09	1.36	1.33	2.46	2.83
18464	1206	4.26	18.02	-0.09			2.26	2.63
18464	1206	4.26	18.02	-0.09			2.13	2.49
18464	1206	4.26	18.02	-0.09			2.53	2.89
18463	1311	4.18	17.80	-0.09			2.44	2.80
18463	1311	4.18	17.80	-0.09			2.2	2.56
18463	1311	4.18	17.80	-0.09			2.23	2.59
18499	1383	3.51	17.64	0.00	1.44	1.36	2.43	2.70
18499	1383	3.51	17.64	0.00	1.17	1.36	2.34	2.61
18499	1383	3.51	17.64	0.00			2.32	2.59
18499	1383	3.51	17.64	0.00			2.33	2.60
18462	1422	4.26	17.55	-0.09			2.58	2.94
18462	1422	4.26	17.55	-0.09			2.4	2.76
18462	1422	4.26	17.55	-0.09			2.25	2.61
18478	1769	3.56	16.60	-0.13	1.11	1.27	2.52	2.92

Auxiliary Table 2.1. (continued)

Station	Water Depth, m	BWT, °C	$\Delta[CO_3]_{calcite}$ µmol kg^{-1}	$\delta^{18}O_{sw}$ vs SMOW	*C. wuellerstorfi* Mg/Ca, mmol mol^{-1}	*C. wuellerstorfi* Sr/Ca, mmol mol^{-1}	*C. wuellerstorfi* $\delta^{18}O$ vs VPDB	*C. wuellerstorfi* $\delta^{18}O - \delta^{18}O_{sw}$ vs VPDB
18478	1769	3.56	16.60	-0.13			2.47	2.87
18506	2410	2.17	14.14	-0.15	2.04	1.21	2.65	3.08
18506	2410	2.17	14.14	-0.15	1.21	1.23	2.66	3.08
18506	2410	2.17	14.14	-0.15	0.90	1.27	2.65	3.07
18506	2410	2.17	14.14	-0.15			2.59	3.01
18507	2450	2.00	13.96	-0.16	1.42	1.23	2.74	3.18
18507	2450	2.00	13.96	-0.16	1.01	1.26		
18507	2450	2.00	13.96	-0.16	1.12	1.23		
				Makassar Strait				
18534	563	6.90	27.11	-0.14	2.22	1.35	1.91	2.32
18518	620	6.43	26.55	-0.27	2.12	1.38	2.08	2.62
18532	629	6.60	26.51	-0.14	2.57	1.42	1.77	2.18
18517	699	6.14	25.63	-0.28	1.73	1.39		
18545	707	6.07	25.47	-0.16	1.87	1.39	2.08	2.51
18541	739	5.75	24.74	-0.14	1.68	1.40	1.90	2.31
18541	739	5.75	24.74	-0.14	1.69	1.37		
18530	876	5.31	21.09	-0.15	2.05	1.39	2.20	2.62

Red values represent samples not included in this study

Auxiliary Table 2.2. *H. elegans* results

Station	Water Depth, m	BWT, °C	$\Delta[CO_3]_{aragonite}$ µmol kg^{-1}	$\delta^{18}O_{sw}$ vs SMOW	*H. elegans* Mg/Ca, mmol mol^{-1}	*H. elegans* Sr/Ca, mmol mol^{-1}	*H. elegans* $\delta^{18}O$ vs VPDB	*H. elegans* $\delta^{18}O$ - $\delta^{18}O_{sw}$ vs VPDB
				Timor Sea				
18454	131	18.30	99.83	0.20	1.84	3.20	-0.20	-0.13
18454	131	18.30	99.83	0.20	1.51	3.24		
18454	131	18.30	99.83	0.20	1.46	3.26		
18503	354	10.37	13.98	-0.05			2.35	2.67
18489	431	9.01	5.08	-0.05	1.35	2.02	2.70	3.02
18489	431	9.01	5.08	-0.05	0.98	2.28		
18489	431	9.01	5.08	-0.05	0.99	2.16		
18488	555	7.82	-0.36	-0.03	0.87	1.95	3.33	3.63
18488	555	7.82	-0.36	-0.03	1.12	2.11		
18488	555	7.82	-0.36	-0.03	1.04	2.04		
18488	555	7.82	-0.36	-0.03	0.98	2.00		
18488	555	7.82	-0.36	-0.03	1.04	1.98		
18493	599	7.23	-1.2	-0.04	1.06	1.98	3.25	3.56
18493	599	7.23	-1.2	-0.04	0.89	1.99		
18469	704	6.25	-2.97	0.03	0.86	1.32	3.39	3.63
18469	704	6.25	-2.97	0.03				
18501	742	6.13	-3.97	-0.06	1.42	1.78	3.34	3.67
18501	742	6.13	-3.97	-0.06	0.85	1.87		
18501	742	6.13	-3.97	-0.06	0.68	1.27		
18501	742	6.13	-3.97	-0.06	0.74	1.40		
18501	742	6.13	-3.97	-0.06	0.84	1.60		
18501	742	6.13	-3.97	-0.06	0.82	1.69		

Auxiliary Table 2.2. (continued)

Station	Water Depth, m	BWT, °C	$\Delta[CO_3]_{aragonite}$ µmol kg^{-1}	$\delta^{18}O_{sw}$ vs SMOW	*H. elegans* Mg/Ca, mmol mol^{-1}	*H. elegans* Sr/Ca, mmol mol^{-1}	*H. elegans* $\delta^{18}O$ vs VPDB	*H. elegans* $\delta^{18}O$ - $\delta^{18}O_{sw}$ vs VPDB
18501	742	6.13	-3.97	-0.06	1.18	1.76		
18468	803	5.80	-6.31	0.01	0.61	1.45	3.90	4.16
18468	803	5.80	-6.31	0.01	0.76	1.48		
18468	803	5.80	-6.31	0.01	0.5	1.31		
18467	899	4.99	-8.33	0.00	0.7	1.28	3.28	3.55
18467	899	4.99	-8.33	0.00	0.82	1.57		
18467	899	4.99	-8.33	0.00	0.73	1.54		
18466	1004	4.62	-9.82	-0.02	1.02	1.08	4.21	4.50
18466	1004	4.62	-9.82	-0.02				
18466	1004	4.62	-9.82	-0.02				
18465	1082	4.61	-10.96	-0.03	0.76	0.7	3.67	3.97
18465	1082	4.61	-10.96	-0.03	0.54	0.66		
18465	1082	4.61	-10.96	-0.03	0.44	0.89		
18500	1167	4.10	-12.21	-0.10			3.74	4.11
18500	1167	4.10	-12.21	-0.10				
18464	1206	4.26	-12.65	-0.09	0.88	0.69	3.57	3.93
18464	1206	4.26	-12.65	-0.09	0.56	0.67		
18464	1206	4.26	-12.65	-0.09	0.34	0.68		
18464	1206	4.26	-12.65	-0.09	0.38	0.73		
18464	1206	4.26	-12.65	-0.09	0.35	0.60		
18463	1311	4.18	-13.36	-0.09	0.46	0.62	3.54	3.90
18463	1311	4.18	-13.36	-0.09	0.44	0.63		
18499	1383	3.51	-13.87	0.00	0.52	0.74	3.89	4.16

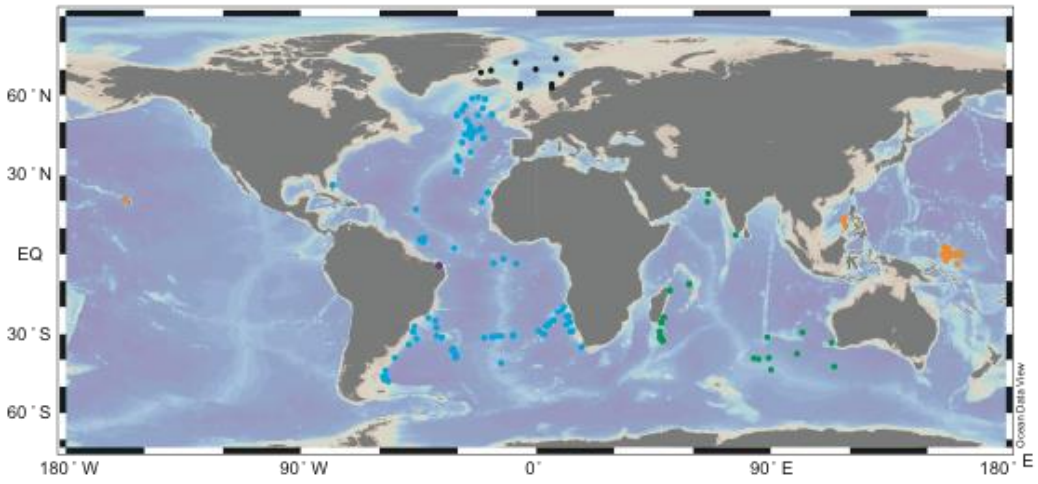
Auxiliary Table 2.2. (continued)

Station	Water Depth, m	BWT, °C	$\Delta[CO_3]_{aragonite}$ µmol kg^{-1}	$\delta^{18}O_{sw}$ vs SMOW	*H. elegans* Mg/Ca, mmol mol^{-1}	*H. elegans* Sr/Ca, mmol mol^{-1}	*H. elegans* $\delta^{18}O$ vs VPDB	*H. elegans* $\delta^{18}O$ - $\delta^{18}O_{sw}$ vs VPDB
18499	1383	3.51	-13.87	0.00	0.46	0.77		
18462	1422	4.26	-14.15	-0.09			3.69	4.05
18462	1422	4.26	-14.15	-0.09				
18478	1769	3.56	-16.82	-0.13			4.02	4.42
18506	2410	2.17	-22.71	-0.15	0.54	0.45	4.09	4.51
18506	2410	2.17	-22.71	-0.15				
18506	2410	2.17	-22.71	-0.15				
18507	2450	2.00	-23.12	-0.16	0.54	0.54	4.07	4.50
18507	2450	2.00	-23.12	-0.16	0.33	0.44		
18507	2450	2.00	-23.12	-0.16				
				Makassar Strait				
18534	563	6.90	-0.66	-0.14	2.45	1.09	3.37	3.78
18534	563	6.90	-0.66		0.87	1.65		
18534	563	6.90	-0.66		0.86	1.61		
18518	620	6.43	-1.48	-0.27	0.99	1.53	2.96	3.50
18518	620	6.43	-1.48		0.92	1.49		
18532	629	6.60	-1.6	-0.14	1.07	1.43	2.88	3.29
18517	699	6.14	-2.84	-0.28	0.68	1.37	3.08	3.63
18517	699	6.14	-2.84		0.73	1.46		
18545	707	6.07	-3.05	-0.16	0.88	1.60	3.54	3.97
18545	707	6.07	-3.05		0.85	1.62		
18541	739	5.75	-3.89	-0.14	0.89	1.34	3.21	3.62
18541	739	5.75	-3.89		0.88	1.58		

Auxiliary Table 2.2. (continued)

Station	Water Depth, m	BWT, °C	$\Delta[CO_3]_{aragonite}$ µmol kg^{-1}	$\delta^{18}O_{sw}$ vs SMOW	*H. elegans* Mg/Ca, mmol mol^{-1}	*H. elegans* Sr/Ca, mmol mol^{-1}	*H. elegans* $\delta^{18}O$ vs VPDB	*H. elegans* $\delta^{18}O$ - $\delta^{18}O_{sw}$ vs VPDB
18536	836	5.65	-7.44	-0.18	0.83	1.21	3.26	3.71
18536	836	5.65	-7.44		0.87	1.18		
18536	836	5.65	-7.44		0.88	1.18		
18530	876	5.31	-8	-0.15	0.9	1.35	3.30	3.72
18530	876	5.31	-8		0.86	1.47		
18530	876	5.31	-8		0.88	1.52		
18537	929	5.38	-8.75	-0.24	0.83	1.20	3.41	3.92
18522	974	4.67	-9.39	-0.07	0.9	1.50	3.60	3.94
18531	1086	4.50	-11.01	-0.15	0.7	0.80	3.40	3.82
18531	1086	4.50	-11.01		0.66	0.79		
18531	1086	4.50	-11.01		0.83	0.71		
18531	1086	4.50	-11.01		0.66	0.77		
18540	1200	4.09	-12.61	-0.41	0.66	0.77	3.52	4.20
18540	1200	4.09	-12.61		0.62	1.10		
18526	1538	3.95	-15	-0.20	0.83	0.70	3.39	3.86
18526	1538	3.95	-15		0.68	0.71		
18526	1538	3.95	-15		0.7	0.73		
18527	1615	3.61	-15.59	-0.17	0.69	0.64	3.50	3.94
18527	1615	3.61	-15.59		0.58	0.72		
18527	1615	3.61	-15.59		0.59	0.75		
18528	1785	3.47	-16.96	0.02	0.58	0.70	3.56	3.81
18528	1785	3.47	-16.96		0.59	0.66		
18528	1785	3.47	-16.96		0.75	0.78		
18525	1822	3.52	-17.26	-0.66	0.5	0.73	3.55	4.48

Red values represent samples not included in this study



Auxiliary Figure 2.1. Locations of published core top samples