

**Supplementary information to :**

**Southern Ocean biological pump over the last glacial cycle from new diatom transfer functions**

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**Diatom species names updated following Algebase recommendations ([www.algeabase.org](http://www.algeabase.org))**

*Actinocyclus ehrenbergii* (Ralfs) was updated to *Actinocyclus octonarius* (Ehrenberg).

*Actinocyclus ingens* (Rattray) was updated to *Actinocyclus rattrayi* (Williams).

*Coscinodiscus tabularis* (Grunow) was updated to *Azpeitia tabularis* (Grunow).

*Corethron criophilum* (Castracane) was updated to *Corethron pennatum* (Grunow).

*Fragilariopsis sublinearis* (Van Heurck) was updated to *Fragilariopsis obliquecostata* (Van Heurck).

*Hemidiscus cuneiformis* (Wallich) was updated to *Actinocyclus cuneiformis* (Wallich).

*Thalassiosira trifulta* (Fryxell) was updated to *Shionodiscus trifultus* (Fryxell).

*Tropidoneis antarctica* (Grunow) was updated to *Membraneis challengerii* (Grunow).

**Full list of diatom species/taxa groups reported in the sediment trap and sediment core datasets**

*Actinocyclus actinochilus* (Ehrenberg)

*Actinocyclus cuneiformis* (Wallich)

*Actinocyclus curvatulus* (Janisch)

*Actinocyclus exiguus* (Fryxell & Semina)

*Actinocyclus octonarius* (Ehrenberg)

*Actinocyclus rattrayi* (Williams)

*Actinocyclus* spp.

*Alveus marinus* (Kaczmarska & Fryxell)

*Amphora copulata* (Schoeman & R.E.M. Archibald)

*Asteromphalus heptactis* (Brébisson)

*Asteromphalus hookeri* (Ehrenberg)

*Asteromphalus hyalinus* (Karsten)

*Asteromphalus parvulus* (Karsten)

*Asteromphalus* spp.

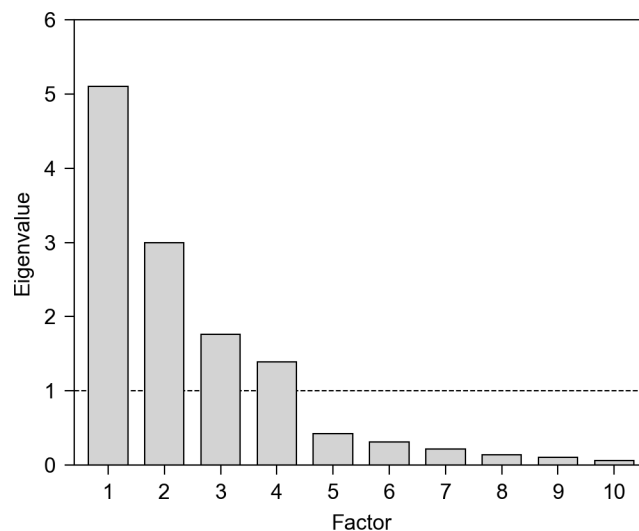
*Azpeitia tabularis* (Grunow)  
*Banquisia belgicae* (Van Heurck)  
*Chaetoceros aequatorialis* var. *antarcticus* (Manguin)  
*Chaetoceros atlanticus* (Cleve)  
*Chaetoceros bulbosus* (Ehrenberg)  
*Chaetoceros criophilus* (Castracane)  
*Chaetoceros decipiens* (Cleve)  
*Chaetoceros diadema* (Ehrenberg)  
*Chaetoceros dichchaeta* (Ehrenberg)  
*Chaetoceros peruvianus* (Brightwell)  
*Chaetoceros radicans* (Schütt)  
*Chaetoceros* subgenus *Hyalochaete*  
*Chaetoceros* subgenus *Hyalochaete* resting spore  
*Chaetoceros* subgenus *Phaeoceros*  
*Cocconeis costata* (Gregory)  
*Cocconeis dallmannii* (Al-Handal, Riaux-Gobin, Romero & Wulff)  
*Cocconeis fasciolata* (Ehrenberg)  
*Cocconeis californica* (Grunow)  
*Cocconeis californica* var. *keruelensis* (Heiden)  
*Cocconeis melchioroides* (Al-Handal, Riaux-Gobin, Romero & Wulff)  
*Cocconeis* spp.  
*Corethron inerme* (Karsten)  
*Corethron pennatum* (Grunow)  
*Coscinodiscus asteromphalus* (Ehrenberg)  
*Coscinodiscus cruvatulus* (Grunow)  
*Coscinodiscus marginatus* (Ehrenberg)  
*Coscinodiscus* spp.  
*Cyclotella* spp.  
*Dactyliosolen antarcticus* (Castracane)  
*Denticulopsis* spp.  
*Diploneis bombus* (Ehrenberg)  
*Eucampia antarctica* (Castracane)  
*Eucampia antarctica* resting spore  
*Eupyxidicula turris* (Greville)  
*Fallacia marnieri* (Manguin)  
*Fragilariopsis bicapitata* (unreferenced)  
*Fragilariopsis curta* (Van Heurck)  
*Fragilariopsis cylindrus* (Grunow)

*Fragilariopsis doliolus* (Wallich)  
*Fragilariopsis kerguelensis* (O'Meara)  
*Fragilariopsis obliquecostata* (Van Heurck)  
*Fragilariopsis panduriformis* (unreferenced)  
*Fragilariopsis pseudonana* (Hasle)  
*Fragilariopsis rhombica* (O'Meara)  
*Fragilariopsis ritsheri* (Hustedt)  
*Fragilariopsis separanda/rhombica*  
*Fragilariopsis separanda* (Hustedt)  
*Fragilariopsis vanheurckii* (Peragallo)  
*Fragilariopsis* spp.  
*Gomphomenopsis littoralis* (unreferenced)  
*Guinardia cylindrus* (Cleve)  
*Guinardia cylindrus* (Cleve)  
*Gyrosigma* spp.  
*Haslea trompii* (Cleve)  
*Leptocylindrus* spp.  
*Licmophora gracilis* (Ehrenberg)  
*Manguinea fusiformis* (Manguin)  
*Melosira adeliae* (Manguin)  
*Membraneis challengerii* (Grunow)  
*Navicula directa* (Smith)  
*Navicula* spp.  
*Nitzschia bicapitata* (Cleve)  
*Nitzschia braarudii* (Hasle)  
*Nitzschia interruptestriata* (Simonsen)  
*Nitzschia kolaczekii* (Grunow)  
*Nitzschia sicala* (Castracane)  
*Nitzschia taeniiformis* (Simonsen)  
*Nitzschia* spp.  
*Odontella weissflogii* (Grunow)  
*Odontella weissflogii* resting spore  
*Paralia sulcata* (Ehrenberg)  
*Paralia* spp.  
*Plagiotropis gaussii* (Heiden)  
*Pleurosigma directum* (Grunow)  
*Pleurosigma* spp.  
*Porosira glacialis* (Grunow)

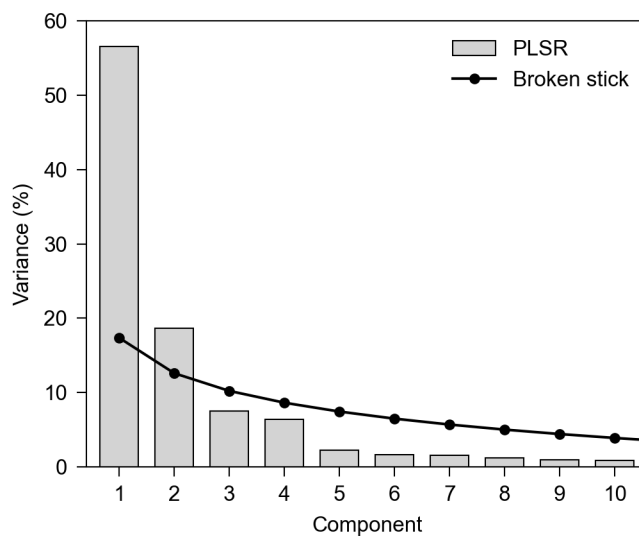
*Porosira pseudodenticulata* (Hustedt)  
*Proboscia alata* (Brightwell)  
*Proboscia inermis* (Castracane)  
*Proboscia truncata* (Karsten)  
*Proboscia* spp.  
*Psammodictyon panduriforme* (Gregory)  
*Pseudogomphonema kamtschaticum* (Grunow)  
*Pseudo-nitzschia heimii* (Manguin)  
*Pseudo-nitzschia lineola* (Cleve)  
*Pseudo-nitzschia heimii/lineola*  
*Pseudo-nitzschia prolongatoides* (Hasle)  
*Pseudo-nitzschia turgiduloides* (Hasle)  
*Rhizosolenia antennata* (Ehrenberg)  
*Rhizosolenia bergonii* (Peragallo)  
*Rhizosolenia chunii* (Karsten)  
*Rhizosolenia costata* (Gersonde)  
*Rhizosolenia crassa* (Schimper ex Karsten)  
*Rhizosolenia curvata* (Zacharias)  
*Rhizosolenia hebetata* (Bailey)  
*Rhizosolenia polydactyla* (Castracane)  
*Rhizosolenia sima* (Castracane)  
*Rhizosolenia simplex* (Karsten)  
*Rhizosolenia styliformis* (Brightwell)  
*Rhizosolenia* spp.  
*Roperia tessellata* (Roper)  
*Rouxia* spp.  
*Shionodiscus gracilis* (Karsten)  
*Shionodiscus gracilis* var. *expectus* (VanLandingham)  
*Shionodiscus frenguelliopsis* (Fryxell & Johansen)  
*Shionodiscus oestrupii* (Ostenfeld)  
*Shionodiscus trifultus* (Fryxell)  
*Stellarima microtrias* (Ehrenberg)  
*Stellarima stellaris* (Roper)  
*Synedropsis laevis* (Heiden)  
*Synedropsis recta* (Hasle, Medlin & Syversten)  
*Synedropsis* spp.  
*Thalassionema nitzschioides* (Grunow)  
*Thalassionema nitzschioides* var. *capitulata* (Schrader)

*Thalassionema nitzschioides* var. *lanceolata* (Grunow)  
*Thalassionema nitzschioides* var. *parva* (Heiden & Kolbe)  
*Thalassiosira antarctica* (Karsten)  
*Thalassiosira decipiens* (Grunow)  
*Thalassiosira eccentrica* (Ehrenberg)  
*Thalassiosira ferelineata* (Hasle & Fryxell)  
*Thalassiosira gracilis* (Karsten)  
*Thalassiosira gracilis* var. *expecta* (Van Landingham)  
*Thalassiosira gravida* (Cleve)  
*Thalassiosira lentiginosa* (Janisch)  
*Thalassiosira leptopus* (Grunow)  
*Thalassiosira lineata* (Jousé)  
*Thalassiosira maculata* (Fryxell & Johansen)  
*Thalassiosira oestrupii* (Ostenfeld)  
*Thalassiosira oliverana* (O'Meara)  
*Thalassiosira scotia* (Fryxell & Hoban)  
*Thalassiosira symmetrica* (Fryxell & Hasle)  
*Thalassiosira tumida* (Janisch)  
*Thalassiosira* spp.  
*Thalassiosira* resting spore  
*Thalassiothrix antarctica* (Schimper)  
*Trachyneis aspera* (Ehrenberg)  
*Trichotoxon reinboldii* (Van Heurck)  
Unidentified centric < 20 µm  
Unidentified centric > 20 µm

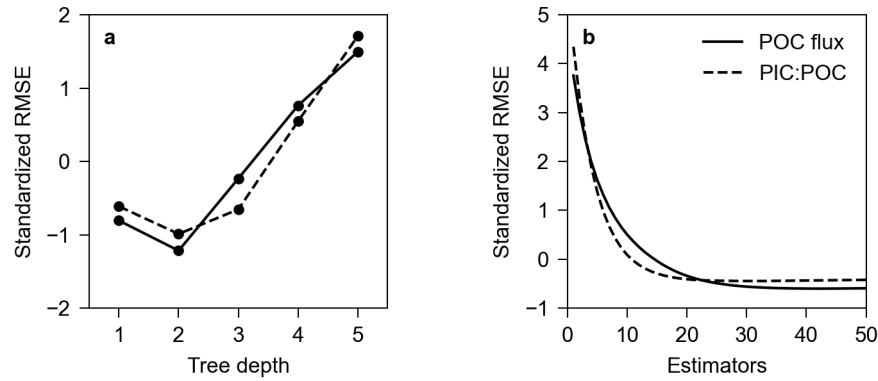
## Supplementary figures



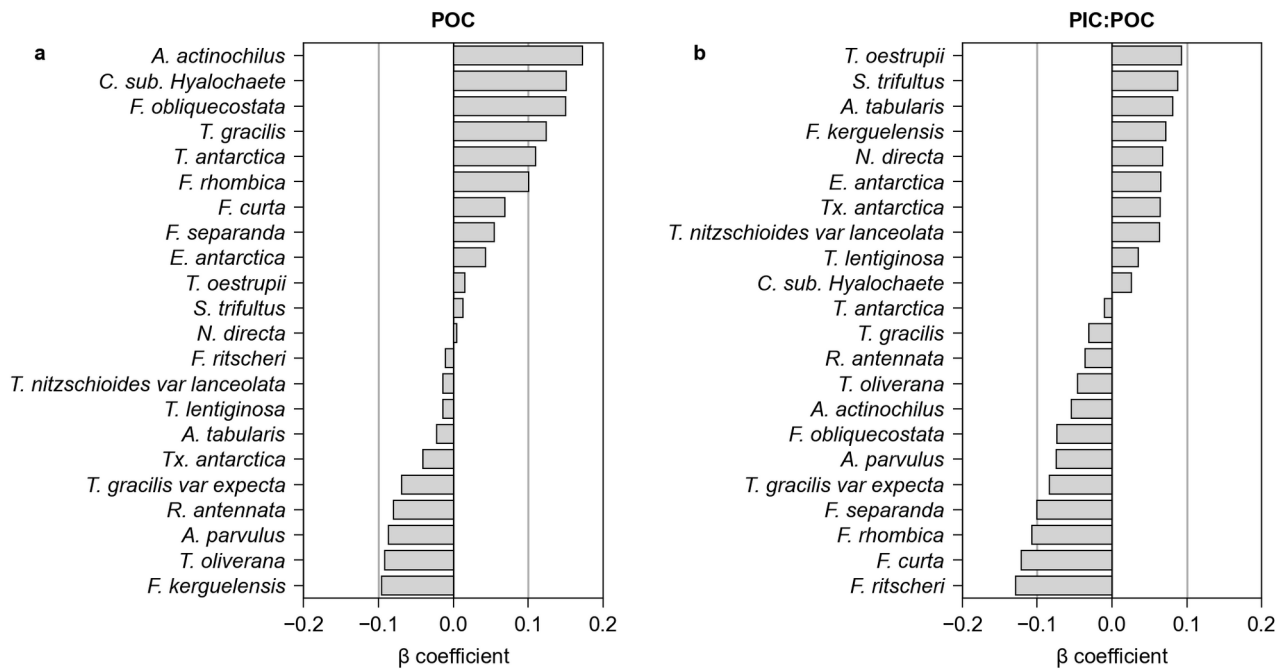
**Figure S1.** Scree plot representing eigenvalues associated with the first 10 components of the factorial analysis. Dotted line denotes the eigenvalue of 1, a threshold used to select the informative factors used in the multiple linear regressions (MLR).



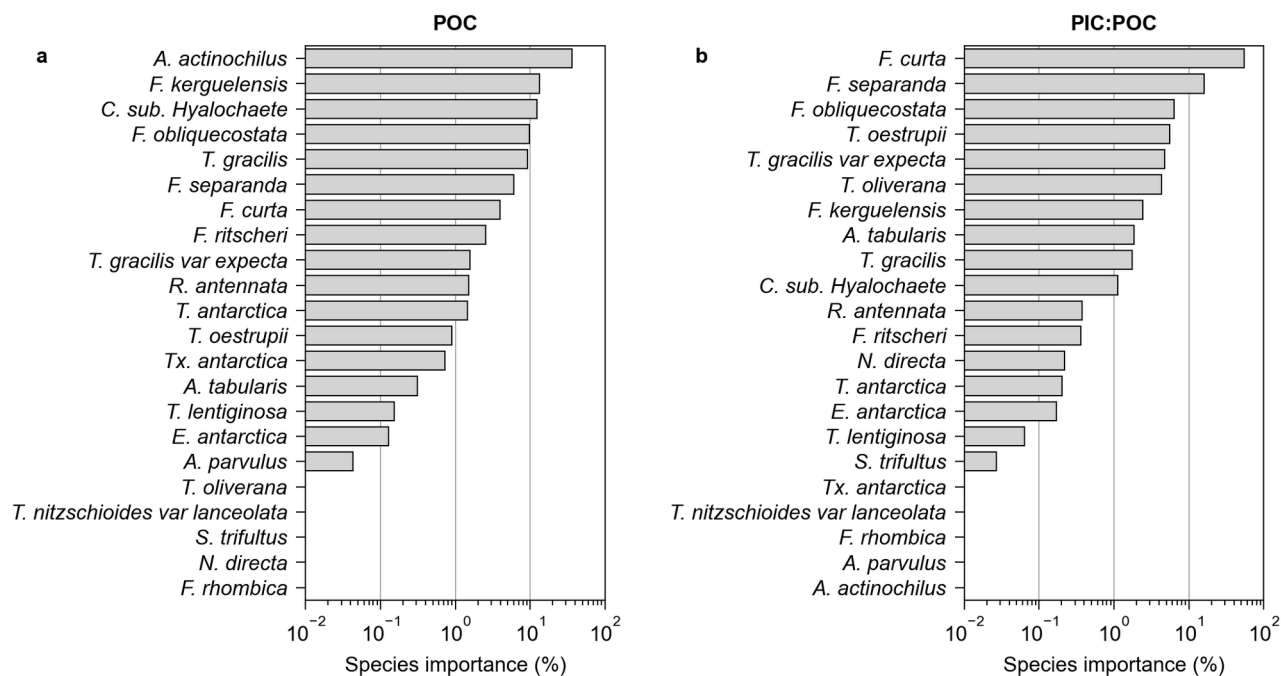
**Figure S2.** Variance explained by the first 10 components of the partial least square regression (PLSR). Line and dots represent variance distribution according to a null broken stick model that evenly distributes a decreasing variance among the components (see materials and methods for explanations). PLSR components explaining more variance than the null model were considered informative and kept for the transfer function calibration.



**Figure S3.** Parameters selection for the gradient boosting regression (GBR). a) Effect of tree depth on the root mean square error (RMSE) of the prediction. b) Effect of the number of estimators on the RMSE. Each line is the mean from the bootstrapping technique (10 000 permutations). RMSE were standardized (mean subtracted, divided by standard deviation) to allow a direct comparison of the two variables.

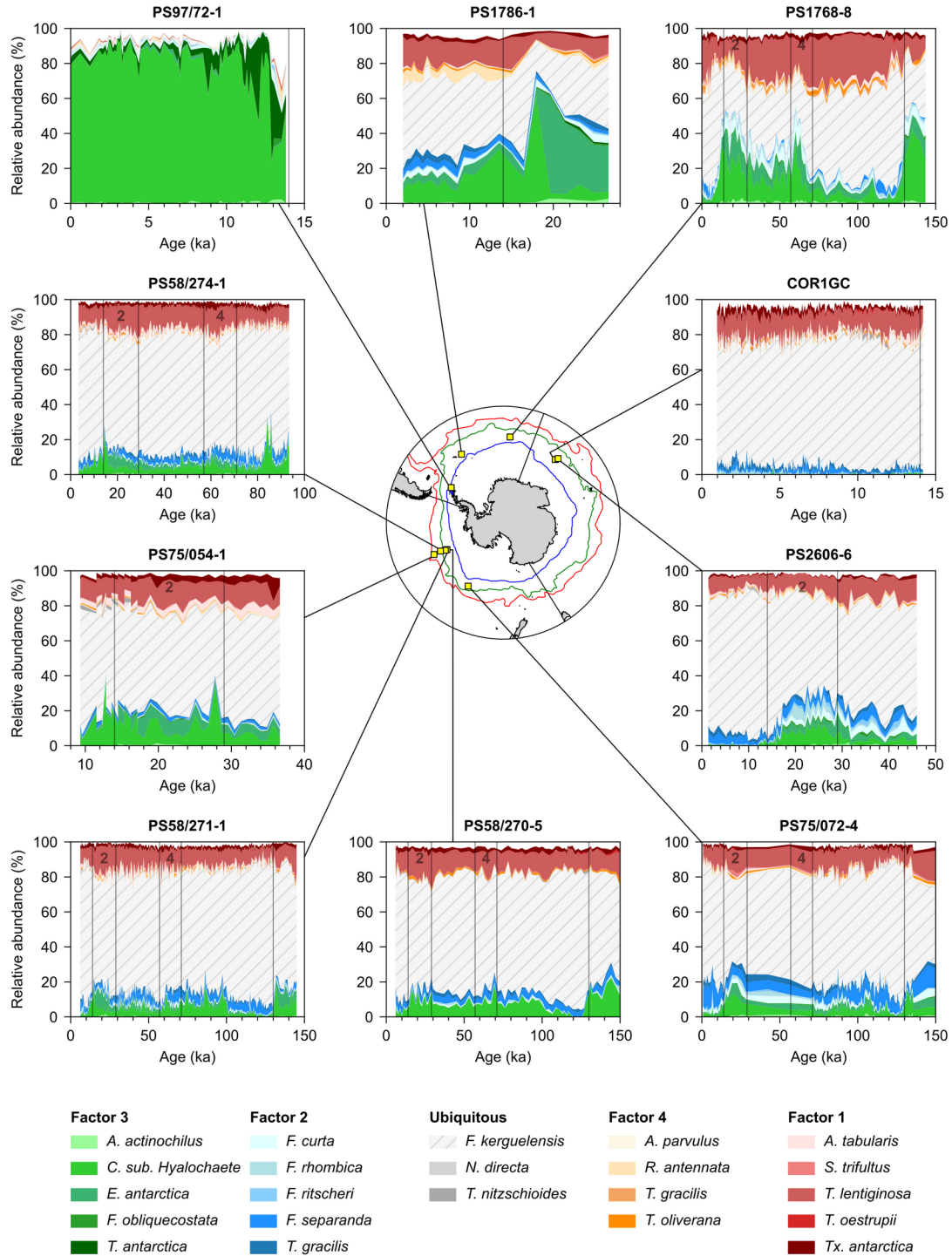


**Figure S4.** Sorted partial correlation coefficients ( $\beta$ ) from the partial least square regression (PLSR) for a) particulate organic carbon (POC) export flux and b) particulate inorganic to organic (PIC:POC) export ratio.



**Figure S5.** Sorted species relative importance in the gradient boosting repression (GBR) models for a) particulate organic carbon (POC) export flux and b) particulate inorganic to organic (PIC:POC) export ratio.





**Figure S6.** Relative abundance of the main diatom species in the sediment cores used to apply the transfer functions. The white area at the top of each panel represents rare species not considered in the transfer functions. Vertical lines and numbers denote marine isotopic stages (MIS). In the central map, colored lines represent hydrological fronts: Subantarctic Front (red), Polar Front (green), sea ice extent (blue).