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A Laboratory Computational Study for the Detection of Acrylamide in Coffee and Chips Products Using FTIR and DFT

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A B S T R A C T

The present study utilizes Fourier-transform infrared spectroscopy (FTIR) and density functional theory (DFT) to demonstrate that a range of products contain significant acrylamide components. The products under consideration are Tora Bika from Indonesia, Mokate from Poland, Chips box from Libya, as well as Averroes and Liz from Egypt. The analysis revealed the presence of acrylamide in all of the products, as indicated by the positive results for functional groups. However, the majority of the samples yielded negative results, indicating the absence of all the required groups. Samples containing the C-N functional group exhibited positive results for acrylamide, with samples C-2, C-10, P-1, P-2, and P-5 demonstrating positive signals. The computational results for acrylamide demonstrated a wavelength of 212.45 nanometers (nm), suggesting the presence of high energy due to the application of heat. Prior to the application of heat, the wavelengths of caffeine and amylose were measured to be 298.74 nm and 778.3 nm, respectively. Subsequent to the application of heat, the impact of acrylamide on the extinction coefficient of caffeine and amylose was examined, exhibiting a shift from 298.74 to 274.56 nm and from 778.3 to 244.88 nm, respectively. This phenomenon is attributed to the heightened energy derived from the roasting and cooking processes conducted at elevated temperatures. The polar moment of caffeine and amylose underwent a substantial shift, changing from 3.43 to 6.76 Debye and 7.09 to 15.42 Debye. This phenomenon is indicative of an increase in the density of the caffeine-amylose complex with acrylamide, which also causes a change in color to darker shades due to the increased density and concentration of acrylamide as a complex.

1 Introduction

During the cooking process, heat application is displayed to play an important role in the protection and quality of foods. This process is shown to increase the sensory characteristics of food, including its taste and texture. However, contemporary food processing has led to concerns about the presence of harmful chemicals. The process of heating food can result in generation of toxins [Tareke et al., 2002].

Consumption of potatoes and coffee is generally considered safe practice. However, it is important to note that some cooking methods may pose potential risk. For example, the preparation of high temperatures of the potato is displayed to obtain carcinogenic by products including acrylamide [Tucker & Featherstone, 2010]. Consumption of fried potatoes is associated with weight gain, type 2 diabetes and increasing risk of heart diseases. Coffee consumption in moderation is displayed to secure; however, it has been observed that consumption of hot coffee can produce potentially harmful substances. In addition, excessive amounts of

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caffeine are associated with adverse effects including ingestion, anxiety, insomnia and gastrointestinal crisis [Mogol & Go¨kmen, 2016].

Coffee is the third most popular drink worldwide, playing an important role in global trade and more benefiting from seventy countries [Corrêa et al., 2021; Hu et al., 2019; Hu et al., 2020; Vignoli et al., 2014]. The production of coffee includes selection of high quality beans and their subsequent processing through drying, roasted and grinding [Soares et al., 2015]. The roasted process makes different types of coffee depending on consumer preferences, [Kucˇera et al., 2016; Worku et al., 2023, Tassew et al., 2021] such as light, medium and dark roasted in Figure (1) [Toci, A.T, et al. 2020]. **bou.hosouna@sebhau.edu.ly**

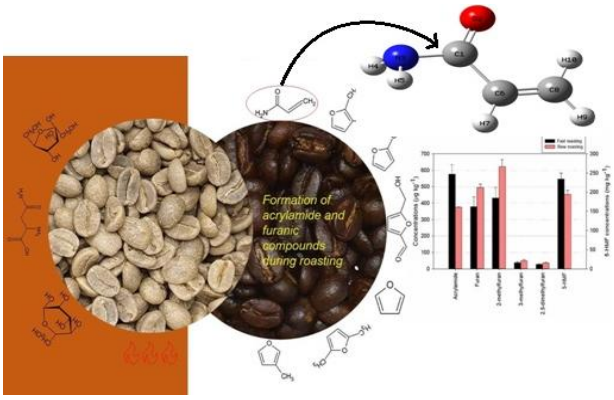

Figure 1: The appearance of Acrylamide after roasting at high temperatures [Hsin-Chieh et al., 2024].

The theme of high temperature processing has been focused on comprehensive research due to its ability to generate harmful compounds that can negatively affect human health [Schouten et al., 2020; Chang et al., 2020]. The presence of acrylamide, a chemical compound associated with the maillard reaction, [Ecile et al., 2016; Boyaci-Gunduz, 2022] is affected by various factors, including the type of coffee bean and the degree and duration of frying [Alsafra et al., 2023; Strocchi et al., 2022].

A comparable example is potato chips, a widely eaten snack, which is produced by subjugating thin potato slices under high temperature frying. The visual appeal of potato chips, which includes factors such as colors and absence of flaws, have adequate effects on consumer acceptance [Pedreschi et al., 2016]. The golden-brown color of the potato is the result of lipid oxidation and chemical reactions that occur during the frying process. These reactions are affected by potato types, oil types and cooking conditions [Marquez & Añon, 1986]. In terms of industrial frying, frequent application of high temperatures during processing of cooking oils may result in a decline in oil quality. Concurrently, this process can achieve the production of sub -products that are entitled to the properties that are considered defective [Hwang, 2019]. The present study will employ a dual approach, which will include laboratory experiments and theoretical computational methods, to certify its findings and the effect of temperature on color changes and increased appearance of acrylamide, as illustrated in Figure (2).

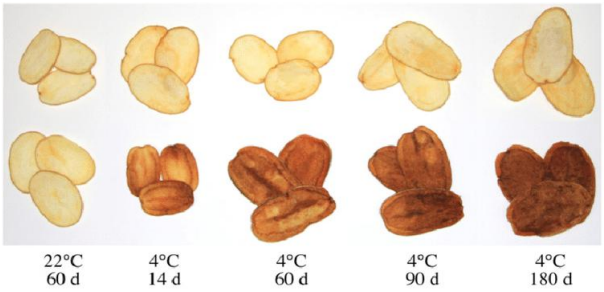

Figure 2: The effect of temperature on color change and the enhanced appearance of Acrylamide [Bhaskar et al., 2010].

The research will employ Fourier Transform Infrared (FTIR) spectroscopy, a technique that measures how much light at different frequencies is absorbed by the sample, allowing for detailed analysis of its properties [Griffiths & de Hasseth, 2007]. Furthermore, computational chemistry will be employed to generate mathematical models for efficient analysis, thereby reducing the necessity for substantial quantities of materials typically utilized in laboratory settings [Krishnan & Kannan, 2021]. This approach has been demonstrated to facilitate the resolution of scientific challenges and promote comprehensive research. Chemical computing works a main role in the field of drug analysis, facilitating the measurement of binding energies and the discernment of the distinct effects manifested by various compounds [Hardin & Drnevich, 1972]. In the absence of empirical research examining the presence of acrylamide in Libya's food products, previous studies investigating the dangers of acrylamide in coffee and potato products are of limited use.

2 Materials and Methods

Practical Part:

Infrared spectroscopy (FTIR) is an extensive instrument in the area of chemical analysis, as it permits the acquisition of critical information regarding useful corporations. In this examine, a Michelson interferometer with a source, beam splitter, and detector might be utilized, using either a Cary 630 or a Shimadzu version. This tool is hired to generate an interferogram, which is then processed by software to yield a molecular spectrum, or "fingerprint," this is specific to the pattern underneath investigation. The key settings encompass the spectral variety, which may be special as a number

of 400-4000 cm^{-1}, for instance, in the context of mid-IR, and a transmittance ranging from -5 to 15%. A selection of corporations operating in the Libyan marketplace turned into surveyed to accumulate a sample of food products intended for evaluation, specifically espresso and potato products. The specific corporations and their respective merchandise are enumerated in Table 1.

Table 1: Presents a Commercial samples used in this study.

	Sample type	product trade name	country of production
C-1	Coffee	Maccofee	Malaysia
C-2	Coffee	Tora Bika	Indonesia
C-3	Coffee	Santos	Indonesia
C-4	Coffee	Mic coffe Espresso	Italy
C-5	Coffee	Italian coffee	Italy
C-6	Coffee	Gulf coffee	Libya
C-7	Coffee	Brazilian coffee	Brazil
C-8	Coffee	Colombian coffee	Colombia
C-9	Coffee	Nestli	Brazil
C-10	Coffee	Mokate	Poland
P-1	Chips	Chips Box	Libya
P-2	Chips	Turquoise Long	Egypt
P-3	Chips	Dorisos	Egypt
P-4	Chips	Tiger	Egypt
P-5	Chips	Lay's	Egypt
P-6	Chips	Corn captain	Libya
P-7	Chips	Tringles	Egypt
P-8	Chips	Pringles	Egypt

They were classified and nominated according to their first Latin letters. Coffee samples were labeled C-1, C-2, C-3, C-4, C-5, C-6, C-7, C-8, and C-9, while potato samples were labeled P-1, P-2, P-3, P-4, P-5, P-6, P-7, and P-8. These products were carefully prepared in plastic containers, especially named for chemical analysis after the fully drying process to ensure complete elimination of any residual moisture. Specific information for each product, including the name of the product, the name of the company, the country of production and the expiration date, was fully recorded on these containers.

The process of preparing the sample was started in a timely manner, due to its transparency in the infrared area, the potassium bromide (KBR) was employed as a stabilizer, enabling the transmission of light and subsequent analysis of the sample. The solid samples to be analyzed are then mixed with powder potassium bromide and subsequently compressed to create a transparent disc that allows the infrared light to pass. The purpose of this configuration is to facilitate the stabilization of the sample during its placement within the infrared spectrometer. Subsequently, each sample is individually analyzed in an FTIR device to achieve results for functional groups within each sample.

Computational Part:

The study of electron behavior is paramount for understanding the properties of specific substances. Historically, quantum mechanical equations were used especially for single-electron system [Esposito, G. et al. 2004]. However, recent progress in mathematical methods has enabled the discovery of estimated solutions to the systems that include several electrons. Quantum computing has effectively challenged traditional classical physics paradigms, which has a profound impact on events such as the blackbody effect and photoelectric effect [Rai-Choudhury, *1997*; Natelson, 2000].

The geometric structures of the complex were created from data provided by the Cambridge Structural Database and adapted to Gaussian 06/09 software, by using B3LYP (Becke, 3-parameter) is a very popular hybrid functional in Density Functional Theory (DFT) by the main key for calculation is (# td b3lyp/sdd nosymm scf=qc geom=connectivity). The purpose of adjusting geometry is to detect the stable point of a molecule, in which it is most stable, usually at the lowest energy level. The configuration of the structure at low energy levels has been demonstrated to facilitate the prevention of issues in reaching the state reaching the state [Natelson, 2000].

Density functional theory (DFT) is a fundamental principle in molecular modeling that facilitates an understanding of various types of events in chemistry and physics [Assadi, et al., 2013]. This is mandatory for analysis of molecular interaction and understanding of chemical reactions [Van & Gdanitz, 2002; Vondrášek, et al., 2005]. The DFT has also been employed in the study of catalysts and tangled systems; however, improper handling of certain concepts can lead to errors [Grimme, 2006; Zimmerli et al., 2004, Grimme, 2004; Von et al., 2004, Tkatchenko & Scheffler, 2009]. Researchers are currently engaged in efforts to increase the accuracy of DFT by modifying existing methods. The study indicates that this quantum chemistry approach can provide a better energy efficiency than traditional methods [Lewars, 2010; Ambraseys, 1988].

[Vignale et al., 1987].

$$\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \left[\sum_{i}^{N}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_{i}^{N} V(\mathbf{r}_i) + \sum_{i<j}^{N} U(\mathbf{r}_i, \mathbf{r}_j)\right]\Psi = E\Psi$$

3 Results

Laboratory Results:

To presents the findings of FTIR spectroscopy analysis, which were divided into two categories: coffee samples, designated by names beginning with the letter C, representing the first letter of the word "coffee," and potato samples, designated by names beginning with the letter P, representing the first letter of the word "potatoes," as outlined in Table 2.

Table 2: shows the results of the analysis demonstrate the presence of acrylamide in certain products, indicated by a positive (+) sign, and its absence, indicated by a negative (-) sign.

	Sample type	product trade name	country of production	Acrylamide detection result
C-1	Coffee	Maccofee	Malaysia	**(-)**
C-2	Coffee	Tora Bika	Indonesia	**(+)**
C-3	Coffee	Santos	Indonesia	**(-)**
C-4	Coffee	Mic coffe Espresso	Italy	**(-)**
C-5	Coffee	Italian coffee	Italy	**(-)**
C-6	Coffee	Gulf coffee	Libya	**(-)**
C-7	Coffee	Brazilian coffee	Brazil	**(-)**
C-8	Coffee	Colombian coffee	Colombia	**(-)**
C-9	Coffee	Nestli	Brazil	**(-)**
C10-	Coffee	Mokate	Poland	**(+)**
P-1	Chips	Chips Box	Libya	**(+)**
P-2	Chips	Turquoise Long	Egypt	**(+)**
P-3	Chips	Dorisos	Egypt	**(-)**
P-4	Chips	Tiger	Egypt	**(-)**
P-5	Chips	Lay's	Egypt	**(+)**
P-6	Chips	Corn captain	Libya	**(-)**
P-7	Chips	Tringles	Egypt	**(-)**
P-8	Chips	Pringles	Egypt	**(-)**

Where the red sign (+) means a positive result in the presence of Acrylamide, and the green sign (-) means a negative result in the absence of Acrylamide.

The infrared spectrum of acrylamide displays in Figure both positive and negative results. The following discussion will clarify the expansion of each functional group that forms acrylamide in samples.

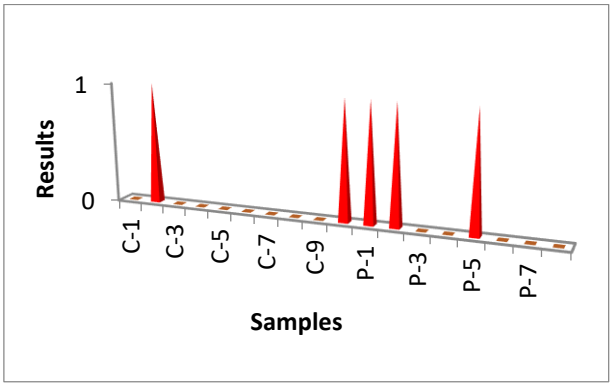

Figure 3: FTIR spectrum of the positive and negative samples in the presence of Acrylamide compound.

As evidenced by the samples (C-2, C-10, P-1, P-2, and P-5) containing acrylamide, positive spectral signals were detected for all functional groups complementary to the acrylamide compound as painted in Figure 3.
The presence of acrylamide was confirmed in two coffee products, Indonesian Tora Bika C -2 and Polish Mokate C -10, as indicated by the presence of functional groups characteristic characteristic in infrared spectrum as painted in (Figures 4 and 5). However, the remaining coffee products (C-1, C-3, C-4, C-5, C-6, C-7, C-8, and C-9) demonstrated negative results, suggesting the absence of some functional groups of acrylamide and as a result, confirms its non-conservations in these products.

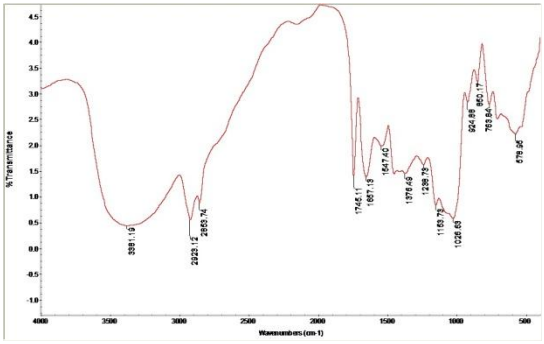

Figure 4: FTIR spectrum of sample C-2.

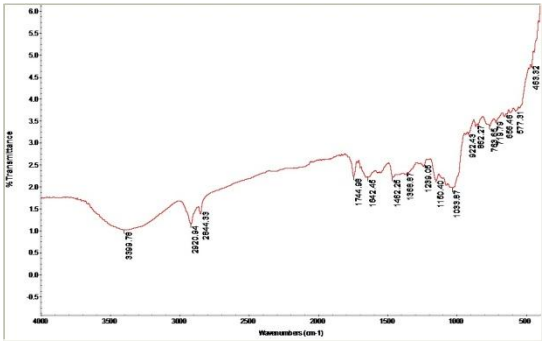

Figure 5: FTIR spectrum of sample C-10.

In the case of potato products, especially built by box chips, Libya (P -1), built by Fairuz Long, Egypt (P -2), and finally produced by Egypt (P -5), the results were also positive, confirming the presence of acrylamide with all its functional groups in the infrared spectrum. As Figures are displayed in 6, 7, and 8 respectively. But the remaining potato products (P -8, P -7, P -6, P -4, and P -3) demonstrated negative results, refuting the hypothesis that some functional groups of acrylamide are present. This result does not provide certain evidence for the presence of acrylamide in these products.

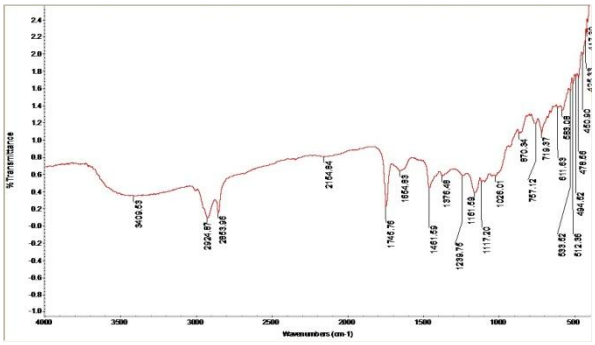

Figure 6: FTIR spectrum of sample P-1

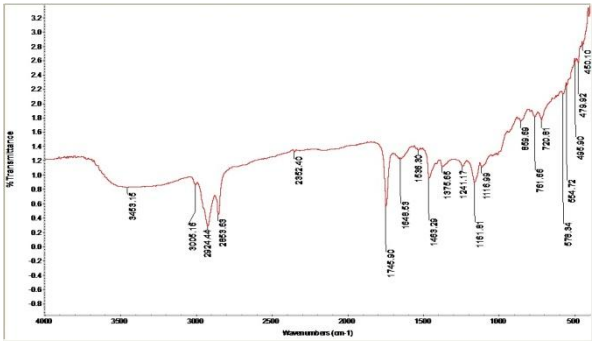

Figure 7: FTIR spectrum of sample P-2.

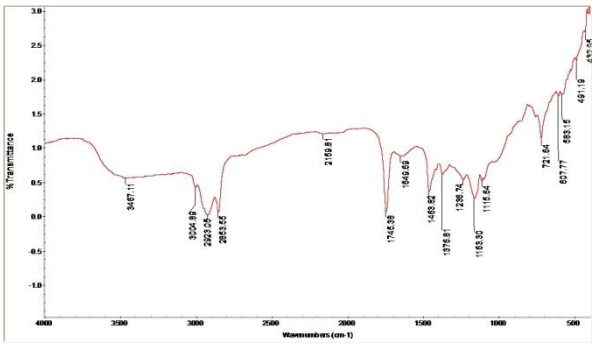

Figure 8: FTIR spectrum of sample P-5.

Computational Results

In this section, the interaction of acrylamide with coffee and potato complexes was presented and evaluated, and the computational effect of connecting acrylamide was observed. The results of the study are as follows:

In this section, UV spectral analysis of primary chemical structures of caffeine ($C_8N_4O_2H_{10}$), key compounds of coffee and amilos ($C_{12}O_{11}H_{21}$) were examined as individual compounds and in combination with acrylamide (C_3NOH_5). As the Figures are illustrated in 9, 10, 11, 12, 13 and 14, acrylamide, caffeine, and amylose, when coffee is roasted and potatoes are cooked at high temperatures. As the Figures are illustrated in 15, 16, 17 and 18, the formation of caffeine- acrylamide complexes and amylose- acrylamide complexes is performed.

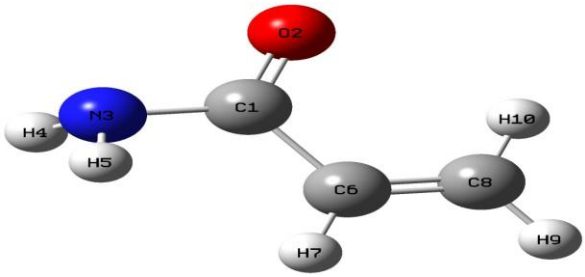

Figure 9: Computational spatial structure of Acrylamide.

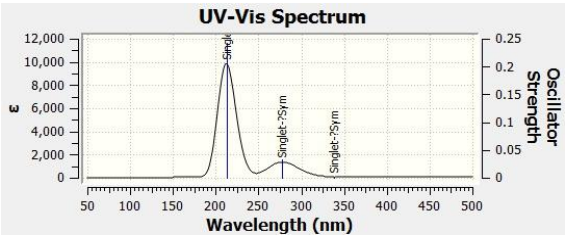

Figure 10: UV-vis spectrum of Acrylamide.

As displayed in Figure 11, the UV spectrum of acrylamide displays an absorption band in the wavelength of 212.45 (nm), it is a sign of its high energy. Therefore, it can be concluded that these wavelength levels are seen only on high energy, which is the direct result of high temperatures. It is an early physical factor that has a significant impact on the growth seen in energy. The polar moment value of the molecule was determined for 4.68 Debye. Concurrently, individual compounds as wavelength spectra of caffeine and amylose demonstrated high wavelengths, indicating low energy, at low temperatures before the process of roasting and cooking, as displayed in Figures 12, 13 and Figures 14, 15 for amylase.

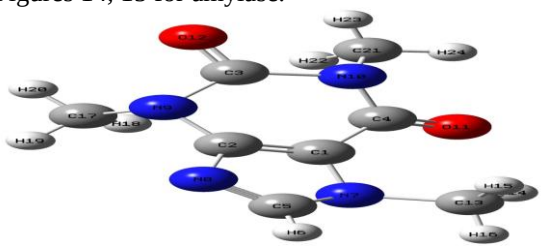

Figure 11: Computational spatial structure of Caffeine.

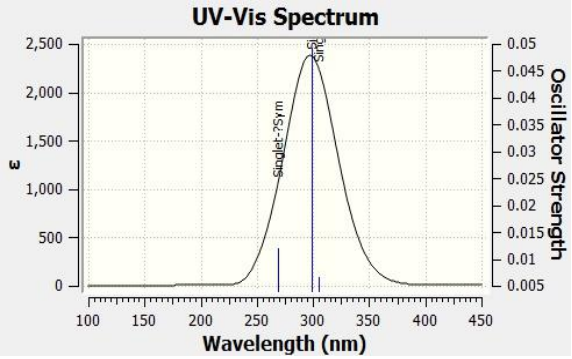

Figure 12: UV-vis spectrum of Caffeine.

As seen, caffeine's UV spectrum performed the highest degree of absorption at a wavelength of 298.74 nm, which corresponds to natural absorption before heating and roasting processes. Its polar moment value was scheduled to be 3.437042 Debye.

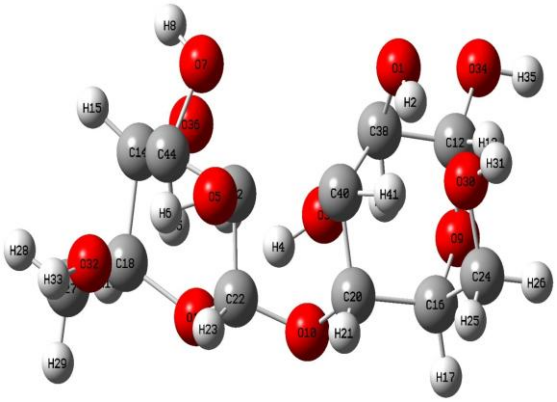

Figure 13: Computational spatial structure of the Amylose complex.

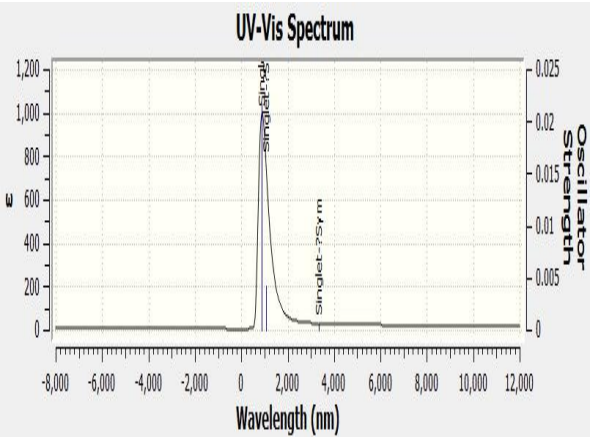

Figure 14: UV-vis spectrum of the Amylose compound.

As seen, the UV spectrum of amylose performed the highest degree of absorption at a wavelength of 778.3 nm, which corresponds to natural absorption before heating and cooking processes. The value of its polar moment was fixed at 7.09 Debye.

It has been established through several studies referred to the presence of acrylamide has a significant impact on the presence of coffee and potato roasting at high temperatures, the changes in the optical density of the caffeine. This phenomenon responsible for high energy levels generated by the roasting process has been observed to transfer caffeine's absorption spectrum from 298.74 nm to 274.56 nm. In addition, 6.76 Debye was observed from 3.43 Debye, indicating sufficient increase in the density of the complex intervention between caffeine and acrylamide compounds. This change in the polar moment is concomitant with a shift in a dark color, which is attributed to an increase in the concentration of the complex after the presence of the acrylamide compound as an intervention compound adjacent to the caffeine. This observation is supported by the results of UV-Vis spectrum analysis, as depicted in Figure (17). In addition, the change in extinction of amylose from 778.3 to 244.88 nm is sufficient, providing certain evidence to the coefficient of extinction of acrylamide to the extent that affects the primary ingredient of potatoes. This change is responsible for an increase in energy generated by the cooking process at elevated temperatures. In addition, a change was seen in the polar moment. The Figures presented in Figure 17 reveal a significant increase in the density of the intervention complex between amylose and acrylamide compounds, from 7.09 to 15.42 Debye and. This increase in density is responsible for changes in color from light to darkness, indicating an increase in concentration of acrylamide compound after its appearance as an intervention compound adjacent to amylose. This observation is supported by the results of UV-VIS spectrum analysis, providing a quantitative measurement of changes in complex density.

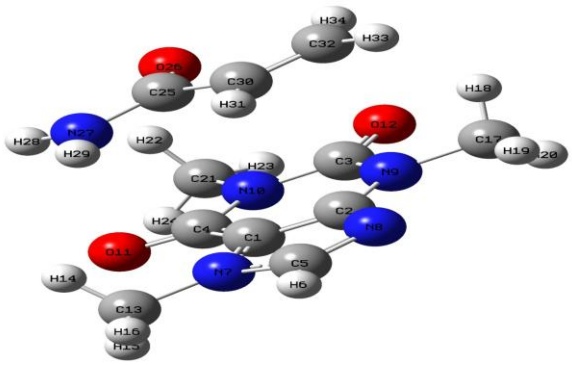

Figure 15: The computational spatial structure of the complex between Acrylamide and Caffeine.

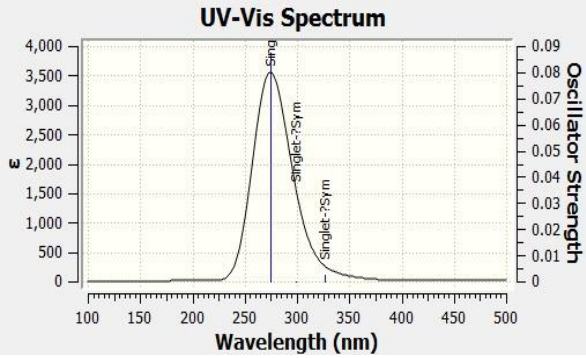

Figure 16: UV-vis spectrum of the complex between Acrylamide and Caffeine.

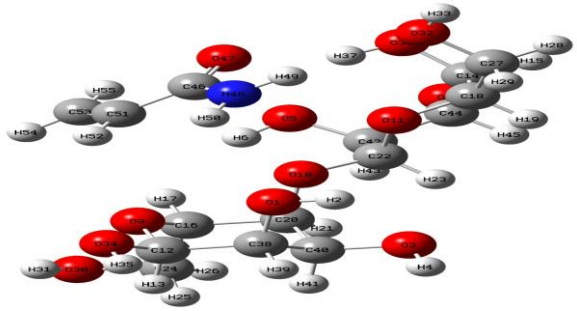

Figure 17: Computational spatial structure of the complex between acrylamide and Amylose.

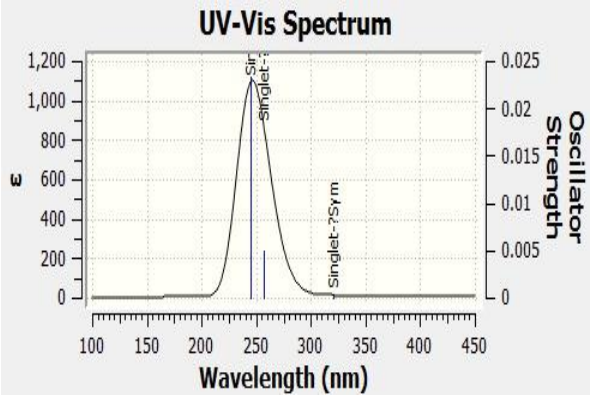

Figure 18: UV-vis spectrum of the intercalated complex between Acrylamide and Amylose.

A thorough examination of the ultraviolet spectral calculations well-known shows a precise congruence with the infrared spectral effects. This phenomenon can be attributed to the effect of acrylamide at the absorption coefficients and caffeine concentrations in coffee and potatoes.

4 Discussion

The immediate removal of products linked to acrylamide from the Libya market is required, along with a ban on producing toxic items by all companies. All commercial ties with these companies must end right away. Also the number of testing centers at international airports and border crossings needs to increase, especially for products like potato chips and modern coffee.

5 Conclusions

1. The conclusions obtained from the Fourier-Transform Infrared Spectroscopy (FTIR) and the density functional theory (DFT) indicated the presence of acrylamide functional groups in many products. The products under consideration include Tora Bika from Indonesia, Mokate from Poland, Chips Box from Libya and Long and Late from Ferozing Long and Le. All samples displayed a positive response to the presence of functional groups, reflecting the presence of acrylamide. However, the remaining samples displayed a negative response to all functional groups.
2. C-N functional group samples were examined, and the presence of acrylamide was confirmed. The results indicated that C-2, C-10, P-1, P-2, and P-5 conducted a positive test. Computer results for acrylamide demonstrated a wavelength of 212.45 nm, which suggests the generation of vital energy through heat application. Concurrent, the measurement of caffeine and amylose was recorded at 298.74 nm and 778.3 nm respectively before the heat application.

Following the application of heat, it was observed that the acrylamide compound had an impact on changes in the absorption of caffeine and amylose, decreasing to 298.74 and 778.3 nm respectively, decreased to 274.56 and 244.88 nm. This phenomenon is attributed to an increase in energy as a result of the roasting and cooking process conducted at high temperatures. In addition, the polar moments of caffeine and amylose performed a change from 3.43 to 6.76 Debye and 7.096819 to 15.42 Debye. This discovery suggests an increase in the density of the complex formed between caffeine and amylose. It is believed that an increase in the density and concentration of a competitive complex acrylamide is believed to be responsible for changes seen in a darker color from a mild shade.

Acknowledgements

We would like to express our gratitude to all the importing companies that facilitated the acquisition of these products. Additionally, we would like to acknowledge the Chemistry Department at Sebha University for providing us with advanced measuring instruments and computers. These instruments and computers were instrumental in modeling the atomic structures of the components utilized in these products.

Conflict of interest: The authors declare that there are no conflicts of interest

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