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Prediction of specialty coffee cup quality based on near infrared spectra of green coffee beans

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ABSTRACT

The growing global demand for specialty coffee increases the need for improved coffee quality assessment methods. Green bean coffee quality analysis is usually carried out by physical (e.g. black beans, immature beans) and cup quality (e.g. acidity, flavour) evaluation. However, these evaluation methods are subjective, costly, time consuming, require sample preparation and may end up in poor grading systems. This calls for the development of a rapid, low-cost, reliable and reproducible analytical method to evaluate coffee quality attributes and eventually chemical compounds of interest (e.g. chlorogenic acid) in coffee beans. The aim of this study was to develop a model able to predict coffee cup quality based on NIR spectra of green coffee beans. NIR spectra of 86 samples of green *Arabica* beans of varying quality were analysed. Partial least squares (PLS) regression method was used to develop a model correlating spectral data to cupping score data (cup quality).

The selected PLS model had a good predictive power for total specialty cup quality and its individual quality attributes (overall cup preference, acidity, body and aftertaste) showing a high correlation coefficient with *r*-values of 90, 90,78, 72 and 72, respectively, between measured and predicted cupping scores for 20 out of 86 samples. The corresponding root mean square error of prediction (RMSEP) was 1.04, 0.22, 0.27, 0.24 and 0.27 for total specialty cup quality, overall cup preference, acidity, body and aftertaste, respectively. The results obtained suggest that NIR spectra of green coffee beans are a promising tool for fast and accurate prediction of coffee quality and for classifying green coffee beans into different specialty grades. However, the model should be further tested for coffee samples from different regions in Ethiopia and test if one generic or region-specific model should be developed.
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1. Introduction

The specialty coffee market is constantly growing, which is driven by changing consumers preferences [1]. Specialty coffee refers to the highest quality of green coffee beans, has a known geographical origin, and mostly includes coffee beans certified as e.g. organic coffee (coffee grown without chemical fertilizer and pesticides), fair trade (promotes greater economic incentives via fair price and direct trade) and rainforest alliance (integrates biodiversity conservations, community development and suitable agricultural practices to ensure sustainable farm management) [2]. High quality green coffee beans show little or no physical defects (e.g. black beans, immature beans, floaters, broken beans, insect damage and other foreign materials such as seeds of shade trees) and, when roasted, have a distinctive character in the cup and high cup tasting scores [3,4]. As such, the success of specialty coffee brings along a need for more reliable and objective quality assessment methods.

The increasing consumption of specialty coffee [1] creates a strong potential and opportunity for coffee-producing countries. An increasing demand for such coffees on the world market resulted in a segmentation of the coffee market and higher prices are paid for specialty coffees [5]. For instance, specialty coffee beans receive a premium price of ca. 20–50% compared to regular coffee beans. Certification also raises coffee prices (e.g. organic and fair trade generate premium of about ca. 9%) [6]. Ethiopia is one of the top ten coffee-producing countries in the world and the largest exporter in Africa [6]. The country produces specialty coffees with a wide range of flavours [7]. Currently, specialty coffee accounts for ca. 20% of Ethiopia's coffee export and there is potential to boost its share in the world market even further [8].

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Table 1
Overview of 86 coffee samples used for model development and validation with measured values of quality attributes.

No.	Sample identifier	District	Altitude[a]	Processing method	Preliminary total quality	Preliminary cup quality	Total specialty cup quality	Overall cup preference[b]	Acidity	Body	Aroma	Flavour	Aftertaste
1	741DP	Limu Kosa	Mid	Dry	79.00	45.00	81.50	7.25	7.50	7.25	7.50	7.50	7.25
2	7440SW	Limu Kosa	Mid	Semi-washed	73.00	48.00	81.75	7.25	7.75	7.50	7.25	7.25	7.50
3	74110DP	Limu Kosa	Mid	Dry	79.00	45.00	81.50	7.25	7.50	7.25	7.25	7.50	7.25
4	74148SW	Limu Kosa	Mid	Semi-washed	85.00	48.00	82.00	7.50	7.75	7.50	7.25	7.50	7.00
5	74148WP	Limu Kosa	Mid	Washed	74.00	45.00	80.25	7.00	7.25	7.25	7.50	7.25	7.00
6	74165DP	Limu Kosa	Mid	Dry	76.00	42.00	80.25	7.00	7.25	7.25	7.25	7.50	7.00
7	74165SW	Limu Kosa	Mid	Semi-washed	79.00	45.00	81.00	7.25	7.50	7.25	7.25	7.25	7.25
8	74165WP	Limu Kosa	Mid	Washed	74.00	45.00	82.25	7.25	7.75	7.50	7.25	7.50	7.50
9	75227DP	Limu Kosa	Mid	Dry	76.00	42.00	79.50	7.00	7.75	7.25	7.00	7.25	7.00
10	AFATAF1WP	Mana	Mid	Washed	77.00	45.00	80.75	7.25	7.50	7.50	7.25	7.25	7.00
11	CHOCE-C-WP	Goma	Mid	Washed	71.00	45.00	81.75	7.25	7.75	7.50	7.50	7.50	7.25
12	CHOCE-F1WP	Goma	Mid	Washed	82.00	45.00	82.75	7.50	6.75	7.50	7.50	7.50	7.50
13	COMB DP1	Limu Kosa	Mid	Dry	82.00	45.00	83.50	7.75	8.00	7.75	7.50	7.50	7.50
14	COMB DP2	Limu Kosa	Mid	Dry	82.00	45.00	81.50	7.25	8.00	7.50	7.25	7.25	7.25
15	COMB DP3	Limu Kosa	Mid	Dry	79.00	45.00	83.00	7.50	8.00	7.75	7.50	7.50	7.50
16	COMB WP	Limu Kosa	Mid	Washed	73.00	48.00	76.75	6.50	8.00	6.50	6.50	6.50	6.50
17	DAWA-NC	Goma	High	Washed	71.00	45.00	80.25	7.00	8.00	7.00	7.50	7.25	7.00
18	DEBF1WP	Limu Kosa	Mid	Washed	83.00	51.00	85.25	8.00	7.75	7.75	7.50	8.25	8.00
19	DOYO-NC	Goma	High	Washed	75.00	51.00	86.00	8.50	7.75	8.00	7.50	8.00	7.50
20	HAROF2DP	Mana	High	Dry	88.00	48.00	84.25	7.75	7.75	7.75	7.50	7.75	7.75
21	HF2DP	Mana	High	Dry	88.00	51.00	86.75	8.50	7.75	8.00	8.00	8.25	8.00
22	HF2SW	Mana	High	Semi-washed	82.00	48.00	85.75	8.00	7.75	7.75	7.75	8.25	8.00
23	HF2WP	Mana	High	Washed	83.00	51.00	85.75	8.00	7.75	8.00	7.75	8.25	7.75
24	HF4DP	Mana	High	Dry	91.00	51.00	86.50	8.50	7.50	8.00	8.00	8.25	7.75
25	HF4SW	Mana	High	Semi-washed	81.00	45.00	85.00	8.00	7.75	7.75	7.75	8.00	7.75
26	HF4WP	Mana	High	Washed	81.00	48.00	84.25	7.75	7.75	7.75	7.75	8.00	7.50
27	HUDAF1WP	Goma	High	Washed	86.00	51.00	85.00	8.25	7.75	7.75	7.50	8.00	7.75
28	ILBUF1DP	Goma	Mid	Dry	85.00	48.00	84.00	7.75	9.00	8.00	7.50	7.50	7.50
29	KENTERF1WP	Mana	High	Washed	81.00	48.00	80.50	7.25	9.00	7.25	7.25	7.25	7.00
30	LF1DP	Mana	Low	Dry	82.00	45.00	83.50	7.75	9.00	7.50	7.50	7.75	7.75
31	LF1SW	Mana	Low	Semi-washed	79.00	48.00	83.50	7.50	8.75	7.75	7.50	7.50	7.75
32	LF1WP	Mana	Low	Washed	81.00	48.00	83.25	7.50	8.25	7.75	7.50	7.75	7.50
33	LF3DP	Mana	Low	Dry	82.00	45.00	82.25	7.50	9.00	7.50	7.50	7.50	7.50
34	LF3SW	Mana	Low	Semi-washed	78.00	48.00	83.25	7.50	8.50	7.75	7.50	7.50	7.50
35	LF3WP	Mana	Low	Washed	75.00	45.00	82.00	7.50	8.00	7.50	7.50	7.50	7.50
36	LF5SW	Mana	Low	Semi-washed	85.00	48.00	83.75	7.75	9.00	7.75	7.50	7.75	7.50
37	LF5DP	Mana	Low	Dry	79.00	45.00	83.25	7.75	8.25	7.50	7.50	7.50	7.50
38	LF5WP	Mana	Low	Washed	81.00	48.00	83.50	7.50	8.50	7.75	7.50	7.75	7.50
39	LPS1WP	Limu Kosa	Mid	Washed	80.00	48.00	84.00	7.75	8.25	7.50	8.00	7.50	7.75
40	LPS3WP	Limu Kosa	Mid	Washed	75.00	51.00	85.75	8.00	9.00	7.75	8.25	8.00	7.75
41	MF1WP	Mana	Mid	Semi-washed	84.00	48.00	82.50	7.50	9.00	7.50	7.50	7.50	7.25
42	OMOF1WP	Goma	Mid	Washed	85.00	48.00	86.50	8.25	8.75	8.25	7.75	8.00	8.00
43	PSAF6WP	Limu Kosa	Mid	Washed	75.00	51.00	84.00	7.75	9.00	8.00	7.50	7.75	7.50
44	PSHUF1WP	Goma	High	Washed	88.00	51.00	83.75	8.00	8.75	7.50	7.50	7.75	7.50
45	SHGF2WP	Limu Kosa	Mid	Washed	88.00	51.00	85.75	8.00	7.75	7.75	7.75	8.25	8.00
46	HF1-FH-D	Mana	High	Dry	82.00	45.00	90.25	9.00	8.00	9.00	7.75	9.00	9.00
47	HF1-FH-M	Mana	High	Dry	91.00	54.00	92.25	8.75	8.50	9.00	9.00	9.00	9.00
48	HF1-FH-O	Mana	High	Dry	91.00	54.00	92.00	9.00	7.25	9.00	9.00	9.00	9.00
49	HF1-SH-D	Mana	High	Dry	85.00	51.00	87.00	8.50	7.50	7.75	9.00	7.75	7.50
50	HF1-SH-M	Mana	High	Dry	88.00	48.00	85.50	8.25	8.50	7.75	8.00	7.75	7.75
51	HF1-SH-O	Mana	High	Dry	88.00	54.00	92.00	9.00	8.00	9.00	9.00	9.00	9.00
52	HF1-TH-M	Mana	High	Dry	88.00	51.00	89.50	8.50	7.50	8.50	8.50	8.50	9.00
53	HF1-TH-O	Mana	High	Dry	85.00	48.00	84.00	8.00	7.25	7.75	7.75	7.50	7.50
54	HF2-FH-D	Mana	High	Dry	85.00	48.00	84.75	7.50	8.50	8.25	7.50	7.50	7.50
55	HF2-FH-M	Mana	High	Dry	82.00	48.00	85.25	8.25	8.00	8.25	7.75	7.75	7.50
56	HF2-FH-O	Mana	High	Dry	85.00	51.00	89.00	8.50	8.00	8.50	8.50	8.75	8.25
57	HF2-SH-M	Mana	High	Dry	85.00	48.00	85.50	8.25	8.25	8.25	8.75	7.50	7.50
58	HF3-FH-D	Mana	High	Dry	85.00	51.00	86.50	8.00	8.00	9.00	8.00	8.00	7.75
59	HF3-FH-M	Mana	High	Dry	85.00	51.00	90.25	8.75	8.00	9.00	8.25	9.00	8.50
60	HF3-SH-M	Mana	High	Dry	85.00	48.00	86.25	8.75	8.00	8.75	7.75	7.75	7.75
61	HF3-SH-O	Mana	High	Dry	88.00	54.00	92.50	9.00	8.00	9.00	9.00	9.00	9.00
62	HF3-TH-M	Mana	High	Dry	91.00	54.00	90.25	8.75	7.75	8.75	8.75	8.50	8.75
63	HF4-TH-M	Mana	High	Dry	88.00	51.00	86.25	8.00	7.75	7.75	8.50	7.75	8.50
64	HF5-FH-D	Mana	High	Dry	91.00	51.00	85.50	8.00	7.00	8.00	8.00	8.00	7.75

Table 1 (*continued*)

No.	Sample identifier	District	Altitude[a]	Processing method	Preliminary total quality	Preliminary cup quality	Total specialty cup quality	Overall cup preference[b]	Acidity	Body	Aroma	Flavour	Aftertaste
65	HF5-FH-M	Mana	High	Dry	85.00	51.00	87.50	8.50	7.75	8.50	8.50	8.00	8.50
66	DUR-NC	Goma	High	Washed	78.00	54.00	88.00	8.50	8.00	8.50	7.75	8.50	8.25
67	744WP	Limu Kosa	Mid	Washed	81.00	48.00	82.25	7.25	7.50	7.50	7.25	7.50	7.50
68	74112WP	Limu Kosa	Mid	Washed	71.00	42.00	79.75	7.00	7.00	7.25	7.00	7.50	7.00
69	74158DP	Limu Kosa	Mid	Dry	85.00	48.00	83.25	7.50	8.00	7.75	7.50	7.50	7.50
70	HF1WP	Mana	High	Washed	85.00	51.00	85.50	8.00	8.00	7.75	7.75	8.25	7.75
71	HF5DP	Mana	High	Dry	88.00	51.00	85.50	8.25	8.00	7.75	8.00	8.00	7.75
72	HF5SW	Mana	High	Semi-washed	84.00	54.00	86.50	8.00	8.00	8.00	8.00	8.25	8.00
73	LF2DP	Mana	Low	Dry	85.00	48.00	83.50	7.75	7.75	7.50	7.50	7.75	7.75
74	LF4DP	Mana	Low	Dry	82.00	45.00	82.75	7.50	7.75	7.50	7.50	7.50	7.50
75	LF4WP	Mana	Low	Washed	78.00	45.00	81.50	7.25	7.50	7.25	7.50	7.50	7.25
76	DURF1DP	Goma	High	Dry	91.00	57.00	87.50	8.25	8.25	8.25	8.00	8.25	8.00
77	OMOF2DP	Goma	High	Dry	91.00	51.00	85.75	8.00	8.00	8.00	7.75	8.00	8.00
78	DEBF2WP	Limu Kosa	Mid	Washed	87.00	51.00	85.00	8.00	8.00	8.00	7.50	8.00	7.75
79	HUNDA-NC-WP	Goma	High	Washed	76.00	48.00	84.75	8.50	8.00	7.50	8.00	7.75	7.50
80	MPS1WP	Mana	Mid	Washed	74.00	51.00	85.00	8.00	8.00	8.00	8.00	7.25	7.75
81	HF5WP	Mana	High	Washed	83.00	51.00	85.00	8.00	8.00	7.75	7.75	8.00	7.75
82	GPS3	Goma	Mid	Washed	85.00	51.00	84.75	8.00	7.75	8.00	8.00	7.50	7.75
83	HF5-FH-O	Mana	High	Dry	85.00	51.00	87.25	9.00	9.00	8.00	7.50	8.00	7.75
84	MF4SW	Mana	Mid	Semi-washed	84.00	48.00	83.50	7.75	7.75	7.50	7.50	7.75	7.75
85	744SW	Limu Kosa	Mid	Semi-washed	79.00	45.00	81.75	7.50	7.50	7.50	7.25	7.50	7.25
86	MF1SW	Mana	Mid	Semi-washed	84.00	48.00	84.00	7.75	7.75	7.75	7.50	7.75	7.75

[a] High altitude: >1750 m asl, Mid altitude: 1550–1750 m asl and Low altitude: <1550 m asl.
[b] Overall cup preference, acidity, body, aroma, flavour and aftertaste are a part of specialty cup quality attributes. Samples 1–66 are calibration samples and samples 67–86 are prediction samples.

The assessment of coffee quality is a key step in price setting and determines its export potential in coffee-producing countries. Consequently, it is of major importance to many coffee roasters and distributors [9]. Currently, physical and cup quality analysis are the key tools for coffee quality assessment. Physical quality of green coffee beans is associated with the presence of defects found in certain coffee batches such as deviations in odour, colour, size and shape of beans. Cup quality characteristics are attributes of coffee that can be distinguished by senses and can be assessed organoleptically by professional coffee tasters, based on established terminologies for cup quality analysis (e.g. flavour, acidity and body and cup cleanness). Based on these quality attributes the grading system for coffee varies and follows specific guidelines of the producing country [9].

In the Ethiopian system, physical and cup quality analysis enable experts to evaluate total preliminary coffee quality, which is used to classify coffee beans into different grades (Table 2). Coffee beans graded from grade one to three (total preliminary quality $>70\%$) are grouped into specialty coffee. Coffee beans from these three grades are further classified into different specialty grades, which are called: Q1, Q2 and commercial (Table 3). However, such methods of assessing coffee quality are rather subjective [10]. In addition, they are costly, require sample preparation and are time consuming. They are also difficult to implement when many samples need to be analysed during peak coffee production. Therefore, there is a need for a rapid, low-cost, reliable and reproducible analytical method as an alternative tool to evaluate coffee quality attributes and, eventually, other chemical compounds presents in coffee beans.

Near-infrared spectroscopy (NIRS) has gained broad acceptance for food quality evaluation [4]. It is rapid, reliable, simple and cheap, does not require use of chemicals and requires little sample preparation as well as low instrumental maintenance [11–13]. Several studies have shown the potential applicability of NIRS as an alternative technique to analyse coffee quality. NIRS has been used for the discrimination of Arabica coffee from Robusta [14–19], immature from mature as well as defective from non-defective coffee beans [17,20–22]. It was also reported that NIRS could be used successfully for authentication of coffee origin [23,24], detection of coffee adulteration [25–28], quantification of theobromine, theophylline, ash and lipid content of roasted coffee beans [29–32]. Some other studies also indicated the feasibility of predicting coffees cup quality attributes from roasted coffee beans using NIRS [33].

However, NIRS-based coffee cup quality prediction has been mainly focused on roasted beans and only a few studies used green coffee beans for coffee discrimination between defective and non-defective beans and to evaluate physical bean quality

Table 2
Overview of Ethiopian Commodity Exchange (ECX) preliminary quality parameters and contribution to a total score of 100 points.Source: [36].

Preliminary quality analysis		Grade categories and total points	
		Grade	Total points
Physical quality (40)	Primary defects (10)	Grade 1	91–100
	Secondary defects (10)	Grade 2	81–90
	Shape and make (10)	Grade 3	71–80
	Odour (5)	Grade 4	63–70
	Colour (5)	Grade 5	58–62
		Grade 6	50–57
		Grade 7	40–49
Cup quality (60)	Cup cleanness (15)	Grade 8	31–39
	Acidity (15)	Grade 9	20–30
	Body (15)	Under grade	15–19
	Flavour (15)		
Preliminary total quality	(100)	Grade 1–3 qualifies for specialty coffee	

Table 3
Overview of ECX specialty cup quality parameters, and contribution to a total score of 100 points and specialty coffee categories.Source: [36].

Specialty cup quality atrributes	Specialty coffee categories and points	
	Grade	Total points
Cup cleanness (10)	Specialty 1 (Q1)	85–100
Acidity (10)		
Body (10)	Specialty 2 (Q2)	80–84.75
Flavour (10)		
Aroma (10)	Commercial (Grade 3)	71–80
After taste (10)		
Uniformity (10)		
Sweetness (10)		
Balance (10)		
Overall cup preference (10)		
Total specialty cup quality (100)		

[21,34,35]. Many countries, organisations and companies could benefit from a reliable NIRS-based coffee quality assessment starting from green beans. However, to the best of our knowledge, prediction of coffee cup quality from NIRS spectra of green coffee bean has not yet been reported. Therefore, the objective of the present study was to develop a NIRS-based model for the prediction of coffee cup quality from green coffee beans using partial least squares regression.

2. Material and methods

2.1. Description of the study site

The coffee samples were collected from three districts (Mana, Goma and Limu Kosa) of the Jimma zone, Oromia regional state of Ethiopia. They are known as the predominant *Coffea arabica* growing areas of the Jimma zone. Sample collection was carried out from October 2012 to December 2013 during the peak harvesting season.

2.2. Coffee samples and cup quality analysis

The data set used in the present study comprised 86 coffee samples with varying cup quality characteristics as the coffee samples were collected from different environments (low, mid and high altitude) (Table 1). Only fully ripe, red coloured coffee cherries were harvested by hand picking and then subjected to dry, washed and semi-washed processing methods.

2.2.1. Dry processing method

The coffee cherries were directly sundried on raised beds without pre-treatment until they reached a moisture content of ca. 11.5%. The dried coffee cherries were dehusked using coffee hulling machine (Coffee huller, McKinnon, Scotland) at Jimma University College of Agriculture and Veterinary Medicine. Subsequently, the coffee beans were packed in plastic bags and stored at room temperature in the laboratory prior to analysis

2.2.2. Washed processing method

Red coffee cherries were mechanically de-pulped using a coffee pulper (Aagaard pregrader, McKinnon, Brazil) followed by 48 h fermentation and mucilage removal. Subsequently, the washed coffee beans were sundried on raised beds until a moisture content of ca. 11.5% was reached. Finally dry beans were mechanically hulled (Coffee huller, Pinhalense, Brazil) to remove parchment at TechnoServe organization, Jimma branch, that provides technical support for small-scale farmers to improve coffee quality. Subsequently, the coffee beans were stored in plastic bags at room temperature in the laboratory prior to analysis.

2.2.3. Semi-washed processing method

This method consists of a shortened washed processing whereby the fermentation step is omitted. The coffee cherries were introduced into a demucilaging machine (Mucilage remover, Pinhalense, Brazil) to remove pulp and mucilage. The de-mucilated coffee beans were subsequently washed and sundried on raised beds until a moisture content of ca. 11.5%. Finally, parchemnt was removed using a hulling machine (Coffee huller, Pinhalense, Brazil). Subsequently, the coffee beans were stored in plastic bags at room temperature in the laboratory prior to analysis.

From each sample, 500 g green beans were delivered to the Ethiopian Commodity Exchange (ECX), Jimma Branch, for physical and cup quality evaluation. A team of three professional who operate commercially in the ECX carried out the cup taste analysis. During the preparation of the actual cup tasting, 100 g green beans of each sample was roasted at 160–200 °C for six minutes using a sample roasting machine (Probat, 4 Barrel Roaster, Germany) allowing medium roasting of the coffee. The roasted beans were tipped out into a cooling tray and rapidly cooled by blowing cold air through the beans for four minutes. Then the roasted beans were ground with a coffee grinding machine (Mahlkonig Guatemala SB, K32SB2, Germany) with medium adjustment. For cup quality analysis, 13.75 g of ground coffee was diluted in a cup of 250 ml of hot water (93 °C) at the time of pouring onto the ground coffee to prepare an infusion. Five cups of brewed coffee for each coffee sample were prepared for analysis and three cuppers tasted each of the five cups. Subsequently, the average score of each cupper was taken as replication. The preliminary total quality scoring comprises physical (40/100) and cup quality (60/100) scores (Table 2). The criteria commonly used to evaluate the physical quality of coffee beans include the presence of defects: primary and secondary defects, shape and make, odour and colour. Santos et al. [13] described primary defects (e.g. full black and sour beans) and secondary defects (e.g. partial black, insect damaged and broken beans). For cup quality assessment, acidity, body, flavour and cup cleanness were considered and the sum of these four cup quality attributes gives a total cup quality with a score between 0 and 60. Hence, the sum of both cup and physical quality ranges between 0 and 100 and is used to classify the samples into different grades (grade 1 = 91–100, grade 2 = 81–90, grade 3 = 71–80 and grade 4 = 63–70) (Table 2). Coffee grades ranging from 1 to 3 were further assessed as specialty coffee based on overall cup preference, acidity, body, aroma, flavour, aftertaste, uniformity, cup cleanness, sweetness and balance each on a scale ranging from 0 to 10 (Table 3). Based on the total specialty coffee scores, samples were further grouped into specialty 1 (Q1) $\geq$ 85, specialty 2 (Q2) (80–84.75) and a regular commercial coffee (71–80) [36].

2.3. NIR spectra measurement and analysis

A Fourier Transform-NIR spectrometer (Tango, Brücker, Belgium) was used to obtain three replicated spectra. Green coffee samples were ground to a size smaller than 5 mm and 15 g of each sample was used for analysis. The samples were irradiated with tungsten (5 V/7 W) as source of near infrared light. The spectra were recorded in the wavenumber range between 4000 and 11,500 cm^{-1} with a spectral resolution of 8 cm^{-1} and the reflectance was detected by an Indium Gallium Arsenide (InGaAs) diode. The measurement was performed at room temperature.

Pre-processing of original NIR spectra to remove unwanted information, such as spectral noise, was a crucial step prior to model development since it deteriorates the quality of the model [22,37]. As such, specific pre-processing methods were identified

Table 4
Summary of NIR model parameters for preliminary and specialty cup quality attributes

Coffee quality attributes	Number of spectra		Selected data points	Wavelength range (cm^{-1})	Data pre-processing
	Cross validation data set ($n=66$)	Prediction data set ($n=20$)			
Preliminary cup quality	184	60	906	8916–6940; 6420–5020 and 4252–4016	First derivatives+Vector normalisation
Preliminary total quality	195	60	975	8916–5020	Subtraction of straight line
Total specialty cup quality	182	60	1009	8944–8524 and 8028–4420	MSC[a]
Individual specialty cup quality attributes					
Overall cup preference	179	60	1055	10,028–10,012; 9268–9252; 8968–5468 and 4712–4040	First derivatives+MSC
Acidity	173	60	892	1540–11,528; 8944–8524 and 7544–4420	Vector normalisation
Body	176	60	714	8944–8524; 8028–7124 and 5940–4420	First derivatives+MSC
Aroma	192	60	619	8944–8524; 6904–6380 and 5940–4420	First derivatives
Flavour	185	60	1136	11,540–11,528 and 8944–4420	First derivatives+Vector Normalisation
Aftertaste	180	60	682	11,540–11,528; 8944–8524; 8028–7268 and 5940–4420	First derivatives+Vector Normalisation

[a] Multiplicative scatter correction.

by the OPUS QUANT software for each coffee quality attribute (Table 4). Thus, suitable processing methods were selected based on the lowest root mean square error of cross validation (RMSECV). Derivatives and vector normalisation methods were used for preliminary cup quality, flavour and aftertaste, subtractions of straight line for preliminary total quality, multiplicative scatter correction for total specialty cup quality, first derivatives and multiplicative scatter correction for overall cup preference and body, vector normalisation for acidity and first derivatives for aroma.

To establish a linear relationship between spectral data and cupping scores, Partial Least Squares (PLS) regression analysis was performed [38,39] with OPUS QUANT software version 7.2 (Brücker, Belgium). The coffee samples were divided into calibration ($n=66$) and prediction ($n=20$) samples (Table 4). The calibration samples were randomly selected and used for model development using the leave-one-out cross-validation procedure. The procedure was repeated untill all calibration data sets were left one by one. Prediction samples (i.e. samples not used for model development) were used for external validation of the developed model. The optimum number of factors were determined on the basis of the lowest RMSECV value [40].

The performance of the developed PLS model was evaluated in terms of RMSECV, root mean square error of external validation (prediction) (RMSEP), residual prediction deviation (RPD), coefficient of determination for cross validation (R^2_{cv}) and correlation coefficient (r) for external validation [22,37,41]. For a good model, the value of RMSECV and RMSEP needs to be as low as possible and gives high R^2 and RPD values. The value of RMSECV and RMSEP refers to the quantitative measure for the precision of the predicted samples in cross and external validation, respectively.

3. Results

Means and ranges of measured cupping scores of all coffee quality attributes for cross-validation and prediction samples are shown in Table 5. Quality analysis (both preliminary and specialty cup quality) R^2_{cv}, RMSECV and RPD values of the cross validation data set ranged between 48–89, 0.19–3.63 and 1.39–3.02, respectively. In the prediction data set the corresponding values were 0.01–90, 0.22–4.82 and 0.74–2.25, respectively for r, RMSEP and RPD (Table 5).

Preliminary total quality had lower R^2_{cv} (48) compared to preliminary cup quality ($R^2_{cv}=67$) and total specialty cup quality ($R^2_{cv}=81$) (Table 5, Fig. 1). For the specialty cup quality attributes, the highest R^2_{cv} was found for overall cup preference ($R^2_{cv}=89$), followed by acidity ($R^2_{cv}=83$), total specialty cup quality ($R^2_{cv}=81$), aftertaste ($R^2_{cv}=80$) and body ($R^2_{cv}=78$) (Table 5, Fig. 1). Flavour ($R^2_{cv}=66$) and aroma ($R^2_{cv}=59$), on the other hand, had the lowest R^2_{cv} values (Table 5, Fig. 2).

The RMSECV values for preliminary cup quality, preliminary total quality, total specialty cup quality, overall cup preference, acidity, body, aroma, flavour and aftertaste were 1.73, 3.63,1.31, 0.19, 0.21, 0.22, 0.33,0.29 and 0.22, respectively (Figs. 1 and 2). The highest RPD value of a cross-validation data set, was obtained for overall cup preference (3.02), followed by acidity (2.44), total specialty cup quality (2.27), aftertaste (2.25), body (2.13). Preliminary cup quality (1.73), flavour (1.71) aroma (1.57) and total preliminary quality (1.39) relatively had lowest RPD values (Table 5, Fig. 1).

For the prediction data set, the PLS models for overall cup preference and total specialty cup quality had the highest coefficient of correlation, ($r=90$), followed by acidity (78), aftertaste (72) and body (72). Preliminary cup quality (27) and aroma (0.01),

Table 5
Statistics for cross validation and prediction (external validation) data for preliminary and specialty coffee quality.

Coffee quality attributes	Cross validation data set						Prediction data set				
	Number of factors	Mean	Range	R^2_{cv}	RMSECV	RPD	Mean	Range	r	RMSEP	RPD
Preliminary cup quality	8	48.4	42–54	67	1.72	1.73	49.2	42–57	27	3.51	1.01
Preliminary total quality	4	82.2	71–91	48	3.63	1.39	82.9	71–91	59	4.82	1.24
Total specialty cup quality	9	84.7	76.8–92.5	81	1.31	2.27	84.2	79.5–87.5	90	1.04	1.98
Individual specialty cup quality attributes											
Overall cup preference	10	7.9	6.5–9.0	89	0.19	3.02	7.9	7.0–9.0	90	0.22	2.25
Acidity	4	8.0	6.75–9.0	83	0.21	2.44	7.9	7.0–9.0	78	0.27	1.56
Body	8	7.9	6.5–9.0	78	0.22	2.13	7.7	7.3–8.3	72	0.24	1.12
Aroma	3	7.8	6.5–9.0	59	0.33	1.57	7.6	7.0–8.0	0.01	0.40	0.74
Flavour	10	7.8	6.5–9.0	66	0.29	1.71	7.8	7.3–8.3	59	0.29	1.01
Aftertaste	10	7.7	6.5–9.0	80	0.22	2.25	7.7	7.0–8.0	72	0.27	0.96

RMSECV: Root Mean Square Error of Cross Validation; RMSEP: Root Mean Square Error of Prediction; RPD: Residual Predictive Deviation; R^2_{cv}: coefficient of determination in cross validation and r: coefficient of correlation in prediction data set

on the other hand, had the lowest coefficient of correlation.

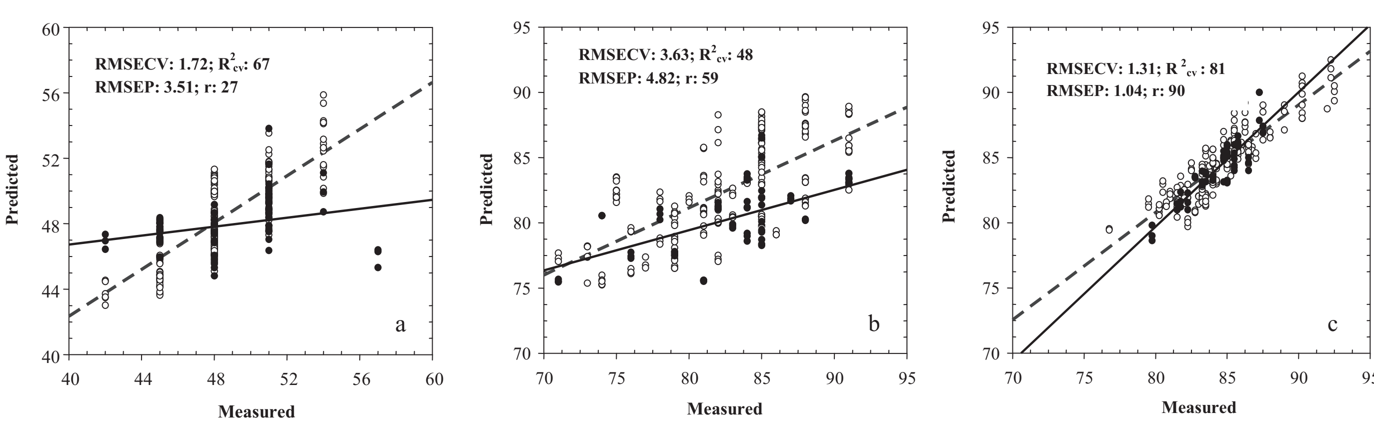
The PLS model of total specialty cup quality and that of individual specialty coffee quality attributes had the lowest RMSEP values compared to preliminary total and preliminary cup quality PLS models. The highest RMSEP value (4.82) was found in preliminary total quality while the lowest value (0.22) was observed in overall cup preference. In the same data set, overall cup preference had the highest RPD (2.25) while the lowest values were observed in aroma and aftertaste (Fig. 2).

4. Discussion

Different PLS models were developed on the basis of NIR spectra of green coffee beans to predict several coffee quality properties. Very promising results were obtained for total specialty cup quality and its individual quality attributes (overall cup preference, acidity, body, flavour and aftertaste) compared to results obtained for preliminary quality. The PLS models of total specialty cup quality, overall cup preference, acidity, body, flavour and aftertaste had, in general, higher R^2_{cv}, lower RMSECV and higher RPD values compared to the corresponding values of preliminary cup quality and preliminary total quality.

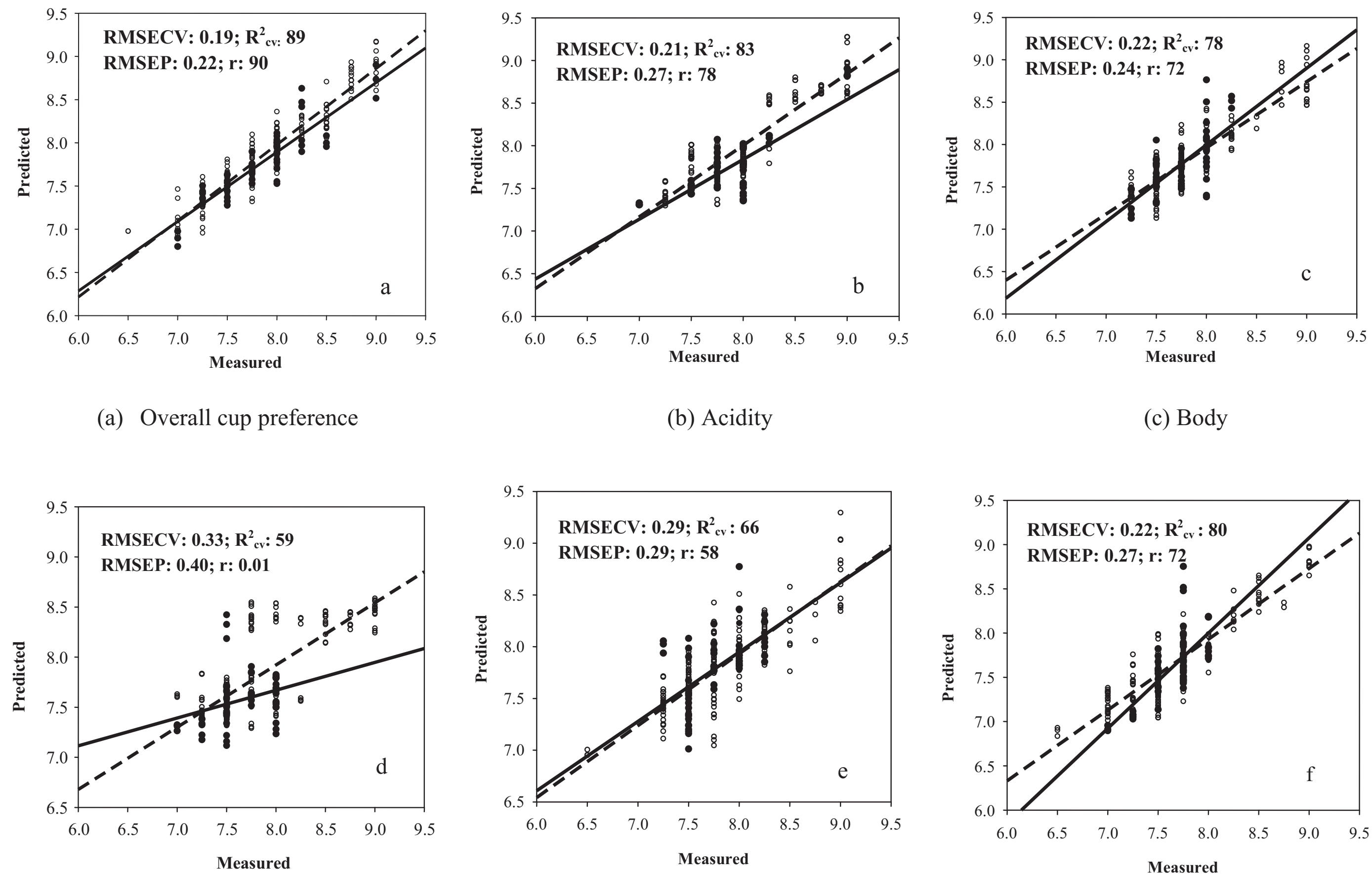
The correlation between measured and predicted cupping scores for total specialty cup quality (r=90), overall cup preferences (r=90), acidity, body and aftertaste were also high, which was, not the case for total preliminary quality (r=59) (Fig. 1b and c). This lower prediction efficiency ("closeness" of the model result to the measured value) for total preliminary quality was most likely due to physical quality parameters (e.g. defects, odour and colour), which are possibly more difficult to detect via NIRS [42]. Thought the defects could not be recognised individually, Barbin et al. [42] indicated that NIRS is still a potential tool to enable fast, simple and quantitative evaluations of green coffees. The higher RPD and the lower RMSEP for total and individual specialty cup quality attributes compared to preliminary quality also showed the promising predictive capabilities of the developed models. Aroma, on the other hand, had higher RMSECV, RMSEP and lower R^2_{cv} values compared to other specialty quality attributes. This indicates that the model had far less power to predict the aroma content, probably due to the complex nature of the attribute and because *Coffea arabica* contains over 40 major aroma components [43]. Further complicating aroma content prediction is the fact that the aroma is a result of a number of chemical reactions that occur during roasting [44].

Numerous efforts have already been carried to use NIRS as alternative technique to determine coffee quality attributes and to analyse its chemical composition and also reported that the techniques is even better than other analytical techniques such as HPLC (e.g. chlorogenic acid and caffeine) [45]. Ribeiro et al. [33] indicated that NIRS can be used to establish the relationship between coffee cup quality attributes and the chemical composition of roasted coffee beans. The authors also developed a model from roasted beans to predict coffee cup quality attributes (e.g. overall



(a) Preliminary cup quality (b) Preliminary total quality (c) Total specialty cup quality

Fig. 1. Measured vs. predicted scores of preliminary cup quality (a), preliminary total quality (b) and total specialty cup quality (c); data set for cross validation (empty bullets; dashed line) and for predictions (full bullets, full line). RMSECV: Root Mean Square Error of Cross Validation; RMSEP: Root Mean Square Error of Prediction, R^2_{cv}: coefficient of determination in cross validation and r: coefficient of correlation for prediction data set. (a) Preliminary cup quality. (b) Preliminary total quality. (c) Total specialty cup quality.



(a) Overall cup preference (b) Acidity (c) Body

(d) Aroma (e) Flavour (f) Aftertaste

Fig. 2. Measured vs. predicted scores of overall cup preference (a), acidity (b), body (c), aroma (d), flavour (e) and aftertaste (f); data set for cross validation (empty bullets; dashed line) and for predictions (full bullets, full line). RMSECV: Root Mean Square Error of Cross Validation; RMSEP: Root Mean Square Error of Prediction, R^2_{cv}: coefficient of determination in cross-validation and *r*: coefficient of correlation in prediction data set. (a) Overall cup preference. (b) Acidity. (c) Body. (d) Aroma (e) Flavour (f) Aftertaste.

cup preference, acidity, body, flavour and cleanliness).Our study developed a model from green beans with a higher R^2_{cv} and a lower RMSEP value for all cup quality attributes (overall cup preference, acidity and body) except for flavour, which had a lower R^2_{cv}. The reason for such discrepancy might be due to the number of samples used for model development and external validation. The number of samples has an impact on the quality of the model developed (e.g. the higher the number of samples the better predictive power of the model). In our study a total of 86 coffee samples were used, while Ribeiro et al. [33] used 51 samples.

The current study also indicates the potentiality of directly using green coffee beans to evaluate coffee quality. Prediction of coffee quality from green coffee beans is faster and cheaper than from roasted coffee beans. Apart from individual quality attributes our study developed promising models for total specialty cup quality, which can be used for classifying coffees into different specialty grades. For instance, out of 11 samples in “specialty 1”, nine of them are correctly predicted and two samples were predicted as “specialty 2” by our developed model. All eight samples found in “specialty 2” were predicted correctly. This showed that NIRS can potentially also be used to distinguish specialty coffees.

5. Conclusions

Specialty cup quality could be predicted well by the developed NIR-based prediction model. Prediction of total preliminary quality was relatively poor, perhaps indicating that the physical quality assessment cannot easily be done by NIR spectra of green beans. The NIR-based technique proved promising to predict some individual quality attributes such as overall preference, acidity and body. However, there is a need for improvement for total preliminary quality, flavour and aroma. Our model for total specialty cup quality holds potential as a rapid and reliable classification method for assigning coffees into different specialty grades. Hence coffee quality analysis with NIR spectra of green coffee beans is promising. However, the developed models need to be tested now further on independent data sets from other Ethiopian regions to test stability and accuracy of the models.

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