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Sensory profile of Italian Espresso brewed Arabica Specialty Coffee under three roasting profiles with chemical and safety insight on roasted beans

Fosca Vezzulli,[1]* Terenzio Bertuzzi,[2] Silvia Rastelli,[2] Annalisa Mulazzi[2] & Milena Lambri[1]

1 Department for Sustainable Food Process DiSTAS, Università Cattolica del Sacro Cuore, Via Emilia Parmense 84, Piacenza 29122, Italy
2 Department of Animal, Nutrition and Food Sciences DiANA, Università Cattolica del Sacro Cuore, Via Emilia Parmense 84, Piacenza 29122, Italy

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Summary Specialty coffee (SC) has been showing an increasing interest from the consumers which appreciate its traceability and the peculiar flavours from each single origin. Additionally, the processes to which coffee fruits underwent to get green coffee characterise the beans in terms of macromolecules acting as substrates during the roasting. This work evaluates via sensory analysed eight SC, roasted at light, medium, and dark level, submitted to Italian espresso extraction, to assess how different roasting levels exalt the expected cup profile obtained by the suppliers via cupping in origin countries. Finally, roasted beans were characterised for physico-chemical features (pH, titratable acidity, caffeine, melanoidins, polyphenols and acrylamide). Sensory analysis demonstrated that the intermediate roasting level and espresso extraction match better attributes from in-origin cupping. Melanoidins (mmol g^{-1} coffee d.b.) was able to discriminate among roasting levels (light 0.12 ± 0.01; medium 0.13 ± 0.003; dark 0.14 ± 0.01; $\alpha = 0.05$). Acrylamide analyses ensured compliance with the food safety standards (light 301.9 ± 37.2 ppb; medium 126.1 ± 19ppb; dark 107.9 ± 22.5ppb). Physico-chemical features were able to cluster samples from different origins within the same roasting level ($\alpha = 0.05$). Results showed correlations ($\alpha = 0.01$) between sensory analysis and physico-chemical values: direct for caffeine and astringency, reverse for perceived acidity in relation to astringency, roasted, dried fruits and nutty notes.

Keywords Acrylamide, caffeine, polyphenols, roasting, sensory analysis, sensory profile, specialty coffee.

Introduction

Particularly in the last two decades, coffee market permitted consumers to appreciate the connection between origin, processes and taste of different single-origin coffee (Teuber, 2010; Specialty Coffee Association, 2018c), and the certified quality (Farah *et al.*, 2006) of those products started to be mostly required (Credence Research, 2018). From the selected species of the genus Coffea, the variety and the terroir of the harvesting country (Aguilar *et al.*, 2012; Costantini & Bucelli, 2014), going through the post-harvest processing to obtain coffee beans (Illy & Viani, 2005), up to the different roasting systems and sensory profiles of a cup of coffee, it can straightforwardly be understood the complexity and the huge number of variables involved to obtain high-quality coffee (Andueza *et al.*, 2003; Joët *et al.*, 2009; Piccino *et al.*, 2014; Barbosa *et al.*, 2019; Chen *et al.*, 2019; Rodriguez *et al.*, 2020).

In this panorama, specialty coffee (SC) has been started to become a new positive trend in the world coffee market, with helpful reflections on producers' life conditions and improvement of productions quality (Kilian *et al.*, 2005). SC as defined by Coffee Quality Institute and Specialty Coffee Association is traceable and well identified lots of coffee, evaluated first as green and roasted beans to ensure the absence of primary defects, quakers and up to five secondary defects, then submitted as roasted and ground coffee to a standard extraction and lastly cupped to be scored in terms of sensory quality. People in charge of this quality control procedure are certified experts known as Arabic Q-Graders (Specialty Coffee Association,

*Correspondent: Fax: +39 0523 599232; e-mail: fosca.vezzulli@unicatt.it

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2018b, 2018d). Besides the availability of more efficient industrial plants and the parallel increased potentiality of data recording and process monitoring, a big improvement in cropping, selection, processing, roasting and extraction processes has been done, leading to a quick development in the SC sector. Many studies on these topics indeed are aimed to evaluate quality indicators and to assess the authenticity of raw material (Maeztu *et al.*, 2001; Piccino *et al.*, 2014; Toci & Farah, 2014; Zhang *et al.*, 2019; Wadood *et al.*, 2020; Núñez *et al.*, 2021).

Further, detailed studies and scientific approaches about industrial coffee roasting to exalt the most green's features (Barbosa *et al.*, 2019) and to evaluate changings in given and perceived quality under different extraction systems are missing (Barroso *et al.*, 2016; Hamdouche *et al.*, 2016; Kwak *et al.*, 2017). Such a knowledge may also be spent on an industrial scale along with the definition of a set of routine analytical methods scientifically based that are suitable to monitor the roasting profiles and to detect the main quality markers of the roasted powder and of the final coffee brew.

Indeed, during post-harvesting and roasting processes, enzymatic modifications, fermentations, caramelisation, non-enzymatic browning, thermal degradations and pyrolysis, along with the Maillard reactions (Illy & Viani, 2005), are all responsible for the final cup profile (Farah *et al.*, 2006; Barbosa *et al.*, 2019). Some of these reactions are directly involved in beneficial compounds' metabolic pathways like polyphenols (Frei & Higdon, 2003), antioxidant compound attributable to melanoidins group (Moreira *et al.*, 2012) and caffeine, of which daily intake coffee is one of the main sources. On the other hand, also hazardous low molecular weight compounds deriving from specific pathways of Maillard reactions and thermal degradation are produced during roasting, namely acrylamide (Benford *et al.*, 2015; Schouten *et al.*, 2020). In this respect, the analysis of acrylamide, caffeine, titratable acidity, melanoidins and polyphenols should be used as chemical quality control tool to support and complement sensory analysis of brewed coffee in the evaluation of perceived quality levels of beverage related to changes in the roasting profiles.

All that considered, this work deals with eight samples of Arabica SC that, after being roasted at three different levels, were assessed for the consistency between the experimental sensory profile obtained from sensory analysis of espresso extraction and the expected profile got from technical sheets of green coffee to evaluate which roasting level better allows the perception of the expected sensory attributes. Roasted beans are then physico-chemically analysed following methods feasible for small-medium roasting company to get measurable quality markers.

Materials and methods

Coffee samples

The analysis had been conducted on eight different micro lots of green Arabica SC from five different producing countries from 2018/2019 crop as detailed in Table 1. Four micro lots belonged to washed coffees, the other four were naturals including semi-washed/honey processes according to the CQI Protocol for cupping. These eight micro lots have been roasted as detailed below using a Giesen W6A drum roaster applying three roasting profiles (light-medium-dark) (Appendix S1), giving rise to twenty-four independent samples.

Producers' description of coffee samples' sensory profile

Overall scores and scores for each descriptor obtained from in-origin cupping (Specialty Coffee Association, 2018b) and reported in technical sheets of the SCs are listed in Table 2.

Herein, one by one, a brief qualitative description of every sample is given:

- *Brazil semi washed*: Light aroma with cherry, sugar cane, tangerine, black currant and vanilla notes; high sweetness. Cherry, sugar cane, tangerine, black currant, vanilla and dried fruit in aftertaste.
- *Brazil Full Bloom*: medium-to-high aroma with chocolate and roasted nuts notes, silky and syrupy body; milk chocolate in aftertaste.
- *Dominican Republic AA*: intense aroma with caramel, red and yellow fruits in aftertaste; sweet. Juicy and light body. Apricot, caramel and sugarcane in aftertaste.
- *El Salvador natural*: pineapple, lemon, apricot, cherry, red apple and dark chocolate in both aroma and aftertaste. Nuts in aftertaste.
- *El Salvador*: citrus, dried fruits, peach, sugar, apple and nuts in aroma. Citrus, grapefruit, peach, sugar, nuts and chocolate in aftertaste.
- *Kenia AB*: intense aroma with floral, peach, banana, orange, tea and chocolate notes; juicy body. Floral, sugar cane, banana and orange notes in aftertaste.
- *Guatemala*: orange, lemon, yellow fruit, cherry, caramel and milk chocolate notes in both aroma and aftertaste.
- *Guatemala Geisha*: jasmine, apricot, tangerine notes in both aroma and aftertaste.

Roasting process

Roasting process had been conducted on a 6-kg professional drum roasting machine (Giesen coffee roasters W6A), with traditional conductive/convective heat

Table 1 Characterisation of green coffee samples by origin, variety, altitude, post harvesting processes and physical parameters

Sample	Origin/name	Process	Region	Farm	Harvesting altitude (m)	Variety	Screen	Density (g L^{-1})	Moisture (%)
1	Kenia AB	Washed Sun-dried	Nyeri Country	Ibutiti	1700	N/A*	16/18	866	9.7
2	Brazil FB	Natural	Minas Gerais	Tabuoes Boa vista	1140–1150	Bourbon, Mundo Novo	16/18	834	8.7
3	Guatemala G	Washed	San Marcos	El Platillo	1260	Geisha	18/19	800	10.8
4	El Salvador N	Natural Honey	Cordillera Apaneca Ilamatepec	San Juan Bosco	1400–1600	Pacas Bourbon	16/18	846	10.7
5	Dom. Republic	Natural	Barahona	Toral	1000	Caturra, Typica	N/A	828	9.5
6	Brazil SW	Pulped natural	Chiapada Diamantina	Sitio Santana II	1380	Red & yellow Catuai	16/18	853	10.7
7	Guatemala B/C/C	Washed	Los Humitos Amatitlan	Los Humitos	1400–1600	Bourbon Caturra Catuai	16/18	834	10.4
8	El Salvador W	Washed	Cordillera Apaneca Ilamatepec	Santa Gregoria	1350–1500	Pacas 80% Catimor 20%	16/18	820	10.4

*N/A not available.

Table 2 Overall and scores by classes given during in-origin cupping and reported in technical sheets of each lot

	Guatemala Geisha	Guatemala	Kenia AB	El Salvador	El Salvador natural	Dominican Republic AA	Brazil full bloom	Brazil semi washed
Aroma	8.25	8	8	8	8.5	8	8.5	7.75
Taste	8.25	8	8	8.25	8.5	8	9	7.75
Acidity	8.25	8	8	8.25	8.25	8	8.5	7.5
Aftertaste	7.75	8	8	7.75	8.25	7.75	8.5	7.5
Body	8.25	8	8	7.75	8.25	7.75	8.5	7.75
Balance	8.25	8	8	8	8.25	7.75	9	7.5
Uniformity	10	10	10	10	10	10	10	10
Sweetness	10	10	10	10	10	10	10	10
Clean cup	10	10	10	10	10	10	10	10
Overall	8	8.25	8	8	8.25	7.75	8.5	7.5
TOT	87	86.25	86	86	88.25	85	90.5	83.25

exchange system led by a 0–100% modulable burner fed by LPG from domestic distribution. Roasting process parameters were in continuum recorded on Cropster Roasting Intelligence (Cropster GmbH, Innsbruc, Austria) software. The air flow during all roasts was stable adjusted (drum inner pressure at 103 Pa). Drum speed was set at 49 Hz. Setpoint of the exhausted air was at 235 °C. Coffee was dropped in the preheated drum at 180 °C ± 1 °C, with burner off before the charge of raw beans. At the turning point of temperature plot, the burner was turned on to manage a proper roasting profile.

The roasting process was performed to obtain three different roasting levels for each micro lot (Appendix S1), modulating the development time ratio on total roasting time. Samples were taken after 5 min of cooling from the mass of roasted coffee for the three roasting levels (Table 3). Moreover, 15 g of each coffee was taken from the drum of the roasting machine by sampler probe at minute 3:00 and at minute 5:00 during the light roast of every green coffee. Samples were immediately tested for weight, moisture and density with Sinar BeanPro 6070 (SINAR Technology, Camberley, UK) (Table 4), stored in triple-layer (PET+PETmet+PE) barrier bags with unidirectional valve, and then welded.

Italian espresso extraction

A traditional Italian espresso coffee was prepared with professional espresso machine (Sanremo Café Racer) using softened water from a Brita Purity C150 (30% bypass) to obtain acceptable total and carbonate hardness according to SCA water control chart.

Coffee was ground on Marlkonig E65s, set to obtain the proper percolation (30 mL in 25″). Extraction was made at 91 °C, with 6″ at one bar of prewetting, to get a final brew ratio of 1:2 (g g^{-1}). Coffee was professionally ground and extracted by the authorised SCA trainer (AST) (Specialty Coffee Association, 2018a) for barista and brewing module.

Table 3 Time/temperature parameters for the three roasting levels. Additional samples at 3′ and 5′ are obtained only from light roasting to check acrylamide behaviour. In brackets are reported the numerical code used to identify roasting levels

		Light roasted (0)				Medium roasted (1)				Dark roasted (2)				3′ roasted		5′ roasted	
Sample	Origin/name	Yellow (min)	First crack (min)	Time (min)	End t (°C)	Yellow (min)	First crack (min)	Time (min)	End t (°C)	Yellow (min)	First crack (min)	Time (min)	End t (°C)	Time (min)	T (°C)	Time (min)	T (°C)
1	Kenia AB	3:34	5:43	07:01	198.1	4:01	5:14	07:11	203.3	3:58	5:29	07:36	207.2	03:00	136.7	05:00	170.1
2	Brazil FB	3:35	4:52	07:08	196.9	3:45	5:41	07:07	197.3	3:20	5:15	07:32	207.1	03:00	137.3	05:00	172.3
3	Guatemala G	N/A*	5:45	06:49	195.7	N/A	6:02	07:14	201.2	N/A	6:08	07:50	206.9	03:00	140.4	05:00	173.5
4	El Salvador N	N/A	6:11	07:07	194.9	4:05	6:04	07:40	199	3:54	5:58	08:01	205.3	03:00	134.6	05:00	169.4
5	Dom. Republic	3:59	5:58	07:25	194.9	3:48	5:37	07:25	200	3:56	5:39	07:39	204.1	03:00	130.5	05:00	164.3
6	Brazil SW	4:13	6:27	05:54	191.3	N/A	6:05	06:59	196.3	4:23	5:59	07:00	203.7	03:00	139.7	05:00	179.7
7	Guatemala B/C/C	3:53	6:01	06:52	187.9	4:01	6:06	06:40	192.9	4:01	6:00	07:08	198.1	03:00	128.2	05:00	165.4
8	El Salvador W	3:55	5:51	06:44	194.7	3:44	6:02	07:17	200.3	3:56	5:59	07:39	204.3	03:00	137.9	05:00	170.9

*N/A not available.

Sensory analysis

Within 2 weeks from the roasting date, coffee samples were submitted for sensory analysis. The twenty-four samples were split into three groups of eight samples each, homogeneous for roasting level. Tasting was performed from lighter to darker roasted group to prevent draft effect given by bitter compounds.

A panel of six coffee tasters (three of them certified Q-Arabica Graders, two expert panellists from I.i.a.c. (Istituti Italiano Assaggiatori Caffè) and a food technologist with a second-level master in sensory analysis) was asked to fill in M34 Trialcard Plus form (Appendix S2) by ‘Centro Studi Assaggiatori – Italian tasters’. The validation and replicability power of the panel were evaluated via analytical replicate. Panel calibration was made by checking the results obtained from the evaluation of a reference 100% arabica coffee not included in samples list and considering the median as panel central value. Data were recorded with ADS System by Horizon Design and Centro Studi Assaggiatori Brescia.

Acrylamide and caffeine analysis

For caffeine determination, 2.25 g of coffee was extracted with 50 mL of distilled water for 30 min, in a thermostatic bath. The extract was cooled at room temperature, paper filtered and consequently micro-filtered using syringe filters (0.45 µm), diluted 100 times and transferred in vial for the chromatographic determination. Separation was performed using a reverse phase C-8 Select B column and isocratic elution with CH3CN: acidified water (2% acetic acid) = 10:90. UV detector was set at 275 nm (Fajara & Susanti, 2017). Quantification was made with external calibration.

Acrylamide was tested at 5 points of the roasting process. All the samples were ground and were extracted according to Bertuzzi *et al.*, 2017. A Quechers separation, clean-up of the extract on Al_2O_3 and HLB 60 cc (60 mg) column (Oasis Waters, Milan, IT), was performed. Separation and quantification by LC-MS/MS were performed using an X-Select HSS T3 2.5 µm column, gradient elution with acidified water and acetonitrile. Ionisation was performed by ESI and the cation (72 *m*/*z*) was fragmented by argon collision, and then detected and quantified as ion fragments (55 and 44 *m*/*z*). Quantification was made with internal standard d3-acrylamide from Sigma-Aldrich (St. Louis, MO, USA).

pH, acidity, total phenolics and melanoidin analysis of roasted SCs

For pH and acidity analysis, the extract described for caffeine, after filtration, was split into two aliquots of 15 mL

Table 4 Physical characterisation of samples after roasting. Roasting was performed on a 2.5-kg batch of green coffee. Inlet temperature was constant between 180 and 181 °C

Sample	Process	Roasting level	Final density (g L^{-1})	Moisture (%)	Final weight (g)	Roasting time (min)	Final T (°C)	Weight loss (%)
Kenia AB	Washed	Light	502	1.7	2200	06:52	187.9	12.0
Kenia AB	Washed	Medium	483	1.5	2167	06:40	192.9	13.3
Kenia AB	Washed	Dark	436	1.5	2142	07:08	198.1	14.3
Brazil FB	Natural	Light	434	1.6	2191	05:54	191.3	12.4
Brazil FB	Natural	Medium	476	1.5	2170	06:59	196.3	13.2
Brazil FB	Natural	Dark	410	1.4	2143	07:00	203.7	14.3
Guatemala G	Washed	Light	385	1.7	2168	06:49	195.7	13.3
Guatemala G	Washed	Medium	397	1.5	2118	07:14	201.2	15.3
Guatemala G	Washed	Dark	416	1.4	2090	07:50	206.9	16.4
El Salvador N	Natural	Light	408	1.6	2153	07:01	198.1	13.9
El Salvador N	Natural	Medium	416	1.5	2116	07:11	203.3	15.4
El Salvador N	Natural	Dark	439	1.5	2093	07:36	207.2	16.3
Dominican Republic	Natural	Light	429	1.6	2177	07:08	196.9	12.9
Dominican Republic	Natural	Medium	423	1.6	2150	07:07	197.3	14.0
Dominican Republic	Natural	Dark	380	1.4	2115	07:32	207.1	15.4
Brazil SW	Pulped natural	Light	442	1.5	2156	07:25	194.9	13.8
Brazil SW	Pulped natural	Medium	442	1.5	2125	07:25	200.0	15.0
Brazil SW	Pulped natural	Dark	416	1.5	2112	07:39	204.1	15.5
Guatemala B/C/C	Washed	Light	469	1.7	2171	07:07	194.9	13.2
Guatemala B/C/C	Washed	Medium	457	1.6	2136	07:40	199.0	14.6
Guatemala B/C/C	Washed	Dark	429	1.4	2102	08:01	205.3	15.9
El Salvador W	Washed	Light	436	1.7	2168	06:44	194.7	13.3
El Salvador W	Washed	Medium	442	1.5	2127	07:17	200.3	14.9
El Salvador W	Washed	Dark	403	1.5	2105	07:39	204.3	15.8

each and then directly tested. Automatic combined system formed by a pH-meter and an automatic titrator (CRISON MICRO TT 2050, Carpi, Modena, Italy) was calibrated with standard solutions, and then used for samples analysis. Potentiometric titration was performed with NaOH 0.1 N. Samples were analysed in duplicate and results were expressed as percentage of equivalent chlorogenic acid on roasted ground coffee mass.

For melanoidins quantification, 10 g of ground coffee was suspended with 100 mL of distilled water, covered with a watch glass to prevent solvent loss during extraction (30 min, in a thermostatic bath at 100 °C). Samples were cooled at room temperature, then vacuum microfiltered using 1.2 µm paper membrane filters on a glass filter. 0.5 mL of the extract was diluted in 10 mL of distilled water and put into poly-carbonate cuvette for UV-Visible spectrometry (1-cm optical path). Absorbance at λ = 420 nm was read in duplicate on a Shimadzu UV-1601 spectrophotometer (Shimadzu Europe, Duisburg, Germany) (Bravo *et al*., 2013). Before tests, the instrument was double zeroed using distilled water as blank. Melanoidins were expressed as mmol g^{-1} coffee dry base (d.b.) using molar extinction coefficient of 0.97 ± 0.07 L $mmol^{-1}$ cm^{-1} at 420 nm as reported by Martins and van Boekel (2003).

Total phenolics were analysed according to Singleton and Rossi (1965). A volume of 100 µL of the same filtrate used for melanoidin was added of 0.5 mL of Folin-Ciocalteau reactive, 5 mL of a water solution at 20% of Na_2CO_3, and then made up to volume in a 50-mL graduated flask, mixed and stored in a dark place at room temperature for 30 min. Blank was prepared in the same way. After storing, samples were put into polycarbonate cuvette for UV-Visible spectrometry (1-cm optical path). Absorbance at λ = 700 nm was read in duplicate on a Shimadzu UV-1601 spectrophotometer (Shimadzu Europe). Before tests, the instrument was double zeroed using the blank. The concentration of total phenolics was calculated with external calibration and reported as percentage of grams of chlorogenic acid equivalents on roasted coffee (w/w).

Statistical analysis

All the data were subjected to Microsoft Excel 2003 and multivariate analysis of variance (ANOVA). Correlations between process, chemical and sensory parameters were performed by Pearson's test. Factorial analysis with PCA elaboration was applied to highlight relationships within variables and between variables and samples, which were clustered as for origin, process and roasting level. Statistical elaboration was carried out by IBM SPSS Statistics 27 (IBM Corporation, New York, NY, USA).

Results and discussion

Regarding the roasting process, all the eight samples followed the expected trends in terms of decrease of density, moisture and weight when passing from a light, to a medium, to a dark roasting and compared with green beans. This confirms the loss of water and organic matter together with the increase in volume.

Sensory profile of SC espresso and its correlations with parameters from roasted SC

Spider-graphs reported in Fig. 1 outlines the overall vision on how SC is perceived by consumers in the south European countries (Sepúlveda *et al.*, 2016) where there is rooted belief about coffee consumption and on the descriptors that must be founded in espresso coffee (Ferini *et al.*, 2020). Going through different origins, samples of SCs here studied were really appreciated for the presence of remarkable aromas and the extremely low level of the defective ones (Specialty Coffee Association, 2016). This confirmed both the overall high quality of the raw beans and the suitable roasting applied. The sensory profile provided a comparison among the perceptions scored for the three roasting modalities which matched with data from technical sheets and literature (Hoffmann, 2018).

The Kenyan coffee was the only one representing washed coffee from Africa in the set; it was expected to be differently characterised from other samples. Roasting modulation enhanced the peculiar characteristics of that coffee, scored 86 by the producer (Table 2). The region is well known for the high quality of its coffees, finesse of their cup and the impressive acidity, complexity and brightness, fruity and berry notes, all harmonised by good sweetness. Aftertaste and aroma were characterised by orange, peach, banana and floral notes, juicy body, tea and cocoa fragrance and can sugar-like sweetness. As well shown by the spider graph (Fig. 1), acidity was better perceived in medium roasted cup because in the lighter, it was a little masked by an astringent mouthfeel given by chlorogenic acids. The intense floral and fruity notes have always been recognised as well as the strong and pleasant olfactive and retro-olfactive components.

The two Brazilian samples were from different producing regions with altitude and climate (Table 1) providing the best condition for harvesting of different varieties. The beans' peculiar characteristics properly exalted the low and elegant acidity, heavy round body, chocolaty sweetness and nutty flavours as outlined from spider graph in Fig. 1. Natural coffees from Minas Gerais, scored 86 points at Q-Grading (Table 2), were characterised by high and balanced intensity of all the descriptors, with a stress on the excellent velvety body; aroma was described as

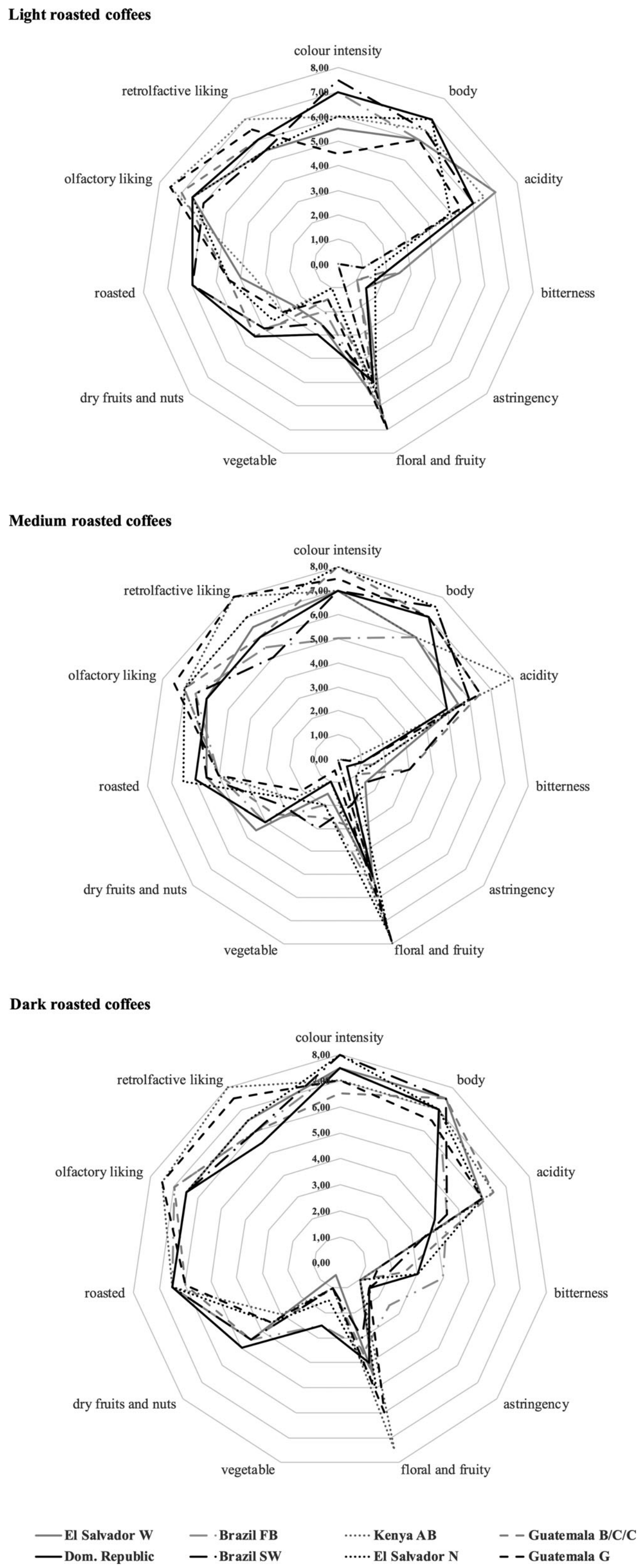

Figure 1 Spider graphs from sensory analysis of espresso brewed SCs clustered by roasting level.

medium to intense with remarkable chocolate and roasted nuts notes, and aftertaste and flavours were that of milk chocolate. Panellists were more aligned with these traits for the medium and dark roasted coffees than for light roasted sample, which was also discriminated for the pleasant and intense acidity and lower body than the other two (Fig. 1). The second Brazilian sample, from one of the Nordic producing region called Chiapada Diamantina, was described as well balanced, but with weaker intensity and complexity if compared with the previous one (Table 2). Panellists properly discriminated the differences in quality and intensity between the two coffees, showing a decrease in floral and fruity notes as the roasting degree increased, and even the second sample was more attractive in all the roasting versions. This last point was powerful to demonstrate how the traditional consumption of less complex coffees, usually blended with different Robusta percentages, remarkably influences the acceptance of espressos characterised by unusual tastes and aromas (Sepúlveda *et al.*, 2016).

Guatemala is known to produce a wide assortment of different coffees, from light, sweet and floral, to heavy, fruity chocolatey full cups (Hoffmann, 2018). The two samples of Guatemala green coffee were both wet processed but from different harvesting regions (Table 1) far one to the other and used to cultivate differnet varieties of Arabica coffee. Guatemala coffee from San Marcos is a Geisha variety, washed processed, scored 87 (Table 2) at Q-Grading, has been reported as excellent for body, balance, taste and aroma, and a little less impressive for aftertaste lasting and complexity. The main descriptors for these characteristics are jasmine, apricot, tangerine and aromatic herbs. Panellists evaluated this coffee as described by the producer, but the different roasts discriminated cups for the intensity of roast taste, intensity of floral and fruity notes, body and acidity (Fig. 1). Medium roasted coffee gave a more complex cup, thanks to a proper development of all the aromatic and volatile compounds in the beans that, conversely, in lighter roasting level were present as aromatic precursors and in darker were already degraded by the thermal treatment. Opposite to what provided by the producer, the intensity for the retro-olfactive perception ranged from medium to high through the roasting levels, with a maximum for the medium roasted. The second sample was from volcano Amatitlan area. This washed micro lot was different, thanks to the special mix of three varieties harvested, cropped and processed all together from the origin. At Q-Grading, this coffee has been scored 86.25 (Table 2), characterised by notes, both for aroma and taste, of citrus, yellow fruits, cherry, caramel, and milk chocolate. From our results (Fig. 1), this sample seemed not to meet the expectation: the panel found low intense notes of the descriptors mentioned and did not score as high as supposed also for the balance. As already said for the Brazil semi-washed sample, the less complexity was considered more attractive in all the roasting versions if compared with the Geisha variety.

The peculiarity of the two samples from El Salvador is that they came from the same region and were harvested and processed by the same producer in two different farms following once washed and once natural process (Table 1). These two micro lots were composed respectively of two varieties, but the most abundant is Pacas. Those were some of the best examples of what Central American coffee is (Hoffmann, 2018): as ‘milds’, the generic name for these coffees says, they are elegant, sweet, clean and balanced with complex malic, lactic and citric acidity that also impacts on body and tactile sensation. The first sample considered is the natural one; it was scored 88.25 by the Q-graders (Table 2) and the cup should be characterised by aromas of pineapple, apricot, cherry, lemon, and dark chocolate, all found also in taste and aftertaste accompanied by nut notes. As provided by panel (Fig. 1), the roasting level that, in quantity and quality, matched better than the expected profile of coffees was the medium one. In this case, light roasted coffee seemed to be considered as a little underdeveloped or backed due to lack of good acidity, balance and retro olfactive good notes. The discrimination between roasting levels has been properly done by the intensity of roasted notes. The second sample, that is, the washed one, was characterised by more citrus and light fruits notes, sugary sweetness, and some nutty and dry fruit hint. This lot scored 86 points (Table 2) at cupping, and the higher marks were given to taste and acidity as expected for washed coffee yet. Body and aftertaste was not outstanding but however good and pleasant. As the radar graph shows (Fig. 1), panellists agreed with all the notes provided for this coffee when light and medium roasts were analysed. Body increased its intensity only in the dark roasted cup when also all the other descriptors connected to darker coffees appear; on behalf all, the positive floral, fruity, and nutty notes were masked by the roasted taste and aroma. As provided for Brazilian and Guatemalan coffee, this loss of complexity exalted the average appreciation of the sample.

Lastly, considering the Dominican sample, from many descriptions available about coffees from this origin and especially from Barahona island, this micro lot was expected to have typical attributes characterising coffee from islands (Hoffmann, 2018). The lot was scored 85 points at Q-Grading (Table 2), mild and clean cup, full of different aromas, with good balanced acidity. From the producer, it was described as intense in positive odours of yellow and red fruits, caramel, juicy, clean and delicate at taste with apricots, caramel, and cane sugar aftertaste. By the panellists (Fig. 1), there was generally a good discrimination of the three roasting levels by increased perception of roasted taste, bitterness, spicy notes, body, odour intensity and darkness of 'crema' colour from light to dark roast; at the counter part, a decrease in astringency, acidity and vegetable notes was observed. Light and medium roasted references exalted the most expected characteristics provided for this micro lot.

Acrylamide and caffeine behaviour during and after roasting of SCs

The bell pattern of acrylamide concentration during roasting (Fig. 2) was obtained by data from quantitative analysis on samples of the eight coffee lots taken from roaster at five different moments of the process (Table 3). After 5-min of roasting in a range of temperatures between 164.3 and 173.5 °C, six out of the eight coffees showed acrylamide concentration above 400 ppb (i.e. the limit stated by EU (2017)). Then, acrylamide rapidly decreased due to the prevalence of breakdown pathways, as already evidenced by different authors (Bertuzzi *et al.*, 2020; Schöneich *et al.*, 2020). Although SC is usually light roasted, such a behaviour did not throw safety issues for the final consumers; in fact, by data (Table 5) relative to acrylamide concentration for the three roasting levels, it is higher in the light, lower in medium and dark one, but always under 400 ppb. Additionally, a reduction in the human intake at the consumption stage is guaranteed from every extraction method (Alves *et al.*, 2010).

As expected, no significant changes in the concentration of caffeine were recorded (Table 5). This might be justified by the loss of water and organic matter and the sublimation of a fraction of caffeine during roasting (Illy & Viani, 2005); reversely, concentration defers among different coffee lots due to variety and origin variability (Hečimović *et al.*, 2011).

pH, acidity, total phenolics and melanoidins of roasted SCs

Regarding pH, all the values were around 5.58 ± 0.22 (Table 5) aligned with the expected average pH value for brewed coffee that ranges from 5.2 to 5.8 (Massimi *et al.*, 2005). Results from different roasting levels (Table 5) demonstrated how the pH followed the same trend: lower in light and medium roasted than in dark coffees with no significant differences between washed and natural coffees. In the subset of natural coffees, the weaker difference in pH between the two milder roasting processes may reflect acidic fraction modification of these samples due to their distinctive fermentation pathway and possible occurrence of off-fermentations (Lima Filho *et al.*, 2013).

Furthermore, titratable acidity could properly discriminate light roasted from dark. As already been provided by Ginz *et al.* (2000), this could be due to the progressive rising in the degradation rate of the organic acids during the early stage of roasting. Thanks to different thermolability values of these acids, pH could gradually increase from light to dark roasts (Table 5), when roasting is performed by applying the same profile. As a consequence, titratable acidity showed to be inversely related to pH (Table 5), confirming the progressive breakdown and evaporation of organic acids when the amount of thermal energy increased, moving from light to dark roast.

The concentration in phenolic compounds of roasted coffees has been expressed (Table 5) as a percentage weight by weight of equivalent chlorogenic acid,

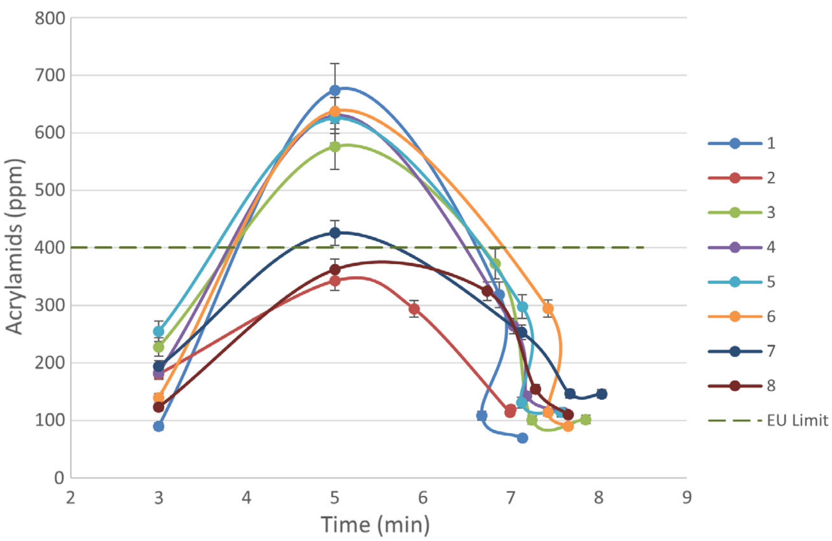

Figure 2 Acrylamide trend during roasting.

Table 5 Chemical characterisation of roasted beans. Roasting was performed on a 2.5-kg batch of green coffee. Inlet temperature was constant between 180 and 181 °C. Waller-Duncan test (α = 0.05) was conducted within roasting level to discriminate samples (lower case) and among averages to discriminate roasting levels (upper case)

		Roasting		
Analysis	**Sample**	**Light**	**Medium**	**Dark**
Caffeine (% w/w d.b.)	Kenia AB	1.14 ± 0.02 bc	1.02 ± 0.02 c	1.25 ± 0.03 e
	Brazil FB	1.12 ± 0.02 b	1.21 ± 0.02 e	1.12 ± 0.02 c
	Guatemala G	1.00 ± 0.02 a	0.92 ± 0.02 a	0.81 ± 0.02 a
	El Salvador N	1.49 ± 0.03 f	1.10 ± 0.02 d	1.22 ± 0.02 de
	Dom. Republic	1.39 ± 0.03 e	1.26 ± 0.03 e	1.16 ± 0.02 cd
	Brazil SW	1.16 ± 0.02 bc	1.00 ± 0.02 bc	1.26 ± 0.03 e
	Guatemala B/C/C	1.22 ± 0.02 cd	0.94 ± 0.02 ab	1.59 ± 0.03 f
	El Salvador W	1.25 ± 0.02 d	1.13 ± 0.02 d	1.03 ± 0.02 b
	Average	1.22 ± 0.16 A	1.20 ± 0.32 A	1.18 ± 0.21 A
pH	Kenia AB	5.14 ± 0.05 a	5.28 ± 0.26 a	5.30 ± 0.24 a
	Brazil FB	5.36 ± 0.05 ab	5.57 ± 0.28 a	5.90 ± 0.11 b
	Guatemala G	5.52 ± 0.22 bc	5.65 ± 0.04 a	5.75 ± 0.04 b
	El Salvador N	5.71 ± 0.09 c	5.70 ± 0.03 a	5.84 ± 0.11 b
	Dom. Republic	5.51 ± 0.01bc	5.51 ± 0.01 a	5.76 ± 0.06 b
	Brazil SW	5.54 ± 0.08 bc	5.48 ± 0.23 a	5.88 ± 0.07 b
	Guatemala B/C/C	5.44 ± 0.06 abc	5.69 ± 0.21 a	5.66 ± 0.07 b
	El Salvador W	5.52 ± 0.24 bc	5.65 ± 0.16 a	5.82 ± 0.08 b
	Average	5.47 ± 0.18 A	5.57 ± 0.19 A	5.76 ± 0.21 B
Acidity (g chlorogenic eq per kg coffee d.b.)	Kenia AB	53.9 ± 0.7 d	47.2 ± 3.5 b	46.9 ± 3.4 c
	Brazil FB	40.9 ± 0.4 bc	34.6 ± 3.4 a	28.7 ± 0.5 a
	Guatemala G	42.6 ± 0.9 bc	36.7 ± 0.5 a	33.2 ± 0.6 ab
	El Salvador N	39.6 ± 0.7 b	37.1 ± 0.8 a	32.8 ± 2.5 ab
	Dom. Republic	31.1 ± 1.9 a	39.5 ± 0.9 ab	38.3 ± 0.4 b
	Brazil SW	40.6 ± 1.0 bc	36.4 ± 4.2 a	30.5 ± 0.6 a
	Guatemala B/C/C	42.8 ± 0.5 bc	35.7 ± 1.9 a	37.3 ± 1.0 b
	El Salvador W	44.4 ± 1.7 c	42.2 ± 1.3 ab	36.5 ± 0.7 b
	Average	42.0 ± 6.17 B	38.7 ± 4.8 AB	33.6 ± 10.5 A
Acrylamide (ppb)	Kenia AB	318.4 ± 22.3 ab	108.3 ± 7.6 a	69.2 ± 4.8 a
	Brazil FB	294.0 ± 20.6 ab	113.4 ± 7.9 ab	119.5 ± 8.4 cd
	Guatemala G	372.1 ± 26.1 b	100.3 ± 7.0 a	101.6 ± 7.1 bc
	El Salvador N	263.9 ± 18.5 a	142.8 ± 10.0 bc	113.5 ± 7.9 bc
	Dom. Republic	297.8 ± 20.8 ab	130.7 ± 9.2 abc	113.8 ± 7.9 bc
	Brazil SW	294.5 ± 20.6 ab	113.4 ± 7.9 ab	89.3 ± 6.3 ab
	Guatemala B/C/C	253.1 ± 17.7 a	146.2 ± 10.2 c	146.0 ± 10.2 d
	El Salvador W	324.5 ± 22.7 ab	154.0 ± 10.8 c	110.2 ± 7.7 bc
	Average	301.9 ± 37.2 B	126.1 ± 19.9 A	107.9 ± 22.5 A
Melanoidins (mmol g^{-1} coffee d.b.)	Kenia AB	0.12 ± 0.01 e	0.13 ± 0.01 d	0.14 ± 0.01 d
	Brazil FB	0.13 ± 0.01 c	0.12 ± 0.01 bc	0.14 ± 0.01 c
	Guatemala G	0.11 ± 0.01 b	0.13 ± 0.01 c	0.13 ± 0.01 a
	El Salvador N	0.12 ± 0.01 d	0.13 ± 0.01 e	0.14 ± 0.01 b
	Dom. Republic	0.11 ± 0.01 a	0.11 ± 0.01 a	0.13 ± 0.01 a
	Brazil SW	0.12 ± 0.01 d	0.13 ± 0.01 e	0.14 ± 0.01 c
	Guatemala B/C/C	0.11 ± 0.01 a	0.12 ± 0.01 b	0.14 ± 0.01 e
	El Salvador W	0.12 ± 0.01 c	0.14 ± 0.01 f	0.14 ± 0.01 c
	Average	0.12 ± 0.01 A	0.13 ± 0.003 B	0.14 ± 0.01 C
Polyphenols (% w/w d.b.)	Kenia AB	4.99 ± 0.01 c	5.55 ± 0.04 f	1.54 ± 0.03 a
	Brazil FB	5.17 ± 0.03 d	5.41 ± 0.02 e	4.63 ± 0.01 e
	Guatemala G	6.22 ± 0.04 e	4.95 ± 0.01 d	5.40 ± 0.01 g
	El Salvador N	6.21 ± 0.01 e	2.55 ± 0.01 a	2.48 ± 0.01 b
	Dom. Republic	4.40 ± 0.16 b	4.18 ± 0.01 b	4.67 ± 0.02 f
	Brazil SW	5.05 ± 0.01 cd	5.59 ± 0.01 f	5.49 ± 0.01 h
	Guatemala B/C/C	3.16 ± 0.01 a	4.86 ± 0.01 c	4.53 ± 0.01 d
	El Salvador W	5.02 ± 0.01 c	5.79 ± 0.01 g	4.41 ± 0.01 c
	Average	5.03 ± 0.95 B	4.86 ± 1.03 AB	4.15 ± 1.35 A

responsible for the majority of the antioxidant power of a coffee extract (Bekedam *et al.*, 2008). In this respect, samples followed the trend suggested by Schouten *et al.* (2020), that is, coffees got the highest antioxidant power which is likely given by both the ratio between high and low molecular weight phenolics and the relative extent of degraded or new-formed antioxidant molecules. Actually, data from these authors and results from this work (Table 5) confirm the average decrease in phenolic concentration going from light to darker roasting level.

As reported by Martins and van Boekel (2003), melanoidins gradually increased in each sample when roasting led to a darker colour (Table 5), as higher temperatures and longer times promote final stages of Maillard and caramelisation reactions (Moreira *et al.*, 2012). Melanoidin concentration was capable of discriminating among the roasting levels with the same trend for washed and natural samples. In particular, a proportional increase in concentration was shown when darker roasts were achieved (Table 5).

Correlations between sensory profile of espresso SC and chemical data of roasted beans

From data obtained with Pearson test (Appendix S3), some noticeable interdependences were available between chemical and sensory perceptions. Acrylamide, that was more abundant in light roasted coffees (Fig. 1 and Table 5), showed a positive correlation ($P < 0.05$) with the perception of astringency which characterises the light roasted SCs for the larger preservation of chlorogenic compounds, and with floral/fruity notes also widely reported in milder thermal treatments (Perrone *et al.*, 2010). Caffeine, as described by Poole and Tordoff (2017), can serve as a bitter compound, and also gives tactile perceptions: this was true for samples where a superior caffeine content (Appendix S3) occurred along with bigger body, higher bitterness and astringency perceptions ($P < 0.05$). The low pH, as an estimator for the acidity of the brewed coffee (Cangussu *et al.*, 2020), was correlated ($P < 0.05$) with the perceivable acidity, the floral/fruity notes, the hedonic level, the vegetable notes and with the lack of balance and palatability. This last consideration led to confirm the well-known lower acceptability of light roasted single origin coffees by espresso coffee consumers due to the low pH (Cangussu *et al.*, 2020). Additionally, the perceived acidity, that is generally higher where astringency and roasted notes of dried fruits and nuts are low (Farah *et al.*, 2006), shows an inverse correlation ($P < 0.05$) with the olfactory acceptability of the samples.

Finally, also physical parameters (Table 1 and 3) were correlated with some sensory perceptions: in particular, the green moisture and the green density impacted the cup profile, modulating the visual, the olfactory and the tactile properties of the coffee brew. In detail, the green density was positively correlated ($P < 0.05$) with the vegetable and bitter notes and negatively ($P < 0.05$) with positive retro-olfactory perceptions. In high-density green coffee lots, thanks to the higher mass per unit of volume leading to a lower heat transfer rate, the bean development during roasting is limited, especially when the roasting degree is light, leading to vegetable notes in cup; conversely, if dark roasts are performed, more bitter compounds are produced as a result of the abundance of vegetal structures undergoing pyrolytic reactions (Balzer, 2008).

Conclusion

In conclusion, the eight lots of Arabica SC proved to be comparable in sensory attributes, both quantitative and qualitative, with the cup profile given after official in-origin cupping session when prepared via Italian espresso extraction and tasted by a trained panel. Medium roasting level appeared to be the most suitable to exalt coffee sensory attributes under espresso preparation. Physico-chemical analyses were capable of outlining similarities and dissimilarities in the final products obtained from the three different roasting processes and, potentially, to obtain reliable parameters to assess the conformity of roasting final products with a given quality standard. Further studies may be carried out to identify possible correlations between physico-chemical traits of green and roasted beans, and cup profile.

Conflict of interest

All authors declare no conflict of interest.

Author contribution

Fosca Vezzulli: Conceptualization (lead); Data curation (lead); Methodology (equal); Writing-original draft (lead). **Terenzio Bertuzzi:** Methodology (equal); Writing-review & editing (equal). **Silvia Rastelli:** Data curation (equal). **Annalisa Mulazzi:** Data curation (equal). **Milena Lambri:** Supervision (lead); Writing-review & editing (equal).

Ethical statement

Ethics approval was not required for this research.

Peer review

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Data availability statement

Research data are available in article supplementary materials and from the authors on request.

References

NOTE: this paper reports the method used and validated for the acrylamide extraction.
NOTE: this document reports the limits and the risk assessment on acrylamide in food.
NOTE: this book reports the state of art on several aspect of coffee harvesting, post harvesting, roasting and serving processes, acting as a baseline for further studies.
NOTE: this paper reports the trend followed by acids present in green coffee during roasting, useful to sustain the sensory profile modification under different roasting processes.

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Supporting Information

Additional Supporting Information may be found in the online version of this article:

Appendix S1. Roasting profiles.

Appendix S2. TrialCard Plus Form.

Appendix S3. Pearson's correlation tables.