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INVESTIGATIONS ON THERMAL DEGRADATION OF PHYTOCHEMICALS FROM LAVENDER EXTRACT

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The importance of lavender as a source of essential oils has been well recognized. This study reports the phytochemical profile of lavender extract in terms of chlorophylls, total carotenoids, polyphenols and flavonoids, related to antioxidant activity. The extract displayed a high polyphenolic and flavonoids content, with an antioxidant activity of 2.28±0.18 mMol Trolox/g D.W. The fractional conversion and first order kinetic models were found suitable for predicting the changes that occur in the selected phytochemicals. Kinetic and thermodynamic parameters were calculated confirming the irreversible degradation of phytochemicals. Both the temperature and duration of heating significantly impacted the content in bioactive compounds.

Keywords: lavender, chlorophylls, carotenoids, thermal treatment, kinetic

Introduction

Lavenders are aromatic evergreen shrubs from *Lamiaceae* family that have been traditionally used as culinary herbs and medicine for headaches, digestive troubles, burns, skin sores and insect bites (Pereira *et al*., 2015). Nowadays, the plant is extensively cultivated as ornamental plants for garden, landscape use, potpourris and essential oil production to fragrance, cosmetic, pharmaceutical, food and flavor industries (Zuzarte *et al*., 2008). *Lavandula* genus comprises 39 species and several hybrids of woody perennial plants, some of which have long been grown for their essential oil (Urwin and Mailer, 2008).

Lavender (*Lavandula angustifolia*) is rich in essential oils, extensively studied and found to have many functional effects including antimicrobial, insecticidal (Da Camara *et al*., 2015), antioxidant activity (Chrysargyris *et al*., 2016), and anticholinesterase inhibition (Ferreira *et al*., 2006). The economic value of

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Lavandula spp. predominantly relates to the properties of their essential oils, which are strictly regulated by international ISO standards and are used both cosmetically and therapeutically for centuries (Gonçalves and Romano, 2013). Lavender essential oils are extensively used in the manufacturing of soaps, perfumes, food flavors and other products. The content in essential oils depends on species. For example, the essential oil from *Lavandula angustifolia* is dominated by linalool and linalool acetate, whereas linalol, 1,8-cineole and camphor can be found in *Lavandula latifolia* (Munõz-Bertomeu *et al*., 2008). *Lavandula*×*intermedia*, a hybrid from *L. angustifolia* and *L. latifolia*, contains linalol, linalool acetate, camphor and 1,8-cineole as major constituents (Desautels *et al*., 2009). Terpenes are the largest and most diverse family of natural products. Within these compounds both primary and secondary metabolites (hormones, carotenoids, chlorophylls and sterols), necessary for plant growth and survival, can be found (Raut and Karuppayil, 2014). However, less is known about the phytochemicals content of lavender extracts from the perspectives of using in food industry as an ingredient. Therefore, until date no attempts have been made in analyzing the chlorophylls, carotenoids, flavonoids, volatile compounds and fatty acids profile of the lavender. The interest in phytochemicals related to vegetables diet is namely due to phytochemicals bioactivity, since it has been demonstrated that they have biological properties consistent with cancer prevention, such as antioxidant and antimutagenic activities, action modulating the activity of xenobiotic enzymes, and the induction of apoptotic events in cancer cell lines (Aparicio-Ruiz *et al*., 2010). Phenolic antioxidants have several positive effects on human health such as the anticarcinogenic and anti-inflammatory effects (Usenik *et al*., 2008). The use of plant extracts as functional ingredients in various food, beverage and cosmetic applications is gaining growing interest among scientists, as well as among consumers and food manufacturers (Komes *et al*., 2011). However, phytochemicals, which are often responsible for the color of plants and foodstuffs of vegetable origin (Aparicio-Ruiz *et al*., 2010), are highly susceptible to degradation to various factors during processing, resulting in color changes in food, associated by consumers with quality loss. In recent years, the microencapsulation techniques aiming to develop proper environment for different susceptible bioactive in a stable wall matrix as a means of protecting functional compounds from processing conditions (like oxygen, pH, ionic strength, and temperature) and improving the bioavailability have gained significant interest. However, before microencapsulation, the knowledge of the thermal degradation mechanisms based on mathematical models is essential for predicting the behavior of biologically active compounds during industrial processing, from the perspective of minimal nutritional and functional losses. Vieira *et al.* (2016) highlighted the importance of mathematical models that can be used to predict the thermal degradation considering several conditions without conducting long experimental procedures. Therefore, in order to predict the nutritional and functional changes during industrial processing, studies are needed to estimate the kinetic and thermodynamic parameters under different environmental conditions. Hereto, this study aims to investigate the lavender extract from the perspective of the comprehensive

phytochemical profile, involving the chlorophylls (*a*, *b* and total), total carotenoids, total polyphenolic and flavonoids content (TPC and TFC, respectively), and antioxidant activity. Furthermore, the study involved assessing the kinetics of thermal degradation of the chlorophylls, total carotenoids, TPC and TFC in the ethanolic lavender extract, in relation with antioxidant activity loss in the temperature range of 75°C to 100°C. Moreover, our study aims to demonstrate the thermal sensitivity of selected bioactives from lavender, less studied until now, from the perspective of microencapsulation and developing food-grade functional ingredients.

Materials and methods

Reagents

Folin-Ciocalteu's phenol reagent, sodium carbonate (Na_2CO_3), sodium nitrite ($NaNO_2$), aluminum chloride ($AlCl_3$), sodium hydroxide (NaOH), methanol, gallic acid, catechin, DPPH (1,1-diphenyl-2 picrylhydrazyl), 6-Hydroxy-2,5,7,8-tetramethylchromane-2-carboxylic acid (Trolox) were purchased from Sigma-Aldrich (Steinheim, Germany).

Plant material

The aerial parts of lavender (*Lavandula angustifolia* Mill.) were collected from natural populations occurring throughout the south-eastern regions of Romania. The plant material was air-dried at 40°C and powdered.

Pigments extraction

The phytochemicals were extracted from the powdered lavender by adding 10 ml of n-hexan:acetone (3:1) to 2 g of powder. The mixture was homogenized by using an Ultra-Turrax homogenizer (IKA Werke, Labortechnik, Staufen, Germany) for 2 min, followed by ultrasonication for 30 minutes. After centrifugation at 8000x*g* for 10 min at 4°C, the residue was re-extracted with 10 mL of n-hexan:acetone solutions (3:1, v/v) and the extraction was repeated four times. The extract was concentrated at 40°C to dryness, dissolved in 10 mL ethanol (70%) and filtered through 0.45 μm membranes.

Chlorophylls measurements

For chlorophylls and carotenoids measurements, the absorbance was measured at 645 nm, 663 nm and 470 nm. In order to calculate Chl *a*, Chl *b*, total chlorophyll (tot Chl) and total carotenoids, Arnon's equations were used (Arnon, 1949), as follow:

$$\text{Chl } a = 0.0127 \times A_{663} - 0.00269 \times A_{645} \quad (1)$$

$$\text{Chl } b = 0.0229 \times A_{645} - 0.00468 \times A_{663} \quad (2)$$

$$\text{tot Chl} = 0.0202 \times A_{645} + 0.00802 \times A_{663} \quad (3)$$

$$\text{Carotenoids} = (1000 \times A_{470} - 2.13\ \text{Chl } a - 97.63\ \text{Chl } b)/209 \quad (4)$$

The results were expressed as mg/g of extract (mg/g D.W.).

Determination of total polyphenolic content

Total phenol content (TPC) was determined using Folin–Ciocalteu reagent. In brief, 1 mL of Folin–Ciocalteu reagent was added to 0.1 mL of extract, followed by addition of 0.8 mL of sodium carbonate (6%) and 1 mL of distilled water. After incubation for 30 minutes, the absorbance was measured at 765 nm. Gallic acid was used as the standard and the results were expressed in mg of gallic acid equivalents (GAE) per g D.W.

Determination of total flavonoids content

Total flavonoids content (TFC) was determined by adding 1 mL of distilled water and 0.075 mL of sodium nitrite (5%) to 0.25 mL of extract. After incubation for 5 min in the dark at room temperature, 0.15 mL of $AlCl_3$ 10%, 0.5 mL of sodium chloride (1 M) and 1 mL of distilled water was added to solution and incubated for more 10 min in the dark at room temperature. The absorbance was measured at 510 nm against blank sample. Catechin was used as the standard and the results were expressed in mg of catechin equivalents (CE) per g D.W.

Antioxidant activity

The DPPH radical scavenging assay was conducted according to the method described by Guo *et al.* (2018) with slight modification. Briefly, 0.1 mL of extract was mixed with 3.9 mL of DPPH methanolic solution (1.5×10^{-4} M). The mixture was shaken vigorously and stored for 30 min in dark conditions at approximately 25°C. The absorbance of the reaction mixture was then measured at 515 nm using a UV-Vis spectrophotometer. The antioxidant activity was expressed as mMol Trolox/g D.W. using a calibration curve.

Heat treatment

For the kinetic studies, 0.3 mL of extract solutions were filled in Eppendorf tubes (1 cm diameter) and heated in the temperature range of 75°C to 100°C for different treatment times (0-40 min) in a thermostatic water bath (Digibath-2 BAD 4, RaypaTrade, Barcelona, Spain). After the thermal treatment, the Eppendorf tubes were immediately cooled in ice in order to prevent further degradation.

Mathematical models and kinetic analysis

The degradation kinetics of phytochemicals content in lavender extract was fitted to a first-order fractional conversion kinetic model as described by Turturică *et al.* (2016). The degradation kinetics of antioxidant capacity was described by fitting the first order kinetic model (Eq. 5) to the experimental data:

$$\frac{A}{A_0} = e^{-kt} \tag{5}$$

where A is the antioxidant activity to be estimated, the subscript 0 indicates the initial value of the antioxidant activity, t is the heating time, and k is the rate constant at temperature T (1/min).

The Arrhenius model was used to describe the temperature dependence of both degradation rate constants as described by (Eq. 6):

$$k = k_{ref}\, exp\left[-\frac{E_a}{R}\left(\frac{1}{T}\right)\right] \tag{6}$$

where E_a is the activation energies (kJ/mol), k_{ref} is the reaction constant at the infinite temperature (1/min), T is the absolute temperature (K), and R the universal gas constant (8.314 J/mol·K). The kinetic parameters E_a were estimated by a linear regression of the natural logarithm of the degradation rate constant versus the reciprocal of the absolute temperature. The validity of these equations was evaluated based on the linearity of the graph, regression coefficients and residual analysis.

Thermodynamic parameters

The thermodynamic parameters were estimated as described earlier by Vieira *et al.* (2016).

Statistical analysis of data

All experiments were performed in triplicate with duplicate samples. The results were expressed in terms of average values. Statistical analysis of data was performed using the data analysis tool pack of the Microsoft Excel software.

Results and discussion

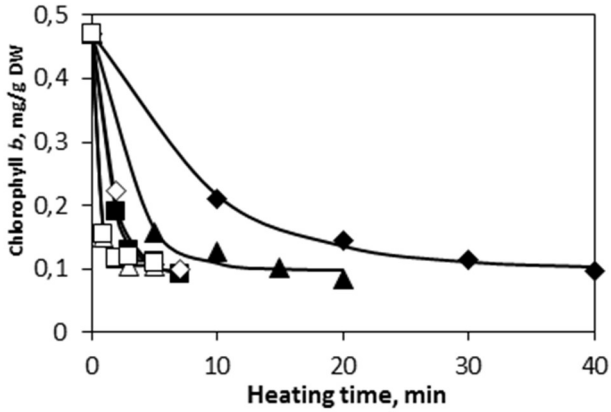
Phytochemicals content of the lavender extract

The extract showed TPC value of 3.29±0.08 mg GAE/g D.W. and TFC of 2.36±0.75 mg CE/g D.W. The chlorophyll *a* content was 471.74±10.25 µg/g D.W., whereas chlorophyll *b* and total chlorophyll showed a content of 239.86±8.89 µg/g D.W. and 625.85±15.18 µg/g D.W. The extract showed a content of total carotenoids of 126.18±5.86 mg/g D.W. The extract showed a high polyphenolic and flavonoids content, with an antioxidant activity of 2.28±0.18 mMol Trolox/g D.W. The significant TPC and TFC content led to an antioxidant activity of 2.28±0.18 mMol Trolox/g D.W. Comparison with data from literature was difficult, since lavender is very well studied for its content in essential oils and less for polyphenolic, chlorophylls or carotenoids content. However, Xylia *et al.* (2017) suggested a TPC of 12.23 mg GAE/g of lavender oil and an antioxidant activity expressed as DPPH radical scavenging activity of 19.88 mg/mL. Komes *et al.* (2011) studied the phenolic composition and antioxidant activity of some medicinal plants, including lavender, as affected by the extraction time and hydrolysis and reported a content of flavan-3-ols of 2.42±0.34 mg catechin/L and 3.30±1.02 mg catechin/L in non-hydrolyzed extract obtained after 5 and 15 min of extraction, whereas a higher content of 4.94±0.29 mg catechin/L was suggested in hydrolyzed extract of lavender. These authors detected significant concentration of rosmarinic, caffeic and ferulic acids, whereas luteolin was the main flavone found in the hydrolyzed extract.

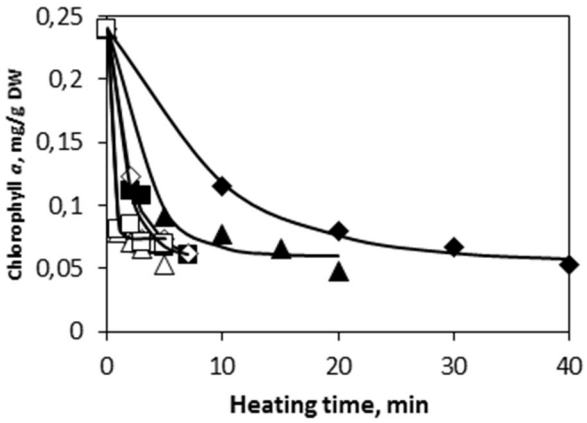
The influence of thermal treatment on phytochemical content

Chlorophyll pigments are responsible for the green color of plants and foodstuffs of vegetable origin (Aparicio-Ruiz *et al*., 2010). Chlorophylls are highly susceptible to degradation during processing, resulting in color changes in food. Within the temperature range, the different temperature-time combinations caused a sequential reduction in phytochemicals content (Figure 1). For example, the chlorophyll *a*

content decreased by 78% after 40 minutes at 75°C and with 71% after 5 minutes at 100°C (Figure 1 a). Chlorophyll *b* was more heat sensitive, with a reduction of 80% and 78%, respectively (Figure 1 b).



(a)



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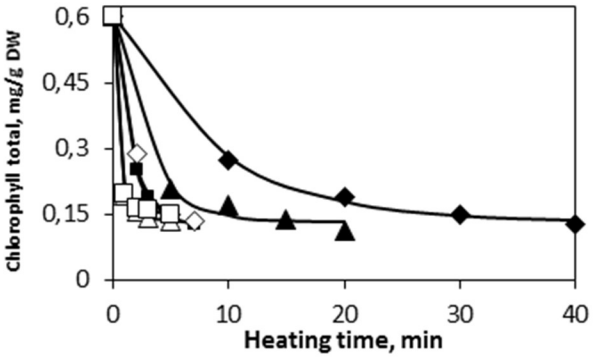
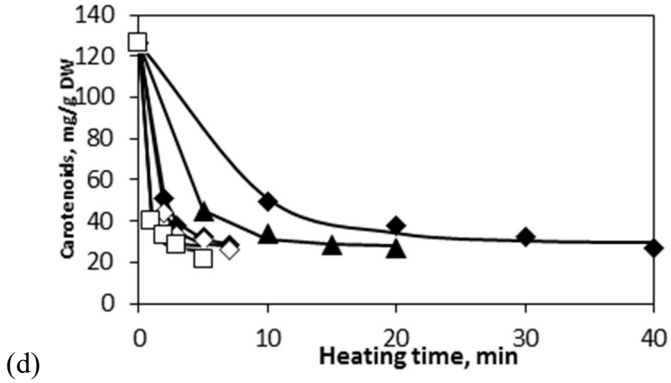


(c)



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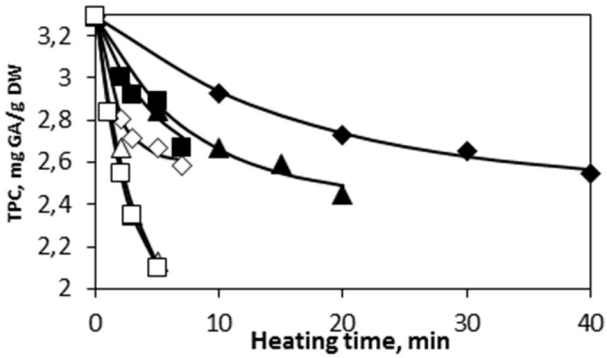

(e)

Figure 1. Isothermal degradation of chlorophyll *a* (a), chlorophyll *b* (b), chlorophylls total (c), carotenoids (d) and TPC (e) in lavender flower extracts, treated at different temperatures (◆ 75°C, ▲80°C, ■ 85°C, ◇90°C, △95°C and □ 100°C). The lines represent the fractional conversion kinetic model fits to experimental data.

For total chlorophylls, a thermal treatment at 80°C for 20 min resulted in significant loss, with approximately 82%, whereas increasing temperature at 100°C for 5 min caused a reduction with 75% (Figure 1 c). Marangoni (1996) developed a complete kinetic scheme that includes the degradation of chlorophyll to pheophytin, chlorophyllide, pheophorbide, and ultimately colourless chlorophyll breakdown products. Aparicio-Ruiz *et al.* (2010) proposed a degradation mechanism involving reactions that alter the structure of the isocyclic ring of pheophytin, originating intermediary products such as pyropheophytin, 13^2-OH-pheophytin, and 15^1-OH-lactone-pheophytin, and reactions that affect the porphyrin ring, producing colourless compounds.

Heating caused a significant decrease in total carotenoids content (Figure 1 d). Therefore, heating at 75°C for 40 min caused a decrease by about 79%, whereas after 5 min of heating at 100°C, a decrease of about 83% in total carotenoids content in the extract was found. Benlloch-Tinoco *et al.* (2015) suggested a reduction in total carotenoids by 67±7% in case of pasteurized kiwi puree during storage, highlighting that neoxanthin (loss of 91%) and lutein (loss of 62%) were the most and the least thermolabile compounds. The thermal degradation of

carotenoids mechanism was described by Zepka *et al.* (2009), involving parallel irreversible and reversible coupled reactions of the initial all-*trans*-β-cryptoxanthin and all-*trans*-β-carotene to yield, respectively, degradation compounds and mono-*cis* isomers. However, thermal behavior seems to be influenced by both experimental conditions and food matrices.

Figure 1 e shows the heat-induced changes in TPC at different temperatures as a function of heating time. TPC showed a similar trend in the whole temperature studied, with reduction varying between 22 and 24% at temperatures ranging from 75 to 90°C after 40 min and 5 min, respectively. Nambi *et al.* (2016) studied the effect of blanching (70 to 95°C) on TPC in selected vegetables and reported that with increasing the time and temperature, the reduction in polyphenolic compounds increased drastically. Blanching for short duration (3 min) reduced the total phenolic contents significantly (15–20 % at 70° C and 50–52 % at 90° C). The loss in TPC may be explained by the breakdown of phenolic components (Turkmen *et al.*, 2005) and/or dissolution of polyphenols into the cooking water (Chuah *et al*., 2008).

Similar reduction in TPC during thermal treatment of different vegetables like broccoli, cabbage, colored peppers, Irish York cabbage, kale, leek, peas, shallots, spinach, squash, swamp cabbage, tomato and some of selected cruciferous vegetables has been previously reported (Ismail *et al*., 2004; Gonçalves *et al*., 2010; Jaiswal *et al*., 2012).

With regard to the effect of thermal treatment on TFC, no significant differences in the flavonoids content were observed, regardless the applied time-temperature combinations, suggesting a high thermostability of the selected bioactives. For example, heating at 75°C for 30 min caused a reduction by about 9% in TFC, whereas after 3 min at 100°C, 15% from TFC was lost.

Thermal treatment had a significant impact on antioxidant activity, with losses of approx. 54% at 75°C after 40 minutes and 92% at 100°C after 3 minutes (Figure *2*).

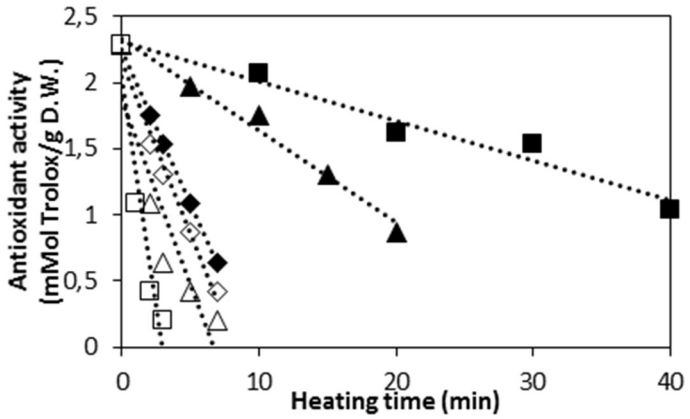

Figure 2. Isothermal degradation of antioxidant activity in lavender extracts, treated at different temperatures (◆ 75°C, ▲80°C, ■ 85°C, ◇90°C, △95°C and □ 100°C). The data were processed as the arithmetic mean of three sets of analytical experiments.

Similar reducing trend have been reported in many vegetables by Chuah *et al.* (2008), Ismail *et al.* (2004), and Zhang and Hamauzu (2004). The loss in antioxidant activity is related to degradation of certain types of phenolic compounds, chlorophylls and carotenoids in the extract.

Kinetics of thermal degradation of phytochemicals in lavender extract

In lavender extract, kinetic parameters for chlorophyll *a*, chlorophyll *b*, total chlorophyll, carotenoids, TPC and antioxidant activity at constant pH (6.5) and at different temperatures ranging from 75 to 100°C for present heating time (0-40 min), have been studied by spectrophotometric analysis. Degradation kinetic of the phytochemicals content in lavender extract was modelled using fractional conversion and first order kinetic models. For each tested phytochemical compound, a good correlation between experimental and predicted values were obtained, considering the wide sample variability and that a single set of parameters was used at each temperature for all experiments (data not shown).

The heat induced changes in chlorophyll *a*, chlorophyll *b*, total chlorophyll, carotenoids and TPC was described in terms of degradation rate constants (1/min) and degradation energy of activation (E_a) (Table 1). These parameters are often used to estimate the shelf life of nutritional quality, and in developing processing systems that maintain phytochemicals compounds and antioxidant activity in fruit and vegetable products.

As it can be seen from Table 1, the *k* values for chlorophyll *a* increases with increasing temperature, from 10.83±1.15x10^{-2} 1/min at 75°C to 297.81±11.99x10^{-2} 1/min at 100°C, whereas for chlorophyll *b*, the *k* was 17 times higher at 100°C when compared with 75°C, suggesting a lower thermal stability at higher temperature. In lavender extract, chlorophyll *b* degrades faster in temperature range of 75-90°C when compared to chlorophyll *a*, which degrades more rapidly at temperatures of 95-100°C (Table 1).

The carotenoids degrade faster at lower temperature compared with chlorophyll *a*, with *k* value of 11.39±0.99x10^{-2} 1/min at 75°C and comparable with chlorophyll *b* at higher temperature, with *k* value of 232.54±17.14 x10^{-2} 1/min (Table 1).

The first-order kinetic model has been reported for chlorophylls degradation during the fermentation processing of food matrices such as pickles, olives, and coleslaw (Weemaes *et al.,* 1999) and during heat treatment of spinach puree (Koca *et al*., 2007), broccoli juice (Gaur Rudra *et al*., 2007), green peas (Al-Zubaidy and Khalil, 2007). For example, Koca *et al*. (2007) reported lower values for chlorophyll *a* thermal degradation at 100°C of 0.1330±0.0269 1/min at pH 5.5 and 0.0182±0.0033 1/min at pH 7.5, respectively. For chlorophyll *b*, these authors reported significant lower *k* values of 0.0053±0.0008 1/min at pH 5.5 and 0.0016±0.0001 1/min at pH 7.5, respectively. However, these authors suggested that chlorophyll *a* degraded faster than chlorophyll *b* at 5.5, 6.5 and 7.5 pH for each temperature applied.

Gaur Rudra *et al.* (2007) reported that an excellent agreement between experimental and calculated values demonstrating the applicability of the first-

order rate kinetic equation to describe the degradation of chlorophylls of coriander and mint puree during thermal processing. These authors tested a higher temperature range, from 105 to 145°C at different pH and reported *k* values varying from 0.00623 1/min at 105°C and pH 5.5 to 0.04831 1/min at 145°C and pH 7.5 for chlorophyll *a* in thermally processed coriander puree.

Table 1. Estimated kinetic parameters of phytochemicals thermal degradation in lavender flower extract

Compounds	**Temperature (°C)**	**k, 1/min (x10^{-2})**	***E$_a$* (kJ/Mol)**
Chlorophyll *a*	75	10.83±1.15	139.69±15.22
	80	32.05±8.32	
	85	52.24±12.10	
	90	61.07±15.90	
	95	229.98±5.97	
	100	297.81±11.99	
Chlorophyll *b*	75	11.58±0.96	123.49±18.24
	80	34.92±6.18	
	85	61.82±15.86	
	90	70.90±6.49	
	95	208.71±9.72	
	100	220.82±16.23	
Total chlorophyll	75	11.39±0.99	126.69±17.38
	80	34.23±6.70	
	85	61.65±2.58	
	90	66.30±15.76	
	95	213.09±17.88	
	100	232.54±17.14	
Carotenoids	75	15.05±2.01	114.18±11.44
	80	34.79±3.24	
	85	74.35±4.22	
	90	90.95±8.09	
	95	184.43±4.65	
	100	212.73±3.79	
TPC	75	5.80±0.90	94.65±8.19
	80	12.94±3.30	
	85	20.35±8.91	
	90	30.82±10.19	
	95	38.79±9.50	
	100	58.69±1.54	
Antioxidant activity	75	1.86±0.09	153.66±16.61
	80	4.69±0.87	
	85	17.87±1.28	
	90	23.49±2.37	
	95	34.01±1.27	
	100	77.35±3.78	

Activation energies (E_a) were calculated on the basis of linear regression analysis of natural logarithms of rate constants against reciprocal absolute temperature. The E_a values were 139.69±15.22 kJ/mol, 123.49±18.24 kJ/mol, 126.69±17.38 kJ/mol and 114.18±11.44 kJ/mol for chlorophyll *a*, *b*, total chlorophylls and carotenoids, respectively. The corresponding E_a value for TPC was 94.65±8.19 kJ/mol, whereas for antioxidant activity 153.66±16.61 kJ/mol. Higher activation energy implies that a smaller temperature change is required to degrade a specific compound more rapidly. Therefore, it can be suggested that polyphenols were the most heat stable at pH 6.5.

Koca *et al.* (2007) reported activation energies of 14.0±0.71 kcal/mol, 11.7±1.44 kcal/mol and 4.80±0.91 kcal/mol for chlorophyll *a* and 10.0±1.22 kcal/mol, 11.0±0.24 kcal/mol and 6.84±0.29 kcal/mol for chlorophyll *b* at pH 5.5, 6.5 and 7.5, respectively. Gaur Rudra *et al.* (2007) suggested lower E_a values for chlorophylls thermal degradation in pureed coriander leaves, ranged from 28.48 kJ/mol for chlorophyll *a,* 43.019 kJ/mol for chlorophyll *b* and 38.48 kJ/mol for total chlorophylls at pH 6.3. It seems that chlorophylls are more susceptible to thermal degradation in lavender extract.

Thermodynamic parameters

Table 2 shows the activation enthalpy ($\Delta H^{\#}$), the free energy of inactivation ($\Delta G^{\#}$) and the activation entropy ($\Delta S^{\#}$) for chlorophylls, carotenoids and TPC at temperatures ranging from 75°C to 100°C.

The free energy of degradation ($\Delta G\#$), representing the difference between the activated state and reactants as reported by Al-Zubaidy and Khalil (2007) showed values ranging from 9.21 to 8.86 J/mol for chlorophyll *a*, 9.19 to 8.96 J/mol for chlorophyll *b* and 9.19 to 8.94 J/mol for total chlorophylls, respectively. The corresponding values for carotenoids ranged from 9.11 J/mol at 75°C to 8.97 J/mol at 100°C, whereas for TPC, $\Delta G\#$ values did not vary significantly with temperature increase, with values of 9.39 J/mol and 9.37 J/mol when increasing temperature from 75 to 100°C. The positive sign implies that thermal degradation of phytochemicals in flower lavender extract is a nonspontaneous reaction. Vikram *et al.* (2005) suggested that the activation enthalpy ($\Delta H^{\#}$) is a measure of the energy barrier that must be overcome by the reacting molecules, being correlated with the strength of the broken or/and new formed bonds of the transition state from the reactant.

As it can be seen from Table 2, $\Delta H^{\#}$ had positive sign, implying an endothermic state between activated complex and reactant. $\Delta H^{\#}$ values varied between 11.01 kJ/mol for chlorophyll *a* at 75°C to 6.36 kJ/mol for TPC at 100°C.

The activation entropy ($\Delta S^{\#}$) had negative values for all phytochemicals (Table 2), highlighting that the heat-induced transition state has a lower structural freedom than the reactants, while the thermal degradation process is irreversible.

Table 2. Thermodynamic parameters obtained for phytochemical degradation in lavender extract

Compounds	Temperature °C	$\Delta H^{\#}$ (kJ/mol)	$\Delta S^{\#}$ (kJ/mol/K)	$\Delta G^{\#}$ (J/mol)
Chlorophyll *a*	75	11.01±1.78	-233.06±10.48	9.21±1.04
	80	10.97±1.36	-224.72±10.74	9.02±1.11
	85	10.92±1.02	-221.36±11.43	9.01±1.21
	90	10.88±0.99	-220.68±15.47	9.09±1.03
	95	10.84±1.02	-210.29±16.95	8.82±0.99
	100	10.80±1.03	-208.76±16.32	8.86±0.87
Chlorophyll *b*	75	9.45±1.04	-236.98±17.84	9.19±0.77
	80	9.41±0.78	-228.42±11.47	9.00±0.89
	85	9.37±1.74	-224.28±11.31	8.96±1.23
	90	9.33±1.08	-223.73±11.65	9.05±1.36
	95	9.28±1.48	-215.32±13.47	8.85±1.45
	100	9.24±1.49	-215.42±14.74	8.96±0.99
Total chlorophyll	75	9.77±1.74	-236.19±19.34	9.19±1.01
	80	9.73±1.05	-227.68±18.42	9.01±1.09
	85	9.69±1.11	-223.40±11.12	8.96±0.87
	90	9.65±0.48	-223.40±11.36	9.07±0.75
	95	9.60±0.78	-214.28±17.43	8.84±1.07
	100	9.56±1.09	-214.13±15.41	8.94±1.06
Total carotenoids	75	8.52±0.56	-237.47±13.21	9.11±0.82
	80	8.48±0.57	-231.09±13.58	9.00±0.81
	85	8.44±0.79	-225.34±14.74	8.91±1.01
	90	8.39±0.98	-224.22±14.71	8.97±1.32
	95	8.35±1.06	-218.88±19.78	8.89±1.36
	100	8.31±1.12	-218.22±11.20	8.97±0.92
TPC	75	6.57±0.49	-251.01±11.02	9.39±0.91
	80	6.52±0.87	-244.84±11.08	9.29±1.04
	85	6.48±0.79	-241.71±11.06	9.30±1.11
	90	6.44±0.87	-238.60±19.47	9.30±1.12
	95	6.40±0.47	-237.15±15.48	9.36±1.51
	100	6.36±0.65	-234.17±14.11	9.37±1.28

Conclusions

A phytochemical profile of the lavender extract, comprising evaluation of chlorophylls carotenoids, polyphenols, flavonoids, and antioxidant activity was highlighted, from the perspective of using the extracts as functional ingredient. The high antioxidant activity of extracts lavender was correlated with a higher content in polyphenols and flavonoids.

Our results supported the hypothesis that temperature and duration of heating significantly reduced the content in bioactive components. Kinetic modeling revealed that, the changes in bioactive components could be predicted by fractional conversion and first order kinetic models. The kinetic parameters, rate constant values, activation energy and thermodynamic parameters, in terms of free energy

of degradation, activation enthalpy, and entropy were calculated for all bioactive compounds. No significant influence was found on the flavonoids content, whereas the results highlighted the lower degradation rate of total polyphenols in the whole temperature range studied.

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