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Chemical Fingerprinting of Various Tea and Coffee Types Using SEM, UV-Visible and FTIR Spectroscopy

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Abstract

Chemical fingerprinting provides a robust approach for characterizing and differentiating various types of tea and coffee based on their unique chemical profiles. In this study, Scanning Electron Microscopy (SEM), UV-Visible (UV-Vis) and Fourier Transform Infrared (FTIR) Spectroscopy were employed to analyze and compare chemical fingerprint various types of tea and coffee samples. The study analyzed green tea, black tea, chamomile tea and coffee samples due to their distinct composition and sources of natural antioxidant properties. SEM results showed the surface morphology for all samples is varied indicating the differences in the nature of raw material, processing, composition and surface characteristics of samples. UV-Vis spectroscopy revealed distinct patterns of chromophores observed in the UV region 250-300 nm associated with key compounds such as phenolic substances, flavonoids, methylxanthine compounds and caffeine. Additionally, FTIR spectroscopy demonstrated the fingerprint spectra and functional groups for all samples such as N-H stretching, O-H stretching, C=C aromatic ring and C-O stretching vibrations revealing compositional variations such as polysaccharides, polyphenols, sugars, caffeine, fatty acids and amino acids. The results recorded clear distinctions among various tea and coffee types. This study highlights the potential of combining SEM, UV-Vis and FTIR spectroscopy as a non-destructive, cost-effective, and comprehensive toolkit for the chemical profiling of various foods, offering valuable insights for quality assessment, authentication, and adulteration detection in the food industry.

1. Introduction

Tea and coffee have become the most popular drinking beverages around the world. Generally, tea is classified into three types based on the level of fermentation: unfermented varieties such as green and white tea, partially fermented oolong tea, and fully fermented black tea [1]. Green tea does not undergo the enzymatic oxidation process, allowing the natural scent of tea leaves to be preserved. On the other hand, black tea is produced through a full fermentation process, which involves enzymatic oxidation during this stage [2]. Coffee is categorized into two types which are ground coffee and instant coffee [3]. Coffee quality is influenced by genetics. post harvest

processing and brewing methods [4]. The biological properties of tea and coffee are primarily attributed to its polyphenol contents (such as flavonoids, catechins and tannins) as well as caffeine and other bioactive compounds [3]. These compounds are able to scavenge free radicals, allowing tea and coffee to demonstrate potent antioxidant properties as shown in both in vitro and in vivo studies [5].

Tea contains abundantly bioactive components. Catechin is the most studied compound in the tea. The content of catechin in dry matter of brewed green tea is about 30-42%. These compounds are distinguished by di- or tri-hydroxyl groups on ring B and meta-5,7-dihydroxy groups on ring A [6]. Catechins consist of three hydrocarbon rings and are structurally categorized into esterified catechins such as epigallocatechin-3-gallate (EGCG) and epicatechin-3-gallate (ECG) and non-esterified catechins such as epigallocatechin (EGC) and epicatechin (EC) [7].

On the other hand, caffeine is a widely known compound in coffee. Caffeine is a psychostimulant that contributes to the "waking" effect of coffee [8]. Apart from caffeine, coffee also contains other bioactive compounds such as chlorogenic acid (CGA), cafestol, and kahweol. These compounds showed significant biological and pharmacological properties on human health [9]. Polyphenols, such as feruloylquinic acid, dicaffeoylquinic acid, and the lactones of CGA have been reported to be present in significant amounts in coffee brew [10]. Several studies have documented the presence of phenolic acids in green coffee (primarily chlorogenic acid) and in roasted coffee (various other phenolic acids). However, only a few studies have specifically examined the flavonoid content in the final product [11].

Fingerprinting analysis has become widely popular in recent years for authenticating and ensuring the quality of food and herbal products. Spectroscopic and chromatographic techniques provide distinct spectra and chromatograms with detailed information on the characteristics of a sample. Fourier Transform Infrared (FTIR) spectroscopy is a fast, non-destructive and reliable method to characterize the macromolecular composition of biological matrix including food. This analytical approach offers a single measurement of the complete chemical fingerprint of the analysed sample [12]. Ultraviolet-visible (UV-Vis) spectroscopy were employed to characterize the water extract of tea leaves [13]. In addition, this technique has been used for caffeine quantification, simultaneous determination of methylxanthines, and tea classification [14, 15, 16]. However, there is a lack of comparative studies between tea and coffee using techniques such as UV-Vis and FTIR spectroscopy for fingerprinting purposes. Therefore, in this study, UV-Vis and FTIR spectroscopy were employed for chemical fingerprinting different types of tea and coffee in order to identify their unique chemical profiles. The UV-Vis and FTIR spectroscopy are ideal for the authentication and classification studies of various plants or herbs, owing to their simple sample preparation process and widely accessible equipment [16]. Furthermore, this integrative spectroscopic approach provides a more comprehensive chemical fingerprint comparison across various tea types (green, black, chamomile) and coffee, which are closely related in the context of food authentication and quality control.

2. Material and Method

Analytical grade of solvent ethanol was used as an extraction solvent (Merck, distributor Selangor). Green tea, black tea, chamomile tea and coffee were purchased in the local market, Malaysia. Filter paper Whatman No.1 was purchased from Modernlab, Penang.

2.1 Preparation of Tea and Coffee Extracts

The extraction of tea and coffee was performed using this method [17] with slight modifications. About 5 g green tea, black tea, chamomile tea and coffee samples were extracted with 100 mL ethanol on a water bath at 60°C for 20 minutes. The extracts were filtered using filter paper Whatman No.1 and the solvent was evaporated using a rotatory vacuum evaporator at 40°C. Each extract was stored in the chiller at 4°C until further use.

2.2 Scanning Electron Microscopy (SEM)

Scanning electron microscopy was conducted to investigate the morphological characteristics of the different types of tea and coffee using SEM JEOL JSM-6490LA, Japan operating at 50 kV. The SEM images with a magnification of 500 x were recorded. The samples were performed in triplicates.

2.3 UV- Visible Measurement

The UV-Visible spectra data were acquired using Jenway UV 6705 spectrophotometer, equipped with a deuterium lamp for the UV region and a tungsten-iodine lamp for the visible region. Ten mm quartz cuvettes were applied to contain the samples and blank. The used blank solution is ethanol. The wavelength was scanned from 200-500 nm at 1 nm intervals, with a measurement speed fixed at 400 nm/min. The baseline autocorrection was performed prior to the analysis of each sample. The samples were performed in triplicates. Spectral interpretation was carried out by analyzing characteristic absorption bands and comparing them with literature-reported values and standard reference spectra.

2.4 ATR-FTIR Measurement

ATR-FTIR measurement was conducted following the method described by [18] using a Shimadzu IRPrestige-21 Fourier Infrared Spectrophotometer (Tokyo, Japan). The instrument featured an air-cooled ceramic infrared light source and DLATGS (Deuterated Triglycine Sulfate doped with L-Alanine) detector. Spectral data for the sample were recorded within the range of 4000 cm^{-1} to 500 cm^{-1}. The sample was placed directly on the diamond prism for measurement. The IR resolution was set to 4 cm^{-1} and 16 inferograms were co-added before performing the Fourier transformation. Data processing, including baseline correction, normalization and smoothing was carried out using Shimadzu IRsolution version 1.40 (Shimadzu Corporation) software. The baseline autocorrection was applied prior to each sample measurement. Spectral interpretation was carried out by analyzing characteristic absorption bands and comparing them with literature-reported values and standard reference spectra. The samples were performed in triplicates.

3. Results and Discussion

The surface structure of the raw powdered different types of tea and coffee was assessed using SEM imaging. Fig 1 shows that tea and coffee have different surface morphologies. Fig 1(a) revealed a fibrous and wavy structure, typical of plant cell walls, with ridges and grooves running across the surface. The scattered particulate matter may indicate surface impurities or residual particles from the tea production process. The fibrous network suggests the presence of cellulose and lignin, which form the primary structure of plant materials. Minor cracks and surface irregularities could be a result of drying or processing steps, such as grinding or heating [19]. The rough and irregular surface image in Fig 1 (b) reflects the natural structure of tea leaves, which is influenced by their cellular makeup and drying process. The presence of folds, grooves, and fibrous textures may be indicative of the plant's vascular system and cell wall structure. The micrograph may capture the effects of tea processing, such as rolling, drying, or oxidation, on the surface morphology. These processes might break cell walls or cause structural deformation, visible in the image. The exposed or disrupted surfaces might relate to the release of bioactive compounds during brewing. Surface area plays a crucial role in determining the rate of compound release [20]. On the other hand, Fig 1 (c) showed a highly irregular surface with prominent ridges, folds and voids. These features suggest a porous or fibrous material, which might contribute to its functional properties, such as adsorption capacity, surface area, or mechanical strength. The structural characteristics are the cracks and cavities visible on the surface might indicate fragility or structural weakness, possibly due to processing methods or the material's composition [21]. Meanwhile, Fig 1 (d) shows the surface appears rough and irregular, with numerous protuberances and cavities of varying sizes. There are observable particle-like structures distributed across the surface, possibly indicating the presence of aggregated material or particulate debris. The structural features are circular and irregular voids are evident, which may suggest the material has undergone processes like cracking, aggregation, or pore formation. These features indicate a porous structure, which could influence the material's properties, such as permeability or surface activity [22]. The surface morphology of tea and coffee displays distinct differences which tea has a more fibrous and less porous surface whereas coffee exhibits a rougher, more porous structure. These findings revealed the different nature of raw material, processing, composition and surface characteristics different types of tea and coffee.

The UV-Vis spectra different types of tea and coffee extracts ranging from 200- 500 nm are shown in Fig 2. The absorption peaks of UV-Vis spectra were broad and mainly related to $\pi \rightarrow \pi^*$, and $n \rightarrow \delta^*$ electronic transitions of chromophores and auxochromes in tea and coffee extracts. The absorption bands were observed in the UV region 250-300 nm, which correlates with flavonoids and methylxanthine compounds in black and green tea, including caffeine (with maxima at 280 nm, as reported by [15], catechin and related compounds (maxima at 275 nm, according to [23]), and other phenolic compounds [24]. As observed in Fig 2, the maximum absorbance peaks for green tea and black tea at 275 nm, which specifically is associated with the C=O chromophore of caffeine and the conjugated unsaturation system of catechins [17]. The maximum absorption peak for chamomile tea was found at 319 nm, which is probably linked to aromatic compounds of polyphenols. Additional significant peak was observed at 237 and 283 nm, indicating the existence of aromatic compounds or conjugated systems, especially phenolic compounds and flavonoids. The UV-Vis spectra of coffee showed maximum absorption around 280 nm, indicating the presence of caffeine. These spectral features closely align with the known chemical profiles of each sample, confirming the presence of characteristic bioactive compounds such as caffeine, catechins, and polyphenols in the respective tea and coffee types.

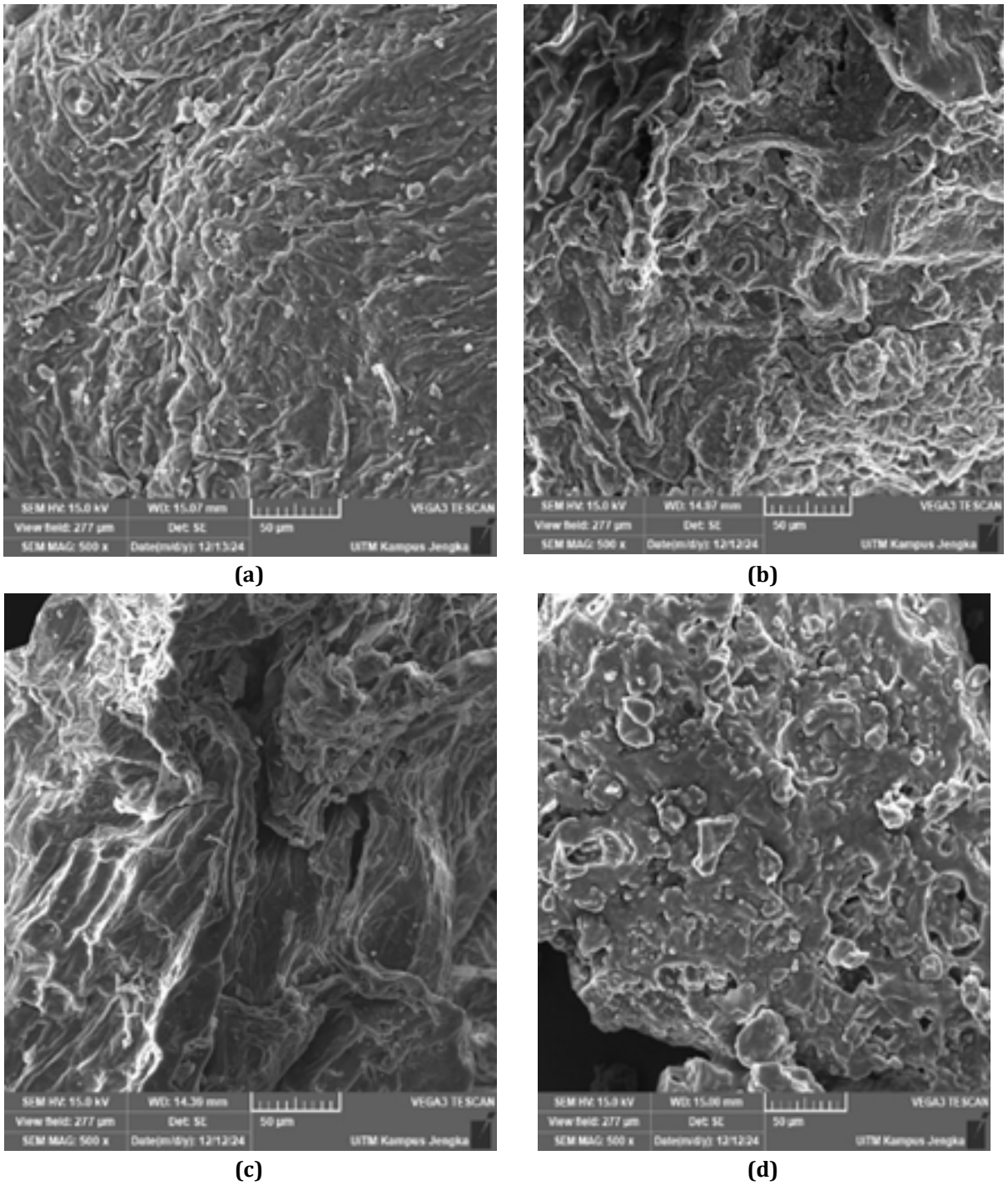


Fig. 1 *SEM image various types of tea and coffee (a) Green tea; (b) Black tea; (c) Chamomile tea; (d) Coffee*

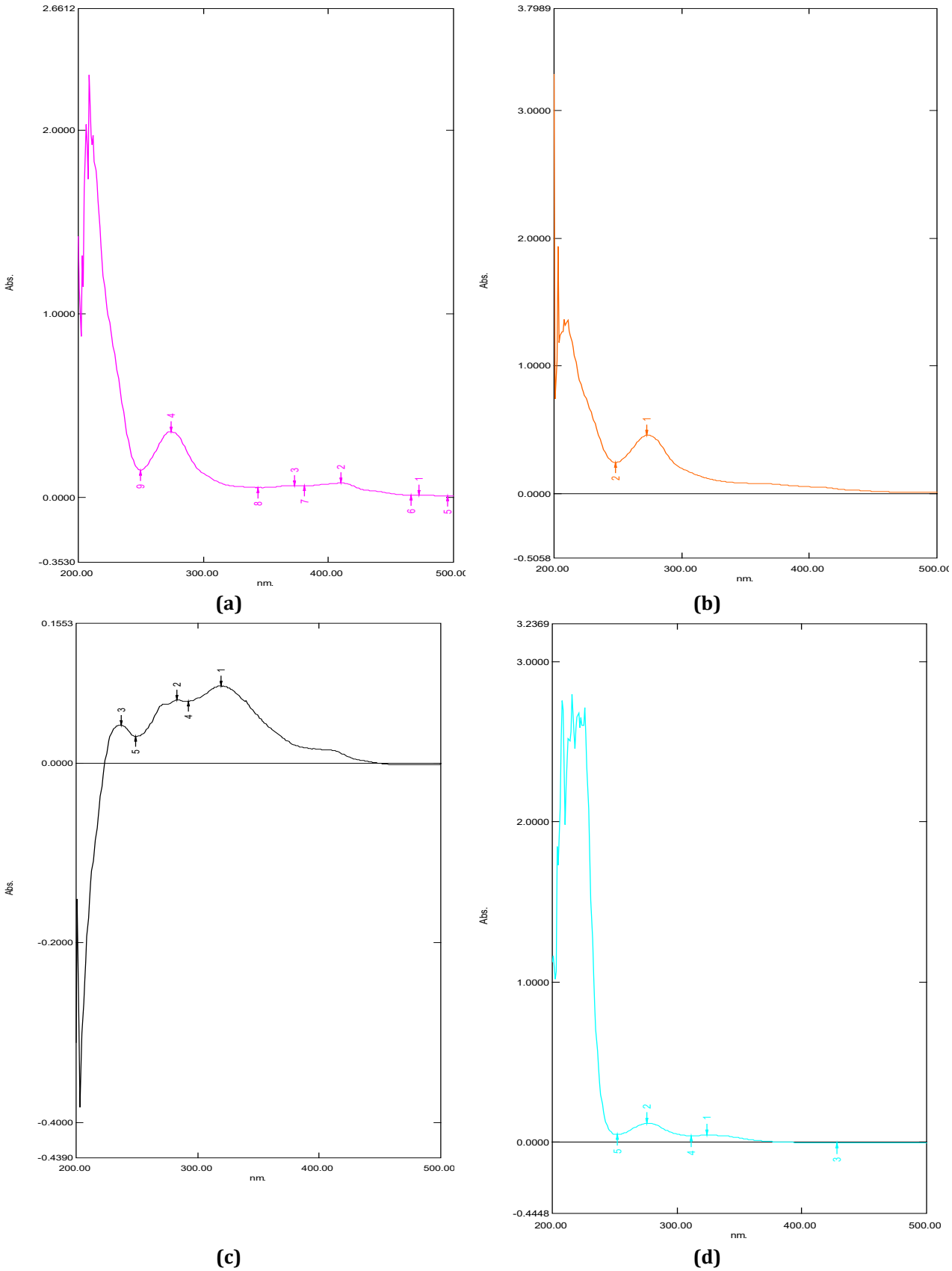
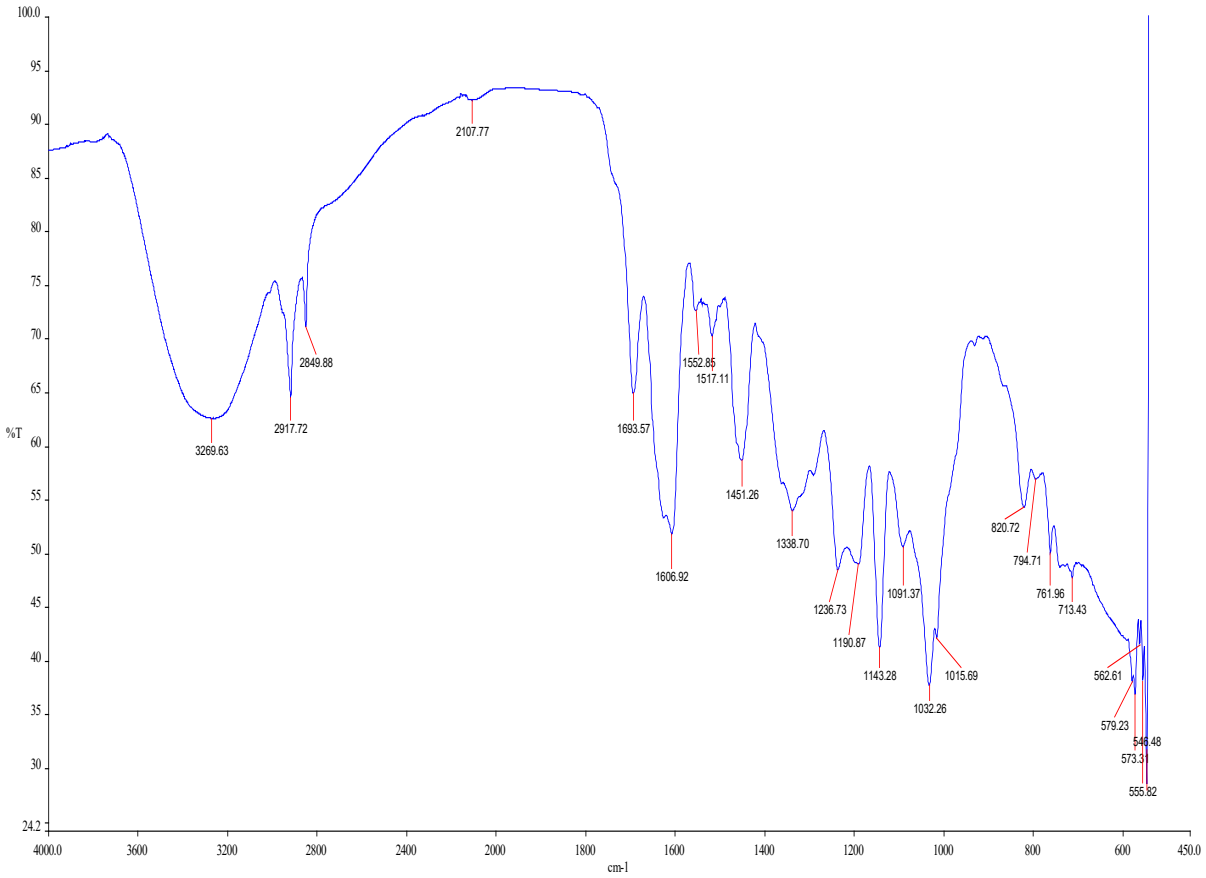
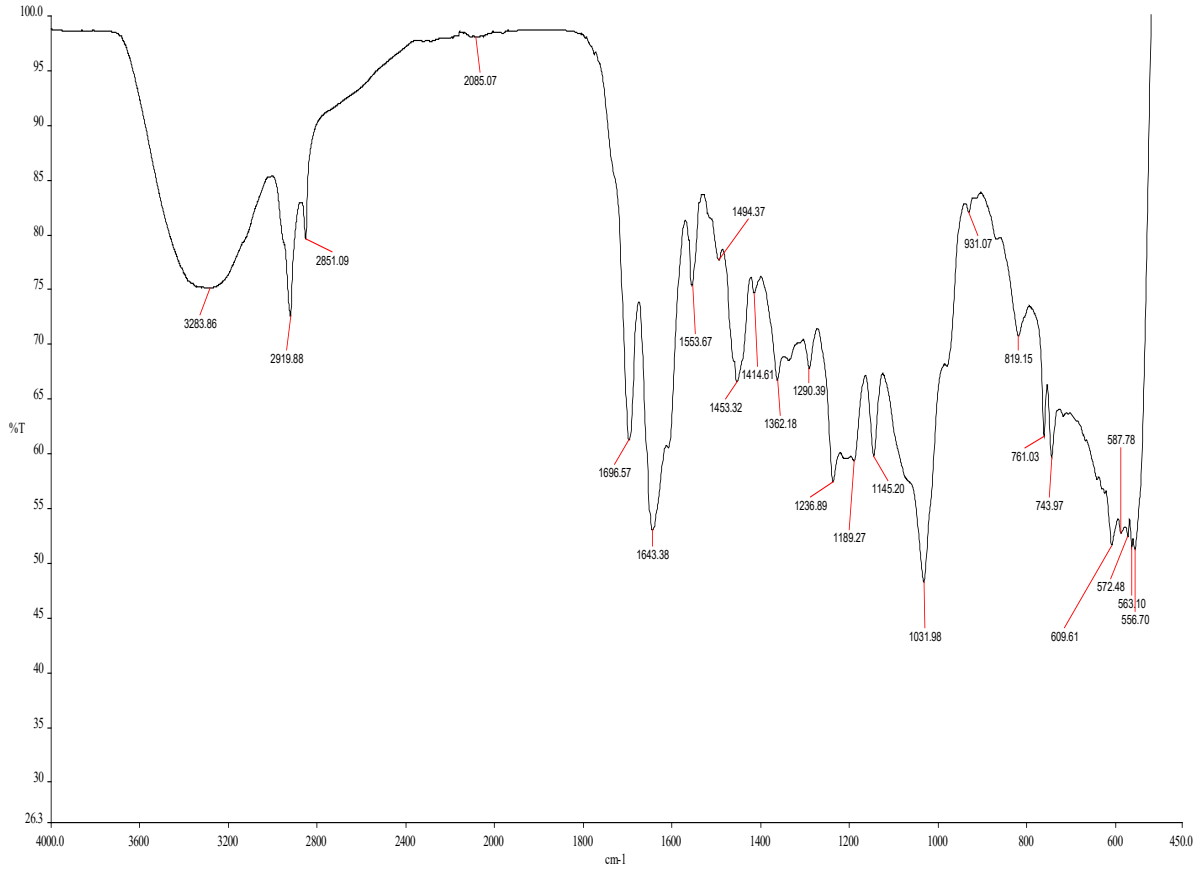


Fig. 2 *UV-Visible spectra various types of tea and coffee (a) Green tea; (b) Black tea; (c) Chamomile tea; (d) Coffee extracts*

The FTIR spectra of tea and coffee extracts were analysed to obtain the spectral fingerprint of each sample and are shown in Fig 3. Spectra are recorded in the region 4000-450 cm^{-1}. Generally, the spectra between 1400-650 cm^{-1} are fingerprint regions which can differentiate the profile of each sample. The stretching vibrations of the O-H broadband were observed at the region of 3200-3600 cm^{-1} in all tea extracts, indicating the presence of a hydroxyl group in polysaccharides, polyphenols, and sugars [25, 26]. Coffee extract showed a distinct peak at 3462 cm^{-1}, corresponding to N-H stretching vibrations, indicating the presence an amine functional group commonly associated with caffeine. This observation is consistent with the UV-Vis spectra, which exhibited characteristic absorption bands attributed to the electronic transitions of caffeine. Two sharp peaks at region 2924- 2854 cm^{-1} in tea and coffee extracts showed the stretching vibration of C-H saturated carbon corresponded to C-H methylene groups from the lipid-saturated hydrocarbon chain [26, 27]. The presence of sharp absorption bands at region 1640-1746 cm^{-1} corresponded to carbonyl (C=O), which could suggest the presence of polyphenols, fatty acids, and amino acids [26]. Two sharp peaks were observed at region 1600 and 1450 cm^{-1} associated with the existence of a C=C aromatic ring in green tea, black tea and coffee extracts. The presence of a C-H bending peak at 1376 and 1377 cm^{-1} were found in chamomile tea and coffee extracts. The observed peaks at 1143 and 1145 cm^{-1} in green tea and black tea represents the existence of C-O stretching vibrations. The peaks at region 1160 cm^{-1} represented the existence of C-N stretching vibration in the coffee extract. The FTIR peaks corresponding to the O-H stretching, C=C aromatic ring and C-O stretching vibrations in green and black tea indicate the presence of catechin as the primary compound [28]. These findings were further supported by the characteristic absorption bands in the UV-Vis spectra, which displayed π–π* transitions associated with conjugated aromatic systems in the catechin structure.



(a)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1696.57
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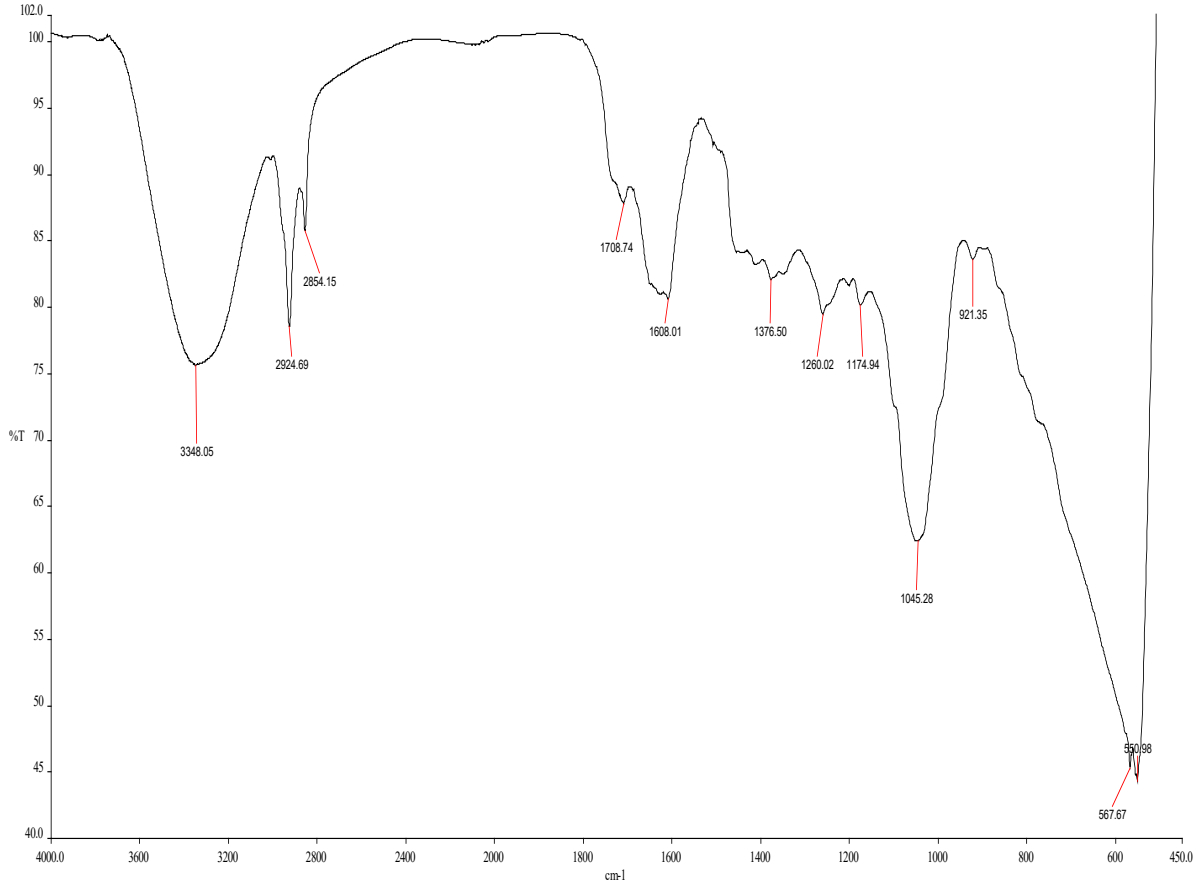
(b)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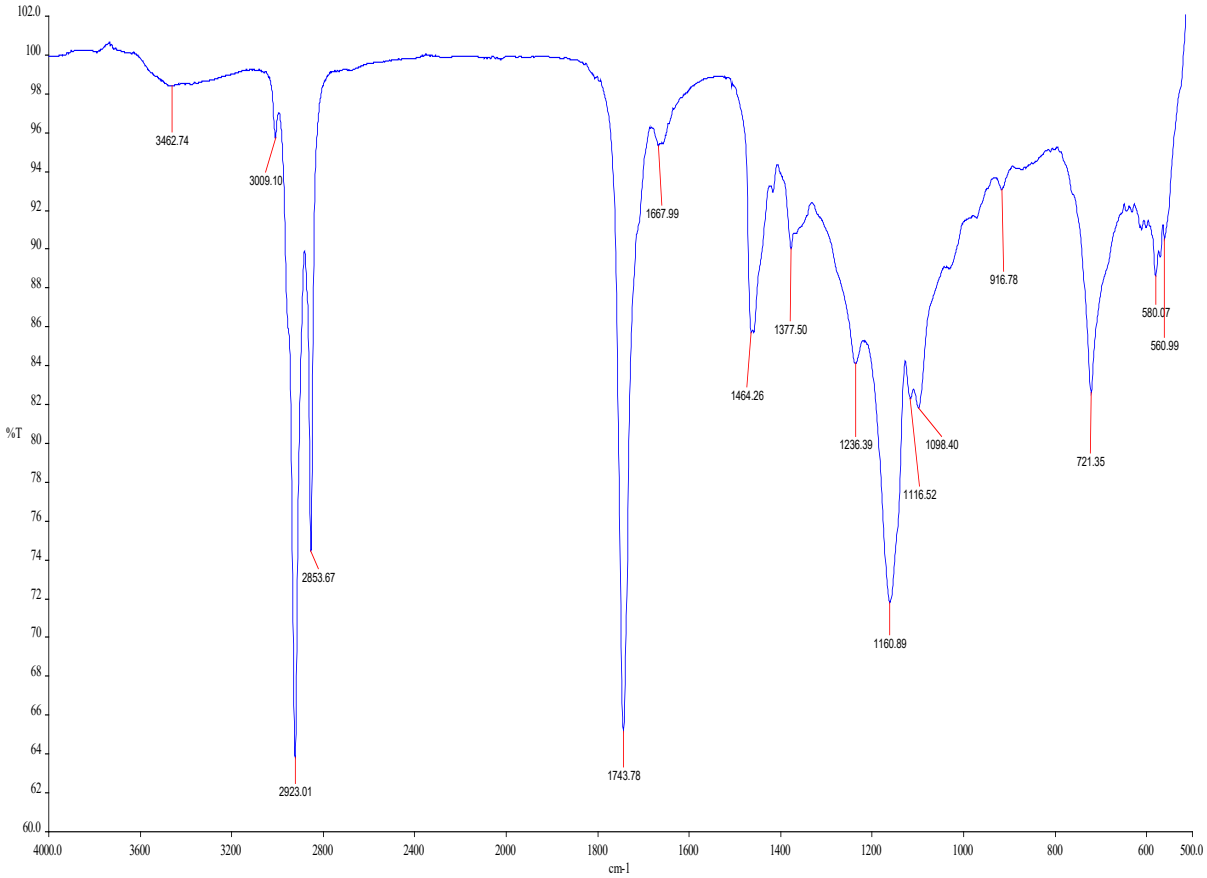
(c)



(d)

Fig. 3 *FTIR spectra various types of tea and coffee (a) Green tea; (b) Black tea; (c) Chamomile tea; (d) Coffee extracts*

4. Conclusion

In conclusion, the comparison chemical fingerprint of green tea, black tea, chamomile tea and coffee extracts were observed as analysed through SEM, UV-Vis and FTIR spectroscopy, which revealed clear distinctions among the samples. Green tea and black tea extracts demonstrated comparable spectral profiles, suggesting a similarity in their chemical composition. In contrast, chamomile tea extract exhibited a unique fingerprint, and coffee extract showed distinct chemical fingerprint as compared to other samples. These findings highlight the potential spectroscopic techniques for distinguishing and characterizing the unique chemical profiles of different food products. Furthermore, these methods can be applied in food authentication and quality control, aiding in the verification of product authenticity, monitoring quality, and ensuring regulatory compliance throughout the supply chain. Further investigation on the integration of chemometric approaches and machine learning algorithms should be conducted to enhance the classification accuracy and spectroscopic data analysis.

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Conflict of Interest

The authors declare that there is no conflict of interest regarding the publication of the paper.

Author Contribution

The authors confirm contribution to the paper as follows: ***study conception and design:*** *AAMB;* ***data collection:*** *SMM, NNANA, AYMNH, NAFMF, NHAMS, NAR;* ***analysis and interpretation of results:*** *AAMB, SMM, NNANA, AYMNH, NAFMF, NHAMS, NAR;* ***draft manuscript preparation:*** *AAMB, MHMZ, SMM, NNANA, AYMNH, NAFMF, NHAMS, NAR. All authors reviewed the results and approved the final version of the manuscript.*

References

[1] Chan, E. W., Soh, E. Y., Tie, P. P., & Law, Y. P. (2011). Antioxidant and antibacterial properties of green, black, and herbal teas of Camellia sinensis. *Pharmacognosy research*, *3*(4), 266.

[2] Liczbiński, P., & Bukowska, B. (2022). Tea and coffee polyphenols and their biological properties based on the latest in vitro investigations. *Industrial Crops and Products, 175*, 114265.

[3] Thomson, J. (2022). Massive, strange white structures appear on Utah's Great Salt Lake. *Newsweek*.

[4] de Melo Pereira, G. V., de Carvalho Neto, D. P., Júnior, A. I. M., Vásquez, Z. S., Medeiros, A. B., Vandenberghe, L. P., & Soccol, C. R. (2019). Exploring the impacts of postharvest processing on the aroma formation of coffee beans–A review. *Food Chemistry, 272*, 441-452.

[5] Wiseman, S. A., Balentine, D. A., & Frei, B. (1997). Antioxidants in tea. *Critical Reviews in Food Science & Nutrition, 37(8),* 705-718.

[6] Khan, N., & Mukhtar, H. (2007). Tea polyphenols for health promotion. *Life Sciences, 81(7),* 519-533.

[7] Ravindranath, M., Sumobay, C., Ramasamy, V., Muthugounder, S., Selvan, S., Brosman, S., & Morton, D. (2007). Response of lymph node and organ metastasized melanoma cells to green tea catechins (EGCG, EGC & ECG) differs markedly from that of prostate and epithelial ovarian carcinomas. *Cancer Research, 67(9*), 5538-5538.

[8] Clark, I., & Landolt, H. P. (2017). Coffee, caffeine, and sleep: A systematic review of epidemiological studies and randomized controlled trials. *Sleep Medicine Reviews, 31*, 70-78.

[9] Açıkalın, B., & Sanlier, N. (2021). Coffee and its effects on the immune system. *Trends in Food Science & Technology, 114*, 625-632.

[10] Fujimoto, H., Narita, Y., Iwai, K., Hanzawa, T., Kobayashi, T., Kakiuchi, M., ... & Toko, K. (2021). Bitterness compounds in coffee brew measured by analytical instruments and taste sensing system. *Food Chemistry, 342*, 128228.

[11] Lee, M., McGeer, E. G., & McGeer, P. L. (2016). Quercetin, not caffeine, is a major neuroprotective component in coffee. *Neurobiology of Aging, 46*, 113-123.

[12] Ahmad, A., & Ayub, H. (2022). Fourier transform infrared spectroscopy (FTIR) technique for food analysis and authentication. In Nondestructive quality assessment techniques for fresh fruits and vegetables (pp. 103-142). Singapore: Springer Nature Singapore.

[13] Wang, Y., Xian, J., Xi, X., & Wei, X. (2013). Multifingerprint and quality control analysis of tea polysaccharides. *Carbohydrate Polymers, 92(1),* 583–590.

[14] Belay, A., Ture, K., Redi, M., & Asfaw, A. (2008). Measurement of caffeine in coffee beans with UV/vis spectrometer. *Food Chemistry, 108(1),* 310-315.

[15] López-Martínez, L., López-de-Alba, P. L., García-Campos, R., & De León-Rodríguez, L. M. (2003). Simultaneous determination of methylxanthines in coffees and teas by UV-Vis spectrophotometry and partial least squares. *Analytica Chimica Acta, 493(1)*, 83-94.

[16] Arifah, M. F., Hastuti, A. A. M. B. H., & Rohman, A. (2022). Utilization of UV-visible and FTIR spectroscopy coupled with chemometrics for differentiation of Indonesian tea: an exploratory study. *Indonesian Journal of Pharmacy, 33(2)*, 200-207.

[17] Atomssa, T., & Gholap, A. V. (2015). Characterization and determination of catechins in green tea leaves using UV-visible spectrometer. *Journal Engineering Technology Research, 7(1),* 22-31.

[18] Badiazaman, A. A. M., Mohd, K. S., Zin, N. B. M., Mohamad, H., & Aziz, A. N. (2023). HPTLC profiling and FTIR fingerprinting coupled with chemometric analysis of Malaysian stingless bee propolis. *Jurnal Teknologi, 85(2)*, 121-131.

[19] Kumar, S., & Singh, P. (2021). SEM characterization of plant-based biosorbents for environmental applications. *Environmental Science and Technology, 32(4),* 675–689.

[20] Lee, H., Park, J., & Kim, S. (2020). Morphological changes in tea leaves during processing: Insights from SEM studies. *Springer Nature, 45(6),* 921–933.

[21] Chen, J., Wang, F., & Li, Z. (2023). Structural properties of tea-based adsorbents: An SEM analysis. *Applied Sciences, 23(13),* 1984–1992

[22] Ali, R., & Zhang, L. (2022). Surface morphology of tea leaf materials: Implications for bioactive compound release. *Journal of Plant Science, 14(2),* 112–120.

[23] Sarkar, D., Das, S., & Pramanik, A. (2014). A solution spectroscopy study of tea polyphenol and cellulose: Effect of surfactants. *RSC Advances, 4(68),* 36196–36205

[24] Boulet, J. C., Ducasse, M. A., & Cheynier, V. (2017). Ultraviolet spectroscopy study of phenolic substances and other major compounds in red wines: relationship between astringency and the concentration of phenolic substances. *Australian Journal of Grape and Wine Research, 23(2),* 193–199

[25] Esteki, M., Memarbashi, N., & Simal-Gandara, J. (2022). Classification and authentication of tea according to their geographical origin based on FT-IR fingerprinting using pattern recognition methods. *Journal of Food Composition and Analysis, 106,* 104321.

[26] Thummajitsakul, S., Samaikam, S., Tacha, S., & Silprasit, K. (2020). Study on FTIR spectroscopy, total phenolic content, antioxidant activity and anti-amylase activity of extracts and different tea forms of Garcinia schomburgkiana leaves. *LWT, 134*, 110005.
[27] Ou, Q., Li, J., Yang, X., Yang, W., Liu, G., & Shi, Y. (2021). Identification of Pu'er raw tea with different storage years by infrared spectroscopy. *Journal of Food Processing and Preservation*, *45(12),* e16103.
[28] Xia, J., Wang, D., Liang, P., Zhang, D., Du, X., Ni, D., & Yu, Z. (2020). Vibrational (FT-IR, Raman) analysis of tea catechins based on both theoretical calculations and experiments. *Biophysical Chemistry*, *256*, 106282.