Responses of marine phytoplankton communities to environmental changes:

new insights from a niche classification scheme

Wupeng Xiao,[1] Edward A Laws,[2] Yuyuan Xie,[1] Lei Wang,[3]

Xin Liu,[1]* Jixin Chen,[1] Bingzhang Chen,[4] Bangqin Huang[1]*

[1]State Key Laboratory of Marine Environmental Science / Fujian Provincial Key Laboratory for Coastal Ecology and Environmental Studies / College of the Environment and Ecology, Xiamen University, Xiamen, China.

[2]Department of Environmental Sciences, School of the Coast & Environment, Louisiana State University, Baton Rouge, Louisiana 70803, USA.

[3]Laboratory of Marine Biology and Ecology, Third Institute of Oceanography, State Oceanic Administration, Xiamen, China.

[4]Department of Mathematics and Statistics, University of Strathclyde, Glasgow, UK.

*Corresponding authors:

Dr. Bangqin Huang, tel: 86-592-2187783, email: bqhuang@xmu.edu.cn

Dr. Xin Liu, tel: 86-592-2181151, email: liuxin1983@xmu.edu.cn

1   **Abstract**

2   Predicting changes of phytoplankton communities in response to global warming

3   is one of the challenges of ecological forecasting. One of the constraints is the paucity

4   of general principles applicable to community ecology. Based on a synecological

5   analysis of a decadal-scale database, we created a niche habitat classification scheme

6   relating nine phytoplankton groups to fifteen statistically refined realized niches

7   comprised of three niche dimensions: temperature, irradiance, and nitrate

8   concentrations. The niche scheme assigned the nine phytoplankton groups to three

9   types of niches: a cold type, a warm type, and a type associated with high irradiance

10   and high nitrate concentrations. The fact that phytoplankton groups in cold niches

11   were governed by irradiance and those in warm niches by nitrate is consistent with

12   general ecological theories, but the fact that diatoms were the only dominant group in

13   high-irradiance, high-nitrate niches challenges the idea based on autecological studies

14   that diatoms are generally better adapted to low-irradiance, high-nutrient conditions.

15   When combined with an irradiance model, the niche scheme revealed that

16   photoinhibition of *Prochlorococcus*, which is predicted from autecological studies, is

17   a function of temperature. We used the niche scheme to predict the responses of

18   phytoplankton communities to environmental changes due to seawater warming and

19   eutrophication. The results of the study suggest that a synecological analysis of large

20   databases from field studies facilitates identification of general principles of

21   community ecology that can be used to forecast responses of biological communities

22   to environmental changes.

23   **Keywords**: Phytoplankton community; climate change; synecology; niche

24   classification scheme; South China Sea.

25   **1. Introduction**

26   Whether general ecological principles will emerge from studies of community

27   ecology is a question that has been debated for at least several decades (Eppley 1972,

28   Lawton 1999), but especially after the concept of a *periodic table of niches*, analogous

29   to the periodic table of elements, was proposed by Pianka (1974). The desire to

30   generate such general theories has been stimulated by concerns over the impact of

31   climate change on biological communities (Mcgill et al. 2006). Winemiller et al.

32   (2015) state that "A universal periodic table of niches is unlikely, but instead

33   alternative niche schemes could be developed for making predictions for different

34   groups of organisms in different regions, or for addressing different kinds of

35   problems." They have proposed feasible methods for creating niche schemes from a

36   functional traits perspective as opposed to pairwise species interactions with no

37   environmental context (Winemiller et al. 2015). They suggest use of a niche scheme

38   that involves 1440 possible niches consisting of five niche dimensions, including

39   habitat (4 levels), life history (5 levels), trophic position (6 levels), defense (2 levels),

40   and metabolism (6 levels). However, it is doubtful that a niche scheme based on so

41   many possibilities is going to be of much practical use. So many niches violate a

42   general principle of science, Occam's Razor, which argues that the number of entities

43   (e.g., niches) should not to be multiplied beyond necessity (Baker 2007).

44   In practical applications, the choice of niche dimensions is very much a function

45   of the anticipated application of the niche scheme. To develop a niche scheme that can

46   be used to predict the response of a biological community to climate change, it seems

47   reasonable to begin by using habitat as the niche dimension and ignore the other four

48   dimensions mentioned by Winemiller et al. (2015). The reason is that it is primarily

49   the habitat that we believe climate change will affect, and the distribution of habitats

50   in the future may, in many cases, amount to a rearrangement of habitats in the

51   contemporary environment (Irwin et al. 2012). If the habitats associated with a

52   large-scale field study are sufficiently comprehensive, it may be possible to define a

53   niche table and associated ecological communities that would make possible an

54   informed assessment of the impact of climate change on the composition of

55   communities if future habitats can be characterized with sufficient accuracy.

56   Predicting future changes from niche schemes is of fundamental importance in

57   the case of marine phytoplankton, which are essential components of most marine

58   biogeochemical cycles and food webs (Falkowski et al. 1998) and are likely to

59   undergo significant changes in terms of biomass, community structure, and diversity

60   in response to sea surface warming and ocean acidification (Barton et al. 2010, Boyce

61   et al. 2010, Follows et al. 2007, Gao et al. 2012). However, phytoplankton as a whole

62   are evolutionarily and ecologically diverse and include tens of thousands of species

63   (Sournia et al. 1991). Assigning all species to a variety of niches based on

64 autecological information would be very challenging, and tests conducted with

65 several species or functional types may not adequately represent natural

66 phytoplankton communities (Mutshinda et al. 2017). Hence there is still much

67 uncertainty about the extent to which the impacts of climate change on natural

68 phytoplankton communities can be generalized from autecological studies. An

69 informed assessment of the likely impact of climate change on phytoplankton

70 communities is more likely to result from a synecological study that identifies

71 practical niche schemes in which information about whole phytoplankton

72 communities can be the basis of niche assignments.

73　　One approach to developing such niche schemes based on synecological

74 information is to use simplified indicators to characterize phytoplankton community

75 composition. Phytoplankton community composition estimated from CHEMTAX on

76 the basis of specific marker pigments is one such indicator (Mackey et al. 1996).

77 CHEMTAX is remarkable for its ability to characterize the whole phytoplankton

78 community from picoplankton to large colonies at one time (Mackey et al. 1996).

79 Although the information is limited to taxonomic characterizations at the class level,

80 its advantage is that it facilitates analysis of large datasets.

81　　To create a niche scheme that is useful for predicting phytoplankton community

82 responses to climate change, we used a large-scale field dataset collected from the

83 South China Sea (SCS), the largest marginal sea in the Western Pacific. The dataset

84 contained the full size range of phytoplankton communities estimated from

85 CHEMTAX and covered a wide range of environmental conditions that characterize

86 their habitats. Biogeographic distribution patterns of phytoplankton based on this

87 dataset have been published previously (Xiao et al. 2018b), but there has been no

88 prognosticative analysis of the impact of climate change on the SCS phytoplankton

89 communities. Here, we systematically interpolated the data and developed a niche

90 scheme relating phytoplankton communities to changes of three habitat-related niche

91 dimensions: temperature, irradiance, and nitrate concentrations. Our goal was to

92 predict the response of the composition of phytoplankton communities to future

93 environmental changes using the niche classification scheme.

94 **2. Materials and methods**

95 *2.1. Data sources*

96   We previously compiled a dataset based on 5338 samples that were analyzed for

97 phytoplankton community composition and associated environmental parameters. The

98 samples were collected during 20 cruises in the SCS conducted from February 2004

99 to July 2015 (Chen et al. 2014, Chen et al. 2011, Han et al. 2012, Huang et al. 2010,

100 Wang et al. 2016, Wang et al. 2018, Wang et al. 2015, Xiao et al. 2018b, Yang et al.

101 2015, Zeng et al. 2015). The relative contributions of nine phytoplankton groups to

102 the total chlorophyll *a* (TChl *a*, the sum of monovinyl chlorophyll *a* and divinyl

103 chlorophyll *a*) were calculated using the CHEMTAX program based on thirteen

104 diagnostic   pigments   that   were   determined   by   high-performance   liquid

105   chromatography (HPLC) (for details, see Xiao et al., 2018b). The nine phytoplankton

106   groups included dinoflagellates (Dino), diatoms (Diat), haptophytes_8 (Hapt_8),

107   haptophytes_6 (Hapt_6), chlorophytes (Chlo), cryptophytes (Cryp), *Prochlorococcus*

108   (Proc), *Synechococcus* (Syne), and prasinophytes (Pras).

109   For the present analysis, we excluded the coastal region where the bottom depth

110   was less than 50 m because the nutrient sources and hydrological conditions in the

111   coastal region are complex (Han et al. 2012) and the irradiance data are less reliable

112   (Lee et al. 2007). We focused on the dynamics of phytoplankton communities in the

113   upper mixed layer, where global warming effects are likely to be greatest (Six et al.

114   2007). Similar to other regions worldwide (Johnson et al. 2006, Karl and Church 2014,

115   Laws 2013), high cell abundance, biomass, and relative abundances (contributions to

116   TChl *a*) of most of the dominant groups were generally highest in the upper mixed

117   layer in our study area (Fig. S1).

118   Among the environmental factors that define niche dimensions, we focused on

119   temperature (°C), irradiance at depth (mol quanta m^{-2} d^{-1}), and nitrate concentrations

120   (μmol L^{-1}) because these factors have been demonstrated to be the most important

121   determinants of phytoplankton community structure in the SCS (Ho et al. 2015, Xiao

122   et al. 2018b). Xiao et al. (2018b) have described details of the acquisition and quality

123   control of these parameters. Because the present analysis focused on the upper mixed

124   layer, the relative abundance of each group and the values of each environmental

125   factor were averaged over the mixed layer by trapezoidal integration with the

126   exception of the mean irradiance in the euphotic zone ($\bar{E}$), which was computed as

127   follows:

128 $$\frac{1}{MLD}\int_0^{MLD} E_0 e^{-k_d z}\, dz = \frac{E_0}{k_d MLD}(1 - e^{-k_d MLD}) \tag{1}$$

129   where

130 $$k_d = \ln(0.01)/Z_e \tag{2}$$

131   where z is the integration variable representing depth (m) in the mixed layer, *MLD* is

132   the mixed layer depth, and k_d is the light attenuation coefficient. Z_e is the depth of the

133   euphotic zone, calculated according to Lee et al. (2007); E_0 is the monthly surface

134   photosynthetically active radiation (400–700 nm) obtained from the standard

135   MODIS-Aqua   Level-3   products   at   9   km-pixel   resolution

136   (http://oceandata.sci.gsfc.nasa.gov/MODISA).

137   After being averaged over the mixed layer, the total number of samples was 689,

138   among which 140 samples had no nitrate data. The result is that we had 549 samples

139   in all analyses if nitrate was incorporated.

140   *2.2. Data interpolation for individual niche schemes*

141   The mean temperature, mean irradiance, and mean nitrate in the mixed layer

142   were in the ranges of 20.6–31.2 °C, 1.9–47.4 mol quanta m^{-2} d^{-1}, and 0.001–8.6 µmol

143   L^{-1}, respectively. To investigate the succession of phytoplankton communities along

144   each niche dimension in the mixed layer, we assigned each sample to different

145 intervals of each niche dimension. The number of intervals was 1 greater than the

146 number of boundaries because the first and last interval included all values less than

147 the lowest boundary and greater than the highest boundary, respectively. The interval

148 boundaries of temperature and irradiance were specified to vary every 2 °C in the

149 range 22–30 °C and every 5 mol quanta m^{-2} d^{-1} in the range 5–40 mol quanta m^{-2} d^{-1},

150 respectively. The interval boundaries for nitrate, 0.1, 0.3, 0.5, and 1 μmol L^{-1}, were

151 uneven because the distribution of nitrate concentrations was highly right skewed (Fig.

152 S2). The mean relative abundance of each group and the standard error (SEM,

153 standard deviation divided by the square root of the number of data) were calculated

154 within each specified interval. Although information about realized niches that were

155 obtained via machine learning methods (Generalized Additive Models and Maximum

156 Entropy Models) based on raw data in the upper 150 m has already been described in

157 Xiao et al. (2018b), the present analysis was different in that the data interpolation

158 was based on mean values in the upper mixed layer and thus no complex statistical

159 methods were needed.

160 *2.3. Data reduction, ordination, and classification for a three-dimensional niche*

161 *scheme*

162   In order to create a three-dimensional niche scheme that was useful for

163 characterizing the dynamics of the phytoplankton communities, the samples were

164 divided into a series of bins on the basis of different intervals of temperature,

165   irradiance, and nitrate. The interval boundaries of each niche dimension were the

166   same as the individual niches. These bins represented $\sum_1^5 C_5^i \times \sum_1^8 C_8^j \times \sum_1^4 C_4^k =$

167   118,575 possible three-dimensional niche divisions, where the C_n^m are the number

168   of combinations of n interval boundaries taken m at a time, and the summation is over

169   the number of interval boundaries for temperature (5), irradiance (8), and nitrate (4).

170   The calculations began with one interval boundary for each environmental parameter,

171   and hence there was a minimum of $2^3 = 8$ possible niches and a maximum of $6 \times 9 \times 5 =$

172   270 possible niches. We defined niches for which we had fewer than 3 samples as

173   empty niches and niches with at least 3 samples as realized niches. For each niche

174   division, we removed the empty niches and carried out a one-way analysis of variance

175   on the remaining niches in which we compared the normalized between-niche sum of

176   squares (between-niche variance) to the normalized within-niche sum of squares

177   (within-niche variance) for each of the nine phytoplankton groups. We concluded that

178   the relative abundance of a phytoplankton group varied significantly between niches

179   if the ratio of the between-niche variance to the within-niche variance (V_w)

180   significantly exceeded 1.0 based on an F test. We considered that the division into

181   niches was informative if the smallest F statistic (F_{min}) among the 9 phytoplankton

182   groups exceeded the critical value. The critical value of the F statistic was associated

183   with a type I error rate (p) of 0.005 to ensure that the overall type I error rate was

184   <0.05, i.e., $1 - (0.995)^9 = 0.044$.

185   For the initial case of 8 possible niches, the corresponding candidate boundaries

186 for temperature, irradiance, and nitrate generated $C_5^1 \times C_8^1 \times C_4^1 = 160$ possible

187 combinations. We removed combinations for which the number of empty niches was

188 more than 1. For the 51 remaining combinations, we determined the optimum

189 combination of niche boundaries by varying the boundaries until $F_{\min}$ was a maximum.

190 The computer program that determined the optimum niche boundaries of 8 possible

191 niches is presented as 'R Program 1' in the Supplementary Information.

192   To determine whether further subdivision of the niches was informative, we

193 calculated the within-niche sum of squares with and without one more niche division.

194 We then calculated the statistic F' as follows:

195 $$F' = \frac{(S_{wa} - S_{wb})/(D_{wa} - D_{wb})}{S_{wb}/(D_{wb})} \qquad (3)$$

196 where S_w is the within-niche sum of squares, b and a represent the realized niches

197 with and without one more niche division, and D_{wb} and D_{wa} are the associated degrees

198 of freedom. The additional niche division was judged to have significantly reduced

199 the V_w if the p value associated with F' was <0.005 for the group that had the largest F

200 statistic ($F_{\max}$) among the 9 phytoplankton groups. We chose the combination of niche

201 boundaries that produced the smallest p value. This process was repeated until no

202 significant reduction of the V_w could be achieved by further subdivision of the niches

203 (Table S1). Computer programs that obtained the statistical information of all

204 subdivisions of the optimum niche division of 8 possible niches and determined the

205 final optimum niche division are presented as 'R Program 2' and 'R Program 3',

206   respectively, in the Supplementary Information.

207   The realized niches of the last niche division were selected to create the final

208   three-dimensional niche scheme using a Canonical Correspondence Analysis (CCA)

209   and clustering analysis based on the mean relative abundance of each phytoplankton

210   group and mean values of the associated environmental factors within each niche. A

211   Monte Carlo permutation test was used to test the significance of the correlation

212   between each environmental factor and community composition, and the results

213   showed that all the three environmental factors passed this test ($p < 0.05$ for all cases).

214   The scores of the groups along the first two canonical axes of the CCA were used for

215   clustering analysis. Ward's minimum variance clustering was conducted based on the

216   Euclidean distances among the standardized values of the first two canonical axes.

217   The number of clusters was determined by a scree plot that showed the changes of the

218   within-clusters sum of squares (Fig. S4). The CCA was done using the '*cca*' function

219   of the R package 'vegan' (Borcard et al. 2011). The parameter 'scale' was set as

220   'TRUE' to standardize the environmental factors to zero mean and unit variance. The

221   function '*ordicluster*' in the R package 'vegan' was used to overlay a cluster

222   dendrogram onto the ordination diagram. All analyses were done using R version

223   3.4.4 (R Development Core Team 2018).

224   **3. Results**

225   *3.1. Individual niche schemes*

226   The phytoplankton communities displayed some clear patterns in response to

227   changes in each niche dimension (Fig. 1). With increasing temperature, the relative

228   abundances of *Prochlorococcus*, *Synechococcus*, haptophytes_6, and dinoflagellates

229   increased, whereas those of other groups decreased (Fig. 1a). The system changed

230   from communities dominated by haptophytes_8 and diatoms at low temperatures to

231   communities dominated by *Prochlorococcus* and *Synechococcus* at high temperatures

232   (Fig. 1a). With increasing irradiance, the relative abundance of *Synechococcus*

233   increased greatly, the relative abundances of haptophytes_6 and dinoflagellates

234   increased slightly, and the relative abundances of haptophytes_8, prasinophytes,

235   cryptophytes, and chlorophytes decreased (Figs. 1b). The relative abundance of

236   *Prochlorococcus* was a unimodal function of irradiance with a peak at roughly 10–20

237   mol quanta m^{-2} d^{-1}, whereas that of diatoms was a bimodal function of irradiance,

238   with peaks at roughly 0–5 and 30–40 mol quanta m^{-2} d^{-1} (Fig. 1b). With increasing

239   nitrate concentrations, the relative abundances of diatoms, haptophytes_8,

240   cryptophytes, and chlorophytes increased, whereas those of other groups decreased

241   (Fig. 1c). Most of the trends were nonlinear, and some were clearly not monotonic

242   (Fig. 1). The implication is that these niche dimensions may not act alone but instead

243   may interact.

244   *3.2. Three-dimensional niche scheme*

245   When two levels of each of the three niche dimensions were combined, the

246   boundaries of 26 °C, 20 mol quanta m^{-2} d^{-1}, and 0.3 μmol L^{-1} for temperature,

247   irradiance, and nitrate, respectively, resulted in a largest F_{min} of 5.83 ($p = 6.75\times10^{-6}$)

248   (Fig. 2a). These boundaries defined the optimum niche division of 8 possible niches.

249   If any of the niche intervals increased, the number of possible niches increased in

250   proportion to the number of intervals, but the proportion of empty niches also

251   increased (Fig. 2b). At the same time, the F_{min} decreased with increasing numbers of

252   possible niches (Fig. 2c). The implication is that the significance of the niche division

253   declined with increasing numbers of intervals. As a result, increasing the number of

254   niches increased the percentage of non-significant niche divisions in which the

255   relative abundances of all nine of the phytoplankton groups did not vary significantly

256   (Fig. 2c). For the significant niche divisions, the value of the smallest V_w initially

257   declined as the number of niches increased, but then became constant or increased

258   after the number of possible niches reached about 50 (Fig. 2d). Haptophytes_8 was

259   the group that resulted in the F_{max} for all niche divisions (Fig. S3), and this group was

260   abundant in our study area (Fig. 1). The largest number of possible niches that

261   significantly reduced the V_w of haptophytes_8 was 24 (Tables S1 and S2). The

262   corresponding optimum niche boundaries were 26 and 28 for temperature (°C), 5, 15,

263   and 20 for irradiance (mol quanta m^{-2} d^{-1}), and 0.3 for nitrate (μmol L^{-1}). This

264   division of niche space produced 15 realized niches (Tables S1 and S2). Although

265   these niches were divided according to statistics associated with haptophytes_8, the

266   percentages of the total variance of each of the other eight phytoplankton groups that

267   were accounted for by the 15 realized niches were quite high (76%–96%) (Table S3).

268   We used the mean values of the 15 realized niches (Table S2) to create a

269   three-dimensional niche scheme. No significant correlations were found between all

270   pairs of environmental factors based on their mean values ($p > 0.05$ for all cases).

271   The CCA revealed that the 15 niches explained 81% of the variance of the

272   phytoplankton communities, almost all of which was contributed by the first two

273   canonical axes (Fig. 3). The ordination diagram based on the first two canonical axes

274   created a clear niche classification scheme for the phytoplankton communities (Fig. 3).

275   The first canonical axis was contributed mainly by nitrate, and the second canonical

276   axis by temperature-related factors (temperature and irradiance). The scree plot

277   showed that there was an "elbow" at the three-cluster solution, the suggestion being

278   that clusters >3 did not have a substantial impact on the total within-cluster sum of

279   squares. The dendrogram of the nine phytoplankton groups also showed three major

280   branches. One branch was linked to the diatom group, which was assigned to the two

281   niches with high values of both irradiance and nitrate concentration. The other two

282   branches divided the other eight groups into a cold type and a warm type. The cold

283   type included haptopytes_8, prasinophytes, cryptophytes, and chlorophytes, which

284   were linked to the niches associated with low temperature and irradiance. The warm

285   type included *Prochlorococcus*, *Synechococcus*, dinoflagellates, and haptophytes_6,

286   which were related to the niches associated with high temperature and irradiance. The

287   cold type groups were first classified along irradiance, whereas the warm type groups

288　were first classified along nitrate. Among the warm type groups, *Synechococcus* was

289　close to the niches with the highest irradiance level (20–45 mol quanta m^{-2} d^{-1}),

290　whereas *Prochlorococcus* was mostly linked to the niches with intermediate

291　irradiance (5–20 mol quanta m^{-2} d^{-1}) at temperatures higher than 26 °C and the niche

292　with the highest irradiance level at lower temperatures. In addition, *Prochlorococcus*

293　was more negatively correlated with nitrate than *Synechococcus* (Fig. 3). Because the

294　number of samples in each niche varied from 5 to 277 (Table S2), we randomly

295　picked five samples from those niches that had more than five samples to calculate the

296　average. We then used those mean values to create a three-dimensional niche scheme.

297　The randomization was repeated 10 times, and the resulting niche schemes were

298　almost the same as in Fig. 3. One such example is presented in Fig. S5.

299　**4. Discussion**

300　*4.1. Practical considerations limit the number of niches*

301　　We found that increasing the number of possible niches decreased the F_{min} and

302　increased the fraction of non-significant niche divisions (Fig. 2c). In addition, the

303　decreasing trend of the V_w of all nine phytoplankton groups stopped after the number

304　of possible niches reached about 50 (Fig. 2d). These results reflect the fact that the

305　need to increase niches decreased with increasing numbers of possible niches, and

306　there was a maximum number of niches above which further subdivision of the niches

307　did not significantly reduce the estimate of the V_w for all nine of the phytoplankton

308   groups. Increasing the number of possible niches is the analog of adding more terms

309   to a polynomial function to describe a curvilinear function. Because there is

310   invariably some noise in data, at some point adding more terms to the polynomial

311   amounts to fitting noise as opposed to the underlying relationship (Laws 1997). Based

312   on similar logic, too fine a division of niches may amount to fitting noise. The reason

313   is that temperature, irradiance, and nitrate do not explain all of the variability of

314   phytoplankton community composition, so further subdividing the niche dimension

315   amounts to fitting variability that is probably explained by factors other than these

316   three environmental variables. In the case of polynomial regression, there is a

317   straightforward way to decide when the function is fitting noise. The strategy is to

318   find the point when the F statistic is lower than the critical F value (Laws 1997).

319   Similarly, we used an F statistic (F') on the basis of decreases in V_w to decide how

320   many niches to create. Our procedure selected 15 realized niches that resulted from 24

321   possible niches that consisted of 3 temperature levels, 4 irradiance levels, and 2 nitrate

322   levels as the last significant niche division (Table S1). Such a small number of niches

323   suggests that there is a practical limit to the number of niches that can be used for

324   groups of organisms in specific regions.

325   *4.2. Simplified niche scheme meets the goal of Occam's Razor*

326   Using the 15 realized niches, we created a three-dimensional niche classification

327   scheme that related phytoplankton communities to the niches via CCA and clustering

328   analysis (Fig. 3). The CCA results revealed that the 15 niches accounted for 81% of

329   the variability of the phytoplankton community composition. Such a high percentage

330   of the variance accounted for was possible because the number of niches was small

331   and the community information was represented by only nine groups at the class level

332   rather than a much larger number of species. The simplification (i.e., reducing the

333   number) of niches decreased the between-niche sum of squares (S_b) that the CCA

334   explained, whereas the simplification of communities may have decreased the S_w that

335   the CCA ignored but would show up as S_b with more niches being created. A CCA

336   analysis using the 549 raw samples produced a figure (Fig. S6) with a shape similar to

337   Fig. 3, but the percentage of the variance explained was much lower, and it was not

338   easy to distinguish the niches of the phytoplankton groups. Our results suggest that

339   simplification of both niches and communities is key to developing a niche scheme

340   that is able to yield realistic estimates of how phytoplankton communities might

341   respond to the impact of climate change. This simplification is the goal of Occam's

342   Razor, which aims to make the analysis no more complicated than necessary, or

343   equivalently, keep the analysis as simple as possible (Baker 2007). The idea of

344   representing the phytoplankton communities in terms of a small number of groups

345   rather than a large number of species is a common practice in food web models (Laws

346   2008), ocean biogeochemical models (Hood et al. 2006), and trait-based approaches

347   (Litchman et al. 2007). There is evidence that emergent simplicity in the microbial

348   community assemblage at higher levels of organization is a generic property of large,

349   diverse systems (Goldford et al. 2017). There are also precedents for holding the

350   number of habitats to single digits. For instance, Bala et al. (2005) have broken down

351   climate zones into 7 categories to address the effect of climate on the distribution of

352   vegetation. Manipulation experiments also tend to follow the principle of Occam's

353   Razor and keep the number and levels of variables small (Burson et al. 2018,

354   Lewandowska et al. 2014). Our analysis is therefore a useful guide for experiments

355   aimed at discerning how phytoplankton communities will respond to climate change.

356   *4.3. Synecological findings support known ecological theories*

357   Our niche scheme separated two critical ecological systems from each other, the

358   River-dominated Ocean Margin (RiOMar) and the Ocean-dominated Margin (OceMar)

359   (Dai et al. 2013). These systems are characterized by the left side and the right side of

360   the scheme, respectively (Fig. 3). Phytoplankton communities are regulated mainly by

361   nitrate and irradiance in the RiOMar system and by temperature-related factors in the

362   OceMar system (Fig. 3). The scheme has also revealed two types of groups in the

363   OceMar system, a cold type and a warm type (Fig. 3). We found that the groups of the

364   cold type were divided primarily by irradiance, whereas those of the warm type were

365   divided primarily by nitrate (Fig. 3). These results are consistent with the general

366   view that temperature influences plankton mainly by changing metabolic rates

367   (related to the balance of photosynthesis and respiration) in cold waters and mainly by

368   affecting nutrient supply in warm waters (Lewandowska et al. 2014). Because

369 temperature and nutrient supply are often negatively correlated in the open ocean

370 (Finkel et al. 2010), our results are also consistent with the theoretical resource

371 competition model for phytoplankton communities, which assumes that the species

372 interaction shifts from competition for light to competition for nutrients as nutrient

373 supplies decrease and vice versa (Huisman and Weissing 1995). These consistencies

374 indicate that our niche classification scheme is sufficiently general and may be

375 broadly applicable.

376 *4.4. Synecological findings challenge some views based on autecological studies*

377 Our niche scheme clearly assigned diatoms to the niches with both high nitrate

378 concentrations and high light intensity (Fig. 3). Culture studies have suggested that

379 diatoms are generally better adapted to low irradiances under high-nutrient and

380 strong-mixing conditions (Falkowski 1980). Our analysis does not support this

381 paradigm. The reason for this disagreement might be that our approach was

382 synecological rather than autecological. Our field database included the relative

383 abundances of a full range of sizes of phytoplankton at the class level. Synecology

384 considers that the competitive ability of a group depends not only on the physiological

385 response of the group itself but also on that of other groups (Walter and Hengeveld

386 2000). Under very low-light conditions, other groups, especially haptophytes_8, could

387 outcompete diatoms (Fig. 1c) at low temperatures, such as a well-mixed water column

388 in the winter (Schoemann et al. 2005). However, light-sufficient and nutrient-rich

389   environments in the SCS reflect the impact of the eutrophic and highly stratified Pearl

390   River freshwater plumes in the northern SCS during warm seasons, and under such

391   variable and co-limiting conditions diatoms tend to outperform other groups (Ning et

392   al. 2004). Similar results have been found in the East China Sea (Liu et al. 2016, Xiao

393   et al. 2018a) and in competition experiments using natural phytoplankton

394   communities as inocula (Burson et al. 2018). We therefore suggest that the results of

395   autecological studies of a limited number of species without consideration of

396   inter-species interactions can be misleading with respect to predictions of effects in

397   the real ocean.

398   Although photoinhibition of *Prochlorococcus* has been reported previously

399   (Chen et al. 2014, Flombaum et al. 2013, Six et al. 2007, Xie et al. 2018, Zinser et al.

400   2007), our niche scheme revealed that *Prochlorococcus* was linked to a high

401   irradiance niche at low temperatures but to intermediate irradiance niches at high

402   temperatures (Fig. 3). The implication is that the irradiance niche of *Prochlorococcus*

403   depends on temperature. All phytoplankton are adversely affected if the irradiance to

404   which they are exposed becomes too great (Litchman and Klausmeier 2008). This

405   effect is generally characterized as photoinhibition and is related to the production of

406   reactive oxygen species (Nishiyama et al. 2006). Because this study was of a

407   synecological rather than autecological nature, a decline of the relative abundance of a

408   group of phytoplankton at high irradiance could be related to photoinhibition, or it

409   could simply mean that other groups of phytoplankton were better able to exploit high

410   irradiances. To incorporate the effects of high irradiance in our synecological study,

411   we used a model that has been used to describe photoinhibition in autecological

412   research (Platt 1980, Xie et al. 2015), but with the caveat that the model is purely

413   descriptive and is not meant to imply cause-and-effect. The model was formulated as

414   follows:

415    $$P = a + P_m(1 - e^{-E\alpha/P_m})e^{-bE\alpha/P_m} \tag{4}$$

416   In Equation (4), P is the relative abundance of a phytoplankton group, and E is the

417   explanatory variable irradiance. The parameter a is the intercept, and α is the initial

418   slope of the P vs. E curve. P_m is the light-saturated relative abundance of the group in

419   the absence of "photoinhibition", and b is a dimensionless "photoinhibition"

420   parameter. The combination of $b\alpha/P_m$ reflects the strength of "photoinhibition".

421   We fitted the model at three temperature intervals, low (24–26 °C), medium

422   (26–28 °C), and high (28–30 °C) (Fig. 4). The irradiance model provided further

423   evidence that "photoinhibition" of *Prochlorococcus* existed at all temperatures (Fig.

424   4). This 'photoinhibition' may be due to the fact that *Synechococcus* did better than

425   *Prochlorococcus* at high irradiance (Fig. S7). The "photoinhibition" at moderate and

426   high temperatures was the same, but it was twice as high at those temperatures as at

427   low temperatures, and the threshold at which light became inhibitory was lower at

428   moderate   and   high   temperatures   (Fig.   4).   These   results   indicate   that   the

429   "photoinhibition" effect on *Prochlorococcus* is a saturation function of temperature.

430   This saturation function very likely resulted from the fact that the relative abundances

431   of other groups such as *Synechococcus* and diatoms were lower at low temperatures

432   than at higher temperatures (Fig. S7). This discovery suggests that, from a

433   synecological standpoint, one cannot assume that the "photoinhibition" of

434   *Prochlorococcus* is a fixed trait but should take temperature as an important covariate

435   when predicting climate change effects.

436   *4.5. Responses of phytoplankton communities to environmental changes*

437   Our niche scheme provided an opportunity to make inferences about possible

438   effects of environmental changes on phytoplankton communities. Global warming is

439   expected to lead to increases of sea surface temperature, greater thermal stratification

440   of the upper water column, and a reduction of nutrient inputs to the mixed layer from

441   sub-nutricline waters (shallower mixed layers and less upwelling) in the coming

442   century (Doney et al. 2012). There is also evidence that warming could bring more

443   frequent and extreme rain events (Wentz et al. 2007), which would increase the

444   impact of land runoff on coastal waters. Anthropogenic nutrient pollution would add

445   to the eutrophication of coastal waters caused by these freshwater plumes (Anderson

446   et al. 2002). Under such conditions, the cold type groups such as haptophytes_8,

447   prasinophytes, cryptophytes, and chlorophytes would presumably be at a disadvantage

448   because they were assigned to the low-temperature, low-irradiance niches (Fig. 3).

449   The diatom group was linked to the high-nitrate and high-irradiance niches (Fig. 3).

450   The impact on diatoms would therefore be mixed: they would benefit from higher

451   irradiance in nutrient-replete waters, such as most coastal regions, seasonally mixed

452   shelf seas, and eutrophic freshwater plumes, but they would be adversely affected by

453   the higher temperatures (fewer nutrients) in nutrient-limited waters such as the

454   seasonally stratified shelf seas and oligotrophic open ocean.

455   The warm type groups, including *Prochlorococcus*, *Synechococcus*,

456   dinoflagellates, and haptophytes_6, would benefit from sea-surface warming. This

457   would be especially true for *Prochlorococcus* and *Syenchococcus*. However, the

458   relative competitive ability of these two picophytoplankton would depend on the

459   nutrient status of their habitat. In mesotrophic environments such as stratified shelf

460   seas, mixed open oceans, and mesotrophic freshwater plumes, *Synechococcus* would

461   benefit more than *Prochlorococcus* because its irradiance and nitrate niches are higher

462   than those of *Prochlorococcus* (Fig. 3) and the effect of "photoinhibition" on

463   *Prochlorococcus* would be twice as great if the temperature increased by more than 2

464   °C (Fig. 4). This is very likely to happen by the year 2100 because at that time a

465   temperature rise of 2 °C compared to the pre-industrial era has been predicted by

466   scenarios of the Representative Concentration Pathways (RCP) 4.5−8.5 in most of the

467   ocean, especially in high latitudes of the northern hemisphere (Gattuso et al. 2015,

468   Stocker et al. 2013). In stratified oligotrophic waters, *Prochlorococcus* would have an

469   advantage over other groups because the negative effect of temperature on other

470   groups would be enhanced, but the "photoinhibition" effect on *Prochlorococcus*

471   would be the same (Fig. 4).

472   Changes of phytoplankton communities can have large impacts on aquatic

473   ecosystems and global biogeochemical cycles (Litchman et al. 2007). Whether the

474   observed results are unique for the SCS or are widespread among other marine

475   ecosystems remains to be determined. Our analyses were based on a synthesis of a

476   large-scale field database spanning more than 10 years rather than on a few cases. A

477   caveat of our niche classification scheme is that the sample sizes varied greatly

478   between niches. Although this did not change our results because we used only mean

479   values, there is still a need to collect more field observations to expand the sample

480   sizes. Another caveat is that our inferences on responses of phytoplankton

481   communities to climate changes were based solely on a CCA analysis, which is

482   qualitative and does not reveal causation. Controlled experiments are needed to test

483   whether our results are reproducible. Also, we did not consider the other four niche

484   dimensions proposed by Winemiller et al. (2015), including life history, trophic

485   position, defense, and metabolism. These four dimensions may collectively be

486   associated with ocean acidification (Gao et al. 2012), nutrient ratios (Klausmeier et al.

487   2004), grazing by zooplankton (Edwards and Richardson 2004, Lewandowska et al.

488   2014), and losses to viruses or pathogens (Burson et al. 2018). However, because the

489   percent of the total variance accounted for by the 15 realized niches was 76−99% for

490   all nine phytoplankton groups (Table S3), addition of more dimensions would be

491   unlikely to greatly improve the explanatory capability of the niche classification

492   scheme. Furthermore, our purpose was to identify the important and available niche

493   dimensions and try to keep things simple according to the principle of Occam's Razor.

494   If one other niche dimension is invoked, the number of niches will be immediately

495   doubled, and of course the number of niches becomes a geometric series as more

496   dimensions are added.

497   **5. Conclusions**

498   This study provided a novel approach for selecting optimum niche numbers and

499   niche boundaries to produce a simplified phytoplankton niche classification scheme

500   that characterizes the full size range of phytoplankton communities. The main

501   conclusions can be summarized as follows:

502   • There is a practical limit to how many niches the niche table contains for the

503   purpose of predicting the responses of phytoplankton communities to climate

504   changes.

505   • The simplified niche scheme supported general ecological theories, such as

506   physical and metabolic pathways of warming effects on plankton and

507   theoretical resource competition models for phytoplankton communities.

508   • The niche scheme also challenged some concepts based on autecological

509   studies on two phytoplankton groups, diatoms and *Prochlorococcus*, and

510   thereby enabled more informed predictions of their fates under future climate

511   change scenarios.

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References

Anderson, D.M., Glibert, P.M. and Burkholder, J.M. (2002) Harmful algal blooms and eutrophication: nutrient sources, composition, and consequences. Estuaries 25(4), 704-726.

Baker, A. (2007) Occam's Razor in science: a case study from biogeography. Biology and Philosophy 22(2), 193-215.

Bala, G., Caldeira, K., Mirin, A., Wickett, M. and Delire, C. (2005) Multi-century changes to global climate and carbon cycle: Results from a coupled climate and carbon cycle model. Journal of Climate 18(21), 4531-4544.

Barton, A.D., Dutkiewkz, S., Flierl, G., Bragg, J. and Follows, M.J. (2010) Patterns of diversity in marine phytoplankton. Science 327(5972), 1509-1511.

Borcard, D., Gillet, F. and Legendre, P. (2011) Numerical ecology with R, Springer, New York.

Boyce, D.G., Lewis, M.R. and Worm, B. (2010) Global phytoplankton decline over the past century. Nature 466(7306), 591-596.

Burson, A., Stomp, M., Greenwell, E., Grosse, J. and Huisman, J. (2018) Competition for nutrients and light: testing advances in resource competition with a natural phytoplankton community. Ecology 0(0), 1-11.

Chen, B., Liu, H., Huang, B. and Wang, J. (2014) Temperature effects on the growth rate of marine picoplankton. Marine Ecology Progress Series 505, 37-47.

Chen, B., Wang, L., Song, S., Huang, B., Sun, J. and Liu, H. (2011) Comparisons of picophytoplankton abundance, size, and fluorescence between summer and winter in northern South China Sea. Continental Shelf Research 31(14), 1527-1540.

Dai, M., Cao, Z., Guo, X., Zhai, W., Liu, Z., Yin, Z., Xu, Y., Gan, J., Hu, J. and Du, C. (2013) Why are some marginal seas sources of atmospheric CO_2? Geophysical Research Letters 40(10), 2154-2158.

Doney, S.C., Ruckelshaus, M., Duffy, J.E., Barry, J.P., Chan, F., English, C.A., Galindo, H.M., Grebmeier, J.M., Hollowed, A.B. and Knowlton, N. (2012) Climate change impacts on marine ecosystems. Annual Review of Marine Science 4(1), 11-37.

Edwards, M. and Richardson, A.J. (2004) Impact of climate change on marine pelagic phenology and trophic mismatch. Nature 430(7002), 881-884.

Eppley, R.W. (1972) Temperature and phytoplankton growth in the sea. Fishery Bulletin 70(4), 1063-1085.

Falkowski, P.G. (1980) Light-shade adaptation in marine phytoplankton, Springer, New York.

Falkowski, P.G., Barber, R.T. and Smetacek, V. (1998) Biogeochemical controls and feedbacks on ocean primary production. Science 281(5374), 200-207.

Finkel, Z.V., Beardall, J., Flynn, K.J., Quigg, A., Rees, T.A.V. and Raven, J.A. (2010) Phytoplankton in a changing world: cell size and elemental stoichiometry. Journal of Plankton Research 32(1), 119-137.

Flombaum, P., Gallegos, J.L., Gordillo, R.A., Rincón, J., Zabala, L.L., Jiao, N., Karl,

D.M., Li, W.K.W., Lomas, M.W. and Veneziano, D. (2013) Present and future global distributions of the marine Cyanobacteria *Prochlorococcus* and *Synechococcus*. Proceedings of the National Academy of Sciences of the United States of America 110(24), 9824-9829.

Follows, M.J., Dutkiewicz, S., Grant, S. and Chisholm, S.W. (2007) Emergent biogeography of microbial communities in a model ocean. Science 315(5820), 1843-1846.

Gao, K., Xu, J., Gao, G., Li, Y. and Hutchins, D.A. (2012) Rising CO_2 and increased light exposure synergistically reduce marine primary productivity. Nature Climate Change 2(7), 519-523.

Gattuso, J.P., Magnan, A., Billé, R., Cheung, W.W., Howes, E.L., Joos, F., Allemand, D., Bopp, L., Cooley, S.R. and Eakin, C.M. (2015) Contrasting futures for ocean and society from different anthropogenic CO_2 emissions scenarios. Science 349(6243), aac4722.

Goldford, J.E., Lu, N., Bajic, D., Estrela, S., Tikhonov, M., Sanchez-Gorostiaga, A., Segre, D., Mehta, P. and Sanchez, A. (2017) Emergent simplicity in microbial community assembly. Science 361(6401), 469-474.

Han, A., Dai, M., Kao, S., Gan, J., Li, Q., Wang, L., Zhai, W. and Wang, L. (2012) Nutrient dynamics and biological consumption in a large continental shelf system under the influence of both a river plume and coastal upwelling. Limnology and Oceanography 57(2), 486-502.

Ho, T.Y., Pan, X., Yang, H.H., George, T.F.W. and Shiah, F.K. (2015) Controls on temporal and spatial variations of phytoplankton pigment distribution in the Northern South China Sea. Deep Sea Research Part II: Topical Studies in Oceanography 117(6), 65-85.

Hood, R.R., Laws, E.A., Armstrong, R.A., Bates, N.R., Brown, C.W., Carlson, C.A., Chai, F., Doney, S.C., Falkowski, P.G. and Feely, R.A. (2006) Pelagic functional group modeling: Progress, challenges and prospects. Deep-Sea Research Part II: Topical Studies in Oceanography 53(5), 459-512.

Huang, B., Hu, J., Xu, H., Cao, Z. and Wang, D. (2010) Phytoplankton community at warm eddies in the northern South China Sea in winter 2003/2004. Deep Sea Research Part II: Topical Studies in Oceanography 57(19–20), 1792-1798.

Huisman, J. and Weissing, F.J. (1995) Competition for nutrients and light in a mixed water column: a theoretical analysis. American Naturalist 146(4), 536-564.

Irwin, A.J., Nelles, A.M. and Finkel, Z.V. (2012) Phytoplankton niches estimated from field data. Limnology and Oceanography 57(3), 787-797.

Johnson, Z.I., Zinser, E.R., Coe, A., McNulty, N.P., Woodward, E.M.S. and Chisholm, S.W. (2006) Niche partitioning among *Prochlorococcus* ecotypes along ocean-scale environmental gradients. Science 311(5768), 1737-1740.

Karl, D.M. and Church, M.J. (2014) Microbial oceanography and the Hawaii Ocean Time-series programme. Nature Reviews Microbiology 12(10), 699-713.

Klausmeier, C.A., Litchman, E., Daufresne, T. and Levin, S.A. (2004) Optimal nitrogen-to-phosphorus stoichiometry of phytoplankton. Nature 429(6988), 171-174.

611 Laws, E.A. (1997) Mathematical methods for oceanographers: an introduction, John
612   Wiley & Sons, New York.
613 Laws, E.A. (2008) Food-web structure and planktonic predator-prey relationships in
614   two eutrophic european lakes: Stability constraints on carbon fluxes. Limnology
615   and Oceanography 53(2), 760-772.
616 Laws, E.A. (2013) Evaluation of in situ phytoplankton growth rates: a synthesis of
617   data from varied approaches. Annual Review of Marine Science 5(1), 247-268.
618 Lawton, J.H. (1999) Are there general laws in ecology? Oikos 84(2), 177-192.
619 Lee, Z., Weidemann, A., Kindle, J., Arnone, R., Carder, K.L. and Davis, C. (2007)
620   Euphotic zone depth: Its derivation and implication to ocean‐color remote
621   sensing. Journal of Geophysical Research: Oceans 112, C03009.
622 Lewandowska, A.M., Boyce, D.G., Hofmann, M., Matthiessen, B., Sommer, U. and
623   Worm, B. (2014) Effects of sea surface warming on marine plankton. Ecology
624   Letters 17(5), 614-623.
625 Litchman, E. and Klausmeier, C.A. (2008) Trait-based community ecology of
626   phytoplankton. Annual Review of Ecology, Evolution, and Systematics, 615-639.
627 Litchman, E., Klausmeier, C.A., Schofield, O.M. and Falkowski, P.G. (2007) The role
628   of functional traits and trade-offs in structuring phytoplankton communities:
629   scaling from cellular to ecosystem level. Ecology Letters 10(12), 1170-1181.
630 Liu, X., Xiao, W., Landry, M.R., Chiang, K.-P., Wang, L. and Huang, B. (2016)
631   Responses of phytoplankton communities to environmental variability in the
632   East China Sea. Ecosystems 19(5), 832-849.
633 Mackey, M.D., Mackey, D.J., Higgins, H.W. and Wright, S.W. (1996) CHEMTAX - A
634   program for estimating class abundances from chemical markers: Application to
635   HPLC measurements of phytoplankton. Marine Ecology Progress Series
636   144(1-3), 265-283.
637 Mcgill, B.J., Enquist, B.J., Weiher, E. and Westoby, M. (2006) Rebuilding community
638   ecology from functional traits. Trends in Ecology and Evolution 21(4), 178-185.
639 Mutshinda, C.M., Finkel, Z.V., Widdicombe, C.E. and Irwin, A.J. (2017)
640   Phytoplankton traits from long-term oceanographic time-series. Marine Ecology
641   Progress Series 576, 11-25.
642 Ning, X., Chai, F., Xue, H., Cai, Y., Liu, C., Zhu, G. and Shi, J. (2004)
643   Physical-biological oceanographic coupling influencing phytoplankton and
644   primary production in the South China Sea. Journal of Geophysical Research:
645   Oceans 110(C5), 215-255.
646 Nishiyama, Y., Allakhverdiev, S.I. and Murata, N. (2006) A new paradigm for the
647   action of reactive oxygen species in the photoinhibition of photosystem II.
648   Biochimica et Biophysica Acta 1757(7), 742-749.
649 Pianka, E.R. (1974) Evolutionary ecology, Harper and Row, New York.
650 Platt, T. (1980) Photoinhibition of photosynthesis in natural assemblages of marine
651   phytoplankton. Journal of Marine Research 38(57), 341-345.
652 R Development Core Team (2018) R: a language and environment for statistical
653   computing. Vienna, Austria: R Foundation for Statistical Computing.
654 Schoemann, V., Becquevort, S., Stefels, J., Rousseau, V. and Lancelot, C. (2005)

655   Phaeocystis blooms in the global ocean and their controlling mechanisms: a
656   review. Journal of Sea Research 53(1), 43-66.

657 Six, C., Finkel, Z.V., Irwin, A.J. and Campbell, D.A. (2007) Light variability
658   illuminates niche-partitioning among marine picocyanobacteria. Plos One 2(12),
659   e1341.

660 Sournia, A., Chrdtiennotdinet, M.J. and Ricard, M. (1991) Marine phytoplankton:
661   how many species in the world ocean? Journal of Plankton Research 13(5),
662   1093-1099.

663 Stocker, T.F., Qin, D., Plattner, G.-K., Tignor, M., Allen, S.K., Boschung, J., Nauels,
664   A., Xia, Y., Bex, V. and Midgley, P.M. (2013) Climate change 2013: The physical
665   science basis, Cambridge University Press, Cambridge.

666 Walter, G.H. and Hengeveld, R. (2000) The structure of the two ecological paradigms.
667   Acta Biotheoretica 48(1), 15-46.

668 Wang, L., Huang, B., Chiang, K.P., Liu, X., Chen, B., Xie, Y., Xu, Y., Hu, J. and Dai,
669   M. (2016) Physical-biological coupling in the western South China Sea: The
670   response of phytoplankton community to a mesoscale cyclonic eddy. Plos One
671   11(4), e0153735.

672 Wang, L., Huang, B., Laws, E.A., Zhou, K., Liu, X., Xie, Y. and Dai, M. (2018)
673   Anticyclonic eddy edge effects on phytoplankton communities and particle
674   export in the northern South China Sea. Journal of Geophysical Research:
675   Oceans, C23110.

676 Wang, L., Huang, B., Liu, X. and Xiao, W. (2015) The modification and optimizing of
677   the CHEMTAX running in the South China Sea. Acta Oceanologica Sinica 34(2),
678   124-131.

679 Wentz, F.J., Lucrezia, R., Kyle, H. and Carl, M. (2007) How much more rain will
680   global warming bring? Science 317(5835), 233-235.

681 Winemiller, K.O., Fitzgerald, D.B., Bower, L.M. and Pianka, E.R. (2015) Functional
682   traits, convergent evolution, and periodic tables of niches. Ecology Letters 18(8),
683   737-751.

684 Xiao, W., Liu, X., Irwin, A.J., Laws, E.A., Wang, L., Chen, B., Zeng, Y. and Huang, B.
685   (2018a) Warming and eutrophication combine to restructure diatoms and
686   dinoflagellates. Water Research 128, 206-216.

687 Xiao, W., Wang, L., Laws, E., Xie, Y., Chen, J., Liu, X., Chen, B. and Huang, B.
688   (2018b) Realized niches explain spatial gradients in seasonal abundance of
689   phytoplankton groups in the South China Sea. Progress in Oceanography 162,
690   223-239.

691 Xie, Y., Huang, B., Lin, L., Laws, E.A., Wang, L., Shang, S., Zhang, T. and Dai, M.
692   (2015) Photosynthetic parameters in the northern South China Sea in relation to
693   phytoplankton community structure. Journal of Geophysical Research: Oceans
694   120(6), 4187-4204.

695 Xie, Y., Laws, E.A., Yang, L. and Huang, B. (2018) Diel patterns of variable
696   fluorescence and carbon fixation of picocyanobacteria
697   *Prochlorococcus*-dominated phytoplankton in the South China Sea basin.
698   Frontiers in Microbiology 9, 1598.

699 Yang, L., Wang, D., Huang, J., Wang, X., Zeng, L., Shi, R., He, Y., Xie, Q., Wang, S.
700   and Chen, R. (2015) Toward a mesoscale hydrological and marine
701   meteorological observation network in the South China Sea. Bulletin of the
702   American Meteorological Society 96(7), 1117-1135.
703 Zeng, L., Wang, Q., Xie, Q., Shi, P., Yang, L., Shu, Y., Chen, J., Sui, D., He, Y. and
704   Chen, R. (2015) Hydrographic field investigations in the Northern South China
705   Sea by open cruises during 2004–2013. Science Bulletin 60(6), 607-615.
706 Zinser, E.R., Johnson, Z.I., Coe, A., Karaca, E., Veneziano, D. and Chisholm, S.W.
707   (2007) Influence of light and temperature on *Prochlorococcus* ecotype
708   distributions in the Atlantic Ocean. Limnology and Oceanography 52(5),
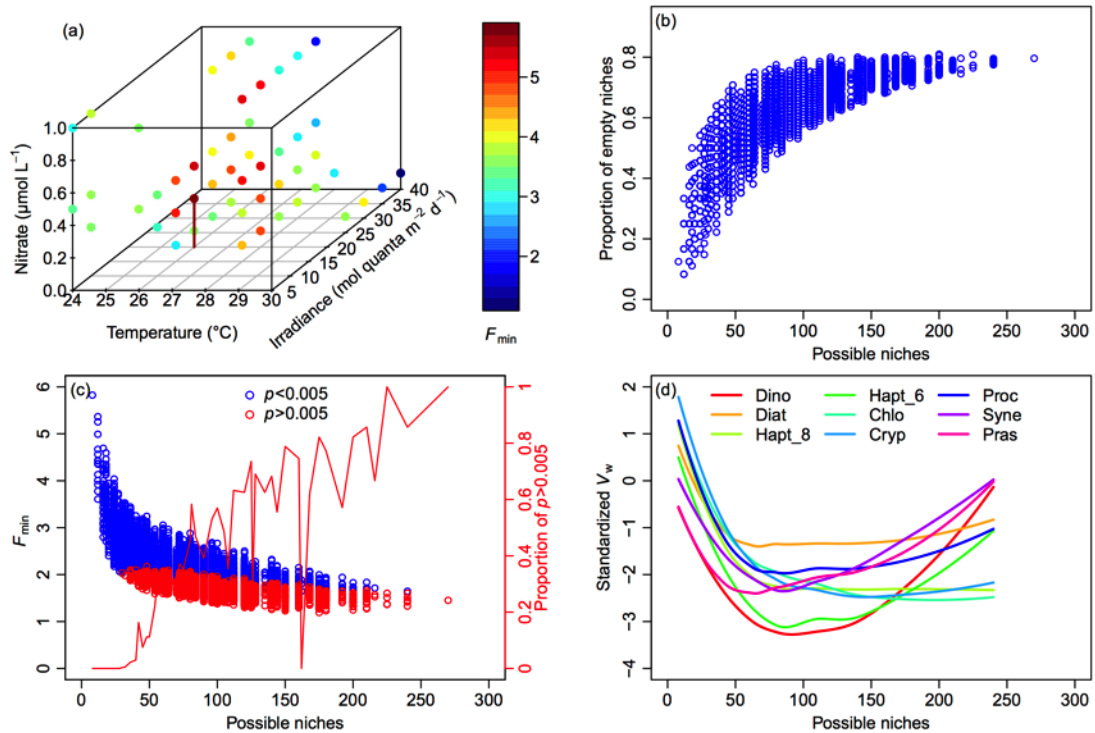709   2205-2220.

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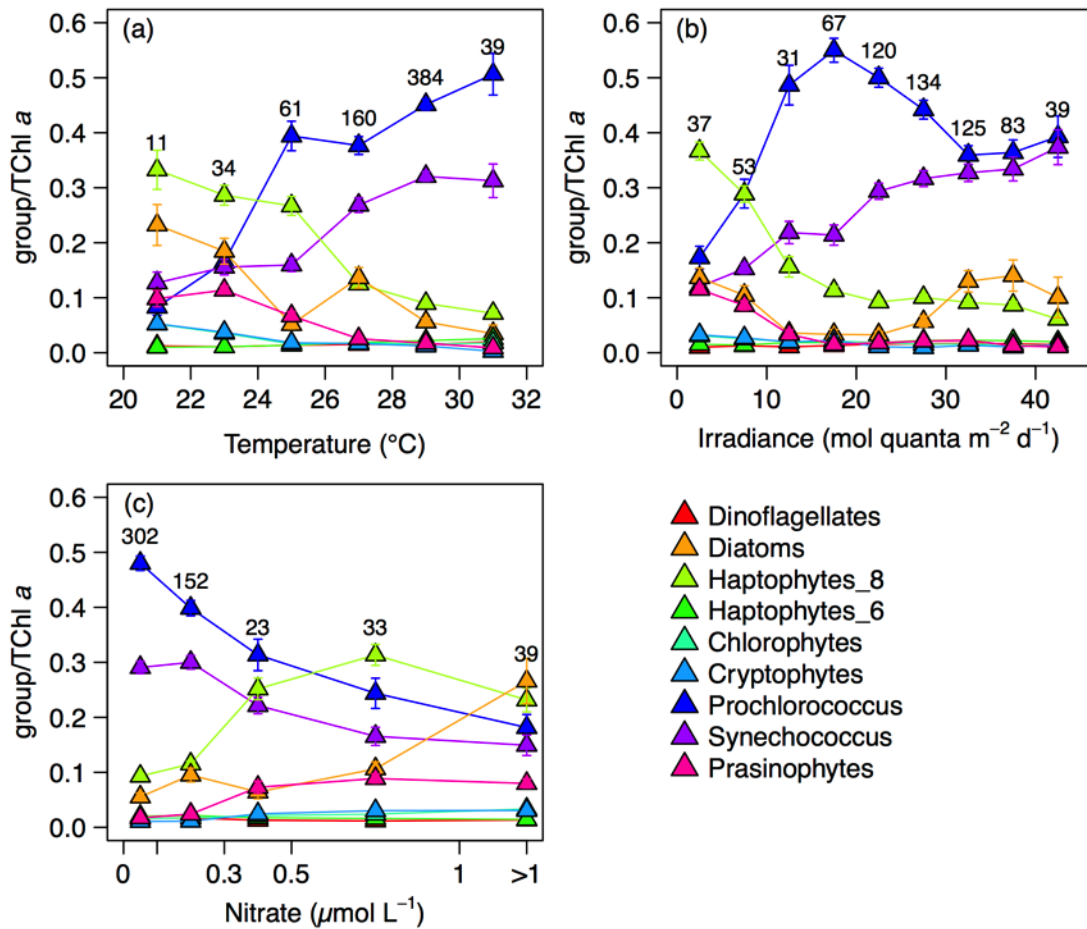
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712 **Fig. 1** Relative abundances of phytoplankton groups as a function of individual niche

713 dimensions in the upper mixed layer. Error bars are the SEM. Digits above each bin

714 show sample sizes. The total number of samples was 689 for (**a**) and (**b**) and 549 for

715 (**c**).

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Fig. 2 Statistical information for deciding where to draw the boundaries between niches and how many niches to create. (**a**) The F_{min} resulted from 8 possible niches versus niche boundaries; the optimum boundaries were marked in a dark red line; the niche divisions with more than one empty niche were removed. (**b**) The proportion of empty niches versus the numbers of all possible niches. (**c**) The F_{min} and the proportion of non-significant niche divisions ($p > 0.005$) versus the numbers of all possible niches. (**d**) Loess curves between the smallest standardized V_w (within-niche variance) and the numb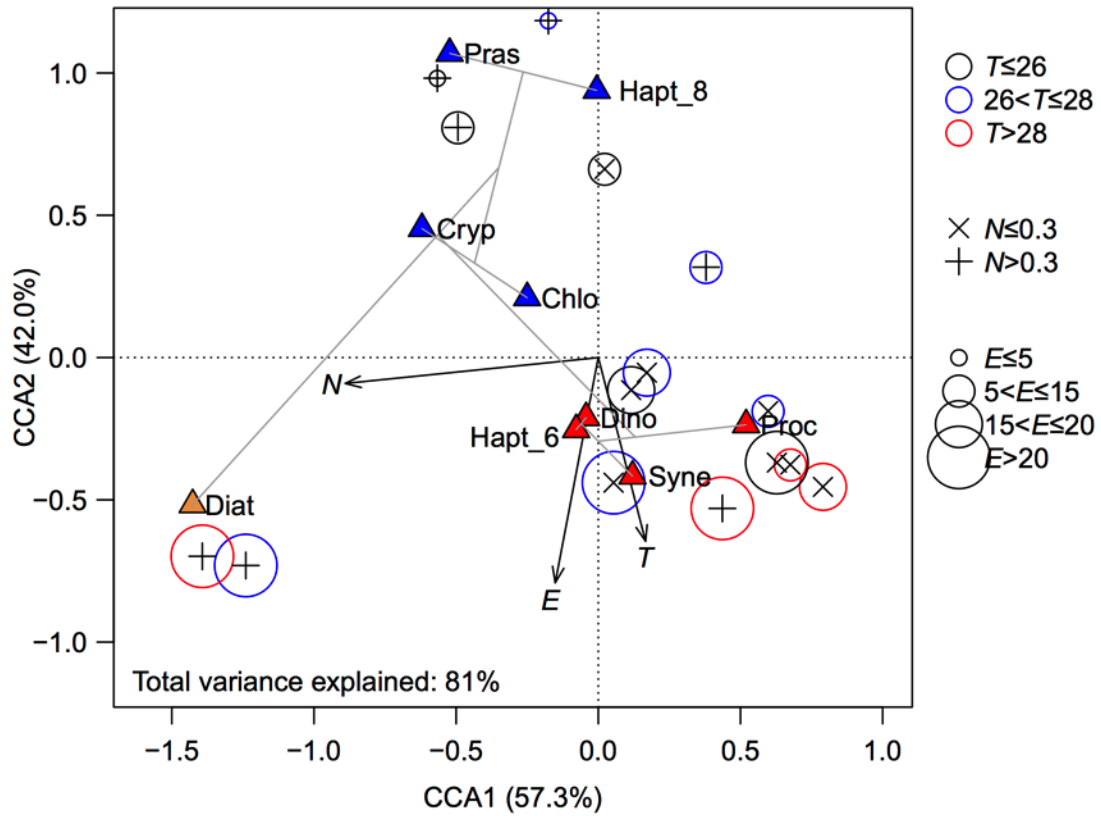ers of all possible niches; the niche divisions in which the relative abundances of all of the nine phytoplankton groups did not vary significantly (marked in red in (**c**)) were removed. Statistical information for drawing these figures were obtained by 'R Program 1' (**a**) and 'R Program 2' (**b**−**d**) in the Supplementary Information.

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**Fig. 3** A three-dimensional niche classification scheme produced by CCA and clustering analysis based on mean values of 15 niches. Every circle is a niche and every triangle is a phytoplankton group. Sample sizes of the niches are presented in Table S2. The dendrogram was overlaid by grey segments. Colored triangles showed three clusters of phytoplankton groups determined by clustering analysis. T: temperature (°C); E: irradiance (mol quanta m^{-2} d^{-1}); N: nitrate (μmol L^{-1}).

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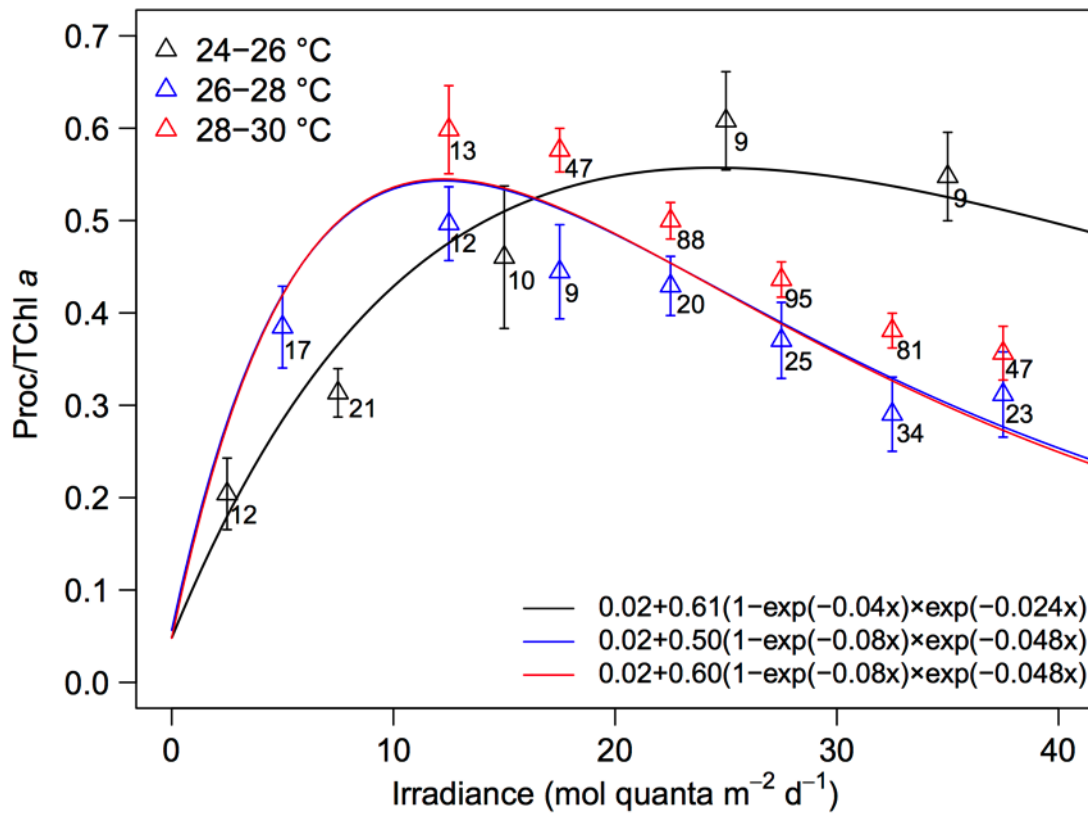
Fig. 4 The relative abundance of *Prochlorococcus* as a function of irradiance at different temperature intervals. Digits next to triangles show sample sizes. The vertical axis is the mean and SEM of the relative abundance at each combined bin of temperature and irradiance.

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