

How to interpret palaeoclimate CLAMP estimates – is it a number value or an interval range?

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Palaeoclimatic estimates derived from CLAMP are usually presented as an exact value/number. However, in order to be correct, palaeoclimatic estimates derived from the CLAMP calibration datasets including physiognomic and meteorological characteristics of living vegetation must be expressed as intervals. This study introduces a method for calculating confidence intervals of CLAMP estimates. These intervals are generated separately for each palaeoclimate parameter and dataset of modern calibration sites and will help to interpret the obtained CLAMP results in a statistically sound way.

• Key words: palaeoclimate, proxy-data, estimate, CLAMP, STDEV residual, confidence interval.

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Currently, two different proxies for palaeoclimatic analysis using the plant fossil record are widely used. One is the physiognomic approach such as Leaf Margin Analysis (LMA) and Climate Leaf Analysis Multivariate Program (CLAMP) (e.g., Wolfe 1979, Wolfe & Spicer 1999, Spicer 2011–2016) while the other is based on the nearest living relative principle (NLR; Coexisting Approach, CA, e.g., Mosbrugger & Utescher 1997, Utescher & Mosbrugger 1997–2016). These two classes of techniques are quite different in their methodology. Both approaches produce comparable outcomes – palaeoclimate estimates, which may be correlated and discussed (e.g., Kvaček 2007, Grim & Denk 2012, Utescher *et al.* 2014, Teodoridis & Kvaček 2015). By necessity, the results of CA are presented as specific ranges of coexistence intervals for each studied climatic/palaeoclimatic parameters – Mean Annual Temperature (MAT), Coldest Month Mean Temperature (CMMT), Warmest Month Mean Temperature (WMMT), Mean Annual Precipitation (MAP) (see Mosbrugger & Utescher 1997, Utescher *et al.* 2014). However, the estimates derived from CLAMP are most often presented and interpreted as an exact value/number, *i.e.* a single (point) estimate, or as the value/number plus-minus a value of the STDEV residuals (e.g., Uhl *et al.* 2007, Teodoridis *et al.* 2009).

This paper introduces a statistically sound concept for calculating the interval of CLAMP estimates. This range or

interval is defined separately for each palaeoclimate parameter and set of modern calibration sites. This concept will allow a more meaningful interpretation of CLAMP results.

CLAMP – a brief methodological description

Climate Leaf Analysis Multivariate Program (CLAMP) is based on a multivariate statistical technique to quantitatively determine palaeoclimate parameters based on the leaf physiognomy of woody dicotyledonous flowering plants. CLAMP was first introduced by Wolfe (1993) and subsequently this technique has been refined mainly by Wolfe & Spicer (1999), Spicer (2000, 2007), Spicer *et al.* (2004, 2009), and Teodoridis *et al.* (2011). Generally, the CLAMP technique employs 31 different leaf physiognomic characteristics to estimate 11 climatic parameters, *i.e.* MAT (Mean Annual Temperature), WMMT (Warmest Month Mean Temperature), CMMT (Coldest Month Mean Temperature), GROWSEAS (Length of the Growing Season), GSP (Growing Season Precipitation), MMGSP (Mean Monthly Growing Season Precipitation), 3-WET (Precipitation during 3 Consecutive Wettest Months), 3-DRY (Precipitation during 3 Consecutive Driest Months),

RH (Relative Humidity), SH (Specific Humidity) and ENTHAL (Enthalpy). Mathematically, this method is based on Canonical Correspondence Analysis (CCA) – see Ter Braak (1986) performed by the software CANOCO for Windows Version 4.5 or automatically by an on-line application (see below), which reduces this multidimensional space (31 leaf physiognomic characteristics and 11 climatic parameters) to fewer, typically four-dimensional space and for each site is estimated vector score (AX1-4, ENV AX1-4), which represents its position in this space (position along the climate vector). The relationship between the climate vector scores and the observed climate values for those sites is represented by 2nd order polynomial regression CLAMP physiognomic datasets from 144, 162, 173 and 189 modern sites mainly from SE Asia, Northern America and India and their relevant modern gridded meteorological calibration datasets corrected for the exact altitude of the sampling site (New *et al.* 2002, Spicer *et al.* 2009), *i.e.*, Physg3ar, Physg3br, PhysgAsia1, PhysgIndia1, GRIDMet3a, GRIDMet3b, GRIDMetAsia1 and GRIDMetIndia1, were published by Spicer *et al.* (2009), Jacques *et al.* (2011), Srivastava *et al.* (2012) – see Appendix 1. Teodoridis *et al.* (2011, 2012) developed a special statistical tool, which helps to select relevant CLAMP physiognomic/meteorological datasets. All the mentioned reference files and datasets can be freely downloadable from the CLAMP website (Spicer 2011–2016) – see Appendix 1. Recently Yang *et al.* (2015) presented a new calibration dataset from 378 natural or naturalized vegetation sites from all continents except Antarctica including biomes from tropical to taiga, over a range of elevations from 0.5 m to over 3000 m a.s.l. The study verified the generally assumed correlation between leaf form and climate used by CLAMP and/or LMA. The CLAMP analysis including the new updates is now automated by the on-line application developed by Yang *et al.* (2011) on the CLAMP website (Spicer 2011–2016).

Methodology

As mentioned above, the CLAMP technique is based on Canonical Correspondence Analysis (CCA – Ter Braak 1986). Generally, one of the basic assumptions of any statistical techniques working with a sample is that the sample is randomly selected. It is clear that in some cases this assumption has to be applied with some limitations as is usual in natural science. There is no unlimited number of sites in the world, where vegetation and meteorological data are available as a source for the calibration datasets of CLAMP because of the vegetation has to have a primary character or with less influence of human being. Randomness in this sample is assumed as there is

no impact of any vegetation or meteorological deviation and sample represents variability of the whole population of sites. For the CLAMP technique the randomness of the sample is limited by some more aspects, which are summarized by R. Spicer on the CLAMP website under the heading “Uncertainties in CLAMP” (Spicer 2011–2016). The CLAMP uncertainties are divided into four main categories, *i.e.* (a) taphonomic uncertainties bound on fossil assemblage altered during the process of transport, deposition and fossilization, (b) errors associated with climatic measurements, (c) uncertainties derived from environmental and ecosystem “noise” (individual plant responses to specific environmental constrains), and (d) errors originated during sampling and scoring (for more details see Spicer 2011–2016). Nevertheless, it has to be assumed that in the CLAMP sample (calibration datasets) all types of vegetation and their climate aspects are covered and the sample is not systematically deviated by any effects. This is why the CLAMP technique can still be taken as a model, which is based on the random selection of natural or naturalized vegetation sites from which a relationship between modern meteorological and physiognomic data is estimated, which is compared with physiognomic data encountered in a fossil leaf assemblage. The crucial assumption for using CCA (engine of the CLAMP technique) is the randomness of sample of the input (calibration) datasets (see Ter Braak 1986, p. 1168) irrespective of subsequent interpretation of the character of the CLAMP results (*i.e.*, number or interval). The variability in calibration datasets causes the variability of the results (CLAMP estimates), which should not be presented as single points (number estimation), but as an interval that considers the specific level of confidence of the result.

Using STDEV Residuals value to build the CLAMP interval estimate

Values of the STDEV Residuals are normally generated from the “result lists” (see Table 1) and are completely independent of the CLAMP results derived from the studied fossil flora/its physiognomic characteristic. What are these values? How can they be used for the interpretation of CLAMP results? Values of the STDEV Residuals represent the Standard Deviation of differences between observed values of meteorological data from modern sites (GRID-files see Appendix 1) and predicted values (estimates) by CLAMP (*i.e.*, the standard deviation of the distance of the real point of meteorological measurements on the modern site and the regression line expressing predicted “palaeoclimatic” values by CLAMP), in fact this value is “the Standard deviation of the deviation”. Mathematical expression of

Table 1. Values of the STDEV Residuals for the CLAMP palaeoclimate parameters derived from the modern CLAMP calibration datasets (Appendix 1).

CLAMP palaeoclimate parameters [unit]	Calibration datasets / values of the STDEV Residuals							
	Physg3brcAZ + GRIDMet3arAZ (144)		Physg3arcAZ + GRIDMet3brAZ (173)		PhysgAsia1 + GRIDMetAsia1 (189)		Physg3brcAZIndia1 + GRIDMet3brAZIndia1 (162)	
	STDEV Residuals	2x STDEV Residuals	STDEV Residuals	2x STDEV Residuals	STDEV Residuals	2x STDEV Residuals	STDEV Residuals	2x STDEV Residuals
MAT [°C]	1.17	2.33	1.63	3.25	1.25	2.51	1.35	2.70
WMMT [°C]	1.39	2.78	1.77	3.54	1.51	3.02	1.65	3.31
CMMT [°C]	1.88	3.77	2.12	4.25	2.57	5.15	2.16	4.32
GROWSEAS [month]	0.69	1.39	0.77	1.54	0.74	1.48	0.72	1.44
GSP [cm]	20.17	40.35	19.48	38.97	21.77	43.53	30.73	61.46
MMGSP [cm]	2.61	5.22	2.50	5.01	2.53	5.07	3.10	6.20
3-WET [cm]	14.63	29.25	13.37	26.74	13.90	27.80	17.25	34.50
3-DRY [cm]	3.20	6.39	3.54	7.09	4.12	8.25	4.22	8.43
RH [%]	5.08	10.15	6.28	12.56	6.04	12.09	6.28	12.56
SH [g/kg]	1.00	2.01	1.00	2.00	1.18	2.36	1.15	2.29
ENTHAL 0.1*[kJ/kg]	0.45	0.91	0.44	0.89	0.54	1.09	0.52	1.04

Table 2. Margin of error of the Confidence Intervals calculated for each palaeoclimate parameters and modern CLAMP calibration datasets (Appendix 1).

CLAMP palaeoclimate parameters [unit]	CLAMP calibration datasets			
	Physg3brcAZ + GRIDMet3arAZ (144)	Physg3arcAZ + GRIDMet3brAZ (173)	PhysgAsia1 + GRIDMetAsia1 (189)	Physg3brcAZIndia1 + GRIDMet3brAZIndia1 (162)
MAT [°C]	3.9	5.3	4.4	4.6
WMMT [°C]	4.8	5.8	5.2	5.4
CMMT [°C]	6.6	7.4	8.1	7.4
GROWSEAS [month]	2.1	2.4	2.3	2.1
GSP [cm]	59.4	56.5	67.5	87.1
MMGSP [cm]	7.1	6.7	8.3	9.1
3-WET [cm]	43.9	42.5	41.8	54.7
3-DRY [cm]	11.2	11.3	14.6	13.2
RH [%]	16.7	20.3	18.4	18.9
SH [g/kg]	3.2	3.1	3.7	3.5
ENTHAL 0.1*[kJ/kg]	1.5	1.5	1.7	1.6

the interval based on the STDEV Residual values is followed in Eqs 1, 2:

Eq (1):

$$El_{w,x} = E_{w,x} - \sqrt{\frac{\sum_{x=1}^n \sqrt{(E_{w,x} - O_{w,x})^2}}{n-1}},$$

Eq (2):

$$Eu_{w,x} = E_{w,x} + \sqrt{\frac{\sum_{x=1}^n \sqrt{(E_{w,x} - O_{w,x})^2}}{n-1}},$$

where $E_{w,x}$ is the numerical CLAMP value (estimate) of the studied (meteorological) parameter w at modern site x

and $O_{w,x}$ is observed value of the studied (meteorological) parameter w at modern site x and n is the total number of studied sites used. The “real point” of meteorological measurements on modern sites, *i.e.* real values of the measured meteorological parameters on the sites, where a “primary” vegetation has grown, belongs to CLAMP uncertainties, which arise from the way climate data are recorded and gridded, climate alters over time, variations in local microclimates and how plants respond to them, and how well leaf physiognomy data from a given site are collected and converted to the CLAMP scoring scheme (Spicer *et al.* 2009, see Measuring CLAMP uncertainties on CLAMP website – Spicer 2011–2016).

Table 3. Palaeoclimatic estimates based on the CLAMP and the Coexistence Approach (CA) techniques from the selected late Eocene to early Miocene floras of the Bohemian Massif.

Age	Locality	Floristic references	Palaeoclimatic estimates						
			Coexistence Approach (CA)				CLAMP		
			MAT [°C]	WMMT [°C]	CMMT [°C]	Reference	MAT [°C]	Value/point estimate	STDEV Residual Interval
Early Miocene	Mydlovary Formation	Knobloch (1986), Knobloch & Kvaček (1996)	15.7–16.5	24.9–26.0	4.5–5.8	Teodoridis & Kvaček (2015)	13.9	12.7–15.1	10.0–17.8
	Cypris Formation	Bůžek <i>et al.</i> (1996)	15.7–17.0	24.9–27.5	5.6–13.3	Teodoridis & Kvaček (2015)	13.1	11.8–14.4	8.7–17.5
	Břešťany	Kvaček & Teodoridis (2007), Teodoridis & Kvaček (2006)	16.5–18.9	24.7–27.5	4.8–12.2	Mach <i>et al.</i> (2014)	14.5	13.3–15.7	10.6–18.4
Late Oligocene	Hlavačov Gravel and Sand	Teodoridis (2002)	15.7–17.0	24.3–27.0	2.2–8.3	Teodoridis & Kvaček (2015)	8.5	7.3–9.7	4.6–12.4
	Matrý	Radoň (2001), Soukupová (2004)	11.2–15.6	24.0–26.8	(–1.6)–5.0		13.6	12.0–15.2	8.3–18.9
Early Oligocene	Markvartice–Veselíčko	Bůžek <i>et al.</i> (1976)	14.6–18.5	24.7–25.9	2.2–12.2		11.9	10.6–13.2	7.5–16.3
	Sulečice–Berand	Kvaček & Walther (1995)	15.6–18.3	24.7–27.5	5.0–10.9		12.4	11.2–13.6	8.5–16.3
	Hrazený	Kvaček <i>et al.</i> (2015)	14.6–18.9	24.7–28.3	5.0–12.2		11.3	10.1–12.5	7.4–15.2
	Kundratice	Kvaček & Walther (1998)	14.6–18.5	24.7–25.9	5.0–11.0	Kvaček <i>et al.</i> (2014)	12.1	10.9–13.3	8.2–16.0
	Bechlejšovice	Kvaček & Walther (2004)	14.6–17.4	24.7–28.1	7.7–10.9		11.1	9.9–12.3	7.2–15.0
Late Eocene	Roudníky	Kvaček <i>et al.</i> (2014)	13.6–18.0	23.6–27.1	1.8–10.0		10	8.8–11.2	6.1–13.9
	Kučlín	Kvaček & Teodoridis (2011)	16.5–18.0	24.7–27.1	7.7–10.0	Kvaček & Teodoridis (2011)	16.8	15.5–18.1	12.4–21.2
	Staré Sedlo	Knobloch <i>et al.</i> (1996)	15.7–23.9	25.6–28.1	5.0–12.6	Teodoridis <i>et al.</i> (2012)	16.2	14.9–17.5	11.8–20.6

Using STDEV Residuals values as interval estimate is incorrect because its construction lacks any component of confidence.

Using Confidence Interval as the CLAMP estimate

The upper and lower limits of the interval ($E_{w,x}^{reg}$, $Eu_{w,x}^{reg}$) equal to the value of $(1-\alpha)$ % confidence level (usually we use 90% or 95% confidence level) derived from the regression relation between “vector score” and the relevant observed CLAMP climatic parameter. The limits were calculated following equations Eq 3, 4 as $E_{w,x}$ (estimated CLAMP value) \pm margin of error:

Eq (3):

$$CLAMP_{w,x}^{reg} = E_{w,x} - t_{1-\frac{\alpha}{2}}(n-2) \cdot$$

$$\sqrt{\frac{S_R}{n-2}} \cdot \sqrt{1 + \frac{1}{n} + \frac{(v_x - \bar{v})^2}{(n-1)s_v^2}},$$

Eq (4):

$$CLAMP_{w,x}^{reg} = E_{w,x} + t_{1-\frac{\alpha}{2}}(n-2) \cdot$$

$$\sqrt{\frac{S_R}{n-2}} \cdot \sqrt{1 + \frac{1}{n} + \frac{(v_x - \bar{v})^2}{(n-1)s_v^2}},$$

where $E_{w,x}$ is the estimated CLAMP value of the studied (meteorological) parameter w at the modern site x , $t_{1-\alpha/2}$ is a Student’s t-distribution quantile, S_R is the residual sum of squares (differences between observed values of meteorological data from modern sites and predicted values), $v_{w,x}$ is the value of the vector score for parameter w of the relevant modern site x , s_v^2 is the dispersion of the vector score values for parameter w , and n is the total number of studied sites used. Contrary to the above-mentioned STDEV residuals, this interval of range considers more factors. The middle part of the formula (Eqs 3 and 4) contains STDEV but it is multiplied by two other components:

1. “ $t_{1-\alpha/2}(n-2)$ ” is Student’s distribution quantile, which depends on two parameters – α is the level of the used con-

Table 3. continued

Age	Locality	Palaeoclimatic estimates						CLAMP calibration dataset selected via application <i>sensu</i> Teodoridis <i>et al.</i> (2012)
		CLAMP						
		WMMT [°C]			CMMT [°C]			
		Value/point estimate	STDEV Residual Interval	Confidence Interval	Value/point estimate	STDEV Residual Interval	Confidence Interval	
Early Miocene	Mydlovary Formation	25.3	23.9–26.7	20.5–30.1	4.1	2.2–6.0	–2.5–10.7	144
	Cypris Formation	25.1	23.4–26.8	19.9–30.3	2.9	0.3–5.5	–5.2–11.0	189
	Břešťany	21.4	20.0–22.8	16.6–26.2	8.9	7.0–10.8	2.3–15.5	144
Late Oligocene	Hlavačov Gravel and Sand	21.3	19.9–22.7	16.5–26.1	–3.3	–5.2–(–1.4)	–100–3.4	144
	Matrý	20.7	18.9–22.5	14.9–26.5	7.4	5.2–9.6	0.0–14.8	173
Early Oligocene	Markvartice–Veselíčko	23.5	21.8–25.2	18.3–28.7	1.8	–0.8–4.4	–6.3–9.9	189
	Suletice–Berand	24.8	23.4–26.2	20.0–29.6	1.6	–0.3–3.5	–5.0–8.2	144
	Hrazený	22.1	20.7–23.5	17.3–26.9	1.7	–0.2–3.6	–4.9–8.3	144
	Kundratice	23.5	22.1–24.9	18.7–28.3	2.4	0.5–4.3	–4.2–9.0	144
	Bechlejevce	21.1	19.7–22.5	16.3–25.9	2.1	0.2–4.0	–4.5–8.7	144
	Roudníky	21.6	20.2–23.0	16.8–26.4	0	–1.9–1.9	–6.6–6.6	144
Late Eocene	Kučlín	26.1	24.4–27.8	20.9–31.3	8.1	5.5–10.7	0.0–16.2	189
	Staré Sedlo	25.9	24.2–27.6	20.7–31.1	6.3	3.7–8.9	–1.8–14.4	189

confidence (expressed as $1 - \alpha$) and n is the number of observations. The confidence level of 90% roughly equals 1.65 and the confidence level of 95% is about 2.0. The level of confidence 95% corresponds to Spicer’s original recommendation to multiple 2 times the value of the STDEV to obtain an interval covering 95 % of the data (see Measuring CLAMP uncertainties on CLAMP website).

$$2. \sqrt{1 + \frac{1}{n} + \frac{(v_x - \bar{v})^2}{(n-1)s_v^2}}$$

is usually close to 1 (especially

for large samples as we use in CLAMP analysis) and if the value of the vector score is nearest to the mean value of the calibration file (the studied locality is not an outlier), a range of estimated interval is narrow and this part has not high influence on the width of the interval. Towards the ends of the regression line, near the limits of the calibrated physiognomic space, uncertainties rise, so any fossil site lying at the extremes of the calibration has larger, poorly quantified uncertainties. Although the CLAMP analysis is robust, it is not recommended to use its results (estimates) for extreme sites/localities due to its uncertainties. In other

cases, where localities do not produce extreme values, a simplified table can be used with estimated values based on the interval range at 95% confidence level (see Table 2).

To obtain an accurate limit of the Confidence Interval for specific physiognomic characteristics of fossil sites it is possible to use a “Copy & Paste” application (see Appendix 2). The limit values of the confidence interval will automatically appeared in a result table of Appendix 2, when values of the vector score for each palaeoclimatic parameters from the result files (*i.e.*, Res3arcAZ, Res3brcAZ, ResAsia1 and RES3BRCIndia1 – see Appendix 3) are input into a vector score’s table of Appendix 2.

Discussion

A comparison of results based on the STDEV Residuals and Confidence intervals are presented in Fig. 1. There is evidence that the confidence interval is wider and covers almost all “regression” points. The results correspond to a previous statement made on the CLAMP website (Spicer

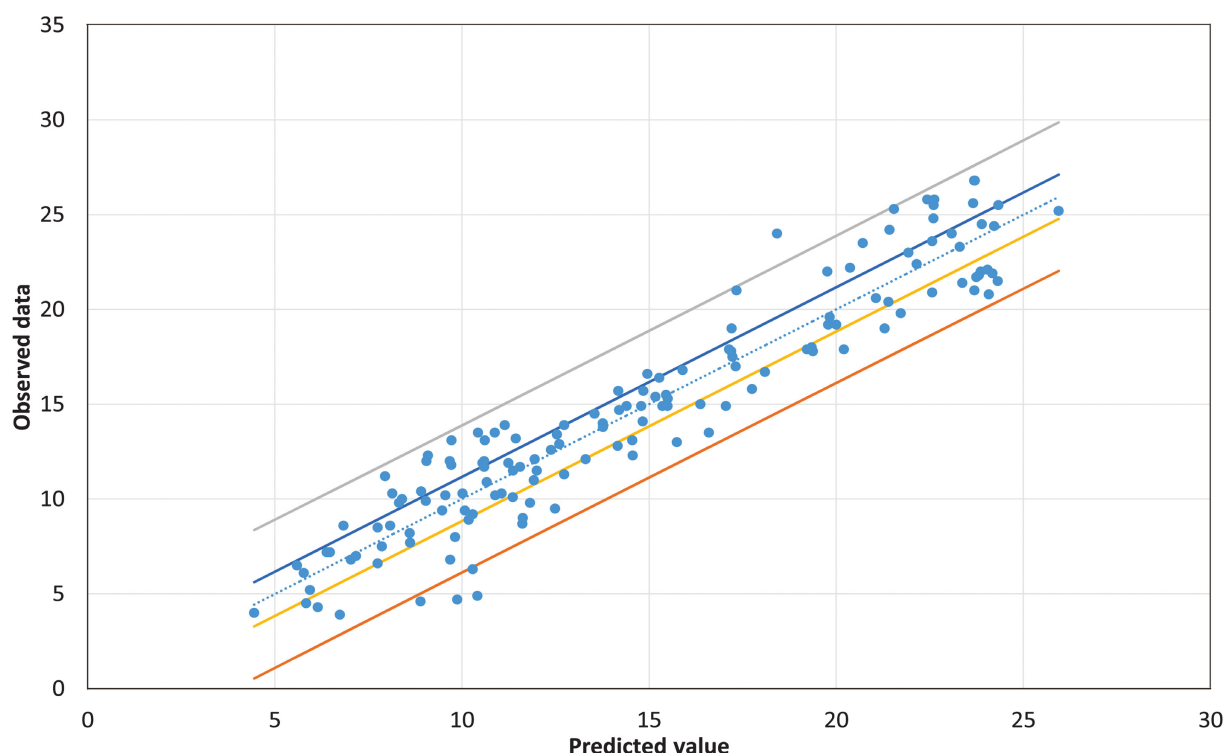


Figure 1. A relation of the observed MAT value and predicted MAT derived from the CLAMP calibration dataset Physg3brcAZ + GRIDMet3brAZ including 144 sampling site. Symbols: dotted line – regression line, yellow and blue lines – upper and lower limits of the STDEV Residuals Interval, red and grey lines – upper and lower limits of the Confidence Interval.

2011–2016): “The scatter of the sites about the regression model line is usually expressed in terms of standard deviations, with ± 2 standard deviations encompassing 95% of the data. The standard deviation in this measure, however, calculates uncertainty from the point of view of active samples and not passive ones as is the case with fossils and only in respect of the vector score rather than the observed climate data.” Table 1 and Fig. 1 show values of STDEV Residuals multiplied by 2 that correspond in fact to a rounded value of 97.5% confidence limit of Normal or Student distribution. To see a real impact of the application of the confidence intervals in CLAMP estimates we re-evaluated several published CLAMP results based on Czech fossil plant assemblages from late Eocene to early Miocene including published climatic estimates of CA (see Table 3). We have no ambition here to discuss the “palaeoclimatic” relevance of the CA and CLAMP estimates presented in Table 3.

Conclusion

We can summarize the main results of the presented study as follows:

1. CLAMP estimates presented as simple values/numbers are statistically unsound and ought to be expressed as variabilities derived from the modern calibration datasets.

2. Expressing CLAMP estimates as interval range calculated by confidence intervals results in the most accurate and reliable estimates corresponding to the 95% confidence level.

3. This confidence intervals produce a more accurate and reliable range than the interval from a simple value/number plus-minus value of the STDEV Residuals or plus-minus doubled value of the STDEV Residuals.

4. The new “Copy & Paste” application allows defining specific accurate range intervals based on physiognomic characteristics of the studied fossil site.

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