

n-Alkanes in tomato (*Solanum lycopersicum* L.) seed oil: the cultivar effect

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Abstract

Three cultivars of tomato (*Solanum lycopersicum* L. cv 'Principe Borghese', 'Rebellion F1' and 'San Marzano') were separately grown in three greenhouses in Southern Italy to investigate the *n*-alkane (saturated linear hydrocarbons) composition of the tomato seed oil (TSO). The oil was obtained by Soxhlet-petroleum ether extraction. One-way ANOVA and principal component analysis were applied to differentiate the three cultivars. 14 components were identified. Tomato seed oil contained mainly odd-chain carbon number *n*-alkanes (79.09% - 89.35%), and among them, *n*-C25, *n*-C21 and *n*-C23 were prevalent in all cultivars. The Σ odd chain carbon number / Σ even chain carbon number ratio was 8.39 in 'Principe Borghese', 3.78 in 'Rebellion F1' and 7.60 in 'San Marzano'. Relevant differences in the quantitative composition were observed among the oils 'San Marzano' contained the lowest *n*-alkane quantity (100.67 mg/kg) whereas 'Principe Borghese' contained 347.33 mg/kg.

Keywords

n-alkanes
Minor components
Principe Borghese
Rebellion
San Marzano
Saturated linear
hydrocarbons
Unsaponifiable fraction
Vegetable oil

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Introduction

The unsaponifiable fraction of a vegetable oil is contained in low quantity (1-2%) but has a great importance from the point of view of the biological properties of its constituents and for the possibility of using it to characterize each vegetable oil. More than two hundreds of components are present in the unsaponifiable fraction. *n*-Alkanes are endogenous to plants and are thinking to be the result of decarboxylation of long chains fatty acids (Webster *et al.*, 2000). *n*-Alkanes are non polar organic compounds naturally present in the unsaponifiable fraction of a vegetable oil. They are aliphatic saturated hydrocarbons made up of carbon and hydrogen and with a linear carbon chain following the empiric formula C_nH_{2n+2} . Refining reduces the *n*-alkane content. Benitez-Sánchez *et al.* (2003) studied the hydrocarbons (*n*-alkenes and *n*-alkanes) in hazelnut oil and found that refined oils have half the *n*-alkanes compared to the crude oils.

From the point of view of the edibility of a vegetable oil it is important to report that intakes of biogenic hydrocarbons are normally within the range of 10-100 mg/person/day (0.17 – 1.7 mg/kg body weight /day) and the intake of hydrocarbons from all

sources has been estimated to be normally about 240 mg/person/day (4 mg/kg body weight/day) (EMEA, 1995).

From the point of view of the industrial use of a vegetable oil, it is important to report that *n*-alkanes are very stable compounds and scarcely reactive with other substances, for this reason they used to be known as paraffins, which in Latin means "with a scarce chemical affinity". They are good fuels, insoluble in water and float on water. Aerobic alkane degraders activate alkane molecules using O_2 as a reactant. The alkane-activating monooxygenase overcomes the low reactivity of the hydrocarbon by producing reactive oxygen species (Singh *et al.*, 2012).

The food production process, packaging and environmental pollution can contaminate foods, in particular vegetable oils and fats because of their chemico-physical compatibility with linear hydrocarbons. Many studies have been conducted on the presence of paraffins and hydrocarbons in foodstuffs (Neukom *et al.*, 2002; Moret *et al.*, 2003; Fiorini *et al.*, 2008; Biedermann *et al.*, 2009). Methods have been optimized to detect mineral oil saturated hydrocarbons in vegetable oil (Moret *et al.* 2011) and in fatty foods (Zurfluh *et al.*, 2014).

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As a consequence it is very important to know the endogenous *n*-alkane content and composition of each vegetable oil and in particular of TSO, which has great potential for the large quantity obtainable at low cost, in particular by considering that, currently tomato seeds are considered a waste product.

The importance of this paper is related to the concept that as a vegetable edible oil contains a low *n*-alkane content whereas a vegetable oil as a source of biofuel production contains a higher *n*-alkane content, it is necessary to know the *n*-alkane content of the TSO to evaluate its potentiality.

Minor components of tomato seed oil such as policosanol (Giuffrè and Capocasale, 2015) and sterols (Giuffrè and Capocasale, 2016a) in addition to other edible properties of the tomato seed oil (Giuffrè and Capocasale, 2016b) were previously studied. The aim of this research is to determine the effect of three tomato cultivars on *n*-alkane composition of tomato seed oil at greenhouses grown in Calabria (South Italy). To our knowledge, this is the first paper studying these arguments.

Materials and Methods

Plant material

Three tomato cultivars were grown in three greenhouses at Roccella Ionica (South East Calabria, Southern Italy). Plants were spaced 70 cm within the row and 80 cm between the rows. Irrigation was conducted every 48 hr on the basis of the effective evaporation and transpiration. A manual and random collection of fruits was conducted at full ripeness (mid-June 2014). Fruits were washed with water and chopped. Chopped fruits were passed through a bored metal grid (\varnothing 1.5 mm) to separate pulp from a mixture of seeds and peel. Seeds were separated from peel by floatation and sedimentation in a plastic tank filled with water.

Chemicals

Standard samples: *n*-C19 nondecane (99%), *n*-C20 eicosane (99%), *n*-C21 heneicosane (98%), *n*-C23 tricosane (\geq 99.5%), *n*-C24 tetracosane (99%), *n*-C25 pentacosane (99%), C26 hexacosane (96%), *n*-C27 heptacosane (99%), *n*-C28 octacosane (99%), *n*-C29 nonacosane (99%), *n*-C32 dotriacontane (97%), were from Sigma-Aldrich (Steinheim-Germany); *n*-C30 triacontane (purissimum), *n*-C31 hentriacontane (purissimum) were from Fluka. *n*-C12 dodecane (99%) as internal standard was from Sigma-Aldrich. Silica gel 60 for column chromatography, 70 to 230 meshes, (Merck, reference 7734) was from Merck (Germany). All other reagents were from Panreac

(Barcelona, Spain).

Tomato seed oil extraction

The extraction was conducted as follows: drying in the dark at room temperature for one month until complete water losses; coarse grinding of seeds by a home coffee grinder; Soxhlet extraction, firstly with petroleum ether (bp = 40-60°C) overnight in a static extraction at room temperature and in the dark, secondly at the minimum boiling point of the solvent until complete oil recovery (two hours); solvent evaporation in a Rotavapor (25°C, under vacuum); oil filtration in a paper filter; storage in a 50 mL brown glass bottles at room temperature and in the dark; oil analysis within 7 days from extraction.

n-Alkanes analysis

n-Alkanes were determined as described in Annex XVII of the CONSLEG 2003 for olive oil analysis (Consleg, 2003). TSO was previously submitted to saponification. The unsaponifiable fraction was fractionated in a glass chromatographic column using silica gel as a stationary phase and hexane as an eluent. The first eluted fraction (0-30 mL) containing alkane was analyzed.

One μ L of sample diluted in *n*-heptane was injected into the Fisons GC 8000 gas chromatograph equipped with a capillary column SE 54 (30 m length x 0.32 mm ID, 0.5 μ m film thickness, Mega, Milan - Italy). The oven was programmed as follows: 100°C (1 min), increase of 4°C/min up to 300°C (10 min). The injector and detector temperatures were 280°C and 310°C respectively. Helium was used as a carrier gas (10 psi). Auxiliary gases were hydrogen at 15 psi and air at 22 psi. The split/splitless injector was operated in the split mode.

Statistical analysis

One-way ANOVA was performed by SPSS software version 15.0 (SPSS Inc., Chicago, IL, U.S.A.) using multiple range means comparison by the Tukey test ($p < 0.05$). Principal component analysis was performed by the software XLSTAT version 2009.1.01.

Results and Discussion

The unsaponifiable content (1.25% in 'Principe Borghese', 1.49% in 'Rebellion F1' and 1.29% in 'San Marzano' TSO) was described in a previous paper on policosanol composition (Giuffrè and Capocasale, 2015). In that paper, the lowest oil content was found in 'Rebellion F1' (19.83%, w/w on dried seeds), in higher amount with respect to the oil content obtained

Table 1. *n*-Alkane composition (%) of tomato seed oil (mean values \pm standard Deviation). Means in the same row with different lowercase letters differ significantly. Significance level: *** $p < 0.001$

Alkane chain length	Principe Borghese	Rebellion F1	San Marzano	Sign.
<i>n</i> -C19	1.58a \pm 0.01	1.61a \pm 0.02	0.25b \pm 0.01	***
<i>n</i> -C 20	2.79c \pm 0.04	4.16b \pm 0.06	5.11a \pm 0.04	***
<i>n</i> -C 21	28.77b \pm 0.10	8.20c \pm 0.10	44.05a \pm 0.03	***
<i>n</i> -C 22	0.75a \pm 0.03	0.43b \pm 0.03	0.32c \pm 0.01	***
<i>n</i> -C 23	10.17b \pm 0.06	11.16a \pm 0.03	5.31c \pm 0.04	***
<i>n</i> -C 24	1.47c \pm 0.03	4.35a \pm 0.05	1.62b \pm 0.02	***
<i>n</i> -C 25	35.10b \pm 0.18	42.06a \pm 0.17	18.80c \pm 0.05	***
<i>n</i> -C 26	1.12a \pm 0.01	1.00b \pm 0.03	0.49c \pm 0.02	***
<i>n</i> -C 27	2.92c \pm 0.13	5.22a \pm 0.03	3.73b \pm 0.10	***
<i>n</i> -C 28	1.31b \pm 0.04	4.04a \pm 0.05	1.40b \pm 0.01	***
<i>n</i> -C 29	5.02c \pm 0.03	9.46b \pm 0.09	10.07a \pm 0.05	***
<i>n</i> -C 30	1.52c \pm 0.03	3.28a \pm 0.04	2.25b \pm 0.04	***
<i>n</i> -C 31	5.79b \pm 0.10	1.38c \pm 0.03	6.17a \pm 0.06	***
<i>n</i> -C 32	1.69b \pm 0.02	3.65a \pm 0.04	0.43c \pm 0.02	***
Total (%)	100.00	100.00	100.00	
Σ Odd Chain Number	89.35a \pm 0.12	79.09c \pm 0.04	88.39b \pm 0.03	***
Σ Even Chain Number	10.65c \pm 0.12	20.91a \pm 0.04	11.61b \pm 0.03	***
<i>n</i> C19- <i>n</i> C29	91.00c \pm 0.15	91.70a \pm 0.06	91.15b \pm 0.08	***
<i>n</i> C30- <i>n</i> C32	9.00a \pm 0.15	8.30c \pm 0.06	8.85b \pm 0.08	***

by a mechanical system (17-18% w/w on dried seeds) from different cultivars (Giuffrè *et al.*, 2015) and in higher amount with respect the oil obtained by a mechanical system (10-12% w/w on wet seeds) from different cultivars (Giuffrè *et al.*, 2016).

n-Alkane content

The *n*-alkane composition expressed as a percentage and as an absolute value is shown in Tables 1 and 2. In TSO, 14 *n*-alkanes were detected ranging from *n*-C19 to *n*-C32. Seven *n*-alkanes had an odd-chain carbon number (*n*-C19, *n*-C21, *n*-C23, *n*-C25, *n*-C27, *n*-C29, *n*-C31) and seven had an even-chain carbon number (*n*-C20, *n*-C22, *n*-C24, *n*-C26, *n*-C28, *n*-C30, *n*-C32). The highest *n*-alkane content was in ('Principe Borghese' 347.33 \pm 4.04 mg/kg), the second was in 'Rebellion F1' (216.33 \pm 3.05 mg/kg), (Table 2). 'San Marzano' seed oil contained the lowest *n*-alkane amount (106.70 \pm 0.58 mg/kg), such as 3.25 times lower than in 'Principe Borghese' and 2.03 times lower than in 'Rebellion F1'.

Little information is available about *n*-alkane content in vegetable oils: in olive oil from the Extremadura region of Spain from 18.69 to 37.32 mg/kg were found (Osorio Bueno *et al.*, 2005); in olive oil from Croatia 40.15-61.67 mg/kg were found (Koprivnjak and Conte, 1996; Koprivnjak *et al.*, 1997); 17-25 mg/kg were found in raw avocado pulp oil (Giuffrè, 2005). In a study conducted on the *n*-alkanes in retail samples of edible oils, the following contents were found: 105-166 mg/kg in sunflower, 22-82 mg/kg in sesame, 26-33 mg/kg in

corn, 7-30 mg/kg in walnut, 27-40 mg/Kg in peanut, 14 mg/Kg in hazelnut, 21 mg/kg in pistachio, 74 mg/kg in mustard seed, 61 mg/kg in safflower, 52 mg/kg in grapeseed and 17 mg/kg in soybean (Mc Gills *et al.*, 1993).

León-Camacho *et al.* (2001) found 157.55 ppm of total *n*-alkanes in Austrian crude amaranth oil after a Soxhlet-hexane extraction, with the odd-chain compounds accounting for 99.95 ppm and the even chained compounds accounting for 57.60 ppm. Herchi *et al.* (2009) studied the hydrocarbon fraction of three linseed oils produced in Tunisia and after chloroform extraction and they found that the *n*-alkane content decreased drastically to the first 21 days after flowering and then remained the constant from day 21 to day 56. The most represented components were *n*C27, *n*C25 and *n*C23.

The *n*-alkane with the shortest chain length of linum seed oil was *n*C22. The rate of absorption by the gut of linear alkanes (*n*-alkanes) and branched alkanes has been shown to decrease as the carbon number increases. *n*-Alkanes with carbon number chain > C29 are not significantly absorbed (EMEA, 1995). In TSOs studied in this paper, the sum (%) of *n*C19-*n*C29 is 91.00-91.70% of the total and reciprocally the sum of *n*C30-*n*C32 is 8.30-9.00% (Table 1). If considered as an absolute value, in TSO the sum *n*C19-*n*C29 was 316.06 mg/kg in 'Principe Borghese', 198.37 in 'Rebellion F1' and 97.20 in 'San Marzano' (Table 2) and consequently the sum *n*C30-*n*C32 was 31.27 in 'Principe Borghese', 17.97 in 'Rebellion F1' and 9.40 in 'San Marzano'. The

Table 2. *n*-Alkane composition (mg/kg) of tomato seed oil (mean values \pm standard Deviation). Means in the same row with different lowercase letters differ significantly. Significance level: *** $p < 0.001$

Alkane chain length	Principe Borghese	Rebellion F1	San Marzano	Sign.
<i>n</i> -C19	5.48a \pm 0.10	3.48b \pm 0.06	0.30c \pm 0.00	***
<i>n</i> -C 20	9.69a \pm 0.15	9.01b \pm 0.19	5.50c \pm 0.03	***
<i>n</i> -C 21	99.92a \pm 1.29	17.74b \pm 0.38	47.00c \pm 0.25	***
<i>n</i> -C 22	2.62a \pm 0.12	0.93b \pm 0.05	0.30c \pm 0.00	***
<i>n</i> -C 23	35.31a \pm 0.43	24.15b \pm 0.39	5.70c \pm 0.03	***
<i>n</i> -C 24	5.11b \pm 0.04	9.41a \pm 0.12	1.70c \pm 0.01	***
<i>n</i> -C 25	121.91a \pm 1.95	90.99b \pm 1.33	20.00c \pm 0.11	***
<i>n</i> -C 26	3.89a \pm 0.02	2.17b \pm 0.06	0.50c \pm 0.00	***
<i>n</i> -C 27	10.14b \pm 0.38	11.29a \pm 0.10	4.00c \pm 0.03	***
<i>n</i> -C 28	4.55b \pm 0.13	8.74a \pm 0.19	1.50c \pm 0.01	***
<i>n</i> -C 29	17.45b \pm 0.29	20.46a \pm 0.34	10.70c \pm 0.06	***
<i>n</i> -C 30	5.29b \pm 0.09	7.09a \pm 0.13	2.40c \pm 0.01	***
<i>n</i> -C 31	20.12a \pm 0.33	2.98b \pm 0.08	6.60c \pm 0.03	***
<i>n</i> -C 32	5.86b \pm 0.09	7.90a \pm 0.15	0.50c \pm 0.00	***
Total content (mg/Kg)	347.33a \pm 4.04	216.33b \pm 3.05	106.70c \pm 0.58	***
Σ Odd Chain Number	310.33a \pm 3.80	171.09b \pm 2.46	94.30c \pm 0.51	***
Σ Even Chain Number	37.00b \pm 0.46	45.24a \pm 0.60	12.40c \pm 0.07	***
Odd Chain / Even Chain	8.39a \pm 0.11	3.78c \pm 0.01	7.60b \pm 0.02	***
<i>n</i> C19- <i>n</i> C29	316.06a \pm 3.93	198.37b \pm 2.79	97.20c \pm 0.53	***
<i>n</i> C30- <i>n</i> C32	31.27a \pm 0.50	17.97b \pm 0.30	9.50c \pm 0.05	***
<i>n</i> C19 <i>n</i> C29 / <i>n</i> C30 <i>n</i> C32	10.11a \pm 0.19	11.04b \pm 0.08	10.23c \pm 0.11	***

ratio of *n*C19-*n*C29 / *n*C30-*n*C32 was similar in all cultivars (Table 2).

Webster *et al.* (2000), reported that in commercially available extra virgin olive oil found a predominance of *n*C23 and *n*C25. This allowed the discrimination between olive oil, crude sunflower oil and crude rapeseed oil, the latter showing a predominance of *n*C29 and *n*C31. Lanzón *et al.* (1994) found in 250 Spanish virgin olive oils a predominance of *n*C25, *n*C27, *n*C29 and *n*C31. This confirms how important is the influence of biotic factors (specie and cultivar) and of the abiotic factors (soil, harvest date, harvest year, fertilizers, temperature, microclimatic conditions, geographical origin, etc.) on the vegetable oil production. From this point of view, the TSO produced in Calabria can be distinguished from its high content of *n*C21, *n*C23, *n*C25 and *n*C29. This profile is characteristic for TSO oil even if each cultivar presented its own profile (Tables 1, 2).

Odd chain carbon number *n*-alkanes / even chain carbon number *n*-alkanes

The Σ odd-chain carbon number saturated *n*-alkanes to Σ even-chain carbon number saturated *n*-alkanes ratio was calculated in the range from *n*C19 to *n*C32, with the following formula: sum of the odd-chain carbon number saturated *n*-alkanes / sum of the even-chain carbon number saturated *n*-alkanes.

The odd-chain carbon number saturated *n*-alkanes had a biogenic origin whereas the even-chain carbon number saturated *n*-alkanes had an anthropogenic origin: mineral oils (Grundböck *et al.*, 2010),

paraffins (Grob *et al.*, 2001), air pollution (Singh *et al.*, 2012) and soil pollution (Lee *et al.*, 2008). As a consequence, a low odd-to-even predominance, or a ratio equal or lower than 1 can be used as parameters to detect contamination in vegetable oils.

Previous studies have proved that terrestrial plants are characterized by an odd-long-chain carbon number predominance in *n*-alkanes (Eglinton and Hamilton, 1967; Rieley *et al.*, 1991; Bianchi and Canuel, 2011; Reddy *et al.*, 2000). The *n*-alkane composition of TSO confirms these results, in fact, a characteristic long chain odd-carbon predominance was observed in all cultivars: 79.09% in 'Rebellion F1', 88.39% in 'San Marzano' and 89.35% in 'Principe Borghese' (Table 1).

The *n*-alkane composition of TSO confirms these results, in fact, a characteristic long chain odd-carbon predominance was observed in all cultivars: 79.09% in Rebellion F1, 88.39% in San Marzano and 89.35% in Principe Borghese (Table 1). The three most represented *n*-alkanes were *n*-C21, *n*-C25 and *n*-C23. The ratio of odd-chain carbon number *n*-alkanes to even-chain carbon number *n*-alkanes was 8.39 in 'Principe Borghese', 3.78 in 'Rebellion F1' and 7.61 in 'San Marzano'. Those results showed in TSO of the 'Principe Borghese' and 'San Marzano' a ratio doubled that in 'Rebellion F1'.

ANOVA analysis and correlation matrix

Cultivars were compared ($p < 0.05$) and the results were considered horizontally. The significantly highest *n*-alkanes were *n*C21 in 'San Marzano' (44.05%), *n*C25 in 'Rebellion F1' (42.06%), *n*C25

Table 3. Correlation data matrix of *n*-alkane parameters expressed as a percentage of the total *n*-alkane content

Variables	<i>n</i> -C 19	<i>n</i> -C 20	<i>n</i> -C 21	<i>n</i> -C 22	<i>n</i> -C 23	<i>n</i> -C 24	<i>n</i> -C 25	<i>n</i> -C 26	<i>n</i> -C 27	<i>n</i> -C 28	<i>n</i> -C 29	<i>n</i> -C 30	<i>n</i> -C 31	<i>n</i> -C 32	Σ Odd Chain	Σ Even Chain	<i>n</i> C19- <i>n</i> C29	<i>n</i> C19- <i>n</i> C28
<i>n</i> -C19	1																	
<i>n</i> -C 20	-0.798	1																
<i>n</i> -C 21	-0.831	0.328	1															
<i>n</i> -C 22	0.684	-0.985	-0.163	1														
<i>n</i> -C 23	0.990	-0.706	-0.901	0.576	1													
<i>n</i> -C 24	0.476	0.150	-0.885	-0.316	0.594	1												
<i>n</i> -C 25	0.962	-0.603	-0.951	0.459	0.991	0.698	1											
<i>n</i> -C 26	0.980	-0.902	-0.705	0.815	0.943	0.293	0.889	1										
<i>n</i> -C 27	0.187	0.443	-0.702	-0.589	0.322	0.953	0.448	-0.011	1									
<i>n</i> -C 28	0.492	0.133	-0.893	-0.299	0.608	1.000	0.711	0.309	0.947	1								
<i>n</i> -C 29	-0.577	0.953	0.026	-0.991	-0.458	0.443	-0.332	-0.728	0.694	0.428	1							
<i>n</i> -C 30	0.117	0.505	-0.649	-0.644	0.254	0.929	0.384	-0.082	0.997	0.922	0.743	1						
<i>n</i> -C 31	-0.576	-0.033	0.933	0.202	-0.684	-0.993	-0.778	-0.403	-0.911	-0.995	-0.335	-0.879	1					
<i>n</i> -C 32	0.809	-0.290	-0.999	0.124	0.882	0.903	0.938	0.676	0.729	0.910	0.014	0.679	-0.947	1				
Σ Odd Chain	-0.442	-0.188	0.866	0.352	-0.563	-0.999	-0.670	-0.256	-0.964	-0.998	-0.477	-0.943	0.988	-0.885	1			
Σ Even Chain	0.442	0.188	-0.866	-0.352	0.563	0.999	0.670	0.256	0.964	0.998	0.477	0.943	-0.988	0.885	-1.000	1		
<i>n</i> C19- <i>n</i> C29	0.332	0.304	-0.800	-0.462	0.459	0.987	0.577	0.138	0.989	0.985	0.579	0.976	-0.962	0.823	-0.993	0.993	1	
<i>n</i> C30- <i>n</i> C32	-0.332	-0.304	0.800	0.462	-0.459	-0.987	-0.577	-0.138	-0.989	-0.985	-0.579	-0.976	0.962	-0.823	0.993	-0.993	-1.000	1

in ‘Principe Borghese’ (35.10%), (Table 1). The significantly highest *n*-alkanes were *n*C21 in San Marzano (44.05%), *n*C25 in Rebellion F1 (42.06%), *n*C25 in Principe Borghese (35.10%), (Table 1). ‘Principe Borghese’ showed the significantly highest percentage content of *n*C22 (0.75%), *n*C26 (1.12%). ‘Rebellion F1’ showed the significantly highest percentage content of *n*C23 (11.16%), *n*C24 (4.35%), *n*C25 (42.06%), *n*C27 (5.22%), *n*C28 (4.04%), *n*C30 (3.28%) and *n*C32 (3.65%). ‘San Marzano’ had the significantly highest *n*C20 (5.11%), *n*C21 (44.05%), *n*C29 (10.07%) and *n*C31 (6.17%) (Table 1).

San Marzano had the significantly highest *n*C20 (5.11%), *n*C21 (44.05%), *n*C29 (10.07%) and *n*C31 (6.17%), (Table 1). The highest correlation between *n*-alkanes expressed as a percentage was found among *n*C28 and *n*-C24 ($R = 1.000$). *n*C24 was found to be positively correlated with the Σ even-chain carbon number *n*-alkanes ($R = 0.999$) and negatively correlated with Σ odd-chain carbon number *n*-alkanes ($R = -0.999$), (Table 3).

Principal component analysis

Principal Component Analysis (PCA) was performed on the three cultivars and 21 parameters listed in Table 2 were included in the test. Only two Eigen values were obtained for each studied parameter which were higher than 1.00. All the values of all the parameters accounted for 100% of the cumulative

variance. The Eigen values and the percentage of total variance were 16.05 (76.40%) and 4.96 (23.60%). Visualization of the discriminatory among cultivars on the plane of the first two functions led to a fairly good separation from the different groups.

The orthogonality between *n*C21 and *n*C22, *n*C20 and *n*C31, *n*C22 and *n*C32, indicated the independence of these variables. The relative position of each cultivar in Fig.1a evidenced the high separation of the cultivars. ‘Rebellion F1’ was in the left top corner, ‘San Marzano’ was in the right top corner and ‘Principe Borghese’ was in the right bottom corner (Figure 1a).

The similar vector direction of the relative value data set shows the sum of odd-chain *n*-alkanes increased at the expense to *n*C24 and *n*C28, whereas the sum of even chain *n*-alkanes was highly correlated with *n*C24 and *n*C28 (Figure 1b).

Conclusions

The *n*-alkane length and concentration of chains is characteristic for each vegetable specie. The *n*-alkane analysis and the appliance of chemometrics to the *n*-alkane data matrix showed that cultivar highly significantly influenced the *n*-alkane composition of TSO. The ‘Principe Borghese’, ‘Rebellion F1’ and ‘San Marzano’ cultivars showed three different compositions both in qualitative and

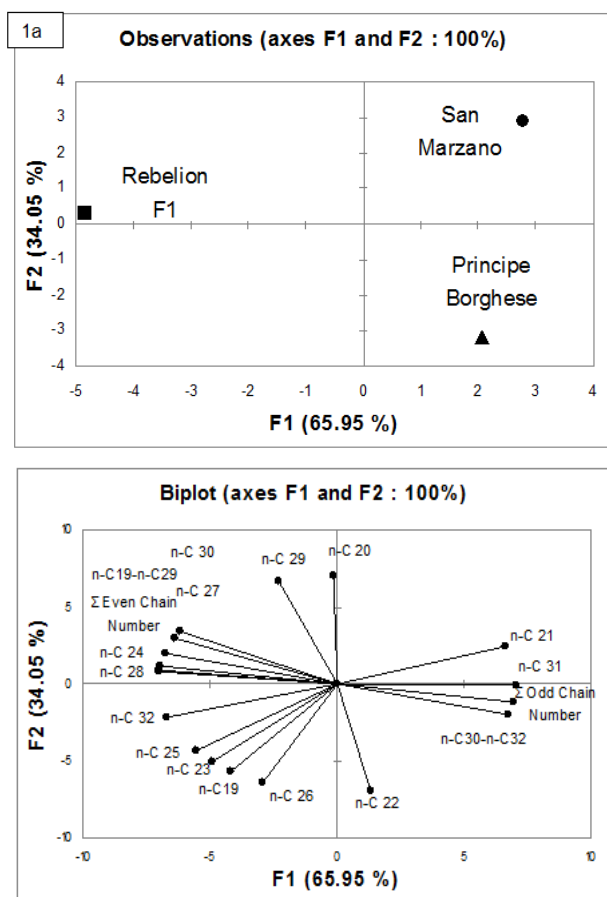


Figure 1. (a) PCA of the TSO studied *n*-alkane composition (%): (1a) relative position of the cultivars; (b) relationship between variables

in quantitative terms. Odd-chain carbon number saturated *n*-alkanes were largely the most represented saturated linear aliphatic hydrocarbons in the TSO, as expected for a terrestrial plant. The *n*C25, *n*C21, *n*C23 and *n*C29 were the most represented *n*-alkanes in the TSO of all cultivars. *n*-Alkane composition is useful to distinguish both the seed oil of different tomato cultivars and the TSO from other vegetable oils. The study of the *n*-alkane composition in the TSO increases the knowledge of an unusual vegetable oil which could be used both as an edible oil or as a source for biofuel production. In relation to the total *n*-alkane content, 'Principe Borghese' and 'Rebellion F1' produced an oil with a better attitude for a biodiesel use, whereas the 'San Marzano' TSO showed better edible characteristics. In relation to the total *n*-alkane content, Principe Borghese and Rebellion F1 produced an oil with a better attitude for a biodiesel use, whereas the San Marzano TSO showed better edible characteristics.

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