Supplemental document accompanying submission to *Optics Express*

Title: High latitude Southern Ocean phytoplankton have distinctive bio-optical properties

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High latitude Southern Ocean phytoplankton have distinctive bio-optical prorperties: supplemental document

Weight-specific pigment absorption spectra. The weight-specific absorption spectra for pigments from Clementson & Wojtasiewicz [1] were used to reconstruct the absorption spectra for each sample of the same pigment in solution. The spectra were first wavelength shifted by correcting for the differences in refractive index between the solvent and water by using the ratio between the refractive index between the solvent and water as per Baird et al. [2] and Garcia et al. [3]. Next the spectra for each pigment were shifted to the *in-vivo* position, matching the positions of Bricaud et al. [4] and Bidigare et al. [5]. The refractive index ratios and wavelength shifts (in nm) for each pigment are in Table S1. The final wavelength-shifted absorption spectra for each pigment are presented in Figure S1.

Table S1. Wavelength of the absorption maxima (λ_{max}), weight-specific absorption coefficient at the maxima ($a^*_{sol,i}$), refractive index multiplier and wavelength shift applied to the pigment weight-specific absorption coefficients from the Clementson and Wojtasiewicz [1] dataset. Pigments included are chlorophyll *a* (Chl*a*), divinyl chlorophyll *a* (DVChl*a*), chlorophyll *b* (Chl*b*), chlorophyllide *a* (Chlde*a*), pheophorbide *a* (Pheophyb*a*), pheophytin *a* (Pheophy*a*), chlorophyll *c*2 (Chl*c*2), chlorophyll *c*3 (Chl*c*3), fucoxanthin (Fuco), 19'-butanoloxyfucoxanthin (19BF), 19'-hexanoloxyfucoxanthin (19HF), peridinin (Peri), neoxanthin (Neox), prasinoxanthin (Pras), violaxanthin (Viol), antheraxanthin (Anth), diadinoxanthin (Diad), diatoxanthin (Diat), zeaxanthin (Zeax), lutein (Lut), alloxanthin (Allox), β,β-carotene (β,β-caro).

Pigment	λ_{max} (nm)	$a^*_{sol,i}$ (m^2 mg^{-1})	Refractive Index Multiplier	Wavelength Shift (nm)
Chl*a*	440	0.0232	1.017	+ 2
Chl*a*	676	0.0200	1.017	+ 2
DVChl*a*	450	0.0274	1.017	+ 4
Chl*b*	466	0.0329	1.017	0
Chlde*a*	418	0.0392	1.017	0
Chlde*a*	676	0.0277	1.017	0
Pheophyb*a*	416	0.0366	1.017	0
Pheophyb*a*	676	0.0167	1.017	0
Pheophy*a*	416	0.0269	1.017	0
Pheophy*a*	676	0.0122	1.017	0
Chl*c*2	462	0.0877	1.017	+ 10
Chl*c*3	462	0.0772	1.017	+ 2
Fuco	490	0.0359	1.023	+ 30
19BF	488	0.0367	1.023	+ 32
19HF	488	0.0361	1.023	+ 32
Peri	504	0.0296	1.023	+ 18
Neox	488	0.0502	1.023	0
Pras	490	0.0368	1.023	+ 26
Viol	488	0.0556	1.023	+ 38
Anth	488	0.0533	1.023	+ 32
Diad	462	0.0594	1.023	+ 4
Diat	462	0.0598	1.023	0

Zeax	462	0.0528	1.023	0
Lut	462	0.0561	1.023	+ 6
Allox	462	0.0585	1.023	- 2
β,β-caro	462	0.0568	1.017	0

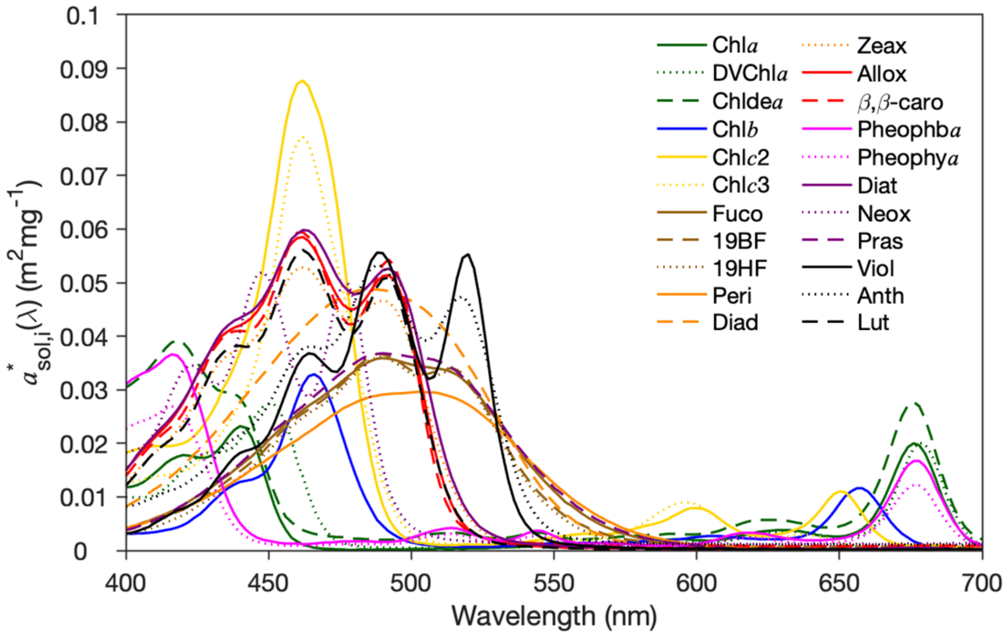

Figure S1. Pigment weight-specific absorption coefficients from Clementson and Wojtasiewicz [1] after correction for the refractive index of the solvent and wavelength shifted to *in-vivo* absorption positions, see text and Table S1. Pigments include chlorophyll *a* (Chl*a*), divinyl chlorophyll *a* (DVChl*a*), chlorophyllide *a* (Chlde*a*), chlorophyll *b* (Chl*b*), chlorophyll *c*2 (Chl*c*2), chlorophyll *c*3 (Chl*c*3), fucoxanthin (Fuco), 19'-butanoloxyfucoxanthin (19BF), 19'-hexanoloxyfucoxanthin (19HF), peridinin (Peri), diadinoxanthin (Diad), zeaxanthin (Zeax), alloxanthin (Allox), β,β-carotene (β,β-caro), pheophorbide *a* (Pheophyb*a*), pheophytin *a* (Pheophy*a*), diatoxanthin (Diat), neoxanthin (Neox), prasinoxanthin (Pras), violaxanthin (Viol), antheraxanthin (Anth), lutein (Lut).

Power Law Relationships between $a_\phi(\lambda)$ and [Tchl*a*]. To investigate changes to the phytoplankton absorption spectral shapes as a function of chlorophyll *a*, power law functions were fit to log-transformed $a_\phi(\lambda)$ and log-transformed [Tchl*a*] as per Equation S1 at 2 nm intervals between 400-700 nm.

$$a_\phi(\lambda) = C(\lambda) \times [Tchla]^{E(\lambda)} \qquad \text{Eq. S1}$$

These relationships were derived for all ACE data, as well as subsets of the data from low latitudes (40-60 °S), and high latitudes (> 60 °S). The constants ($C(\lambda)$), exponents ($E(\lambda)$), coefficient of determination (R^2) and p-value are provided in supplementary files:

Data_File_1.csv – Parameters from the power law function fit to data from all latitudes

Data_File_2.csv – Parameters from the power law function fit to data from low latitudes (40-60 °S)

Data_File_3.csv - Parameters from the power law function fit to data from high latitudes (> 60 °S)

Note that the chlorophyll-specific phytoplankton absorption ($a^*_\phi(\lambda)$) can be derived using the same coefficients as per Equation S2:

$$a^*_\phi(\lambda) = C(\lambda) \times [Tchla]^{E(\lambda)-1} \quad \text{Eq. S2}$$

References

1. L. A. Clementson and B. Wojtasiewicz, "Dataset on the in vivo absorption characteristics and pigment composition of various phytoplankton species," Data in brief, **25**, 104020 (2019)
2. M. E. Baird, M. Mongin, F. Rizwi, L. K. Bay, N. E. Cantin, M. Soja-Wozniak and J. Skerratt, "A mechanistic model of coral bleaching due to temperature-mediated light-driven reactive oxygen build-up in zooxanthellae," Ecol. Model., **386**, 20-37 (2018)
3. L. Garcia-Rubio, "Refractive index effects on the absorption spectra of macromolecules," Macromolecules, **25**, 2608-2613 (1992)
4. A. Bricaud, H. Claustre, J. Ras and K. Oubelkheir, "Natural variability of phytoplanktonic absorption in oceanic waters: Influence of the size structure of algal populations," J. Geophys. Res. Ocean., **109** (2004)
5. R. R. bidigare, M. E. Ondrusek, J. H. Morrow and D. A. Kiefer, "In-vivo absorption properties of algal pigments," in *Ocean Optics X*, vol. 1302 (International Society for Optics and Photonics, 1990), pp. 290-302.