Data Article

Dataset on the absorption characteristics of extracted phytoplankton pigments

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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-c3, chlorophyll-c2) 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,e-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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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 (\(a(\lambda)\), \(\text{m}^{-1}\)) 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):

\[
a(\lambda) = \frac{2.3 \ OD(\lambda)}{0.01}
\]

Finally, the concentration specific absorption coefficients (\(a'(\lambda)\), \(\text{m}^2 \text{g}^{-1}\)) 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 absorbance 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) pheophorbide-a, (f) pheophytin-a, (g) chlorophyll-c3, (h) chlorophyll-c2.
Fig. 2. Concentration-specific absorption spectra of (a) peridinin, (b) 19'-butanoyloxyfucoxanthin, (c) fucoxanthin, (d) neoxanthin, (e) prasinoxanthin, (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) gyrooxanthin diester, (t) echinenone, (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-c3, and chlorophyll-c2.

| Name of pigment          | Source | Lot/Batch number | Solvent     | Main absorption peaks (nm) | Concentration specific absorption coefficient (m² mg⁻¹) |
|--------------------------|--------|------------------|-------------|----------------------------|------------------------------------------------------|
| Chlorophyll-a            | Sigma  | RCBK2207V        | 90% acetone | 431 663 412 382 617        | 0.0233 0.0202 0.0179 0.0122 0.0040                   |
| Chlorophyll-b            | Sigma  | SLBF7339V        | 90% acetone | 458 646                     | 0.0330 0.0118                                        |
| DV chlorophyll-a         | DHI    | 112              | 90% acetone | 439 663                     | 0.0276 0.0203                                        |
| Chlorophyllide-a         | DHI    | 125              | 90% acetone | 411 665 615 535 506        | 0.0387 0.0272 0.0053 0.0029 0.0028                   |
| Phaeophorbide-a          | DHI    | 105              | 90% acetone | 410 666 505 535 608        | 0.0363 0.0166 0.0039 0.0034 0.0031                   |
| Phaeophytin-a            | DHI    | 107              | 90% acetone | 410 665 505 535 607        | 0.0266 0.0119 0.0027 0.0024 0.0021                   |
| Chlorophyll-c3           | DHI    | 122              | 90% acetone | 452 584 626                 | 0.0766 0.0085 0.0024                                 |
| Chlorophyll-c2           | DHI    | 129              | 90% acetone | 444 630 580                 | 0.0880 0.0113 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, diatocxanthin, zeaxanthin, lutein, canthaxanthin, gyroxanthin diester, echinenone, b,α-carotene, b,b-carotene).

| Name of pigment          | Source | Lot/Batch number | Solvent      | Main absorption peaks (nm) | Concentration specific absorption coefficient (m² mg⁻¹) |
|--------------------------|--------|------------------|--------------|----------------------------|------------------------------------------------------|
| Peridinin                | DHI    | 111              | 100% ethanol | 474                        | 0.0293                                               |
| 19'-Butanoyloxyfucoxanthin | DHI    | 122              | 100% ethanol | 447 471                    | 0.0362 0.0335                                        |
| Fucoxanthin              | DHI    | 119              | 100% ethanol | 449                        | 0.0355                                               |
| Neoxanthin               | DHI    | 122              | 100% ethanol | 438 466 413                 | 0.0508 0.0489 0.0333                                 |
| Prasinoxanthin           | DHI    | 110              | 100% ethanol | 453 471                    | 0.0367 0.0337                                        |
| 19'-keto-hexanoyloxyfucoxanthin | DHI | 101              | 100% ethanol | 448 471                    | 0.0365 0.0337                                        |
| Violaxanthin             | DHI    | 138              | 100% ethanol | 441 471 417                 | 0.0555 0.0552 0.0365                                 |
| 19'-hexanoyloxyfucoxanthin | DHI    | 116              | 100% ethanol | 446 471                    | 0.0367 0.0339                                        |

(continued on next page)
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].

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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.

References

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Table 2 (continued)

| Name of pigment           | Source | Lot/Batch number | Solvent     | Main absorption peaks (nm) | Concentration specific absorption coefficient (m² mg⁻¹) |
|---------------------------|--------|------------------|-------------|----------------------------|--------------------------------------------------------|
| Astaxanthin               | DHI    | 105              | 100% acetone| 477                        | 0.0486                                                 |
| Diadinoxanthin            | DHI    | 117              | 100% ethanol| 447                        | 0.0588                                                 |
|                           |        |                  |             | 477                        | 0.0535                                                 |
|                           |        |                  |             | 426                        | 0.0402                                                 |
| Dinoxanthin               | DHI    | 103              | 100% ethanol| 442                        | 0.0468                                                 |
|                           |        |                  |             | 471                        | 0.0458                                                 |
|                           |        |                  |             | 417                        | 0.0316                                                 |
| Antheraxanthin            | DHI    | 127              | 100% ethanol| 446                        | 0.0523                                                 |
|                           |        |                  |             | 475                        | 0.0464                                                 |
|                           |        |                  |             | 423                        | 0.0369                                                 |
| Alloxanthin               | DHI    | 112              | 100% ethanol| 453                        | 0.0583                                                 |
|                           |        |                  |             | 482                        | 0.0511                                                 |
| Myxoxanthophyll           | DHI    | 106              | 100% acetone| 477                        | 0.0486                                                 |
|                           |        |                  |             | 508                        | 0.0427                                                 |
|                           |        |                  |             | 452                        | 0.0333                                                 |
|                           |        |                  |             | 481                        | 0.0524                                                 |
| Diatoxanthin              | DHI    | 133              | 100% ethanol| 452                        | 0.0596                                                 |
|                           |        |                  |             | 481                        | 0.0524                                                 |
| Zeaxanthin                | DHI    | 131              | 100% ethanol| 452                        | 0.0524                                                 |
|                           |        |                  |             | 479                        | 0.0464                                                 |
|                           |        |                  |             | 474                        | 0.0508                                                 |
|                           |        |                  |             | 423                        | 0.0381                                                 |
| Lutein                    | DHI    | 128              | 100% ethanol| 446                        | 0.0559                                                 |
|                           |        |                  |             | 474                        | 0.0508                                                 |
|                           |        |                  |             | 423                        | 0.0381                                                 |
| Canthaxanthin             | DHI    | 131              | 100% ethanol| 478                        | 0.0458                                                 |
| Gyroxanthin diester       | DHI    | 105              | 100% ethanol| 445                        | 0.0538                                                 |
|                           |        |                  |             | 472                        | 0.0473                                                 |
| Echinenone                | DHI    | 121              | 100% ethanol| 461                        | 0.0488                                                 |
| β,β-carotene              | DHI    | 126              | 100% acetone| 488                        | 0.0600                                                 |
|                           |        |                  |             | 476                        | 0.0544                                                 |
|                           |        |                  |             | 480                        | 0.0492                                                 |
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