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Data Article

Dataset on the absorption characteristics of extracted phytoplankton pigments



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ABSTRACT

This article presents the raw and analysed data on the absorption features of 30 pigments commonly occurring in phytoplankton. All unprocessed absorption spectra are given between 350 and 800 nm. The presented data also gives information on the wavelength of the main absorption peaks together with associated magnitudes of the concentration-specific absorption coefficient.

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1. Data

The unprocessed measurement data for the absorption spectra of chlorophylls (chlorophyll-*a*, chlorophyll-*b*, DV chlorophyll-*a*, chlorophyllide-*a*, phaeophorbide-*a*, phaeophytin-*a*, chlorophyll-*c*3, chlorophyll-*c*2) and carotenoids (peridinin, 19'-butanoyloxyfucoxanthin, fucoxanthin, neoxanthin, prasinoxanthin, 19'-keto-hexanoyloxyfucoxanthin, violaxanthin, 19'-hexanoyloxyfucoxanthin, astaxanthin, diadinoxanthin, dinoxanthin, antheraxanthin, alloxanthin, myxoxanthophyll, diatoxanthin, zeaxanthin, lutein, canthaxanthin, gyroxanthin diester, echinenone, β , ϵ -carotene, β , β -carotene) are given in separate files ([Appendix A](#); `carotenoids_concentration_specific_spectra.txt`, `chlorophylls_concentration_specific_spectra.txt`). [Figs. 1 and 2](#) present pigment-specific absorption spectra for each of the analysed pigments and [Tables 1 and 2](#) list the location of the main absorption peaks and the magnitude of the pigment-specific absorption coefficients at these local maxima for chlorophylls and carotenoids, respectively.

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Specifications table

Subject area	Biology
More specific subject area	Phytoplankton biology; Marine biology; Marine bio-optics
Type of data	Tables, figures, separate .txt files with entire measured spectra
How data was acquired	UV-VIS double-beam spectrophotometer (GBC Scientific Equipment Ltd., Cintra 404); software: Cintral ver. 2.2
Data format	Analysed
Experimental factors	Pigments were dissolved in either 100% ethanol or 90% acetone as received from DHI (Denmark) or Sigma Aldrich prior to the measurements being made.
Experimental features	The absorption spectra were measured in a 1-cm quartz-glass cuvette using a dual-beam spectrophotometer against the pure solvent as a blank. The spectra were measured over the 350–800 nm spectral range in 1.3 nm increments.
Data source location	Hobart, TAS, Australia
Data accessibility	All data are provided in this article
Related research article	Baird, M.E., Mongin, M., Rizwi, F., Bay, L.K., Cantin, N.E., Soja-Woźniak, M., Skerratt, J., 2018. A mechanistic model of coral bleaching due to temperature-mediated light-driven reactive oxygen build-up in zooxanthellae. <i>Ecol. Model.</i> 386, 20–37 [1].

Value of the data

- This dataset is unique in that it provides the absorption characteristics together with a pigment concentration for 30 different pigments. From this, concentration-specific absorption coefficients are obtained which can be used for both phytoplankton and bio-optical studies.
- The dataset can be used in models pertaining to phytoplankton behavior or for theoretical experiments.
- The dataset can be used to both compare to in situ experimental results or to help explain experimental results.
- The dataset can be base for theoretical experiments in phytoplankton physiology or ecology and marine bio-optics.

2. Experimental design, materials, and methods

Pigment standards for chlorophyll-*a* and chlorophyll-*b* were prepared from extracts purchased from Sigma-Aldrich (www.sigmaaldrich.com), while other pigment standards were obtained from DHI (www.dhigroup.com). The source and the batch/lot number of each pigment are given in [Tables 1 and 2](#). The standards were in either 90% acetone, 100% acetone or 100% ethanol ([Table 1](#), [Table 2](#)). The final concentrations of the standards were measured by HPLC (High Performance Liquid Chromatography) with the CSIRO method [2], which is a modified version of the [3] technique, using C₈ column and binary gradient system with an elevated column temperature. Pigments were identified by their retention time and their absorption spectra from the photo-diode array detector. Next, the pigment concentrations were determined through peak integration performed in Empower[®] software.

The absorption spectra of the pigment standards were measured in a 1-cm quartz-glass cuvette using a Cintra 404 (GBC Scientific Equipment Ltd.) UV-VIS dual-beam spectrophotometer against the pure solvent as a blank. The spectra were measured over the 350–800 nm spectral range in 1.3 nm increments. The absorbance (*OD*) obtained from the measurements was converted to an absorption coefficient ($a(\lambda)$, m⁻¹) by multiplying the appropriate baseline-corrected optical density values of each standard by 2.3 and dividing by the optical path length/cuvette thickness (0.01 m):

$$a(\lambda) = \frac{2.3 OD(\lambda)}{0.01} \quad (1)$$

Finally, the concentration specific absorption coefficients ($a^*(\lambda)$, m² g⁻¹) were calculated by dividing each absorption coefficient by the respective pigment concentration.

Data presented in [Figs. 1 and 2](#) and in [Tables 1 and 2](#) were null-point corrected by subtracting the absorption coefficient value at 750 nm assuming no absorption of pigments in the NIR region of the

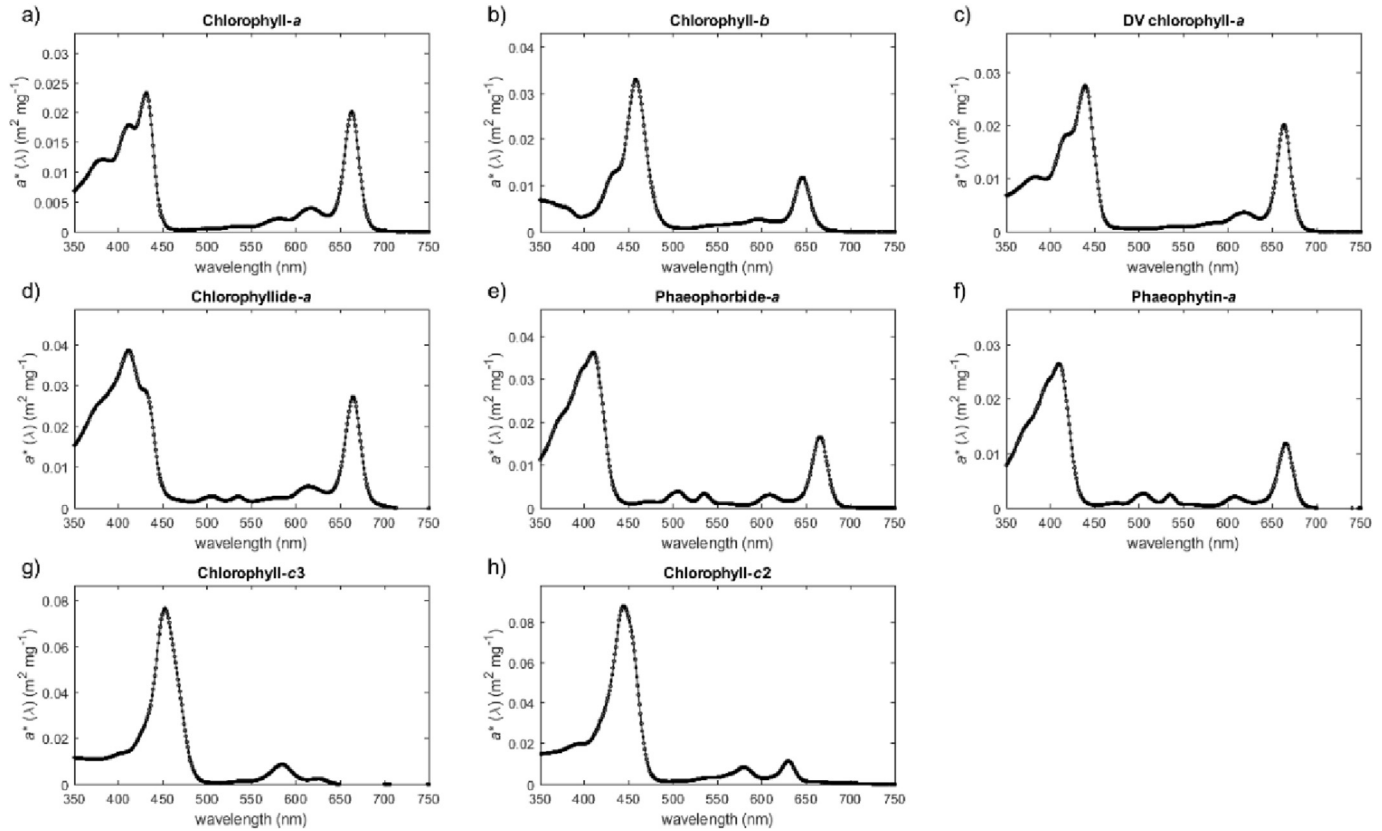


Fig. 1. Concentration-specific absorption spectra of (a) chlorophyll-a, (b) chlorophyll-b, (c) DV chlorophyll-a, (d) chlorophyllide-a, (e) phaeophorbide-a, (f) phaeophytin-a, (g) chlorophyll-c3, (h) chlorophyll-c2.

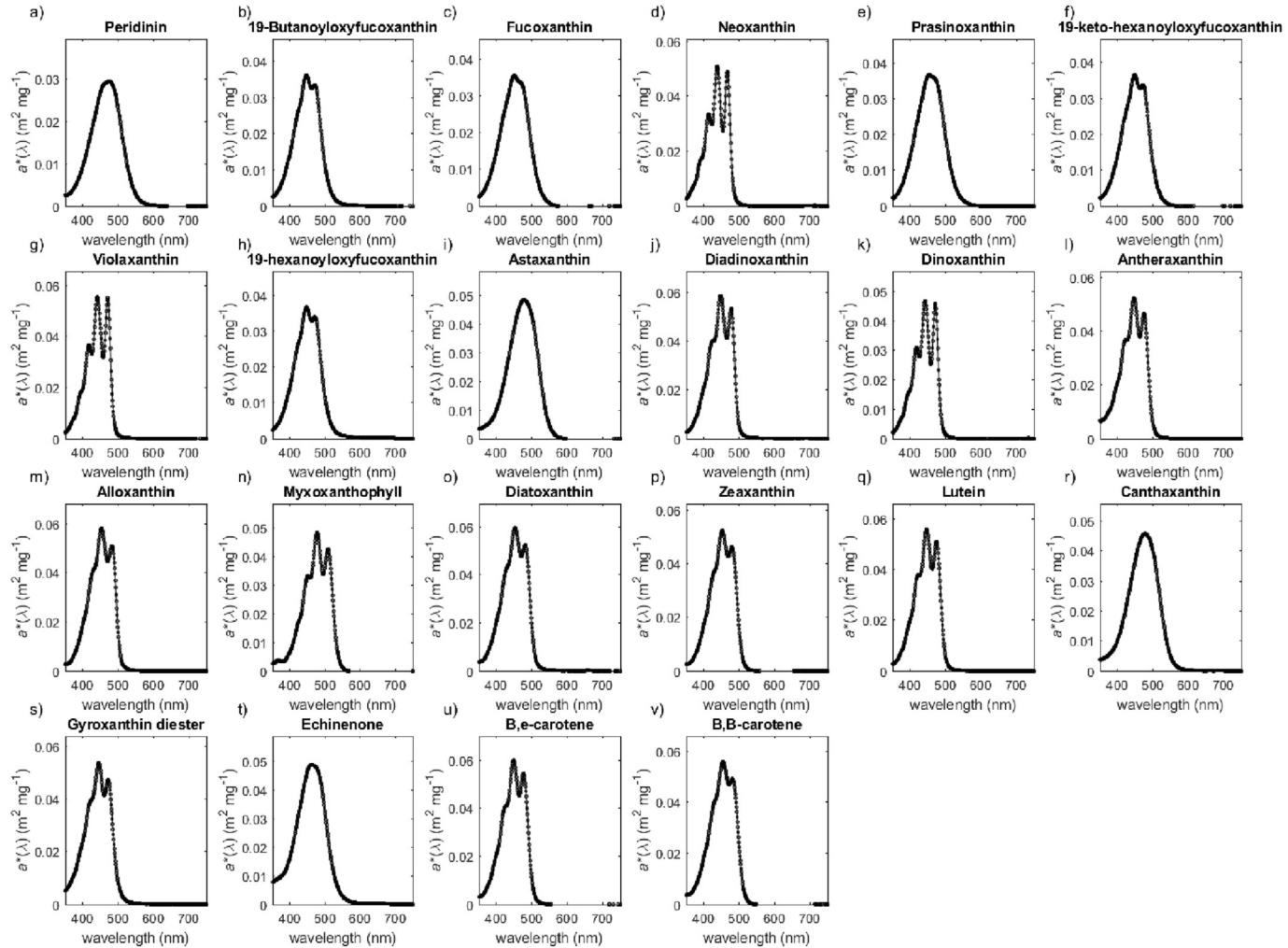


Fig. 2. Concentration-specific absorption spectra of (a) peridinin, (b) 19'-butanoyloxyfucoxanthin, (c) fucoxanthin, (d) neoxanthin, (e) prasincoxanthin, (f) 19'-keto-hexanoyloxyfucoxanthin, (g) violaxanthin, (h) 19'-hexanoyloxyfucoxanthin, (i) astaxanthin, (j) diadinoxanthin, (k) dinoxanthin, (l) antheraxanthin, (m) alloxanthin, (n) myxoxanthophyll, (o) diatoxanthin, (p) zeaxanthin, (q) lutein, (r) canthaxanthin, (s) gyroxanthin diester, (t) echinonone, (u) β,ϵ -carotene, (v) β,β -carotene.

Table 1

Location of the main absorption peaks and the associated magnitude of the concentration specific absorption coefficient for chlorophyll-*a*, chlorophyll-*b*, DV chlorophyll-*a*, chlorophyllide-*a*, phaeophorbide-*a*, phaeophytin-*a*, chlorophyll-*c*3, and chlorophyll-*c*2.

Name of pigment	Source	Lot/Batch number	Solvent	Main absorption peaks (nm)	Concentration specific absorption coefficient ($\text{m}^2 \text{mg}^{-1}$)
Chlorophyll- <i>a</i>	Sigma	BCBK2207V	90% acetone	431	0.0233
				663	0.0202
				412	0.0179
				382	0.0122
				617	0.0040
Chlorophyll- <i>b</i>	Sigma	SLBF7339V	90% acetone	458	0.0330
DV chlorophyll- <i>a</i>	DHI	112	90% acetone	439	0.0276
Chlorophyllide- <i>a</i>	DHI	125	90% acetone	663	0.0203
				411	0.0387
				665	0.0272
				615	0.0053
				535	0.0029
Phaeophorbide- <i>a</i>	DHI	105	90% acetone	506	0.0028
				410	0.0363
				666	0.0166
				505	0.0039
				535	0.0034
Phaeophytin- <i>a</i>	DHI	107	90% acetone	608	0.0031
				410	0.0266
				665	0.0119
				505	0.0027
				535	0.0024
Chlorophyll- <i>c</i> 3	DHI	122	90% acetone	607	0.0021
				452	0.0766
				584	0.0085
Chlorophyll- <i>c</i> 2	DHI	129	90% acetone	626	0.0024
				444	0.0880
				630	0.0113
				580	0.0083

Table 2

Location of the main absorption peaks and the associated magnitude of the concentration-specific absorption coefficient for carotenoids (peridinin, 190-butanoyloxyfucoxanthin, fucoxanthin, neoxanthin, prasinoxanthin, 190-keto-hexanoyloxyfucoxanthin, violaxanthin, 190-hexanoyloxyfucoxanthin, astaxanthin, diadinoxanthin, dinoxanthin, antheraxanthin, alloxanthin, myxoxanthophyll, diatoxanthin, zeaxanthin, lutein, canthaxanthin, gyroxanthin diester, echinenone, b, ϵ -carotene, b,b-carotene).

Name of pigment	Source	Lot/Batch number	Solvent	Main absorption peaks (nm)	Concentration specific absorption coefficient ($\text{m}^2 \text{mg}^{-1}$)
Peridinin	DHI	111	100% ethanol	474	0.0293
19'-Butanoyloxyfucoxanthin	DHI	122	100% ethanol	447	0.0362
				471	0.0335
				449	0.0355
Fucoxanthin	DHI	119	100% ethanol	438	0.0508
Neoxanthin	DHI	122	100% ethanol	466	0.0489
				413	0.0333
				453	0.0367
Prasinoxanthin	DHI	110	100% ethanol	448	0.0365
19'-keto-hexanoyloxyfucoxanthin	DHI	101	100% ethanol	471	0.0337
				441	0.0555
				471	0.0552
Violaxanthin	DHI	138	100% ethanol	417	0.0365
19'-hexanoyloxyfucoxanthin	DHI	116	100% ethanol	446	0.0367
				471	0.0339

(continued on next page)

Table 2 (continued)

Name of pigment	Source	Lot/Batch number	Solvent	Main absorption peaks (nm)	Concentration specific absorption coefficient ($\text{m}^2 \text{mg}^{-1}$)
Astaxanthin	DHI	105	100% acetone	477	0.0486
Diadinoxanthin	DHI	117	100% ethanol	447 477 426	0.0588 0.0535 0.0402
Dinoxanthin	DHI	103	100% ethanol	442 471 417	0.0468 0.0458 0.0316
Antheraxanthin	DHI	127	100% ethanol	446 475 423	0.0523 0.0464 0.0369
Alloxanthin	DHI	112	100% ethanol	453 482	0.0583 0.0511
Myxoxanthophyll	DHI	106	100% acetone	477 508 452	0.0486 0.0427 0.0333
Diatoxanthin	DHI	133	100% ethanol	452 481	0.0596 0.0524
Zeaxanthin	DHI	131	100% ethanol	452 479	0.0524 0.0464
Lutein	DHI	128	100% ethanol	446 474 423	0.0559 0.0508 0.0381
Canthaxanthin	DHI	131	100% ethanol	478	0.0458
Gyroxanthin diester	DHI	105	100% ethanol	445 472	0.0538 0.0473
Echinenone	DHI	121	100% ethanol	461	0.0488
β,ϵ -carotene	DHI	126	100% acetone	488 476	0.0600 0.0544
β,β -carotene	DHI	126	100% acetone	454 480	0.0559 0.0492

spectrum [4]. The spectra were also interpolated to yield absorption coefficients between 350 and 750 nm with the resolution of 1 nm using linear interpolation method (MATLAB, *interp1.m*).

Due to differences in the organic solvent and water refractive index (i.e. 1.352 for acetone, 1.361 for ethanol and 1.330 for water), the spectra may be wavelength-adjusted by using the ratio between the refractive index of the solvent and the water as done by [1].

Acknowledgements

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Transparency document

Transparency document associated with this article can be found in the online version at <https://doi.org/10.1016/j.dib.2019.103875>.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.dib.2019.103875>.

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