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Estimation of black tea quality by analysis of chemical composition and colour difference of tea infusions

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Abstract

Chemical composition, colour differences of black tea infusions and their relationships with sensory quality assessed by tea tasters were analysed. There were significant correlations between the individual quality attributes. Content of caffeine, nitrogen, amino acids, polyphenols, gallocatechin (GC), epigallocatechin (EGC), catechin (C), epicatechin (EC), epicatechin gallate (ECG), catechin gallate (CG), total catechins, theaflavin (TF) and theaflavin-3′-gallate (TF3′G) and infusion colour indicators of ΔL, Δa, Δb and ΔE were significantly correlated to total quality score (TQS). The parameters correlating significantly with the TQS were classified into four groups. Group 1 was compounds containing nitrogen, group 2 phenol compounds, group 3 tea pigments and group 4 infusion colour indicators. Four principal components were screened from the four groups as independent variables for constructing regression equations for estimation of black tea quality by principal component analysis. The regression of the TQS upon the principal components gives a highly significant relationship.

Keywords: *Camellia sinensis*; Black tea; Quality; Chemical composition; Infusion colour; HPLC; Principal component analysis; Regression

1. Introduction

Teas are usually classified as black tea, green tea, Oolong tea, yellow tea, white tea and dark compressed tea. Black tea is the most important one consumed across the world. Black tea quality depends mainly on the components and colour of the tea infusions and tea prices vary greatly, depending on the quality which has traditionally been assessed by a tea taster who has developed a language of his own to describe various quality attributes of a tea infusion. This language is sometimes difficult to comprehend by consumers. It is necessary to develop objective methods to identify the tea quality, chemically or physically.

Attempts have been made by tea researchers to explain black tea quality chemically. Roberts and Smith (1963) showed that theaflavin content is an important chemical compound in determining black tea quality. Hilton and Ellis (1972) and Cloughley (1980) confirmed that there was a close linear regressive relation between theaflavin content and broker's valuation of Central African black tea. Regression analysis of tasters' preferences for black teas against green tea leaf chemical components showed positive and significant correlations for (−)epicatechin gallate (ECG), (−)epigallocatechin gallate (EGCG) and caffeine (Obanda, Owuor, & Taylor, 1997). Wright, Mphargwe, Nyirenda, and Apostolides (2000) showed that fresh leaf (−)epicatechin (EC) and ECG content together correlated well with the total score of black tea and the total theaflavin content of black tea correlated significantly with the value of the tea. Liang and Xu (2001) showed that theaflavin makes a greater contribution to the brightness of black tea infusion than theaflavin gallates but theaflavin gallates have stronger ability to form tea cream than theaflavin.

Researchers have endeavoured to develop chemical and physical methods for identifying tea quality. Capillary electrophoresis, electronic tongue and lipid membrane taste sensor have been applied to tea quality estimation (Horie & Kohata, 1998; Ivarsson, Homin, Hojer, Krantz-Rulcker, & Winquist, 2001; Ivarsson & Kikkawa et al, 2001; Legin, Rudnitskaya, Vlasov, Natale, Davide, & D'Amico, 1997). However, these techniques have not been widely used in commercial practices of tea pro-

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duction and marketing. It is still necessary to search for other ways to solve tea quality estimation problems.

Black tea is a fermented tea. During the black tea fermentation, an enzymatic oxidation of tea polyphenols, especially tea catechins takes place, leading to formation of a series of coloured chemical compounds, such as theaflavins (TFs) and thearubigins (TRs), which are responsible for the characteristics of the black tea liquors. In assessment of tea quality or tea price, professional tea tasters mainly consider the tea liquor characteristics (Biswas & Biswas, 1971). Understanding the relationship of infusion constituents and liquor colour to quality of the black tea would be interesting for development of methods to identify black tea quality, chemically and physically. The present paper is set to analyse chemical composition and colour differences of black tea infusions and their correlation with sensory quality attributes assessed by tea tasters, so as to provide useful information for developing mathematical models to estimate black tea quality.

2. Materials and methods

2.1. Materials

Seventeen samples of black tea were collected from the major estates across China (Table 1). Equipment for infusion chemical composition analysis was high performance liquid chromatograph (HPLC) (model Shimadzu SCL-10A, Shimadzu Cooperation, Tokyo, Japan) and for infusion colour difference analysis was an automatic colour difference meter (model TC-PIIG, Beijing Optical Instrument Factory, Beijing, China). Catechins and TFs [theaflavins, including theaflavin (TF), theaflavin-3-gallate (TF3G), theaflavin-3′-gallate (TF3′G), theaflavin-3,3′-digallate(TF3,3′DG)] for HPLC references were provided by Dr. Takeda from the National Research Institute of Vegetables, Ornamental Plants and Tea of Japan. The other chemical reagents used were of HPLC grade (Jinmei Biotech Coporation, Tianjin, China), except where stated otherwise.

2.2. Methods

2.2.1. Sensory quality assessment of tea samples

Three grammes of tea sample were infused with 150 ml freshly boiled water for 5 min. The tea quality was estimated and scored by professional tea tasters SY Gong and ZL Gu from the Department of Tea Science at Zhejiang University. The grading system was based on a total score of 100, of which 10% was awarded for the appearance of dry tea, 30% for the tea aroma, 15% for the infusion colour, 35% for the taste and 10% for the infused leaves. The grading system is commonly used to evaluate black tea quality in China.

2.2.2. Analysis of chemical constituents of tea infusions

2.2.2.1. HPLC analysis of ascorbic acid, caffeine, catechins and theaflavins. Three grammes of tea sample were infused with 150 ml freshly boiled distilled water in a boiling water bath for 10 min. The infusion was filtered through "Double-ring" no.102 filter paper (Xinhua Paper Industry Co. Ltd, Hangzhou, China) and 0.2 μm

Table 1
Sensory quality score of the black tea samples assessed by the tea tasters ($n=2$, Mean±1 S.D.[a])

Samples No.	Estate	Appearance	Aroma	Liquor colour	Taste	Infused leaf	TQS[b]
1	Guangxi Lingyun	9.2±0.1	23.7±0.3	13.8±0.1	28.7±0.2	9.2±0.1	84.6±0.8
2	Zhejiang Huzhou	7.0±0.2	19.5±0.3	10.5±0.3	22.8±0.3	6.7±0.2	66.5±0.6
3	Zhejiang Huzhou	6.4±0.1	20.4±0.2	11.4±0.4	26.6±0.4	6.5±0.1	71.3±0.9
4	Zhejiang Huzhou	6.2±0.1	19.8±0.4	11.0±0.2	25.9±0.4	6.4±0.1	69.3±1.0
5	Yunnan Menghai	6.6±0.2	23.1±0.3	12.9±0.3	27.0±0.6	6.8±0.3	76.4±1.1
6	Yunnan Menghai	6.8±0.1	23.4±0.2	12.6±0.3	27.3±0.4	7.1±0.1	77.2±1.3
7	Chongqing Fuling	8.0±0.3	24.3±0.4	11.3±0.2	28.7±0.3	8.0±0.2	80.3±1.3
8	Yunnan Menghai	8.0±0.1	21.0±0.5	11.3±0.4	25.6±0.3	7.8±0.4	73.6±1.1
9	Yunnan Menghai	8.3±0.1	20.4±0.6	11.7±0.3	26.3±0.3	8.1±0.2	74.8±1.3
10	Yunnan Menghai	7.8±0.2	23.4±0.3	12.0±0.2	27.7±0.4	7.7±0.4	78.6±1.3
11	Yunnan Fengqing	8.0±0.1	25.8±0.6	12.8±0.4	30.5±0.2	8.2±0.2	85.2±1.5
12	Yunnan Fengqing	8.8±0.3	26.4±0.4	12.8±0.3	29.8±0.1	8.6±0.3	86.3±1.3
13	Guangxi Longbei	8.6±0.2	24.9±0.1	13.1±0.3	28.4±0.2	8.5±0.1	83.4±1.1
14	Zhejiang Hangzhou	8.2±0.1	24.0±0.1	12.3±0.2	27.3±0.3	8.2±0.2	80.0±1.0
15	Zhejiang Hangzhou	6.6±0.2	22.2±0.3	10.8±0.3	25.9±0.4	6.8±0.2	72.3±1.2
16	Zhejiang Hangzhou	8.1±0.4	22.8±0.4	12.3±0.2	28.4±0.4	7.8±0.2	79.4±0.9
17	Zhejiang Hangzhou	8.3±0.2	24.6±0.4	12.6±0.2	29.1±0.3	8.0±0.1	82.6±1.3
Average		7.7±0.9	22.9±2.1	12.1±0.9	27.4±1.8	7.7±0.8	77.7±5.8

[a] S.D., standard deviation
[b] TQS, total quality score.

Milipore filter before injecting into the HPLC. HPLC was carried out according to the method described in a previous paper (Liang, Ma, Lu & Wu, 2001) and the chromatographic conditions were as follows:

Injection volume:	10 μl
Column:	5μ-Diamonsil™ C_{18}, 4.6 mm×250 mm
Column temperature:	40°
Mobile phase:	Solvent A: acetonitrile/acetic acid/ water (6:1:193, v); Solvent B: acetonitrile/acetic acid/ water (60:1:139, v)
Gradient:	100% (v) solvent A to 100% (v) solvent B by linear gradient during first 45 min and then 100% (v) solvent B till 60 min.
Flow rate:	1 ml min^{-1}
Detector:	Shimadzu SPD ultraviolet detector, 280 nm

2.2.2.2. Analysis of amino acids, nitrogen. Contents of amino acids and nitrogen in the earlier tea infusions were determined by a spectra-photometric method with ninhydrin dying and Kjeldalhl's method (Zhong, 1989), respectively.

2.2.2.3. Analysis of tea polyphenols. Content of tea polyphenols in the above tea infusions was determined by the spectrophotometric method described by Zhong (1989). One millilitre of the earlier filtered tea extract was transferred into a 25-ml volumetric flask to react with 5 ml dyeing solution (containing 3.6×10^{-3} M $FeSO_4$ and 3.5×10^{-3} M potassium sodium tartrate, $KNaC_4H_4O_6$), 4 ml distilled water and 15 ml buffer (0.067 M Na_2HPO_4 and 0.067 M KH_2PO_4). Absorbance (E_1) at 540 nm of the reaction solution was determined in a 1 cm light-path cell by a spectrophotometer (Lengguang model-752, Lengguang Optical Instrument Ltd. Co., Shanghai, China). Absorbance (E_2) at 540 nm of a control reaction solution (containing 5 ml distilled water, 5 ml dyeing solution and 15 ml buffer) was determined as earlier. The content of tea polyphenols was calculated by the following equation:

$$\text{Polyphenols}\left(\text{mg g}^{-1}\right) = (E_1 - E_2) \times 3.9133 \times 150/3$$

E1: Absorbance of the tested solution at 540 nm; E2: Absorbance of the control solution at 540 nm; 3.913: Constant, meaning that polyphenols concentration was 3.913 mg ml^{-1} when absorbance at 540 nm was 1.0 under the earlier conditions; 150/3: constant, meaning that 3 g of tea sample was extracted in 150 ml water

2.2.3. *Analysis of colour difference of tea infusions*

The infusion colour difference analysis was carried out in a TC-PIIG automatic colour difference meter (Beijing Optical Instrument Factory, Beijing, China). The white plate supplied by the TC-PIIG automatic colour difference meter was used as background. To diminish the errors arising from different determination conditions, such as different equipment and temperatures, distilled water was used as control and the infusion colour difference indicators of ΔL, Δa, Δb and ΔE, which represent the light–dark (ΔL), red–green (Δa), yellow–blue (Δb) and total colour differences (ΔE) in the three dimensional colour coordinate system between the tea infusion and the distilled water were read and printed out directly by the TC-PIIG automatic colour difference metre.

2.2.4. *Data analysis*

The tests in the present paper were duplicated for each sample and mean values of the duplicated tests are presented. The contents of chemical constituents were calculated and based on the dry tea weight. Linear regressive analysis and principal component analysis were carried out on software of SPSS for Windows (version 10.0; SPSS Inc. 1999).

3. Results and discussion

3.1. *Sensory quality of various tea samples*

Total quality scores (TQS) of the seventeen tested tea samples ranged from 66.5 to 86.3 with a mean value of 77.7, in which the two samples from Yunnan Fengqing (No. 12 & No. 11) had the highest total quality score and the two samples from Zhejiang Huzhou (No. 2 & No. 4) had the lowest total quality score (Table 1). Linear correlation analysis showed that there were significant linear relationships between the individual tea quality attributes, and the total quality score was significantly correlated to the individual tea quality attributes (Table 2). This suggests that a good tea should have good individual quality attributes. Various attributes of teas may be compensated by blending. For example, a good blended tea may be obtained by blending a tea of strong taste and weak aroma with a tea of weak taste and strong aroma. That is why a tea manufacturer blends his special brand tea with materials produced from various origins and seasons.

3.2. *Chemical compositions and their relationship with sensory quality*

Chemical composition varied greatly from sample to sample. The coefficients of variation of ascorbic acid, epigallocatechin gallate (EGCG) and theaflavin-3-gallate (TF3G) were greater than 100%. The coefficients of

Table 2
Linear correlation coefficient between quality attributes of black tea $n=17$

	Appearance	Aroma	Liquor	Taste	Infused
Aroma	0.591*				
Liquor	0.588*	0.715**			
Taste	0.578*	0.881**	0.729**		
Infused	0.979**	0.671**	0.671**	0.664**	
TQS[a]	0.780**	0.935**	0.830**	0.930**	0.849**

[a] TQS, total quality score.
* $P<0.05$
** $P<0.01$

variation of epigallocatechin (EGC), epicatechin (EC), gallocatechin gallate (GCG), epicatechin gallate (ECG), catechin gallate (CG), theaflavin (TF), theaflavin-3′-gallate (TF3′G), theaflavin-3,3′-digallate (TF3,3′DG) and total theaflavins (TFs) ranged from 53.0 to 95.1% and those of caffeine, nitrogen, amino acids, polyphenols, gallocatechin (GC), catechin (C) and total catechins were below 50% (Table 3). The results showed that concentration of polyphenols was highest in black tea and caffeine was the next. Our previous research showed that EGCG was the most important catechin in the unfermented green tea and its concentration was 29.8 mg g^{-1} (Liang, Ma, Lu, & Wu, 2001), while the present study showed that GC was the most important catechin in the black tea. The average concentration of EGCG in the black teas shown in Table 3 was 2.51 mg g^{-1}, being 8.4% of that in green tea. This suggests that EGCG was mostly oxidized during black tea fermentation.

Linear correlation analysis showed that concentrations of caffeine, nitrogen, amino acids, polyphenols, C, ECG and total catechins were correlated positively and significantly with various individual quality attributes and total quality scores (Table 4). GC, EGC, EC, CG, TF and TF3′G were positively and significantly correlated with total quality score (Table 4). There were positive and significant correlations of the concentration of TF3,3′DG, total TFs with the scores of tea appearance and infused leaf while correlations between the concentrations of TF3,3′DG, total TFs and the total quality score were not statistically significant. The concentrations of ascorbic acid, EGCG and GCG were not significantly correlated with individual quality attributes or the total quality score (Table 4).

3.3. Infusion colour difference indicators and their correlation with sensory quality

The result of tea infusion colour difference analysis showed that the black tea infusions had minus values of ΔL (Table 5), suggesting that the black tea infusions were darker than water. The ΔL value was negatively correlated to the total quality score, appearance and infused leaf, respectively (Table 6). Values of Δa and Δb

Table 3
Infusion constituents of black tea samples ($n=2$, mg g^{-1})

Sample No.	Ascorbic acid	Caffeine	Nitrogen	Amino acids	Polyphenol	Tea catechins							Total catechins	Theaflavins (TFs)				Total TFs
						GC	EGC	C	EC	EGCG	GCG	ECG	CG		TF	TF3G	TF3′G	TF3,3′DG	
1	1.26	58.7	47.8	34.6	131	29.6	0.64	6.44	3.03	2.69	0.49	9.38	2.95	55.3	1.30	0.13	2.22	3.81	7.45
2	1.21	35.3	37.8	18.3	50.2	7.59	0.33	2.40	0.36	0.72	0.07	0.61	1.00	13.1	0.23	0.04	0.40	0.51	1.17
3	0.61	36.7	34.9	18.6	56.7	6.86	0.66	0.90	0.51	1.14	0.18	0.89	0.95	12.1	0.56	0.05	0.91	0.81	2.33
4	0.51	36.0	32.4	18.1	63.8	5.81	0.66	1.04	0.56	1.31	0.19	1.14	0.92	11.7	0.60	0.06	0.83	0.78	2.26
5	0.61	39.9	34.6	21.0	79.7	11.4	1.96	5.26	4.94	1.05	0.20	6.76	2.52	34.1	0.74	0.03	0.79	0.97	2.53
6	0.85	43.9	36.7	21.9	67.5	11.5	1.49	4.56	3.60	0.84	0.14	5.50	2.47	30.1	1.27	2.01	2.15	0.99	6.42
7	0.91	42.9	37.8	28.9	117	10.8	3.57	6.21	4.08	11.9	1.78	6.48	2.68	47.5	5.02	1.07	6.14	4.72	17.0
8	0.98	45.9	38.6	24.9	97.8	15.8	1.59	5.07	4.52	1.76	0.22	7.61	2.79	39.3	3.25	0.84	3.04	3.15	10.3
9	7.21	41.2	35.6	25.9	95.0	12.6	1.65	5.56	5.49	2.06	0.56	7.69	3.69	39.3	2.48	0.40	3.29	4.21	10.4
10	2.39	44.1	38.0	30.3	92.1	14.1	3.61	3.02	3.56	1.88	0.20	5.53	3.90	35.8	5.85	6.50	8.76	4.00	25.1
11	0.87	53.2	46.3	38.6	106	17.4	3.02	5.88	4.50	2.00	0.27	7.91	3.39	44.3	3.16	0.68	2.28	1.10	7.22
12	0.71	49.5	42.0	41.0	123	11.3	4.30	8.36	7.71	2.85	0.48	13.55	5.13	53.6	5.22	1.68	5.99	3.48	16.4
13	0.68	52.3	41.7	50.4	116	14.7	4.94	7.22	3.73	3.53	0.67	7.01	2.55	44.3	4.49	0.43	5.42	5.88	16.2
14	0.50	43.6	36.6	35.9	99.5	7.20	3.02	8.54	8.18	2.16	0.39	9.99	4.14	43.6	4.02	0.82	4.88	1.86	11.6
15	1.00	38.9	34.2	21.2	54.5	7.36	0.66	2.58	0.46	1.40	0.21	0.83	0.94	14.4	0.56	0.03	0.79	0.95	2.33
16	1.77	53.8	41.8	27.6	90.3	10.8	0.82	3.65	0.68	2.74	0.53	2.15	1.56	22.9	1.10	0.03	1.73	2.30	5.15
17	4.56	54.8	46.2	29.4	83.8	14.2	0.35	4.41	0.61	2.55	0.33	1.94	0.72	25.1	0.16	0.25	1.01	0.06	1.47
Average	1.57	45.3	39.0	28.6	89.6	12.3	1.96	4.77	3.32	2.51	0.41	5.59	2.49	33.3	2.35	0.89	2.98	2.33	8.54
S.D.[a]	1.76	7.22	4.6	9.1	24.8	5.60	1.49	2.29	2.51	2.55	0.39	3.79	1.32	14.6	1.96	1.57	2.43	1.75	6.88
CV%[b]	112	15.9	11.8	31.8	26.7	45.6	76.0	48.0	75.6	102	95.1	67.8	53.0	43.7	83.4	176	81.5	75.1	80.6

[a] S.D., standard deviation
[b] CV, coefficient of variation.

Table 4
Linear correlation coefficients between the infusion chemical constituent and tea quality attributes ($n=17$)

Quality attributes	Ascorbic acid	Caffeine	Nitrogen	Amino acid	Polyphenols	Tea catechins								Total catechins	Theaflavins				Total TFs
						GC	EGC	C	EC	EGCG	GCG	ECG	CG		TF	TF3G	TF3′G	TF3,3′DG	
Appearance	0.290	0.806**	0.763**	0.792**	0.886**	0.668**	0.443	0.758**	0.484*	0.343	0.413	0.677**	0.593*	0.806**	0.538*	0.115	0.520*	0.653**	0.530*
Aroma	−0.170	0.697**	0.633**	0.786**	0.685**	0.382	0.656**	0.720**	0.501*	0.351	0.336	0.613**	0.534*	0.692**	0.535*	0.239	0.485*	0.292	0.453
Liquor	−0.010	0.782**	0.663**	0.650**	0.649**	0.681**	0.334	0.620**	0.410	−0.035	0.033	0.592*	0.447	0.653**	0.186	0.068	0.195	0.262	0.204
Taste	−0.017	0.759**	0.659**	0.691**	0.707**	0.456	0.501*	0.547*	0.358	0.378	0.385	0.514*	0.440	0.625**	0.429	0.166	0.390	0.293	0.373
Infused	0.208	0.827**	0.762**	0.831**	0.931**	0.721**	0.493*	0.810**	0.546*	0.356	0.426	0.746**	0.645**	0.875**	0.561*	0.120	0.529*	0.656**	0.542*
TQS[a]	0.007	0.854**	0.765**	0.842**	0.840**	0.594*	0.584*	0.760**	0.509*	0.343	0.371	0.686**	0.583*	0.796**	0.519*	0.183	0.483*	0.432	0.471

[a] TQS, total quality score.
* $P<0.05$

of black tea infusions were on the positive scales (Table 5), suggesting that the black tea infusions were red and yellow in colour. The Δa,Δb andΔE were positively and significantly correlated with black tea appearance, infused leaf and total quality, respectively. The Δb was also significantly correlated with liquor score (Table 6), suggesting that infusion of high quality black tea was deeper in red and yellow colour than that of low quality tea. Table 7 shows that TF, TF3′G, TF3,3′DG and total TFs (including TF, TF3G, TF3′G, TF3,3′DG) were positively correlated with Δa, Δb andΔE, but negatively correlated with ΔL. This suggests that a high quality black tea may have a high concentration of red and yellow tea pigments, among which TFs are an important group, leading to a higher value of Δa, Δb and ΔE, but lower ΔL (Tables 1, 5 & 6).

3.4. Regressive relationship of chemical composition and infusion colour to total quality score

TQS is the most important parameter for evaluating the tea and it is significantly correlated with the individual quality attributes (Table 2). It will be interesting for estimating tea quality if mathematic models can be constructed using the TQS as dependent variable and the chemical and infusion colour indicators as independent variables.

To obtain a few indicators useful for establishing a mathematic model for estimation of the black tea quality, principal component analysis (PCA) was applied to screen the data set. The PCA with the earlier 17 factors, which had significant correlation with TQS showed that the cumulative variance of the first four principal components accounted for 93.6% of the total variance of the data set (Table 8). According to the absolute value of the component score (Table 9), the representative indicator of the first component is total catechins (component score = 0.916), the second is nitrogen (component score = 0.781), the third is ΔL (component score = 0.547) and the fourth is TF3′G (component score = 0.453). Regression of the TQS upon the four principal components produces the following highly significant relationship ($R^2=0.816$; $P<0.001$):

$$\text{TQS} = 44.90 + 0.16\ \text{Total catechins} + 0.66\ \text{Nitrogen} - 0.02\Delta L + 0.35\text{TF3}'\text{G} \quad (\text{Model 1})$$

In which the standard error of estimate is 2.88.

The principal component scores in Table 9 for total catechins, Δb, polyphenols, and amino acids (component 1) do not differ greatly, neither do those for nitrogen and caffeine (component 2); regressions of the TQS upon the these components were tried. The regressions

Table 5
Infusion colour difference indicators of the black tea samples ($n=2$)

Sample No.	ΔL	Δa	Δb	ΔE
1	−39.51	19.08	49.69	66.29
2	−19.72	6.42	40.63	45.62
3	−25.40	10.26	42.95	50.94
4	−28.54	11.12	44.45	53.98
5	−27.08	12.61	47.39	56.02
6	−25.49	11.26	46.89	54.55
7	−27.17	13.67	44.58	53.97
8	−44.10	30.43	51.04	74.01
9	−38.30	27.38	50.89	69.33
10	−39.77	30.39	52.38	72.88
11	−33.06	19.46	51.01	63.82
12	−47.01	33.87	51.49	77.51
13	−75.62	44.03	58.88	105.47
14	−37.26	27.70	51.32	69.21
15	−21.90	8.34	42.27	48.33
16	−38.23	18.00	46.50	62.83
17	−34.44	19.18	47.38	61.64
Average	−35.45	20.19	48.22	63.91
S.D.[a]	12.99	10.52	4.55	14.27

[a] S.D., standard deviation.

Table 6
Linear coefficients between infusion colour difference indicators and quality attributes of black tea ($n=17$)

Quality attributes	ΔL	Δa	Δb	ΔE
Appearance	−0.622**	0.674**	0.640**	0.631**
Aroma	−0.347	0.367	0.447	0.382
Liquor	−0.427	0.338	0.547*	0.436
Taste	−0.267	0.239	0.326	0.269
Infused leaf	−0.613**	0.655**	0.673**	0.632**
Total quality score	−0.564*	0.575*	0.640**	0.582*

* $P<0.05$
** $P<0.01$

Table 7
Linear correlation coefficients between content of TFs and infusion color difference indicators ($n=17$)

	TF	TF3G	TF3′G	TF3,3′DG	Total TFs
ΔL	−0.558*	−0.130	−0.527*	−0.724**	−0.560*
Δa	0.734**	0.339	0.700**	0.727**	0.719**
Δb	0.668**	0.328	0.625**	0.668**	0.657**
ΔE	0.637**	0.228	0.602*	0.730**	0.632**

* $P<0.05$
** $P<0.01$

of Δb, caffeine, ECG and TF, whose scores ranked next to those in the model 1, produce the following equation ($R^2=0.880$; $P<0.001$; standard error of estimate = 2.33):

Table 8
Total variance distribution by principal component analysis

Component	Total	% Of variance	Cumulative%
1	11.0	64.8	64.8
2	2.59	15.2	78.0
3	1.61	9.47	89.5
4	7.02E-1	4.13	93.6
5	4.70 E-1	2.76	96.4
6	2.17 E-1	1.28	97.6
7	1.49 E-1	8.79 E-1	98.5
8	8.26 E-2	4.86 E-1	99.0
9	6.78 E-2	0.399 E-1	99.4
10	4.35 E-2	2.56 E-1	99.6
11	2.77 E-2	1.63 E-1	99.8
12	1.51 E-2	8.91 E-2	99.9
13	1.03 E-2	6.07 E-2	99.9
14	4.62 E-3	2.72 E-2	100
15	1.49 E-3	8.75 E-3	100
16	8.62 E-4	5.07 E-3	100
17	−5.28 E-17	−3.11 E-3	100

Table 9
Component score of various components

Component	1	2	3	4
Total catechins	0.916	6.32E-2	6.32E-2	2.83E-2
Δb	0.902	3.30 E-2	−0.295 E-2	−0.183 E-2
Polyphenols	0.902	2.31 E-1	1.88 E-1	1.34 E-1
Amino acids	0.901	1.79 E-1	−1.94 E-1	2.35 E-2
Δa	0.880	7.71 E-2	−3.92 E-1	−1.30 E-1
ECG	0.873	−1.35 E-1	4.08 E-1	−1.81 E-1
C	0.861	−1.03 E-2	3.07 E-1	−2.38 E-1
ΔE	0.850	4.80 E-2	−4.88 E-1	−1.68 E-1
CG	0.833	−339 E-1	3.40 E-1	1.70 E-2
EGC	0.819	−4.17 E-1	−1.46 E-1	1.75 E-1
TF	0.813	−4.37 E-1	5.40 E-2	3.62 E-1
ΔL	−0.796	−1.32 E-1	5.47 E-1	1.66 E-1
EC	0.766	−4.24 E-1	3.86 E-1	−2.69 E-1
TF3G	0.751	−4.32 E-1	−1.09 E-1	4.53 E-1
Nitrogen	0.509	7.81 E-1	9.70 E-2	1.82 E-1
Caffeine	0.625	7.30 E-1	1.13 E-2	7.67 E-2
GC	0.520	6.89 E-1	2.41 E-1	9.70 E-2

$$\text{TQS} = 53.98 - 0.16\Delta b + 0.61\ \text{caffeine} + 0.42\text{ECG} + 0.75\text{TF}\ \text{(Model 2)}$$

If total catechins and nitrogen in model 1 were replaced by polyphenols and caffeine respectively, the regression equation would be:

$$\text{TQS} = 47.55 + 0.07\ \text{polyphenols} + 0.54\ \text{caffeine} + 0.06\Delta L + 0.59\text{TF3}'\text{G}\ \text{(Model 3)}$$

($R^2=0.859$; $P<0.001$; standard error of estimate = 2.53).

Table 10
Linear correlation coefficients between individual chemical constituents ($n=17$[a])

Constituent	Caffeine	Nitrogen	Amino acids	Polyphenols	ECG	Total catechins	TF	TF3′G	ΔL	Δb
Caffeine		0.923**	0.708**	0.732**	0.429*	0.601**	0.216	0.201	−0.559**	0.568**
Nitrogen	0.923**		0.636**	0.638**	0.342	0.522*	0.138	0.105	−0.399	0.403
Amino acids	0.708**	0.636**		0.804**	0.668**	0.750**	0.665**	0.597**	−0.827**	0.835**
Polyphenols	0.732**	0.638**	0.804**		0.811**	0.938**	0.672**	0.611**	−0.654**	0.712**
GC	0.764**	0.759**	0.454*	0.683**	0.458*	0.646**	0.144	0.146	−0.374	0.469*
EGC	0.222	0.134	0.765**	0.630**	0.673**	0.680**	0.909**	0.837**	−0.640**	0.724**
C	0.541*	0.445*	0.775**	0.804**	0.893**	0.895**	0.599**	0.503*	−0.553*	0.679**
EC	0.168	0.065	0.533*	0.612**	0.926**	0.796**	0.693**	0.593**	−0.374	0.624**
ECG	0.429	0.342	0.668**	0.811**		0.931**	0.682**	0.584**	−0.494*	0.691**
CG	0.283	0.201	0.579**	0.700**	0.929**	0.837**	0.799**	0.738**	−0.424*	0.673**
Total catechins	0.601**	0.522*	0.750**	0.938**	0.931**		0.708**	0.634**	−0.549*	0.716**
TF	0.216	0.138	0.665**	0.672**	0.682**	0.708**		0.959**	−0.558**	0.668**
TF3′G	0.201	0.105	0.597**	0.611**	0.584**	0.634**	0.959**		−0.527**	0.625**
ΔL	−0.559**	−0.399	−0.827**	−0.654**	−0.494*	−0.549*	−0.558**	−0.527**		−0.896**
Δa	0.477*	0.332	0.806**	0.680**	0.650**	0.647**	0.734**	0.700**	−0.924**	0.937**
Δb	0.568**	0.403	0.835**	0.712**	0.691**	0.716**	0.668**	0.625**	−0.896**	
ΔE	0.534*	0.376	0.843**	0.669**	0.573**	0.608**	0.637**	0.602**	−0.987**	0.948**

[a] Correlation coefficients between the variables used in constructed model 1-model 4 and the constituents which were correlated significantly with the total quality (see Tables 4 and 6) were listed. The original data comes from Tables 3 and 5.
* $P<0.05$
** $P<0.01$

When amino acids and caffeine replace total catechins and nitrogen of model 1, the regression equation is produced as model 4:

$$\text{TQS} = 49.63 + 0.43\text{ amino acids} + 0.47\text{ caffeine} + 0.19\Delta L + 0.46\text{TF3}'\text{G (Model 4)}$$

($R^2=0.918$; $P<0.001$; standard error of estimate = 1.93).

The parameters which are correlated significantly with the total tea quality score in Tables 4 and 6 can be classified into four groups. Group 1 is compounds containing nitrogen, including amino acids and caffeine as well as nitrogen itself. Group 2 is phenol compounds including polyphenols, GC, EGC, C, EC, ECG, CG and total catechins. Group 3 is tea pigments, i.e. TF and TF3′G (Table 4). Group 4 is infusion colour indicators, including ΔL, Δa, Δb and ΔE (Table 6). Table 10 shows that the individual parameters within each group are correlated with each other. Furthermore, parameters between the groups are also correlated with each other except for nitrogen and caffeine (Tables 7 & 10). In the models 1 to 3, one component was chosen from each group by the principal component analysis. Although there is no principal component from Group 2 (phenol compounds), the model 4 regression equation is highly significant because amino acids, ΔL and TF3′G are correlated significantly with polyphenols, GC, EGC, C, EC, ECG, CG and total catechins, respectively (Table 10).

In consideration of the effect of the principal components on tea quality, chemical compounds from Groups 1 and 2 are important taste constituents in the tea infusions while those from Group 3 affect both tea taste and infusion colour. The parameters of Group 4 are infusion colour indicators. It can be considered that the above regression equations estimate black tea quality by yielding information about the variation of taste and colour of the tea infusions and they will be interesting for estimating black tea quality and designing quality estimation equipment of black tea.

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