

Supplemental Material:

**Origin of Xylitol in Chewing Gum: A Compound-Specific
Isotope Technique for the Differentiation of Corn and Wood
Based Xylitol by LC-IRMS**

Köster, Daniel.¹, Wolbert, Jens-Benjamin¹, Schulte, Marcel S.², Jochmann, Maik A.¹, Schmidt,
Torsten C.^{1,3}

¹ Instrumental Analytical Chemistry, University of Duisburg-Essen, Universitätsstr. 5, 45141
Essen, Germany

² Biofilm Centre, University of Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

³ University of Duisburg-Essen, Centre for Water and Environmental Research (ZWU)
Universitätsstr. 5, 45141 Essen, Germany

Setting a threshold for assigning an unknown xylitol sample to wood or corn origin

For the calculation of the one-sided prediction intervals as threshold values for a decision between C3 and C4 based xylitol, the values of the single measurements ($n=3$ for each sample) shown in Figure 4 of the article for the xylitol extracted from chewing gum were used (Except for gum MWH which showed intermediate $\delta^{13}\text{C}$ values between C3 and C4) to calculate the lower, respectively the upper limit of these confidence intervals as given by:

$$\delta^{13}\text{C}_{\text{corn, lower}} = \overline{\delta^{13}\text{C}_{\text{corn}}} - t_{\alpha, df} \times s_{\text{corn}} \times \sqrt{1 + \frac{1}{n_{\text{corn}}}}$$

$$\delta^{13}\text{C}_{\text{wood, upper}} = \overline{\delta^{13}\text{C}_{\text{wood}}} + t_{\alpha, df} \times s_{\text{wood}} \times \sqrt{1 + \frac{1}{n_{\text{wood}}}}$$

With

$\overline{\delta^{13}\text{C}_{\text{corn}}}$	mean $\delta^{13}\text{C}$ of samples from corn origin
$\overline{\delta^{13}\text{C}_{\text{wood}}}$	mean $\delta^{13}\text{C}$ of samples from wood origin
n_{corn}	number of samples from corn origin
n_{wood}	number of samples from wood origin
s_{corn}	standard deviation of $\delta^{13}\text{C}$ values from corn samples
s_{wood}	standard deviation of $\delta^{13}\text{C}$ values from wood samples
$t_{\alpha, df}$	t value for a given confidence level $1-\alpha$ and $n-1$ degrees of freedom

Setting $\alpha = 0.01$ the following results were calculated:

	$\overline{\delta^{13}\text{C}}$	s	n	df	$t_{0.01}$	Limit of the confidence interval (‰)
Wood (C3)	-20.69	1.08	39	38	2.428	-18.03
Corn (C4)	-11.11	1.54	15	14	2.624	-15.29

The threshold values for origin assignment: If the $\delta^{13}\text{C}$ for xylitol in an unknown sample falls below -18.03 ‰ a wood origin can be assumed accepting an α of 0.01. In contrast a value of an unknown sample above -15.29 ‰ can be assumed to be of C4 plant or corn origin accepting an α error of 0.01.