

# Analysis Report

Sample ID: Orange\_juice\_100\_training\_20211119

## Information/Declaration provided by customer:

Customer: **Woolworths.Food**

Type of Sample: Orange, Juice from Concentrate

*Disclaimer: this information will affect the applicability and validity of analyses and results.*

Preparation: Sample preparation was performed by an external service provider

Measuring Date: 19-Nov-2021 10:19:22

Reporting Date: 06-Dec-2021 14:56:46, Version 3.0.11, 9 pages

## Results Summary

Type of Analysis	Analysis ID	Result	Status
<b>Classification Analysis</b>			
Fruit-Type Model	JU-1001-01/0195	OS/MN/BOS <sup>1</sup>	-
Orange, Variety	JU-1003-01/0195	OS <sup>2</sup>	-
Orange, Product Type	JU-1004-01/0195	OS-S <sup>3</sup>	-
Orange, Origin	JU-1002-01/0195	? <sup>4</sup>	-
<b>Targeted Analysis</b>			
Quantification (A.I.J.N.)	JU-QA-02/3261	-	●
Quantification (NMR-Reference)	JU-QC-01/0301	-	●
<b>Verification Analysis</b>			
Univariate Verification	JU-2005-01/0195	In-Model	●
Multivariate Verification	JU-2005-01/0195	In-Model	●
Blend Sinensis/Reticulata	JU-CSR-01/0189	C.Sinensis	●
Fruit Content Verification	JU-3002-01/0196	-	●

1 = Type of Fruit "Orange/Mandarin/Blood-Orange" was assigned.

2 = Variety "Orange" was assigned.

3 = Type of Product "Direct Juice" was assigned.

4 = No Origin could be assigned.

The data analysis is performed at Bruker BioSpin GmbH (Reinstetten, Germany) according to testing method AA-72-01-06 (SGF-Profiling 3.0.11), released on 04-Dec-2020 (DIN EN ISO/IEC 17025:2018 Accreditation Certificate D-PL-19229-01-00 of Bruker BioSpin GmbH). All results solely refer to the tested sample as provided by the customer.

SGF-Profiling™ is co-developed by Bruker BioSpin GmbH and SGF International e.V.



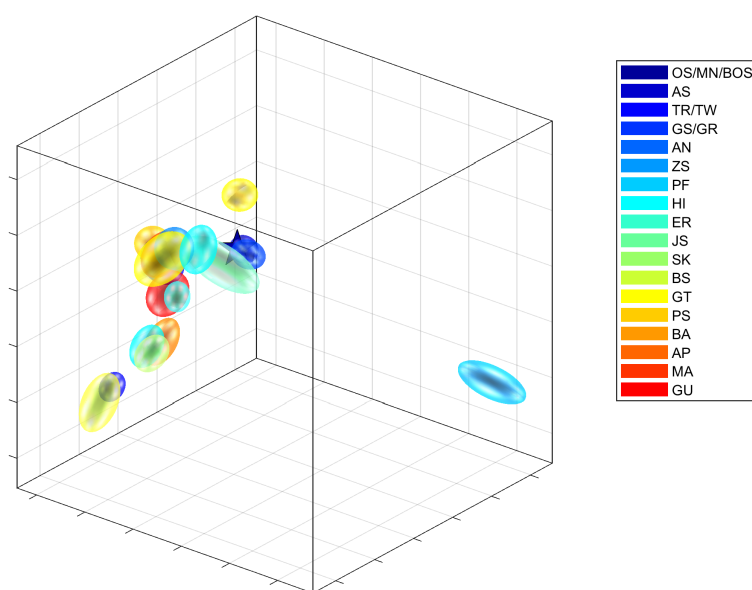
## Fruit-Type Model

(Classification, Analysis ID: JU-1001-01/0195)

Type of Fruit "Orange/Mandarin/Blood-Orange" was assigned.

Following classes are available:

OS/MN/BOS = Orange/Mandarin/Blood-Orange, AS = Apple, TR/TW = Grape, GS/GR = Grapefruit, AN = Pineapple, ZS = Lemon, PF = Peach, HI = Raspberry, ER = Strawberry, JS = Black Currant, SK = Sour Cherry, BS = Pear, GT = Pomegranate, PS = Passion Fruit, BA = Banana, AP = Apricot, MA = Mango, GU = Guava



	p-Values	
OS/MN/BOS		0.75
AS	< 0.0001	
TR/TW	< 0.0001	
GS/GR	< 0.001	
AN	< 0.0001	
ZS	< 0.0001	
PF	< 0.0001	
HI	< 0.0001	
ER	< 0.0001	
JS	< 0.0001	
SK	< 0.0001	
BS	< 0.0001	
GT	< 0.0001	
PS	< 0.001	
BA	< 0.0001	
AP	< 0.0001	
MA	< 0.0001	
GU	< 0.0001	

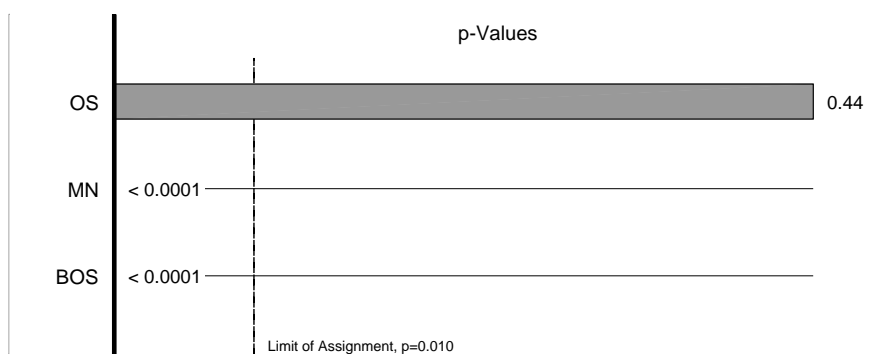
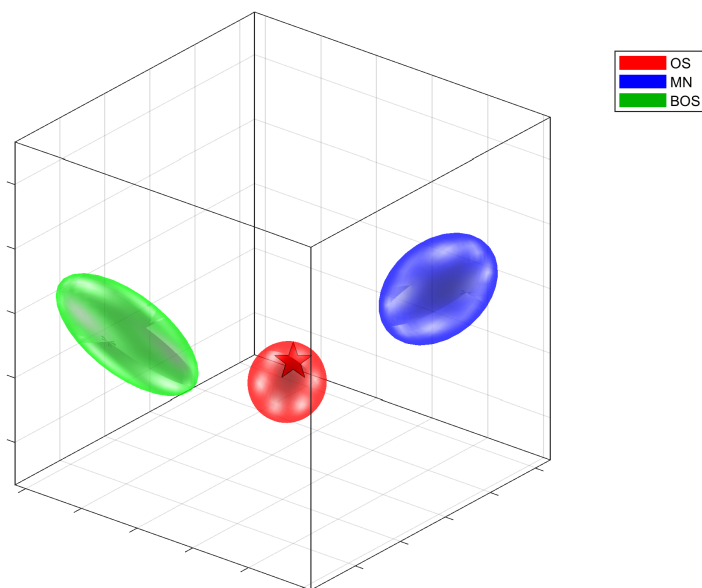
Limit of Assignment, p=0.010

## Orange, Variety

(Classification, Analysis ID: JU-1003-01/0195)

Variety "Orange" was assigned.

Following classes are available:  
OS = Orange, MN = Mandarin, BOS = Blood Orange

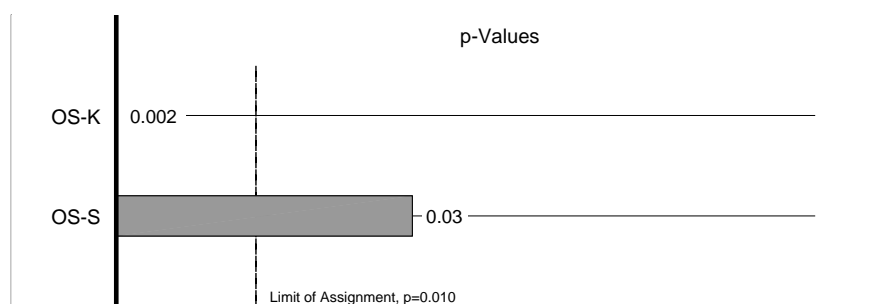
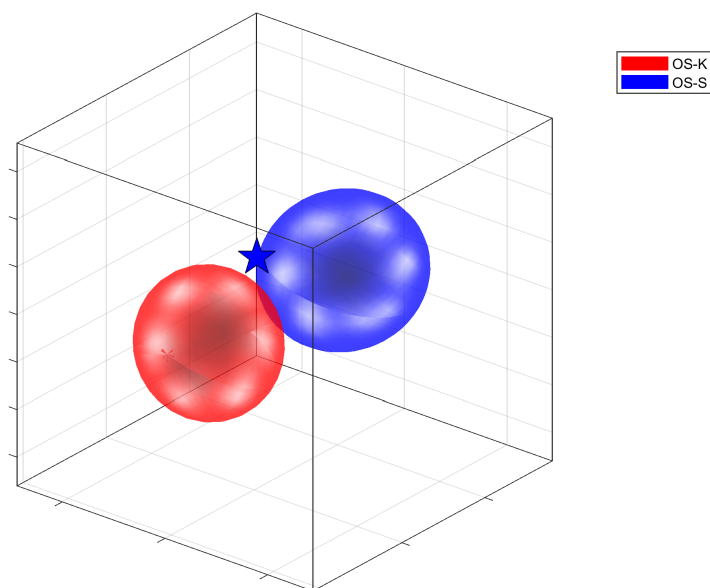


## Orange, Product Type

(Classification, Analysis ID: JU-1004-01/0195)

Type of Product "Direct Juice" was assigned.

Following classes are available:  
OS-K = Concentrate, OS-S = Direct Juice



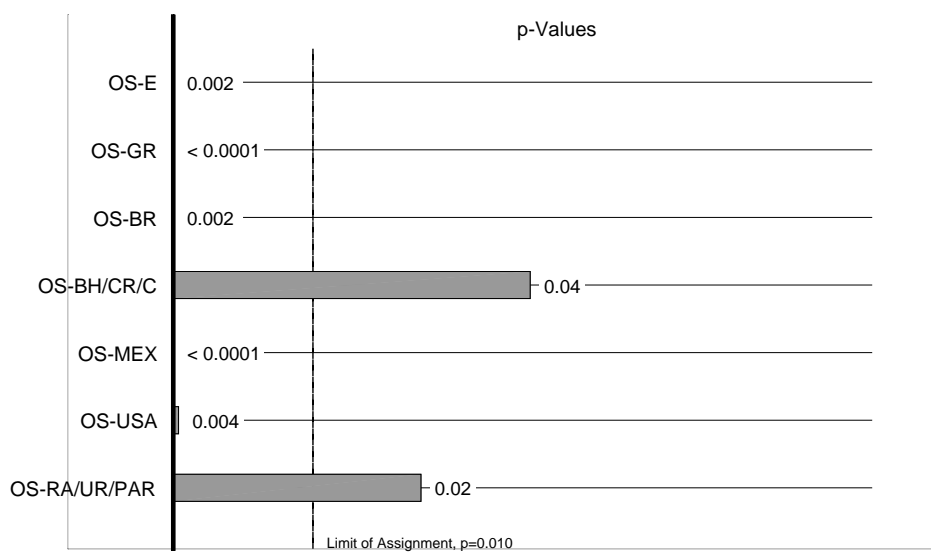
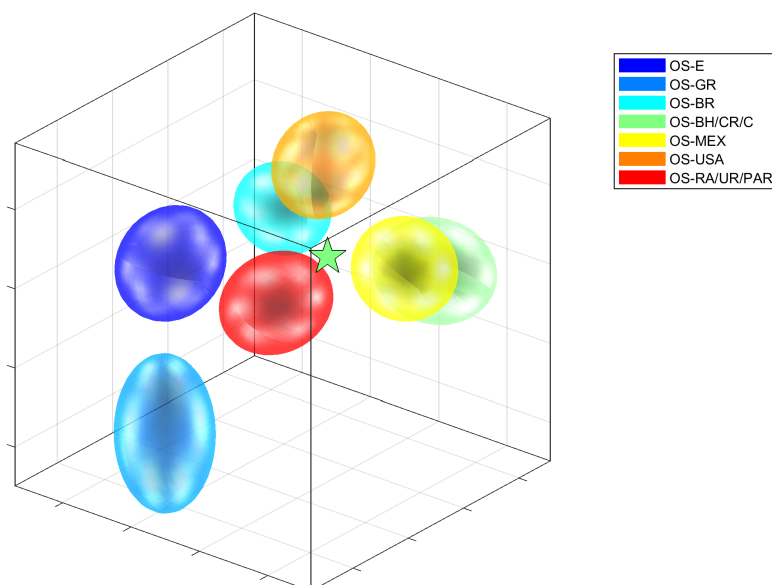
## Orange, Origin

(Classification, Analysis ID: JU-1002-01/0195)

No Origin could be assigned.

Following classes are available:

OS-E = Spain, OS-GR = Greece, OS-BR = Brazil, OS-BH/CR/C = Belize/Costa Rica/Cuba, OS-MEX = Mexico, OS-USA = U.S.A., OS-RA/UR/PAR = Argentina/Uruguay/Paraguay



## Verification Models

Applied Model: Orange

### Univariate Verification

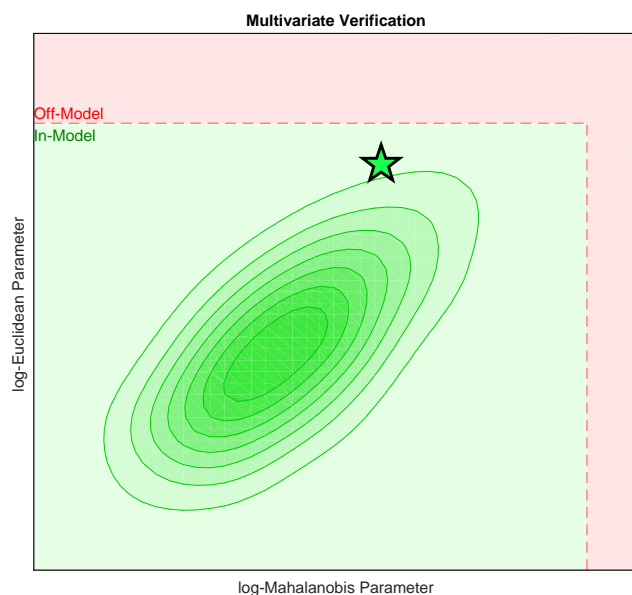
(Verification, Analysis ID: JU-2005-01/0195)

**Result:** No deviation was detected in univariate verification (In-Model).

### Multivariate Verification

(Verification, Analysis ID: JU-2005-01/0195)

**Result:** No deviation was detected in multivariate verification (In-Model).



## Blend Citrus Sinensis/Reticulata

(Analysis ID: JU-CSR-01/0189)

Based on the current database of Citrus sinensis and Citrus reticulata **no significant hint for a possible mixture** could be detected. For a final conclusion, counterchecking with further appropriate analytical methods is suggested.

### Fruit Content

(Fruit Content, Analysis ID: JU-3002-01/0196)

Applied Model: Orange

Origin of Fruit	Consistent with 100%
All origins	Yes





















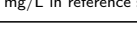
## Targeted Analysis


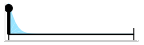



In the following tables the results of the quantitative analysis are given and compared to the A.I.J.N. reference ranges (if available). Parameters labelled with \* are determined by regression analysis. Parameters labelled with \*\* are calculated parameters. For concentrated products, results are expressed for juice strength (corresponding Brix for orange is 11.2). The displayed distributions of the SGF-Profiling NMR reference database refer to group *Orange*.

- consistent with A.I.J.N.
- outside the A.I.J.N. limits ( $\pm 10\%$ )
- outside the A.I.J.N. limits
- no A.I.J.N. reference range

## Quantification Results:

(Analysis-ID: JU-QA-02/3261)

Compound	Value	Unit	LOQ	A.I.J.N. (Orange)			SGF-Profiling Database n = 2378
				Flag	min	max	
ethanol	58	mg/L	10	●	-	3000	<10  874
lactic acid	<50	mg/L	50	●	-	200	<50  146
5-hydroxymethylfurfural	<5	mg/L	5	●	-	10	<5 mg/L in reference set
Tit. Acidity pH 7*	141	meq/l	-	○	-	-	73  215
Tit. Acidity pH 8.1*	151	meq/l	-	●	90	240	78  222
Tit. Acidity (pH 7, tartaric acid)*	10.8	g/l	-	○	-	-	5.4  16.2
Tit. Acidity (pH 7, malic acid)*	9.7	g/l	-	○	-	-	4.8  14.4
Tit. Acidity (pH 8.1, citric acid)*	9.6	g/l	-	●	5.8	15.4	5.0  14.2
citric acid	11.2	g/L	0.2	●	6.3	17.0	5.9  15.6
malic acid	1.8	g/L	0.5	●	0.8	3.0	0.6  2.7
potassium*	1715	mg/l	-	●	1300	2500	1405  2174
magnesium*	104	mg/l	-	●	70	160	84  121
glucose	26.1	g/L	0.5	●	20.0	35.0	16.0  31.1
fructose	29.0	g/L	0.5	●	20.0	35.0	18.0  32.5
glucose/fructose ratio**	0.90	-	-	●	0.85	1.00	0.82  1.06
sucrose	36.9	g/L	0.2	●	10.0	50.0	27.8  56.6
% sucrose**	40	%	1	●	-	50	33  58
total sugar**	92.1	g/L	2.0	○	-	-	67.3  111.8
4-aminobutanoic acid	256	mg/L	50	●	180	500	144  513
alanine	62	mg/L	5	●	60	205	40  153
arginine	599	mg/L	100	●	400	1000	328  1044
proline	500	mg/L	50	●	450	2090	192  1703
acetaldehyde	<5	mg/L	5	○	-	-	<5 mg/L in reference set

Compound	Value	Unit	LOQ	A.I.J.N. (Orange)			SGF-Profiling Database n = 2378
				Flag	min	max	
benzaldehyde	<5	mg/L	5	○	-	-	<5 mg/L in reference set
benzoic acid	<20	mg/L	20	○	-	-	<20 mg/L in reference set
formic acid	8	mg/L	5	○	-	-	<5  22
galacturonic acid	<150	mg/L	150	○	-	-	<150  169
methanol	26	mg/L	10	○	-	-	<10  90
phlorin	<10	mg/L	10	○	-	-	<10  69
sorbic acid	<10	mg/L	10	○	-	-	<10 mg/L in reference set
succinic acid	26	mg/L	10	○	-	-	15  44

## General Remarks

### Classification Models

The aim of a classification model is to assign a specific sample to its most probable group. The group is chosen from a list of proposed groups. This assignment does not guarantee that the sample is exclusively a member of this group.

The 3D-discrimination diagram shows available groups (ellipsoids) in the projection space of the NMR-profiles with maximized discrimination. The star represents the actual sample.

In most cases these models are discriminating in multidimensional spaces. For such models human perceptibility and options for graphical representation are limited. Misperception is possible in certain cases. The mathematically correct probability for any group membership is represented by p-values which are calculated in the complete space. Typically values higher than 0.05 or 0.01 will accept the hypothesis of group membership. Expert interpretation is necessary before deducing any conclusions.

Only groups listed in the respective models can be considered. Therefore models (especially models of origin) are not applicable for blends and origins which are not listed in the corresponding model.

### Verification Models

Verification models are non-targeted analyses comparing the whole NMR-Profile of a specific sample with one corresponding group of reference spectra (database). All spectra data points are taken into account irrespective of whether the signals are caused by already identified molecules or not.

There are different possible reasons for any deviation from the group of reference spectra. If there are detected deviations, this does not automatically mean, that the sample is adulterated. Expert interpretation is necessary before deducing any conclusions.

In some cases for a single spectrum different models are calculated and respective results are proposed. Correct interpretation of the results implies choosing the most appropriate one based on the context and background of the sample.

In the univariate analysis, the NMR spectrum is checked for any unusual low or high signal intensities for a given sample, while taking into account the natural variability of a respective reference group. Multivariate models also take into account the relation between different signals in the NMR spectrum.

### Fruit Content Verification

The consistency with the declared or expected legal fruit content for a sample is checked based on the comparison of selected signal intensities of the NMR-spectra with the signal intensities of reference spectra (database). Where appropriate, a refined evaluation for specific origin is done. In some cases for a single spectrum different models are calculated and respective results are proposed. Expert interpretation is necessary before deducing any conclusions. It is part of a correct interpretation to choose the most appropriate model based on the context and background of the sample.

### Quantification Results

Obtained quantification levels of parameters are compared to AIJN-CoP-guide values if available and consistency is indicated by an extra traffic light flag. Depending on the type of juice, different compounds are quantifiable. Quantitative values are compared to the SGF-Profiling database if the number of reference values in there is sufficiently large (visualised by distribution). Expert interpretation is necessary before deducing any conclusions.

### Regression Results

Some analytical figures are determined by regression analyses because they are not directly quantifiable from any peak in the spectrum. The calibration to obtain valid regression results is based on typical reference spectra. Therefore regression results could be erroneous in cases where any deviation has been detected in another applied model or if the product shows estimation of fruit content significantly lower than 100%. In both cases, no results can be given based on mathematic principles.

### Citrus Sinensis/Citrus Reticulata

A specific research for spectral properties characteristic for citrus reticulata is carried out. Based on statistical evaluation a possible or probable mixture of citrus reticulata with citrus sinensis is evaluated. Due to very large biological variation inside the species citrus reticulata the applied statistical model is not designed to detect the addition of citrus reticulata in amounts up to 10-20 %, but the risk of false positive results is minimized.