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ANALYSIS OF THE EXTRACTION PROCESS OF EUGENOL FROM PEPPER (Pimenta dioica L.) USING QUANTUM CHEMISTRY

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ABSTRACT

Pepper belongs to the Myrtaceae family, known for its berries called pimenta de dioica; it is one of the oldest spices in the world, used for its culinary and medicinal qualities. Eugenol was obtained by hydrodistillation and isolated with cyclohexane from pepper berries. Eugenol, cyclohexane, and water were characterized by quantum chemistry and electron transfer coefficient (ETC). The hyperchem simulator and semi-empirical method PM3 (SE-PM3) were used for quantum calculations of HOMO, LUMO, electrostatic potential (EP), ETC. The results of the quantum simulation coincide with the entire process and experimental result in the laboratory. From 5 grams of pepper, 10,645 milligrams of Eugenol were obtained on average. The most important thing is that the theoretical calculations agree with the laboratory results.

KEYWORDS
Eugenol, allspice, quantum-chemistry, In silico laboratory

INTRODUCTIÓN

Pepper belongs to the Myrtaceae family, known for its berries called pimenta de doica; it is one of the oldest spices in the world, used for its culinary and medicinal qualities.
Recent studies represent eugenol as a selective antitumor and antiproliferative agent, an excellent antioxidant, anticancer agent, and antimicrobial molecule. Researchers emphasize the processing, chemistry, applications of pepper, and impending modes of green and sustainable technologies, as well as the development of value-added products such as eugenol. Premachandran (2022).
Eugenol 60–90% in berries and>90% in pepper leaves is the main component of this plant. Premachandran (2022), eugenol is the majority component present in essential oils, followed by methyl-eugenol. Rodriguez (2022).
The methods to obtain the essential oil of Pimenta dioica L. have been studied, as well as the chemical profile of the oil and its biological properties, which include its effects on humans, plants, animals, insects, and microorganisms. As a result of these studies, the extraction process and operating conditions significantly impact the bioactivity of these molecules. Consequently, it is essential to select the correct combination of variables to improve the extraction and functionality of the essential oil. Avila (2022).
The essential oil of Pimenta dioica L. and its main compound (eugenol) were tested for their antibacterial potency against eight Gram-negative and Gram-positive bacteria involved in food poisoning and evaluated for their ability to inhibit mechanisms as well as motility in Pseudomonas aeruginosa, the production of violacein by Chromobacterium violaceum and the formation of biofilms on stainless steel and glass surfaces. ALrashidi (2022). Eugenol has potential: anti-inflammatory, antioxidant, antibacterial, antifungal, antiproliferative, hypoglycemic, hypotensive, anticarcinogenic, antivenom, larvicidal, and insecticidal potential. Rodrigues (2022), Barros (2022).
Researchers evaluated the biological efficacy of Hypocreales fungi (Purpureocillium lilacinum and Trichoderma harzianum) and allspice essential oil (Pimenta dioica (L.) Merrill) as nematode biocontrol agents in plantain crops. Alvarez-Ortega (2022). As an alternative to anti-inflammatory treatment, the essential oil blend is pharmacologically safe as it is non-toxic and non-mutagenic. Padilla (2022).
Statistical analysis showed that there are significant differences between root treatments. Smaller amounts of nematodes of the genera Scutellonema sp. and Rotylenchulus sp. T. harzianum presented in the treatment with 720 and 340 nematodes, respectively; in soil, populations of Scutellonema sp. and Helicotylenchus sp. they were minor. P. lilacinum plus T. harzianum were recorded in the treatment with 795 and 395 nematodes, respectively. The highest plant height, basal diameter, and leaf area were recorded in the allspice treatment with 177.85 centimeters in height Alvarez-Ortega (2022).
The current works report the bioefficacy of silver nanoparticles derived from the Pimenta dioica L. leaf (Pd@AgNPs) and the leaf extract obtained through different solvents against the larvae of malaria, filarial, and dengue vectors. Kumar (2022). The potential larvicidal activity of Pd@AgNPs was observed against the larvae of Aedes aegypti, (LC50, 2,605; LC90, 5,084 ppm), Anopheles stephensi (LC50, 3,269; LC90, 7,790 ppm) and Culex quinquefasciatus (LC50, 5,373; LC90).,

14,738 ppm) without affecting the non-target organism. Kumar (2022).

In terms of human activity, allspice essential oil has been shown to reduce ear inflammation by more than 65%. The anti-inflammatory activity of allspice essential oil is enhanced when combined with sweet orange peel and cumin essential oils. With this mixture, it is possible to reduce the inflammation of the edema by more than 85%, similar to indomethacin. Padilla (2022).

On the other hand, historically successful anticancer herbs and clinical oncology drugs paved the way to cracking cancer. Shortly, safer and more effective natural herbal medicines could systematically treat common solid tumors. Ko (2022).

Studies have been conducted with high-purity copper oxide nanoparticles synthesized using Pimenta dioica L. leaf extract as a reducing and stabilizing agent. Pillai (2022).

The objective was to evaluate a suitable procedure for the extraction of eugenol from the berries of the dioca pepper for its better use in the food and medicinal industry.

MATERIAL AND METHODS

Raw material.

For the development of this work, the fruits of the allspice tree (Pimenta dioica L.) were used, collected in August-September 2021 in the Sierra Norte of the state of Puebla (figure 1).

Figure 1. A) Pepper on the tree. B) Approach. C) Dried pepper.

Eugenol was obtained in three stages:

Laboratory procedure.

Stage 1. Obtaining eugenol by hydro distillation.

The extraction of essential oil from the fruit of the allspice tree was carried out by hydrodistillation. 5 g of allspice fruit flour (previously ground) was placed in a ball flask with 100 ml of purified water. This mixture was kept in recirculation for five h at a temperature of 70 °C. The distillate (mixture of water and eugenol) was obtained with this recirculation.

Stage 2. Isolation of eugenol from the distillate.

Isolation of eugenol was carried out according to the methodology of Khalil et al. (2017) with the following modifications.

A) The distillate obtained in the previous stage was placed in a separation funnel.

B) Technical grade cyclohexane (J.T. Baker) was added in a 10:50 ratio, cyclohexane to the separatory funnel

C) This mixture was shaken to cause molecular shocks. This mixture was done in the extraction funnel with the lid.

Two phases were observed:

1. Transparent phase corresponding to cyclohexane-eugenol at the top.
2. Opaque phase corresponding to the distillate-eugenol at the bottom.

These phases were separated and collected in an Erlenmeyer flask (figure 2). This procedure was performed twice to recover the most considerable amount of eugenol from the distillate.

Figure 2. Left to right. From separation to obtaining eugenol.

Stage 3. Desiccated. Then, to facilitate the recovery of the eugenol, 50 g of anhydrous sodium sulfate (J.T. Baker) was added to the flask containing the cyclohexane and eugenol as drying material, and the remaining solution was passed through the filtered paper to separate the excess sodium sulfate. Furthermore, allow the recovery of cyclohexane and eugenol. Next, the Erlenmeyer flask and the filter paper were rinsed with 10 ml of cyclohexane, allowing the maximum amount of eugenol to be recovered. Using a water bath, we isolated the eugenol and evaporated the cyclohexane contained in the filtrate.

Quantum chemistry.

Computational quantum chemistry has had a boom in recent decades. As we begin to reach the limits of classical computing, quantum computing has become a technology that has captured the imagination of the scientific world. Bauer (2020). For this investigation, we use the electron transfer coefficient theory. Gonzalez-Perez (2017).

An electron transfer coefficient is a number that tells us how many times a molecule needs its electrostatic potential for an electron to go from HOMO to LUMO.

We use the semi-empirical method PM3 (SE-PM3) to calculate all properties and quantum characteristics of molecules.

The equations involved in the electron transfer coefficient theory are:

Bg = |HOMO – LUMO| Equation 1

EP = | (d-) - (d+) | Equation 2

ETC = Bg/EP Equqtion 3

Where:

Bg = Band gap.

EP = Electrostatic Potential.

ETC = Electron Transfer Coefficient.

δ = Electron density. González-Pérez (2017), González-Pérez et al. (2022)

RESULTS AND DISCUSSION.

Quantum chemistry in silico.

In the table, the competition between the three compounds is presented. In the first part, the calculations of the three pure substances are stated. It is observed that the most stable substance is eugenol due to its lowest ETC value. It is followed by water and finally cyclohexane.

Table 1. Quantum chemical competition (ETCs) of water and cyclohexane vs. Eugenol.

DATA	Nombre	Reducer	Oxidizing	HOMO	LUMO	Bg	δ–	δ+	EP	ETC
564	Cyclohexane	CHN	CHN	-11.288	3.476	14.764	-0.012	0.094	0.106	139.279
104	Eugenol	EUG	EUG	-8.858	0.299	9.157	-0.094	0.184	0.278	32.939
47	Water	H_2O	H_2O	-12.316	4.059	16.375	-0.127	0.171	0.298	54.950
Option 1	Cyclohexane vs. Eugenol	CHN	EUG	-11.288	0.299	11.587	-0.012	0.184	0.196	59.115
Option 2	Cyclohexane vs. Water	CHN	H_2O	-11.288	3.476	14.764	-0.012	0.171	0.183	80.675
Option 3	Eugenol vs. Cyclohexane	EUG	CHN	-8.858	3.476	12.334	-0.094	0.094	0.188	65.606
Option 4	Eugenol vs. Water	EUG	H_2O	-8.858	4.059	12.917	-0.094	0.171	0.265	48.743
Option 5	Water vs. Cyclohexane	H_2O	CHN	-12.316	3.476	15.792	-0.127	0.094	0.221	71.457
Option 6	Water vs. Eugenol	H_2O	EUG	-12.316	0.299	12.615	-0.127	0.184	0.311	40.563

The most minor of all interactions with an ETC is the pure substance eugenol. This observation tells us that eugenol will be preserved despite all interactions. The laboratory extraction method is suitable.

It is followed by the water-eugenol interaction, option 6 (brown). The laboratory method agrees with the theory because the extraction with water was done first. In turn, theory and practice are reinforced with option 4.

Another coincidence between the laboratory method and the in-sillico theory is options 1 (blue) and 5 (purple), which refer to the interactions of eugenol and cyclohexane.

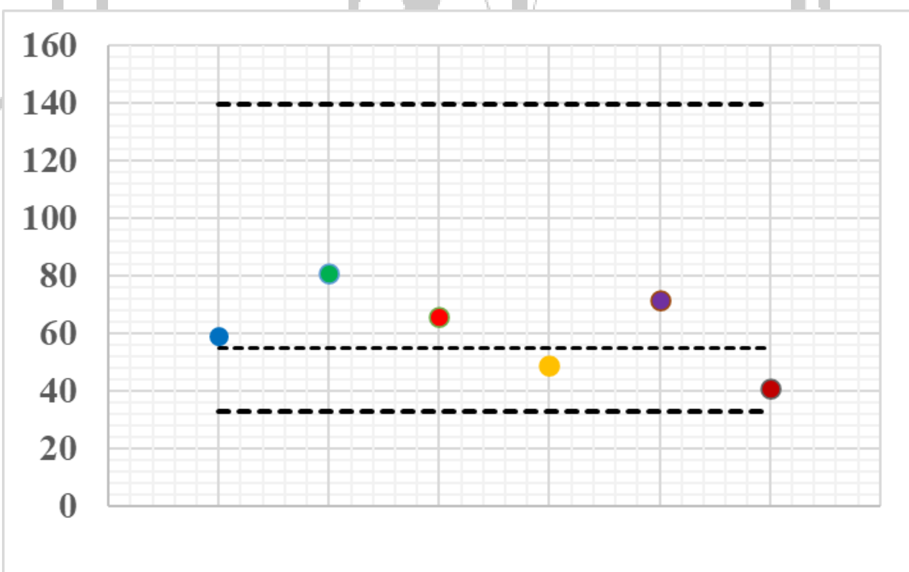

Figure 3. Quantum well bottoms of the quantum-chemical interactions of water, cyclohexane, and eugenol. The brown dot represents the bottom of the most bottomless well of interactions. This Water-eugenol interaction has the highest affinity of all the interactions.

Laboratory.

Five grams of pepper were used, and 10,645 milligrams of eugenol were obtained.

CONCLUSIONS

We extracted eugenol from allspice berries with water and cyclohexanol.

We characterize eugenol, cyclohexane, and water with quantum chemistry and the electron transfer coefficient.

Extraction with water and isolation with cyclohexane was done.

From 5 grams of pepper and 10,645 milligrams of eugenol were obtained on average.

The most important thing is that the theoretical calculations agree with the laboratory results.

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