**Probing heavy metal binding to phycobiliproteins**

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The raw data associated with the publication entitled “Probing heavy metal binding to phycobiliproteins”. Native mass spectrometry, absorbance spectroscopy and fluorescence spectroscopy data. Phycobiliproteins extracted and purified from cyanobacteria were incubated with heavy metal ions including iron, copper, zinc and silver. The effects on oligomer assembly, absorbance and fluorescence where measured. Data files are organised into folders according to their corresponding figures.

The following files have been archived:

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| **File name** | **File description** (Short description of content, sample size, format, any linking between different types of data, i.e. survey and interviews/focus groups) |
| **Native Mass Spectrometry** | |
| APC\_1um\_Fig1.raw | Native mass spectra of APC protein at 1 μM (hexamer, 6 μM bilin). Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| PC\_1um\_Fig1.raw | Native mass spectra of PC protein at 1 μM (hexamer, 9 μM bilin). Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| APC\_only\_Fig3.raw | Native mass spectra of APC protein at 1 μM. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| APC\_Fe\_10eqv.raw  APC\_Fe\_20eqv.raw  APC\_Fe\_40eqv.raw | Native mass spectra of APC protein incubated with 10, 20 and 40 equivalents of Fe salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| APC\_FeNTA\_10eqv.raw  APC\_FeNTA\_20eqv.raw  APC\_FeNTA\_5eqv.raw | Native mass spectra of APC protein incubated with 5, 10 and 20 equivalents of Fe:NTA salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| APC\_Cu\_5eqv.raw  APC\_Cu\_10eqv.raw  APC\_Cu\_20eqv.raw | Native mass spectra of APC protein incubated with 5, 10 and 20 equivalents of Cu salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| APC\_Ag\_1eqv.raw  APC\_Ag\_2eqv.raw  APC\_Ag\_5eqv.raw | Native mass spectra of APC protein incubated with 1, 2 and 5 equivalents of Ag salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| APC\_Zn\_5eqv.raw  APC\_Zn\_10eqv.raw  APC\_Zn\_20eqv.raw | Native mass spectra of APC protein incubated with 5, 10 and 20 equivalents of Zn salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| PC\_only\_Fig4.raw | Native mass spectra of PC protein at 2.7 μM (hexamer, 24 μM bilin). Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| PC\_Ag\_0-5eqv.raw  PC\_Ag\_0-25eqv.raw | Native mass spectra of PC protein incubated with 0.25 and 0.5 equivalents of Ag salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| PC\_Cu\_0-5eqv.raw  PC\_Cu\_0-25eqv.raw | Native mass spectra of PC protein incubated with 0.25, 0.5 equivalents of Cu salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| 1475-9\_extract\_only\_Fig6.raw | Native mass spectra of phycobiliprotein extract from 1475/9 (*Arthrospira Maxima*) containing APC and PC protein. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| 1475-9\_extract\_Fe\_5eqv.raw | Native mass spectra of phycobiliprotein extract from 1475/9 (*Arthrospira Maxima*) containing APC and PC protein incubated with 5 equivalents of Fe salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| 1475-9\_extract\_Cu\_5eqv.raw | Native mass spectra of phycobiliprotein extract from 1475/9 (*Arthrospira Maxima*) containing APC and PC protein incubated with 5 equivalents of Cu salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| 1475-9\_extract\_Zn\_5eqv.raw | Native mass spectra of phycobiliprotein extract from 1475/9 (*Arthrospira Maxima*) containing APC and PC protein incubated with 5 equivalents of Zn salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| 1475-9\_extract\_Ag\_1-25eqv.raw | Native mass spectra of phycobiliprotein extract from 1475/9 (*Arthrospira Maxima*) containing APC and PC protein incubated with 1.25 equivalents of Ag salt. Raw data file(s) from Orbitrap Eclipse Tribrid mass spectrometer. |
| **Absorbance and fluorescence spectroscopy** | |
| APC\_absorbance\_with\_metals.txt | Absorbance spectroscopy spectra of APC protein incubated with metal salts (Fe, Cu, Zn and Ag). Raw data file from a Biowave 3 spectrophotometer. |
| APC\_absorbance\_with\_metals.xlsx | Absorbance spectroscopy spectra of APC protein incubated with metal salts (Fe, Cu, Zn and Ag). Combined Excel file with data from a Biowave 3 spectrophotometer. |
| APC\_fluorescence\_only.csv  APC\_fluorescence\_Fe60.csv  APC\_fluorescence\_Cu60.csv  APC\_fluorescence\_Zn60.csv  APC\_fluorescence\_Ag60.csv | Fluorescence spectroscopy spectra of APC protein incubated with metal salts (Fe, Cu, Zn and Ag). Raw data files from a Cary Eclipse fluorescence spectrophotometer. |
| APC\_fluorescence\_with\_metals.xlsx | Fluorescence spectroscopy spectra of APC protein incubated with metal salts (Fe, Cu, Zn and Ag). Combined Excel file with data from a Agilent Cary Eclipse fluorescence spectrophotometer. |
| PC\_absorbance\_only.txt  PC\_absorbance\_Cu60.txt  PC\_absorbance\_Ag60.txt | Absorbance spectroscopy spectra of PC protein incubated with metal salts (Cu and Ag). Raw data files from Jenway 7200 spectrophotometer. |
| PC\_absorbance\_with\_metals.xlsx | Absorbance spectroscopy spectra of PC protein incubated with metal salts (Cu and Ag). Combined Excel file with data from Jenway 7200 spectrophotometer. |
| PC\_fluorescence\_only.csv  PC\_fluorescence\_Cu60.csv  PC\_fluorescence\_Ag60.csv | Fluorescence spectroscopy spectra of PC protein incubated with metal salts (Cu and Ag). Raw data files from a Cary Eclipse fluorescence spectrophotometer. |
| PC\_fluorescence\_with\_metals.xlsx | Fluorescence spectroscopy spectra of PC protein incubated with metal salts (Cu and Ag). Combined Excel file with data files from a Cary Eclipse fluorescence spectrophotometer. |