

1 **Modern sea surface productivity and temperature estimations**
2 **off Chile as detected by coccolith accumulation rates**

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11
12 **Abstract**
13

14 Recent coccoliths from 74 surface sediment samples recovered from the southeastern
15 Pacific off Chile were examined quantitatively to investigate modern regional gradients
16 of sea surface productivity and temperature. All findings are based on coccolith
17 accumulations rates. Therefore an approach was designed to estimate recent
18 sedimentation rates based on ^{210}Pb and bulk chemistry analyses of the same set of surface
19 samples. Highest total coccolith accumulation rates were found off north-central Chile,
20 where seasonal upwelling takes place. Based on a multiple linear regression between
21 calculated coccolith accumulation rates and World Ocean Atlas derived sea surface
22 temperatures, a calibration model to reconstruct annual average temperatures of the
23 uppermost 75 m of the water column is provided. The model was cross-validated and the
24 SST estimates were compared with SST observed and SST estimates based on diatoms
25 and planktic foraminifera, showing a good correlation.

26

27 **1. Introduction**

28

29 Coccolithophores, one of the main open ocean primary producers, have a broad fossil
30 record, which makes them an outstanding biostratigraphical group and gives them
31 potential for paleontological study of ecosystem response to global change. As a basic
32 requisite for their application as paleoceanographic proxies it is necessary to maximize
33 the retrieval of paleoecological information from coccolithophore species, and to enhance
34 the understanding of their ecology as a plankton group. Knowing how the present-day
35 environment influences their spatial and temporal distribution, we could use the fossil
36 record of such organisms to reconstruct the state and variation of past environments
37 (Kucera et al., 2005).

38 One of the modern ocean's most productive upwelling conditions occur all along the
39 Chilean margin (Strub et al., 1998; Abrantes et al., 2007). In coastal upwelling domains,
40 the dominant primary producers are diatoms, although coccolithophores are also
41 significant contributors to the total phytoplankton community (e.g., Mitchell-Innes and
42 Winter, 1987; Giraudeau et al., 2000; Boeckel and Baumann, 2004). However, there are
43 very few modern studies on coccolithophores ecology and calibration to climate proxies
44 in the Southeast (SE) Pacific, and most of them are based on plankton samples (e.g.,
45 Beaufort et al., 2007; Beaufort et al., 2008; Beaufort et al., 2011) or on sediment trap
46 samples (e.g., González et al., 2004; Köbrich, 2008). So far, only a small number of
47 surface sediment studies were performed by Saavedra-Pellitero et al. (i.e., 2010; 2011). In
48 such studies the ecological optima of the most important species of coccolithophores in

49 the Pacific sector was studied in order to produced feasible transfer functions to
50 reconstruct climate changes in the past. In this work the focus was on coccolithophore
51 surface sediment assemblages since they represent the former living communities and
52 with that, the overlying surface water conditions (Andruleit et al., 2004). While relative
53 abundances indicate dominance of a certain ecological habitat, absolute fluxes represent
54 more realistic living conditions in the water column, thus providing a more detailed
55 reconstruction of hydrography (Ravelo et al., 1990). Coccolith accumulation rate (CAR)
56 data could furthermore complement and in some cases improve upon the relative
57 abundance data, whereas also comparing with modern flux estimates derived from
58 sediment trap studies.

59

60 The estimation of past environmental parameters using micropaleontological data has
61 become a very useful tool from the development of statistical transfer function techniques
62 (IKM - Imbrie and Kipp Method) in which the authors originally used planktonic
63 foraminifera (Imbrie and Kipp, 1971; Klován and Imbrie, 1971). It provides quantitative
64 estimations of hydrographical parameters (e.g., sea surface temperature, SST) preserved
65 in the recent sedimentary record (e.g., CLIMAP 1976, 1981, Ortiz and Mix 1997, Pisias
66 et al., 1997; Mix et al., 1999; Kucera et al., 2005; Morey et al., 2005; Abrantes et al.,
67 2007). Different statistical techniques were already applied to coccolith census counts
68 from surface sediments of the North and Equatorial Pacific (Geitzenauer et al., 1977;
69 Roth and Coulbourn, 1982; Roth, 1994), of the North Atlantic (Geitzenauer et al., 1977)
70 as well as of the Benguela upwelling system (Giraudeau and Rogers, 1994). However the
71 different sample coverage, the different taxonomies (of traditional broad species) as well

72 as the exclusion of species in some of those investigations prevented any transfer function
73 to be properly defined. Consequently, a well established calibration of modern
74 coccolithophore assemblages to surface mixed-layer temperatures has only been
75 previously achieved at a few locations. These were performed at the Benguela and the
76 Peru-Chile upwelling systems (Giraudeau and Rogers, 1994; Saavedra-Pellitero et al.,
77 2010; 2011) and differ from ours by being based on species relative abundances. The
78 main goal of the present study was to investigate whether the modern regional gradients
79 of sea surface productivity and temperature can be detected by studying (a) coccolith
80 accumulation rates and (b) coccolithophore derived temperature estimates.

81

82 **1.1. Regional setting**

83

84 The SE Pacific is dominated by the Peru-Chile current system (Strub et al., 1998), one of
85 the most productive eastern boundary systems in the world. Off southern Chile, cool
86 waters from the Antarctic Circumpolar Current reach the continent and split in two
87 branches, the southward-flowing Cape Horn Current and the northward-flowing Peru
88 Current (Fig. 1A). Coastal upwelling, driven by persistent southerly winds along the coast
89 brings cold and nutrient-rich waters to the sea surface along the coast of Chile and Peru
90 towards the equator (Wyrki, 1981; Bryden and Brady, 1985; Strub et al., 1998).
91 Phytoplankton biomass is high throughout the year in this coastal upwelling system
92 (Rojas de Mendiola, 1981). However, from 15°S to 30°S, minimum chlorophyll
93 seasonality offshore Chile is observed, despite strong seasonality in wind forcing between
94 20°S and 30°S. South of this area, chlorophyll reaches maxima during austral summer

95 and minima in austral winter, in phase with the seasonal wind forcing (Thomas et al.,
96 2004).
97 Precipitation patterns in Chile, the most important climate factor driving continental
98 erosion, show one of the most pronounced latitudinal gradients on Earth (Kaiser, 2005;
99 Hebbeln et al., 2007). Rainfall rates rapidly increases from almost zero in the hyper-arid
100 Atacama desert (north of 27°S) over intermediate precipitation in the semi-arid
101 Mediterranean-type climate of central Chile (from 31°S to 37°S) to year round humid
102 conditions with extraordinary high annual precipitation south of 42°S (Miller, 1976; New
103 et al., 2002). Major atmospheric circulation patterns, specifically the SE Pacific
104 anticyclone in the north and the rain-bearing Southern Westerlies in the south, are
105 responsible for this marked N-S gradient along Chile (Hebbeln et al., 2007, see Fig. 1B).
106 However, expected differences in mass accumulation rates along the Chilean continental
107 margin depend not only on the different hydrological regimes, but also on the topography
108 of margin and on the latitudinal variability of primary productivity and upwelling (Muñoz
109 et al., 2004).

110

111 **2. Material and Methods**

112

113 For this study we considered 74 out of 106 surface sediment samples located from
114 22.80°S to 44.28°S and from 70.49°W to 75.86°W offshore Chile. Previous studies
115 (Saavedra-Pellitero et al., 2010; 2011) allowed us to select the best preserved samples and
116 to exclude the samples where coccoliths were poorly preserved. The uppermost
117 centimetre from the undisturbed surface sediment samples (boxcores and multicores), has

118 been used for the analyses reported here. They were retrieved during Genesis III Cruise,
119 RR9702A onboard the American R/V Roger Revelle and during R/V SONNE Cruise SO-
120 156 Valparaiso-Talcahuano (Hebbeln and cruise participants, 2001) onboard the German
121 R/V Sonne.

122

123 **2.1. Coccolith counts and estimations of CARs**

124 Coccolith absolute abundance counts were already available from a previous study
125 (Saavedra-Pellitero et al., 2010) although only relative abundances were published in that
126 paper. Slides for coccolith counts were prepared using the standard settling methodology
127 of Flores and Sierro (1997). Coccolith identification was done using a Leica DMRXE and
128 a Nikon Eclipse 80i polarized microscopes at a magnification of X1000, occasionally
129 X1250. In order to ensure statistical reliability a minimum of 400 coccoliths per sample
130 were counted. This procedure allowed us to estimate the total number of coccoliths per
131 gram of sediment for each of the coccolithophore species and species CARs. We
132 followed the taxonomy established by Hine and Weaver (1998), Bown and Young (1998)
133 and the internet site www.nannotax.org. Some additional considerations were also taken
134 into account (i.e., the group of *Gephyrocapsa* <3µm defined by Flores et al., 1997). The
135 formula used to calculate CARs is:

$$136 \text{ CAR} = [(n \cdot R^2 \cdot V^2) / (r^2 \cdot g \cdot v)] \cdot DBD \cdot SR$$

137 where n is the number of coccoliths counted in a random light microscope scanned area;
138 R is the radius of the Petri dish used; V is the volume of the water added to the dry
139 sediment; r is the radius of the visual field used in the counting; g is the dry sediment

140 weight; v is the volume of mixture withdrawn with the micropipette; DBD is the
141 estimated dry density of the sediment, and SR is the linear sedimentation rate.

142

143

144 **2.2. Sedimentation rate estimates and dry bulk densities**

145

146 Sedimentation rates (SRs) and sediment dry bulk densities (DBD) are required to
147 estimate CARs. However the lack of these measurements for the majority of the samples
148 considered in this study led us to design an approach to estimate them. To calculate the
149 SR along the Chilean continental margin, we considered the recent SR data based on
150 ^{210}Pb (Muñoz et al., 2004; Fig. 2A) available from a subset of samples spanning across a
151 broad range of sedimentation regimes which correspond to some of the samples studied
152 here (Figs. 1B and 2, Table 1). Owing to the fact that the samples cover very distinct
153 areas and stations are quite sparsely distributed, we normalized the number of coccoliths
154 per gram of sediment instead of directly interpolating the SR data from Muñoz et al.
155 (2004; see Fig. 2). This designed approach consists of comparing the bulk chemistry
156 analyses done by inductively coupled plasma atomic emission spectrometry (ICP-MS,
157 Stuut et al., 2007), with the SR based on ^{210}Pb (Muñoz et al., 2004) using multiple
158 regression analysis. Mesh grids were created for Al, Fe, K, Mg, and Ti derived by ICP-
159 MS measurements with Matlab™ and the values for the 17 stations indicated in Table 1
160 were used for the calibration.

161

162 Stepwise multiple regression is a systematic method for choosing predictors (or
163 independent variables) of a particular dependent variable on the basis of statistical criteria
164 (Howitt and Cramer, 2008). This procedure determines which independent variable is the
165 best predictor, the second best predictor, etc. After regressing our independent or
166 predictor variables (Al, Fe, K, Mg, and Ti ICP-MS values, in our case) against the
167 dependent variable (SR, in our case) with Matlab™ software, we found out that only Ti is
168 positively correlated to SR ($R^2=0.61$, Fig. 2B and supplementary material). This
169 relationship reflects the recent sedimentation patterns on the Chilean continental slope. A
170 lack of significant precipitation limits the denudation in the Atacama Desert (Stuut et al.,
171 2007) restricting the sediment supply to the Chilean margin and therefore the high SRs
172 and Ti contents offshore North Chile. On the contrary, humid conditions and stronger
173 erosion in South Chile (Miller, 1976) favors the higher SR and Ti contents at the
174 southernmost surface sediment samples. The linear equation obtained allowed us to
175 estimate SR from Ti measurements for the specific case of the study area.

$$176 \quad SR=(0.1089 \cdot Ti)-0.274$$

177 This formula provided a way to estimate SR for the surface sediment samples studied
178 (Table 2, Fig. 3A) with a root mean squared error (RMSE) of 0.047 for the 64 samples
179 where ICP-MS were performed, all of them GeoB samples. Concerning the 10 non-GeoB
180 stations of the database (RR-), euclidean distances between each station and the GeoB
181 stations were calculated and the smallest one was chosen. For the four samples located
182 further offshore, different SR values were considered (Table 1).

183 To estimate sediment DBDs, the closest value from Muñoz et al. (2004) was chosen
184 (Table 1 for original measurements and Table 2 for estimates), except for the four further
185 offshore stations, where the same criteria as for SR was followed.

186

187 **2.3. Oceanographic variables of the surface waters**

188

189 The modern oceanographic properties chosen for this work are sea surface temperature
190 (SST in °C, Locarnini et al., 2006), sea surface salinity (SSS in PSU, Antonov et al.,
191 2006), nitrate (micromole/l), phosphate (micromole/l), silicate (micromole/l, all data from
192 Garcia et al., 2006) and chlorophyll concentrations (microgram/l, Levitus, 1982;
193 Conkright and Boyer, 2002) expressed as an annual average from 0 m to 75 m water
194 depth. In addition, depth of the mixing layer (m) and primary productivity (mg C/m²/day)
195 were considered. All these parameters were obtained from the World Ocean Atlas 2005,
196 from the World Ocean Atlas 2001 Data Sets, National Oceanographic Data Centre,
197 Washington DC (see <http://ingrid.ldgo.columbia.edu/SOURCES/.NOAA/.NODC>), and
198 from Ocean Productivity
199 (<http://www.science.oregonstate.edu/ocean.productivity/index.php>).

200 Euclidean distances between each station and World Ocean Atlas database (1° grid) were
201 calculated and the smallest one was chosen using Matlab™. All the contour maps were
202 generated using Ocean Data View (ODV) software (Schlitzer, 2011). The main model
203 was generated with R software (for further details see section 3.2) and ordination was
204 performed using the Vegan package for R (Oksanen et al., 2006).

205

206 **3. Results**

207 **3.1. Coccolith accumulation rates**

208

209 Maximum numbers of $2.21 \cdot 10^9$ coccoliths/g and highest CARs of $6.9 \cdot 10^7$
210 coccoliths/cm²/yr are reached at different locations in the northernmost stations while
211 minimum numbers of $2.10 \cdot 10^6$ coccoliths/g and CARs of $9.2 \cdot 10^4$ coccoliths/cm²/yr are
212 reached offshore southern Chile (44.06°S, 75.13°W, Fig. 3B, C).

213 The 14 most common taxa or groups of coccoliths regarded in this study are
214 *Calciosolenia* spp., *Calcidiscus leptoporus*, *Coccolithus pelagicus*, *Emiliana huxleyi*,
215 *Florisphaera profunda*, *Gephyrocapsa muellerae*, *Gephyrocapsa oceanica*,
216 *Helicosphaera carteri*, *Rhabdosphaera clavigera*, small *Gephyrocapsa* (*Gephyrocapsa*
217 <3µm), *Syracosphaera* spp., *Umbellosphaera* spp., *Umbilicosphaera* spp. and *Oolithotus*
218 spp. In the following we briefly describe the main features observed in the contour maps
219 (Fig. 4) ranging from highest CARs average to lowest ones for each coccolithophore taxa.
220 Small *Gephyrocapsa* is the most abundant group (average of $1.94 \cdot 10^6$ coccoliths/cm²/yr)
221 which reaches abundances of $1.69 \cdot 10^7$ coccoliths/cm²/yr at 26°S, although high numbers
222 are also recorded in other parts of the Chilean upwelling area (Fig. 4A). *C. leptoporus*
223 shows an average CAR of $1.48 \cdot 10^6$ coccoliths/cm²/yr. Maximum CARs of up to $1.5 \cdot 10^7$
224 coccoliths/cm²/yr for this species are reached in the samples located in the north of the
225 study area and decrease towards the South (Fig. 4B). An average of $1.3 \cdot 10^6$
226 coccoliths/cm²/yr was estimated for *F. profunda* (Fig. 4C). CARs for this lower photic
227 zone dweller fluctuates considerably, decreasing broadly southwards; maximum values
228 are reached at 26°S ($1.08 \cdot 10^7$ coccoliths/cm²) and minimum at the southernmost locations

229 offshore Chile ($8.59 \cdot 10^3$ coccoliths/cm²/yr). *E. huxleyi*, with an average of $1.21 \cdot 10^6$
230 coccoliths/cm²/yr, displays a similar distribution pattern to small *Gephyrocapsa* with
231 maximum CAR of $8.81 \cdot 10^6$ coccoliths/cm² (Fig. 4D).
232 *G. muelleriae* occurs in average CARs of $1.10 \cdot 10^6$ coccoliths/cm²/yr. This species
233 fluctuates along the Chilean upwelling region; it reaches a maximum of $7.42 \cdot 10^6$
234 coccoliths/cm²/yr in the northern part of the study area and high CARs at the
235 southernmost locations (Fig. 4E). *G. oceanica*, with an average of $1.08 \cdot 10^6$
236 coccoliths/cm²/yr, reaches maximum CARs ($9.74 \cdot 10^6$ coccoliths/cm²/yr) at the northern
237 part of the study area and progressively decreases southwards (Fig. 4F).
238 *H. carteri* shows average CARs of $5.24 \cdot 10^5$ coccoliths/cm²/yr. Maximum CARs of this
239 species are clearly reached in central and north offshore Chile ($6.19 \cdot 10^6$
240 coccoliths/cm²/yr, Fig. 4G). *C. pelagicus* reaches average CARs of $9.73 \cdot 10^4$
241 coccoliths/cm²/yr and its maxima ($7.19 \cdot 10^5$ coccoliths/cm²/yr) at the southernmost
242 locations of the Chilean upwelling (Fig. 4H). *Umbellosphaera* spp. shows average CARs
243 of $8.86 \cdot 10^3$ coccoliths/cm²/yr with maximum of $2.47 \cdot 10^5$ coccoliths/cm²/yr (Fig. 4I).
244 Results corresponding to the rest of the coccolithophore species are not listed here either
245 owing to their low numbers or to the non-relevance for the SST estimates. This refers to
246 *Syracosphaera* spp. (average of $3.67 \cdot 10^4$ coccoliths/cm²/yr), *Oolithotus* spp. (average of
247 $1.98 \cdot 10^4$ coccoliths/cm²/yr), *Umbilicosphaera* spp. (average of $1.06 \cdot 10^5$
248 coccoliths/cm²/yr), *R. clavigera* (average of $5.19 \cdot 10^3$ coccoliths/cm²/yr) and
249 *Calciosolenia* spp. (average of $4.18 \cdot 10^3$ coccoliths/cm²/yr).

250

251 **3.2. Statistical analysis and SST transfer function**

252 A preliminary detrended correspondence analysis (DCA) on the coccolithophore
 253 assemblage resulted in a gradient shorter than 2 Standard Deviation (SD) units,
 254 suggesting a linear response (ter Braak, 1987). Then, principal component analysis (PCA)
 255 was used to analyze the relationship between coccolithophore assemblage and
 256 environmental properties, where the latter variables have been entered passively, and to
 257 identify outlying samples with unusual assemblages (ter, Braak, 1987). There were no
 258 unusual samples, as indicated by the PCA. The significance of PCA axes was assessed
 259 using the broken-stick model, resulting in just one significant axis explaining 78.9% of
 260 the variance, and being highly correlated with SST. These results are in agreement with
 261 Saavedra-Pellitero (2011) who found out that SST was the dominant oceanographic
 262 parameter controlling certain coccolithophore species (grouped into a factor) offshore
 263 Chile. CARs were square transformed to standardize their variances. Rare species were
 264 downweighted because the square root transformation increases their weight and they can
 265 have undue influence on the ordination. To establish a SST-sensitive transfer function
 266 based on CAR, we performed a multiple linear regression. The number of parameters in
 267 the fitted model were determined using a Akaike's information criterion. Thus, the
 268 species eventually included in the minimal adequate model were: *F. profunda* (F.pro), *H.*
 269 *carteri* (H.car), *G. muelleriae* (G.mue), *Umbellosphaera* spp. (Umbe) and *C. pelagicus*
 270 (C.pel). The minimal adequate regression and final calibration model showed a residual
 271 standard error of 0.803 on 66 degrees of freedom and adjusted R² of 0.7021. We obtained
 272 the following equation to estimate SST using CARs:

$$\begin{aligned}
 273 \quad SST = & 12.98 + [0.0015557 \cdot (F.pro) + 0.0011031 \cdot (H.car) - 0.0009193 \cdot (G.mue) - \\
 274 \quad & 0.0032570 \cdot (Umbe) - 0.0024363 \cdot (C.pel)]
 \end{aligned}$$

275 A root mean squared error of prediction (RMSEP) was assessed by (bootstrapping and
276 jackknifing) cross-validation (99 permutation cycles) in order to assess the predictive
277 power of our transfer function (Table 3). The final model was examined for potential
278 outliers, because these can strongly affect transfer function coefficients and may
279 markedly decrease the predictive ability of the model. Outliers were identified as samples
280 having an absolute residual (observed minus estimated) higher than the SD of the
281 environmental variable of interest and a low influence on the model indicated by Cook's
282 D (Cook's $D < 4/n$, Fig 5D). Based on this criterion, the samples GeoB 7108 and RR 52
283 mc3 were excluded.

284 The SST residuals (the difference between the observed minus the estimated SST) were
285 tested for homoscedasticity (constant variance). This condition ensures that the best-
286 fitting line works well for all relevant values of SST estimated, not just in certain areas.
287 In the scatter plot of the standardized residuals against the SST estimated values (Fig. 5C)
288 the spread in the residuals stays almost the same throughout, addressing the
289 homoscedasticity condition. In general, the SST residuals are relatively low (most of
290 them are between -1 and 1) and without any significant correlation or trend with the
291 estimated SSTs (Fig. 5A). Our results based on CARs reveal good reproducibility of the
292 SST World Ocean Atlas 2005 (see Fig. 6 and supplementary material). Even though we
293 regarded annual averages to avoid any influence of seasonality, seasonal changes in
294 oceanographic conditions can strongly influence the coccolithophore fluxes. Therefore
295 SST residuals were also compared with the SST difference between summer and winter
296 in the study area (Fig. 7A). A slight trend can be observed between SST difference and
297 SST residuals (Fig. 7B)

298

299 **4. Discussion**

300 **4.1. CARs estimates**

301 Coccolith distribution patterns and coccolith numbers from surface sediment samples are
302 dependent on coccolithophore productivity, on dissolution and on dilution by terrigenous
303 material, which influences sedimentation rates. Due to the enormous differences in mass
304 accumulation rates along the Chilean continental margin, CARs complement and in some
305 cases improve the relative data to reconstruct gradients in coccolithophore productivity
306 off Chile. Highest total CARs are found in the stations located off north-central Chilean
307 coast (22.8°S-30°S, Fig. 3), where seasonal upwelling takes place (18°S-27°S; Strub et al.,
308 1998) and where Abrantes et al. (2007) observed samples barren of diatoms. However, a
309 marked decrease in CARs is observed further offshore at surface sediment samples
310 around ~23°S (Fig. 3C). At these locations high numbers of coccoliths per gram of
311 sediment are noted (Fig. 3B), yet CARs notably decrease with respect to more coastal
312 samples at similar latitude, probably driven by low SRs estimates. High coccolithophore
313 diversity is also recorded off north-central Chilean continental margin, as displayed by
314 the presence of different coccolith bearing species (i.e., small *Gephyrocapsa*, *C.*
315 *leptoporus*, *E. huxleyi*, *G. muelleriae* and *G. oceanica*) together with other coccolith forms
316 (e.g., *F. profunda*, *H. carteri* and *Umbellosphaera* spp.). Offshore central-south Chile,
317 upwelling-favorable conditions occur from late spring to early fall, corresponding to the
318 most persistent upwelling extending from 35°S to 38°S (Strub et al., 1998). Due to the
319 fact that underneath these high productive zones degradational processes of organic
320 matter may favor enhanced carbonate dissolution (Boeckel and Baumann, 2004), samples

321 barren of coccolithophores or highly affected by dissolution (which were excluded in our
322 model) are mainly located in areas from 35.5°S to 39°S (Saavedra-Pellitero et al., 2010).
323 A drop in the total CARs and in all the species numbers are observed in the area from
324 36.5°S to 38°S (Fig. 3) nearby the persistent upwelling cell off point Concepción (Strub et
325 al., 1998) coincident with the highest diatom abundance values (valves/g) and organic
326 carbon recorded in the same region by Abrantes et al. (2007). The only coccoliths
327 recorded in this area (around ~36°S) belong to *F. profunda* and *G. oceanica*, and in a
328 lesser extent *E. huxleyi*, small *Gephyrocapsa*. and *G. muelleriae*. The tongue of low-
329 salinity water characteristic from the fjord region off south Chile (e.g., Lamy et al., 2002)
330 has been recognized by maxima in the abundance of freshwater diatoms (Abrantes et al.,
331 2007) and by the factors derived from the coccolith percentage dataset (Saavedra-
332 Pellitero et al., 2010), but is not clearly defined by the CARs. The most prominent
333 coccolithophore species in this area are *C. pelagicus* and *G. muelleriae*, but small
334 placoliths, such as small *Gephyrocapsa* and *E. huxleyi* are also present.

335

336 A comparison of the observed CARs with the coccolith flux collected from a sediment
337 trap located offshore Chile (30°S, 73°11'W, Fig. 4) showed that numbers differ, although
338 they are still comparable. A total CAR of $6.8 \cdot 10^6$ coccoliths/cm²/yr, was obtained for the
339 closest surface sediment sample in our dataset (29.72°S, 72.17°W), a minimum flux of
340 $9.86 \cdot 10^6$ coccoliths/cm²/yr was estimated during El Niño conditions (1997-1998) and an
341 average of $1.59 \cdot 10^8$ coccoliths/cm²/yr during non-El Niño conditions (1993-1994;
342 Köbrich, 2008); at least the calculated CAR is in the order of the minimum flux during El
343 Niño conditions. Owing to the fact that the surface sediment sample was not retrieved

344 directly underneath the mooring location and that dissolution processes are likely to
345 affect primarily deep sediments, differences between the CAR estimates and the sediment
346 trap fluxes appear to be reasonable. In addition, the sediment trap recorded seasonal and
347 annual variations while the surface sediment samples provided averaged data on a wider
348 time interval of tens to hundreds of years.

349

350 **4.2. Reliability of the SST reconstruction**

351 The present SST estimation is adding to a series of previously published transfer
352 functions in the SE Pacific realm based on data from different siliceous and calcareous
353 microfossils, with the innovation of using species CARs from surface sediment samples
354 instead of relative abundances. The results of our SST transfer function based on CARs
355 reveal good reproducibility of the SST World Ocean Atlas 2005 (Locarnini et al., 2006)
356 data; the estimated and measured SST values are highly correlated ($R^2=0.723$, Fig. 8B).
357 We improved the spatial resolution offshore Chile, especially compared with previous
358 works based on radiolarian census (Pisias et al., 1997; Pisias et al., 2006) and planktonic
359 foraminifera (Mix et al., 1999; Feldberg and Mix, 2002; Kucera et al., 2005; Morey et al.,
360 2005) which considered very few samples for the whole study area (see Fig. 8A).
361 Abrantes et al. (2007) added some samples to previously collected databases (e.g.,
362 Schuette and Schrader, 1979; Romero and Hebbeln, 2003) and successfully obtained a
363 SST diatom transfer function based directly on species percentages. Many of those
364 samples were also used by Saavedra-Pellitero et al. (2011) to estimate SST using
365 multivariate statistical analyses performed on modern coccolithophore census data from
366 15°N to 50.6°S and from 71°W to 93°W. With our work we covered an existing gap in

367 the north-central Chilean coast (from ~23°S to ~33°S) due to the lack of preserved
368 diatoms in the samples (Fig. 8A).

369 A comparison of the SST estimates derived from our model (using CARs) with previous
370 SST transfer functions based on planktonic foraminifera (Kucera et al., 2005) and
371 diatoms (Abrantes et al., 2007) was performed and they resulted in close agreement (Fig.
372 8A). Nevertheless, even if the three reconstructions follow the same trend, our SST
373 estimates are always lower than the other two because we considered an annual SST
374 average from 0 m to 75 m water depth, instead of 0 m (chosen for diatoms) or 10 m
375 (chosen for planktonic foraminifera) SST annual averages. Those differences are indeed
376 higher offshore north-central Chile and become smaller offshore central-south Chile,
377 specifically at intense upwelling areas (e.g., around 36°S, Fig. 8A). The underestimation
378 of SST further offshore Chile around ~23°S (Figs. 6C and 8A) would be linked to the
379 calculation of SR at those locations. A SST average (from 0 m to 75 m) was considered
380 due to the fact that coccolithophore production can also happen at deeper depths (e.g., *F.*
381 *profunda*); this choice also allowed us directly to compare with the SST estimates based
382 on coccolith percentages (Saavedra-Pellitero et al., 2011). Both reconstructions based on
383 coccolithophores follow the same trend as the SST observed, although the SST CAR
384 estimates fits better (see Fig. 8A), especially from ~26°S to ~36°S. In any case, it should
385 be noted that SST estimates using different coccolith datasets and statistical approaches
386 offshore Chile resulted in close agreement, as shown by the high correlation ($R^2=0.71$)
387 between the SST coccolith percentage estimates and the SST CAR estimates
388 (supplementary material).

389 Focusing more on the CAR transfer function, it can be noted that negative SST residuals
390 indicate that the model overestimated the mean annual SST while positive residuals
391 indicate that the model estimates underestimated this parameter. Although SST residuals
392 calculated here are low, the contour map of SST residuals (Fig. 6C) shows that our model
393 tends to underestimate SSTs at the northernmost locations and overestimate SSTs at the
394 southernmost ones together with those stations from the area between $\sim 34.5^{\circ}\text{S}$ and
395 $\sim 36.5^{\circ}\text{S}$ which are under the influence of the persistent upwelling region described by
396 Strub et al. (1998). Abrantes et al. (2007) also got SST overestimates and SST
397 underestimates at the northern- and southernmost locations of our study area, but not
398 offshore central Chile. This can be just explained by the ecological dominance of diatoms
399 over coccolithophores and/or by coccolith carbonate preservation which could affect
400 coccolithophore species composition in the upwelling region near Concepción (from 35°S
401 to 38°S). The slight trend observed between SST summer-winter difference and SST
402 residuals (Fig. 7B) suggest that samples with SST underestimates (high positive
403 residuals) are more affected by seasonality than samples with SST overestimates (low
404 negative residuals). Therefore seasonality has, to some extent, an influence on the warm-
405 water and cold-water coccolithophore taxa preserved in the surface sediment samples.
406 Even considering the limitations of our regional approach, both the total and species CAR
407 estimates give a general idea of the number of coccoliths/cm²/yr preserved in the surface
408 sediments offshore Chile, an upwelling region mainly dominated by diatoms, and
409 furthermore allowed us to obtain an accurate SST reconstruction.

410

411 **5. Conclusions**

412 In this study the modern regional gradients of sea surface productivity and temperature
413 offshore Chile were detected by studying (a) coccolith accumulation rates (CARs) and (b)
414 coccolithophore derived sea surface temperature (SST) estimates. The main findings are
415 as follows:

416 (1) CARs, calculated by using estimated sedimentation rates based on recent ^{210}Pb and
417 bulk chemistry analyses of surface samples from the Chilean margin, clearly reveal that
418 the accumulation of coccolithophores shows a strong statistical relationship to SST.
419 Rigorous numerical methods have been used to quantify the inherent error of the model
420 and to assess the reliability of the quantitative reconstruction for the average temperatures
421 of the uppermost 75 m of the water column.

422 (2) Total CARs and species CARs reflect the regional upwelling conditions along the
423 Chilean continental margin. Highest total CARs were found off north-central Chile,
424 where seasonal upwelling occurs.

425 (3) There are five key coccolithophore species which as show by our model record SST
426 information; these are *Florisphaera profunda*, *Helicosphaera carteri*, *Gephyrocapsa*
427 *muelleriae*, *Umbellosphaera* spp. and *Coccolithus pelagicus*.

428 (4) Differences between observed and estimated SST coincide with a persistent upwelling
429 region between $\sim 34.5^\circ\text{S}$ and $\sim 36.5^\circ\text{S}$, yielding warmer temperatures than expected.

430 (5) In short, our results demonstrate the good reconstructive skill of observed SSTs and
431 are in close agreement to a series of previously published SST transfer functions in the
432 Southeast Pacific realm based on species percentages from different siliceous and
433 calcareous microfossils.

434

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446

447

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Figure. 1. A. Map of the Pacific and adjacent areas showing major surface currents (after Tomczak and Godfrey, 2003; modified from Lamy and Kaiser, 2009). The study area has been indicated with yellow rectangle.

B. Sea Surface Temperature (SST in °C, Locarnini et al., 2006) expressed as an annual average from 0 m to 75 m water depth and annual mean precipitation (mm/yr) over parts of South America in 2000 (Beck et al., 2005).

The location of the sampling stations offshore Chile corresponding to recent sedimentation (SR) data available based on ^{210}Pb (Muñoz et al., 2004) is indicated with blue crosses, the sampling stations corresponding to ICP-MS measurements (Stuut et al., 2007) with black dots, and the 74 sea surface sediment samples used in this study with red dots.

Figure1
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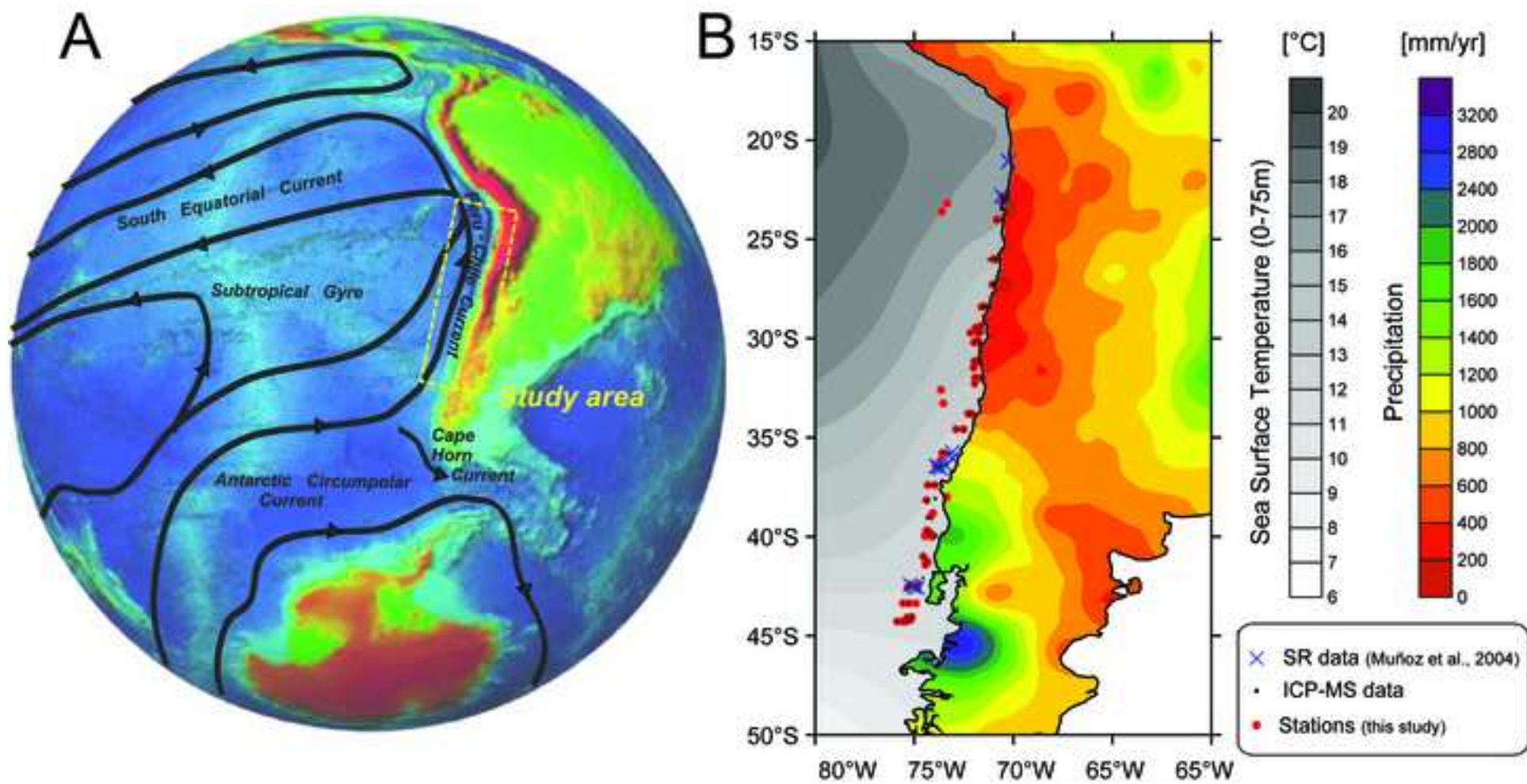


Figure 2. A. Sedimentation Rates (cm/yr) used in this work, from Muñoz et al. (2004), Lamy et al. (1999) and Ho et al. (2012).
B. Sedimentation Rates (cm/yr) from Muñoz et al. (2004) versus Ti (‰) values from the bulk chemistry analyses done by inductively coupled plasma atomic emission spectrometry (ICP-MS; Stuu et al. 2007).
C. Dry bulk densities (g/cm^3) used in this work, from Muñoz et al. (2004), Hebbeln et al. (2004), Klump et al. (2004), Muñoz and Nuñez pers. comm.

Figure 2
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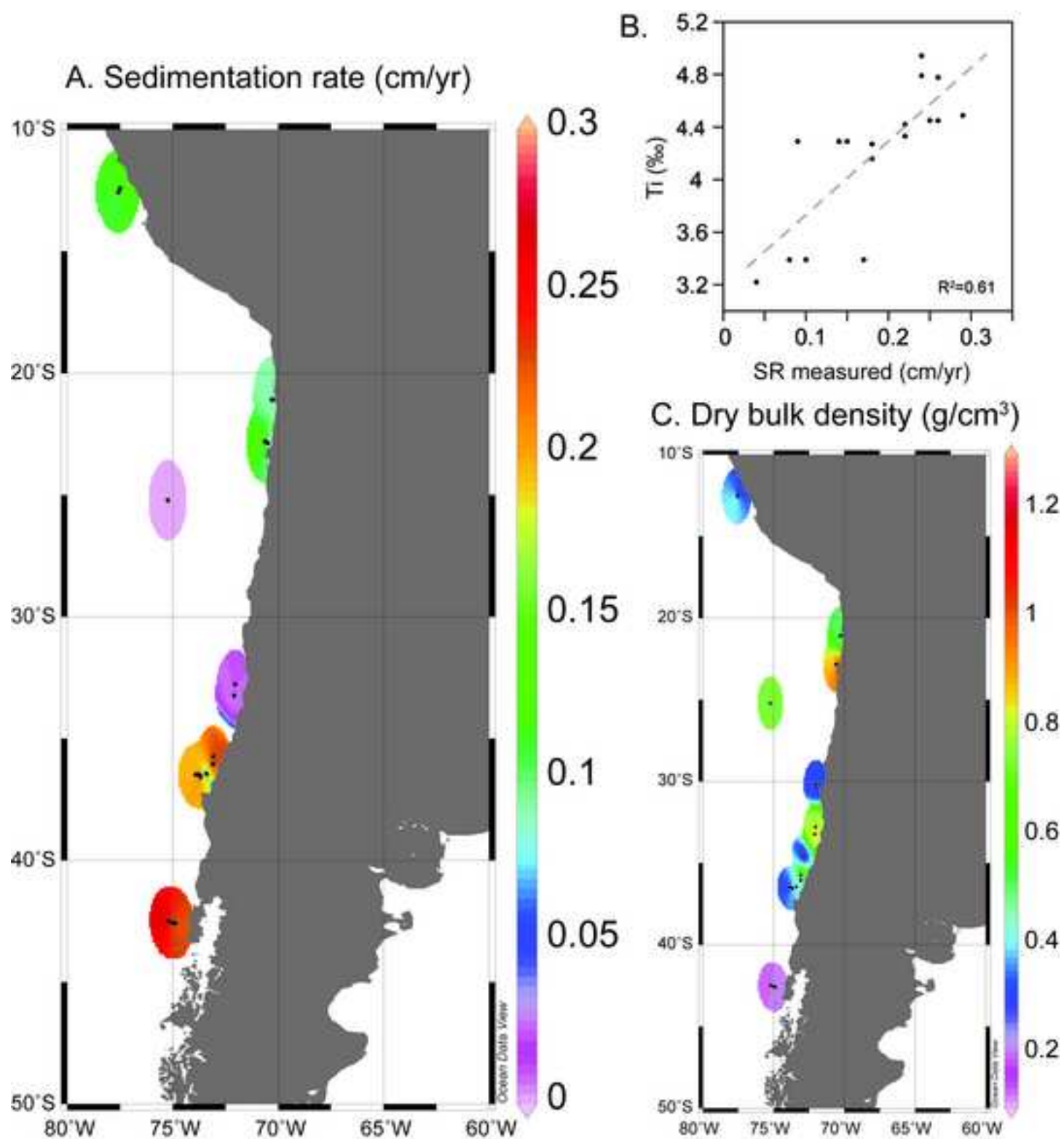


Figure 3. A. Sedimentation Rate estimates (cm/yr) for the study area using the present approach explained within the text. B. Total number of coccoliths per gram of sediment. C. Coccolith Accumulation Rate (CAR, coccoliths/cm²/yr). The 74 surface sediment sample locations are indicated here with black dots.

Figure3
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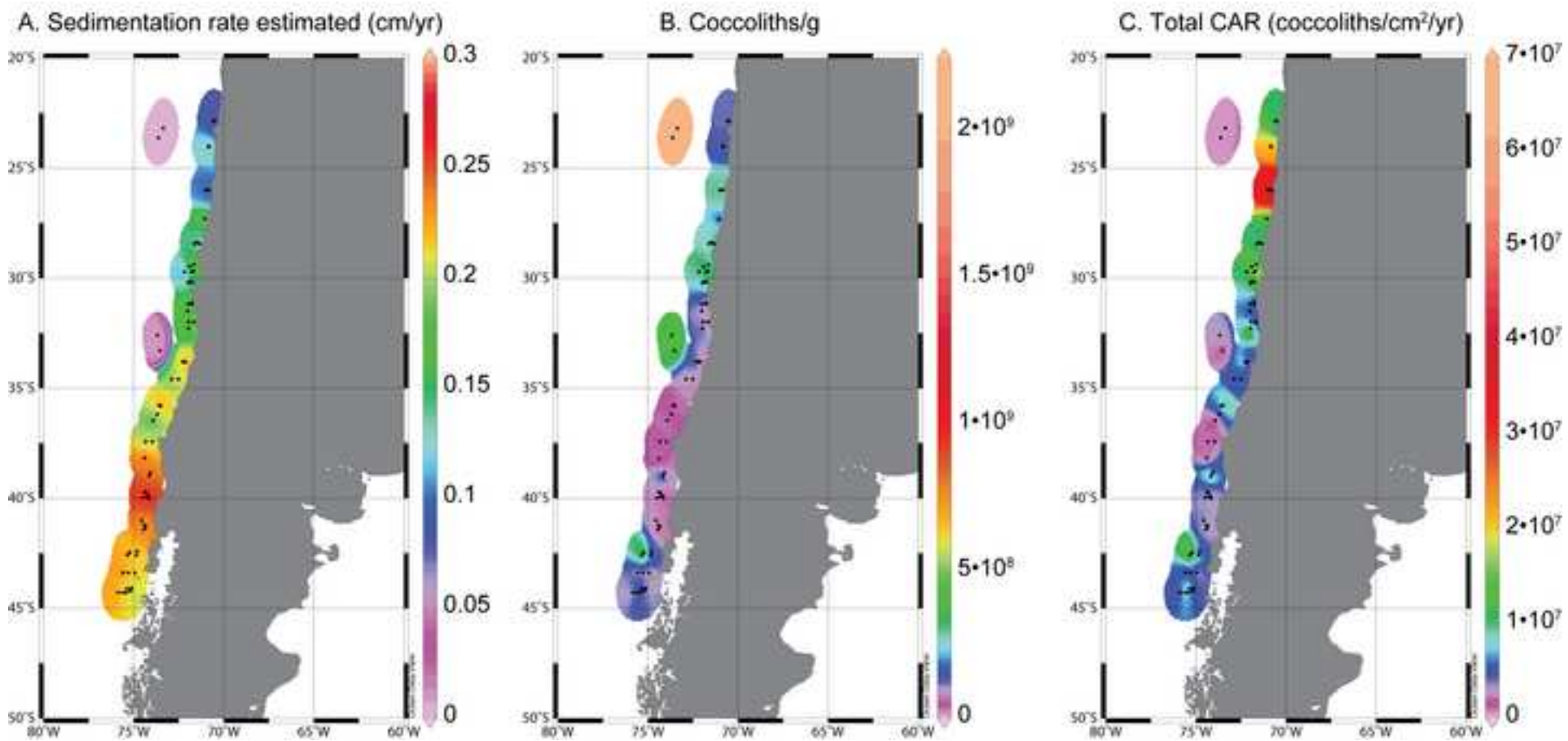
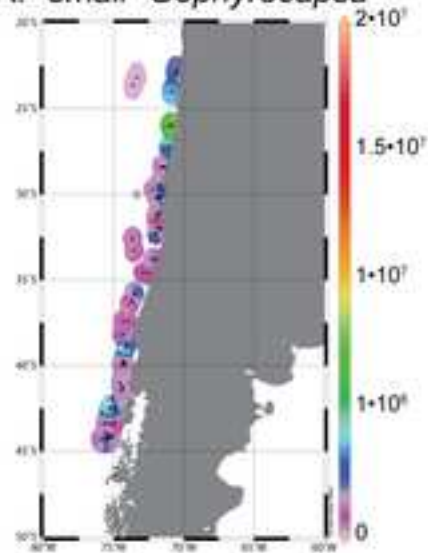


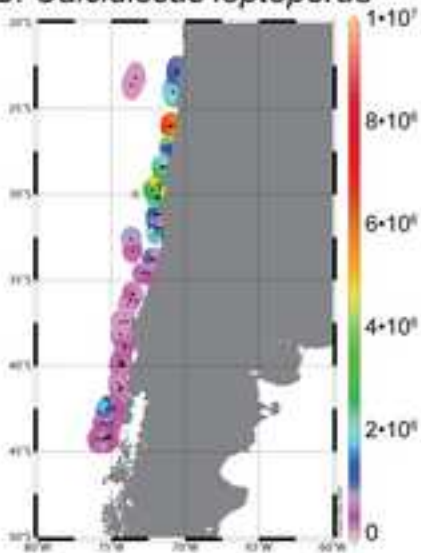
Figure 4. Distribution maps of Coccolith Accumulation Rates for the more important taxa or groups of coccoliths considered in the study area: A. “small” *Gephyrocapsa*, B. *Calcidiscus leptoporus*, C. *Florisphaera profunda*, D. *Emiliana huxleyi*, E. *Gephyrocapsa muellerae*, F. *Gephyrocapsa oceanica*, G. *Helicosphaera carteri*, H. *Coccolithus pelagicus* and I. *Umbellosphaera* spp. Stations are indicated with black dots. The gray star indicates the location of the sediment trap deployed off Chile (30°S, 73°11'W; González et al., 2004; Köbrich, 2008).

Figure4
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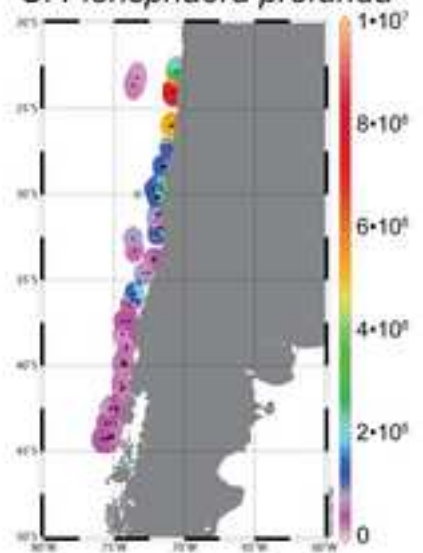
A. "small" *Gephyrocapsa*



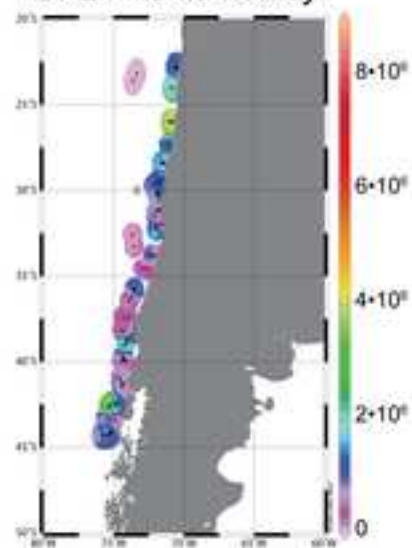
B. *Calcidiscus leptoporus*



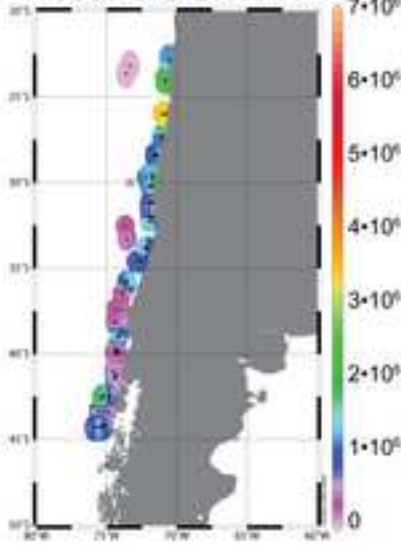
C. *Florisphaera profunda*



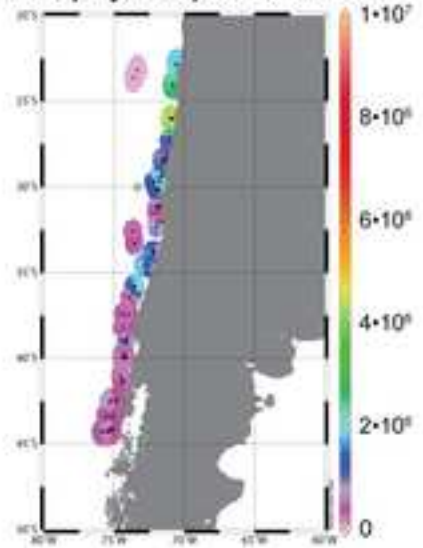
D. *Emiliana huxleyi*



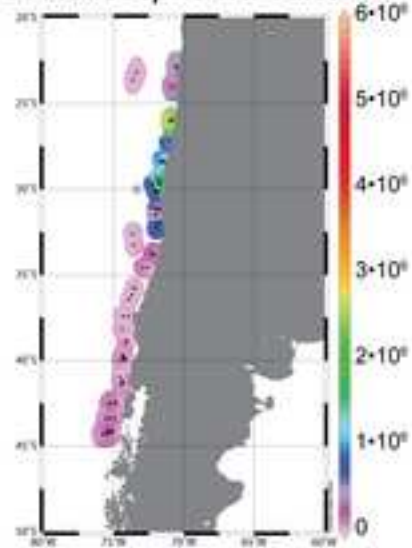
E. *Gephyrocapsa muelleriae*



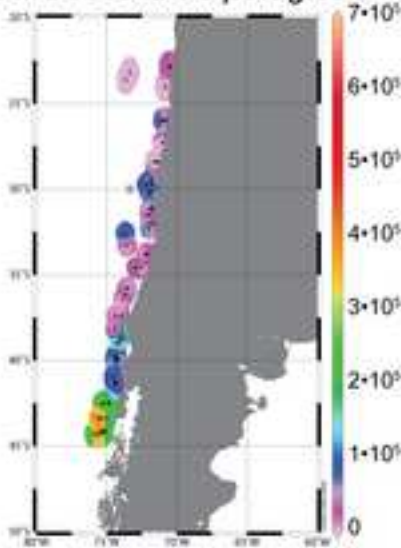
F. *Gephyrocapsa oceanica*



G. *Helicosphaera carteri*



H. *Coccolithus pelagicus*



I. *Umbellosphaera* spp.

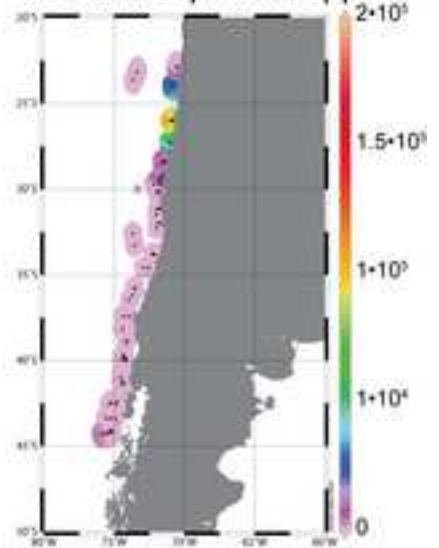


Figure 5. A. SST residuals versus SST estimated. B. Normal Q-Q. C. Scale location. D. SST residuals versus leverage.

Figure5
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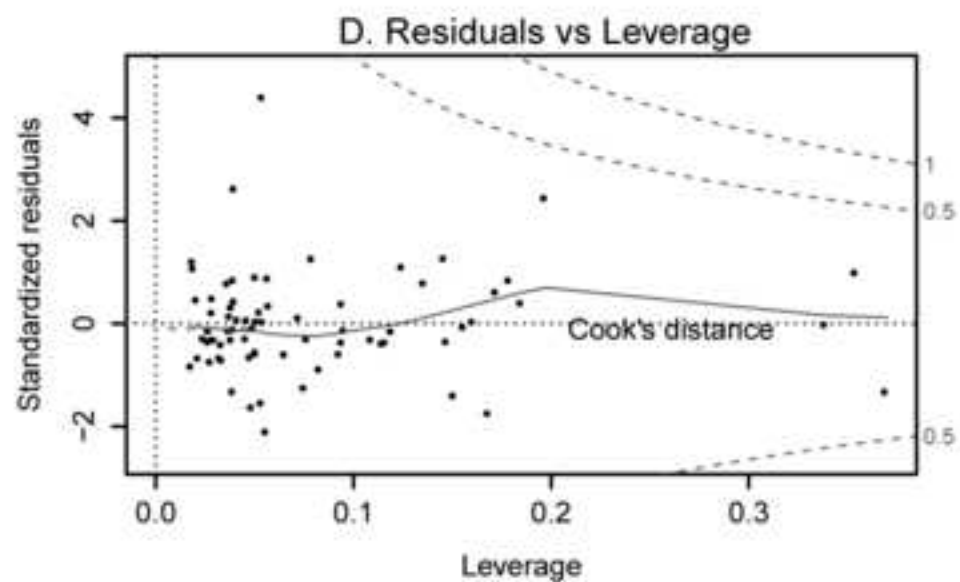
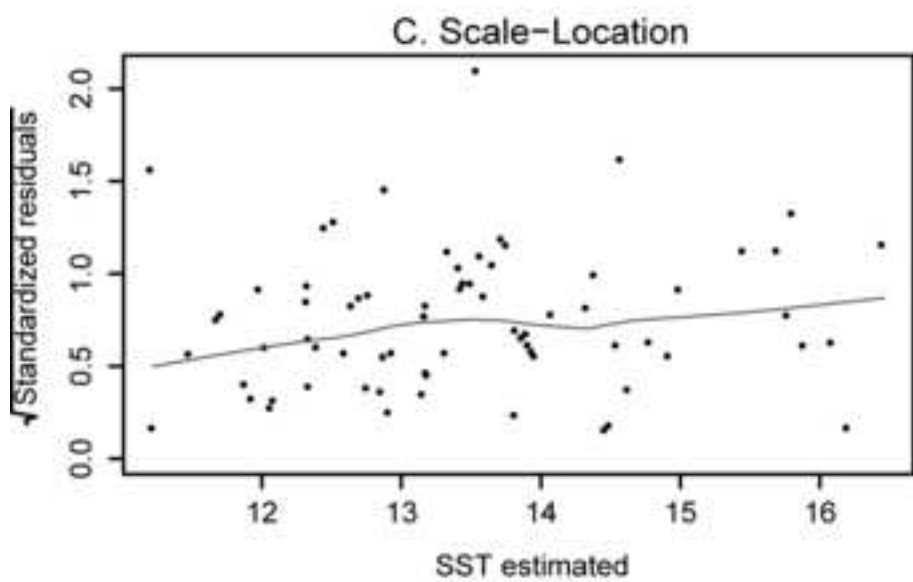
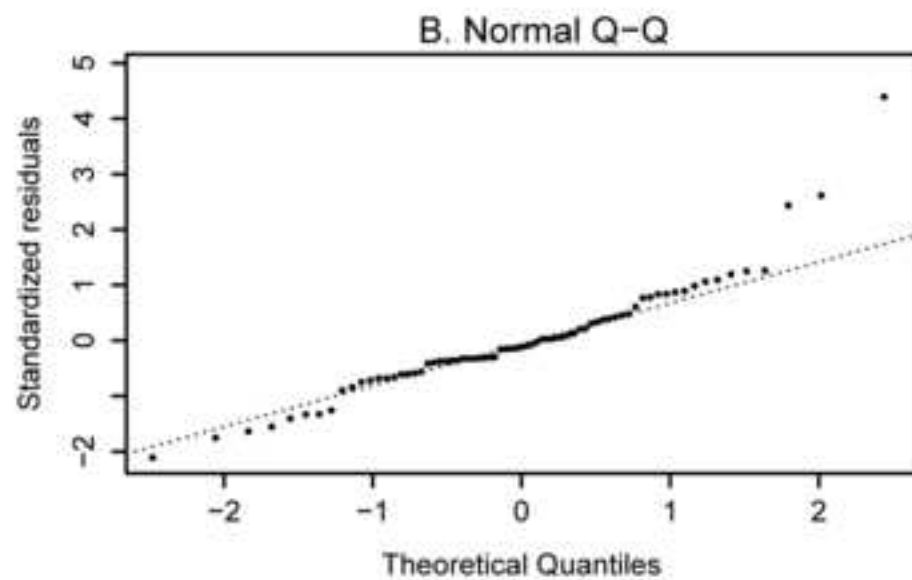
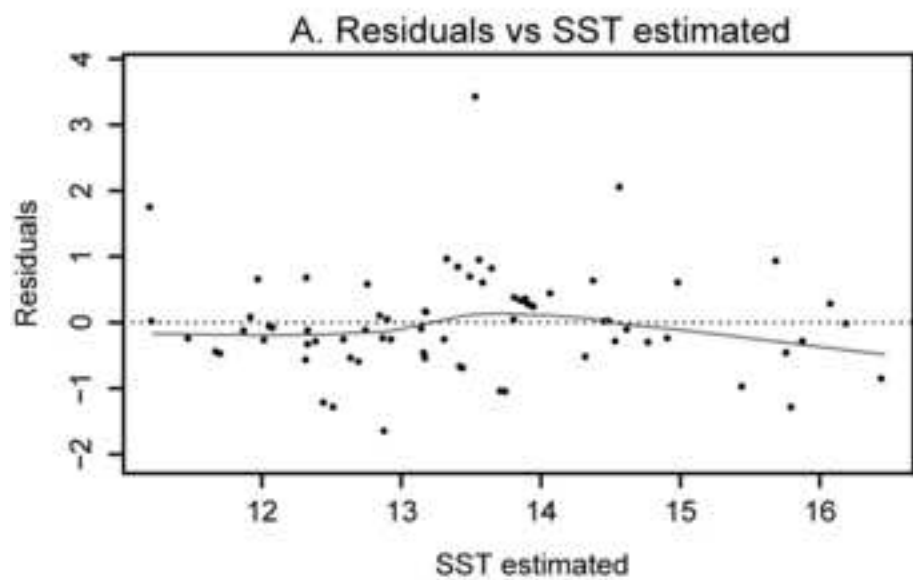


Figure 6. A. Annual 0-75 m SST average observed (in °C, from WOA05, Locarnini et al., 2006). B. Annual average 0-75 m SST estimated (in °C). C. Sea Surface Temperature residuals (SST estimated-SST observed). Stations are indicated with black dots.

Figure6
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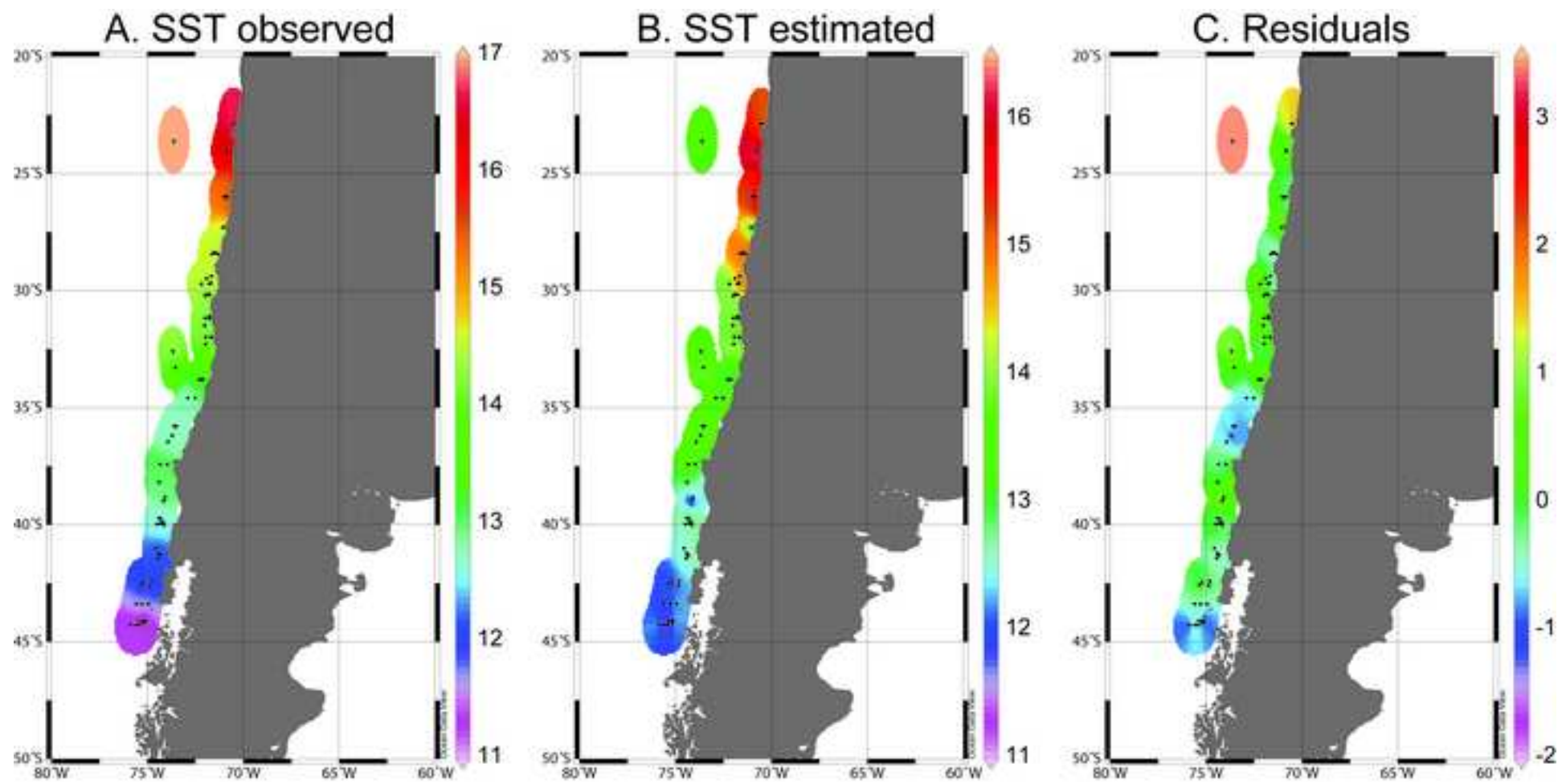


Figure 7. A. SST summer - SST winter (in °C). Data retrieved from WOA05 (Locarnini et al., 2006). The one-degree grid is indicated with black dots and stations with white dots. B. SST summer - SST winter versus SST residuals.

Figure7

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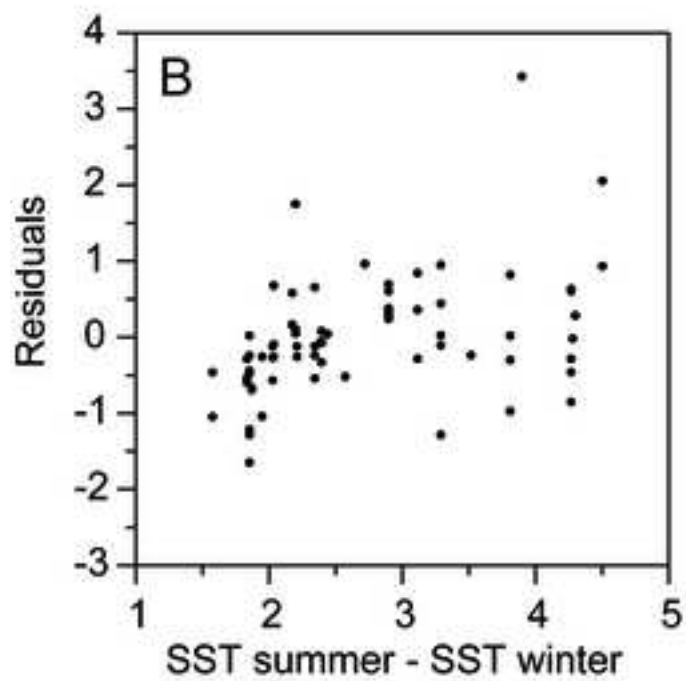
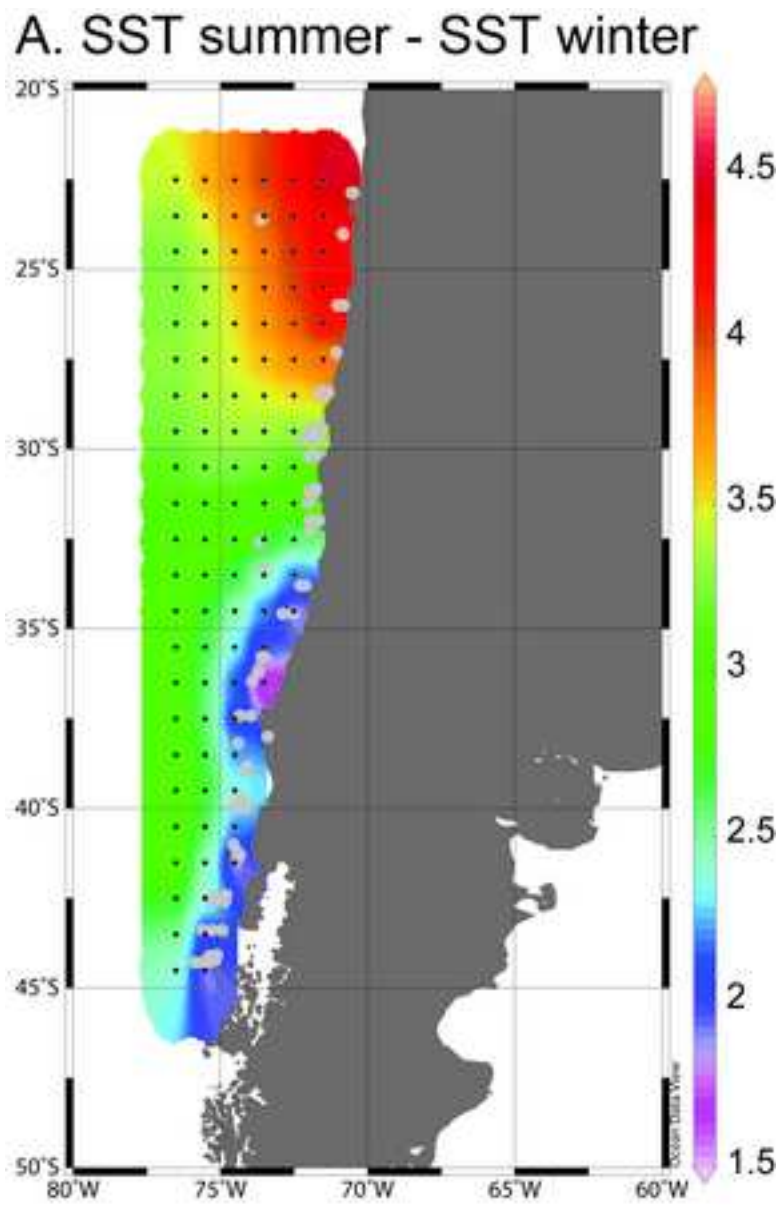
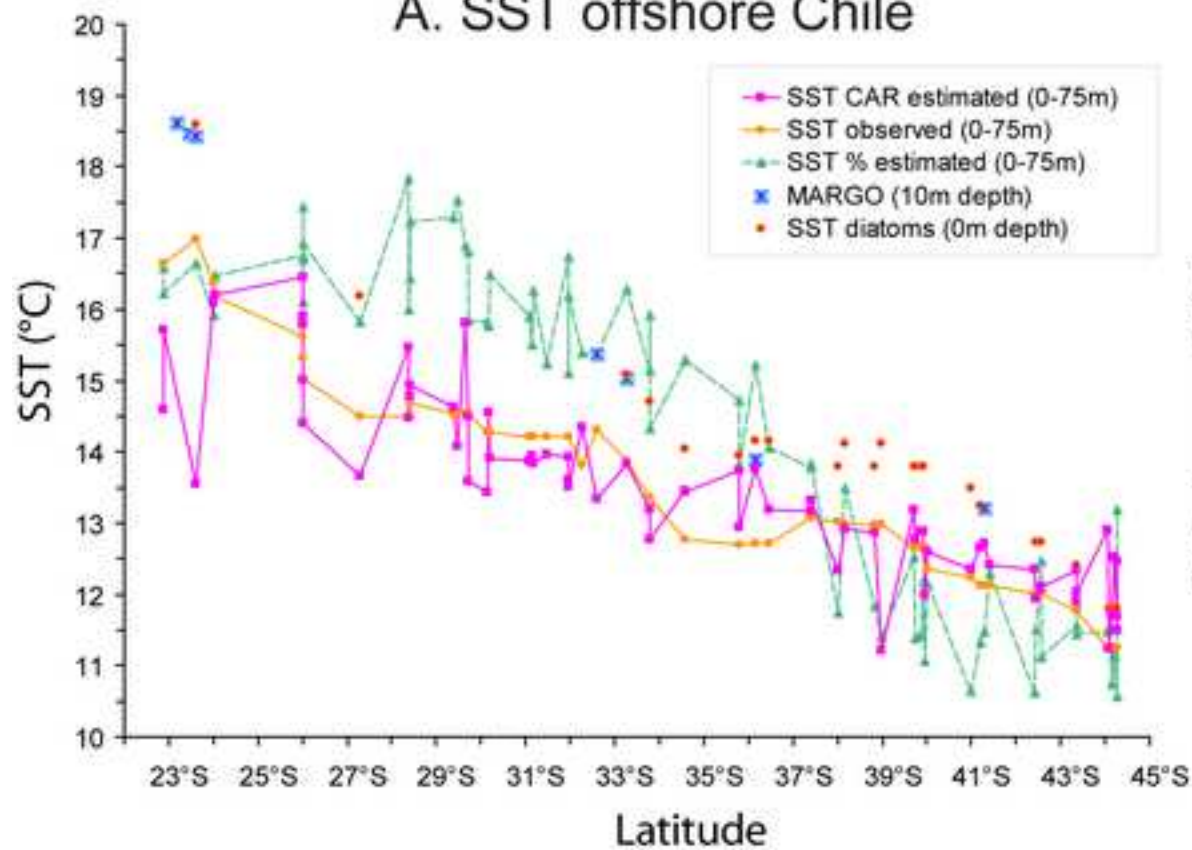


Figure 8. A. Sea Surface Temperature reconstruction (SST in °C, 0-75 m) using Coccolith Accumulation Rates (CARs) indicated with squares and pink line, SST observed (0-75 m, from WOA05, Locarnini et al., 2006) indicated with circles and orange line, SST reconstruction (0-75 m) using coccolithophore percentages (Saavedra-Pellitero et al., 2011) indicated with dashed line and green triangles, SST reconstruction with foraminifera at 10m (Kucera et al., 2005) indicated with blue squares with an asterisk inside and SST reconstruction with diatoms at 0 m depth (Abrantes et al., 2007). B. SST estimated versus SST observed (both in °C). The line represents the best fitting linear regression.

Figure8

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A. SST offshore Chile



B. SST estimated vs SST observed

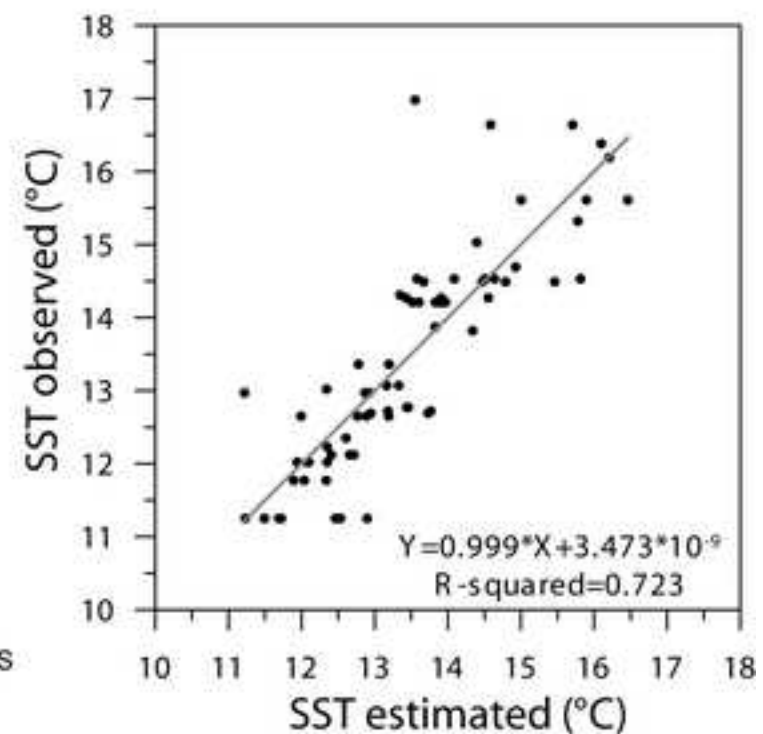


Table 1. Station, geographical position, measured sedimentation rate (SR, in cm/yr), authors of SR measurements, measurements of dry bulk density (DBD, in g/cm³), authors of DBD measurements, Al, Fe, K, Mg and Ti (‰) values selected from the bulk chemistry analyses done by inductively coupled plasma atomic emission spectrometry (ICP-MS; Stuet et al. 2007). Underlined stations were used for the SR-Ti approach.

Table 2. List of studied samples including geographical position as well as estimated Sedimentation Rates (SR, in cm/yr), estimated Dry Bulk Densities (DBDs, in g/cm³) and observed annual Sea Surface Temperature (SST in °C) average from 0 m to 75 m water depth (Locarnini et al., 2006). Asteriks indicate samples in which coccolithophore studies were not performed; for further details, see Saavedra-Pellitero et al. (2010). GeoB samples were retrieved during R/V SONNE Cruise SO-156 and RR samples during Genesis III Cruise RR9702A.

Table 3. Root mean squared error (RMSE), adjusted R², F-statistic, degrees of freedom and p-value of the 5 component model. Root mean squared error of prediction (RMSEP) of the model assessed by bootstrapping and jackknifing.

Table1
[Click here to download Table: TABLE 1 table dry bulk densities and SR Measured.xls](#)

| Station | Longitude | Latitude | SR measured (cm/yr) | | Author (SR) | DBD measured (g/cm3) | | Author (DBD) | Al (‰) | Fe (‰) | K (‰) | Mg (‰) | Ti (‰) |
|------------------|-----------|----------|---------------------|--------|--------------------|----------------------|------------------------------|--------------|--------|--------|-------|--------|--------|
| Sta. A | -77.5 | -12.4 | 0.13 | ±0.02 | Muñoz et al., 2004 | 0.18 | Muñoz et al., 2004 | | | | | | |
| Sta. C | -77.6 | -12.6 | 0.1 | ±0.01 | Muñoz et al., 2004 | 0.53 | Muñoz et al., 2004 | | | | | | |
| Sta. 6 | -70.2 | -21.1 | 0.1 | ±0.01 | Muñoz et al., 2004 | 0.45 | Muñoz et al., 2004 | 48.11 | 60.36 | 19.70 | 17.01 | 3.390 | |
| Sta. 7 | -70.3 | -21.1 | 0.08 | ±0.01 | Muñoz et al., 2004 | 0.54 | Muñoz et al., 2004 | 48.11 | 60.36 | 19.70 | 17.01 | 3.390 | |
| GeoB 7104 | -70.5 | -22.9 | 0.04 | ±0.01 | Muñoz et al., 2004 | 1.22 | Muñoz et al., 2004 | 46.21 | 31.41 | 12.86 | 15.15 | 3.220 | |
| GeoB 7106 | -70.6 | -22.8 | 0.17 | ±0.003 | Muñoz et al., 2004 | 0.67 | Muñoz et al., 2004 | 48.11 | 60.36 | 19.70 | 17.01 | 3.390 | |
| 5d | -73.1 | -35.7 | 0.24 | ±0.05 | Muñoz et al., 2004 | 0.75 | Muñoz et al., 2004 | 83.39 | 43.47 | 14.08 | 13.96 | 4.943 | |
| 4c | -73.1 | -36.0 | 0.26 | ±0.03 | Muñoz et al., 2004 | 0.44 | Muñoz et al., 2004 | 80.86 | 41.90 | 13.29 | 14.55 | 4.778 | |
| GeoB 7160 | -73.1 | -36.0 | 0.24 | ±0.07 | Muñoz et al., 2004 | 0.42 | Muñoz et al., 2004 | 80.93 | 42.09 | 13.31 | 14.61 | 4.791 | |
| 26A | -73.4 | -36.4 | 0.09 | ±0.01 | Muñoz et al., 2004 | 0.32 | Muñoz et al., 2004 | 74.93 | 43.41 | 10.40 | 15.24 | 4.291 | |
| 26B | -73.4 | -36.4 | 0.14 | ±0.02 | Muñoz et al., 2004 | 0.55 | Muñoz et al., 2004 | 74.93 | 43.41 | 10.40 | 15.24 | 4.290 | |
| GeoB 7161 | -73.4 | -36.4 | 0.15 | ±0.01 | Muñoz et al., 2004 | 0.30 | Muñoz et al., 2004 | 74.93 | 43.41 | 10.40 | 15.24 | 4.290 | |
| 3 | -73.7 | -36.5 | 0.26 | ±0.10 | Muñoz et al., 2004 | 0.51 | Muñoz et al., 2004 | 77.43 | 43.71 | 12.72 | 14.42 | 4.448 | |
| GeoB 7162 | -73.7 | -36.6 | 0.25 | ±0.04 | Muñoz et al., 2004 | 0.31 | Muñoz et al., 2004 | 77.44 | 43.67 | 12.68 | 14.43 | 4.450 | |
| GeoB 7166 | -73.8 | -36.5 | 0.18 | ±0.02 | Muñoz et al., 2004 | 0.33 | Muñoz et al., 2004 | 73.45 | 43.94 | 12.58 | 15.23 | 4.270 | |
| GeoB 7167 | -73.9 | -36.5 | 0.18 | ±0.02 | Muñoz et al., 2004 | 0.23 | Muñoz et al., 2004 | 72.10 | 42.56 | 12.40 | 15.86 | 4.159 | |
| GeoB 7177 | -74.8 | -42.6 | 0.22 | ±0.01 | Muñoz et al., 2004 | 0.20 | Muñoz et al., 2004 | 62.83 | 41.54 | 0.00 | 18.81 | 4.331 | |
| GeoB 7174 | -75.0 | -42.5 | 0.22 | ±0.02 | Muñoz et al., 2004 | 0.23 | Muñoz et al., 2004 | 64.60 | 41.96 | 0.00 | 18.36 | 4.421 | |
| GeoB 7175 | -75.2 | -42.5 | 0.29 | ±0.04 | Muñoz et al., 2004 | 0.17 | Muñoz et al., 2004 | 66.40 | 42.38 | 0.00 | 17.59 | 4.489 | |
| GeoB 7139 | -72.0 | -30.2 | - | - | | 0.30 | Muñoz, pers. comm. | | | | | | |
| GeoB 7155 | -72.9 | -34.6 | - | - | | 0.27 | Muñoz, pers. comm. | | | | | | |
| GIK 17748-2 | -72.0 | -32.8 | 0.009 | | Lamy et al., 1999 | 0.77 | Hebbeln et al., 2004 | | | | | | |
| GIK 3302-1 | -72.1 | -33.2 | 0.006 | | Lamy et al., 1999 | 0.85 | Klump et al., 2004 | | | | | | |
| GeoB 3388-1 | -75.2 | -25.2 | 0.0003 | | Ho et al., 2012 | 0.74 | Núñez Ricardo, pers comm. | | | | | | |

Table2

[Click here to download Table: TABLE 2 SR calculated.xls](#)

| Station | Longitude | Latitude | Estimated SR | Estimated DBI | SST average (0-75 m) | Station | Longitude | Latitude | Estimated SR | Estimated DBI | SST average (0-75 m) |
|-----------|-----------|----------|--------------|---------------|----------------------|---------------|-----------|----------|--------------|---------------|----------------------|
| GeoB 7108 | -70.6 | -22.8 | 0.077 | 0.670 | 16.64 | GeoB 7211 | -74.3 | -39.9 | 0.255 | 0.170 | 12.65 |
| GeoB 7104 | -70.5 | -22.9 | 0.077 | 1.220 | 16.64 | RR 20 mc4 | -74.5 | -40.0 | 0.255 | 0.170 | 12.65 |
| GeoB 7103 | -70.5 | -22.9 | 0.077 | 1.220 | 16.64 | RR 22 mc3 | -74.1 | -40.0 | 0.255 | 0.200 | 12.35 |
| RR 52 mc3 | -73.4 | -23.2 | 0.0003 | 0.740 | 16.98 | GeoB 7197 | -74.6 | -41.0 | 0.240 | 0.170 | 12.23 |
| RR 50 mc2 | -73.6 | -23.6 | 0.0003 | 0.740 | 16.98 | GeoB 7195 | -74.4 | -41.2 | 0.234 | 0.200 | 12.12 |
| GeoB 7114 | -70.8 | -24.0 | 0.113 | 1.220 | 16.38 | RR 24 mc3 | -74.3 | -41.3 | 0.234 | 0.200 | 12.12 |
| GeoB 7112 | -70.8 | -24.0 | 0.148 | 1.220 | 16.19 | GeoB 7194 | -74.4 | -41.4 | 0.234 | 0.200 | 12.12 |
| GeoB 7118 | -70.8 | -26.0 | 0.100 | 1.220 | 15.61 | GeoB 7172 | -74.8 | -42.4 | 0.227 | 0.200 | 12.02 |
| GeoB 7122 | -70.8 | -26.0 | 0.100 | 1.220 | 15.61 | GeoB 7175 | -75.2 | -42.5 | 0.215 | 0.170 | 12.02 |
| GeoB 7119 | -70.9 | -26.0 | 0.100 | 1.220 | 15.32 | GeoB 7179 | -75.3 | -42.6 | 0.229 | 0.170 | 12.02 |
| GeoB 7121 | -70.9 | -26.0 | 0.100 | 1.220 | 15.61 | GeoB 7177 | -74.8 | -42.6 | 0.197 | 0.200 | 12.02 |
| GeoB 7116 | -71.0 | -26.0 | 0.100 | 1.220 | 15.03 | GeoB 7182 | -74.9 | -43.4 | 0.212 | 0.200 | 11.77 |
| GeoB 7123 | -71.1 | -27.3 | 0.196 | 0.300 | 14.49 | GeoB 7181 | -75.3 | -43.4 | 0.212 | 0.230 | 11.77 |
| GeoB 7127 | -71.5 | -28.4 | 0.158 | 0.300 | 14.49 | GeoB 7180 | -75.6 | -43.4 | 0.242 | 0.170 | 11.77 |
| GeoB 7131 | -71.5 | -28.4 | 0.145 | 0.300 | 14.49 | GeoB 7183 | -75.1 | -44.1 | 0.218 | 0.200 | 11.25 |
| GeoB 7129 | -71.3 | -28.4 | 0.103 | 0.300 | 14.49 | GeoB 7192 | -75.4 | -44.1 | 0.217 | 0.230 | 11.25 |
| GeoB 7130 | -71.6 | -28.4 | 0.138 | 0.300 | 14.69 | GeoB 7186 | -75.2 | -44.2 | 0.197 | 0.200 | 11.25 |
| GeoB 7133 | -71.6 | -29.4 | 0.213 | 0.300 | 14.53 | GeoB 7187 | -75.2 | -44.2 | 0.194 | 0.200 | 11.25 |
| GeoB 7132 | -71.9 | -29.5 | 0.142 | 0.300 | 14.53 | GeoB 7189 | -75.4 | -44.3 | 0.216 | 0.230 | 11.25 |
| GeoB 7135 | -71.7 | -29.7 | 0.164 | 0.300 | 14.53 | GeoB 7191 | -75.6 | -44.3 | 0.209 | 0.230 | 11.25 |
| GeoB 7134 | -71.8 | -29.7 | 0.143 | 0.300 | 14.53 | GeoB 7190 | -75.9 | -44.3 | 0.232 | 0.230 | 11.25 |
| GeoB 7136 | -72.2 | -29.7 | 0.082 | 0.300 | 14.53 | GeoB 7115 (*) | -70.6 | -24.0 | | | |
| GeoB 7138 | -71.9 | -30.1 | 0.128 | 0.300 | 14.27 | GeoB 7140 (*) | -71.8 | -31.0 | | | |
| GeoB 7137 | -71.7 | -30.2 | 0.172 | 0.300 | 14.27 | RR 44 mc2 (*) | -73.0 | -35.8 | | | |
| GeoB 7139 | -72.0 | -30.2 | 0.115 | 0.300 | 14.27 | GeoB 7159 (*) | -73.2 | -35.8 | | | |
| GeoB 7141 | -71.8 | -31.1 | 0.176 | 0.300 | 14.21 | GeoB 7160 (*) | -73.1 | -36.0 | | | |
| GeoB 7144 | -72.0 | -31.2 | 0.176 | 0.300 | 14.21 | RR 39 mc2 (*) | -73.6 | -36.2 | | | |
| GeoB 7142 | -71.8 | -31.2 | 0.176 | 0.300 | 14.21 | GeoB 7161 (*) | -73.4 | -36.4 | | | |
| GeoB 7149 | -72.0 | -31.5 | 0.158 | 0.300 | 14.21 | GeoB 7163 (*) | -73.6 | -36.4 | | | |
| GeoB 7146 | -71.6 | -32.0 | 0.202 | 0.300 | 14.21 | GeoB 7166 (*) | -73.8 | -36.5 | | | |
| GeoB 7148 | -71.9 | -32.0 | 0.174 | 0.300 | 14.21 | RR 34 mc5 (*) | -73.4 | -36.5 | | | |
| GeoB 7147 | -71.7 | -32.0 | 0.202 | 0.300 | 14.21 | GeoB 7162 (*) | -73.7 | -36.5 | | | |
| GeoB 7150 | -72.0 | -32.3 | 0.157 | 0.770 | 13.82 | GeoB 7170 (*) | -74.1 | -37.4 | | | |
| RR 48 mc4 | -73.7 | -32.6 | 0.009 | 0.770 | 14.31 | RR 31 mc2 (*) | -75.4 | -37.7 | | | |
| RR 46 mc1 | -73.5 | -33.3 | 0.006 | 0.850 | 13.87 | RR 29 mc2 (*) | -75.7 | -37.8 | | | |
| GeoB 7152 | -72.1 | -33.8 | 0.203 | 0.270 | 13.36 | GeoB 7205 (*) | -73.7 | -38.0 | | | |
| GeoB 7153 | -72.2 | -33.8 | 0.234 | 0.270 | 13.36 | GeoB 7204 (*) | -73.8 | -38.0 | | | |
| GeoB 7154 | -72.3 | -33.8 | 0.201 | 0.270 | 13.36 | GeoB 7203 (*) | -74.0 | -38.0 | | | |
| GeoB 7156 | -72.5 | -34.6 | 0.207 | 0.270 | 12.77 | GeoB 7201 (*) | -74.1 | -38.1 | | | |
| GeoB 7155 | -72.9 | -34.6 | 0.194 | 0.270 | 12.77 | GeoB 7202 (*) | -73.9 | -38.1 | | | |
| GeoB 7158 | -73.5 | -35.8 | 0.219 | 0.750 | 12.69 | GeoB 7200 (*) | -74.1 | -38.2 | | | |
| GeoB 7157 | -73.6 | -35.8 | 0.218 | 0.750 | 12.69 | GeoB 7199 (*) | -74.3 | -38.2 | | | |
| RR 42 mc1 | -73.7 | -36.2 | 0.197 | 0.327 | 12.72 | GeoB 7219 (*) | -73.6 | -39.8 | | | |
| GeoB 7167 | -73.9 | -36.5 | 0.179 | 0.227 | 12.72 | RR 25 mc2 (*) | -75.9 | -39.9 | | | |
| GeoB 7171 | -74.0 | -37.4 | 0.202 | 0.313 | 13.07 | GeoB 7218 (*) | -73.9 | -39.9 | | | |
| GeoB 7169 | -74.3 | -37.4 | 0.199 | 0.227 | 13.07 | GeoB 7216 (*) | -73.9 | -40.1 | | | |
| GeoB 7207 | -73.4 | -38.0 | 0.220 | 0.313 | 13.02 | RR 27 mc4 (*) | -75.9 | -40.5 | | | |
| GeoB 7198 | -74.4 | -38.2 | 0.239 | 0.313 | 12.97 | GeoB 7173 (*) | -74.6 | -42.1 | | | |
| GeoB 7215 | -74.1 | -38.8 | 0.239 | 0.313 | 12.97 | GeoB 7174 (*) | -75.0 | -42.5 | | | |
| GeoB 7209 | -74.2 | -39.0 | 0.239 | 0.313 | 12.97 | RR 12 mc2 (*) | -76.3 | -43.4 | | | |
| GeoB 7212 | -74.4 | -39.7 | 0.255 | 0.170 | 12.65 | RR 14 mc2 (*) | -76.5 | -43.5 | | | |
| GeoB 7213 | -74.3 | -39.7 | 0.255 | 0.170 | 12.65 | RR 08 mc6 (*) | -76.7 | -46.4 | | | |
| GeoB 7214 | -74.2 | -39.9 | 0.255 | 0.170 | 12.65 | RR 06 mc4 (*) | -76.6 | -46.9 | | | |

Table3[Click here to download Table: Table 3 Error of the model.xls](#)

| Prediction model (5 components) | |
|--|----------------|
| RMSE | 0.803 |
| Adjusted R-squared | 0.702 |
| F-statistic | 34.470 |
| Degrees of freedom | 66 |
| p-value | $< 2.2e^{-16}$ |
| RMSEP _{jackknifing} | 0.848 |
| RMSEP _{bootstrapping} | 0.869 |