The following supplements accompany the article

A structural equation modeling approach to the diversity–productivity relationship of Wadden Sea phytoplankton

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SUPPLEMENT 1

Overview of the main model parameters

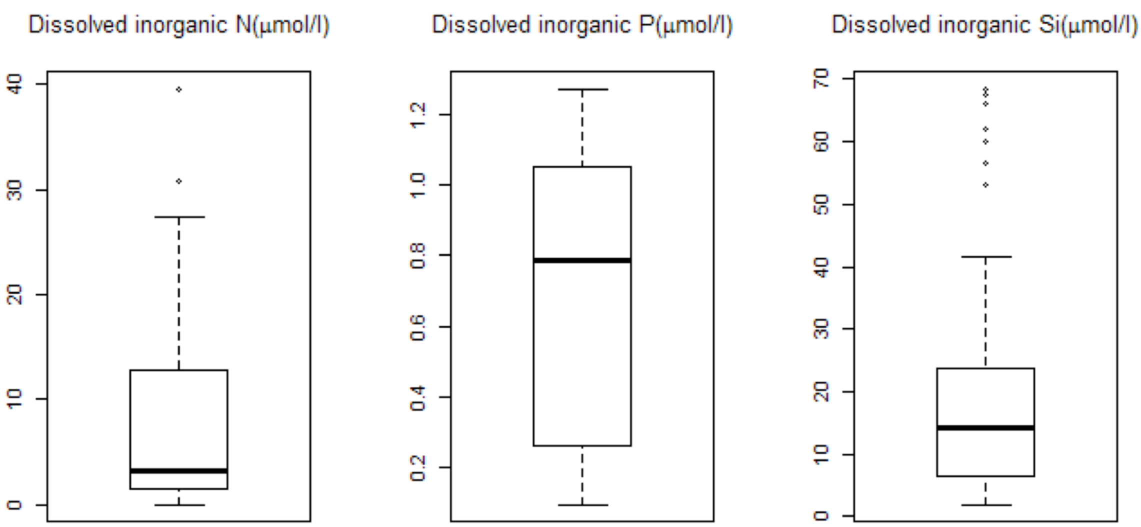

Fig. S 1: Boxplots of dissolved inorganic nutrient (nitrogen, phosphorus, silicate) concentrations.

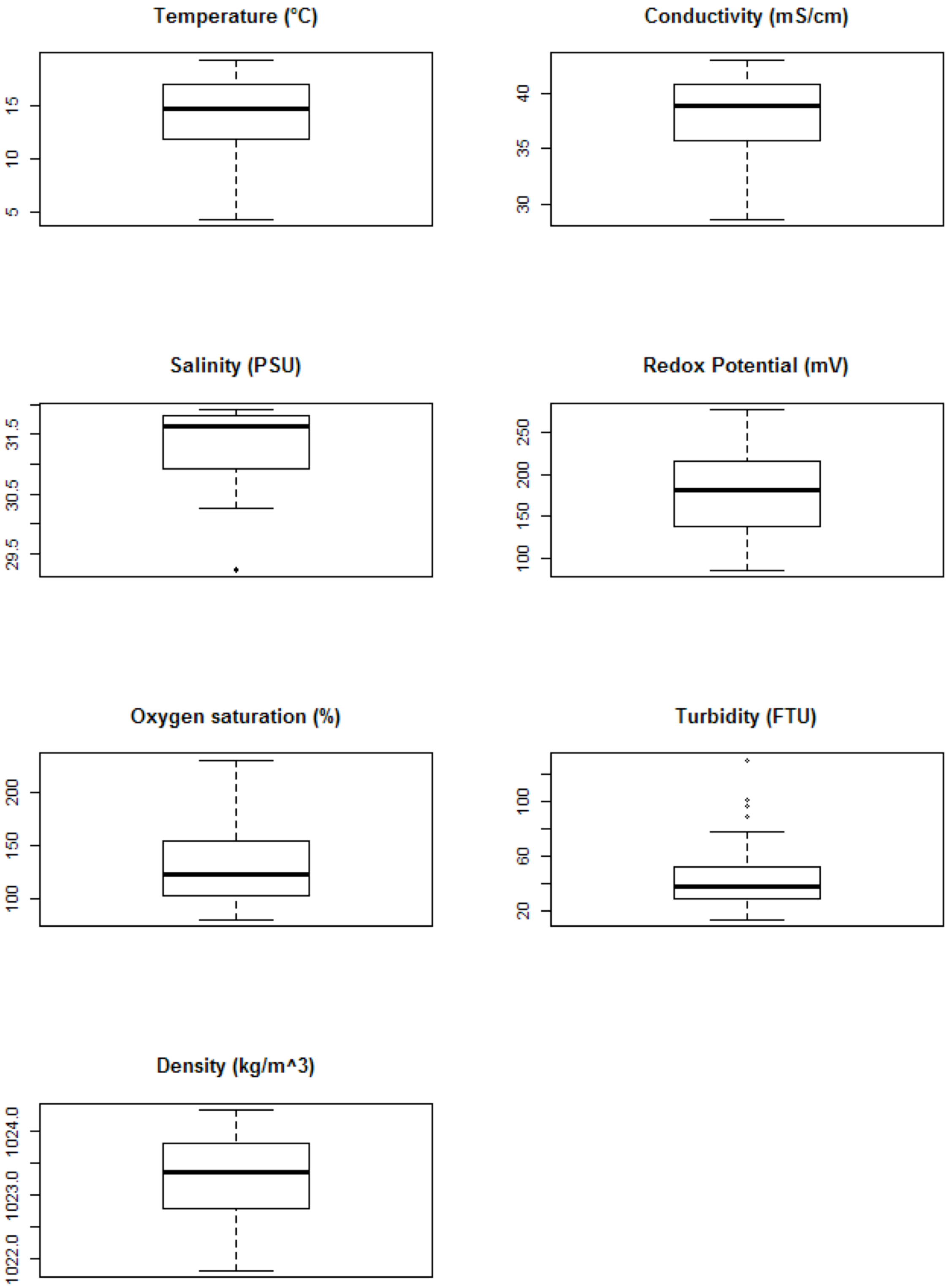

Fig. S 2: Boxplots of environmental parameters.

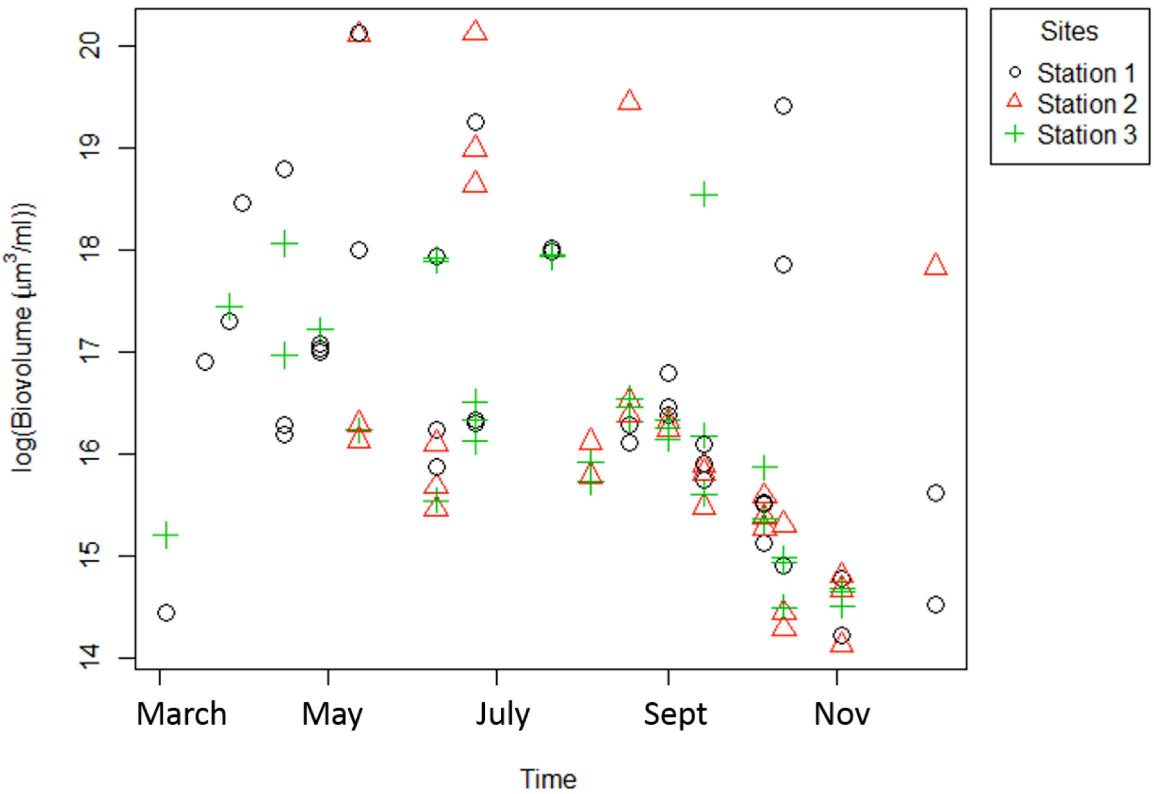

Fig. S 3: Log-transformed phytoplankton biovolume measurements showing seasonal patterns for the 3 sites over the sampling period.

SUPPLEMENT 2

R output: Correlation matrix of environmental parameters

```
> rcorr(as.matrix(dat_pca,type="spearman"))
         Standort windvel  Wdir   PAR Press  Temp  Cond  Sal Density O2_sat  Turb Redox
Standort     1.00    0.00  0.04  0.07 -0.05  0.09  0.09 0.01   -0.09  -0.27 -0.06  0.39
windvel      0.00    1.00  0.77  0.24  0.04  0.30  0.35 0.45    0.00   0.02  0.46 -0.10
Wdir         0.04    0.77  1.00  0.50  0.02  0.42  0.47 0.43   -0.17  -0.16  0.26 -0.05
PAR          0.07    0.24  0.50  1.00  0.05  0.59  0.62 0.41   -0.35  -0.45 -0.31  0.04
Press       -0.05    0.04  0.02  0.05  1.00  0.04  0.06 0.20    0.10   0.12  0.34  0.07
Temp         0.09    0.30  0.42  0.59  0.04  1.00  0.99 0.40   -0.77  -0.19  0.02  0.02
Cond         0.09    0.35  0.47  0.62  0.06  0.99  1.00 0.52   -0.68  -0.15  0.02  0.06
Sal          0.01    0.45  0.43  0.41  0.20  0.40  0.52 1.00    0.26   0.17  0.02  0.27
Density     -0.09    0.00 -0.17 -0.35  0.10 -0.77 -0.68 0.26    1.00   0.32  0.00  0.14
O2_sat      -0.27    0.02 -0.16 -0.45  0.12 -0.19 -0.15 0.17    0.32   1.00  0.32  0.19
Turb        -0.06    0.46  0.26 -0.31  0.34  0.02  0.02 0.02    0.00   0.32  1.00  0.03
Redox        0.39   -0.10 -0.05  0.04  0.07  0.02  0.06 0.27    0.14   0.19  0.03  1.00

n
         Standort windvel Wdir PAR Press Temp Cond Sal Density O2_sat Turb Redox
Standort      101     101  101 101    95   95   95  95      95     95   95    95
windvel       101     101  101 101    95   95   95  95      95     95   95    95
Wdir          101     101  101 101    95   95   95  95      95     95   95    95
PAR           101     101  101 101    95   95   95  95      95     95   95    95
Press          95      95   95  95   101   95   95  95      95     95   95    95
Temp           95      95   95  95    95  101   95  95      95     95   95    95
Cond           95      95   95  95    95   95  101  95      95     95   95    95
Sal            95      95   95  95    95   95   95 101      95     95   95    95
Density        95      95   95  95    95   95   95  95     101     95   95    95
O2_sat         95      95   95  95    95   95   95  95      95    101   95    95
Turb           95      95   95  95    95   95   95  95      95     95  101    95
Redox          95      95   95  95    95   95   95  95      95     95   95   101

P
         Standort windvel Wdir   PAR    Press  Temp   Cond   Sal    Density O2_sat Turb   Redox
Standort          0.9685  0.6623 0.4891 0.6068 0.3706 0.3997 0.9155 0.3788  0.0094 0.5830 0.0000
```

```
windvel  0.9685          0.0000 0.0158 0.6813 0.0034 0.0005 0.0000 0.9797  0.8405 0.0000 0.3575
Wdir     0.6623   0.0000        0.0000 0.8111 0.0000 0.0000 0.0000 0.0971  0.1140 0.0111 0.6541
PAR      0.4891   0.0158 0.0000        0.6558 0.0000 0.0000 0.0000 0.0005  0.0000 0.0026 0.6926
Press    0.6068   0.6813 0.8111 0.6558        0.7332 0.5532 0.0564 0.3180  0.2521 0.0007 0.5076
Temp     0.3706   0.0034 0.0000 0.0000 0.7332        0.0000 0.0000 0.0000  0.0684 0.8467 0.8651
Cond     0.3997   0.0005 0.0000 0.0000 0.5532 0.0000        0.0000 0.0000  0.1446 0.8321 0.5515
Sal      0.9155   0.0000 0.0000 0.0000 0.0564 0.0000 0.0000        0.0097  0.0944 0.8131 0.0080
Density  0.3788   0.9797 0.0971 0.0005 0.3180 0.0000 0.0000 0.0097         0.0018 0.9982 0.1830
O2_sat   0.0094   0.8405 0.1140 0.0000 0.2521 0.0684 0.1446 0.0944 0.0018         0.0015 0.0723
Turb     0.5830   0.0000 0.0111 0.0026 0.0007 0.8467 0.8321 0.8131 0.9982  0.0015        0.7395
Redox    0.0000   0.3575 0.6541 0.6926 0.5076 0.8651 0.5515 0.0080 0.1830  0.0723 0.7395
```

R output: Factor Analysis

```
> fit <- factanal(dat_compl, 3, rotation="varimax")
> print(fit, digits=2, cutoff=.3, sort=TRUE)

Call:
factanal(x = dat_compl, factors = 3, rotation = "varimax")

Uniquenesses:
Standort  windvel     Wdir      PAR    Press     Temp     Cond      Sal
    0.99     0.00     0.32     0.61     0.96     0.00     0.00     0.00
 Density   O2_sat     Turb    Redox
    0.00     0.89     0.74     0.87

Loadings:
         Factor1 Factor2 Factor3
PAR       0.56
Temp      0.98
Cond      0.95
Density  -0.86            0.50
windvel           0.98
Wdir              0.76
Sal                       0.92
Standort
Press
```

```
O2_sat
Turb              0.49
Redox                     0.33

               Factor1 Factor2 Factor3
SS loadings       3.13    1.97    1.50
Proportion Var    0.26    0.16    0.12
Cumulative Var    0.26    0.42    0.55

Test of the hypothesis that 3 factors are sufficient.
The chi square statistic is 539.58 on 33 degrees of freedom.
The p-value is 6.67e-93
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SUPPLEMENT 3

Structural Equation Modeling - approach and evaluation

Structural equation models (SEM) are a multivariate statistical method allowing for the simultaneous analysis of networks of interactions between several variables while accounting for direct as well as indirect relationships and measurement error.

Given the hierarchical structure of most ecological processes underlying observable patterns, structural equation models represent a convenient means for the analysis of biological information (Grace 2006, Arhonditsis et al. 2006). One useful feature of SEMs is the possibility to model relationships between abstract variables or concepts such as biodiversity or ecosystem health, which are not directly measurable, but commonly represented by a number of indices. By means of so called latent variables these can be incorporated in the model structure while accounting for uncertainties or error associated with the measurements of their respective indicator or manifest variables.

Structural equation models consist of two components. The so called measurement model, which comprises the links between each latent variable and their according indicator or manifest variable(s), and the structural model reflecting the direct and indirect relationships between the latent constructs. Latent constructs which only predict other latent variables are called exogenous variables, whereas variables, which depend on at least one causal pathway from any other latent construct are termed endogenous variables.

Indicator variables can be divided into two groups: reflective indicators that are assumed to be affected by the same underlying concept, i.e. latent construct, or formative indicators which can be multidimensional and are defined to cause or affect the current state of the latent construct. We only employed measurement models of the reflective type, as it is implied by the combination of highly correlated indicator variables (Haenlein & Kaplan 2004) and seemed to be most meaningful within the biological context.

Two different approaches are commonly used: covariance-based (CB) SEM (Joreskog 1973) and more recently partial least squares (PLS) SEM (Lohmöller 1989).

CB-SEM intends to reproduce the covariance matrix in the original data as closely as possible with a number of structural equations assumed to reflect the underlying mechanisms of the relationships between the measured parameters. Maximum likelihood or least squares estimation is then used to minimise the difference between the observed and modelled covariances. Several authors have published comprehensive descriptions of the methodological details of this approach (Grace 2006).

PLS SEM combines features of multivariate statistical methods such as factor and principal component analysis with multiple regression (Haenlein & Kaplan 2004, Abdi 2007) using iterative regression processes and bootstrapping to maximise the explained variance of the endogenous latent constructs. Thus, the method is able to overcome limitations of these first generation statistical tools, which are for example the constrained degree of model complexity and the ignorance of measurement error in predictor variables in regression models. Detailed descriptions of the development and use of the PLS algorithm are given in the literature (Vinzi 2010, Hair et al. 2011, Hair Jr et al. 2014).

In contrast to CB-SEM, which is usually applied as a confirmatory tool for validating a priori defined hypotheses and theoretical concepts, PLS SEM can serve as a more exploratory method aiming to maximise the explained variance in the observed data (Hair Jr et al. 2014). Apart from this rather conceptual difference, we chose PLS SEM over CB SEM due to its less strict assumptions regarding data distribution, sample size and the number of indicator variables required for each of the latent constructs (Hair et al. 2011). Further reading on the differences and adequate application of the two approaches can be found in the literature (Chin 2010, Hair et al. 2011).

Model evaluation:

As PLS SEM does not make any distributional assumptions, traditional parametric-based techniques for significance testing and overall goodness-of-fit measures are not suited for this approach. Instead, model performance is usually evaluated by means of nonparametric measures for the amount of explained variance and predictive power of the model, while jack-knifing or bootstrapping procedures are applied for uncertainty analysis (Chin 2010, Götz et al. 2010).

Model evaluation is usually done in two steps. First, the reliability and validity of the measurement part of the model is assessed, i.e. whether the measured indicator variables adequately represent the latent construct, followed by the evaluation of the structural pathways of the model.

Two conditions for the adequate definition of the measurement model are discriminant and convergent validity. These measures indicate whether the indicator variables associated with a certain latent construct do adequately represent this concept, i.e. whether the latent construct shows stronger correlations with its own measures than with the measures of another latent construct or another construct itself. If these two conditions are not met, the two constructs might not be conceptually distinguishable or the chosen indicator variables do not represent the two concepts very well.

The following measures are commonly reported for the evaluation of measurement models.

Factor loadings are the correlations of each indicator with the latent variable. They indicate how much of the indicator's variance can be explained by the latent construct. Values of > 0.7 imply a proportion of explained variance of more than 50%, which is regarded as acceptable.

Average variance extracted (AVE) (Fornell & Larcker 1981) measures the amount of variance a latent variable shares with its indicators relative to the amount of measurement error. AVE values of > 0.5 indicate that more than half of the variance in the indicators is accounted for and are generally accepted.

$$AVE = \frac{\sum_i \lambda_i^2}{\sum_i \lambda_i^2 + \sum_i \operatorname{var}(\varepsilon_i)},$$

where λ_i is the loading of an indicator variable i of a latent variable and ε_i stands for the amount of measurement error associated with indicator variabel i.

Composite reliability (Fornell & Larcker 1981) is a measure of scale reliability which assesses the internal consistency of a construct, i.e. the mutual association of indicators, which are assigned to the same latent construct. Composite reliability is given for values > 0.6.

$$\rho = \frac{\left(\sum_i \lambda_{ij}\right)^2}{\left(\sum_i \lambda_{ij}\right)^2 + \sum_i \operatorname{var}(\varepsilon_{ij})},$$

where λ_i is the loading of an indicator variable i of a latent variable, ε_i stands for the measurement error of indicator variabel i and j represents the index over all measurement models.

Cronbach's Alpha is also a reliability measure of internal consistency assessing the amount of systematic variance within a construct. This measure should also obtain minimum values of 0.6 to imply reliability of the latent construct.

$$\alpha = \frac{N}{(N-1)} * \left(1 - \frac{\sum_1^N \sigma_i^2}{\sigma_t^2}\right),$$

where N is the number of indicators assigned to a latent construct, σ_i^2 represents the variance of indicator variable i and σ_t^2 stands for the variance of the sum of all the assigned indicator scores. Cronbach's alpha varies between 0 and 1. Values > 0.6 are generally accepted.

The **Fornell-Larcker criterion** states that the discriminant validity, i.e. lower correlation between indicator variables associated with different latent constructs, is proven if a latent variable's AVE is larger than the squared correlations of this latent variable with all other latent constructs.

The following table lists the above mentioned measurement model evaluation criteria with their according minimum acceptance thresholds:

Evaluation Measure	Accepted minimum value
Factor Loadings	> 0.7
Average Variance Extracted (AVE)	> 0.5
Composite Reliability	> 0.6
Cronbach's Alpha	> 0.6

For the assessment of the structural part of a PLS SEM and overall model performance three criteria are commonly used.

The **Stone-Geisser criterion (Q^2)** is obtained using a blindfolding procedure implemented in most PLS SEM softwares, in which a number of data points are removed and replaced by a missing value algorithm. Q^2 values below or equal to zero indicate predictive power as good as random or worse. If Q^2 values are larger than zero, a model is considered to have predictive validity. Values of 0.02, 0.15 and 0.35 indicate small, medium and large predictive relevance of an exogenous construct.

$$Q_j^2 = 1 - \frac{\sum_k E_{jk}}{\sum_k O_{jk}},$$

where E_{jk} represent the squares of the prediction error, which is calculated as the difference between the true values of the omitted observations and the values predicted by the model. O_{jk} stands for the squares of the trivial prediction error which is provided by the mean of the remaining data from the blindfolding procedure.

The **effect size (f^2)** measures the change in the R^2 value of an endogenous variable when a particular exogenous construct is excluded from the model and therefore indicates how substantive the effect of this predictor is. Again, effect sizes of 0.02, 0.15 and 0.35 are considered to be of small, medium and large impact (Cohen 1988).

$$f^2 = \frac{R_{incl}^2 - R_{excl}^2}{1 - R_{incl}^2},$$

where R^2_{incl} is the dependent variable's determination coefficient calculated while including the independent latent variabel of interest, R^2_{excl} respectively is obtained from model estimation without the independent latent variable.

The **explained variance (R^2)** values reflect the share of variance in a latent variable explained by its causal predecessor variables and can be interpreted as in normal regression as a measure for the explanatory power of a particular model. Its values can range from 0 to 1. For PLS structural equation models there are no defined thresholds, which identify a model as acceptable as this partly depends on the nature of the underlying data.

For further reading on model evaluation criteria see Chin 2010 and Götz et al. 2010.

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