SUPPLEMENTARY DATA

Table S1. Confusion matrix of the PLS-DA shown in figure 2 (E-nose measurements). N = number of samples; TPR = true positive ratio; FPR=false positive ratio; TNR= true negative ratio; FNR=false negative ratio; Err= total error; P= Precision = total positive (TP)/total positive + false positive.

Confusion matrix	**N**	**TPR**	**FPR**	**TNR**	**FNR**	**Err**	**P**
Fortified CT	3	1	0	1	0	0	1
Fortified RT	3	1	0	1	0	0	1
Sweet CT	3	1	0	1	0	0	1
Sweet RT	3	1	0	1	0	0	1
Confusion table	*Actual class*						
Predicted as	Fortified CT	Fortified RT	Sweet CT	Sweet CT			
Fortified CT	3	0	0	0			
Fortified RT	0	3	0	0			
Sweet CT	0	0	3	0			
Sweet RT	0	0	0	3			
Confusion matrix (CV)	**N**	**TPR**	**FPR**	**TNR**	**FNR**	**Err**	**P**
Fortified CT	3	0	0	1	1	0.25	NaN
Fortified RT	3	0.66	0.33	0.66	0.33	0.33	0.4
Sweet CT	3	1	0.11	0.88	0	0.08	0.75
Sweet RT	3	1	0	1	0	0	1
Confusion table (CV)	*Actual class*						
Predicted as	Fortified CT	Fortified RT	Sweet CT	Sweet CT			
Predicted as Fortified CT	0	0	0	0			
Predicted as Fortified RT	3	2	0	0			
Predicted as Sweet CT	0	1	3	0			
Predicted as Sweet RT	0	0	0	3			

Table S2. Confusion matrix of the PLS-DA shown in figure 3 (NIR measurements). N = number of samples; TPR = true positive ratio; FPR=false positive ratio; TNR= true negative ratio; FNR=false negative ratio; Err= total error; P= Precision = total positive (TP)/total positive + false positive.

Confusion matrix	**N**	**TPR**	**FPR**	**TNR**	**FNR**	**Err**	**P**
Fortified CT	3	1	0	1	0	0	1
Fortified RT	3	1	0	1	0	0	1
Sweet CT	3	1	0	1	0	0	1
Sweet RT	3	1	0	1	0	0	1

Confusion table	*Actual class*			
Predicted as	Fortified CT	Fortified RT	Sweet CT	Sweet CT
Fortified CT	3	0	0	0
Fortified RT	0	3	0	0
Sweet CT	0	0	3	0
Sweet RT	0	0	0	3

Confusion matrix (CV)	**N**	**TPR**	**FPR**	**TNR**	**FNR**	**Err**	**P**
Fortified CT	3	1	0	1	0	0	1
Fortified RT	3	1	0	1	0	0	1
Sweet CT	3	1	0	1	0	0	1
Sweet RT	3	1	0	1	0	0	1

Confusion table (CV)	*Actual class*			
Predicted as	Fortified CT	Fortified RT	Sweet CT	Sweet CT
Predicted as Fortified CT	3	0	0	0
Predicted as Fortified RT	0	3	0	0
Predicted as Sweet CT	0	0	3	0
Predicted as Sweet RT	0	0	0	3