Computers and Electronics in Agriculture 103 (2014) 122–126

Contents lists available at ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

Application note

CUBA: An internet-based software application for berry anthocyanins units' conversion for viticulturists, oenologists and physiologists

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ARTICLE INFO

Article history:
Received 23 October 2013
Received in revised form 12 February 2014
Accepted 24 February 2014

Keywords:
Viticulture
Grapes
Wine colour
Phenolic maturity
Fruits
Vitis vinifera

ABSTRACT

In viticulture and especially for red wine production it is important to know the grape quality. Anthocyanins, the red pigments of berry skins that define the colour of wines, are good indicators of the so-called phenolic maturity of grapes. We provided an easily accessible mean to convert anthocyanins units acquired by different analytical methods. It is available as a free internet-based tool accessible from all supports, computers, tablets and smartphones. The usefulness of this software tool was illustrated by simulation of the influence of berry mass and skin mass per area on the anthocyanin content of the must.

1. Introduction

There are numerous online tools for unit conversions of physical measurements (e.g. http://www.onlineconversion.com/). More recently appeared free downloads for various unit conversion applications adapted to mobile supports, smartphones, PDAs and tablets. Still, there are neither online tools nor software available for some specific domains of application. A good example is viticulture and oenology. Indeed, the vast majority of red grape cultivars accumulate anthocyanins only in the berry skin (Conde et al., 2007). This is why there are four different ways of expressing anthocyanin content in berries and grapes (Fig. 1). As described in Ben Ghozlen et al. (2010) where a first scheme for unit conversion was presented, these are the following. (1) Anthocyanin content expressed on skin mass basis ($Anth_m$). This is the preferred basis for cell biology (Ojeda et al., 2002), enzymology and genetics research when different types of anthocyanin are looked for (Dai et al., 2011). It is often obtained by skin peeling and subsequent HPLC analysis (e.g. Castellarin et al., 2007; Falcão et al., 2008; Hilbert et al., 2003; Ortega-Regules et al., 2006). (2) Physiologists prefer to follow the accumulation of total or individual anthocyanins per whole berry ($Anth_b$). This kinetics per organ is a good indicator of phenological stages (e.g. Ginestar et al., 1998; Ojeda et al., 2002; Ollé et al., 2011). (3) Oenologists and wine producers are interested more by the final product at harvest that is the total anthocyanin content per mass of grapes ($Anth_g$) or per volume of must ($Anth_v$), which will define the final colour of wine (Conde et al., 2007). The vast majority of available data on grape anthocyanins are on that latter basis because winery laboratories and analytical laboratories alike obtain them by extracting whole berry or cluster samples (Iland et al., 2004). (4) The last basis for anthocyanin expression is the one obtained by nondestructive optical measurements. By definition, optical measurements can only provide a surface area-based estimation of anthocyanins ($Anth_a$). This type of

Abbreviations: $Anth_a$, berry surface area-based content of anthocyanins; $Anth_b$, anthocyanins content expressed per berry; $Anth_m$, anthocyanin content expressed on skin mass basis; $Anth_g$, anthocyanin content per mass of grapes; $Anth_v$, anthocyanin content per volume of must; BM, berry mass; BV, berry volume; SMA, skin mass per area; SVR, surface-to-volume ratio.

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http://dx.doi.org/10.1016/j.compag.2014.02.012
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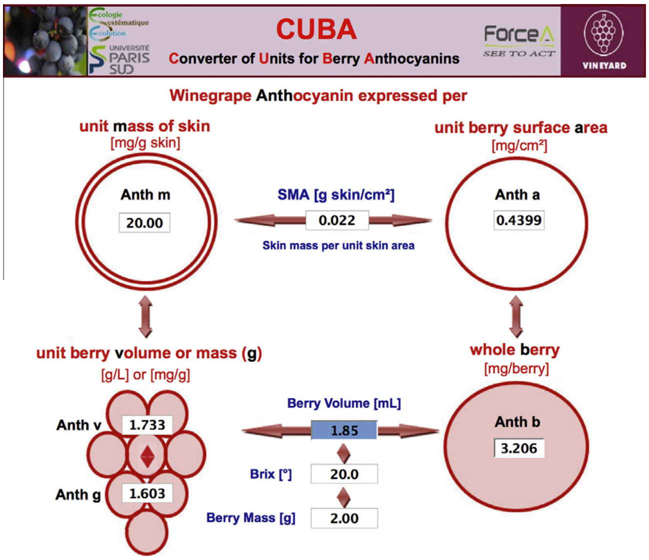

Fig. 1. Print screen of the CUBA web page.

measurement is gaining importance with the introduction of proximal sensors in viticulture, like the Multiplex based on fluorescence (Ben Ghozlen et al., 2010) or prototypes based on NIR spectroscopy (Cozzolino et al., 2006; Geraudie et al., 2010; Nicolaï et al., 2007).

To help overcome this problem of variations in units used we designed a freely accessible internet-based software tool to help viticulturists and oenologists transform easily the anthocyanin content data coming from different sources. We were especially motivated by the need to compare the newly introduced nondestructive optical measurements to standard extraction-based methods and standard oenological practice. This tool can also be useful for researchers who would like to simulate anthocyanin accumulation under the effect of various environmental variables (temperature, water availability, irradiance) on berry characteristics (berry mass, skin thickness) and how they will influence the final grape and wine quality.

2. Basis for calculation

The four basis for anthocyanin content expression are linked by known relationships that are dependent on berry characteristics. Only four intrinsic berry characteristics need to be known to calculate the six parameters linking the four types of anthocyanin contents (Fig. 1) (cf. also Appendix A). First, the skin thickness, or better to say skin mass per area (SMA) that encompasses both the thickness and the specific gravity of the skin (by analogy to the often used leaf mass per area – LMA) is needed to transform $Anth_m$ to $Anth_a$, and vice versa. Second, the knowledge of berry shape and third of berry volume (BV) are needed. Berry shape can be approximated to a sphere without making a large error, especially for widespread international cultivars like Merlot, Cabernet Sauvignon and Pinot Noir. Alternatively, two dimensions of the berry can be acquired for the calculation of an ellipsoid. The latter has been restricted to basic research (Agati et al., 2007), so the approximation of berries to spheres is retained for the time being in CUBA. Hence, only berry volume is needed to calculate the surface (skin containing anthocyanins) to volume (whole berry) ratio (SVR). The average volume of berries needs to be either known or calculated from the berry mass (BM), which is more often available, and its specific gravity. Berry sugar content is routinely measured as the main grape quality attribute, so, the specific gravity, the fourth needed berry characteristics, is easily obtained from tables relating sugar content to specific gravity measured either by refractometry (°Brix) or hydrometry (EEC Commission, 1990). It can be noted that by taking an average specific gravity of 1.0817 for grapes at harvest, corresponding to 20 °Brix (11.4% potential alcohol) the error would be less than 5% for most grapes, more or less mature. For all four remaining parameters (or ratios) linking the units only the knowledge of berry volume is needed (cf. table in Appendix A). Most interestingly, for the transformation of optically obtained estimates of $Anth_a$ to oenologically relevant grapes anthocyanin content $Anth_v$ the average berry volume is sufficient. The latter is used to calculate SVR that links the two without the knowledge of SMA (Appendix A).

3. Description of the software

CUBA is an abbreviation for the software 'Converter of Units of Berry Anthocyanins'. The web page can be accessed from: http://max2.ese.u-psud.fr/cuba. The graphical interface consists presently of only one page. The theoretical base and formulas used for calculations can be found in Ben Ghozlen et al. (2010) and in Appendix A.

There are nine numerical fields on the CUBA page that can all, but one, be changed by the user. When the value of one field is changed all values for all other fields are automatically recalculated and displayed. The exception is the field for BV (blue[1] rectangle on Fig. 1) that bears values that cannot be changed by the operator and that are always calculated from BM and degree Brix.

The CUBA web page is based on three classical technologies for web development: HTML, CSS and JavaScript.

HTML (Hypertext Markup Language) is one of the most popular languages used for structuring content in web pages: texts, images, interactive forms or other contents. Further information about the syntax of this language can be found at World Wide Web Consortium (http://www.w3.org/TR/html-markup/syntax.html%23doctype-syntax).

CSS (Cascading Style Sheets) is a language for managing the presentation of contents written in HTML. It is used to apply visual styles and tell the browser (Chrome, Safari, Internet Explorer or Firefox) how to display different elements depending on the size of the screen on which it is viewed. CUBA can be used via personal computers or mobile platforms like tablets or smartphones. More details about CSS can also be found at World Wide Web Consortium (http://www.w3.org/Style/CSS/).

JavaScript is an interpreted computer programming language running on web browsers. It is useful for all interactive functionalities. It is used in CUBA to calculate the values of the different fields based on the conversion formulas (cf. Appendix A). Complete documentation on JavaScript is available on the web site of the Mozilla Foundation that manages this language (https://developer.mozilla.org/en-US/docs/Web/JavaScript?redirectlocale=en-US&redirectslug=JavaScript).

3.1. Programming for simulations

Simulations were performed using an object-oriented software LabVIEW 7.1 (National Instruments, Le Blanc-Mesnil, France). Same parameters and functions (cf. Appendix A) were used in the LabVIEW software module like the one used in CUBA. The only difference was the use of one-column-data arrays instead of single value in the nine fields of CUBA. When the user changes the values of one field by defining the number of data points, the starting

[1] Please note that Fig. 1 will appear in B/W in print and color in the web version. Based on this, please approve the footnote 1 which explains this.

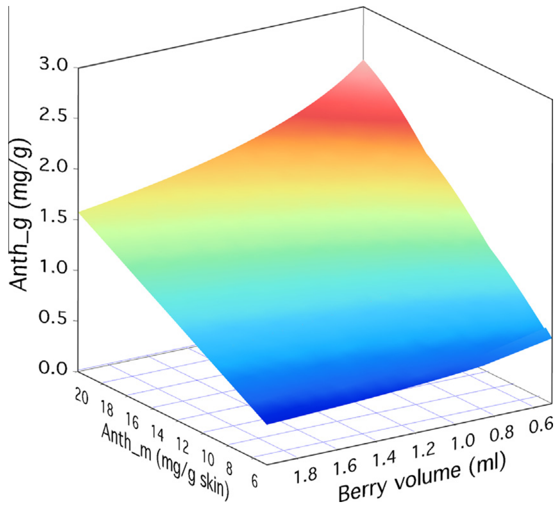

Fig. 2. Result of the simulation of the influence of skin anthocyanin content ($Anth_m$) and berry volume (BV) on anthocyanins in the must ($Anth_g$). Physiological ranges of $Anth_m$ and BV were used (cf. Table S1).

value and the increment step, all values for all other fields are automatically recalculated and displayed as columns. A multi-column table could be saved containing the results of all fields for further display. Igor 6.2 (WaveMetrics, Lake Oswego, Oregon) was used for graphical presentation of simulation data (Figs. 2 and 3). The range of values for berry size, $Anth_m$ and fixed parameters like SMA, were used based on literature data (Table S1).

4. Results and discussion

The concentration of anthocyanins in the must ($Anth_g$ or $Anth_v$) is the aspect that concerns most producers and users of grapes or juice and, hence, it is the variable most often measured and quoted in scientific literature (Coombe, 1992). However, for those who wish to interpret changes in anthocyanins during berry development, the amount per berry gives valuable additional information. But, as mentioned above, the knowledge of berry weight is needed to calculate either $Anth_g$ or $Anth_b$ from $Anth_a$. Although one can regret that it is sometimes omitted from reports on anthocyanins concentration (Coombe, 1992) it is still frequently recorded in wineries performing grape quality analysis and can therefore be used in CUBA. For wineries that do not perform analysis other than total weight and grape sugar content, if they adopt grape quality analysis they should include the hundred-berry weight measurement.

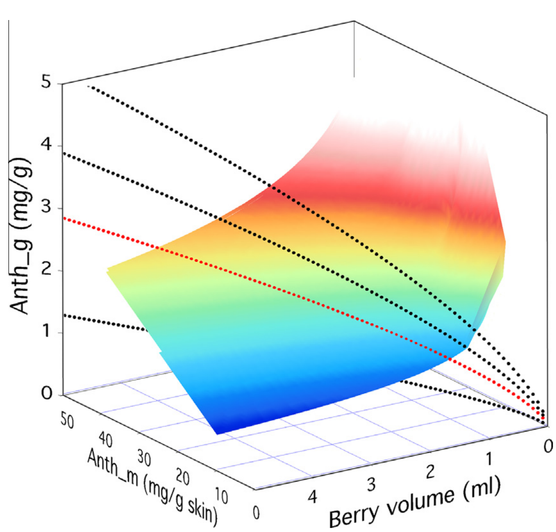

Fig. 3. Result of the same simulation as in Fig. 2 but using wider ranges for $Anth_m$ and BV, and repeated for four values of SMA (dotted curves). From bottom to top, SMA was 0.01, 0.22 (the default value in CUBA, used in Fig. 2), 0.03 and 0.04 g skin/cm^2. For clarity, only the response surface for 0.22 g skin/cm^2 is presented.

The importance of assessing the real $Anth_m$ (or $Anth_a$) during berry maturation to define the optimal date for grape harvesting cannot be overstressed (e.g. Guidoni et al., 2008). It is important to alleviate the effect of BV changes at the end of maturation and to recalculate $Anth_m$ from $Anth_g$, the latter being measured in most laboratories. So, CUBA will be very useful for the calculation of the real kinetics of anthocyanins accumulation.

4.1. Simulations of physiological changes

During grape maturation the interplay of vine nitrogen availability, soil water availability, light and temperature, which are all influenced by each other, will define the final berry size and composition (Bell and Henschke, 2005). In the majority of studies, low light reduced berry weight, while low temperatures increased berry size (cf. Dai et al., 2011). Still, water availability to the vine is the major factor defining berry size (Esteban et al., 2002; Ojeda et al., 2002). So, thanks to a moderate water stress and sun exposure, at the same technological maturity (°Brix) and phenolic maturity ($Anth_m$), smaller berries will have a larger anthocyanin content in the must ($Anth_g$). Fig. 2 illustrates in detail the response of $Anth_g$ to changes in skin content of anthocyanins and changes in berry volume by applying CUBA relationships. It can be seen that for winegrapes the physiological range of $Anth_m$ (5–25 mg/g skin) (cf. Table S1) has a larger influence on potential $Anth_g$ than the physiological range of BV (0.5–2 g). As usually acknowledged (cf. literature citations above), the decrease in berry size is favourable to $Anth_g$, but $Anth_g$ increases more steeply with size decrease at higher $Anth_m$ than at lower $Anth_m$. Also, the size effect will have a stronger influence for cultivars with small berries (Merlot Noir, Cabernet Sauvignon) than for cultivars with larger berries (Grenache) (Fig. 3). For the latter, the usual practice to induce water stress that decreases berry size in order to obtain larger $Anth_g$ (Ojeda et al., 2002) might not be as efficient as to increase directly $Anth_m$ by over-maturation, high light during maturation or lower temperature.

Further, it has been shown that water deficits increased the amount of skin tannins and anthocyanins ($Anth_m$) independently of the effect on berry size (Roby et al., 2004) probably by changing the SMA. Because of this, the skin fraction is sometimes calculated (Keller et al., 1998a; Mane et al., 2007), but the separation into the contribution of the berry size and the SMA is rarely acknowledged. The most striking example is the comparison of Pinot Noir and Meunier where an almost double SMA (skin thickness) compensates for the almost half $Anth_m$ content in the skin, leading to an equivalent $Anth_g$ in the two cultivars (Mane et al., 2007). CUBA actually allows one to calculate SMA from literature data (Table S1). Fig. 3 thus illustrates a wider range of $Anth_m$ and BV encompassing cultivars with large berries, including table grape, for a variety of SMAs in addition to the default starting value of 0.22 g skin/cm^2 used in CUBA. This simulation illustrates the preponderant influence of SMA for the final $Anth_g$, often neglected in the literature.

5. Conclusions and outlook

Like any other software, CUBA will be further developed in the future. For example, the approximation of a berry by a sphere can be replaced by an ellipsoid that would need the information on both equatorial and meridian dimensions. Although the error of approximating an ellipsoid berry to a sphere is small (less than 3% underestimation of the surface area even for a 50% difference in the two axes of a prolate spheroid) it could be introduced in the future as a cultivar selectable constant. More importantly, cultivar selectable constant for SMA could also be added, once more data per cultivar become available. The CUBA software will be useful for the transformation of units in order to produce adequate variable for process-based simulation models (Martre et al., 2011). Towards that aim treatments of arrays of data could be introduced in addition to single values. Still, our intention is to keep the software interface as simple as possible for the majority of users, and to keep that simple version available even after future developments. Naturally, the CUBA software can be used for other berries than grapes, like blueberries, or other fruits as long they are bearing anthocyanins only in the skin. To allow the evolution of the software in the direction of needs of potential users a possibility for them to post comments and suggestions will be added in the future.

Works of Ewart and Kliewer (1977), Guidoni et al. (2002), Hrazdina et al. (1984), Keller et al. (1998b), Kontoudakis et al. (2011), Tuccio et al. (2011) and Yokotsuka et al. (1999) are cited in supplementary material.

Acknowledgements

This work was partially supported by the European project no 311775 InnoVine and by the CNRS. We are indebted to the web master of ESE Nicolas Moulonguet for his help with the installation of CUBA.

Appendix A

A.1. Formulas used for the calculations in CUBA

By approximating a berry to a sphere
Volume (V) = $4/3\pi R^3$
and
Surface (S) = $4\pi R^2$
Therefore, the surface-to-volume ratio (SVR) is
$\mathrm{SVR} = \mathrm{S/V} = 3\ (3/(4\pi))^{-1/3}\ \mathrm{BV}^{-1/3}$
The total soluble solids (°Brix) of berries is used to calculate the berry volume (BV) from berry mass (BM) according to standard tables (EEC Commission, 1990)
BM = BV (0.98845 + 0.0046645 °Brix)
Other relations used were:
$\mathrm{Anth_a} = \mathrm{SMA\ Anth_m}$
$\mathrm{Anth_v} = \mathrm{SVR\ Anth_a}$
$\mathrm{Anth_b} = \mathrm{BV\ Anth_v}$
$\mathrm{Anth_b} = \mathrm{BM\ Anth_g}$
$\mathrm{Anth_g} = \mathrm{BV/BM\ Anth_v}$

See also the summary table that follows.

A.2. Summary table of conversion parameters

The variable in the first column is obtained by multiplying the variable in the first row by the parameter in the table cell at the column-row intersection.

	$\mathrm{Anth_a}$	$\mathrm{Anth_m}$	$\mathrm{Anth_b}$	$\mathrm{Anth_g}$	$\mathrm{Anth_v}$
$\mathrm{Anth_a}$	1	SMA	1/(SVR*BV)	BM/(SVR*BV)	1/SVR
$\mathrm{Anth_m}$	1/SMA	1	1/(BV*SVR*SMA)	BM/(SVR*SMA*BV)	1/(SVR*SMA)
$\mathrm{Anth_b}$	SVR*BV	BV*SVR*SMA	1	BM	BV
$\mathrm{Anth_g}$	SVR*BV/BM	SVR*SMA*BV/BM	1/BM	1	BV/BM
$\mathrm{Anth_v}$	SVR	SVR*SMA	1/BV	BM/BV	1

Appendix B. Supplementary materials

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.compag.2014.02.012.

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Table S1. Berry attributes from selected literature (**in bold characters**) with anthocyanin contents in missing units recalculated by the CUBA tool (in *italic*). Discrepancies among literature data can arise from several types of causes: type of extraction solvent (e.g. artificial wine vs. 1N acidified ethanol), duration of extraction, extinction coefficients used for calculations or expression as malvidin-3-glucoside equivalent. When a range of value is given in the reference the extreme values are calculated by CUBA and reported.

$Anth_m$ (mg/g skin FW)	**$Anth_a$ (mg/cm^2)**	**$Anth_v$ (g/L berry)**	**$Anth_b$ (mg/berry)**	**SMA or (RSM)[1] (g/cm^2) or (%)**	**Berry Mass (g)**	**Cultivar**	**Reference**
2.91 – 9.41	*0.064 – 0.207*	*0.417 – 1.351*	**0.17 – 0.55**	*0.022* **(13)**	**0.44**	Cabernet Sauvignon	[15]
0.83 – 2.68	*0.027 – 0.088*	*0.116 – 0.376*	**0.17 – 0.55**	*0.033* **(13)**	**1.58**		
2.13 – 6.90	*0.064 – 0.207*	*0.417 – 1.351*	**0.17 – 0.55**	*0.030* **(18)**	**0.44**		
0.59 – 1.92	*0.027 – 0.088*	*0.116 – 0.376*	**0.17 – 0.55**	*0.046* **(18)**	**1.58**		
6 – 12	*0.132 – 0.264*	*0.526 – 1.052*	**1 – 2**	*0.022*[2]	**0.98 – 1.93**	Shiraz	[12]
1.34 – 6.69	*0.029 – 0.147*	*0.120 – 0.600*	**0.2 – 1.0**	0.022[3]	**1.8**	Cabernet Sauvignon	[17]
0.97 – 4.87	*0.021 – 0.107*	*0.074 – 0.372*	**0.2 – 1.0**	0.022[3]	**2.9**		
1.66 – 14.13	*0.036 – 0.311*	*0.166 – 1.414*	**0.2 – 1.7**	0.022[3]	**1.3**	Merlot	[17]
1.34 – 11.37	*0.029 - 0.250*	*0.120 – 1.021*	**0.2 – 1.7**	0.022[3]	**1.8**		
13.15 – 17.54	*0.290 – 0.386*	*1.352 – 1.667*	**1.5 – 2.0**	0.022[3]	**1.2**	Shiraz	[13]
10.86 – 14.48	*0.239 – 0.318*	*1.014 – 1.352*	**1.5 – 2.0**	0.022[3]	**1.6**		
25 – 40	*0.462 – 0.74*	*1.996 – 3.195*	**2.4 – 3.8**	*0.0185* **(8)**	**1.2**	Cabernet Sauvignon	[8] [9]
25 – 40	*0.638 – 1.02*	*2.752 – 4.404*	**3.3 – 5.3**	*0.0255* **(11)**	**1.2**		

$Anth_m$ (mg/g skin FW)	**$Anth_a$ (mg/cm^2)**	**$Anth_g$ (mg/g berry)**	**$Anth_b$ (mg/berry)**	**SMA or (RSM)[1] (g/cm^2) or (%)**	**Berry Mass (g)**	**Cultivar**	**Reference (& notes)**
6.15 – 9.36	*0.135 – 0.206*	**0.502 – 0.764**	*0.949 – 1.444*	0.022[3]	**1.89**	Nebbiolo	[5]
6.37 – 9.69	*0.140 – 0.213*	**0.502 – 0.764**	*1.054 – 1.604*	0.022[3]	**2.01**		
4.21 – 7.14	*0.093 – 0.157*	**0.36 – 0.61**	*0.594 – 1.006*	*0.022*[3]	**1.65**	Nebbiolo	[4]
4.57 – 7.74	*0.101 – 0.170*	**0.36 – 0.61**	*0.756 – 1.281*	*0.022*[3]	**2.10**		
2.75 – 5.75	*0.060 – 0.126*	*0.261 – 0.546*	*0.313 – 0.655*	0.022[3]	**1.2**	Cabernet Sauvignon	[3]
2.75 – 5.75	*0.060 – 0.126*	*0.237 – 0.496*	*0.379 – 0.794*	0.022[3]	**1.6**		
17 – 25 (DW)				**0.04**	**1.3 – 1.7**	Merlot	[6]
8.5 – 12.5 @50%FW	*0.340 – 0.500*	*1.307 – 1.923*	*2.223 – 3.269*	**0.04**	**1.7**		
3.4 – 5 @80%FW	*0.136 –0.200*	*0.571 – 0.841*	*0.743 – 1.093*	**0.04**	**1.3**		
6.8	*0.152*	**0.6**	**0.9**	*0.0222*	**1.5**	Chaunac	[7]
8.70 – 10.98	*0.191 – 0.242*	**0.811 – 1.024**	*1.030 – 1.300*	0.022[3]	**1.27**	Shiraz	[10]
9.37 – 11.71	*0.204 – 0.258*	**0.811 – 1.024**	*1.249 – 1.577*	0.022[3]	**1.54**		
2.962 – 3.736	*0.132 – 0.167*	**0.541 – 0.683**	*0.758 – 0.956*	*0.0446* **(18.3)**	**1.4**	Aleatico	[16]
2.962 – 3.736	*0.105 – 0.132*	**0.430 – 0.542**	*0.602 – 0.759*	*0.0354* **(14.5)**	**1.4**		
6.191	*0.2420*	**1.242**	*0.850*	*0.0391*	**0.685**	Cab. Sauv.	[14]
4.777	*0.1810*	**0.879**	*0.708*	*0.0379*	**0.805**	Merlot	(Known °Brix
8.222	*0.2302*	**1.065**	*1.002*	*0.0280*	**0.943**	Syrah	were used for
8.658	*0.2199*	**0.824**	*1.450*	*0.0254*	**1.758**	Monastrell	calculations[4])
6.3	*0.1386*	**0.632**	*0.632*	*0.0220* **(10)**	*1*	Pinot Noir	[11]
3.3	*0.1320*	**0.602**	*0.602*	*0.0400* **(18.2)**	*1*	Meunier	
5.94 – 6.94	*0.131 – 0.152*	**0.6 – 0.7**	**0.6 – 0.7**	0.022[3]	**1**	Cabernet Sauvignon	[1]
3.27– 3.81	*0.131 – 0.152*	**0.6 – 0.7**	**0.6 – 0.7**	0.040	**1**		
4.91	**0.108**	*0.466*	*0.560*	0.022[3]	**1.20**	Mixed data for	[2]
6.09	**0.134**	*0.578*	*0.694*	0.022[3]	**1.20**	Cab. Sauv.	
4.91	**0.108**	*0.412*	*0.717*	0.022[3]	**1.74**	Sylvaner and	
6.09	**0.134**	*0.511*	*0.890*	0.022[3]	**1.74**	Zinfandel	

[1]RSM, Relative Skin Mass (% skin of berry fresh weight).

[2]SMA calculated from skin mass divided by skin surface (obtained from berry mass) [4; 12].

[3]Anth calculations made using the CUBA default value for SMA.

[4]When °Brix was not specified, a °Brix of 20 was used for the calculation of the berry volume from berry mass.

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