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Impact of brewing water type on the physicochemical, antioxidant, and sensory quality of cold brew coffee

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Abstract

Cold brew coffee has gained popularity due to its smoother flavour, lower acidity, and reduced bitterness compared with hot-brewed coffee. However, scientific evidence on the influence of brewing water composition on cold brew quality remains limited. Variations in water pH and mineral content may substantially affect extraction efficiency, chemical composition, and product consistency, highlighting the need for guidance on water selection. This study evaluated the effects of seven brewing water types (mineral, drinking, alkaline, reverse osmosis, tap, distilled, and deionized) on the physicochemical (colour, pH, total soluble solids, and caffeine), antioxidant (total phenolic content, total flavonoid content, DPPH radical scavenging activity, and ferric reducing antioxidant power), and sensory (aroma, acidity, bitterness, aftertaste, and overall acceptability) properties of cold brew coffee prepared from light- and dark-roasted beans under controlled conditions. Brewing water type significantly influenced physicochemical and antioxidant properties ($p < 0.05$). Light-roasted coffee brewed with mineral water exhibited higher pH (5.47), total phenolic content (16.60 mg GAE/g), and total flavonoid content (6.28 mg QE/g), indicating enhanced extraction of bioactive compounds. Alkaline water produced greater antioxidant activity for both roasting levels, with DPPH radical scavenging activity ranging from 5.82–8.29%, while tap water resulted in a higher caffeine content (161.18–201.41 mg/100 mL). Sensory attributes showed no significant differences among water types ($p > 0.05$); however, reverse osmosis water achieved higher overall acceptability scores. Multivariate analyses (PCA and PLSR) confirmed that water composition strongly influenced extraction behavior and antioxidant functionality, whereas sensory preference was not directly associated with phenolic concentration. These findings demonstrate the critical role of brewing water chemistry in determining cold brew coffee quality and provide quantitative guidance for water selection.

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1. Introduction

Cold brew coffee has emerged as a prominent segment of the global coffee market, driven by consumer preference for its smoother flavor profile, lower perceived acidity, and reduced bitterness compared with conventionally hot-brewed coffee. Unlike traditional brewing methods, cold brew coffee is prepared by steeping ground coffee in cold or room-temperature water for prolonged periods, typically 12–24 h, commonly using immersion systems such as a French press (1). The low-temperature, extended extraction fundamentally alters mass transfer kinetics and solubility behavior of coffee constituents, resulting in a beverage characterized by modified acidity perception, reduced harshness, and a distinct chemical profile.

Coffee quality is governed by multiple interacting variables, including bean origin, roasting degree, grind size, coffee-to-water ratio, and extraction time. Among these, water composition represents a critical yet comparatively underexplored factor, particularly in cold brew systems. As water accounts for more than 98% of the final beverage, its physicochemical characteristics directly influence extraction efficiency and chemical equilibria. Parameters such as pH, alkalinity, hardness, and dissolved mineral content modulate the solubility and stability of key coffee components, including caffeine, chlorogenic acids, phenolic compounds, and volatile aroma compounds. Mineral ions may enhance extraction through buffering capacity and complexation effects, thereby influencing flavor perception, whereas distilled or low-mineral water may result in limited solubilization and a relatively flat sensory profile (2). In cold extraction, divalent ions such as Mg^{2+} and Ca^{2+} may influence solute release differently, where Mg^{2+} can enhance extraction via interactions with polar/phenolic compounds, while Ca^{2+} may reduce efficiency through less favorable complex formation. Conversely, excessive alkalinity may shift acid–base equilibria and alter perceived acidity and balance. *Coffea liberica* was selected because it is widely cultivated in Malaysia due to favorable climatic conditions, despite being less commercially favored than *Coffea arabica* and *Coffea canephora*. Previous studies also indicate that its green beans exhibit higher antioxidant activity compared to these commonly studied coffee species (3).

Despite the rapid expansion of the cold brew market over the past decade, systematic scientific investigations examining the influence of brewing water chemistry on cold extraction remain limited. Most available studies have focused on hot brewing methods, such as espresso or drip filtration, where elevated temperatures accelerate diffusion and alter degradation pathways of thermolabile compounds (3,4). Given the substantial differences in temperature, extraction kinetics, and solubility dynamics between hot and cold brewing systems, findings from hot-brew studies cannot be directly extrapolated to cold brew. This gap highlights the need for controlled, quantitative evaluation of how water composition specifically modulates physicochemical, antioxidant, and sensory characteristics under cold extraction conditions.

Therefore, the present study systematically evaluated the effects of seven commonly used water types—mineral, drinking, alkaline, reverse osmosis, tap, distilled, and deionized water—on the quality attributes of cold brew coffee prepared from light- and dark-roasted beans. The investigation encompassed physicochemical parameters (colour, pH, total soluble solids, and caffeine content), antioxidant properties (total phenolic content, total flavonoid content, DPPH radical scavenging activity, and ferric reducing antioxidant power), and sensory characteristics (aroma, acidity, bitterness, aftertaste, and overall acceptability). Multivariate analyses were further employed to elucidate the relationships between water

composition and extraction behaviour. By providing quantitative evidence on the role of brewing water chemistry in determining cold brew coffee quality, this study aims to establish scientifically grounded guidance for water selection and contribute to improved flavour consistency, functional value, and quality control in specialty coffee production.

2. Materials and Method

2.1. Material

Light- and dark-roasted *Coffea liberica* coffee beans were obtained from My Liberica Coffee (Malaysia). Cold brew coffee was prepared using seven different types of brewing water: mineral water (Evian, Spritzer, Cactus), drinking water (Summer, Sea Master), alkaline water (Cuckoo Hot & Cold Water Purifier, CP-KN501HW), reverse osmosis (RO) water (Coway, CHP-5721L), tap water, distilled water, and deionized water. Brewed coffee samples were filtered using Whatman No. 102 filter paper.

Chemicals used for physicochemical and antioxidant analyses included hydrochloric acid (HCl), sodium hydroxide (NaOH), methanol (analytical grade), methanol (HPLC grade), sodium bicarbonate, gallic acid, phosphoric acid (0.05%, v/v), sodium nitrite ($NaNO_2$), aluminium chloride ($AlCl_3$), quercetin, sodium acetate trihydrate, glacial acetic acid, 2,4,6-tripyridyl-s-triazine (TPTZ), ferric chloride ($FeCl_3$), ascorbic acid, DPPH (2,2-diphenyl-1-picrylhydrazyl), and Folin–Ciocalteu reagent. All chemicals were of analytical grade unless otherwise stated.

2.2. Sample Preparation

Cold brew coffee was prepared using ground *Coffea liberica* beans at a coffee-to-water ratio of 1:10 (w/v) (1). Briefly, 10 g of ground coffee was placed into a sterile glass jar, followed by the addition of 100 mL of pre-cooled brewing water (4 °C, monitored using a calibrated food-grade thermometer). The water types used were mineral (Evian, Spritzer, Cactus), drinking (Summer, Sea Master), alkaline, reverse osmosis, tap, distilled, and deionized water.

Immediately after water addition, the jars were inverted manually 10 times to ensure homogeneous mixing [4]. The jars were sealed, wrapped with aluminium foil to prevent light exposure, and stored at 4 °C for 24 h for extraction. After brewing, the samples were filtered through Whatman No. 102 filter paper to remove fine particles and stored at 4°C until analysis.

2.3. Colour Analysis

Colour parameters (L*, a*, b*) were measured using a laboratory colorimeter (1). Samples were equilibrated to room temperature prior to analysis and transferred into clean, transparent cuvettes free of bubbles or foam. The instrument was calibrated using distilled water, and measurements were conducted in L*a*b* mode. Three readings were recorded per sample, and mean values were calculated to evaluate the influence of brewing water on colour characteristics.

2.4. pH Measurement

The pH of cold brew samples was measured using a calibrated pH meter (1). Calibration was performed using standard buffer solutions at pH 6, 7, and 8. Approximately 10 mL of each sample was analysed in triplicate, and results were expressed as mean ± standard deviation.

2.5. Total Soluble Solids (TSS) Analysis

Total soluble solids were determined using a digital refractometer and expressed as °Brix (5). The instrument was calibrated with distilled water (0.0 °Brix). A few drops of each sample were placed on the clean prism surface, and readings were recorded after stabilisation. Measurements were performed in triplicate.

2.6. Caffeine Analysis

Caffeine content was determined using high-performance liquid chromatography (HPLC) equipped with a reverse-phase C18 column (150 × 4.6 mm, 5 µm). Filtered samples (0.20 µm membrane filter) were transferred into 2 mL vials, and 10 µL was injected into the system. Caffeine was analyzed using HPLC under isocratic elution conditions. The mobile phase consisted of 70% water and 30% methanol, delivered at a constant flow rate of 1.0 mL/min throughout the analysis. The total run time was 15 min. The column temperature was maintained at 25°C. Detection was performed at 272 nm using a UV-Vis detector. Caffeine was identified by comparing retention times with a commercial standard, and quantification was conducted using calibration curves. Results were expressed as mg/100 mL of coffee extract (6).

2.7. Total Phenolic Content (TPC)

TPC was determined using the Folin–Ciocalteu method (6). Briefly, 100 µL of coffee extract was mixed with 200 µL of Folin–Ciocalteu reagent. After 3 min, 0.5 mL of sodium carbonate solution was added, followed by dilution to 3 mL with distilled water. The mixture was incubated in the dark at room temperature for 30 min. Absorbance was measured at 765 nm using a UV-Vis spectrophotometer. Gallic acid (15.63–250 mg/L) was used to construct the calibration curve. Results were expressed as mg gallic acid equivalents (GAE)/g ground coffee.

2.8. Total Flavonoid Content (TFC)

TFC was determined using the aluminium chloride colorimetric method (1). Coffee extract (50 µL) was mixed with 150 µL of 0.5 M $NaNO_2$, 150 µL of 0.3 M $AlCl_3$, and 3.4 mL methanol. After 5 min, 1 mL of 1 M NaOH was added. Absorbance was measured at 506 nm. Quercetin was used as the calibration standard, and results were expressed as mg quercetin equivalents (QE)/g coffee sample.

2.9. DPPH (2,2-Diphenyl-1-picrylhydrazyl) Radical Scavenging Assay

DPPH radical scavenging activity was determined according to (6). Briefly, 1 mL of coffee extract was mixed with 3 mL DPPH solution and incubated in the dark at room temperature for 30 min. Absorbance was measured at 517 nm against methanol as blank. Ascorbic acid (20–100 mg/L) was used for calibration. Radical scavenging activity was calculated as:

$$\text{Inhibition (\%)} = \frac{\mathrm{A_{control}} - \mathrm{A_{sample}}}{\mathrm{A_{control}}} \times 100$$

where $A_{control}$ is the absorbance without extract and A_{sample} is the absorbance with coffee extract.

2.10. FRAP (Ferric Reducing Antioxidant Power) Assay

FRAP reagent was prepared by mixing acetate buffer (300 mM, pH 3.6), TPTZ solution, and 20 mM $FeCl_3$ in a ratio of 10:1:1. The acetate buffer was prepared by dissolving 3.1 g sodium acetate trihydrate in 16 mL glacial acetic acid and adjusting to 1 L with distilled water. Coffee extract (50 µL) was mixed with 3 mL FRAP reagent and incubated for 30 min. Absorbance was measured at 593 nm (1). Ascorbic acid was used as standard, and results were expressed as µmol ascorbic acid equivalents (AAE)/mL.

2.11. Sensory Evaluation Analysis of Cold Brew Coffee

Sensory evaluation was conducted following ethical approval (FERC/FSG/25/152(UG)). A total of 50 untrained panellists participated. Samples were equilibrated to room temperature prior to evaluation. Four water treatments (mineral, drinking, alkaline, and reverse osmosis) for both light- and dark-roasted coffee were selected for sensory assessment. Samples were coded with random three-digit numbers and served in randomised order. Panellists evaluated aroma, acidity, bitterness, aftertaste, and overall acceptability using a 9-point hedonic scale (1 = dislike extremely; 9 = like extremely). Panellists rinsed their mouths with water between samples. Data were collected and subjected to statistical analysis.

2.12. Statistical Analysis

All physicochemical and antioxidant analyses were conducted in triplicate. Data were expressed as mean ± standard deviation. Two-way analysis of variance (ANOVA) was performed at a significance level of $p < 0.05$ using IBM SPSS Statistics (version 30), and Tukey's HSD test was applied as the post hoc analysis for multiple comparisons. Multivariate analyses, including principal component analysis (PCA) and partial least squares regression (PLSR), were performed using XLSTAT (version 2019) to evaluate correlations among physicochemical, antioxidant, and sensory attributes and to determine the influence of brewing water composition on extraction behaviour.

3. Results and Discussion

3.1. Physicochemical Properties of Cold Brew Coffee Brewed with Different Brew Water Types

As presented in Table 1, significant differences ($p < 0.05$) were observed in L*, a*, and b* values among water types and roast levels. For light roasted samples, L* values ranged from 19.93–23.40. Distilled water produced the lowest L* value (19.93 ± 2.67), indicating a darker appearance relative to other waters. In contrast, mineral, drinking, alkaline, reverse osmosis (RO), tap, and deionized waters showed comparable lightness. The relatively narrow L* range suggests that under cold extraction conditions (4°C), pigment solubilisation is limited regardless of water composition. Since cold brew avoids thermal acceleration of Maillard-derived melanoidin solubilisation, colour development primarily reflects roast-induced chemical changes rather than extraction temperature (7).

For dark roasted coffee, L* values ranged from 20.34–24.75 and were generally lower than light roast counterparts, confirming the dominant effect of roasting intensity. Extended roasting promotes melanoidin formation prior to extraction, explaining the darker appearance independent of brewing water (7). Across both roast levels, b* values were consistently higher than a* values, indicating greater yellowness than redness. This suggests preferential extraction of yellow-brown chromophoric compounds under cold brewing

conditions. Variations in a* and b* among water types likely reflect differences in ionic strength influencing pigment solubility and complexation.

Table 1. Colour Characteristics (L*, a*, b*) of Cold Brew Coffee with Different Brew Water Types.

Analysis	Brew Water Types	Cold Brew Coffee	
		Light Roasted	Dark Roasted
L*	Mineral	22.29 ± 0.45^{Ba}	23.97 ± 1.0^{Aa}
	Drinking	23.03 ± 0.19^{Ba}	24.37 ± 1.40^{Aa}
	Alkaline	21.79 ± 0.86^{Bab}	24.75 ± 0.10^{Aa}
	Reverse Osmosis	23.10 ± 0.22^{Aa}	20.34 ± 1.57^{Bb}
	Tap	23.40 ± 0.22^{Aa}	20.52 ± 0.65^{Ba}
	Distilled	19.93 ± 2.67^{Bb}	24.47 ± 0.48^{Aa}
	Deionized	22.42 ± 0.17^{Aa}	23.72 ± 1.68^{Aa}
a*	Mineral	0.33 ± 0.12^{Ac}	0.08 ± 0.22^{Ba}
	Drinking	0.33 ± 0.08^{Ac}	0.03 ± 0.11^{Ba}
	Alkaline	0.32 ± 0.13^{Ac}	0.01 ± 0.09^{Ba}
	Reverse Osmosis	1.70 ± 0.02^{Aa}	0.07 ± 0.22^{Ba}
	Tap	0.64 ± 0.09^{Ab}	0.18 ± 0.03^{Ba}
	Distilled	0.71 ± 0.07^{Ab}	0.11 ± 0.06^{Ba}
	Deionized	0.63 ± 0.09^{Ab}	0.04 ± 0.03^{Ba}
b*	Mineral	1.10 ± 0.12^{Ab}	1.06 ± 0.23^{Aa}
	Drinking	1.12 ± 0.13^{Ab}	1.13 ± 0.23^{Aa}
	Alkaline	1.31 ± 0.14^{Aab}	1.13 ± 0.09^{Aa}
	Reverse Osmosis	1.48 ± 0.05^{Aa}	1.16 ± 0.04^{Ba}
	Tap	0.99 ± 0.13^{Bb}	1.24 ± 0.08^{Aa}
	Distilled	1.48 ± 0.24^{Aa}	1.07 ± 0.22^{Aa}
	Deionized	1.09 ± 0.07^{Ab}	1.01 ± 0.10^{Aa}

Each value is expressed as mean ± value standard deviation (n = 3).
* A-B, within the same row, with different superscript letters are significantly different at $p<0.05$.
* a-c, within the same column, with different superscript letters are significantly different at $p<0.05$.

The pH of light roasted samples ranged from 5.32–5.47 (Table 2), with mineral water yielding the highest value (5.47 ± 0.10; $p < 0.05$). The buffering capacity of bicarbonates and divalent ions in mineral water likely contributed to partial neutralisation of organic acids during extraction (8). Dark roasted samples exhibited significantly higher pH values (5.76–6.06) compared to light roasted coffee ($p < 0.05$). This aligns with established roasting chemistry, where chlorogenic acids degrade during prolonged roasting, reducing acidity (7). Therefore, roast level exerted a stronger influence on pH than water type.

TSS values ranged from 2.35–3.53 °Brix and differed significantly among water types ($p < 0.05$). For light roast coffee, mineral and drinking waters produced the highest TSS (~3.53 °Brix), whereas RO water yielded the lowest (2.35 ± 0.07 °Brix). The absence of divalent cations (Mg^{2+}, Ca^{2+}) in RO water likely reduced complexation with coffee solutes, resulting in lower extraction efficiency (9). Dark roasted samples generally showed lower TSS compared to light roasted samples. This may be attributed to thermal degradation of certain soluble compounds during roasting, reducing extractable solids despite increased bean porosity.

Table 2. pH, Total Soluble Solid, and Caffeine Content (mg/100 mL) of Cold Brew Coffee with Different Brew Water Types.

Analysis	Brew Water Types	Cold Brew Coffee	
		Light Roasted	Dark Roasted
pH	Mineral	5.47 ± 0.10^{Ba}	6.06 ± 0.20^{Aa}
	Drinking	5.32 ± 0.02^{Bb}	5.81 ± 0.01^{Aab}
	Alkaline	5.35 ± 0.01^{Bab}	5.82 ± 0.01^{Aab}
	Reverse Osmosis	5.38 ± 0.01 ^{Bab}	5.79 ± 0.01 ^{Aab}
	Tap	5.34 ± 0.00 ^{Bab}	5.78 ± 0.01 ^{Aab}
	Distilled	5.33 ± 0.00 ^{Bab}	5.76 ± 0.01 ^{Ab}
	Deionized	5.32 ± 0.00 ^{Bab}	5.76 ± 0.00 ^{Ab}
Total Soluble Solid	Mineral	3.53 ± 0.12 ^{Aa}	2.72 ± 0.26 ^{Bab}
	Drinking	3.53 ± 0.26 ^{Aa}	2.82 ± 0.12 ^{Bab}
	Alkaline	2.85 ± 0.21^{Abc}	2.63 ± 0.15 ^{Aab}
	Reverse Osmosis	2.35 ± 0.07^{Ac}	2.70 ± 0.00 ^{Aab}
	Tap	2.90 ± 0.00 ^{Ab}	2.57 ± 0.31 ^{Ab}
	Distilled	3.00 ± 0.00 ^{Ab}	3.00 ± 0.17 ^{Aab}
	Deionized	3.2 ± 0.14 ^{Aab}	3.03 ± 0.12^{Aa}
Caffeine Content (mg/100 mL)	Mineral	146.85 ± 11.52^{Ab}	142.74 ± 12.17^{Ac}
	Drinking	155.68 ± 2.01^{Bab}	228.77 ± 29.34^{Aa}
	Alkaline	155.66 ± 0.53^{Aab}	142.40 ± 1.86^{Bc}
	Reverse Osmosis	150.31 ± 0.47^{Ab}	155.38 ± 2.55^{Abc}
	Tap	161.18 ± 0.99^{Ba}	201.41 ± 3.23^{Aab}
	Distilled	154.56 ± 0.20^{Bab}	161.81 ± 2.25^{Abc}
	Deionized	153.30 ± 0.56^{Ab}	138.45 ± 1.36^{Bc}

* Each value is expressed as mean ± value standard deviation (n = 3).
* A-B, within the same row, with different superscript letters are significantly different at p<0.05.
* a-c, within the same column, with different superscript letters are significantly different at p<0.05.

Caffeine levels in light roasted coffee ranged from 146.85–161.18 mg/100 mL. Tap water produced the highest value (161.18 ± 0.99 mg/100 mL), whereas mineral water yielded the lowest (146.85 ± 11.52 mg/100 mL). The presence of divalent cations in mineral water may promote competitive extraction of non-caffeine compounds, reducing relative caffeine solubility (9). Dark roasted samples exhibited a wider caffeine range (138.45–228.77 mg/100 mL), with drinking and tap water producing notably higher concentrations. Although caffeine is thermostable (10), structural changes in darker roasted beans (increased porosity) may facilitate greater extraction efficiency. Importantly, higher TSS did not necessarily correspond to higher caffeine levels, indicating selective extraction mechanisms influenced by water composition. These interpretations are based on observed trends in the present preliminary comparative assessment. A comprehensive water characterization shall be required in future work to experimentally verify these mechanisms and to strengthen the fundamental understanding of the observed extraction behavior.

3.2. Antioxidant Properties of Cold Brew Coffee Brewed with Different Brew Water Types

Antioxidant content was evaluated using TPC, TFC, DPPH, and FRAP assays (Tables 3 and 4). Light roasted samples showed significantly higher TPC (14.59–16.60 mg GAE/g) than dark roasted samples (4.57–7.71 mg GAE/g; $p < 0.05$). Mineral and alkaline waters enhanced phenolic extraction, likely due to ionic interactions stabilising chlorogenic acids [8]. The substantial reduction in TPC for dark roast coffee reflects thermal degradation and transformation of phenolics into melanoidins during roasting (7). Light roasted coffee

exhibited TFC values of 3.86–6.28 mg QE/g, whereas dark roasted samples were markedly lower (0.13–0.50 mg QE/g). RO water produced the lowest TFC among light roast samples, reinforcing the importance of moderate ionic strength for optimal flavonoid extraction (9).

Table 3. The Total Phenolic Content (mg GAE/g) and Total Flavonoid Content (mg QE/g) of Cold Brew Coffee with Different Brew Water Types.

Analysis	Brew Water Types	Cold Brew Coffee	
		Light Roasted	Dark Roasted
Total Phenolic Content (mg GAE/g)	Mineral	16.60 ± 0.01^{Aa}	5.90 ± 2.22^{Ba}
	Drinking	15.80 ± 0.13^{Aab}	4.64 ± 0.41^{Ba}
	Alkaline	16.26 ± 0.09^{Aa}	7.43 ± 0.14^{Ba}
	Reverse Osmosis	14.59 ± 0.14^{Abc}	7.71 ± 0.15^{Ba}
	Tap	14.59 ± 1.11^{Ac}	7.00 ± 0.14^{Ba}
	Distilled	15.20 ± 0.17^{Aabc}	4.57 ± 0.14^{Ba}
	Deionized	15.93 ± 0.33^{Aab}	5.43 ± 0.14^{Ba}
Total Flavonoid Content (mg QE/g)	Mineral	6.28 ± 0.98^{Aa}	0.17 ± 0.01^{Bbc}
	Drinking	6.22 ± 0.98^{Aa}	0.13 ± 0.02^{Bc}
	Alkaline	5.32 ± 0.38^{Aab}	0.50 ± 0.19^{Ba}
	Reverse Osmosis	3.86 ± 0.58^{Ab}	0.31 ± 0.07^{Ba}
	Tap	5.54 ± 0.43^{Aab}	0.24 ± 0.01^{Bbc}
	Distilled	5.62 ± 0.07^{Aa}	0.26 ± 0.01^{Bbc}
	Deionized	5.67 ± 0.46^{Aa}	0.29 ± 0.02^{Ba}

* Each value is expressed as mean ± value standard deviation (n = 3).
* A-B, within the same row, with different superscript letters are significantly different at $p<0.05$.
* a-c, within the same column, with different superscript letters are significantly different at $p<0.05$.

For light roasted coffee, DPPH ranged from 5.36–8.29% inhibition, with alkaline and RO water showing higher activity. FRAP values ranged from 16.11–21.67 mg AAE/g, again highest for alkaline water. Interestingly, antioxidant activity did not strictly follow TPC trends. Although mineral water produced higher TPC, alkaline and RO waters exhibited stronger DPPH and FRAP responses. This suggests that antioxidant performance depends not only on phenolic quantity but also on ionization state, molecular structure, and redox environment (9). Dark roasted samples consistently showed lower antioxidant content across all assays, confirming that phenolic degradation outweighs potential antioxidant contribution from melanoidins under cold extraction conditions.

Table 4. The Radical Scavenging Activity (%inhibition) and Reducing Antioxidants Power (mg AAE/g) of Cold Brew Coffee with Different Brew Water Types

Analysis	Brew Water Types	Cold Brew Coffee	
		Light Roasted	Dark Roasted
DPPH Assay (%inhibition)	Mineral	6.57 ± 2.29^{Aab}	6.06 ± 0.20^{Aa}
	Drinking	5.36 ± 0.41^{Bb}	5.81 ± 0.01^{Aab}
	Alkaline	8.29 ± 0.15^{Aa}	5.82 ± 0.01^{Bab}
	Reverse Osmosis	8.00 ± 0.14^{Aa}	5.79 ± 0.01^{Aab}
	Tap	6.00 ± 0.14^{Ab}	5.78 ± 0.01^{Bab}
	Distilled	7.29 ± 0.15^{Aab}	5.76 ± 0.01^{Bb}
	Deionized	6.29 ± 0.15^{Ab}	5.76 ± 0.00^{Bb}
FRAP Assay (mg AAE/g)	Mineral	16.88 ± 0.22^{Ab}	8.00 ± 0.06^{Ba}
	Drinking	16.60 ± 0.17^{Ab}	6.44 ± 0.08^{Ba}
	Alkaline	21.67 ± 0.29^{Aa}	7.44 ± 0.09^{Ba}
	Reverse Osmosis	19.78 ± 1.32^{Aa}	7.54 ± 0.12^{Ba}
	Tap	16.71 ± 0.22^{Ab}	7.60 ± 0.20^{Ba}
	Distilled	17.49 ± 0.22^{Ab}	6.85 ± 0.31^{Ba}
	Deionized	16.11 ± 0.10^{Ab}	6.55 ± 0.21^{Ba}

* Each value is expressed as mean ± value standard deviation (n = 3).
* A-B, within the same row, with different superscript letters are significantly different at $p<0.05$.
* a-b, within the same column, with different superscript letters are significantly different at $p<0.05$.

3.3. Sensory Evaluation Analysis of Cold Brew Coffee with Different Brew Water Types

Despite significant physicochemical and antioxidant differences, no statistically significant differences ($p > 0.05$) were observed among water types for aroma, acidity, bitterness, aftertaste, or overall acceptability (Figure 1). The results indicated that variation in brewing water composition used during brewing the cold brew coffee were not strongly influenced the sensory perception (11). However, reverse osmosis water consistently showed slightly higher overall acceptability for both roast levels. The limited sensory differentiation suggests that cold brewing produces a relatively uniform extraction profile, masking subtle chemical differences (12). The low mineral content of RO water may reduce ionic interactions that contribute to bitterness or astringency, resulting in a cleaner flavour profile (13). Roast level appeared to exert a stronger influence on flavour dominance than water chemistry.

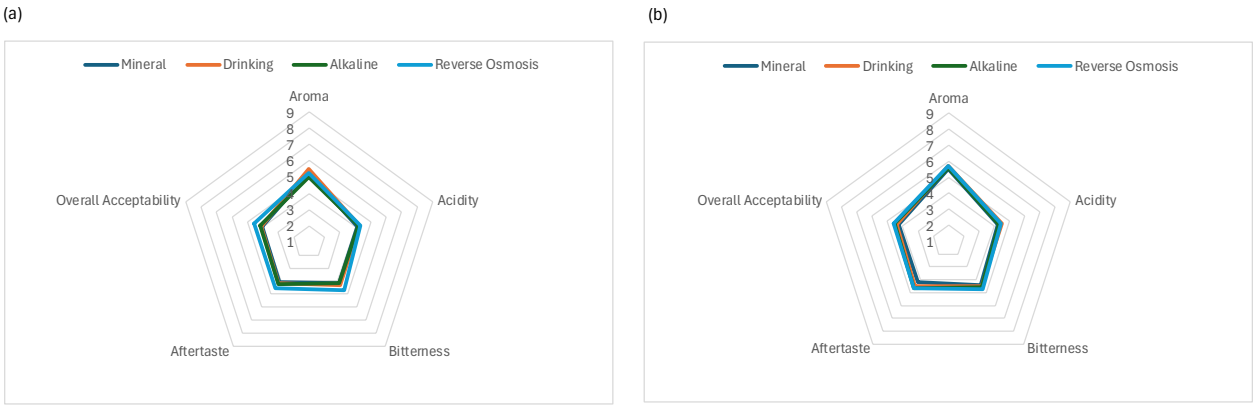

Figure 1. (a) Spider web of sensory evaluation analysis for light roasted coffee, and (b) spider web of sensory evaluation analysis for dark roasted coffee.

3.4. Correlation of Physicochemical and Antioxidants Analysis and Sensory Analysis of Cold Brew Coffee via SPSS

Pearson's correlation analysis provided further insight into the interrelationships among physicochemical and antioxidant variables and clarified the mechanistic pathways underlying extraction behaviour. In light-roasted cold brew coffee (Table 5), pH exhibited a strong negative correlation with caffeine ($r = -0.881$, $p < 0.05$), indicating that higher pH conditions were associated with reduced caffeine concentration. This relationship suggests that water buffering capacity and ionic composition influence selective solubilisation of alkaloids versus phenolic acids. Previous studies have reported that mineral ions, particularly Ca^{2+} and Mg^{2+}, preferentially interact with acidic and phenolic constituents, potentially altering the extraction equilibrium of caffeine under low-temperature conditions (8,9). Total soluble solids (TSS) were positively correlated with total phenolic content (TPC) and total flavonoid content (TFC), confirming that phenolic compounds represent a substantial fraction of extractable solids in cold brew systems (11,14). Furthermore, significant positive correlations between DPPH radical scavenging activity and FRAP values reinforce that phenolic constituents are the principal contributors to antioxidant functionality, consistent with established coffee chemistry literature (7).

Table 5. Correlation between physicochemical and antioxidants properties of Light Roasted Cold Brew Coffee.

Analysis	pH	TSS	L*	a*	b*	Caffeine Content	TPC	TFC	DPPH	FRAP
pH	1	0.259	0.33	-0.128	-0.010	-0.881*	0.639**	0.367*	0.421	-0.132
TSS		1	0.043	-0.724**	-0.388*	-0.200	0.531**	0.428*	-0.389*	-0.606**
L*			1	0.133	-0.503**	-0.013	-0.080	-0.019	-0.246	-0.178
a*				1	0.469**	-0.007	-0.512**	-0.493**	0.235	0.259
b*					1	-0.227	-0.087	-0.333	0.511**	0.406*
Caffeine content						1	-0.708**	-0.301	-0.519**	0.118
TPC							1	0.412*	0.225	-0.151
TFC								1	-0.173	-0.331
DPPH									1	0.572**
FRAP										1

** and * correspond to significance of correlation at the 0.05 level (2-tailed), respectively

In contrast, correlation patterns in dark-roasted samples (Table 6) differed markedly. pH demonstrated a strong positive correlation with FRAP ($r = 0.776$, $p < 0.01$), suggesting that redox potential in darker roasts may be influenced not only by residual phenolics but also by Maillard-derived melanoidins, which possess metal-chelating and reducing properties (7). Interestingly, TPC showed a weaker or even negative association with FRAP in dark roast samples, indicating that antioxidant mechanisms shift as roasting intensity increases. These findings support the hypothesis that cold brew extraction from dark roasted beans reflects a more complex interplay between degraded phenolics and newly formed high-molecular-weight compounds rather than simple phenolic-driven antioxidant activity (7,11). Collectively,

the correlation analysis demonstrates that roast level modulates the influence of water chemistry on extraction dynamics.

Table 6. Correlation between physicochemical and antioxidants properties of Dark Roasted Cold Brew Coffee.

Analysis	pH	TSS	L*	a*	b*	Caffeine Content	TPC	TFC	DPPH	FRAP
pH	1	0.090	2.66	-0.201	-0.210	-0.370	-0.223	-0.291	0.283	0.776**
TSS		1	0.331	0.105	-0.150	-0.070	-0.051	-0.070	0.119	0.141
L*			1	0.340	-0.383*	0.116	0.163	-0.058	-0.198	0.065
a*				1	0.132	0.164	0.176	-0.038	-0.344	-0.319
b*					1	0.032	0.228	0.110	0.056	-0.161
Caffeine content						1	0.185	-0.350	-0.244	-0.335
TPC							1	-0.207	-0.362*	-0.459*
TFC								1	0.461*	0.087
DPPH									1	0.769*
FRAP										1

** and * correspond to significance of correlation at the 0.05 level (2-tailed), respectively

3.5. Correlation of Physicochemical and Antioxidants Analysis and Sensory Analysis of Cold Brew Coffee via PCA

Principal component analysis (PCA) was performed to visualise multivariate relationships among physicochemical and antioxidant variables and to determine clustering patterns according to brewing water type (15). As shown in Figure 2A, the first two principal components (PC1 and PC2) for light-roasted cold brew coffee explained more than 70% of the total variance, indicating strong structural organisation of the dataset. Variables associated with phenolic extraction—namely total phenolic content (TPC) and total flavonoid content (TFC) (Table 3)—clustered closely with total soluble solids (TSS) and pH (Table 2), suggesting that these parameters are governed by similar extraction mechanisms. This clustering supports the hypothesis that moderate mineral content enhances solubilisation and stabilisation of chlorogenic acids and related phenolic compounds through ionic interactions and buffering effects (8,9).

Caffeine (Table 2) was positioned separately from phenolic and antioxidant variables in Figure 2A, indicating that caffeine extraction is influenced by distinct physicochemical drivers, primarily diffusion kinetics and intrinsic solubility rather than redox-related interactions (10). Although antioxidant assays (DPPH and FRAP; Table 3) were associated with phenolic variables, their vectors did not completely overlap with TPC and TFC, suggesting that antioxidant performance is not solely concentration-dependent but also influenced by structural characteristics and ionisation state of extracted compounds (11).

For dark-roasted coffee (Figure 2B), PCA revealed a different clustering pattern. While PC1 and PC2 similarly explained the majority of variance (>70%), antioxidant variables showed stronger alignment with pH and certain water types, particularly alkaline and mineral waters. This observation reflects the compositional shift induced by roasting. As shown in Table 3,

dark-roasted samples exhibited substantially lower TPC and TFC compared with light roast samples, indicating degradation of chlorogenic acids during roasting (7). Consequently, antioxidant activity in dark roast coffee may be more strongly associated with Maillard-derived melanoidins than with native phenolics. The separation of water types in Figure 2B further demonstrates that roasting modifies the interaction between water mineral composition and extractable compounds, leading to distinct multivariate profiles.

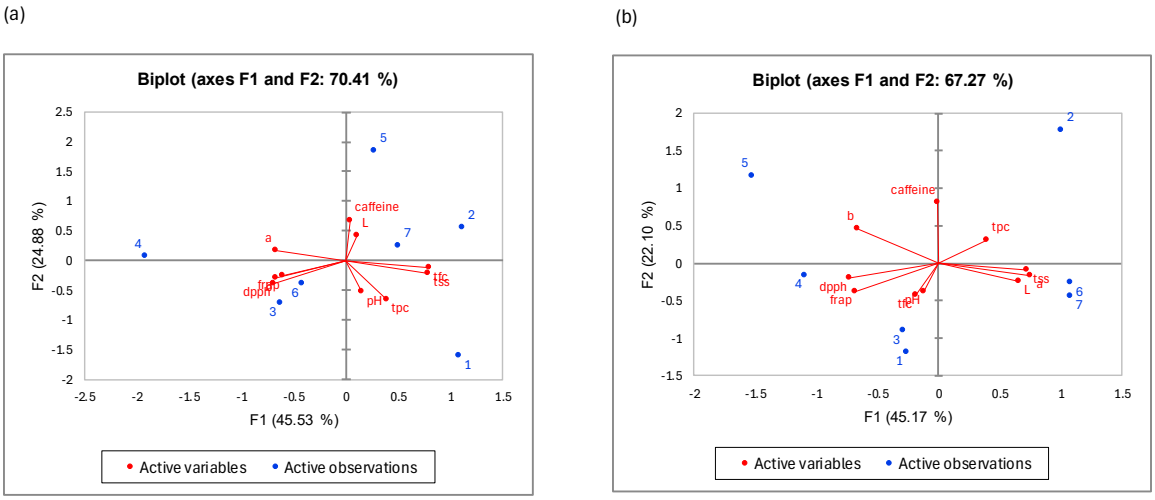

Figure 2. (a) Correlation of physicochemical and antioxidants analysis for light roasted coffee, and (b) correlation of physicochemical and antioxidants analysis for dark roasted coffee, ** 1 = Mineral, 2 = Drinking, 3 = Alkaline, 4 = Reverse Osmosis, 5 = Tap, 6 = Distilled, 7 = Deionized*

Principal component analysis (PCA) was applied to sensory data to elucidate relationships among sensory attributes and to determine whether brewing water type influenced perceptual differentiation. The PCA biplots for light- and dark-roasted cold brew coffee are presented in Figure 3a and 3b, respectively.

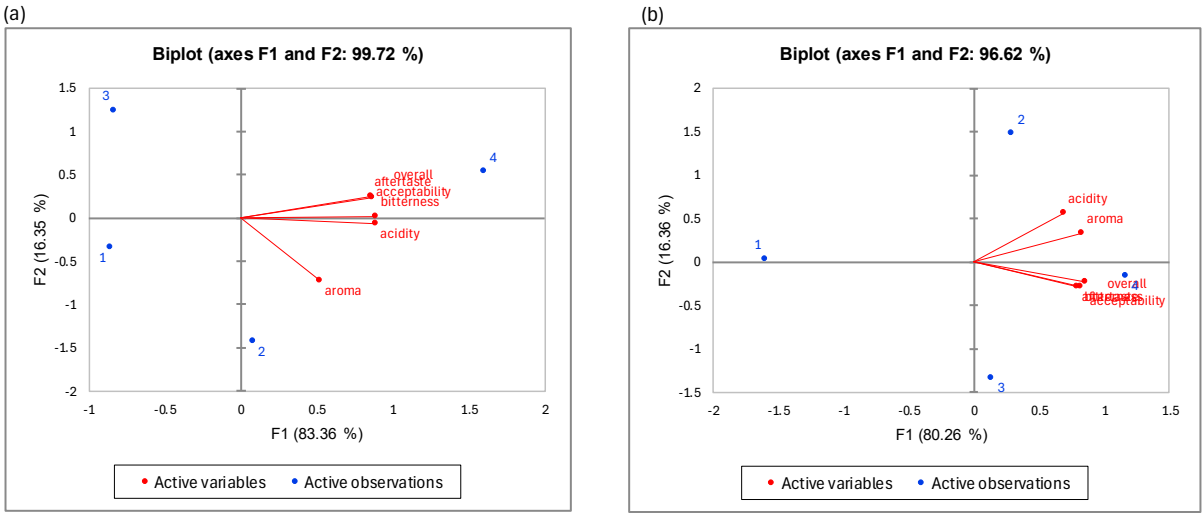

Figure 3. (a) Correlation of sensory evaluation analysis for light roasted coffee, and (b) correlation of sensory evaluation analysis for dark roasted coffee, ** 1 = mineral, 2 = drinking, 3 = alkaline, 4 = reverse osmosis*

For light-roasted coffee (Figure 3a), the first two principal components (F1 and F2) explained 99.72% of the total variance, with F1 accounting for 83.36% and F2 for 16.35%. Such a high cumulative variance indicates strong dimensional reduction and confirms that sensory variability among samples can be effectively interpreted within a two-dimensional space. Along F1, overall acceptability, bitterness, aftertaste, and acidity loaded positively and were closely aligned, indicating strong positive intercorrelations among these attributes. This alignment suggests that in light roast cold brew, bitterness and aftertaste contribute positively to overall liking rather than negatively, which is consistent with previous findings that cold extraction reduces harsh bitterness while maintaining desirable flavour complexity (12,13).

Aroma, however, was positioned separately along the negative direction of F2, indicating partial independence from taste-related attributes. This separation may reflect the distinct chemical origin of aroma compounds, which are largely volatile Maillard and Strecker-derived compounds formed during roasting (7), whereas bitterness and acidity are primarily associated with caffeine and organic acids. The divergence implies that water composition exerts limited influence on volatile-driven aroma perception under cold extraction conditions, as low temperatures reduce volatilisation and aroma release (12).

Regarding treatment distribution, reverse osmosis water (4) was positioned on the positive side of F1 and in close proximity to overall acceptability and bitterness vectors, indicating a tendency toward slightly higher preference scores. In contrast, alkaline water (3) was located further from the main sensory cluster, suggesting minor differentiation. Mineral (1) and drinking water (2) were distributed more centrally, indicating comparable sensory profiles. However, despite these positional tendencies, the clustering pattern supports earlier statistical results showing no significant differences ($p > 0.05$) among treatments. The PCA therefore confirms that sensory variability in light-roasted cold brew is minimal across water types, even though chemical differences were analytically significant (Tables 2–4).

For dark-roasted coffee (Figure 3b), F1 and F2 explained 96.62% of the total variance (80.26% and 16.36%, respectively), again indicating strong model adequacy. In contrast to light roast, acidity and aroma loaded positively along F1, while overall acceptability, bitterness, and aftertaste were closely grouped but slightly separated along F2, similar to (16). This shift suggests that in dark roast cold brew, perceptual drivers differ, likely due to compositional changes induced by roasting. Dark roasting reduces chlorogenic acids and increases formation of melanoidins and other Maillard reaction products (7), altering the balance between acidity and bitterness perception.

Drinking water (2) was positioned furthest along the positive F2 direction, indicating relatively stronger association with acidity perception (17). Reverse osmosis water (4) clustered near overall acceptability, bitterness, and aftertaste, again suggesting a slight preference tendency, possibly due to reduced ionic interactions that might otherwise enhance harsh or metallic notes (8,9). Mineral (1) and alkaline water (3) showed moderate dispersion without strong directional alignment, reinforcing the limited sensory differentiation among water types.

Importantly, in both roast levels, vectors for overall acceptability closely followed bitterness and aftertaste rather than acidity. This indicates that under cold brew conditions, controlled bitterness contributes positively to flavour balance. Cold extraction is known to suppress excessive acid extraction and reduce perceived sharpness compared with hot

brewing (12), which may explain why acidity was not a dominant driver of liking despite measurable pH differences (Table 2).

Overall, the PCA results in Figure 3 demonstrate that although brewing water significantly influenced physicochemical and antioxidant parameters, its effect on sensory perception was comparatively modest. The dominant factor governing sensory structure remains roast level, consistent with established coffee chemistry literature (7,12). Water composition may subtly modulate extraction balance, but under cold brewing conditions (4°C, extended extraction time), perceptual differences appear attenuated.

3.6. Relationship Between Physicochemical, Antioxidants, And Sensory Properties of Cold Brew Coffee

Integrating the physicochemical results (Table 2), antioxidant data (Tables 3 and 4), correlation matrices (Tables 5 and 6), and multivariate analyses (Figure 2) provides a comprehensive understanding of how water chemistry and roast level interact to shape cold brew coffee quality. Water containing moderate mineral concentrations, particularly mineral and alkaline waters, enhanced phenolic and flavonoid extraction in light-roasted coffee (Table 3). This effect can be attributed to ionic complexation between divalent cations (Ca^{2+}, Mg^{2+}) and phenolic acids, which improves solubilisation and stabilisation under cold extraction conditions (8,9). The positive correlations between TPC, TFC, TSS, and antioxidant assays observed in Table 5 reinforce that phenolic compounds constitute a substantial fraction of extractable solids and are primary contributors to antioxidant activity in light roast samples. However, antioxidant activity (DPPH and FRAP) did not always increase proportionally with TPC (Table 4). For instance, alkaline water demonstrated comparatively strong DPPH and FRAP values despite moderate phenolic levels, indicating that antioxidant performance depends not only on concentration but also on molecular structure, redox potential, and ionisation state (11). Such findings highlight that extraction efficiency and functional activity are related but not identical parameters.

Roast level emerged as a dominant modulator of water effects. As shown in Table 4, dark-roasted coffee exhibited markedly reduced TPC and TFC compared with light roast samples, reflecting thermal degradation of chlorogenic acids and formation of high-molecular-weight melanoidins (7). Correlation analysis in Table 6 indicated stronger associations between pH and FRAP in dark roast coffee, suggesting that redox behaviour in these samples may be influenced by Maillard reaction products rather than native phenolics. Under cold brewing conditions, which minimise thermal degradation during extraction, these roast-dependent compositional differences become particularly evident.

Interestingly, despite significant differences ($p < 0.05$) in chemical composition and antioxidant properties across water types, sensory evaluation (Figure 1) revealed no significant differences in aroma, acidity, bitterness, aftertaste, or overall acceptability. Reverse osmosis water exhibited slightly higher overall acceptability scores, although these differences were not statistically significant. This suggests that while water chemistry influences measurable chemical characteristics, the resulting changes may not be sufficiently pronounced to exceed the sensory perception threshold of the panelists. Furthermore, the use of semi-trained panelists may have limited the ability to detect subtle sensory differences among samples. Therefore, cold brew extraction appears to produce a relatively balanced sensory profile that may mask compositional variability, resulting in a comparatively moderate impact of water chemistry on perceived sensory quality (12,13).

3.7. Correlation of Physicochemical and Antioxidants Analysis and Sensory Analysis of Cold Brew Coffee via PSLR

Partial least squares regression (PLSR) was conducted to determine the relative importance of measured variables in explaining overall quality variation among brewing water types (18). The PLSR loading and VIP plots are presented in Figure 4, while corresponding physicochemical and antioxidant data are summarised in Tables 2–4.

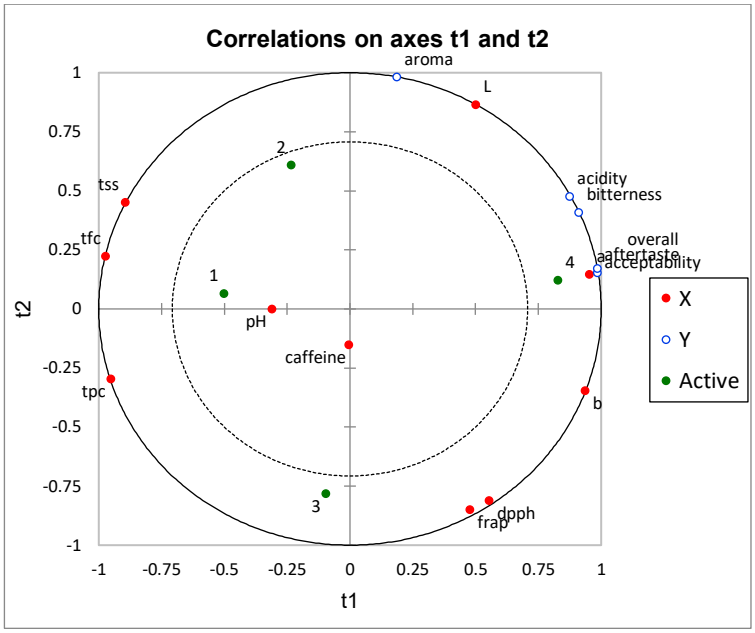

Figure 4. PSLR plot of cold brew coffee, ** 1 = Mineral, 2 = Drinking, 3 = Alkaline, 4 = Reverse Osmosis*

According to Table 7, variables with VIP scores greater than 1.0 included TPC, TFC, and colour parameters (L*, a*, b*), identifying phenolic-related extraction and chromophoric compounds as primary discriminators among water types. This finding is consistent with PCA results (Figure 2), where phenolic variables contributed strongly to principal component separation. The prominence of colour parameters further supports that pigment extraction, likely associated with phenolic oxidation products and melanoidins, is sensitive to water composition.

In contrast, DPPH and FRAP exhibited moderate VIP values, indicating that antioxidant assays reflect cumulative compositional effects rather than acting as independent predictive markers. Caffeine and pH displayed relatively low VIP values (< 0.5), suggesting that although statistically different among water types (Table 2), they contribute less to overall multivariate differentiation. This is noteworthy because caffeine is often regarded as a defining coffee component; however, in the context of cold brew, phenolic composition and pigment extraction appear to be more influential in distinguishing quality profiles.

Collectively, the PLSR model confirms that brewing water composition primarily modulates phenolic and chromophoric extraction rather than alkaloid content. When interpreted alongside PCA (Figure 2) and correlation analyses (Tables 5 and 6), the multivariate approach provides robust statistical evidence that water mineral composition is a critical determinant of cold brew coffee chemistry, with roast level acting as an interactive factor that modifies extraction pathways.

Table 7: Variable Important in the Projection (VIP) of Cold Brew Coffee via PSLR.

Variable	VIP	Standard deviation	Lower bound (95%)	Upper bound (95%)
TPC	1.496	0.366	0.332	2.660
a*	1.431	0.727	-0.884	3.746
TFC	1.266	0.838	-1.401	3.933
b*	1.151	0.603	-0.767	3.070
L*	1.148	0.716	-1.129	3.426
DPPH	0.377	0.858	-2.353	3.106
FRAP	0.241	0.898	-2.616	3.098
pH	0.419	0.311	-0.570	1.407
Caffeine	0.105	0.428	-1.256	1.466

4. Conclusions

This study confirms that brewing water composition significantly modulates the physicochemical and antioxidant properties of cold brew coffee, while exerting minimal influence on sensory perception under controlled conditions. Waters with moderate mineral content enhanced phenolic and flavonoid extraction, particularly in light-roasted coffee, whereas alkaline and reverse osmosis waters demonstrated comparatively stronger antioxidant responses in selected assays. Tap and drinking waters promoted higher caffeine extraction, indicating selective solubility behaviour influenced by ionic strength.

Roast level markedly influenced water–extraction interactions. Light-roasted beans, with higher retention of chlorogenic acids, were more responsive to mineral composition, whereas antioxidant activity in dark-roasted samples appeared more associated with Maillard-derived compounds than native phenolics. Multivariate analyses (PCA and PLSR) identified phenolic content and colour attributes as the primary drivers of compositional differentiation, while caffeine and pH contributed less substantially.

Despite significant chemical differences, sensory attributes did not differ significantly among water types, indicating that cold brew processing yields a chemically variable yet sensorially stable beverage. Overall, these findings provide mechanistic evidence for the role of water chemistry in shaping cold brew quality and offer practical guidance for optimising extraction without compromising consumer acceptance.

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Author Contributions

N.S.Z Methodology, Software, Formal analysis, Investigation, Writing - Original Draft, Visualization; N.A.A. Software, Validation, Visualization; N.A. Validation, Investigation; S.R.R. Validation, Formal analysis; L.J.S. Resources, Writing - Review & Editing; A.N. Writing - Review & Editing; F.E.H. Writing - Review & Editing, Visualization; E.K.S. Conceptualization, Methodology, Validation, Resources, Writing - Review & Editing, Visualization, Supervision,

Project administration, Funding acquisition. All authors have read and agreed to the published version of the manuscript.

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Institutional Review Board Statement

This study was conducted in accordance with the ethical standards of the institution and received approval from the Faculty Ethics Review Committee (FERC) of the Faculty of Applied Sciences, Universiti Teknologi MARA (UiTM), Malaysia. Ethical approval was granted under reference numbers FERC/FSG/25/152(UG) for the sensory evaluation.

Data Availability Statement

Available data are presented in the manuscript.

Conflicts of Interest

The authors declare no conflicts of interest.

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