Supplementary information for Ganssen et al, submitted to Climate of the Past.

Outlier detection for ISA data: a comparison of different methods.

In the study presented here Individual Specimen Analyis (ISA) oxygen isotope data are used to infer a range of calcification temperatures for a given species. It is commonly known that the range is particular sensitive to outliers, as it is defined by subtracting the maximum from the minimum value, and therefore critically depends on the two most extreme values. Since the resulting range of oxygen isotope ISA values is important for our conclusions, we consider it necessary to give special attention to this aspect of the data-analysis. We here compare different methods for outlier detection, and the impact of these analyses on the extreme values.

Various methods or approaches exist to detect outliers in data, i.e. data points having an anomalous value. Basically one could test or assume the data are normally distributed and exclude data based on the mean value +/- a range defined for example using the variance of each data-set, or one does not make the assumption that the data are normally distributed and uses methods that do not require this assumption. In addition to both methods one could follow two different approaches again; either one excludes consistently a few data values (e.g. based on a given percentile) in the tails of the distribution, or only exclude extreme values in case there is a firm basis for this. One cannot state a priori which of these methods is the best to be applied for the present study, and therefore we compare different approaches to see what would be the impact of the different methods.

Four different methods are compared:

1). Ranges resulting from the raw data values;

2). Ranges resulting from excluding data outside the mean value +/- two standard deviations;

3). Ranges resulting from excluding values using the Inter Quartile Range (IQR) of the data; i.e. outside the range [Q1-k*IQR, Q3+k*IQR] in which IQR = Q3-Q1, and k a given positive value often chosen to be 1.5 by commonly used software packages;

4). Ranges resulting from excluding values using the Median Absolute Deviation (MAD) of the data; i.e. outside the range [M-k*MAD; M+k*MAD]. Since for a normal distribtion it can be shown that the standard deviation of the data equals 1.4826*MAD, we will use k = 3.8189 for the detection of anomalous values. Hence we exclude data outside the range [M-3.8189*MAD; M+3.8189*MAD]; M being the median value of the data-set.

Method 3 was selected for application for Figure 3.

Comparison of outlier detection methods
***Globigerinoides ruber* box - core transect Somalia**
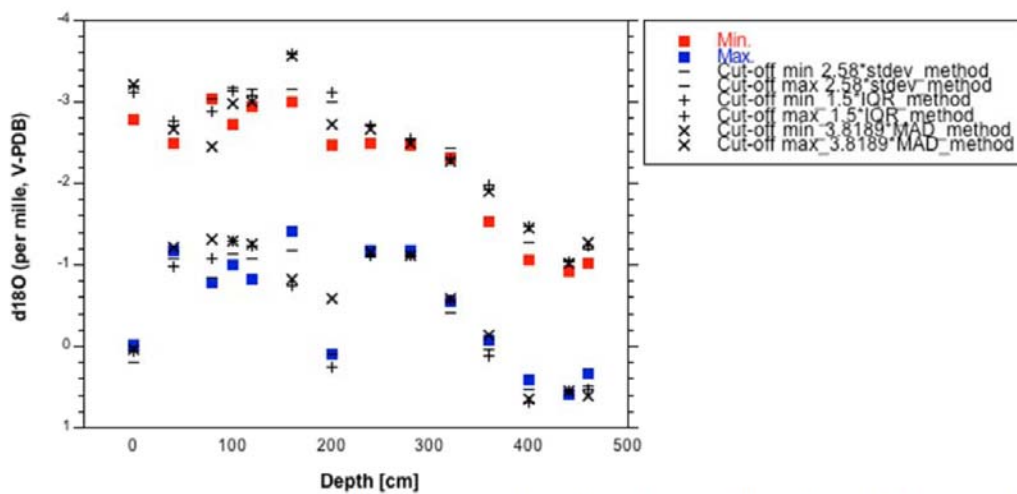**902B - 906B**
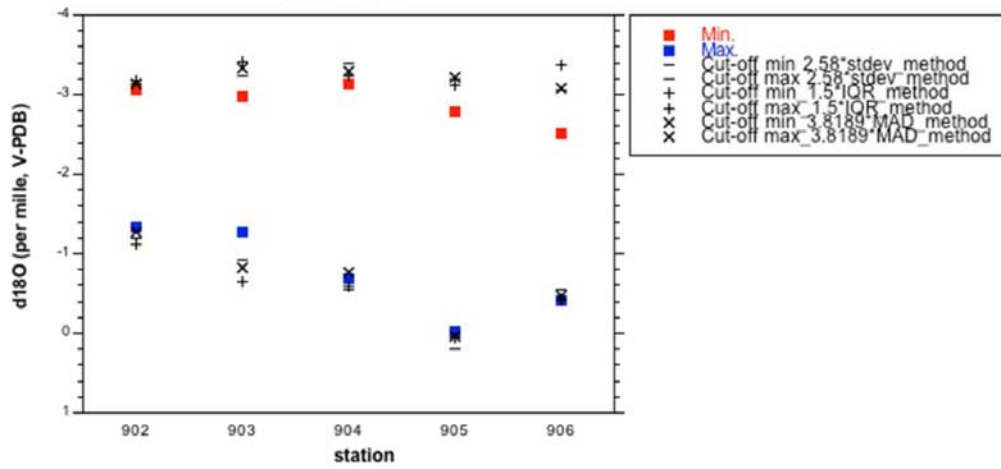
Supplementary Figure 1. Comparison of outlier detection methods applied to G. ruber (355 - 400 μm) d18O core tope data Somalia transect. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.
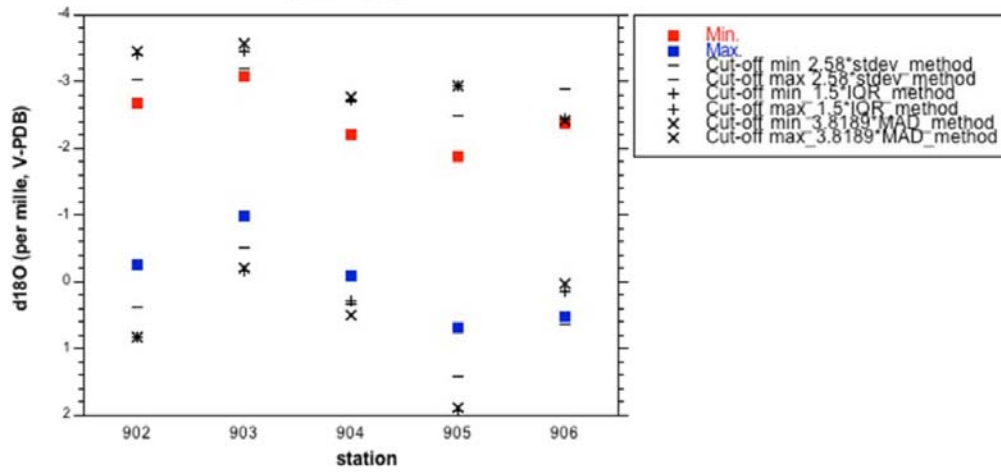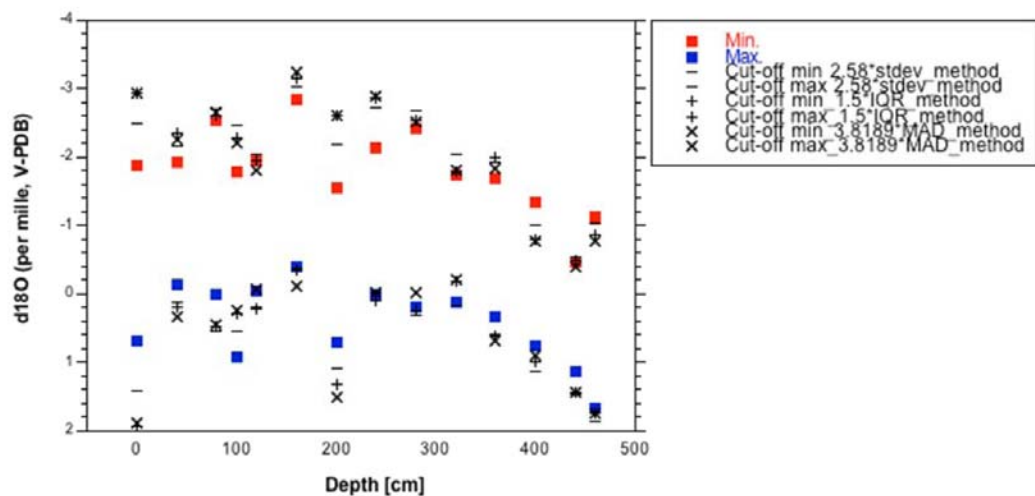
Supplementary Figure 2. Comparison of outlier detection methods applied to G. bulloides(300 - 355 μm) d18O core tope data Somalia transect. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.

Comparison of outlier detection methods
Globigerinoides ruber - 905P

Supplementary Figure 3. Comparison of outlier detection methods applied to G. ruber (335 - 400 μm) d18O 905P data. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.
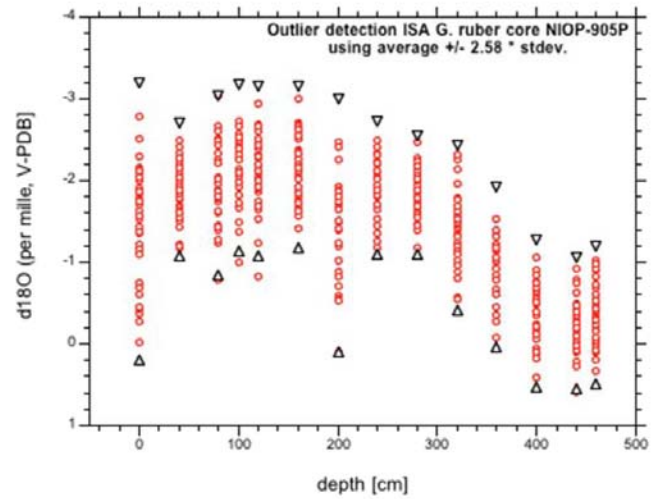
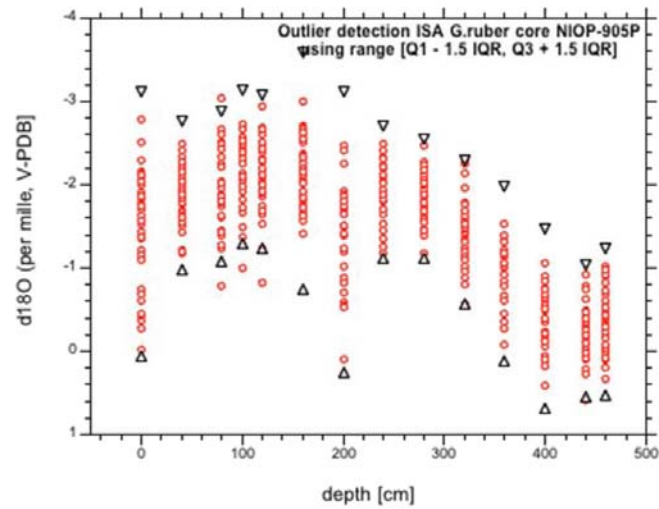## Comparison of outlier detection methods
Globigerina bulloides - 905P

Supplementary Figure 4. Comparison of outlier detection methods applied to G. boilloides (300 - 355 µm) d18O 905P data. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.

Supplementary Figure 5. Visualisation of the four outlier correction methodologies for down core $\delta^{18}O$ range for (a-c) *G.ruber* (red circles) and (d-f) *G.bulloides* (blue circles), triangles represent cut off points. Method 1: Raw data range; Method 2: resulting from excluding data outside the mean value +/- two standard deviations; Method 3: from excluding values using the Inter Quartile Range (IQR) and Method 4: excluding values using the Median Absolute Deviation (MAD).
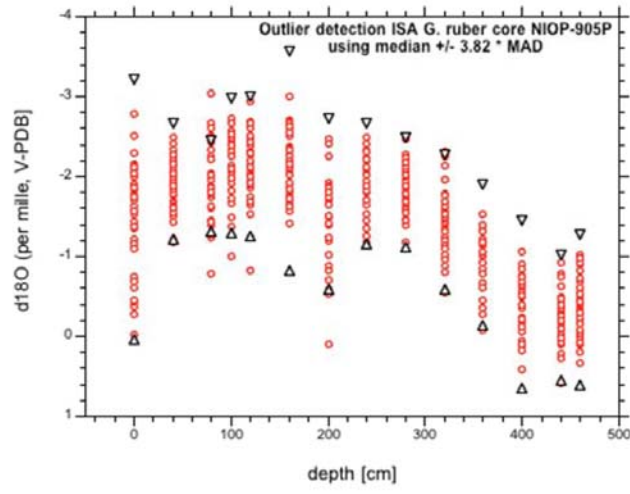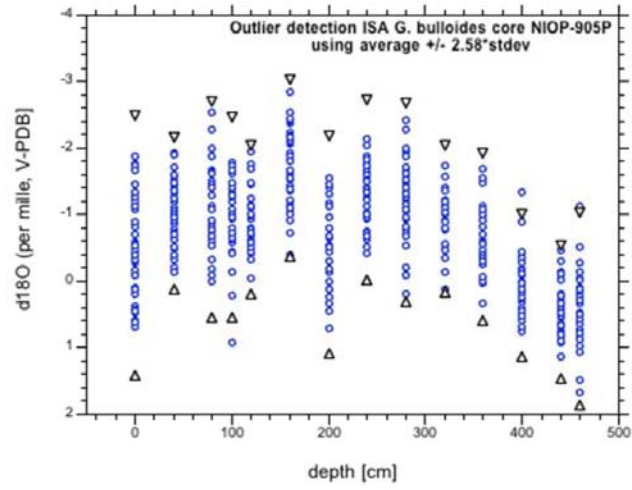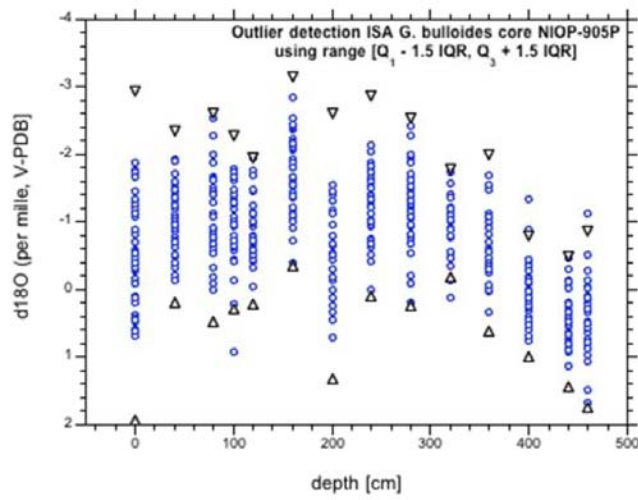
a)

b)

c)

Outlier detection ISA G. ruber core NIOP-905P
using median +/- 3.82 * MAD

d)

Outlier detection ISA G. bulloides core NIOP-905P
using average +/- 2.58*stdev

e)

Outlier detection ISA G. bulloides core NIOP-905P
using range [Q_1 - 1.5 IQR, Q_3 + 1.5 IQR]

f)

Outlier detection ISA G. bulloides core NIOP 905P
using median +/-3.82* MAD